



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2021 – 10:58 AM EST

PDB ID : 5V2C
Title : RE-REFINEMENT OF CRYSTAL STRUCTURE OF PHOTOSYSTEM II COMPLEX
Authors : Wang, J.; Wiwczar, J.M.; Brudvig, G.W.
Deposited on : 2017-03-03
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 : 2.17.1
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) : 2.17.1

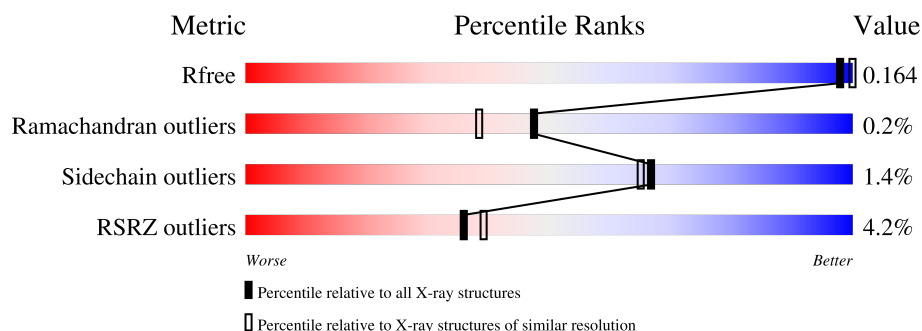
1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	A	344	<div> <div>%</div> <div> <div></div> <div>95%</div> <div></div> </div> <div>..</div> </div>
1	a	344	<div> <div>%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>..</div> </div>
2	B	506	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div>.</div> </div>
2	b	506	<div> <div>6%</div> <div> <div></div> <div>96%</div> <div></div> </div> <div>.</div> </div>
3	C	458	<div> <div>%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div>..</div> </div>
3	c	458	<div> <div>3%</div> <div> <div></div> <div>97%</div> <div></div> </div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	342	% 98% .
4	d	342	% 97% .
5	E	83	6% 94% ..
5	e	83	10% 96% ..
6	F	44	7% 75% 23% .
6	f	44	5% 68% 5% 27%
7	H	65	6% 95% 5%
7	h	65	5% 94% 6%
8	I	38	8% 97% .
8	i	38	5% 97% .
9	J	40	15% 98% .
9	j	40	12% 95% ..
10	K	37	97% .
10	k	37	97% .
11	L	37	8% 92% 8%
11	l	37	11% 97% .
12	M	36	6% 92% 6% .
12	m	36	8% 92% 6% .
13	O	245	6% 97% .
13	o	245	10% 96% .
14	T	32	6% 84% 9% 6%
14	t	32	3% 91% 6%
15	U	104	2% 90% 7%
15	u	104	% 91% 7%
16	V	137	97% .

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	41	
18	x	41	
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
24	CLA	A	606	X	-	-	-
24	CLA	A	607	X	-	-	-
24	CLA	A	609	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	609	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-
24	CLA	C	506	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	511	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	407	X	-	-	-
24	CLA	a	408	X	-	-	-
24	CLA	a	410	X	-	-	-
24	CLA	b	602	X	-	-	-
24	CLA	b	603	X	-	-	-
24	CLA	b	604	X	-	-	-
24	CLA	b	605	X	-	-	-
24	CLA	b	606	X	-	-	-
24	CLA	b	607	X	-	-	-
24	CLA	b	608	X	-	-	-
24	CLA	b	609	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	c	501	X	-	-	-
24	CLA	c	502	X	-	-	-
24	CLA	c	503	X	-	-	-
24	CLA	c	504	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-
28	SQD	h	105	-	-	-	X
30	GOL	C	528	-	X	-	-
30	GOL	O	307	-	-	-	X
30	GOL	o	303	-	-	-	X
30	GOL	v	205	-	-	-	X
31	LMT	C	533	-	-	-	X
31	LMT	j	103	-	-	-	X
33	PG4	B	642	-	-	-	X
33	PG4	B	643	-	-	-	X
33	PG4	C	534	-	-	-	X
33	PG4	b	637	-	-	-	X
33	PG4	e	103	-	-	-	X
33	PG4	e	104	-	-	-	X
34	PGE	B	646	-	-	-	X
34	PGE	B	650	-	-	-	X
34	PGE	D	415	-	-	-	X
34	PGE	E	105	-	-	-	X
34	PGE	E	107	-	-	-	X
34	PGE	E	108	-	-	-	X
34	PGE	H	110	-	-	-	X
34	PGE	O	309	-	-	-	X
34	PGE	V	215	-	-	-	X
34	PGE	b	639	-	-	-	X
34	PGE	b	644	-	-	-	X
34	PGE	b	645	-	-	-	X
34	PGE	b	646	-	-	-	X
34	PGE	b	647	-	-	-	X
34	PGE	c	536	-	-	-	X
34	PGE	c	539	-	-	-	X
34	PGE	c	540	-	-	-	X
34	PGE	f	105	-	-	-	X
34	PGE	h	109	-	-	-	X
34	PGE	i	106	-	-	-	X
34	PGE	o	307	-	-	-	X
35	P6G	C	541	-	-	-	X
35	P6G	E	110	-	-	-	X
36	EDO	B	656	-	-	-	X
36	EDO	C	542	-	-	-	X
36	EDO	V	218	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	EDO	c	542	-	-	-	X
38	HTG	C	530	-	-	-	X
38	HTG	C	531	-	-	-	X
39	1PE	B	653	-	-	-	X
39	1PE	V	217	-	-	-	X

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 57584 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	4	0
			2639	1730	434	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2639	1730	434	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765
a	279	PRO	ARG	conflict	UNP P51765

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	11	0
			4032	2646	671	702	13			
2	b	506	Total	C	N	O	S	0	10	0
			4037	2649	670	705	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	SER	-	expression tag	UNP D0VWR1
B	507	ASP	-	expression tag	UNP D0VWR1
b	506	SER	-	expression tag	UNP D0VWR1
b	507	ASP	-	expression tag	UNP D0VWR1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	5	0
			3508	2297	585	613	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	c	458	Total	C	N	O	S	0	4	0
			3553	2324	592	624	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLU	-	expression tag	UNP D0VWR7
C	17	ALA	-	expression tag	UNP D0VWR7
C	18	ALA	-	expression tag	UNP D0VWR7
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	16	GLU	-	expression tag	UNP D0VWR7
c	17	ALA	-	expression tag	UNP D0VWR7
c	18	ALA	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2731	1810	445	464	12			
4	d	342	Total	C	N	O	S	0	2	0
			2741	1815	448	466	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		0	3	0
			676	441	110	125				
5	e	81	Total	C	N	O		0	2	0
			668	436	107	125				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	65	Total	C	N	O	S	0	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			
8	i	38	Total	C	N	O	S	0	0	0
			314	211	48	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	39	Total	C	N	O	S	0	2	0
			294	197	46	50	1			
9	j	39	Total	C	N	O	S	0	0	0
			281	187	43	50	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLU	MET	conflict	UNP Q7DGD4
j	2	GLU	MET	conflict	UNP Q7DGD4

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054
k	33	LEU	PHE	conflict	UNP P19054
k	39	TRP	VAL	conflict	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	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	2	0
			315	211	49	54	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	2	0
			286	190	42	53	1			
12	m	35	Total	C	N	O	S	0	2	0
			289	193	42	52	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312
m	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	245	Total	C	N	O	S	0	6	0
			1904	1192	317	391	4			
13	o	245	Total	C	N	O	S	0	5	0
			1902	1189	320	389	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	2	ALA	-	expression tag	UNP D0VWR2
O	3	ALA	-	expression tag	UNP D0VWR2
o	2	ALA	-	expression tag	UNP D0VWR2
o	3	ALA	-	expression tag	UNP D0VWR2

- 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	2	0
			271	190	36	42	3			
14	t	30	Total	C	N	O	S	0	2	0
			271	190	36	42	3			

- 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	S	0	2	0
			786	499	130	157				
15	u	97	Total	C	N	O	S	0	0	0
			774	491	129	154				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1077	683	181	209	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	1	0
			219	145	37	34	3			
17	y	29	Total	C	N	O	S	0	1	0
			220	146	37	33	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	S	0	1	0
			300	201	47	51	1			
18	x	40	Total	C	N	O	S	0	0	0
			295	196	47	51	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	initiating methionine	UNP D0VWR4

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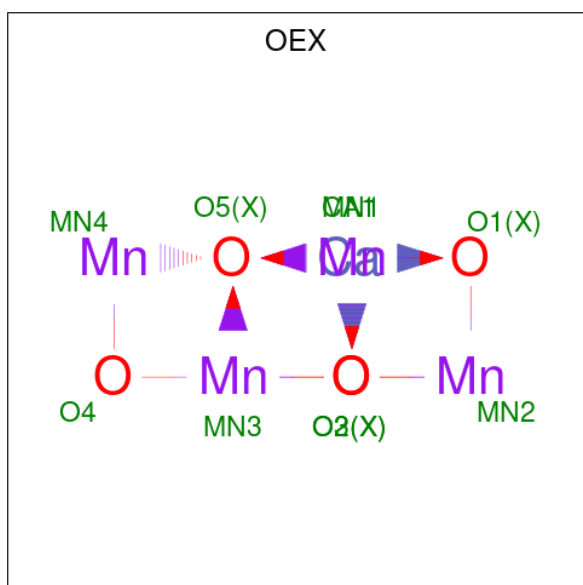
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Chain	Residue	Modelled	Actual	Comment	Reference
x	1	MET	-	initiating methionine	UNP D0VWR4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			
19	z	62	Total	C	N	O	S	0	0	0
			479	328	72	77	2			

- Molecule 20 is 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		
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

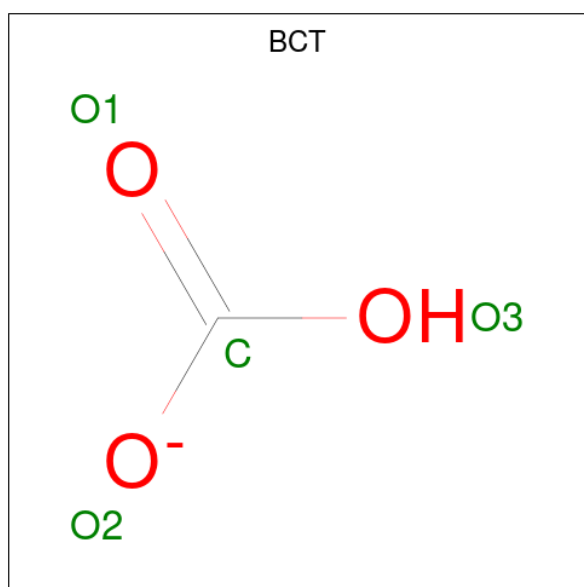
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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

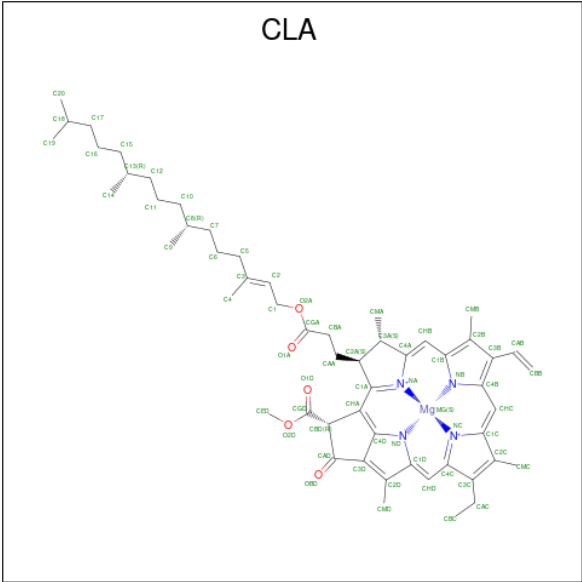
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	V	1	Total	Cl	0	0
			1	1		
22	a	2	Total	Cl	0	0
			2	2		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	C	O	0	0
			4	1	3		
23	a	1	Total	C	O	0	0
			4	1	3		
23	m	1	Total	C	O	0	1
			8	2	6		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	B	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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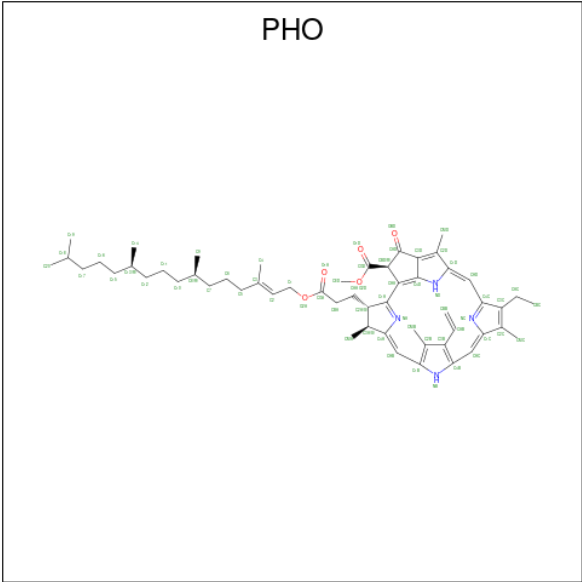
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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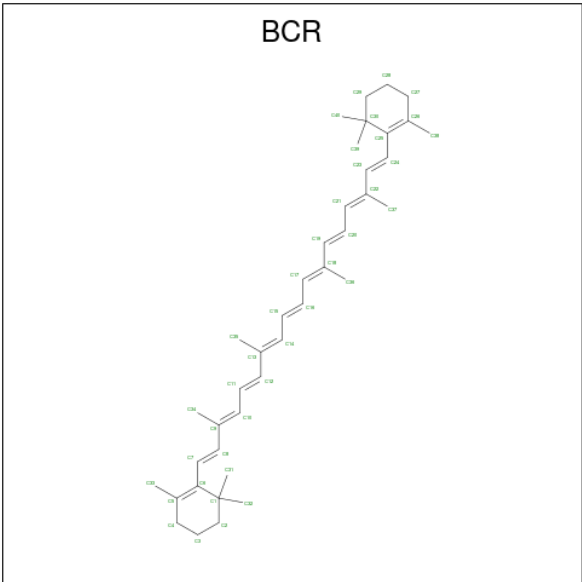
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



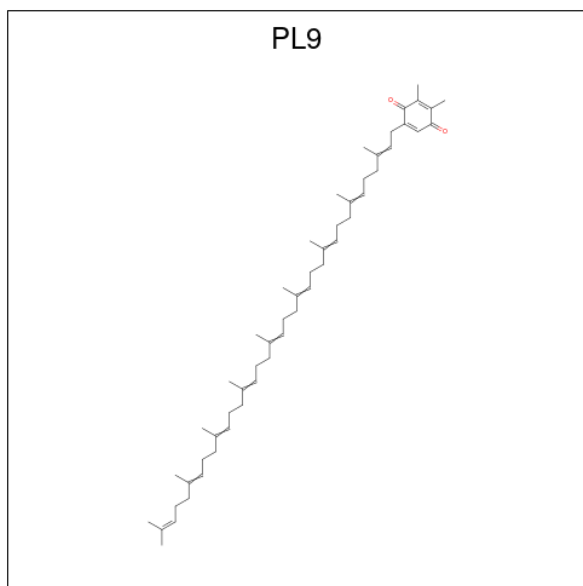
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



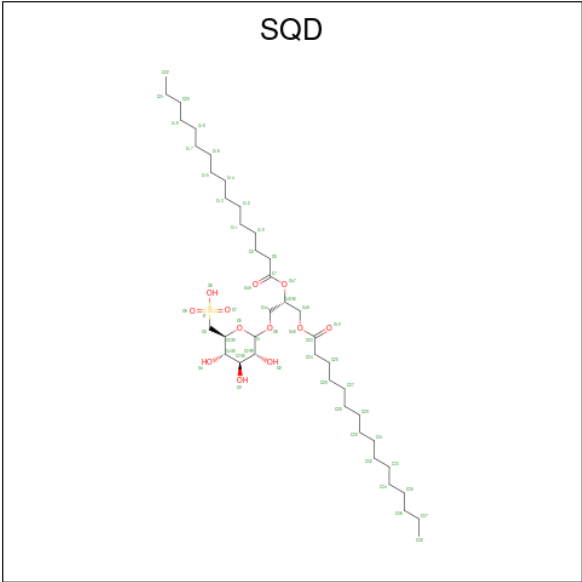
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total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

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



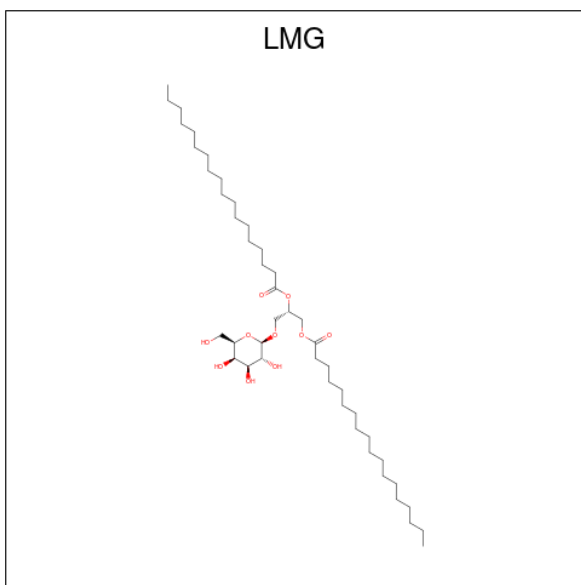
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	h	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		
28	x	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			51	41	10		
29	B	1	Total	C	O	0	0
			55	45	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			51	41	10		
29	C	1	Total	C	O	0	0
			55	45	10		
29	J	1	Total	C	O	0	0
			47	37	10		
29	a	1	Total	C	O	0	0
			51	41	10		
29	b	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	c	1	Total	C	O	0	0
			51	41	10		
29	d	1	Total	C	O	0	0
			55	45	10		
29	j	1	Total	C	O	0	0
			47	37	10		
29	z	1	Total	C	O	0	0
			55	45	10		

- Molecule 30 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total 6	C 3	O 3	0	0
30	D	1	Total 6	C 3	O 3	0	0
30	D	1	Total 6	C 3	O 3	0	0
30	F	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	O	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	T	1	Total 6	C 3	O 3	0	0
30	U	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	V	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	a	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0

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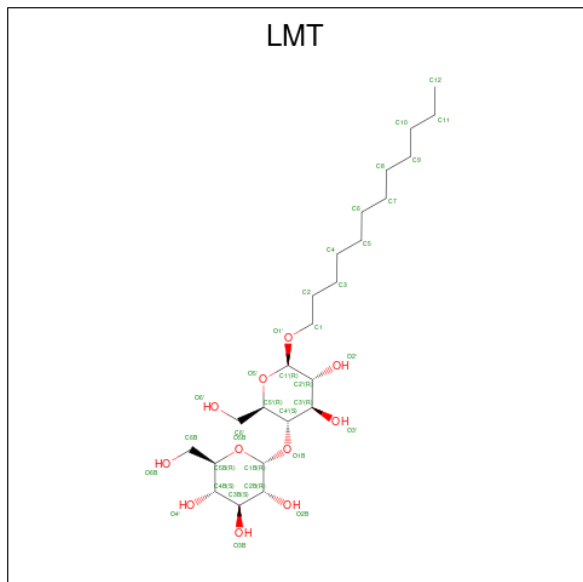
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	b	1	Total 6	C 3	O 3	0	0
30	c	1	Total 6	C 3	O 3	0	0
30	c	1	Total 6	C 3	O 3	0	0
30	c	1	Total 6	C 3	O 3	0	0
30	c	1	Total 6	C 3	O 3	0	0
30	d	1	Total 6	C 3	O 3	0	0
30	d	1	Total 6	C 3	O 3	0	0
30	e	1	Total 6	C 3	O 3	0	0
30	f	1	Total 6	C 3	O 3	0	0
30	f	1	Total 6	C 3	O 3	0	0
30	m	1	Total 6	C 3	O 3	0	0
30	o	1	Total 6	C 3	O 3	0	0
30	o	1	Total 6	C 3	O 3	0	0
30	o	1	Total 6	C 3	O 3	0	0
30	t	1	Total 6	C 3	O 3	0	0
30	u	1	Total 6	C 3	O 3	0	0
30	u	1	Total 6	C 3	O 3	0	0
30	v	1	Total 6	C 3	O 3	0	0

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

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



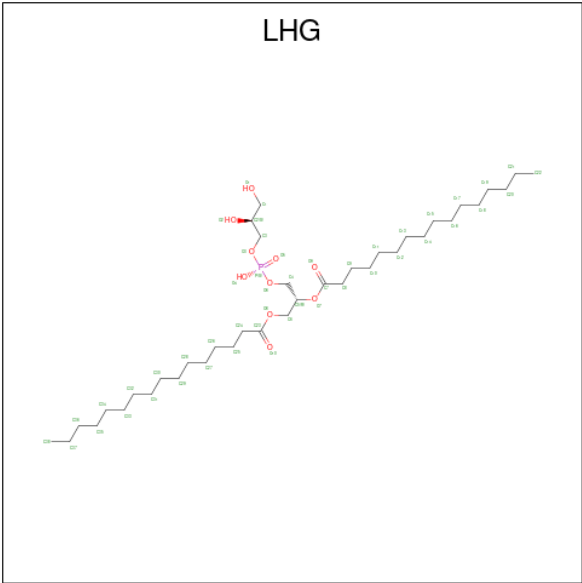
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	C	1	Total	C	O	0	0
			35	24	11		
31	F	1	Total	C	O	0	0
			35	24	11		
31	I	1	Total	C	O	0	0
			35	24	11		
31	J	1	Total	C	O	0	0
			35	24	11		

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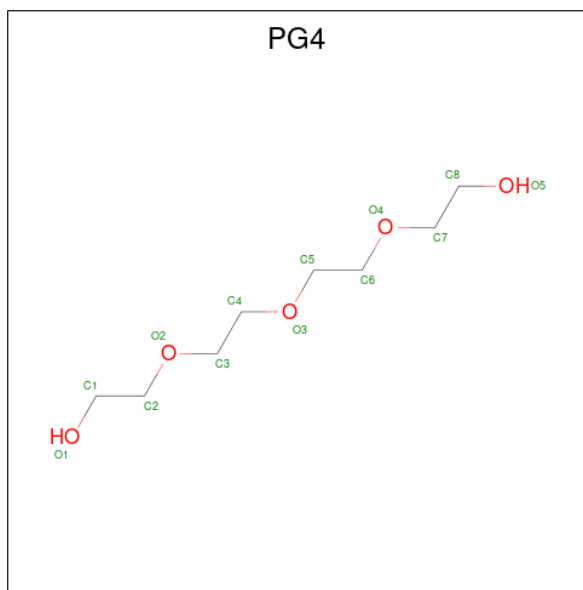
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	Y	1	Total	C	O	0	0
			35	24	11		
31	a	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			35	24	11		
31	c	1	Total	C	O	0	0
			35	24	11		
31	f	1	Total	C	O	0	0
			35	24	11		
31	j	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			35	24	11		
31	u	1	Total	C	O	0	0
			35	24	11		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			42	31	10	1		
32	B	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	a	1	Total	C	O	P	0	0
			41	30	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	B	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	C	1	Total	C	O	0	0
			13	8	5		
33	D	1	Total	C	O	0	0
			13	8	5		
33	E	1	Total	C	O	0	0
			13	8	5		
33	E	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	H	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		

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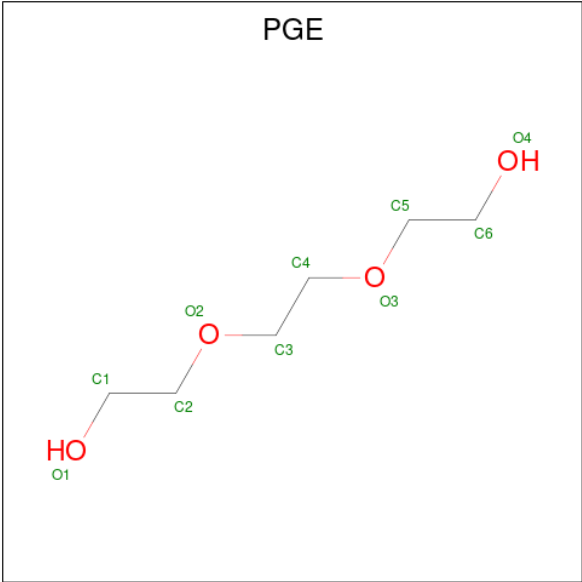
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	I	1	Total	C	O	0	0
			13	8	5		
33	I	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	J	1	Total	C	O	0	0
			13	8	5		
33	K	1	Total	C	O	0	0
			13	8	5		
33	U	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	V	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	X	1	Total	C	O	0	0
			13	8	5		
33	a	1	Total	C	O	0	0
			13	8	5		
33	a	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	b	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	c	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		
33	c	1	Total	C	O	0	0
			13	8	5		
33	d	1	Total	C	O	0	0
			13	8	5		
33	e	1	Total	C	O	0	0
			13	8	5		
33	e	1	Total	C	O	0	0
			13	8	5		
33	h	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	i	1	Total	C	O	0	0
			13	8	5		
33	j	1	Total	C	O	0	0
			13	8	5		
33	l	1	Total	C	O	0	0
			13	8	5		
33	x	1	Total	C	O	0	0
			13	8	5		

- Molecule 34 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			7	4	3		
34	A	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	B	1	Total	C	O	0	0
			10	6	4		
34	C	1	Total	C	O	0	0
			10	6	4		
34	C	1	Total	C	O	0	0
			10	6	4		
34	D	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	E	1	Total C O 10 6 4	0	0
34	E	1	Total C O 10 6 4	0	0
34	E	1	Total C O 10 6 4	0	0
34	E	1	Total C O 10 6 4	0	0
34	H	1	Total C O 10 6 4	0	0
34	H	1	Total C O 10 6 4	0	0
34	H	1	Total C O 10 6 4	0	0
34	H	1	Total C O 10 6 4	0	0
34	I	1	Total C O 10 6 4	0	0
34	J	1	Total C O 10 6 4	0	0
34	J	1	Total C O 10 6 4	0	0
34	J	1	Total C O 10 6 4	0	0
34	O	1	Total C O 10 6 4	0	0
34	O	1	Total C O 10 6 4	0	0
34	O	1	Total C O 10 6 4	0	0
34	T	1	Total C O 7 4 3	0	0
34	V	1	Total C O 10 6 4	0	0
34	V	1	Total C O 10 6 4	0	0
34	Y	1	Total C O 10 6 4	0	0
34	a	1	Total C O 10 6 4	0	0
34	a	1	Total C O 10 6 4	0	0

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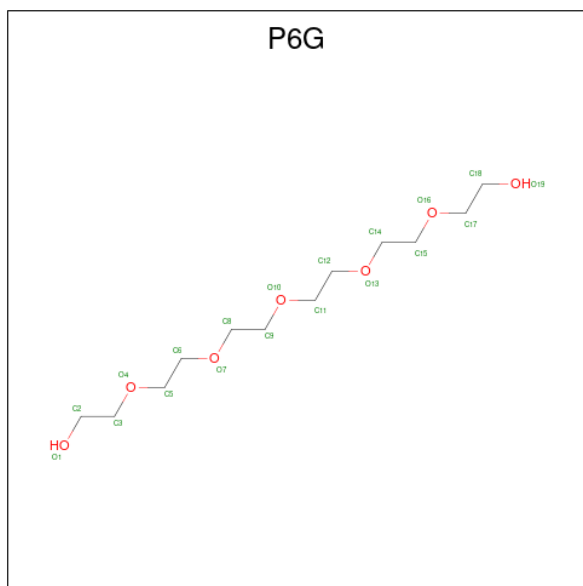
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	b	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	c	1	Total	C	O	0	0
			10	6	4		
34	f	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	h	1	Total	C	O	0	0
			10	6	4		
34	i	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	i	1	Total	C	O	0	0
			10	6	4		
34	j	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	o	1	Total	C	O	0	0
			10	6	4		
34	t	1	Total	C	O	0	0
			10	6	4		
34	t	1	Total	C	O	0	0
			7	4	3		
34	x	1	Total	C	O	0	0
			10	6	4		

- Molecule 35 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	A	1	Total	C	O	0	0
			19	12	7		
35	A	1	Total	C	O	0	0
			19	12	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
35	B	1	Total	C	O	0	0
			19	12	7		
35	B	1	Total	C	O	0	0
			19	12	7		
35	C	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	D	1	Total	C	O	0	0
			19	12	7		
35	E	1	Total	C	O	0	0
			19	12	7		
35	I	1	Total	C	O	0	0
			19	12	7		
35	T	1	Total	C	O	0	0
			19	12	7		
35	b	1	Total	C	O	0	0
			19	12	7		
35	b	1	Total	C	O	0	0
			19	12	7		
35	c	1	Total	C	O	0	0
			19	12	7		
35	d	1	Total	C	O	0	0
			19	12	7		
35	d	1	Total	C	O	0	0
			19	12	7		
35	j	1	Total	C	O	0	0
			19	12	7		

- Molecule 36 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	A	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	C	1	Total	C	O	0	0
			4	2	2		
36	D	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	H	1	Total	C	O	0	0
			4	2	2		
36	I	1	Total	C	O	0	0
			4	2	2		
36	J	1	Total	C	O	0	0
			4	2	2		
36	O	1	Total	C	O	0	0
			4	2	2		
36	V	1	Total	C	O	0	0
			4	2	2		

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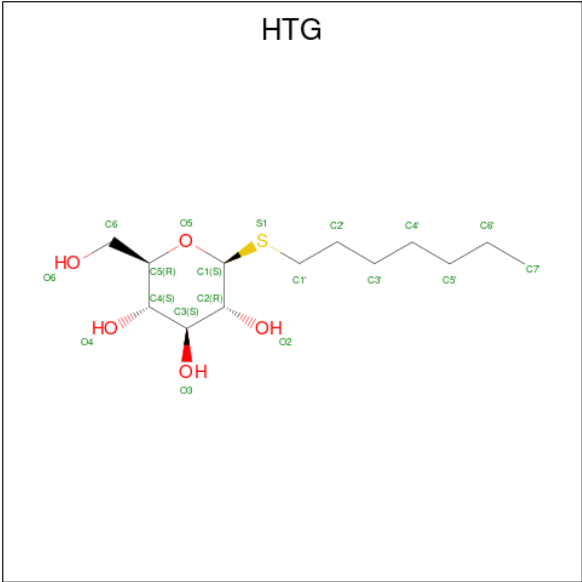
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	1	Total C O 4 2 2	0	0
36	a	1	Total C O 4 2 2	0	0
36	c	1	Total C O 4 2 2	0	0
36	d	1	Total C O 4 2 2	0	0
36	e	1	Total C O 4 2 2	0	0
36	i	1	Total C O 4 2 2	0	0
36	o	1	Total C O 4 2 2	0	0
36	o	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	B	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	b	1	Total Ca 1 1	0	0
37	c	1	Total Ca 1 1	0	0
37	h	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

- Molecule 38 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: C₁₃H₂₆O₅S).



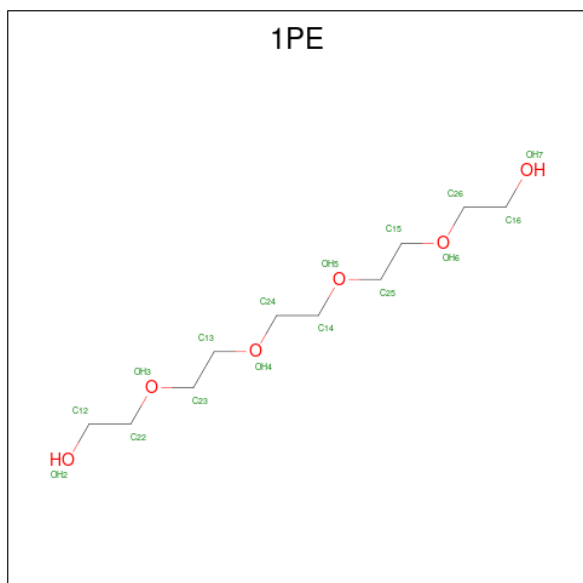
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	H	1	Total	C	O	S	0	0
			19	13	5	1		
38	O	1	Total	C	O	S	0	0
			19	13	5	1		
38	V	1	Total	C	O	S	0	0
			19	13	5	1		
38	a	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	h	1	Total	C	O	S	0	0
			19	13	5	1		
38	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 39 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



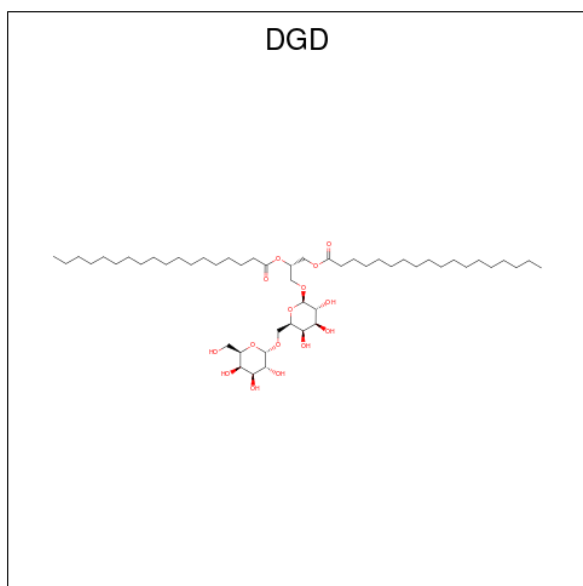
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		
39	L	1	Total	C	O	0	0
			16	10	6		
39	V	1	Total	C	O	0	0
			16	10	6		
39	e	1	Total	C	O	0	0
			16	10	6		
39	j	1	Total	C	O	0	0
			16	10	6		
39	x	1	Total	C	O	0	0
			16	10	6		

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



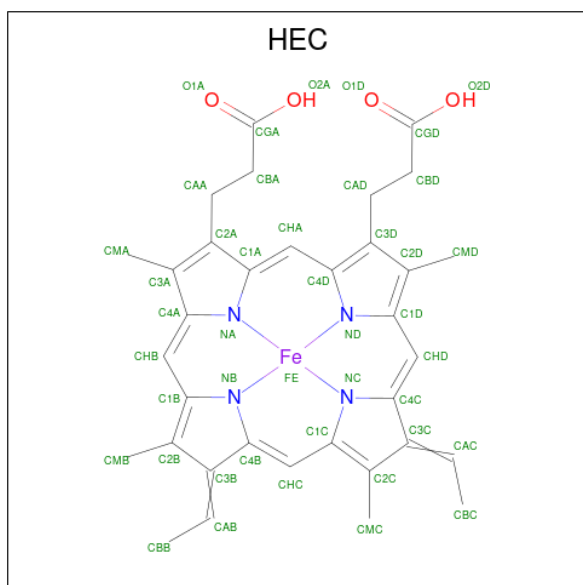
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
40	C	1	Total	C	O	0	0
			62	47	15		
40	C	1	Total	C	O	0	0
			56	41	15		
40	C	1	Total	C	O	0	0
			62	47	15		
40	D	1	Total	C	O	0	0
			66	51	15		
40	H	1	Total	C	O	0	0
			62	47	15		

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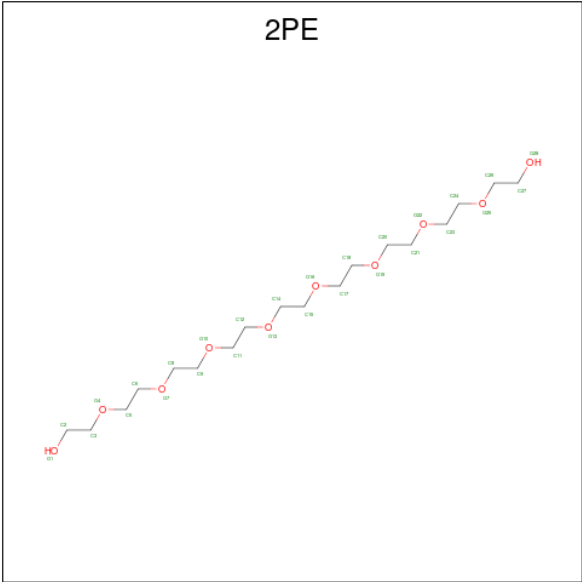
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	f	1	Total	Mg	0	0
			1	1		
42	j	1	Total	Mg	0	0
			1	1		

- Molecule 43 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



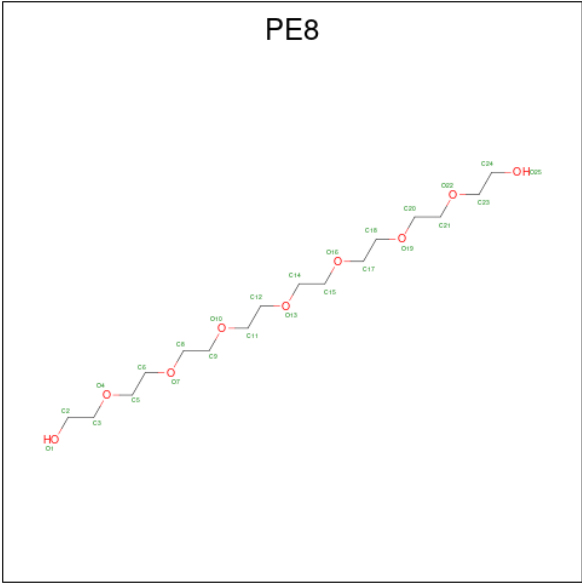
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
43	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
43	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 44 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
44	V	1	Total	C	O	0	0
			28	18	10		

- Molecule 45 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (three-letter code: PE8) (formula: C₁₆H₃₄O₉).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
45	i	1	Total	C	O	0	0
			25	16	9		

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
46	A	191	Total O 191 191	0	0
46	B	413	Total O 413 413	0	0
46	C	320	Total O 320 320	0	0
46	D	169	Total O 170 170	0	1
46	E	57	Total O 57 57	0	0
46	F	17	Total O 17 17	0	0
46	H	63	Total O 63 63	0	0
46	I	16	Total O 16 16	0	0
46	J	17	Total O 17 17	0	0
46	K	15	Total O 15 15	0	0
46	L	23	Total O 23 23	0	0
46	M	33	Total O 33 33	0	0
46	O	254	Total O 254 254	0	0
46	T	27	Total O 27 27	0	0
46	U	112	Total O 112 112	0	0
46	V	149	Total O 149 149	0	0
46	Y	6	Total O 6 6	0	0
46	X	10	Total O 10 10	0	0
46	Z	4	Total O 4 4	0	0
46	a	177	Total O 177 177	0	0
46	b	421	Total O 421 421	0	0
46	c	329	Total O 329 329	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
46	d	188	Total 189	O 189	0	1
46	e	46	Total 46	O 46	0	0
46	f	15	Total 15	O 15	0	0
46	h	52	Total 52	O 52	0	0
46	i	22	Total 22	O 22	0	0
46	j	12	Total 12	O 12	0	0
46	k	9	Total 9	O 9	0	0
46	l	23	Total 23	O 23	0	0
46	m	24	Total 24	O 24	0	0
46	o	246	Total 246	O 246	0	0
46	t	17	Total 17	O 17	0	0
46	u	140	Total 140	O 140	0	0
46	v	154	Total 154	O 154	0	0
46	y	7	Total 7	O 7	0	0
46	x	8	Total 8	O 8	0	0
46	z	1	Total 1	O 1	0	0

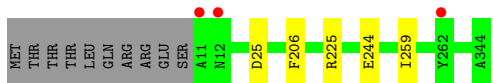
3 Residue-property plots

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

- Molecule 1: Photosystem II protein D1



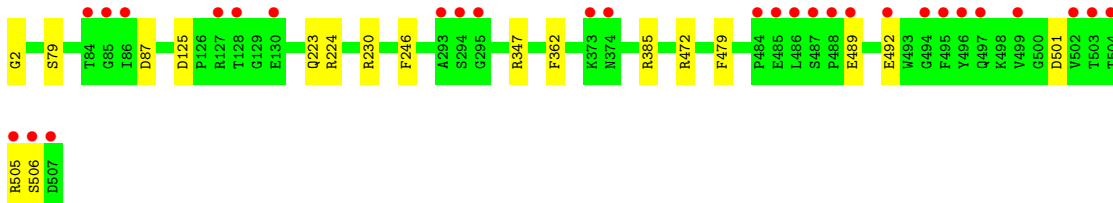
- Molecule 1: Photosystem II protein D1



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 2: Photosystem II CP47 reaction center protein



- Molecule 3: Photosystem II CP43 reaction center protein

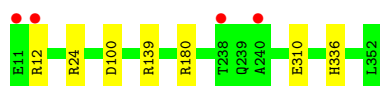




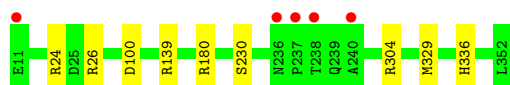
- Molecule 3: Photosystem II CP43 reaction center protein



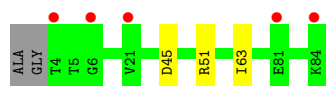
- Molecule 4: Photosystem II D2 protein



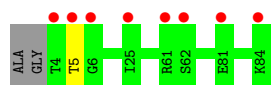
- Molecule 4: Photosystem II D2 protein



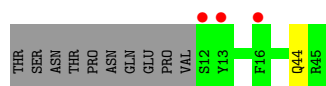
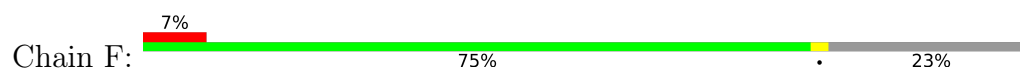
- Molecule 5: Cytochrome b559 subunit alpha



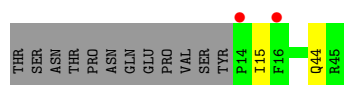
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



- Molecule 6: Cytochrome b559 subunit beta



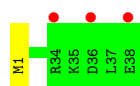
- Molecule 7: Photosystem II reaction center protein H



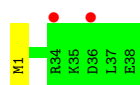
- Molecule 7: Photosystem II reaction center protein H



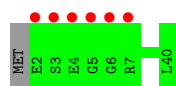
- Molecule 8: Photosystem II reaction center protein I



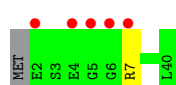
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



- Molecule 9: Photosystem II reaction center protein J



- Molecule 10: Photosystem II reaction center protein K

Chain K:  97% .




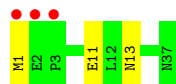
- Molecule 10: Photosystem II reaction center protein K

Chain k:  97% .



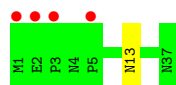
- Molecule 11: Photosystem II reaction center protein L

Chain L:  8% 92% 8% .




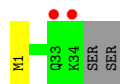
- Molecule 11: Photosystem II reaction center protein L

Chain l:  11% 97% .




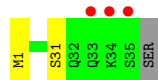
- Molecule 12: Photosystem II reaction center protein M

Chain M:  6% 92% 6% .



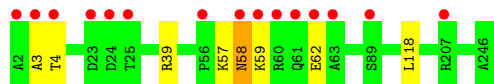
- Molecule 12: Photosystem II reaction center protein M

Chain m:  8% 92% 6% .

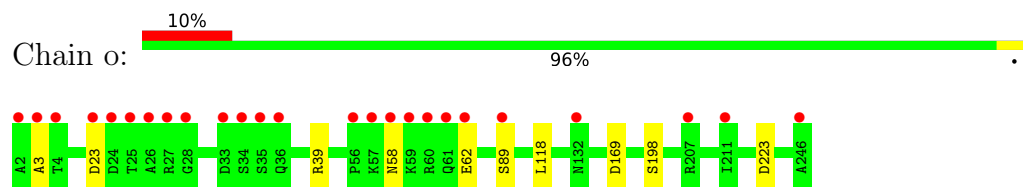


- Molecule 13: Photosystem II manganese-stabilizing polypeptide

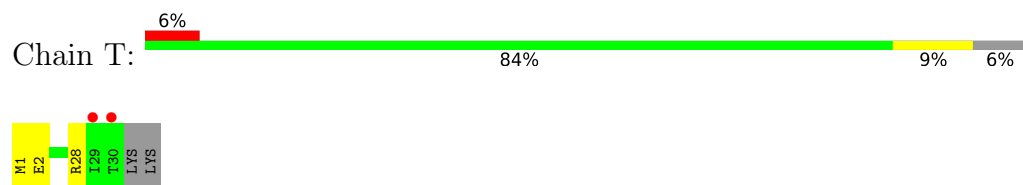
Chain O:  6% 97% .



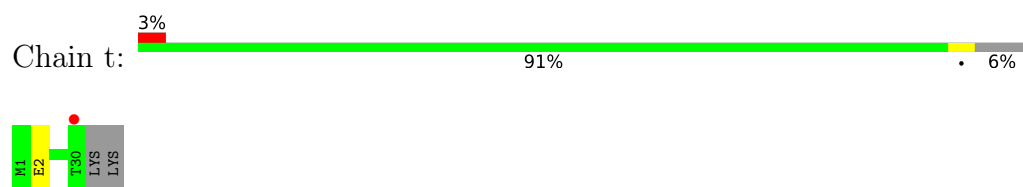
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



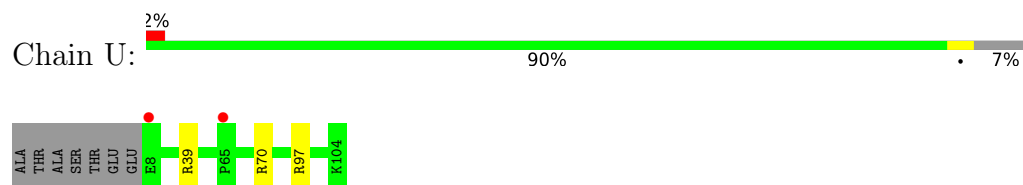
- Molecule 14: Photosystem II reaction center protein T



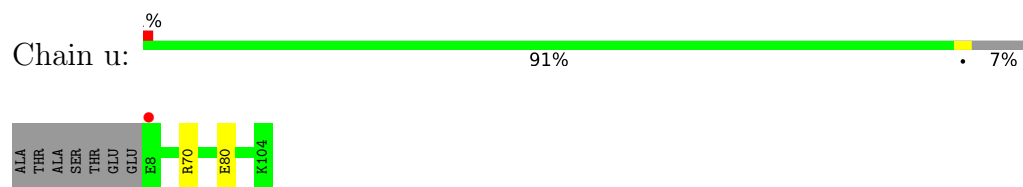
- Molecule 14: Photosystem II reaction center protein T



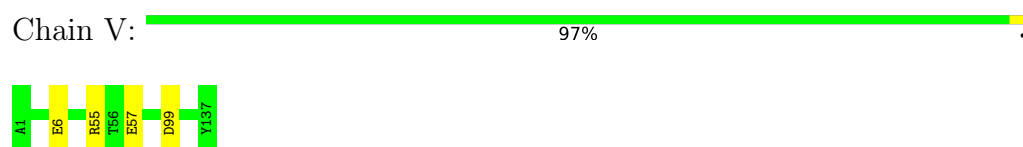
- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 16: Cytochrome c-550

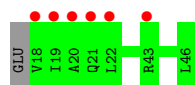


- Molecule 16: Cytochrome c-550

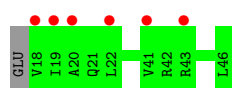




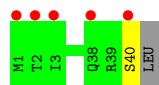
- Molecule 17: Photosystem II reaction center protein Ycf12



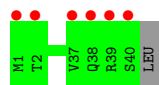
- Molecule 17: Photosystem II reaction center protein Ycf12



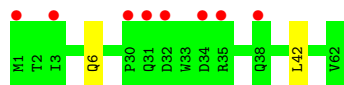
- Molecule 18: Photosystem II reaction center protein X



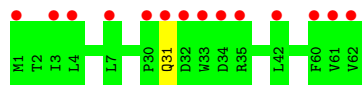
- Molecule 18: Photosystem II reaction center protein X



- Molecule 19: Photosystem II reaction center protein Z



- Molecule 19: Photosystem II reaction center protein Z



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	178.62 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (178.62-1.90) 99.9 (20.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.092 , 0.163 0.095 , 0.164	Depositor DCC
R_{free} test set	31202 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 81.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	57584	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage'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: BCT, DGD, 1PE, LMT, FE2, MHS, FME, MG, HTG, LHG, BCR, OEX, CLA, PG4, PL9, 2PE, PHO, EDO, P6G, PE8, LMG, CA, CL, HEC, SQD, GOL, PGE, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	2/2736 (0.1%)	0.88	4/3730 (0.1%)
1	a	0.93	0/2736	0.87	7/3730 (0.2%)
2	B	0.98	2/4205 (0.0%)	0.88	9/5727 (0.2%)
2	b	0.94	3/4207 (0.1%)	0.88	7/5731 (0.1%)
3	C	0.92	1/3636 (0.0%)	0.83	6/4950 (0.1%)
3	c	0.83	1/3679 (0.0%)	0.84	6/5008 (0.1%)
4	D	0.98	1/2816 (0.0%)	0.90	4/3836 (0.1%)
4	d	0.92	1/2829 (0.0%)	0.86	8/3852 (0.2%)
5	E	0.92	0/704	0.93	3/959 (0.3%)
5	e	0.86	0/693	0.83	0/944
6	F	0.84	0/284	0.71	0/387
6	f	0.74	0/265	0.74	0/360
7	H	1.01	2/544 (0.4%)	0.89	0/739
7	h	0.88	1/535 (0.2%)	0.75	0/728
8	I	0.90	0/311	0.81	0/419
8	i	0.86	0/311	0.83	0/419
9	J	0.87	0/306	0.74	0/413
9	j	0.75	0/287	0.77	0/388
10	K	0.80	0/303	0.75	0/416
10	k	0.75	0/303	0.77	0/416
11	L	1.00	1/319 (0.3%)	0.93	0/433
11	l	0.93	0/328	0.87	0/446
12	M	0.99	0/279	0.83	0/380
12	m	0.98	1/275 (0.4%)	0.88	0/375
13	O	0.90	0/1953	0.92	1/2649 (0.0%)
13	o	0.90	1/1948 (0.1%)	0.94	6/2641 (0.2%)
14	T	1.21	1/266 (0.4%)	1.06	1/362 (0.3%)
14	t	1.07	2/266 (0.8%)	0.91	0/362
15	U	0.85	0/803	0.92	2/1088 (0.2%)
15	u	0.98	1/785 (0.1%)	0.90	0/1064
16	V	0.95	3/1104 (0.3%)	0.89	3/1498 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.86	0/1096	0.84	4/1487 (0.3%)
17	Y	0.76	0/223	0.80	0/299
17	y	0.71	0/224	0.83	0/299
18	X	0.77	0/306	0.82	0/413
18	x	0.83	0/298	0.83	0/402
19	Z	0.74	0/490	0.79	0/669
19	z	0.73	0/490	0.70	0/669
All	All	0.92	24/43143 (0.1%)	0.87	71/58688 (0.1%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	66	GLY	C-O	7.92	1.36	1.23
7	H	66	GLY	C-OXT	7.84	1.38	1.23
14	t	2	GLU	CB-CG	-7.21	1.38	1.52
15	u	80	GLU	CD-OE2	-6.83	1.18	1.25
16	V	57	GLU	CG-CD	6.71	1.62	1.51
1	A	65	GLU	CD-OE2	6.36	1.32	1.25
16	V	6	GLU	CG-CD	6.25	1.61	1.51
14	t	2	GLU	CD-OE2	-6.12	1.19	1.25
13	o	198	SER	CB-OG	-6.09	1.34	1.42
16	V	57	GLU	CD-OE1	6.09	1.32	1.25
7	h	61	SER	CB-OG	-6.06	1.34	1.42
2	B	307	GLU	CD-OE2	-5.91	1.19	1.25
14	T	2	GLU	CD-OE2	-5.74	1.19	1.25
12	m	31	SER	CB-OG	5.64	1.49	1.42
2	b	2	GLY	N-CA	5.58	1.54	1.46
3	c	344	SER	CB-OG	5.51	1.49	1.42
3	C	275	SER	CB-OG	5.46	1.49	1.42
4	D	310	GLU	CD-OE2	-5.39	1.19	1.25
1	A	244	GLU	CD-OE1	5.31	1.31	1.25
2	B	340	TRP	CE2-CZ2	-5.15	1.30	1.39
11	L	11	GLU	CD-OE1	5.06	1.31	1.25
2	b	347[A]	ARG	CZ-NH2	-5.06	1.26	1.33
2	b	347[B]	ARG	CZ-NH2	-5.06	1.26	1.33
4	d	230	SER	CB-OG	5.04	1.48	1.42

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	139	ARG	NE-CZ-NH1	14.27	127.43	120.30
4	D	139	ARG	NE-CZ-NH2	-9.74	115.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	357	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	a	225[A]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	a	225[B]	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	a	225[A]	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	a	225[B]	ARG	NE-CZ-NH2	-8.60	116.00	120.30
4	d	100	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	225[A]	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	225[B]	ARG	NE-CZ-NH1	-7.49	116.56	120.30
2	B	444	ARG	NE-CZ-NH2	-7.49	116.56	120.30
3	C	460	ASP	CB-CG-OD1	7.47	125.02	118.30
2	B	224	ARG	NE-CZ-NH2	7.46	124.03	120.30
4	d	139	ARG	NE-CZ-NH2	-7.26	116.67	120.30
2	b	385	ARG	NE-CZ-NH2	-7.14	116.73	120.30
2	B	224	ARG	NE-CZ-NH1	-7.07	116.76	120.30
13	o	39[A]	ARG	NE-CZ-NH1	7.04	123.82	120.30
13	o	39[B]	ARG	NE-CZ-NH1	7.04	123.82	120.30
3	c	460	ASP	CB-CG-OD1	6.97	124.57	118.30
4	d	139	ARG	NE-CZ-NH1	6.90	123.75	120.30
3	c	390	ARG	NE-CZ-NH1	6.86	123.73	120.30
13	O	39	ARG	NE-CZ-NH2	6.70	123.65	120.30
2	b	224	ARG	NE-CZ-NH1	-6.61	117.00	120.30
2	B	444	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	25	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	b	125	ASP	CB-CG-OD1	6.28	123.95	118.30
13	o	39[A]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
13	o	39[B]	ARG	NE-CZ-NH2	-6.09	117.25	120.30
14	T	28	ARG	NE-CZ-NH2	6.05	123.33	120.30
4	D	100	ASP	CB-CG-OD1	5.98	123.68	118.30
16	v	55[A]	ARG	NE-CZ-NH1	5.97	123.28	120.30
16	v	55[B]	ARG	NE-CZ-NH1	5.97	123.28	120.30
13	o	223	ASP	CB-CG-OD1	5.92	123.63	118.30
4	d	24	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	a	25	ASP	CB-CG-OD2	-5.84	113.04	118.30
3	C	473	ASP	CB-CG-OD1	5.82	123.53	118.30
1	a	25	ASP	CB-CG-OD1	5.76	123.48	118.30
16	v	55[A]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
16	v	55[B]	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	b	230	ARG	NE-CZ-NH1	5.72	123.16	120.30
16	V	55[A]	ARG	NE-CZ-NH1	5.69	123.14	120.30
16	V	55[B]	ARG	NE-CZ-NH1	5.69	123.14	120.30
5	E	51	ARG	NE-CZ-NH1	5.68	123.14	120.30
4	D	24	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	87	ASP	CB-CG-OD1	5.59	123.33	118.30
2	b	224	ARG	NE-CZ-NH2	5.55	123.08	120.30
4	d	304	ARG	NE-CZ-NH1	5.52	123.06	120.30
3	C	197	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	A	25	ASP	CB-CG-OD1	5.49	123.24	118.30
3	C	473	ASP	CB-CG-OD2	-5.48	113.37	118.30
2	B	357	ARG	NE-CZ-NH2	-5.47	117.56	120.30
3	c	449	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	B	477	ASP	CB-CG-OD1	5.45	123.21	118.30
3	c	460	ASP	CB-CG-OD2	-5.45	113.40	118.30
3	c	390	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	a	206	PHE	CB-CG-CD1	5.42	124.59	120.80
4	d	26	ARG	NE-CZ-NH1	5.41	123.01	120.30
3	C	357	ARG	NE-CZ-NH2	-5.41	117.60	120.30
3	C	357	ARG	NE-CZ-NH1	5.39	123.00	120.30
2	B	402	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
16	V	99	ASP	CB-CG-OD1	5.38	123.14	118.30
15	U	39	ARG	NE-CZ-NH1	5.35	122.98	120.30
2	B	230	ARG	NE-CZ-NH1	5.33	122.97	120.30
4	d	24	ARG	NE-CZ-NH2	-5.31	117.65	120.30
5	E	45	ASP	CB-CG-OD1	5.30	123.07	118.30
15	U	97	ARG	NE-CZ-NH2	-5.29	117.66	120.30
2	b	501	ASP	CB-CG-OD1	5.25	123.03	118.30
4	d	100	ASP	CB-CG-OD2	-5.23	113.60	118.30
3	c	150	ASP	CB-CG-OD1	5.09	122.89	118.30
5	E	63	ILE	CG1-CB-CG2	-5.07	100.24	111.40
13	o	169	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	41	31
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	41	31
2	B	513/506 (101%)	508 (99%)	5 (1%)	0	100	100
2	b	514/506 (102%)	505 (98%)	9 (2%)	0	100	100
3	C	454/458 (99%)	444 (98%)	9 (2%)	1 (0%)	47	38
3	c	460/458 (100%)	446 (97%)	11 (2%)	3 (1%)	22	12
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	82/83 (99%)	82 (100%)	0	0	100	100
5	e	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	29 (97%)	0	1 (3%)	4	0
7	H	65/65 (100%)	58 (89%)	7 (11%)	0	100	100
7	h	64/65 (98%)	59 (92%)	4 (6%)	1 (2%)	9	2
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	39/40 (98%)	39 (100%)	0	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	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	34/36 (94%)	34 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	249/245 (102%)	242 (97%)	3 (1%)	4 (2%)	9	2
13	o	248/245 (101%)	239 (96%)	8 (3%)	1 (0%)	34	24
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	97/104 (93%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
18	x	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5280/5362 (98%)	5161 (98%)	106 (2%)	13 (0%)	47	38

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	O	59	LYS
3	C	416	SER
3	c	416[A]	SER
3	c	416[B]	SER
13	o	3	ALA
13	O	3	ALA
13	O	4	THR
3	c	19	ASN
7	h	65	LEU
1	A	259	ILE
6	f	15	ILE
1	a	259	ILE

5.3.2 Protein sidechains ⓘ

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/279 (98%)	271 (99%)	2 (1%)	84	84
1	a	273/279 (98%)	272 (100%)	1 (0%)	91	91
2	B	413/404 (102%)	407 (98%)	6 (2%)	65	62
2	b	414/404 (102%)	403 (97%)	11 (3%)	44	38
3	C	357/357 (100%)	354 (99%)	3 (1%)	81	82
3	c	361/357 (101%)	352 (98%)	9 (2%)	47	41
4	D	277/276 (100%)	275 (99%)	2 (1%)	84	84
4	d	278/276 (101%)	276 (99%)	2 (1%)	84	84
5	E	75/72 (104%)	75 (100%)	0	100	100
5	e	74/72 (103%)	73 (99%)	1 (1%)	67	65
6	F	28/38 (74%)	27 (96%)	1 (4%)	35	26
6	f	26/38 (68%)	25 (96%)	1 (4%)	33	24
7	H	56/54 (104%)	53 (95%)	3 (5%)	22	13
7	h	55/54 (102%)	52 (94%)	3 (6%)	21	12
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	34 (100%)	0	100	100
9	J	29/28 (104%)	29 (100%)	0	100	100
9	j	27/28 (96%)	26 (96%)	1 (4%)	34	25
10	K	30/30 (100%)	29 (97%)	1 (3%)	38	29
10	k	30/30 (100%)	29 (97%)	1 (3%)	38	29
11	L	36/35 (103%)	34 (94%)	2 (6%)	21	11
11	l	37/35 (106%)	36 (97%)	1 (3%)	44	38
12	M	32/32 (100%)	32 (100%)	0	100	100
12	m	31/32 (97%)	31 (100%)	0	100	100
13	O	212/206 (103%)	208 (98%)	4 (2%)	57	53
13	o	211/206 (102%)	206 (98%)	5 (2%)	49	43
14	T	27/28 (96%)	27 (100%)	0	100	100
14	t	27/28 (96%)	27 (100%)	0	100	100
15	U	86/89 (97%)	85 (99%)	1 (1%)	71	70
15	u	84/89 (94%)	83 (99%)	1 (1%)	71	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	23/23 (100%)	23 (100%)	0	100	100
17	y	23/23 (100%)	23 (100%)	0	100	100
18	X	34/34 (100%)	33 (97%)	1 (3%)	42	35
18	x	33/34 (97%)	33 (100%)	0	100	100
19	Z	52/52 (100%)	50 (96%)	2 (4%)	33	24
19	z	52/52 (100%)	51 (98%)	1 (2%)	57	53
All	All	4381/4376 (100%)	4315 (98%)	66 (2%)	67	62

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

Mol	Chain	Res	Type
1	A	229	GLU
1	A	238	LYS
2	B	223[A]	GLN
2	B	223[B]	GLN
2	B	246	PHE
2	B	479	PHE
2	B	489	GLU
2	B	492	GLU
3	C	289	PHE
3	C	315	MET
3	C	418	ASN
4	D	12	ARG
4	D	180	ARG
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
7	H	49	TYR
10	K	10	LYS
11	L	1	MET
11	L	13	ASN
13	O	57	LYS
13	O	58	ASN
13	O	62	GLU
13	O	118	LEU
15	U	70	ARG
18	X	40	SER

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Mol	Chain	Res	Type
19	Z	6	GLN
19	Z	42	LEU
1	a	244	GLU
2	b	79	SER
2	b	223[A]	GLN
2	b	223[B]	GLN
2	b	246	PHE
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	489	GLU
2	b	492	GLU
2	b	505	ARG
2	b	506	SER
3	c	16	GLU
3	c	19	ASN
3	c	145[A]	SER
3	c	145[B]	SER
3	c	289	PHE
3	c	355	THR
3	c	418	ASN
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	180	ARG
4	d	329	MET
5	e	5	THR
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
7	h	49	TYR
9	j	7	ARG
10	k	10	LYS
11	l	13	ASN
13	o	23	ASP
13	o	58	ASN
13	o	62	GLU
13	o	89	SER
13	o	118	LEU
15	u	70	ARG
19	z	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	261	GLN
1	A	315	ASN
1	A	338	ASN
2	B	53	ASN
2	B	281	GLN
2	B	331	ASN
3	C	25	ASN
3	C	201	ASN
3	C	373	ASN
4	D	83	ASN
4	D	98	GLN
4	D	332	GLN
6	F	44	GLN
11	L	13	ASN
13	O	82	GLN
13	O	124	ASN
13	O	130	GLN
13	O	147	ASN
16	V	34	GLN
16	V	118	HIS
19	Z	58	ASN
1	a	315	ASN
1	a	338	ASN
2	b	53	ASN
2	b	281	GLN
2	b	331	ASN
2	b	338	GLN
3	c	19	ASN
3	c	201	ASN
3	c	373	ASN
4	d	61	HIS
4	d	83	ASN
4	d	332	GLN
6	f	44	GLN
11	l	13	ASN
13	o	124	ASN
13	o	132	ASN
13	o	147	ASN
18	x	38	GLN
19	z	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1[A]	-	8,9,10	0.91	0	7,9,11	0.99	0
4	MHS	D	336	4	7,11,12	0.82	0	6,14,16	2.64	4 (66%)
8	FME	i	1	8	8,9,10	0.49	0	7,9,11	1.45	1 (14%)
14	FME	T	1[B]	-	8,9,10	0.47	0	7,9,11	1.19	1 (14%)
14	FME	T	1[A]	-	8,9,10	0.60	0	7,9,11	1.29	2 (28%)
12	FME	m	1[B]	-	8,9,10	0.95	0	7,9,11	1.84	3 (42%)
14	FME	t	1[B]	-	8,9,10	0.66	0	7,9,11	1.06	0
12	FME	M	1	12	8,9,10	1.52	1 (12%)	7,9,11	1.55	1 (14%)
12	FME	m	1[A]	-	8,9,10	0.61	0	7,9,11	1.53	2 (28%)
4	MHS	d	336	4	7,11,12	1.17	0	6,14,16	1.96	1 (16%)
8	FME	I	1	8	8,9,10	0.75	0	7,9,11	1.09	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1[A]	-	-	0/7/9/11	-
4	MHS	D	336	4	-	0/5/6/8	0/1/1/1
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1[B]	-	-	2/7/9/11	-
14	FME	T	1[A]	-	-	0/7/9/11	-
12	FME	m	1[B]	-	-	3/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1[B]	-	-	2/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
12	FME	m	1[A]	-	-	1/7/9/11	-
4	MHS	d	336	4	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	0/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	M	1	FME	CA-N	-3.01	1.42	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	336	MHS	CM-ND1-CG	5.06	131.17	124.44
4	d	336	MHS	CM-ND1-CG	4.39	130.28	124.44
12	M	1	FME	CG-CB-CA	2.91	121.03	112.95
12	m	1[B]	FME	CB-CG-SD	-2.90	97.90	113.48
8	i	1	FME	O-C-CA	-2.74	117.61	124.78
12	m	1[A]	FME	O-C-CA	-2.40	118.48	124.78
14	T	1[A]	FME	CG-CB-CA	2.35	119.47	112.95
14	T	1[B]	FME	O-C-CA	-2.26	118.85	124.78
14	T	1[A]	FME	O-C-CA	-2.25	118.89	124.78
4	D	336	MHS	CB-CA-C	-2.24	107.27	111.47
8	I	1	FME	O-C-CA	-2.12	119.21	124.78
4	D	336	MHS	NE2-CE1-ND1	-2.11	109.13	112.26
4	D	336	MHS	CD2-NE2-CE1	2.10	109.06	105.78
12	m	1[A]	FME	C-CA-N	-2.10	105.94	109.73
12	m	1[B]	FME	CG-CB-CA	-2.05	107.25	112.95
12	m	1[B]	FME	O1-CN-N	-2.03	119.93	125.27

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1[B]	FME	CB-CG-SD-CE
14	t	1[B]	FME	CB-CG-SD-CE
12	m	1[B]	FME	CB-CG-SD-CE
14	T	1[B]	FME	C-CA-CB-CG
14	t	1[B]	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
12	m	1[A]	FME	CA-CB-CG-SD
12	m	1[B]	FME	C-CA-CB-CG
12	m	1[B]	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 447 ligands modelled in this entry, 18 are monoatomic - leaving 429 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
29	LMG	C	526	-	55,55,55	1.05	2 (3%)	63,63,63	1.51	8 (12%)
38	HTG	b	632	-	19,19,19	0.97	1 (5%)	23,24,24	1.67	7 (30%)
34	PGE	t	105	-	6,6,9	0.67	0	5,5,8	0.49	0
38	HTG	C	522	-	19,19,19	1.09	1 (5%)	23,24,24	1.90	3 (13%)
34	PGE	T	104	-	6,6,9	1.04	0	5,5,8	0.54	0
31	LMT	m	102	-	36,36,36	0.98	1 (2%)	47,47,47	1.67	7 (14%)
30	GOL	D	402	-	5,5,5	0.78	0	5,5,5	1.28	1 (20%)
31	LMT	m	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.09	5 (10%)
24	CLA	d	404	-	59,73,73	1.49	10 (16%)	67,113,113	2.34	19 (28%)
24	CLA	B	603	-	59,73,73	1.79	11 (18%)	67,113,113	2.08	15 (22%)
34	PGE	c	539	-	9,9,9	0.64	0	8,8,8	0.38	0
34	PGE	E	106	-	9,9,9	0.69	0	8,8,8	0.60	0
34	PGE	h	108	-	9,9,9	0.60	0	8,8,8	0.43	0
33	PG4	l	103	-	12,12,12	0.65	0	11,11,11	0.50	0
33	PG4	V	212	-	12,12,12	0.71	0	11,11,11	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	GOL	D	412	-	5,5,5	0.61	0	5,5,5	0.66	0
29	LMG	A	613	-	51,51,55	0.98	3 (5%)	59,59,63	1.02	3 (5%)
32	LHG	e	101	-	41,41,48	1.13	2 (4%)	44,47,54	1.18	4 (9%)
34	PGE	O	310	-	9,9,9	0.60	0	8,8,8	0.36	0
38	HTG	C	531	-	19,19,19	1.31	2 (10%)	23,24,24	1.01	2 (8%)
39	1PE	e	105	-	15,15,15	0.64	0	14,14,14	0.54	0
34	PGE	a	423	-	9,9,9	0.59	0	8,8,8	0.44	0
34	PGE	V	215	-	9,9,9	0.87	0	8,8,8	0.63	0
38	HTG	a	418	-	19,19,19	1.35	3 (15%)	23,24,24	1.84	8 (34%)
40	DGD	H	103	-	63,63,67	1.07	7 (11%)	77,77,81	1.22	11 (14%)
33	PG4	I	103	-	12,12,12	0.73	0	11,11,11	0.58	0
34	PGE	B	645	-	9,9,9	0.72	0	8,8,8	0.68	0
36	EDO	B	655	-	3,3,3	0.43	0	2,2,2	0.50	0
34	PGE	b	641	-	9,9,9	0.39	0	8,8,8	0.74	0
40	DGD	D	408	-	67,67,67	1.22	4 (5%)	81,81,81	1.61	10 (12%)
38	HTG	C	532	-	19,19,19	1.16	2 (10%)	23,24,24	1.79	5 (21%)
31	LMT	B	622	-	36,36,36	0.80	1 (2%)	47,47,47	1.45	7 (14%)
28	SQD	A	622	-	53,54,54	1.36	4 (7%)	62,65,65	1.52	9 (14%)
24	CLA	c	507	46	59,73,73	1.82	11 (18%)	67,113,113	2.14	18 (26%)
36	EDO	e	106	-	3,3,3	0.41	0	2,2,2	0.50	0
34	PGE	o	306	-	9,9,9	0.61	0	8,8,8	0.24	0
35	P6G	D	418	-	18,18,18	0.75	0	17,17,17	0.60	0
24	CLA	b	605	-	59,73,73	1.76	14 (23%)	67,113,113	2.78	21 (31%)
26	BCR	C	514	-	41,41,41	1.29	4 (9%)	56,56,56	1.85	13 (23%)
30	GOL	c	529	-	5,5,5	1.01	0	5,5,5	1.36	1 (20%)
39	1PE	V	217	-	15,15,15	0.94	0	14,14,14	1.01	1 (7%)
24	CLA	b	611	46	59,73,73	1.61	9 (15%)	67,113,113	2.40	23 (34%)
29	LMG	c	519	-	51,51,55	1.01	3 (5%)	59,59,63	1.39	8 (13%)
24	CLA	c	512	-	59,73,73	1.81	12 (20%)	67,113,113	2.30	21 (31%)
29	LMG	b	621	-	51,51,55	1.03	3 (5%)	59,59,63	1.66	7 (11%)
24	CLA	c	511	3	59,73,73	1.63	12 (20%)	67,113,113	2.09	20 (29%)
33	PG4	B	643	-	12,12,12	0.55	0	11,11,11	0.56	0
31	LMT	c	521	-	36,36,36	0.83	0	47,47,47	1.63	12 (25%)
30	GOL	u	201	-	5,5,5	0.72	0	5,5,5	1.10	0
26	BCR	C	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.62	11 (19%)
32	LHG	a	419	-	40,40,48	1.21	3 (7%)	43,46,54	1.38	6 (13%)
35	P6G	j	106	-	18,18,18	0.80	0	17,17,17	0.75	0
27	PL9	A	611	-	55,55,55	1.35	7 (12%)	68,69,69	2.10	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	HTG	c	522	-	19,19,19	0.72	0	23,24,24	1.44	3 (13%)
24	CLA	C	506	-	59,73,73	1.64	10 (16%)	67,113,113	2.27	17 (25%)
33	PG4	c	535	-	12,12,12	0.86	0	11,11,11	0.68	0
33	PG4	X	101	-	12,12,12	0.66	0	11,11,11	0.51	0
33	PG4	B	637	-	12,12,12	0.80	0	11,11,11	0.55	0
30	GOL	c	528	-	5,5,5	0.57	0	5,5,5	0.62	0
38	HTG	C	529	-	19,19,19	1.20	2 (10%)	23,24,24	2.27	4 (17%)
24	CLA	c	502	-	59,73,73	1.59	12 (20%)	67,113,113	2.38	17 (25%)
34	PGE	b	644	-	9,9,9	0.63	0	8,8,8	0.38	0
24	CLA	a	408	46	54,68,73	1.62	9 (16%)	61,107,113	2.37	18 (29%)
32	LHG	D	411	-	48,48,48	0.87	2 (4%)	51,54,54	0.84	3 (5%)
38	HTG	C	521	-	19,19,19	0.94	1 (5%)	23,24,24	1.05	1 (4%)
33	PG4	e	103	-	12,12,12	0.58	0	11,11,11	0.51	0
33	PG4	B	642	-	12,12,12	0.82	0	11,11,11	0.64	0
38	HTG	O	303	-	19,19,19	1.58	2 (10%)	23,24,24	1.07	2 (8%)
33	PG4	i	101	-	12,12,12	0.58	0	11,11,11	0.41	0
38	HTG	B	624	-	19,19,19	1.01	1 (5%)	23,24,24	1.90	5 (21%)
34	PGE	Y	102	-	9,9,9	0.79	0	8,8,8	0.62	0
26	BCR	b	618	-	41,41,41	1.14	3 (7%)	56,56,56	1.49	7 (12%)
34	PGE	A	620	-	6,6,9	0.64	0	5,5,8	0.90	0
26	BCR	A	610	-	41,41,41	1.23	5 (12%)	56,56,56	1.52	14 (25%)
31	LMT	Y	101	-	36,36,36	0.58	0	47,47,47	1.24	5 (10%)
35	P6G	B	651	-	18,18,18	0.52	0	17,17,17	0.67	0
36	EDO	B	656	-	3,3,3	1.06	0	2,2,2	0.21	0
33	PG4	c	532	-	12,12,12	0.90	0	11,11,11	0.81	0
24	CLA	b	602	46	59,73,73	1.81	10 (16%)	67,113,113	2.38	23 (34%)
30	GOL	a	415	-	5,5,5	1.09	0	5,5,5	1.12	1 (20%)
25	PHO	A	608	-	67,69,69	1.53	13 (19%)	85,99,99	1.79	17 (20%)
24	CLA	b	614	-	59,73,73	1.80	10 (16%)	67,113,113	2.16	16 (23%)
34	PGE	b	638	-	9,9,9	1.00	0	8,8,8	0.71	0
32	LHG	E	101	-	41,41,48	1.11	2 (4%)	44,47,54	1.14	3 (6%)
24	CLA	D	404	-	59,73,73	1.56	12 (20%)	67,113,113	2.24	20 (29%)
35	P6G	b	649	-	18,18,18	0.55	0	17,17,17	0.53	0
24	CLA	b	617	-	54,68,73	1.75	13 (24%)	61,107,113	2.62	22 (36%)
39	1PE	x	104	-	15,15,15	0.62	0	14,14,14	0.41	0
24	CLA	a	410	-	59,73,73	1.61	10 (16%)	67,113,113	2.31	22 (32%)
20	OEX	a	402	1,3,46	0,15,15	0.00	-	-	-	-
24	CLA	c	510	-	59,73,73	1.85	16 (27%)	67,113,113	2.10	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	GOL	B	626	-	5,5,5	0.82	0	5,5,5	0.70	0
34	PGE	o	308	-	9,9,9	0.69	0	8,8,8	0.56	0
35	P6G	T	105	-	18,18,18	0.68	0	17,17,17	0.96	0
24	CLA	c	509	-	59,73,73	1.70	11 (18%)	67,113,113	2.15	16 (23%)
31	LMT	I	101	-	36,36,36	0.89	1 (2%)	47,47,47	1.52	9 (19%)
33	PG4	B	636	-	12,12,12	0.57	0	11,11,11	0.59	0
34	PGE	c	538	-	9,9,9	0.91	0	8,8,8	0.88	0
24	CLA	B	616	-	59,73,73	1.46	10 (16%)	67,113,113	2.08	14 (20%)
26	BCR	C	525	-	41,41,41	1.13	3 (7%)	56,56,56	1.68	11 (19%)
34	PGE	D	415	-	9,9,9	0.59	0	8,8,8	0.41	0
34	PGE	f	105	-	9,9,9	0.58	0	8,8,8	0.26	0
31	LMT	F	102	-	36,36,36	1.09	3 (8%)	47,47,47	1.26	5 (10%)
34	PGE	i	106	-	9,9,9	0.83	0	8,8,8	0.64	0
35	P6G	d	416	-	18,18,18	0.64	0	17,17,17	0.59	0
30	GOL	B	625	-	5,5,5	0.69	0	5,5,5	1.86	2 (40%)
32	LHG	A	618	-	41,41,48	1.22	2 (4%)	44,47,54	1.21	5 (11%)
31	LMT	f	101	-	36,36,36	0.94	1 (2%)	47,47,47	1.33	5 (10%)
30	GOL	v	206	-	5,5,5	0.31	0	5,5,5	0.52	0
33	PG4	X	102	-	12,12,12	0.85	0	11,11,11	0.79	0
33	PG4	B	638	-	12,12,12	0.81	0	11,11,11	0.76	0
38	HTG	B	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.34	3 (13%)
29	LMG	B	621	-	51,51,55	1.09	4 (7%)	59,59,63	1.67	8 (13%)
25	PHO	a	409	-	67,69,69	1.65	11 (16%)	85,99,99	1.62	19 (22%)
34	PGE	j	105	-	9,9,9	0.64	0	8,8,8	0.59	0
30	GOL	t	101	-	5,5,5	1.24	0	5,5,5	1.10	1 (20%)
33	PG4	K	102	-	12,12,12	0.62	0	11,11,11	0.50	0
38	HTG	c	531	-	19,19,19	1.15	2 (10%)	23,24,24	1.87	7 (30%)
35	P6G	E	110	-	18,18,18	0.77	0	17,17,17	0.53	0
30	GOL	C	524	-	5,5,5	0.79	0	5,5,5	1.03	0
34	PGE	o	307	-	9,9,9	0.78	0	8,8,8	0.55	0
24	CLA	b	607	-	49,63,73	1.70	10 (20%)	55,101,113	2.24	20 (36%)
26	BCR	a	411	-	41,41,41	1.20	4 (9%)	56,56,56	1.34	6 (10%)
36	EDO	A	625	-	3,3,3	0.63	0	2,2,2	0.40	0
40	DGD	C	518	-	63,63,67	0.79	2 (3%)	77,77,81	1.10	6 (7%)
24	CLA	B	611	46	59,73,73	1.58	9 (15%)	67,113,113	2.48	24 (35%)
34	PGE	h	109	-	9,9,9	0.70	0	8,8,8	0.45	0
30	GOL	B	627	-	5,5,5	0.69	0	5,5,5	0.88	0
33	PG4	b	635	-	12,12,12	0.84	0	11,11,11	0.78	0
36	EDO	E	112	-	3,3,3	0.60	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	c	513	-	59,73,73	1.73	11 (18%)	67,113,113	2.24	17 (25%)
30	GOL	f	104	-	5,5,5	0.76	0	5,5,5	1.23	0
34	PGE	i	105	-	9,9,9	0.66	0	8,8,8	0.68	0
24	CLA	D	403	46	59,73,73	1.76	9 (15%)	67,113,113	2.10	14 (20%)
30	GOL	v	204	-	5,5,5	1.16	0	5,5,5	0.88	0
28	SQD	a	413	-	53,54,54	1.12	4 (7%)	62,65,65	2.14	12 (19%)
29	LMG	j	101	42	47,47,55	1.00	3 (6%)	55,55,63	1.04	3 (5%)
24	CLA	C	501	-	59,73,73	1.71	12 (20%)	67,113,113	2.62	17 (25%)
25	PHO	D	401	-	67,69,69	1.77	16 (23%)	85,99,99	1.72	16 (18%)
36	EDO	H	112	-	3,3,3	0.50	0	2,2,2	0.37	0
30	GOL	B	635	-	5,5,5	0.78	0	5,5,5	1.17	0
32	LHG	B	632	-	48,48,48	0.80	2 (4%)	51,54,54	1.30	7 (13%)
24	CLA	c	506	-	59,73,73	1.60	12 (20%)	67,113,113	2.09	19 (28%)
30	GOL	v	207	-	5,5,5	0.50	0	5,5,5	0.34	0
36	EDO	J	109	-	3,3,3	0.43	0	2,2,2	0.34	0
34	PGE	J	108	-	9,9,9	0.57	0	8,8,8	0.52	0
28	SQD	a	424	-	53,54,54	1.31	3 (5%)	62,65,65	2.01	14 (22%)
30	GOL	V	206	-	5,5,5	0.56	0	5,5,5	0.19	0
24	CLA	B	617	-	54,68,73	1.76	12 (22%)	61,107,113	2.38	21 (34%)
26	BCR	t	102	-	41,41,41	1.13	3 (7%)	56,56,56	1.98	18 (32%)
36	EDO	E	111	-	3,3,3	0.67	0	2,2,2	0.39	0
29	LMG	a	414	-	51,51,55	0.85	2 (3%)	59,59,63	1.26	5 (8%)
34	PGE	H	109	-	9,9,9	0.53	0	8,8,8	0.48	0
26	BCR	B	619	-	41,41,41	1.19	5 (12%)	56,56,56	1.45	8 (14%)
30	GOL	o	303	-	5,5,5	0.76	0	5,5,5	0.65	0
28	SQD	b	633	-	53,54,54	1.43	5 (9%)	62,65,65	1.99	16 (25%)
33	PG4	x	102	-	12,12,12	0.64	0	11,11,11	0.37	0
30	GOL	B	628	-	5,5,5	0.76	0	5,5,5	1.66	1 (20%)
39	1PE	j	107	-	15,15,15	0.63	0	14,14,14	0.63	0
34	PGE	B	647	-	9,9,9	0.70	0	8,8,8	0.67	0
30	GOL	c	525	-	5,5,5	0.46	0	5,5,5	1.43	1 (20%)
26	BCR	B	620	-	41,41,41	1.14	3 (7%)	56,56,56	1.37	7 (12%)
28	SQD	A	616	-	53,54,54	1.18	4 (7%)	62,65,65	1.56	10 (16%)
24	CLA	b	608	46	59,73,73	1.61	10 (16%)	67,113,113	1.79	12 (17%)
33	PG4	E	103	-	12,12,12	0.64	0	11,11,11	0.53	0
32	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.18	3 (5%)
30	GOL	b	628	-	5,5,5	0.83	0	5,5,5	0.42	0
35	P6G	I	106	-	18,18,18	0.64	0	17,17,17	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PGE	E	109	-	9,9,9	0.84	0	8,8,8	0.58	0
31	LMT	C	533	-	36,36,36	0.68	1 (2%)	47,47,47	1.09	1 (2%)
26	BCR	B	618	-	41,41,41	0.98	0	56,56,56	1.54	10 (17%)
32	LHG	D	409	-	48,48,48	0.83	2 (4%)	51,54,54	1.48	5 (9%)
34	PGE	O	309	-	9,9,9	0.81	0	8,8,8	0.99	1 (12%)
34	PGE	t	104	-	9,9,9	0.83	0	8,8,8	0.70	0
26	BCR	d	406	-	41,41,41	1.48	4 (9%)	56,56,56	2.20	17 (30%)
24	CLA	B	606	-	59,73,73	1.72	11 (18%)	67,113,113	2.53	24 (35%)
38	HTG	b	631	-	19,19,19	1.32	2 (10%)	23,24,24	1.71	6 (26%)
27	PL9	d	407	-	55,55,55	1.27	8 (14%)	68,69,69	1.32	10 (14%)
24	CLA	D	405	-	59,73,73	1.59	8 (13%)	67,113,113	2.25	16 (23%)
33	PG4	J	105	-	12,12,12	0.69	0	11,11,11	0.37	0
30	GOL	f	103	42	5,5,5	0.67	0	5,5,5	0.89	0
24	CLA	B	610	-	59,73,73	1.46	7 (11%)	67,113,113	2.42	19 (28%)
36	EDO	o	311	-	3,3,3	0.48	0	2,2,2	0.28	0
24	CLA	B	614	-	59,73,73	1.61	10 (16%)	67,113,113	2.14	16 (23%)
33	PG4	i	104	-	12,12,12	0.51	0	11,11,11	0.41	0
30	GOL	T	101	-	5,5,5	0.94	0	5,5,5	0.86	0
33	PG4	B	640	-	12,12,12	0.67	0	11,11,11	0.43	0
30	GOL	T	103	-	5,5,5	0.73	0	5,5,5	0.70	0
36	EDO	O	311	-	3,3,3	0.67	0	2,2,2	0.29	0
31	LMT	M	101	-	36,36,36	0.96	3 (8%)	47,47,47	1.80	15 (31%)
38	HTG	b	623	-	19,19,19	1.21	2 (10%)	23,24,24	1.58	5 (21%)
30	GOL	m	103	-	5,5,5	0.28	0	5,5,5	0.57	0
31	LMT	t	103	-	36,36,36	0.85	0	47,47,47	1.40	8 (17%)
24	CLA	C	502	-	59,73,73	1.53	9 (15%)	67,113,113	2.29	18 (26%)
24	CLA	B	602	46	59,73,73	1.77	11 (18%)	67,113,113	2.87	25 (37%)
26	BCR	k	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.65	11 (19%)
40	DGD	c	517	-	58,58,67	1.00	4 (6%)	72,72,81	1.12	3 (4%)
41	HEM	E	113	6,5	27,50,50	1.08	1 (3%)	17,82,82	3.78	8 (47%)
31	LMT	J	103	-	36,36,36	0.93	1 (2%)	47,47,47	1.56	9 (19%)
35	P6G	d	415	-	18,18,18	0.69	0	17,17,17	0.96	1 (5%)
26	BCR	c	515	-	41,41,41	1.25	2 (4%)	56,56,56	1.65	12 (21%)
32	LHG	D	410	-	48,48,48	0.87	2 (4%)	51,54,54	0.98	1 (1%)
28	SQD	l	102	-	53,54,54	1.30	4 (7%)	62,65,65	1.86	14 (22%)
30	GOL	v	205	-	5,5,5	0.44	0	5,5,5	0.59	0
36	EDO	o	310	-	3,3,3	0.62	0	2,2,2	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	SQD	a	417	-	53,54,54	1.25	4 (7%)	62,65,65	1.26	5 (8%)
33	PG4	I	104	-	12,12,12	0.50	0	11,11,11	0.48	0
35	P6G	B	652	-	18,18,18	0.83	0	17,17,17	1.10	1 (5%)
34	PGE	h	107	-	9,9,9	0.77	0	8,8,8	0.69	0
38	HTG	V	204	-	19,19,19	0.97	1 (5%)	23,24,24	2.71	7 (30%)
35	P6G	A	624	-	18,18,18	0.59	0	17,17,17	0.55	0
32	LHG	d	410	-	48,48,48	0.80	2 (4%)	51,54,54	1.11	3 (5%)
24	CLA	C	505	-	59,73,73	1.81	12 (20%)	67,113,113	2.24	16 (23%)
30	GOL	O	302	-	5,5,5	1.49	1 (20%)	5,5,5	0.94	0
28	SQD	h	105	-	53,54,54	1.43	6 (11%)	62,65,65	1.53	9 (14%)
24	CLA	B	607	-	49,63,73	1.65	12 (24%)	55,101,113	2.59	17 (30%)
29	LMG	B	634	-	55,55,55	1.25	3 (5%)	63,63,63	1.42	12 (19%)
24	CLA	C	508	-	54,68,73	1.75	12 (22%)	61,107,113	2.51	17 (27%)
24	CLA	b	615	-	59,73,73	1.60	11 (18%)	67,113,113	2.04	20 (29%)
33	PG4	U	202	-	12,12,12	0.69	0	11,11,11	0.47	0
24	CLA	C	512	-	59,73,73	1.64	12 (20%)	67,113,113	2.07	21 (31%)
36	EDO	V	218	-	3,3,3	0.91	0	2,2,2	0.21	0
24	CLA	b	603	-	59,73,73	1.68	9 (15%)	67,113,113	2.14	18 (26%)
30	GOL	O	304	-	5,5,5	0.43	0	5,5,5	0.52	0
31	LMT	j	103	-	36,36,36	0.74	1 (2%)	47,47,47	1.43	4 (8%)
33	PG4	H	106	-	12,12,12	0.73	0	11,11,11	0.63	0
30	GOL	b	630	-	5,5,5	0.46	0	5,5,5	0.31	0
33	PG4	e	104	-	12,12,12	0.60	0	11,11,11	0.56	0
30	GOL	A	615	-	5,5,5	0.53	0	5,5,5	1.05	0
34	PGE	E	104	-	9,9,9	0.56	0	8,8,8	0.46	0
23	BCT	a	406	21	0,3,3	0.00	-	0,3,3	0.00	-
30	GOL	d	413	-	5,5,5	0.77	0	5,5,5	0.92	0
33	PG4	b	636	-	12,12,12	0.77	0	11,11,11	0.68	0
24	CLA	b	609	-	59,73,73	1.58	10 (16%)	67,113,113	2.23	19 (28%)
33	PG4	V	213	-	12,12,12	0.71	0	11,11,11	0.63	0
39	1PE	B	654	-	15,15,15	0.77	0	14,14,14	0.90	0
30	GOL	v	203	-	5,5,5	0.75	0	5,5,5	0.64	0
34	PGE	V	214	-	9,9,9	0.63	0	8,8,8	0.30	0
43	HEC	v	202	16	26,50,50	1.03	2 (7%)	18,82,82	1.94	7 (38%)
28	SQD	F	104	-	53,54,54	1.43	5 (9%)	62,65,65	2.09	17 (27%)
43	HEC	V	203	16	26,50,50	1.22	3 (11%)	18,82,82	1.78	5 (27%)
26	BCR	b	619	-	41,41,41	1.27	5 (12%)	56,56,56	1.78	14 (25%)
23	BCT	m	104[B]	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	PG4	J	104	-	12,12,12	0.59	0	11,11,11	0.31	0
24	CLA	B	604	-	59,73,73	1.69	10 (16%)	67,113,113	2.33	17 (25%)
34	PGE	c	536	-	9,9,9	0.61	0	8,8,8	0.27	0
34	PGE	A	621	-	9,9,9	0.73	0	8,8,8	0.48	0
40	DGD	C	516	-	63,63,67	0.89	5 (7%)	77,77,81	1.29	10 (12%)
34	PGE	B	650	-	9,9,9	0.63	0	8,8,8	0.38	0
33	PG4	C	538	-	12,12,12	0.76	0	11,11,11	0.55	0
35	P6G	D	416	-	18,18,18	0.72	0	17,17,17	0.60	0
35	P6G	b	648	-	18,18,18	0.62	0	17,17,17	0.74	0
36	EDO	c	542	-	3,3,3	0.62	0	2,2,2	0.39	0
24	CLA	B	613	-	59,73,73	1.45	8 (13%)	67,113,113	1.80	12 (17%)
30	GOL	d	402	-	5,5,5	0.62	0	5,5,5	0.96	1 (20%)
24	CLA	C	507	46	59,73,73	1.72	11 (18%)	67,113,113	2.24	18 (26%)
40	DGD	c	516	-	63,63,67	0.90	3 (4%)	77,77,81	1.10	4 (5%)
31	LMT	u	203	-	36,36,36	1.28	4 (11%)	47,47,47	1.67	9 (19%)
30	GOL	a	416	-	5,5,5	0.62	0	5,5,5	0.79	0
24	CLA	A	606	-	59,73,73	1.71	9 (15%)	67,113,113	2.11	18 (26%)
33	PG4	C	535	-	12,12,12	0.95	0	11,11,11	0.83	0
33	PG4	I	102	-	12,12,12	0.61	0	11,11,11	0.42	0
33	PG4	C	534	-	12,12,12	0.72	0	11,11,11	0.41	0
28	SQD	x	101	-	53,54,54	1.26	4 (7%)	62,65,65	1.83	11 (17%)
34	PGE	b	639	-	9,9,9	0.62	0	8,8,8	0.44	0
26	BCR	c	527	-	41,41,41	1.04	2 (4%)	56,56,56	1.40	9 (16%)
33	PG4	V	209	-	12,12,12	0.85	0	11,11,11	1.01	1 (9%)
24	CLA	c	505	-	59,73,73	1.56	10 (16%)	67,113,113	2.32	17 (25%)
34	PGE	H	111	-	9,9,9	0.66	0	8,8,8	0.39	0
30	GOL	C	527	-	5,5,5	0.48	0	5,5,5	0.29	0
34	PGE	b	640	-	9,9,9	0.64	0	8,8,8	0.31	0
30	GOL	V	208	-	5,5,5	0.48	0	5,5,5	0.46	0
30	GOL	o	305	-	5,5,5	0.68	0	5,5,5	0.97	0
40	DGD	C	517	-	57,57,67	0.88	3 (5%)	71,71,81	1.09	2 (2%)
24	CLA	C	510	-	59,73,73	1.69	11 (18%)	67,113,113	2.19	19 (28%)
34	PGE	B	649	-	9,9,9	0.89	0	8,8,8	0.55	0
44	2PE	V	216	-	27,27,27	0.92	0	26,26,26	0.69	0
30	GOL	O	306	-	5,5,5	1.26	1 (20%)	5,5,5	1.12	1 (20%)
33	PG4	a	421	-	12,12,12	0.63	0	11,11,11	0.62	0
38	HTG	H	101	-	19,19,19	1.11	2 (10%)	23,24,24	1.56	5 (21%)
29	LMG	C	519	-	51,51,55	1.12	3 (5%)	59,59,63	1.52	7 (11%)
38	HTG	C	530	-	19,19,19	1.05	1 (5%)	23,24,24	1.19	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	PGE	x	103	-	9,9,9	0.60	0	8,8,8	0.58	0
34	PGE	c	540	-	9,9,9	0.67	0	8,8,8	0.46	0
33	PG4	H	105	-	12,12,12	0.74	0	11,11,11	0.48	0
24	CLA	C	503	-	59,73,73	1.75	11 (18%)	67,113,113	2.36	17 (25%)
26	BCR	b	620	-	41,41,41	1.00	2 (4%)	56,56,56	1.39	4 (7%)
34	PGE	I	105	-	9,9,9	0.96	0	8,8,8	0.75	0
24	CLA	b	613	-	59,73,73	1.75	13 (22%)	67,113,113	2.14	16 (23%)
30	GOL	A	614	-	5,5,5	1.17	0	5,5,5	0.88	0
34	PGE	B	644	-	9,9,9	0.57	0	8,8,8	0.44	0
34	PGE	E	105	-	9,9,9	0.73	0	8,8,8	0.47	0
38	HTG	c	530	-	19,19,19	1.69	3 (15%)	23,24,24	1.24	3 (13%)
30	GOL	b	629	-	5,5,5	0.67	0	5,5,5	1.11	0
33	PG4	D	414	-	12,12,12	0.66	0	11,11,11	0.51	0
33	PG4	a	420	-	12,12,12	0.57	0	11,11,11	0.38	0
30	GOL	b	625	-	5,5,5	0.52	0	5,5,5	1.54	1 (20%)
33	PG4	B	641	-	12,12,12	0.72	0	11,11,11	0.61	0
30	GOL	C	523	-	5,5,5	0.68	0	5,5,5	2.18	2 (40%)
30	GOL	U	201	-	5,5,5	0.53	0	5,5,5	1.10	0
24	CLA	B	615	-	49,63,73	1.78	8 (16%)	55,101,113	2.34	19 (34%)
40	DGD	c	518	-	63,63,67	0.91	3 (4%)	77,77,81	0.98	6 (7%)
30	GOL	e	102	-	5,5,5	0.69	0	5,5,5	0.81	0
29	LMG	C	520	-	51,51,55	1.26	3 (5%)	59,59,63	1.27	9 (15%)
27	PL9	D	407	-	55,55,55	1.43	8 (14%)	68,69,69	1.36	6 (8%)
24	CLA	C	513	-	59,73,73	1.66	10 (16%)	67,113,113	2.39	21 (31%)
34	PGE	o	309	-	9,9,9	0.84	0	8,8,8	0.71	0
36	EDO	X	104	-	3,3,3	0.95	0	2,2,2	0.48	0
27	PL9	a	412	-	55,55,55	1.35	2 (3%)	68,69,69	1.79	14 (20%)
29	LMG	d	412	-	55,55,55	1.05	3 (5%)	63,63,63	1.17	5 (7%)
34	PGE	a	422	-	9,9,9	0.67	0	8,8,8	0.73	0
40	DGD	h	104	-	63,63,67	1.12	5 (7%)	77,77,81	1.26	8 (10%)
30	GOL	V	201	-	5,5,5	1.03	0	5,5,5	0.49	0
38	HTG	B	631	-	19,19,19	1.10	3 (15%)	23,24,24	1.20	2 (8%)
33	PG4	c	533	-	12,12,12	0.59	0	11,11,11	0.48	0
34	PGE	b	642	-	9,9,9	0.66	0	8,8,8	0.20	0
40	DGD	d	408	-	67,67,67	1.32	4 (5%)	81,81,81	1.76	10 (12%)
29	LMG	J	101	42	47,47,55	0.74	2 (4%)	55,55,63	0.90	2 (3%)
24	CLA	c	501	-	59,73,73	1.51	8 (13%)	67,113,113	2.53	16 (23%)
34	PGE	O	308	-	9,9,9	0.99	0	8,8,8	1.28	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMT	M	102	-	36,36,36	0.90	0	47,47,47	1.57	2 (4%)
24	CLA	d	405	-	59,73,73	1.80	12 (20%)	67,113,113	2.18	18 (26%)
24	CLA	b	610	-	59,73,73	1.71	11 (18%)	67,113,113	2.31	18 (26%)
24	CLA	b	616	-	59,73,73	1.76	8 (13%)	67,113,113	2.27	17 (25%)
34	PGE	b	643	-	9,9,9	0.86	0	8,8,8	0.62	0
35	P6G	D	417	-	18,18,18	0.64	0	17,17,17	0.88	1 (5%)
31	LMT	a	401	-	36,36,36	0.83	1 (2%)	47,47,47	1.42	4 (8%)
31	LMT	b	622	-	36,36,36	0.84	1 (2%)	47,47,47	1.42	5 (10%)
34	PGE	c	537	-	9,9,9	0.54	0	8,8,8	0.35	0
34	PGE	H	108	-	9,9,9	0.60	0	8,8,8	0.60	0
38	HTG	o	301	-	19,19,19	2.03	2 (10%)	23,24,24	1.08	1 (4%)
24	CLA	B	605	-	59,73,73	1.63	10 (16%)	67,113,113	2.58	25 (37%)
33	PG4	b	634	-	12,12,12	0.81	0	11,11,11	0.68	0
30	GOL	u	202	-	5,5,5	0.81	0	5,5,5	0.39	0
30	GOL	c	526	-	5,5,5	0.39	0	5,5,5	0.84	0
30	GOL	V	207	-	5,5,5	0.76	0	5,5,5	0.81	0
38	HTG	c	523	-	19,19,19	0.92	2 (10%)	23,24,24	1.49	5 (21%)
41	HEM	e	107	6,5	27,50,50	0.84	1 (3%)	17,82,82	1.94	4 (23%)
26	BCR	H	102	-	41,41,41	1.07	3 (7%)	56,56,56	1.76	17 (30%)
36	EDO	C	542	-	3,3,3	0.51	0	2,2,2	0.37	0
34	PGE	J	106	-	9,9,9	0.63	0	8,8,8	0.34	0
20	OEX	A	601	1,3,46	0,15,15	0.00	-	-	-	-
35	P6G	A	623	-	18,18,18	0.69	0	17,17,17	0.56	0
33	PG4	B	639	-	12,12,12	0.90	0	11,11,11	0.73	0
30	GOL	y	101	-	5,5,5	0.66	0	5,5,5	0.69	0
24	CLA	C	509	-	59,73,73	1.47	8 (13%)	67,113,113	2.23	19 (28%)
38	HTG	B	630	-	19,19,19	1.09	2 (10%)	23,24,24	1.59	8 (34%)
33	PG4	V	210	-	12,12,12	0.91	0	11,11,11	0.78	0
36	EDO	a	425	-	3,3,3	0.61	0	2,2,2	0.06	0
30	GOL	b	627	-	5,5,5	1.23	1 (20%)	5,5,5	1.34	1 (20%)
29	LMG	c	520	-	51,51,55	1.18	3 (5%)	59,59,63	1.19	5 (8%)
45	PE8	i	107	-	24,24,24	0.69	0	23,23,23	0.69	0
32	LHG	d	411	-	48,48,48	1.00	3 (6%)	51,54,54	0.84	2 (3%)
24	CLA	C	504	46	54,68,73	1.81	13 (24%)	61,107,113	2.20	17 (27%)
34	PGE	C	540	-	9,9,9	0.60	0	8,8,8	0.33	0
26	BCR	T	102	-	41,41,41	1.05	4 (9%)	56,56,56	1.62	11 (19%)
34	PGE	J	107	-	9,9,9	0.68	0	8,8,8	0.54	0
24	CLA	B	608	46	59,73,73	1.57	8 (13%)	67,113,113	2.16	19 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	GOL	C	528	-	5,5,5	0.67	0	5,5,5	3.00	3 (60%)
28	SQD	A	612	-	53,54,54	1.12	4 (7%)	62,65,65	2.16	14 (22%)
33	PG4	C	536	-	12,12,12	0.69	0	11,11,11	0.65	0
34	PGE	B	648	-	9,9,9	0.86	0	8,8,8	0.73	0
34	PGE	b	645	-	9,9,9	0.54	0	8,8,8	0.41	0
26	BCR	h	103	-	41,41,41	1.14	4 (9%)	56,56,56	1.76	16 (28%)
35	P6G	c	541	-	18,18,18	0.51	0	17,17,17	0.42	0
33	PG4	V	211	-	12,12,12	1.02	0	11,11,11	0.81	0
30	GOL	B	629	-	5,5,5	0.91	0	5,5,5	0.38	0
24	CLA	d	403	46	59,73,73	1.67	9 (15%)	67,113,113	1.93	16 (23%)
23	BCT	A	605	21	0,3,3	0.00	-	0,3,3	0.00	-
36	EDO	i	108	-	3,3,3	0.43	0	2,2,2	0.42	0
24	CLA	c	508	-	54,68,73	1.63	10 (18%)	61,107,113	2.54	19 (31%)
33	PG4	b	637	-	12,12,12	0.78	0	11,11,11	0.56	0
30	GOL	b	626	-	5,5,5	0.79	0	5,5,5	0.77	0
23	BCT	m	104[A]	-	0,3,3	0.00	-	0,3,3	0.00	-
39	1PE	L	101	-	15,15,15	0.68	0	14,14,14	0.67	0
25	PHO	d	401	-	67,69,69	1.60	11 (16%)	85,99,99	1.87	17 (20%)
26	BCR	D	406	-	41,41,41	1.43	5 (12%)	56,56,56	1.96	12 (21%)
34	PGE	B	646	-	9,9,9	0.54	0	8,8,8	0.48	0
30	GOL	B	633	-	5,5,5	1.24	1 (20%)	5,5,5	1.25	0
30	GOL	D	413	-	5,5,5	0.56	0	5,5,5	0.84	0
34	PGE	E	108	-	9,9,9	0.56	0	8,8,8	0.40	0
24	CLA	b	604	-	59,73,73	1.62	10 (16%)	67,113,113	2.25	20 (29%)
24	CLA	b	612	-	59,73,73	1.45	11 (18%)	67,113,113	2.32	19 (28%)
33	PG4	C	537	-	12,12,12	0.66	0	11,11,11	0.57	0
34	PGE	b	647	-	9,9,9	0.59	0	8,8,8	0.42	0
24	CLA	B	612	-	59,73,73	1.56	10 (16%)	67,113,113	2.44	17 (25%)
33	PG4	H	104	-	12,12,12	0.62	0	11,11,11	0.34	0
24	CLA	c	503	-	59,73,73	1.55	10 (16%)	67,113,113	1.94	17 (25%)
30	GOL	O	307	-	5,5,5	0.50	0	5,5,5	0.21	0
30	GOL	F	101	42	5,5,5	0.52	0	5,5,5	0.73	0
32	LHG	d	409	-	48,48,48	0.85	3 (6%)	51,54,54	1.37	6 (11%)
33	PG4	h	106	-	12,12,12	0.57	0	11,11,11	0.48	0
33	PG4	d	414	-	12,12,12	0.72	0	11,11,11	0.45	0
35	P6G	C	541	-	18,18,18	0.66	0	17,17,17	0.43	0
33	PG4	A	619	-	12,12,12	0.71	0	11,11,11	0.61	0
34	PGE	h	110	-	9,9,9	0.79	0	8,8,8	0.68	0
30	GOL	o	304	-	5,5,5	0.50	0	5,5,5	0.86	0
24	CLA	b	606	-	59,73,73	1.81	9 (15%)	67,113,113	2.47	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	GOL	V	205	-	5,5,5	0.92	0	5,5,5	1.09	0
34	PGE	H	110	-	9,9,9	0.56	0	8,8,8	0.34	0
24	CLA	A	609	-	59,73,73	1.52	9 (15%)	67,113,113	2.40	20 (29%)
30	GOL	O	305	-	5,5,5	0.45	0	5,5,5	0.34	0
24	CLA	A	607	46	54,68,73	1.54	10 (18%)	61,107,113	2.27	16 (26%)
33	PG4	H	107	-	12,12,12	0.70	0	11,11,11	0.50	0
38	HTG	b	624	-	19,19,19	1.51	2 (10%)	23,24,24	1.32	2 (8%)
39	1PE	B	653	-	15,15,15	0.61	0	14,14,14	0.41	0
24	CLA	a	407	-	59,73,73	1.52	7 (11%)	67,113,113	2.12	19 (28%)
24	CLA	c	504	46	54,68,73	1.85	13 (24%)	61,107,113	2.29	18 (29%)
36	EDO	B	657	-	3,3,3	0.65	0	2,2,2	0.06	0
33	PG4	c	534	-	12,12,12	0.54	0	11,11,11	0.43	0
34	PGE	C	539	-	9,9,9	0.92	0	8,8,8	0.86	0
33	PG4	X	103	-	12,12,12	0.76	0	11,11,11	0.54	0
36	EDO	d	417	-	3,3,3	0.70	0	2,2,2	0.40	0
33	PG4	i	102	-	12,12,12	0.57	0	11,11,11	0.52	0
26	BCR	c	514	-	41,41,41	1.21	5 (12%)	56,56,56	1.70	14 (25%)
36	EDO	B	658	-	3,3,3	0.46	0	2,2,2	0.44	0
34	PGE	b	646	-	9,9,9	0.66	0	8,8,8	0.51	0
34	PGE	E	107	-	9,9,9	0.77	0	8,8,8	0.76	0
33	PG4	E	102	-	12,12,12	0.61	0	11,11,11	0.58	0
29	LMG	z	101	-	55,55,55	1.03	2 (3%)	63,63,63	1.18	5 (7%)
26	BCR	K	101	-	41,41,41	0.97	1 (2%)	56,56,56	1.49	11 (19%)
33	PG4	i	103	-	12,12,12	0.64	0	11,11,11	0.48	0
36	EDO	I	107	-	3,3,3	0.75	0	2,2,2	0.20	0
33	PG4	j	104	-	12,12,12	0.70	0	11,11,11	0.72	0
38	HTG	h	101	-	19,19,19	1.17	2 (10%)	23,24,24	1.75	5 (21%)
24	CLA	B	609	-	59,73,73	1.47	8 (13%)	67,113,113	2.12	15 (22%)
24	CLA	C	511	3	59,73,73	1.67	8 (13%)	67,113,113	2.01	18 (26%)
36	EDO	D	419	-	3,3,3	0.71	0	2,2,2	0.08	0
31	LMT	A	617	-	36,36,36	1.10	2 (5%)	47,47,47	1.58	9 (19%)

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
29	LMG	C	526	-	-	27/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	HTG	b	632	-	-	2/10/30/30	0/1/1/1
34	PGE	t	105	-	-	1/4/4/7	-
38	HTG	C	522	-	-	4/10/30/30	0/1/1/1
34	PGE	T	104	-	-	1/4/4/7	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
30	GOL	D	402	-	-	2/4/4/4	-
31	LMT	m	101	-	-	5/21/61/61	0/2/2/2
24	CLA	d	404	-	3/3/20/25	2/37/135/135	-
24	CLA	B	603	-	3/3/20/25	5/37/135/135	-
34	PGE	c	539	-	-	1/7/7/7	-
34	PGE	E	106	-	-	3/7/7/7	-
34	PGE	h	108	-	-	4/7/7/7	-
33	PG4	l	103	-	-	3/10/10/10	-
33	PG4	V	212	-	-	5/10/10/10	-
30	GOL	D	412	-	-	4/4/4/4	-
29	LMG	A	613	-	-	20/46/66/70	0/1/1/1
32	LHG	e	101	-	-	26/46/46/53	-
34	PGE	O	310	-	-	5/7/7/7	-
38	HTG	C	531	-	-	7/10/30/30	0/1/1/1
39	1PE	e	105	-	-	7/13/13/13	-
34	PGE	a	423	-	-	2/7/7/7	-
34	PGE	V	215	-	-	4/7/7/7	-
38	HTG	a	418	-	-	7/10/30/30	0/1/1/1
40	DGD	H	103	-	-	10/51/91/95	0/2/2/2
33	PG4	I	103	-	-	5/10/10/10	-
34	PGE	B	645	-	-	5/7/7/7	-
36	EDO	B	655	-	-	0/1/1/1	-
34	PGE	b	641	-	-	3/7/7/7	-
40	DGD	D	408	-	-	30/55/95/95	0/2/2/2
38	HTG	C	532	-	-	2/10/30/30	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
28	SQD	A	622	-	-	25/49/69/69	0/1/1/1
24	CLA	c	507	46	3/3/20/25	2/37/135/135	-
36	EDO	e	106	-	-	1/1/1/1	-
34	PGE	o	306	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	P6G	D	418	-	-	7/16/16/16	-
24	CLA	b	605	-	3/3/20/25	7/37/135/135	-
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
30	GOL	c	529	-	-	2/4/4/4	-
39	1PE	V	217	-	-	5/13/13/13	-
24	CLA	b	611	46	3/3/20/25	5/37/135/135	-
29	LMG	c	519	-	-	19/46/66/70	0/1/1/1
24	CLA	c	512	-	3/3/20/25	8/37/135/135	-
29	LMG	b	621	-	-	13/46/66/70	0/1/1/1
24	CLA	c	511	3	3/3/20/25	2/37/135/135	-
33	PG4	B	643	-	-	5/10/10/10	-
31	LMT	c	521	-	-	8/21/61/61	0/2/2/2
30	GOL	u	201	-	-	0/4/4/4	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
32	LHG	a	419	-	-	22/45/45/53	-
35	P6G	j	106	-	-	8/16/16/16	-
27	PL9	A	611	-	-	9/53/73/73	0/1/1/1
38	HTG	c	522	-	-	4/10/30/30	0/1/1/1
24	CLA	C	506	-	3/3/20/25	11/37/135/135	-
33	PG4	c	535	-	-	4/10/10/10	-
33	PG4	X	101	-	-	3/10/10/10	-
33	PG4	B	637	-	-	4/10/10/10	-
30	GOL	c	528	-	-	4/4/4/4	-
38	HTG	C	529	-	-	5/10/30/30	0/1/1/1
24	CLA	c	502	-	3/3/20/25	3/37/135/135	-
34	PGE	b	644	-	-	3/7/7/7	-
24	CLA	a	408	46	3/3/19/25	5/31/129/135	-
32	LHG	D	411	-	-	8/53/53/53	-
38	HTG	C	521	-	-	4/10/30/30	0/1/1/1
33	PG4	e	103	-	-	4/10/10/10	-
33	PG4	B	642	-	-	5/10/10/10	-
38	HTG	O	303	-	-	1/10/30/30	0/1/1/1
33	PG4	i	101	-	-	7/10/10/10	-
38	HTG	B	624	-	-	4/10/30/30	0/1/1/1
34	PGE	Y	102	-	-	4/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2
34	PGE	A	620	-	-	2/4/4/7	-
26	BCR	A	610	-	-	2/29/63/63	0/2/2/2
31	LMT	Y	101	-	-	11/21/61/61	0/2/2/2
35	P6G	B	651	-	-	7/16/16/16	-
36	EDO	B	656	-	-	1/1/1/1	-
33	PG4	c	532	-	-	6/10/10/10	-
24	CLA	b	602	46	3/3/20/25	15/37/135/135	-
30	GOL	a	415	-	-	0/4/4/4	-
25	PHO	A	608	-	-	2/53/103/103	0/5/6/6
24	CLA	b	614	-	3/3/20/25	0/37/135/135	-
34	PGE	b	638	-	-	3/7/7/7	-
32	LHG	E	101	-	-	16/46/46/53	-
24	CLA	D	404	-	3/3/20/25	4/37/135/135	-
35	P6G	b	649	-	-	10/16/16/16	-
24	CLA	b	617	-	3/3/19/25	6/31/129/135	-
39	1PE	x	104	-	-	9/13/13/13	-
24	CLA	a	410	-	3/3/20/25	9/37/135/135	-
24	CLA	c	510	-	3/3/20/25	5/37/135/135	-
30	GOL	B	626	-	-	0/4/4/4	-
34	PGE	o	308	-	-	5/7/7/7	-
35	P6G	T	105	-	-	12/16/16/16	-
24	CLA	c	509	-	3/3/20/25	7/37/135/135	-
31	LMT	I	101	-	-	7/21/61/61	0/2/2/2
33	PG4	B	636	-	-	4/10/10/10	-
34	PGE	c	538	-	-	2/7/7/7	-
24	CLA	B	616	-	2/2/20/25	6/37/135/135	-
26	BCR	C	525	-	-	2/29/63/63	0/2/2/2
34	PGE	D	415	-	-	6/7/7/7	-
34	PGE	f	105	-	-	2/7/7/7	-
31	LMT	F	102	-	-	6/21/61/61	0/2/2/2
34	PGE	i	106	-	-	4/7/7/7	-
35	P6G	d	416	-	-	8/16/16/16	-
30	GOL	B	625	-	-	2/4/4/4	-
32	LHG	A	618	-	-	23/46/46/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	f	101	-	-	3/21/61/61	0/2/2/2
30	GOL	v	206	-	-	2/4/4/4	-
33	PG4	X	102	-	-	4/10/10/10	-
33	PG4	B	638	-	-	6/10/10/10	-
38	HTG	B	623	-	-	3/10/30/30	0/1/1/1
29	LMG	B	621	-	-	12/46/66/70	0/1/1/1
25	PHO	a	409	-	-	2/53/103/103	0/5/6/6
34	PGE	j	105	-	-	4/7/7/7	-
30	GOL	t	101	-	-	0/4/4/4	-
33	PG4	K	102	-	-	4/10/10/10	-
38	HTG	c	531	-	-	8/10/30/30	0/1/1/1
35	P6G	E	110	-	-	11/16/16/16	-
30	GOL	C	524	-	-	0/4/4/4	-
34	PGE	o	307	-	-	5/7/7/7	-
24	CLA	b	607	-	3/3/18/25	3/25/123/135	-
26	BCR	a	411	-	-	0/29/63/63	0/2/2/2
36	EDO	A	625	-	-	0/1/1/1	-
40	DGD	C	518	-	-	10/51/91/95	0/2/2/2
24	CLA	B	611	46	3/3/20/25	4/37/135/135	-
34	PGE	h	109	-	-	4/7/7/7	-
30	GOL	B	627	-	-	2/4/4/4	-
33	PG4	b	635	-	-	5/10/10/10	-
36	EDO	E	112	-	-	0/1/1/1	-
24	CLA	c	513	-	3/3/20/25	1/37/135/135	-
30	GOL	f	104	-	-	4/4/4/4	-
34	PGE	i	105	-	-	4/7/7/7	-
24	CLA	D	403	46	3/3/20/25	5/37/135/135	-
30	GOL	v	204	-	-	1/4/4/4	-
28	SQD	a	413	-	-	19/49/69/69	0/1/1/1
29	LMG	j	101	42	-	9/42/62/70	0/1/1/1
24	CLA	C	501	-	3/3/20/25	4/37/135/135	-
25	PHO	D	401	-	-	2/53/103/103	0/5/6/6
36	EDO	H	112	-	-	1/1/1/1	-
30	GOL	B	635	-	-	0/4/4/4	-
32	LHG	B	632	-	-	12/53/53/53	-
24	CLA	c	506	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	v	207	-	-	2/4/4/4	-
36	EDO	J	109	-	-	0/1/1/1	-
34	PGE	J	108	-	-	4/7/7/7	-
28	SQD	a	424	-	-	22/49/69/69	0/1/1/1
30	GOL	V	206	-	-	0/4/4/4	-
24	CLA	B	617	-	3/3/19/25	8/31/129/135	-
26	BCR	t	102	-	-	2/29/63/63	0/2/2/2
36	EDO	E	111	-	-	1/1/1/1	-
29	LMG	a	414	-	-	25/46/66/70	0/1/1/1
34	PGE	H	109	-	-	5/7/7/7	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	GOL	o	303	-	-	2/4/4/4	-
28	SQD	b	633	-	-	17/49/69/69	0/1/1/1
33	PG4	x	102	-	-	3/10/10/10	-
30	GOL	B	628	-	-	0/4/4/4	-
39	1PE	j	107	-	-	5/13/13/13	-
34	PGE	B	647	-	-	2/7/7/7	-
30	GOL	c	525	-	-	2/4/4/4	-
26	BCR	B	620	-	-	1/29/63/63	0/2/2/2
28	SQD	A	616	-	-	18/49/69/69	0/1/1/1
24	CLA	b	608	46	3/3/20/25	2/37/135/135	-
33	PG4	E	103	-	-	4/10/10/10	-
32	LHG	l	101	-	-	13/53/53/53	-
30	GOL	b	628	-	-	0/4/4/4	-
35	P6G	I	106	-	-	10/16/16/16	-
34	PGE	E	109	-	-	4/7/7/7	-
31	LMT	C	533	-	-	12/21/61/61	0/2/2/2
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
32	LHG	D	409	-	-	7/53/53/53	-
34	PGE	O	309	-	-	5/7/7/7	-
34	PGE	t	104	-	-	2/7/7/7	-
26	BCR	d	406	-	-	2/29/63/63	0/2/2/2
24	CLA	B	606	-	3/3/20/25	4/37/135/135	-
38	HTG	b	631	-	-	2/10/30/30	0/1/1/1
27	PL9	d	407	-	-	2/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	D	405	-	3/3/20/25	7/37/135/135	-
33	PG4	J	105	-	-	6/10/10/10	-
30	GOL	f	103	42	-	1/4/4/4	-
24	CLA	B	610	-	3/3/20/25	1/37/135/135	-
36	EDO	o	311	-	-	1/1/1/1	-
24	CLA	B	614	-	3/3/20/25	2/37/135/135	-
33	PG4	i	104	-	-	5/10/10/10	-
30	GOL	T	101	-	-	0/4/4/4	-
33	PG4	B	640	-	-	5/10/10/10	-
30	GOL	T	103	-	-	3/4/4/4	-
36	EDO	O	311	-	-	1/1/1/1	-
31	LMT	M	101	-	-	2/21/61/61	0/2/2/2
38	HTG	b	623	-	-	2/10/30/30	0/1/1/1
30	GOL	m	103	-	-	0/4/4/4	-
31	LMT	t	103	-	-	7/21/61/61	0/2/2/2
24	CLA	C	502	-	3/3/20/25	5/37/135/135	-
24	CLA	B	602	46	3/3/20/25	12/37/135/135	-
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
40	DGD	c	517	-	-	15/46/86/95	0/2/2/2
41	HEM	E	113	6,5	-	1/6/54/54	-
31	LMT	J	103	-	-	10/21/61/61	0/2/2/2
35	P6G	d	415	-	-	8/16/16/16	-
26	BCR	c	515	-	-	0/29/63/63	0/2/2/2
32	LHG	D	410	-	-	9/53/53/53	-
28	SQD	l	102	-	-	18/49/69/69	0/1/1/1
30	GOL	v	205	-	-	2/4/4/4	-
36	EDO	o	310	-	-	0/1/1/1	-
28	SQD	a	417	-	-	15/49/69/69	0/1/1/1
33	PG4	I	104	-	-	4/10/10/10	-
35	P6G	B	652	-	-	7/16/16/16	-
34	PGE	h	107	-	-	4/7/7/7	-
38	HTG	V	204	-	-	2/10/30/30	0/1/1/1
35	P6G	A	624	-	-	9/16/16/16	-
32	LHG	d	410	-	-	9/53/53/53	-
24	CLA	C	505	-	3/3/20/25	3/37/135/135	-
30	GOL	O	302	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	h	105	-	-	26/49/69/69	0/1/1/1
24	CLA	B	607	-	3/3/18/25	4/25/123/135	-
29	LMG	B	634	-	-	18/50/70/70	0/1/1/1
24	CLA	C	508	-	3/3/19/25	4/31/129/135	-
24	CLA	b	615	-	3/3/20/25	11/37/135/135	-
33	PG4	U	202	-	-	3/10/10/10	-
24	CLA	C	512	-	3/3/20/25	4/37/135/135	-
36	EDO	V	218	-	-	1/1/1/1	-
24	CLA	b	603	-	3/3/20/25	4/37/135/135	-
30	GOL	O	304	-	-	0/4/4/4	-
31	LMT	j	103	-	-	9/21/61/61	0/2/2/2
33	PG4	H	106	-	-	4/10/10/10	-
30	GOL	b	630	-	-	0/4/4/4	-
33	PG4	e	104	-	-	4/10/10/10	-
30	GOL	A	615	-	-	2/4/4/4	-
34	PGE	E	104	-	-	1/7/7/7	-
30	GOL	d	413	-	-	4/4/4/4	-
33	PG4	b	636	-	-	6/10/10/10	-
24	CLA	b	609	-	3/3/20/25	1/37/135/135	-
33	PG4	V	213	-	-	4/10/10/10	-
39	1PE	B	654	-	-	5/13/13/13	-
30	GOL	v	203	-	-	0/4/4/4	-
34	PGE	V	214	-	-	4/7/7/7	-
43	HEC	v	202	16	-	0/6/54/54	-
28	SQD	F	104	-	-	18/49/69/69	0/1/1/1
43	HEC	V	203	16	-	0/6/54/54	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
33	PG4	J	104	-	-	2/10/10/10	-
24	CLA	B	604	-	3/3/20/25	4/37/135/135	-
34	PGE	c	536	-	-	3/7/7/7	-
34	PGE	A	621	-	-	3/7/7/7	-
40	DGD	C	516	-	-	17/51/91/95	0/2/2/2
34	PGE	B	650	-	-	2/7/7/7	-
33	PG4	C	538	-	-	2/10/10/10	-
35	P6G	D	416	-	-	9/16/16/16	-
35	P6G	b	648	-	-	7/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	EDO	c	542	-	-	1/1/1/1	-
24	CLA	B	613	-	3/3/20/25	2/37/135/135	-
30	GOL	d	402	-	-	2/4/4/4	-
24	CLA	C	507	46	2/2/20/25	7/37/135/135	-
40	DGD	c	516	-	-	17/51/91/95	0/2/2/2
31	LMT	u	203	-	-	12/21/61/61	0/2/2/2
30	GOL	a	416	-	-	2/4/4/4	-
24	CLA	A	606	-	3/3/20/25	5/37/135/135	-
33	PG4	C	535	-	-	3/10/10/10	-
33	PG4	I	102	-	-	6/10/10/10	-
33	PG4	C	534	-	-	5/10/10/10	-
28	SQD	x	101	-	-	23/49/69/69	0/1/1/1
34	PGE	b	639	-	-	3/7/7/7	-
26	BCR	c	527	-	-	1/29/63/63	0/2/2/2
33	PG4	V	209	-	-	5/10/10/10	-
24	CLA	c	505	-	3/3/20/25	2/37/135/135	-
34	PGE	H	111	-	-	3/7/7/7	-
30	GOL	C	527	-	-	2/4/4/4	-
34	PGE	b	640	-	-	3/7/7/7	-
30	GOL	V	208	-	-	4/4/4/4	-
30	GOL	o	305	-	-	2/4/4/4	-
40	DGD	C	517	-	-	14/45/85/95	0/2/2/2
24	CLA	C	510	-	3/3/20/25	3/37/135/135	-
34	PGE	B	649	-	-	3/7/7/7	-
44	2PE	V	216	-	-	14/25/25/25	-
30	GOL	O	306	-	-	0/4/4/4	-
33	PG4	a	421	-	-	4/10/10/10	-
38	HTG	H	101	-	-	3/10/30/30	0/1/1/1
29	LMG	C	519	-	-	15/46/66/70	0/1/1/1
38	HTG	C	530	-	-	3/10/30/30	0/1/1/1
34	PGE	x	103	-	-	2/7/7/7	-
34	PGE	c	540	-	-	4/7/7/7	-
33	PG4	H	105	-	-	4/10/10/10	-
24	CLA	C	503	-	3/3/20/25	4/37/135/135	-
26	BCR	b	620	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	I	105	-	-	2/7/7/7	-
24	CLA	b	613	-	3/3/20/25	3/37/135/135	-
30	GOL	A	614	-	-	0/4/4/4	-
34	PGE	B	644	-	-	3/7/7/7	-
34	PGE	E	105	-	-	4/7/7/7	-
38	HTG	c	530	-	-	3/10/30/30	0/1/1/1
30	GOL	b	629	-	-	2/4/4/4	-
33	PG4	D	414	-	-	5/10/10/10	-
33	PG4	a	420	-	-	3/10/10/10	-
30	GOL	b	625	-	-	3/4/4/4	-
33	PG4	B	641	-	-	4/10/10/10	-
30	GOL	C	523	-	-	1/4/4/4	-
30	GOL	U	201	-	-	1/4/4/4	-
24	CLA	B	615	-	3/3/18/25	4/25/123/135	-
40	DGD	c	518	-	-	14/51/91/95	0/2/2/2
30	GOL	e	102	-	-	0/4/4/4	-
29	LMG	C	520	-	-	17/46/66/70	0/1/1/1
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
24	CLA	C	513	-	3/3/20/25	8/37/135/135	-
34	PGE	o	309	-	-	5/7/7/7	-
36	EDO	X	104	-	-	0/1/1/1	-
27	PL9	a	412	-	-	10/53/73/73	0/1/1/1
29	LMG	d	412	-	-	25/50/70/70	0/1/1/1
34	PGE	a	422	-	-	5/7/7/7	-
40	DGD	h	104	-	-	10/51/91/95	0/2/2/2
30	GOL	V	201	-	-	0/4/4/4	-
38	HTG	B	631	-	-	3/10/30/30	0/1/1/1
33	PG4	c	533	-	-	5/10/10/10	-
34	PGE	b	642	-	-	3/7/7/7	-
40	DGD	d	408	-	-	31/55/95/95	0/2/2/2
29	LMG	J	101	42	-	6/42/62/70	0/1/1/1
24	CLA	c	501	-	3/3/20/25	4/37/135/135	-
34	PGE	O	308	-	-	5/7/7/7	-
31	LMT	M	102	-	-	7/21/61/61	0/2/2/2
24	CLA	d	405	-	3/3/20/25	6/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	610	-	3/3/20/25	2/37/135/135	-
24	CLA	b	616	-	2/2/20/25	4/37/135/135	-
34	PGE	b	643	-	-	3/7/7/7	-
35	P6G	D	417	-	-	8/16/16/16	-
31	LMT	a	401	-	-	9/21/61/61	0/2/2/2
31	LMT	b	622	-	-	9/21/61/61	0/2/2/2
34	PGE	c	537	-	-	4/7/7/7	-
34	PGE	H	108	-	-	5/7/7/7	-
38	HTG	o	301	-	-	0/10/30/30	0/1/1/1
24	CLA	B	605	-	3/3/20/25	5/37/135/135	-
33	PG4	b	634	-	-	3/10/10/10	-
30	GOL	u	202	-	-	0/4/4/4	-
30	GOL	c	526	-	-	0/4/4/4	-
30	GOL	V	207	-	-	0/4/4/4	-
38	HTG	c	523	-	-	3/10/30/30	0/1/1/1
41	HEM	e	107	6,5	-	1/6/54/54	-
26	BCR	H	102	-	-	0/29/63/63	0/2/2/2
36	EDO	C	542	-	-	1/1/1/1	-
34	PGE	J	106	-	-	3/7/7/7	-
35	P6G	A	623	-	-	9/16/16/16	-
33	PG4	B	639	-	-	4/10/10/10	-
30	GOL	y	101	-	-	2/4/4/4	-
24	CLA	C	509	-	3/3/20/25	7/37/135/135	-
38	HTG	B	630	-	-	4/10/30/30	0/1/1/1
33	PG4	V	210	-	-	7/10/10/10	-
36	EDO	a	425	-	-	1/1/1/1	-
30	GOL	b	627	-	-	0/4/4/4	-
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
45	PE8	i	107	-	-	14/22/22/22	-
32	LHG	d	411	-	-	10/53/53/53	-
24	CLA	C	504	46	3/3/19/25	4/31/129/135	-
34	PGE	C	540	-	-	4/7/7/7	-
26	BCR	T	102	-	-	2/29/63/63	0/2/2/2
34	PGE	J	107	-	-	3/7/7/7	-
24	CLA	B	608	46	3/3/20/25	1/37/135/135	-
30	GOL	C	528	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	SQD	A	612	-	-	11/49/69/69	0/1/1/1
33	PG4	C	536	-	-	5/10/10/10	-
34	PGE	B	648	-	-	3/7/7/7	-
34	PGE	b	645	-	-	4/7/7/7	-
26	BCR	h	103	-	-	0/29/63/63	0/2/2/2
35	P6G	c	541	-	-	4/16/16/16	-
33	PG4	V	211	-	-	3/10/10/10	-
30	GOL	B	629	-	-	0/4/4/4	-
24	CLA	d	403	46	3/3/20/25	5/37/135/135	-
36	EDO	i	108	-	-	0/1/1/1	-
24	CLA	c	508	-	3/3/19/25	2/31/129/135	-
33	PG4	b	637	-	-	5/10/10/10	-
30	GOL	b	626	-	-	0/4/4/4	-
39	1PE	L	101	-	-	5/13/13/13	-
25	PHO	d	401	-	-	3/53/103/103	0/5/6/6
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
34	PGE	B	646	-	-	4/7/7/7	-
30	GOL	B	633	-	-	4/4/4/4	-
30	GOL	D	413	-	-	2/4/4/4	-
34	PGE	E	108	-	-	2/7/7/7	-
24	CLA	b	604	-	3/3/20/25	4/37/135/135	-
24	CLA	b	612	-	3/3/20/25	3/37/135/135	-
33	PG4	C	537	-	-	6/10/10/10	-
34	PGE	b	647	-	-	3/7/7/7	-
24	CLA	B	612	-	3/3/20/25	3/37/135/135	-
33	PG4	H	104	-	-	3/10/10/10	-
24	CLA	c	503	-	3/3/20/25	2/37/135/135	-
30	GOL	O	307	-	-	2/4/4/4	-
30	GOL	F	101	42	-	2/4/4/4	-
32	LHG	d	409	-	-	7/53/53/53	-
33	PG4	h	106	-	-	3/10/10/10	-
33	PG4	d	414	-	-	3/10/10/10	-
35	P6G	C	541	-	-	8/16/16/16	-
33	PG4	A	619	-	-	3/10/10/10	-
34	PGE	h	110	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	o	304	-	-	4/4/4/4	-
24	CLA	b	606	-	3/3/20/25	3/37/135/135	-
30	GOL	V	205	-	-	0/4/4/4	-
34	PGE	H	110	-	-	4/7/7/7	-
24	CLA	A	609	-	3/3/20/25	11/37/135/135	-
30	GOL	O	305	-	-	2/4/4/4	-
24	CLA	A	607	46	3/3/19/25	3/31/129/135	-
33	PG4	H	107	-	-	4/10/10/10	-
38	HTG	b	624	-	-	5/10/30/30	0/1/1/1
39	1PE	B	653	-	-	4/13/13/13	-
24	CLA	a	407	-	3/3/20/25	2/37/135/135	-
24	CLA	c	504	46	3/3/19/25	4/31/129/135	-
36	EDO	B	657	-	-	0/1/1/1	-
33	PG4	c	534	-	-	6/10/10/10	-
34	PGE	C	539	-	-	3/7/7/7	-
33	PG4	X	103	-	-	4/10/10/10	-
36	EDO	d	417	-	-	1/1/1/1	-
33	PG4	i	102	-	-	4/10/10/10	-
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
36	EDO	B	658	-	-	1/1/1/1	-
34	PGE	b	646	-	-	4/7/7/7	-
34	PGE	E	107	-	-	4/7/7/7	-
33	PG4	E	102	-	-	8/10/10/10	-
29	LMG	z	101	-	-	31/50/70/70	0/1/1/1
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
33	PG4	i	103	-	-	6/10/10/10	-
36	EDO	I	107	-	-	0/1/1/1	-
33	PG4	j	104	-	-	8/10/10/10	-
38	HTG	h	101	-	-	5/10/30/30	0/1/1/1
24	CLA	B	609	-	3/3/20/25	1/37/135/135	-
24	CLA	C	511	3	3/3/20/25	0/37/135/135	-
36	EDO	D	419	-	-	0/1/1/1	-
31	LMT	A	617	-	-	8/21/61/61	0/2/2/2

All (1097) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	OBD-CAD	8.12	1.33	1.22
38	o	301	HTG	C1'-S1	-7.89	1.71	1.81
27	a	412	PL9	C7-C3	7.55	1.59	1.51
24	b	614	CLA	OBD-CAD	7.07	1.32	1.22
24	C	505	CLA	OBD-CAD	6.86	1.31	1.22
25	D	401	PHO	C3B-C2B	6.27	1.50	1.37
24	B	606	CLA	C2-C3	6.19	1.47	1.33
24	b	616	CLA	C3D-C2D	6.17	1.50	1.39
24	C	511	CLA	C3D-C2D	6.10	1.50	1.39
40	D	408	DGD	O2G-C1B	6.07	1.51	1.34
24	B	615	CLA	C1B-NB	-6.04	1.29	1.35
24	b	616	CLA	OBD-CAD	6.02	1.30	1.22
24	B	603	CLA	OBD-CAD	6.02	1.30	1.22
24	A	606	CLA	OBD-CAD	5.97	1.30	1.22
27	A	611	PL9	C7-C3	5.96	1.57	1.51
24	B	602	CLA	O2A-CGA	5.91	1.50	1.33
24	B	615	CLA	CHC-C1C	5.85	1.50	1.35
24	b	602	CLA	O2D-CGD	5.79	1.47	1.33
24	b	606	CLA	O2D-CGD	5.78	1.47	1.33
24	c	509	CLA	OBD-CAD	5.78	1.30	1.22
24	a	410	CLA	CHC-C1C	5.74	1.49	1.35
24	c	507	CLA	OBD-CAD	5.74	1.30	1.22
24	b	606	CLA	C2-C3	5.70	1.46	1.33
24	B	611	CLA	C3D-C2D	5.67	1.49	1.39
26	d	406	BCR	C30-C25	-5.67	1.46	1.53
40	d	408	DGD	O2G-C1B	5.65	1.50	1.34
24	c	504	CLA	C3D-C2D	5.62	1.49	1.39
28	F	104	SQD	O48-C23	5.62	1.49	1.33
24	C	512	CLA	C3D-C2D	5.60	1.49	1.39
24	c	512	CLA	C3D-C2D	5.58	1.49	1.39
24	b	613	CLA	OBD-CAD	5.52	1.30	1.22
24	c	510	CLA	C3D-C2D	5.46	1.49	1.39
38	O	303	HTG	C1'-S1	-5.46	1.74	1.81
24	c	510	CLA	OBD-CAD	5.45	1.29	1.22
24	b	606	CLA	C3C-C2C	5.44	1.48	1.36
24	C	504	CLA	C4B-NB	-5.44	1.30	1.35
24	B	604	CLA	C3C-C2C	5.43	1.48	1.36
24	b	610	CLA	OBD-CAD	5.42	1.29	1.22
24	C	507	CLA	C3D-C2D	5.42	1.49	1.39
24	B	605	CLA	C2-C3	5.40	1.45	1.33
24	b	614	CLA	C3C-C2C	5.34	1.48	1.36
24	b	602	CLA	O2A-CGA	5.33	1.48	1.33
24	c	507	CLA	C3D-C2D	5.32	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	526	LMG	O7-C10	5.32	1.49	1.34
24	C	508	CLA	C3C-C2C	5.31	1.48	1.36
24	C	501	CLA	C3D-C2D	5.30	1.48	1.39
24	b	605	CLA	C2-C3	5.26	1.45	1.33
24	c	513	CLA	C3D-C2D	5.25	1.48	1.39
28	l	102	SQD	O8-S	5.23	1.66	1.47
24	d	404	CLA	CHC-C1C	5.23	1.48	1.35
24	C	513	CLA	C3B-C2B	5.21	1.47	1.40
24	B	603	CLA	CHC-C1C	5.20	1.48	1.35
24	B	602	CLA	C3B-C2B	5.18	1.47	1.40
24	D	405	CLA	C3D-C2D	5.15	1.48	1.39
24	B	613	CLA	CHC-C1C	5.14	1.48	1.35
24	d	403	CLA	CHC-C1C	5.13	1.48	1.35
24	b	607	CLA	C3B-C2B	5.13	1.47	1.40
24	d	405	CLA	C3D-C2D	5.13	1.48	1.39
24	b	608	CLA	C3D-C2D	5.12	1.48	1.39
24	b	603	CLA	CHC-C1C	5.11	1.48	1.35
28	x	101	SQD	O48-C23	5.10	1.48	1.33
24	c	513	CLA	C3B-C2B	5.10	1.47	1.40
29	C	520	LMG	O8-C28	5.09	1.48	1.33
24	b	605	CLA	CHC-C1C	5.09	1.48	1.35
24	C	508	CLA	C3B-C2B	5.08	1.47	1.40
24	C	509	CLA	OBD-CAD	5.08	1.29	1.22
24	C	512	CLA	CHC-C1C	5.04	1.47	1.35
24	c	501	CLA	C3B-C2B	5.03	1.47	1.40
24	B	604	CLA	C3D-C2D	5.02	1.48	1.39
24	c	513	CLA	OBD-CAD	5.02	1.29	1.22
38	c	530	HTG	O2-C2	5.02	1.54	1.43
28	b	633	SQD	O47-C7	5.02	1.48	1.34
24	C	503	CLA	CHC-C1C	4.99	1.47	1.35
24	d	403	CLA	C1C-NC	-4.99	1.30	1.37
24	C	501	CLA	OBD-CAD	4.98	1.29	1.22
24	B	602	CLA	C3D-C2D	4.98	1.48	1.39
25	a	409	PHO	C3B-C2B	4.97	1.47	1.37
40	d	408	DGD	O1G-C1A	4.97	1.47	1.33
25	A	608	PHO	C3B-C2B	4.96	1.47	1.37
29	C	520	LMG	O7-C10	4.95	1.48	1.34
24	C	513	CLA	CHC-C1C	4.94	1.47	1.35
24	d	403	CLA	OBD-CAD	4.93	1.29	1.22
24	b	610	CLA	O2D-CGD	4.93	1.45	1.33
24	c	510	CLA	C3B-C2B	4.93	1.47	1.40
28	h	105	SQD	O48-C23	4.89	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	OBD-CAD	4.89	1.29	1.22
28	A	622	SQD	O47-C7	4.88	1.48	1.34
25	a	409	PHO	CHB-C1B	4.88	1.48	1.38
24	C	506	CLA	O2D-CGD	4.87	1.45	1.33
32	a	419	LHG	O8-C23	4.87	1.47	1.33
32	A	618	LHG	O7-C7	4.87	1.48	1.34
24	b	603	CLA	OBD-CAD	4.86	1.29	1.22
24	b	613	CLA	C3D-C2D	4.86	1.48	1.39
28	b	633	SQD	O8-S	4.85	1.64	1.47
24	c	507	CLA	CHC-C1C	4.85	1.47	1.35
28	h	105	SQD	O47-C7	4.84	1.47	1.34
29	C	519	LMG	O8-C28	4.84	1.47	1.33
28	h	105	SQD	O8-S	4.83	1.64	1.47
24	A	606	CLA	C3C-C2C	4.83	1.47	1.36
24	a	410	CLA	C3D-C2D	4.82	1.48	1.39
24	b	616	CLA	C3B-C2B	4.81	1.47	1.40
29	c	520	LMG	O8-C28	4.79	1.47	1.33
28	F	104	SQD	O47-C7	4.78	1.47	1.34
24	B	609	CLA	C3D-C2D	4.78	1.48	1.39
24	B	613	CLA	OBD-CAD	4.78	1.29	1.22
24	c	508	CLA	C3D-C2D	4.78	1.48	1.39
28	A	622	SQD	O48-C23	4.77	1.47	1.33
29	B	621	LMG	O8-C28	4.77	1.47	1.33
29	B	634	LMG	O8-C28	4.75	1.47	1.33
24	B	607	CLA	CHC-C1C	4.75	1.47	1.35
24	b	615	CLA	O2A-CGA	4.74	1.47	1.33
24	c	503	CLA	CHC-C1C	4.73	1.47	1.35
24	B	617	CLA	C3D-C2D	4.73	1.47	1.39
24	b	616	CLA	C3C-C2C	4.73	1.46	1.36
24	c	511	CLA	OBD-CAD	4.72	1.28	1.22
28	b	633	SQD	O48-C23	4.72	1.47	1.33
28	A	622	SQD	O8-S	4.71	1.64	1.47
28	a	417	SQD	O48-C23	4.71	1.47	1.33
24	C	508	CLA	CHC-C1C	4.70	1.47	1.35
24	C	507	CLA	O2D-CGD	4.68	1.44	1.33
28	a	424	SQD	O47-C7	4.68	1.47	1.34
24	B	614	CLA	CHC-C1C	4.67	1.46	1.35
38	b	624	HTG	C1'-S1	-4.67	1.75	1.81
24	C	506	CLA	C3D-C2D	4.66	1.47	1.39
24	C	502	CLA	C3D-C2D	4.66	1.47	1.39
24	d	405	CLA	OBD-CAD	4.66	1.28	1.22
24	a	408	CLA	C3D-C2D	4.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	424	SQD	O8-S	4.65	1.64	1.47
24	B	612	CLA	CHC-C1C	4.65	1.46	1.35
40	D	408	DGD	O1G-C1A	4.65	1.46	1.33
32	A	618	LHG	O8-C23	4.64	1.46	1.33
24	b	610	CLA	CHC-C1C	4.64	1.46	1.35
24	D	405	CLA	CHC-C1C	4.64	1.46	1.35
24	b	612	CLA	C3B-C2B	4.64	1.46	1.40
32	e	101	LHG	O8-C23	4.63	1.46	1.33
24	b	608	CLA	C3C-C2C	4.62	1.46	1.36
24	a	408	CLA	OBD-CAD	4.61	1.28	1.22
24	B	608	CLA	C3D-C2D	4.61	1.47	1.39
24	C	510	CLA	C3D-C2D	4.61	1.47	1.39
24	C	502	CLA	CHC-C1C	4.60	1.46	1.35
24	c	511	CLA	C3D-C2D	4.60	1.47	1.39
26	D	406	BCR	C30-C25	-4.60	1.47	1.53
24	C	513	CLA	C3D-C2D	4.60	1.47	1.39
28	x	101	SQD	O8-S	4.58	1.63	1.47
29	d	412	LMG	O8-C28	4.58	1.46	1.33
24	C	505	CLA	C3C-C2C	4.57	1.46	1.36
24	b	604	CLA	C3D-C2D	4.55	1.47	1.39
24	c	507	CLA	C3C-C2C	4.55	1.46	1.36
24	b	611	CLA	C3D-C2D	4.54	1.47	1.39
24	A	607	CLA	CHC-C1C	4.54	1.46	1.35
29	B	634	LMG	O7-C10	4.54	1.47	1.34
24	c	512	CLA	OBD-CAD	4.53	1.28	1.22
24	a	407	CLA	OBD-CAD	4.53	1.28	1.22
24	d	404	CLA	C3D-C2D	4.53	1.47	1.39
32	e	101	LHG	O7-C7	4.53	1.47	1.34
24	b	611	CLA	C3C-C2C	4.52	1.46	1.36
29	c	520	LMG	O7-C10	4.52	1.47	1.34
28	a	424	SQD	O48-C23	4.52	1.46	1.33
24	b	615	CLA	OBD-CAD	4.52	1.28	1.22
26	c	515	BCR	C1-C6	-4.50	1.47	1.53
24	c	512	CLA	CHC-C1C	4.49	1.46	1.35
24	C	504	CLA	OBD-CAD	4.48	1.28	1.22
24	C	503	CLA	O2D-CGD	4.46	1.44	1.33
24	b	604	CLA	CHC-C1C	4.46	1.46	1.35
24	b	603	CLA	C3D-C2D	4.44	1.47	1.39
24	C	510	CLA	OBD-CAD	4.44	1.28	1.22
24	c	502	CLA	O2D-CGD	4.44	1.44	1.33
24	A	609	CLA	C3D-C2D	4.43	1.47	1.39
24	b	614	CLA	O2D-CGD	4.42	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	F	104	SQD	O8-S	4.41	1.63	1.47
24	C	511	CLA	C3C-C2C	4.41	1.46	1.36
24	c	512	CLA	C3C-C2C	4.40	1.46	1.36
24	c	503	CLA	O2D-CGD	4.40	1.43	1.33
24	b	611	CLA	CHC-C1C	4.39	1.46	1.35
24	c	503	CLA	C3D-C2D	4.39	1.47	1.39
24	C	501	CLA	C3C-C2C	4.35	1.46	1.36
24	b	604	CLA	C3C-C2C	4.35	1.46	1.36
24	C	504	CLA	C3D-C2D	4.35	1.47	1.39
25	d	401	PHO	CHC-C1C	4.35	1.47	1.38
24	b	617	CLA	C3D-C2D	4.35	1.47	1.39
24	A	607	CLA	C3D-C2D	4.34	1.47	1.39
24	C	510	CLA	O2D-CGD	4.34	1.43	1.33
24	A	606	CLA	C3D-C2D	4.33	1.47	1.39
32	E	101	LHG	O8-C23	4.32	1.46	1.33
24	b	602	CLA	C3D-C2D	4.32	1.47	1.39
32	a	419	LHG	O7-C7	4.30	1.46	1.34
24	C	503	CLA	OBD-CAD	4.29	1.28	1.22
24	b	609	CLA	C3D-C2D	4.29	1.47	1.39
24	b	608	CLA	CHC-C1C	4.27	1.45	1.35
28	a	417	SQD	O47-C7	4.26	1.46	1.34
24	C	501	CLA	CHC-C1C	4.26	1.45	1.35
24	c	512	CLA	C3B-C2B	4.26	1.46	1.40
27	D	407	PL9	C36-C37	-4.26	1.39	1.53
24	C	503	CLA	C3C-C2C	4.26	1.45	1.36
29	A	613	LMG	O7-C10	4.26	1.46	1.34
24	c	508	CLA	C3C-C2C	4.25	1.45	1.36
24	B	608	CLA	CHC-C1C	4.25	1.45	1.35
24	c	505	CLA	C3C-C2C	4.25	1.45	1.36
28	a	417	SQD	O8-S	4.25	1.62	1.47
29	z	101	LMG	O8-C28	4.24	1.45	1.33
24	c	507	CLA	O2D-CGD	4.23	1.43	1.33
24	c	502	CLA	C3D-C2D	4.21	1.47	1.39
28	A	612	SQD	O8-S	4.21	1.62	1.47
24	c	509	CLA	C3D-C2D	4.20	1.47	1.39
24	B	611	CLA	C3C-C2C	4.20	1.45	1.36
24	b	617	CLA	CHC-C1C	4.18	1.45	1.35
24	B	606	CLA	O2D-CGD	4.18	1.43	1.33
24	C	505	CLA	C1B-NB	-4.18	1.31	1.35
24	B	604	CLA	CHC-C1C	4.18	1.45	1.35
28	A	616	SQD	O48-C23	4.17	1.45	1.33
28	a	413	SQD	O8-S	4.17	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	OBD-CAD	4.16	1.28	1.22
24	D	405	CLA	C3C-C2C	4.15	1.45	1.36
29	z	101	LMG	O7-C10	4.15	1.46	1.34
32	E	101	LHG	O7-C7	4.15	1.46	1.34
24	B	602	CLA	CHC-C1C	4.15	1.45	1.35
24	b	614	CLA	C3D-C2D	4.15	1.46	1.39
24	B	617	CLA	OBD-CAD	4.15	1.28	1.22
25	d	401	PHO	C3C-C2C	4.14	1.45	1.36
24	c	504	CLA	C4B-NB	-4.14	1.31	1.35
24	D	403	CLA	CHC-C1C	4.13	1.45	1.35
24	A	609	CLA	CHC-C1C	4.13	1.45	1.35
24	B	617	CLA	C3B-C2B	4.12	1.46	1.40
24	B	610	CLA	CHC-C1C	4.12	1.45	1.35
29	c	519	LMG	O8-C28	4.12	1.45	1.33
24	B	612	CLA	C3D-C2D	4.11	1.46	1.39
28	A	616	SQD	O47-C7	4.11	1.45	1.34
24	a	408	CLA	CHC-C1C	4.10	1.45	1.35
24	C	512	CLA	O2A-CGA	4.08	1.45	1.33
24	A	606	CLA	CHC-C1C	4.08	1.45	1.35
24	B	608	CLA	C3B-C2B	4.08	1.46	1.40
24	C	511	CLA	C3B-C2B	4.08	1.46	1.40
24	C	502	CLA	C3C-C2C	4.08	1.45	1.36
24	C	505	CLA	C3D-C2D	4.08	1.46	1.39
24	b	602	CLA	CHC-C1C	4.08	1.45	1.35
24	B	611	CLA	CHC-C1C	4.07	1.45	1.35
24	B	610	CLA	C3D-C2D	4.07	1.46	1.39
24	B	614	CLA	C3D-C2D	4.07	1.46	1.39
24	c	506	CLA	CHC-C1C	4.06	1.45	1.35
24	B	616	CLA	OBD-CAD	4.06	1.28	1.22
24	C	507	CLA	CHC-C1C	4.06	1.45	1.35
24	B	604	CLA	OBD-CAD	4.06	1.28	1.22
25	a	409	PHO	CHD-C1D	4.06	1.46	1.38
24	C	506	CLA	C3B-C2B	4.05	1.46	1.40
25	d	401	PHO	CHB-C1B	4.05	1.46	1.38
24	B	603	CLA	C3C-C2C	4.04	1.45	1.36
24	C	510	CLA	C3C-C2C	4.04	1.45	1.36
24	c	508	CLA	CHC-C1C	4.02	1.45	1.35
24	c	503	CLA	C3B-C2B	4.02	1.46	1.40
24	c	501	CLA	C3D-C2D	4.01	1.46	1.39
28	l	102	SQD	O48-C23	4.01	1.45	1.33
40	h	104	DGD	O5D-C1E	4.01	1.47	1.40
24	c	513	CLA	C3C-C2C	4.01	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	614	CLA	C3C-C2C	4.00	1.45	1.36
24	b	605	CLA	C1D-C2D	4.00	1.51	1.42
24	B	606	CLA	C3D-C2D	4.00	1.46	1.39
24	b	609	CLA	C3C-C2C	4.00	1.45	1.36
24	D	403	CLA	C3C-C2C	3.99	1.45	1.36
28	x	101	SQD	O47-C7	3.99	1.45	1.34
24	c	513	CLA	O2D-CGD	3.99	1.42	1.33
29	j	101	LMG	O7-C10	3.97	1.45	1.34
24	b	604	CLA	OBD-CAD	3.97	1.27	1.22
25	A	608	PHO	CHC-C1C	3.96	1.46	1.38
24	b	617	CLA	C3B-C2B	3.96	1.45	1.40
24	c	509	CLA	C3B-C2B	3.96	1.45	1.40
25	D	401	PHO	CHD-C1D	3.95	1.46	1.38
24	C	501	CLA	C3B-C2B	3.95	1.45	1.40
25	D	401	PHO	CHB-C1B	3.95	1.46	1.38
24	c	512	CLA	O2D-CGD	3.95	1.42	1.33
24	C	508	CLA	C3D-C2D	3.95	1.46	1.39
24	b	605	CLA	O2D-CGD	3.94	1.42	1.33
24	a	407	CLA	C3C-C2C	3.94	1.45	1.36
24	C	510	CLA	CHC-C1C	3.93	1.45	1.35
24	B	609	CLA	C3C-C2C	3.93	1.45	1.36
24	C	510	CLA	C3B-C2B	3.93	1.45	1.40
24	d	405	CLA	C3C-C2C	3.93	1.45	1.36
24	d	405	CLA	CHC-C1C	3.93	1.45	1.35
24	c	504	CLA	C3C-C2C	3.93	1.45	1.36
38	C	531	HTG	C1'-S1	-3.92	1.76	1.81
24	c	505	CLA	CHC-C1C	3.92	1.45	1.35
24	c	505	CLA	C3B-C2B	3.91	1.45	1.40
24	B	610	CLA	C3B-C2B	3.90	1.45	1.40
24	c	502	CLA	CHC-C1C	3.89	1.44	1.35
28	A	612	SQD	O47-C7	3.88	1.45	1.34
24	b	613	CLA	O2D-CGD	3.88	1.42	1.33
24	B	617	CLA	CHC-C1C	3.87	1.44	1.35
27	A	611	PL9	O1-C4	-3.87	1.14	1.23
24	C	511	CLA	OBD-CAD	3.87	1.27	1.22
24	C	507	CLA	C3C-C2C	3.86	1.44	1.36
24	C	503	CLA	C3B-C2B	3.86	1.45	1.40
24	b	603	CLA	C3B-C2B	3.85	1.45	1.40
24	B	607	CLA	C3C-C2C	3.85	1.44	1.36
24	c	513	CLA	CHC-C1C	3.85	1.44	1.35
24	b	615	CLA	C4B-NB	-3.84	1.31	1.35
29	C	519	LMG	O7-C10	3.84	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B	634	LMG	O1-C1	3.84	1.46	1.40
32	d	411	LHG	O7-C7	3.84	1.45	1.34
28	A	616	SQD	O8-S	3.83	1.61	1.47
25	a	409	PHO	C3C-C2C	3.83	1.44	1.36
24	B	615	CLA	O2A-CGA	3.82	1.44	1.33
24	b	611	CLA	C3B-C2B	3.82	1.45	1.40
24	c	509	CLA	C3C-C2C	3.82	1.44	1.36
29	C	526	LMG	O8-C28	3.82	1.44	1.33
24	c	509	CLA	O2D-CGD	3.81	1.42	1.33
24	C	507	CLA	OBD-CAD	3.81	1.27	1.22
24	c	504	CLA	C1D-C2D	3.81	1.51	1.42
24	A	607	CLA	OBD-CAD	3.80	1.27	1.22
24	C	509	CLA	CHC-C1C	3.79	1.44	1.35
24	B	604	CLA	O2A-CGA	3.79	1.44	1.33
24	c	508	CLA	C3B-C2B	3.78	1.45	1.40
24	D	404	CLA	OBD-CAD	3.78	1.27	1.22
24	b	614	CLA	CHC-C1C	3.78	1.44	1.35
24	A	609	CLA	OBD-CAD	3.77	1.27	1.22
24	c	506	CLA	C3C-C2C	3.77	1.44	1.36
24	B	603	CLA	C3D-C2D	3.77	1.46	1.39
24	D	403	CLA	C3D-C2D	3.77	1.46	1.39
24	C	507	CLA	C3B-C2B	3.77	1.45	1.40
38	b	631	HTG	C1'-S1	-3.76	1.76	1.81
24	b	606	CLA	C3D-C2D	3.76	1.46	1.39
24	B	616	CLA	CHC-C1C	3.76	1.44	1.35
27	D	407	PL9	C41-C39	3.76	1.59	1.51
24	C	511	CLA	O2D-CGD	3.76	1.42	1.33
24	b	609	CLA	OBD-CAD	3.76	1.27	1.22
24	b	602	CLA	C3C-C2C	3.76	1.44	1.36
24	b	613	CLA	CHC-C1C	3.76	1.44	1.35
24	B	605	CLA	OBD-CAD	3.75	1.27	1.22
24	B	605	CLA	CHC-C1C	3.75	1.44	1.35
25	d	401	PHO	OBD-CAD	3.75	1.28	1.22
24	c	501	CLA	C3C-C2C	3.75	1.44	1.36
25	A	608	PHO	CHB-C1B	3.75	1.46	1.38
24	b	614	CLA	O2A-CGA	3.74	1.44	1.33
24	C	513	CLA	C3C-C2C	3.74	1.44	1.36
24	B	610	CLA	C3C-C2C	3.73	1.44	1.36
24	d	403	CLA	C3B-C2B	3.73	1.45	1.40
24	c	504	CLA	OBD-CAD	3.72	1.27	1.22
24	B	612	CLA	OBD-CAD	3.72	1.27	1.22
24	b	610	CLA	C3D-C2D	3.72	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C3C-C2C	3.71	1.44	1.36
28	l	102	SQD	O47-C7	3.71	1.44	1.34
24	C	504	CLA	C1B-NB	3.70	1.38	1.35
24	c	508	CLA	O2A-CGA	3.70	1.44	1.33
24	A	606	CLA	O2D-CGD	3.69	1.42	1.33
24	b	606	CLA	O2A-CGA	3.69	1.44	1.33
24	b	607	CLA	CHC-C1C	3.69	1.44	1.35
24	b	603	CLA	C3C-C2C	3.69	1.44	1.36
24	c	501	CLA	CHC-C1C	3.68	1.44	1.35
24	D	405	CLA	O2D-CGD	3.68	1.42	1.33
24	c	510	CLA	O2D-CGD	3.68	1.42	1.33
24	b	604	CLA	C3B-C2B	3.68	1.45	1.40
24	A	609	CLA	C3C-C2C	3.67	1.44	1.36
24	b	609	CLA	CHC-C1C	3.67	1.44	1.35
24	d	405	CLA	C1C-NC	-3.67	1.32	1.37
24	B	606	CLA	CHC-C1C	3.66	1.44	1.35
24	B	602	CLA	O2D-CGD	3.66	1.42	1.33
40	d	408	DGD	O3G-C1D	3.65	1.46	1.40
24	C	509	CLA	C3D-C2D	3.65	1.46	1.39
24	C	511	CLA	CHC-C1C	3.65	1.44	1.35
40	h	104	DGD	O1G-C1A	3.65	1.44	1.33
24	B	610	CLA	O2D-CGD	3.65	1.42	1.33
24	c	510	CLA	CHC-C1C	3.65	1.44	1.35
24	B	617	CLA	C1C-NC	-3.65	1.32	1.37
24	D	404	CLA	C1B-NB	3.65	1.38	1.35
24	b	612	CLA	CHC-C1C	3.65	1.44	1.35
24	C	513	CLA	O2D-CGD	3.64	1.42	1.33
24	c	503	CLA	OBD-CAD	3.64	1.27	1.22
25	D	401	PHO	OBD-CAD	3.63	1.28	1.22
24	a	407	CLA	C3D-C2D	3.63	1.45	1.39
24	B	609	CLA	C3B-C2B	3.63	1.45	1.40
24	C	506	CLA	CHC-C1C	3.63	1.44	1.35
25	a	409	PHO	CHC-C1C	3.61	1.45	1.38
24	a	410	CLA	C3C-C2C	3.61	1.44	1.36
32	l	101	LHG	O8-C23	3.60	1.43	1.33
24	B	608	CLA	O2D-CGD	3.60	1.42	1.33
24	B	605	CLA	C3D-C2D	3.60	1.45	1.39
24	c	504	CLA	CHC-C1C	3.60	1.44	1.35
29	c	519	LMG	O7-C10	3.59	1.44	1.34
24	A	606	CLA	C4B-NB	3.59	1.38	1.35
29	a	414	LMG	O7-C10	3.58	1.44	1.34
43	V	203	HEC	C3B-C2B	-3.58	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	O2D-CGD	3.58	1.41	1.33
26	C	514	BCR	C10-C9	-3.58	1.31	1.35
31	u	203	LMT	O1'-C1'	3.57	1.46	1.40
24	b	607	CLA	C3D-C2D	3.56	1.45	1.39
24	b	607	CLA	C4B-NB	3.56	1.38	1.35
24	b	613	CLA	C3C-C2C	3.55	1.44	1.36
40	c	517	DGD	O1G-C1A	3.55	1.43	1.33
24	a	407	CLA	CHC-C1C	3.53	1.44	1.35
24	C	512	CLA	O2D-CGD	3.52	1.41	1.33
24	c	506	CLA	C1C-NC	-3.52	1.32	1.37
24	b	608	CLA	C1D-C2D	3.52	1.50	1.42
24	c	505	CLA	OBD-CAD	3.51	1.27	1.22
24	c	507	CLA	C1D-C2D	3.51	1.50	1.42
24	C	505	CLA	C3B-C2B	3.51	1.45	1.40
24	A	607	CLA	O2D-CGD	3.50	1.41	1.33
24	B	612	CLA	C1B-NB	3.50	1.38	1.35
24	b	611	CLA	OBD-CAD	3.50	1.27	1.22
38	C	530	HTG	C1'-S1	-3.49	1.77	1.81
26	D	406	BCR	C1-C6	-3.49	1.49	1.53
24	c	509	CLA	O2A-CGA	3.49	1.43	1.33
24	b	616	CLA	O2A-CGA	3.49	1.43	1.33
24	b	606	CLA	CHC-C1C	3.49	1.43	1.35
24	B	605	CLA	O2A-CGA	3.48	1.43	1.33
24	b	605	CLA	C1B-NB	3.48	1.38	1.35
24	d	403	CLA	C3D-C2D	3.48	1.45	1.39
24	c	512	CLA	O2A-CGA	3.47	1.43	1.33
24	c	513	CLA	O2A-CGA	3.47	1.43	1.33
24	c	504	CLA	O2D-CGD	3.47	1.41	1.33
27	d	407	PL9	C36-C37	-3.46	1.42	1.53
24	c	510	CLA	C3C-C2C	3.46	1.44	1.36
24	C	503	CLA	C3D-C2D	3.45	1.45	1.39
24	b	603	CLA	C1D-C2D	3.45	1.50	1.42
24	c	502	CLA	OBD-CAD	3.45	1.27	1.22
24	c	506	CLA	O2D-CGD	3.45	1.41	1.33
24	C	502	CLA	O2D-CGD	3.44	1.41	1.33
24	c	509	CLA	CHC-C1C	3.44	1.43	1.35
24	C	506	CLA	C3C-C2C	3.44	1.44	1.36
24	C	511	CLA	C1B-CHB	3.44	1.50	1.41
24	B	603	CLA	O2D-CGD	3.44	1.41	1.33
40	c	518	DGD	O1G-C1A	3.44	1.43	1.33
24	B	609	CLA	O2A-CGA	3.43	1.43	1.33
24	D	404	CLA	CHC-C1C	3.42	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	CHC-C1C	3.42	1.43	1.35
41	E	113	HEM	C4D-C3D	3.41	1.50	1.42
24	c	511	CLA	O2D-CGD	3.41	1.41	1.33
24	B	610	CLA	OBD-CAD	3.41	1.27	1.22
24	B	607	CLA	OBD-CAD	3.41	1.27	1.22
24	a	407	CLA	C1D-C2D	3.41	1.50	1.42
24	B	603	CLA	C3B-C2B	3.41	1.45	1.40
24	B	616	CLA	O2D-CGD	3.41	1.41	1.33
25	D	401	PHO	C3C-C2C	3.41	1.44	1.36
24	B	607	CLA	C3D-C2D	3.40	1.45	1.39
32	d	411	LHG	O8-C23	3.40	1.43	1.33
24	d	405	CLA	C1D-C2D	3.39	1.50	1.42
28	a	417	SQD	C6-S	-3.39	1.64	1.77
25	A	608	PHO	O2D-CGD	3.39	1.41	1.33
25	D	401	PHO	C4A-NA	-3.39	1.27	1.35
24	b	617	CLA	C3C-C2C	3.39	1.43	1.36
24	b	617	CLA	O2D-CGD	3.38	1.41	1.33
24	b	605	CLA	C3D-C2D	3.38	1.45	1.39
24	C	505	CLA	CHC-C1C	3.38	1.43	1.35
24	B	606	CLA	C1D-C2D	3.38	1.50	1.42
25	D	401	PHO	C3D-C2D	3.37	1.48	1.39
24	B	616	CLA	C3D-C2D	3.37	1.45	1.39
24	B	613	CLA	C3C-C2C	3.36	1.43	1.36
24	b	615	CLA	CHC-C1C	3.36	1.43	1.35
24	B	608	CLA	OBD-CAD	3.36	1.27	1.22
27	D	407	PL9	C38-C39	-3.36	1.24	1.33
24	b	612	CLA	C3C-C2C	3.36	1.43	1.36
24	a	408	CLA	C3C-C2C	3.36	1.43	1.36
24	B	606	CLA	O2A-CGA	3.35	1.43	1.33
29	A	613	LMG	O8-C28	3.35	1.43	1.33
24	b	602	CLA	OBD-CAD	3.35	1.27	1.22
24	C	504	CLA	O2D-CGD	3.34	1.41	1.33
38	C	532	HTG	C1'-S1	-3.34	1.77	1.81
24	C	504	CLA	C1C-NC	-3.34	1.32	1.37
28	a	413	SQD	O47-C7	3.34	1.43	1.34
24	C	503	CLA	O2A-CGA	3.34	1.43	1.33
24	C	504	CLA	C3C-C2C	3.34	1.43	1.36
29	B	621	LMG	O7-C10	3.33	1.43	1.34
24	b	609	CLA	C3B-C2B	3.33	1.45	1.40
40	h	104	DGD	O2G-C1B	3.32	1.43	1.34
40	c	516	DGD	O1G-C1A	3.31	1.43	1.33
38	c	530	HTG	C1'-S1	-3.30	1.77	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	621	LMG	O7-C10	3.30	1.43	1.34
24	d	403	CLA	C3C-C2C	3.28	1.43	1.36
24	C	511	CLA	O2A-CGA	3.28	1.42	1.33
38	H	101	HTG	C1'-S1	-3.28	1.77	1.81
24	B	606	CLA	C1C-NC	-3.28	1.32	1.37
24	b	612	CLA	O2D-CGD	3.27	1.41	1.33
24	d	405	CLA	C1B-NB	-3.27	1.32	1.35
24	d	403	CLA	O2D-CGD	3.27	1.41	1.33
29	d	412	LMG	O7-C10	3.27	1.43	1.34
24	b	608	CLA	C3B-C2B	3.26	1.44	1.40
31	F	102	LMT	O1'-C1'	3.26	1.45	1.40
25	A	608	PHO	C3C-C2C	3.26	1.43	1.36
38	C	521	HTG	C1-S1	-3.26	1.75	1.80
24	b	610	CLA	C1D-C2D	3.25	1.49	1.42
24	b	602	CLA	C3B-C2B	3.24	1.44	1.40
24	b	607	CLA	O2D-CGD	3.22	1.41	1.33
26	d	406	BCR	C1-C6	-3.22	1.49	1.53
24	a	407	CLA	O2D-CGD	3.22	1.41	1.33
24	b	613	CLA	CMB-C2B	-3.22	1.44	1.51
24	c	505	CLA	C1C-C2C	3.22	1.50	1.44
24	C	505	CLA	O2A-CGA	3.21	1.42	1.33
24	C	509	CLA	C3C-C2C	3.20	1.43	1.36
24	c	501	CLA	O2A-CGA	3.20	1.42	1.33
24	B	611	CLA	OBD-CAD	3.20	1.26	1.22
24	B	617	CLA	O2D-CGD	3.20	1.41	1.33
24	c	506	CLA	C3D-C2D	3.19	1.45	1.39
32	D	411	LHG	O8-C23	3.19	1.42	1.33
40	C	517	DGD	O1G-C1A	3.19	1.42	1.33
24	d	405	CLA	C3B-C2B	3.19	1.44	1.40
25	D	401	PHO	O2D-CGD	3.19	1.41	1.33
28	A	612	SQD	C6-S	-3.19	1.65	1.77
24	b	617	CLA	O2A-CGA	3.18	1.42	1.33
25	A	608	PHO	O2A-CGA	3.18	1.42	1.33
31	f	101	LMT	O1'-C1'	3.18	1.45	1.40
24	d	405	CLA	CAA-C2A	-3.17	1.48	1.54
24	B	612	CLA	C3C-C2C	3.17	1.43	1.36
24	b	610	CLA	C3C-C2C	3.17	1.43	1.36
24	c	506	CLA	O2A-CGA	3.16	1.42	1.33
24	c	505	CLA	C1C-NC	-3.16	1.33	1.37
24	c	502	CLA	C3B-C2B	3.16	1.44	1.40
24	C	512	CLA	C3C-C2C	3.15	1.43	1.36
24	C	513	CLA	C1D-C2D	3.15	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C1B-NB	-3.15	1.32	1.35
29	b	621	LMG	O7-C8	-3.15	1.38	1.46
24	C	513	CLA	O2A-CGA	3.15	1.42	1.33
24	b	609	CLA	O2D-CGD	3.14	1.40	1.33
24	D	405	CLA	O2A-CGA	3.14	1.42	1.33
24	c	511	CLA	C3B-C2B	3.13	1.44	1.40
24	c	508	CLA	OBD-CAD	3.13	1.26	1.22
29	C	520	LMG	O1-C1	3.13	1.45	1.40
24	C	509	CLA	O2A-CGA	3.12	1.42	1.33
24	C	509	CLA	C3B-C2B	3.12	1.44	1.40
24	c	508	CLA	O2D-CGD	3.12	1.40	1.33
24	B	609	CLA	CHC-C1C	3.12	1.43	1.35
24	b	617	CLA	C1B-CHB	3.12	1.49	1.41
24	c	511	CLA	O2A-CGA	3.10	1.42	1.33
32	D	410	LHG	O8-C23	3.10	1.42	1.33
24	a	408	CLA	C1C-NC	-3.10	1.33	1.37
24	A	609	CLA	C1B-CHB	3.10	1.49	1.41
24	b	604	CLA	O2D-CGD	3.09	1.40	1.33
25	a	409	PHO	C4A-NA	-3.09	1.27	1.35
38	h	101	HTG	C1-S1	-3.08	1.76	1.80
24	C	505	CLA	O2D-CGD	3.08	1.40	1.33
24	b	610	CLA	C3B-C2B	3.07	1.44	1.40
24	b	609	CLA	C1C-NC	-3.07	1.33	1.37
38	B	624	HTG	C1'-S1	-3.07	1.77	1.81
24	b	603	CLA	O2A-CGA	3.06	1.42	1.33
24	d	404	CLA	O2A-CGA	3.06	1.42	1.33
24	C	508	CLA	OBD-CAD	3.06	1.26	1.22
24	A	607	CLA	C1C-NC	-3.06	1.33	1.37
24	C	506	CLA	OBD-CAD	3.05	1.26	1.22
40	c	516	DGD	O5D-C1E	3.05	1.45	1.40
27	d	407	PL9	C41-C39	3.04	1.57	1.51
38	b	623	HTG	C1-C2	3.04	1.58	1.53
24	B	608	CLA	C1D-C2D	3.03	1.49	1.42
24	b	616	CLA	C1B-NB	3.03	1.37	1.35
40	C	516	DGD	O2G-C1B	3.03	1.42	1.34
24	d	405	CLA	O2A-CGA	3.02	1.42	1.33
24	c	502	CLA	O2A-CGA	3.02	1.42	1.33
32	B	632	LHG	O8-C23	3.02	1.42	1.33
24	C	506	CLA	O2A-CGA	3.02	1.42	1.33
24	C	501	CLA	C4B-NB	-3.00	1.32	1.35
24	c	504	CLA	O2A-CGA	3.00	1.42	1.33
24	A	606	CLA	C1D-C2D	3.00	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	CMB-C2B	-3.00	1.45	1.51
24	b	615	CLA	C3D-C2D	2.99	1.44	1.39
32	l	101	LHG	O7-C7	2.99	1.42	1.34
24	b	613	CLA	C3B-C2B	2.99	1.44	1.40
38	C	529	HTG	O5-C1	2.99	1.47	1.42
24	c	511	CLA	C3C-C2C	2.98	1.43	1.36
26	B	619	BCR	C17-C18	2.98	1.39	1.35
24	b	605	CLA	C3C-C2C	2.98	1.43	1.36
32	D	410	LHG	O7-C7	2.98	1.42	1.34
24	C	512	CLA	C4C-C3C	2.97	1.50	1.45
24	D	404	CLA	C3C-C2C	2.97	1.43	1.36
24	b	610	CLA	O2A-CGA	2.97	1.42	1.33
24	d	404	CLA	C1D-C2D	2.97	1.49	1.42
24	D	403	CLA	O2D-CGD	2.96	1.40	1.33
29	c	520	LMG	O1-C1	2.96	1.45	1.40
24	B	611	CLA	C1C-NC	-2.96	1.33	1.37
24	B	602	CLA	C3C-C2C	2.96	1.43	1.36
24	C	502	CLA	C4B-NB	-2.94	1.32	1.35
24	b	607	CLA	OBD-CAD	2.94	1.26	1.22
25	D	401	PHO	CHC-C4B	2.94	1.47	1.40
24	C	503	CLA	C1C-NC	-2.93	1.33	1.37
25	d	401	PHO	O2D-CGD	2.93	1.40	1.33
40	c	518	DGD	O2G-C1B	2.93	1.42	1.34
24	b	616	CLA	CHC-C1C	2.93	1.42	1.35
24	D	403	CLA	C4B-CHC	2.92	1.49	1.41
28	a	413	SQD	O48-C23	2.92	1.41	1.33
24	A	606	CLA	C3B-C2B	2.92	1.44	1.40
24	d	403	CLA	O2A-CGA	2.92	1.41	1.33
40	D	408	DGD	O5D-C1E	2.92	1.45	1.40
24	c	506	CLA	C1C-C2C	2.91	1.50	1.44
40	H	103	DGD	O5D-C1E	2.91	1.45	1.40
24	B	609	CLA	OBD-CAD	2.90	1.26	1.22
24	B	603	CLA	C1B-CHB	2.90	1.49	1.41
24	A	607	CLA	C4B-NB	-2.90	1.32	1.35
40	c	517	DGD	O2G-C1B	2.90	1.42	1.34
27	a	412	PL9	C6-C5	2.90	1.50	1.35
29	j	101	LMG	O8-C28	2.90	1.41	1.33
38	a	418	HTG	C1'-S1	-2.90	1.77	1.81
27	d	407	PL9	C38-C39	-2.89	1.26	1.33
24	B	613	CLA	C3D-C2D	2.89	1.44	1.39
24	D	404	CLA	C1C-C2C	2.89	1.50	1.44
24	C	504	CLA	O2A-CGA	2.89	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	C1C-NC	-2.88	1.33	1.37
24	B	606	CLA	OBD-CAD	2.88	1.26	1.22
24	B	607	CLA	C3B-C2B	2.88	1.44	1.40
31	b	622	LMT	O3B-C3B	2.88	1.49	1.43
29	d	412	LMG	O1-C1	2.88	1.45	1.40
38	h	101	HTG	C1'-S1	-2.87	1.77	1.81
24	a	408	CLA	O2D-CGD	2.87	1.40	1.33
26	a	411	BCR	C36-C18	2.87	1.56	1.50
24	B	603	CLA	C4B-NB	2.87	1.37	1.35
24	b	617	CLA	C1D-C2D	2.87	1.49	1.42
24	b	609	CLA	O2A-CGA	2.86	1.41	1.33
24	c	502	CLA	C1C-NC	-2.86	1.33	1.37
24	b	617	CLA	C1C-NC	-2.86	1.33	1.37
24	d	404	CLA	C3B-C2B	2.86	1.44	1.40
24	b	613	CLA	O2A-CGA	2.86	1.41	1.33
24	b	615	CLA	C3C-C2C	2.85	1.42	1.36
24	B	605	CLA	O2D-CGD	2.85	1.40	1.33
24	b	602	CLA	C4B-CHC	2.85	1.48	1.41
24	c	505	CLA	O2D-CGD	2.85	1.40	1.33
28	A	616	SQD	C6-S	-2.83	1.66	1.77
24	b	615	CLA	O2D-CGD	2.83	1.40	1.33
24	B	610	CLA	O2A-CGA	2.83	1.41	1.33
31	A	617	LMT	O1'-C1'	2.83	1.45	1.40
24	c	506	CLA	OBD-CAD	2.82	1.26	1.22
27	D	407	PL9	C18-C19	2.82	1.39	1.33
24	B	604	CLA	C3B-C2B	2.82	1.44	1.40
24	C	508	CLA	C1C-C2C	2.82	1.50	1.44
24	B	605	CLA	C1C-C2C	2.82	1.50	1.44
40	c	517	DGD	O5D-C1E	2.82	1.45	1.40
24	B	613	CLA	O2D-CGD	2.81	1.40	1.33
24	b	608	CLA	O2D-CGD	2.81	1.40	1.33
24	b	607	CLA	C3C-C2C	2.81	1.42	1.36
40	C	517	DGD	O2G-C1B	2.81	1.42	1.34
24	b	615	CLA	C1B-CHB	2.81	1.48	1.41
29	b	621	LMG	O8-C28	2.80	1.41	1.33
24	D	404	CLA	O2D-CGD	2.80	1.40	1.33
24	c	502	CLA	C1B-CHB	2.80	1.48	1.41
24	b	609	CLA	C1D-C2D	2.80	1.48	1.42
24	C	508	CLA	O2A-CGA	2.80	1.41	1.33
38	c	531	HTG	C1'-S1	-2.79	1.77	1.81
24	B	617	CLA	C1B-CHB	2.79	1.48	1.41
26	c	514	BCR	C30-C25	-2.79	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3C-C2C	2.78	1.42	1.36
24	B	603	CLA	C1D-C2D	2.78	1.48	1.42
40	d	408	DGD	O5D-C1E	2.78	1.44	1.40
24	D	405	CLA	C1B-CHB	2.78	1.48	1.41
24	c	501	CLA	OBD-CAD	2.78	1.26	1.22
24	B	608	CLA	C1B-CHB	2.77	1.48	1.41
26	c	514	BCR	C8-C9	2.77	1.51	1.45
24	c	501	CLA	C4B-NB	-2.77	1.32	1.35
27	A	611	PL9	C6-C5	2.77	1.49	1.35
24	B	616	CLA	C4C-C3C	2.76	1.49	1.45
25	a	409	PHO	C3D-C2D	2.76	1.46	1.39
40	C	516	DGD	O1G-C1A	2.76	1.41	1.33
31	I	101	LMT	O1'-C1'	2.76	1.44	1.40
24	a	408	CLA	C1D-C2D	2.75	1.48	1.42
24	b	605	CLA	O2A-CGA	2.75	1.41	1.33
32	D	409	LHG	O8-C23	2.74	1.41	1.33
24	D	404	CLA	CMB-C2B	-2.74	1.45	1.51
26	t	102	BCR	C29-C30	-2.74	1.47	1.54
24	B	614	CLA	O2D-CGD	2.74	1.39	1.33
24	B	616	CLA	O2A-CGA	2.73	1.41	1.33
24	c	504	CLA	CHD-C4C	2.73	1.48	1.41
26	A	610	BCR	C21-C22	2.73	1.39	1.35
24	c	507	CLA	C1B-CHB	2.73	1.48	1.41
24	B	617	CLA	C3C-C2C	2.73	1.42	1.36
38	c	523	HTG	C1'-S1	-2.72	1.78	1.81
24	B	612	CLA	C4C-C3C	2.72	1.49	1.45
40	c	516	DGD	O2G-C1B	2.72	1.42	1.34
24	C	507	CLA	C1B-CHB	2.71	1.48	1.41
24	b	605	CLA	OBD-CAD	2.71	1.26	1.22
24	B	614	CLA	O2A-CGA	2.70	1.41	1.33
24	B	617	CLA	O2A-CGA	2.70	1.41	1.33
24	d	405	CLA	C4B-NB	-2.70	1.32	1.35
31	a	401	LMT	O1'-C1'	2.70	1.44	1.40
26	c	514	BCR	C1-C6	-2.70	1.50	1.53
24	D	404	CLA	O1D-CGD	2.69	1.28	1.21
24	C	503	CLA	C1C-C2C	2.68	1.49	1.44
38	C	532	HTG	C1-S1	-2.68	1.76	1.80
31	m	102	LMT	O4'-C4B	2.68	1.49	1.43
24	C	502	CLA	OBD-CAD	2.67	1.26	1.22
24	B	614	CLA	C3B-C2B	2.67	1.44	1.40
28	A	622	SQD	C6-S	-2.66	1.67	1.77
24	D	404	CLA	C3D-C2D	2.66	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	514	BCR	C30-C25	-2.66	1.50	1.53
24	b	613	CLA	C4B-CHC	2.66	1.48	1.41
38	c	530	HTG	C1-C2	2.66	1.58	1.53
25	a	409	PHO	O2D-CGD	2.66	1.39	1.33
30	O	302	GOL	O1-C1	2.66	1.53	1.42
24	c	510	CLA	CMC-C2C	-2.65	1.45	1.50
24	B	605	CLA	C3C-C2C	2.65	1.42	1.36
24	c	505	CLA	C3D-C2D	2.65	1.44	1.39
26	a	411	BCR	C8-C9	2.65	1.51	1.45
24	C	501	CLA	C1C-C2C	2.65	1.49	1.44
25	d	401	PHO	CHD-C1D	2.64	1.43	1.38
24	B	615	CLA	C1B-CHB	2.64	1.48	1.41
24	a	410	CLA	C1B-CHB	2.63	1.48	1.41
24	C	502	CLA	C3B-C2B	2.63	1.44	1.40
24	d	405	CLA	O2D-CGD	2.63	1.39	1.33
24	C	504	CLA	C3B-C2B	2.63	1.44	1.40
27	A	611	PL9	C2-C3	2.63	1.41	1.34
38	c	531	HTG	O5-C1	2.63	1.46	1.42
38	o	301	HTG	C1-C2	2.62	1.57	1.53
24	b	610	CLA	CMC-C2C	-2.62	1.45	1.50
26	B	619	BCR	C24-C25	2.62	1.54	1.45
26	H	102	BCR	C8-C9	2.62	1.51	1.45
24	c	505	CLA	O2A-CGA	2.61	1.41	1.33
26	b	618	BCR	C8-C9	2.61	1.51	1.45
29	J	101	LMG	O7-C10	2.61	1.41	1.34
24	d	404	CLA	CMB-C2B	-2.60	1.46	1.51
24	C	508	CLA	C1D-C2D	2.60	1.48	1.42
26	B	620	BCR	C23-C22	2.60	1.51	1.45
24	B	609	CLA	O2D-CGD	2.60	1.39	1.33
28	A	612	SQD	O48-C23	2.60	1.40	1.33
24	B	614	CLA	C1B-NB	2.60	1.37	1.35
25	D	401	PHO	O2A-C1	-2.59	1.38	1.46
24	d	404	CLA	C3C-C2C	2.59	1.42	1.36
40	H	103	DGD	O1G-C1A	2.59	1.40	1.33
28	h	105	SQD	O6-C1	2.59	1.44	1.40
24	a	408	CLA	C1B-CHB	2.59	1.48	1.41
40	H	103	DGD	O5D-C6D	2.58	1.48	1.43
24	b	611	CLA	O2D-CGD	2.58	1.39	1.33
25	d	401	PHO	CHB-C4A	2.58	1.46	1.40
24	C	505	CLA	C4C-C3C	2.58	1.49	1.45
40	H	103	DGD	O2G-C1B	2.58	1.41	1.34
24	a	410	CLA	O2A-CGA	2.58	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	403	CLA	O2A-CGA	2.57	1.40	1.33
24	C	507	CLA	CBD-CGD	-2.57	1.44	1.52
24	b	607	CLA	C4B-CHC	2.57	1.48	1.41
24	B	615	CLA	C3C-C2C	2.57	1.42	1.36
27	D	407	PL9	C6-C5	2.57	1.48	1.35
32	D	411	LHG	O7-C7	2.57	1.41	1.34
25	A	608	PHO	CHC-C4B	2.57	1.46	1.40
24	c	506	CLA	C1B-CHB	2.57	1.48	1.41
24	B	614	CLA	C1D-C2D	2.56	1.48	1.42
24	C	504	CLA	CHC-C1C	2.56	1.41	1.35
26	b	619	BCR	C24-C25	2.56	1.54	1.45
24	c	508	CLA	C1D-C2D	2.56	1.48	1.42
24	C	510	CLA	C1D-C2D	2.55	1.48	1.42
32	d	409	LHG	O8-C23	2.54	1.40	1.33
40	C	518	DGD	O1G-C1A	2.54	1.40	1.33
24	a	410	CLA	C1D-C2D	2.54	1.48	1.42
38	B	631	HTG	O5-C1	2.54	1.46	1.42
24	B	605	CLA	C1D-C2D	2.54	1.48	1.42
26	d	406	BCR	C32-C1	-2.54	1.48	1.53
24	c	513	CLA	C4B-CHC	2.54	1.48	1.41
26	C	514	BCR	C8-C9	2.54	1.51	1.45
24	A	609	CLA	C4B-CHC	2.54	1.48	1.41
26	D	406	BCR	C14-C13	2.54	1.39	1.35
24	c	510	CLA	C4B-CHC	2.54	1.48	1.41
25	d	401	PHO	C4A-NA	-2.53	1.29	1.35
24	B	609	CLA	C1D-C2D	2.53	1.48	1.42
24	c	511	CLA	CHD-C4C	2.53	1.48	1.41
24	b	614	CLA	C1D-C2D	2.52	1.48	1.42
31	B	622	LMT	O1'-C1'	2.52	1.44	1.40
24	c	507	CLA	C3B-C2B	2.52	1.43	1.40
24	B	602	CLA	C1D-C2D	2.52	1.48	1.42
28	a	413	SQD	C6-S	-2.52	1.68	1.77
26	A	610	BCR	C40-C30	-2.51	1.48	1.53
24	b	612	CLA	C1D-C2D	2.51	1.48	1.42
32	d	411	LHG	O8-C6	-2.51	1.39	1.45
24	C	508	CLA	O2D-CED	-2.51	1.39	1.45
24	B	607	CLA	C1C-C2C	2.51	1.49	1.44
24	A	607	CLA	C3C-C2C	2.51	1.42	1.36
25	a	409	PHO	OBD-CAD	2.51	1.26	1.22
24	b	608	CLA	CMB-C2B	-2.51	1.46	1.51
26	c	514	BCR	C23-C22	2.50	1.51	1.45
24	b	604	CLA	O2A-CGA	2.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	603	CLA	C1B-CHB	2.50	1.47	1.41
29	a	414	LMG	O8-C28	2.50	1.40	1.33
24	b	606	CLA	C1D-C2D	2.50	1.48	1.42
31	M	101	LMT	O4'-C4B	2.50	1.48	1.43
24	C	501	CLA	C1C-NC	-2.50	1.34	1.37
24	B	604	CLA	C1D-C2D	2.50	1.48	1.42
24	D	403	CLA	C1D-C2D	2.49	1.48	1.42
24	b	613	CLA	CMC-C2C	-2.49	1.45	1.50
24	B	607	CLA	C1B-CHB	2.49	1.47	1.41
38	B	630	HTG	C1'-S1	-2.49	1.78	1.81
24	a	407	CLA	CMD-C2D	-2.49	1.45	1.51
24	c	512	CLA	C4B-NB	2.49	1.37	1.35
25	a	409	PHO	O2A-CGA	2.48	1.40	1.33
38	V	204	HTG	O5-C1	2.48	1.46	1.42
24	b	607	CLA	C1B-NB	2.48	1.37	1.35
24	b	613	CLA	C1D-C2D	2.48	1.48	1.42
26	A	610	BCR	C23-C22	2.48	1.51	1.45
24	B	606	CLA	C3B-C2B	2.47	1.43	1.40
26	h	103	BCR	C27-C26	2.47	1.55	1.51
24	b	605	CLA	O2A-C1	-2.47	1.39	1.46
24	B	617	CLA	C2-C3	2.47	1.38	1.33
26	c	515	BCR	C8-C9	2.46	1.51	1.45
24	c	502	CLA	C3C-C2C	2.46	1.41	1.36
28	b	633	SQD	C6-S	-2.46	1.68	1.77
40	c	518	DGD	O2G-C2G	-2.46	1.40	1.46
25	D	401	PHO	O2A-CGA	2.45	1.40	1.33
24	C	512	CLA	C3B-C2B	2.45	1.43	1.40
24	b	614	CLA	CMB-C2B	-2.45	1.46	1.51
24	d	403	CLA	C1B-CHB	2.45	1.47	1.41
24	b	612	CLA	O2A-CGA	2.45	1.40	1.33
32	d	410	LHG	O7-C7	2.45	1.41	1.34
25	A	608	PHO	OBD-CAD	2.45	1.26	1.22
38	C	522	HTG	C1'-S1	-2.45	1.78	1.81
24	b	616	CLA	O2D-CGD	2.44	1.39	1.33
24	c	502	CLA	O2A-C1	-2.44	1.39	1.46
24	C	507	CLA	O2A-CGA	2.44	1.40	1.33
24	B	611	CLA	C3B-C2B	2.44	1.43	1.40
31	A	617	LMT	O3B-C3B	2.44	1.48	1.43
24	C	503	CLA	O2D-CED	-2.44	1.39	1.45
27	D	407	PL9	O1-C4	2.44	1.28	1.23
26	K	101	BCR	C30-C25	-2.44	1.50	1.53
24	b	603	CLA	O2D-CGD	2.43	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	516	DGD	O5D-C1E	2.43	1.44	1.40
24	B	602	CLA	MG-NC	-2.43	2.00	2.06
26	T	102	BCR	C38-C26	-2.43	1.46	1.50
24	B	616	CLA	C1B-NB	-2.43	1.33	1.35
31	m	101	LMT	O1'-C1'	2.43	1.44	1.40
24	C	512	CLA	OBD-CAD	2.43	1.25	1.22
40	D	408	DGD	O3G-C1D	2.42	1.44	1.40
27	d	407	PL9	C15-C14	-2.42	1.44	1.50
24	c	501	CLA	C1B-CHB	2.42	1.47	1.41
38	a	418	HTG	C1-S1	-2.42	1.77	1.80
24	c	509	CLA	C1C-NC	-2.41	1.34	1.37
24	B	612	CLA	O2D-CGD	2.41	1.39	1.33
24	C	512	CLA	C1B-CHB	2.41	1.47	1.41
24	B	613	CLA	CHD-C4C	2.40	1.48	1.41
24	B	613	CLA	C1D-C2D	2.40	1.48	1.42
24	B	615	CLA	OBD-CAD	2.40	1.25	1.22
24	b	612	CLA	C1C-C2C	2.40	1.49	1.44
24	d	404	CLA	C1C-NC	-2.40	1.34	1.37
24	c	505	CLA	C1D-C2D	2.40	1.48	1.42
26	B	619	BCR	C35-C13	2.39	1.55	1.50
24	c	510	CLA	C1D-C2D	2.39	1.48	1.42
24	B	607	CLA	C1B-NB	-2.39	1.33	1.35
24	b	605	CLA	C1B-CHB	2.39	1.47	1.41
24	b	612	CLA	C1B-CHB	2.39	1.47	1.41
26	H	102	BCR	C12-C13	2.38	1.51	1.45
24	b	612	CLA	OBD-CAD	2.38	1.25	1.22
25	d	401	PHO	C1D-ND	-2.38	1.33	1.38
24	c	506	CLA	C3B-C2B	2.38	1.43	1.40
24	B	606	CLA	O1D-CGD	2.36	1.27	1.21
27	A	611	PL9	C11-C9	-2.36	1.46	1.51
24	C	513	CLA	OBD-CAD	2.36	1.25	1.22
24	c	512	CLA	C4C-C3C	2.36	1.49	1.45
25	d	401	PHO	C3D-C2D	2.36	1.45	1.39
25	D	401	PHO	C3D-C4D	-2.36	1.36	1.43
38	a	418	HTG	O2-C2	2.35	1.48	1.43
24	c	506	CLA	CHD-C4C	2.35	1.47	1.41
24	B	612	CLA	C3B-C2B	2.35	1.43	1.40
24	B	606	CLA	C4B-CHC	2.35	1.47	1.41
28	l	102	SQD	O5-C1	2.35	1.47	1.41
28	x	101	SQD	C6-S	-2.35	1.68	1.77
24	B	603	CLA	C1C-NC	-2.35	1.34	1.37
43	V	203	HEC	C4D-CHA	-2.35	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	505	CLA	CMD-C2D	-2.34	1.46	1.51
24	D	404	CLA	C3B-C2B	2.34	1.43	1.40
43	v	202	HEC	C3B-C4B	2.34	1.47	1.43
24	c	510	CLA	CHD-C4C	2.34	1.47	1.41
40	C	516	DGD	O5D-C6D	-2.34	1.39	1.43
24	c	512	CLA	C1D-C2D	2.34	1.47	1.42
32	d	409	LHG	O7-C5	-2.34	1.40	1.46
27	D	407	PL9	C51-C49	-2.33	1.44	1.50
29	B	621	LMG	O10-C28	-2.33	1.15	1.22
29	C	519	LMG	O7-C8	-2.33	1.40	1.46
24	B	604	CLA	C4-C3	-2.33	1.44	1.50
28	h	105	SQD	C6-S	-2.33	1.68	1.77
24	b	611	CLA	O2D-CED	-2.33	1.39	1.45
24	c	512	CLA	C1B-CHB	2.33	1.47	1.41
25	A	608	PHO	C3D-C2D	2.32	1.45	1.39
30	B	633	GOL	O2-C2	2.32	1.50	1.43
24	C	501	CLA	C4B-CHC	2.32	1.47	1.41
26	b	619	BCR	C5-C6	2.32	1.38	1.34
24	b	617	CLA	C2-C3	2.32	1.38	1.33
24	b	604	CLA	C1C-C2C	2.31	1.49	1.44
25	D	401	PHO	CHC-C1C	2.31	1.43	1.38
26	b	618	BCR	C40-C30	-2.31	1.49	1.53
32	D	409	LHG	C24-C23	2.31	1.57	1.50
24	C	506	CLA	C1C-C2C	2.31	1.49	1.44
31	J	103	LMT	O1'-C1'	2.31	1.44	1.40
24	C	506	CLA	C1B-CHB	2.31	1.47	1.41
24	B	604	CLA	C1C-NC	-2.30	1.34	1.37
38	b	632	HTG	O5-C1	2.30	1.46	1.42
24	B	612	CLA	CMD-C2D	-2.30	1.46	1.51
31	F	102	LMT	C4B-C5B	2.30	1.57	1.53
25	D	401	PHO	C1C-C2C	2.30	1.50	1.45
24	C	512	CLA	C1C-C2C	2.30	1.49	1.44
27	d	407	PL9	C2-C1	-2.30	1.38	1.44
24	b	604	CLA	C3A-C2A	-2.29	1.48	1.54
24	c	511	CLA	CMD-C2D	-2.29	1.46	1.51
26	b	620	BCR	C12-C13	2.29	1.50	1.45
26	C	525	BCR	C1-C6	-2.29	1.50	1.53
24	b	612	CLA	C3D-C2D	2.29	1.43	1.39
27	A	611	PL9	C48-C49	2.29	1.38	1.32
26	d	406	BCR	C8-C9	2.28	1.50	1.45
24	C	510	CLA	C1C-C2C	2.28	1.49	1.44
24	c	503	CLA	C3C-C2C	2.28	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	C4C-C3C	2.28	1.49	1.45
24	c	509	CLA	C1C-C2C	2.28	1.49	1.44
24	A	607	CLA	C4B-CHC	2.28	1.47	1.41
26	D	406	BCR	C2-C3	-2.27	1.47	1.52
30	O	306	GOL	O2-C2	2.27	1.50	1.43
24	c	513	CLA	MG-NA	-2.27	2.00	2.06
24	b	609	CLA	C1B-CHB	2.27	1.47	1.41
26	C	525	BCR	C30-C25	-2.27	1.50	1.53
24	A	609	CLA	O2A-CGA	2.27	1.40	1.33
28	b	633	SQD	O6-C1	2.27	1.44	1.40
25	A	608	PHO	C4A-NA	-2.26	1.29	1.35
24	C	507	CLA	C1C-C2C	2.26	1.48	1.44
24	C	513	CLA	C1B-CHB	2.26	1.47	1.41
31	u	203	LMT	C1B-C2B	2.26	1.59	1.52
24	B	612	CLA	O2A-CGA	2.26	1.39	1.33
24	b	608	CLA	O2A-CGA	2.26	1.39	1.33
26	C	515	BCR	C12-C13	2.26	1.50	1.45
40	c	517	DGD	O5D-C6D	-2.25	1.39	1.43
24	b	608	CLA	C1B-CHB	2.25	1.47	1.41
29	A	613	LMG	O1-C1	2.25	1.44	1.40
31	F	102	LMT	O4'-C4B	2.25	1.48	1.43
24	c	504	CLA	C1C-NC	-2.24	1.34	1.37
24	C	508	CLA	O2D-CGD	2.24	1.38	1.33
24	b	617	CLA	C1B-NB	2.24	1.37	1.35
24	c	503	CLA	C1B-CHB	2.23	1.47	1.41
24	c	511	CLA	C1B-CHB	2.23	1.47	1.41
26	h	103	BCR	C21-C22	-2.23	1.32	1.35
24	c	504	CLA	C3B-C2B	2.23	1.43	1.40
24	c	509	CLA	C1B-CHB	2.23	1.47	1.41
24	b	605	CLA	C4B-NB	-2.23	1.33	1.35
24	D	405	CLA	C1C-NC	-2.23	1.34	1.37
38	B	631	HTG	C1'-S1	-2.22	1.78	1.81
24	c	503	CLA	O2D-CED	-2.22	1.40	1.45
32	B	632	LHG	O7-C7	2.22	1.40	1.34
24	c	508	CLA	CMD-C2D	-2.22	1.46	1.51
24	C	512	CLA	C1D-C2D	2.22	1.47	1.42
24	a	410	CLA	OBD-CAD	2.22	1.25	1.22
24	b	602	CLA	C1C-C2C	2.21	1.48	1.44
24	A	607	CLA	C1D-C2D	2.21	1.47	1.42
24	C	508	CLA	CMD-C2D	-2.21	1.46	1.51
24	c	507	CLA	C1C-C2C	2.21	1.48	1.44
24	C	510	CLA	C4C-C3C	2.21	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	A	611	PL9	C6-C1	2.21	1.52	1.48
27	d	407	PL9	C6-C5	2.20	1.46	1.35
24	B	615	CLA	C1C-NC	-2.20	1.34	1.37
24	c	510	CLA	C1B-CHB	2.20	1.47	1.41
32	d	409	LHG	P-O4	-2.20	1.45	1.55
40	C	517	DGD	O5D-C1E	2.20	1.43	1.40
24	C	507	CLA	C4B-NB	-2.20	1.33	1.35
24	c	506	CLA	C1B-NB	-2.20	1.33	1.35
26	C	514	BCR	C15-C14	2.20	1.50	1.43
24	b	611	CLA	C1C-NC	-2.20	1.34	1.37
24	a	410	CLA	O2A-C1	-2.20	1.40	1.46
24	C	501	CLA	C1D-C2D	2.20	1.47	1.42
24	B	602	CLA	C1C-NC	-2.19	1.34	1.37
38	b	631	HTG	O4-C4	2.19	1.48	1.43
24	B	617	CLA	C1D-C2D	2.19	1.47	1.42
24	b	612	CLA	C1C-NC	-2.19	1.34	1.37
26	c	527	BCR	C8-C9	2.18	1.50	1.45
24	b	605	CLA	C1C-NC	-2.18	1.34	1.37
24	B	602	CLA	C2-C3	2.18	1.38	1.33
29	c	519	LMG	O7-C8	-2.18	1.41	1.46
38	B	630	HTG	O2-C2	2.18	1.48	1.43
26	a	411	BCR	C20-C21	2.18	1.50	1.43
24	C	509	CLA	C1D-C2D	2.18	1.47	1.42
24	B	615	CLA	CBA-CGA	2.18	1.57	1.50
24	C	508	CLA	C1B-CHB	2.18	1.47	1.41
24	b	607	CLA	O2A-CGA	2.17	1.39	1.33
26	T	102	BCR	C21-C22	2.17	1.38	1.35
24	c	510	CLA	CAA-C2A	-2.17	1.50	1.54
26	b	619	BCR	C34-C9	2.17	1.55	1.50
26	T	102	BCR	C14-C13	-2.17	1.32	1.35
24	B	602	CLA	CBD-CGD	-2.16	1.45	1.52
24	a	410	CLA	C1C-NC	-2.16	1.34	1.37
38	O	303	HTG	C1-C2	2.16	1.57	1.53
29	J	101	LMG	O8-C28	2.16	1.39	1.33
31	C	533	LMT	O1'-C1'	2.16	1.43	1.40
24	b	610	CLA	C1C-C2C	2.16	1.48	1.44
24	b	614	CLA	C1C-NC	-2.16	1.34	1.37
26	h	103	BCR	C19-C18	2.16	1.50	1.45
26	T	102	BCR	C15-C14	2.16	1.50	1.43
26	D	406	BCR	C26-C25	2.16	1.38	1.34
24	C	505	CLA	C4B-CHC	2.16	1.47	1.41
24	B	607	CLA	O2A-CGA	2.16	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C1A-NA	-2.16	1.33	1.37
24	D	404	CLA	C1B-CHB	2.16	1.47	1.41
24	c	513	CLA	C1B-CHB	2.15	1.47	1.41
27	d	407	PL9	C45-C44	2.15	1.56	1.50
25	A	608	PHO	C1C-NC	-2.15	1.34	1.38
24	C	502	CLA	C1B-CHB	2.15	1.47	1.41
40	h	104	DGD	O4E-C4E	2.15	1.48	1.43
38	B	631	HTG	C1-S1	-2.15	1.77	1.80
26	k	101	BCR	C30-C25	-2.15	1.50	1.53
24	b	605	CLA	C1C-C2C	2.15	1.48	1.44
28	F	104	SQD	C3-C2	2.14	1.57	1.52
24	c	507	CLA	C1C-NC	-2.14	1.34	1.37
24	C	501	CLA	O2A-CGA	2.14	1.39	1.33
24	D	404	CLA	C4B-CHC	2.14	1.46	1.41
24	b	606	CLA	C1C-C2C	2.14	1.48	1.44
24	C	502	CLA	O2A-CGA	2.13	1.39	1.33
24	C	510	CLA	C1B-CHB	2.13	1.46	1.41
40	H	103	DGD	O4E-C4E	2.13	1.48	1.43
40	C	518	DGD	O2G-C2G	-2.13	1.41	1.46
24	d	404	CLA	O2D-CGD	2.12	1.38	1.33
38	B	623	HTG	C1-C2	2.12	1.57	1.53
29	j	101	LMG	O7-C8	-2.12	1.41	1.46
24	b	608	CLA	C1B-NB	2.12	1.37	1.35
24	C	513	CLA	C1C-NC	-2.12	1.34	1.37
24	c	513	CLA	C1C-C2C	2.12	1.48	1.44
24	c	509	CLA	C4C-C3C	2.11	1.48	1.45
24	b	615	CLA	CMB-C2B	-2.11	1.47	1.51
24	A	609	CLA	MG-NA	-2.11	2.01	2.06
24	b	602	CLA	C1D-C2D	2.11	1.47	1.42
24	b	615	CLA	C1D-C2D	2.11	1.47	1.42
24	b	614	CLA	C3B-C2B	2.11	1.43	1.40
24	C	505	CLA	C1C-NC	-2.11	1.34	1.37
25	D	401	PHO	C1D-ND	-2.11	1.34	1.38
41	e	107	HEM	C4D-C3D	2.11	1.47	1.42
28	h	105	SQD	C46-C45	2.11	1.57	1.50
24	d	404	CLA	C4B-CHC	2.11	1.46	1.41
24	b	610	CLA	C1C-NC	-2.11	1.34	1.37
24	c	510	CLA	O2A-CGA	2.10	1.39	1.33
32	d	410	LHG	O8-C23	2.10	1.39	1.33
24	C	509	CLA	O2D-CGD	2.10	1.38	1.33
26	c	514	BCR	C12-C13	2.10	1.50	1.45
24	a	408	CLA	CMB-C2B	-2.10	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	620	BCR	C29-C28	-2.10	1.47	1.52
24	C	512	CLA	CHD-C4C	2.10	1.47	1.41
24	C	504	CLA	CAC-C3C	-2.10	1.45	1.51
24	c	512	CLA	CHD-C4C	2.10	1.47	1.41
24	c	504	CLA	C1C-C2C	2.10	1.48	1.44
24	c	503	CLA	O2A-CGA	2.10	1.39	1.33
24	c	510	CLA	CMD-C2D	-2.10	1.46	1.51
24	b	611	CLA	C4B-CHC	2.09	1.46	1.41
40	h	104	DGD	O2E-C2E	2.09	1.47	1.43
24	B	613	CLA	O2A-CGA	2.09	1.39	1.33
26	A	610	BCR	C31-C1	-2.09	1.49	1.53
26	b	619	BCR	C19-C18	2.09	1.50	1.45
43	v	202	HEC	C3C-C2C	-2.09	1.38	1.40
32	a	419	LHG	C4-C5	2.09	1.57	1.50
24	B	611	CLA	C1D-C2D	2.09	1.47	1.42
24	D	405	CLA	C4B-NB	2.09	1.37	1.35
24	B	616	CLA	C1C-C2C	2.08	1.48	1.44
26	h	103	BCR	C24-C25	2.08	1.52	1.45
24	B	616	CLA	CHD-C4C	2.08	1.47	1.41
43	V	203	HEC	CAA-C2A	-2.08	1.48	1.52
24	c	502	CLA	C4B-CHC	2.08	1.46	1.41
26	a	411	BCR	C27-C26	2.08	1.55	1.51
26	A	610	BCR	C20-C21	2.08	1.49	1.43
38	C	529	HTG	C1-C2	2.08	1.57	1.53
38	b	624	HTG	O5-C1	2.08	1.45	1.42
24	B	614	CLA	C1B-CHB	2.08	1.46	1.41
27	D	407	PL9	C31-C29	2.08	1.55	1.51
40	H	103	DGD	O6E-C1E	2.08	1.47	1.41
26	C	525	BCR	C8-C9	2.07	1.50	1.45
38	c	523	HTG	C1-S1	-2.07	1.77	1.80
24	B	617	CLA	C1C-C2C	2.07	1.48	1.44
30	b	627	GOL	O3-C3	2.07	1.51	1.42
31	M	101	LMT	C3B-C2B	2.07	1.57	1.52
31	M	101	LMT	O2'-C2'	2.07	1.47	1.43
24	C	503	CLA	C4B-CHC	2.07	1.46	1.41
38	C	531	HTG	O5-C1	2.07	1.45	1.42
40	C	516	DGD	O1G-C1G	-2.07	1.40	1.45
24	C	501	CLA	CMB-C2B	-2.07	1.47	1.51
24	A	607	CLA	O2A-CGA	2.07	1.39	1.33
27	d	407	PL9	C50-C49	-2.07	1.44	1.50
26	b	618	BCR	C12-C13	2.06	1.50	1.45
29	B	621	LMG	O7-C8	-2.06	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	620	BCR	C15-C14	2.06	1.49	1.43
24	C	510	CLA	CMC-C2C	-2.06	1.46	1.50
24	b	613	CLA	C1C-NC	-2.06	1.34	1.37
24	b	615	CLA	CHD-C4C	2.06	1.47	1.41
24	c	510	CLA	CMB-C2B	-2.06	1.47	1.51
24	c	508	CLA	C1B-CHB	2.05	1.46	1.41
31	j	103	LMT	O1'-C1'	2.05	1.43	1.40
24	b	604	CLA	C4C-C3C	2.05	1.48	1.45
28	F	104	SQD	C4-C5	2.05	1.57	1.53
25	a	409	PHO	CHD-C4C	2.05	1.45	1.40
26	B	619	BCR	C19-C18	2.05	1.50	1.45
38	b	623	HTG	O4-C4	2.05	1.47	1.43
24	A	606	CLA	C2-C3	2.05	1.37	1.33
24	B	603	CLA	C4B-CHC	2.05	1.46	1.41
24	B	607	CLA	O2D-CGD	2.04	1.38	1.33
24	C	504	CLA	CMB-C2B	-2.04	1.47	1.51
24	C	506	CLA	C1D-C2D	2.04	1.47	1.42
24	b	613	CLA	C1B-CHB	2.04	1.46	1.41
24	A	609	CLA	CMB-C2B	-2.04	1.47	1.51
24	b	617	CLA	C4B-CHC	2.04	1.46	1.41
24	B	607	CLA	CMA-C3A	-2.04	1.48	1.53
26	b	619	BCR	C30-C25	-2.04	1.51	1.53
26	H	102	BCR	C23-C22	2.04	1.50	1.45
24	c	510	CLA	C1C-C2C	2.04	1.48	1.44
24	b	606	CLA	C5-C3	2.03	1.55	1.51
24	c	511	CLA	CMC-C2C	-2.03	1.46	1.50
24	B	607	CLA	C1D-C2D	2.03	1.47	1.42
26	t	102	BCR	C16-C17	2.03	1.49	1.43
24	B	605	CLA	CBD-CGD	-2.03	1.46	1.52
25	A	608	PHO	CHD-C1D	2.03	1.42	1.38
24	c	503	CLA	C1D-C2D	2.03	1.47	1.42
25	d	401	PHO	C3B-C4B	2.03	1.47	1.43
40	H	103	DGD	O6D-C1D	2.03	1.47	1.41
25	A	608	PHO	CAA-C2A	-2.02	1.50	1.54
26	c	527	BCR	C5-C6	2.02	1.37	1.34
24	a	410	CLA	C4C-C3C	2.02	1.48	1.45
24	c	502	CLA	C1C-C2C	2.02	1.48	1.44
24	C	504	CLA	CHD-C4C	2.02	1.46	1.41
26	t	102	BCR	C23-C22	2.02	1.50	1.45
26	b	620	BCR	C1-C6	-2.02	1.51	1.53
24	B	611	CLA	O2A-CGA	2.01	1.39	1.33
26	B	619	BCR	C12-C13	2.01	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	O2A-CGA	2.01	1.39	1.33
31	u	203	LMT	O5B-C5B	2.00	1.49	1.44
38	H	101	HTG	C1-S1	-2.00	1.77	1.80
31	u	203	LMT	C4B-C5B	2.00	1.57	1.53

All (2264) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	E	113	HEM	CAD-CBD-CGD	11.43	131.84	112.67
24	c	508	CLA	C4D-C3D-CAD	-11.16	102.24	108.47
24	c	502	CLA	C4D-C3D-CAD	-10.91	102.38	108.47
24	C	508	CLA	C4D-C3D-CAD	-10.27	102.74	108.47
24	A	609	CLA	C4D-C3D-CAD	-9.59	103.12	108.47
24	B	602	CLA	C4D-C3D-CAD	-9.12	103.39	108.47
28	a	413	SQD	O6-C1-C2	9.07	122.46	108.30
24	B	610	CLA	C2C-C1C-NC	9.03	118.43	109.97
38	V	204	HTG	O5-C1-C2	-8.88	99.14	110.31
24	d	404	CLA	C2C-C1C-NC	8.87	118.28	109.97
40	d	408	DGD	O3G-C1D-C2D	8.83	122.09	108.30
24	c	501	CLA	C4D-C3D-CAD	-8.80	103.56	108.47
24	C	501	CLA	C2C-C1C-NC	8.74	118.16	109.97
28	F	104	SQD	O6-C1-C2	8.63	121.78	108.30
31	M	102	LMT	C1-O1'-C1'	8.58	128.06	113.84
24	B	612	CLA	C2C-C1C-NC	8.54	117.98	109.97
38	C	529	HTG	C1'-S1-C1	8.54	116.06	100.09
24	C	502	CLA	C4D-C3D-CAD	-8.47	103.75	108.47
24	c	501	CLA	C2C-C1C-NC	8.37	117.82	109.97
24	b	605	CLA	C2C-C1C-NC	8.30	117.75	109.97
24	C	501	CLA	O2D-CGD-CBD	8.29	126.00	111.27
24	C	503	CLA	C4D-C3D-CAD	-8.28	103.85	108.47
24	C	505	CLA	C2C-C1C-NC	8.22	117.67	109.97
24	C	504	CLA	C2C-C1C-NC	8.18	117.64	109.97
24	B	610	CLA	C4D-C3D-CAD	-8.14	103.93	108.47
24	B	611	CLA	C4D-C3D-CAD	-8.12	103.94	108.47
24	b	609	CLA	C2C-C1C-NC	8.10	117.56	109.97
24	B	605	CLA	C5-C3-C2	-8.09	104.74	121.12
24	B	614	CLA	C4D-C3D-CAD	-8.07	103.97	108.47
26	d	406	BCR	C40-C30-C25	-8.06	97.22	110.30
24	B	608	CLA	C2C-C1C-NC	8.01	117.48	109.97
24	D	405	CLA	C4D-C3D-CAD	-8.00	104.01	108.47
24	c	504	CLA	C2C-C1C-NC	7.98	117.44	109.97
24	c	508	CLA	C2C-C1C-NC	7.92	117.39	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	O2D-CGD-O1D	-7.91	108.37	123.84
24	c	505	CLA	C3C-C4C-NC	7.87	119.40	110.57
24	B	616	CLA	C2C-C1C-NC	7.86	117.33	109.97
24	D	403	CLA	C2C-C1C-NC	7.86	117.33	109.97
24	C	506	CLA	C2C-C1C-NC	7.82	117.30	109.97
24	b	611	CLA	C2C-C1C-NC	7.78	117.26	109.97
24	b	616	CLA	C2C-C1C-NC	7.72	117.21	109.97
24	c	512	CLA	C2C-C1C-NC	7.71	117.20	109.97
24	B	604	CLA	C2C-C1C-NC	7.70	117.18	109.97
24	B	605	CLA	C1-C2-C3	-7.67	112.78	126.04
24	C	509	CLA	C2C-C1C-NC	7.59	117.08	109.97
24	B	607	CLA	C2C-C1C-NC	7.49	116.99	109.97
24	a	410	CLA	C2C-C1C-NC	7.49	116.99	109.97
24	C	513	CLA	C4D-C3D-CAD	-7.49	104.29	108.47
24	b	610	CLA	C3C-C4C-NC	7.48	118.96	110.57
24	C	507	CLA	C2C-C1C-NC	7.47	116.97	109.97
40	D	408	DGD	O2G-C1B-C2B	7.46	127.58	111.50
24	D	404	CLA	C2C-C1C-NC	7.42	116.92	109.97
24	b	612	CLA	C2C-C1C-NC	7.41	116.91	109.97
24	b	617	CLA	C2C-C1C-NC	7.38	116.89	109.97
24	b	613	CLA	C3C-C4C-NC	7.36	118.83	110.57
24	B	606	CLA	C3C-C4C-NC	7.36	118.82	110.57
24	A	609	CLA	C2C-C1C-NC	7.35	116.86	109.97
24	B	609	CLA	C2C-C1C-NC	7.34	116.84	109.97
26	D	406	BCR	C40-C30-C25	-7.30	98.45	110.30
24	b	617	CLA	C3C-C4C-NC	7.26	118.72	110.57
24	c	511	CLA	C2C-C1C-NC	7.24	116.75	109.97
24	C	510	CLA	C4D-C3D-CAD	-7.15	104.48	108.47
24	B	602	CLA	C2C-C1C-NC	7.14	116.66	109.97
24	a	408	CLA	C2C-C1C-NC	7.11	116.63	109.97
27	A	611	PL9	C3-C4-C5	7.10	127.83	118.60
24	c	502	CLA	C2C-C1C-NC	7.09	116.62	109.97
24	B	605	CLA	C2C-C1C-NC	7.09	116.61	109.97
24	a	410	CLA	C4D-C3D-CAD	-7.09	104.52	108.47
24	B	617	CLA	C2C-C1C-NC	7.08	116.61	109.97
24	c	513	CLA	C2C-C1C-NC	7.05	116.57	109.97
24	C	508	CLA	C2C-C1C-NC	7.04	116.57	109.97
24	b	604	CLA	C2C-C1C-NC	7.03	116.56	109.97
24	b	605	CLA	C3C-C4C-NC	6.99	118.41	110.57
24	A	607	CLA	C2C-C1C-NC	6.97	116.50	109.97
24	a	408	CLA	C3C-C4C-NC	6.95	118.37	110.57
28	a	424	SQD	O9-S-C6	6.94	115.18	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C4D-C3D-CAD	-6.91	104.62	108.47
24	c	507	CLA	C2C-C1C-NC	6.89	116.43	109.97
24	b	604	CLA	C4D-C3D-CAD	-6.89	104.63	108.47
24	D	405	CLA	C2C-C1C-NC	6.86	116.40	109.97
28	A	612	SQD	C1-O5-C5	-6.85	100.24	113.69
24	b	614	CLA	C2C-C1C-NC	6.84	116.38	109.97
24	B	606	CLA	C2C-C1C-NC	6.84	116.38	109.97
24	C	503	CLA	C3C-C4C-NC	6.82	118.21	110.57
24	B	602	CLA	O2A-C1-C2	6.80	126.51	108.64
24	b	603	CLA	C3C-C4C-NC	6.79	118.19	110.57
24	a	407	CLA	C2C-C1C-NC	6.78	116.33	109.97
24	C	506	CLA	C4D-C3D-CAD	-6.78	104.69	108.47
24	b	610	CLA	C2C-C1C-NC	6.75	116.29	109.97
24	B	612	CLA	C4D-C3D-CAD	-6.69	104.74	108.47
27	a	412	PL9	C7-C3-C4	6.69	122.31	116.88
24	d	404	CLA	C1C-C2C-C3C	-6.64	99.97	106.96
24	c	509	CLA	C2C-C1C-NC	6.63	116.19	109.97
27	A	611	PL9	C7-C3-C2	6.63	132.01	123.30
24	B	611	CLA	C3C-C4C-NC	6.62	118.00	110.57
24	b	605	CLA	C4D-C3D-CAD	-6.61	104.78	108.47
24	b	602	CLA	C2C-C1C-NC	6.61	116.16	109.97
29	C	519	LMG	O8-C28-C29	6.56	132.50	111.91
24	C	507	CLA	C3C-C4C-NC	6.55	117.92	110.57
24	b	612	CLA	C4D-C3D-CAD	-6.54	104.82	108.47
24	a	407	CLA	C4D-C3D-CAD	-6.49	104.85	108.47
24	d	405	CLA	C2C-C1C-NC	6.49	116.05	109.97
41	E	113	HEM	C1D-C2D-C3D	-6.48	102.49	107.00
24	b	605	CLA	C5-C3-C2	-6.47	108.02	121.12
38	C	522	HTG	C1'-S1-C1	6.42	112.10	100.09
24	b	610	CLA	C4D-C3D-CAD	-6.41	104.90	108.47
24	b	606	CLA	C3C-C4C-NC	6.40	117.75	110.57
29	B	621	LMG	O7-C10-C11	6.40	125.29	111.50
28	x	101	SQD	O8-S-C6	6.39	115.92	105.74
24	c	505	CLA	C2C-C1C-NC	6.38	115.95	109.97
28	l	102	SQD	O6-C1-C2	6.36	118.23	108.30
24	B	611	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	c	504	CLA	C3B-C4B-NB	6.34	117.40	109.21
24	C	513	CLA	C3C-C4C-NC	6.32	117.66	110.57
24	B	606	CLA	C4D-C3D-CAD	-6.32	104.95	108.47
24	b	602	CLA	O2D-CGD-CBD	6.28	122.42	111.27
26	C	525	BCR	C7-C8-C9	-6.25	116.79	126.23
24	D	404	CLA	C4D-C3D-CAD	-6.25	104.98	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	605	CLA	C1-C2-C3	-6.25	115.23	126.04
24	C	508	CLA	C3C-C4C-NC	6.24	117.57	110.57
24	c	510	CLA	C4D-C3D-CAD	-6.22	105.00	108.47
24	c	510	CLA	C3C-C4C-NC	6.22	117.55	110.57
24	B	612	CLA	C3C-C4C-NC	6.21	117.54	110.57
24	B	614	CLA	C2C-C1C-NC	6.20	115.78	109.97
24	c	505	CLA	CAC-C3C-C4C	6.20	132.85	124.81
24	C	510	CLA	C2C-C1C-NC	6.19	115.77	109.97
24	B	602	CLA	O2D-CGD-CBD	6.18	122.25	111.27
24	c	509	CLA	C3C-C4C-NC	6.16	117.48	110.57
40	d	408	DGD	O2G-C1B-C2B	6.16	124.78	111.50
28	A	612	SQD	C1-C2-C3	-6.14	97.20	110.00
24	c	503	CLA	C4D-C3D-CAD	-6.13	105.05	108.47
24	c	503	CLA	C2C-C1C-NC	6.13	115.71	109.97
24	A	607	CLA	C4D-C3D-CAD	-6.13	105.05	108.47
38	B	624	HTG	C1'-S1-C1	6.12	111.54	100.09
24	c	501	CLA	O2D-CGD-O1D	-6.11	111.89	123.84
24	B	613	CLA	C4D-C3D-CAD	-6.10	105.07	108.47
24	d	404	CLA	C3B-C4B-NB	6.10	117.09	109.21
24	C	513	CLA	C2C-C1C-NC	6.09	115.67	109.97
24	a	408	CLA	C4D-C3D-CAD	-6.07	105.08	108.47
24	B	609	CLA	C3C-C4C-NC	6.07	117.38	110.57
24	B	615	CLA	C2C-C1C-NC	6.07	115.66	109.97
24	c	513	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
31	c	521	LMT	O1B-C4'-C3'	6.05	123.37	107.28
24	b	617	CLA	C4D-C3D-CAD	-6.05	105.10	108.47
24	b	613	CLA	C2C-C1C-NC	6.04	115.63	109.97
25	D	401	PHO	CMD-C2D-C1D	6.03	134.35	125.06
24	c	506	CLA	C3C-C4C-NC	6.01	117.31	110.57
28	A	612	SQD	O9-S-C6	6.01	114.08	106.94
24	A	606	CLA	C2C-C1C-NC	6.01	115.60	109.97
24	C	503	CLA	C2C-C1C-NC	6.01	115.60	109.97
24	c	504	CLA	C1C-C2C-C3C	-6.00	100.65	106.96
24	b	616	CLA	C1C-C2C-C3C	-5.98	100.67	106.96
24	B	607	CLA	C1C-C2C-C3C	-5.96	100.69	106.96
24	b	611	CLA	C3C-C4C-NC	5.95	117.25	110.57
28	a	413	SQD	O9-S-C6	5.95	114.02	106.94
24	B	602	CLA	CMC-C2C-C1C	5.95	134.10	125.04
38	c	531	HTG	C1'-S1-C1	5.94	111.20	100.09
24	A	607	CLA	CAC-C3C-C4C	5.94	132.51	124.81
24	c	501	CLA	C3B-C4B-NB	5.93	116.88	109.21
24	b	614	CLA	C3C-C4C-NC	5.92	117.21	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	424	SQD	O47-C7-C8	5.89	124.20	111.50
24	b	609	CLA	C3C-C4C-NC	5.88	117.16	110.57
24	C	501	CLA	C4D-C3D-CAD	-5.87	105.19	108.47
24	b	607	CLA	C4D-C3D-CAD	-5.87	105.19	108.47
24	C	502	CLA	C2C-C1C-NC	5.86	115.47	109.97
24	B	616	CLA	C3C-C4C-NC	5.86	117.14	110.57
24	B	610	CLA	C3C-C4C-NC	5.84	117.13	110.57
24	b	611	CLA	C4D-C3D-CAD	-5.84	105.21	108.47
24	c	513	CLA	CMC-C2C-C1C	5.84	133.93	125.04
24	b	609	CLA	C4D-C3D-CAD	-5.83	105.22	108.47
24	b	606	CLA	C5-C3-C2	-5.82	109.34	121.12
28	b	633	SQD	O6-C1-C2	5.82	117.39	108.30
24	c	510	CLA	C2C-C1C-NC	5.81	115.42	109.97
24	B	602	CLA	C3C-C4C-NC	5.81	117.09	110.57
24	b	606	CLA	C4D-C3D-CAD	-5.80	105.23	108.47
24	c	513	CLA	C3C-C4C-NC	5.80	117.08	110.57
24	B	603	CLA	C3C-C4C-NC	5.80	117.07	110.57
24	b	602	CLA	C3C-C4C-NC	5.79	117.07	110.57
24	C	503	CLA	CHD-C4C-C3C	-5.78	116.33	124.84
31	m	102	LMT	O1'-C1'-C2'	5.77	117.32	108.30
24	b	607	CLA	C2C-C1C-NC	5.77	115.38	109.97
24	C	512	CLA	C2C-C1C-NC	5.76	115.37	109.97
32	D	409	LHG	O8-C23-O10	-5.76	109.06	123.59
24	D	405	CLA	C3C-C4C-NC	5.75	117.02	110.57
24	C	504	CLA	C1C-C2C-C3C	-5.75	100.92	106.96
24	B	616	CLA	C3B-C4B-NB	5.74	116.63	109.21
24	B	609	CLA	C4D-C3D-CAD	-5.74	105.27	108.47
24	B	605	CLA	C3C-C4C-NC	5.72	116.99	110.57
26	t	102	BCR	C31-C1-C6	5.69	119.54	110.30
24	b	617	CLA	O2D-CGD-CBD	5.69	121.38	111.27
24	c	507	CLA	C3C-C4C-NC	5.69	116.95	110.57
24	d	403	CLA	C4D-C3D-CAD	-5.67	105.31	108.47
24	C	502	CLA	C3B-C4B-NB	5.67	116.54	109.21
25	A	608	PHO	C3C-C4C-NC	5.66	119.06	110.28
24	D	403	CLA	C1C-C2C-C3C	-5.66	101.01	106.96
24	c	506	CLA	C3B-C4B-NB	5.65	116.52	109.21
24	C	505	CLA	C3C-C4C-NC	5.64	116.89	110.57
24	b	615	CLA	C2C-C1C-NC	5.63	115.25	109.97
24	A	607	CLA	C3C-C4C-NC	5.63	116.88	110.57
24	B	614	CLA	C3C-C4C-NC	5.62	116.88	110.57
24	D	403	CLA	C3B-C4B-NB	5.62	116.47	109.21
24	A	606	CLA	C4A-NA-C1A	-5.61	104.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	526	LMG	O7-C10-C11	5.60	123.56	111.50
24	B	605	CLA	C4D-C3D-CAD	-5.59	105.35	108.47
24	C	506	CLA	C3C-C4C-NC	5.58	116.83	110.57
24	B	607	CLA	C3B-C4B-NB	5.58	116.43	109.21
40	D	408	DGD	O3G-C1D-C2D	5.58	117.02	108.30
24	b	605	CLA	C4-C3-C5	-5.58	105.88	115.27
32	a	419	LHG	O7-C7-C8	5.58	123.52	111.50
26	k	101	BCR	C39-C30-C25	-5.56	101.28	110.30
38	V	204	HTG	C1-O5-C5	-5.55	102.35	112.58
24	c	506	CLA	C2C-C1C-NC	5.54	115.17	109.97
25	A	608	PHO	C4C-C3C-C2C	-5.54	100.65	106.78
24	c	508	CLA	C3C-C4C-NC	5.54	116.78	110.57
24	c	511	CLA	CMC-C2C-C1C	5.54	133.47	125.04
24	B	603	CLA	C2C-C1C-NC	5.54	115.16	109.97
24	b	606	CLA	C2C-C1C-NC	5.53	115.16	109.97
24	B	612	CLA	C1C-C2C-C3C	-5.53	101.14	106.96
24	a	408	CLA	C3B-C4B-NB	5.52	116.35	109.21
24	C	506	CLA	C1C-C2C-C3C	-5.52	101.15	106.96
24	B	602	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
24	B	604	CLA	CMC-C2C-C1C	5.52	133.44	125.04
24	C	501	CLA	C1C-C2C-C3C	-5.52	101.16	106.96
24	A	606	CLA	C4D-C3D-CAD	-5.52	105.39	108.47
24	b	613	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
24	a	410	CLA	C3C-C4C-NC	5.51	116.75	110.57
24	B	604	CLA	O2D-CGD-CBD	5.50	121.05	111.27
24	C	509	CLA	C4D-C3D-CAD	-5.50	105.41	108.47
24	C	512	CLA	C3B-C4B-NB	5.49	116.31	109.21
24	C	510	CLA	C3C-C4C-NC	5.49	116.73	110.57
24	C	508	CLA	C1C-C2C-C3C	-5.49	101.19	106.96
24	B	604	CLA	O2D-CGD-O1D	-5.48	113.13	123.84
24	C	511	CLA	O2D-CGD-CBD	5.48	121.00	111.27
24	b	616	CLA	C4D-C3D-CAD	-5.47	105.42	108.47
25	d	401	PHO	C3C-C4C-NC	5.46	118.75	110.28
29	B	621	LMG	O7-C10-O9	-5.45	110.53	123.70
25	A	608	PHO	CMD-C2D-C1D	5.43	133.43	125.06
24	B	607	CLA	O2D-CGD-CBD	5.40	120.87	111.27
24	c	511	CLA	C1C-C2C-C3C	-5.40	101.28	106.96
28	b	633	SQD	O9-S-C6	5.39	113.34	106.94
24	B	617	CLA	C3C-C4C-NC	5.39	116.61	110.57
28	a	413	SQD	C1-O5-C5	-5.38	103.13	113.69
24	C	511	CLA	C2C-C1C-NC	5.38	115.01	109.97
24	B	607	CLA	C4A-NA-C1A	-5.37	104.29	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	410	CLA	C3B-C4B-NB	5.35	116.12	109.21
29	B	621	LMG	O8-C28-C29	5.34	128.68	111.91
24	c	505	CLA	C4D-C3D-CAD	-5.34	105.49	108.47
24	B	615	CLA	CHD-C4C-C3C	-5.33	117.00	124.84
29	b	621	LMG	O8-C28-C29	5.32	128.62	111.91
24	B	611	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
28	a	424	SQD	C44-O6-C1	5.29	124.08	113.74
28	A	612	SQD	O47-C7-C8	5.29	122.91	111.50
28	h	105	SQD	O7-S-C6	5.29	113.22	106.94
24	b	614	CLA	CAC-C3C-C4C	5.28	131.67	124.81
24	D	404	CLA	C3C-C4C-NC	5.28	116.50	110.57
24	B	615	CLA	C4D-C3D-CAD	-5.27	105.53	108.47
24	B	612	CLA	CMC-C2C-C1C	5.27	133.06	125.04
24	B	617	CLA	O2D-CGD-CBD	5.26	120.61	111.27
24	B	617	CLA	C4D-C3D-CAD	-5.26	105.54	108.47
24	c	509	CLA	CAC-C3C-C4C	5.25	131.62	124.81
24	b	604	CLA	C3B-C4B-NB	5.24	115.99	109.21
24	C	509	CLA	CAC-C3C-C4C	5.24	131.61	124.81
29	b	621	LMG	O7-C10-C11	5.23	122.78	111.50
24	b	603	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
24	c	501	CLA	C1C-C2C-C3C	-5.21	101.48	106.96
24	C	503	CLA	C3B-C4B-NB	5.20	115.94	109.21
24	b	602	CLA	CHD-C4C-C3C	-5.20	117.19	124.84
24	B	606	CLA	CHD-C4C-C3C	-5.19	117.20	124.84
31	I	101	LMT	O1B-C4'-C3'	5.19	121.08	107.28
25	d	401	PHO	C4C-C3C-C2C	-5.19	101.04	106.78
25	a	409	PHO	CMD-C2D-C1D	5.18	133.04	125.06
24	A	606	CLA	C3C-C4C-NC	5.18	116.38	110.57
25	d	401	PHO	C2C-C1C-NC	5.18	117.60	109.79
24	C	512	CLA	C3C-C4C-NC	5.17	116.37	110.57
30	C	528	GOL	C3-C2-C1	5.17	131.81	111.70
24	D	404	CLA	C3B-C4B-NB	5.16	115.89	109.21
24	b	612	CLA	CMC-C2C-C1C	5.16	132.90	125.04
24	b	612	CLA	C1C-C2C-C3C	-5.16	101.53	106.96
24	d	405	CLA	C3C-C4C-NC	5.16	116.36	110.57
25	d	401	PHO	CMD-C2D-C1D	5.16	133.00	125.06
26	b	618	BCR	C7-C8-C9	-5.15	118.45	126.23
28	x	101	SQD	O9-S-C6	5.15	113.06	106.94
24	b	605	CLA	CAC-C3C-C4C	5.14	131.48	124.81
24	c	508	CLA	C3B-C4B-NB	5.13	115.85	109.21
24	C	503	CLA	CMC-C2C-C1C	5.13	132.85	125.04
24	c	512	CLA	C3B-C4B-NB	5.12	115.83	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	621	LMG	O7-C10-O9	-5.12	111.33	123.70
24	b	617	CLA	CAC-C3C-C4C	5.11	131.44	124.81
24	d	403	CLA	C2C-C1C-NC	5.11	114.76	109.97
24	b	608	CLA	C3C-C4C-NC	5.11	116.30	110.57
24	c	513	CLA	C1C-C2C-C3C	-5.08	101.61	106.96
28	l	102	SQD	O7-S-C6	5.06	112.96	106.94
24	C	505	CLA	C4D-C3D-CAD	-5.06	105.65	108.47
27	a	412	PL9	C3-C4-C5	5.06	125.18	118.60
24	B	602	CLA	OBD-CAD-C3D	-5.06	119.59	127.98
24	b	614	CLA	C4D-C3D-CAD	-5.06	105.65	108.47
24	d	404	CLA	C3C-C4C-NC	5.05	116.24	110.57
24	b	613	CLA	CAC-C3C-C4C	5.05	131.36	124.81
24	c	512	CLA	O2D-CGD-CBD	5.05	120.24	111.27
24	d	404	CLA	C4D-C3D-CAD	-5.04	105.66	108.47
25	A	608	PHO	C2C-C1C-NC	5.04	117.39	109.79
24	b	611	CLA	CAC-C3C-C4C	5.03	131.34	124.81
24	b	615	CLA	O2D-CGD-CBD	5.03	120.20	111.27
24	C	501	CLA	C3B-C4B-NB	5.02	115.70	109.21
24	b	616	CLA	CMC-C2C-C1C	5.02	132.68	125.04
28	A	622	SQD	O9-S-C6	5.01	112.89	106.94
24	b	610	CLA	O2D-CGD-O1D	-4.99	114.08	123.84
28	F	104	SQD	O9-S-C6	4.99	112.86	106.94
24	b	612	CLA	CHD-C4C-C3C	-4.99	117.51	124.84
24	c	512	CLA	C4D-C3D-CAD	-4.98	105.69	108.47
24	c	512	CLA	C3C-C4C-NC	4.98	116.16	110.57
28	a	413	SQD	O8-S-C6	4.98	113.68	105.74
38	C	532	HTG	C1-O5-C5	4.98	121.76	112.58
24	B	608	CLA	C3B-C4B-NB	4.98	115.64	109.21
32	e	101	LHG	O7-C7-C8	4.97	122.22	111.50
40	c	517	DGD	O2G-C1B-C2B	4.97	122.21	111.50
24	c	502	CLA	C1C-C2C-C3C	-4.97	101.73	106.96
24	C	509	CLA	C3B-C4B-NB	4.96	115.62	109.21
24	D	403	CLA	C4D-C3D-CAD	-4.96	105.70	108.47
24	B	610	CLA	C3B-C4B-NB	4.96	115.62	109.21
28	A	612	SQD	O6-C1-C2	4.95	116.04	108.30
29	c	519	LMG	O8-C28-C29	4.95	127.44	111.91
24	C	508	CLA	C3B-C4B-NB	4.95	115.61	109.21
24	D	403	CLA	C3C-C4C-NC	4.95	116.12	110.57
24	C	511	CLA	C4D-C3D-CAD	-4.94	105.71	108.47
25	D	401	PHO	C3C-C4C-NC	4.94	117.94	110.28
24	b	608	CLA	C4D-C3D-CAD	-4.93	105.72	108.47
28	A	622	SQD	C44-O6-C1	4.93	123.37	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	O2D-CGD-CBD	4.92	120.02	111.27
24	b	617	CLA	O2A-CGA-CBA	4.92	127.36	111.91
31	a	401	LMT	C1'-O5'-C5'	4.92	123.34	113.69
24	B	607	CLA	C3C-C4C-NC	4.92	116.09	110.57
24	b	612	CLA	C3C-C4C-NC	4.92	116.08	110.57
24	B	603	CLA	CHD-C4C-C3C	-4.91	117.62	124.84
24	b	608	CLA	C2C-C1C-NC	4.90	114.56	109.97
24	d	403	CLA	C3C-C4C-NC	4.90	116.06	110.57
24	C	509	CLA	C3C-C4C-NC	4.89	116.06	110.57
24	c	506	CLA	CHD-C4C-C3C	-4.89	117.65	124.84
24	b	612	CLA	C3B-C4B-NB	4.89	115.53	109.21
24	d	405	CLA	C3B-C4B-NB	4.88	115.53	109.21
28	b	633	SQD	O5-C1-C2	-4.88	100.02	110.35
28	F	104	SQD	O3-C3-C2	4.88	121.62	110.35
24	d	405	CLA	CAC-C3C-C4C	4.87	131.13	124.81
24	b	610	CLA	O2D-CGD-CBD	4.87	119.92	111.27
38	C	522	HTG	C1-O5-C5	4.87	121.56	112.58
24	C	507	CLA	CHD-C4C-C3C	-4.86	117.69	124.84
24	b	604	CLA	C3C-C4C-NC	4.86	116.03	110.57
24	B	606	CLA	C5-C3-C2	-4.85	111.30	121.12
24	B	603	CLA	C3B-C4B-NB	4.85	115.48	109.21
29	C	526	LMG	C1-C2-C3	-4.85	99.90	110.00
24	c	508	CLA	C1C-C2C-C3C	-4.85	101.86	106.96
24	c	509	CLA	C4D-C3D-CAD	-4.83	105.77	108.47
24	B	605	CLA	C3B-C4B-NB	4.83	115.46	109.21
24	b	613	CLA	C4C-C3C-C2C	-4.83	99.86	106.90
27	D	407	PL9	C40-C39-C41	4.83	123.39	115.27
24	c	512	CLA	C1C-C2C-C3C	-4.82	101.88	106.96
24	b	606	CLA	CHD-C4C-C3C	-4.82	117.75	124.84
24	B	611	CLA	C4C-C3C-C2C	-4.82	99.87	106.90
24	a	407	CLA	CAC-C3C-C4C	4.82	131.06	124.81
24	b	609	CLA	C3B-C4B-NB	4.81	115.43	109.21
24	B	607	CLA	CMC-C2C-C1C	4.81	132.36	125.04
24	C	511	CLA	C3B-C4B-NB	4.80	115.42	109.21
24	B	604	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
24	B	606	CLA	C4-C3-C2	-4.80	111.36	123.68
24	B	606	CLA	C1-C2-C3	-4.80	117.74	126.04
24	b	613	CLA	C3B-C4B-NB	4.80	115.41	109.21
32	d	409	LHG	O8-C23-O10	-4.79	111.50	123.59
29	b	621	LMG	O8-C28-O10	-4.79	111.50	123.59
24	C	512	CLA	CAC-C3C-C4C	4.79	131.02	124.81
24	c	507	CLA	C3B-C4B-NB	4.78	115.39	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	501	CLA	CMC-C2C-C1C	4.78	132.31	125.04
26	B	619	BCR	C40-C30-C25	-4.78	102.55	110.30
24	b	613	CLA	C4D-C3D-CAD	-4.78	105.81	108.47
29	a	414	LMG	O7-C10-C11	4.76	121.76	111.50
24	c	505	CLA	C4C-C3C-C2C	-4.75	99.97	106.90
24	c	503	CLA	CHD-C4C-C3C	-4.75	117.85	124.84
24	B	608	CLA	C3C-C4C-NC	4.75	115.90	110.57
24	b	603	CLA	C2C-C1C-NC	4.75	114.42	109.97
24	B	609	CLA	CHD-C4C-C3C	-4.75	117.86	124.84
41	E	113	HEM	CBD-CAD-C3D	-4.74	103.74	112.48
24	b	617	CLA	CHD-C4C-C3C	-4.74	117.87	124.84
25	D	401	PHO	C4C-C3C-C2C	-4.73	101.54	106.78
24	d	405	CLA	CHD-C4C-C3C	-4.73	117.89	124.84
28	A	616	SQD	O47-C7-C8	4.72	121.66	111.50
27	A	611	PL9	C7-C8-C9	-4.71	118.95	126.79
31	j	103	LMT	C1-O1'-C1'	4.71	121.64	113.84
24	C	511	CLA	C3C-C4C-NC	4.71	115.85	110.57
24	b	602	CLA	C4D-C3D-CAD	-4.70	105.85	108.47
24	c	505	CLA	CHD-C4C-C3C	-4.70	117.93	124.84
24	b	614	CLA	C3B-C4B-NB	4.69	115.27	109.21
24	c	501	CLA	O2D-CGD-CBD	4.69	119.60	111.27
24	B	604	CLA	C3C-C4C-NC	4.69	115.83	110.57
24	C	502	CLA	CMC-C2C-C1C	4.68	132.17	125.04
24	B	611	CLA	CAC-C3C-C4C	4.67	130.88	124.81
24	b	605	CLA	C4-C3-C2	-4.67	111.69	123.68
24	b	606	CLA	CMC-C2C-C1C	4.67	132.16	125.04
40	d	408	DGD	C3G-O3G-C1D	4.67	122.86	113.74
24	C	505	CLA	CAC-C3C-C4C	4.67	130.87	124.81
24	c	511	CLA	C3C-C4C-NC	4.66	115.80	110.57
24	B	607	CLA	C4D-C3D-CAD	-4.66	105.87	108.47
26	C	514	BCR	C23-C24-C25	-4.66	114.12	127.20
32	E	101	LHG	O7-C7-C8	4.65	121.53	111.50
24	B	604	CLA	C3B-C4B-NB	4.64	115.22	109.21
24	B	607	CLA	CHD-C4C-C3C	-4.64	118.01	124.84
24	A	606	CLA	CAC-C3C-C4C	4.64	130.83	124.81
28	b	633	SQD	C4-C3-C2	4.63	118.91	110.82
24	b	603	CLA	O2D-CGD-O1D	-4.63	114.79	123.84
24	b	610	CLA	C3B-C4B-NB	4.63	115.19	109.21
24	d	405	CLA	O2D-CGD-CBD	4.63	119.49	111.27
38	H	101	HTG	C1-O5-C5	4.63	121.11	112.58
24	D	405	CLA	C3B-C4B-NB	4.62	115.19	109.21
24	b	607	CLA	C3C-C4C-NC	4.62	115.75	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	613	CLA	C2C-C1C-NC	4.62	114.30	109.97
24	c	507	CLA	CHD-C4C-C3C	-4.60	118.07	124.84
24	B	610	CLA	C1C-C2C-C3C	-4.60	102.12	106.96
24	B	609	CLA	C3B-C4B-NB	4.59	115.15	109.21
38	h	101	HTG	O5-C1-C2	4.58	116.08	110.31
26	T	102	BCR	C20-C21-C22	-4.58	120.77	127.31
24	b	608	CLA	C3B-C4B-NB	4.58	115.13	109.21
24	c	511	CLA	CHD-C4C-C3C	-4.58	118.10	124.84
24	B	602	CLA	C3D-CAD-CBD	4.58	113.63	107.61
24	B	606	CLA	C4C-C3C-C2C	-4.57	100.24	106.90
24	B	613	CLA	C3C-C4C-NC	4.56	115.69	110.57
40	C	517	DGD	O2G-C1B-O1B	-4.56	112.68	123.70
26	C	514	BCR	C24-C23-C22	-4.56	119.35	126.23
27	A	611	PL9	C53-C6-C1	4.56	124.31	114.99
24	B	612	CLA	C3B-C4B-NB	4.55	115.10	109.21
24	C	507	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
31	B	622	LMT	O1'-C1'-C2'	4.55	115.41	108.30
24	C	506	CLA	CHD-C4C-C3C	-4.55	118.15	124.84
24	B	615	CLA	C3C-C4C-NC	4.55	115.67	110.57
25	a	409	PHO	C2C-C1C-NC	4.54	116.64	109.79
24	C	506	CLA	CMC-C2C-C1C	4.54	131.95	125.04
24	B	617	CLA	CAC-C3C-C4C	4.54	130.70	124.81
24	c	502	CLA	CHD-C4C-C3C	-4.53	118.17	124.84
24	C	510	CLA	CMC-C2C-C1C	4.52	131.93	125.04
24	C	510	CLA	CAC-C3C-C4C	4.52	130.67	124.81
41	e	107	HEM	CBA-CAA-C2A	-4.52	104.16	112.49
24	c	504	CLA	CMC-C2C-C1C	4.51	131.91	125.04
24	C	501	CLA	C3C-C4C-NC	4.51	115.63	110.57
24	C	510	CLA	CHD-C4C-C3C	-4.51	118.21	124.84
24	b	615	CLA	O2D-CGD-O1D	-4.51	115.03	123.84
24	b	615	CLA	C3C-C4C-NC	4.50	115.62	110.57
24	C	513	CLA	O2D-CGD-CBD	4.49	119.25	111.27
24	b	616	CLA	CMB-C2B-C3B	4.49	133.08	124.68
24	C	511	CLA	CHD-C4C-C3C	-4.48	118.25	124.84
24	D	404	CLA	C1C-C2C-C3C	-4.48	102.25	106.96
26	C	514	BCR	C7-C8-C9	-4.48	119.47	126.23
24	d	403	CLA	CHD-C4C-C3C	-4.48	118.26	124.84
24	B	604	CLA	CHD-C4C-C3C	-4.47	118.26	124.84
24	c	502	CLA	C3C-C4C-NC	4.47	115.58	110.57
24	c	501	CLA	C3C-C4C-NC	4.46	115.58	110.57
24	C	504	CLA	C3B-C4B-NB	4.46	114.98	109.21
24	b	617	CLA	C4C-C3C-C2C	-4.46	100.40	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	CHD-C4C-C3C	-4.45	118.30	124.84
24	C	513	CLA	CAC-C3C-C4C	4.45	130.58	124.81
24	A	609	CLA	C3C-C4C-NC	4.44	115.56	110.57
28	A	616	SQD	O6-C1-C2	4.44	115.23	108.30
24	c	503	CLA	C3C-C4C-NC	4.43	115.54	110.57
24	c	502	CLA	C3B-C4B-NB	4.43	114.94	109.21
24	c	502	CLA	CMC-C2C-C1C	4.42	131.78	125.04
28	F	104	SQD	O8-S-C6	4.42	112.78	105.74
24	c	513	CLA	C4D-C3D-CAD	-4.42	106.01	108.47
24	B	608	CLA	C4A-NA-C1A	-4.42	104.72	106.71
40	C	517	DGD	O2G-C1B-C2B	4.41	121.01	111.50
28	a	413	SQD	C1-C2-C3	-4.41	100.81	110.00
26	b	619	BCR	C37-C22-C23	4.41	125.02	118.08
26	t	102	BCR	C39-C30-C25	-4.41	103.15	110.30
24	b	605	CLA	C3B-C4B-NB	4.40	114.89	109.21
24	B	608	CLA	C4D-C3D-CAD	-4.40	106.02	108.47
24	a	408	CLA	CHD-C4C-C3C	-4.40	118.38	124.84
24	c	509	CLA	CHD-C4C-C3C	-4.40	118.38	124.84
40	C	516	DGD	O2G-C1B-C2B	4.39	120.97	111.50
28	x	101	SQD	O47-C7-C8	4.39	120.95	111.50
29	C	519	LMG	O7-C10-C11	4.38	120.95	111.50
24	C	513	CLA	CHD-C4C-C3C	-4.38	118.39	124.84
24	b	610	CLA	C4C-C3C-C2C	-4.38	100.51	106.90
24	B	605	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
24	B	608	CLA	C1C-C2C-C3C	-4.37	102.36	106.96
26	T	102	BCR	C7-C8-C9	-4.37	119.64	126.23
24	C	509	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
26	d	406	BCR	C30-C25-C26	-4.36	116.47	122.61
24	c	504	CLA	C3C-C4C-NC	4.35	115.45	110.57
24	B	616	CLA	CMC-C2C-C1C	4.34	131.65	125.04
24	c	507	CLA	C4D-C3D-CAD	-4.34	106.05	108.47
24	c	503	CLA	C3B-C4B-NB	4.34	114.82	109.21
24	C	502	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
24	A	606	CLA	C3B-C4B-NB	4.33	114.81	109.21
26	d	406	BCR	C40-C30-C39	4.33	121.82	108.53
24	C	506	CLA	O2D-CGD-CBD	4.33	118.96	111.27
26	C	515	BCR	C3-C4-C5	-4.32	106.36	114.08
24	B	603	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
24	C	513	CLA	CMB-C2B-C3B	4.32	132.76	124.68
31	b	622	LMT	O1'-C1'-C2'	4.31	115.03	108.30
24	B	609	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
24	A	609	CLA	CED-O2D-CGD	4.30	125.66	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	617	LMT	C1-O1'-C1'	4.30	120.96	113.84
43	v	202	HEC	CBD-CAD-C3D	-4.29	104.57	112.49
24	b	616	CLA	C1B-CHB-C4A	-4.29	121.62	130.12
24	b	606	CLA	C4-C3-C2	-4.28	112.70	123.68
24	b	615	CLA	C3B-C4B-NB	4.27	114.72	109.21
26	h	103	BCR	C38-C26-C25	-4.26	119.74	124.53
29	B	634	LMG	O7-C10-C11	4.26	120.68	111.50
24	c	510	CLA	CHD-C4C-C3C	-4.26	118.58	124.84
28	a	417	SQD	O48-C23-C24	4.26	125.28	111.91
24	C	512	CLA	C4D-C3D-CAD	-4.26	106.10	108.47
24	B	616	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
24	A	607	CLA	CHD-C4C-C3C	-4.25	118.59	124.84
24	A	609	CLA	OBD-CAD-C3D	-4.24	120.93	127.98
24	a	408	CLA	C4C-C3C-C2C	-4.24	100.71	106.90
28	a	424	SQD	O6-C1-C2	4.24	114.93	108.30
28	x	101	SQD	C1-O5-C5	4.24	122.01	113.69
24	A	609	CLA	C4A-NA-C1A	-4.24	104.80	106.71
28	l	102	SQD	O47-C7-C8	4.24	120.64	111.50
24	C	505	CLA	C3B-C4B-NB	4.24	114.69	109.21
24	a	407	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
26	c	514	BCR	C7-C8-C9	-4.23	119.84	126.23
24	d	405	CLA	C4D-C3D-CAD	-4.23	106.11	108.47
26	c	515	BCR	C32-C1-C6	-4.23	103.44	110.30
24	c	512	CLA	C1-C2-C3	-4.23	118.73	126.04
31	A	617	LMT	O2'-C2'-C1'	4.22	120.30	110.05
24	b	605	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
24	b	603	CLA	C3B-C4B-NB	4.21	114.66	109.21
27	a	412	PL9	C53-C6-C1	4.21	123.59	114.99
24	b	616	CLA	C3C-C4C-NC	4.20	115.28	110.57
28	A	612	SQD	O8-S-C6	4.20	112.44	105.74
24	B	603	CLA	O2D-CGD-CBD	4.20	118.72	111.27
24	B	615	CLA	O2A-CGA-O1A	-4.19	113.01	123.59
24	b	602	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
24	b	602	CLA	C2A-C1A-CHA	-4.19	116.53	123.86
24	c	507	CLA	CAC-C3C-C4C	4.19	130.24	124.81
24	d	403	CLA	C3B-C4B-NB	4.19	114.62	109.21
24	B	602	CLA	C1C-C2C-C3C	-4.19	102.56	106.96
26	t	102	BCR	C38-C26-C25	-4.18	119.83	124.53
24	c	512	CLA	CHD-C4C-C3C	-4.18	118.69	124.84
24	B	603	CLA	C4C-C3C-C2C	-4.18	100.80	106.90
24	b	605	CLA	CMC-C2C-C1C	4.18	131.40	125.04
24	a	407	CLA	C3B-C4B-NB	4.17	114.61	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C3B-C4B-NB	4.17	114.60	109.21
24	C	505	CLA	CHD-C4C-C3C	-4.17	118.71	124.84
24	A	609	CLA	C3B-C4B-NB	4.17	114.60	109.21
24	B	617	CLA	C3B-C4B-NB	4.16	114.59	109.21
25	d	401	PHO	O2D-CGD-CBD	4.16	118.66	111.27
26	C	514	BCR	C28-C27-C26	-4.16	106.65	114.08
24	C	505	CLA	O2D-CGD-O1D	-4.16	115.71	123.84
24	b	611	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
24	B	610	CLA	CMC-C2C-C1C	4.15	131.36	125.04
24	B	612	CLA	CAC-C3C-C4C	4.14	130.19	124.81
26	b	619	BCR	C28-C27-C26	-4.14	106.68	114.08
24	b	604	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
24	B	616	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
24	c	509	CLA	C3B-C4B-NB	4.14	114.57	109.21
24	b	605	CLA	CHD-C4C-C3C	-4.14	118.75	124.84
26	K	101	BCR	C37-C22-C23	4.14	124.59	118.08
24	C	502	CLA	OBD-CAD-C3D	-4.13	121.12	127.98
27	d	407	PL9	C40-C39-C41	4.13	122.22	115.27
24	b	617	CLA	O2A-CGA-O1A	-4.13	113.17	123.59
38	V	204	HTG	C1-C2-C3	-4.13	102.43	110.59
24	C	501	CLA	CMC-C2C-C1C	4.12	131.31	125.04
24	A	609	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
32	d	409	LHG	O8-C23-C24	4.11	124.82	111.91
24	a	407	CLA	C3C-C4C-NC	4.11	115.19	110.57
24	b	611	CLA	CHD-C4C-C3C	-4.11	118.79	124.84
28	b	633	SQD	O47-C7-C8	4.11	120.36	111.50
32	D	409	LHG	O8-C23-C24	4.11	124.80	111.91
24	b	612	CLA	O2D-CGD-CBD	4.11	118.56	111.27
24	b	609	CLA	CHD-C4C-C3C	-4.10	118.81	124.84
24	B	614	CLA	C1D-CHD-C4C	4.10	127.97	122.56
24	C	503	CLA	C4C-C3C-C2C	-4.10	100.92	106.90
24	b	611	CLA	CED-O2D-CGD	4.10	125.20	115.94
24	B	608	CLA	CMC-C2C-C1C	4.10	131.28	125.04
24	A	607	CLA	C4-C3-C5	4.09	122.16	115.27
25	a	409	PHO	C3C-C4C-NC	4.09	116.62	110.28
24	B	605	CLA	C4-C3-C2	-4.09	113.19	123.68
24	B	613	CLA	O2D-CGD-CBD	4.08	118.53	111.27
24	C	505	CLA	C4C-C3C-C2C	-4.08	100.96	106.90
24	C	513	CLA	C4C-C3C-C2C	-4.07	100.96	106.90
31	u	203	LMT	O1'-C1'-C2'	4.07	114.65	108.30
24	c	507	CLA	O2D-CGD-CBD	4.07	118.49	111.27
24	c	506	CLA	C4D-C3D-CAD	-4.06	106.21	108.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	606	CLA	C3B-C4B-NB	4.06	114.45	109.21
24	b	611	CLA	CMC-C2C-C1C	4.05	131.21	125.04
24	b	609	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
27	a	412	PL9	O1-C4-C3	-4.05	116.26	120.72
24	b	603	CLA	C4C-C3C-C2C	-4.04	101.01	106.90
28	A	622	SQD	C45-O47-C7	4.04	127.74	117.79
26	b	620	BCR	C40-C30-C25	-4.04	103.75	110.30
24	C	513	CLA	C2A-C1A-CHA	-4.04	116.80	123.86
41	E	113	HEM	CBA-CAA-C2A	-4.03	105.05	112.49
25	d	401	PHO	C4-C3-C5	4.03	122.05	115.27
29	c	519	LMG	O7-C10-C11	4.02	120.17	111.50
38	c	523	HTG	C1'-S1-C1	4.02	107.62	100.09
28	l	102	SQD	O48-C46-C45	4.02	120.14	108.43
24	B	617	CLA	CHD-C4C-C3C	-4.02	118.93	124.84
25	D	401	PHO	C2B-C1B-NB	4.01	115.84	109.79
25	A	608	PHO	C1C-NC-C4C	-4.01	98.96	106.51
24	b	616	CLA	CHD-C4C-C3C	-4.01	118.94	124.84
28	a	413	SQD	O5-C1-C2	-4.01	101.87	110.35
26	c	527	BCR	C7-C8-C9	-4.01	120.18	126.23
24	b	617	CLA	C3B-C4B-NB	4.01	114.39	109.21
24	a	410	CLA	CAC-C3C-C4C	4.00	130.01	124.81
24	B	602	CLA	C3B-C4B-NB	4.00	114.38	109.21
24	b	603	CLA	O2D-CGD-CBD	4.00	118.37	111.27
31	m	102	LMT	O5'-C1'-O1'	-3.99	100.52	109.97
43	V	203	HEC	CBD-CAD-C3D	-3.99	105.13	112.49
24	C	509	CLA	CMC-C2C-C1C	3.99	131.11	125.04
24	b	604	CLA	CMC-C2C-C1C	3.98	131.11	125.04
24	a	410	CLA	CHD-C4C-C3C	-3.98	118.98	124.84
41	e	107	HEM	CAD-CBD-CGD	3.98	119.35	112.67
24	D	405	CLA	CHD-C4C-C3C	-3.98	118.99	124.84
24	b	602	CLA	OBD-CAD-C3D	-3.98	121.38	127.98
24	b	615	CLA	CMC-C2C-C1C	3.98	131.10	125.04
26	C	514	BCR	C20-C21-C22	-3.98	121.63	127.31
25	d	401	PHO	C1C-NC-C4C	-3.98	99.02	106.51
24	a	408	CLA	CAC-C3C-C4C	3.97	129.97	124.81
25	A	608	PHO	CAC-C3C-C4C	3.97	129.56	125.22
28	x	101	SQD	O48-C23-C24	3.97	124.38	111.91
24	c	504	CLA	C7-C6-C5	-3.97	102.57	113.36
26	b	619	BCR	C40-C30-C25	-3.96	103.87	110.30
24	C	501	CLA	CHD-C4C-C3C	-3.96	119.01	124.84
24	D	403	CLA	CHD-C4C-C3C	-3.96	119.02	124.84
26	B	618	BCR	C7-C8-C9	-3.96	120.25	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	j	103	LMT	C3B-C4B-C5B	3.96	117.30	110.24
24	c	509	CLA	C4C-C3C-C2C	-3.96	101.13	106.90
24	b	610	CLA	CHD-C4C-C3C	-3.95	119.03	124.84
24	B	613	CLA	CAC-C3C-C4C	3.95	129.94	124.81
24	D	403	CLA	CAC-C3C-C4C	3.95	129.94	124.81
24	C	513	CLA	OBD-CAD-C3D	-3.95	121.43	127.98
24	B	617	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
24	b	615	CLA	CHD-C4C-C3C	-3.94	119.04	124.84
24	C	505	CLA	CMC-C2C-C1C	3.94	131.04	125.04
24	B	605	CLA	C6-C5-C3	-3.94	103.12	113.45
28	b	633	SQD	O48-C23-C24	3.94	124.27	111.91
24	d	403	CLA	C4C-C3C-C2C	-3.94	101.16	106.90
26	d	406	BCR	C38-C26-C25	-3.93	120.11	124.53
24	B	604	CLA	C4D-C3D-CAD	-3.93	106.28	108.47
24	b	614	CLA	CHD-C4C-C3C	-3.93	119.07	124.84
24	b	602	CLA	CMC-C2C-C1C	3.92	131.01	125.04
24	b	606	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
24	b	617	CLA	CMB-C2B-C3B	3.92	132.01	124.68
31	u	203	LMT	O5B-C1B-C2B	3.92	118.65	110.35
24	a	410	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
24	C	507	CLA	CMC-C2C-C1C	3.91	130.99	125.04
31	f	101	LMT	O5'-C5'-C6'	3.91	116.15	106.44
26	D	406	BCR	C7-C8-C9	-3.91	120.33	126.23
24	D	404	CLA	C1B-CHB-C4A	-3.90	122.39	130.12
24	b	606	CLA	O2D-CGD-CBD	3.90	118.19	111.27
31	u	203	LMT	O5B-C5B-C6B	3.90	116.12	106.44
24	B	608	CLA	CHD-C4C-C3C	-3.89	119.12	124.84
24	b	602	CLA	CAC-C3C-C4C	3.89	129.86	124.81
27	A	611	PL9	C37-C36-C34	-3.89	100.19	112.98
24	D	404	CLA	C3A-C2A-C1A	-3.89	95.52	101.34
24	b	607	CLA	C2A-C1A-CHA	-3.89	117.06	123.86
24	B	607	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
24	C	507	CLA	C4A-NA-C1A	-3.88	104.96	106.71
24	b	606	CLA	C4C-C3C-C2C	-3.88	101.24	106.90
26	b	620	BCR	C7-C8-C9	-3.88	120.37	126.23
28	l	102	SQD	O2-C2-C1	3.88	119.47	110.05
24	c	503	CLA	CMC-C2C-C1C	3.88	130.95	125.04
24	b	603	CLA	CMB-C2B-C3B	3.88	131.94	124.68
26	d	406	BCR	C31-C1-C6	-3.88	104.01	110.30
26	D	406	BCR	C37-C22-C23	3.87	124.18	118.08
31	m	102	LMT	C1'-O5'-C5'	-3.87	106.09	113.69
24	C	505	CLA	CMB-C2B-C3B	3.87	131.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CAC-C3C-C4C	3.87	129.83	124.81
24	d	405	CLA	C4C-C3C-C2C	-3.86	101.27	106.90
24	C	507	CLA	C3B-C4B-NB	3.86	114.20	109.21
28	a	424	SQD	O8-S-C6	3.86	111.89	105.74
24	a	407	CLA	CMC-C2C-C1C	3.86	130.91	125.04
24	B	606	CLA	C3B-C4B-NB	3.86	114.20	109.21
24	B	617	CLA	O2A-CGA-O1A	-3.85	113.86	123.59
24	B	610	CLA	CHD-C4C-C3C	-3.85	119.17	124.84
24	C	502	CLA	CAC-C3C-C4C	3.85	129.81	124.81
40	c	516	DGD	O2G-C1B-C2B	3.85	119.80	111.50
31	J	103	LMT	C1B-O5B-C5B	3.85	121.24	113.69
24	b	606	CLA	C1-C2-C3	-3.85	119.39	126.04
24	b	607	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
24	c	513	CLA	CMB-C2B-C3B	3.84	131.87	124.68
24	b	605	CLA	C6-C5-C3	-3.84	103.38	113.45
24	C	506	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
26	c	514	BCR	C24-C23-C22	-3.84	120.44	126.23
24	c	510	CLA	CAC-C3C-C4C	3.83	129.78	124.81
24	b	604	CLA	O2D-CGD-CBD	3.83	118.07	111.27
30	C	523	GOL	O2-C2-C1	3.83	125.99	109.12
24	c	511	CLA	C3B-C4B-NB	3.82	114.15	109.21
28	a	413	SQD	O47-C7-C8	3.82	119.74	111.50
24	D	405	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
40	D	408	DGD	C2G-O2G-C1B	3.82	127.19	117.79
24	b	607	CLA	CHD-C4C-C3C	-3.82	119.23	124.84
24	b	610	CLA	CAC-C3C-C4C	3.82	129.76	124.81
24	C	509	CLA	CHD-C4C-C3C	-3.81	119.23	124.84
26	D	406	BCR	C32-C1-C6	3.81	116.48	110.30
24	D	405	CLA	O2D-CGD-CBD	3.81	118.03	111.27
24	D	404	CLA	C2A-C1A-CHA	-3.80	117.21	123.86
24	c	506	CLA	C4C-C3C-C2C	-3.80	101.36	106.90
29	c	520	LMG	C4-C3-C2	3.80	117.45	110.82
25	a	409	PHO	O2D-CGD-CBD	3.79	118.01	111.27
25	d	401	PHO	O2D-CGD-O1D	-3.78	116.45	123.84
31	u	203	LMT	C1B-O5B-C5B	3.78	121.10	113.69
24	A	607	CLA	C3B-C4B-NB	3.77	114.09	109.21
24	B	612	CLA	C2A-C1A-CHA	-3.77	117.26	123.86
26	b	618	BCR	C8-C7-C6	-3.77	116.61	127.20
24	c	501	CLA	CHD-C4C-C3C	-3.77	119.29	124.84
24	C	501	CLA	C2A-C1A-CHA	-3.77	117.26	123.86
24	c	510	CLA	C4C-C3C-C2C	-3.77	101.40	106.90
24	B	610	CLA	CMB-C2B-C3B	3.77	131.73	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	609	CLA	CHD-C4C-C3C	-3.77	119.30	124.84
31	A	617	LMT	O5'-C1'-C2'	-3.76	102.38	110.35
24	C	512	CLA	O2D-CGD-CBD	3.76	117.95	111.27
31	M	101	LMT	O1'-C1'-C2'	3.76	114.17	108.30
24	C	513	CLA	C4-C3-C5	3.76	121.59	115.27
31	F	102	LMT	O4'-C4B-C5B	3.76	118.63	109.30
24	B	615	CLA	CMC-C2C-C1C	3.75	130.76	125.04
24	d	404	CLA	C4-C3-C5	3.75	121.59	115.27
24	B	615	CLA	C3B-C4B-NB	3.75	114.06	109.21
24	c	504	CLA	O2D-CGD-CBD	3.75	117.94	111.27
24	B	603	CLA	C4A-NA-C1A	-3.75	105.02	106.71
24	B	613	CLA	C3B-C4B-NB	3.75	114.05	109.21
24	B	606	CLA	C2A-C1A-CHA	-3.74	117.31	123.86
28	F	104	SQD	C3-C4-C5	3.74	116.91	110.24
29	z	101	LMG	O7-C10-C11	3.74	119.56	111.50
31	C	533	LMT	O1B-C4'-C3'	3.74	117.22	107.28
38	h	101	HTG	O5-C1-S1	-3.74	100.89	109.82
26	a	411	BCR	C7-C8-C9	-3.73	120.60	126.23
31	M	101	LMT	O2B-C2B-C1B	-3.73	100.99	110.05
27	A	611	PL9	O1-C4-C3	-3.73	116.61	120.72
28	b	633	SQD	O3-C3-C4	-3.72	101.75	110.35
38	b	631	HTG	O5-C1-C2	-3.72	105.64	110.31
26	C	525	BCR	C24-C23-C22	-3.72	120.62	126.23
24	B	615	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
24	B	615	CLA	CED-O2D-CGD	3.72	124.34	115.94
26	c	527	BCR	C24-C23-C22	-3.71	120.62	126.23
32	d	410	LHG	O8-C23-O10	-3.71	114.22	123.59
40	c	517	DGD	O2G-C1B-O1B	-3.71	114.73	123.70
27	A	611	PL9	C7-C3-C4	-3.71	113.86	116.88
24	B	611	CLA	OBD-CAD-C3D	-3.70	121.83	127.98
32	B	632	LHG	O7-C7-O9	-3.70	114.75	123.70
24	b	609	CLA	OBD-CAD-C3D	-3.70	121.83	127.98
27	a	412	PL9	C2-C3-C4	-3.70	113.69	118.80
24	C	510	CLA	C3B-C4B-NB	3.70	113.99	109.21
25	A	608	PHO	C3D-C2D-C1D	-3.70	100.49	105.87
24	b	605	CLA	O2D-CGD-CBD	3.69	117.83	111.27
24	b	614	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
24	B	602	CLA	CHB-C4A-NA	3.69	129.61	124.51
24	b	602	CLA	CED-O2D-CGD	3.69	124.28	115.94
24	B	615	CLA	O2D-CGD-CBD	3.68	117.81	111.27
24	b	607	CLA	CAC-C3C-C4C	3.68	129.58	124.81
24	C	501	CLA	CAC-C3C-C4C	3.68	129.58	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	406	BCR	C40-C30-C39	3.67	119.81	108.53
24	C	504	CLA	CMC-C2C-C1C	3.67	130.63	125.04
24	c	505	CLA	C2A-C1A-CHA	-3.67	117.44	123.86
24	B	602	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
24	c	510	CLA	C3B-C4B-NB	3.67	113.95	109.21
38	B	631	HTG	C1'-S1-C1	3.67	106.95	100.09
24	c	506	CLA	CMC-C2C-C1C	3.67	130.62	125.04
24	c	507	CLA	CMC-C2C-C1C	3.67	130.62	125.04
24	C	507	CLA	O2D-CGD-CBD	3.67	117.78	111.27
43	v	202	HEC	CMC-C2C-C1C	-3.67	122.83	128.46
28	a	424	SQD	O48-C23-C24	3.66	123.39	111.91
25	D	401	PHO	CED-O2D-CGD	3.66	124.21	115.94
24	B	615	CLA	O2D-CGD-O1D	-3.65	116.69	123.84
24	B	603	CLA	CMC-C2C-C1C	3.65	130.60	125.04
24	C	502	CLA	CHD-C4C-C3C	-3.65	119.47	124.84
24	b	608	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
28	A	622	SQD	O48-C23-C24	3.64	123.33	111.91
38	b	631	HTG	C4-C3-C2	3.64	117.18	110.82
24	C	507	CLA	C2A-C1A-CHA	-3.64	117.50	123.86
24	D	405	CLA	CAC-C3C-C4C	3.64	129.53	124.81
26	c	515	BCR	C19-C18-C17	-3.64	113.36	118.94
24	d	403	CLA	CBC-CAC-C3C	-3.64	102.41	112.43
24	b	615	CLA	O2A-CGA-O1A	-3.63	114.42	123.59
24	d	405	CLA	C4-C3-C5	3.63	121.38	115.27
38	c	522	HTG	O5-C1-C2	-3.63	105.75	110.31
35	B	652	P6G	O4-C3-C2	3.63	126.00	110.07
26	c	515	BCR	C24-C23-C22	-3.62	120.76	126.23
24	B	606	CLA	O2A-C1-C2	-3.62	99.12	108.64
26	c	515	BCR	C7-C8-C9	-3.62	120.76	126.23
24	b	609	CLA	C4C-C3C-C2C	-3.62	101.62	106.90
24	B	602	CLA	O2A-CGA-CBA	3.62	123.26	111.91
24	B	602	CLA	CAC-C3C-C4C	3.61	129.50	124.81
29	C	519	LMG	O7-C10-O9	-3.61	114.97	123.70
24	c	501	CLA	C2A-C1A-CHA	-3.61	117.55	123.86
24	C	508	CLA	CHD-C4C-C3C	-3.61	119.54	124.84
24	C	513	CLA	O2D-CGD-O1D	-3.61	116.79	123.84
26	h	103	BCR	C40-C30-C25	-3.60	104.45	110.30
26	H	102	BCR	C7-C8-C9	-3.60	120.79	126.23
24	C	512	CLA	CHD-C4C-C3C	-3.60	119.54	124.84
24	b	616	CLA	C3B-C4B-NB	3.60	113.86	109.21
24	C	504	CLA	O2D-CGD-CBD	3.60	117.66	111.27
40	C	518	DGD	O3G-C3G-C2G	-3.59	102.22	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	502	CLA	CAC-C3C-C4C	3.59	129.47	124.81
24	a	407	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
24	b	604	CLA	CHD-C4C-C3C	-3.59	119.56	124.84
31	u	203	LMT	C3B-C4B-C5B	3.59	116.64	110.24
24	D	405	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
40	H	103	DGD	O3G-C1D-C2D	-3.59	102.70	108.30
24	a	408	CLA	O2D-CGD-CBD	3.59	117.64	111.27
24	b	602	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
26	h	103	BCR	C37-C22-C23	3.57	123.71	118.08
29	d	412	LMG	O7-C10-O9	-3.57	115.08	123.70
40	C	516	DGD	O2G-C1B-O1B	-3.57	115.08	123.70
38	c	531	HTG	C1-O5-C5	3.57	119.16	112.58
24	c	507	CLA	C4C-C3C-C2C	-3.55	101.72	106.90
24	b	606	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
28	A	612	SQD	O7-S-C6	-3.55	102.72	106.94
24	B	617	CLA	CED-O2D-CGD	3.55	123.96	115.94
24	C	505	CLA	O2D-CGD-CBD	3.55	117.57	111.27
24	d	404	CLA	CMC-C2C-C1C	3.54	130.44	125.04
24	C	510	CLA	CED-O2D-CGD	3.54	123.95	115.94
24	C	507	CLA	O1D-CGD-CBD	-3.54	117.24	124.48
24	c	503	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
31	f	101	LMT	O4'-C4B-C5B	3.54	118.09	109.30
24	c	504	CLA	CMB-C2B-C3B	3.54	131.30	124.68
26	A	610	BCR	C7-C8-C9	-3.53	120.90	126.23
24	b	604	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
24	b	611	CLA	C4C-C3C-C2C	-3.53	101.75	106.90
24	B	611	CLA	C3B-C4B-NB	3.52	113.77	109.21
24	b	611	CLA	O2D-CGD-CBD	3.52	117.53	111.27
24	a	408	CLA	CMC-C2C-C1C	3.52	130.40	125.04
24	b	614	CLA	C1-C2-C3	-3.52	119.96	126.04
26	B	619	BCR	C29-C28-C27	-3.51	103.52	111.38
26	d	406	BCR	C33-C5-C6	-3.51	120.58	124.53
24	b	605	CLA	C4C-C3C-C2C	-3.51	101.78	106.90
24	B	604	CLA	C2A-C1A-CHA	-3.51	117.73	123.86
26	H	102	BCR	C24-C23-C22	-3.50	120.94	126.23
24	c	507	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
40	d	408	DGD	C2G-O2G-C1B	3.50	126.40	117.79
25	a	409	PHO	C4C-C3C-C2C	-3.50	102.91	106.78
24	B	608	CLA	CMB-C2B-C3B	3.49	131.21	124.68
24	b	603	CLA	CAC-C3C-C4C	3.49	129.34	124.81
24	d	403	CLA	C4-C3-C5	3.49	121.14	115.27
26	c	514	BCR	C23-C24-C25	-3.48	117.43	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CAC-C3C-C4C	3.48	129.32	124.81
24	C	502	CLA	C3D-CAD-CBD	3.48	112.18	107.61
24	b	611	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
24	c	506	CLA	CED-O2D-CGD	3.48	123.80	115.94
28	A	616	SQD	C44-O6-C1	3.47	120.53	113.74
24	c	503	CLA	C2A-C1A-CHA	-3.47	117.79	123.86
31	a	401	LMT	O1'-C1'-C2'	3.47	113.72	108.30
28	h	105	SQD	O47-C7-C8	3.47	118.98	111.50
26	C	515	BCR	C7-C8-C9	-3.47	120.99	126.23
29	c	520	LMG	O1-C1-C2	3.47	113.72	108.30
31	J	103	LMT	O5B-C5B-C4B	3.47	115.99	109.69
24	A	609	CLA	O2D-CGD-CBD	3.46	117.42	111.27
24	B	606	CLA	CMC-C2C-C1C	3.46	130.31	125.04
31	t	103	LMT	C4B-C3B-C2B	3.46	116.87	110.82
24	B	614	CLA	C4C-C3C-C2C	-3.46	101.85	106.90
29	a	414	LMG	C7-O1-C1	-3.46	106.98	113.74
24	C	509	CLA	OBD-CAD-C3D	-3.46	122.24	127.98
24	c	510	CLA	O2A-C1-C2	-3.46	99.55	108.64
40	D	408	DGD	O5D-C6D-C5D	3.46	115.44	109.05
25	D	401	PHO	C2C-C1C-NC	3.45	115.00	109.79
24	C	510	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
26	C	525	BCR	C32-C1-C6	-3.45	104.70	110.30
24	b	611	CLA	C3B-C4B-NB	3.45	113.67	109.21
24	d	405	CLA	CMC-C2C-C1C	3.45	130.29	125.04
28	l	102	SQD	O48-C23-C24	3.44	122.72	111.91
31	f	101	LMT	C1B-O5B-C5B	3.44	120.44	113.69
38	V	204	HTG	O5-C1-S1	3.44	118.04	109.82
24	b	602	CLA	C1-O2A-CGA	3.43	125.45	116.44
38	b	624	HTG	O5-C1-C2	3.43	114.63	110.31
24	D	404	CLA	CHD-C4C-C3C	-3.43	119.80	124.84
24	B	613	CLA	CHD-C4C-C3C	-3.43	119.80	124.84
24	c	505	CLA	CMB-C2B-C3B	3.43	131.09	124.68
24	d	405	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
24	b	611	CLA	O2A-CGA-O1A	-3.42	114.95	123.59
24	C	511	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
31	M	102	LMT	O1'-C1'-C2'	3.42	113.64	108.30
31	b	622	LMT	O1B-C4'-C5'	-3.42	100.08	109.45
24	C	503	CLA	CAC-C3C-C4C	3.42	129.25	124.81
24	B	609	CLA	O2D-CGD-CBD	3.41	117.33	111.27
26	b	619	BCR	C38-C26-C25	-3.41	120.70	124.53
24	b	614	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
24	b	608	CLA	CAC-C3C-C4C	3.41	129.23	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C15-C16-C17	-3.41	116.50	123.47
28	A	616	SQD	O48-C23-C24	3.40	122.59	111.91
24	C	502	CLA	O2D-CGD-O1D	-3.40	117.18	123.84
24	A	606	CLA	CMB-C2B-C3B	3.40	131.04	124.68
29	J	101	LMG	O8-C28-O10	-3.40	115.01	123.59
24	C	506	CLA	CAC-C3C-C4C	3.40	129.22	124.81
24	b	615	CLA	CAC-C3C-C4C	3.40	129.22	124.81
26	b	619	BCR	C29-C28-C27	-3.39	103.80	111.38
27	A	611	PL9	C2-C3-C4	-3.39	114.12	118.80
31	I	101	LMT	C2'-C3'-C4'	-3.39	101.94	109.68
24	C	512	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
40	c	516	DGD	C3B-C2B-C1B	-3.39	101.31	113.62
24	C	503	CLA	CMB-C2B-C3B	3.38	131.01	124.68
31	B	622	LMT	O1B-C4'-C5'	-3.38	100.19	109.45
40	d	408	DGD	C1E-O6E-C5E	3.37	120.31	113.69
24	B	612	CLA	CMB-C2B-C3B	3.37	130.99	124.68
24	a	408	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
24	b	604	CLA	C4-C3-C5	3.37	120.94	115.27
28	a	424	SQD	O5-C5-C4	3.37	115.81	109.69
31	Y	101	LMT	O1B-C4'-C3'	3.37	116.24	107.28
28	F	104	SQD	O7-S-C6	3.37	110.94	106.94
26	B	618	BCR	C16-C15-C14	-3.36	116.59	123.47
28	a	417	SQD	O47-C7-C8	3.36	118.74	111.50
28	h	105	SQD	O48-C46-C45	3.34	118.16	108.43
24	c	509	CLA	C16-C15-C13	-3.34	105.12	115.92
24	c	512	CLA	O2A-CGA-CBA	3.34	122.39	111.91
28	h	105	SQD	O9-S-C6	3.34	110.91	106.94
24	D	405	CLA	C2A-C1A-CHA	-3.34	118.02	123.86
26	b	619	BCR	C37-C22-C21	-3.34	118.25	122.92
38	C	532	HTG	C3-C4-C5	3.33	116.19	110.24
25	a	409	PHO	C1C-C2C-C3C	-3.33	102.68	106.51
32	A	618	LHG	O8-C23-C24	3.33	122.37	111.91
28	b	633	SQD	O47-C45-C46	3.33	120.47	108.40
38	c	523	HTG	O5-C1-C2	-3.33	106.12	110.31
38	a	418	HTG	O2-C2-C3	3.33	118.05	110.35
24	d	405	CLA	C2A-C1A-CHA	-3.33	118.04	123.86
24	b	602	CLA	CHB-C4A-NA	3.33	129.11	124.51
24	b	616	CLA	O2D-CGD-CBD	3.33	117.18	111.27
29	A	613	LMG	O1-C1-C2	3.33	113.50	108.30
24	c	505	CLA	CMC-C2C-C1C	3.33	130.10	125.04
24	D	403	CLA	CBC-CAC-C3C	-3.33	103.26	112.43
31	b	622	LMT	O5'-C5'-C4'	3.32	116.76	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C6-C5-C3	-3.32	104.75	113.45
26	k	101	BCR	C38-C26-C25	-3.32	120.80	124.53
24	c	507	CLA	C2A-C1A-CHA	-3.32	118.06	123.86
26	t	102	BCR	C23-C22-C21	-3.32	113.85	118.94
38	b	623	HTG	O5-C1-C2	3.32	114.49	110.31
26	C	515	BCR	C2-C3-C4	3.32	118.79	111.38
24	C	502	CLA	C3C-C4C-NC	3.32	114.29	110.57
24	c	512	CLA	CHC-C1C-C2C	-3.32	117.55	126.72
24	B	613	CLA	O2D-CGD-O1D	-3.32	117.36	123.84
28	A	616	SQD	C1-O5-C5	-3.32	107.18	113.69
32	B	632	LHG	O4-P-O5	3.31	128.63	112.24
26	C	525	BCR	C20-C21-C22	-3.31	122.58	127.31
24	B	611	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
24	C	511	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
24	a	410	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
24	c	501	CLA	OBD-CAD-C3D	-3.30	122.51	127.98
26	B	618	BCR	C8-C7-C6	-3.29	117.95	127.20
31	b	622	LMT	O5'-C1'-O1'	-3.29	102.17	109.97
26	t	102	BCR	C36-C18-C19	3.29	123.26	118.08
26	T	102	BCR	C19-C18-C17	-3.28	113.90	118.94
24	b	606	CLA	OBD-CAD-C3D	-3.28	122.53	127.98
24	c	509	CLA	CMC-C2C-C1C	3.28	130.04	125.04
29	C	520	LMG	C4-C3-C2	3.28	116.54	110.82
25	A	608	PHO	C2D-C1D-ND	3.27	114.73	109.79
29	C	520	LMG	O7-C10-C11	3.27	118.56	111.50
24	C	506	CLA	C3B-C4B-NB	3.27	113.44	109.21
40	h	104	DGD	O2G-C1B-C2B	3.27	118.54	111.50
31	B	622	LMT	C3B-C4B-C5B	3.27	116.06	110.24
24	C	507	CLA	O2A-CGA-O1A	-3.26	115.35	123.59
29	B	634	LMG	C7-O1-C1	3.26	120.12	113.74
24	C	512	CLA	OBD-CAD-C3D	-3.26	122.57	127.98
27	a	412	PL9	C37-C38-C39	-3.26	119.81	127.66
24	C	513	CLA	C3D-CAD-CBD	3.26	111.90	107.61
38	a	418	HTG	C1-O5-C5	3.26	118.59	112.58
24	C	504	CLA	C3C-C4C-NC	3.26	114.22	110.57
28	l	102	SQD	O8-S-C6	3.26	110.93	105.74
24	B	603	CLA	C4-C3-C5	3.25	120.75	115.27
24	A	609	CLA	C3D-CAD-CBD	3.25	111.89	107.61
24	b	607	CLA	CHC-C1C-C2C	-3.25	117.73	126.72
24	A	606	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
32	A	618	LHG	O8-C23-O10	-3.24	115.42	123.59
38	B	623	HTG	C1-C2-C3	3.24	116.98	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CMC-C2C-C1C	3.24	129.97	125.04
28	x	101	SQD	C3-C4-C5	3.24	116.01	110.24
24	B	609	CLA	CMC-C2C-C1C	3.24	129.97	125.04
24	B	617	CLA	O2A-C1-C2	3.23	117.13	108.64
28	a	424	SQD	O48-C23-O10	-3.23	115.44	123.59
24	B	617	CLA	O2A-CGA-CBA	3.23	122.03	111.91
24	b	609	CLA	C4A-NA-C1A	-3.23	105.26	106.71
38	c	530	HTG	C1'-S1-C1	3.22	106.12	100.09
26	d	406	BCR	C38-C26-C27	3.22	119.80	113.62
24	B	611	CLA	CED-O2D-CGD	3.22	123.22	115.94
40	h	104	DGD	C3E-C4E-C5E	-3.22	104.50	110.24
24	C	503	CLA	C2A-C1A-CHA	-3.22	118.23	123.86
24	B	617	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
24	b	606	CLA	C6-C5-C3	-3.22	105.02	113.45
26	K	101	BCR	C37-C22-C21	-3.21	118.43	122.92
24	b	607	CLA	C3B-C4B-NB	3.21	113.36	109.21
26	C	515	BCR	C24-C23-C22	-3.21	121.39	126.23
26	t	102	BCR	C15-C16-C17	-3.21	116.91	123.47
29	d	412	LMG	O7-C10-C11	3.21	118.41	111.50
40	D	408	DGD	O2G-C1B-O1B	-3.20	115.96	123.70
24	C	512	CLA	C2A-C1A-CHA	-3.20	118.26	123.86
24	c	511	CLA	CAA-C2A-C1A	3.20	122.47	111.97
24	B	614	CLA	CHD-C4C-C3C	-3.20	120.13	124.84
29	C	520	LMG	O8-C28-C29	3.20	121.95	111.91
28	F	104	SQD	O5-C1-C2	-3.20	103.58	110.35
29	c	520	LMG	O7-C10-C11	3.20	118.39	111.50
24	b	606	CLA	C2A-C1A-CHA	-3.19	118.27	123.86
24	a	410	CLA	C5-C3-C2	-3.19	114.65	121.12
26	t	102	BCR	C37-C22-C23	3.19	123.10	118.08
24	A	606	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
26	H	102	BCR	C37-C22-C23	3.19	123.10	118.08
24	B	616	CLA	C11-C10-C8	-3.19	105.62	115.92
24	b	615	CLA	C4D-C3D-CAD	-3.19	106.69	108.47
24	D	404	CLA	CHB-C4A-NA	3.18	128.92	124.51
24	B	614	CLA	O2A-CGA-CBA	3.18	121.90	111.91
26	K	101	BCR	C39-C30-C25	-3.18	105.14	110.30
24	C	508	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
26	H	102	BCR	C29-C28-C27	-3.18	104.28	111.38
24	C	503	CLA	C1C-C2C-C3C	-3.18	103.62	106.96
28	F	104	SQD	O48-C23-C24	3.18	121.88	111.91
31	F	102	LMT	C1B-O5B-C5B	3.18	119.92	113.69
29	c	519	LMG	O1-C7-C8	-3.17	103.24	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	501	CLA	CBC-CAC-C3C	-3.17	103.69	112.43
24	c	508	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
28	F	104	SQD	O8-S-O7	-3.17	103.53	111.27
26	c	515	BCR	C38-C26-C25	-3.17	120.97	124.53
24	a	410	CLA	C2A-C1A-CHA	-3.17	118.32	123.86
24	d	404	CLA	C4A-NA-C1A	-3.17	105.28	106.71
26	d	406	BCR	C32-C1-C6	3.17	115.44	110.30
24	B	604	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
38	V	204	HTG	O2-C2-C1	3.16	116.08	110.27
26	h	103	BCR	C30-C25-C26	-3.16	118.16	122.61
24	b	616	CLA	CHB-C4A-NA	3.16	128.88	124.51
24	C	508	CLA	C2A-C1A-CHA	-3.16	118.33	123.86
31	F	102	LMT	O5'-C5'-C6'	3.16	114.29	106.44
31	J	103	LMT	C1-O1'-C1'	-3.16	108.60	113.84
24	C	510	CLA	C1C-C2C-C3C	-3.16	103.64	106.96
24	B	611	CLA	C3D-CAD-CBD	3.16	111.76	107.61
40	d	408	DGD	O2G-C1B-O1B	-3.16	116.07	123.70
26	C	514	BCR	C8-C7-C6	-3.15	118.35	127.20
24	B	605	CLA	C7-C6-C5	-3.15	104.80	113.36
26	B	620	BCR	C38-C26-C25	-3.15	120.99	124.53
24	c	501	CLA	CMB-C2B-C3B	3.15	130.57	124.68
26	D	406	BCR	C29-C30-C25	3.15	115.33	110.48
24	A	607	CLA	C1C-C2C-C3C	-3.15	103.65	106.96
24	b	612	CLA	CBC-CAC-C3C	-3.14	103.76	112.43
38	B	624	HTG	O5-C1-C2	3.14	114.27	110.31
24	d	404	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
32	D	409	LHG	O7-C7-O9	-3.14	116.11	123.70
38	b	632	HTG	C3-C4-C5	3.14	115.84	110.24
24	b	603	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
25	a	409	PHO	C3D-C2D-C1D	-3.14	101.30	105.87
26	b	619	BCR	C30-C25-C26	-3.14	118.19	122.61
24	A	607	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
26	h	103	BCR	C7-C8-C9	-3.14	121.50	126.23
24	d	404	CLA	O2D-CGD-CBD	3.14	116.84	111.27
24	b	608	CLA	C1D-CHD-C4C	3.13	126.69	122.56
26	a	411	BCR	C37-C22-C21	-3.13	118.53	122.92
28	A	612	SQD	O2-C2-C1	3.13	117.65	110.05
29	c	519	LMG	O8-C28-O10	-3.13	115.69	123.59
29	C	519	LMG	O8-C28-O10	-3.12	115.71	123.59
38	a	418	HTG	O3-C3-C4	-3.12	103.13	110.35
24	b	617	CLA	O2A-C1-C2	3.12	116.83	108.64
24	C	513	CLA	C3B-C4B-NB	3.12	113.24	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	401	PHO	C4-C3-C5	3.12	120.52	115.27
26	C	525	BCR	C37-C22-C23	3.12	122.99	118.08
24	b	612	CLA	C2A-C1A-CHA	-3.12	118.41	123.86
24	b	607	CLA	O2A-CGA-O1A	-3.12	115.73	123.59
24	c	508	CLA	CHD-C4C-C3C	-3.12	120.26	124.84
24	b	609	CLA	O2D-CGD-CBD	3.11	116.80	111.27
24	c	502	CLA	C3D-CAD-CBD	3.11	111.70	107.61
24	A	607	CLA	CMB-C2B-C3B	3.11	130.50	124.68
24	b	616	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
31	A	617	LMT	C1'-O5'-C5'	3.11	119.79	113.69
24	b	612	CLA	OBD-CAD-C3D	-3.11	122.82	127.98
24	b	613	CLA	C2A-C1A-CHA	-3.11	118.42	123.86
38	h	101	HTG	C2'-C1'-S1	-3.11	102.37	112.40
40	c	517	DGD	O1G-C1A-O1A	-3.10	115.76	123.59
24	C	511	CLA	CMC-C2C-C1C	3.10	129.76	125.04
31	J	103	LMT	C3B-C4B-C5B	3.10	115.77	110.24
24	b	606	CLA	CAC-C3C-C4C	3.10	128.83	124.81
24	C	507	CLA	OBD-CAD-C3D	-3.09	122.84	127.98
38	C	529	HTG	C1-O5-C5	3.09	118.28	112.58
24	B	609	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
24	C	505	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
38	B	630	HTG	C4-C3-C2	3.09	116.21	110.82
26	H	102	BCR	C40-C30-C25	-3.09	105.29	110.30
24	B	616	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
31	F	102	LMT	C1'-O5'-C5'	3.09	119.74	113.69
24	c	509	CLA	C1C-C2C-C3C	-3.08	103.71	106.96
38	C	529	HTG	O5-C5-C6	3.08	114.10	106.44
40	H	103	DGD	O1G-C1A-O1A	-3.08	115.81	123.59
26	A	610	BCR	C20-C21-C22	-3.08	122.91	127.31
24	B	611	CLA	CMC-C2C-C1C	3.08	129.73	125.04
28	h	105	SQD	O6-C1-C2	3.08	113.11	108.30
26	t	102	BCR	C7-C8-C9	-3.08	121.58	126.23
40	h	104	DGD	O1G-C1A-O1A	-3.08	115.83	123.59
26	t	102	BCR	C12-C13-C14	-3.08	114.22	118.94
38	B	624	HTG	C1-C2-C3	3.07	116.66	110.59
24	b	610	CLA	CMB-C2B-C3B	3.07	130.43	124.68
24	b	614	CLA	CMC-C2C-C1C	3.07	129.72	125.04
26	d	406	BCR	C28-C27-C26	-3.07	108.59	114.08
24	c	506	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
29	C	519	LMG	O10-C28-C29	-3.07	111.77	123.73
38	c	522	HTG	C1'-S1-C1	3.06	105.82	100.09
26	C	525	BCR	C38-C26-C25	-3.06	121.09	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	612	SQD	O47-C7-O49	-3.06	116.30	123.70
24	c	513	CLA	C2A-C1A-CHA	-3.06	118.51	123.86
26	H	102	BCR	C37-C22-C21	-3.06	118.64	122.92
24	c	504	CLA	CHD-C4C-C3C	-3.06	120.34	124.84
32	A	618	LHG	O8-C6-C5	3.06	117.33	108.43
38	b	632	HTG	C1-O5-C5	3.06	118.22	112.58
29	j	101	LMG	O7-C10-C11	3.05	118.08	111.50
31	M	101	LMT	C1'-O5'-C5'	-3.05	107.69	113.69
28	F	104	SQD	O4-C4-C3	-3.05	103.29	110.35
26	h	103	BCR	C29-C28-C27	-3.05	104.56	111.38
24	C	510	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	A	607	CLA	O2D-CGD-CBD	3.05	116.69	111.27
24	B	614	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
24	d	404	CLA	CHD-C4C-C3C	-3.05	120.36	124.84
29	B	634	LMG	O8-C28-C29	3.05	121.47	111.91
24	c	511	CLA	O2D-CGD-CBD	3.05	116.68	111.27
32	B	632	LHG	O7-C7-C8	3.04	118.06	111.50
26	c	515	BCR	C37-C22-C23	3.04	122.87	118.08
26	H	102	BCR	C20-C21-C22	-3.04	122.97	127.31
38	b	632	HTG	C1'-S1-C1	3.04	105.78	100.09
24	a	410	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
24	B	610	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
28	x	101	SQD	O5-C5-C4	3.04	115.22	109.69
31	f	101	LMT	C1-O1'-C1'	3.04	118.88	113.84
24	b	613	CLA	CMC-C2C-C1C	3.04	129.66	125.04
29	c	520	LMG	O8-C28-C29	3.04	121.43	111.91
26	H	102	BCR	C36-C18-C19	3.03	122.86	118.08
24	A	607	CLA	CMC-C2C-C1C	3.03	129.66	125.04
27	A	611	PL9	C35-C34-C36	3.03	120.37	115.27
26	C	514	BCR	C30-C25-C26	-3.03	118.34	122.61
38	o	301	HTG	C1'-S1-C1	3.03	105.76	100.09
24	a	410	CLA	OBD-CAD-C3D	-3.03	122.95	127.98
25	A	608	PHO	CHC-C1C-C2C	-3.03	118.11	125.73
28	a	417	SQD	O48-C23-O10	-3.03	115.95	123.59
26	c	514	BCR	C20-C21-C22	-3.03	122.99	127.31
24	A	609	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
26	B	619	BCR	C39-C30-C25	3.03	115.21	110.30
26	t	102	BCR	C35-C13-C12	3.03	122.84	118.08
24	b	607	CLA	O2D-CGD-CBD	3.02	116.64	111.27
24	B	615	CLA	C2A-C1A-CHA	-3.02	118.57	123.86
31	Y	101	LMT	O1B-C1B-C2B	3.02	115.92	108.10
24	C	508	CLA	O2D-CGD-CBD	3.02	116.63	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	O2D-CGD-CBD	3.02	116.63	111.27
24	a	408	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
24	C	506	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
24	b	609	CLA	C3D-CAD-CBD	3.01	111.57	107.61
24	B	616	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
24	c	503	CLA	OBD-CAD-C3D	-3.01	122.98	127.98
24	c	511	CLA	C2A-C1A-CHA	-3.01	118.60	123.86
32	d	409	LHG	O7-C7-O9	-3.01	116.43	123.70
24	c	508	CLA	C3D-CAD-CBD	3.01	111.57	107.61
24	C	507	CLA	CAC-C3C-C4C	3.01	128.71	124.81
29	B	634	LMG	C3-C4-C5	3.00	115.60	110.24
24	c	509	CLA	C2A-C1A-CHA	-3.00	118.61	123.86
24	c	513	CLA	C3B-C4B-NB	3.00	113.09	109.21
26	H	102	BCR	C32-C1-C6	3.00	115.17	110.30
31	M	101	LMT	O5'-C5'-C6'	3.00	113.89	106.44
24	b	612	CLA	C1-C2-C3	-3.00	120.86	126.04
31	M	101	LMT	O5'-C1'-O1'	-2.99	102.89	109.97
24	c	504	CLA	C2A-C1A-CHA	-2.99	118.63	123.86
40	d	408	DGD	O1G-C1A-C2A	2.99	121.28	111.91
24	B	607	CLA	C4-C3-C5	2.99	120.30	115.27
26	d	406	BCR	C1-C6-C5	-2.99	118.41	122.61
26	k	101	BCR	C23-C24-C25	-2.99	118.82	127.20
24	b	609	CLA	C2A-C1A-CHA	-2.98	118.64	123.86
31	m	102	LMT	C1B-C2B-C3B	2.98	116.21	110.00
25	D	401	PHO	CMB-C2B-C1B	2.98	129.66	125.06
24	b	611	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
24	B	616	CLA	CAC-C3C-C4C	2.98	128.68	124.81
31	j	103	LMT	O1B-C1B-C2B	2.98	115.82	108.10
28	a	424	SQD	C46-O48-C23	2.98	128.15	117.12
24	b	611	CLA	OBD-CAD-C3D	-2.98	123.04	127.98
24	B	615	CLA	CAC-C3C-C4C	2.98	128.67	124.81
24	c	504	CLA	CHB-C4A-NA	2.98	128.63	124.51
24	C	509	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
38	a	418	HTG	C3-C4-C5	2.98	115.55	110.24
24	D	404	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
30	C	528	GOL	O3-C3-C2	2.97	124.46	110.20
24	d	405	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
31	u	203	LMT	O1B-C1B-C2B	2.97	115.80	108.10
24	b	617	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	a	411	BCR	C28-C27-C26	-2.97	108.77	114.08
26	T	102	BCR	C16-C17-C18	-2.97	123.07	127.31
40	C	518	DGD	O1G-C1A-C2A	2.97	121.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	617	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
26	B	618	BCR	C33-C5-C6	-2.96	121.20	124.53
24	b	610	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
25	a	409	PHO	C1C-NC-C4C	-2.96	100.93	106.51
26	k	101	BCR	C29-C28-C27	2.96	117.99	111.38
26	C	514	BCR	C11-C10-C9	-2.96	123.09	127.31
24	b	607	CLA	C4A-NA-C1A	2.96	108.04	106.71
40	D	408	DGD	O1G-C1A-C2A	2.96	121.19	111.91
31	Y	101	LMT	C3B-C4B-C5B	2.95	115.51	110.24
24	B	605	CLA	O2D-CGD-CBD	2.95	116.52	111.27
24	D	404	CLA	O2D-CGD-CBD	2.95	116.52	111.27
24	c	509	CLA	CED-O2D-CGD	2.95	122.61	115.94
24	b	603	CLA	C2A-C1A-CHA	-2.95	118.70	123.86
28	A	612	SQD	O5-C1-C2	-2.95	104.10	110.35
24	b	615	CLA	CED-O2D-CGD	2.95	122.60	115.94
31	F	102	LMT	C1-O1'-C1'	2.95	118.73	113.84
28	A	622	SQD	O48-C23-O10	-2.95	116.16	123.59
26	C	515	BCR	C36-C18-C19	2.94	122.72	118.08
29	b	621	LMG	C1-O6-C5	-2.94	107.92	113.69
24	b	604	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
24	b	616	CLA	CAC-C3C-C4C	2.94	128.62	124.81
31	I	101	LMT	O3'-C3'-C4'	2.94	117.73	109.94
24	B	611	CLA	CHB-C4A-NA	2.94	128.57	124.51
24	a	407	CLA	CHC-C1C-C2C	-2.93	118.60	126.72
25	D	401	PHO	C3D-C2D-C1D	-2.93	101.59	105.87
25	D	401	PHO	CAC-C3C-C4C	2.93	128.42	125.22
40	D	408	DGD	O3G-C3G-C2G	2.93	117.97	110.90
38	C	529	HTG	O5-C1-C2	-2.93	106.63	110.31
31	M	101	LMT	C1B-C2B-C3B	2.93	116.09	110.00
24	C	501	CLA	CBC-CAC-C3C	-2.93	104.37	112.43
26	c	514	BCR	C39-C30-C25	-2.92	105.56	110.30
26	b	620	BCR	C23-C24-C25	-2.92	118.99	127.20
24	b	602	CLA	C3D-CAD-CBD	2.92	111.45	107.61
26	C	514	BCR	C31-C1-C6	-2.92	105.56	110.30
26	h	103	BCR	C31-C1-C6	-2.92	105.56	110.30
24	B	604	CLA	CMB-C2B-C3B	2.92	130.14	124.68
24	C	507	CLA	CBC-CAC-C3C	-2.92	104.39	112.43
32	e	101	LHG	O8-C23-C24	2.91	121.06	111.91
24	B	611	CLA	C14-C13-C15	-2.91	100.74	111.29
31	M	101	LMT	O4'-C4B-C3B	2.91	117.08	110.35
24	b	608	CLA	CMC-C2C-C1C	2.91	129.47	125.04
28	a	417	SQD	C1-C2-C3	-2.91	103.94	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	523	GOL	C3-C2-C1	-2.90	100.41	111.70
26	c	514	BCR	C37-C22-C23	2.90	122.64	118.08
31	j	103	LMT	C1B-O1B-C4'	2.90	125.14	117.96
30	B	625	GOL	O2-C2-C3	-2.90	96.36	109.12
24	b	612	CLA	CMB-C2B-C3B	2.90	130.10	124.68
24	C	507	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
31	B	622	LMT	C1-O1'-C1'	-2.89	109.04	113.84
24	D	405	CLA	OBD-CAD-C3D	-2.89	123.18	127.98
25	d	401	PHO	C2B-C1B-NB	2.89	114.15	109.79
24	c	503	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
24	C	501	CLA	OBD-CAD-C3D	-2.89	123.18	127.98
24	b	604	CLA	CAC-C3C-C4C	2.89	128.56	124.81
24	B	617	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
24	a	410	CLA	C1-C2-C3	-2.88	121.06	126.04
26	D	406	BCR	C30-C25-C26	-2.88	118.55	122.61
28	A	622	SQD	O6-C1-C2	2.88	112.80	108.30
40	D	408	DGD	O6D-C5D-C6D	2.88	112.48	106.67
40	h	104	DGD	O5D-C6D-C5D	-2.88	103.72	109.05
24	c	502	CLA	O2D-CGD-CBD	2.88	116.39	111.27
31	J	103	LMT	O3'-C3'-C4'	2.88	117.58	109.94
24	B	617	CLA	CMB-C2B-C3B	2.88	130.07	124.68
28	A	616	SQD	O48-C23-O10	-2.88	116.33	123.59
31	m	102	LMT	O5B-C5B-C4B	2.88	114.92	109.69
31	M	101	LMT	O1'-C1-C2	-2.88	99.48	109.56
24	C	512	CLA	C1-O2A-CGA	2.88	123.99	116.44
26	A	610	BCR	C24-C23-C22	-2.87	121.89	126.23
26	B	620	BCR	C37-C22-C23	2.87	122.60	118.08
26	C	515	BCR	C39-C30-C25	-2.87	105.65	110.30
24	a	410	CLA	C3D-CAD-CBD	2.87	111.38	107.61
43	V	203	HEC	CMA-C3A-C2A	2.87	130.34	124.94
24	b	615	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
24	A	609	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
28	b	633	SQD	O48-C23-O10	-2.86	116.37	123.59
24	B	615	CLA	C1-O2A-CGA	2.86	123.95	116.44
24	c	510	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
24	B	614	CLA	CAC-C3C-C4C	2.86	128.52	124.81
33	V	209	PG4	C7-O4-C6	2.86	125.66	113.29
24	b	617	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
32	D	410	LHG	O8-C23-O10	-2.85	116.39	123.59
32	l	101	LHG	O8-C23-O10	-2.85	116.39	123.59
24	B	610	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
24	b	603	CLA	C1B-CHB-C4A	-2.85	124.47	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	A	611	PL9	C37-C38-C39	-2.85	120.80	127.66
24	B	613	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	B	614	CLA	C3B-C4B-NB	2.85	112.89	109.21
24	C	512	CLA	CHC-C1C-C2C	-2.84	118.85	126.72
31	M	101	LMT	C1-O1'-C1'	2.84	118.56	113.84
24	D	405	CLA	CMB-C2B-C3B	2.84	130.00	124.68
26	c	515	BCR	C1-C6-C5	-2.84	118.61	122.61
24	B	614	CLA	C2A-C1A-CHA	-2.84	118.89	123.86
24	B	605	CLA	C4-C3-C5	-2.84	110.49	115.27
43	V	203	HEC	CMD-C2D-C1D	-2.84	124.10	128.46
24	D	404	CLA	CMC-C2C-C1C	2.84	129.36	125.04
28	a	424	SQD	O6-C44-C45	2.84	117.75	110.90
24	B	611	CLA	O2A-CGA-O1A	-2.84	116.43	123.59
24	B	605	CLA	OBD-CAD-C3D	-2.83	123.27	127.98
40	C	516	DGD	C3G-C2G-C1G	-2.83	105.08	111.79
24	c	505	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
25	A	608	PHO	C2B-C1B-NB	2.83	114.07	109.79
26	h	103	BCR	C37-C22-C21	-2.83	118.96	122.92
24	D	403	CLA	CHC-C1C-C2C	-2.83	118.89	126.72
24	c	506	CLA	CHB-C4A-NA	2.83	128.42	124.51
26	c	515	BCR	C8-C7-C6	-2.83	119.26	127.20
24	B	614	CLA	CMB-C2B-C3B	2.83	129.97	124.68
29	C	520	LMG	O1-C1-C2	2.83	112.72	108.30
24	B	606	CLA	C4-C3-C5	-2.83	110.52	115.27
24	d	404	CLA	C3D-CAD-CBD	2.82	111.32	107.61
24	c	504	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
29	C	526	LMG	O3-C3-C4	2.82	116.88	110.35
26	H	102	BCR	C31-C1-C6	-2.82	105.72	110.30
32	l	101	LHG	O7-C7-C8	2.82	117.58	111.50
24	c	511	CLA	CMB-C2B-C3B	2.82	129.95	124.68
26	b	618	BCR	C15-C16-C17	-2.81	117.71	123.47
24	B	608	CLA	C2A-C1A-CHA	-2.81	118.94	123.86
24	c	510	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
24	A	609	CLA	CMC-C2C-C1C	2.81	129.32	125.04
26	t	102	BCR	C24-C23-C22	-2.81	121.99	126.23
29	a	414	LMG	C8-O7-C10	-2.81	110.88	117.79
26	b	618	BCR	C16-C17-C18	-2.81	123.31	127.31
24	c	507	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
26	K	101	BCR	C38-C26-C25	-2.81	121.38	124.53
43	V	203	HEC	CMB-C2B-C1B	-2.80	124.16	128.46
24	C	511	CLA	CAC-C3C-C4C	2.80	128.45	124.81
26	h	103	BCR	C24-C23-C22	-2.80	122.00	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	603	CLA	CMC-C2C-C1C	2.80	129.31	125.04
27	D	407	PL9	C35-C34-C36	2.80	119.98	115.27
24	c	512	CLA	CHB-C4A-NA	2.80	128.38	124.51
40	h	104	DGD	O4E-C4E-C5E	2.80	116.24	109.30
38	C	532	HTG	O5-C5-C4	2.80	114.77	109.69
24	b	603	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	d	401	PHO	CAC-C3C-C4C	2.80	128.27	125.22
38	b	631	HTG	O3-C3-C2	-2.80	103.89	110.35
29	C	519	LMG	O8-C9-C8	2.80	116.57	108.43
24	c	506	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
24	c	508	CLA	OBD-CAD-C3D	-2.79	123.35	127.98
24	B	607	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
26	k	101	BCR	C32-C1-C6	2.79	114.83	110.30
26	k	101	BCR	C20-C21-C22	-2.79	123.33	127.31
24	B	602	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
24	B	605	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	b	612	CLA	CAC-C3C-C4C	2.79	128.43	124.81
24	B	606	CLA	CHB-C4A-NA	2.79	128.37	124.51
29	A	613	LMG	C7-O1-C1	-2.78	108.30	113.74
24	B	605	CLA	CHD-C4C-C3C	-2.78	120.75	124.84
26	B	619	BCR	C30-C25-C26	-2.78	118.69	122.61
24	c	502	CLA	OBD-CAD-C3D	-2.78	123.36	127.98
24	B	612	CLA	CHC-C1C-C2C	-2.78	119.03	126.72
24	B	617	CLA	C4A-NA-C1A	-2.78	105.46	106.71
24	C	507	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	B	611	CLA	CMB-C2B-C3B	2.78	129.87	124.68
24	A	606	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
24	b	606	CLA	C4A-NA-C1A	-2.78	105.46	106.71
31	c	521	LMT	C1B-O1B-C4'	2.77	124.83	117.96
30	c	525	GOL	O1-C1-C2	2.77	123.50	110.20
24	A	607	CLA	CHC-C1C-C2C	-2.77	119.05	126.72
38	C	530	HTG	O5-C5-C6	2.77	113.33	106.44
24	B	609	CLA	C4-C3-C5	2.77	119.93	115.27
24	C	504	CLA	C1D-CHD-C4C	2.77	126.22	122.56
29	C	519	LMG	O1-C7-C8	-2.77	104.21	110.90
24	D	405	CLA	CHB-C4A-NA	2.77	128.34	124.51
28	A	622	SQD	O5-C5-C4	2.77	114.72	109.69
24	C	508	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	B	610	CLA	C4C-C3C-C2C	-2.76	102.87	106.90
26	A	610	BCR	C2-C1-C6	2.76	114.73	110.48
40	H	103	DGD	O5D-C6D-C5D	-2.76	103.94	109.05
41	E	113	HEM	CAA-CBA-CGA	2.76	117.31	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	409	LHG	C6-O8-C23	2.76	127.35	117.12
40	H	103	DGD	C3E-C4E-C5E	-2.76	105.31	110.24
24	A	606	CLA	C4-C3-C5	2.76	119.91	115.27
27	a	412	PL9	C16-C14-C13	-2.76	115.53	121.12
26	A	610	BCR	C37-C22-C23	2.76	122.42	118.08
24	B	614	CLA	C1-C2-C3	-2.76	121.27	126.04
28	A	612	SQD	O9-S-O7	-2.76	104.41	113.95
26	C	514	BCR	C39-C30-C25	-2.76	105.83	110.30
26	h	103	BCR	C36-C18-C19	2.76	122.42	118.08
24	b	605	CLA	CAA-C2A-C1A	2.75	121.00	111.97
29	c	519	LMG	O7-C10-O9	-2.75	117.05	123.70
32	D	409	LHG	C6-O8-C23	2.75	127.30	117.12
40	C	516	DGD	C4E-C3E-C2E	-2.75	106.02	110.82
24	b	604	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
24	b	613	CLA	CMB-C2B-C3B	2.75	129.82	124.68
24	B	602	CLA	CHC-C1C-C2C	-2.75	119.12	126.72
24	C	504	CLA	C7-C6-C5	-2.75	105.90	113.36
26	k	101	BCR	C37-C22-C23	2.74	122.40	118.08
38	b	623	HTG	C2'-C1'-S1	2.74	121.27	112.40
27	d	407	PL9	C10-C9-C11	2.74	119.88	115.27
24	B	607	CLA	OBD-CAD-C3D	-2.74	123.43	127.98
24	d	405	CLA	OBD-CAD-C3D	-2.74	123.43	127.98
26	D	406	BCR	C37-C22-C21	-2.74	119.09	122.92
24	d	403	CLA	C4A-NA-C1A	2.74	107.94	106.71
24	b	603	CLA	C1-C2-C3	-2.74	121.31	126.04
24	a	408	CLA	C4-C3-C5	2.74	119.87	115.27
24	b	613	CLA	OBD-CAD-C3D	-2.73	123.45	127.98
26	T	102	BCR	C39-C30-C25	-2.73	105.87	110.30
24	B	606	CLA	CAA-C2A-C1A	2.73	120.92	111.97
24	b	602	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
31	I	101	LMT	O3B-C3B-C2B	-2.73	104.04	110.35
24	C	504	CLA	CHC-C1C-C2C	-2.73	119.17	126.72
26	a	411	BCR	C23-C24-C25	-2.73	119.54	127.20
24	C	513	CLA	C5-C3-C2	-2.73	115.60	121.12
24	c	505	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
24	c	502	CLA	CHC-C1C-C2C	-2.73	119.18	126.72
31	M	101	LMT	C3'-C4'-C5'	-2.72	104.68	110.93
24	c	503	CLA	CMB-C2B-C3B	2.72	129.77	124.68
24	b	608	CLA	CHD-C4C-C3C	-2.72	120.84	124.84
24	b	606	CLA	C4-C3-C5	-2.72	110.70	115.27
24	b	611	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
24	c	511	CLA	CHB-C4A-NA	2.71	128.26	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
25	a	409	PHO	CMC-C2C-C1C	2.71	129.24	125.06
24	b	605	CLA	CMB-C2B-C3B	2.70	129.74	124.68
26	B	618	BCR	C24-C23-C22	-2.70	122.15	126.23
28	l	102	SQD	C1-C2-C3	-2.70	104.36	110.00
24	c	509	CLA	CHB-C4A-NA	2.70	128.25	124.51
27	d	407	PL9	C20-C19-C21	2.70	119.82	115.27
25	D	401	PHO	C1C-NC-C4C	-2.70	101.42	106.51
29	a	414	LMG	C4-C3-C2	2.70	115.54	110.82
32	d	410	LHG	O8-C23-C24	2.70	120.39	111.91
24	b	617	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
24	C	511	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	B	608	CLA	C1-C2-C3	-2.70	121.37	126.04
32	A	618	LHG	O7-C7-C8	2.70	117.33	111.50
24	B	608	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	c	513	CLA	CHB-C4A-NA	2.70	128.25	124.51
24	d	405	CLA	C5-C3-C2	-2.70	115.65	121.12
28	a	413	SQD	O47-C7-O49	-2.70	117.17	123.70
24	c	512	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	B	609	CLA	CMB-C2B-C3B	2.70	129.73	124.68
24	B	615	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
24	b	615	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
26	H	102	BCR	C38-C26-C25	-2.70	121.50	124.53
29	z	101	LMG	C1-C2-C3	-2.70	104.38	110.00
38	h	101	HTG	O2-C2-C1	2.70	115.22	110.27
24	C	512	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	c	506	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
38	b	632	HTG	O5-C5-C6	2.69	113.13	106.44
24	C	513	CLA	O2A-CGA-CBA	2.69	120.36	111.91
24	C	503	CLA	CAA-C2A-C1A	2.69	120.80	111.97
24	B	608	CLA	O1D-CGD-CBD	-2.69	118.97	124.48
24	C	502	CLA	O2D-CGD-CBD	2.69	116.05	111.27
28	F	104	SQD	C1-C2-C3	-2.69	104.39	110.00
24	C	510	CLA	OBD-CAD-C3D	-2.69	123.52	127.98
24	B	608	CLA	CAC-C3C-C4C	2.69	128.30	124.81
38	c	522	HTG	O2-C2-C1	-2.69	105.33	110.27
24	b	609	CLA	CMC-C2C-C1C	2.69	129.13	125.04
31	c	521	LMT	C2'-C3'-C4'	-2.69	103.55	109.68
26	t	102	BCR	C11-C10-C9	-2.69	123.48	127.31
29	C	526	LMG	O6-C5-C4	2.69	114.57	109.69
28	h	105	SQD	O48-C23-C24	2.68	120.33	111.91
31	c	521	LMT	O3'-C3'-C4'	2.68	117.05	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	h	105	SQD	O3-C3-C4	2.68	116.55	110.35
24	b	614	CLA	C7-C6-C5	-2.68	106.08	113.36
24	C	508	CLA	CMB-C2B-C3B	2.68	129.69	124.68
24	B	611	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
24	b	608	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
38	H	101	HTG	C3-C4-C5	2.68	115.02	110.24
26	A	610	BCR	C8-C7-C6	-2.68	119.68	127.20
24	c	504	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
24	b	604	CLA	C4A-NA-C1A	-2.68	105.50	106.71
29	A	613	LMG	C3-C4-C5	2.68	115.01	110.24
24	C	509	CLA	CHC-C1C-C2C	-2.68	119.32	126.72
31	M	101	LMT	C1B-O1B-C4'	2.67	124.58	117.96
24	d	403	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
24	C	509	CLA	O2A-CGA-O1A	-2.67	116.84	123.59
24	B	603	CLA	C16-C15-C13	-2.67	107.28	115.92
26	h	103	BCR	C2-C1-C6	2.67	114.59	110.48
31	M	101	LMT	C3B-C4B-C5B	-2.67	105.47	110.24
26	h	103	BCR	C33-C5-C4	-2.67	108.49	113.62
24	a	407	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
24	C	508	CLA	C3D-CAD-CBD	2.67	111.12	107.61
24	d	404	CLA	CHB-C4A-NA	2.67	128.20	124.51
31	u	203	LMT	O1B-C1B-O5B	-2.67	103.22	110.67
24	a	407	CLA	CMB-C2B-C3B	2.67	129.67	124.68
29	B	634	LMG	C30-C29-C28	2.66	123.31	113.62
41	e	107	HEM	CBD-CAD-C3D	2.66	117.39	112.48
24	B	612	CLA	C4C-C3C-C2C	-2.66	103.01	106.90
24	b	615	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	b	612	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	t	102	BCR	C28-C27-C26	-2.66	109.32	114.08
27	d	407	PL9	C50-C49-C48	-2.66	114.97	122.65
38	B	630	HTG	C1'-S1-C1	2.66	105.06	100.09
26	A	610	BCR	C39-C30-C25	-2.66	105.99	110.30
38	a	418	HTG	C1-C2-C3	-2.66	105.34	110.59
38	C	530	HTG	C1'-S1-C1	2.65	105.06	100.09
24	b	609	CLA	CAC-C3C-C4C	2.65	128.25	124.81
24	D	404	CLA	CMB-C2B-C3B	2.65	129.64	124.68
31	I	101	LMT	O1'-C1'-C2'	2.65	112.44	108.30
24	C	503	CLA	C3D-CAD-CBD	2.65	111.10	107.61
24	c	511	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
40	D	408	DGD	C3G-O3G-C1D	2.65	118.92	113.74
40	C	516	DGD	C3D-C4D-C5D	-2.65	105.51	110.24
24	C	512	CLA	CMC-C2C-C1C	2.65	129.07	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C4D-C3D-CAD	-2.65	106.99	108.47
31	t	103	LMT	O5B-C5B-C4B	2.64	114.50	109.69
24	B	614	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
26	A	610	BCR	C11-C10-C9	-2.64	123.54	127.31
24	c	512	CLA	C1-O2A-CGA	2.64	123.38	116.44
26	H	102	BCR	C16-C17-C18	-2.64	123.54	127.31
24	D	405	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
24	c	508	CLA	O2D-CGD-CBD	2.64	115.97	111.27
24	C	512	CLA	C1-C2-C3	-2.64	121.47	126.04
24	A	607	CLA	C4A-NA-C1A	2.64	107.89	106.71
31	I	101	LMT	C6B-C5B-C4B	2.64	119.19	113.00
24	c	506	CLA	CAC-C3C-C4C	2.64	128.24	124.81
40	H	103	DGD	O5E-C6E-C5E	-2.64	102.23	111.29
27	D	407	PL9	C40-C39-C38	-2.64	116.91	123.68
24	B	606	CLA	C4A-NA-C1A	2.64	107.89	106.71
25	d	401	PHO	O2A-CGA-O1A	-2.64	116.94	123.59
32	l	101	LHG	O8-C6-C5	2.64	116.11	108.43
24	B	615	CLA	O2A-CGA-CBA	2.64	120.18	111.91
26	H	102	BCR	C16-C15-C14	-2.63	118.08	123.47
24	B	612	CLA	O2D-CGD-CBD	2.63	115.95	111.27
24	c	512	CLA	CAC-C3C-C4C	2.63	128.23	124.81
29	B	634	LMG	C4-C3-C2	2.63	115.42	110.82
31	B	622	LMT	C6B-C5B-C4B	-2.63	106.84	113.00
29	C	520	LMG	O3-C3-C4	-2.63	104.27	110.35
26	B	619	BCR	C37-C22-C23	2.63	122.22	118.08
24	b	610	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
24	c	501	CLA	CHC-C1C-C2C	-2.63	119.45	126.72
38	C	521	HTG	O5-C5-C6	2.63	112.97	106.44
26	h	103	BCR	C11-C10-C9	-2.63	123.56	127.31
38	C	531	HTG	C1'-S1-C1	2.62	105.00	100.09
27	d	407	PL9	C11-C9-C8	-2.62	115.81	121.12
24	B	607	CLA	C3D-CAD-CBD	2.62	111.06	107.61
24	B	602	CLA	C1-C2-C3	-2.62	121.51	126.04
24	c	513	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
26	c	514	BCR	C31-C1-C6	-2.62	106.05	110.30
38	B	623	HTG	O4-C4-C5	2.62	115.80	109.30
24	d	405	CLA	C6-C7-C8	-2.62	107.46	115.92
24	C	510	CLA	O2A-CGA-O1A	-2.62	116.99	123.59
38	c	523	HTG	O5-C5-C4	2.62	114.45	109.69
24	b	612	CLA	C3D-CAD-CBD	2.61	111.05	107.61
24	a	410	CLA	CHB-C4A-NA	2.61	128.13	124.51
24	B	606	CLA	C6-C5-C3	-2.61	106.61	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	O1D-CGD-CBD	-2.61	119.14	124.48
40	h	104	DGD	O1G-C1A-C2A	2.61	120.10	111.91
24	a	408	CLA	C3A-C2A-C1A	-2.61	97.43	101.34
24	D	404	CLA	C2A-C3A-C4A	2.61	106.08	101.87
31	t	103	LMT	O5'-C1'-O1'	-2.61	103.80	109.97
40	C	518	DGD	C6B-C5B-C4B	-2.61	101.20	114.42
25	A	608	PHO	CHD-C4C-C3C	-2.60	119.20	124.49
24	C	503	CLA	O2D-CGD-CBD	2.60	115.89	111.27
43	v	202	HEC	CMA-C3A-C2A	2.60	129.85	124.94
24	b	603	CLA	CED-O2D-CGD	2.60	121.81	115.94
24	b	610	CLA	C1D-CHD-C4C	2.60	125.99	122.56
24	C	502	CLA	C1-C2-C3	-2.60	121.55	126.04
24	C	503	CLA	OBD-CAD-C3D	-2.60	123.67	127.98
24	a	407	CLA	OBD-CAD-C3D	-2.60	123.67	127.98
24	D	404	CLA	CHC-C1C-C2C	-2.60	119.54	126.72
24	b	605	CLA	OBD-CAD-C3D	-2.59	123.68	127.98
24	C	509	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
41	E	113	HEM	CMC-C2C-C3C	2.59	129.52	124.68
25	d	401	PHO	C1C-C2C-C3C	-2.59	103.54	106.51
24	a	410	CLA	C4-C3-C5	2.59	119.62	115.27
24	B	611	CLA	C20-C18-C19	-2.58	98.59	110.51
38	b	631	HTG	O5-C1-S1	2.58	116.00	109.82
24	B	605	CLA	CAA-C2A-C1A	2.58	120.44	111.97
24	C	502	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
41	e	107	HEM	CMC-C2C-C3C	2.58	129.51	124.68
24	b	607	CLA	C1-C2-C3	-2.58	121.58	126.04
24	a	408	CLA	CHC-C1C-C2C	-2.58	119.58	126.72
28	A	616	SQD	O9-S-C6	2.58	110.00	106.94
31	J	103	LMT	O2'-C2'-C3'	-2.58	104.39	110.35
31	J	103	LMT	O1'-C1'-C2'	2.58	112.32	108.30
24	B	602	CLA	C6-C5-C3	2.58	120.21	113.45
26	b	619	BCR	C16-C15-C14	-2.58	118.20	123.47
32	D	409	LHG	C11-C10-C9	-2.57	101.36	114.42
24	B	617	CLA	CMC-C2C-C1C	2.57	128.96	125.04
29	z	101	LMG	C3-C4-C5	2.57	114.83	110.24
31	A	617	LMT	O3B-C3B-C4B	2.57	116.29	110.35
24	b	607	CLA	CMB-C2B-C3B	2.57	129.49	124.68
24	A	609	CLA	C4-C3-C5	2.57	119.59	115.27
38	a	418	HTG	O2-C2-C1	2.57	114.98	110.27
24	b	607	CLA	OBD-CAD-C3D	-2.57	123.72	127.98
24	b	611	CLA	C14-C13-C15	-2.57	102.00	111.29
24	B	602	CLA	C4C-C3C-C2C	-2.56	103.16	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CED-O2D-CGD	2.56	121.73	115.94
24	C	506	CLA	C3D-CAD-CBD	2.56	110.98	107.61
24	b	611	CLA	C1-C2-C3	-2.56	121.61	126.04
24	b	616	CLA	C6-C5-C3	-2.56	106.74	113.45
24	b	610	CLA	CED-O2D-CGD	2.56	121.72	115.94
26	B	618	BCR	C20-C21-C22	-2.56	123.66	127.31
38	c	530	HTG	O5-C5-C4	2.56	114.34	109.69
38	b	623	HTG	O5-C5-C4	2.55	114.33	109.69
40	c	518	DGD	O6E-C5E-C6E	2.55	112.78	106.44
29	B	621	LMG	O8-C28-O10	-2.55	117.15	123.59
24	b	604	CLA	OBD-CAD-C3D	-2.55	123.74	127.98
27	a	412	PL9	O2-C1-C2	-2.55	115.93	121.78
31	m	101	LMT	O2'-C2'-C1'	2.55	116.24	110.05
25	A	608	PHO	O2D-CGD-CBD	2.55	115.80	111.27
25	a	409	PHO	CED-O2D-CGD	2.55	121.70	115.94
38	b	623	HTG	C1-C2-C3	2.55	115.62	110.59
26	H	102	BCR	C19-C18-C17	-2.55	115.03	118.94
32	a	419	LHG	O7-C5-C4	2.54	117.61	108.40
32	d	411	LHG	O8-C23-O10	-2.54	117.18	123.59
40	H	103	DGD	O4E-C4E-C5E	2.54	115.61	109.30
26	c	527	BCR	C37-C22-C21	-2.54	119.36	122.92
24	b	604	CLA	C7-C6-C5	-2.54	106.46	113.36
24	B	611	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
28	h	105	SQD	O2-C2-C1	2.54	116.21	110.05
24	C	507	CLA	CMA-C3A-C4A	2.54	118.59	111.77
24	C	509	CLA	CMB-C2B-C3B	2.54	129.43	124.68
29	z	101	LMG	O1-C7-C8	2.54	117.02	110.90
24	b	616	CLA	C11-C10-C8	-2.54	107.72	115.92
38	b	624	HTG	O4-C4-C3	2.53	116.21	110.35
24	b	611	CLA	CHB-C4A-NA	2.53	128.01	124.51
40	d	408	DGD	C3G-C2G-C1G	-2.53	105.80	111.79
24	C	502	CLA	CMB-C2B-C3B	2.53	129.42	124.68
24	B	604	CLA	CAC-C3C-C4C	2.53	128.09	124.81
24	C	506	CLA	CMB-C2B-C3B	2.53	129.41	124.68
29	B	634	LMG	O8-C28-O10	-2.53	117.22	123.59
27	A	611	PL9	C27-C28-C29	-2.53	121.58	127.66
24	c	512	CLA	C2A-C1A-CHA	-2.52	119.44	123.86
26	c	527	BCR	C20-C21-C22	-2.52	123.71	127.31
28	a	424	SQD	O47-C45-C46	2.52	117.54	108.40
38	B	624	HTG	O5-C5-C4	-2.52	105.11	109.69
27	a	412	PL9	C37-C36-C34	-2.52	104.68	112.98
28	l	102	SQD	C26-C25-C24	-2.52	104.13	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	602	CLA	O1A-CGA-CBA	-2.52	113.90	123.73
24	c	503	CLA	CED-O2D-CGD	2.52	121.63	115.94
26	b	618	BCR	C20-C21-C22	-2.52	123.72	127.31
24	a	410	CLA	C16-C15-C13	2.51	124.03	115.92
31	t	103	LMT	C1-O1'-C1'	2.51	118.00	113.84
26	B	620	BCR	C23-C22-C21	-2.51	115.09	118.94
40	c	518	DGD	C3A-C2A-C1A	-2.51	104.50	113.62
31	t	103	LMT	C1'-C2'-C3'	2.51	115.22	110.00
24	B	612	CLA	C1-C2-C3	-2.51	121.71	126.04
24	d	403	CLA	C2A-C1A-CHA	-2.50	119.48	123.86
31	J	103	LMT	C1B-O1B-C4'	2.50	124.16	117.96
24	B	604	CLA	CHC-C1C-NC	-2.50	120.40	124.20
24	B	616	CLA	CHC-C1C-C2C	-2.50	119.80	126.72
25	a	409	PHO	CMB-C2B-C1B	2.50	128.92	125.06
26	B	618	BCR	C37-C22-C23	2.50	122.02	118.08
24	b	607	CLA	C3D-CAD-CBD	2.50	110.90	107.61
35	d	415	P6G	O16-C17-C18	-2.50	99.08	110.07
26	C	525	BCR	C15-C16-C17	-2.50	118.35	123.47
24	B	612	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
38	B	631	HTG	O5-C1-S1	2.50	115.79	109.82
24	B	613	CLA	C2A-C1A-CHA	-2.50	119.50	123.86
24	B	609	CLA	CAC-C3C-C4C	2.49	128.05	124.81
24	C	508	CLA	C7-C6-C5	-2.49	106.59	113.36
24	c	508	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
26	A	610	BCR	C15-C16-C17	-2.49	118.37	123.47
28	b	633	SQD	C45-O47-C7	2.49	123.93	117.79
29	B	621	LMG	C38-C37-C36	-2.49	101.78	114.42
24	a	410	CLA	CMC-C2C-C1C	2.49	128.83	125.04
40	c	516	DGD	C1D-O6D-C5D	-2.49	108.80	113.69
24	b	606	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
24	b	611	CLA	CAA-CBA-CGA	-2.49	105.98	113.25
24	B	608	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
24	b	617	CLA	CED-O2D-CGD	2.48	121.56	115.94
26	b	619	BCR	C8-C9-C10	-2.48	115.13	118.94
24	C	511	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
24	c	512	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
31	m	102	LMT	O1'-C1-C2	-2.48	100.88	109.56
26	K	101	BCR	C8-C9-C10	-2.48	115.14	118.94
24	C	509	CLA	O2A-CGA-CBA	2.48	119.69	111.91
26	T	102	BCR	C11-C12-C13	-2.48	119.46	126.42
40	C	516	DGD	C1D-O6D-C5D	-2.48	108.83	113.69
26	B	619	BCR	C38-C26-C25	-2.47	121.75	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CED-O2D-CGD	2.47	121.52	115.94
26	t	102	BCR	C7-C6-C5	-2.47	115.48	121.46
24	B	608	CLA	O2D-CGD-CBD	2.47	115.65	111.27
27	A	611	PL9	C22-C21-C19	-2.47	104.86	112.98
26	H	102	BCR	C30-C25-C26	-2.47	119.14	122.61
24	C	506	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
29	j	101	LMG	O8-C28-O10	-2.46	117.38	123.59
26	c	527	BCR	C8-C7-C6	-2.46	120.29	127.20
24	b	609	CLA	C11-C12-C13	-2.46	107.97	115.92
40	d	408	DGD	O6D-C1D-C2D	-2.46	105.14	110.35
24	C	512	CLA	CMB-C2B-C3B	2.46	129.28	124.68
24	C	501	CLA	CHC-C1C-C2C	-2.46	119.92	126.72
26	c	514	BCR	C33-C5-C6	-2.46	121.77	124.53
24	B	603	CLA	CAC-C3C-C4C	2.46	128.00	124.81
27	d	407	PL9	C40-C39-C38	-2.46	117.37	123.68
26	B	620	BCR	C2-C1-C6	2.46	114.26	110.48
25	A	608	PHO	C1-C2-C3	-2.45	121.80	126.04
28	h	105	SQD	O5-C1-C2	2.45	115.54	110.35
24	a	410	CLA	CMB-C2B-C3B	2.45	129.26	124.68
32	a	419	LHG	C25-C24-C23	-2.45	104.71	113.62
24	a	407	CLA	C4A-NA-C1A	-2.45	105.60	106.71
26	C	525	BCR	C16-C17-C18	-2.45	123.81	127.31
24	c	502	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
29	B	621	LMG	O10-C28-C29	-2.45	114.17	123.73
24	C	510	CLA	CHB-C4A-NA	2.45	127.90	124.51
38	H	101	HTG	C1-C2-C3	-2.45	105.75	110.59
24	b	604	CLA	C5-C3-C2	-2.45	116.16	121.12
40	C	518	DGD	C4D-C3D-C2D	-2.45	106.55	110.82
25	d	401	PHO	CHD-C4C-C3C	-2.45	119.52	124.49
24	b	615	CLA	CMB-C2B-C3B	2.45	129.25	124.68
24	b	614	CLA	O2A-CGA-CBA	2.45	119.58	111.91
24	B	617	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
24	b	615	CLA	C4C-C3C-C2C	-2.44	103.33	106.90
29	C	520	LMG	O4-C4-C5	2.44	115.36	109.30
24	C	510	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
24	d	404	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
24	c	510	CLA	CMB-C2B-C3B	2.44	129.25	124.68
24	C	502	CLA	C16-C17-C18	-2.44	104.48	115.98
29	B	634	LMG	O7-C10-O9	-2.44	117.81	123.70
24	a	407	CLA	C5-C3-C2	-2.44	116.19	121.12
38	b	632	HTG	O5-C1-C2	2.44	113.38	110.31
24	c	513	CLA	O2A-CGA-CBA	2.43	119.55	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	401	PHO	CHC-C1C-C2C	-2.43	119.61	125.73
24	b	608	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
24	C	506	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
24	a	410	CLA	O2D-CGD-CBD	2.43	115.58	111.27
24	d	405	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
25	D	401	PHO	C4A-NA-C1A	2.43	110.10	108.14
24	b	616	CLA	OBD-CAD-C3D	-2.43	123.95	127.98
24	a	407	CLA	O2A-CGA-O1A	-2.42	117.47	123.59
25	d	401	PHO	CED-O2D-CGD	2.42	121.42	115.94
24	C	513	CLA	CMC-C2C-C1C	2.42	128.72	125.04
26	T	102	BCR	C36-C18-C19	2.42	121.88	118.08
40	c	516	DGD	CDB-CCB-CBB	-2.42	102.16	114.42
24	B	602	CLA	C11-C10-C8	2.41	123.72	115.92
26	B	619	BCR	C32-C1-C6	-2.41	106.39	110.30
24	b	614	CLA	C17-C16-C15	-2.41	102.17	113.24
31	A	617	LMT	C1B-O5B-C5B	2.41	118.42	113.69
28	a	413	SQD	C45-O47-C7	-2.41	111.86	117.79
24	C	508	CLA	C1D-CHD-C4C	2.41	125.73	122.56
24	b	604	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
24	D	404	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
28	x	101	SQD	O9-S-O7	-2.41	105.62	113.95
29	C	526	LMG	C3-C4-C5	2.40	114.53	110.24
24	B	606	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
24	C	508	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
31	t	103	LMT	C1B-O5B-C5B	2.40	118.39	113.69
40	C	518	DGD	O1G-C1A-O1A	-2.39	117.55	123.59
31	b	622	LMT	C3'-C4'-C5'	2.39	116.41	110.93
24	c	504	CLA	C5-C3-C2	-2.39	116.29	121.12
24	D	405	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
28	b	633	SQD	O6-C44-C45	2.39	116.66	110.90
27	a	412	PL9	C15-C14-C16	2.39	119.28	115.27
24	b	605	CLA	CHC-C1C-C2C	-2.39	120.12	126.72
24	B	611	CLA	C5-C3-C2	-2.39	116.29	121.12
30	C	528	GOL	O1-C1-C2	-2.39	98.76	110.20
26	C	515	BCR	C32-C1-C6	-2.38	106.43	110.30
27	A	611	PL9	O2-C1-C2	-2.38	116.32	121.78
26	A	610	BCR	C28-C27-C26	-2.38	109.82	114.08
38	b	632	HTG	C6-C5-C4	-2.38	107.43	113.00
31	m	101	LMT	C1-O1'-C1'	2.38	117.79	113.84
24	a	407	CLA	C1B-CHB-C4A	-2.38	125.40	130.12
24	B	609	CLA	C11-C12-C13	-2.38	108.23	115.92
28	l	102	SQD	O9-S-O7	-2.38	105.72	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	417	SQD	O6-C1-C2	2.38	112.02	108.30
24	b	609	CLA	C5-C3-C2	-2.38	116.31	121.12
27	D	407	PL9	C53-C6-C1	2.38	119.85	114.99
26	c	515	BCR	C39-C30-C25	-2.38	106.44	110.30
31	M	101	LMT	O5B-C1B-C2B	-2.37	105.32	110.35
24	A	609	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
24	a	410	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
24	C	504	CLA	C5-C3-C2	-2.37	116.32	121.12
38	a	418	HTG	O3-C3-C2	2.37	115.83	110.35
26	b	620	BCR	C1-C6-C5	-2.37	119.28	122.61
31	a	401	LMT	O2'-C2'-C1'	2.37	115.80	110.05
24	a	408	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
24	b	610	CLA	C6-C5-C3	2.37	119.67	113.45
26	B	620	BCR	C31-C1-C6	-2.37	106.46	110.30
26	h	103	BCR	C16-C17-C18	-2.37	123.93	127.31
24	c	507	CLA	OBD-CAD-C3D	-2.37	124.05	127.98
38	b	631	HTG	O4-C4-C5	2.37	115.17	109.30
29	C	526	LMG	O9-C10-C11	-2.37	114.50	123.73
26	K	101	BCR	C15-C16-C17	-2.37	118.63	123.47
29	d	412	LMG	O1-C1-C2	2.36	112.00	108.30
25	d	401	PHO	C5-C3-C2	-2.36	116.33	121.12
24	C	510	CLA	O2D-CGD-CBD	2.36	115.47	111.27
24	C	513	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
24	b	606	CLA	CMB-C2B-C1B	2.36	132.09	128.46
38	b	631	HTG	C1-O5-C5	2.36	116.94	112.58
29	d	412	LMG	O3-C3-C4	2.36	115.81	110.35
38	h	101	HTG	C1-O5-C5	2.36	116.93	112.58
28	A	616	SQD	O47-C7-O49	-2.36	118.00	123.70
38	C	532	HTG	C4-C3-C2	-2.36	106.71	110.82
26	C	515	BCR	C8-C7-C6	-2.36	120.58	127.20
31	a	401	LMT	O5'-C1'-O1'	-2.36	104.39	109.97
24	B	604	CLA	CBC-CAC-C3C	-2.36	105.93	112.43
31	M	101	LMT	O5B-C5B-C4B	2.35	113.97	109.69
27	d	407	PL9	C51-C49-C48	2.35	129.45	122.65
26	c	527	BCR	C36-C18-C17	-2.35	119.63	122.92
29	B	634	LMG	C9-O8-C28	2.35	125.84	117.12
24	B	607	CLA	CED-O2D-CGD	2.35	121.26	115.94
24	B	608	CLA	OBD-CAD-C3D	-2.35	124.07	127.98
24	B	615	CLA	OBD-CAD-C3D	-2.35	124.08	127.98
24	c	501	CLA	C4C-C3C-C2C	-2.35	103.47	106.90
24	c	512	CLA	CBA-CAA-C2A	-2.35	106.93	113.86
28	b	633	SQD	C1-O5-C5	-2.35	109.08	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	411	BCR	C24-C23-C22	-2.35	122.69	126.23
26	D	406	BCR	C15-C16-C17	-2.35	118.67	123.47
24	C	511	CLA	CMB-C2B-C3B	2.35	129.07	124.68
41	E	113	HEM	CMB-C2B-C3B	2.35	129.07	124.68
24	C	505	CLA	C2A-C1A-CHA	-2.35	119.76	123.86
40	d	408	DGD	C4D-C3D-C2D	2.34	114.92	110.82
24	c	507	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
26	A	610	BCR	C15-C14-C13	-2.34	123.97	127.31
24	c	503	CLA	C7-C6-C5	-2.34	107.00	113.36
25	A	608	PHO	C1C-C2C-C3C	-2.34	103.82	106.51
28	a	413	SQD	O9-S-O7	-2.34	105.85	113.95
24	c	508	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
24	B	613	CLA	CMC-C2C-C1C	2.34	128.60	125.04
24	C	502	CLA	CHB-C4A-NA	2.34	127.75	124.51
29	c	519	LMG	C7-O1-C1	2.34	118.31	113.74
26	C	525	BCR	C37-C22-C21	-2.34	119.65	122.92
24	b	605	CLA	C3D-CAD-CBD	2.34	110.68	107.61
24	b	602	CLA	C4-C3-C5	2.34	119.20	115.27
24	C	506	CLA	C1-O2A-CGA	2.34	122.57	116.44
24	A	606	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
26	H	102	BCR	C28-C27-C26	2.33	118.25	114.08
29	d	412	LMG	O6-C5-C4	2.33	113.93	109.69
24	d	403	CLA	CAC-C3C-C4C	2.33	127.84	124.81
26	C	515	BCR	C2-C1-C6	2.33	114.07	110.48
27	a	412	PL9	C7-C8-C9	2.33	130.66	126.79
24	B	612	CLA	C11-C12-C13	-2.33	108.40	115.92
29	C	520	LMG	O8-C28-O10	-2.32	117.72	123.59
28	A	612	SQD	O4-C4-C3	-2.32	104.98	110.35
24	C	501	CLA	CMB-C2B-C3B	2.32	129.02	124.68
28	a	413	SQD	C46-C45-C44	2.32	117.28	111.79
24	B	603	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
26	c	514	BCR	C32-C1-C6	2.32	114.06	110.30
24	B	605	CLA	CED-O2D-CGD	2.32	121.18	115.94
24	c	513	CLA	C4C-C3C-C2C	-2.32	103.52	106.90
31	I	101	LMT	C1B-O5B-C5B	2.32	118.24	113.69
26	c	515	BCR	C15-C16-C17	-2.32	118.73	123.47
24	b	607	CLA	C2A-C3A-C4A	2.32	105.61	101.87
28	A	622	SQD	O47-C7-C8	2.32	116.49	111.50
24	c	508	CLA	CMB-C2B-C3B	2.32	129.01	124.68
24	B	605	CLA	CHB-C4A-NA	2.32	127.71	124.51
24	C	513	CLA	CED-O2D-CGD	2.32	121.17	115.94
24	c	505	CLA	CAA-C2A-C1A	2.31	119.56	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	608	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
24	B	605	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
38	H	101	HTG	C2'-C1'-S1	-2.31	104.94	112.40
26	T	102	BCR	C31-C1-C6	2.31	114.05	110.30
28	l	102	SQD	O47-C7-O49	-2.31	118.12	123.70
26	b	619	BCR	C34-C9-C10	2.31	126.16	122.92
30	b	627	GOL	O3-C3-C2	2.31	121.27	110.20
24	C	504	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
38	c	531	HTG	O2-C2-C3	2.31	115.69	110.35
26	B	618	BCR	C15-C14-C13	-2.31	124.02	127.31
26	t	102	BCR	C40-C30-C25	2.31	114.04	110.30
24	c	513	CLA	O2D-CGD-CBD	2.31	115.37	111.27
24	B	603	CLA	C1C-C2C-C3C	-2.30	104.53	106.96
38	C	532	HTG	O2-C2-C1	2.30	114.50	110.27
24	D	403	CLA	CMC-C2C-C1C	2.30	128.54	125.04
24	A	607	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	B	610	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
26	C	514	BCR	C29-C30-C25	2.30	114.02	110.48
24	b	614	CLA	CMB-C2B-C3B	2.30	128.98	124.68
24	D	404	CLA	CED-O2D-CGD	2.30	121.14	115.94
27	d	407	PL9	C36-C37-C38	-2.30	104.33	111.88
25	A	608	PHO	CHD-C1D-ND	-2.30	119.80	124.58
24	C	512	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
24	c	511	CLA	CHC-C1C-C2C	-2.30	120.37	126.72
26	B	618	BCR	C34-C9-C10	-2.30	119.71	122.92
40	h	104	DGD	O4D-C4D-C3D	-2.29	105.05	110.35
24	b	602	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
26	C	514	BCR	C37-C22-C23	2.29	121.69	118.08
27	d	407	PL9	C7-C3-C4	2.29	118.74	116.88
24	C	510	CLA	C6-C5-C3	2.29	119.46	113.45
26	K	101	BCR	C21-C20-C19	-2.29	116.07	123.22
24	D	403	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
28	a	424	SQD	O47-C7-O49	-2.29	118.17	123.70
28	b	633	SQD	O2-C2-C3	2.29	115.64	110.35
24	b	602	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
28	l	102	SQD	C45-O47-C7	-2.29	112.16	117.79
26	c	527	BCR	C23-C24-C25	-2.29	120.78	127.20
38	H	101	HTG	O2-C2-C1	2.29	114.47	110.27
25	a	409	PHO	CHC-C1C-C2C	-2.29	119.98	125.73
29	z	101	LMG	O1-C1-C2	2.29	111.87	108.30
24	C	513	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
31	A	617	LMT	O5B-C1B-C2B	2.29	115.19	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	B	630	HTG	O5-C1-C2	-2.28	107.44	110.31
38	O	303	HTG	O5-C1-C2	-2.28	107.44	110.31
30	a	415	GOL	O1-C1-C2	2.28	121.15	110.20
24	c	504	CLA	OBD-CAD-C3D	-2.28	124.19	127.98
27	a	412	PL9	C20-C19-C21	2.28	119.11	115.27
32	B	632	LHG	O3-P-O5	-2.28	100.16	109.07
29	C	520	LMG	O6-C5-C6	2.28	112.11	106.44
24	b	617	CLA	C4A-NA-C1A	-2.28	105.68	106.71
24	B	605	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
29	c	519	LMG	C3-C4-C5	2.28	114.30	110.24
24	b	603	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
24	c	505	CLA	C1D-CHD-C4C	2.28	125.56	122.56
38	B	630	HTG	O5-C1-S1	2.28	115.27	109.82
24	b	617	CLA	C1-O2A-CGA	2.28	122.42	116.44
24	c	510	CLA	CMC-C2C-C1C	2.28	128.50	125.04
24	A	606	CLA	CHB-C4A-NA	2.28	127.66	124.51
26	b	619	BCR	C24-C25-C26	2.28	126.97	121.46
24	b	602	CLA	O2A-CGA-CBA	2.27	119.05	111.91
28	F	104	SQD	O47-C7-C8	2.27	116.40	111.50
24	b	610	CLA	CMC-C2C-C1C	2.27	128.50	125.04
38	b	632	HTG	C1-C2-C3	2.27	115.08	110.59
24	c	509	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
24	c	504	CLA	CAC-C3C-C4C	2.27	127.76	124.81
38	B	630	HTG	O2-C2-C3	2.27	115.60	110.35
24	B	615	CLA	CHC-C1C-C2C	-2.27	120.44	126.72
24	C	502	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
24	c	507	CLA	CMB-C2B-C3B	2.27	128.93	124.68
24	C	507	CLA	O2A-CGA-CBA	2.27	119.03	111.91
24	D	403	CLA	CMB-C2B-C3B	2.27	128.92	124.68
39	V	217	1PE	OH3-C22-C12	2.27	120.03	110.07
31	J	103	LMT	C1'-C2'-C3'	2.27	114.72	110.00
24	c	507	CLA	C4-C3-C5	2.27	119.08	115.27
24	C	511	CLA	CED-O2D-CGD	2.27	121.06	115.94
27	D	407	PL9	C22-C23-C24	-2.26	122.21	127.66
24	C	509	CLA	CMD-C2D-C3D	-2.26	120.44	124.68
24	D	405	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
24	b	602	CLA	O2A-C1-C2	2.26	114.58	108.64
26	B	618	BCR	C8-C9-C10	2.26	122.41	118.94
24	c	501	CLA	CAC-C3C-C4C	2.26	127.74	124.81
24	B	610	CLA	C3A-C2A-C1A	-2.26	97.95	101.34
24	b	613	CLA	C11-C12-C13	-2.26	108.61	115.92
24	C	505	CLA	CHC-C1C-NC	-2.26	120.78	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	D	402	GOL	O2-C2-C1	-2.26	99.17	109.12
26	b	618	BCR	C34-C9-C10	-2.26	119.76	122.92
26	d	406	BCR	C23-C24-C25	-2.26	120.86	127.20
27	A	611	PL9	C21-C19-C18	-2.26	116.55	121.12
26	k	101	BCR	C34-C9-C10	2.26	126.08	122.92
30	B	625	GOL	O2-C2-C1	2.25	119.05	109.12
28	F	104	SQD	C46-O48-C23	2.25	125.47	117.12
24	d	404	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
27	a	412	PL9	C22-C21-C19	-2.25	105.56	112.98
24	D	403	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
41	E	113	HEM	CMD-C2D-C1D	2.25	131.93	128.46
24	b	604	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
43	v	202	HEC	CMB-C2B-C3B	-2.25	123.17	125.82
24	B	605	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	a	407	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
26	K	101	BCR	C23-C24-C25	-2.25	120.88	127.20
24	d	404	CLA	CHC-C1C-C2C	-2.25	120.50	126.72
24	d	404	CLA	C5-C3-C2	-2.25	116.56	121.12
26	B	619	BCR	C15-C16-C17	-2.25	118.87	123.47
24	c	505	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
38	C	531	HTG	O2-C2-C1	2.24	114.39	110.27
38	B	630	HTG	C1-O5-C5	2.24	116.72	112.58
24	C	511	CLA	C1-O2A-CGA	2.24	122.33	116.44
24	b	615	CLA	OBD-CAD-C3D	-2.24	124.26	127.98
32	a	419	LHG	O7-C7-O9	-2.24	118.29	123.70
24	b	611	CLA	C20-C18-C19	-2.24	100.19	110.51
24	b	605	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
24	C	510	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
40	C	516	DGD	O3G-C3G-C2G	-2.24	105.50	110.90
24	b	611	CLA	CHC-C1C-C2C	-2.24	120.54	126.72
26	B	620	BCR	C20-C21-C22	-2.24	124.12	127.31
26	t	102	BCR	C1-C6-C7	2.23	122.10	115.78
24	c	510	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
32	E	101	LHG	O7-C7-O9	-2.23	118.31	123.70
26	T	102	BCR	C15-C16-C17	-2.23	118.90	123.47
29	B	621	LMG	C1-O6-C5	-2.23	109.31	113.69
24	c	503	CLA	CHC-C1C-C2C	-2.23	120.55	126.72
28	A	612	SQD	O48-C23-O10	-2.23	117.96	123.59
28	b	633	SQD	C1-C2-C3	-2.23	105.35	110.00
24	c	511	CLA	C5-C3-C2	-2.23	116.60	121.12
24	B	607	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
28	x	101	SQD	O8-S-O7	-2.23	105.83	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	C1C-C2C-C3C	-2.23	104.61	106.96
24	c	511	CLA	C11-C10-C8	-2.23	108.72	115.92
31	c	521	LMT	O4'-C4B-C3B	2.23	115.50	110.35
24	b	602	CLA	C4-C3-C2	-2.23	117.97	123.68
38	b	623	HTG	C1-O5-C5	2.23	116.69	112.58
40	C	516	DGD	C1G-O1G-C1A	2.23	125.37	117.12
24	b	614	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
26	c	515	BCR	C36-C18-C19	2.23	121.58	118.08
24	B	617	CLA	CHC-C1C-C2C	-2.23	120.57	126.72
24	B	606	CLA	O2D-CGD-CBD	2.22	115.22	111.27
43	V	203	HEC	CMB-C2B-C3B	2.22	128.43	125.82
30	B	628	GOL	C3-C2-C1	2.22	120.34	111.70
26	B	620	BCR	C11-C10-C9	-2.22	124.14	127.31
29	C	526	LMG	O8-C28-C29	2.22	118.87	111.91
26	c	527	BCR	C29-C30-C25	2.22	113.89	110.48
24	B	610	CLA	CHC-C1C-C2C	-2.22	120.59	126.72
24	B	611	CLA	CAA-CBA-CGA	-2.22	106.78	113.25
40	c	518	DGD	C6B-C5B-C4B	-2.21	103.18	114.42
24	B	607	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
24	d	403	CLA	CMB-C2B-C3B	2.21	128.82	124.68
26	t	102	BCR	C19-C18-C17	-2.21	115.55	118.94
28	a	424	SQD	O8-S-O7	-2.21	105.87	111.27
24	c	502	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
24	B	609	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
24	c	509	CLA	CMB-C2B-C3B	2.21	128.81	124.68
24	b	606	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
24	D	404	CLA	C4C-C3C-C2C	-2.21	103.68	106.90
24	B	602	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
26	d	406	BCR	C10-C11-C12	-2.21	116.33	123.22
31	c	521	LMT	O1B-C1B-C2B	2.20	113.81	108.10
31	t	103	LMT	O3B-C3B-C4B	-2.20	105.25	110.35
24	c	508	CLA	CHC-C1C-C2C	-2.20	120.63	126.72
24	D	403	CLA	C4A-NA-C1A	-2.20	105.72	106.71
32	D	411	LHG	O8-C23-O10	-2.20	118.03	123.59
32	D	411	LHG	O7-C7-O9	-2.20	118.38	123.70
24	c	509	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
30	b	625	GOL	O2-C2-C1	2.20	118.82	109.12
24	C	508	CLA	CMC-C2C-C1C	2.20	128.39	125.04
38	V	204	HTG	O5-C5-C6	2.20	111.90	106.44
24	B	605	CLA	C1D-CHD-C4C	2.20	125.46	122.56
24	B	615	CLA	C4-C3-C5	2.20	118.97	115.27
24	A	609	CLA	CMB-C2B-C3B	2.20	128.79	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	612	CLA	C4C-C3C-C2C	-2.20	103.69	106.90
24	b	613	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
24	B	605	CLA	CMC-C2C-C1C	2.19	128.38	125.04
25	a	409	PHO	CHD-C4C-C3C	-2.19	120.03	124.49
29	C	526	LMG	C9-C8-C7	-2.19	106.60	111.79
24	b	617	CLA	CMC-C2C-C1C	2.19	128.38	125.04
38	B	630	HTG	O3-C3-C4	-2.19	105.28	110.35
24	B	614	CLA	C7-C6-C5	-2.19	107.41	113.36
24	a	407	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
32	B	632	LHG	O8-C23-O10	-2.19	118.06	123.59
31	B	622	LMT	O1B-C4'-C3'	2.19	113.11	107.28
24	c	503	CLA	CAC-C3C-C4C	2.19	127.65	124.81
24	d	404	CLA	CED-O2D-CGD	2.19	120.89	115.94
26	c	514	BCR	C36-C18-C19	2.19	121.53	118.08
31	c	521	LMT	O5'-C1'-O1'	-2.19	104.79	109.97
40	c	518	DGD	O3G-C3G-C2G	-2.19	105.62	110.90
24	C	504	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
25	a	409	PHO	C4A-NA-C1A	2.19	109.91	108.14
24	C	504	CLA	CAC-C3C-C4C	2.19	127.65	124.81
26	H	102	BCR	C15-C14-C13	2.19	130.43	127.31
24	B	610	CLA	CBC-CAC-C3C	-2.19	106.41	112.43
24	c	506	CLA	C3D-CAD-CBD	2.19	110.48	107.61
29	J	101	LMG	O6-C1-C2	2.18	114.97	110.35
24	B	617	CLA	C5-C3-C2	2.18	125.54	121.12
24	c	505	CLA	O2D-CGD-CBD	2.18	115.15	111.27
25	a	409	PHO	C2D-C1D-ND	2.18	113.08	109.79
24	a	410	CLA	CHC-C1C-C2C	-2.18	120.69	126.72
24	c	506	CLA	CMB-C2B-C3B	2.18	128.76	124.68
26	d	406	BCR	C4-C5-C6	2.18	125.90	122.73
24	C	504	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
28	b	633	SQD	O4-C4-C3	2.18	115.38	110.35
24	B	608	CLA	CHC-C1C-C2C	-2.18	120.70	126.72
28	A	612	SQD	O3-C3-C4	2.18	115.38	110.35
40	C	518	DGD	O3E-C3E-C4E	-2.18	105.32	110.35
26	c	514	BCR	C38-C26-C25	-2.18	122.08	124.53
24	C	501	CLA	C4C-C3C-C2C	-2.17	103.73	106.90
26	c	514	BCR	C12-C13-C14	-2.17	115.61	118.94
24	A	606	CLA	CMC-C2C-C1C	2.17	128.35	125.04
24	b	609	CLA	C6-C7-C8	-2.17	108.90	115.92
24	C	505	CLA	O2A-C1-C2	-2.17	102.93	108.64
26	d	406	BCR	C15-C16-C17	-2.17	119.03	123.47
24	A	606	CLA	CHD-C4C-C3C	-2.17	121.65	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	519	LMG	C6-C5-C4	-2.17	107.92	113.00
40	h	104	DGD	C6D-C5D-C4D	2.17	116.62	112.09
29	B	634	LMG	C1-O6-C5	2.17	117.94	113.69
26	b	618	BCR	C35-C13-C12	2.17	121.49	118.08
32	A	618	LHG	C6-O8-C23	2.17	125.14	117.12
38	c	531	HTG	O5-C1-C2	-2.17	107.59	110.31
30	t	101	GOL	C3-C2-C1	2.16	120.12	111.70
38	c	531	HTG	O3-C3-C2	2.16	115.34	110.35
24	B	606	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
24	D	404	CLA	CAC-C3C-C4C	2.16	127.61	124.81
24	c	508	CLA	CHB-C4A-NA	2.16	127.50	124.51
26	b	619	BCR	C24-C23-C22	-2.16	122.98	126.23
24	B	613	CLA	C1C-C2C-C3C	-2.16	104.69	106.96
38	c	531	HTG	C4-C3-C2	-2.16	107.06	110.82
40	D	408	DGD	C1D-O6D-C5D	-2.16	109.46	113.69
24	b	612	CLA	C7-C6-C5	-2.16	107.50	113.36
24	C	508	CLA	C4A-NA-C1A	-2.16	105.74	106.71
24	C	512	CLA	O2A-CGA-CBA	2.15	118.67	111.91
24	C	512	CLA	C17-C16-C15	-2.15	103.34	113.24
24	b	609	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
24	a	408	CLA	CMB-C2B-C3B	2.15	128.71	124.68
24	b	612	CLA	CHB-C4A-NA	2.15	127.49	124.51
24	B	609	CLA	CHC-C1C-C2C	-2.15	120.77	126.72
31	c	521	LMT	O5'-C1'-C2'	2.15	114.90	110.35
31	c	521	LMT	C3'-C4'-C5'	-2.15	106.00	110.93
24	C	512	CLA	C1C-C2C-C3C	-2.15	104.70	106.96
24	c	506	CLA	C16-C17-C18	2.15	126.11	115.98
26	D	406	BCR	C10-C11-C12	-2.15	116.51	123.22
40	H	103	DGD	C6E-C5E-C4E	2.15	118.03	113.00
24	b	615	CLA	C1-O2A-CGA	2.15	122.08	116.44
34	O	309	PGE	C5-O3-C4	2.15	122.59	113.29
26	c	514	BCR	C15-C14-C13	-2.15	124.25	127.31
26	c	527	BCR	C15-C16-C17	-2.14	119.08	123.47
27	D	407	PL9	C20-C19-C21	2.14	118.88	115.27
38	C	522	HTG	O5-C5-C4	2.14	113.58	109.69
26	A	610	BCR	C23-C24-C25	-2.14	121.19	127.20
32	E	101	LHG	O8-C23-O10	-2.14	118.19	123.59
38	B	624	HTG	O2-C2-C3	-2.14	105.40	110.35
32	e	101	LHG	O7-C7-O9	-2.14	118.53	123.70
27	A	611	PL9	C8-C7-C3	2.14	118.02	111.98
32	B	632	LHG	C6-C5-C4	-2.14	106.73	111.79
25	A	608	PHO	CBA-CAA-C2A	-2.14	107.55	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	j	101	LMG	O2-C2-C1	-2.14	104.85	110.05
31	I	101	LMT	C4B-C3B-C2B	2.14	114.55	110.82
24	b	614	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
24	c	508	CLA	CMC-C2C-C1C	2.13	128.29	125.04
29	B	634	LMG	O2-C2-C3	-2.13	105.41	110.35
26	C	515	BCR	C4-C5-C6	-2.13	119.63	122.73
26	D	406	BCR	C24-C25-C26	2.13	126.63	121.46
24	C	505	CLA	C3D-CAD-CBD	2.13	110.42	107.61
31	A	617	LMT	O1B-C1B-O5B	-2.13	104.71	110.67
28	l	102	SQD	O8-S-O9	-2.13	106.06	111.27
24	c	507	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
24	B	606	CLA	CMB-C2B-C3B	2.13	128.67	124.68
32	d	411	LHG	O7-C7-C8	2.13	116.09	111.50
25	D	401	PHO	CMC-C2C-C1C	2.13	128.34	125.06
26	A	610	BCR	C37-C22-C21	-2.13	119.94	122.92
24	C	510	CLA	C6-C7-C8	-2.13	109.03	115.92
24	B	603	CLA	CAC-C3C-C2C	2.13	131.17	127.53
24	C	512	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
38	c	531	HTG	O5-C5-C6	2.13	111.73	106.44
24	B	610	CLA	CHC-C1C-NC	-2.13	120.97	124.20
40	c	518	DGD	O1G-C1A-C2A	2.13	118.58	111.91
24	d	404	CLA	OBD-CAD-C3D	-2.13	124.45	127.98
25	D	401	PHO	C1C-C2C-C3C	-2.13	104.07	106.51
31	u	203	LMT	O2B-C2B-C1B	2.12	115.21	110.05
24	A	606	CLA	C7-C6-C5	-2.12	107.59	113.36
24	B	611	CLA	O2A-CGA-CBA	2.12	118.56	111.91
24	c	504	CLA	C6-C7-C8	-2.12	109.07	115.92
28	A	622	SQD	O6-C44-C45	-2.12	105.79	110.90
30	c	529	GOL	O3-C3-C2	-2.12	100.06	110.20
24	b	607	CLA	C1-O2A-CGA	2.11	121.99	116.44
32	d	409	LHG	C11-C10-C9	-2.11	103.69	114.42
40	C	516	DGD	CDB-CCB-CBB	-2.11	103.69	114.42
24	c	513	CLA	OBD-CAD-C3D	-2.11	124.47	127.98
38	V	204	HTG	O4-C4-C3	2.11	115.23	110.35
24	B	617	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
24	A	606	CLA	CMD-C2D-C3D	2.11	128.63	124.68
24	B	606	CLA	CHC-C1C-NC	-2.11	121.00	124.20
24	B	604	CLA	CED-O2D-CGD	2.11	120.71	115.94
24	a	408	CLA	CED-O2D-CGD	2.11	120.71	115.94
24	b	617	CLA	CHB-C4A-NA	2.11	127.43	124.51
24	C	504	CLA	CHD-C4C-C3C	-2.11	121.74	124.84
31	I	101	LMT	O6B-C6B-C5B	2.11	118.52	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	c	530	HTG	C1-O5-C5	2.11	116.47	112.58
31	A	617	LMT	O2B-C2B-C3B	-2.11	105.48	110.35
40	H	103	DGD	C1D-O6D-C5D	-2.11	109.55	113.69
24	B	616	CLA	OBD-CAD-C3D	-2.11	124.48	127.98
24	B	604	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
24	C	509	CLA	C16-C17-C18	-2.11	106.05	115.98
24	c	506	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
24	c	510	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
31	m	101	LMT	O1'-C1'-C2'	2.10	111.59	108.30
40	H	103	DGD	C3D-C4D-C5D	-2.10	106.49	110.24
26	b	619	BCR	C7-C8-C9	-2.10	123.06	126.23
28	x	101	SQD	O47-C7-O49	-2.10	118.62	123.70
24	C	503	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
24	c	506	CLA	CHC-C1C-C2C	-2.10	120.91	126.72
26	K	101	BCR	C10-C11-C12	-2.10	116.66	123.22
26	K	101	BCR	C36-C18-C17	-2.10	119.98	122.92
31	M	101	LMT	C2'-C3'-C4'	2.10	114.48	109.68
27	A	611	PL9	C25-C24-C26	2.10	118.80	115.27
24	b	604	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
43	v	202	HEC	CBA-CAA-C2A	-2.10	108.61	112.48
35	I	106	P6G	C17-O16-C15	2.10	122.38	113.29
24	d	405	CLA	CGD-CBD-CAD	-2.10	103.94	110.73
28	x	101	SQD	O48-C23-O10	-2.10	118.30	123.59
24	C	506	CLA	CHB-C4A-NA	2.10	127.41	124.51
24	c	502	CLA	CMB-C2B-C3B	2.10	128.60	124.68
24	c	502	CLA	C4C-C3C-C2C	-2.10	103.84	106.90
31	u	203	LMT	O2'-C2'-C1'	2.09	115.13	110.05
25	A	608	PHO	CMC-C2C-C1C	2.09	128.29	125.06
24	c	506	CLA	O1D-CGD-CBD	2.09	128.77	124.48
32	B	632	LHG	C9-C8-C7	-2.09	106.01	113.62
24	b	603	CLA	C16-C17-C18	-2.09	106.12	115.98
26	c	514	BCR	C8-C7-C6	-2.09	121.33	127.20
38	O	303	HTG	C1'-S1-C1	2.09	104.00	100.09
31	m	102	LMT	O5'-C5'-C6'	2.09	111.64	106.44
28	F	104	SQD	C44-O6-C1	2.09	117.82	113.74
26	D	406	BCR	C8-C7-C6	-2.09	121.33	127.20
24	A	609	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
26	C	525	BCR	C33-C5-C6	-2.09	122.18	124.53
32	d	410	LHG	O2-C2-C1	-2.09	99.92	109.12
38	B	630	HTG	O4-C4-C5	2.09	114.48	109.30
40	H	103	DGD	O2G-C1B-C2B	2.09	116.00	111.50
43	v	202	HEC	C3C-C4C-NC	-2.09	107.00	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C6-C7-C8	-2.09	109.18	115.92
26	A	610	BCR	C35-C13-C14	2.09	125.84	122.92
38	B	623	HTG	C1-O5-C5	2.08	116.42	112.58
25	a	409	PHO	C2B-C1B-NB	2.08	112.93	109.79
24	b	607	CLA	CAA-C2A-C1A	2.08	118.79	111.97
31	t	103	LMT	O1B-C4'-C3'	2.08	112.81	107.28
24	c	511	CLA	O2A-C1-C2	-2.08	103.17	108.64
24	c	511	CLA	C4-C3-C5	2.08	118.77	115.27
32	a	419	LHG	O8-C23-C24	2.08	118.43	111.91
25	D	401	PHO	OBD-CAD-C3D	-2.08	123.52	128.52
24	C	511	CLA	C3A-C2A-C1A	2.08	104.45	101.34
24	c	508	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
28	F	104	SQD	C1-O5-C5	-2.08	109.61	113.69
24	A	609	CLA	CHC-C1C-C2C	-2.08	120.98	126.72
24	c	505	CLA	C16-C15-C13	-2.08	109.21	115.92
27	d	407	PL9	C12-C13-C14	-2.08	122.66	127.66
24	b	616	CLA	CHC-C1C-C2C	-2.07	120.98	126.72
24	c	504	CLA	OBD-CAD-CBD	2.07	128.86	125.89
24	b	615	CLA	C20-C18-C19	2.07	120.07	110.51
26	h	103	BCR	C36-C18-C17	-2.07	120.02	122.92
24	b	610	CLA	C4A-NA-C1A	-2.07	105.77	106.71
24	c	503	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
24	b	613	CLA	O2A-CGA-CBA	2.07	118.41	111.91
24	B	602	CLA	C7-C6-C5	2.07	118.98	113.36
25	D	401	PHO	CHD-C4C-C3C	-2.07	120.28	124.49
24	A	609	CLA	CAC-C3C-C4C	2.07	127.50	124.81
32	e	101	LHG	O8-C23-O10	-2.07	118.37	123.59
24	B	605	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
26	k	101	BCR	C1-C6-C7	2.07	121.63	115.78
26	b	619	BCR	C11-C10-C9	-2.07	124.36	127.31
31	Y	101	LMT	C1B-O1B-C4'	2.07	123.08	117.96
24	C	501	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	c	508	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
28	a	424	SQD	C45-O47-C7	2.06	122.86	117.79
31	c	521	LMT	O6B-C6B-C5B	2.06	118.35	111.29
31	c	521	LMT	C1'-O5'-C5'	2.06	117.73	113.69
27	a	412	PL9	C36-C34-C33	-2.06	116.95	121.12
32	d	409	LHG	C27-C26-C25	-2.06	103.98	114.42
27	A	611	PL9	C20-C19-C21	2.06	118.73	115.27
43	v	202	HEC	CMC-C2C-C3C	2.06	128.24	125.82
24	c	512	CLA	OBD-CAD-C3D	-2.06	124.57	127.98
24	b	606	CLA	C1D-CHD-C4C	2.06	125.27	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	409	PHO	CAC-C3C-C2C	2.05	131.04	127.53
26	a	411	BCR	C39-C30-C25	-2.05	106.97	110.30
24	B	602	CLA	C1-O2A-CGA	2.05	121.83	116.44
26	T	102	BCR	C7-C6-C5	-2.05	116.49	121.46
26	c	515	BCR	C20-C19-C18	-2.05	120.66	126.42
29	b	621	LMG	C4-C3-C2	-2.05	107.24	110.82
26	d	406	BCR	C16-C15-C14	-2.05	119.28	123.47
24	a	408	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
26	k	101	BCR	C1-C6-C5	-2.05	119.73	122.61
28	l	102	SQD	O9-S-C6	2.05	109.37	106.94
31	Y	101	LMT	C4B-C3B-C2B	2.04	114.39	110.82
26	h	103	BCR	C28-C27-C26	2.04	117.73	114.08
40	c	518	DGD	O1G-C1A-O1A	-2.04	118.43	123.59
31	m	101	LMT	C3B-C4B-C5B	2.04	113.89	110.24
24	B	605	CLA	CHC-C1C-C2C	-2.04	121.07	126.72
24	d	403	CLA	CHB-C4A-NA	2.04	127.34	124.51
26	K	101	BCR	C34-C9-C10	2.04	125.78	122.92
24	B	606	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	c	520	LMG	O8-C28-O10	-2.04	118.44	123.59
24	b	602	CLA	CMB-C2B-C1B	2.04	131.60	128.46
24	b	617	CLA	OBD-CAD-C3D	-2.04	124.59	127.98
34	O	308	PGE	O3-C5-C6	2.04	119.04	110.07
24	a	407	CLA	C7-C6-C5	-2.04	107.82	113.36
29	C	520	LMG	C9-O8-C28	2.04	124.67	117.12
24	c	512	CLA	CMB-C2B-C3B	2.04	128.49	124.68
24	C	513	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
24	c	511	CLA	C4D-C3D-CAD	-2.04	107.33	108.47
28	F	104	SQD	O2-C2-C3	2.04	115.05	110.35
24	c	511	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
25	a	409	PHO	CAA-CBA-CGA	-2.03	107.31	113.25
40	C	516	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
24	c	508	CLA	C1D-CHD-C4C	2.03	125.24	122.56
24	c	502	CLA	C1-C2-C3	-2.03	122.53	126.04
24	C	504	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
24	b	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
26	C	514	BCR	C32-C1-C31	2.03	114.76	108.53
26	d	406	BCR	C2-C1-C6	2.03	113.61	110.48
24	b	607	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	A	607	CLA	C1-C2-C3	2.03	129.55	126.04
26	d	406	BCR	C34-C9-C10	-2.03	120.08	122.92
26	T	102	BCR	C35-C13-C12	2.03	121.27	118.08
31	f	101	LMT	C6'-C5'-C4'	-2.03	107.43	113.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	C1D-CHD-C4C	2.03	125.23	122.56
30	d	402	GOL	O2-C2-C1	-2.02	100.20	109.12
29	B	634	LMG	O7-C8-C9	2.02	115.73	108.40
40	H	103	DGD	C6D-C5D-C4D	2.02	116.32	112.09
28	A	616	SQD	O2-C2-C3	2.02	115.03	110.35
38	c	523	HTG	C3-C4-C5	2.02	113.85	110.24
24	c	503	CLA	C4C-C3C-C2C	-2.02	103.95	106.90
30	O	306	GOL	C3-C2-C1	-2.02	103.84	111.70
24	C	511	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	b	613	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
38	a	418	HTG	O5-C5-C4	2.02	113.37	109.69
31	B	622	LMT	O5B-C5B-C6B	2.02	111.46	106.44
26	k	101	BCR	C21-C20-C19	-2.02	116.91	123.22
24	C	511	CLA	CHC-C1C-C2C	-2.02	121.13	126.72
24	c	511	CLA	C1-O2A-CGA	2.02	121.74	116.44
28	F	104	SQD	O48-C23-O10	-2.02	118.50	123.59
25	d	401	PHO	C3D-C2D-C1D	-2.02	102.93	105.87
38	c	523	HTG	C1-O5-C5	2.02	116.30	112.58
31	c	521	LMT	O1'-C1'-C2'	2.02	111.45	108.30
28	a	413	SQD	O2-C2-C1	2.02	114.94	110.05
31	m	101	LMT	O1B-C1B-C2B	2.02	113.32	108.10
28	A	616	SQD	C4-C3-C2	-2.01	107.31	110.82
24	B	612	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
28	b	633	SQD	O2-C2-C1	2.01	114.94	110.05
24	b	609	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
24	b	606	CLA	O2A-C1-C2	-2.01	103.34	108.64
24	A	606	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
24	B	614	CLA	C3D-CAD-CBD	2.01	110.25	107.61
24	b	611	CLA	C3D-CAD-CBD	2.01	110.25	107.61
26	t	102	BCR	C32-C1-C6	-2.01	107.04	110.30
29	B	621	LMG	O5-C6-C5	-2.01	104.39	111.29
24	c	513	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
26	C	525	BCR	C11-C10-C9	-2.01	124.44	127.31
25	a	409	PHO	C7-C6-C5	-2.01	107.90	113.36
24	B	611	CLA	C3A-C2A-C1A	-2.01	98.33	101.34
24	c	507	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
24	C	509	CLA	O2D-CGD-CBD	2.01	114.83	111.27
29	a	414	LMG	O1-C1-C2	2.00	111.43	108.30
24	B	616	CLA	C9-C8-C7	-2.00	104.03	111.29
32	a	419	LHG	C6-O8-C23	2.00	124.54	117.12
35	D	417	P6G	O7-C8-C9	-2.00	101.37	110.39
24	C	503	CLA	CHB-C4A-NA	2.00	127.28	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	621	LMG	C39-C38-C37	-2.00	104.27	114.42
24	b	615	CLA	C5-C3-C2	-2.00	117.07	121.12
24	d	403	CLA	C5-C3-C2	-2.00	117.07	121.12
32	D	411	LHG	O7-C7-C8	2.00	115.81	111.50

All (207) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	606	CLA	NA
24	A	606	CLA	ND
24	A	606	CLA	NC
24	A	607	CLA	NA
24	A	607	CLA	ND
24	A	607	CLA	NC
24	A	609	CLA	NA
24	A	609	CLA	ND
24	A	609	CLA	NC
24	B	602	CLA	NA
24	B	602	CLA	ND
24	B	602	CLA	NC
24	B	603	CLA	NA
24	B	603	CLA	ND
24	B	603	CLA	NC
24	B	604	CLA	NA
24	B	604	CLA	NC
24	B	604	CLA	ND
24	B	605	CLA	NA
24	B	605	CLA	ND
24	B	605	CLA	NC
24	B	606	CLA	NA
24	B	606	CLA	ND
24	B	606	CLA	NC
24	B	607	CLA	NA
24	B	607	CLA	ND
24	B	607	CLA	NC
24	B	608	CLA	NA
24	B	608	CLA	ND
24	B	608	CLA	NC
24	B	609	CLA	NA
24	B	609	CLA	ND
24	B	609	CLA	NC
24	B	610	CLA	NA

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Mol	Chain	Res	Type	Atom
24	B	610	CLA	ND
24	B	610	CLA	NC
24	B	611	CLA	NA
24	B	611	CLA	ND
24	B	611	CLA	NC
24	B	612	CLA	NA
24	B	612	CLA	ND
24	B	612	CLA	NC
24	B	613	CLA	NA
24	B	613	CLA	ND
24	B	613	CLA	NC
24	B	614	CLA	NA
24	B	614	CLA	ND
24	B	614	CLA	NC
24	B	615	CLA	NA
24	B	615	CLA	ND
24	B	615	CLA	NC
24	B	616	CLA	NA
24	B	616	CLA	NC
24	B	617	CLA	NA
24	B	617	CLA	ND
24	B	617	CLA	NC
24	C	501	CLA	NA
24	C	501	CLA	ND
24	C	501	CLA	NC
24	C	502	CLA	NA
24	C	502	CLA	ND
24	C	502	CLA	NC
24	C	503	CLA	NA
24	C	503	CLA	ND
24	C	503	CLA	NC
24	C	504	CLA	NA
24	C	504	CLA	ND
24	C	504	CLA	NC
24	C	505	CLA	NA
24	C	505	CLA	NC
24	C	505	CLA	ND
24	C	506	CLA	NA
24	C	506	CLA	ND
24	C	506	CLA	NC
24	C	507	CLA	NA
24	C	507	CLA	NC

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Mol	Chain	Res	Type	Atom
24	C	508	CLA	NA
24	C	508	CLA	ND
24	C	508	CLA	NC
24	C	509	CLA	NA
24	C	509	CLA	ND
24	C	509	CLA	NC
24	C	510	CLA	NA
24	C	510	CLA	ND
24	C	510	CLA	NC
24	C	511	CLA	NA
24	C	511	CLA	ND
24	C	511	CLA	NC
24	C	512	CLA	NA
24	C	512	CLA	ND
24	C	512	CLA	NC
24	C	513	CLA	NA
24	C	513	CLA	ND
24	C	513	CLA	NC
24	D	403	CLA	NA
24	D	403	CLA	ND
24	D	403	CLA	NC
24	D	404	CLA	NA
24	D	404	CLA	NC
24	D	404	CLA	ND
24	D	405	CLA	NA
24	D	405	CLA	ND
24	D	405	CLA	NC
24	a	407	CLA	NA
24	a	407	CLA	ND
24	a	407	CLA	NC
24	a	408	CLA	NA
24	a	408	CLA	ND
24	a	408	CLA	NC
24	a	410	CLA	NA
24	a	410	CLA	ND
24	a	410	CLA	NC
24	b	602	CLA	NA
24	b	602	CLA	ND
24	b	602	CLA	NC
24	b	603	CLA	NA
24	b	603	CLA	NC
24	b	603	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	604	CLA	NA
24	b	604	CLA	NC
24	b	604	CLA	ND
24	b	605	CLA	NA
24	b	605	CLA	ND
24	b	605	CLA	NC
24	b	606	CLA	NA
24	b	606	CLA	NC
24	b	606	CLA	ND
24	b	607	CLA	NA
24	b	607	CLA	NC
24	b	607	CLA	ND
24	b	608	CLA	NA
24	b	608	CLA	ND
24	b	608	CLA	NC
24	b	609	CLA	NA
24	b	609	CLA	ND
24	b	609	CLA	NC
24	b	610	CLA	NA
24	b	610	CLA	ND
24	b	610	CLA	NC
24	b	611	CLA	NA
24	b	611	CLA	ND
24	b	611	CLA	NC
24	b	612	CLA	NA
24	b	612	CLA	ND
24	b	612	CLA	NC
24	b	613	CLA	NA
24	b	613	CLA	ND
24	b	613	CLA	NC
24	b	614	CLA	NA
24	b	614	CLA	ND
24	b	614	CLA	NC
24	b	615	CLA	NA
24	b	615	CLA	ND
24	b	615	CLA	NC
24	b	616	CLA	NA
24	b	616	CLA	NC
24	b	617	CLA	NA
24	b	617	CLA	ND
24	b	617	CLA	NC
24	c	501	CLA	NA

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Mol	Chain	Res	Type	Atom
24	c	501	CLA	ND
24	c	501	CLA	NC
24	c	502	CLA	NA
24	c	502	CLA	ND
24	c	502	CLA	NC
24	c	503	CLA	NA
24	c	503	CLA	ND
24	c	503	CLA	NC
24	c	504	CLA	NA
24	c	504	CLA	ND
24	c	504	CLA	NC
24	c	505	CLA	NA
24	c	505	CLA	NC
24	c	505	CLA	ND
24	c	506	CLA	NA
24	c	506	CLA	ND
24	c	506	CLA	NC
24	c	507	CLA	NA
24	c	507	CLA	ND
24	c	507	CLA	NC
24	c	508	CLA	NA
24	c	508	CLA	ND
24	c	508	CLA	NC
24	c	509	CLA	NA
24	c	509	CLA	ND
24	c	509	CLA	NC
24	c	510	CLA	NA
24	c	510	CLA	ND
24	c	510	CLA	NC
24	c	511	CLA	NA
24	c	511	CLA	ND
24	c	511	CLA	NC
24	c	512	CLA	NA
24	c	512	CLA	ND
24	c	512	CLA	NC
24	c	513	CLA	NA
24	c	513	CLA	ND
24	c	513	CLA	NC
24	d	403	CLA	NA
24	d	403	CLA	ND
24	d	403	CLA	NC
24	d	404	CLA	NA

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Mol	Chain	Res	Type	Atom
24	d	404	CLA	NC
24	d	404	CLA	ND
24	d	405	CLA	NA
24	d	405	CLA	ND
24	d	405	CLA	NC

All (2168) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C1-C2-C3-C4
24	B	605	CLA	C2-C3-C5-C6
24	B	606	CLA	C1-C2-C3-C4
24	B	607	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O1D
24	B	615	CLA	CHA-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	508	CLA	CHA-CBD-CGD-O1D
24	C	508	CLA	CHA-CBD-CGD-O2D
24	b	605	CLA	C1-C2-C3-C4
24	b	605	CLA	C2-C3-C5-C6
24	b	606	CLA	C1-C2-C3-C4
24	b	606	CLA	C2-C3-C5-C6
24	b	607	CLA	CHA-CBD-CGD-O1D
24	b	607	CLA	CHA-CBD-CGD-O2D
24	b	615	CLA	CHA-CBD-CGD-O1D
24	b	615	CLA	CHA-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O1D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	508	CLA	CHA-CBD-CGD-O1D
24	c	508	CLA	CHA-CBD-CGD-O2D
26	C	525	BCR	C7-C8-C9-C10
26	C	525	BCR	C7-C8-C9-C34
27	A	611	PL9	C9-C11-C12-C13
27	A	611	PL9	C23-C24-C26-C27
28	A	616	SQD	O6-C44-C45-O47
28	F	104	SQD	C2-C1-O6-C44
28	F	104	SQD	O5-C1-O6-C44
28	F	104	SQD	C8-C7-O47-C45
28	a	417	SQD	O6-C44-C45-O47
28	a	424	SQD	C2-C1-O6-C44
28	a	424	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
28	b	633	SQD	C8-C7-O47-C45
28	x	101	SQD	C2-C1-O6-C44
28	x	101	SQD	O5-C1-O6-C44
29	B	634	LMG	O9-C10-O7-C8
29	B	634	LMG	O10-C28-O8-C9
29	B	634	LMG	C29-C28-O8-C9
29	C	519	LMG	O7-C8-C9-O8
29	C	526	LMG	C2-C1-O1-C7
29	C	526	LMG	O6-C1-O1-C7
29	d	412	LMG	C2-C1-O1-C7
29	d	412	LMG	O6-C1-O1-C7
29	d	412	LMG	O9-C10-O7-C8
29	d	412	LMG	C11-C10-O7-C8
29	z	101	LMG	C2-C1-O1-C7
29	z	101	LMG	O6-C1-O1-C7
30	B	633	GOL	C1-C2-C3-O3
30	C	527	GOL	O1-C1-C2-C3
30	O	305	GOL	C1-C2-C3-O3
30	T	103	GOL	O1-C1-C2-C3
30	a	416	GOL	C1-C2-C3-O3
30	c	525	GOL	O1-C1-C2-O2
30	c	525	GOL	O1-C1-C2-C3
30	d	402	GOL	C1-C2-C3-O3
30	d	413	GOL	O1-C1-C2-C3
30	d	413	GOL	C1-C2-C3-O3
30	d	413	GOL	O2-C2-C3-O3
30	f	104	GOL	O1-C1-C2-C3
30	o	303	GOL	O1-C1-C2-C3
30	o	304	GOL	O1-C1-C2-C3
30	o	305	GOL	O1-C1-C2-C3
30	v	205	GOL	O1-C1-C2-O2
30	v	205	GOL	O1-C1-C2-C3
30	v	206	GOL	C1-C2-C3-O3
30	v	206	GOL	O2-C2-C3-O3
30	y	101	GOL	O1-C1-C2-C3
31	F	102	LMT	C2-C1-O1'-C1'
31	J	103	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	Y	101	LMT	C2-C1-O1'-C1'
31	j	103	LMT	O5'-C1'-O1'-C1
31	m	101	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
32	A	618	LHG	C3-O3-P-O4
32	A	618	LHG	C4-O6-P-O3
32	A	618	LHG	C4-O6-P-O5
32	B	632	LHG	C4-O6-P-O4
32	D	410	LHG	C3-O3-P-O4
32	D	410	LHG	C3-O3-P-O5
32	a	419	LHG	C3-O3-P-O4
32	a	419	LHG	C3-O3-P-O5
32	a	419	LHG	C3-O3-P-O6
32	a	419	LHG	C8-C7-O7-C5
32	d	410	LHG	C3-O3-P-O5
32	e	101	LHG	O1-C1-C2-C3
32	l	101	LHG	C4-O6-P-O4
38	B	624	HTG	O5-C1-S1-C1'
38	C	521	HTG	C2'-C1'-S1-C1
38	C	531	HTG	O5-C1-S1-C1'
38	C	531	HTG	C2'-C1'-S1-C1
38	a	418	HTG	C2-C1-S1-C1'
38	a	418	HTG	O5-C1-S1-C1'
38	b	624	HTG	O5-C1-S1-C1'
38	c	522	HTG	C2-C1-S1-C1'
38	c	522	HTG	O5-C1-S1-C1'
38	c	530	HTG	C2'-C1'-S1-C1
38	c	531	HTG	C2-C1-S1-C1'
38	c	531	HTG	O5-C1-S1-C1'
38	c	531	HTG	C2'-C1'-S1-C1
40	D	408	DGD	C2B-C1B-O2G-C2G
40	D	408	DGD	O1B-C1B-O2G-C2G
40	D	408	DGD	C2D-C1D-O3G-C3G
40	d	408	DGD	O1B-C1B-O2G-C2G
40	d	408	DGD	C2D-C1D-O3G-C3G
40	d	408	DGD	C2E-C1E-O5D-C6D
41	E	113	HEM	C3D-CAD-CBD-CGD
31	I	101	LMT	C3'-C4'-O1B-C1B
31	Y	101	LMT	C2B-C1B-O1B-C4'
31	c	521	LMT	C3'-C4'-O1B-C1B
35	c	541	P6G	C14-C15-O16-C17
24	C	501	CLA	CBD-CGD-O2D-CED
24	C	513	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	O1A-CGA-O2A-C1
28	b	633	SQD	O10-C23-O48-C46
28	h	105	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
28	l	102	SQD	O10-C23-O48-C46
28	x	101	SQD	O10-C23-O48-C46
29	C	526	LMG	O10-C28-O8-C9
29	d	412	LMG	O10-C28-O8-C9
29	z	101	LMG	O10-C28-O8-C9
32	A	618	LHG	O10-C23-O8-C6
32	a	419	LHG	O10-C23-O8-C6
40	D	408	DGD	O1A-C1A-O1G-C1G
40	d	408	DGD	O1A-C1A-O1G-C1G
31	J	103	LMT	O5B-C1B-O1B-C4'
33	H	106	PG4	C3-C4-O3-C5
28	F	104	SQD	O49-C7-O47-C45
28	b	633	SQD	O49-C7-O47-C45
29	z	101	LMG	O9-C10-O7-C8
32	a	419	LHG	O9-C7-O7-C5
31	C	533	LMT	C3'-C4'-O1B-C1B
31	j	103	LMT	C2B-C1B-O1B-C4'
24	C	513	CLA	C3-C5-C6-C7
24	b	605	CLA	C3-C5-C6-C7
24	b	615	CLA	C3-C5-C6-C7
24	B	602	CLA	CBA-CGA-O2A-C1
28	A	622	SQD	C24-C23-O48-C46
28	l	102	SQD	C24-C23-O48-C46
29	C	526	LMG	C29-C28-O8-C9
29	d	412	LMG	C29-C28-O8-C9
29	z	101	LMG	C29-C28-O8-C9
32	A	618	LHG	C24-C23-O8-C6
32	a	419	LHG	C24-C23-O8-C6
40	D	408	DGD	C2A-C1A-O1G-C1G
29	B	634	LMG	C11-C10-O7-C8
29	z	101	LMG	C11-C10-O7-C8
40	d	408	DGD	C2B-C1B-O2G-C2G
33	X	102	PG4	C4-C3-O2-C2
29	c	520	LMG	O6-C5-C6-O5
27	A	611	PL9	C25-C24-C26-C27
24	B	617	CLA	C3-C5-C6-C7
24	B	617	CLA	CBA-CGA-O2A-C1
24	b	617	CLA	CBA-CGA-O2A-C1
28	b	633	SQD	C24-C23-O48-C46
28	h	105	SQD	C24-C23-O48-C46
28	x	101	SQD	C24-C23-O48-C46
40	d	408	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	O6-C5-C6-O5
31	j	103	LMT	O5B-C5B-C6B-O6B
31	t	103	LMT	O5'-C5'-C6'-O6'
31	u	203	LMT	C2B-C1B-O1B-C4'
38	B	623	HTG	S1-C1'-C2'-C3'
38	B	631	HTG	C4-C5-C6-O6
28	A	622	SQD	O10-C23-O48-C46
32	e	101	LHG	O10-C23-O8-C6
33	V	213	PG4	O4-C7-C8-O5
32	D	410	LHG	O2-C2-C3-O3
32	d	410	LHG	O2-C2-C3-O3
32	e	101	LHG	C24-C23-O8-C6
24	b	617	CLA	O1A-CGA-O2A-C1
38	H	101	HTG	O5-C5-C6-O6
38	b	632	HTG	O5-C5-C6-O6
31	t	103	LMT	C4'-C5'-C6'-O6'
28	l	102	SQD	C8-C7-O47-C45
28	x	101	SQD	C8-C7-O47-C45
38	h	101	HTG	O5-C5-C6-O6
40	c	516	DGD	C2A-C3A-C4A-C5A
38	C	521	HTG	S1-C1'-C2'-C3'
38	C	522	HTG	S1-C1'-C2'-C3'
38	C	529	HTG	S1-C1'-C2'-C3'
31	C	533	LMT	O5B-C5B-C6B-O6B
31	M	102	LMT	O5'-C5'-C6'-O6'
38	b	624	HTG	O5-C5-C6-O6
33	E	103	PG4	O3-C5-C6-O4
34	i	105	PGE	O2-C3-C4-O3
35	A	623	P6G	O13-C14-C15-O16
39	L	101	1PE	OH6-C15-C25-OH5
24	B	617	CLA	O1A-CGA-O2A-C1
33	B	637	PG4	O2-C3-C4-O3
33	E	102	PG4	O3-C5-C6-O4
33	V	210	PG4	O3-C5-C6-O4
33	h	106	PG4	O3-C5-C6-O4
34	b	638	PGE	O2-C3-C4-O3
34	o	306	PGE	O2-C3-C4-O3
35	A	623	P6G	O10-C11-C12-O13
35	B	652	P6G	O10-C11-C12-O13
35	d	415	P6G	O10-C11-C12-O13
39	B	654	1PE	OH4-C13-C23-OH3
39	j	107	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
45	i	107	PE8	O7-C8-C9-O10
31	J	103	LMT	O5'-C5'-C6'-O6'
31	Y	101	LMT	O5B-C5B-C6B-O6B
31	u	203	LMT	O5B-C5B-C6B-O6B
29	C	520	LMG	C4-C5-C6-O5
29	c	520	LMG	C4-C5-C6-O5
31	A	617	LMT	C4B-C5B-C6B-O6B
38	B	630	HTG	C4-C5-C6-O6
24	B	606	CLA	C2-C3-C5-C6
33	a	420	PG4	O3-C5-C6-O4
34	O	309	PGE	C3-C4-O3-C5
34	V	214	PGE	O2-C3-C4-O3
34	o	308	PGE	O2-C3-C4-O3
35	D	417	P6G	O4-C5-C6-O7
35	c	541	P6G	O10-C11-C12-O13
39	B	654	1PE	OH6-C15-C25-OH5
28	b	633	SQD	O5-C1-O6-C44
40	d	408	DGD	O6E-C1E-O5D-C6D
27	a	412	PL9	C19-C21-C22-C23
33	B	637	PG4	O3-C5-C6-O4
33	C	536	PG4	O2-C3-C4-O3
33	l	103	PG4	O2-C3-C4-O3
34	J	106	PGE	O2-C3-C4-O3
34	x	103	PGE	O2-C3-C4-O3
35	I	106	P6G	O13-C14-C15-O16
35	b	649	P6G	O10-C11-C12-O13
33	c	534	PG4	O3-C5-C6-O4
33	i	101	PG4	O3-C5-C6-O4
34	a	422	PGE	O2-C3-C4-O3
34	i	106	PGE	O2-C3-C4-O3
35	D	418	P6G	O7-C8-C9-O10
35	b	648	P6G	O4-C5-C6-O7
31	j	103	LMT	C4B-C5B-C6B-O6B
31	J	103	LMT	C2B-C1B-O1B-C4'
33	D	414	PG4	O3-C5-C6-O4
33	J	105	PG4	O3-C5-C6-O4
34	I	105	PGE	O2-C3-C4-O3
34	J	108	PGE	O2-C3-C4-O3
35	C	541	P6G	O10-C11-C12-O13
35	b	649	P6G	O4-C5-C6-O7
40	d	408	DGD	O6D-C5D-C6D-O5D
31	c	521	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
33	V	209	PG4	C8-C7-O4-C6
35	A	624	P6G	O7-C8-C9-O10
32	a	419	LHG	C1-C2-C3-O3
32	d	410	LHG	C1-C2-C3-O3
38	B	631	HTG	O5-C5-C6-O6
28	l	102	SQD	O49-C7-O47-C45
28	x	101	SQD	O49-C7-O47-C45
31	I	101	LMT	C4'-C5'-C6'-O6'
33	H	104	PG4	O3-C5-C6-O4
33	c	532	PG4	O3-C5-C6-O4
33	e	103	PG4	O3-C5-C6-O4
33	i	104	PG4	O3-C5-C6-O4
33	j	104	PG4	O2-C3-C4-O3
34	C	540	PGE	O2-C3-C4-O3
35	B	651	P6G	O7-C8-C9-O10
35	T	105	P6G	O13-C14-C15-O16
45	i	107	PE8	O16-C17-C18-O19
24	b	602	CLA	C3-C5-C6-C7
33	e	103	PG4	O4-C7-C8-O5
34	c	536	PGE	O1-C1-C2-O2
34	c	539	PGE	O3-C5-C6-O4
34	h	108	PGE	O1-C1-C2-O2
35	A	624	P6G	O16-C17-C18-O19
39	x	104	1PE	OH7-C16-C26-OH6
24	b	604	CLA	CBD-CGD-O2D-CED
31	M	102	LMT	C4'-C5'-C6'-O6'
35	B	652	P6G	O4-C5-C6-O7
40	C	516	DGD	C1B-C2B-C3B-C4B
33	V	209	PG4	O2-C3-C4-O3
33	i	101	PG4	O2-C3-C4-O3
34	c	538	PGE	O2-C3-C4-O3
24	b	602	CLA	C15-C16-C17-C18
31	C	533	LMT	C4B-C5B-C6B-O6B
31	Y	101	LMT	C4B-C5B-C6B-O6B
38	b	632	HTG	C4-C5-C6-O6
33	B	640	PG4	O2-C3-C4-O3
33	C	538	PG4	O3-C5-C6-O4
34	O	310	PGE	O2-C3-C4-O3
35	j	106	P6G	O4-C5-C6-O7
33	i	102	PG4	O3-C5-C6-O4
33	i	103	PG4	O2-C3-C4-O3
35	E	110	P6G	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
35	I	106	P6G	O7-C8-C9-O10
39	e	105	1PE	OH5-C14-C24-OH4
24	B	616	CLA	C5-C6-C7-C8
28	A	612	SQD	C7-C8-C9-C10
32	E	101	LHG	C7-C8-C9-C10
31	u	203	LMT	O5B-C1B-O1B-C4'
33	j	104	PG4	O3-C5-C6-O4
34	h	107	PGE	O2-C3-C4-O3
35	d	415	P6G	O7-C8-C9-O10
24	C	501	CLA	O1D-CGD-O2D-CED
33	V	213	PG4	O3-C5-C6-O4
33	b	635	PG4	O2-C3-C4-O3
34	o	307	PGE	O2-C3-C4-O3
24	b	602	CLA	C10-C11-C12-C13
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
26	C	515	BCR	C37-C22-C23-C24
33	X	102	PG4	O3-C5-C6-O4
39	B	653	1PE	OH6-C15-C25-OH5
29	C	526	LMG	C10-C11-C12-C13
29	c	519	LMG	C10-C11-C12-C13
40	C	517	DGD	C1B-C2B-C3B-C4B
40	D	408	DGD	C1A-C2A-C3A-C4A
24	C	513	CLA	O1D-CGD-O2D-CED
29	B	634	LMG	O6-C5-C6-O5
31	J	103	LMT	C4'-C5'-C6'-O6'
34	O	308	PGE	O2-C3-C4-O3
35	D	417	P6G	O10-C11-C12-O13
24	A	609	CLA	CBA-CGA-O2A-C1
24	A	606	CLA	C15-C16-C17-C18
24	A	609	CLA	C8-C10-C11-C12
24	B	616	CLA	C10-C11-C12-C13
24	a	410	CLA	C8-C10-C11-C12
24	b	602	CLA	C8-C10-C11-C12
32	D	409	LHG	C23-C24-C25-C26
34	A	621	PGE	O2-C3-C4-O3
35	B	651	P6G	O4-C5-C6-O7
40	D	408	DGD	O6D-C5D-C6D-O5D
24	C	506	CLA	C5-C6-C7-C8
24	C	506	CLA	C10-C11-C12-C13
24	b	615	CLA	C10-C11-C12-C13
24	b	615	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	C10-C11-C12-C13
24	d	405	CLA	C8-C10-C11-C12
34	Y	102	PGE	O2-C3-C4-O3
44	V	216	2PE	C23-C24-O25-C26
30	b	629	GOL	O1-C1-C2-O2
30	d	402	GOL	O2-C2-C3-O3
28	A	616	SQD	C23-C24-C25-C26
28	a	417	SQD	C23-C24-C25-C26
28	h	105	SQD	C23-C24-C25-C26
32	A	618	LHG	C23-C24-C25-C26
32	d	409	LHG	C23-C24-C25-C26
40	c	516	DGD	C1B-C2B-C3B-C4B
40	c	517	DGD	C1A-C2A-C3A-C4A
38	B	630	HTG	O5-C5-C6-O6
24	d	403	CLA	C2C-C3C-CAC-CBC
31	c	521	LMT	O1'-C1-C2-C3
32	d	411	LHG	C12-C13-C14-C15
35	j	106	P6G	O13-C14-C15-O16
31	C	533	LMT	O1'-C1-C2-C3
31	f	101	LMT	O1'-C1-C2-C3
33	B	641	PG4	O3-C5-C6-O4
34	f	105	PGE	O2-C3-C4-O3
35	d	416	P6G	O4-C5-C6-O7
39	j	107	1PE	OH5-C14-C24-OH4
29	z	101	LMG	O6-C5-C6-O5
31	a	401	LMT	O5B-C5B-C6B-O6B
33	J	105	PG4	O2-C3-C4-O3
33	V	211	PG4	O3-C5-C6-O4
34	H	109	PGE	O2-C3-C4-O3
24	C	509	CLA	C8-C10-C11-C12
29	C	519	LMG	C10-C11-C12-C13
33	A	619	PG4	O1-C1-C2-O2
33	B	637	PG4	O1-C1-C2-O2
33	B	639	PG4	O1-C1-C2-O2
33	C	536	PG4	O1-C1-C2-O2
33	I	103	PG4	O4-C7-C8-O5
33	J	105	PG4	O1-C1-C2-O2
33	K	102	PG4	O4-C7-C8-O5
33	b	635	PG4	O4-C7-C8-O5
33	j	104	PG4	O4-C7-C8-O5
34	B	649	PGE	O1-C1-C2-O2
34	E	108	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
34	E	108	PGE	O3-C5-C6-O4
34	H	108	PGE	O1-C1-C2-O2
34	O	308	PGE	O3-C5-C6-O4
34	O	309	PGE	O3-C5-C6-O4
34	c	540	PGE	O3-C5-C6-O4
34	h	107	PGE	O1-C1-C2-O2
34	h	110	PGE	O3-C5-C6-O4
34	o	306	PGE	O3-C5-C6-O4
34	o	308	PGE	O3-C5-C6-O4
35	B	651	P6G	O16-C17-C18-O19
35	E	110	P6G	O16-C17-C18-O19
39	e	105	1PE	OH7-C16-C26-OH6
44	V	216	2PE	O25-C26-C27-O28
33	I	102	PG4	O2-C3-C4-O3
33	B	638	PG4	O3-C5-C6-O4
34	b	645	PGE	O2-C3-C4-O3
24	b	615	CLA	C8-C10-C11-C12
38	C	532	HTG	O5-C5-C6-O6
31	u	203	LMT	C4B-C5B-C6B-O6B
24	D	405	CLA	C11-C10-C8-C7
24	b	602	CLA	C11-C10-C8-C7
40	d	408	DGD	C4D-C5D-C6D-O5D
24	B	602	CLA	C5-C6-C7-C8
24	b	615	CLA	C5-C6-C7-C8
33	A	619	PG4	O2-C3-C4-O3
33	E	102	PG4	O2-C3-C4-O3
33	I	104	PG4	O3-C5-C6-O4
35	E	110	P6G	O7-C8-C9-O10
31	A	617	LMT	O5B-C5B-C6B-O6B
38	b	624	HTG	C4-C5-C6-O6
27	A	611	PL9	C24-C26-C27-C28
27	a	412	PL9	C9-C11-C12-C13
27	a	412	PL9	C14-C16-C17-C18
34	j	105	PGE	C4-C3-O2-C2
28	l	102	SQD	C7-C8-C9-C10
38	C	531	HTG	S1-C1'-C2'-C3'
31	J	103	LMT	O1'-C1-C2-C3
31	Y	101	LMT	O1'-C1-C2-C3
34	b	646	PGE	O2-C3-C4-O3
35	B	652	P6G	O7-C8-C9-O10
39	e	105	1PE	OH6-C15-C25-OH5
32	A	618	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
32	a	419	LHG	O2-C2-C3-O3
24	b	612	CLA	C15-C16-C17-C18
34	B	646	PGE	O2-C3-C4-O3
31	a	401	LMT	C4B-C5B-C6B-O6B
38	H	101	HTG	C4-C5-C6-O6
38	h	101	HTG	C4-C5-C6-O6
31	M	102	LMT	O1'-C1-C2-C3
24	B	612	CLA	C15-C16-C17-C18
24	D	405	CLA	C8-C10-C11-C12
34	c	540	PGE	O2-C3-C4-O3
24	A	609	CLA	O1A-CGA-O2A-C1
27	a	412	PL9	C31-C32-C33-C34
24	c	509	CLA	C8-C10-C11-C12
32	A	618	LHG	C3-O3-P-O6
32	B	632	LHG	C4-O6-P-O3
32	D	410	LHG	C3-O3-P-O6
32	l	101	LHG	C4-O6-P-O3
40	c	517	DGD	C1B-C2B-C3B-C4B
35	D	417	P6G	O13-C14-C15-O16
24	a	410	CLA	CBA-CGA-O2A-C1
38	a	418	HTG	C1'-C2'-C3'-C4'
34	o	309	PGE	O2-C3-C4-O3
35	d	416	P6G	O10-C11-C12-O13
38	c	530	HTG	C4-C5-C6-O6
33	J	104	PG4	O3-C5-C6-O4
40	D	408	DGD	C4D-C5D-C6D-O5D
32	A	618	LHG	C1-C2-C3-O3
32	D	410	LHG	C1-C2-C3-O3
24	c	506	CLA	C15-C16-C17-C18
24	b	611	CLA	CBD-CGD-O2D-CED
31	j	103	LMT	O5B-C1B-O1B-C4'
31	B	622	LMT	C5'-C4'-O1B-C1B
31	m	101	LMT	O1'-C1-C2-C3
31	t	103	LMT	O5B-C5B-C6B-O6B
33	B	641	PG4	O4-C7-C8-O5
33	C	538	PG4	O4-C7-C8-O5
33	D	414	PG4	O1-C1-C2-O2
33	D	414	PG4	O4-C7-C8-O5
33	E	102	PG4	O1-C1-C2-O2
33	I	102	PG4	O4-C7-C8-O5
33	K	102	PG4	O1-C1-C2-O2
33	V	210	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	V	210	PG4	O4-C7-C8-O5
33	X	101	PG4	O1-C1-C2-O2
33	a	420	PG4	O1-C1-C2-O2
33	c	532	PG4	O1-C1-C2-O2
33	c	534	PG4	O4-C7-C8-O5
33	j	104	PG4	O1-C1-C2-O2
34	B	644	PGE	O3-C5-C6-O4
34	B	648	PGE	O3-C5-C6-O4
34	C	540	PGE	O3-C5-C6-O4
34	H	108	PGE	O3-C5-C6-O4
34	O	310	PGE	O1-C1-C2-O2
34	b	638	PGE	O1-C1-C2-O2
34	b	640	PGE	O3-C5-C6-O4
34	b	642	PGE	O1-C1-C2-O2
34	b	642	PGE	O3-C5-C6-O4
34	b	644	PGE	O3-C5-C6-O4
34	f	105	PGE	O3-C5-C6-O4
34	h	107	PGE	O3-C5-C6-O4
34	j	105	PGE	O1-C1-C2-O2
34	o	308	PGE	O1-C1-C2-O2
34	x	103	PGE	O3-C5-C6-O4
35	A	623	P6G	O16-C17-C18-O19
35	C	541	P6G	O1-C2-C3-O4
35	C	541	P6G	O16-C17-C18-O19
35	D	416	P6G	O16-C17-C18-O19
35	I	106	P6G	O1-C2-C3-O4
35	I	106	P6G	O16-C17-C18-O19
35	T	105	P6G	O1-C2-C3-O4
39	B	654	1PE	OH7-C16-C26-OH6
39	j	107	1PE	OH7-C16-C26-OH6
24	b	602	CLA	CBA-CGA-O2A-C1
28	F	104	SQD	C24-C23-O48-C46
29	A	613	LMG	C29-C28-O8-C9
32	E	101	LHG	C24-C23-O8-C6
31	u	203	LMT	O1'-C1-C2-C3
33	B	641	PG4	O2-C3-C4-O3
29	c	519	LMG	C28-C29-C30-C31
35	D	418	P6G	O10-C11-C12-O13
29	A	613	LMG	C19-C20-C21-C22
32	E	101	LHG	C18-C19-C20-C21
35	E	110	P6G	C14-C15-O16-C17
40	D	408	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
24	C	503	CLA	CBD-CGD-O2D-CED
28	h	105	SQD	C8-C7-O47-C45
32	e	101	LHG	C8-C7-O7-C5
38	V	204	HTG	C1'-C2'-C3'-C4'
28	A	612	SQD	C15-C16-C17-C18
28	A	622	SQD	C28-C29-C30-C31
29	B	621	LMG	C31-C32-C33-C34
29	C	526	LMG	C38-C39-C40-C41
29	J	101	LMG	C39-C40-C41-C42
29	a	414	LMG	C11-C12-C13-C14
29	b	621	LMG	C30-C31-C32-C33
29	d	412	LMG	C13-C14-C15-C16
29	d	412	LMG	C29-C30-C31-C32
29	j	101	LMG	C13-C14-C15-C16
31	a	401	LMT	C7-C8-C9-C10
32	E	101	LHG	C15-C16-C17-C18
32	l	101	LHG	C14-C15-C16-C17
38	h	101	HTG	C3'-C4'-C5'-C6'
40	C	516	DGD	C4A-C5A-C6A-C7A
40	C	516	DGD	C7A-C8A-C9A-CAA
40	c	518	DGD	CBA-CCA-CDA-CEA
24	C	506	CLA	C16-C17-C18-C19
24	b	611	CLA	C16-C17-C18-C20
38	c	531	HTG	S1-C1'-C2'-C3'
28	A	622	SQD	C24-C25-C26-C27
28	F	104	SQD	C26-C27-C28-C29
28	l	102	SQD	C26-C27-C28-C29
29	B	634	LMG	C17-C18-C19-C20
29	c	519	LMG	C13-C14-C15-C16
29	j	101	LMG	C15-C16-C17-C18
29	z	101	LMG	C23-C24-C25-C26
31	J	103	LMT	C11-C10-C9-C8
29	B	634	LMG	C9-C8-O7-C10
28	h	105	SQD	O49-C7-O47-C45
32	e	101	LHG	O9-C7-O7-C5
28	A	616	SQD	C34-C35-C36-C37
28	a	424	SQD	C33-C34-C35-C36
29	A	613	LMG	C13-C14-C15-C16
29	C	519	LMG	C39-C40-C41-C42
29	C	520	LMG	C31-C32-C33-C34
29	b	621	LMG	C33-C34-C35-C36
31	t	103	LMT	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	u	203	LMT	C5-C6-C7-C8
31	u	203	LMT	C6-C7-C8-C9
33	a	420	PG4	O2-C3-C4-O3
28	A	612	SQD	C32-C33-C34-C35
28	l	102	SQD	C18-C19-C20-C21
29	C	519	LMG	C16-C17-C18-C19
29	J	101	LMG	C38-C39-C40-C41
29	a	414	LMG	C18-C19-C20-C21
32	d	409	LHG	C27-C28-C29-C30
38	C	529	HTG	C2'-C3'-C4'-C5'
40	C	518	DGD	C8A-C9A-CAA-CBA
40	H	103	DGD	CBB-CCB-CDB-CEB
40	c	517	DGD	C8B-C9B-CAB-CBB
28	A	612	SQD	C11-C12-C13-C14
28	b	633	SQD	C26-C27-C28-C29
29	c	520	LMG	C30-C31-C32-C33
39	x	104	1PE	OH6-C15-C25-OH5
28	x	101	SQD	C33-C34-C35-C36
32	d	411	LHG	C34-C35-C36-C37
32	e	101	LHG	C18-C19-C20-C21
33	D	414	PG4	O2-C3-C4-O3
40	C	518	DGD	CAA-CBA-CCA-CDA
40	c	517	DGD	C5A-C6A-C7A-C8A
24	D	405	CLA	C13-C15-C16-C17
28	l	102	SQD	C9-C10-C11-C12
29	B	634	LMG	C16-C17-C18-C19
29	a	414	LMG	C13-C14-C15-C16
29	c	520	LMG	C15-C16-C17-C18
29	z	101	LMG	C13-C14-C15-C16
29	z	101	LMG	C34-C35-C36-C37
31	B	622	LMT	C7-C8-C9-C10
31	I	101	LMT	C5-C6-C7-C8
32	a	419	LHG	C9-C10-C11-C12
40	D	408	DGD	C4A-C5A-C6A-C7A
24	a	408	CLA	C6-C7-C8-C9
24	b	602	CLA	C11-C10-C8-C9
28	a	424	SQD	C18-C19-C20-C21
28	h	105	SQD	C12-C13-C14-C15
28	x	101	SQD	C12-C13-C14-C15
29	c	519	LMG	C14-C15-C16-C17
29	c	519	LMG	C37-C38-C39-C40
31	F	102	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	u	203	LMT	C4-C5-C6-C7
32	E	101	LHG	C14-C15-C16-C17
32	a	419	LHG	C10-C11-C12-C13
35	d	415	P6G	O13-C14-C15-O16
38	H	101	HTG	C3'-C4'-C5'-C6'
24	b	602	CLA	O1A-CGA-O2A-C1
28	x	101	SQD	C11-C12-C13-C14
30	B	625	GOL	C1-C2-C3-O3
30	B	627	GOL	O1-C1-C2-C3
30	B	633	GOL	O1-C1-C2-C3
30	C	528	GOL	O1-C1-C2-C3
30	D	402	GOL	C1-C2-C3-O3
30	D	412	GOL	C1-C2-C3-O3
30	D	413	GOL	C1-C2-C3-O3
30	F	101	GOL	C1-C2-C3-O3
30	O	302	GOL	C1-C2-C3-O3
30	O	307	GOL	C1-C2-C3-O3
30	V	208	GOL	O1-C1-C2-C3
30	b	625	GOL	O1-C1-C2-C3
30	b	629	GOL	O1-C1-C2-C3
30	c	528	GOL	C1-C2-C3-O3
30	c	529	GOL	O1-C1-C2-C3
30	f	103	GOL	C1-C2-C3-O3
30	f	104	GOL	C1-C2-C3-O3
30	o	304	GOL	C1-C2-C3-O3
28	A	612	SQD	C16-C17-C18-C19
28	a	417	SQD	C27-C28-C29-C30
32	D	411	LHG	C13-C14-C15-C16
34	J	107	PGE	O2-C3-C4-O3
28	A	616	SQD	C18-C19-C20-C21
28	A	616	SQD	C32-C33-C34-C35
28	F	104	SQD	C24-C25-C26-C27
28	a	413	SQD	C29-C30-C31-C32
28	a	424	SQD	C11-C10-C9-C8
28	a	424	SQD	C26-C27-C28-C29
29	C	519	LMG	C32-C33-C34-C35
29	a	414	LMG	C29-C30-C31-C32
29	d	412	LMG	C31-C32-C33-C34
31	t	103	LMT	C4-C5-C6-C7
32	e	101	LHG	C15-C16-C17-C18
33	i	104	PG4	O2-C3-C4-O3
40	C	518	DGD	C2A-C3A-C4A-C5A

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Mol	Chain	Res	Type	Atoms
40	D	408	DGD	C7A-C8A-C9A-CAA
24	c	506	CLA	C16-C17-C18-C20
32	E	101	LHG	C5-C6-O8-C23
33	B	638	PG4	O4-C7-C8-O5
33	H	107	PG4	O1-C1-C2-O2
33	c	533	PG4	O4-C7-C8-O5
34	b	641	PGE	O3-C5-C6-O4
34	b	647	PGE	O3-C5-C6-O4
34	c	537	PGE	O1-C1-C2-O2
34	h	109	PGE	O1-C1-C2-O2
28	x	101	SQD	C18-C19-C20-C21
29	c	519	LMG	C18-C19-C20-C21
31	B	622	LMT	C6-C7-C8-C9
31	C	533	LMT	C3-C4-C5-C6
31	F	102	LMT	C4-C5-C6-C7
32	D	411	LHG	C29-C30-C31-C32
32	E	101	LHG	C26-C27-C28-C29
40	C	517	DGD	CAB-CBB-CCB-CDB
40	c	518	DGD	CCB-CDB-CEB-CFB
28	a	417	SQD	C18-C19-C20-C21
28	b	633	SQD	C9-C10-C11-C12
28	b	633	SQD	C25-C26-C27-C28
31	c	521	LMT	C6-C7-C8-C9
35	D	417	P6G	O7-C8-C9-O10
40	H	103	DGD	C7A-C8A-C9A-CAA
29	C	520	LMG	C10-C11-C12-C13
29	C	520	LMG	C38-C39-C40-C41
29	j	101	LMG	C14-C15-C16-C17
40	D	408	DGD	CBA-CCA-CDA-CEA
29	B	634	LMG	C13-C14-C15-C16
29	c	520	LMG	C38-C39-C40-C41
24	A	609	CLA	C13-C15-C16-C17
24	C	507	CLA	C5-C6-C7-C8
31	M	102	LMT	C2-C1-O1'-C1'
29	B	634	LMG	C18-C19-C20-C21
29	C	519	LMG	C35-C36-C37-C38
29	J	101	LMG	C12-C13-C14-C15
29	c	520	LMG	C16-C17-C18-C19
29	c	520	LMG	C37-C38-C39-C40
31	j	103	LMT	C7-C8-C9-C10
33	d	414	PG4	O2-C3-C4-O3
38	C	530	HTG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
28	F	104	SQD	O10-C23-O48-C46
24	C	506	CLA	C16-C17-C18-C20
32	D	409	LHG	C29-C30-C31-C32
32	d	411	LHG	C29-C30-C31-C32
40	D	408	DGD	C2B-C3B-C4B-C5B
40	H	103	DGD	CBA-CCA-CDA-CEA
40	c	516	DGD	C4B-C5B-C6B-C7B
40	d	408	DGD	C2B-C3B-C4B-C5B
24	B	602	CLA	CBD-CGD-O2D-CED
29	a	414	LMG	C20-C21-C22-C23
35	T	105	P6G	O4-C5-C6-O7
40	C	516	DGD	C4B-C5B-C6B-C7B
28	F	104	SQD	C31-C32-C33-C34
29	B	621	LMG	C34-C35-C36-C37
32	A	618	LHG	C11-C12-C13-C14
40	c	516	DGD	C5B-C6B-C7B-C8B
28	A	622	SQD	C8-C7-O47-C45
32	D	411	LHG	C34-C35-C36-C37
40	D	408	DGD	C7B-C8B-C9B-CAB
31	I	101	LMT	O5'-C5'-C6'-O6'
30	B	625	GOL	O2-C2-C3-O3
30	B	633	GOL	O2-C2-C3-O3
30	D	402	GOL	O2-C2-C3-O3
30	O	302	GOL	O2-C2-C3-O3
30	c	529	GOL	O1-C1-C2-O2
30	d	413	GOL	O1-C1-C2-O2
30	f	104	GOL	O1-C1-C2-O2
30	f	104	GOL	O2-C2-C3-O3
30	o	303	GOL	O1-C1-C2-O2
30	o	304	GOL	O2-C2-C3-O3
30	o	305	GOL	O1-C1-C2-O2
30	y	101	GOL	O1-C1-C2-O2
32	e	101	LHG	O1-C1-C2-O2
24	a	407	CLA	C2C-C3C-CAC-CBC
28	a	424	SQD	C9-C10-C11-C12
29	z	101	LMG	C18-C19-C20-C21
31	B	622	LMT	C3'-C4'-O1B-C1B
31	a	401	LMT	C11-C10-C9-C8
31	u	203	LMT	C2-C3-C4-C5
34	c	537	PGE	O2-C3-C4-O3
40	C	516	DGD	CAA-CBA-CCA-CDA
40	d	408	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
24	A	609	CLA	C16-C17-C18-C19
24	b	603	CLA	C16-C17-C18-C19
38	C	531	HTG	C2'-C3'-C4'-C5'
31	a	401	LMT	C1-C2-C3-C4
29	C	526	LMG	C40-C41-C42-C43
34	b	639	PGE	C6-C5-O3-C4
39	x	104	1PE	OH5-C14-C24-OH4
40	d	408	DGD	O6E-C5E-C6E-O5E
31	J	103	LMT	C1-C2-C3-C4
25	d	401	PHO	C2C-C3C-CAC-CBC
28	a	413	SQD	C10-C11-C12-C13
28	a	413	SQD	C33-C34-C35-C36
31	I	101	LMT	O1'-C1-C2-C3
33	B	641	PG4	C4-C3-O2-C2
40	c	518	DGD	C2A-C3A-C4A-C5A
32	E	101	LHG	O10-C23-O8-C6
28	A	622	SQD	C17-C18-C19-C20
28	b	633	SQD	C34-C35-C36-C37
29	C	520	LMG	C37-C38-C39-C40
35	B	652	P6G	C11-C12-O13-C14
40	D	408	DGD	CEB-CFB-CGB-CHB
31	F	102	LMT	C1-C2-C3-C4
32	B	632	LHG	C12-C13-C14-C15
32	D	409	LHG	C30-C31-C32-C33
32	e	101	LHG	C27-C28-C29-C30
35	D	416	P6G	O13-C14-C15-O16
40	C	516	DGD	C5B-C6B-C7B-C8B
24	C	506	CLA	C13-C15-C16-C17
24	a	410	CLA	C10-C11-C12-C13
24	c	512	CLA	C15-C16-C17-C18
29	A	613	LMG	O10-C28-O8-C9
28	h	105	SQD	C15-C16-C17-C18
31	t	103	LMT	C7-C8-C9-C10
29	a	414	LMG	C10-C11-C12-C13
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
26	K	101	BCR	C5-C6-C7-C8
26	T	102	BCR	C23-C24-C25-C26
26	b	620	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
33	B	636	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	E	103	PG4	O4-C7-C8-O5
33	i	102	PG4	O4-C7-C8-O5
34	A	620	PGE	O2-C3-C4-O3
34	A	621	PGE	O1-C1-C2-O2
34	E	106	PGE	O3-C5-C6-O4
34	H	111	PGE	O3-C5-C6-O4
34	a	422	PGE	O3-C5-C6-O4
34	b	639	PGE	O1-C1-C2-O2
34	b	645	PGE	O3-C5-C6-O4
35	A	623	P6G	O1-C2-C3-O4
35	D	417	P6G	O1-C2-C3-O4
35	D	417	P6G	O16-C17-C18-O19
35	D	418	P6G	O16-C17-C18-O19
35	c	541	P6G	O1-C2-C3-O4
39	x	104	1PE	OH2-C12-C22-OH3
44	V	216	2PE	O1-C2-C3-O4
36	B	656	EDO	O1-C1-C2-O2
36	C	542	EDO	O1-C1-C2-O2
36	d	417	EDO	O1-C1-C2-O2
36	o	311	EDO	O1-C1-C2-O2
29	C	526	LMG	C18-C19-C20-C21
33	U	202	PG4	O3-C5-C6-O4
29	c	520	LMG	C29-C28-O8-C9
24	C	509	CLA	C10-C11-C12-C13
24	d	405	CLA	C15-C16-C17-C18
38	a	418	HTG	C4-C5-C6-O6
29	C	526	LMG	C41-C42-C43-C44
29	z	101	LMG	C32-C33-C34-C35
32	d	409	LHG	C30-C31-C32-C33
35	d	416	P6G	O7-C8-C9-O10
35	j	106	P6G	O10-C11-C12-O13
38	C	522	HTG	O5-C5-C6-O6
29	d	412	LMG	C11-C12-C13-C14
32	D	409	LHG	C27-C28-C29-C30
32	d	411	LHG	C15-C16-C17-C18
24	C	508	CLA	C11-C10-C8-C7
24	a	410	CLA	O1A-CGA-O2A-C1
28	A	622	SQD	C25-C26-C27-C28
34	V	215	PGE	O2-C3-C4-O3
24	b	609	CLA	C13-C15-C16-C17
24	C	502	CLA	C16-C17-C18-C20
28	A	622	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
29	c	519	LMG	O9-C10-O7-C8
29	c	520	LMG	C28-C29-C30-C31
29	C	519	LMG	C29-C28-O8-C9
28	l	102	SQD	C27-C28-C29-C30
40	c	517	DGD	C3A-C4A-C5A-C6A
40	d	408	DGD	C6A-C7A-C8A-C9A
28	h	105	SQD	C24-C25-C26-C27
33	C	534	PG4	O2-C3-C4-O3
28	l	102	SQD	C15-C16-C17-C18
29	A	613	LMG	C12-C13-C14-C15
28	l	102	SQD	C28-C29-C30-C31
33	B	636	PG4	O3-C5-C6-O4
35	C	541	P6G	O13-C14-C15-O16
28	A	622	SQD	C27-C28-C29-C30
34	b	643	PGE	O2-C3-C4-O3
35	b	649	P6G	O13-C14-C15-O16
39	B	653	1PE	OH5-C14-C24-OH4
40	c	516	DGD	C4D-C5D-C6D-O5D
24	b	611	CLA	O1D-CGD-O2D-CED
28	a	413	SQD	C9-C10-C11-C12
31	u	203	LMT	C11-C10-C9-C8
32	D	411	LHG	C17-C18-C19-C20
34	D	415	PGE	O2-C3-C4-O3
35	E	110	P6G	O10-C11-C12-O13
40	c	518	DGD	C9B-CAB-CBB-CCB
29	c	520	LMG	C10-C11-C12-C13
29	c	519	LMG	C11-C10-O7-C8
32	E	101	LHG	C8-C7-O7-C5
28	a	413	SQD	C34-C35-C36-C37
28	l	102	SQD	C10-C11-C12-C13
31	M	102	LMT	C2-C3-C4-C5
33	c	533	PG4	O3-C5-C6-O4
34	h	109	PGE	O2-C3-C4-O3
38	C	531	HTG	C4-C5-C6-O6
24	c	506	CLA	C5-C6-C7-C8
31	B	622	LMT	C2-C3-C4-C5
40	d	408	DGD	C4A-C5A-C6A-C7A
29	a	414	LMG	O9-C10-O7-C8
29	A	613	LMG	C10-C11-C12-C13
29	B	634	LMG	C29-C30-C31-C32
29	b	621	LMG	C35-C36-C37-C38
32	E	101	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
28	A	622	SQD	C2-C1-O6-C44
28	h	105	SQD	C2-C1-O6-C44
32	a	419	LHG	O7-C5-C6-O8
29	J	101	LMG	O6-C5-C6-O5
31	I	101	LMT	O5B-C5B-C6B-O6B
29	z	101	LMG	C15-C16-C17-C18
31	A	617	LMT	O1'-C1-C2-C3
40	d	408	DGD	C5A-C6A-C7A-C8A
33	C	537	PG4	O4-C7-C8-O5
33	V	213	PG4	O1-C1-C2-O2
33	i	103	PG4	O1-C1-C2-O2
34	B	645	PGE	O1-C1-C2-O2
34	V	215	PGE	O1-C1-C2-O2
34	b	643	PGE	O1-C1-C2-O2
24	B	611	CLA	C13-C15-C16-C17
27	a	412	PL9	C4-C3-C7-C8
29	A	613	LMG	C18-C19-C20-C21
29	c	519	LMG	C32-C33-C34-C35
24	C	508	CLA	C11-C10-C8-C9
24	D	405	CLA	C11-C10-C8-C9
31	j	103	LMT	C1-C2-C3-C4
40	c	516	DGD	O6D-C5D-C6D-O5D
28	A	622	SQD	C26-C27-C28-C29
31	Y	101	LMT	C11-C10-C9-C8
33	X	102	PG4	O2-C3-C4-O3
29	c	520	LMG	O10-C28-O8-C9
24	B	611	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C20
24	b	611	CLA	C16-C17-C18-C19
24	c	512	CLA	C16-C17-C18-C19
32	E	101	LHG	O9-C7-O7-C5
29	a	414	LMG	C11-C10-O7-C8
28	F	104	SQD	C9-C10-C11-C12
28	h	105	SQD	C27-C28-C29-C30
24	c	509	CLA	C13-C15-C16-C17
32	d	410	LHG	C3-O3-P-O6
28	h	105	SQD	C31-C32-C33-C34
32	e	101	LHG	C11-C12-C13-C14
33	e	104	PG4	O3-C5-C6-O4
29	j	101	LMG	O6-C5-C6-O5
29	a	414	LMG	C33-C34-C35-C36
35	D	418	P6G	O4-C5-C6-O7

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Mol	Chain	Res	Type	Atoms
40	d	408	DGD	CDA-CEA-CFA-CGA
32	a	419	LHG	C31-C32-C33-C34
28	a	424	SQD	C23-C24-C25-C26
29	a	414	LMG	C35-C36-C37-C38
33	B	643	PG4	O2-C3-C4-O3
33	C	537	PG4	O3-C5-C6-O4
40	c	516	DGD	CAA-CBA-CCA-CDA
31	Y	101	LMT	C1-C2-C3-C4
32	l	101	LHG	C5-C6-O8-C23
31	I	101	LMT	C4-C5-C6-C7
32	d	409	LHG	C29-C30-C31-C32
29	c	519	LMG	C21-C22-C23-C24
34	E	105	PGE	O2-C3-C4-O3
40	c	516	DGD	C4A-C5A-C6A-C7A
29	A	613	LMG	C17-C18-C19-C20
29	c	519	LMG	C16-C17-C18-C19
33	A	619	PG4	O3-C5-C6-O4
33	H	105	PG4	O3-C5-C6-O4
33	B	642	PG4	O2-C3-C4-O3
38	O	303	HTG	C3'-C4'-C5'-C6'
32	B	632	LHG	C13-C14-C15-C16
29	d	412	LMG	O6-C5-C6-O5
33	B	638	PG4	O1-C1-C2-O2
33	B	639	PG4	O4-C7-C8-O5
33	B	642	PG4	O4-C7-C8-O5
33	B	643	PG4	O4-C7-C8-O5
33	C	535	PG4	O1-C1-C2-O2
33	C	535	PG4	O4-C7-C8-O5
33	I	102	PG4	O1-C1-C2-O2
33	V	209	PG4	O4-C7-C8-O5
33	V	212	PG4	O1-C1-C2-O2
33	X	103	PG4	O1-C1-C2-O2
33	a	421	PG4	O1-C1-C2-O2
33	a	421	PG4	O4-C7-C8-O5
33	b	636	PG4	O1-C1-C2-O2
33	b	636	PG4	O4-C7-C8-O5
33	c	532	PG4	O4-C7-C8-O5
33	h	106	PG4	O4-C7-C8-O5
33	i	101	PG4	O4-C7-C8-O5
33	i	104	PG4	O1-C1-C2-O2
33	l	103	PG4	O4-C7-C8-O5
34	B	645	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
34	B	647	PGE	O1-C1-C2-O2
34	C	540	PGE	O1-C1-C2-O2
34	D	415	PGE	O1-C1-C2-O2
34	E	109	PGE	O3-C5-C6-O4
34	H	109	PGE	O1-C1-C2-O2
34	H	109	PGE	O3-C5-C6-O4
34	H	110	PGE	O1-C1-C2-O2
34	H	111	PGE	O1-C1-C2-O2
34	J	107	PGE	O3-C5-C6-O4
34	O	308	PGE	O1-C1-C2-O2
34	O	310	PGE	O3-C5-C6-O4
34	T	104	PGE	O2-C3-C4-O3
34	V	214	PGE	O3-C5-C6-O4
34	b	640	PGE	O1-C1-C2-O2
34	h	108	PGE	O3-C5-C6-O4
34	i	105	PGE	O1-C1-C2-O2
34	o	309	PGE	O3-C5-C6-O4
35	A	624	P6G	O1-C2-C3-O4
35	D	418	P6G	O1-C2-C3-O4
35	b	648	P6G	O16-C17-C18-O19
35	b	649	P6G	O1-C2-C3-O4
35	b	649	P6G	O16-C17-C18-O19
35	j	106	P6G	O16-C17-C18-O19
45	i	107	PE8	O1-C2-C3-O4
28	A	622	SQD	C44-C45-C46-O48
28	a	413	SQD	O6-C44-C45-C46
29	A	613	LMG	C7-C8-C9-O8
29	A	613	LMG	C30-C31-C32-C33
29	B	634	LMG	C7-C8-C9-O8
29	C	519	LMG	C7-C8-C9-O8
29	a	414	LMG	C7-C8-C9-O8
29	b	621	LMG	C39-C40-C41-C42
29	z	101	LMG	C7-C8-C9-O8
32	A	618	LHG	C4-C5-C6-O8
32	a	419	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
40	D	408	DGD	O1G-C1G-C2G-C3G
40	D	408	DGD	C1G-C2G-C3G-O3G
29	z	101	LMG	C12-C13-C14-C15
32	B	632	LHG	C28-C29-C30-C31
32	l	101	LHG	C13-C14-C15-C16
40	C	516	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
28	a	424	SQD	C45-C44-O6-C1
29	C	526	LMG	C8-C7-O1-C1
29	c	520	LMG	C8-C7-O1-C1
29	z	101	LMG	C8-C7-O1-C1
40	C	517	DGD	C2G-C3G-O3G-C1D
40	C	517	DGD	C5D-C6D-O5D-C1E
40	D	408	DGD	C2G-C3G-O3G-C1D
40	c	517	DGD	C5D-C6D-O5D-C1E
28	a	424	SQD	C28-C29-C30-C31
29	C	526	LMG	C42-C43-C44-C45
29	d	412	LMG	C24-C25-C26-C27
24	b	616	CLA	C10-C11-C12-C13
24	A	606	CLA	C2C-C3C-CAC-CBC
28	a	413	SQD	C15-C16-C17-C18
28	x	101	SQD	C35-C36-C37-C38
32	E	101	LHG	C10-C11-C12-C13
33	H	105	PG4	O2-C3-C4-O3
39	L	101	1PE	C12-C22-OH3-C23
31	J	103	LMT	O5B-C5B-C6B-O6B
31	c	521	LMT	O5'-C5'-C6'-O6'
30	a	416	GOL	O2-C2-C3-O3
29	C	519	LMG	O10-C28-O8-C9
40	C	516	DGD	O6E-C5E-C6E-O5E
40	C	517	DGD	C4A-C5A-C6A-C7A
40	d	408	DGD	C7A-C8A-C9A-CAA
28	A	616	SQD	C30-C31-C32-C33
40	c	516	DGD	O6E-C5E-C6E-O5E
27	A	611	PL9	C30-C29-C31-C32
28	a	413	SQD	C31-C32-C33-C34
34	E	109	PGE	O2-C3-C4-O3
38	B	630	HTG	C4'-C5'-C6'-C7'
40	d	408	DGD	C1A-C2A-C3A-C4A
24	A	607	CLA	C11-C12-C13-C15
28	b	633	SQD	C33-C34-C35-C36
29	A	613	LMG	C34-C35-C36-C37
29	d	412	LMG	C14-C15-C16-C17
24	b	604	CLA	C5-C6-C7-C8
31	b	622	LMT	C3'-C4'-O1B-C1B
33	i	102	PG4	O2-C3-C4-O3
39	L	101	1PE	OH5-C14-C24-OH4
28	a	424	SQD	C46-C45-O47-C7
28	b	633	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
24	B	617	CLA	C2-C1-O2A-CGA
24	b	617	CLA	C2-C1-O2A-CGA
35	A	624	P6G	O4-C5-C6-O7
28	a	417	SQD	C31-C32-C33-C34
28	h	105	SQD	C19-C20-C21-C22
29	j	101	LMG	C16-C17-C18-C19
40	c	517	DGD	C7B-C8B-C9B-CAB
24	C	503	CLA	O1D-CGD-O2D-CED
24	c	513	CLA	C10-C11-C12-C13
29	C	526	LMG	C29-C30-C31-C32
29	a	414	LMG	C39-C40-C41-C42
31	C	533	LMT	C7-C8-C9-C10
33	H	107	PG4	O2-C3-C4-O3
40	C	517	DGD	CBB-CCB-CDB-CEB
24	A	609	CLA	C16-C17-C18-C20
32	e	101	LHG	C23-C24-C25-C26
28	A	612	SQD	C28-C29-C30-C31
32	A	618	LHG	C14-C15-C16-C17
33	B	637	PG4	O4-C7-C8-O5
33	B	640	PG4	O4-C7-C8-O5
33	C	534	PG4	O1-C1-C2-O2
33	H	106	PG4	O4-C7-C8-O5
33	V	211	PG4	O1-C1-C2-O2
33	X	102	PG4	O4-C7-C8-O5
33	i	101	PG4	O1-C1-C2-O2
34	j	105	PGE	O3-C5-C6-O4
34	o	307	PGE	O3-C5-C6-O4
34	o	309	PGE	O1-C1-C2-O2
29	z	101	LMG	C21-C22-C23-C24
31	a	401	LMT	C9-C10-C11-C12
40	d	408	DGD	CFB-CGB-CHB-CIB
38	b	623	HTG	C4'-C5'-C6'-C7'
28	a	413	SQD	O6-C44-C45-O47
25	D	401	PHO	C2C-C3C-CAC-CBC
28	A	616	SQD	C19-C20-C21-C22
28	b	633	SQD	C30-C31-C32-C33
29	B	621	LMG	C29-C30-C31-C32
29	c	520	LMG	C31-C32-C33-C34
32	B	632	LHG	C14-C15-C16-C17
28	a	417	SQD	C29-C30-C31-C32
40	c	516	DGD	C9A-CAA-CBA-CCA
40	c	516	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
40	h	104	DGD	CCA-CDA-CEA-CFA
29	B	621	LMG	C30-C31-C32-C33
31	b	622	LMT	C5'-C4'-O1B-C1B
28	h	105	SQD	C32-C33-C34-C35
24	b	602	CLA	C6-C7-C8-C9
29	C	526	LMG	C11-C12-C13-C14
29	C	526	LMG	C33-C34-C35-C36
29	d	412	LMG	C17-C18-C19-C20
38	V	204	HTG	C2'-C3'-C4'-C5'
40	C	517	DGD	C4B-C5B-C6B-C7B
31	J	103	LMT	C6-C7-C8-C9
31	f	101	LMT	C11-C10-C9-C8
32	A	618	LHG	C15-C16-C17-C18
24	b	604	CLA	O1D-CGD-O2D-CED
26	b	620	BCR	C7-C8-C9-C34
32	e	101	LHG	C13-C14-C15-C16
30	C	528	GOL	C1-C2-C3-O3
26	C	515	BCR	C21-C22-C23-C24
28	A	616	SQD	C28-C29-C30-C31
29	d	412	LMG	C40-C41-C42-C43
28	a	424	SQD	C16-C17-C18-C19
29	c	520	LMG	C40-C41-C42-C43
31	C	533	LMT	C9-C10-C11-C12
31	c	521	LMT	C7-C8-C9-C10
33	H	107	PG4	O3-C5-C6-O4
28	l	102	SQD	C29-C30-C31-C32
39	L	101	1PE	OH4-C13-C23-OH3
24	C	509	CLA	C13-C15-C16-C17
24	d	405	CLA	C10-C11-C12-C13
40	H	103	DGD	C9B-CAB-CBB-CCB
28	x	101	SQD	C24-C25-C26-C27
24	b	615	CLA	C16-C17-C18-C20
32	a	419	LHG	O6-C4-C5-C6
34	E	107	PGE	O1-C1-C2-O2
27	d	407	PL9	C39-C41-C42-C43
32	D	410	LHG	C32-C33-C34-C35
40	C	518	DGD	C9B-CAB-CBB-CCB
27	A	611	PL9	C28-C29-C31-C32
29	z	101	LMG	C35-C36-C37-C38
33	j	104	PG4	C8-C7-O4-C6
35	T	105	P6G	O7-C8-C9-O10
29	A	613	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
33	B	639	PG4	O3-C5-C6-O4
40	h	104	DGD	CDB-CEB-CFB-CGB
32	E	101	LHG	C12-C13-C14-C15
38	C	521	HTG	C2'-C3'-C4'-C5'
29	b	621	LMG	C38-C39-C40-C41
31	C	533	LMT	C6-C7-C8-C9
31	m	101	LMT	C9-C10-C11-C12
28	a	424	SQD	C30-C31-C32-C33
28	l	102	SQD	C14-C15-C16-C17
31	b	622	LMT	C2-C3-C4-C5
34	O	309	PGE	O2-C3-C4-O3
40	c	518	DGD	C3B-C4B-C5B-C6B
31	m	101	LMT	C2-C1-O1'-C1'
31	u	203	LMT	C2-C1-O1'-C1'
32	A	618	LHG	C9-C10-C11-C12
24	c	509	CLA	C3-C5-C6-C7
24	C	513	CLA	C8-C10-C11-C12
29	a	414	LMG	C22-C23-C24-C25
31	t	103	LMT	C6-C7-C8-C9
32	l	101	LHG	C32-C33-C34-C35
31	j	103	LMT	O5'-C5'-C6'-O6'
28	a	424	SQD	C25-C26-C27-C28
28	h	105	SQD	C17-C18-C19-C20
31	A	617	LMT	C5-C6-C7-C8
31	B	622	LMT	C4-C5-C6-C7
34	E	107	PGE	O2-C3-C4-O3
40	C	517	DGD	C5B-C6B-C7B-C8B
28	A	616	SQD	O6-C44-C45-C46
28	a	417	SQD	O6-C44-C45-C46
28	b	633	SQD	C44-C45-C46-O48
28	h	105	SQD	O6-C44-C45-C46
40	d	408	DGD	O1G-C1G-C2G-C3G
29	B	621	LMG	C36-C37-C38-C39
34	b	647	PGE	O2-C3-C4-O3
29	a	414	LMG	C19-C20-C21-C22
29	z	101	LMG	C14-C15-C16-C17
34	h	108	PGE	O2-C3-C4-O3
40	h	104	DGD	C9B-CAB-CBB-CCB
40	D	408	DGD	C8A-C9A-CAA-CBA
33	V	212	PG4	O2-C3-C4-O3
35	I	106	P6G	C14-C15-O16-C17
24	c	506	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C2-C3-C5-C6
40	D	408	DGD	CDB-CEB-CFB-CGB
28	h	105	SQD	C25-C26-C27-C28
40	H	103	DGD	C6B-C7B-C8B-C9B
44	V	216	2PE	O10-C11-C12-O13
24	B	602	CLA	C3-C5-C6-C7
30	B	633	GOL	O1-C1-C2-O2
30	C	527	GOL	O1-C1-C2-O2
30	D	412	GOL	O1-C1-C2-O2
30	F	101	GOL	O2-C2-C3-O3
30	O	307	GOL	O2-C2-C3-O3
29	b	621	LMG	C40-C41-C42-C43
40	c	516	DGD	CCA-CDA-CEA-CFA
32	a	419	LHG	O6-C4-C5-O7
40	C	516	DGD	C4D-C5D-C6D-O5D
38	c	531	HTG	C2'-C3'-C4'-C5'
38	b	624	HTG	C1'-C2'-C3'-C4'
31	C	533	LMT	O5'-C5'-C6'-O6'
24	B	611	CLA	C16-C17-C18-C19
31	Y	101	LMT	C2-C3-C4-C5
40	h	104	DGD	O2G-C1B-C2B-C3B
28	a	424	SQD	C14-C15-C16-C17
29	C	520	LMG	C15-C16-C17-C18
31	c	521	LMT	C5-C6-C7-C8
31	j	103	LMT	C2-C3-C4-C5
40	c	518	DGD	C6A-C7A-C8A-C9A
32	e	101	LHG	C26-C27-C28-C29
38	c	531	HTG	C3'-C4'-C5'-C6'
28	A	622	SQD	C16-C17-C18-C19
33	H	106	PG4	O3-C5-C6-O4
34	D	415	PGE	C1-C2-O2-C3
28	b	633	SQD	O47-C45-C46-O48
28	x	101	SQD	O47-C45-C46-O48
29	B	634	LMG	O7-C8-C9-O8
29	z	101	LMG	O1-C7-C8-O7
40	d	408	DGD	O1G-C1G-C2G-O2G
24	D	403	CLA	C2C-C3C-CAC-CBC
29	C	526	LMG	C23-C24-C25-C26
34	B	648	PGE	O2-C3-C4-O3
24	A	607	CLA	C11-C12-C13-C14
24	c	512	CLA	C16-C17-C18-C20
29	B	634	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	C	520	LMG	C40-C41-C42-C43
29	c	519	LMG	C39-C40-C41-C42
40	C	516	DGD	C7B-C8B-C9B-CAB
24	A	609	CLA	C11-C10-C8-C9
39	B	653	1PE	OH4-C13-C23-OH3
32	a	419	LHG	C28-C29-C30-C31
32	a	419	LHG	C29-C30-C31-C32
40	C	517	DGD	CDB-CEB-CFB-CGB
32	A	618	LHG	C24-C25-C26-C27
32	D	411	LHG	C10-C11-C12-C13
33	c	533	PG4	O2-C3-C4-O3
26	B	620	BCR	C5-C6-C7-C8
26	b	618	BCR	C1-C6-C7-C8
26	t	102	BCR	C23-C24-C25-C26
34	J	107	PGE	O1-C1-C2-O2
35	T	105	P6G	O16-C17-C18-O19
39	e	105	1PE	OH2-C12-C22-OH3
24	B	614	CLA	C13-C15-C16-C17
26	A	610	BCR	C36-C18-C19-C20
36	E	111	EDO	O1-C1-C2-O2
33	e	103	PG4	O2-C3-C4-O3
40	C	517	DGD	C3A-C4A-C5A-C6A
26	c	527	BCR	C7-C8-C9-C10
24	b	617	CLA	C5-C6-C7-C8
28	x	101	SQD	C29-C30-C31-C32
29	z	101	LMG	C36-C37-C38-C39
29	A	613	LMG	C14-C15-C16-C17
40	D	408	DGD	C8B-C9B-CAB-CBB
31	m	102	LMT	O5'-C5'-C6'-O6'
24	C	503	CLA	C8-C10-C11-C12
28	A	616	SQD	C27-C28-C29-C30
29	c	519	LMG	C22-C23-C24-C25
32	e	101	LHG	C14-C15-C16-C17
32	l	101	LHG	C10-C11-C12-C13
28	h	105	SQD	O47-C7-C8-C9
24	A	609	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	b	602	CLA	C6-C7-C8-C10
24	b	605	CLA	C6-C7-C8-C10
34	b	645	PGE	C1-C2-O2-C3
33	I	104	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
40	d	408	DGD	CCB-CDB-CEB-CFB
40	h	104	DGD	C5B-C6B-C7B-C8B
33	C	534	PG4	C6-C5-O3-C4
24	c	509	CLA	C15-C16-C17-C18
33	b	636	PG4	O3-C5-C6-O4
34	B	650	PGE	O2-C3-C4-O3
44	V	216	2PE	O13-C14-C15-O16
24	b	605	CLA	C13-C15-C16-C17
28	F	104	SQD	C29-C30-C31-C32
34	t	104	PGE	O2-C3-C4-O3
38	C	522	HTG	O5-C1-S1-C1'
38	c	522	HTG	C2'-C1'-S1-C1
38	h	101	HTG	C2'-C1'-S1-C1
31	C	533	LMT	C1-C2-C3-C4
28	a	413	SQD	C24-C23-O48-C46
28	x	101	SQD	C14-C15-C16-C17
31	m	101	LMT	C2-C3-C4-C5
33	E	102	PG4	C3-C4-O3-C5
33	j	104	PG4	C3-C4-O3-C5
33	B	643	PG4	O1-C1-C2-O2
34	E	109	PGE	O1-C1-C2-O2
34	O	309	PGE	O1-C1-C2-O2
34	h	110	PGE	O1-C1-C2-O2
45	i	107	PE8	O22-C23-C24-O25
33	B	643	PG4	C4-C3-O2-C2
33	C	537	PG4	C1-C2-O2-C3
33	j	104	PG4	C4-C3-O2-C2
34	C	539	PGE	C3-C4-O3-C5
34	h	109	PGE	C3-C4-O3-C5
35	D	417	P6G	C2-C3-O4-C5
35	b	648	P6G	O13-C14-C15-O16
28	F	104	SQD	C11-C10-C9-C8
28	x	101	SQD	C26-C27-C28-C29
29	C	520	LMG	C30-C31-C32-C33
29	J	101	LMG	C35-C36-C37-C38
34	c	537	PGE	C1-C2-O2-C3
34	c	538	PGE	C3-C4-O3-C5
34	c	540	PGE	C1-C2-O2-C3
34	o	309	PGE	C6-C5-O3-C4
35	C	541	P6G	C18-C17-O16-C15
39	V	217	1PE	C23-C13-OH4-C24
39	x	104	1PE	C13-C23-OH3-C22

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Mol	Chain	Res	Type	Atoms
40	C	518	DGD	C2B-C3B-C4B-C5B
45	i	107	PE8	O4-C5-C6-O7
24	A	606	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	510	CLA	CAD-CBD-CGD-O2D
24	C	512	CLA	CAD-CBD-CGD-O2D
24	D	405	CLA	CAD-CBD-CGD-O2D
24	b	611	CLA	CAD-CBD-CGD-O2D
24	c	501	CLA	CAD-CBD-CGD-O2D
24	c	512	CLA	CAD-CBD-CGD-O2D
24	d	405	CLA	CAD-CBD-CGD-O2D
25	A	608	PHO	CAD-CBD-CGD-O2D
28	A	622	SQD	C44-C45-O47-C7
32	a	419	LHG	C4-C5-O7-C7
29	z	101	LMG	C24-C25-C26-C27
32	e	101	LHG	C10-C11-C12-C13
33	B	640	PG4	C5-C6-O4-C7
34	A	620	PGE	C4-C3-O2-C2
34	B	648	PGE	C1-C2-O2-C3
34	b	646	PGE	C4-C3-O2-C2
35	B	652	P6G	C18-C17-O16-C15
38	C	531	HTG	C3'-C4'-C5'-C6'
40	C	516	DGD	C8B-C9B-CAB-CBB
24	c	509	CLA	C10-C11-C12-C13
29	C	520	LMG	C32-C33-C34-C35
33	C	536	PG4	C1-C2-O2-C3
33	i	101	PG4	C6-C5-O3-C4
35	A	623	P6G	C12-C11-O10-C9
35	b	649	P6G	C14-C15-O16-C17
33	b	635	PG4	C4-C3-O2-C2
33	h	106	PG4	C3-C4-O3-C5
34	B	649	PGE	C1-C2-O2-C3
34	B	649	PGE	C6-C5-O3-C4
34	H	108	PGE	C6-C5-O3-C4
35	D	416	P6G	C15-C14-O13-C12
35	E	110	P6G	C5-C6-O7-C8
35	T	105	P6G	C15-C14-O13-C12
35	b	649	P6G	C18-C17-O16-C15
38	C	529	HTG	C4'-C5'-C6'-C7'
40	C	517	DGD	C7A-C8A-C9A-CAA
24	B	609	CLA	C13-C15-C16-C17
33	e	104	PG4	C8-C7-O4-C6

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Mol	Chain	Res	Type	Atoms
34	C	540	PGE	C3-C4-O3-C5
38	B	631	HTG	C4'-C5'-C6'-C7'
45	i	107	PE8	C21-C20-O19-C18
28	A	612	SQD	O6-C44-C45-C46
28	x	101	SQD	C44-C45-C46-O48
29	z	101	LMG	O1-C7-C8-C9
32	e	101	LHG	C2-C3-O3-P
29	C	519	LMG	C11-C10-O7-C8
29	d	412	LMG	C15-C16-C17-C18
34	E	105	PGE	C6-C5-O3-C4
35	d	415	P6G	C15-C14-O13-C12
29	C	526	LMG	C15-C16-C17-C18
31	b	622	LMT	C6-C7-C8-C9
33	j	104	PG4	C5-C6-O4-C7
35	T	105	P6G	C6-C5-O4-C3
39	V	217	1PE	C15-C25-OH5-C14
29	j	101	LMG	C40-C41-C42-C43
33	V	209	PG4	C5-C6-O4-C7
33	b	635	PG4	C3-C4-O3-C5
24	B	603	CLA	CHA-CBD-CGD-O1D
24	B	603	CLA	CHA-CBD-CGD-O2D
24	C	502	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CHA-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	510	CLA	CHA-CBD-CGD-O1D
24	D	403	CLA	CHA-CBD-CGD-O1D
24	b	602	CLA	CHA-CBD-CGD-O1D
24	b	602	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CHA-CBD-CGD-O1D
24	c	502	CLA	CHA-CBD-CGD-O2D
24	c	504	CLA	CHA-CBD-CGD-O1D
24	c	504	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
33	V	212	PG4	C8-C7-O4-C6
34	b	643	PGE	C4-C3-O2-C2
34	c	540	PGE	C3-C4-O3-C5
35	B	652	P6G	C15-C14-O13-C12
28	a	413	SQD	O10-C23-O48-C46
29	b	621	LMG	C29-C30-C31-C32
33	X	101	PG4	C5-C6-O4-C7
33	c	533	PG4	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
33	e	104	PG4	C5-C6-O4-C7
34	B	645	PGE	C3-C4-O3-C5
34	E	107	PGE	C3-C4-O3-C5
34	I	105	PGE	C6-C5-O3-C4
34	O	309	PGE	C4-C3-O2-C2
34	o	308	PGE	C6-C5-O3-C4
35	A	623	P6G	C18-C17-O16-C15
35	I	106	P6G	C18-C17-O16-C15
39	e	105	1PE	C14-C24-OH4-C13
39	x	104	1PE	C16-C26-OH6-C15
33	B	643	PG4	C8-C7-O4-C6
33	H	104	PG4	C6-C5-O3-C4
33	H	105	PG4	C3-C4-O3-C5
33	J	104	PG4	C4-C3-O2-C2
33	b	636	PG4	C6-C5-O3-C4
33	b	637	PG4	C5-C6-O4-C7
34	O	310	PGE	C4-C3-O2-C2
34	o	306	PGE	C6-C5-O3-C4
34	t	105	PGE	C6-C5-O3-C4
35	A	624	P6G	C8-C9-O10-C11
35	T	105	P6G	C11-C12-O13-C14
28	A	612	SQD	O6-C44-C45-O47
28	F	104	SQD	O47-C45-C46-O48
28	h	105	SQD	O6-C44-C45-O47
29	C	520	LMG	O1-C7-C8-O7
29	a	414	LMG	O7-C8-C9-O8
29	z	101	LMG	O7-C8-C9-O8
40	D	408	DGD	O2G-C2G-C3G-O3G
29	b	621	LMG	C32-C33-C34-C35
33	E	103	PG4	C3-C4-O3-C5
45	i	107	PE8	C2-C3-O4-C5
29	C	520	LMG	C11-C12-C13-C14
31	c	521	LMT	C9-C10-C11-C12
30	D	412	GOL	O2-C2-C3-O3
30	O	305	GOL	O2-C2-C3-O3
30	V	208	GOL	O1-C1-C2-O2
30	V	208	GOL	O2-C2-C3-O3
29	A	613	LMG	C22-C23-C24-C25
32	B	632	LHG	C10-C11-C12-C13
33	I	102	PG4	C5-C6-O4-C7
33	E	102	PG4	O4-C7-C8-O5
35	b	648	P6G	O1-C2-C3-O4

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Mol	Chain	Res	Type	Atoms
29	J	101	LMG	C36-C37-C38-C39
32	d	411	LHG	C14-C15-C16-C17
31	b	622	LMT	O5B-C5B-C6B-O6B
34	a	422	PGE	C1-C2-O2-C3
34	H	110	PGE	O2-C3-C4-O3
34	o	308	PGE	C4-C3-O2-C2
35	d	416	P6G	C9-C8-O7-C6
38	c	522	HTG	C2'-C3'-C4'-C5'
24	c	501	CLA	CBD-CGD-O2D-CED
34	b	647	PGE	C1-C2-O2-C3
24	b	616	CLA	C5-C6-C7-C8
24	C	507	CLA	C16-C17-C18-C19
33	V	212	PG4	C1-C2-O2-C3
34	h	110	PGE	C6-C5-O3-C4
24	C	501	CLA	C2A-CAA-CBA-CGA
29	A	613	LMG	O8-C28-C29-C30
40	H	103	DGD	O2G-C1B-C2B-C3B
29	A	613	LMG	C29-C30-C31-C32
31	Y	101	LMT	C3'-C4'-O1B-C1B
40	H	103	DGD	CDB-CEB-CFB-CGB
40	d	408	DGD	C8B-C9B-CAB-CBB
29	B	621	LMG	C12-C13-C14-C15
28	l	102	SQD	C35-C36-C37-C38
33	b	637	PG4	C4-C3-O2-C2
29	B	634	LMG	C4-C5-C6-O5
38	B	624	HTG	C4-C5-C6-O6
29	C	519	LMG	C28-C29-C30-C31
31	A	617	LMT	C4-C5-C6-C7
39	B	654	1PE	C13-C23-OH3-C22
31	F	102	LMT	C9-C10-C11-C12
34	C	539	PGE	O2-C3-C4-O3
40	c	518	DGD	C8A-C9A-CAA-CBA
28	a	413	SQD	C13-C14-C15-C16
28	a	424	SQD	C27-C28-C29-C30
32	d	411	LHG	C18-C19-C20-C21
40	D	408	DGD	CFA-CGA-CHA-CIA
24	B	605	CLA	C3-C5-C6-C7
32	D	411	LHG	C2-C3-O3-P
32	d	411	LHG	C2-C3-O3-P
29	a	414	LMG	C17-C18-C19-C20
40	h	104	DGD	C7A-C8A-C9A-CAA
32	A	618	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
32	B	632	LHG	C4-O6-P-O5
32	D	410	LHG	C4-O6-P-O4
32	d	410	LHG	C3-O3-P-O4
32	l	101	LHG	C4-O6-P-O5
24	D	405	CLA	C16-C17-C18-C19
29	b	621	LMG	C14-C15-C16-C17
32	A	618	LHG	O6-C4-C5-C6
33	C	534	PG4	O4-C7-C8-O5
33	H	105	PG4	O1-C1-C2-O2
33	I	104	PG4	O1-C1-C2-O2
34	D	415	PGE	O3-C5-C6-O4
34	i	105	PGE	O3-C5-C6-O4
38	C	530	HTG	C1'-C2'-C3'-C4'
29	d	412	LMG	C39-C40-C41-C42
34	E	109	PGE	C3-C4-O3-C5
29	a	414	LMG	C31-C32-C33-C34
34	h	107	PGE	C3-C4-O3-C5
24	A	609	CLA	C3-C5-C6-C7
28	F	104	SQD	C19-C20-C21-C22
28	b	633	SQD	C18-C19-C20-C21
28	x	101	SQD	C19-C20-C21-C22
29	j	101	LMG	C39-C40-C41-C42
33	J	105	PG4	C3-C4-O3-C5
34	h	108	PGE	C6-C5-O3-C4
34	t	104	PGE	C4-C3-O2-C2
40	d	408	DGD	C2A-C3A-C4A-C5A
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	b	602	CLA	CAD-CBD-CGD-O1D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
28	A	622	SQD	O5-C5-C6-S
28	a	424	SQD	O5-C5-C6-S
28	x	101	SQD	O5-C5-C6-S
28	b	633	SQD	O47-C7-C8-C9
40	c	517	DGD	C9B-CAB-CBB-CCB
40	c	518	DGD	CDB-CEB-CFB-CGB
34	B	644	PGE	C6-C5-O3-C4
39	x	104	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
24	c	504	CLA	C8-C10-C11-C12
28	F	104	SQD	C18-C19-C20-C21
40	c	517	DGD	C4B-C5B-C6B-C7B
40	h	104	DGD	CBA-CCA-CDA-CEA
29	C	519	LMG	C19-C20-C21-C22
32	D	411	LHG	C30-C31-C32-C33
32	e	101	LHG	C16-C17-C18-C19
33	H	104	PG4	O2-C3-C4-O3
40	d	408	DGD	CBA-CCA-CDA-CEA
24	C	507	CLA	C4-C3-C5-C6
24	B	612	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
38	B	624	HTG	C2-C1-S1-C1'
38	C	522	HTG	C2-C1-S1-C1'
38	b	624	HTG	C2-C1-S1-C1'
34	h	109	PGE	C4-C3-O2-C2
40	H	103	DGD	C3B-C4B-C5B-C6B
40	c	518	DGD	C4A-C5A-C6A-C7A
40	d	408	DGD	C9A-CAA-CBA-CCA
32	e	101	LHG	C11-C10-C9-C8
31	m	102	LMT	C2-C1-O1'-C1'
31	M	101	LMT	O5'-C5'-C6'-O6'
29	C	520	LMG	C14-C15-C16-C17
32	D	410	LHG	C26-C27-C28-C29
34	V	214	PGE	C6-C5-O3-C4
34	o	309	PGE	C4-C3-O2-C2
28	a	413	SQD	C11-C10-C9-C8
29	C	526	LMG	C21-C22-C23-C24
33	I	103	PG4	O3-C5-C6-O4
24	B	617	CLA	C10-C11-C12-C13
35	A	624	P6G	O13-C14-C15-O16
35	B	652	P6G	O13-C14-C15-O16
32	B	632	LHG	C7-C8-C9-C10
28	F	104	SQD	C44-C45-C46-O48
28	a	424	SQD	O6-C44-C45-C46
28	x	101	SQD	C25-C26-C27-C28
29	C	526	LMG	C14-C15-C16-C17
29	d	412	LMG	O1-C7-C8-C9
29	z	101	LMG	C16-C17-C18-C19
29	A	613	LMG	O7-C8-C9-O8
29	d	412	LMG	O1-C7-C8-O7
32	e	101	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
40	D	408	DGD	O1G-C1G-C2G-O2G
31	Y	101	LMT	C5'-C4'-O1B-C1B
33	B	638	PG4	C8-C7-O4-C6
35	d	415	P6G	C8-C9-O10-C11
28	a	417	SQD	C15-C16-C17-C18
29	c	519	LMG	C40-C41-C42-C43
33	i	101	PG4	C1-C2-O2-C3
38	C	530	HTG	C4'-C5'-C6'-C7'
40	d	408	DGD	CAB-CBB-CCB-CDB
31	a	401	LMT	C3-C4-C5-C6
28	h	105	SQD	C45-C44-O6-C1
29	C	520	LMG	C8-C7-O1-C1
40	D	408	DGD	C5D-C6D-O5D-C1E
40	c	517	DGD	C2G-C3G-O3G-C1D
35	D	417	P6G	C14-C15-O16-C17
28	A	616	SQD	O10-C23-O48-C46
31	b	622	LMT	O5B-C1B-O1B-C4'
24	B	612	CLA	C14-C13-C15-C16
24	b	605	CLA	C6-C7-C8-C9
29	a	414	LMG	O10-C28-O8-C9
28	A	622	SQD	C32-C33-C34-C35
28	a	424	SQD	C24-C25-C26-C27
32	d	409	LHG	C11-C10-C9-C8
34	E	106	PGE	C4-C3-O2-C2
35	E	110	P6G	O13-C14-C15-O16
40	C	516	DGD	C2B-C3B-C4B-C5B
24	a	407	CLA	C4C-C3C-CAC-CBC
28	l	102	SQD	C25-C26-C27-C28
29	B	634	LMG	C15-C16-C17-C18
31	A	617	LMT	C7-C8-C9-C10
32	B	632	LHG	C11-C12-C13-C14
32	d	411	LHG	C24-C25-C26-C27
38	a	418	HTG	C4'-C5'-C6'-C7'
29	C	519	LMG	C30-C31-C32-C33
29	b	621	LMG	C36-C37-C38-C39
34	o	307	PGE	C4-C3-O2-C2
29	C	520	LMG	O10-C28-O8-C9
30	T	103	GOL	O1-C1-C2-O2
30	o	304	GOL	O1-C1-C2-O2
29	a	414	LMG	C16-C17-C18-C19
33	e	104	PG4	C3-C4-O3-C5
35	C	541	P6G	C8-C9-O10-C11

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Mol	Chain	Res	Type	Atoms
35	E	110	P6G	C8-C9-O10-C11
35	E	110	P6G	C18-C17-O16-C15
35	c	541	P6G	C18-C17-O16-C15
40	c	516	DGD	C3B-C4B-C5B-C6B
40	h	104	DGD	CBB-CCB-CDB-CEB
34	E	105	PGE	O1-C1-C2-O2
34	J	108	PGE	O3-C5-C6-O4
34	Y	102	PGE	O1-C1-C2-O2
34	H	109	PGE	C3-C4-O3-C5
32	D	409	LHG	C25-C26-C27-C28
33	I	102	PG4	C8-C7-O4-C6
33	I	103	PG4	O2-C3-C4-O3
35	T	105	P6G	C5-C6-O7-C8
38	c	531	HTG	C1'-C2'-C3'-C4'
28	a	424	SQD	C12-C13-C14-C15
33	b	634	PG4	C6-C5-O3-C4
32	A	618	LHG	C11-C10-C9-C8
38	B	630	HTG	C3'-C4'-C5'-C6'
44	V	216	2PE	O22-C23-C24-O25
29	b	621	LMG	C12-C13-C14-C15
33	I	104	PG4	C4-C3-O2-C2
40	C	518	DGD	C3B-C4B-C5B-C6B
40	c	517	DGD	C4A-C5A-C6A-C7A
29	z	101	LMG	C7-C8-O7-C10
34	B	644	PGE	O2-C3-C4-O3
35	T	105	P6G	O10-C11-C12-O13
24	C	509	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	c	509	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
28	A	616	SQD	C29-C30-C31-C32
28	A	622	SQD	C34-C35-C36-C37
33	B	640	PG4	C1-C2-O2-C3
33	E	102	PG4	C5-C6-O4-C7
33	V	210	PG4	O2-C3-C4-O3
34	b	638	PGE	C6-C5-O3-C4
39	B	653	1PE	C12-C22-OH3-C23
32	l	101	LHG	C12-C13-C14-C15
34	O	308	PGE	C1-C2-O2-C3
24	d	403	CLA	C4C-C3C-CAC-CBC
32	E	101	LHG	C25-C26-C27-C28
38	b	631	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
38	B	624	HTG	O5-C5-C6-O6
38	c	530	HTG	O5-C5-C6-O6
28	a	424	SQD	C11-C12-C13-C14
28	l	102	SQD	C12-C13-C14-C15
33	J	105	PG4	O4-C7-C8-O5
33	b	635	PG4	O1-C1-C2-O2
34	a	423	PGE	O3-C5-C6-O4
34	b	644	PGE	O1-C1-C2-O2
34	b	645	PGE	O1-C1-C2-O2
34	b	646	PGE	O1-C1-C2-O2
34	i	106	PGE	O3-C5-C6-O4
35	d	416	P6G	O1-C2-C3-O4
39	L	101	1PE	OH2-C12-C22-OH3
44	V	216	2PE	C9-C8-O7-C6
36	V	218	EDO	O1-C1-C2-O2
36	a	425	EDO	O1-C1-C2-O2
36	e	106	EDO	O1-C1-C2-O2
31	a	401	LMT	O5'-C5'-C6'-O6'
29	B	621	LMG	O8-C28-C29-C30
35	b	649	P6G	C11-C12-O13-C14
33	V	210	PG4	C5-C6-O4-C7
27	a	412	PL9	C39-C41-C42-C43
40	C	517	DGD	C2E-C1E-O5D-C6D
40	c	517	DGD	C2E-C1E-O5D-C6D
33	B	638	PG4	C6-C5-O3-C4
35	T	105	P6G	C18-C17-O16-C15
32	A	618	LHG	O7-C5-C6-O8
33	B	638	PG4	O2-C3-C4-O3
34	a	422	PGE	C6-C5-O3-C4
32	a	419	LHG	C4-O6-P-O3
32	e	101	LHG	C4-O6-P-O3
38	B	623	HTG	C2'-C3'-C4'-C5'
40	d	408	DGD	C7B-C8B-C9B-CAB
45	i	107	PE8	O19-C20-C21-O22
34	H	110	PGE	C3-C4-O3-C5
33	C	534	PG4	C8-C7-O4-C6
35	T	105	P6G	C14-C15-O16-C17
24	c	510	CLA	C8-C10-C11-C12
33	i	103	PG4	C3-C4-O3-C5
24	B	602	CLA	C4-C3-C5-C6
24	B	617	CLA	C6-C7-C8-C10
24	D	404	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	a	408	CLA	C6-C7-C8-C10
32	d	409	LHG	C26-C27-C28-C29
35	j	106	P6G	C6-C5-O4-C3
24	B	616	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	b	612	CLA	C14-C13-C15-C16
32	A	618	LHG	C29-C30-C31-C32
33	E	103	PG4	O2-C3-C4-O3
34	V	215	PGE	C1-C2-O2-C3
33	V	211	PG4	O4-C7-C8-O5
33	i	102	PG4	O1-C1-C2-O2
24	C	513	CLA	CBA-CGA-O2A-C1
33	X	103	PG4	C3-C4-O3-C5
33	E	102	PG4	C6-C5-O3-C4
34	H	111	PGE	O2-C3-C4-O3
35	D	416	P6G	C14-C15-O16-C17
39	e	105	1PE	OH4-C13-C23-OH3
24	b	615	CLA	C16-C17-C18-C19
29	a	414	LMG	C29-C28-O8-C9
30	b	625	GOL	C1-C2-C3-O3
30	v	207	GOL	O1-C1-C2-C3
28	A	622	SQD	C11-C10-C9-C8
28	a	417	SQD	C33-C34-C35-C36
39	j	107	1PE	C12-C22-OH3-C23
34	H	110	PGE	C6-C5-O3-C4
29	C	520	LMG	C18-C19-C20-C21
30	B	627	GOL	O1-C1-C2-O2
30	C	523	GOL	O1-C1-C2-O2
30	b	625	GOL	O2-C2-C3-O3
30	c	528	GOL	O2-C2-C3-O3
24	c	511	CLA	CBA-CGA-O2A-C1
28	A	616	SQD	C24-C23-O48-C46
29	C	520	LMG	C29-C28-O8-C9
31	A	617	LMT	C11-C10-C9-C8
27	a	412	PL9	C2-C3-C7-C8
28	F	104	SQD	C16-C17-C18-C19
28	a	417	SQD	C24-C25-C26-C27
35	D	418	P6G	C15-C14-O13-C12
28	h	105	SQD	C14-C15-C16-C17
33	c	532	PG4	C6-C5-O3-C4
34	Y	102	PGE	C6-C5-O3-C4
29	C	526	LMG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	O	310	PGE	C1-C2-O2-C3
32	A	618	LHG	C7-C8-C9-C10
29	C	526	LMG	C20-C21-C22-C23
34	b	641	PGE	C1-C2-O2-C3
40	C	517	DGD	O6E-C1E-O5D-C6D
40	c	517	DGD	O6E-C1E-O5D-C6D
33	B	642	PG4	O1-C1-C2-O2
34	i	106	PGE	O1-C1-C2-O2
35	E	110	P6G	O1-C2-C3-O4
27	D	407	PL9	C39-C41-C42-C43
24	C	513	CLA	O1A-CGA-O2A-C1
29	A	613	LMG	C32-C33-C34-C35
34	H	108	PGE	C4-C3-O2-C2
27	A	611	PL9	C31-C32-C33-C34
29	j	101	LMG	C36-C37-C38-C39
33	i	103	PG4	C8-C7-O4-C6
40	D	408	DGD	C6A-C7A-C8A-C9A
45	i	107	PE8	C24-C23-O22-C21
24	a	410	CLA	C3-C5-C6-C7
34	H	108	PGE	C1-C2-O2-C3
24	c	510	CLA	C2-C3-C5-C6
34	b	644	PGE	O2-C3-C4-O3
40	C	516	DGD	CAB-CBB-CCB-CDB
31	b	622	LMT	C9-C10-C11-C12
32	A	618	LHG	C30-C31-C32-C33
40	h	104	DGD	C6B-C7B-C8B-C9B
34	J	106	PGE	C4-C3-O2-C2
29	c	519	LMG	C29-C30-C31-C32
28	A	616	SQD	C2-C1-O6-C44
40	c	516	DGD	C2E-C1E-O5D-C6D
28	a	417	SQD	C25-C26-C27-C28
35	A	624	P6G	C12-C11-O10-C9
40	D	408	DGD	CCB-CDB-CEB-CFB
44	V	216	2PE	C24-C23-O22-C21
29	B	634	LMG	C33-C34-C35-C36
44	V	216	2PE	C5-C6-O7-C8
29	d	412	LMG	C42-C43-C44-C45
35	D	416	P6G	C6-C5-O4-C3
34	V	214	PGE	O1-C1-C2-O2
24	B	602	CLA	C8-C10-C11-C12
34	b	642	PGE	O2-C3-C4-O3
40	C	517	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
33	V	213	PG4	O2-C3-C4-O3
44	V	216	2PE	O19-C20-C21-O22
27	A	611	PL9	C4-C3-C7-C8
29	b	621	LMG	C31-C32-C33-C34
35	A	623	P6G	C15-C14-O13-C12
40	h	104	DGD	CCB-CDB-CEB-CFB
24	c	509	CLA	C11-C10-C8-C9
29	C	526	LMG	C36-C37-C38-C39
33	c	535	PG4	C8-C7-O4-C6
34	A	621	PGE	C3-C4-O3-C5
35	b	648	P6G	C5-C6-O7-C8
31	A	617	LMT	C2-C3-C4-C5
31	C	533	LMT	C5-C6-C7-C8
33	c	532	PG4	C8-C7-O4-C6
40	C	516	DGD	C6B-C7B-C8B-C9B
28	A	612	SQD	C30-C31-C32-C33
28	a	417	SQD	C11-C12-C13-C14
34	B	646	PGE	C1-C2-O2-C3
34	a	422	PGE	C3-C4-O3-C5
39	V	217	1PE	C16-C26-OH6-C15
24	C	501	CLA	C16-C17-C18-C20
24	C	507	CLA	C16-C17-C18-C20
24	D	405	CLA	C16-C17-C18-C20
24	c	512	CLA	O2A-C1-C2-C3
28	A	616	SQD	O5-C1-O6-C44
28	h	105	SQD	O5-C1-O6-C44
40	C	516	DGD	O6E-C1E-O5D-C6D
29	c	519	LMG	C36-C37-C38-C39
34	J	108	PGE	C1-C2-O2-C3
39	j	107	1PE	C14-C24-OH4-C13
38	C	531	HTG	O5-C5-C6-O6
45	i	107	PE8	C17-C18-O19-C20
40	d	408	DGD	C1G-C2G-O2G-C1B
24	b	602	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
24	A	609	CLA	C12-C13-C15-C16
24	a	410	CLA	C6-C7-C8-C10
24	b	612	CLA	C12-C13-C15-C16
31	b	622	LMT	C2B-C1B-O1B-C4'
33	i	103	PG4	O4-C7-C8-O5
34	E	106	PGE	O1-C1-C2-O2
34	J	106	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
28	a	413	SQD	C24-C25-C26-C27
40	C	518	DGD	C4A-C5A-C6A-C7A
29	C	526	LMG	C13-C14-C15-C16
34	C	539	PGE	C1-C2-O2-C3
32	l	101	LHG	C17-C18-C19-C20
24	b	617	CLA	C3-C5-C6-C7
38	c	523	HTG	C4-C5-C6-O6
24	C	510	CLA	C8-C10-C11-C12
34	B	645	PGE	C4-C3-O2-C2
40	H	103	DGD	CCB-CDB-CEB-CFB
31	Y	101	LMT	O5'-C5'-C6'-O6'
31	m	102	LMT	C7-C8-C9-C10
34	J	108	PGE	C4-C3-O2-C2
39	x	104	1PE	C14-C24-OH4-C13
24	c	512	CLA	C13-C15-C16-C17
29	C	526	LMG	C32-C33-C34-C35
28	a	417	SQD	C28-C29-C30-C31
29	d	412	LMG	C16-C17-C18-C19
24	B	603	CLA	C13-C15-C16-C17
24	B	604	CLA	C5-C6-C7-C8
29	B	621	LMG	C18-C19-C20-C21
40	C	516	DGD	O1B-C1B-O2G-C2G
40	c	518	DGD	C7A-C8A-C9A-CAA
28	A	612	SQD	C11-C10-C9-C8
38	b	623	HTG	C2'-C3'-C4'-C5'
39	e	105	1PE	C24-C14-OH5-C25
35	j	106	P6G	C15-C14-O13-C12
32	D	411	LHG	C28-C29-C30-C31
40	C	518	DGD	O6D-C5D-C6D-O5D
40	D	408	DGD	C2A-C3A-C4A-C5A
28	A	622	SQD	C18-C19-C20-C21
28	h	105	SQD	C13-C14-C15-C16
35	I	106	P6G	O10-C11-C12-O13
24	B	602	CLA	C2-C3-C5-C6
34	i	105	PGE	C1-C2-O2-C3
34	i	106	PGE	C4-C3-O2-C2
35	A	624	P6G	C6-C5-O4-C3
40	D	408	DGD	CAB-CBB-CCB-CDB
24	C	505	CLA	C11-C10-C8-C9
24	b	604	CLA	C6-C7-C8-C9
33	B	642	PG4	C1-C2-O2-C3
24	c	511	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
32	l	101	LHG	C11-C12-C13-C14
33	C	537	PG4	C3-C4-O3-C5
33	c	534	PG4	C4-C3-O2-C2
38	a	418	HTG	O5-C5-C6-O6
29	C	519	LMG	C20-C21-C22-C23
40	c	517	DGD	C7A-C8A-C9A-CAA
26	K	101	BCR	C1-C6-C7-C8
26	b	620	BCR	C1-C6-C7-C8
26	t	102	BCR	C23-C24-C25-C30
33	U	202	PG4	O1-C1-C2-O2
24	b	616	CLA	C13-C15-C16-C17
33	K	102	PG4	O3-C5-C6-O4
35	d	415	P6G	C18-C17-O16-C15
29	B	621	LMG	C7-C8-C9-O8
32	D	409	LHG	C17-C18-C19-C20
35	C	541	P6G	C5-C6-O7-C8
35	I	106	P6G	C2-C3-O4-C5
36	H	112	EDO	O1-C1-C2-O2
30	A	615	GOL	C1-C2-C3-O3
30	v	204	GOL	O1-C1-C2-C3
32	d	411	LHG	O1-C1-C2-C3
26	A	610	BCR	C17-C18-C19-C20
27	d	407	PL9	C43-C44-C46-C47
33	V	210	PG4	C4-C3-O2-C2
40	c	516	DGD	C5D-C6D-O5D-C1E
29	b	621	LMG	O8-C28-C29-C30
28	A	622	SQD	C11-C12-C13-C14
28	h	105	SQD	C10-C11-C12-C13
34	B	650	PGE	C3-C4-O3-C5
24	a	408	CLA	C11-C12-C13-C14
24	A	606	CLA	C4C-C3C-CAC-CBC
28	A	622	SQD	C12-C13-C14-C15
34	c	536	PGE	O2-C3-C4-O3
35	E	110	P6G	C9-C8-O7-C6
24	B	613	CLA	C8-C10-C11-C12
41	e	107	HEM	C3D-CAD-CBD-CGD
24	B	606	CLA	O1D-CGD-O2D-CED
32	e	101	LHG	C9-C10-C11-C12
38	C	532	HTG	C3'-C4'-C5'-C6'
39	x	104	1PE	OH4-C13-C23-OH3
24	A	606	CLA	C16-C17-C18-C20
32	D	409	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
27	a	412	PL9	C45-C44-C46-C47
33	H	107	PG4	O4-C7-C8-O5
33	b	637	PG4	O1-C1-C2-O2
34	Y	102	PGE	O3-C5-C6-O4
33	X	103	PG4	C8-C7-O4-C6
34	o	307	PGE	C1-C2-O2-C3
24	c	503	CLA	C6-C7-C8-C10
33	J	105	PG4	C8-C7-O4-C6
30	C	528	GOL	O2-C2-C3-O3
30	D	413	GOL	O2-C2-C3-O3
30	U	201	GOL	O1-C1-C2-O2
30	v	207	GOL	O1-C1-C2-O2
35	I	106	P6G	C9-C8-O7-C6
38	a	418	HTG	C2'-C3'-C4'-C5'
35	D	416	P6G	O10-C11-C12-O13
28	A	622	SQD	O47-C45-C46-O48
29	B	621	LMG	O9-C10-O7-C8
29	a	414	LMG	C36-C37-C38-C39
34	b	640	PGE	O2-C3-C4-O3
29	a	414	LMG	C34-C35-C36-C37
35	d	415	P6G	O4-C5-C6-O7
32	d	410	LHG	C26-C27-C28-C29
33	i	104	PG4	C3-C4-O3-C5
29	B	634	LMG	C42-C43-C44-C45
33	U	202	PG4	O2-C3-C4-O3
38	C	529	HTG	C2'-C1'-S1-C1
38	c	523	HTG	O5-C1-S1-C1'
33	I	102	PG4	O3-C5-C6-O4
27	A	611	PL9	C20-C19-C21-C22
27	a	412	PL9	C15-C14-C16-C17
27	a	412	PL9	C20-C19-C21-C22
31	b	622	LMT	C7-C8-C9-C10
35	I	106	P6G	O4-C5-C6-O7
38	C	521	HTG	C3'-C4'-C5'-C6'
24	b	610	CLA	C2-C3-C5-C6
24	c	505	CLA	C2-C3-C5-C6
28	a	413	SQD	C35-C36-C37-C38
24	B	616	CLA	C11-C10-C8-C9
24	D	404	CLA	C14-C13-C15-C16
24	a	410	CLA	C6-C7-C8-C9
24	d	405	CLA	C14-C13-C15-C16
33	c	533	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	d	414	PG4	O1-C1-C2-O2
34	H	109	PGE	C6-C5-O3-C4
33	b	634	PG4	C8-C7-O4-C6
35	D	416	P6G	O7-C8-C9-O10
24	b	616	CLA	C3A-C2A-CAA-CBA
33	x	102	PG4	C4-C3-O2-C2
34	D	415	PGE	C6-C5-O3-C4
35	D	416	P6G	C9-C8-O7-C6
40	c	517	DGD	C6B-C7B-C8B-C9B
40	C	518	DGD	O1G-C1A-C2A-C3A
24	B	605	CLA	CBD-CGD-O2D-CED
24	B	604	CLA	CAD-CBD-CGD-O2D
24	B	605	CLA	CAD-CBD-CGD-O2D
24	B	611	CLA	CAD-CBD-CGD-O2D
24	B	613	CLA	CAD-CBD-CGD-O2D
24	b	605	CLA	CAD-CBD-CGD-O2D
24	b	617	CLA	CAD-CBD-CGD-O2D
24	c	503	CLA	CAD-CBD-CGD-O2D
25	a	409	PHO	CAD-CBD-CGD-O2D
29	B	621	LMG	C13-C14-C15-C16
29	C	519	LMG	O9-C10-O7-C8
29	c	519	LMG	O7-C10-C11-C12
28	A	616	SQD	C33-C34-C35-C36
33	C	535	PG4	O2-C3-C4-O3
33	b	636	PG4	O2-C3-C4-O3
28	A	622	SQD	C19-C20-C21-C22
33	i	103	PG4	O3-C5-C6-O4
40	c	516	DGD	C7A-C8A-C9A-CAA
29	c	520	LMG	C14-C15-C16-C17
40	c	516	DGD	O6E-C1E-O5D-C6D
24	b	602	CLA	C2-C3-C5-C6
33	c	534	PG4	O2-C3-C4-O3
35	B	651	P6G	C9-C8-O7-C6
26	b	620	BCR	C7-C8-C9-C10
31	a	401	LMT	C4'-C5'-C6'-O6'
29	c	520	LMG	C11-C12-C13-C14
29	c	519	LMG	O1-C7-C8-C9
24	C	512	CLA	CAA-CBA-CGA-O2A
29	C	526	LMG	O7-C10-C11-C12
40	c	518	DGD	O1G-C1A-C2A-C3A
24	B	607	CLA	C6-C7-C8-C10
33	C	536	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
35	A	624	P6G	O10-C11-C12-O13
24	B	603	CLA	O2A-C1-C2-C3
24	C	509	CLA	O2A-C1-C2-C3
24	C	512	CLA	O2A-C1-C2-C3
24	C	513	CLA	O2A-C1-C2-C3
24	D	404	CLA	O2A-C1-C2-C3
24	b	603	CLA	O2A-C1-C2-C3
24	d	405	CLA	O2A-C1-C2-C3
25	A	608	PHO	O2A-C1-C2-C3
25	a	409	PHO	O2A-C1-C2-C3
34	b	639	PGE	O3-C5-C6-O4
33	x	102	PG4	O2-C3-C4-O3
35	d	415	P6G	C5-C6-O7-C8
40	c	518	DGD	C2A-C1A-O1G-C1G
44	V	216	2PE	O7-C8-C9-O10
28	x	101	SQD	O48-C23-C24-C25
36	B	658	EDO	O1-C1-C2-O2
36	c	542	EDO	O1-C1-C2-O2
33	X	103	PG4	O3-C5-C6-O4
33	a	421	PG4	O3-C5-C6-O4
24	A	607	CLA	CHA-CBD-CGD-O2D
24	B	602	CLA	CHA-CBD-CGD-O2D
24	B	607	CLA	CHA-CBD-CGD-O2D
24	C	504	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	D	403	CLA	CHA-CBD-CGD-O2D
24	b	603	CLA	CHA-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O2D
24	d	403	CLA	CHA-CBD-CGD-O1D
24	d	403	CLA	CHA-CBD-CGD-O2D
25	D	401	PHO	CHA-CBD-CGD-O1D
25	d	401	PHO	CHA-CBD-CGD-O1D
25	d	401	PHO	CHA-CBD-CGD-O2D
28	a	413	SQD	O47-C7-C8-C9
32	E	101	LHG	O7-C7-C8-C9
33	c	534	PG4	C1-C2-O2-C3
28	l	102	SQD	C30-C31-C32-C33
24	b	608	CLA	C3-C5-C6-C7
33	I	103	PG4	C1-C2-O2-C3
28	a	417	SQD	C26-C27-C28-C29
35	C	541	P6G	C2-C3-O4-C5
28	h	105	SQD	O48-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
33	C	536	PG4	C6-C5-O3-C4
45	i	107	PE8	C6-C5-O4-C3
29	C	526	LMG	C24-C25-C26-C27
28	a	424	SQD	C10-C11-C12-C13
30	A	615	GOL	O2-C2-C3-O3
30	C	528	GOL	O1-C1-C2-O2
30	c	528	GOL	O1-C1-C2-O2
33	H	106	PG4	C5-C6-O4-C7
40	c	518	DGD	O1A-C1A-O1G-C1G
28	A	616	SQD	C7-C8-C9-C10
29	z	101	LMG	C31-C32-C33-C34
33	I	103	PG4	C4-C3-O2-C2
32	A	618	LHG	C26-C27-C28-C29
33	B	639	PG4	O2-C3-C4-O3
35	b	648	P6G	O10-C11-C12-O13
24	A	609	CLA	C6-C7-C8-C9
24	B	617	CLA	C6-C7-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	b	613	CLA	C11-C10-C8-C9
28	F	104	SQD	C33-C34-C35-C36
35	A	623	P6G	O4-C5-C6-O7
24	a	410	CLA	C5-C6-C7-C8
44	V	216	2PE	C12-C11-O10-C9
29	a	414	LMG	C30-C31-C32-C33
33	c	535	PG4	O2-C3-C4-O3
24	C	502	CLA	C16-C17-C18-C19
29	j	101	LMG	C35-C36-C37-C38
35	b	649	P6G	C5-C6-O7-C8
24	c	501	CLA	C2A-CAA-CBA-CGA
24	d	404	CLA	C4C-C3C-CAC-CBC
29	A	613	LMG	C15-C16-C17-C18
32	d	410	LHG	C32-C33-C34-C35
34	B	646	PGE	C3-C4-O3-C5
34	D	415	PGE	C4-C3-O2-C2
24	b	613	CLA	C13-C15-C16-C17
24	B	614	CLA	C16-C17-C18-C19
35	d	416	P6G	C2-C3-O4-C5
33	D	414	PG4	C1-C2-O2-C3
38	B	623	HTG	C3'-C4'-C5'-C6'
30	D	412	GOL	O1-C1-C2-C3
30	T	103	GOL	C1-C2-C3-O3
30	V	208	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	c	528	GOL	O1-C1-C2-C3
33	e	103	PG4	O1-C1-C2-O2
34	E	104	PGE	O3-C5-C6-O4
34	V	215	PGE	O3-C5-C6-O4
33	b	636	PG4	C8-C7-O4-C6
34	O	308	PGE	C3-C4-O3-C5
24	C	512	CLA	CAA-CBA-CGA-O1A
29	C	526	LMG	O9-C10-C11-C12
24	B	602	CLA	CAA-CBA-CGA-O2A
33	B	640	PG4	O3-C5-C6-O4
33	i	101	PG4	C8-C7-O4-C6
34	B	647	PGE	O2-C3-C4-O3
35	b	649	P6G	O7-C8-C9-O10
35	d	416	P6G	C8-C9-O10-C11
35	B	651	P6G	C14-C15-O16-C17
40	C	518	DGD	O1A-C1A-C2A-C3A
29	C	526	LMG	C35-C36-C37-C38
33	K	102	PG4	C6-C5-O3-C4
24	B	602	CLA	C10-C11-C12-C13
32	d	409	LHG	C32-C33-C34-C35
33	V	209	PG4	C4-C3-O2-C2
33	b	637	PG4	O3-C5-C6-O4
28	h	105	SQD	O49-C7-C8-C9
24	C	506	CLA	C15-C16-C17-C18
24	D	403	CLA	C15-C16-C17-C18
32	B	632	LHG	C5-C6-O8-C23
33	b	637	PG4	O2-C3-C4-O3
40	d	408	DGD	C9B-CAB-CBB-CCB
29	z	101	LMG	O7-C10-C11-C12
24	B	616	CLA	C13-C15-C16-C17
24	a	410	CLA	C13-C15-C16-C17
33	C	537	PG4	O2-C3-C4-O3
33	C	537	PG4	C5-C6-O4-C7
34	b	646	PGE	C6-C5-O3-C4
35	A	623	P6G	O7-C8-C9-O10
40	C	516	DGD	C2E-C1E-O5D-C6D
32	B	632	LHG	C17-C18-C19-C20
32	l	101	LHG	C16-C17-C18-C19
33	X	101	PG4	O3-C5-C6-O4
33	x	102	PG4	O3-C5-C6-O4
34	c	536	PGE	C3-C4-O3-C5
39	V	217	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
32	D	410	LHG	C4-O6-P-O5
32	a	419	LHG	C4-O6-P-O5
32	d	410	LHG	C4-O6-P-O5
32	e	101	LHG	C4-O6-P-O5
33	V	212	PG4	O3-C5-C6-O4
34	a	423	PGE	O2-C3-C4-O3
28	a	413	SQD	O49-C7-C8-C9
29	c	519	LMG	O9-C10-C11-C12
38	c	531	HTG	O5-C5-C6-O6
34	E	107	PGE	C6-C5-O3-C4
24	C	509	CLA	C3-C5-C6-C7
26	T	102	BCR	C23-C24-C25-C30
34	c	537	PGE	O3-C5-C6-O4
28	x	101	SQD	C13-C14-C15-C16
29	z	101	LMG	C39-C40-C41-C42
45	i	107	PE8	O10-C11-C12-O13
32	d	410	LHG	C34-C35-C36-C37
34	j	105	PGE	O2-C3-C4-O3
36	O	311	EDO	O1-C1-C2-O2
32	e	101	LHG	O7-C7-C8-C9
33	i	104	PG4	C6-C5-O3-C4
44	V	216	2PE	O16-C17-C18-O19
24	B	603	CLA	C15-C16-C17-C18
31	F	102	LMT	O1'-C1-C2-C3
24	D	403	CLA	C4C-C3C-CAC-CBC
28	a	413	SQD	C32-C33-C34-C35
34	B	645	PGE	O2-C3-C4-O3
34	b	641	PGE	O2-C3-C4-O3
35	d	416	P6G	O13-C14-C15-O16
44	V	216	2PE	O4-C5-C6-O7
28	b	633	SQD	O49-C7-C8-C9
28	h	105	SQD	O10-C23-C24-C25
40	c	518	DGD	O1A-C1A-C2A-C3A
32	d	411	LHG	C13-C14-C15-C16
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	b	606	CLA	CAD-CBD-CGD-O1D
24	b	608	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
28	a	417	SQD	O5-C5-C6-S
29	d	412	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
29	z	101	LMG	C9-C8-O7-C10
32	a	419	LHG	C6-C5-O7-C7
34	o	307	PGE	C6-C5-O3-C4
35	j	106	P6G	C8-C9-O10-C11
24	c	512	CLA	CAA-CBA-CGA-O2A
24	B	604	CLA	C6-C7-C8-C9
24	C	504	CLA	C6-C7-C8-C9
24	a	408	CLA	C11-C10-C8-C9
24	c	510	CLA	C6-C7-C8-C9
39	V	217	1PE	OH6-C15-C25-OH5
40	d	408	DGD	CCA-CDA-CEA-CFA
29	c	520	LMG	C36-C37-C38-C39
31	M	101	LMT	C3-C4-C5-C6
33	V	210	PG4	C6-C5-O3-C4
29	z	101	LMG	O9-C10-C11-C12
32	E	101	LHG	O9-C7-C8-C9
33	B	636	PG4	O4-C7-C8-O5
32	e	101	LHG	C28-C29-C30-C31
34	B	646	PGE	C4-C3-O2-C2
45	i	107	PE8	C18-C17-O16-C15
24	C	505	CLA	CAA-CBA-CGA-O2A
24	c	505	CLA	CAA-CBA-CGA-O2A
28	A	622	SQD	O47-C7-C8-C9
29	a	414	LMG	O7-C10-C11-C12
29	d	412	LMG	O7-C10-C11-C12
33	c	535	PG4	C5-C6-O4-C7
38	b	631	HTG	C4'-C5'-C6'-C7'
29	A	613	LMG	O9-C10-O7-C8
28	a	413	SQD	C12-C13-C14-C15
29	d	412	LMG	C18-C19-C20-C21
24	C	513	CLA	C4-C3-C5-C6
31	u	203	LMT	C3-C4-C5-C6
24	B	604	CLA	C6-C7-C8-C10
24	C	503	CLA	C6-C7-C8-C10
24	C	504	CLA	C6-C7-C8-C10
24	a	408	CLA	C11-C10-C8-C7
24	b	613	CLA	C11-C10-C8-C7
24	c	510	CLA	C6-C7-C8-C10
38	C	529	HTG	C2-C1-S1-C1'
38	c	523	HTG	C2-C1-S1-C1'
24	C	505	CLA	CAA-CBA-CGA-O1A
40	H	103	DGD	O1B-C1B-C2B-C3B

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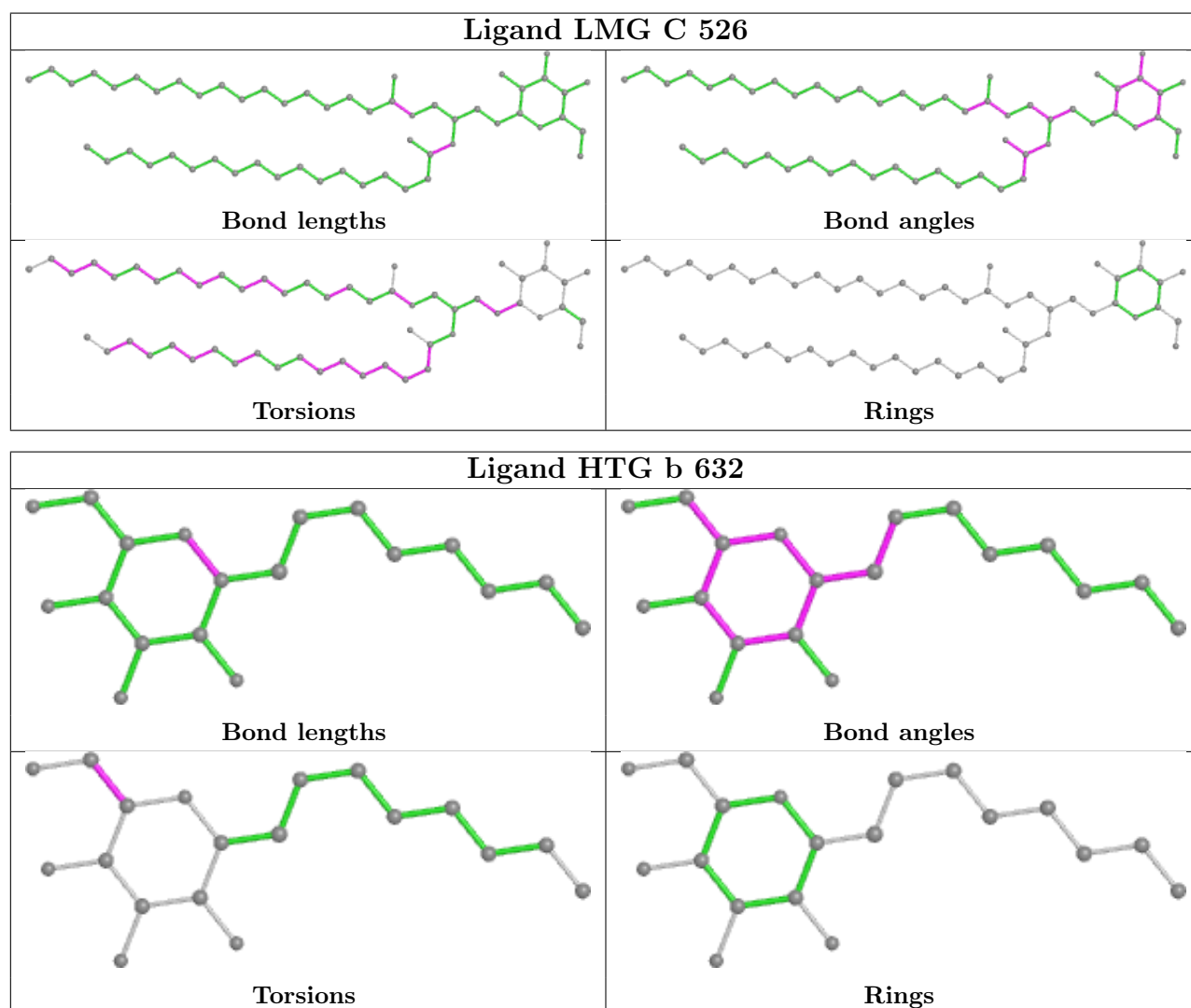
Mol	Chain	Res	Type	Atoms
40	D	408	DGD	C3B-C4B-C5B-C6B
28	x	101	SQD	C32-C33-C34-C35
31	C	533	LMT	C5'-C4'-O1B-C1B
24	c	512	CLA	CAA-CBA-CGA-O1A
29	d	412	LMG	O9-C10-C11-C12
33	b	634	PG4	C5-C6-O4-C7
28	A	612	SQD	O47-C7-C8-C9
33	c	535	PG4	O3-C5-C6-O4
35	B	651	P6G	O13-C14-C15-O16
35	b	648	P6G	O7-C8-C9-O10
31	f	101	LMT	O5'-C1'-O1'-C1
24	c	501	CLA	O1D-CGD-O2D-CED
34	E	105	PGE	C4-C3-O2-C2
35	D	416	P6G	C5-C6-O7-C8
35	j	106	P6G	O7-C8-C9-O10
45	i	107	PE8	O13-C14-C15-O16
28	A	622	SQD	O49-C7-C8-C9
32	e	101	LHG	O9-C7-C8-C9
29	B	621	LMG	C14-C15-C16-C17
33	B	636	PG4	O2-C3-C4-O3
33	c	534	PG4	C8-C7-O4-C6
33	E	102	PG4	C1-C2-O2-C3
33	d	414	PG4	O3-C5-C6-O4
35	D	418	P6G	C12-C11-O10-C9
38	h	101	HTG	S1-C1'-C2'-C3'
33	B	642	PG4	O3-C5-C6-O4
33	c	532	PG4	C1-C2-O2-C3
35	B	651	P6G	O10-C11-C12-O13
24	d	403	CLA	C15-C16-C17-C18
39	B	654	1PE	OH5-C14-C24-OH4
33	a	421	PG4	O2-C3-C4-O3
33	l	103	PG4	O3-C5-C6-O4
28	A	616	SQD	O48-C23-C24-C25
29	a	414	LMG	O8-C28-C29-C30
32	l	101	LHG	O7-C7-C8-C9

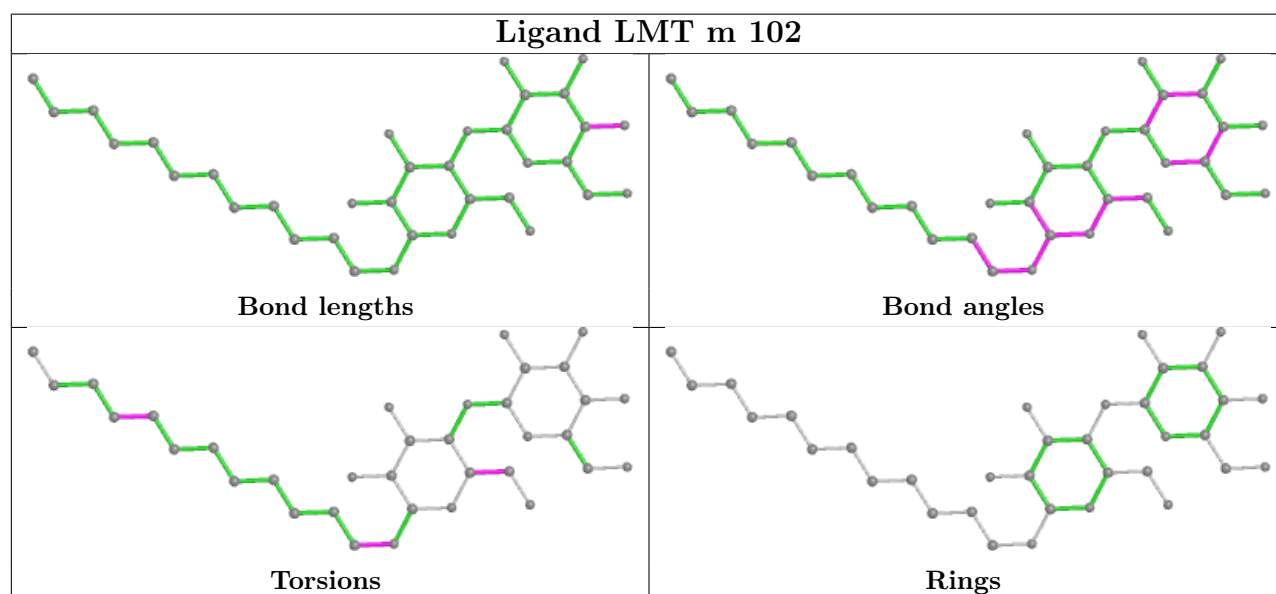
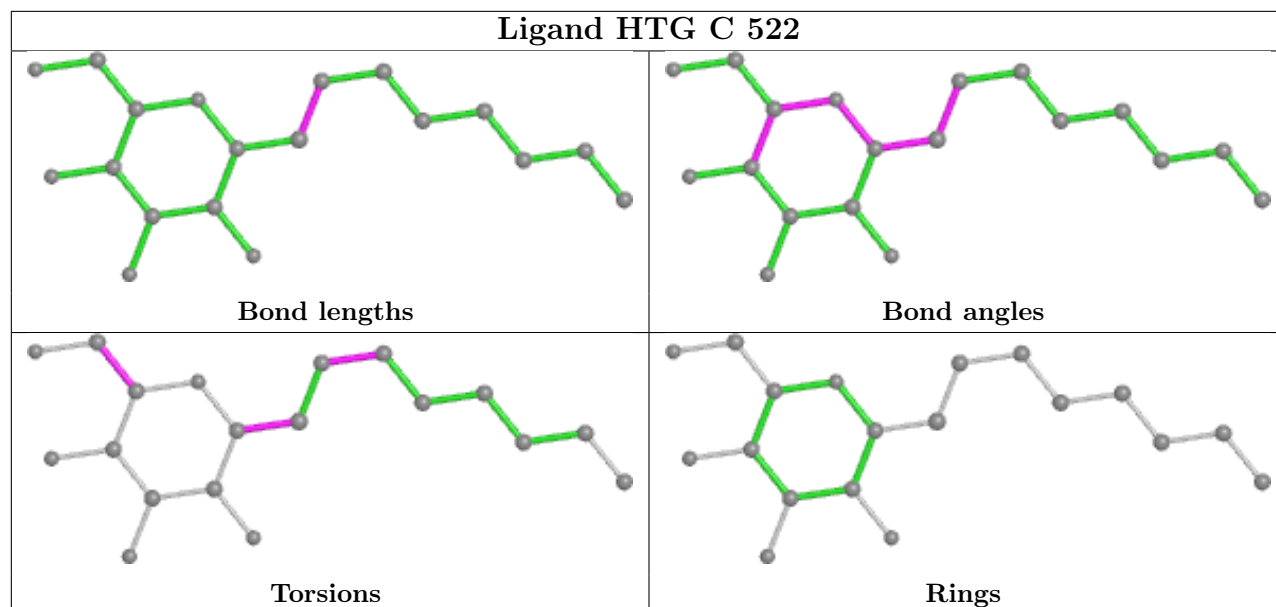
There are no ring outliers.

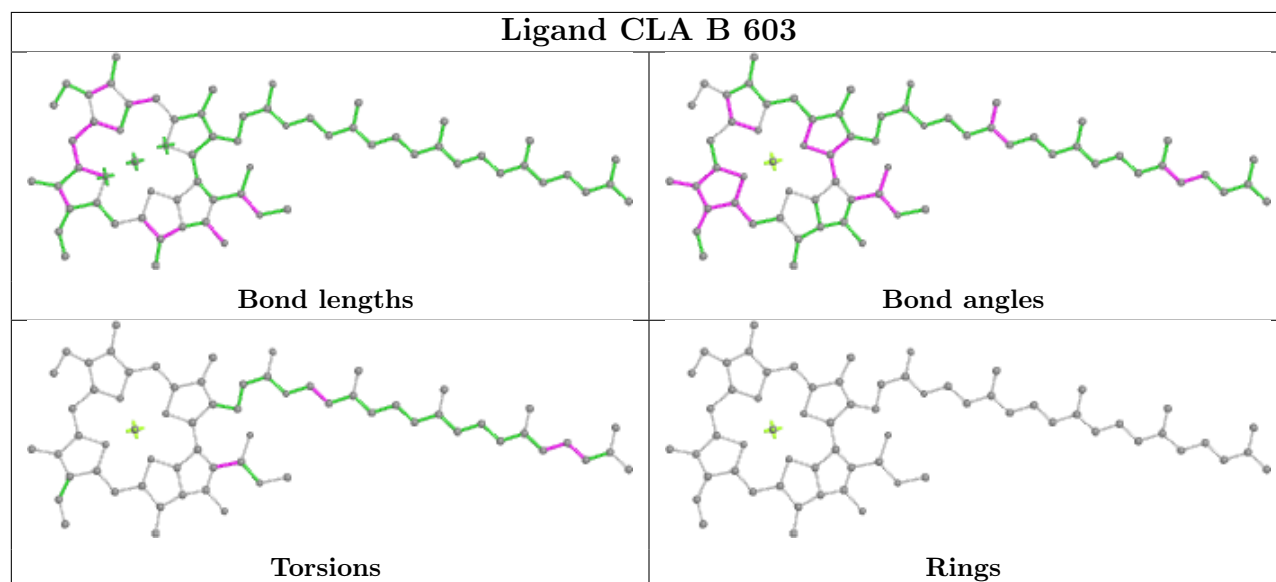
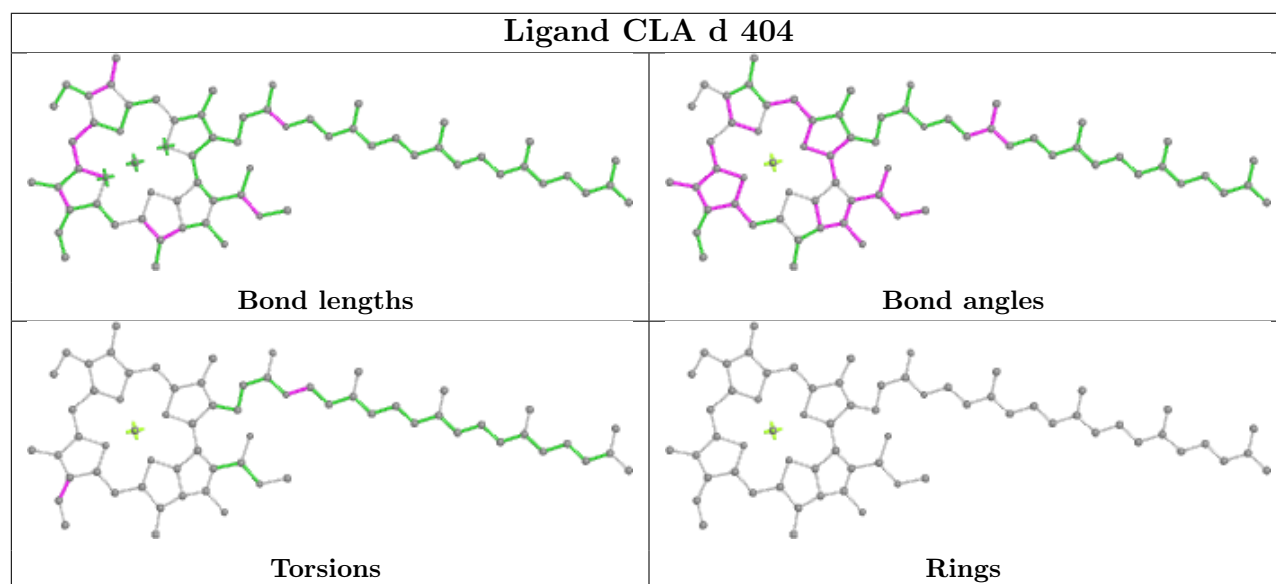
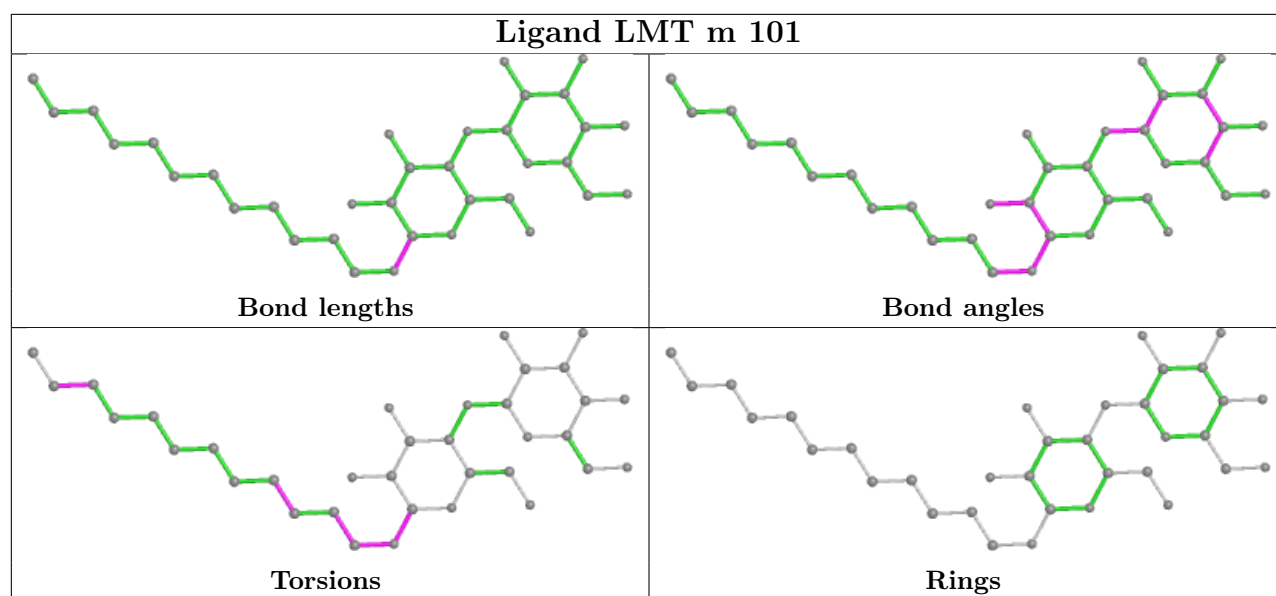
1 monomer is involved in 1 short contact:

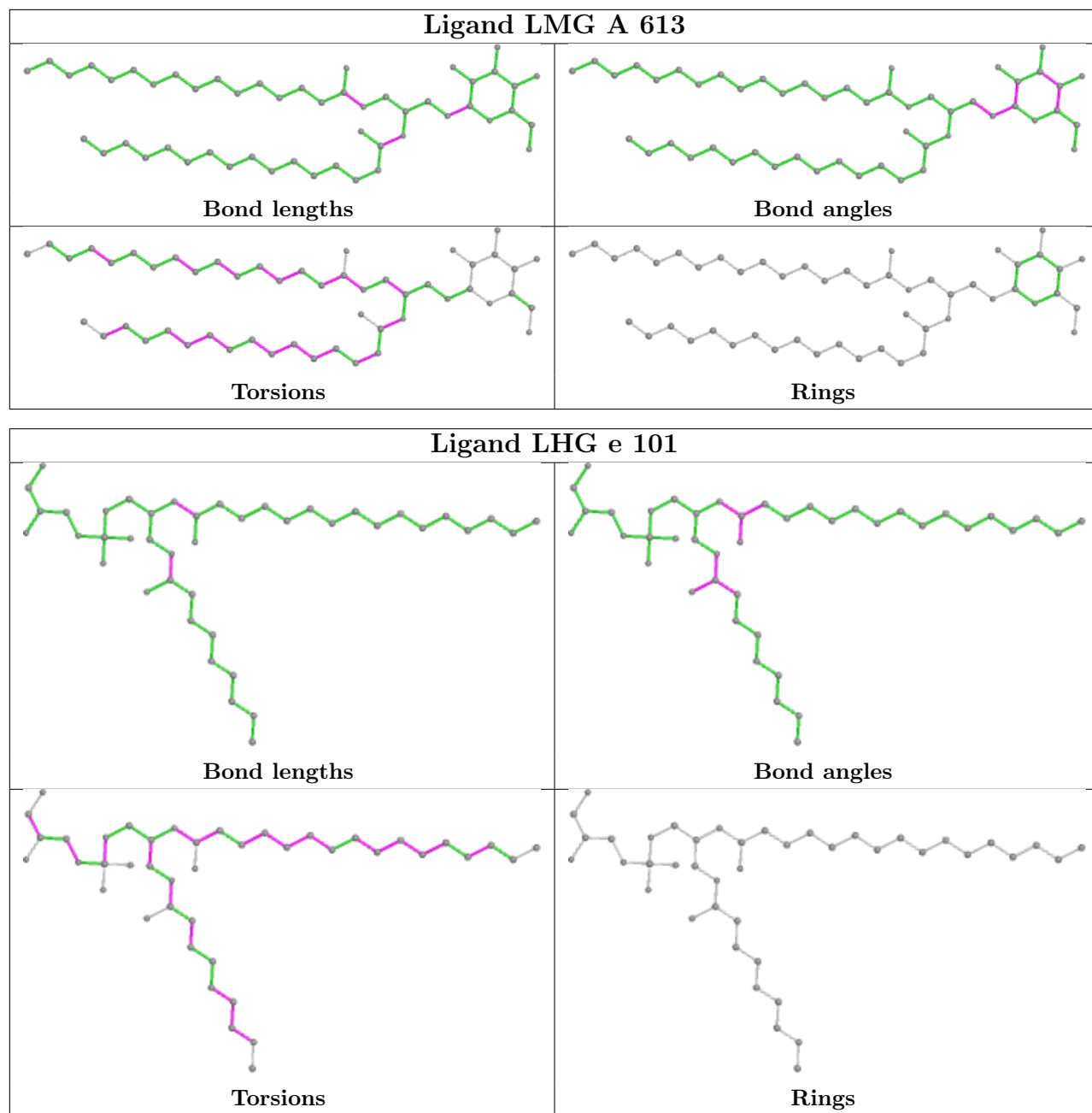
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	d	408	DGD	0	1

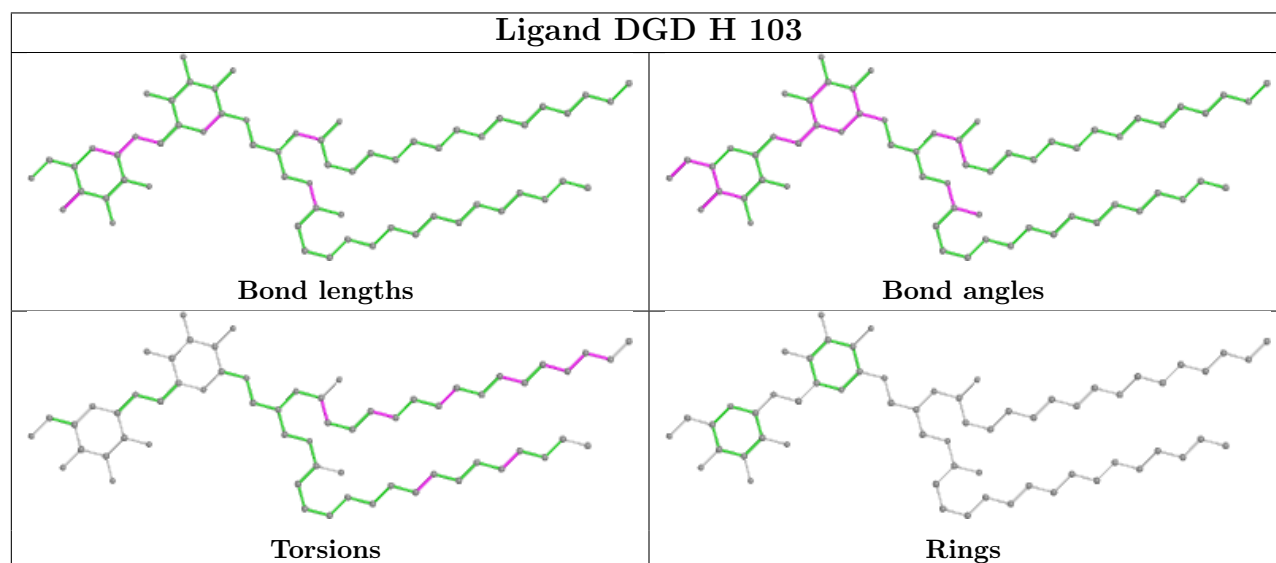
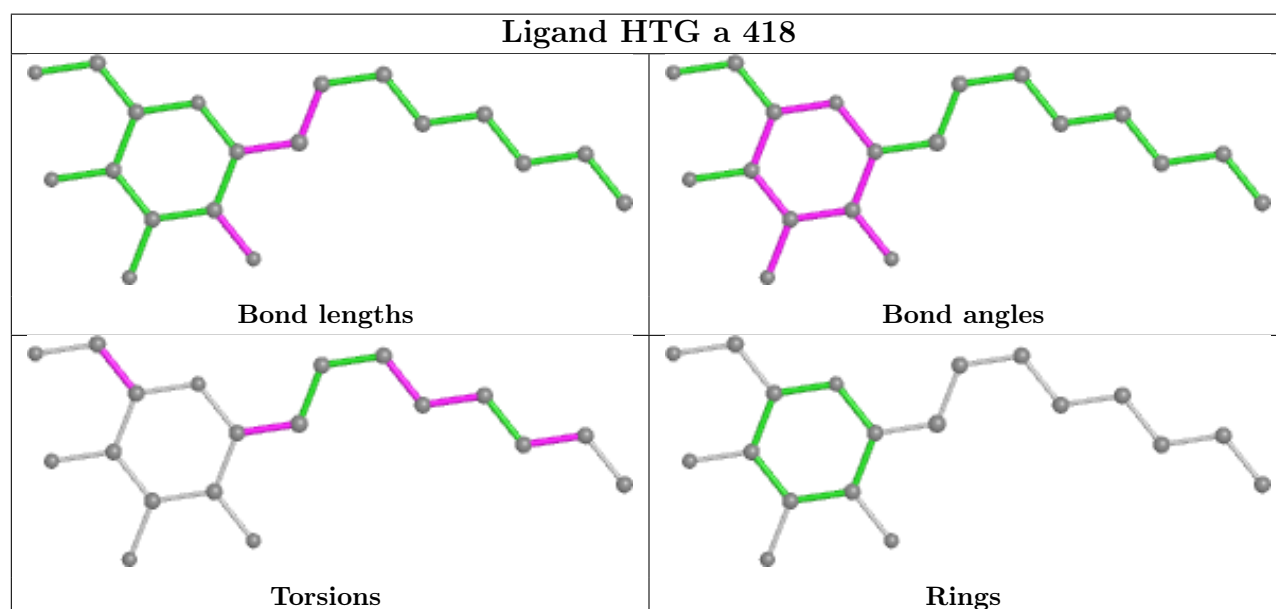
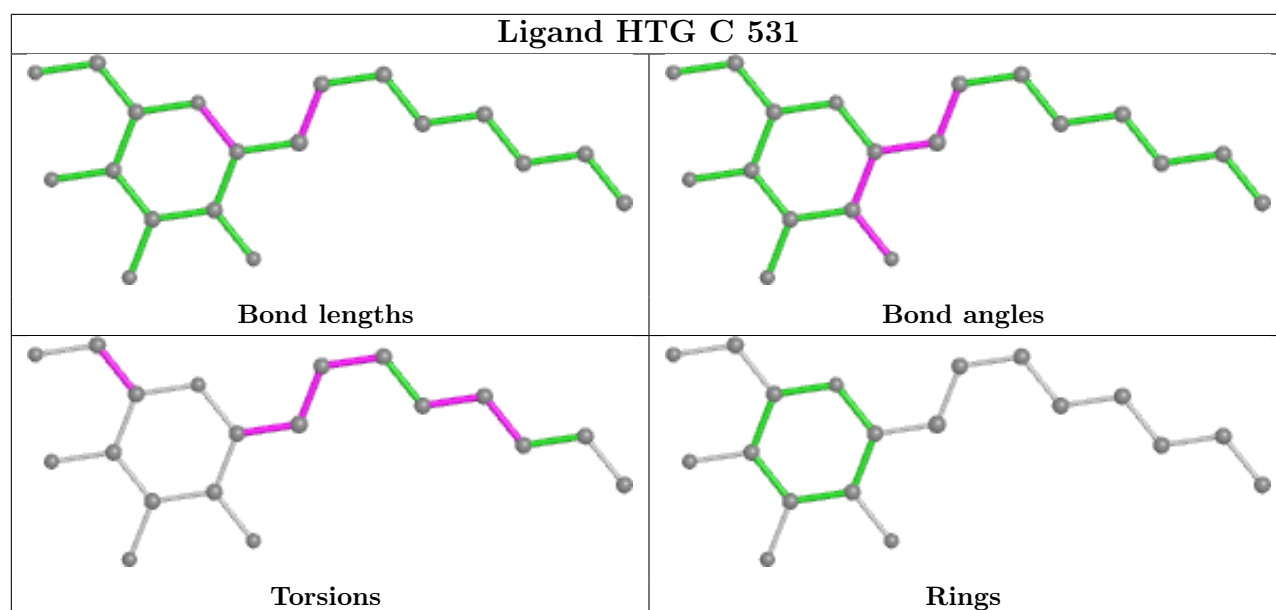
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

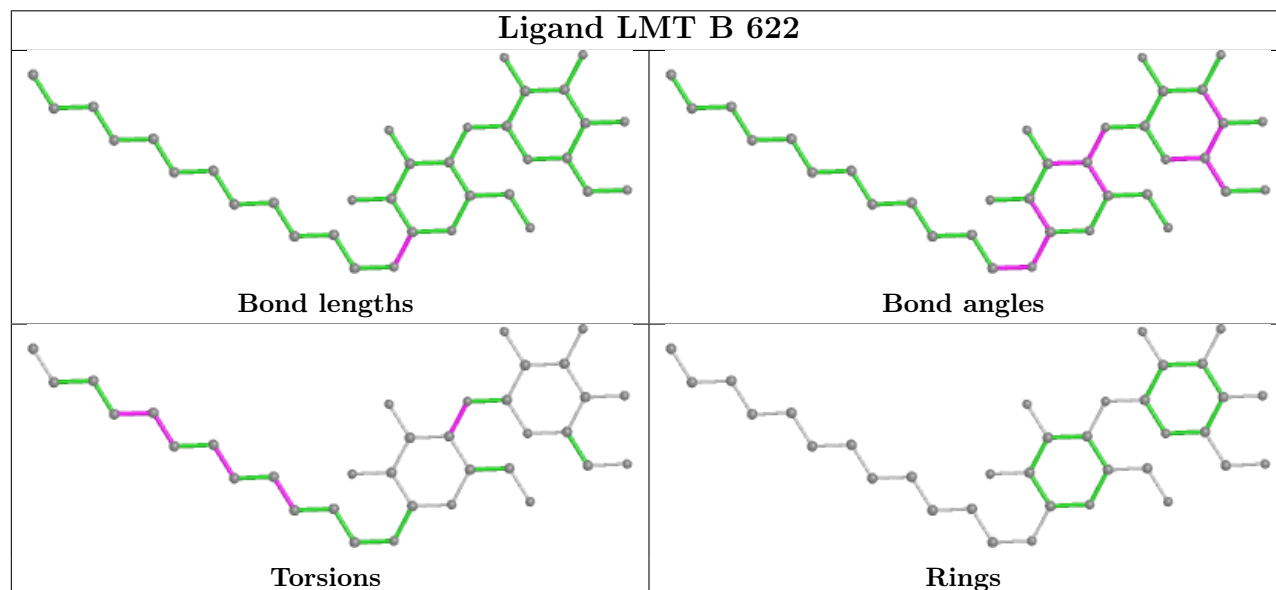
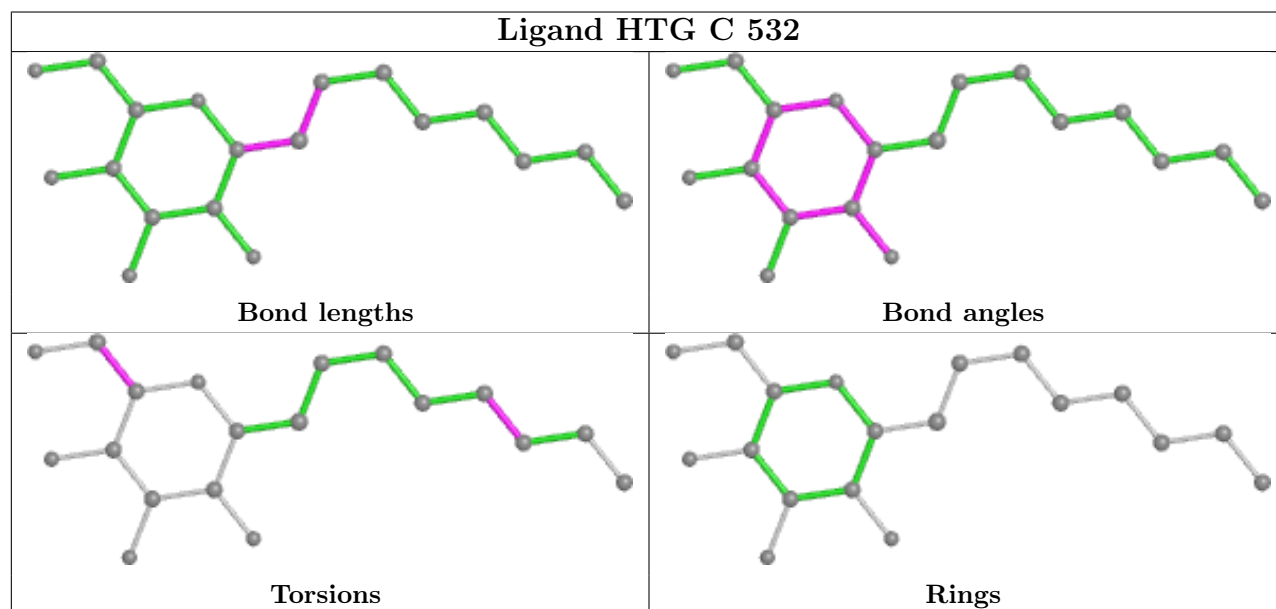
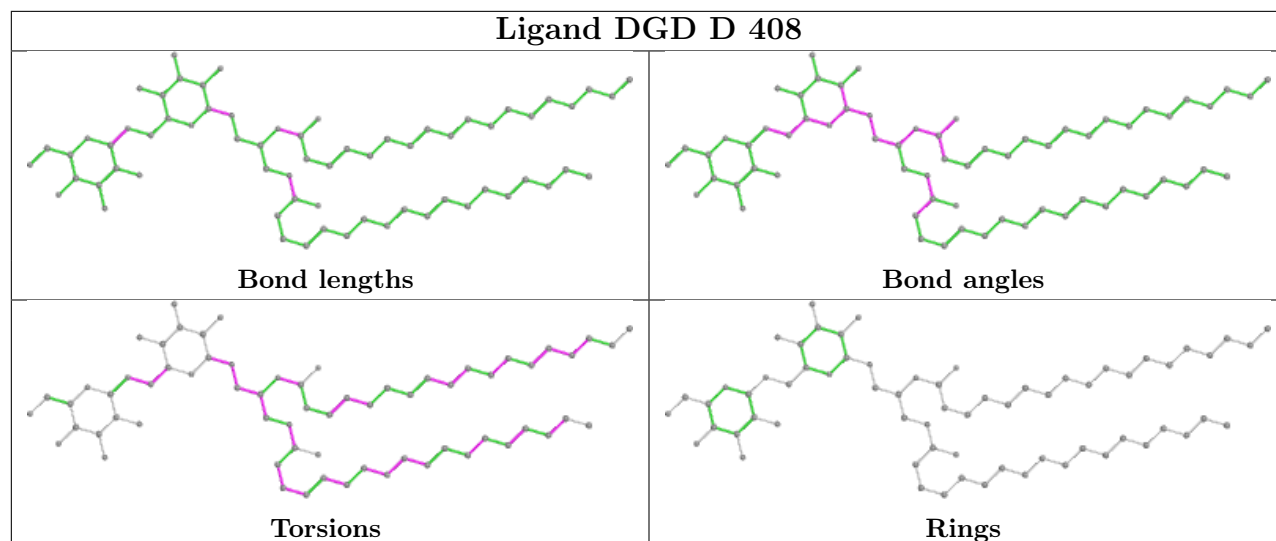


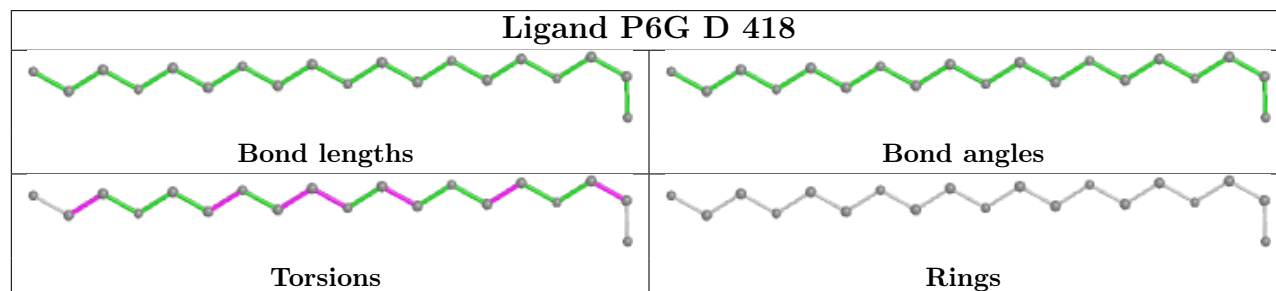
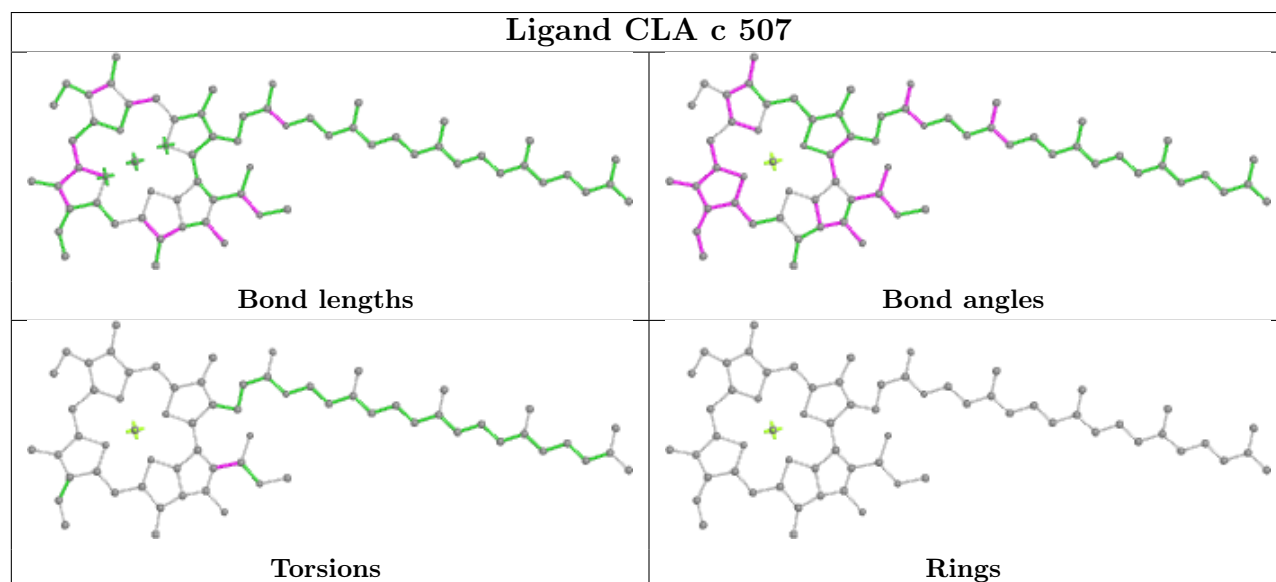
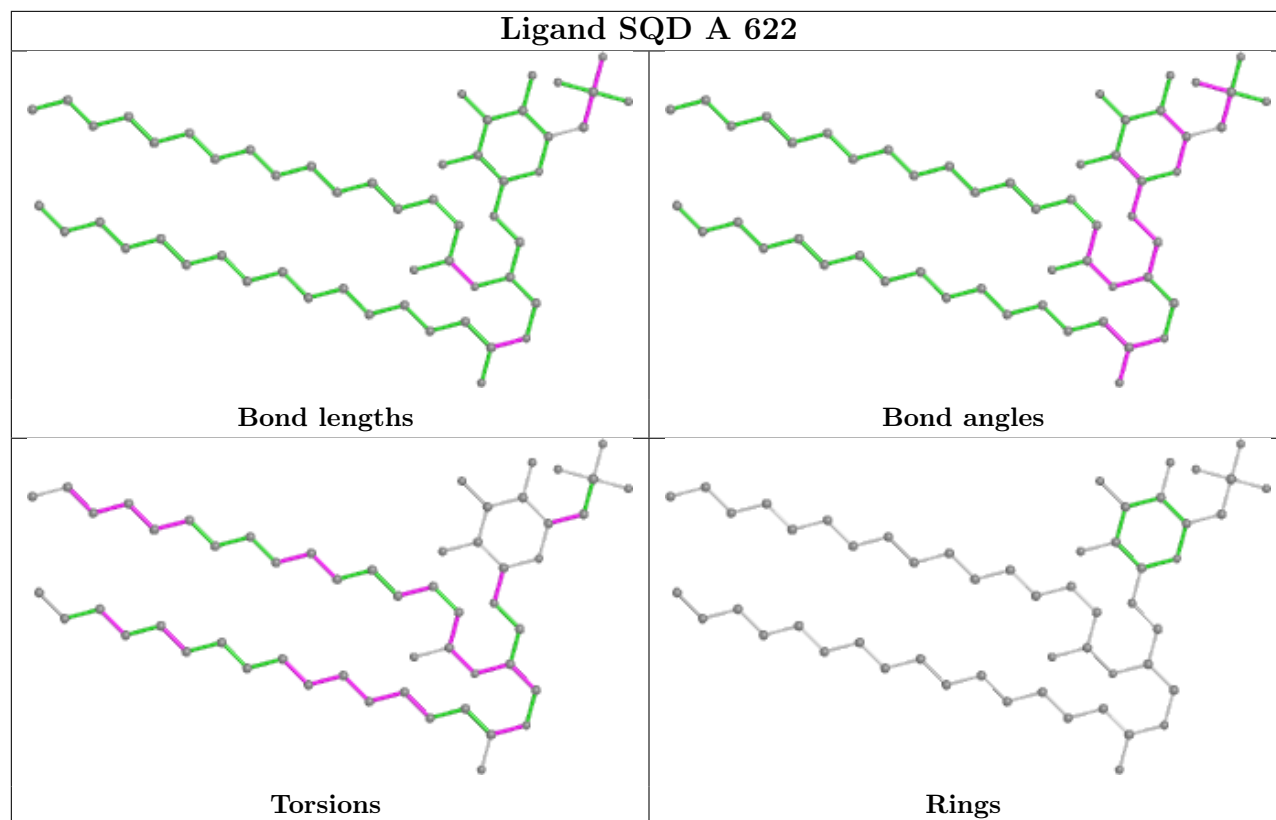




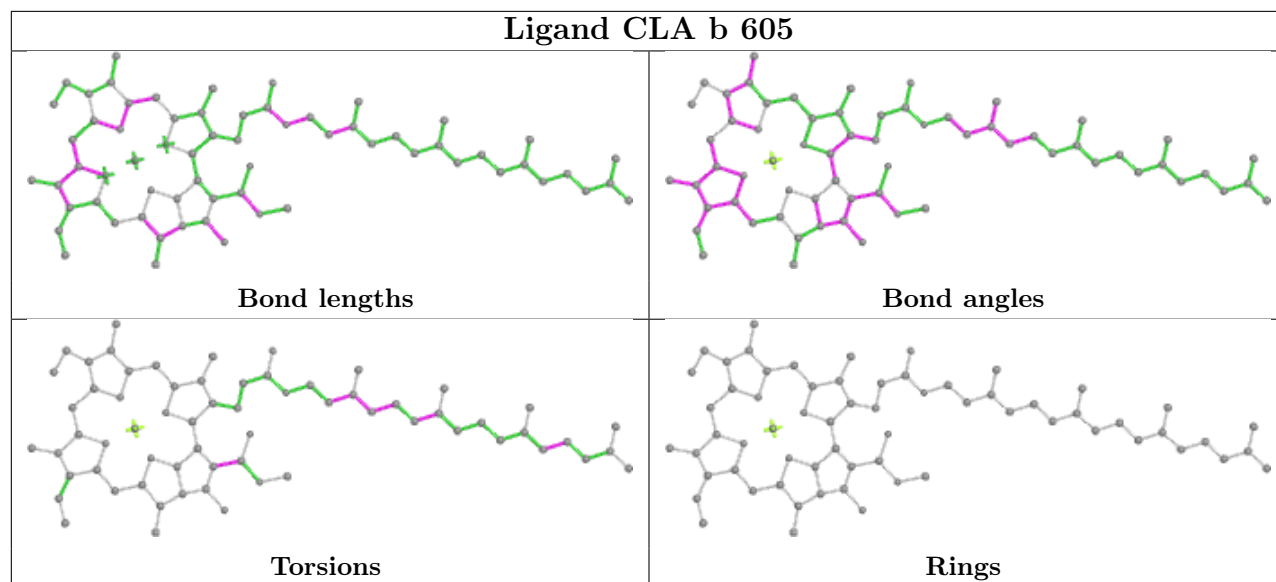




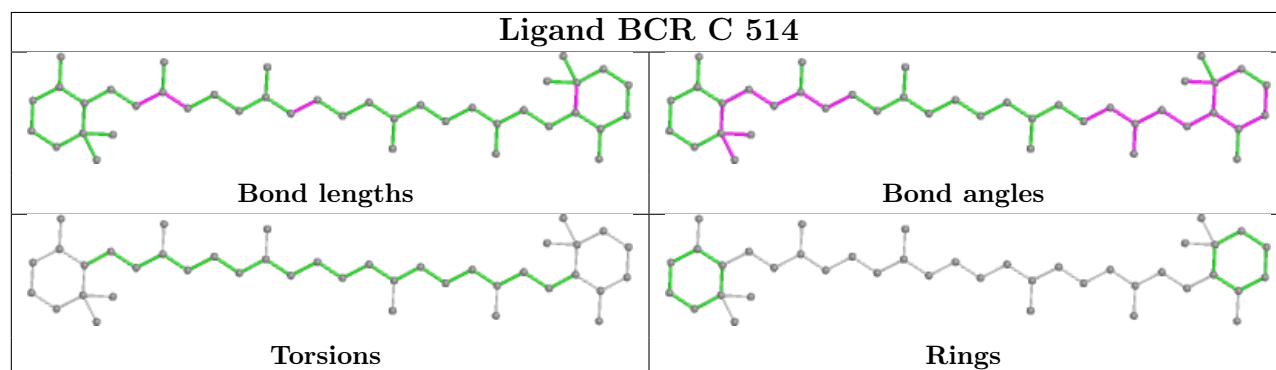




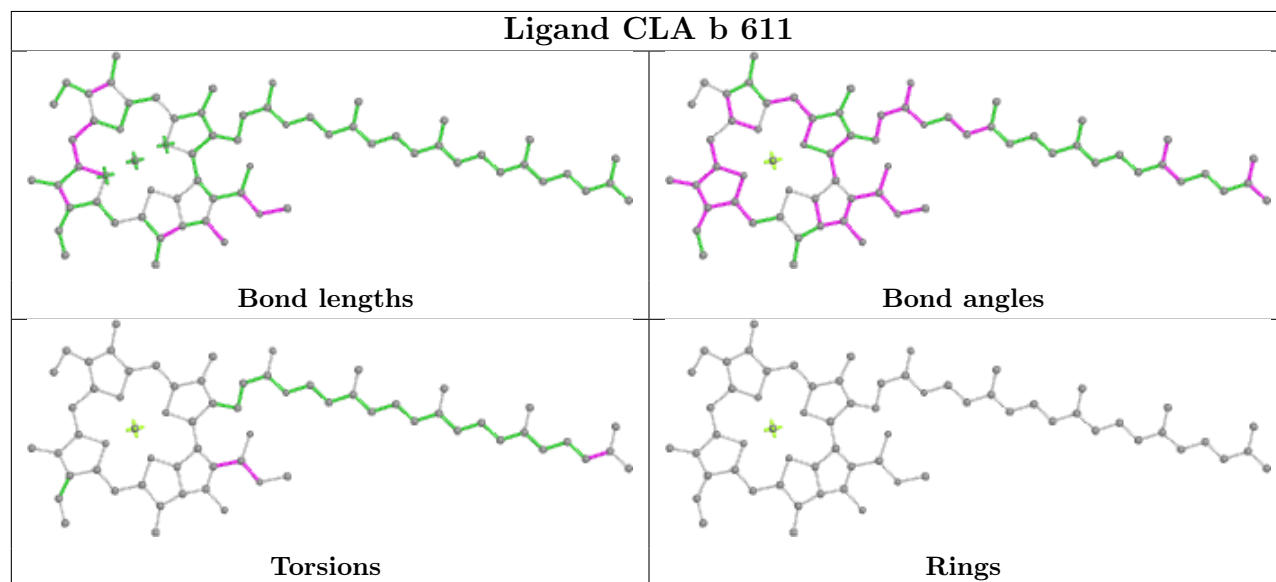
Ligand CLA b 605

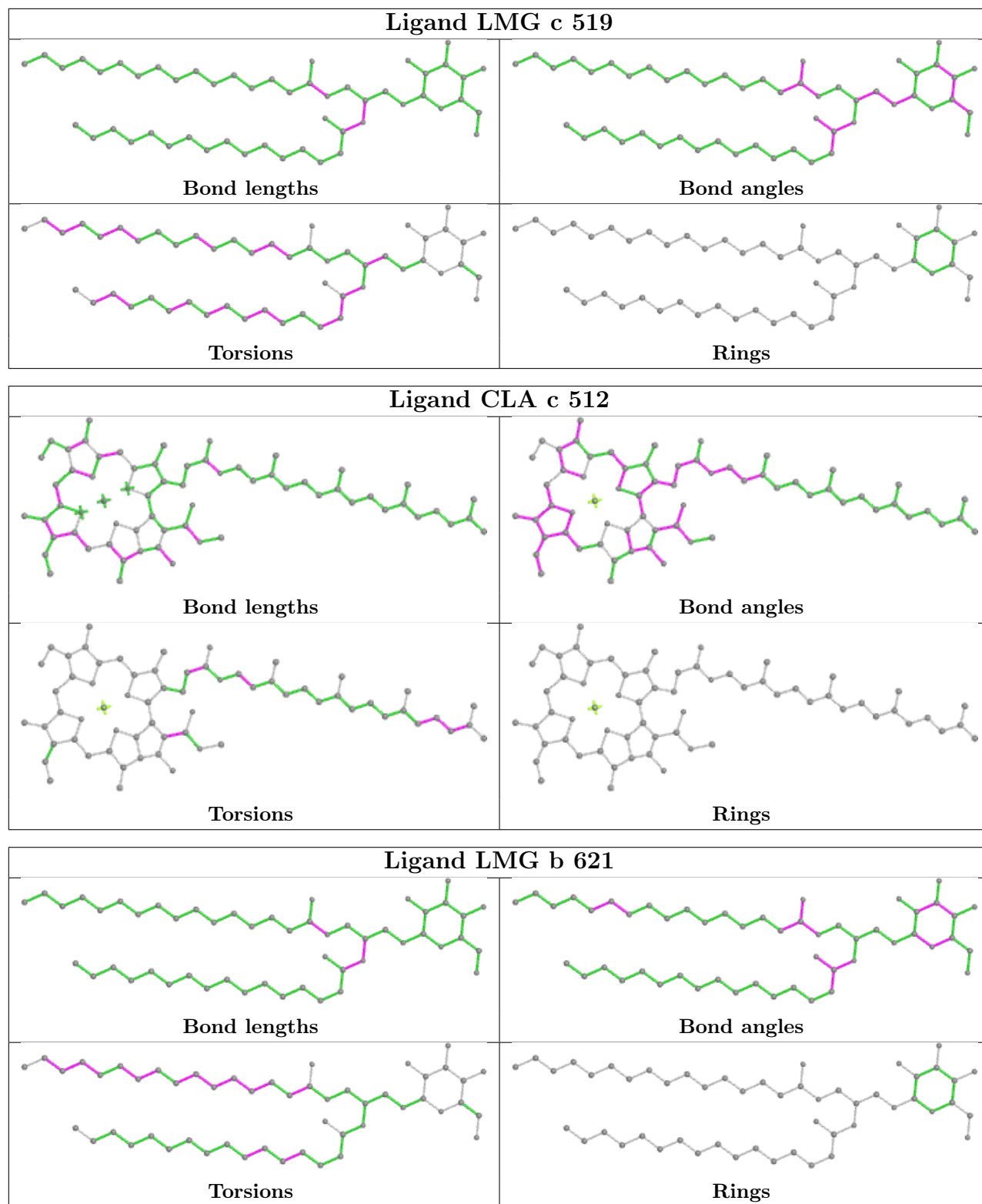


Ligand BCR C 514

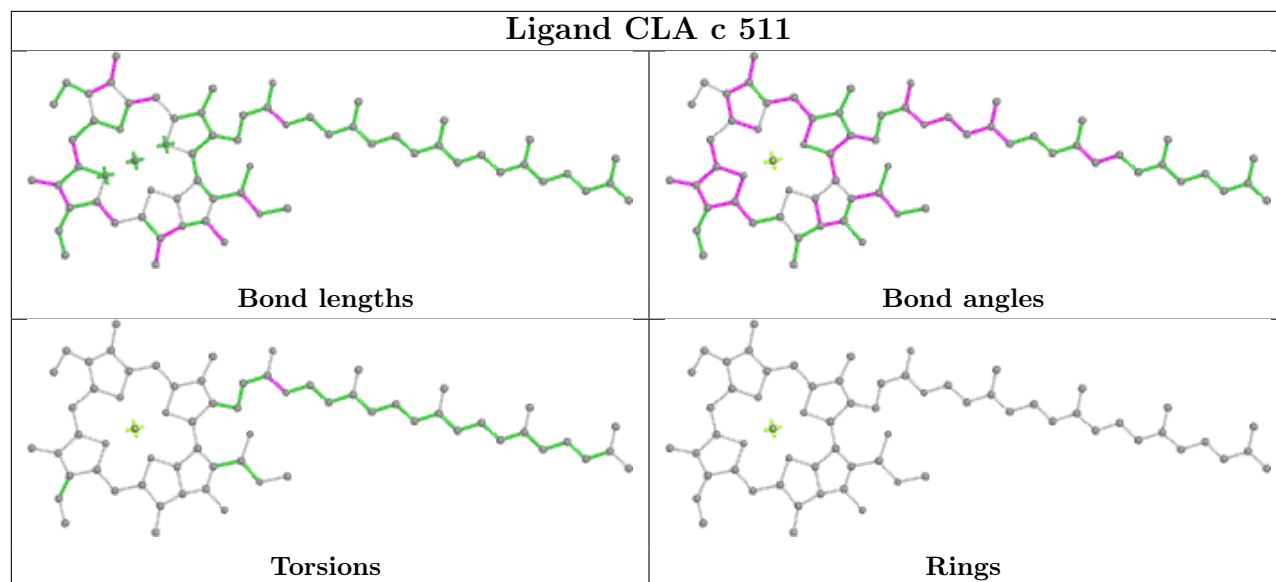


Ligand CLA b 611

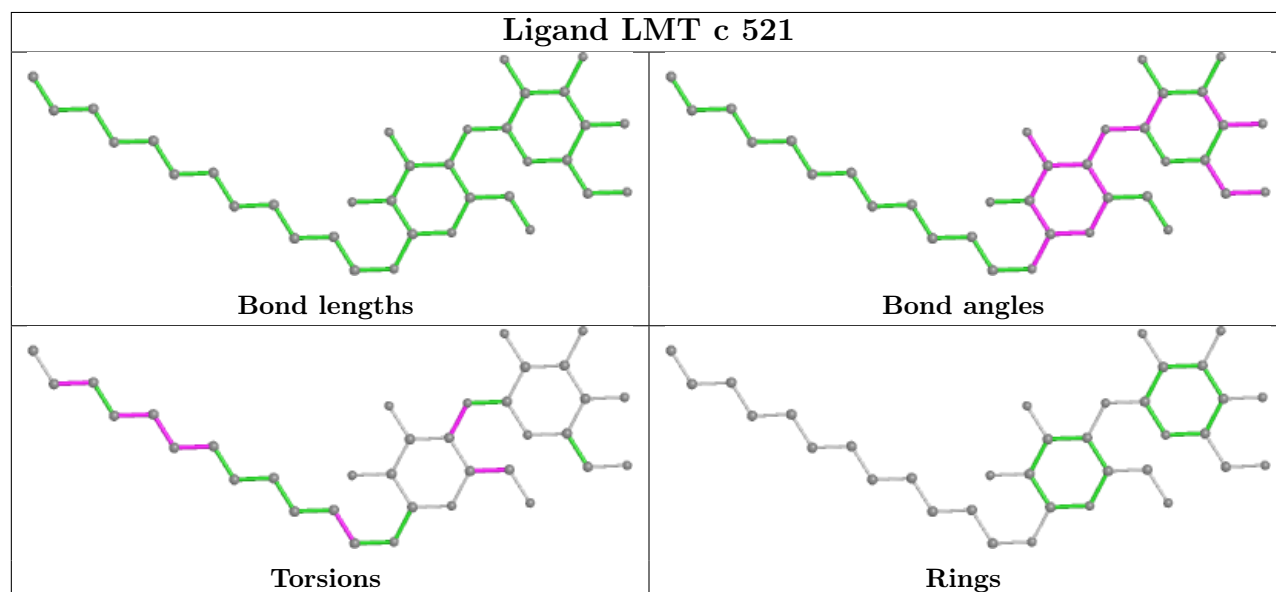




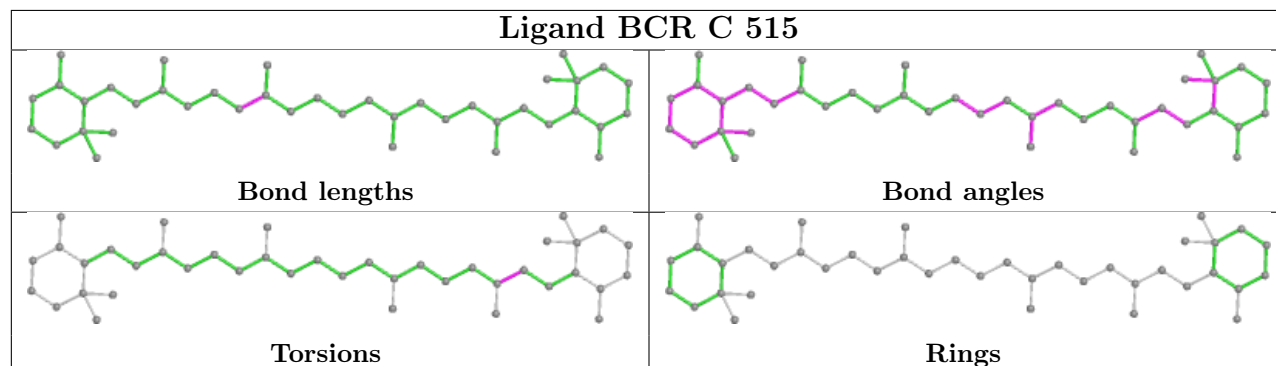
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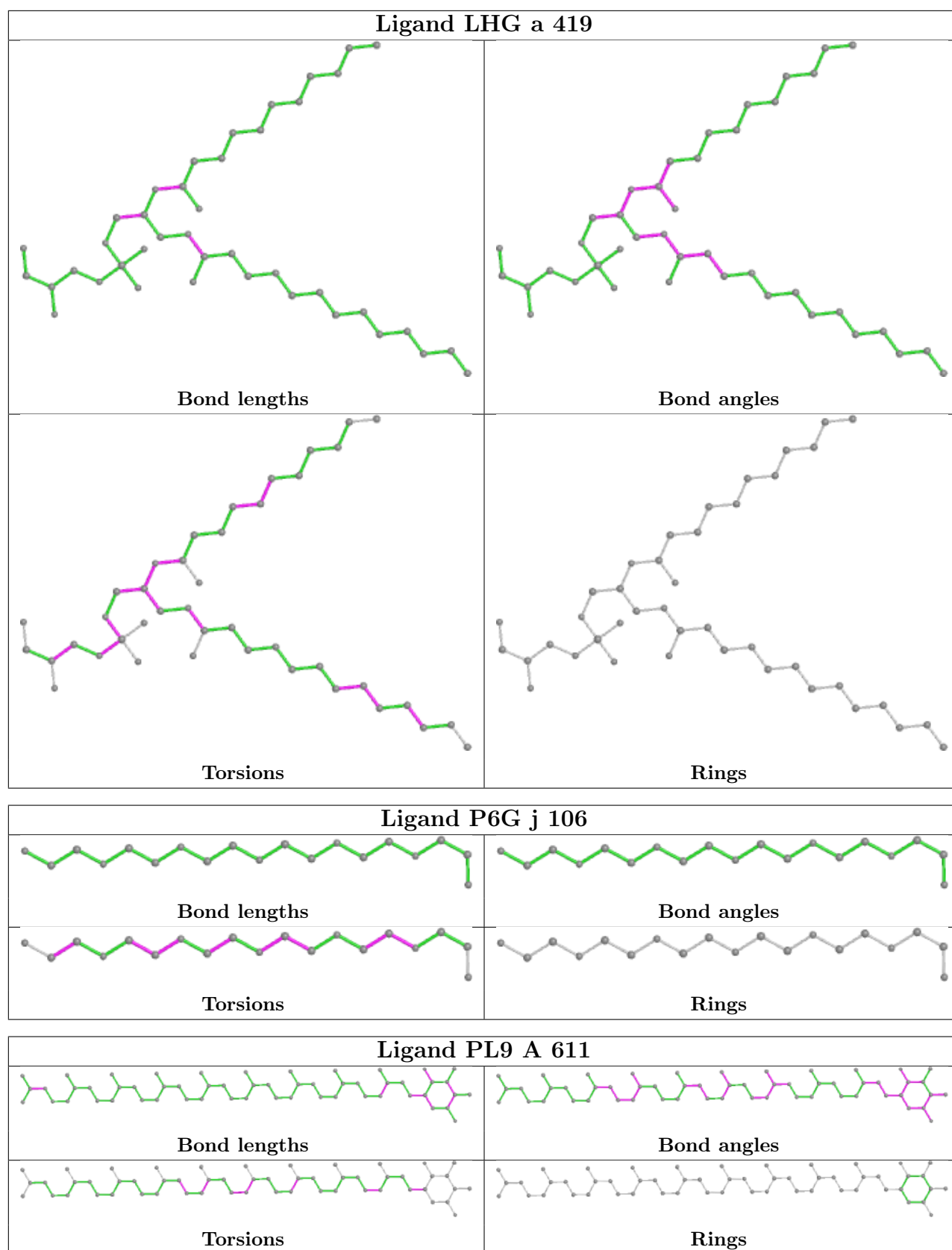


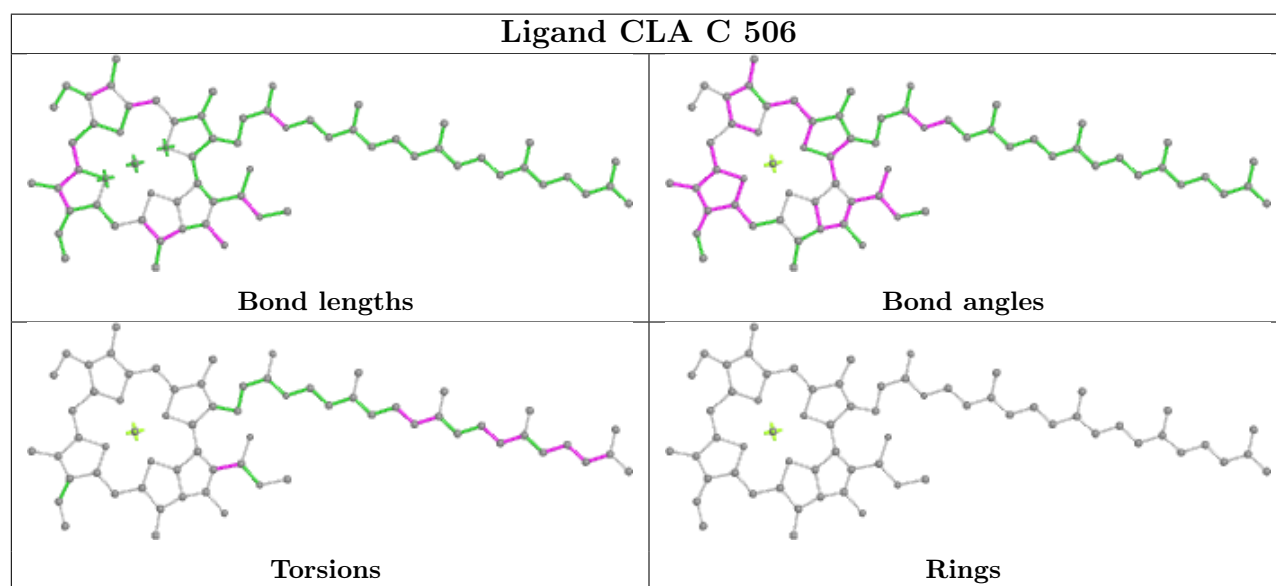
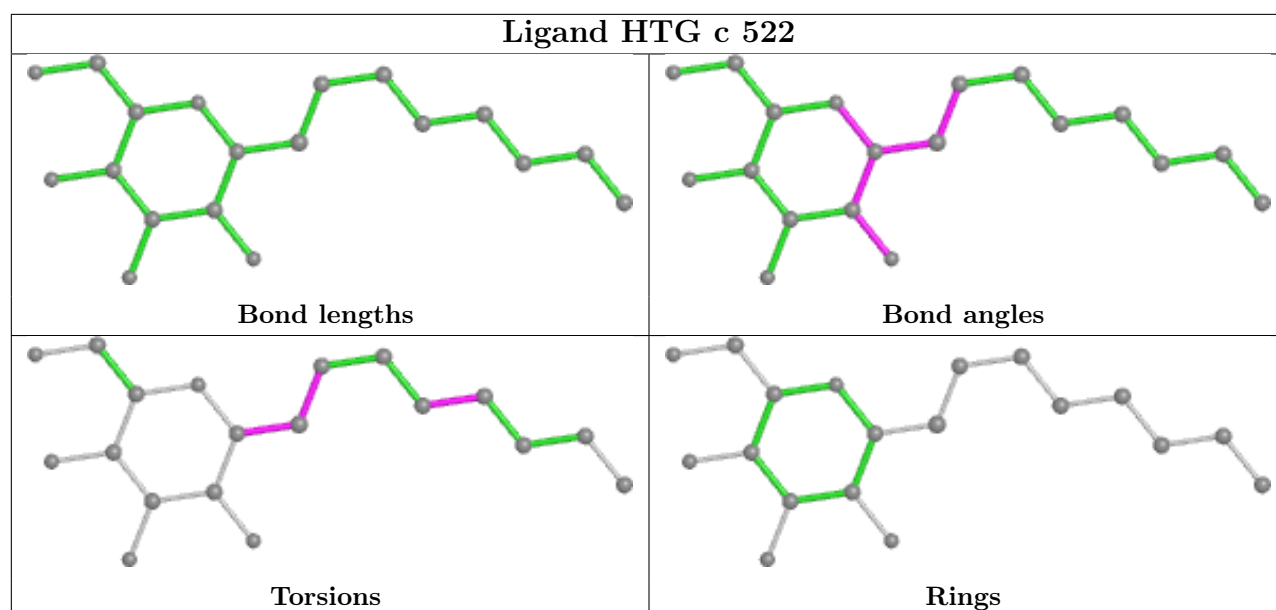
Ligand LMT c 521

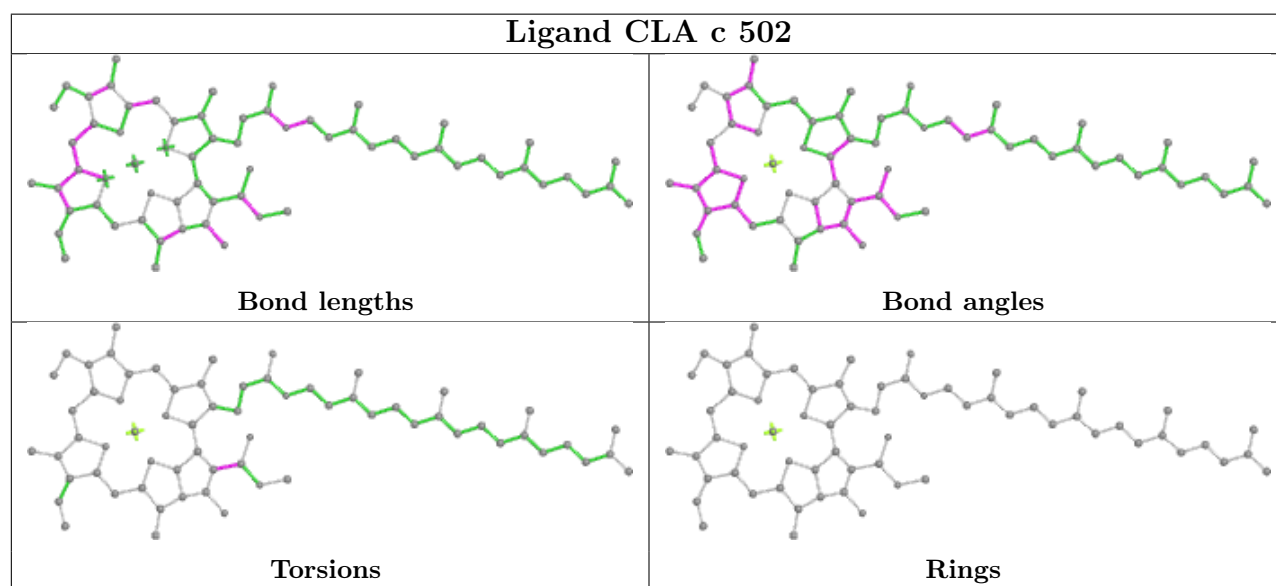
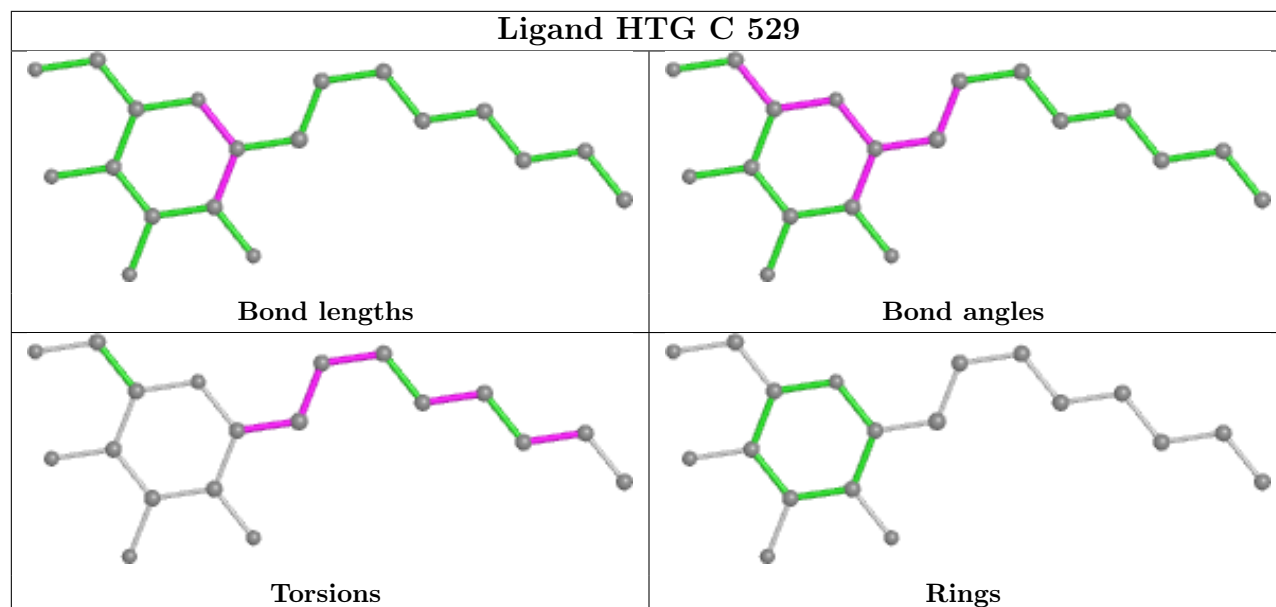


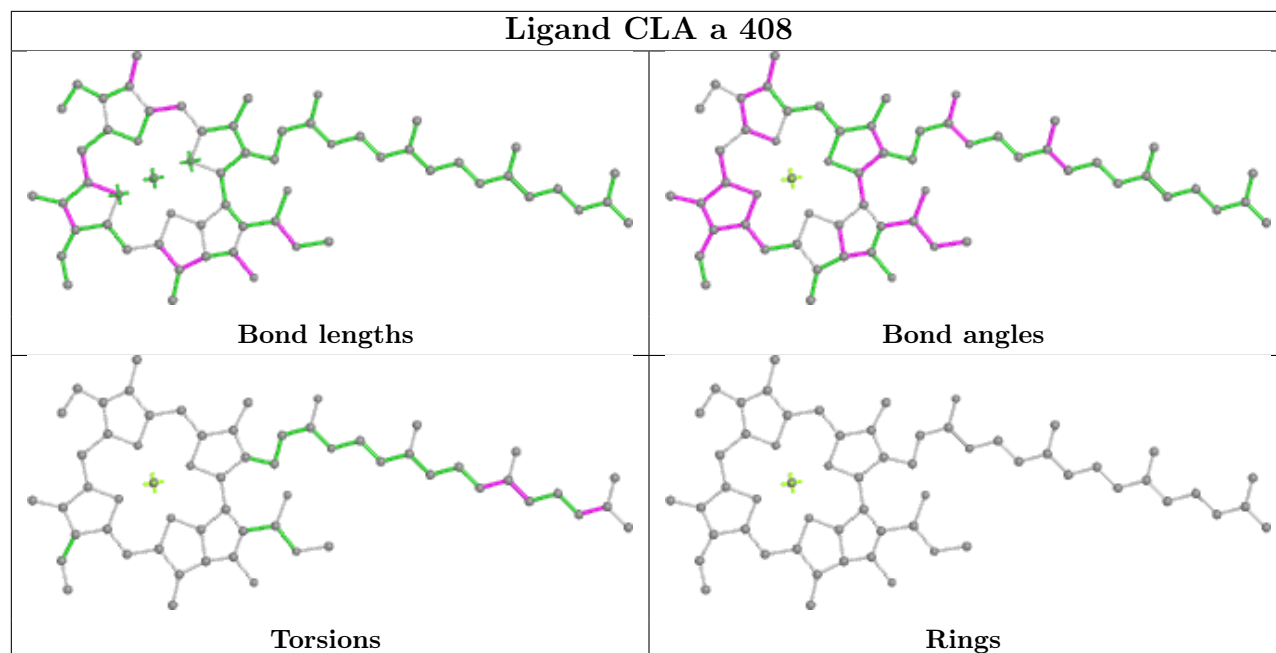
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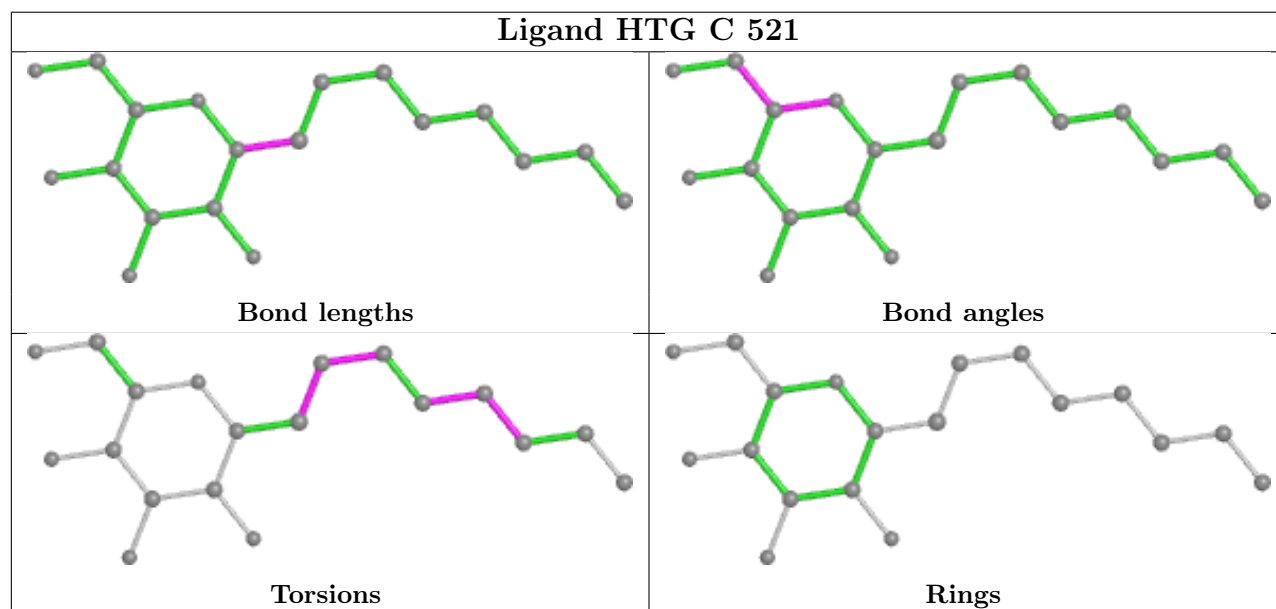
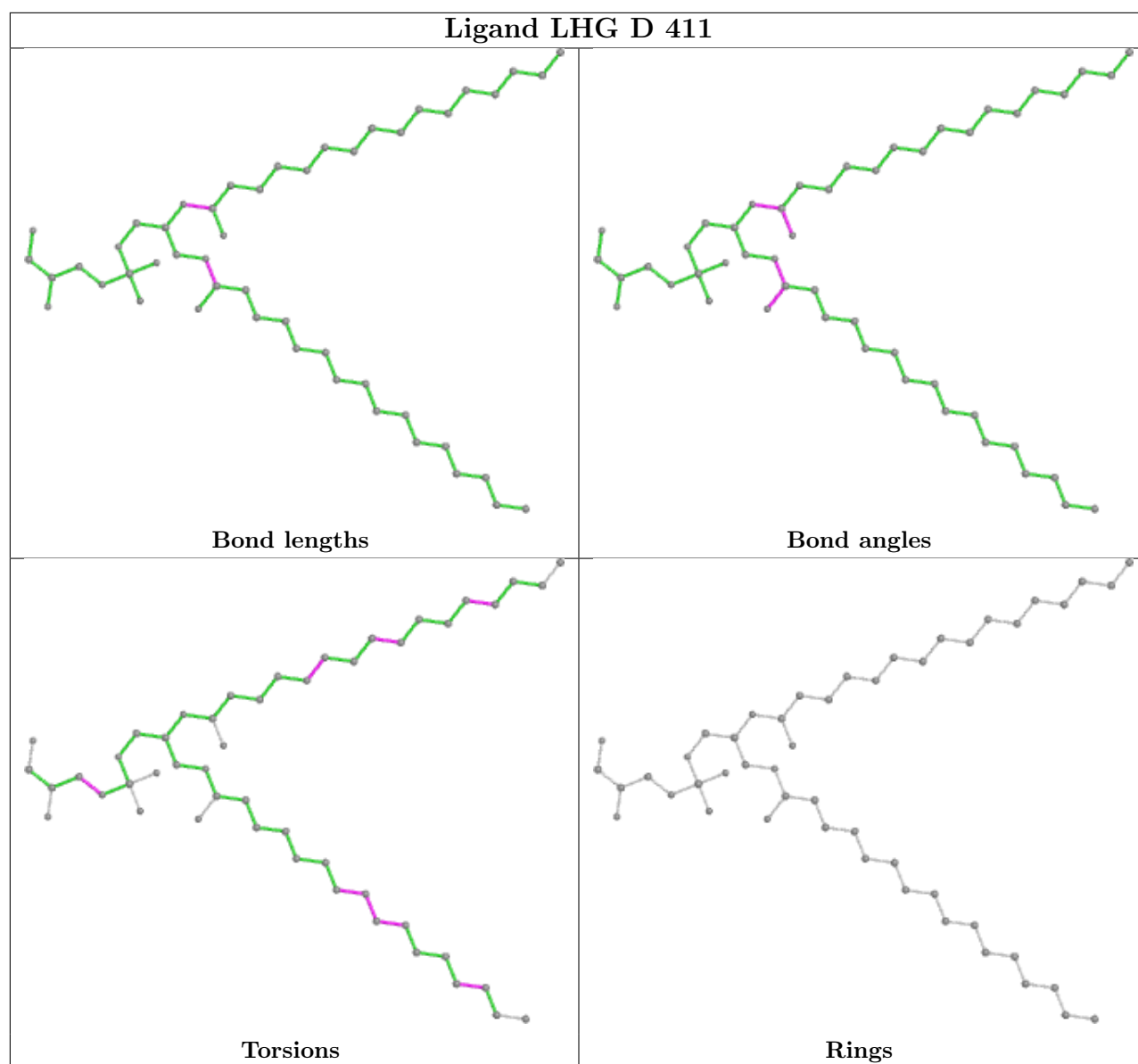


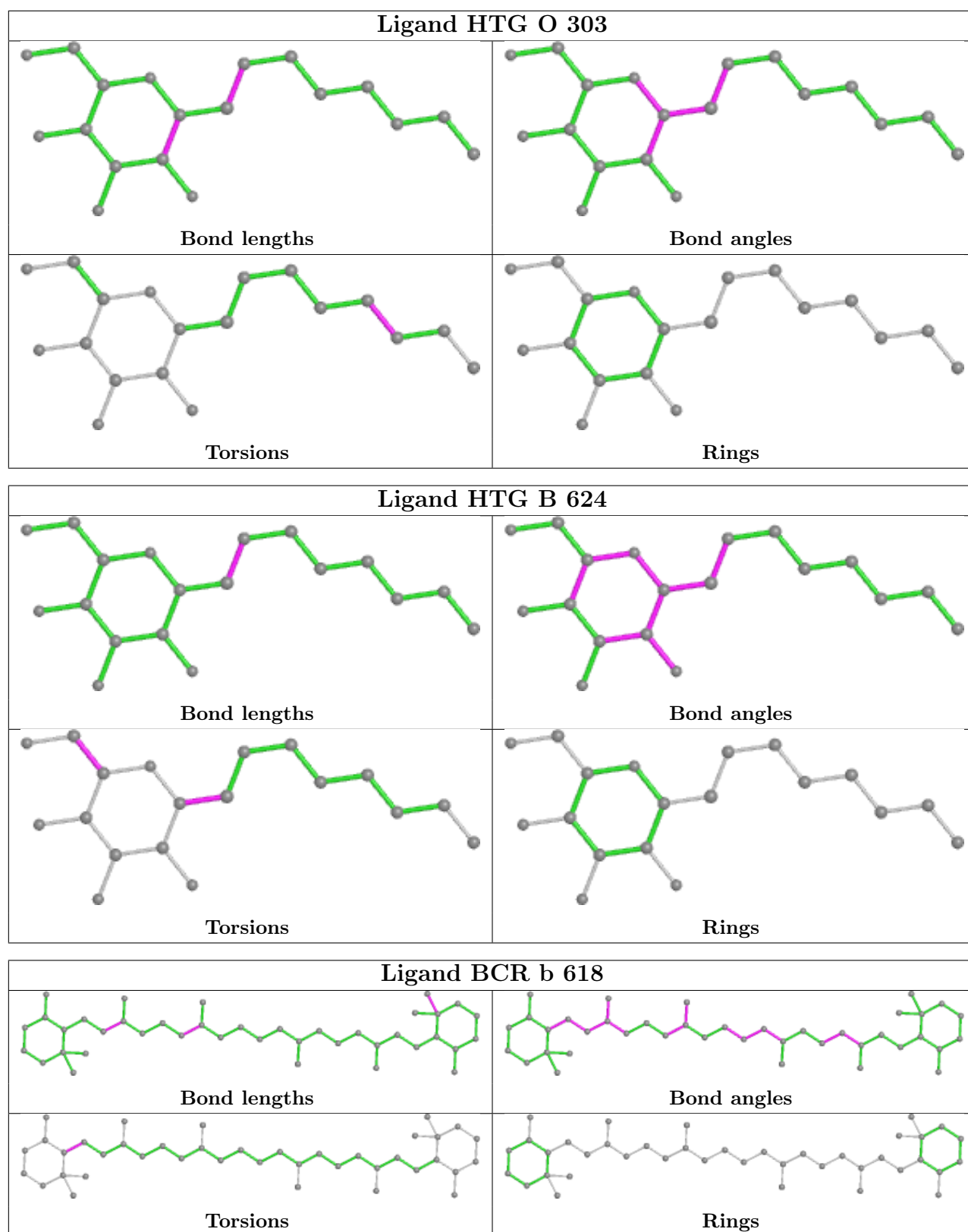


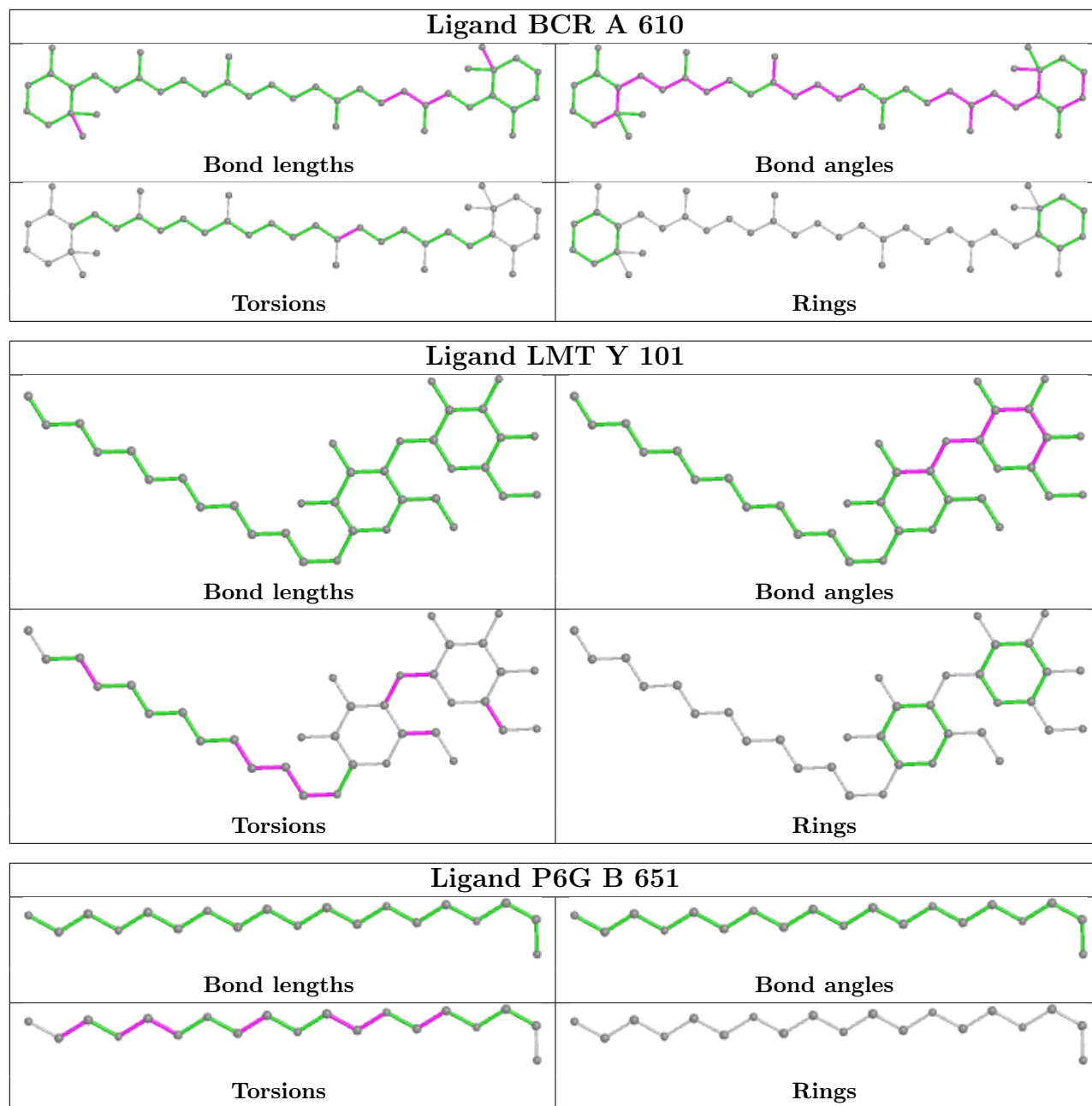




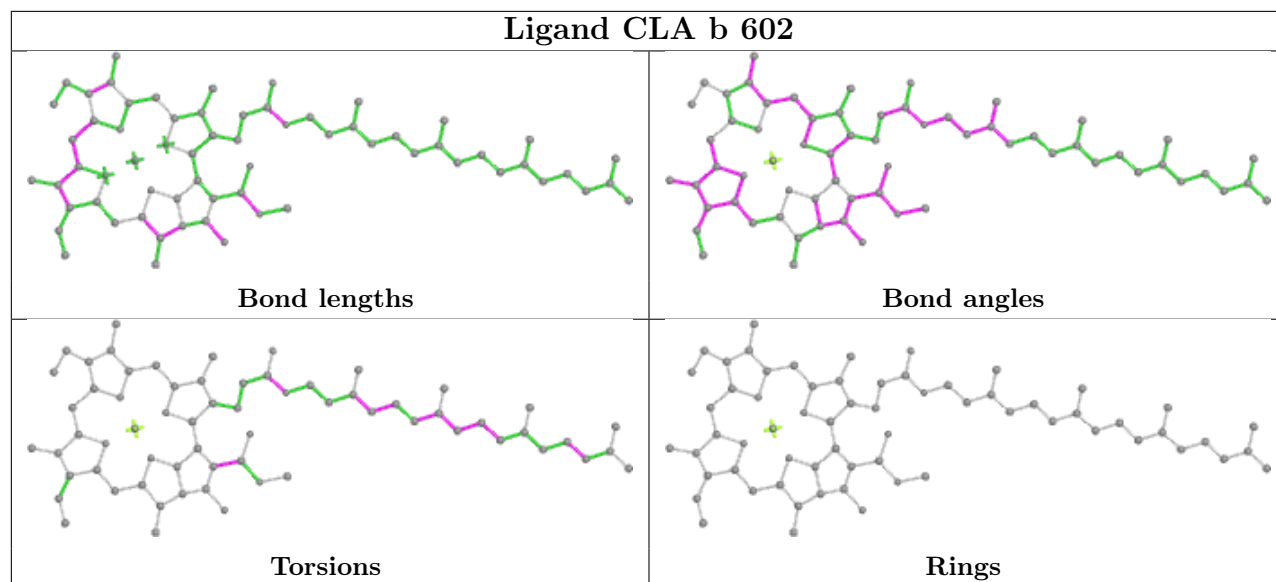




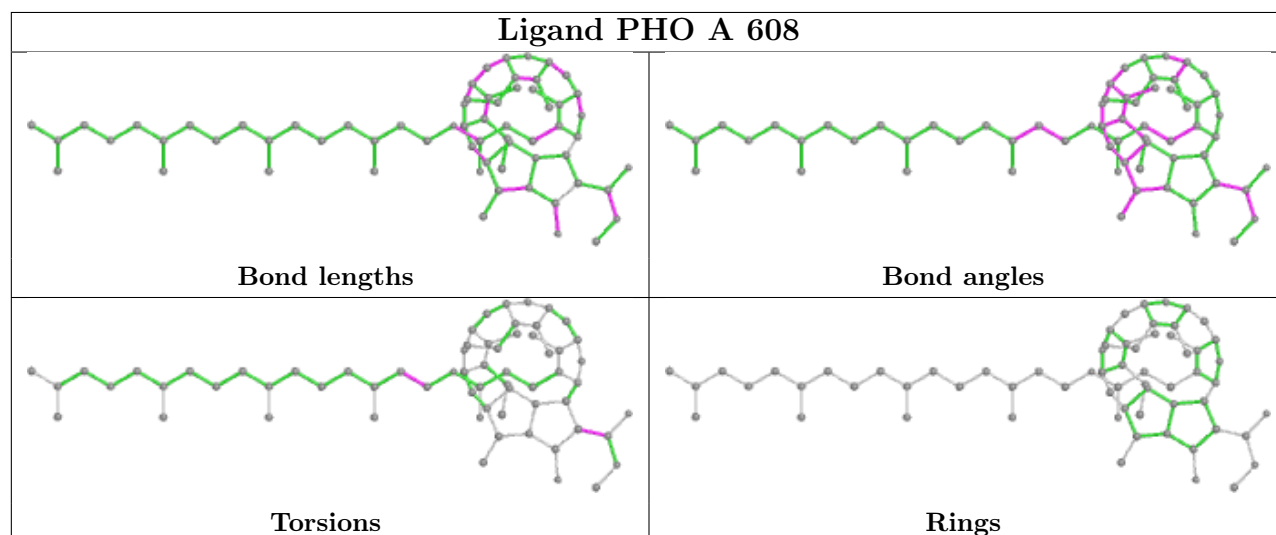




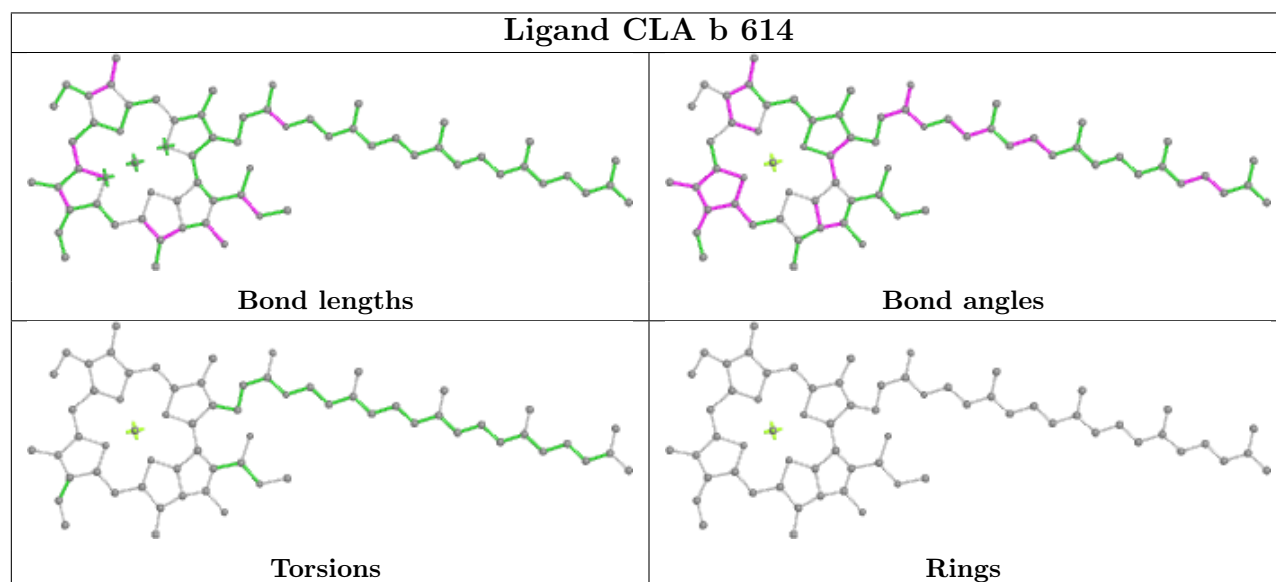
Ligand CLA b 602

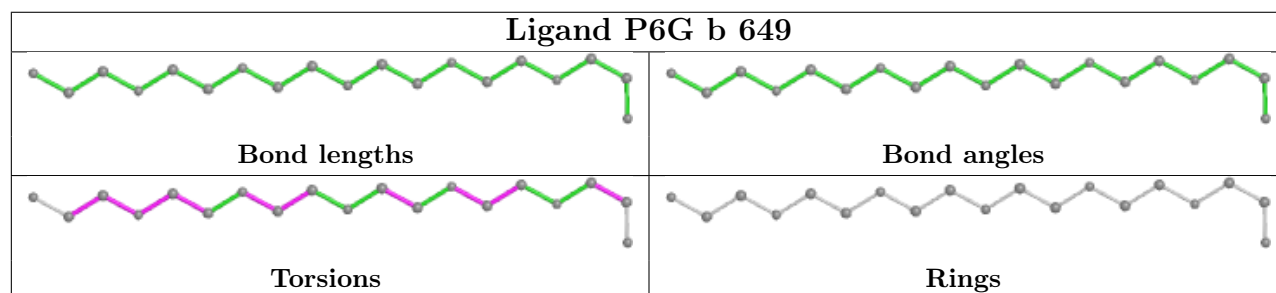
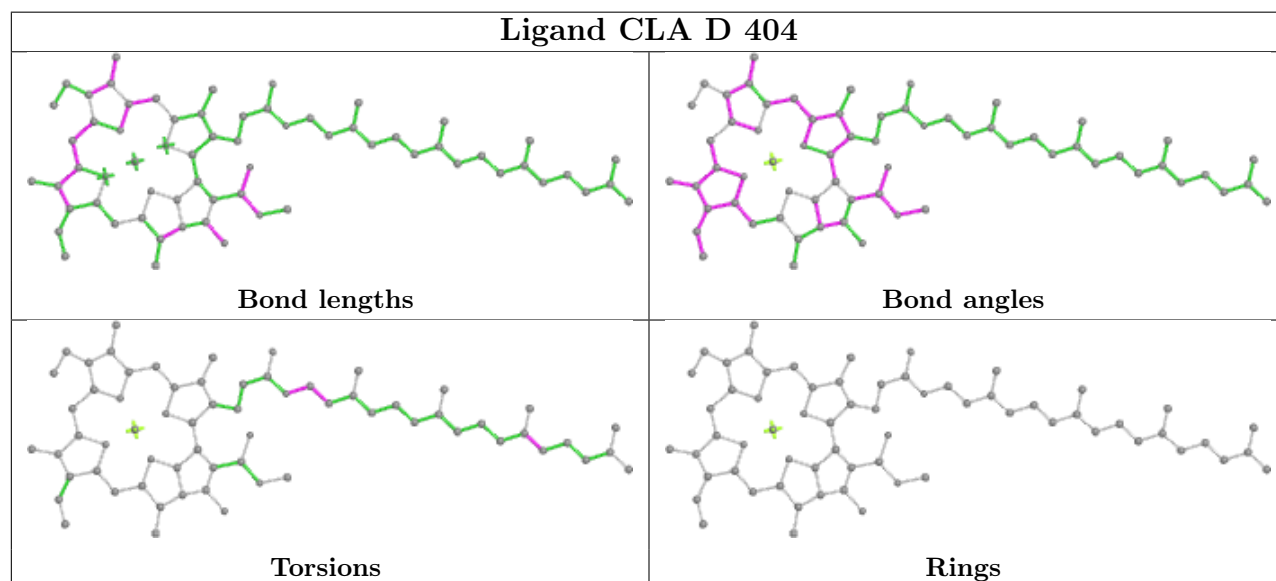
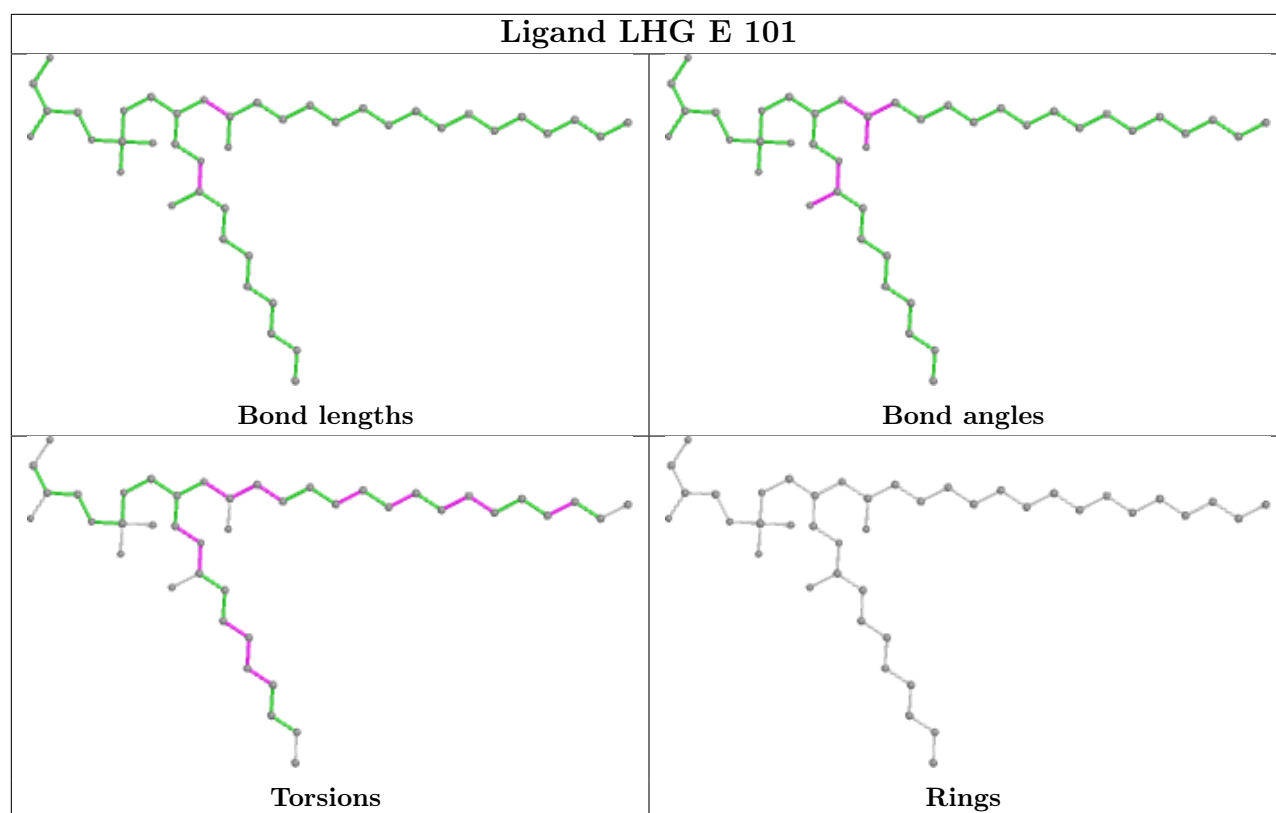


Ligand PHO A 608

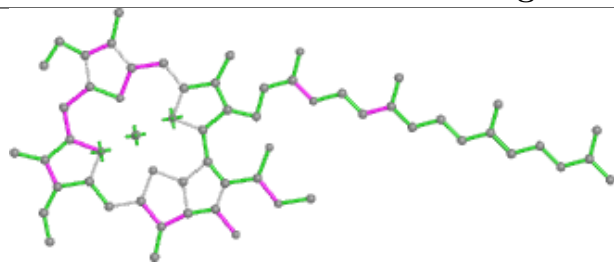


Ligand CLA b 614

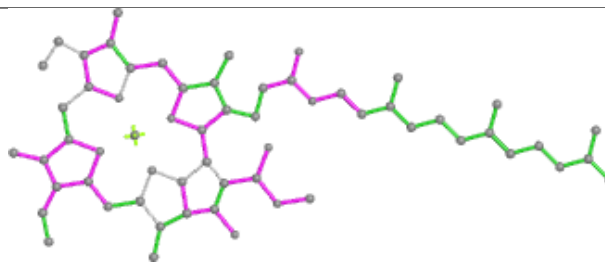




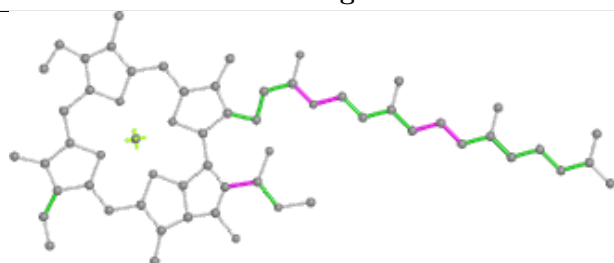
Ligand CLA b 617



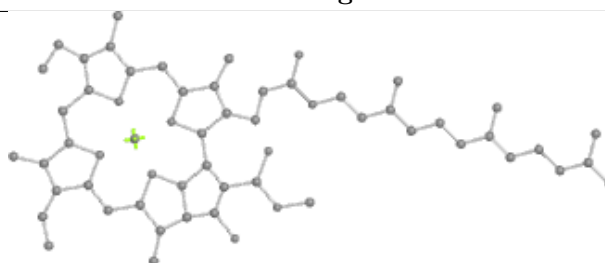
Bond lengths



Bond angles

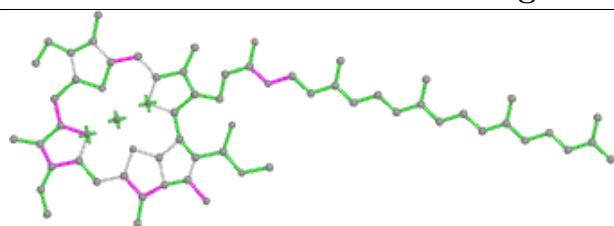


Torsions

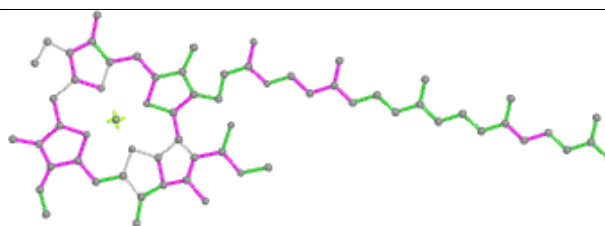


Rings

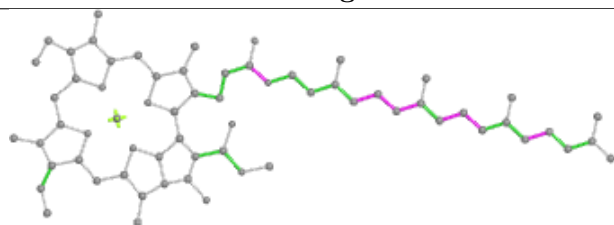
Ligand CLA a 410



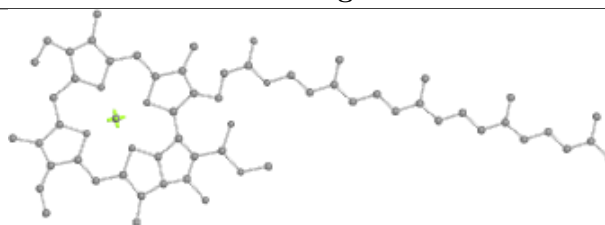
Bond lengths



Bond angles

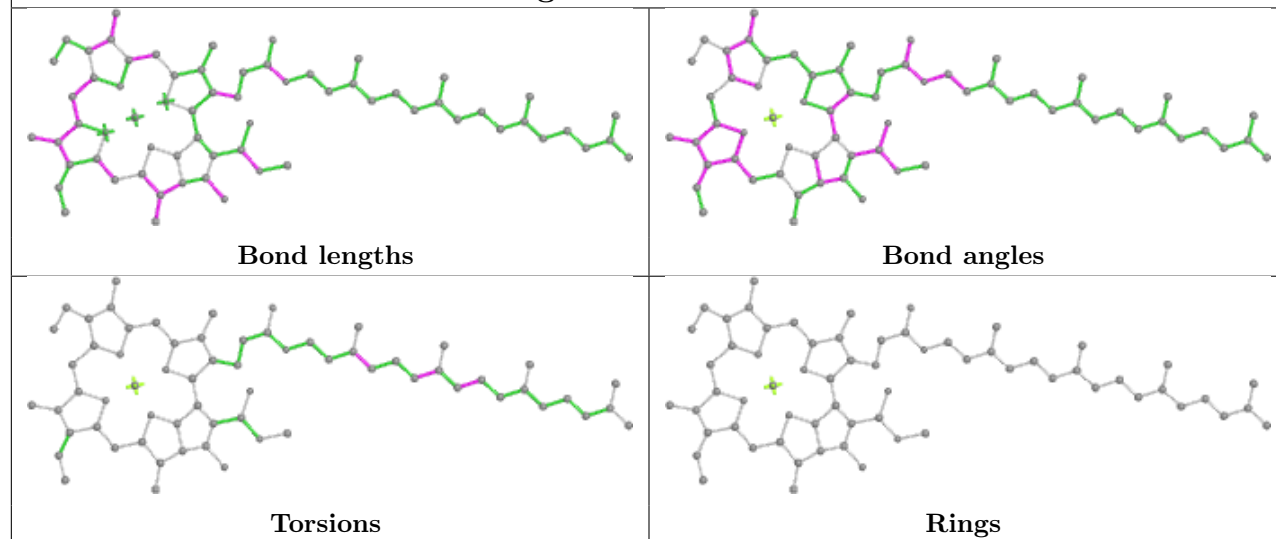


Torsions

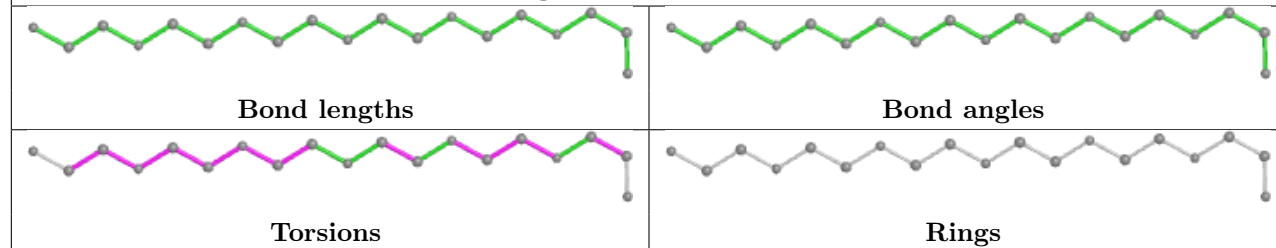


Rings

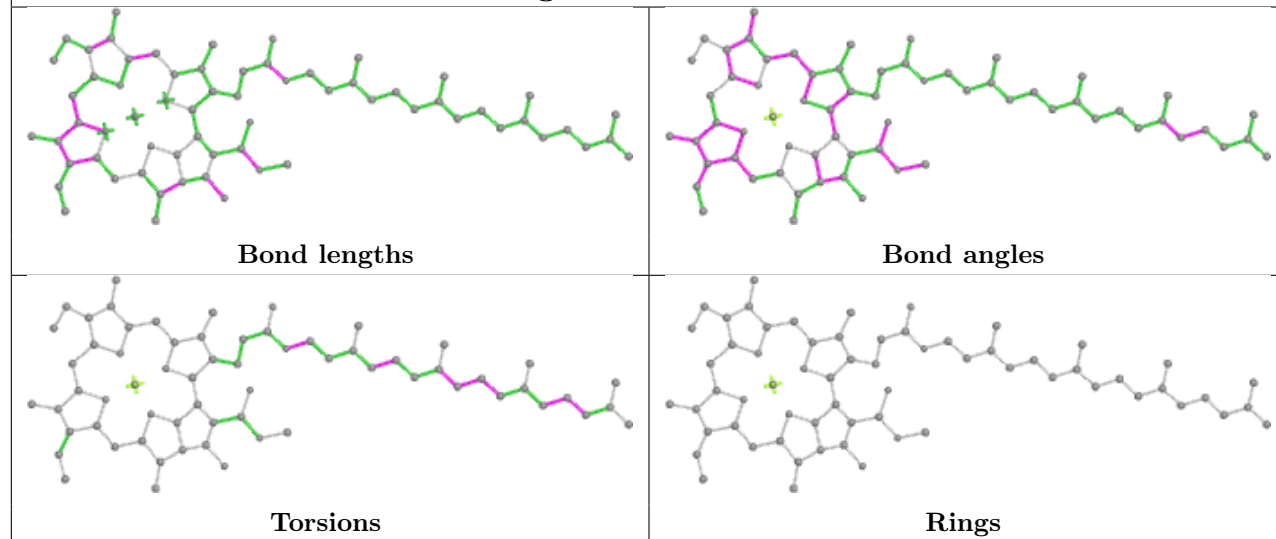
Ligand CLA c 510

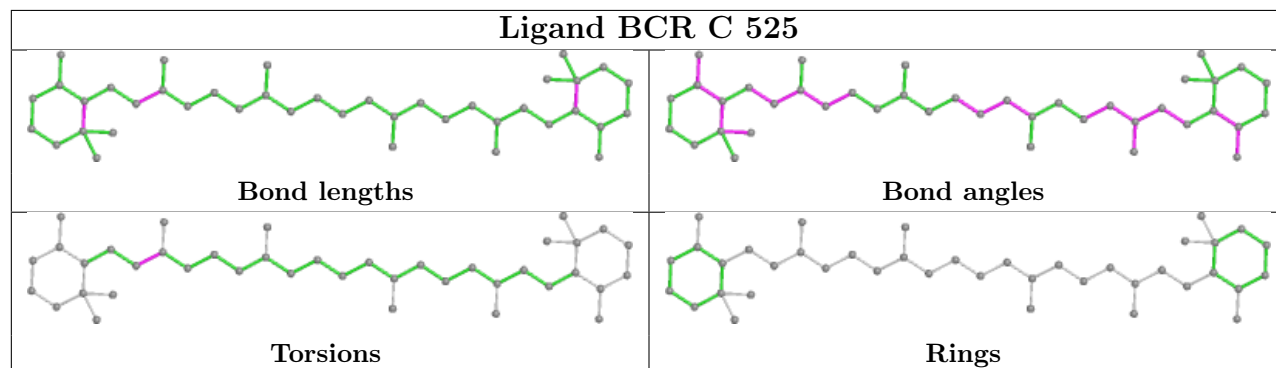
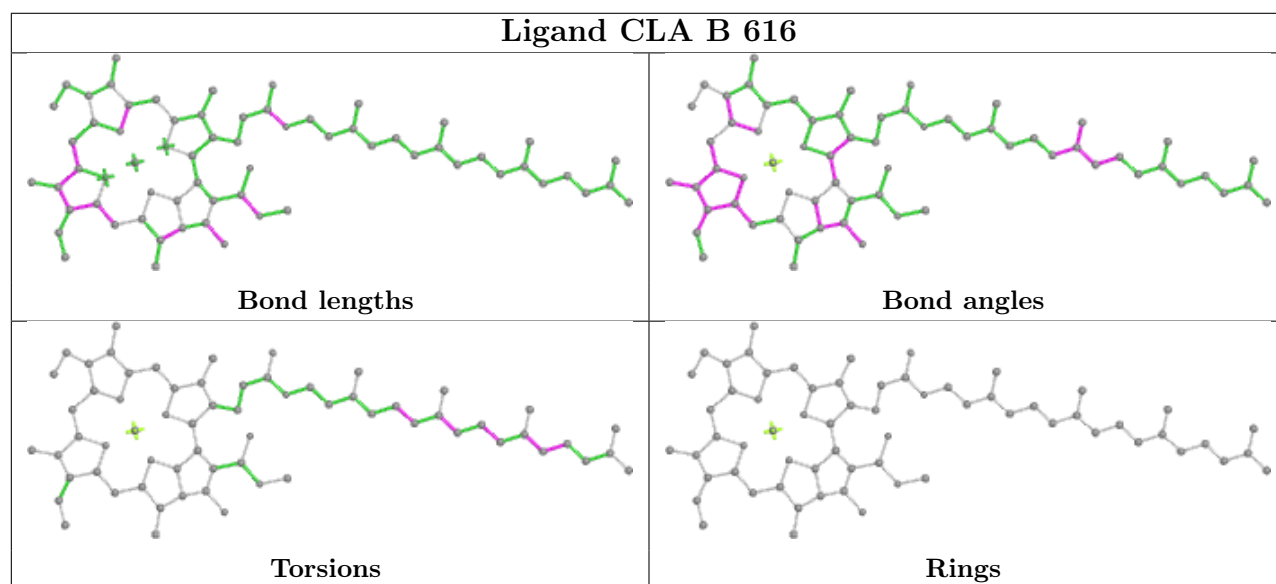
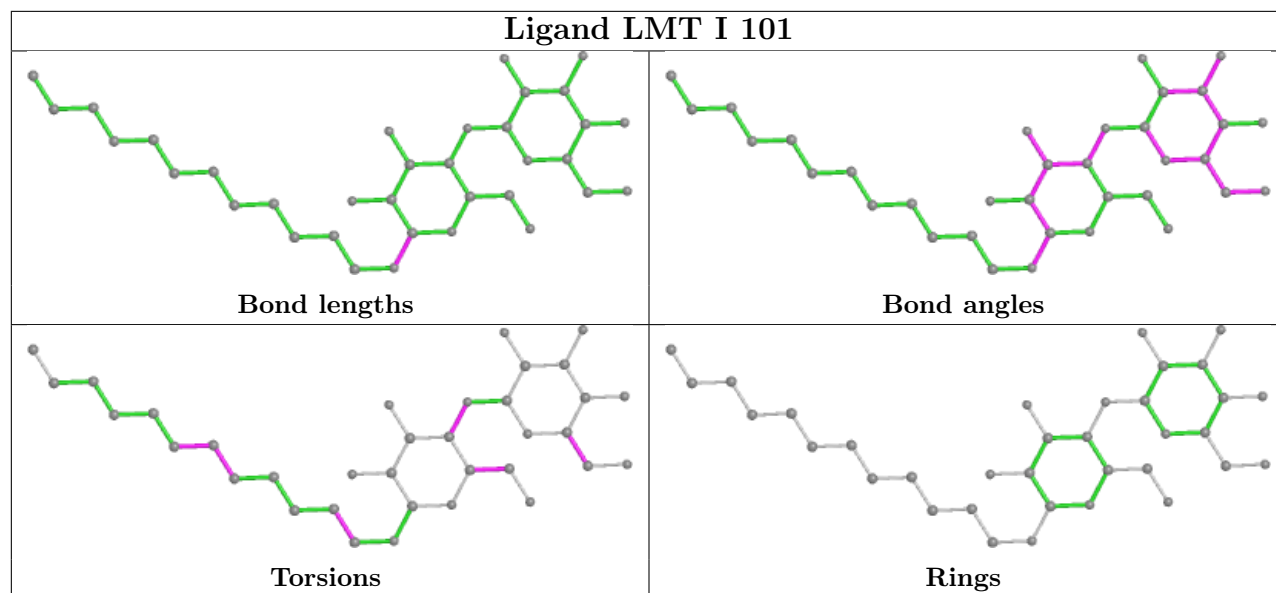


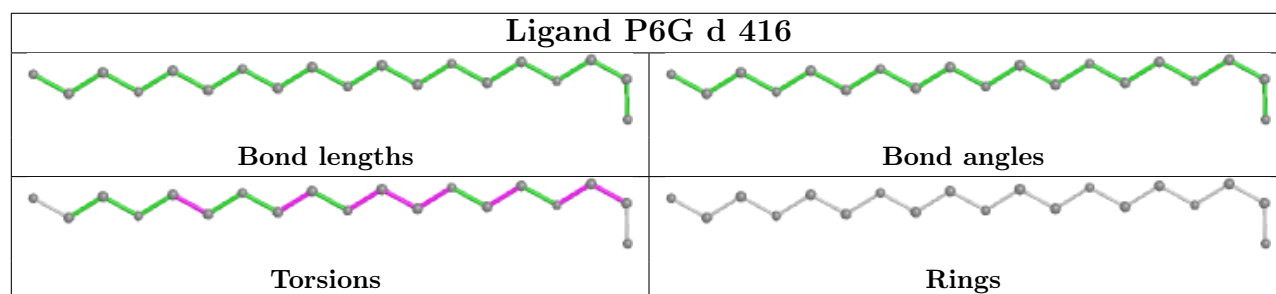
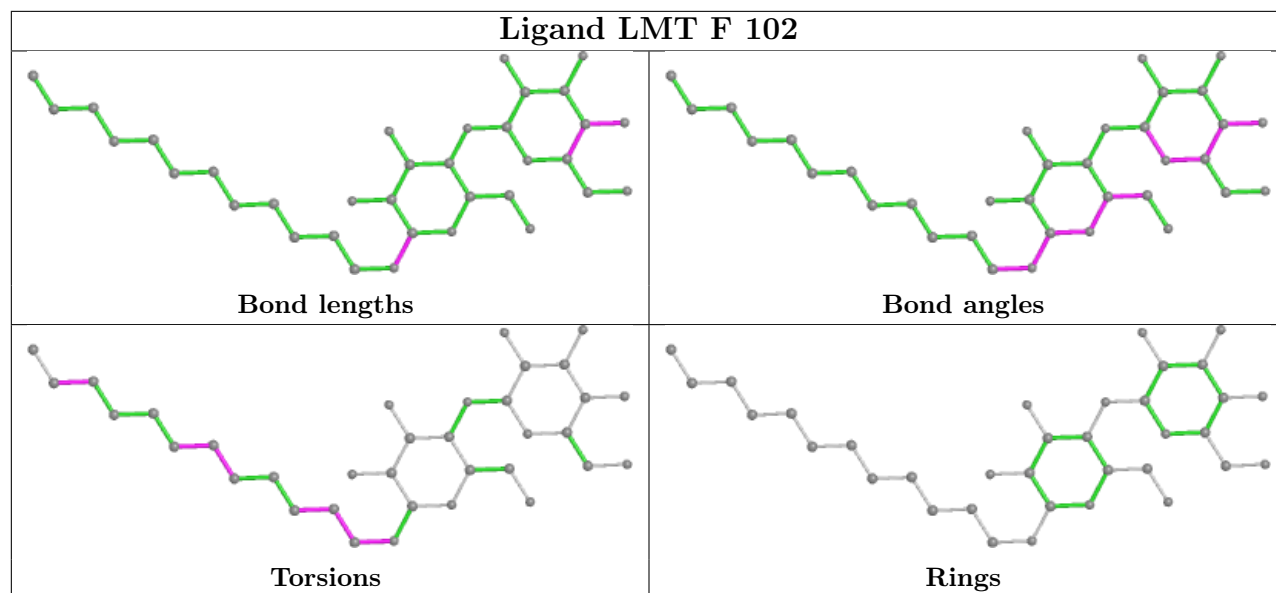
Ligand P6G T 105

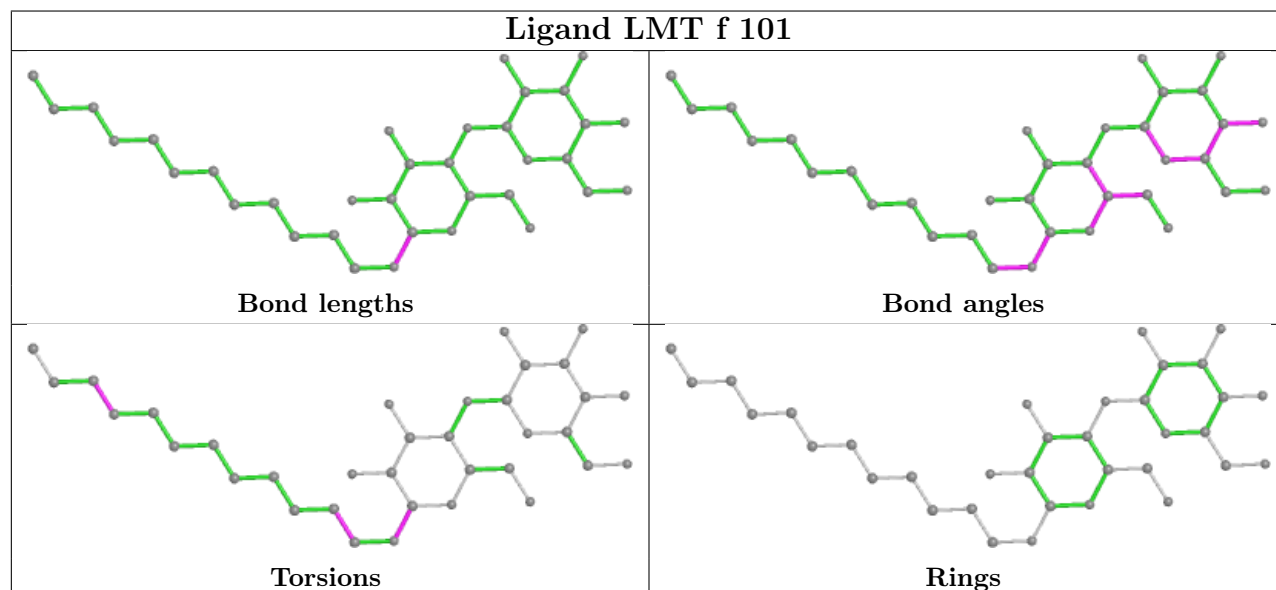
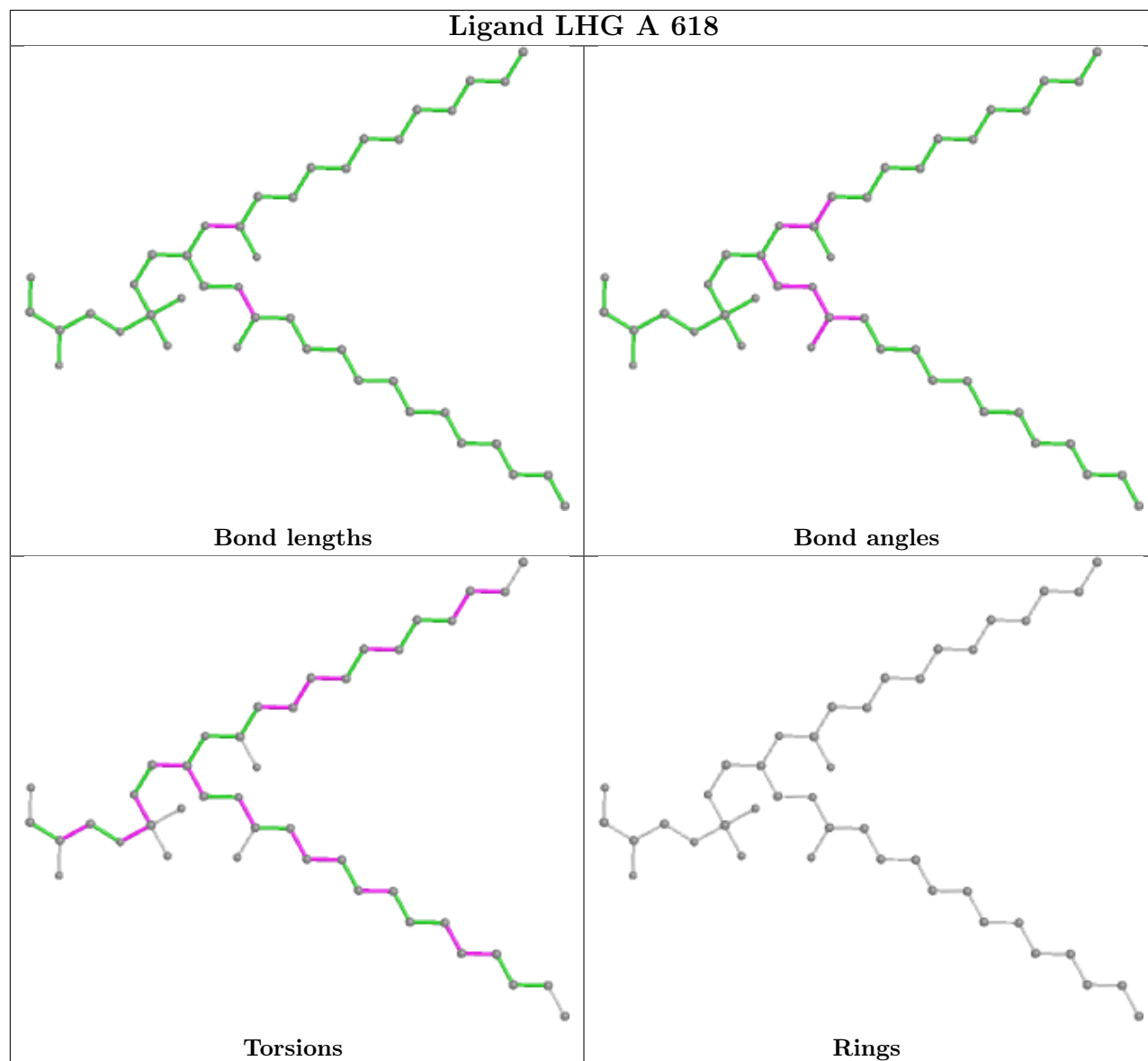


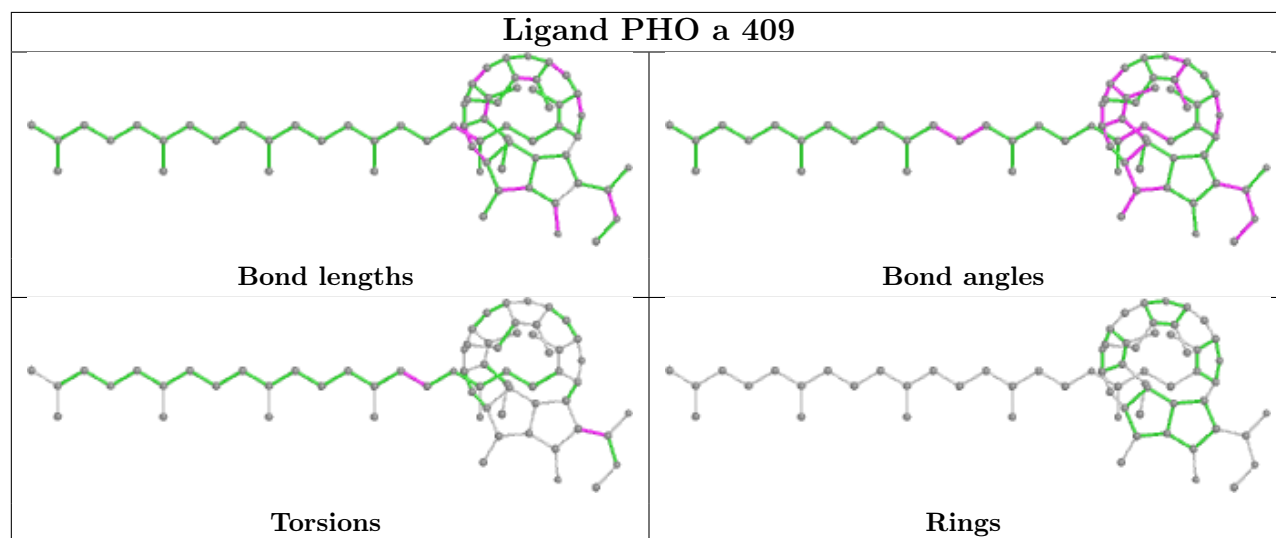
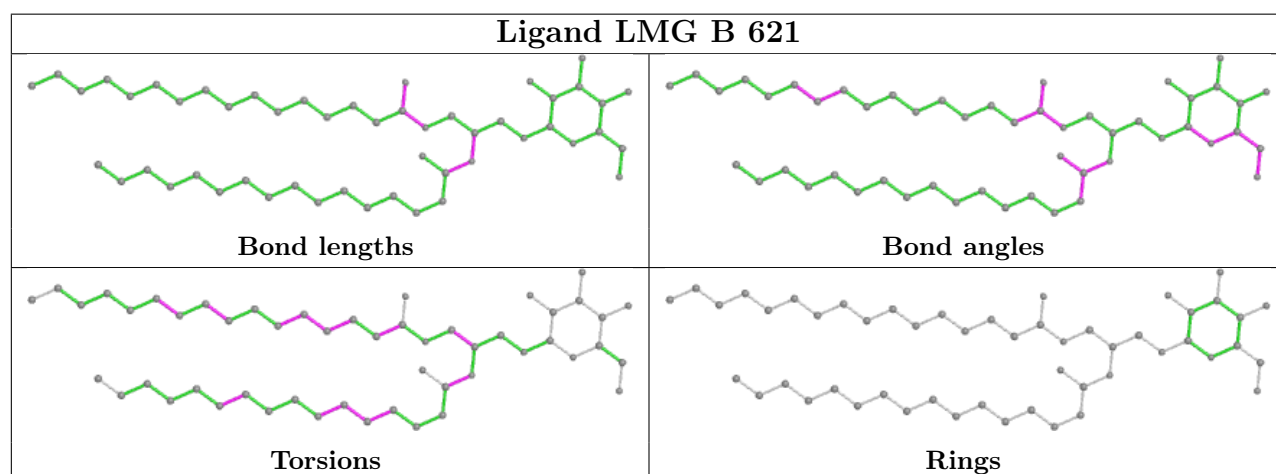
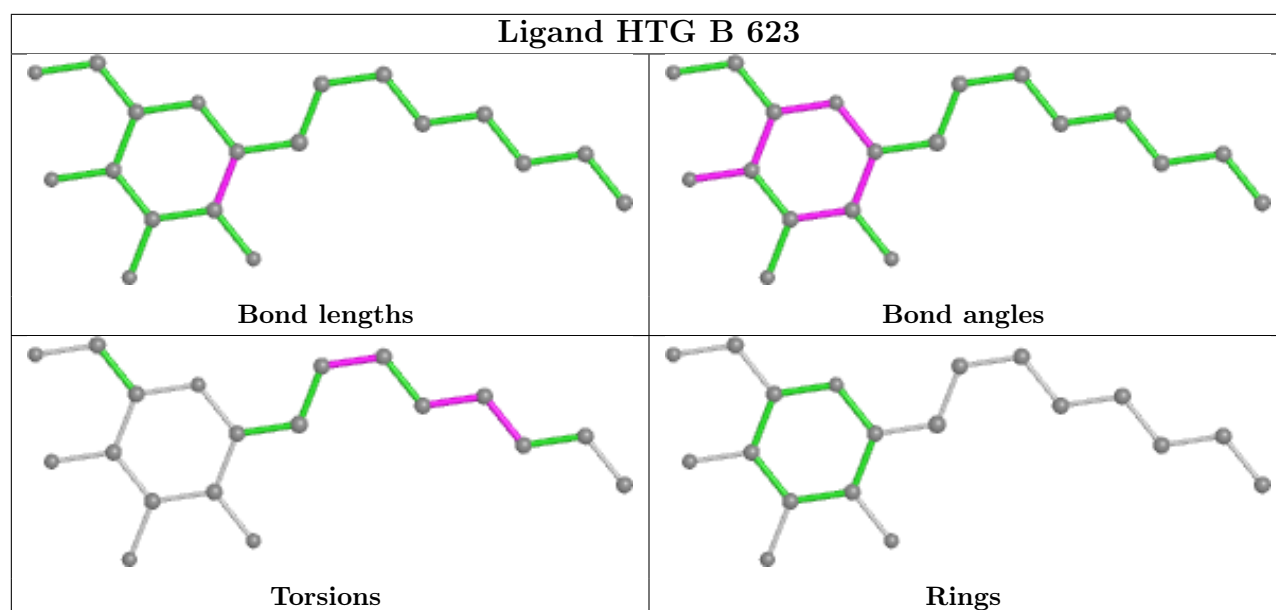
Ligand CLA c 509

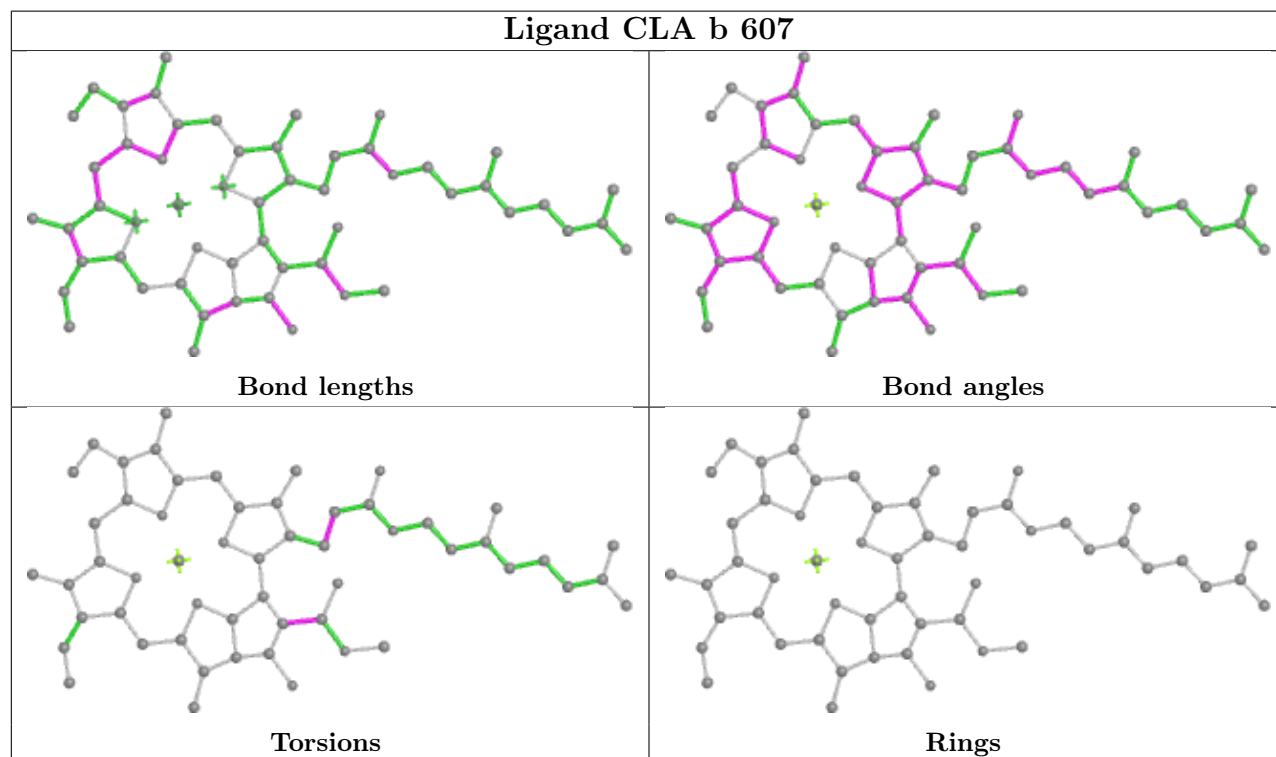
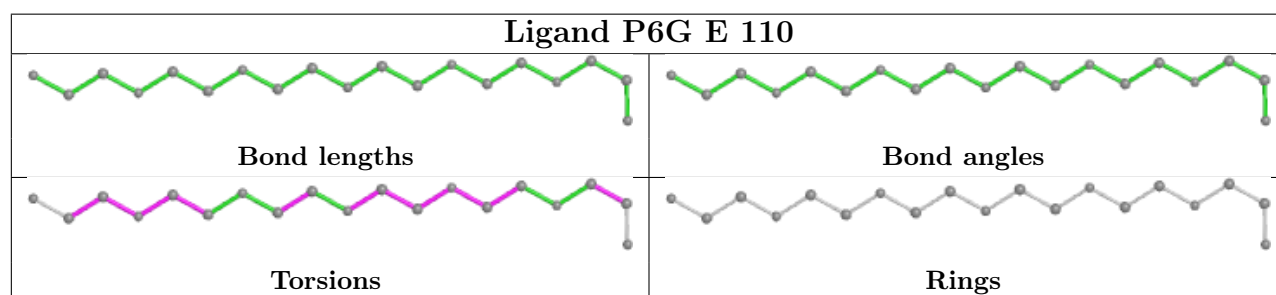
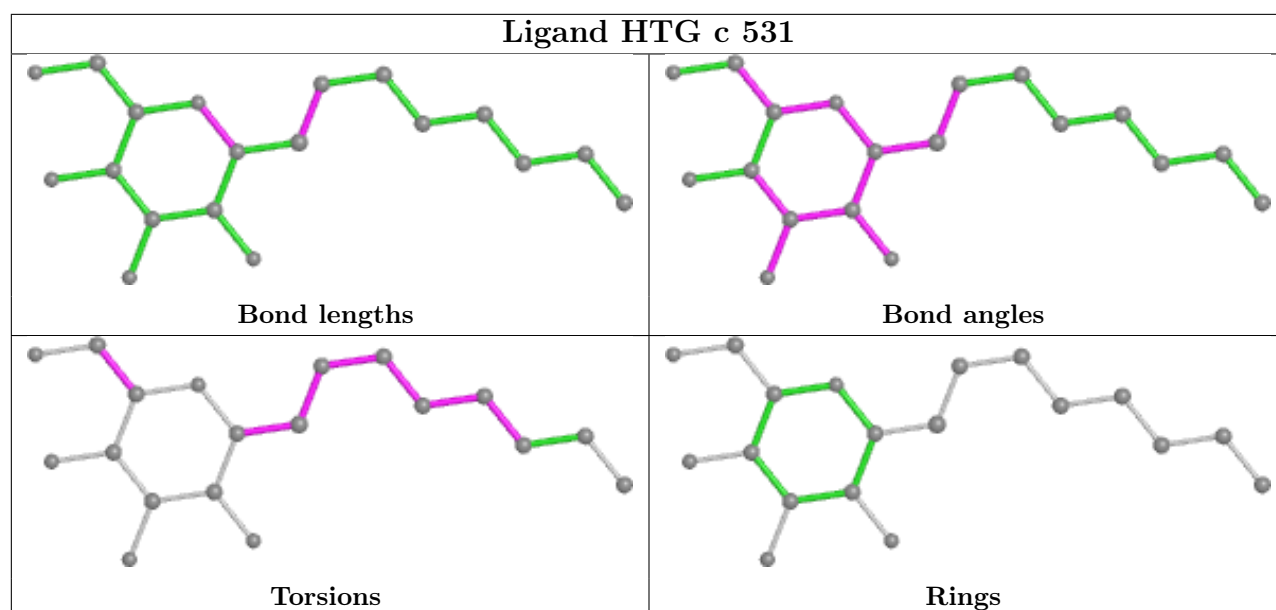




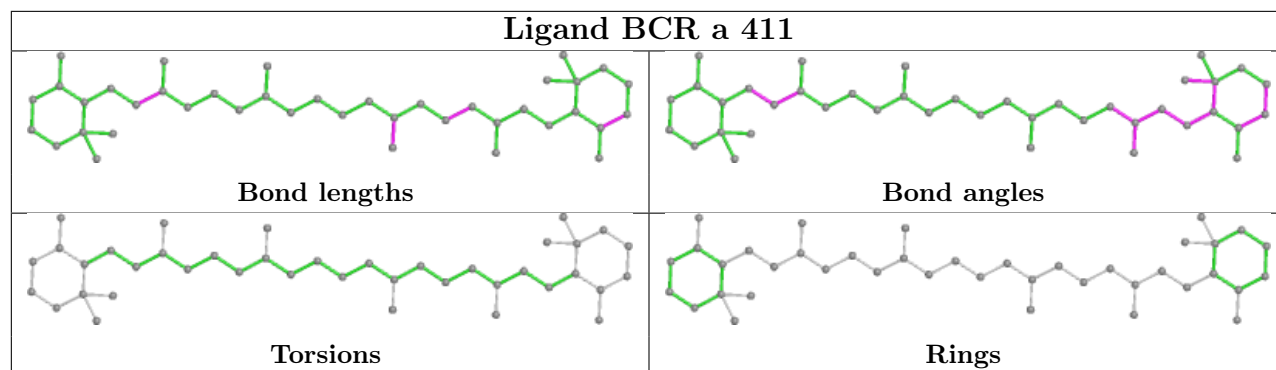




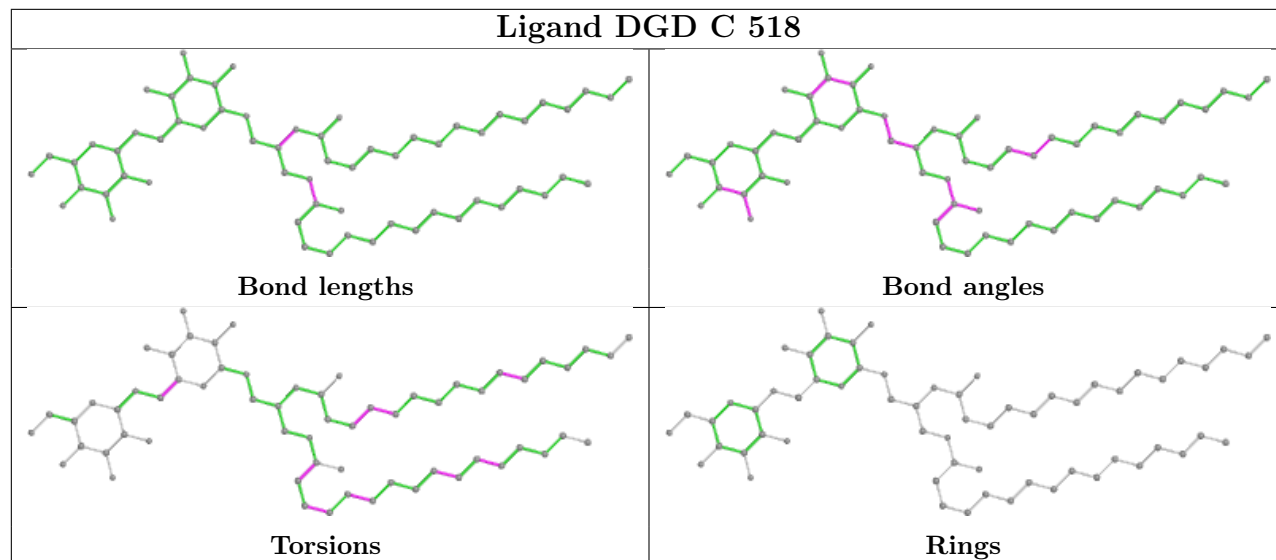




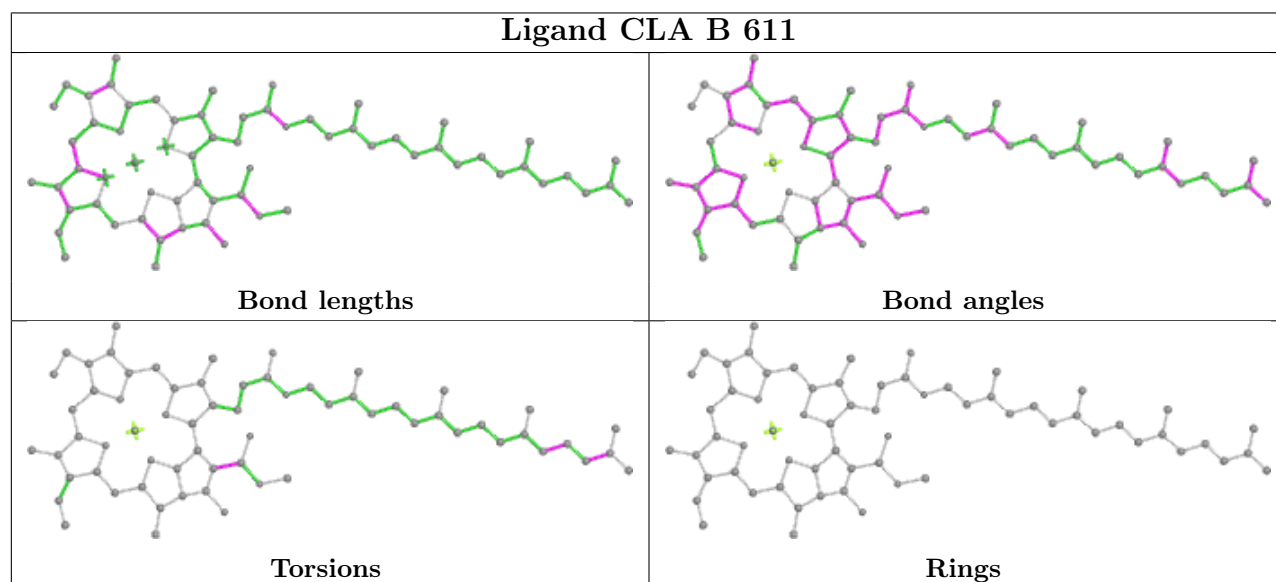
Ligand BCR a 411



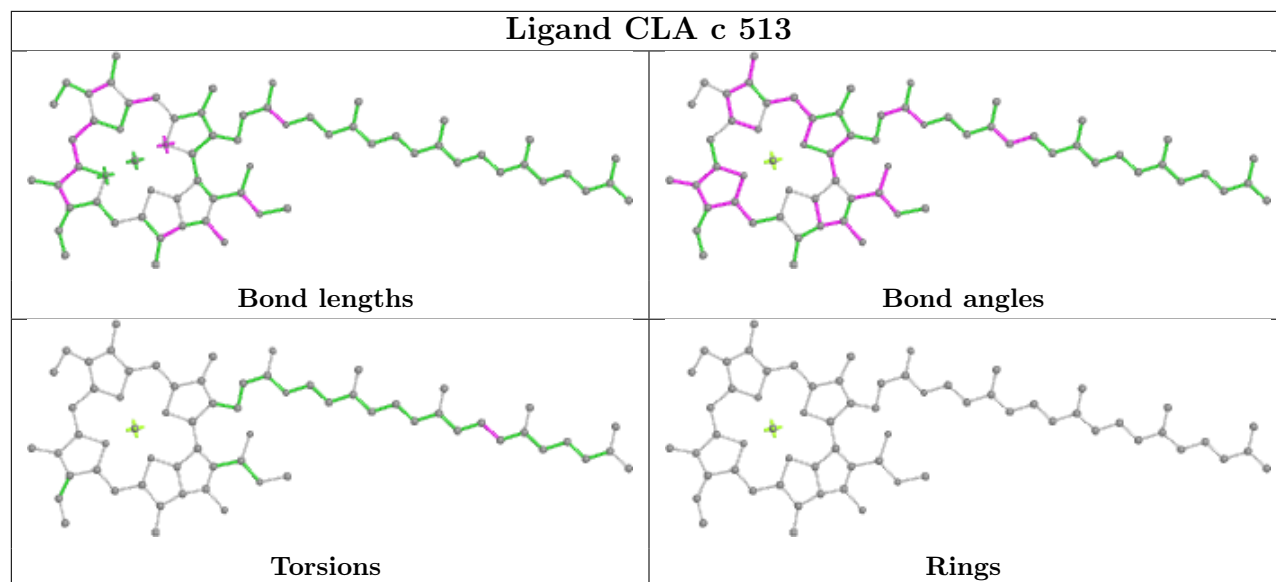
Ligand DGD C 518



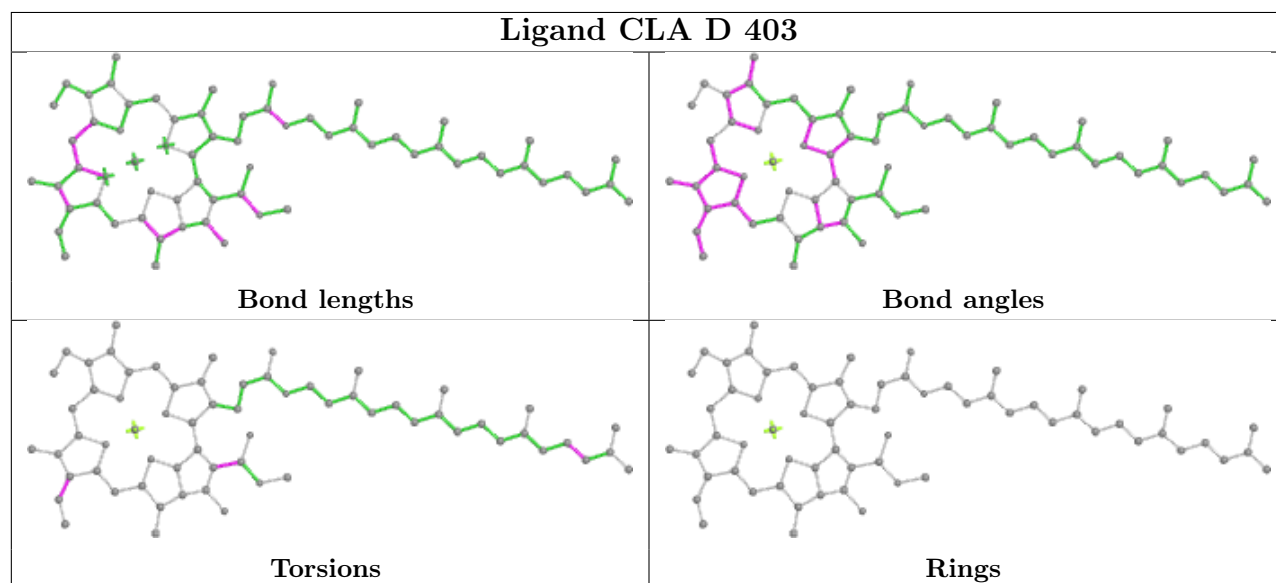
Ligand CLA B 611

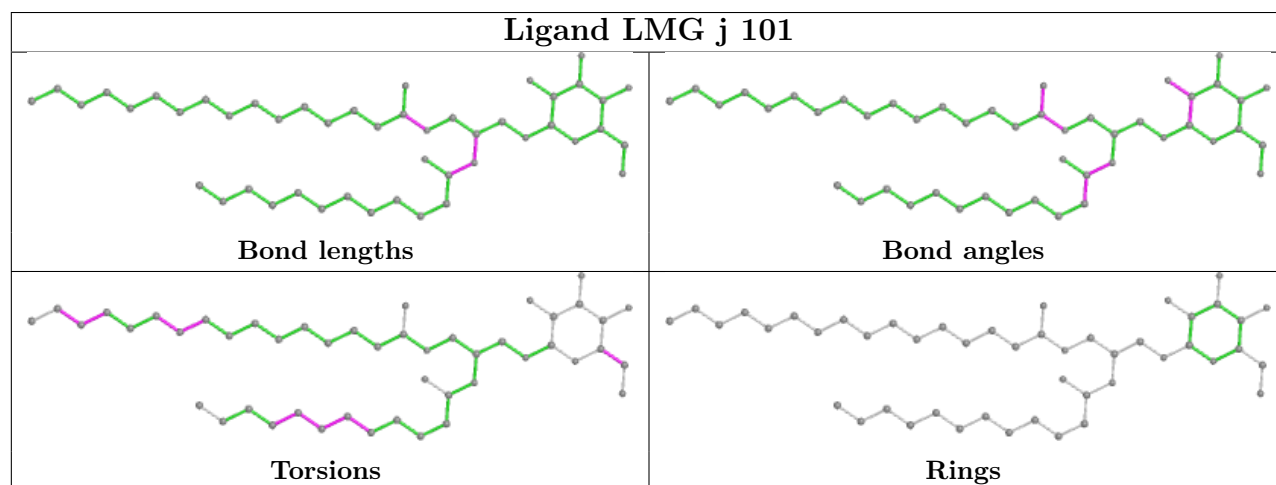
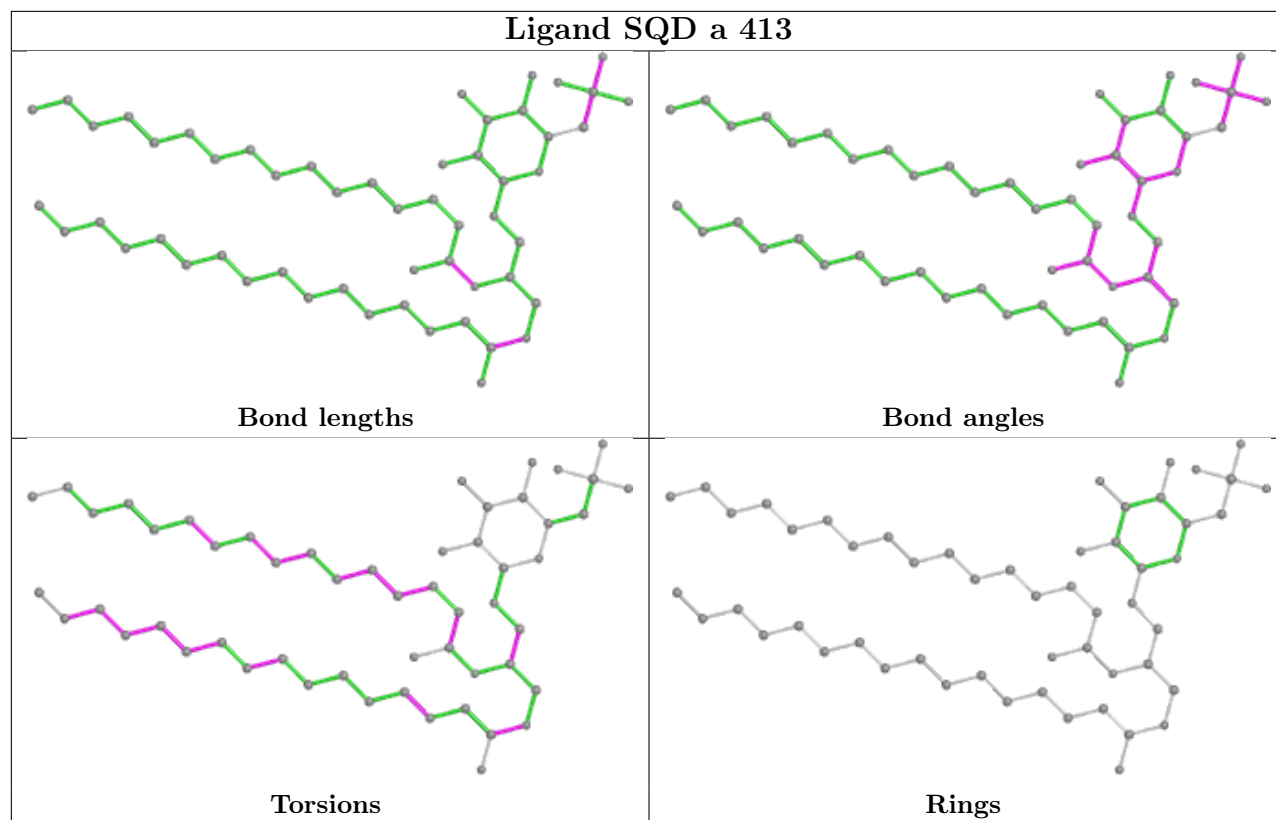


Ligand CLA c 513

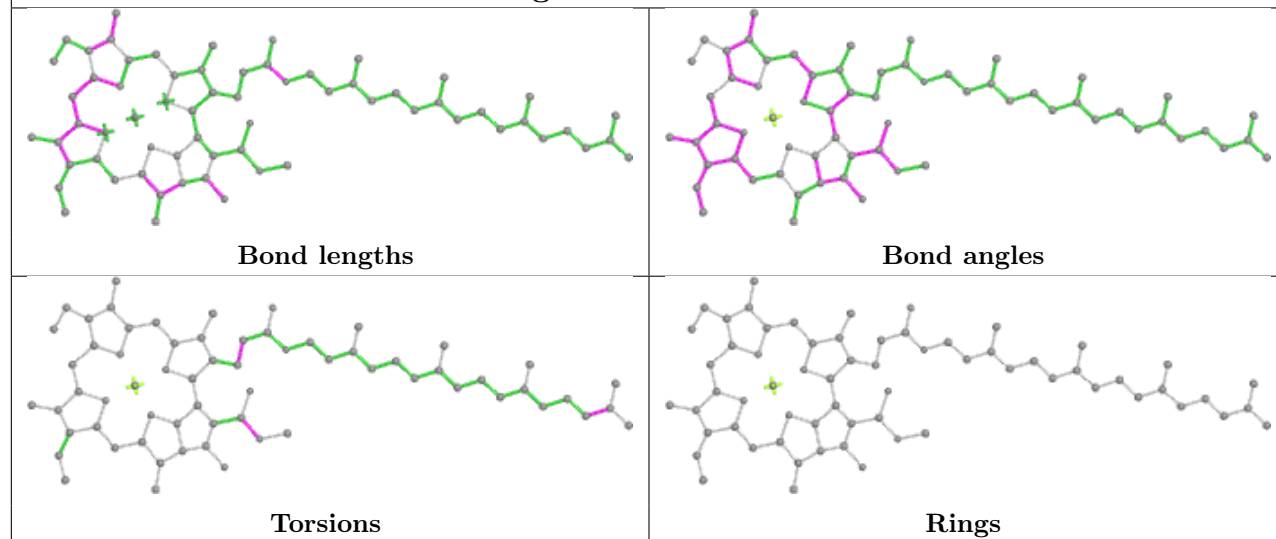


Ligand CLA D 403

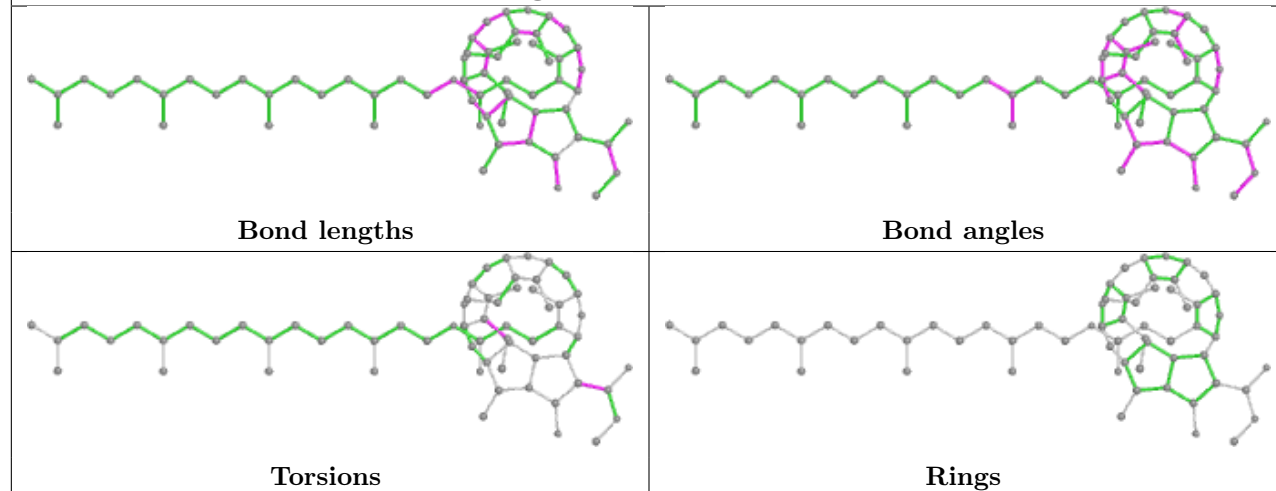


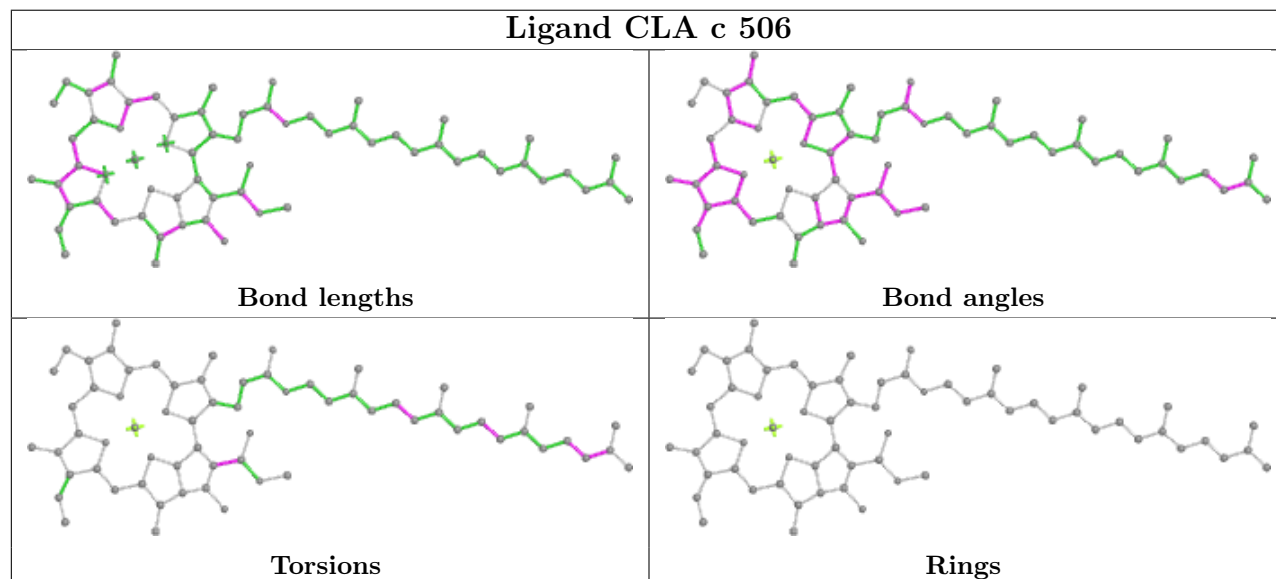
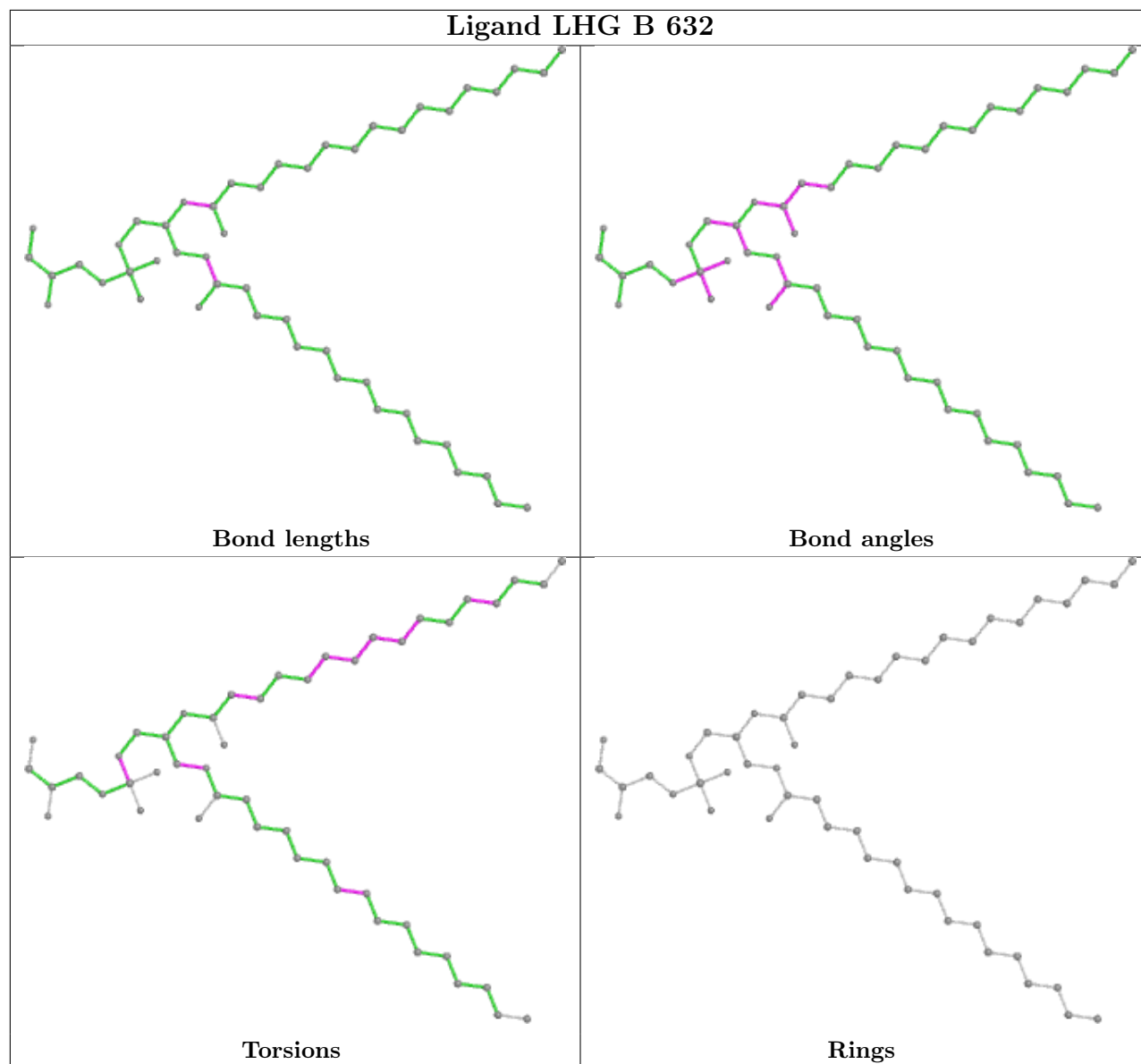


Ligand CLA C 501

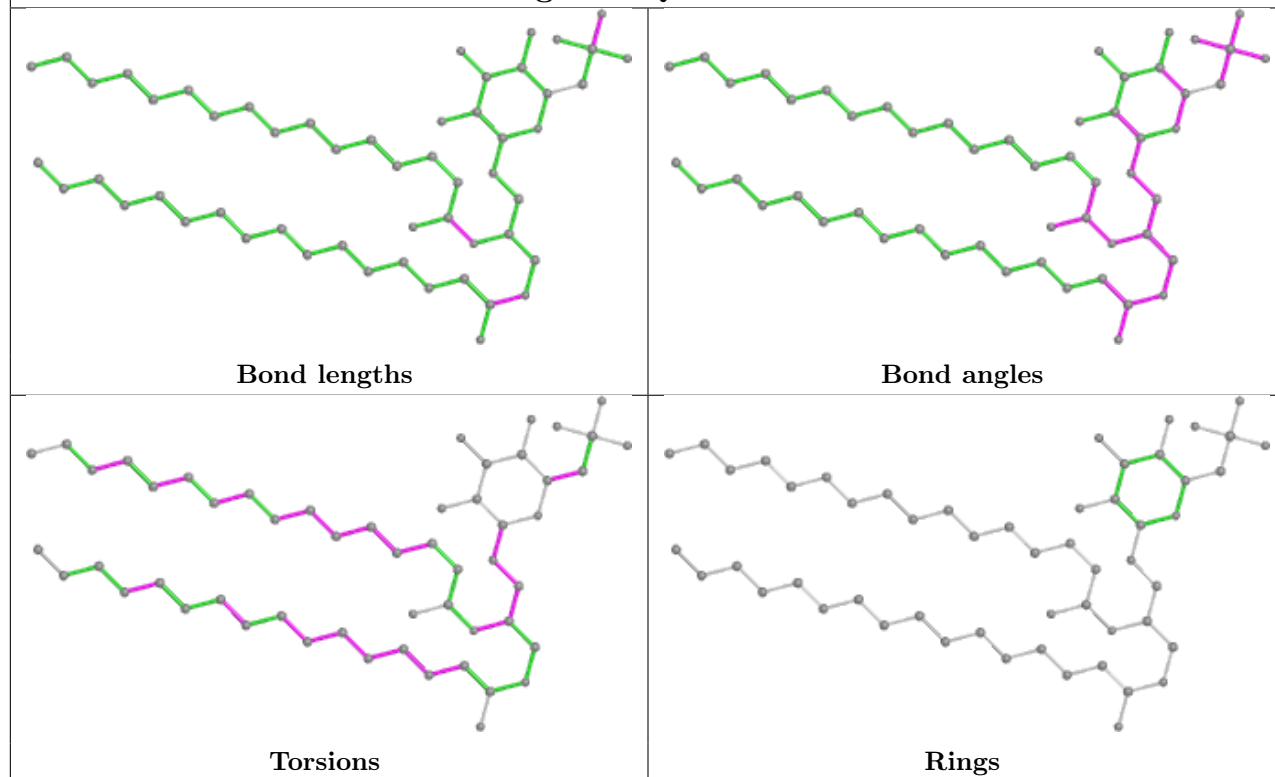


Ligand PHO D 401

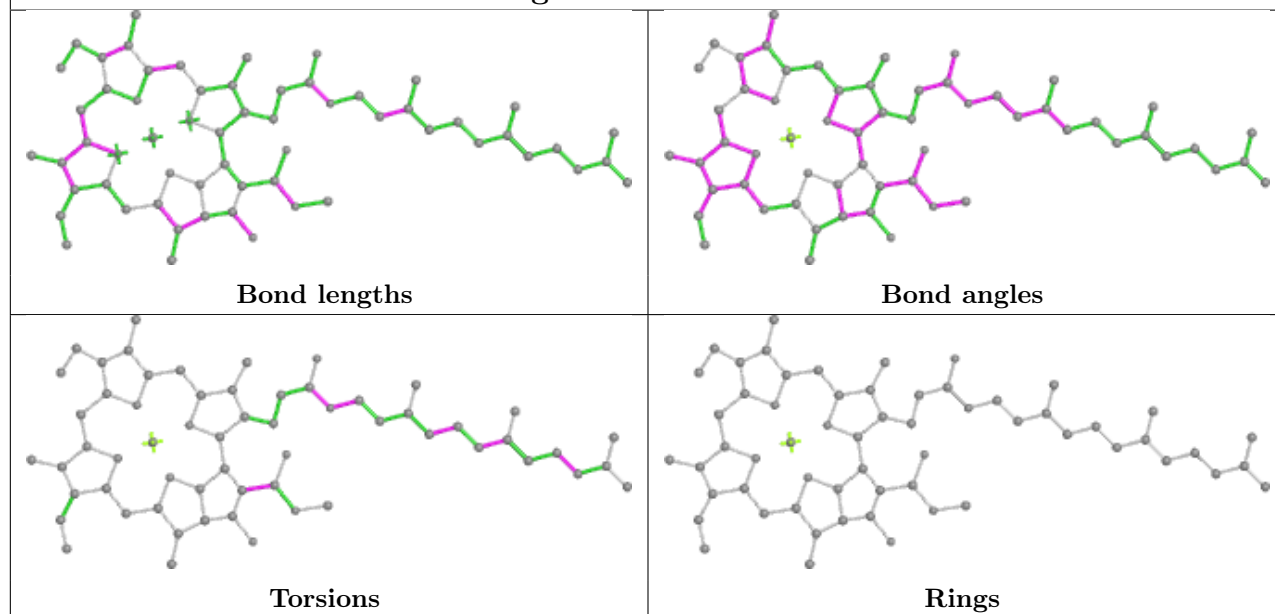


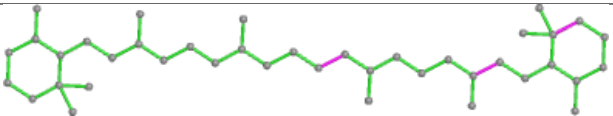
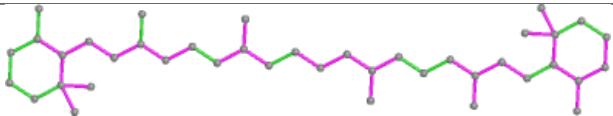
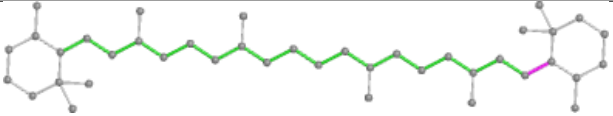
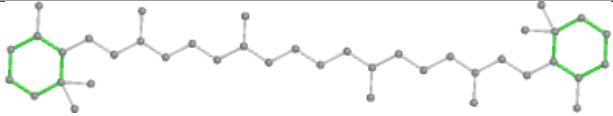


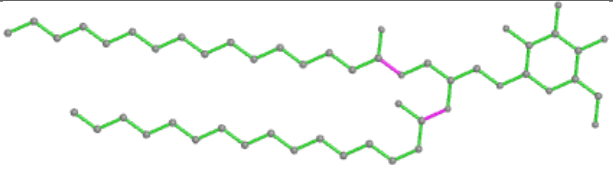
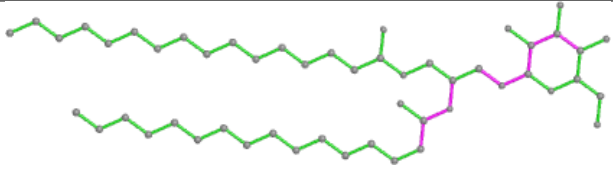
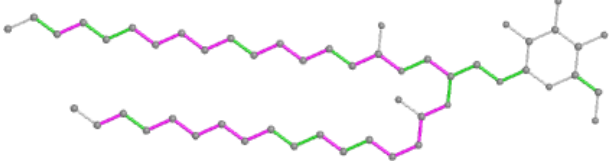
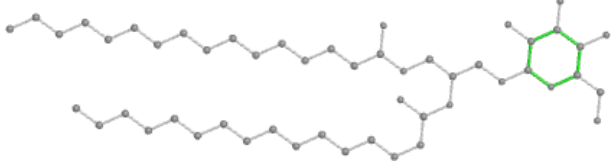
Ligand SQD a 424

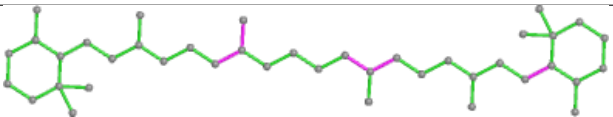
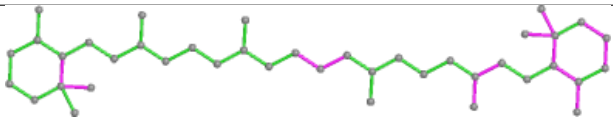

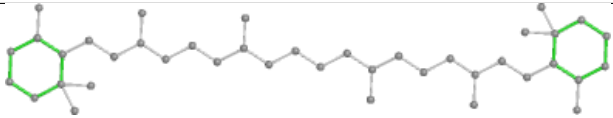


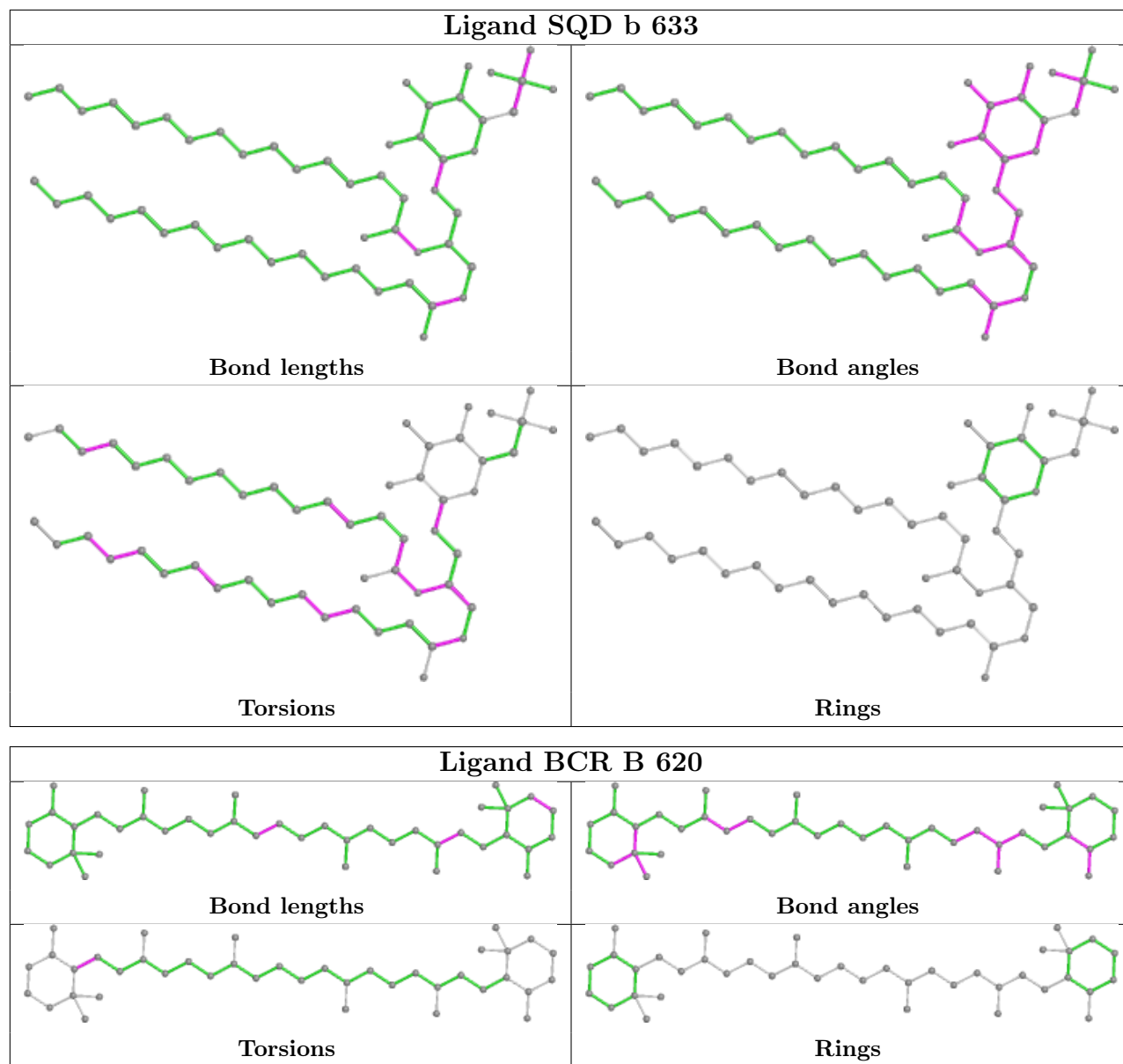
Ligand CLA B 617

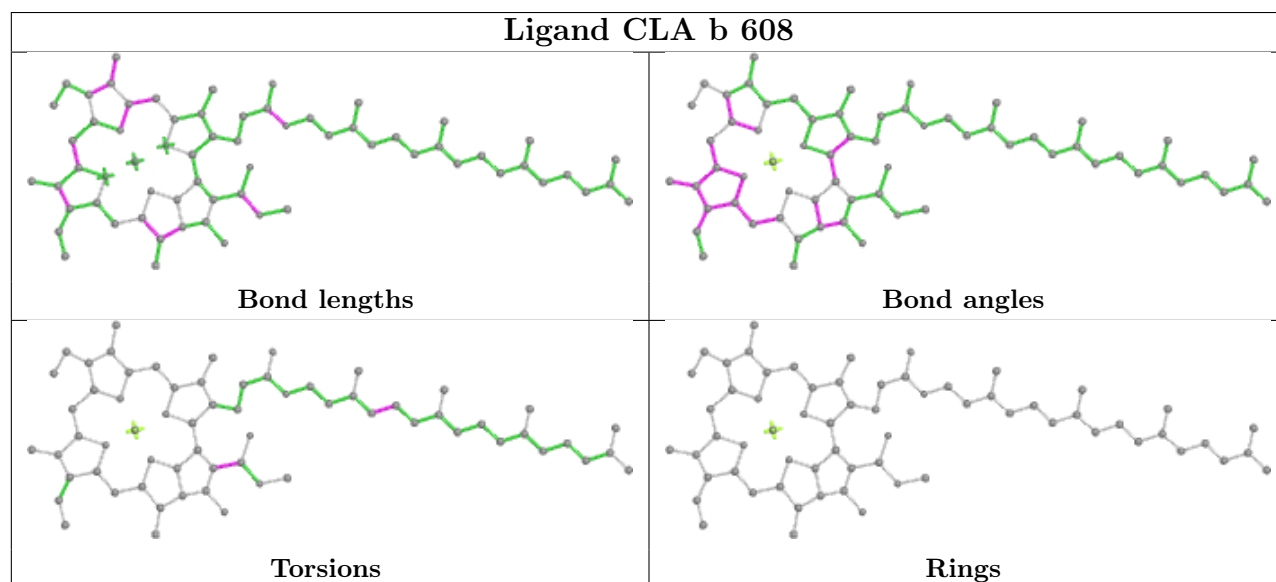
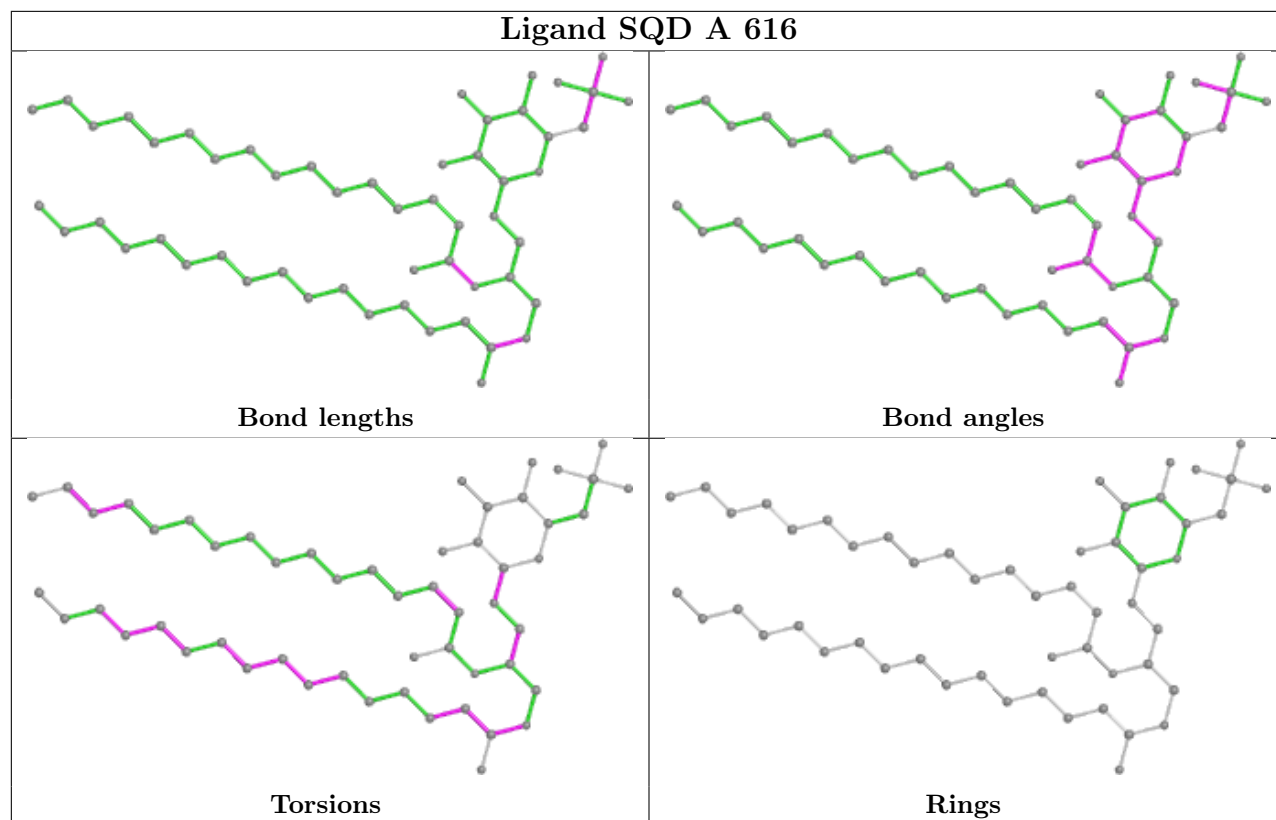


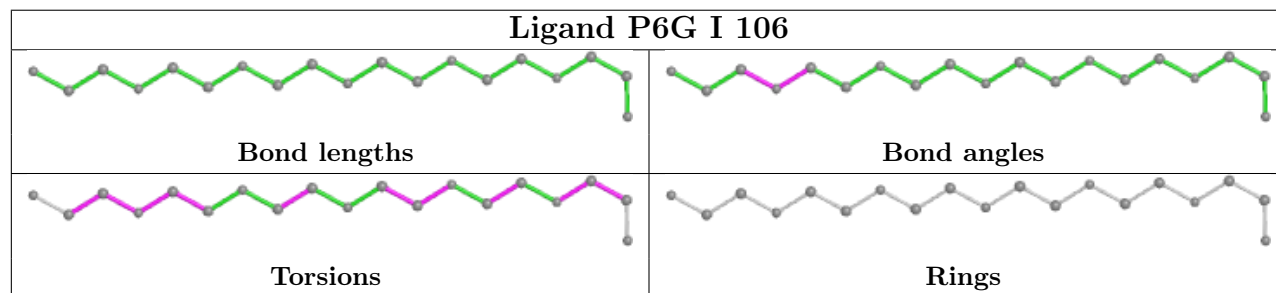
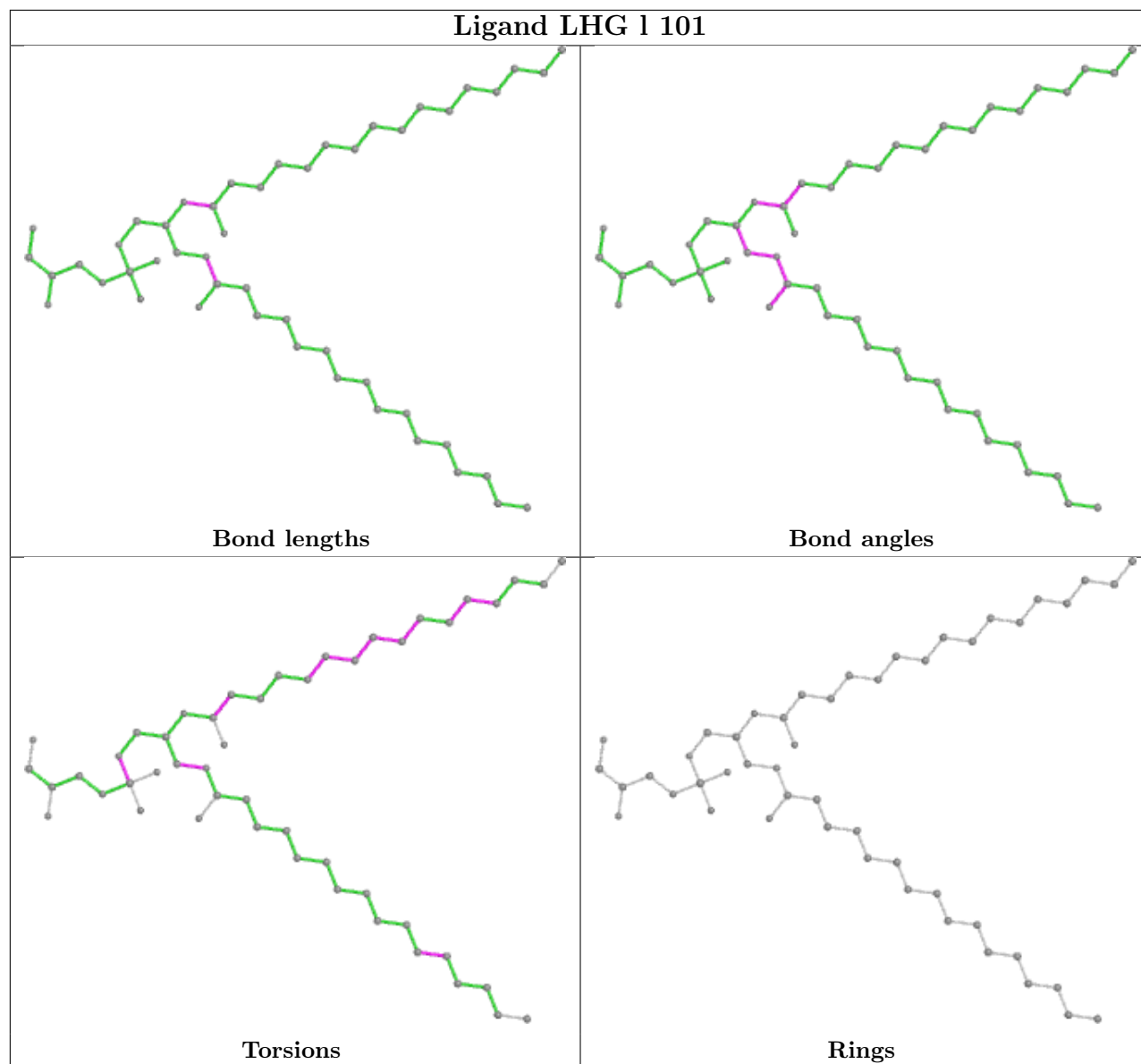
Ligand BCR t 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

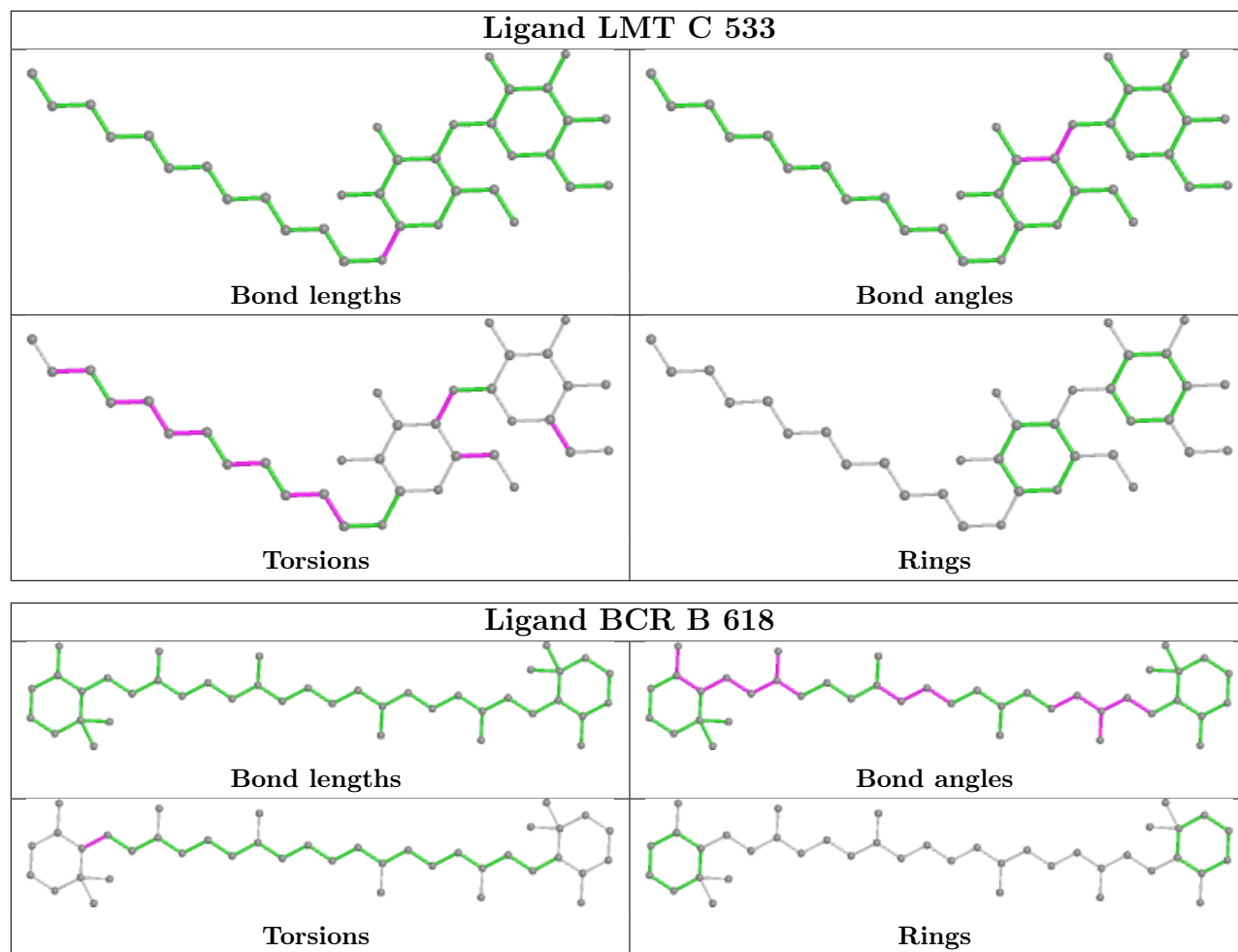
Ligand LMG a 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

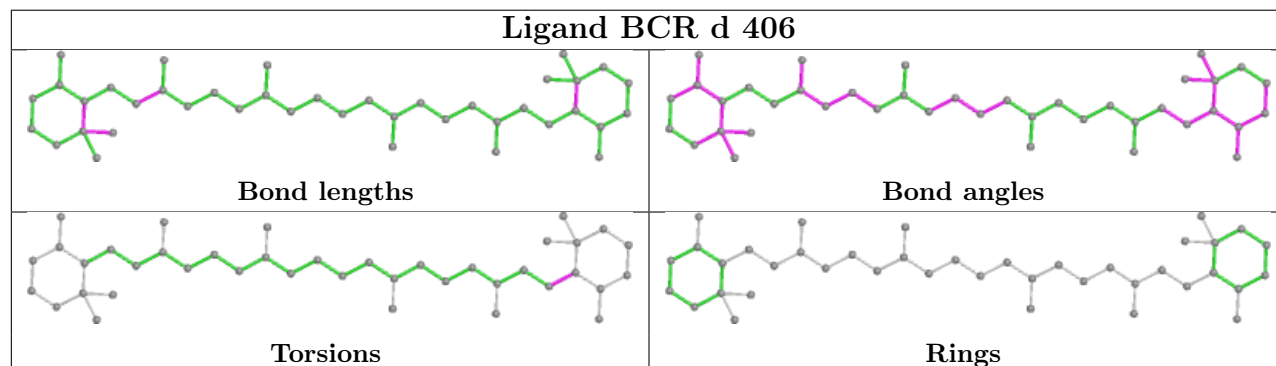
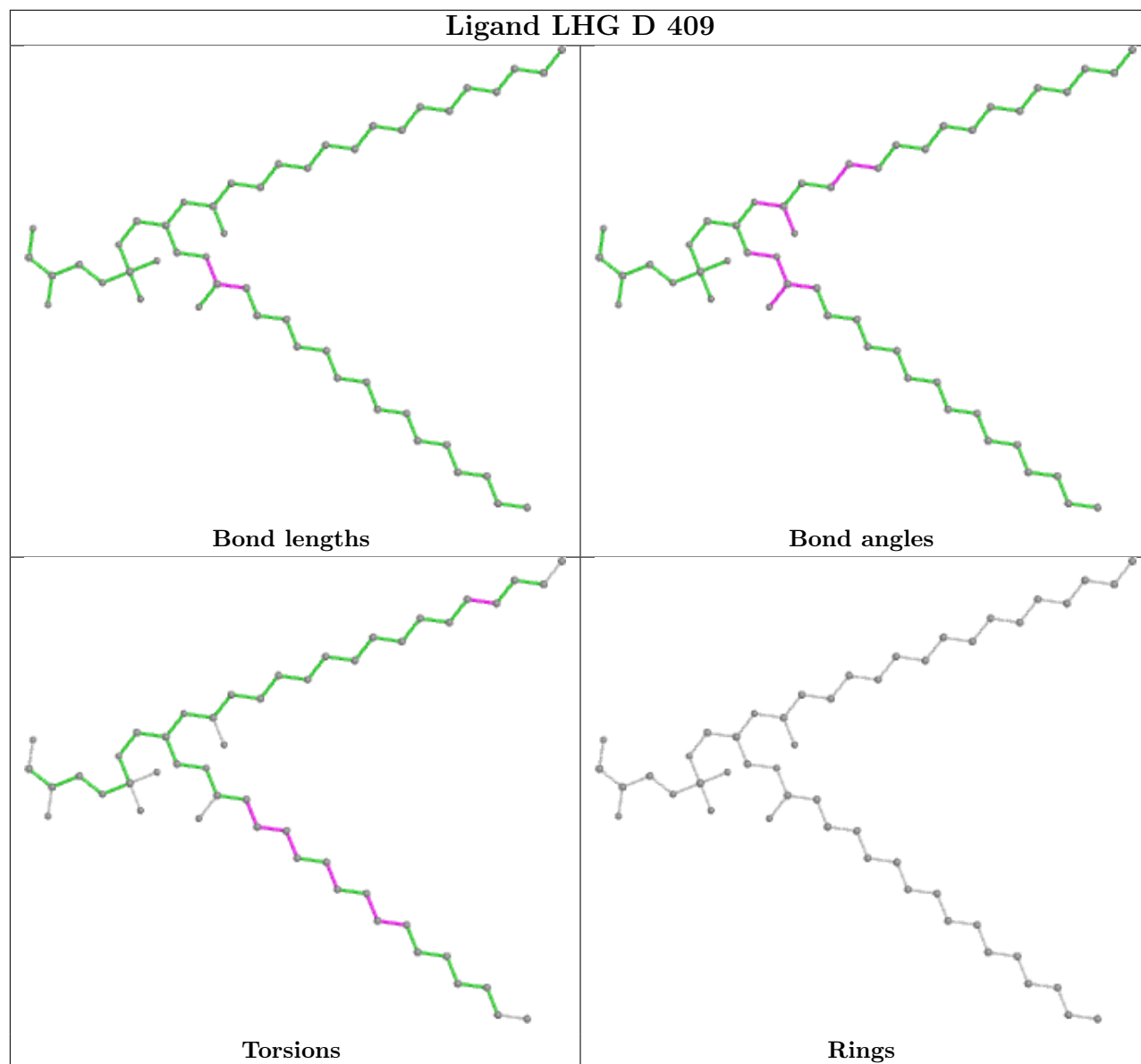
Ligand BCR B 619	
	
Bond lengths	Bond angles
	
Torsions	Rings



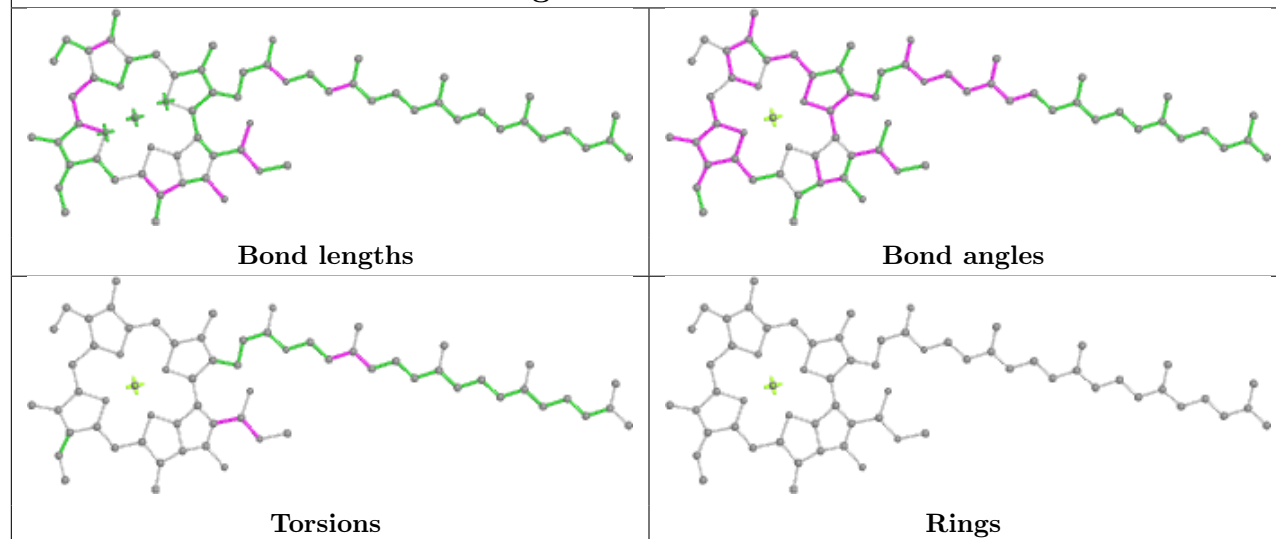




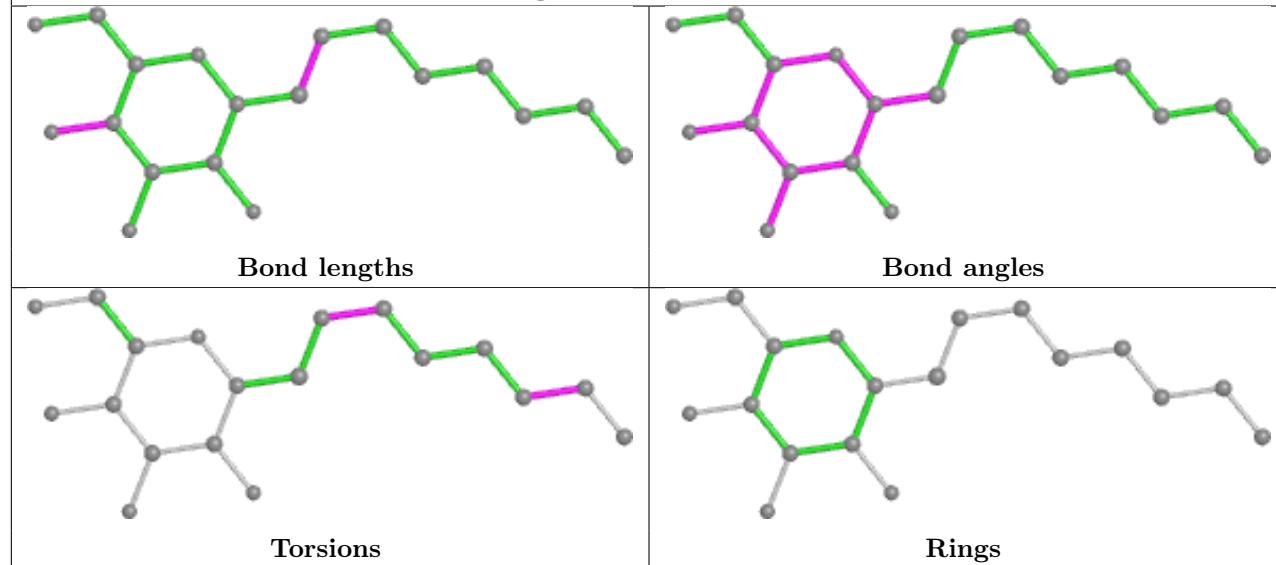




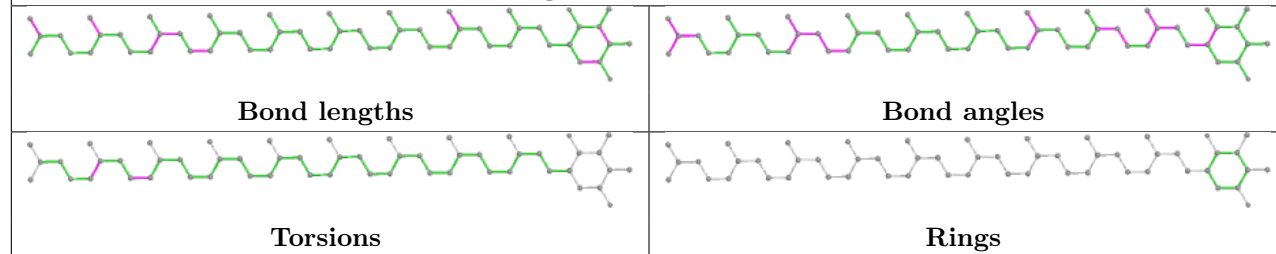
Ligand CLA B 606



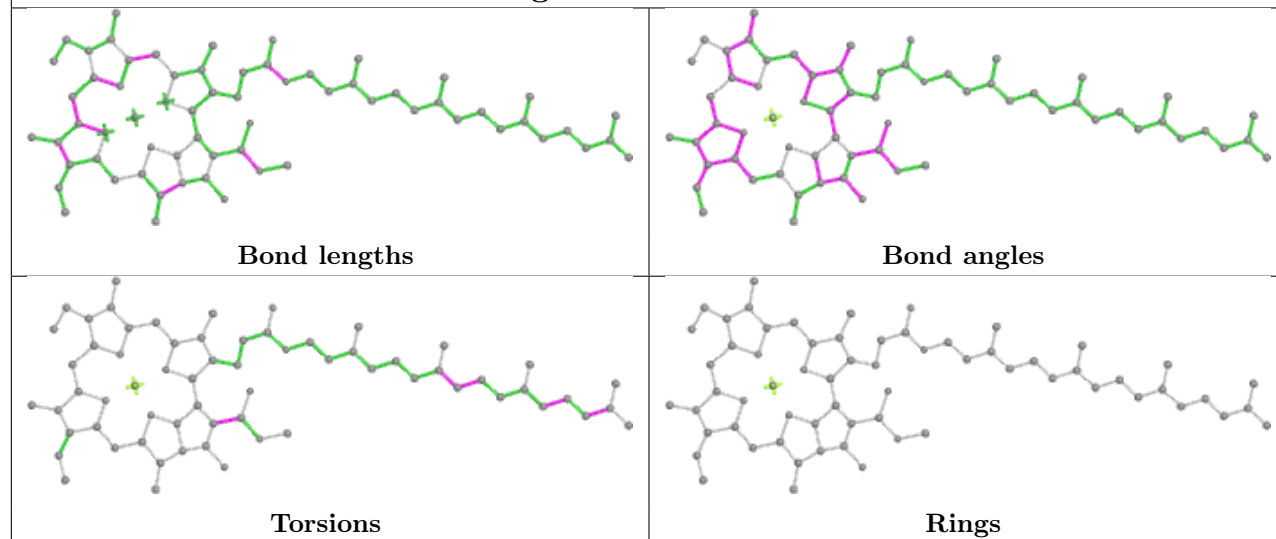
Ligand HTG b 631



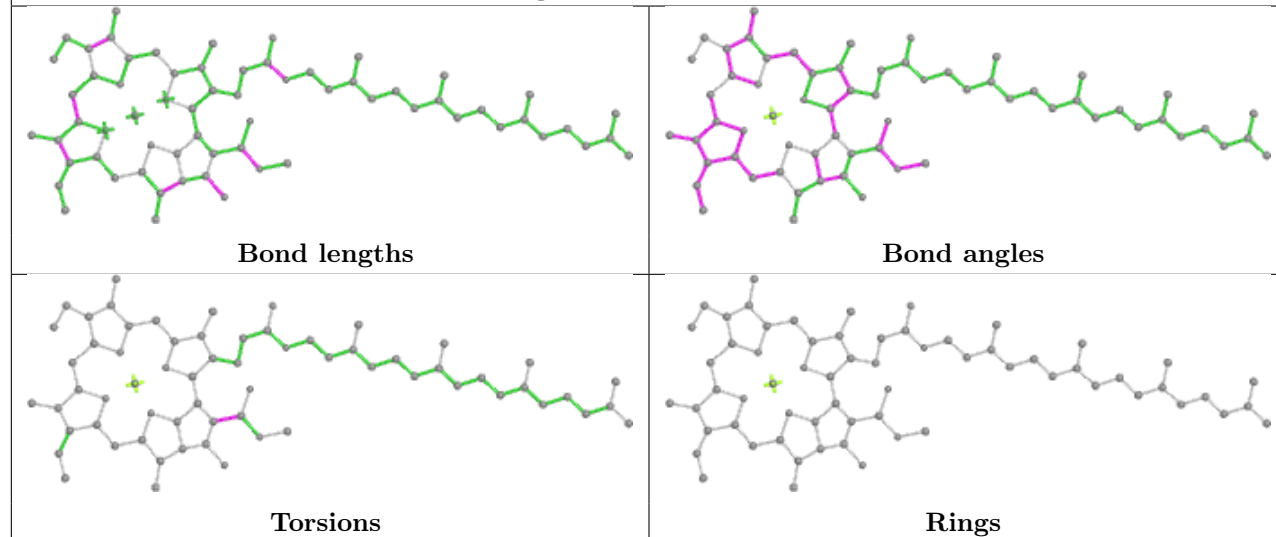
Ligand PL9 d 407



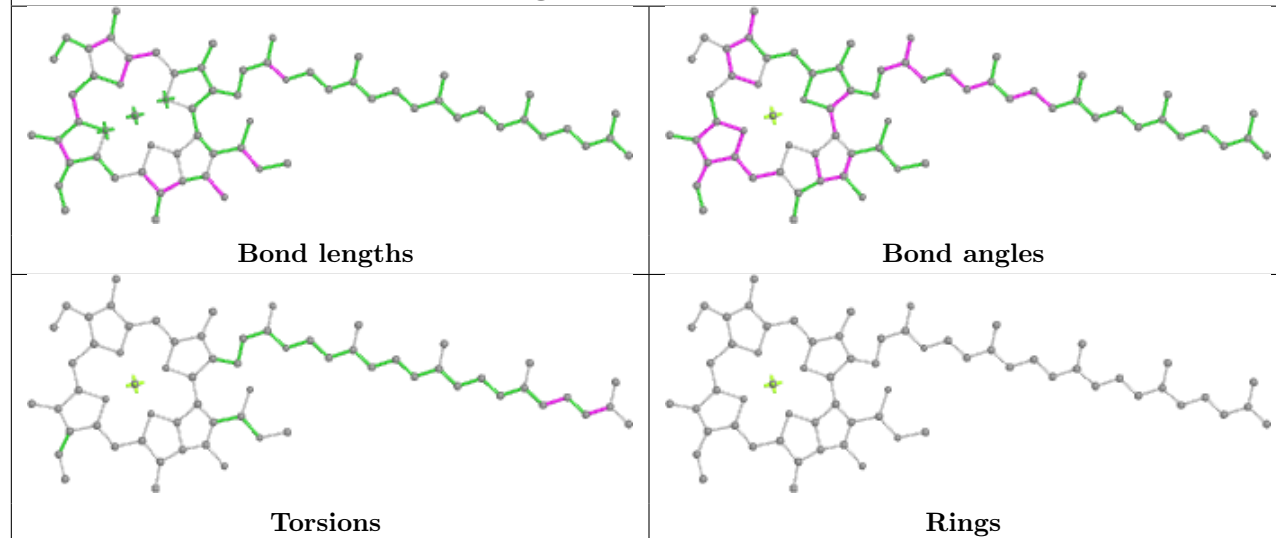
Ligand CLA D 405

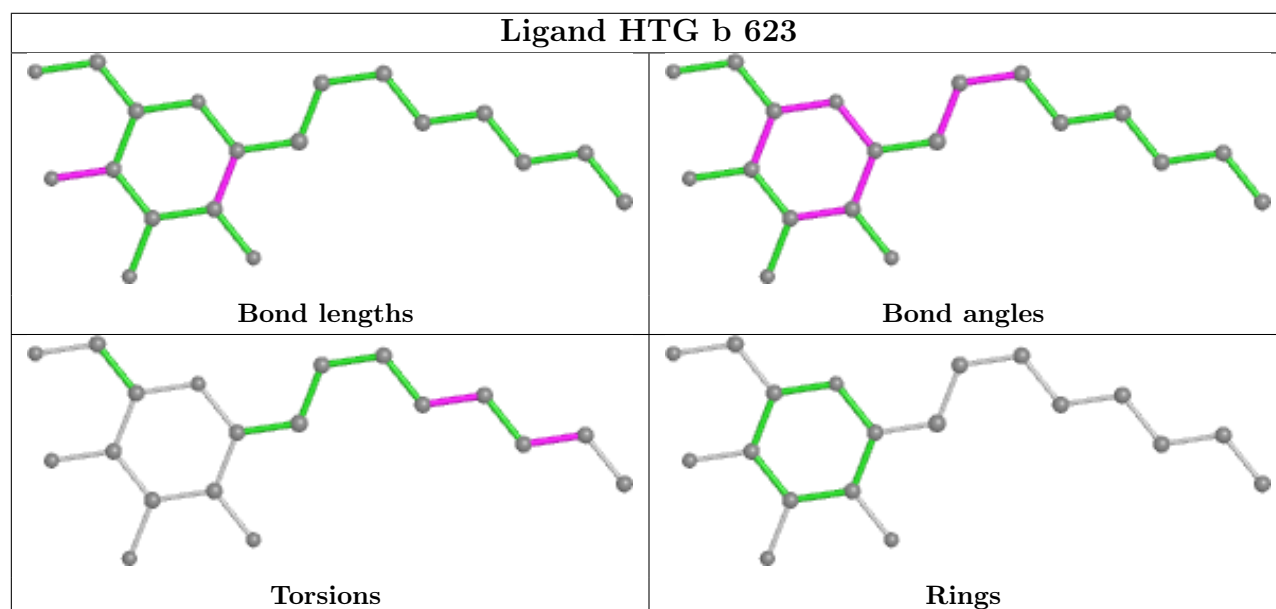
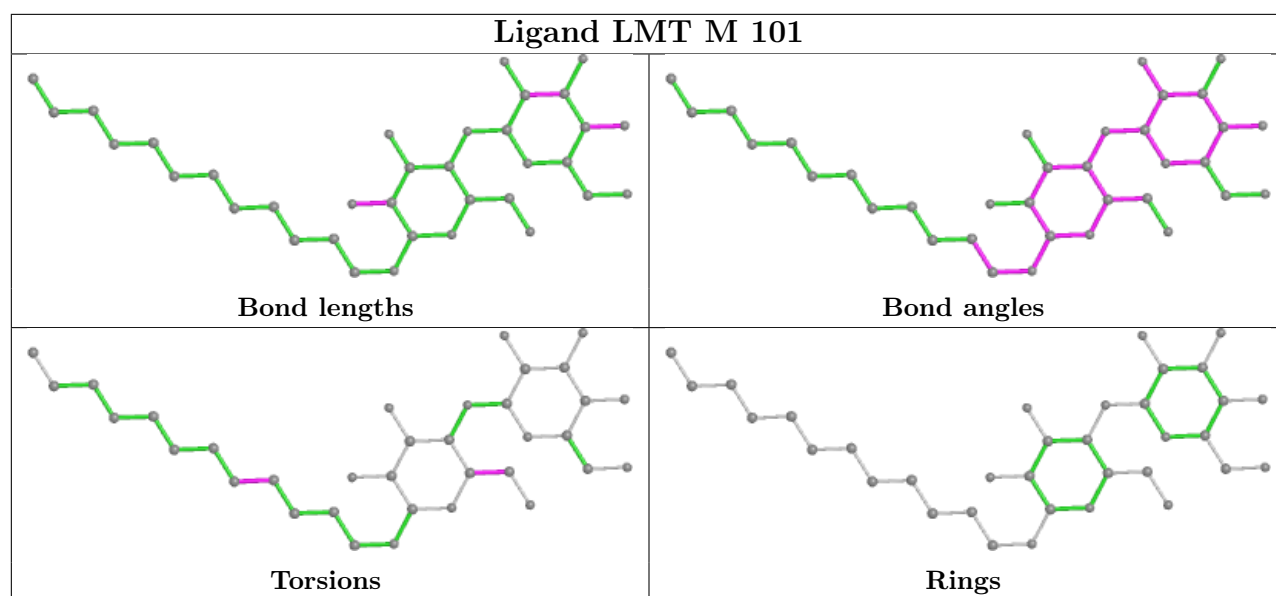


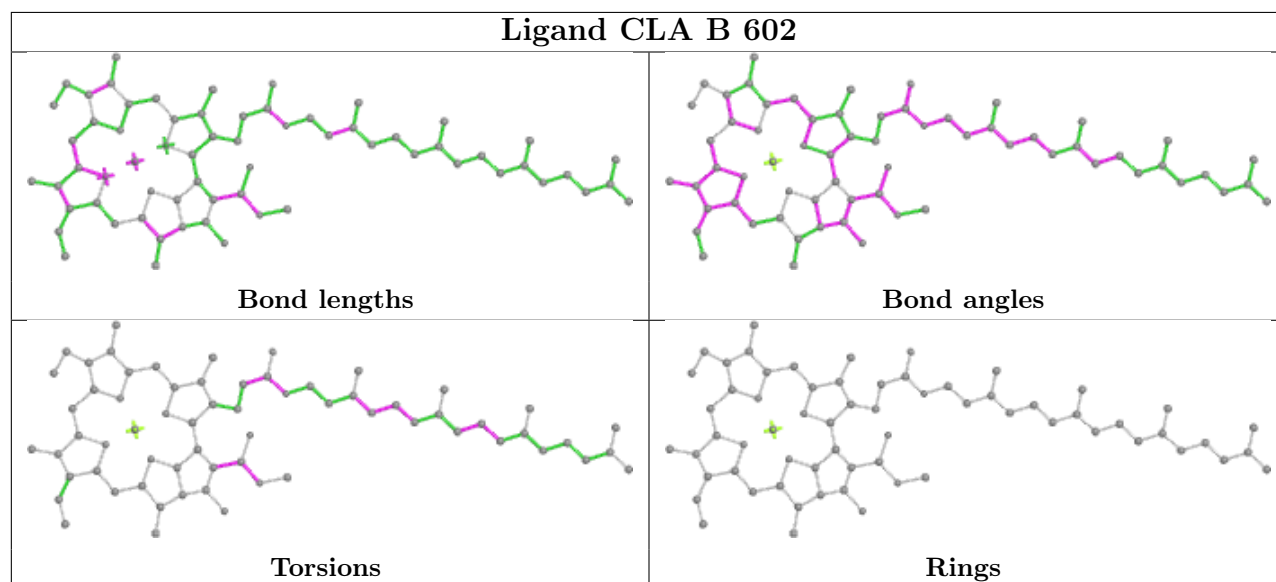
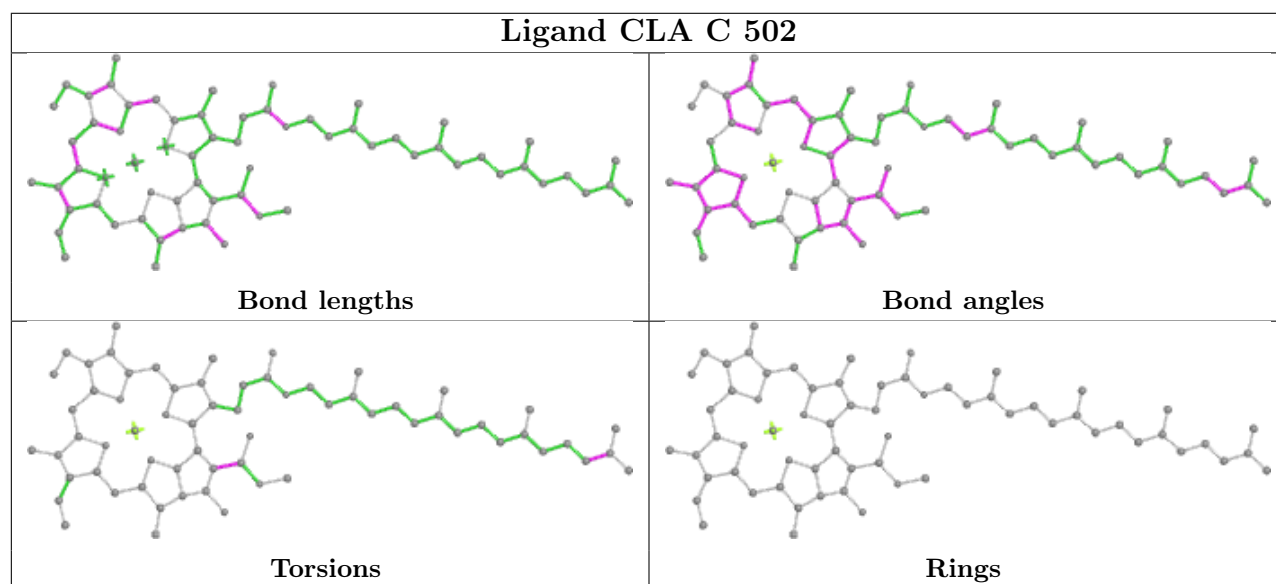
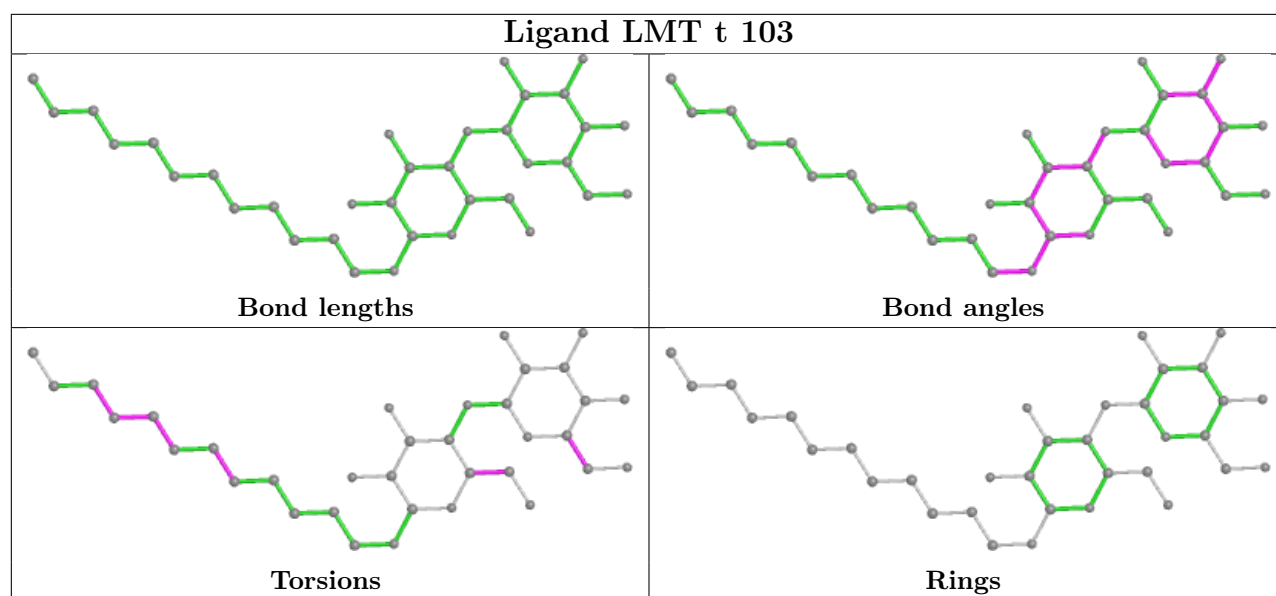
Ligand CLA B 610

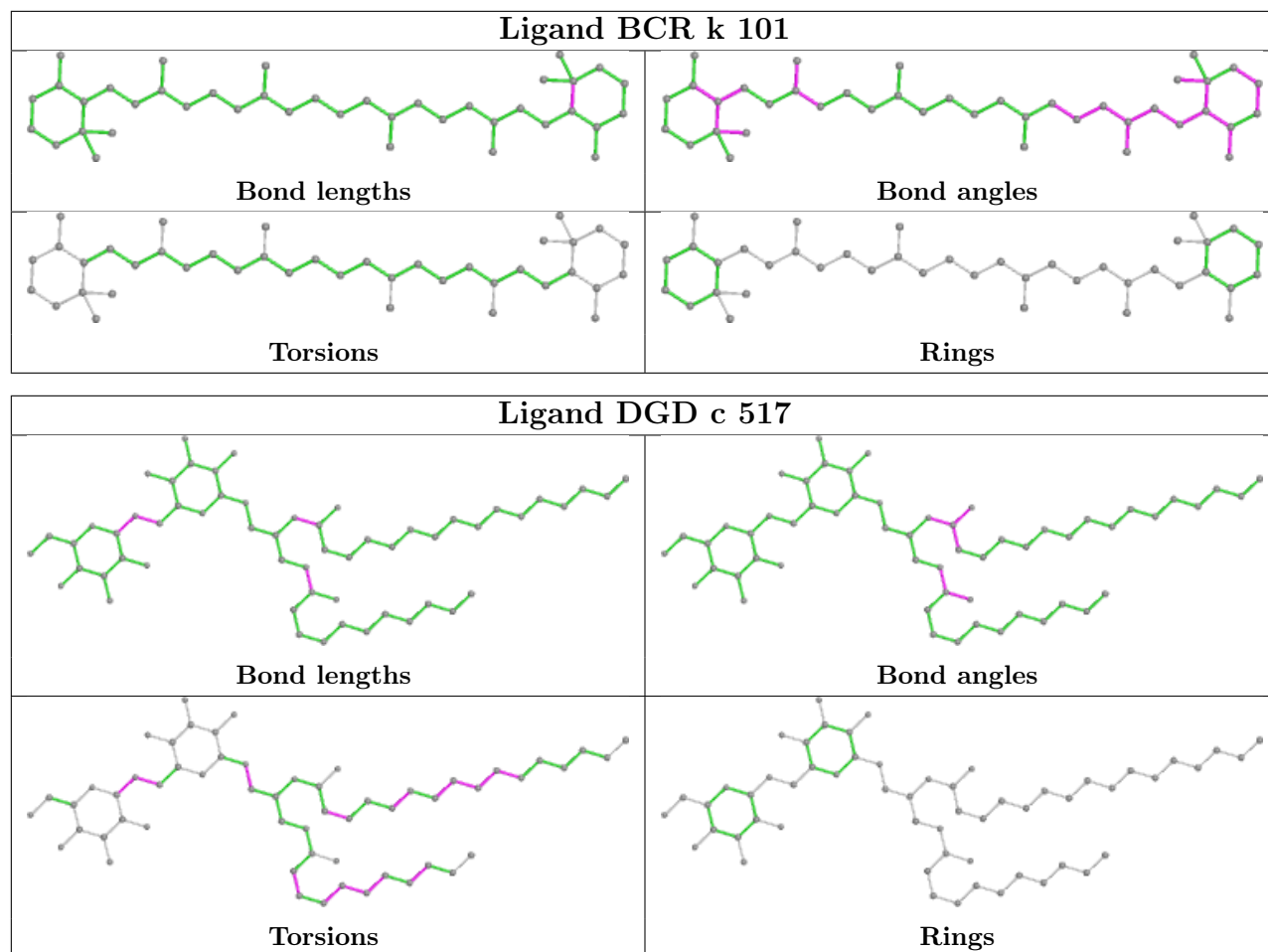


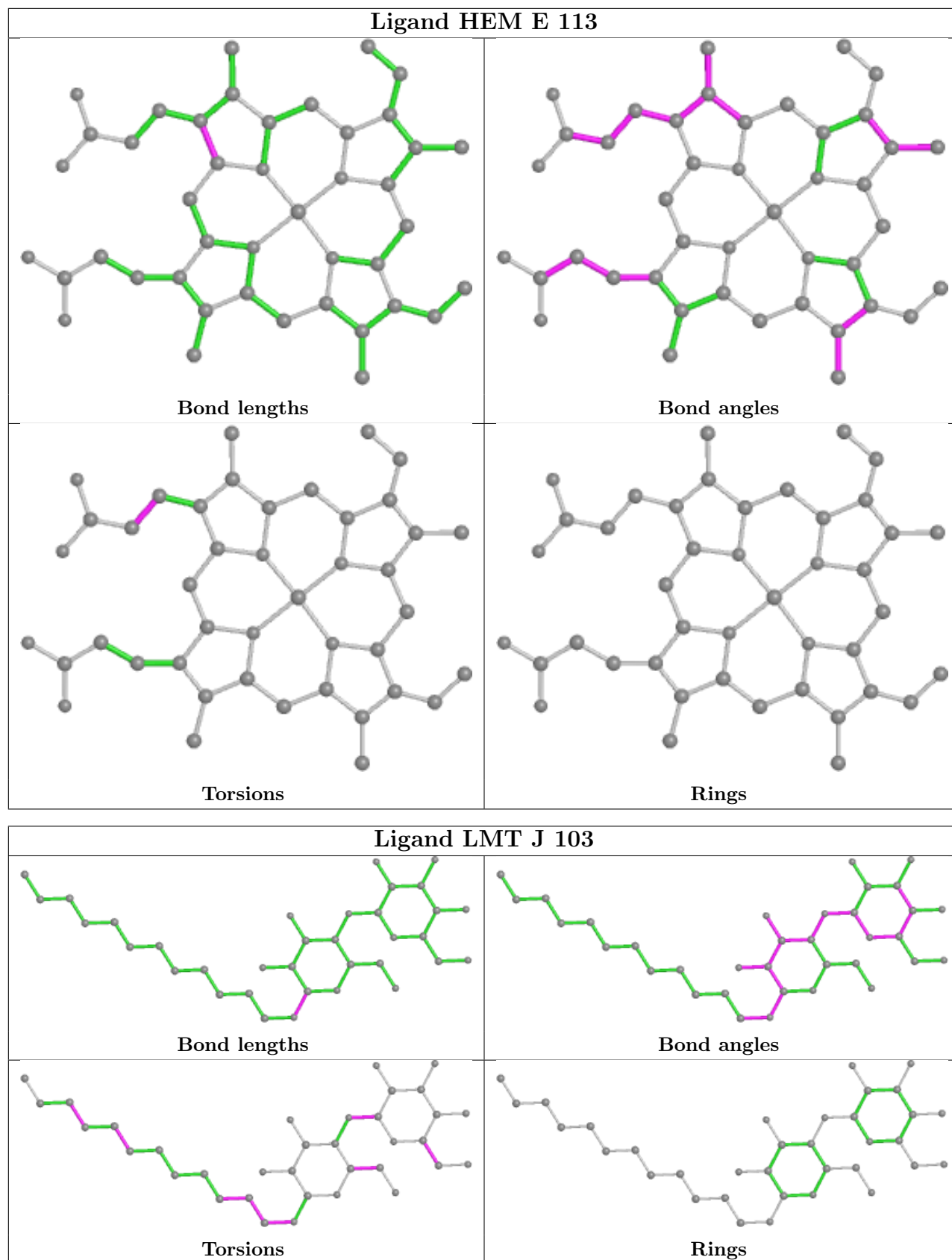
Ligand CLA B 614

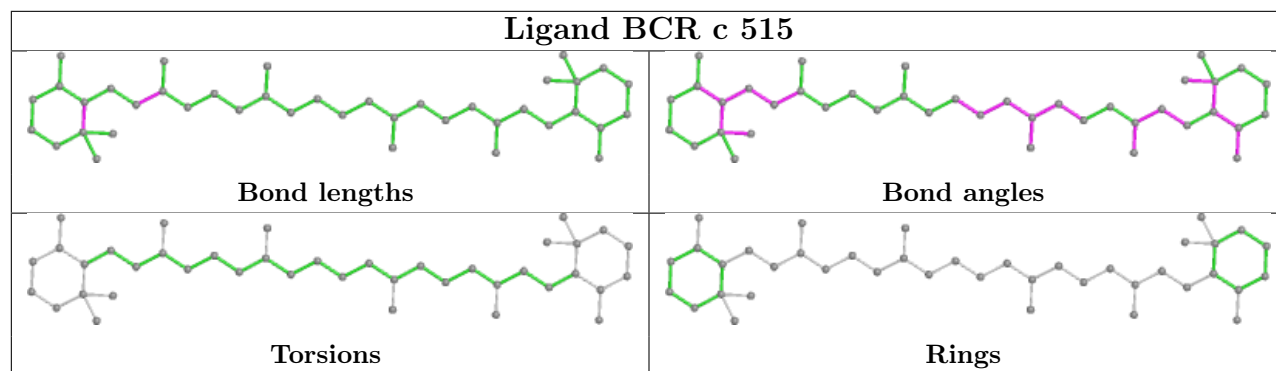
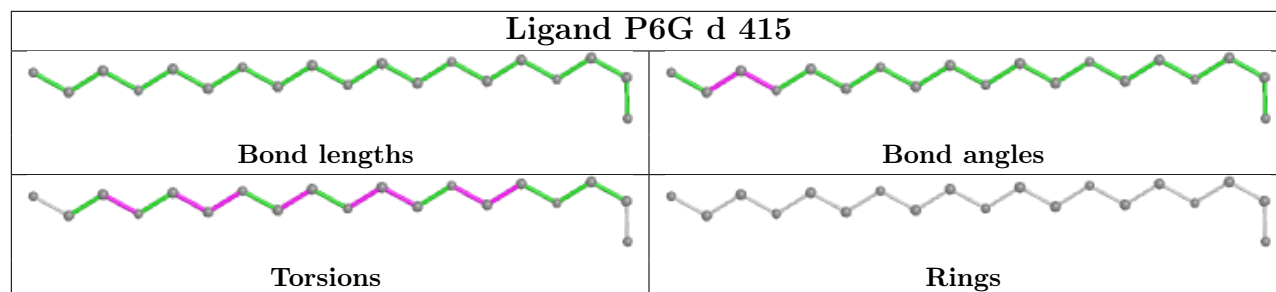


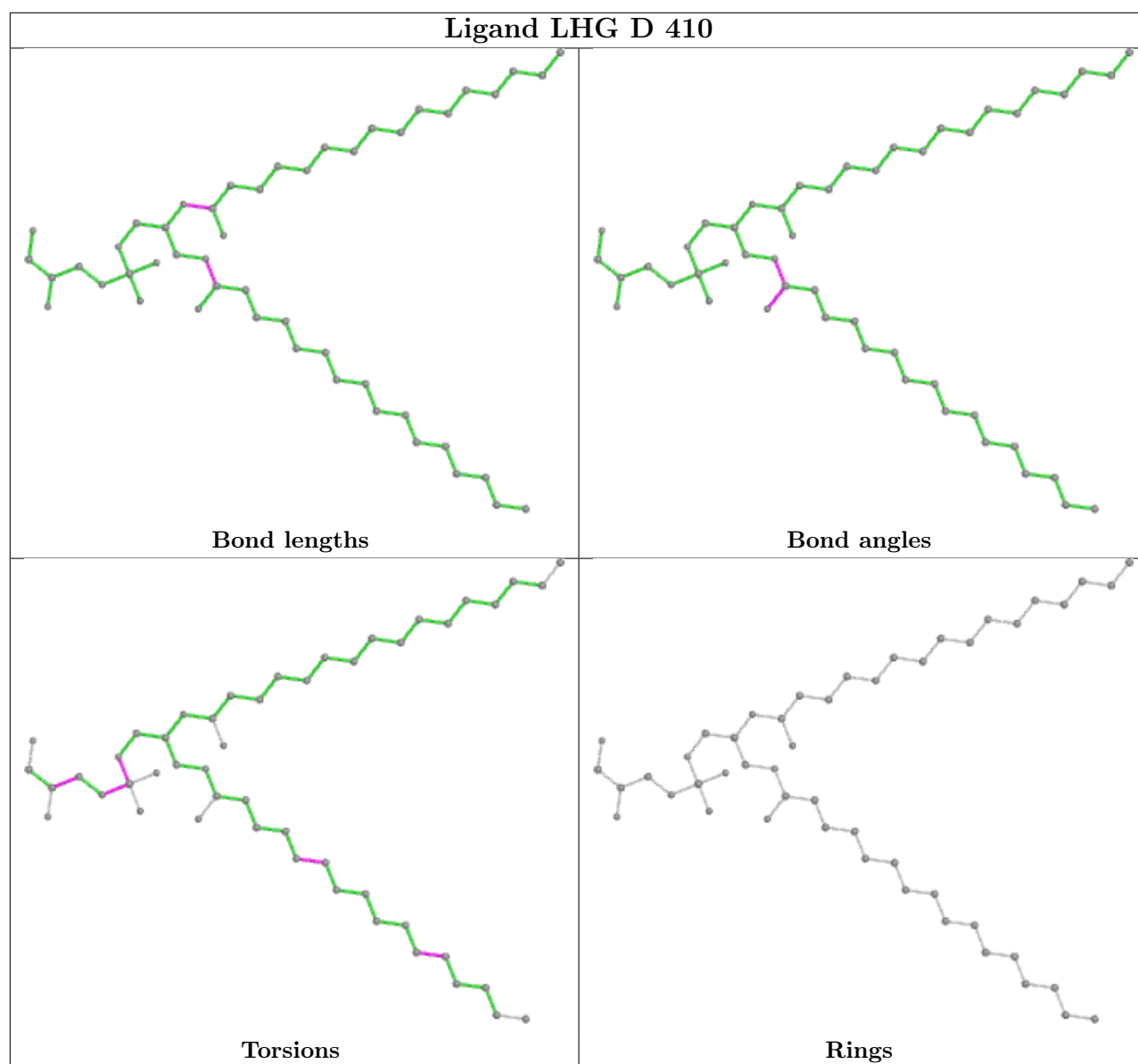


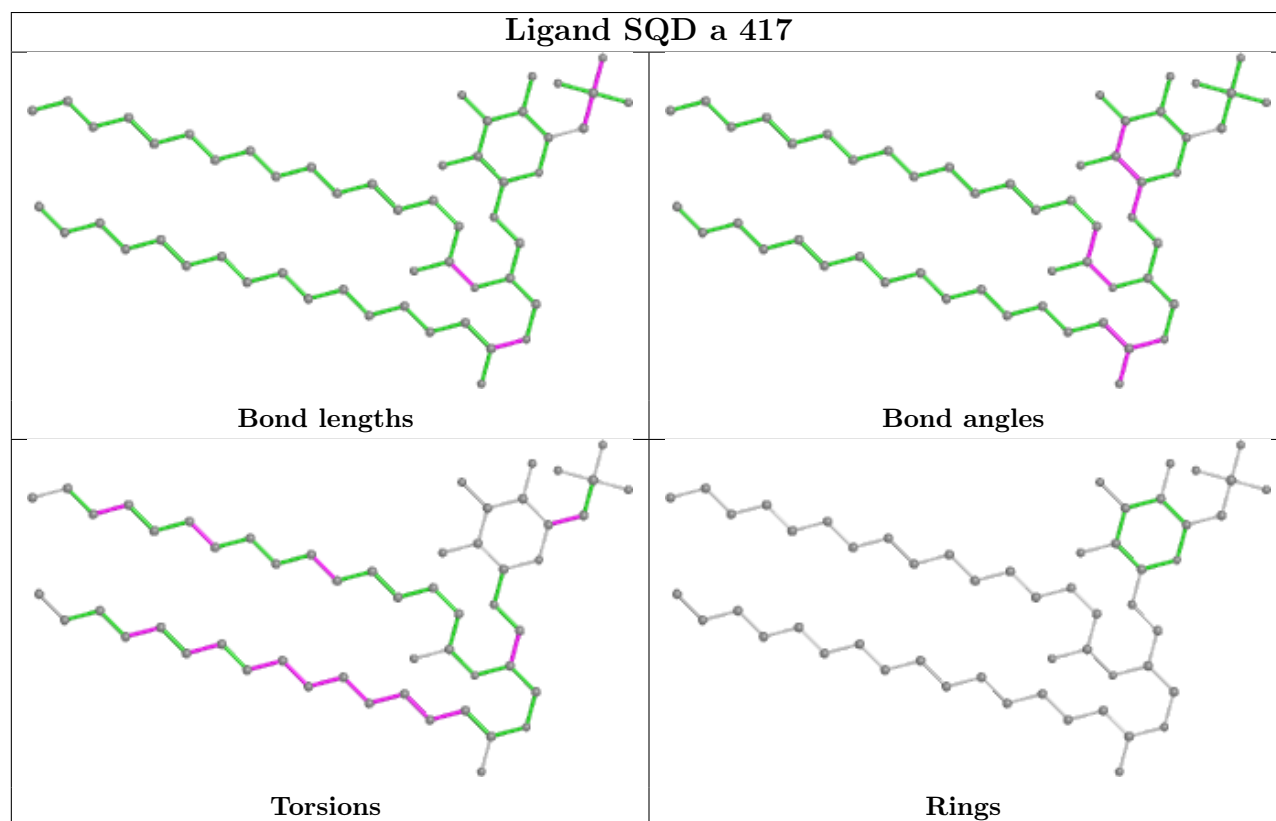
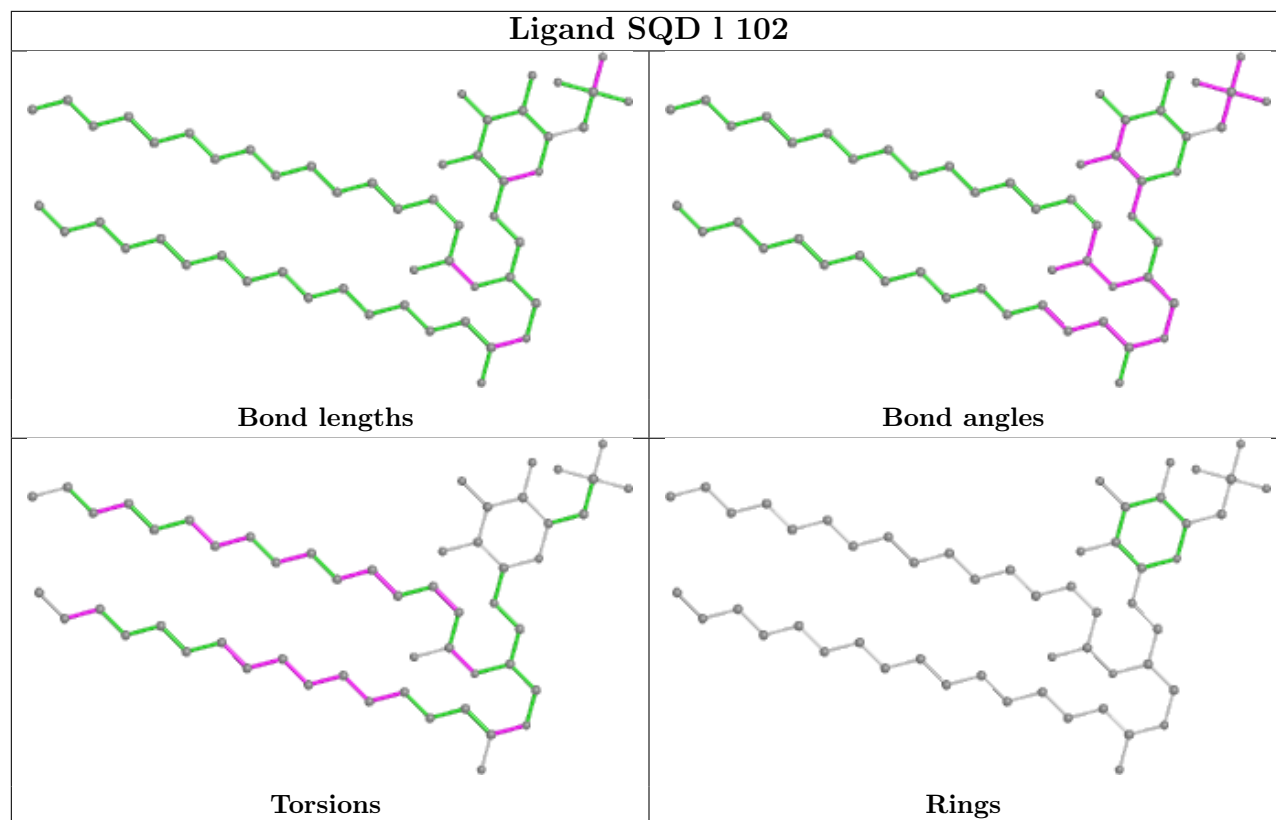


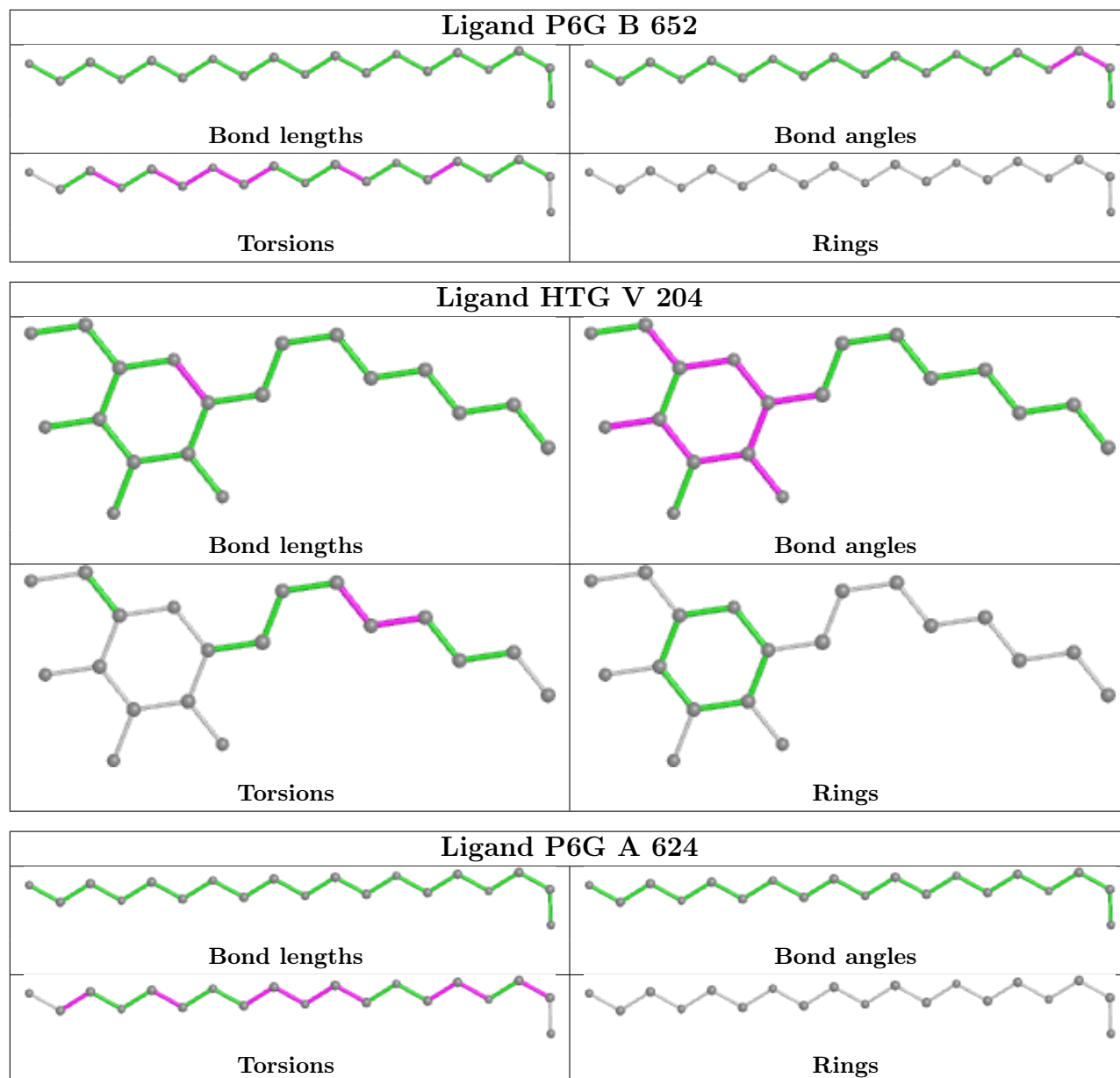




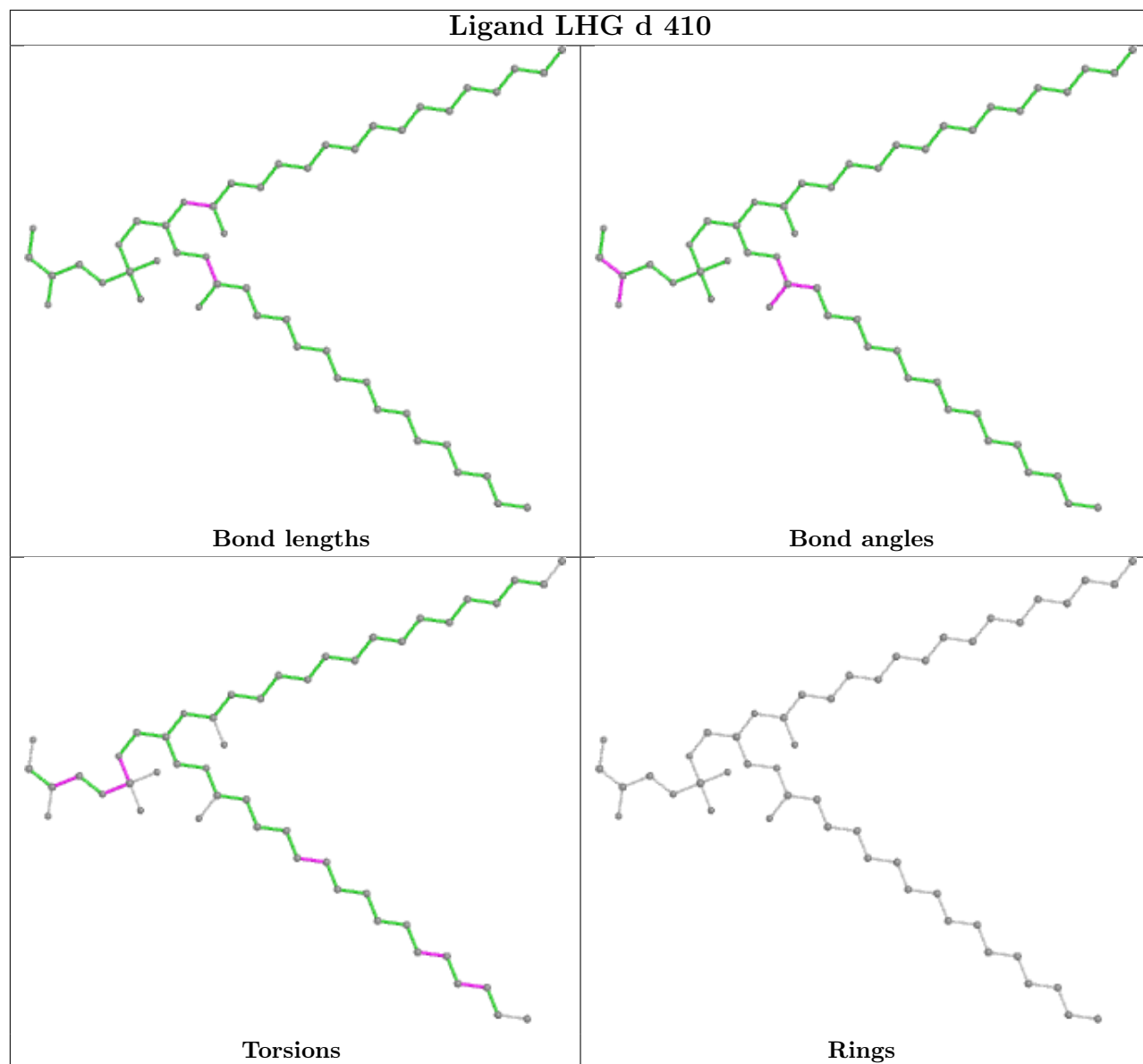




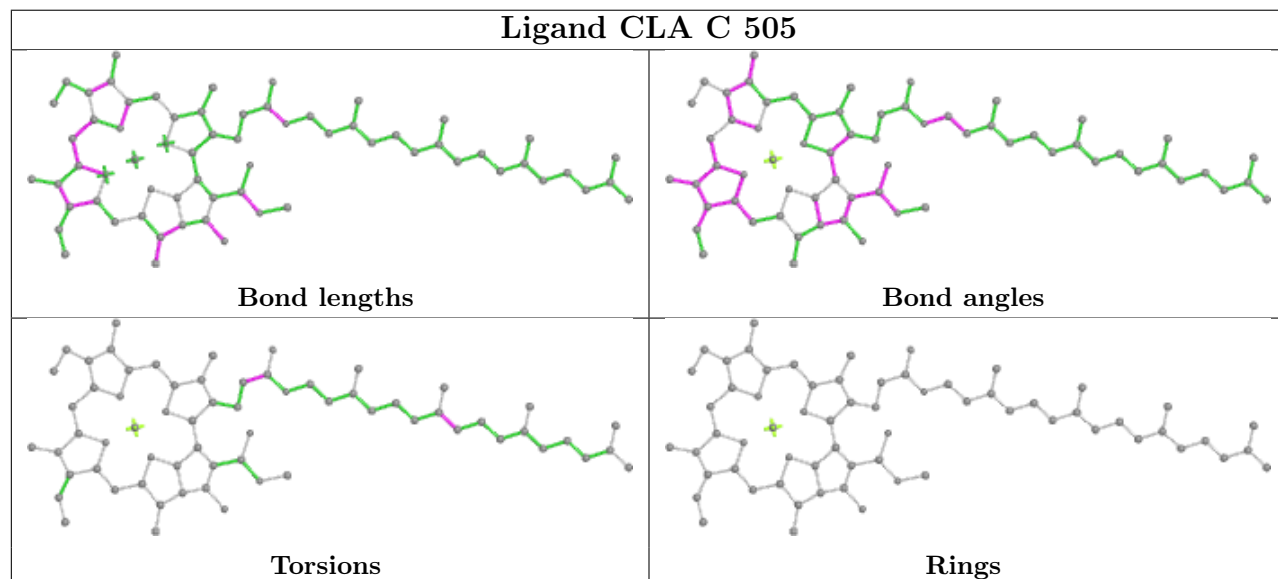


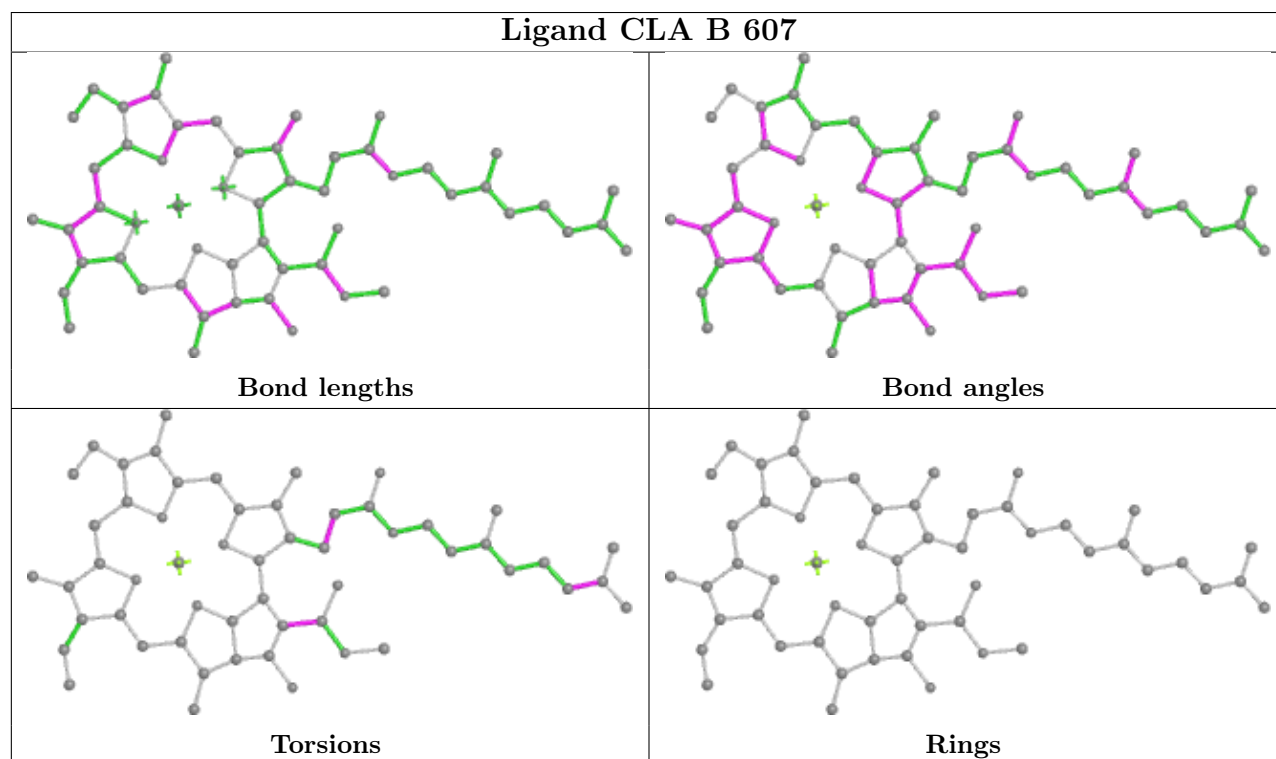
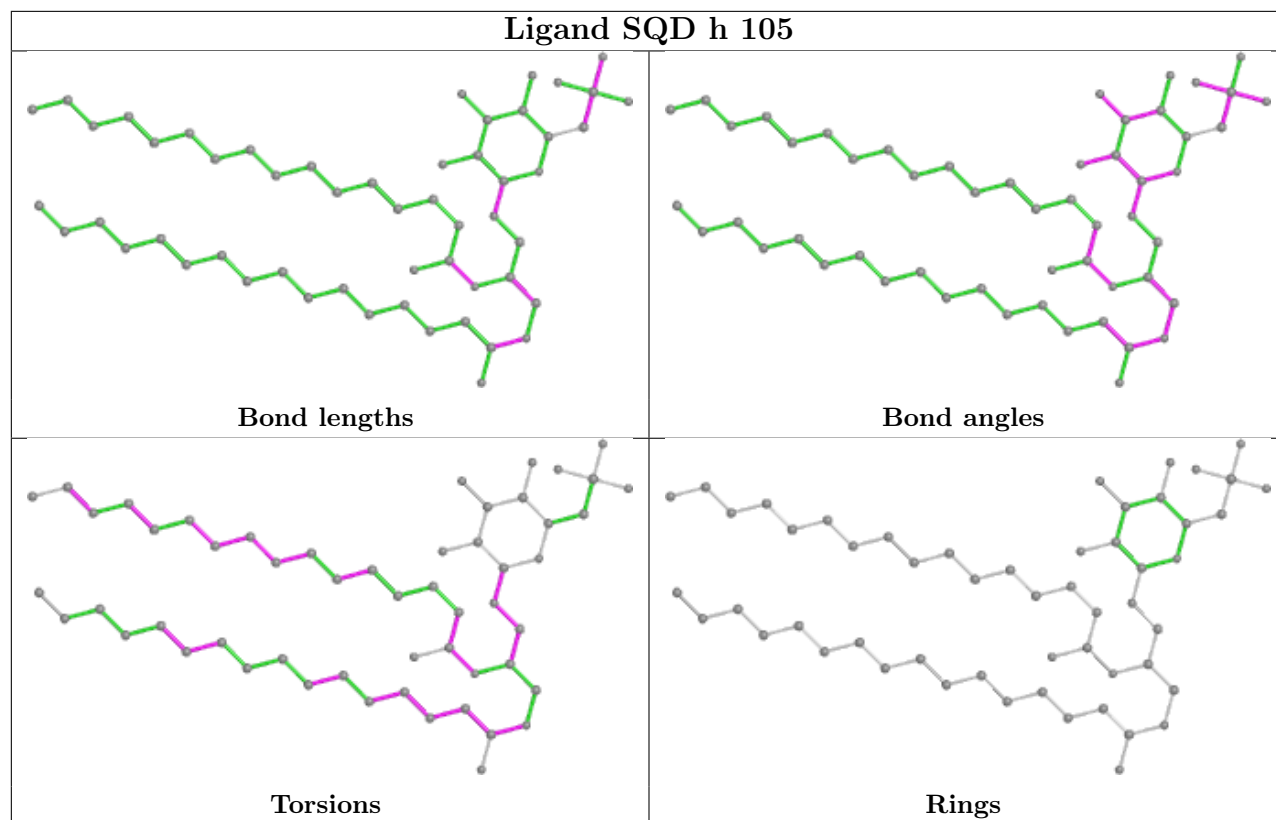


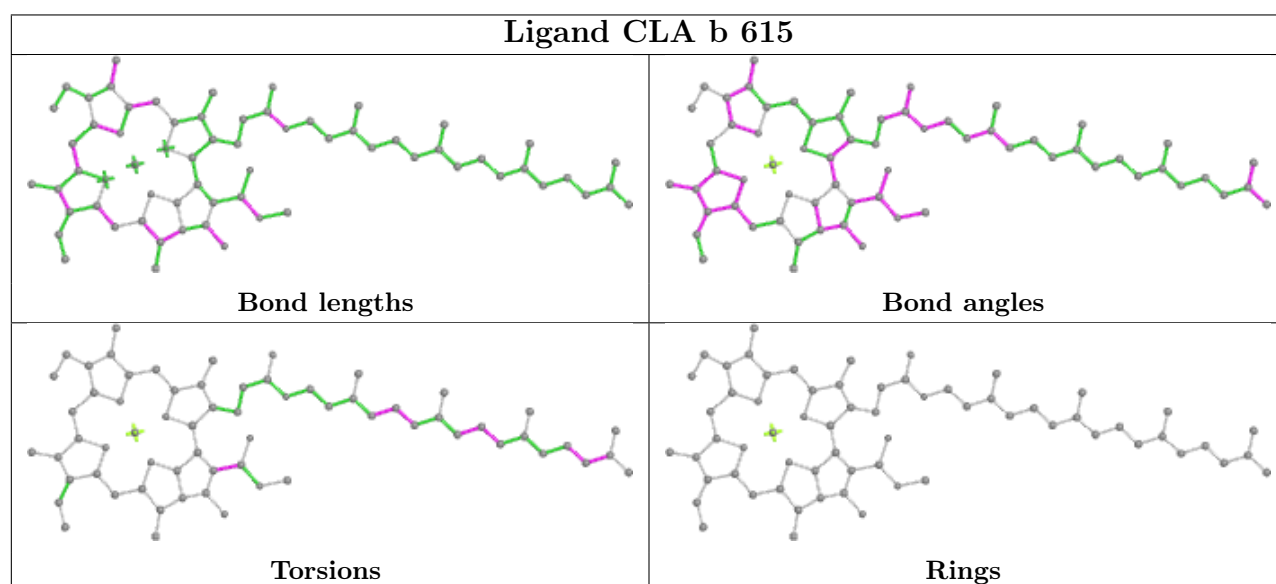
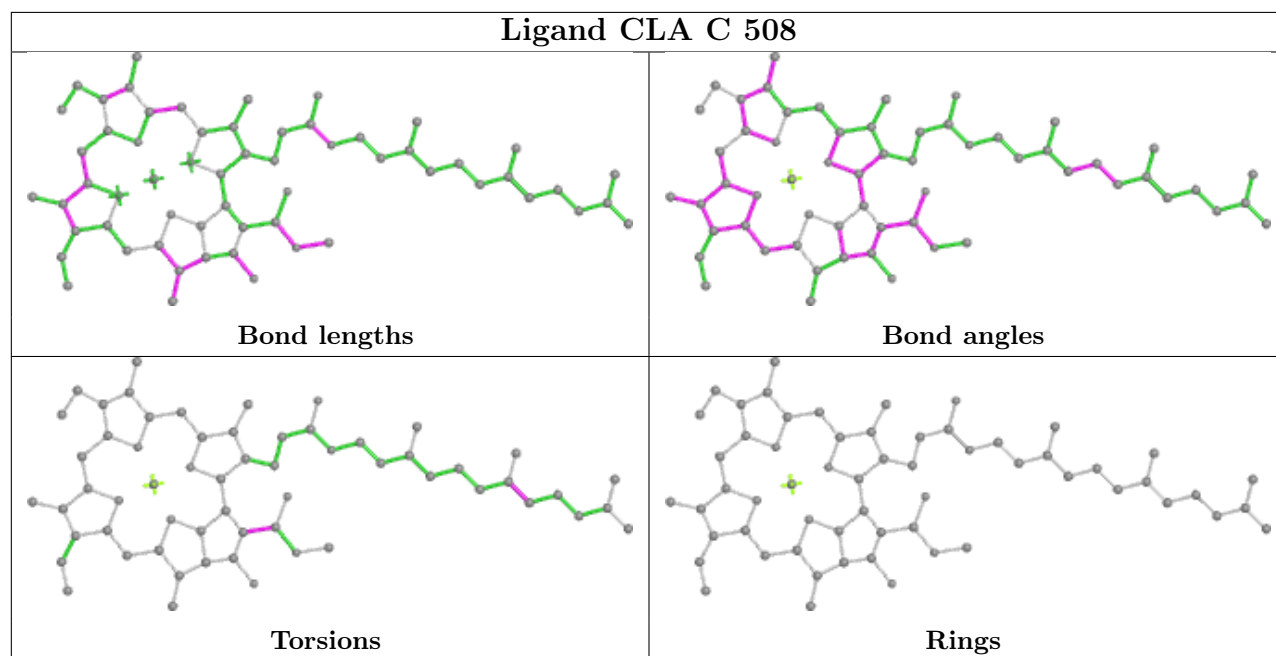
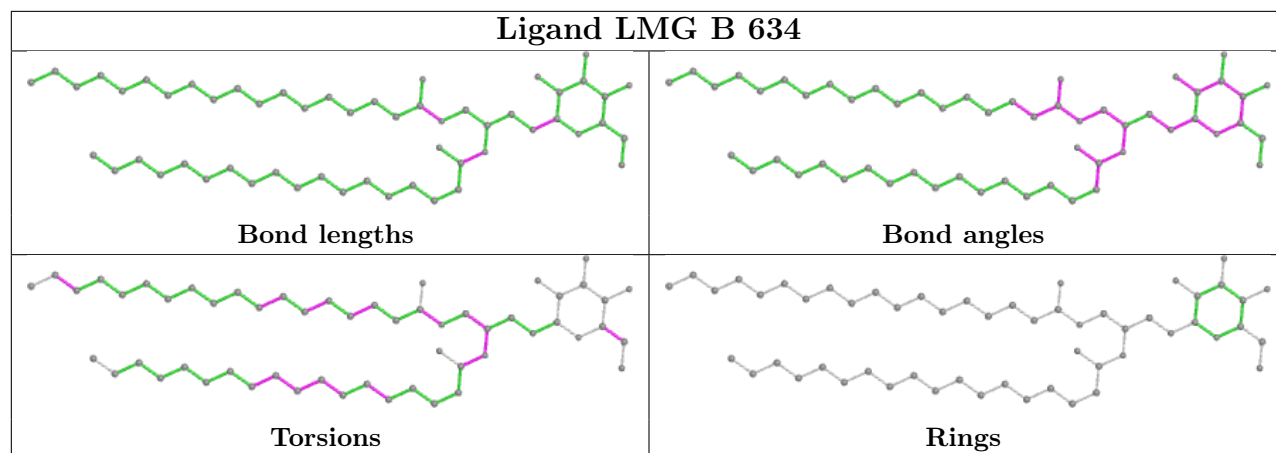
Ligand LHG d 410



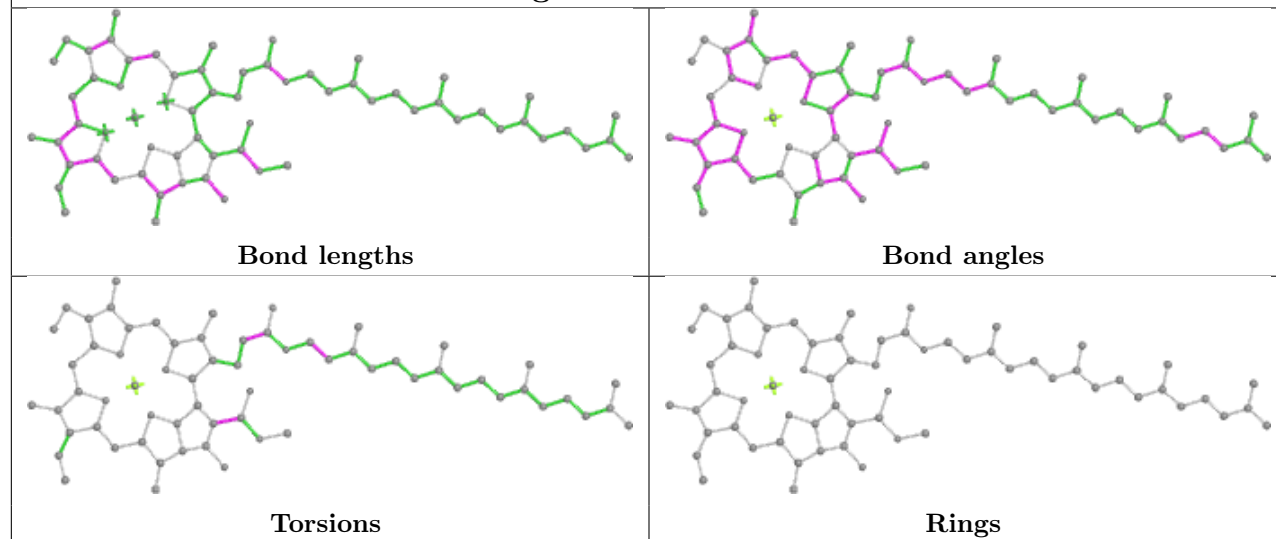
Ligand CLA C 505



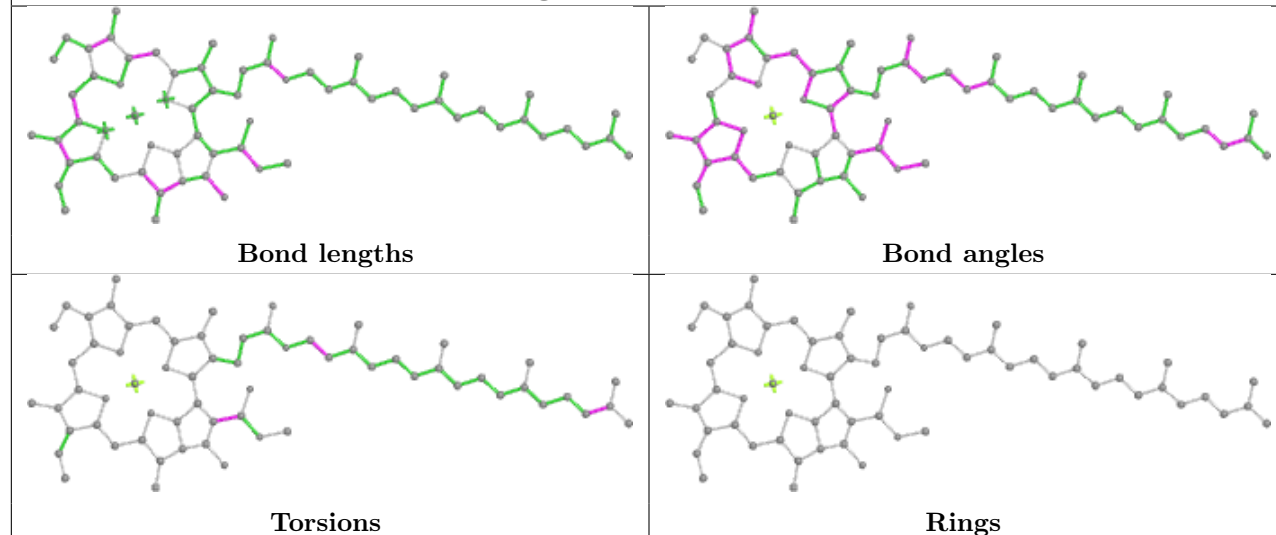




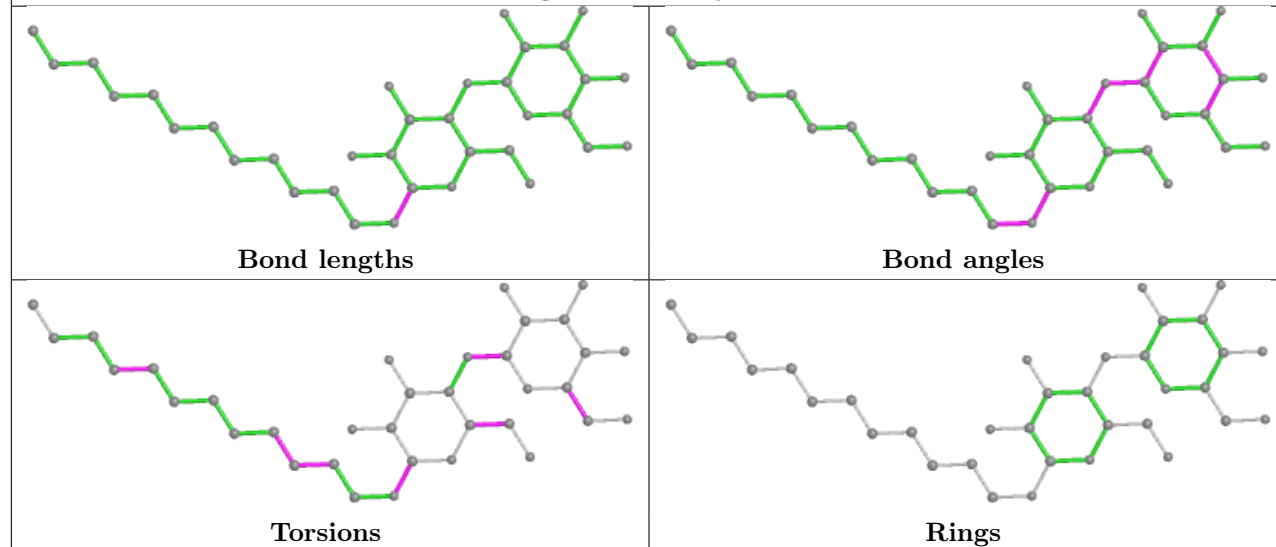
Ligand CLA C 512



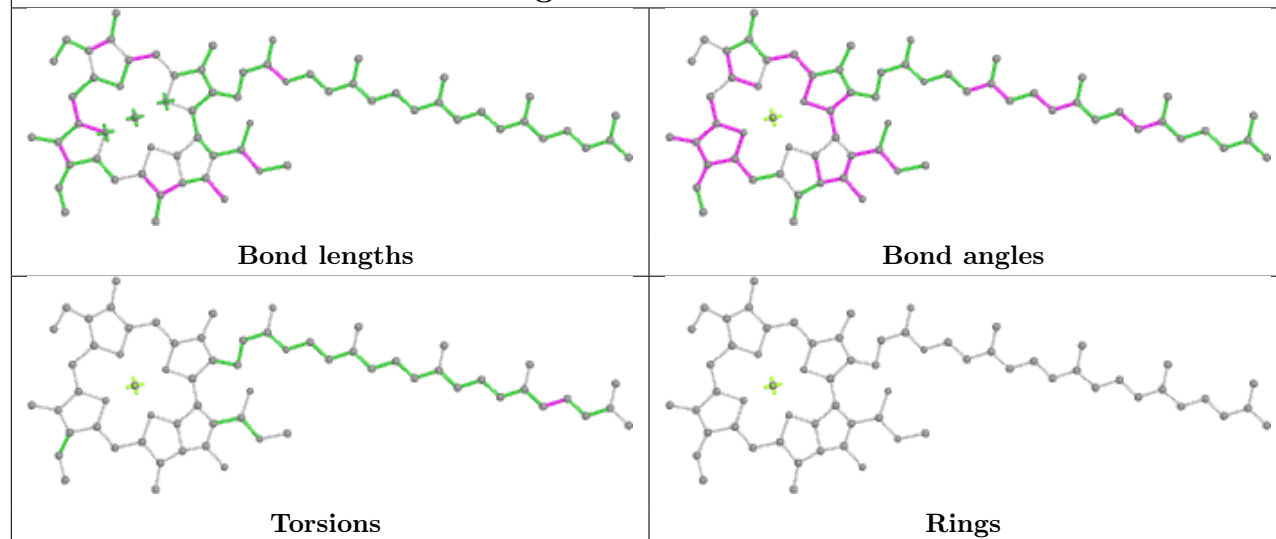
Ligand CLA b 603



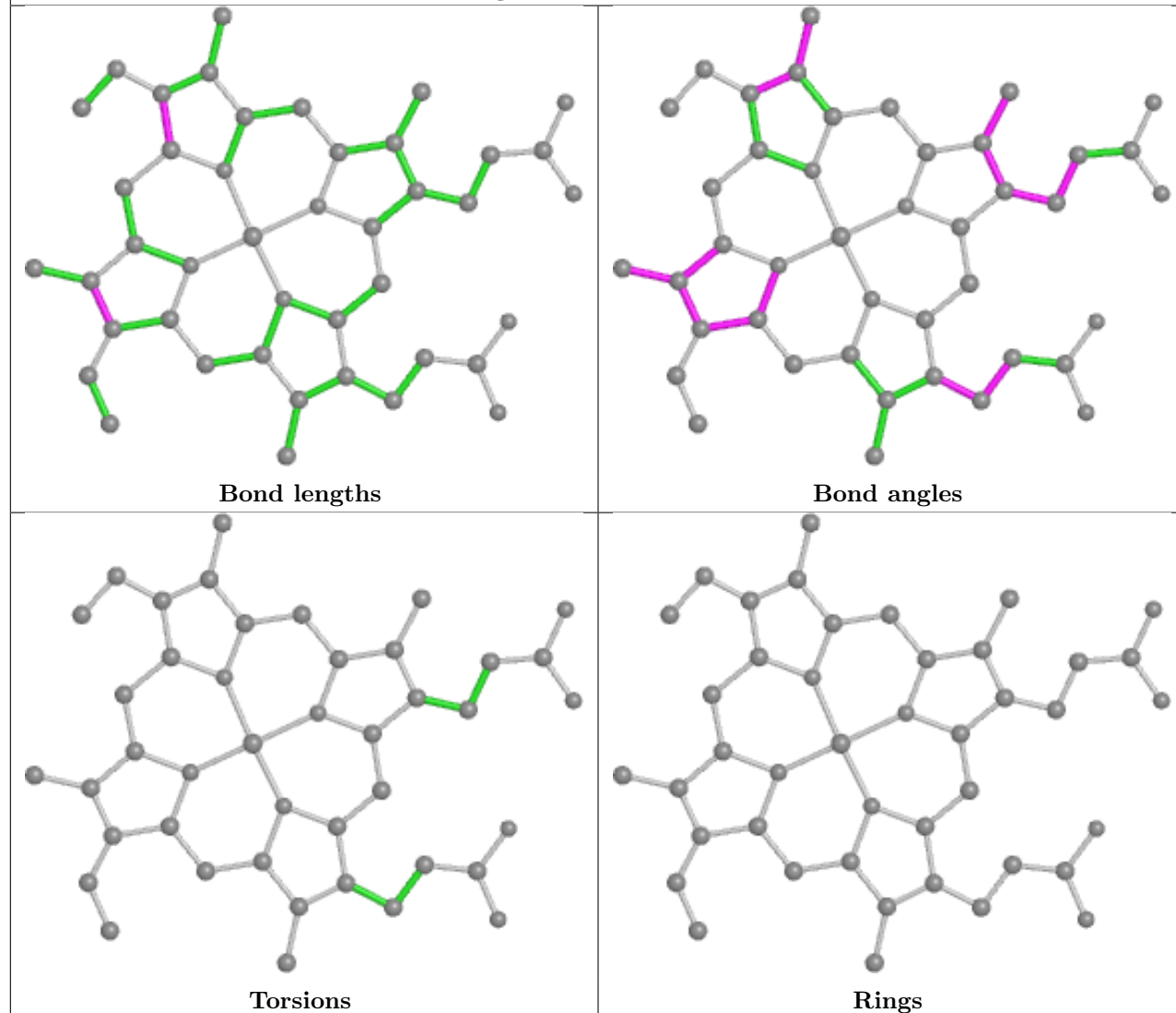
Ligand LMT j 103

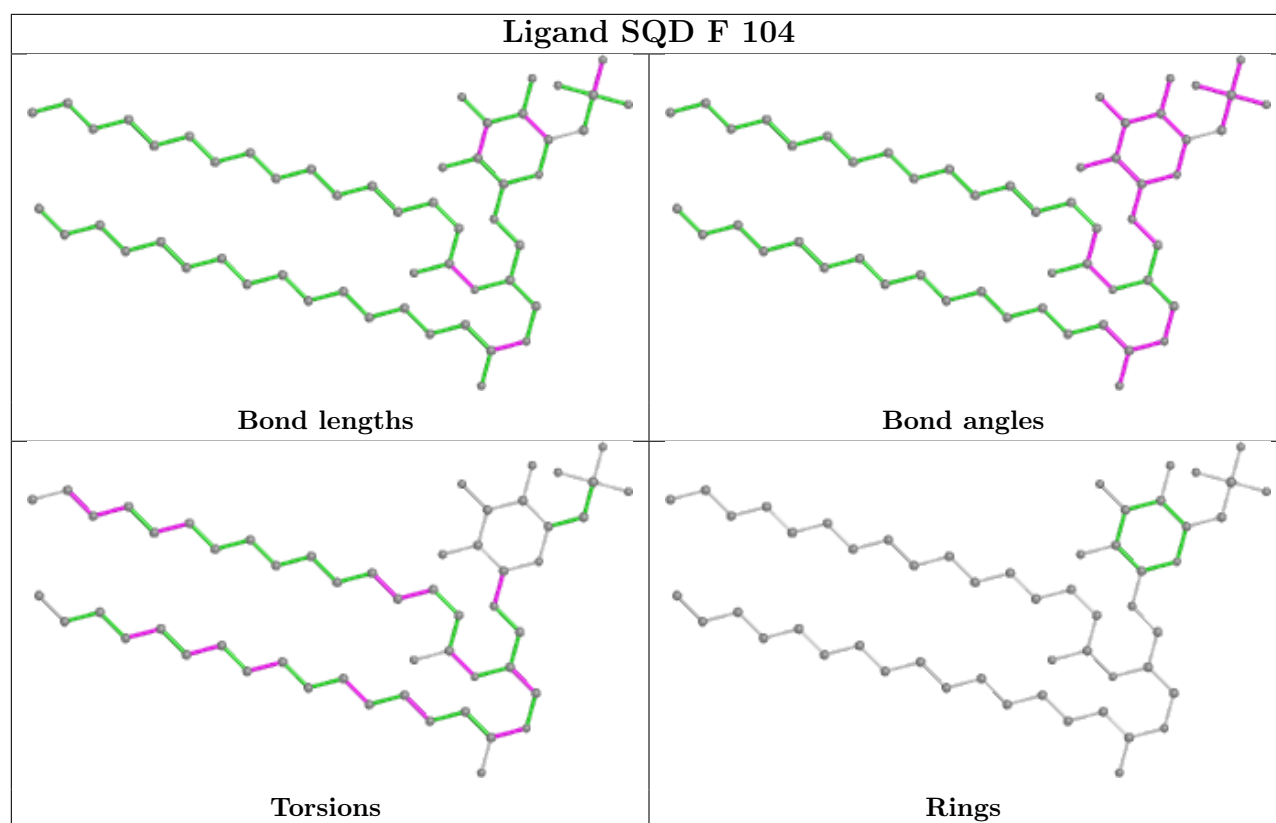


Ligand CLA b 609

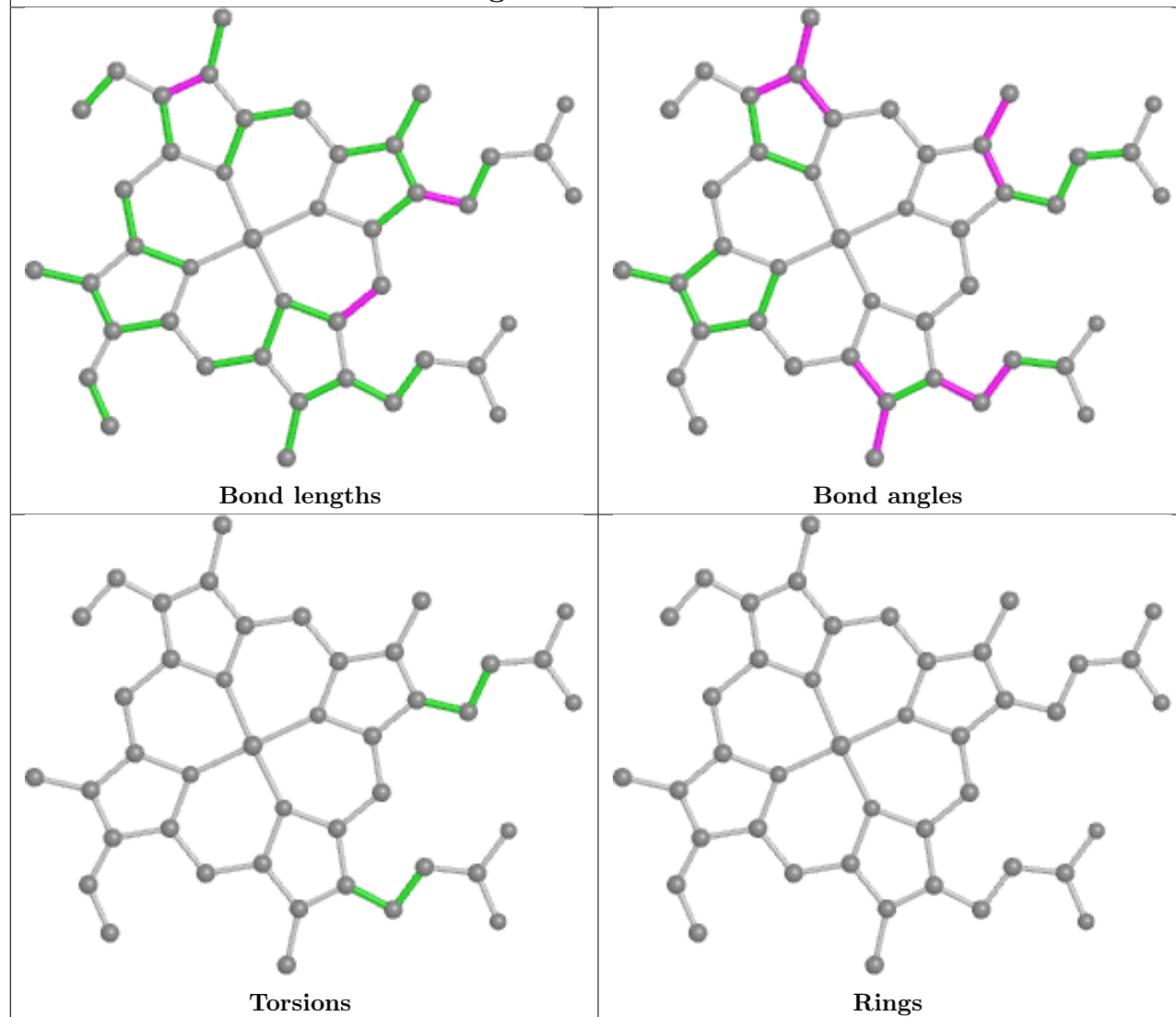


Ligand HEC v 202

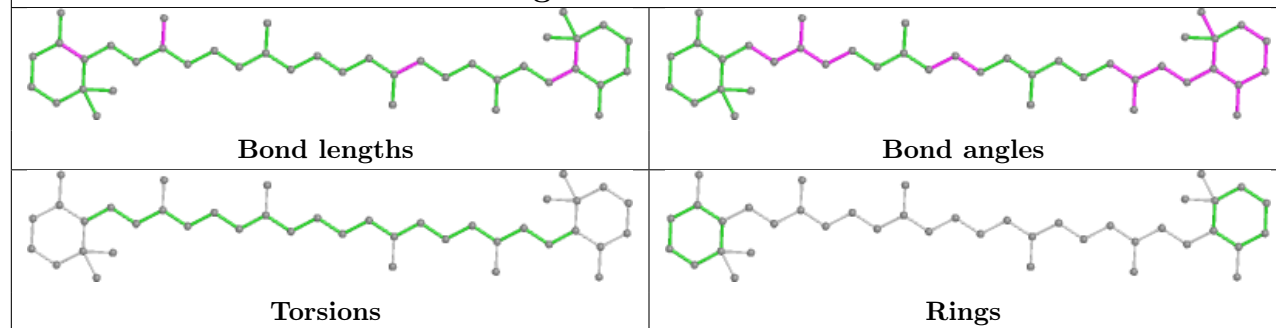




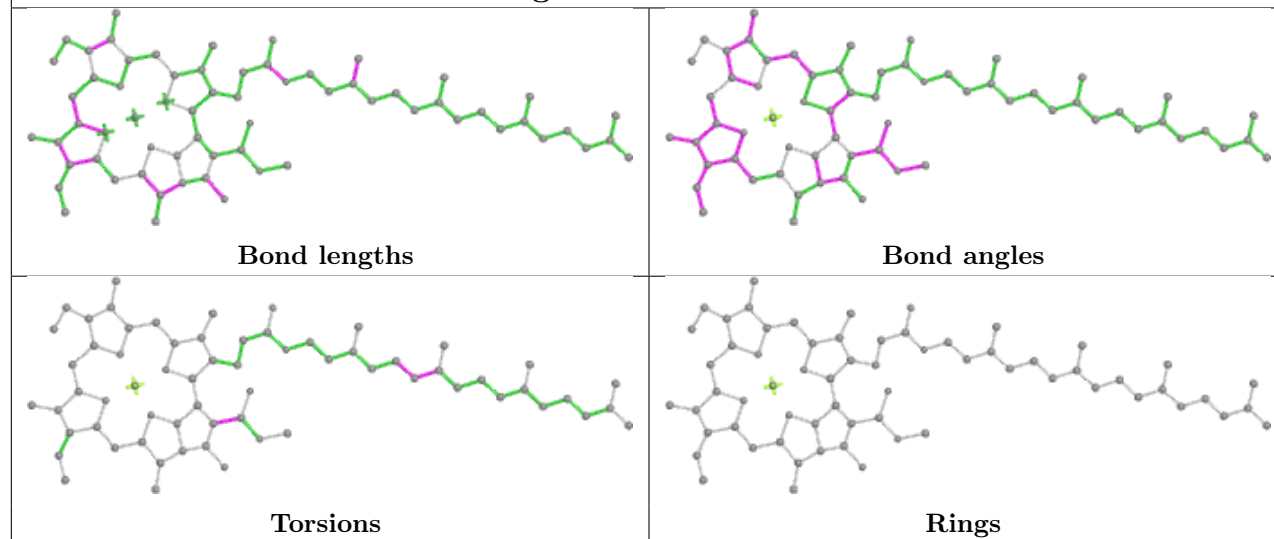
Ligand HEC V 203



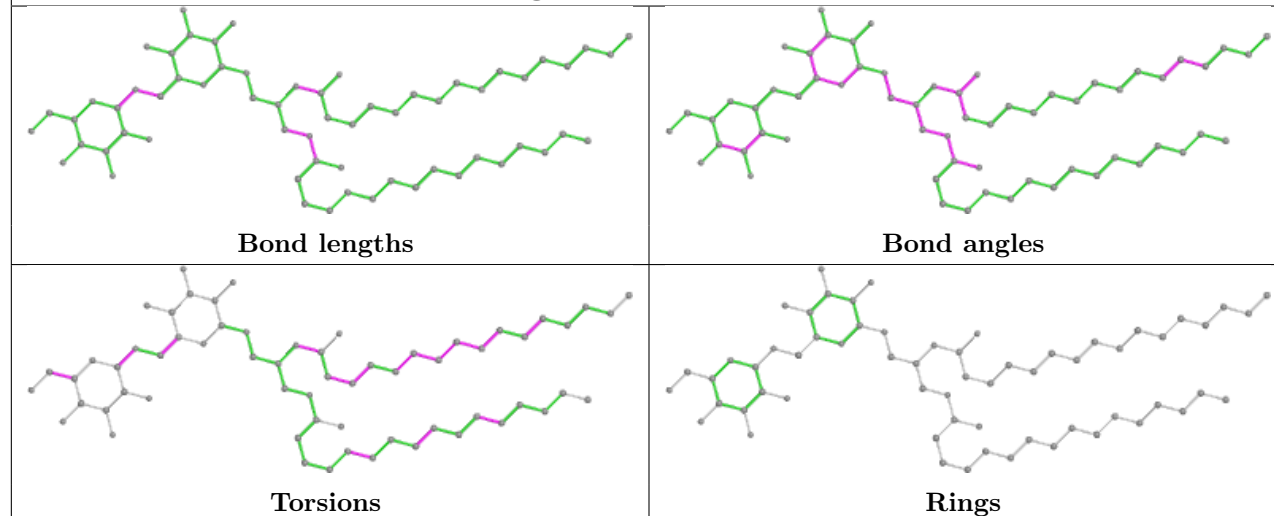
Ligand BCR b 619



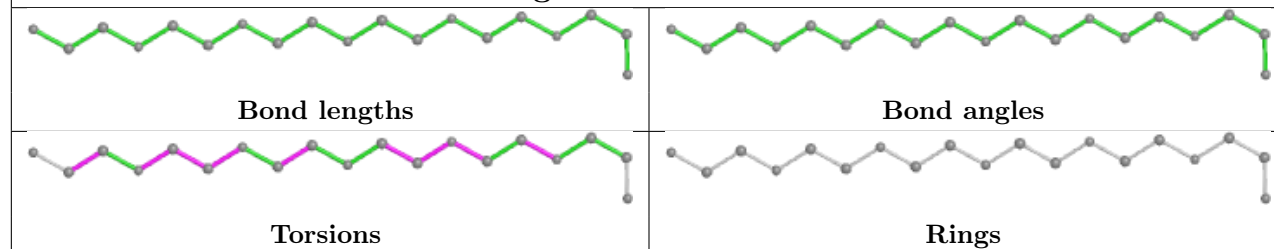
Ligand CLA B 604



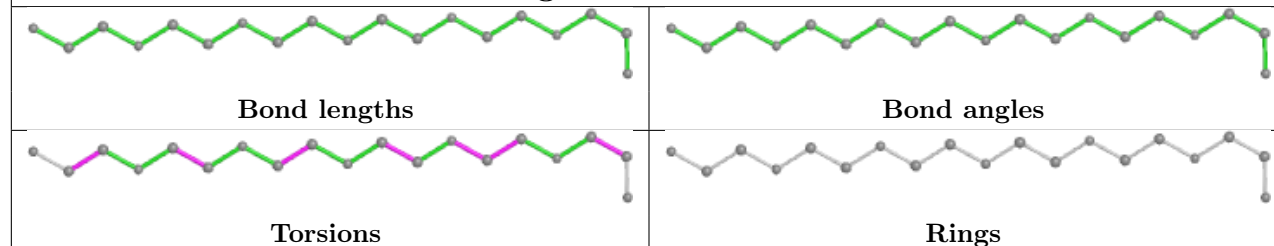
Ligand DGD C 516

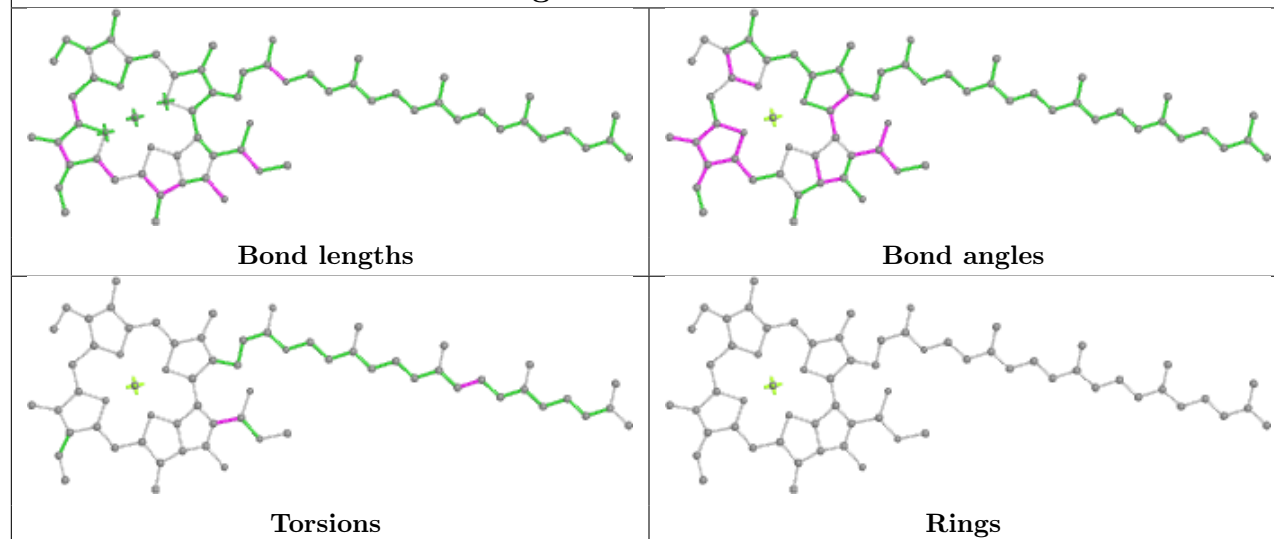
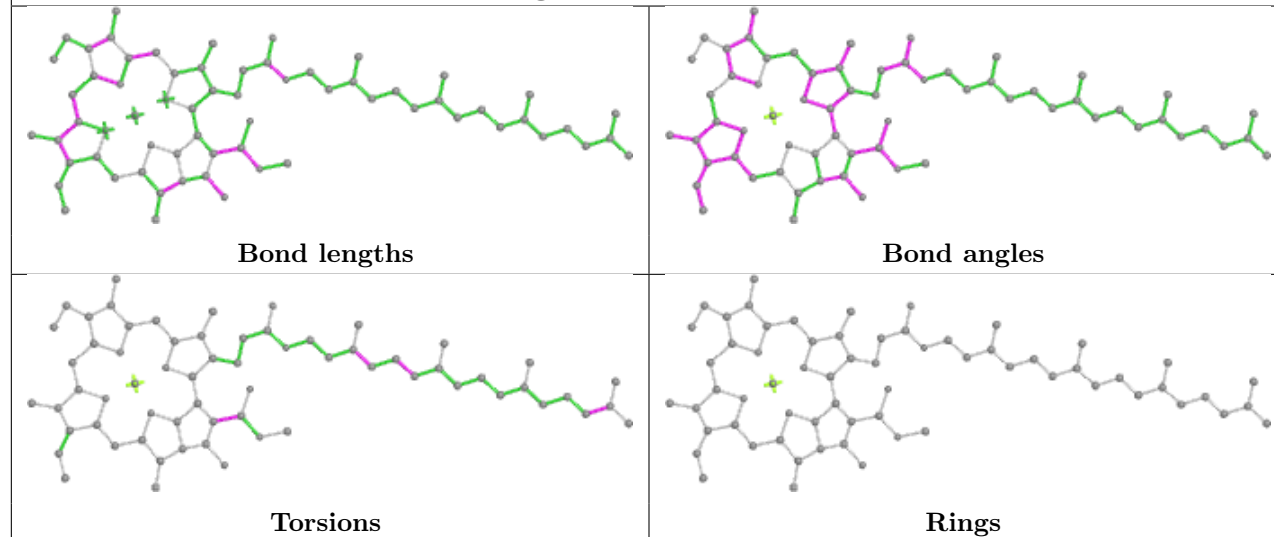
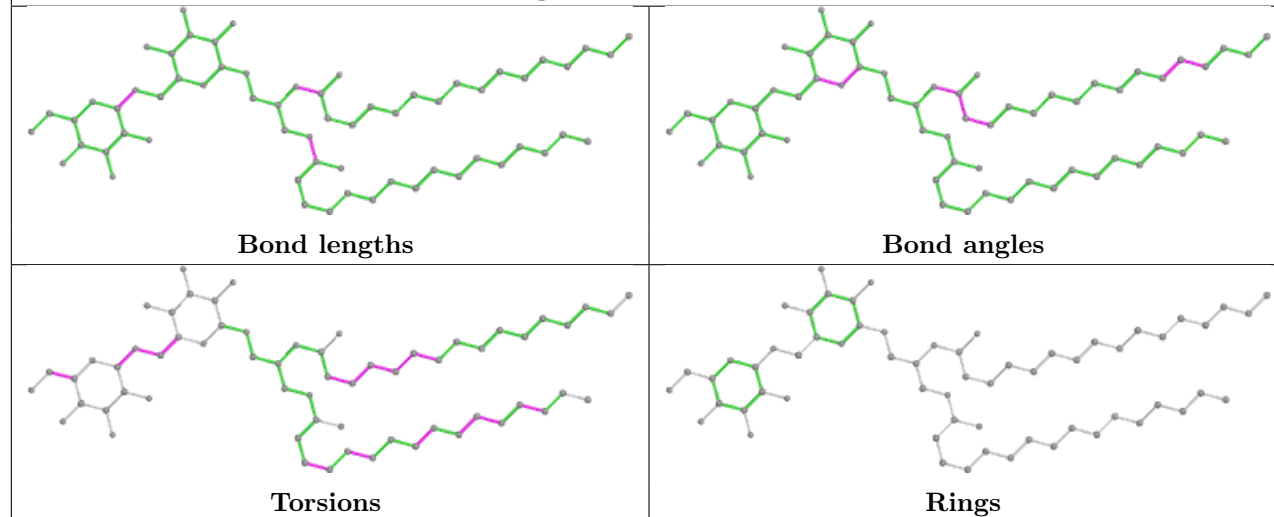


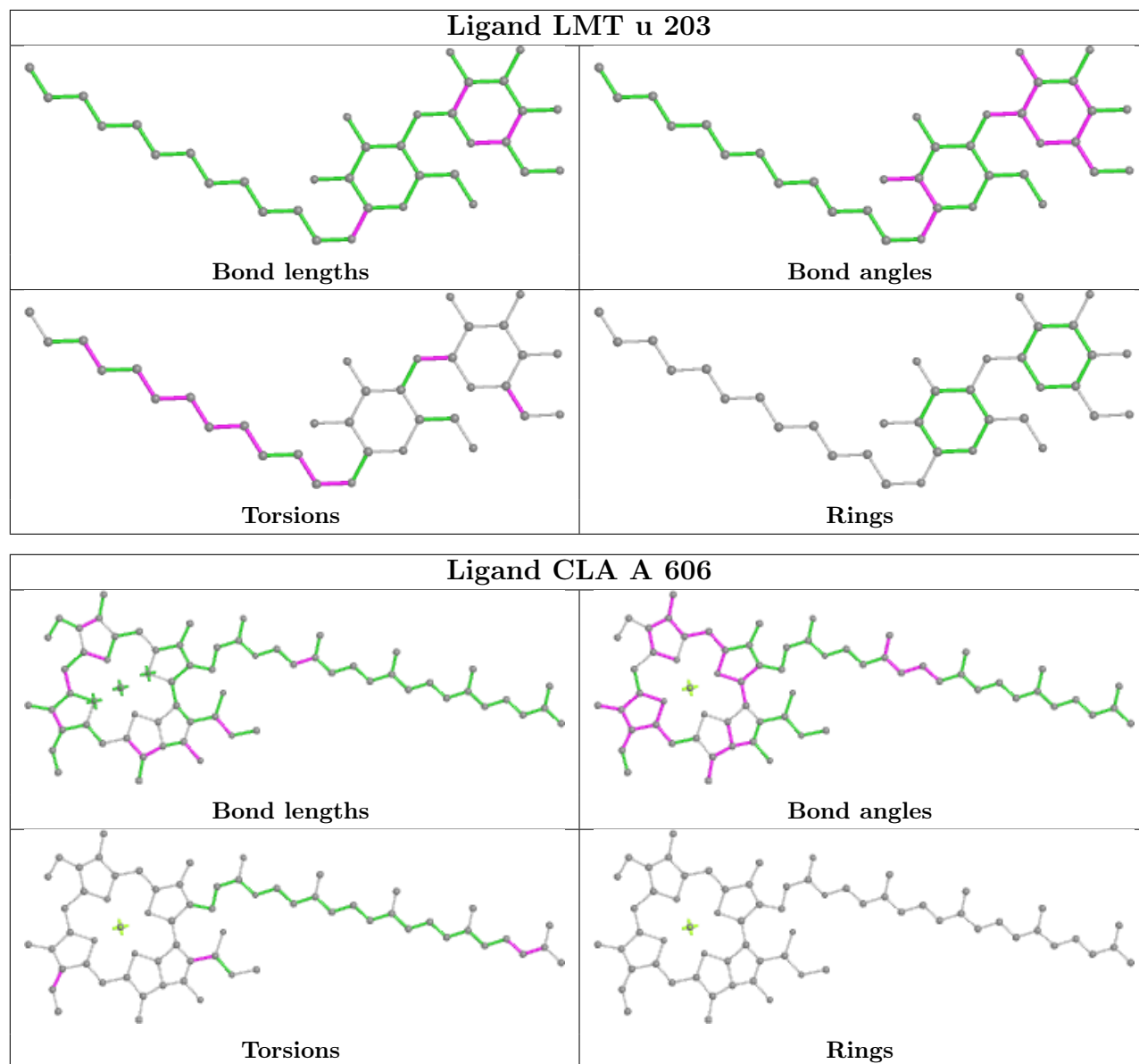
Ligand P6G D 416

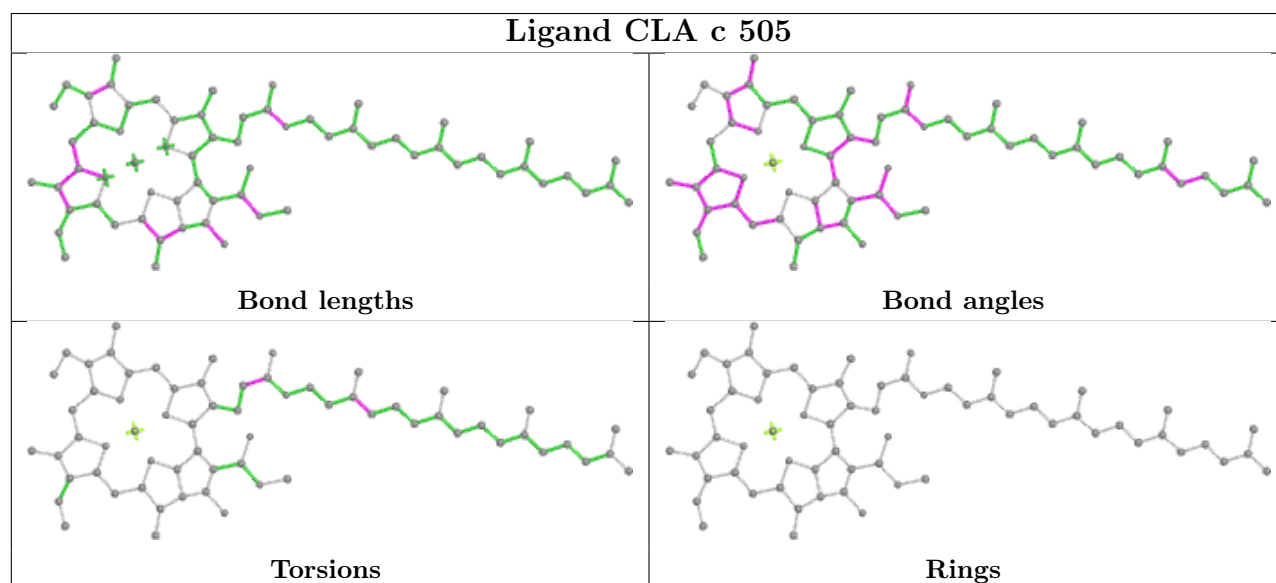
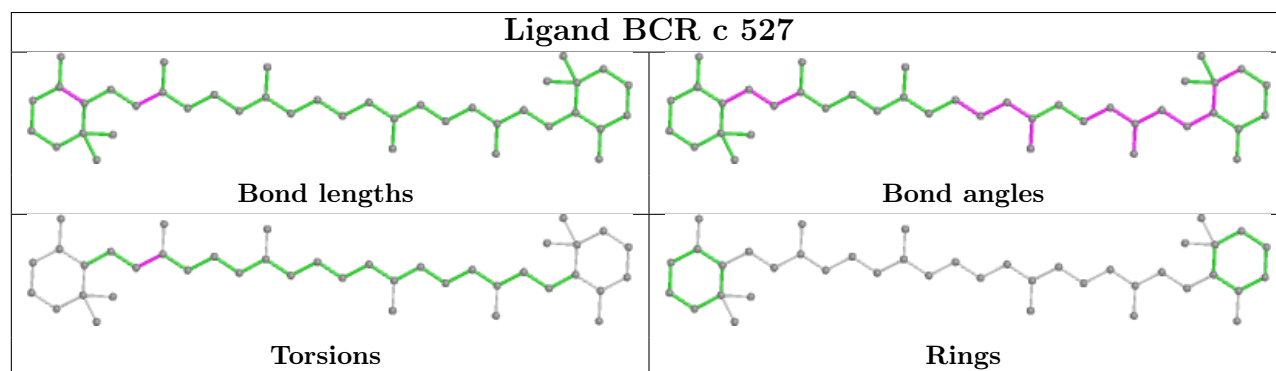
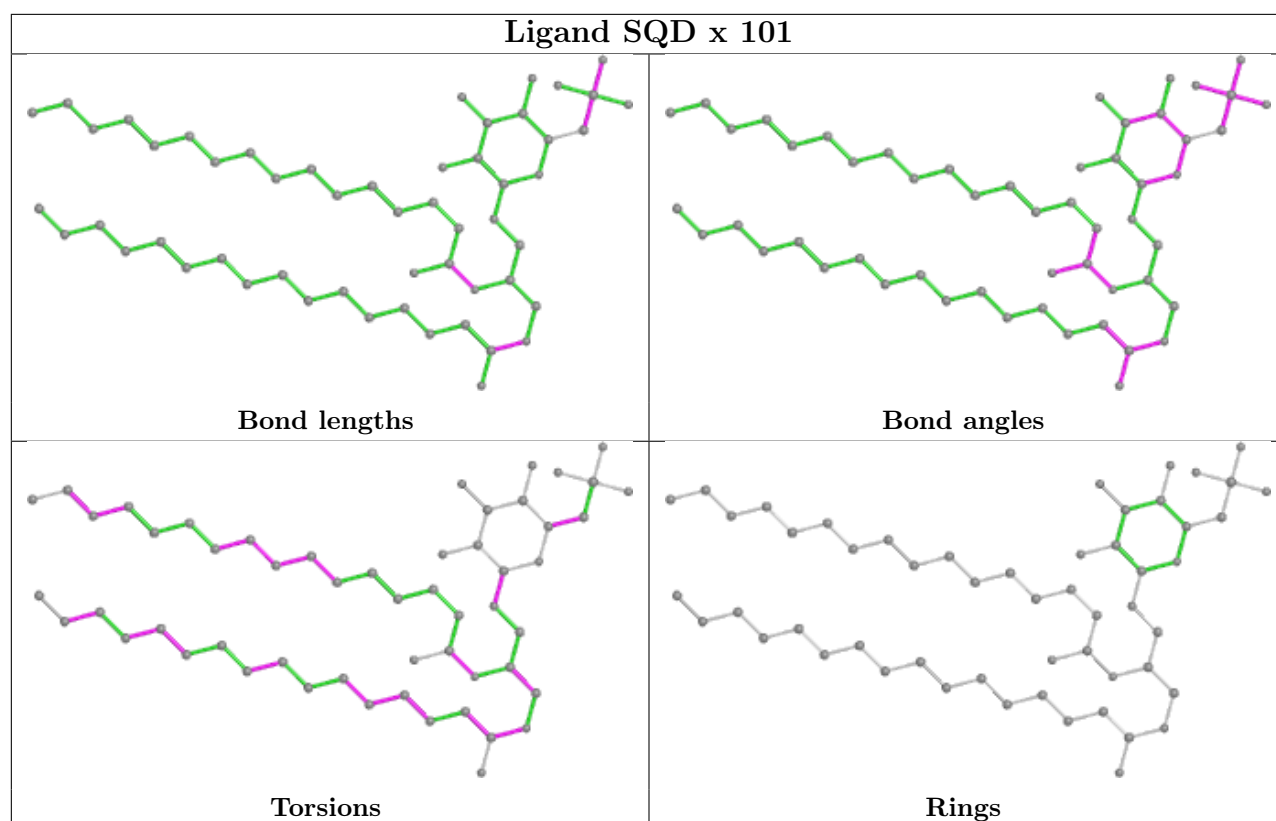


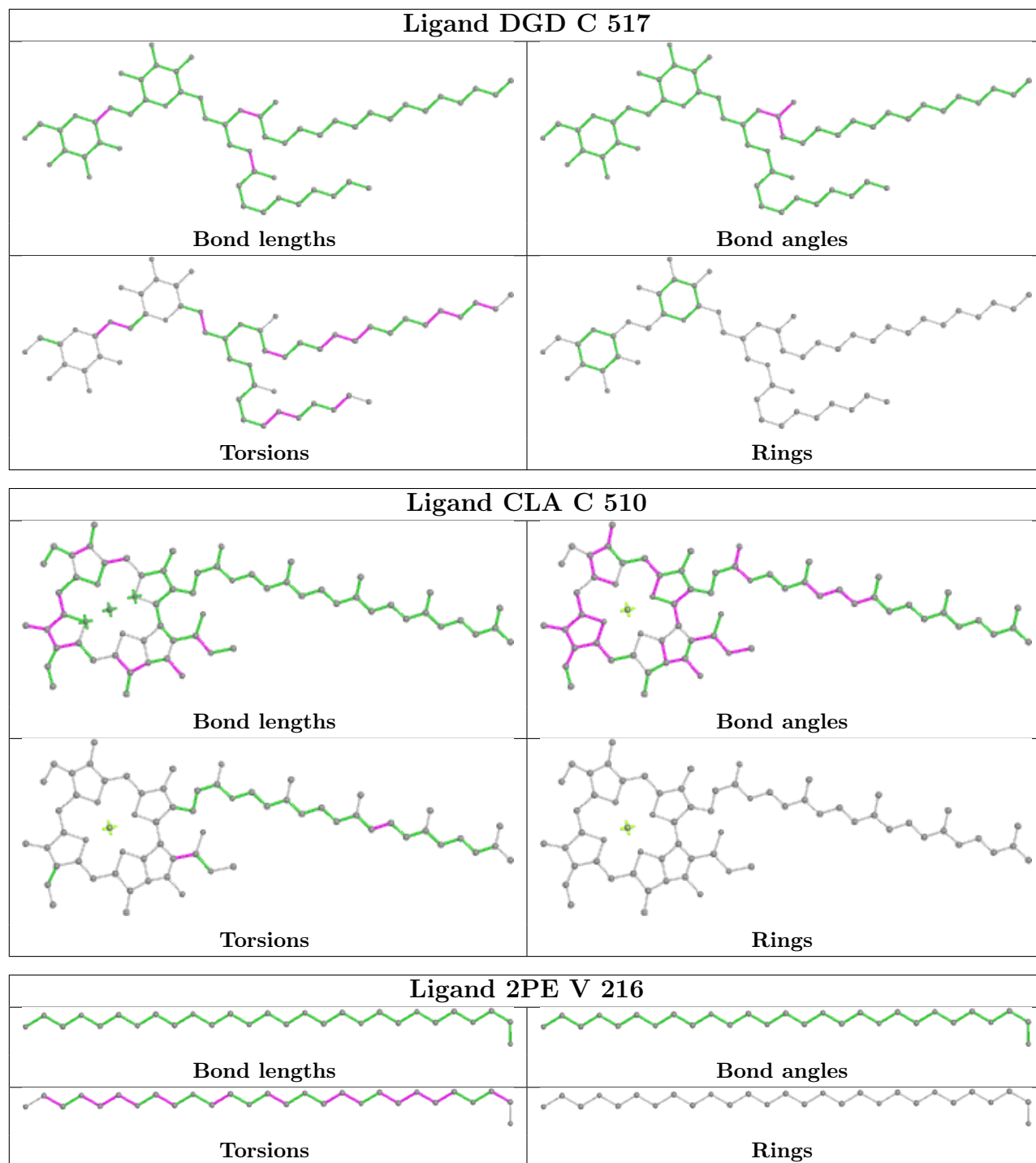
Ligand P6G b 648

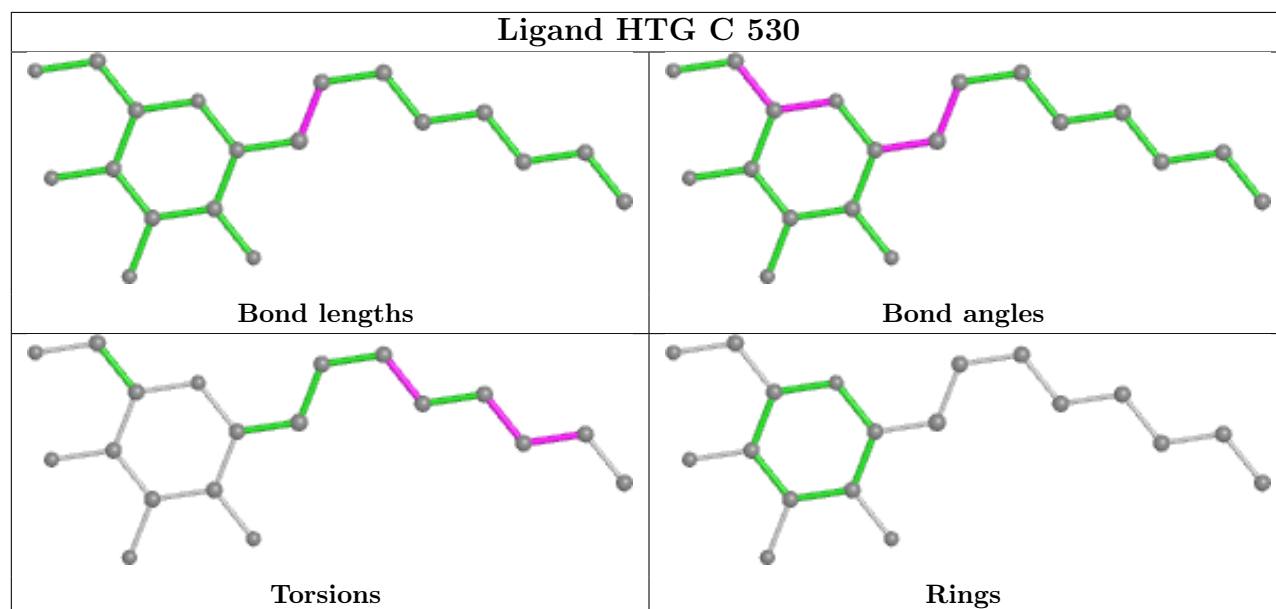
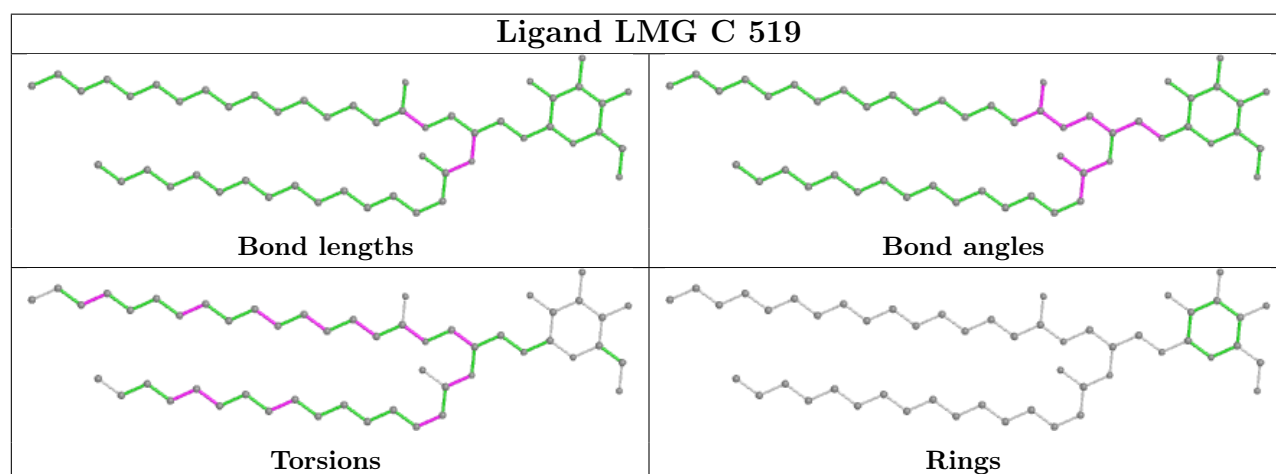
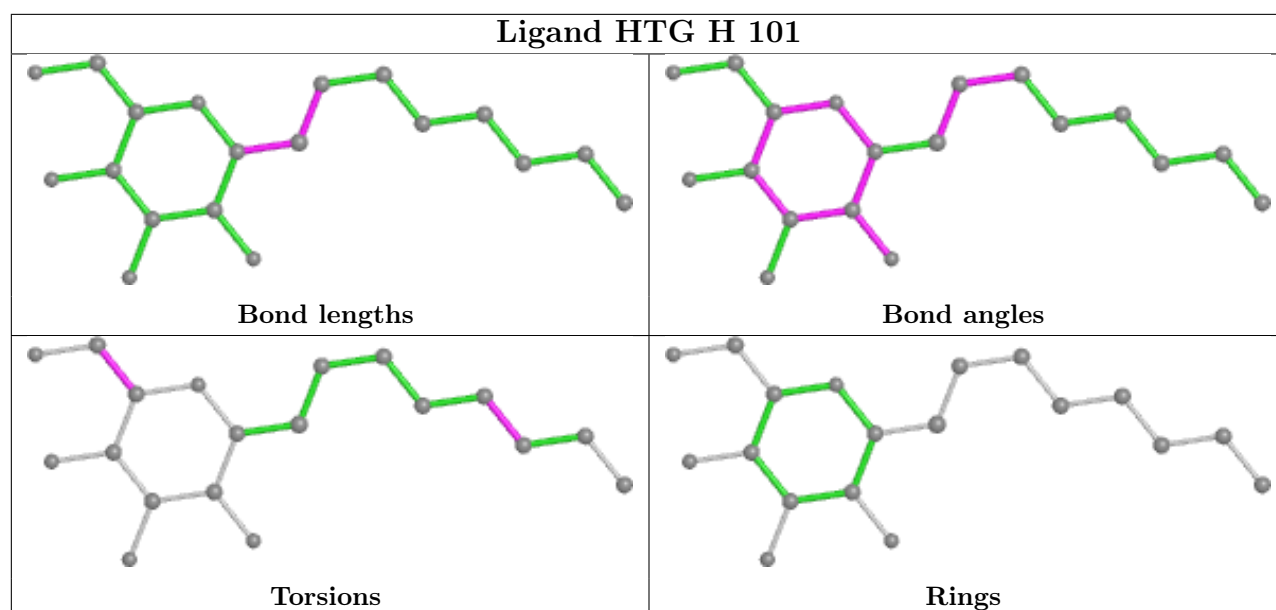


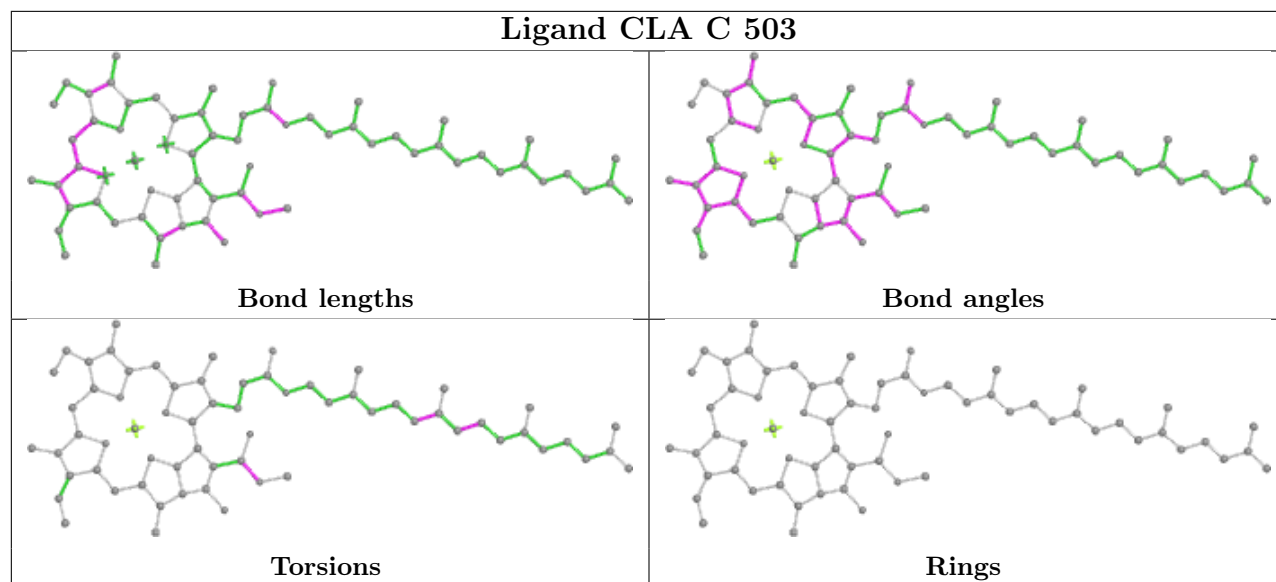
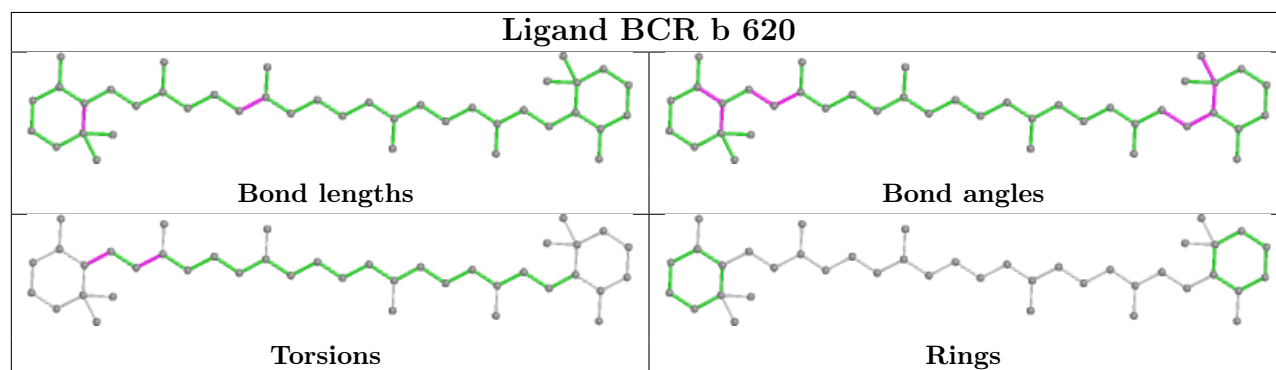
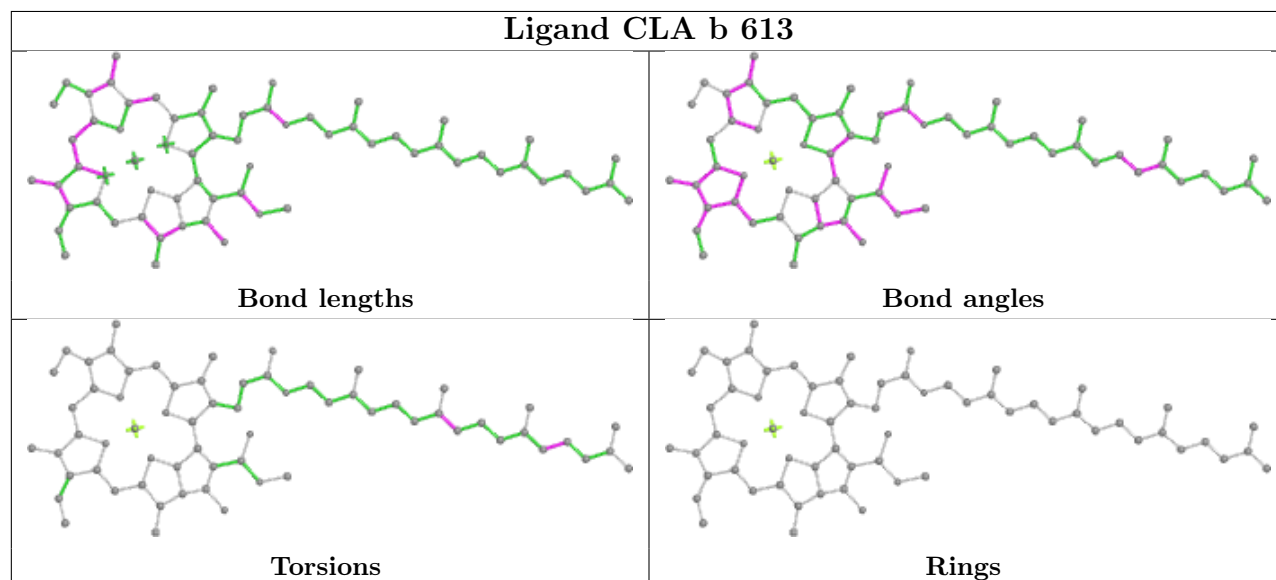
Ligand CLA B 613**Ligand CLA C 507****Ligand DGD c 516**



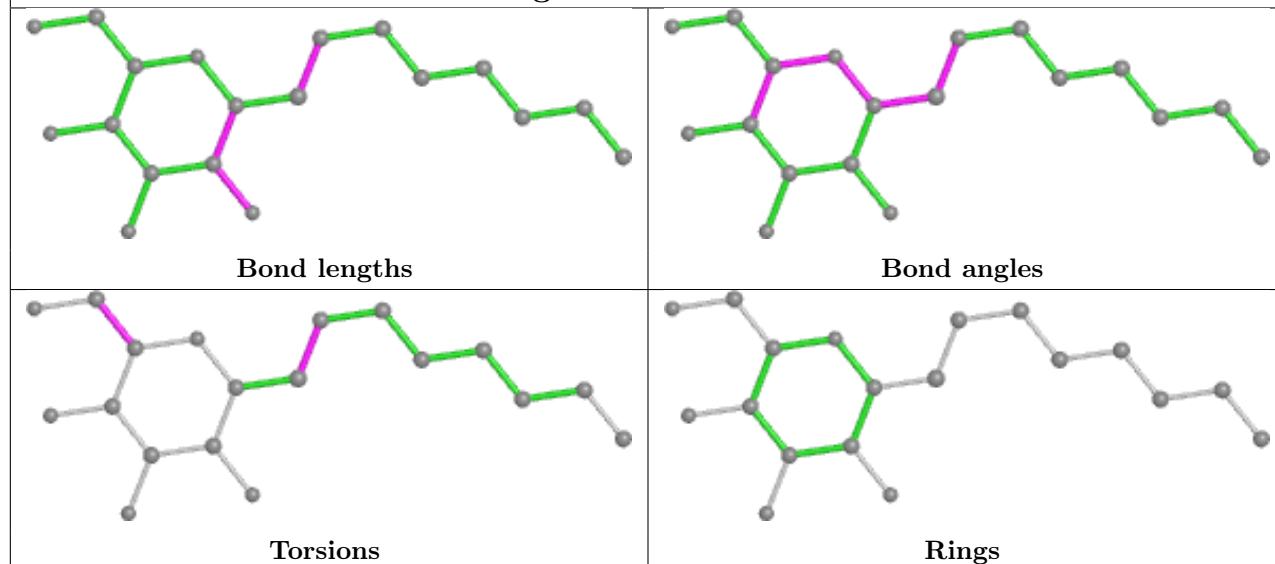




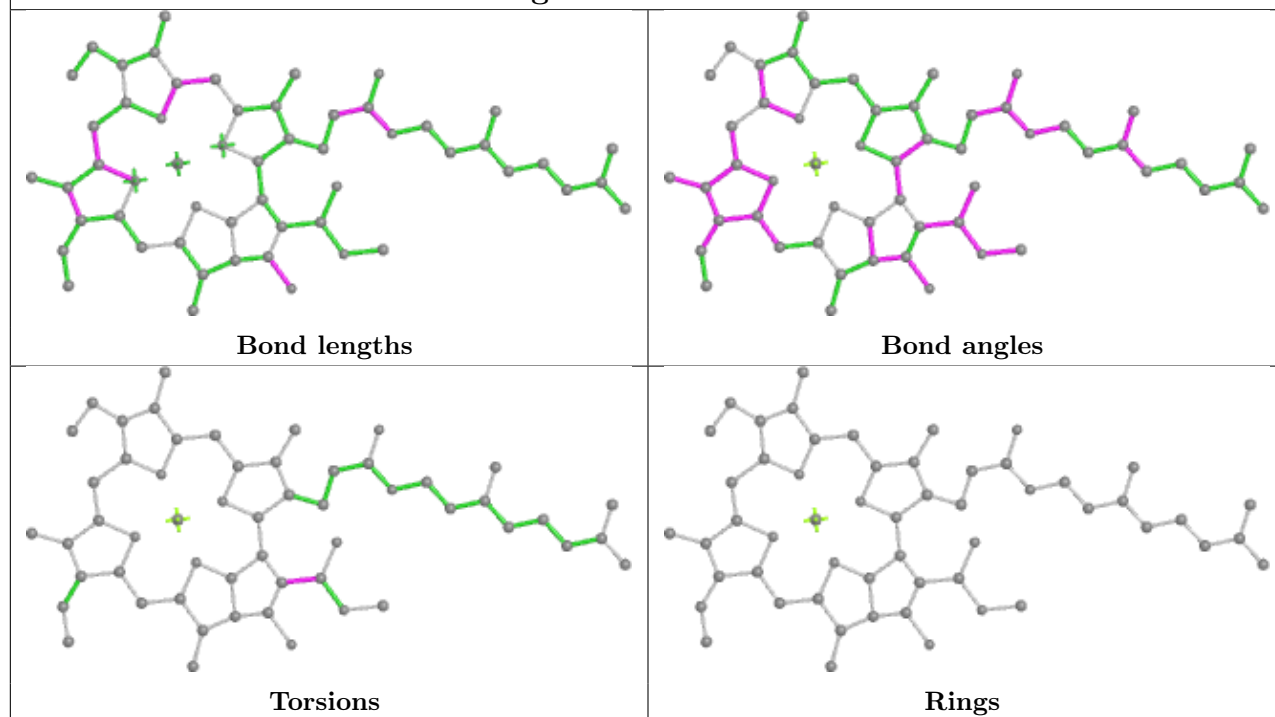


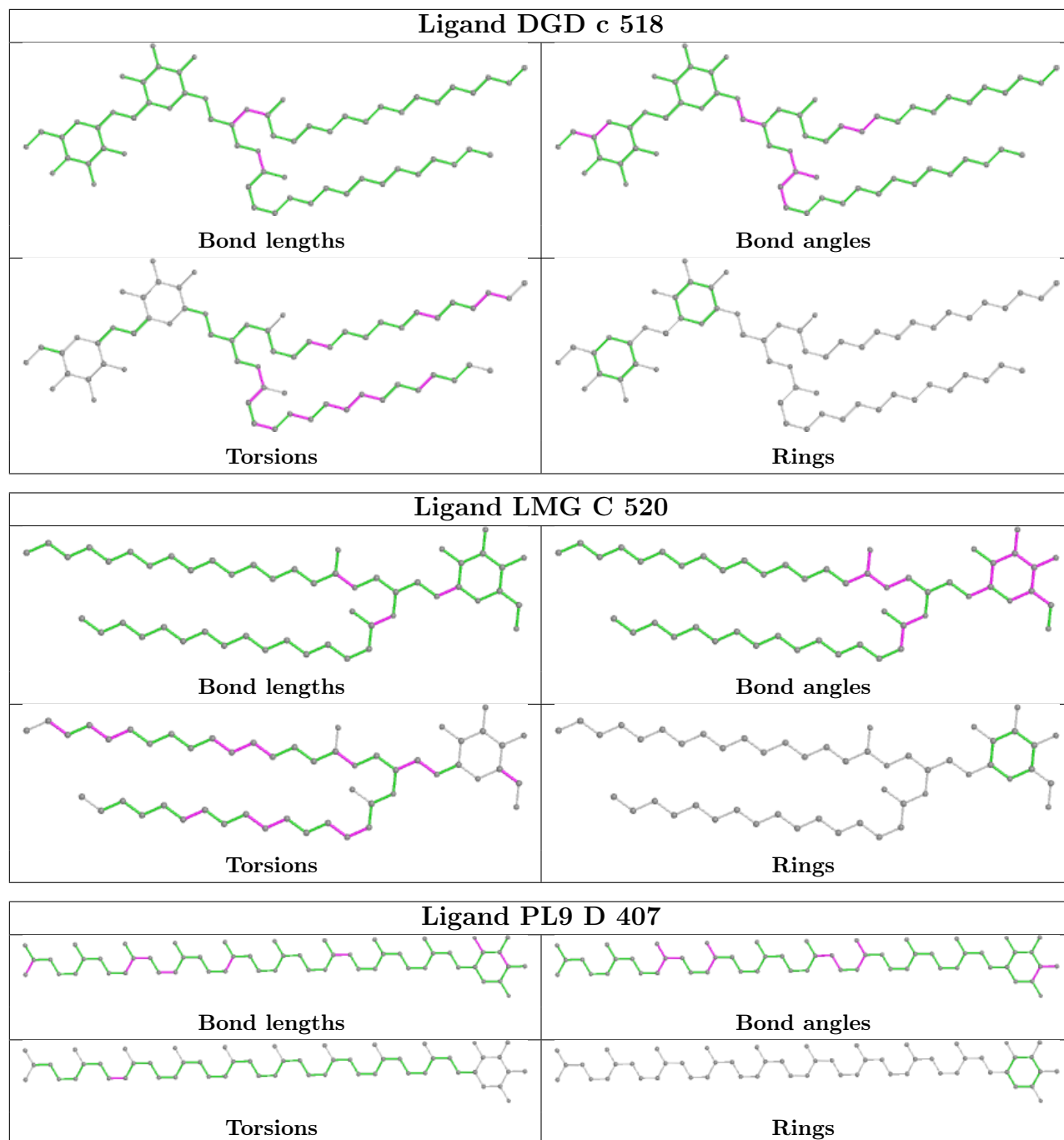
Ligand CLA C 503**Ligand BCR b 620****Ligand CLA b 613**

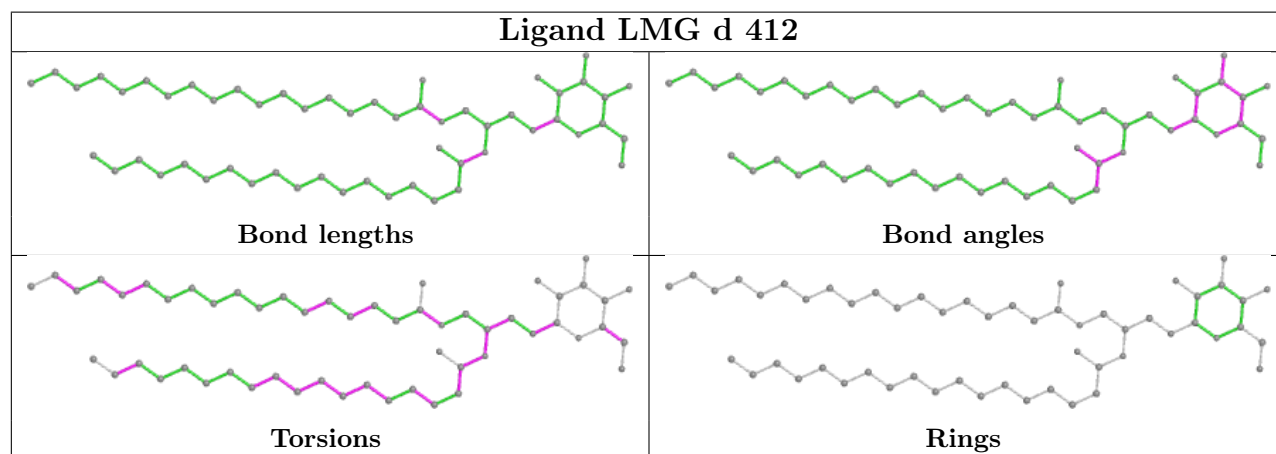
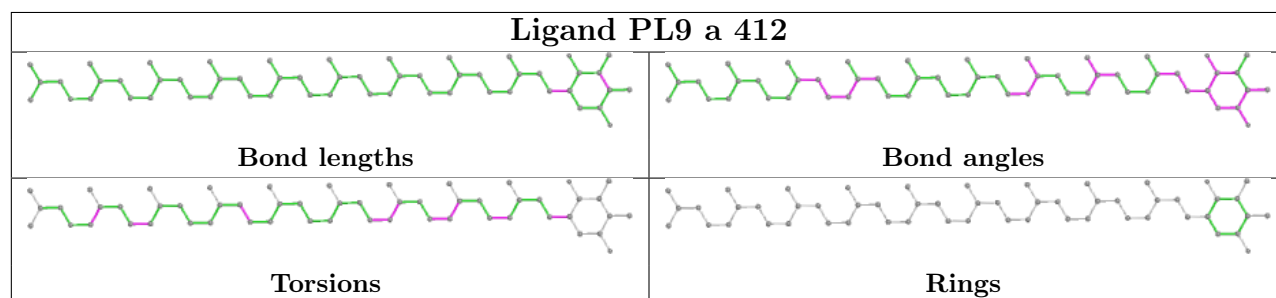
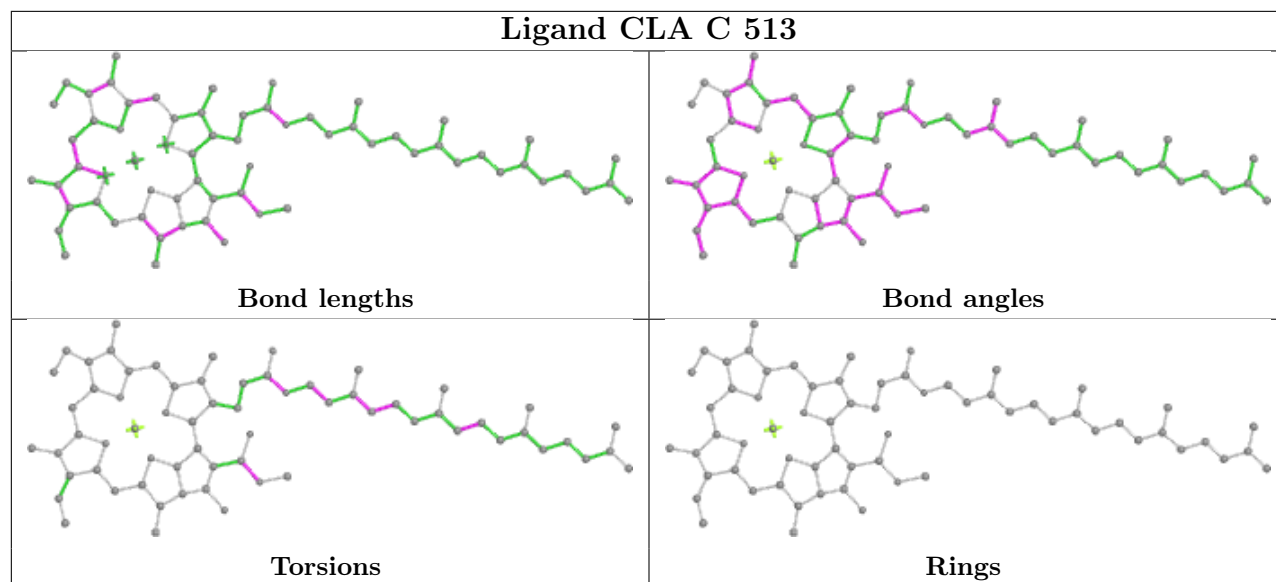
Ligand HTG c 530



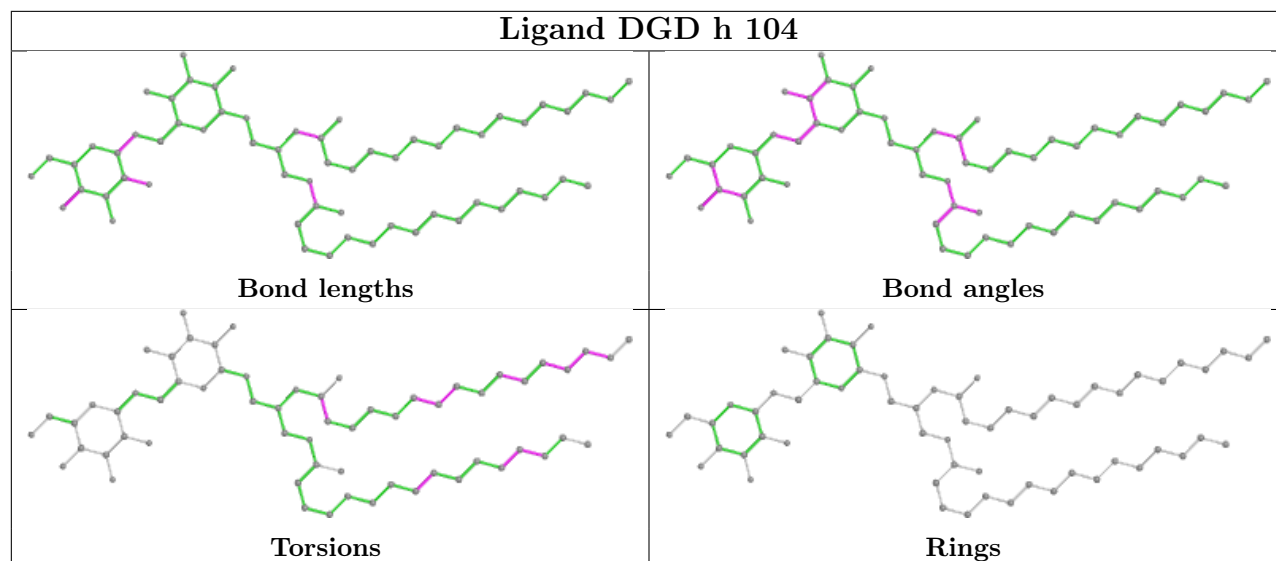
Ligand CLA B 615



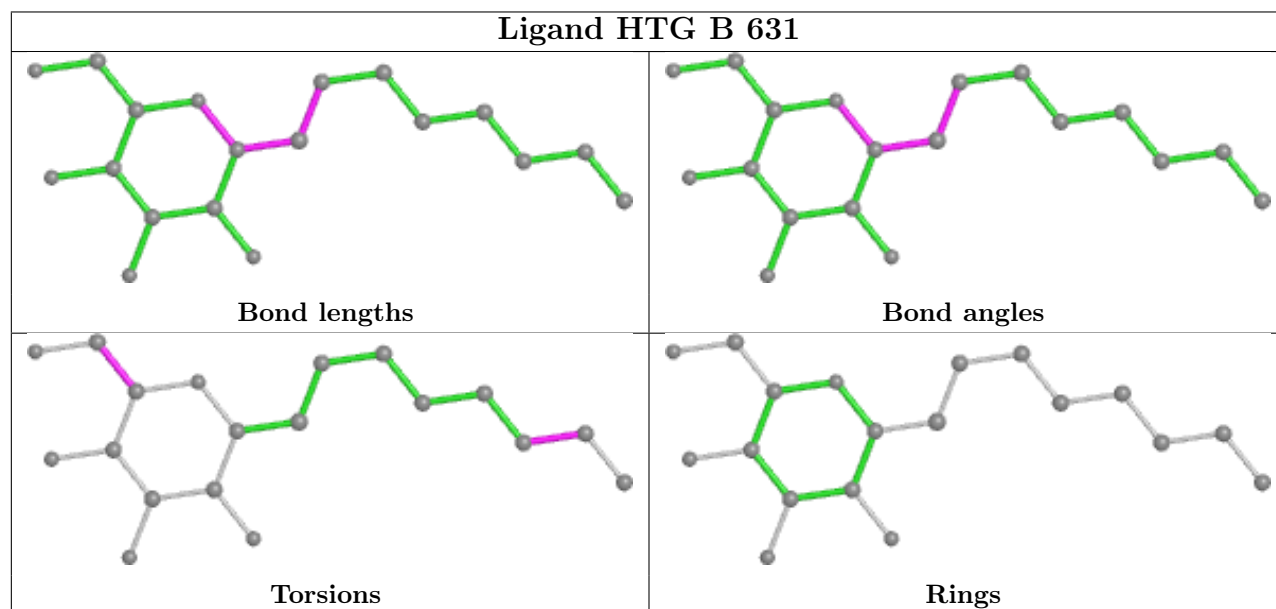




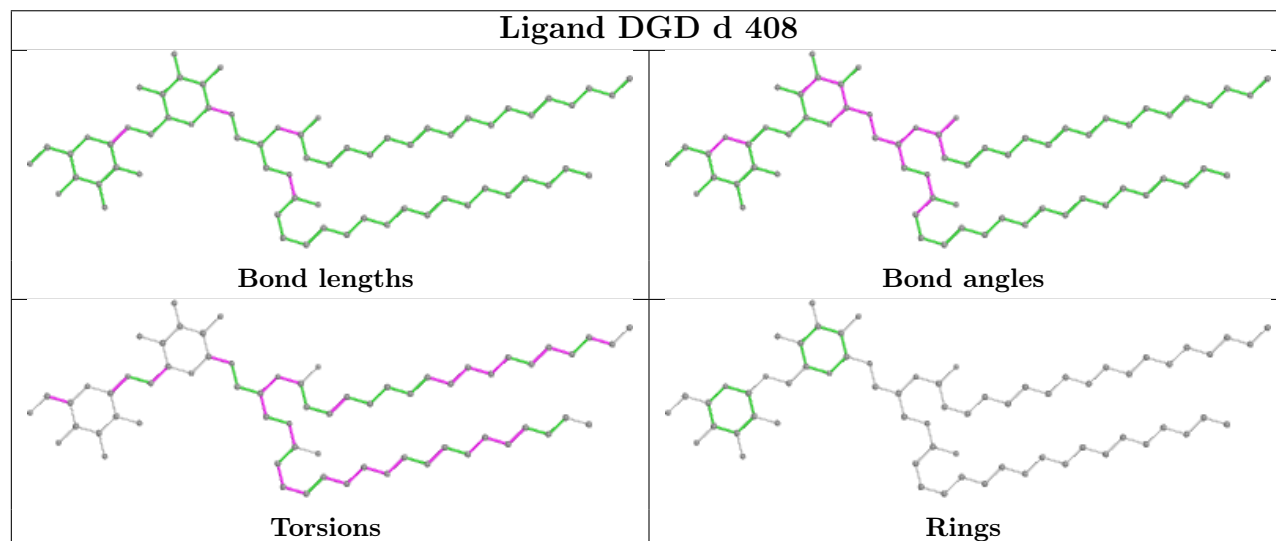
Ligand DGD h 104



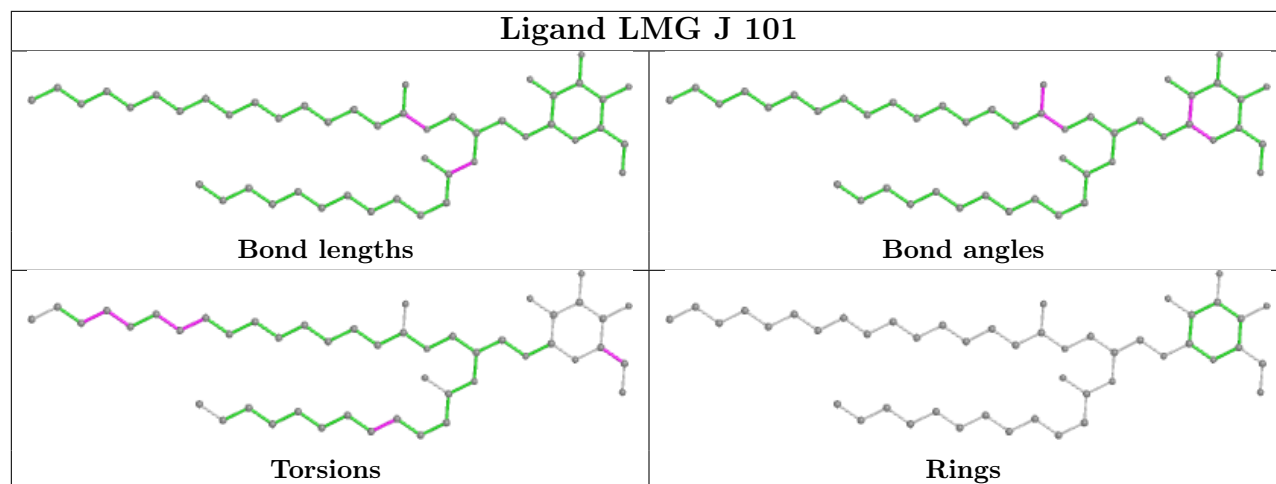
Ligand HTG B 631



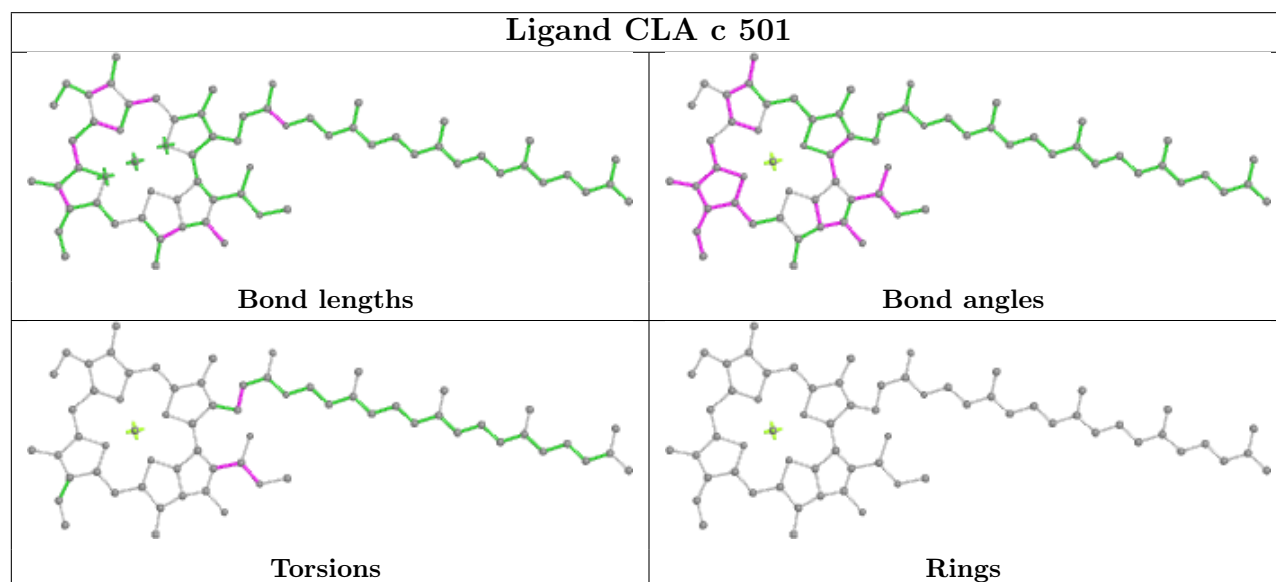
Ligand DGD d 408



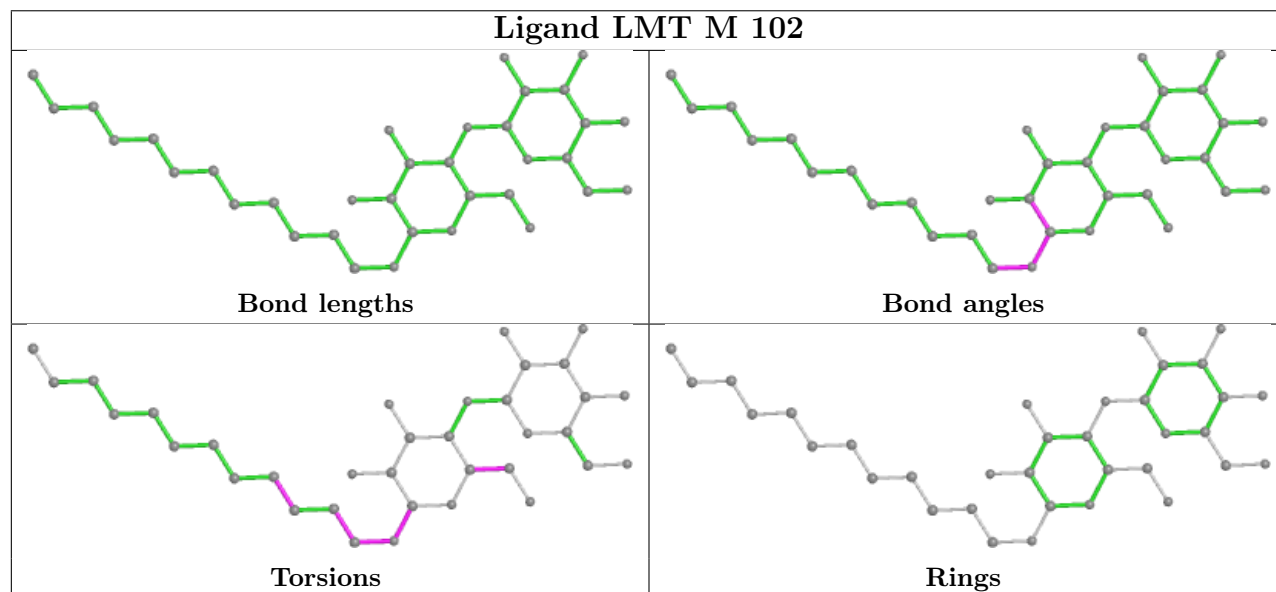
Ligand LMG J 101



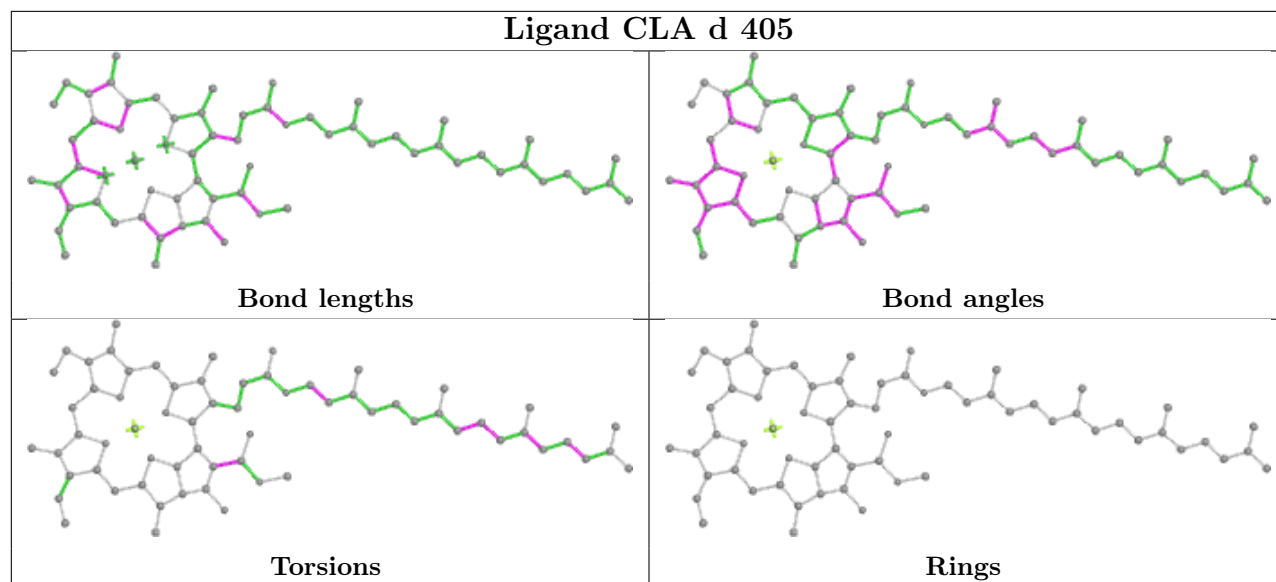
Ligand CLA c 501



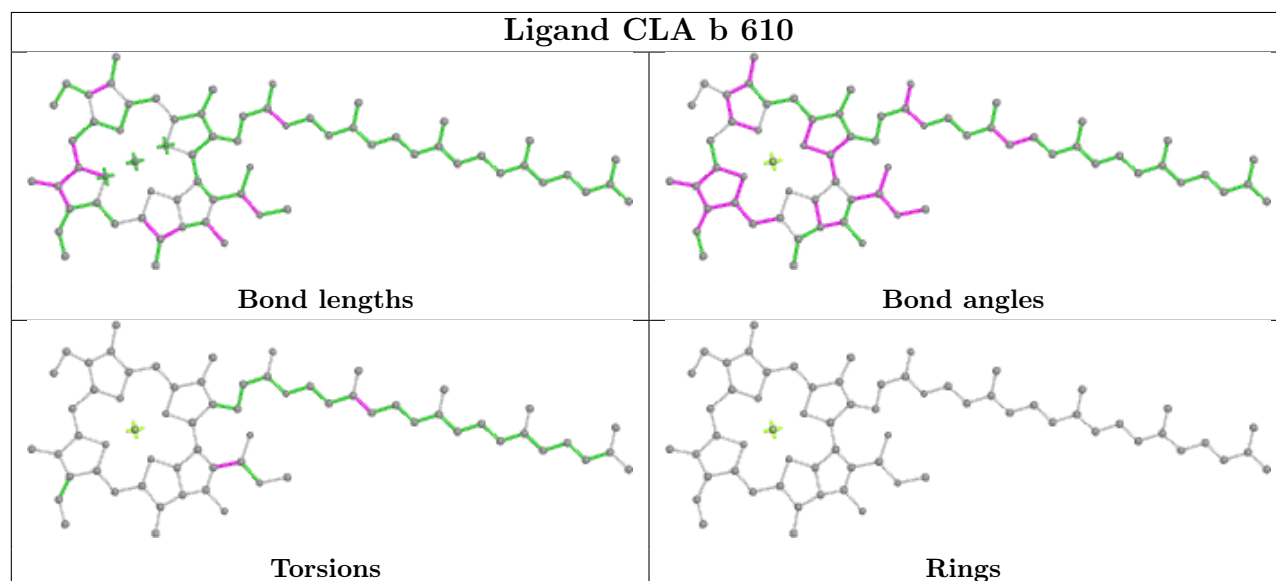
Ligand LMT M 102



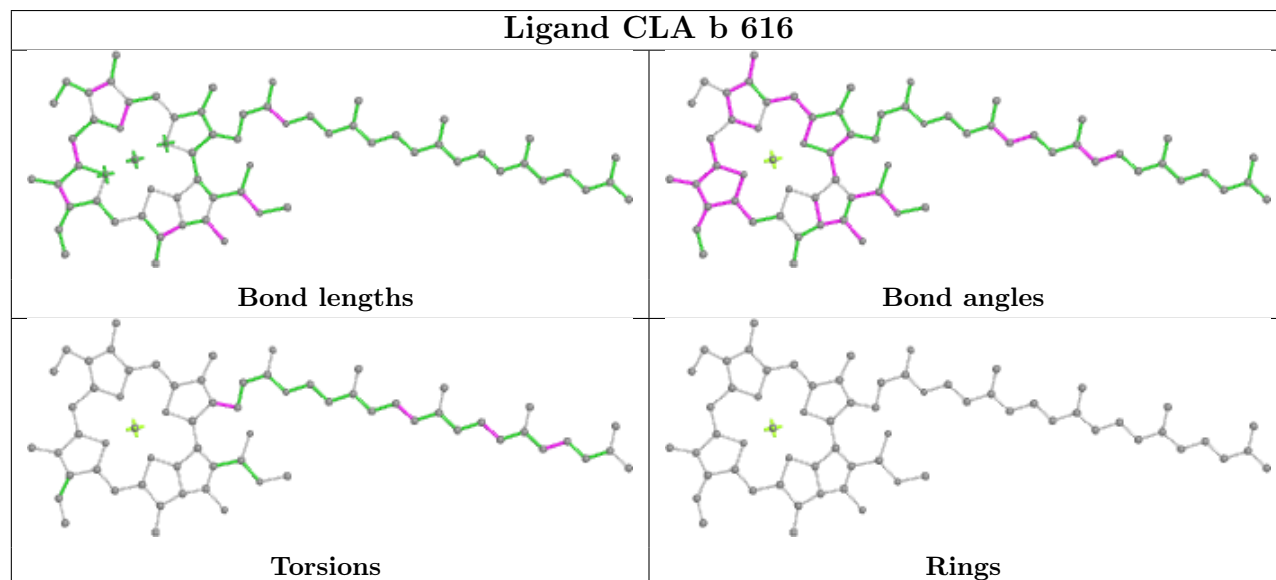
Ligand CLA d 405

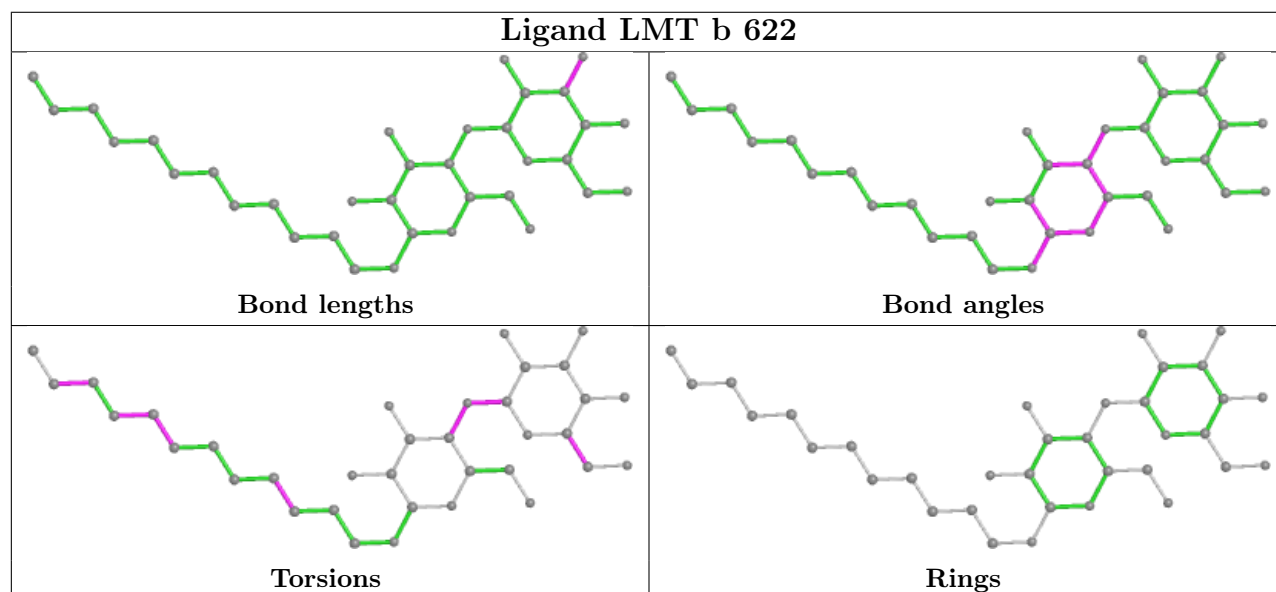
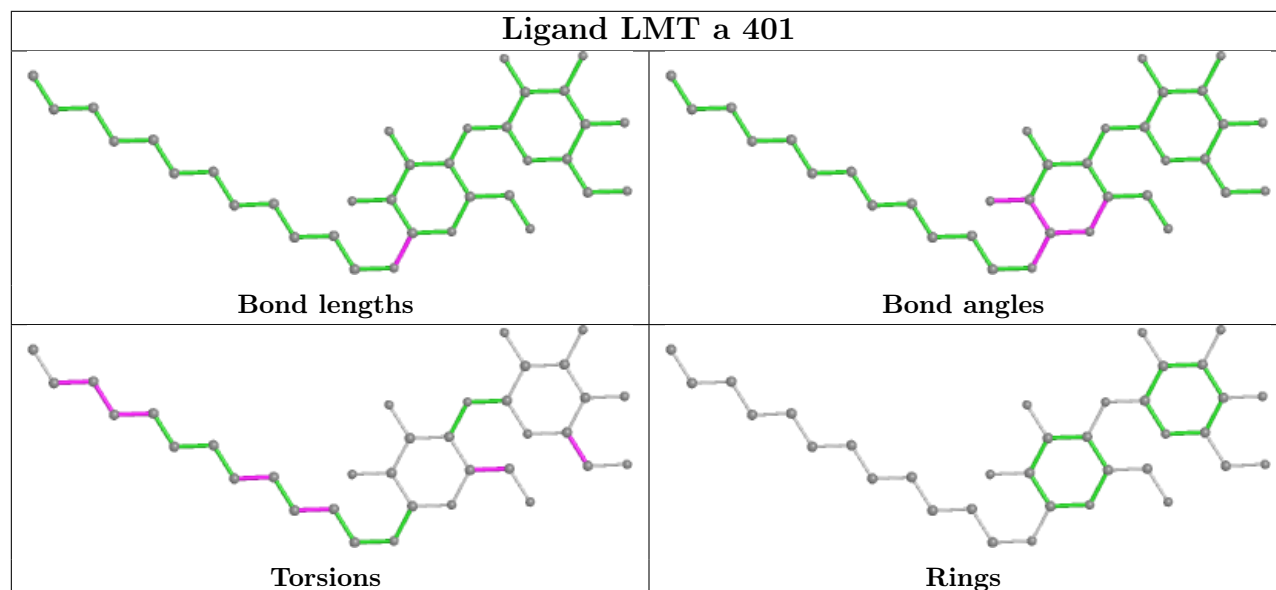
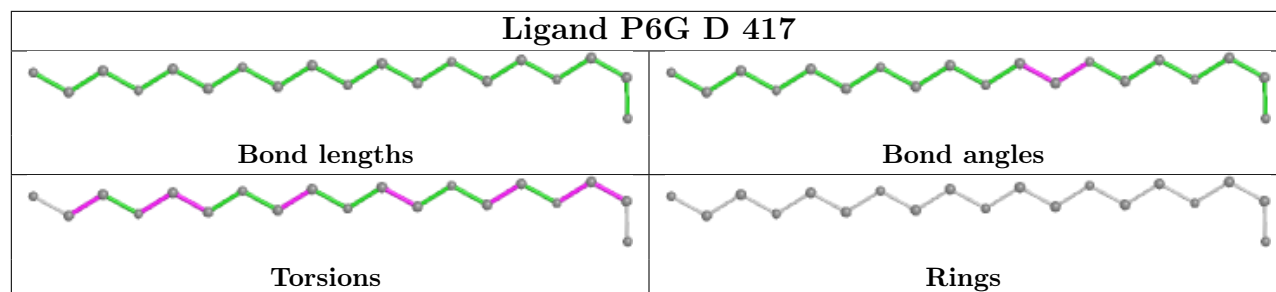


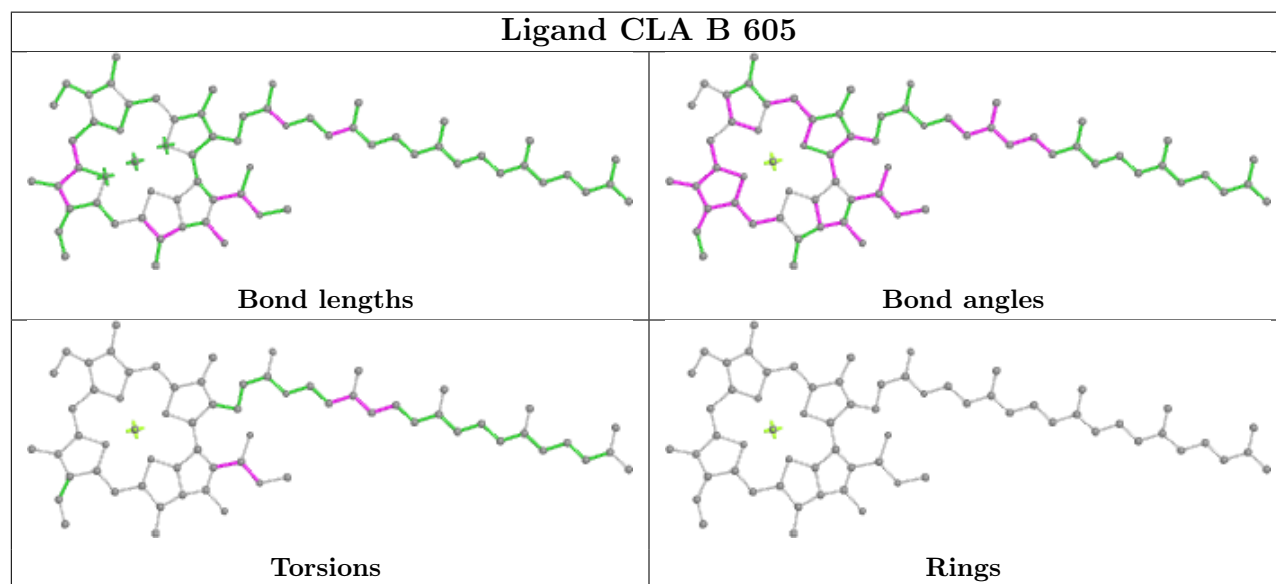
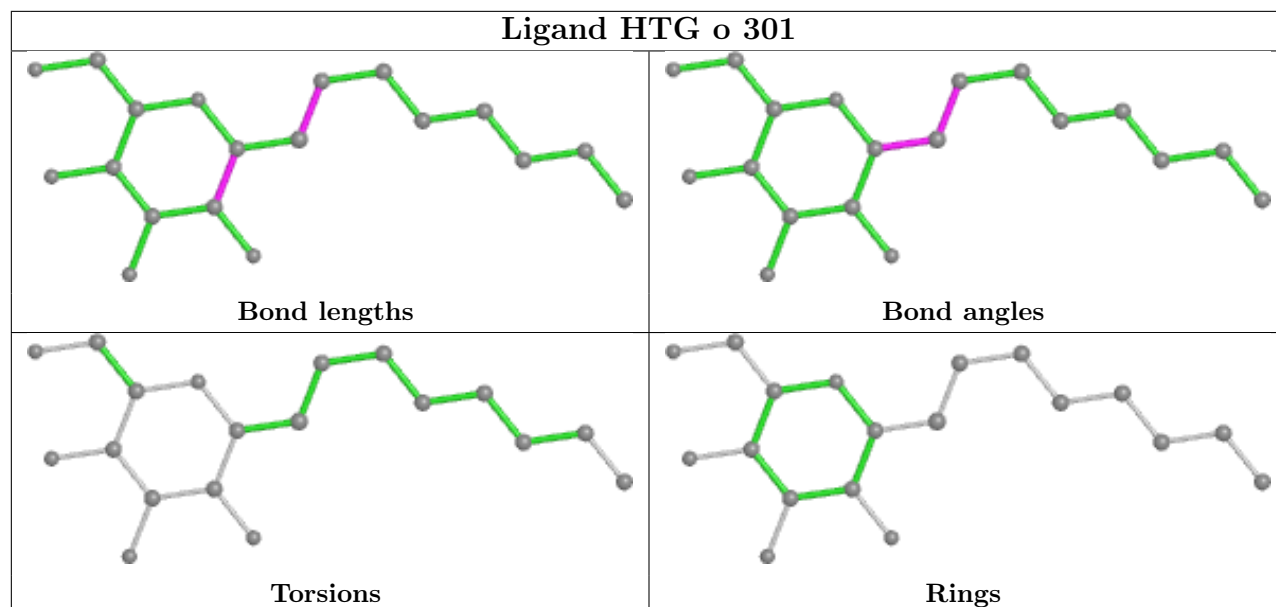
Ligand CLA b 610



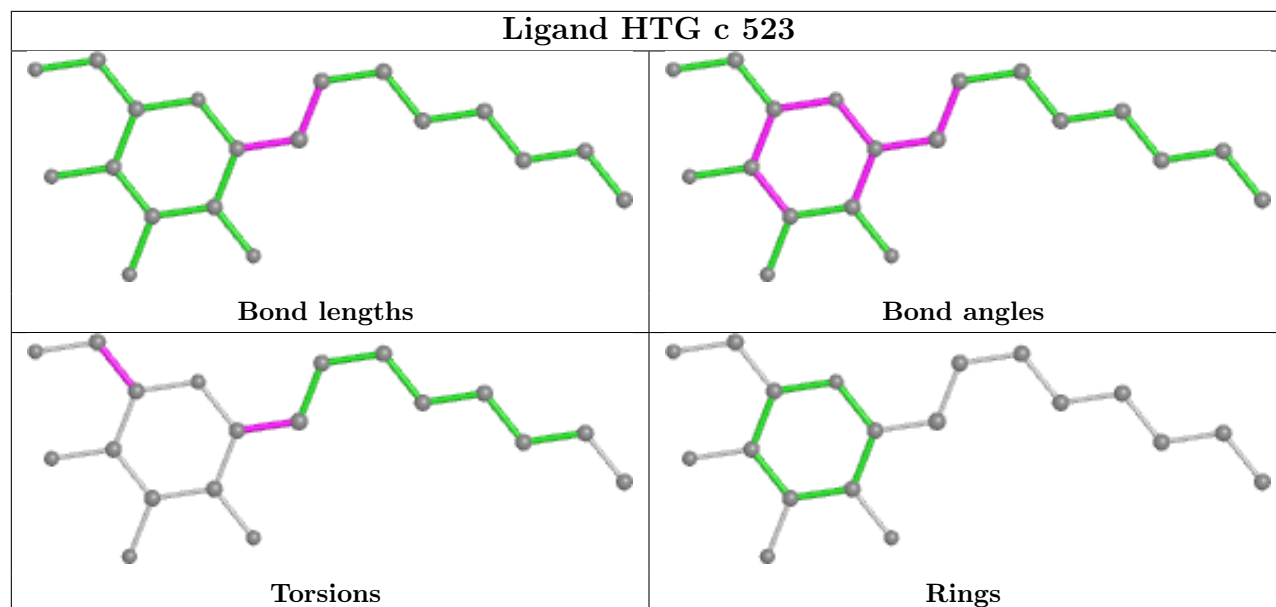
Ligand CLA b 616



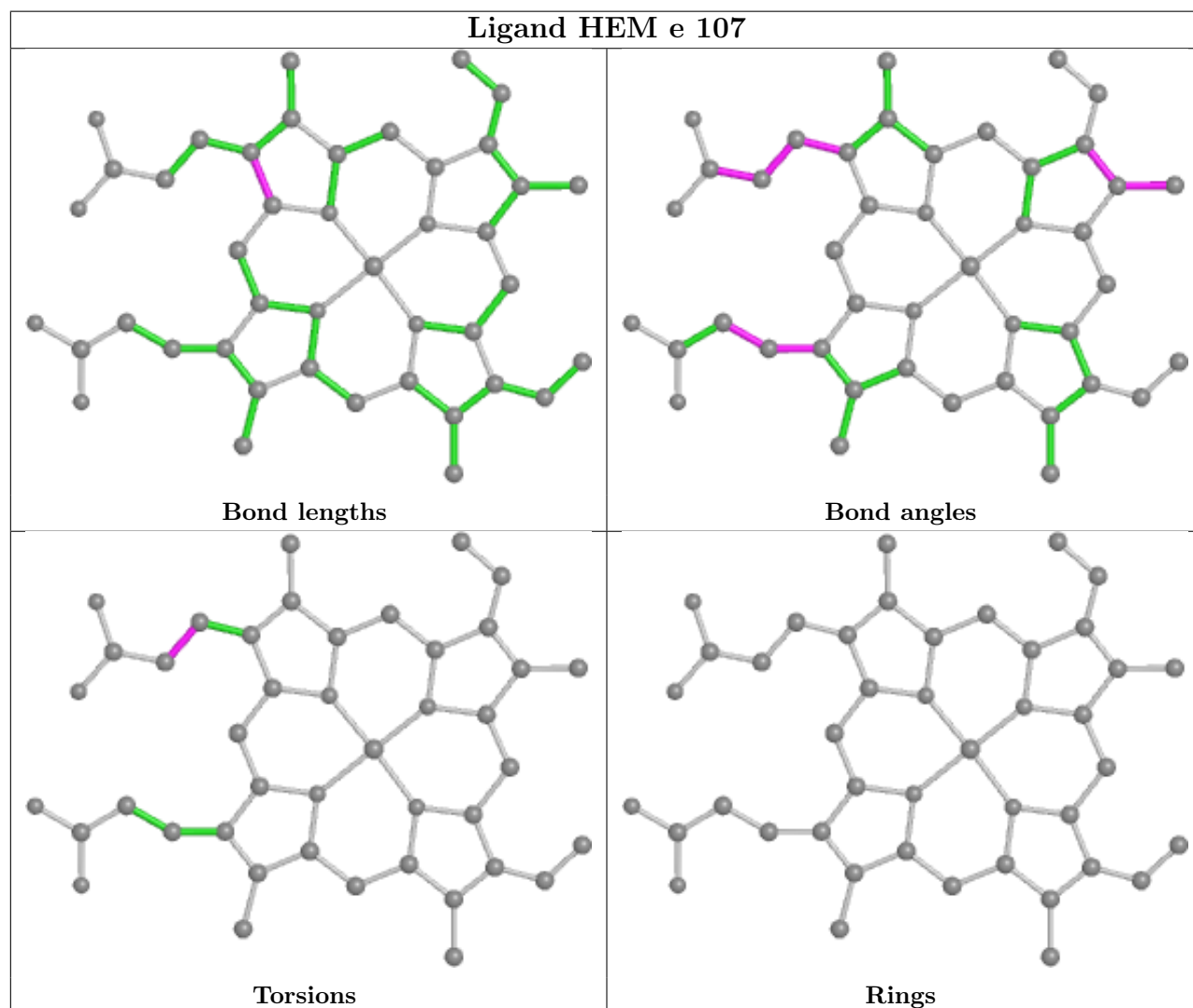


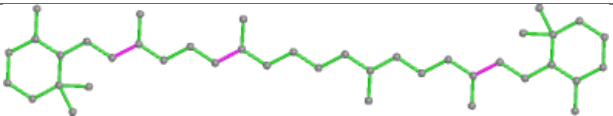
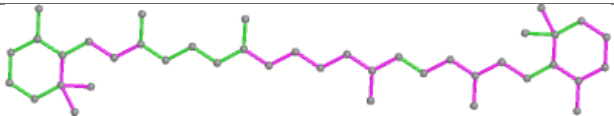
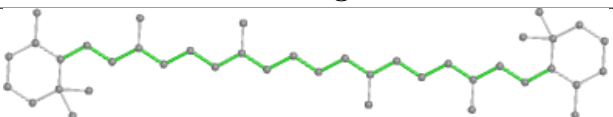
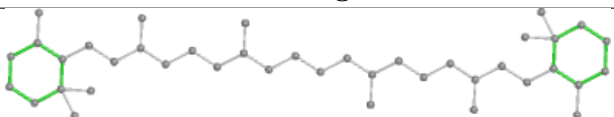


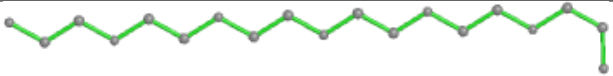
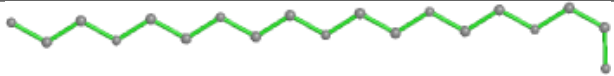
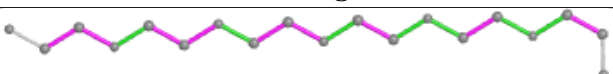
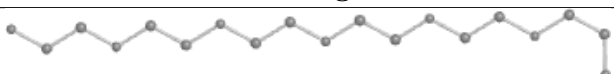
Ligand HTG c 523

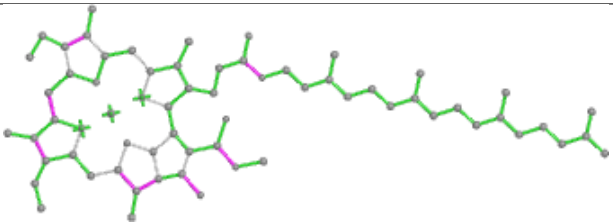
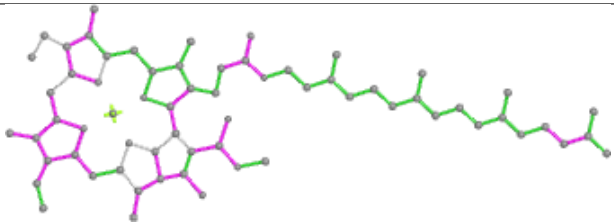
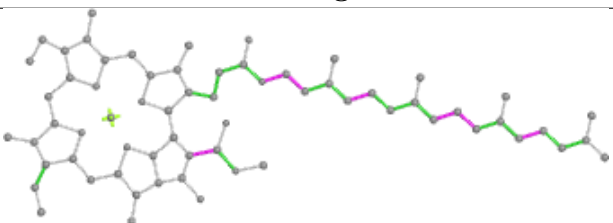
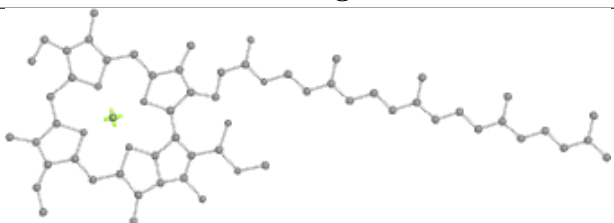


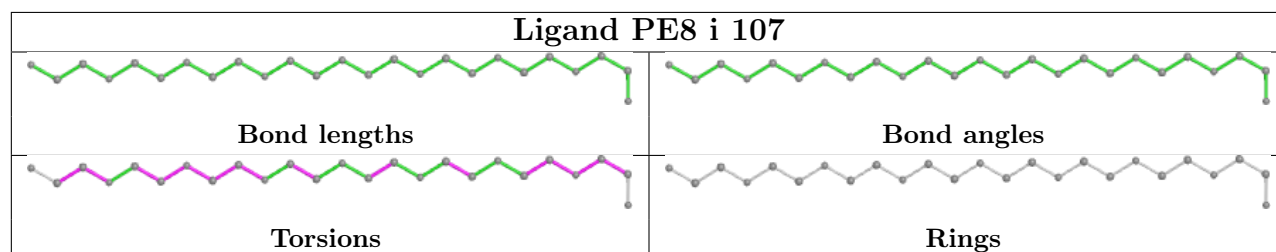
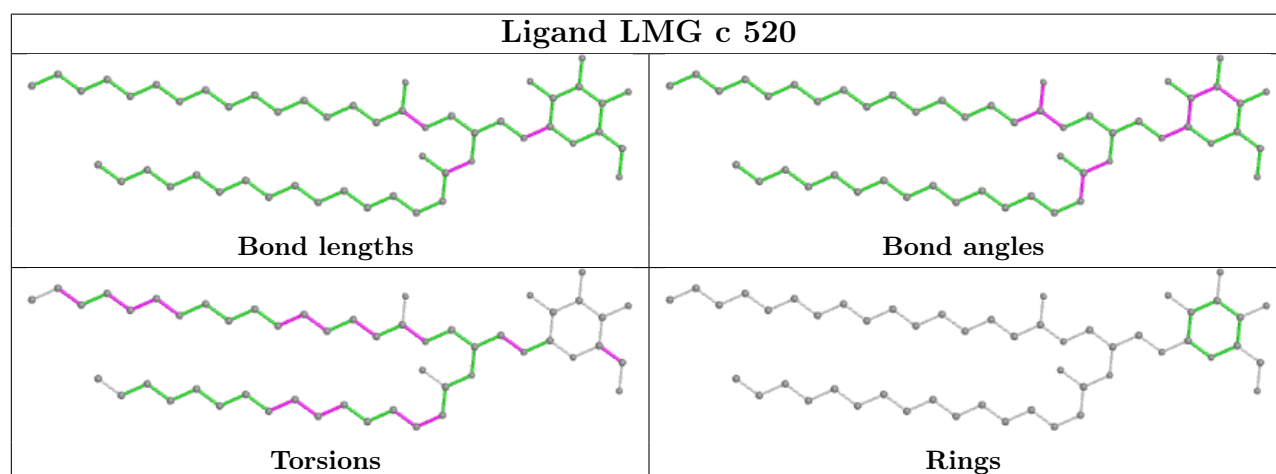
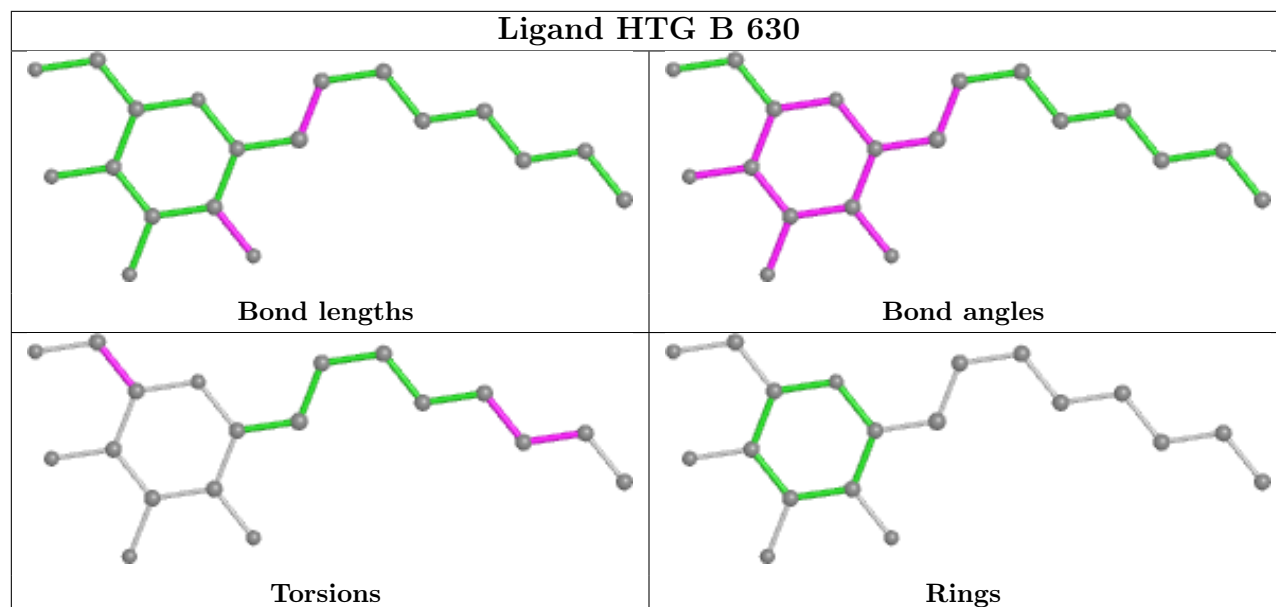
Ligand HEM e 107

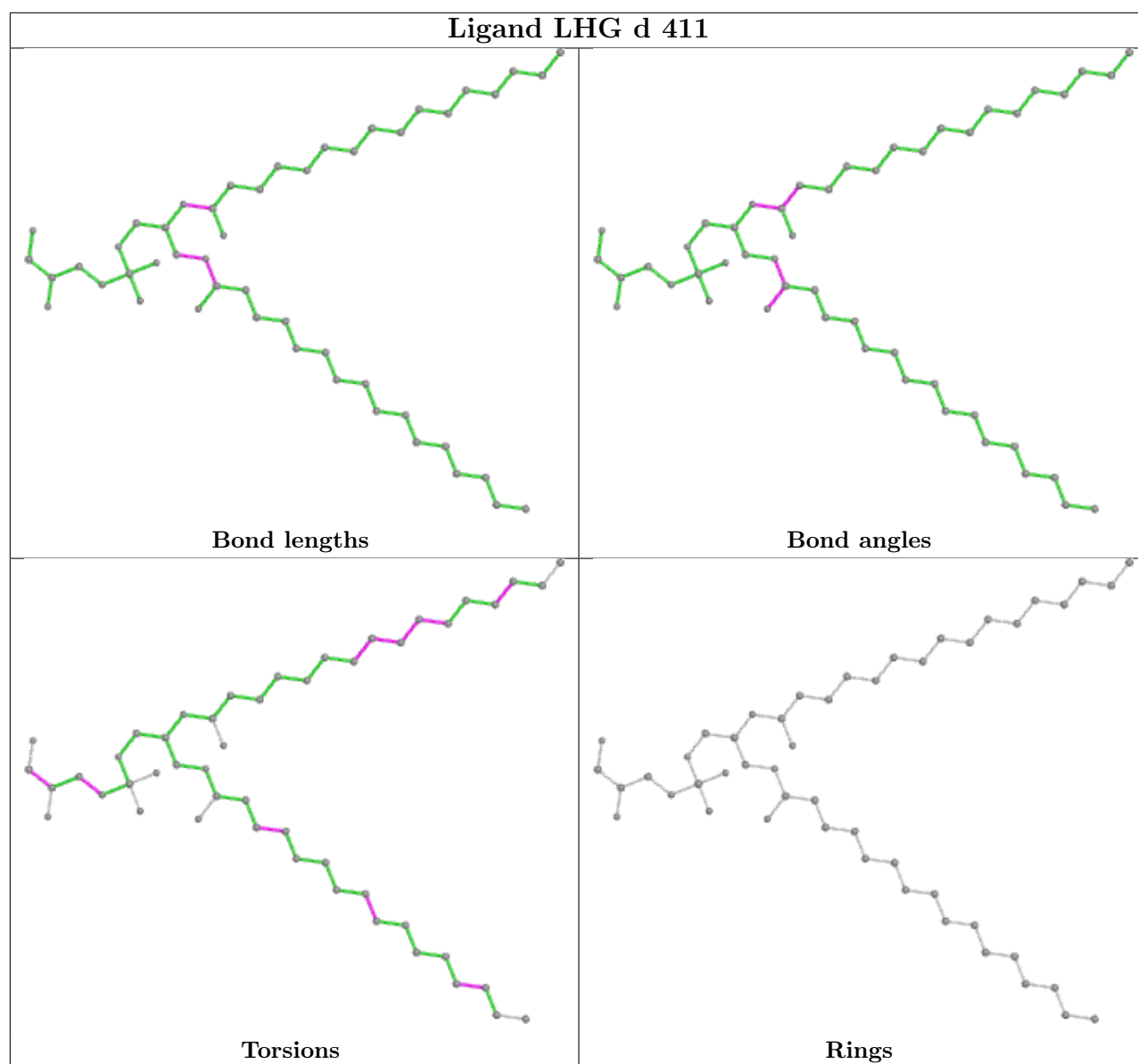


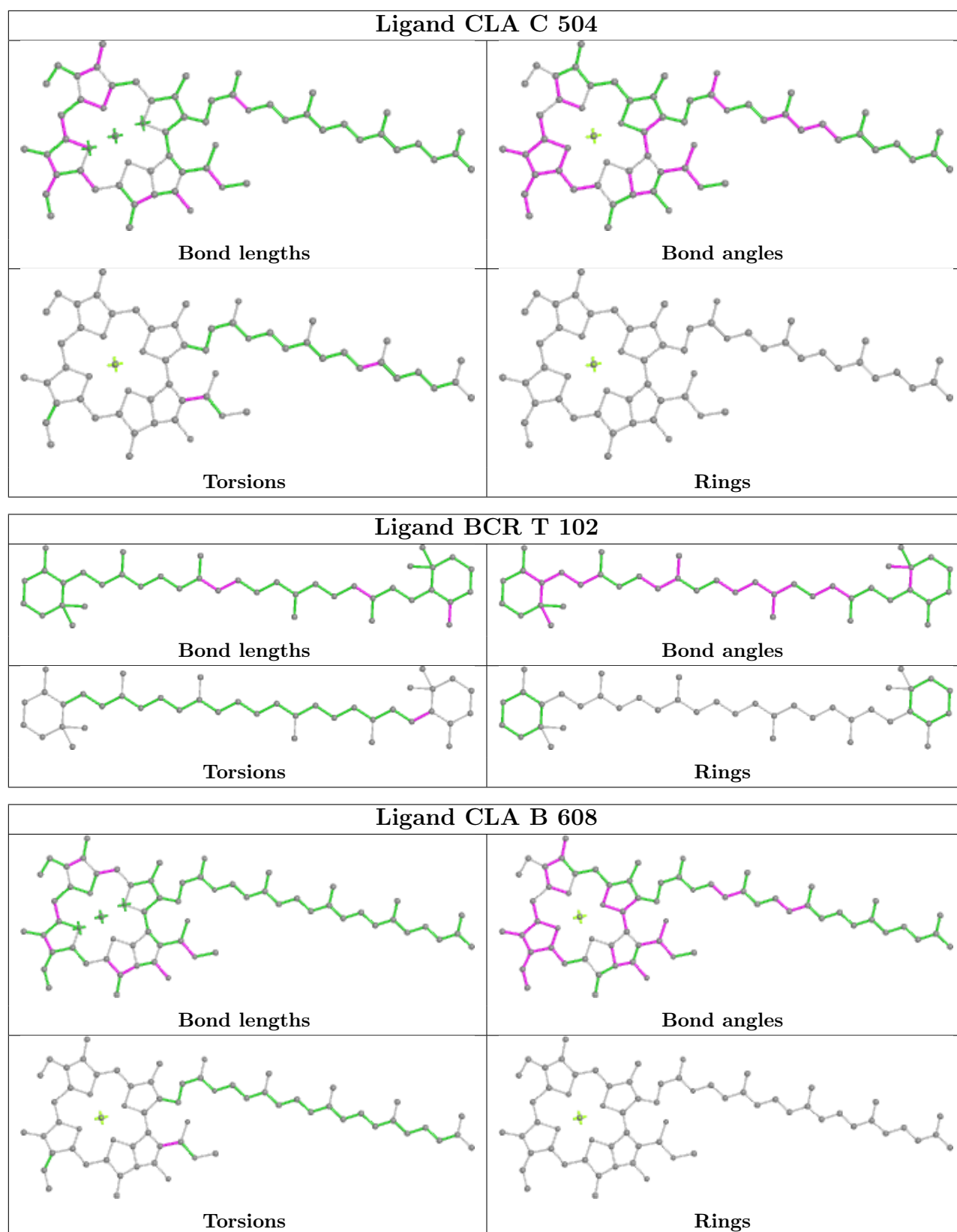
Ligand BCR H 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

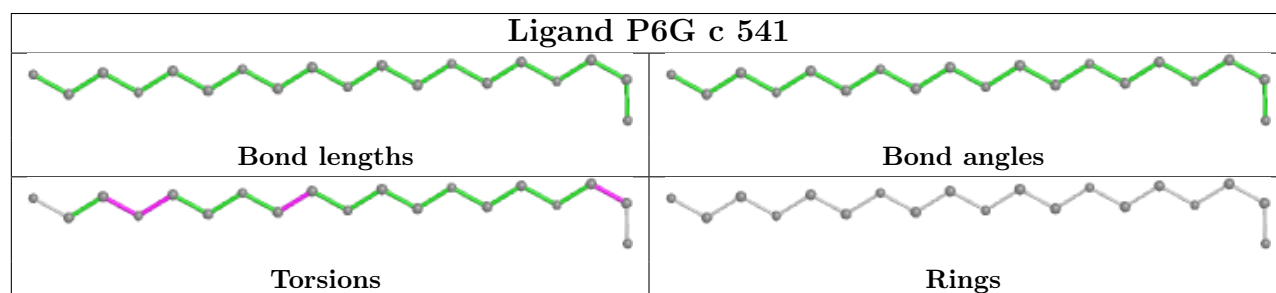
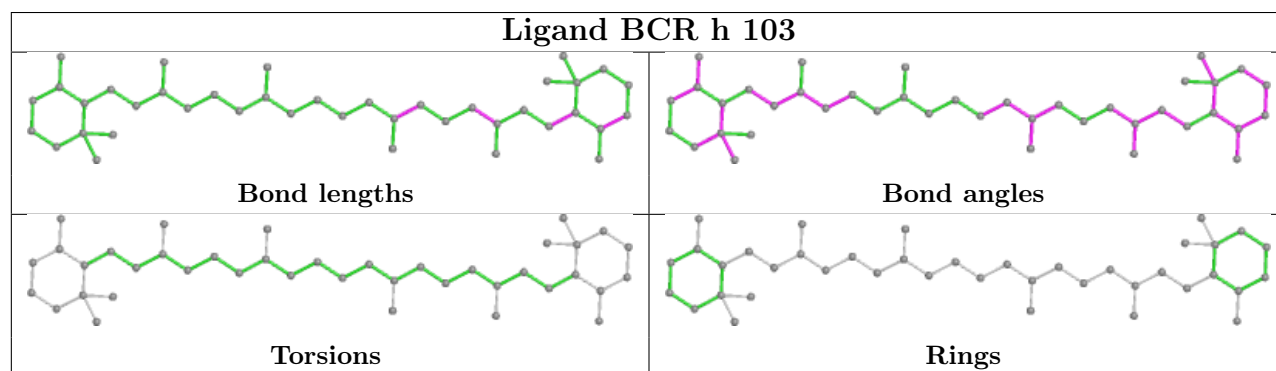
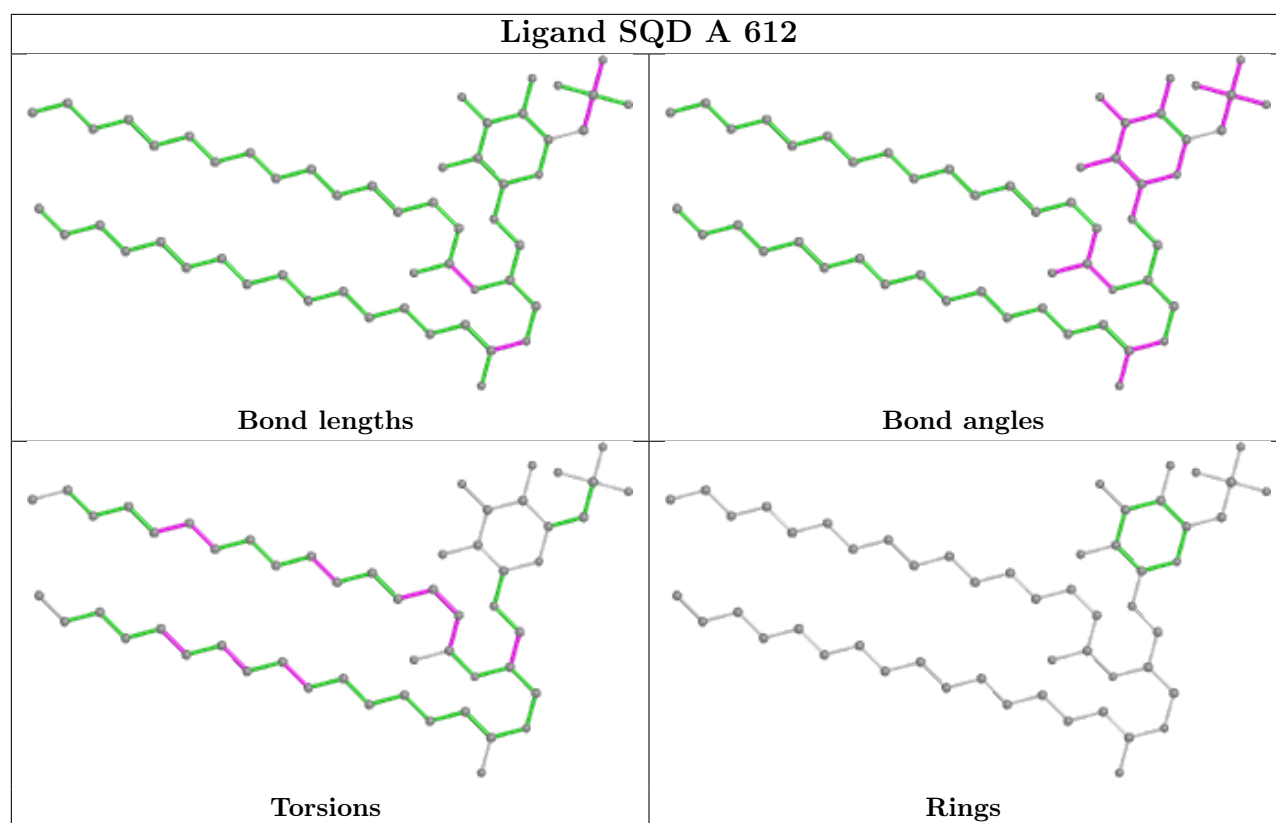
Ligand P6G A 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 509	
	
Bond lengths	Bond angles
	
Torsions	Rings

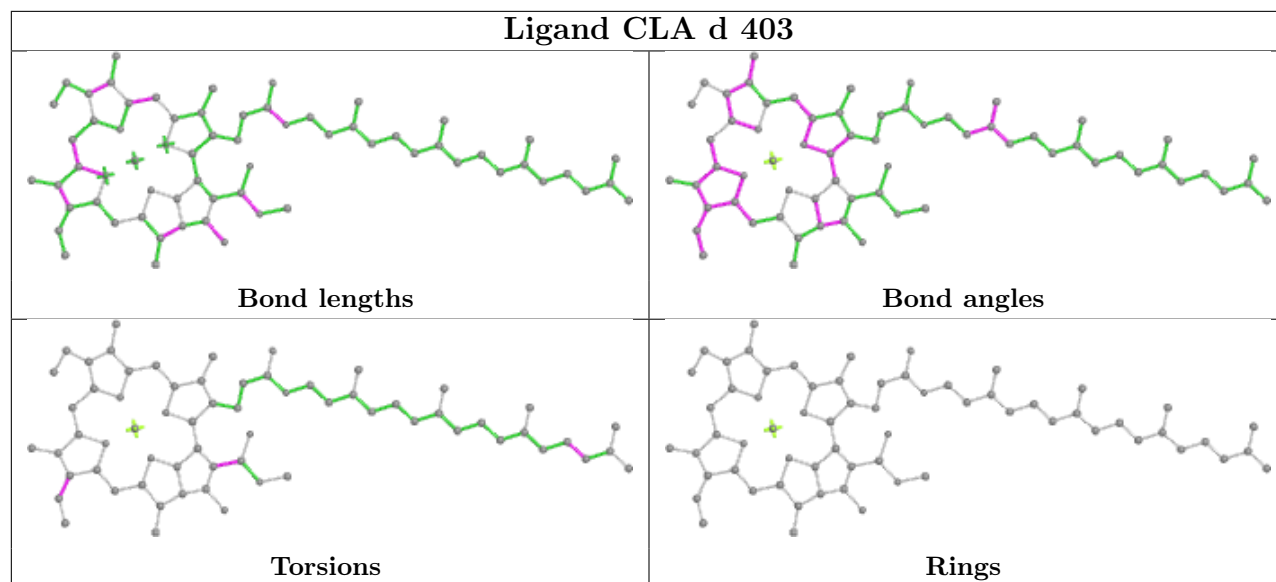




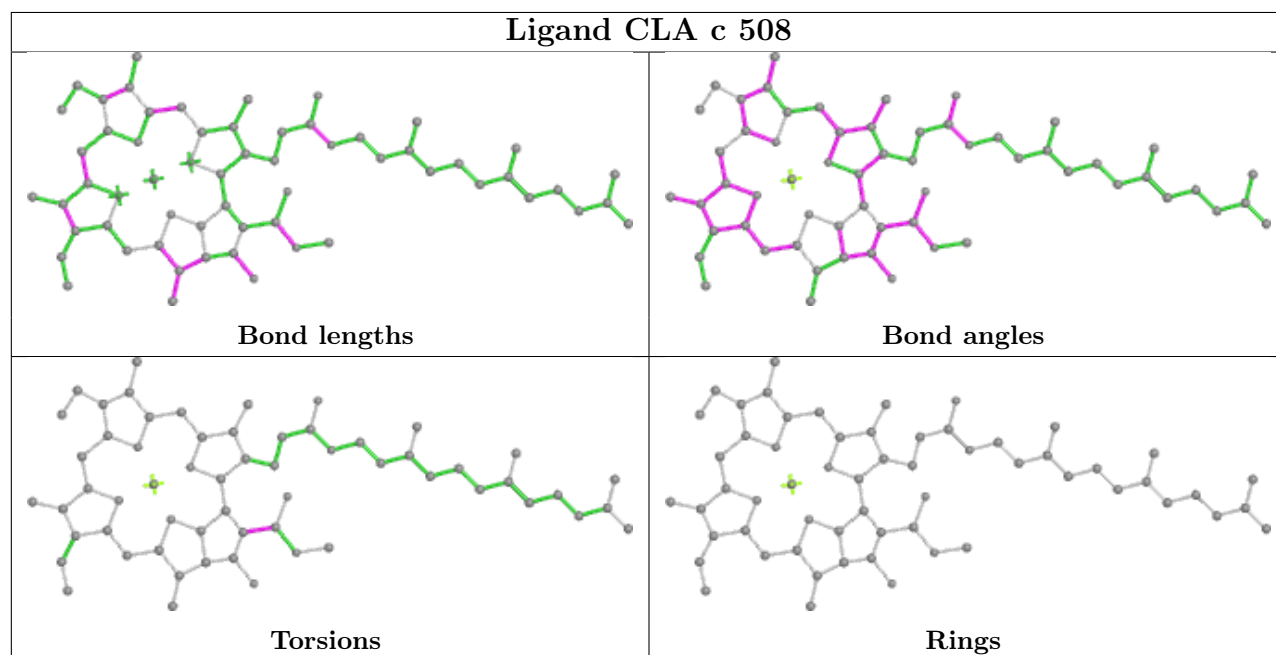




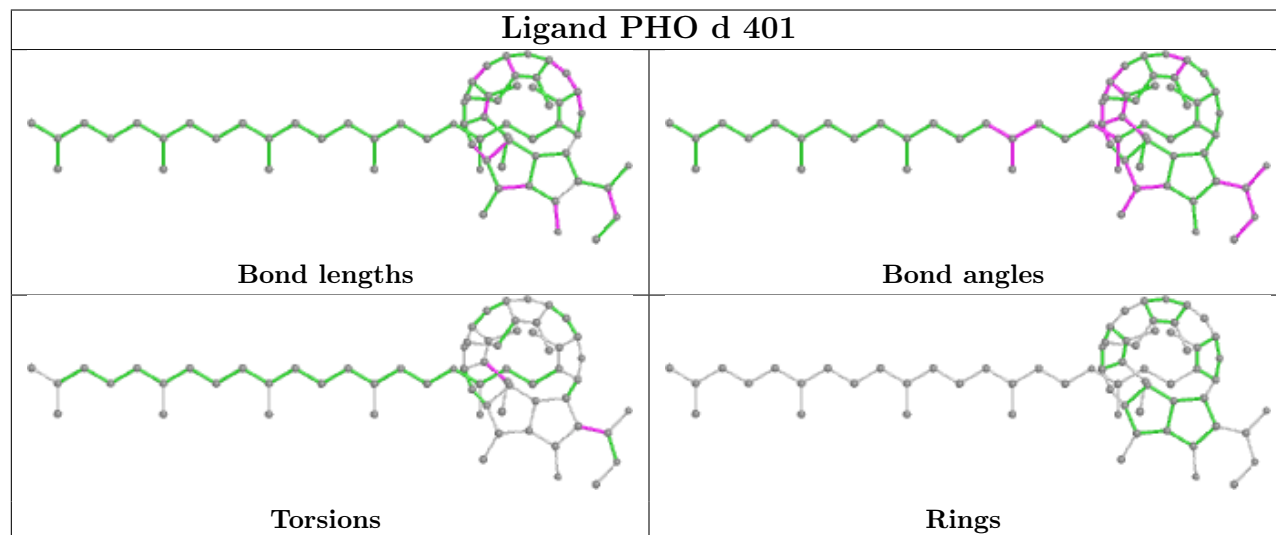
Ligand CLA d 403

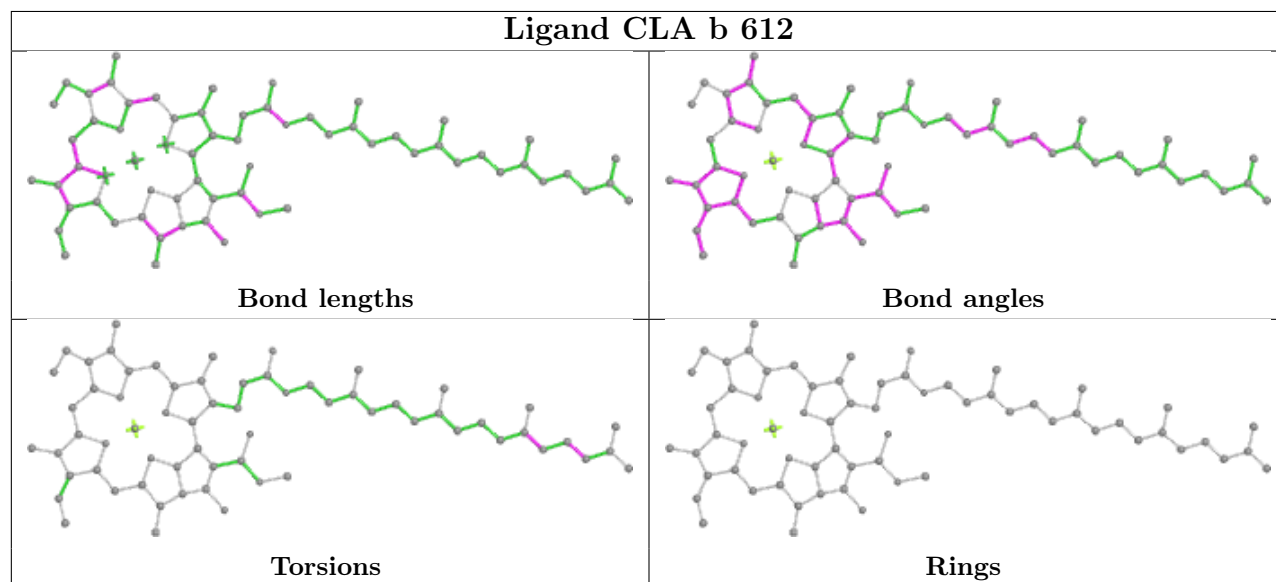
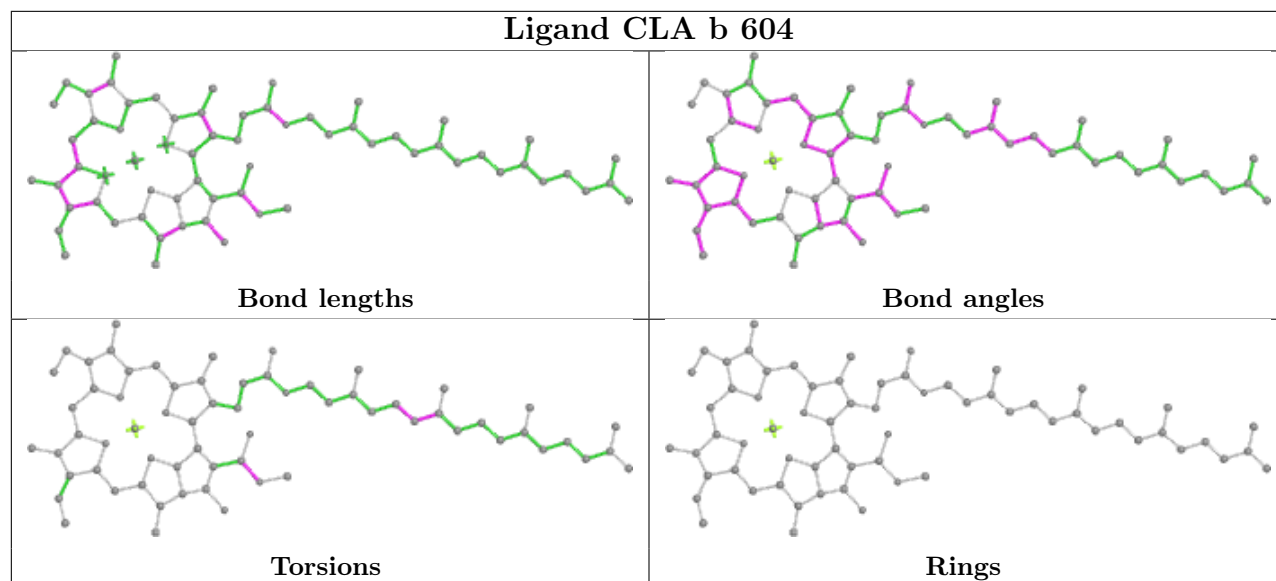
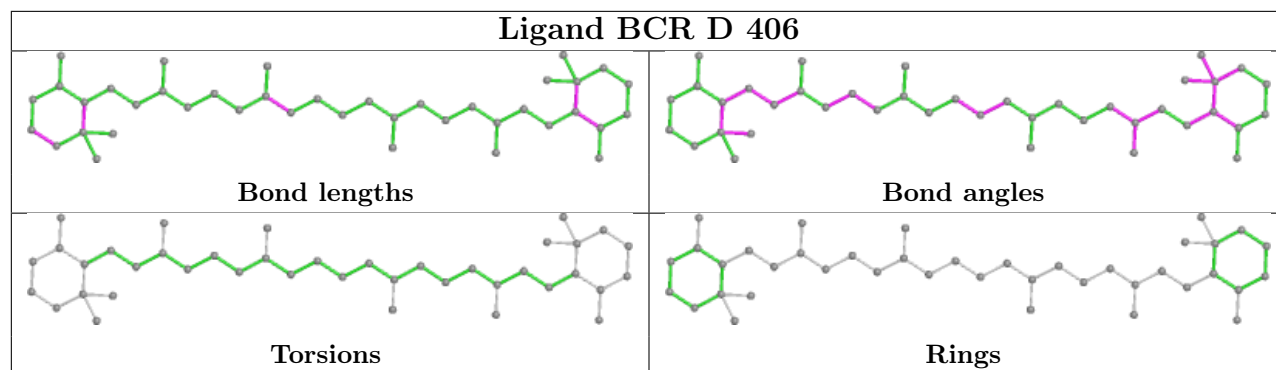


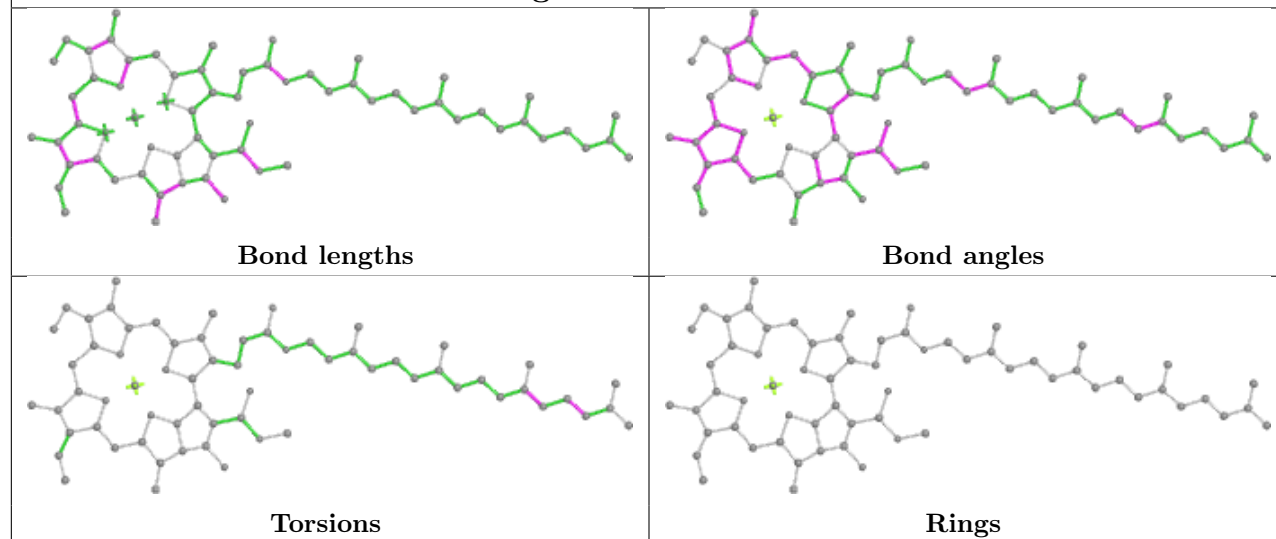
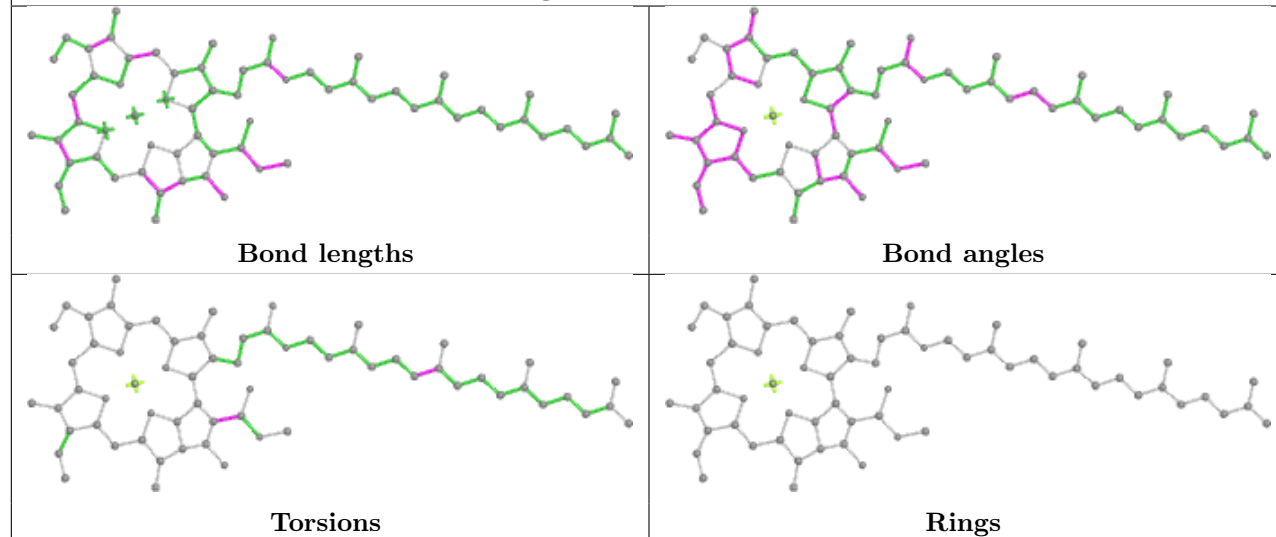
Ligand CLA c 508

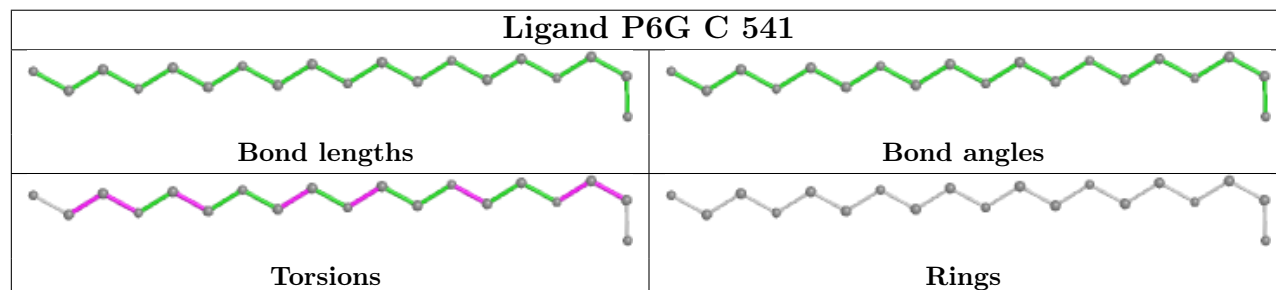
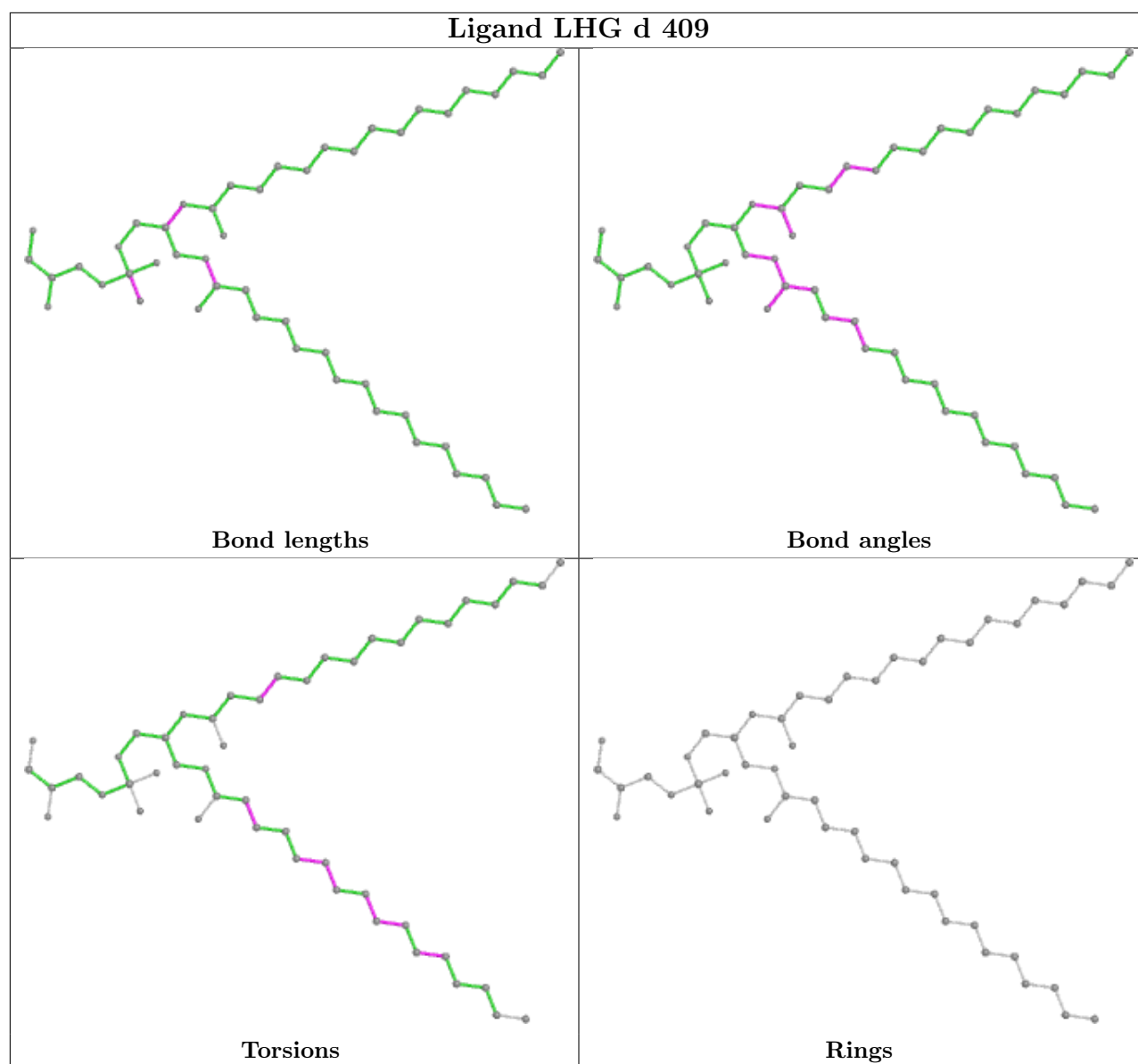


Ligand PHO d 401

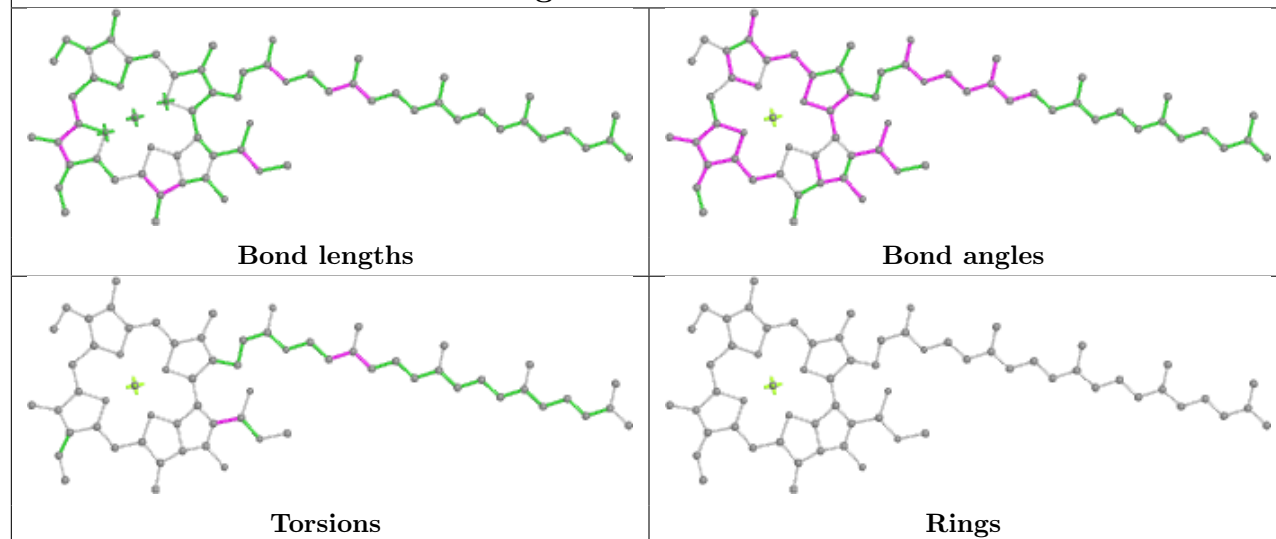




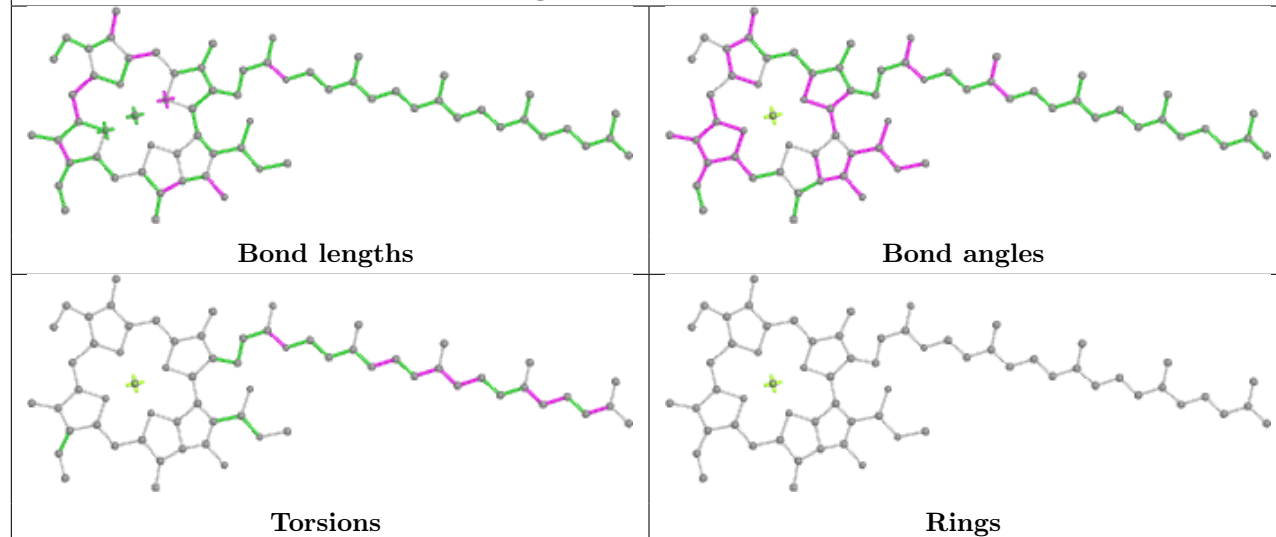
Ligand CLA B 612**Ligand CLA c 503**



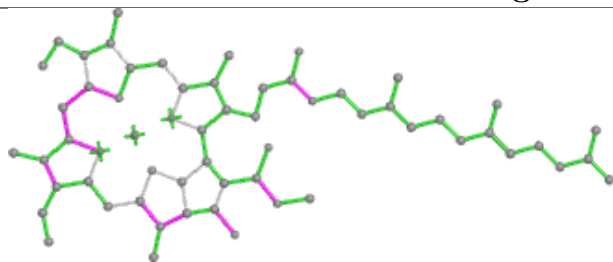
Ligand CLA b 606



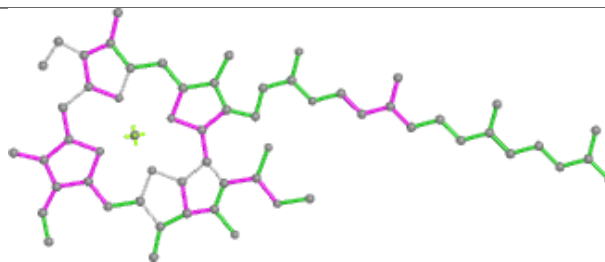
Ligand CLA A 609



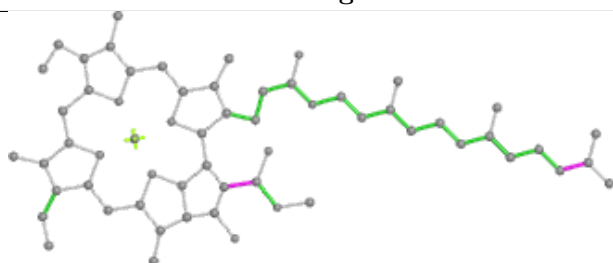
Ligand CLA A 607



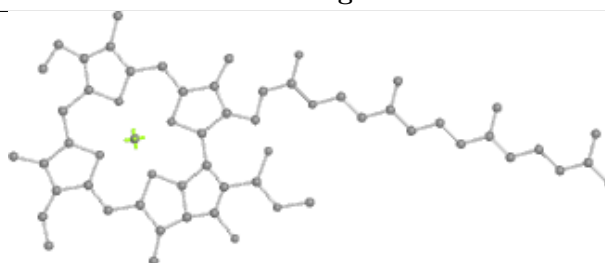
Bond lengths



Bond angles

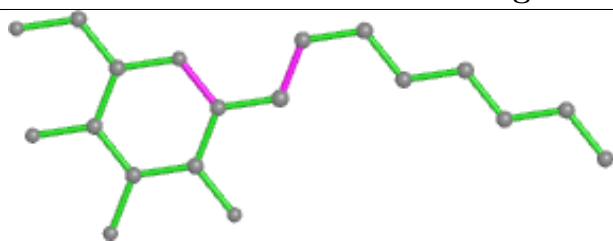


Torsions

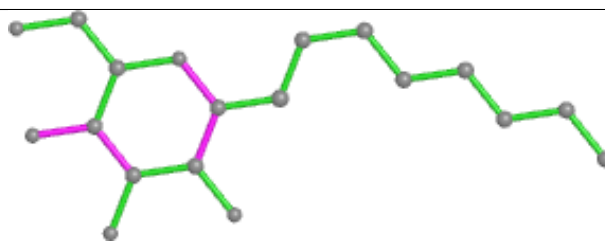


Rings

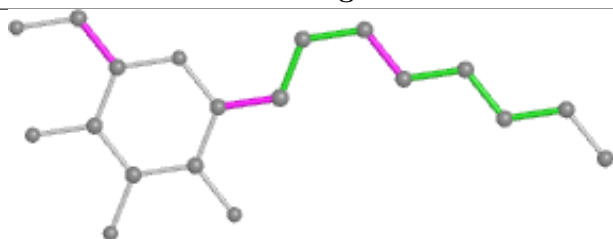
Ligand HTG b 624



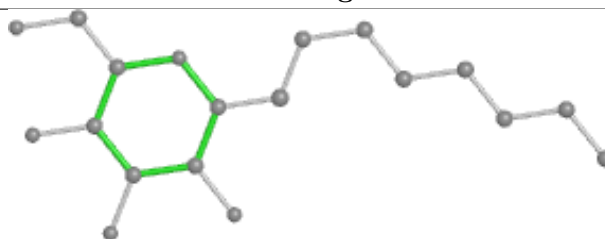
Bond lengths



Bond angles

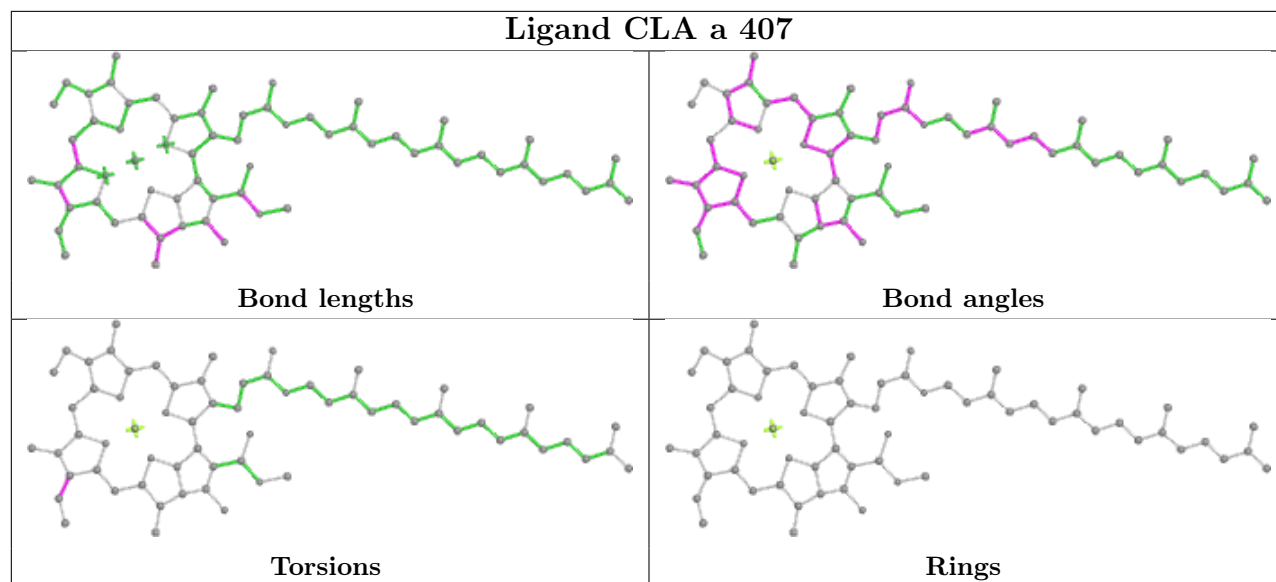


Torsions

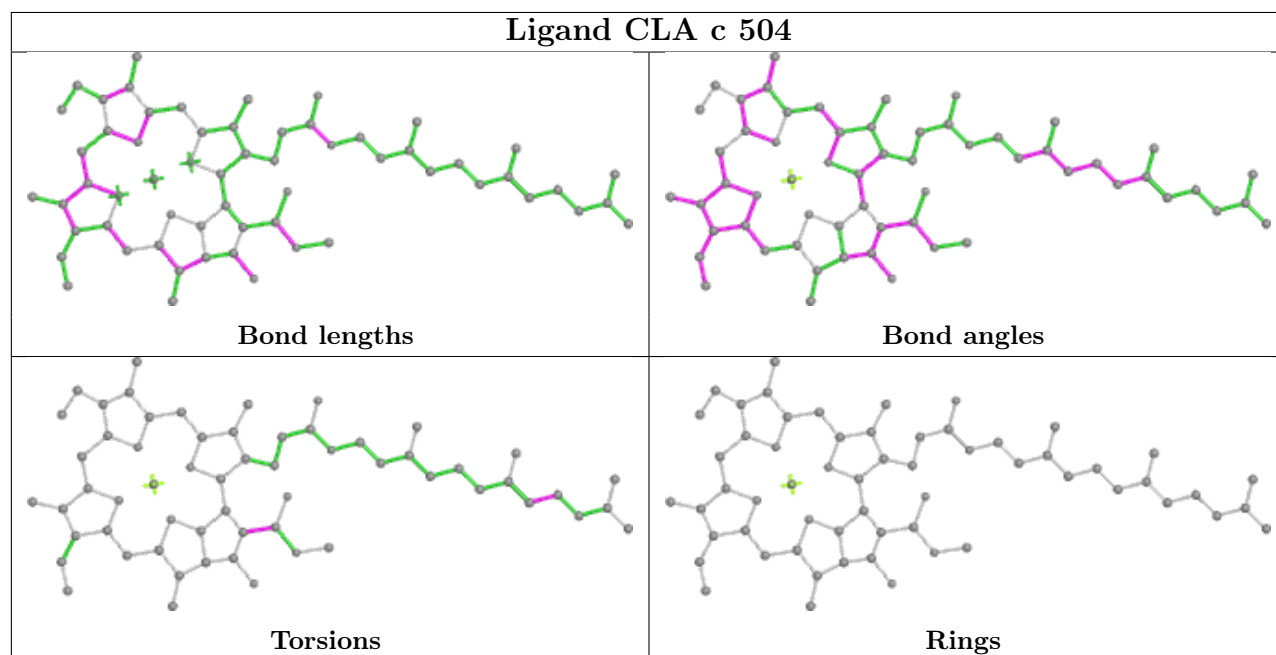


Rings

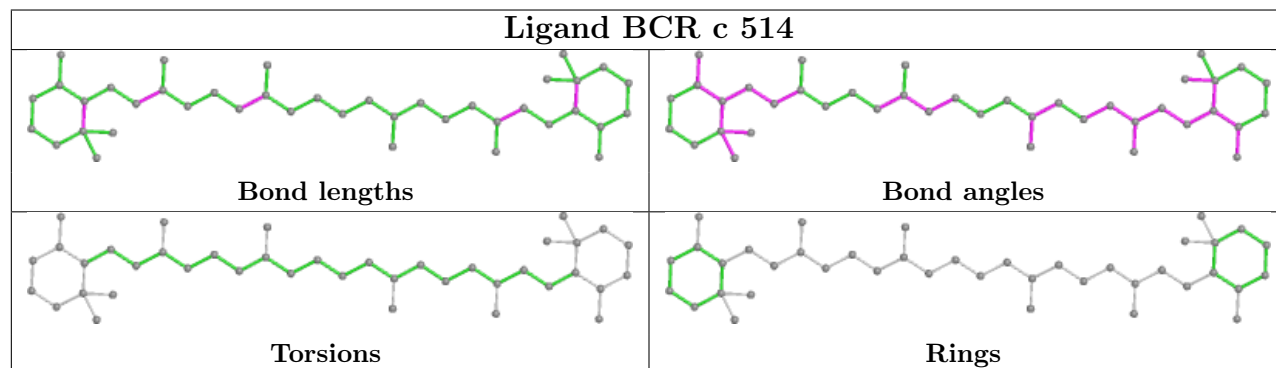
Ligand CLA a 407

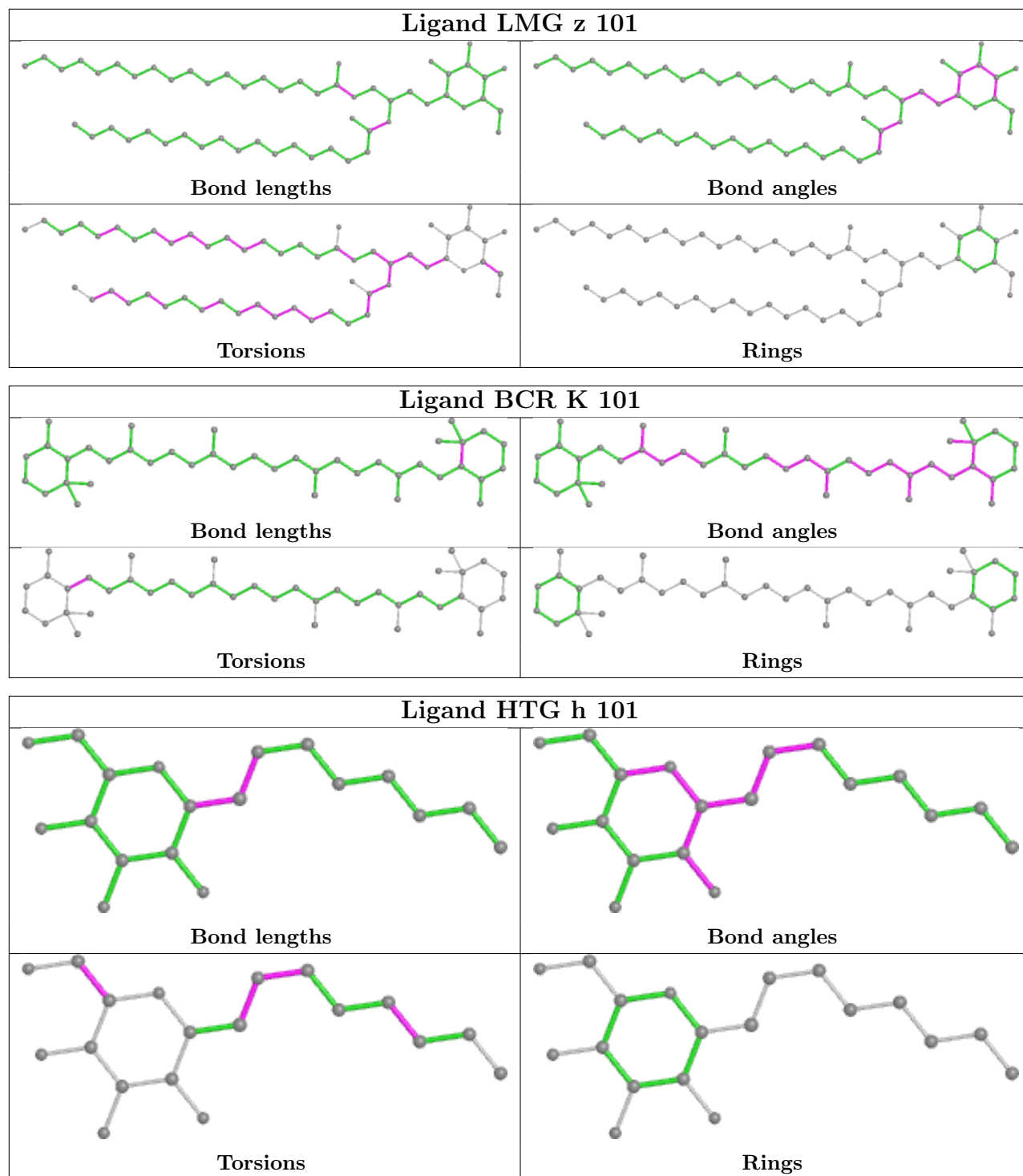


Ligand CLA c 504

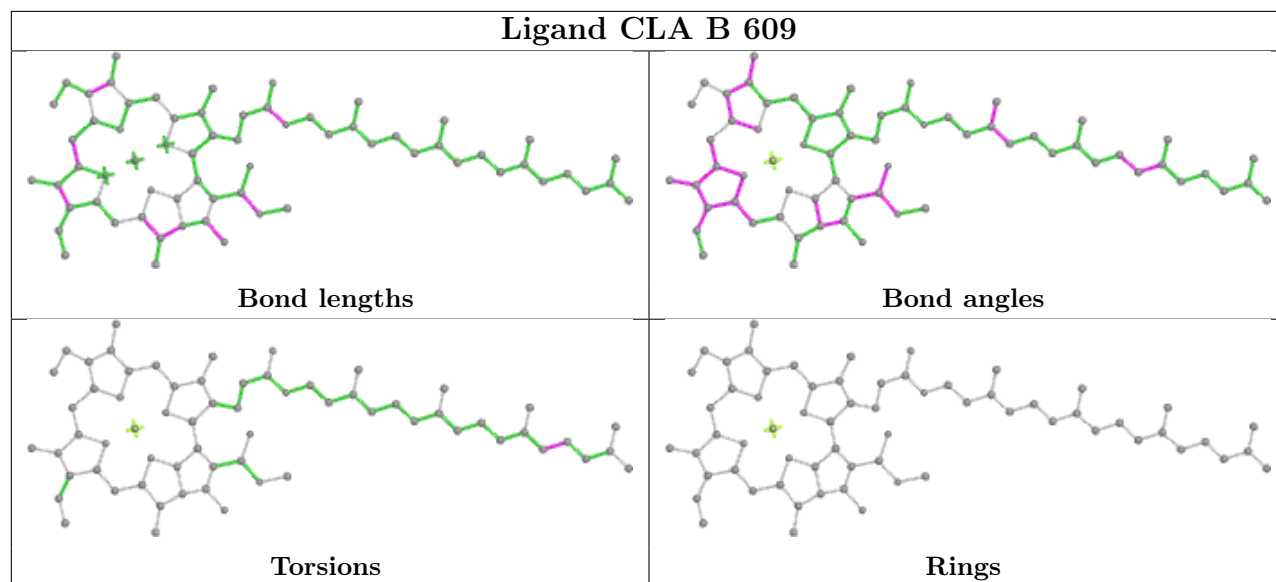


Ligand BCR c 514

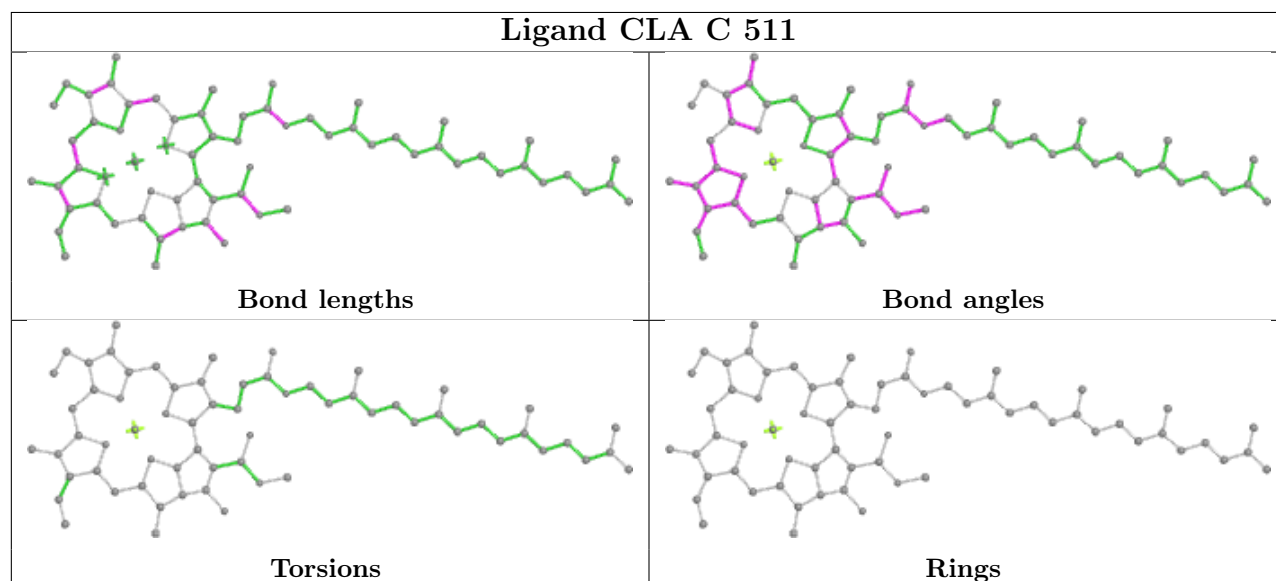




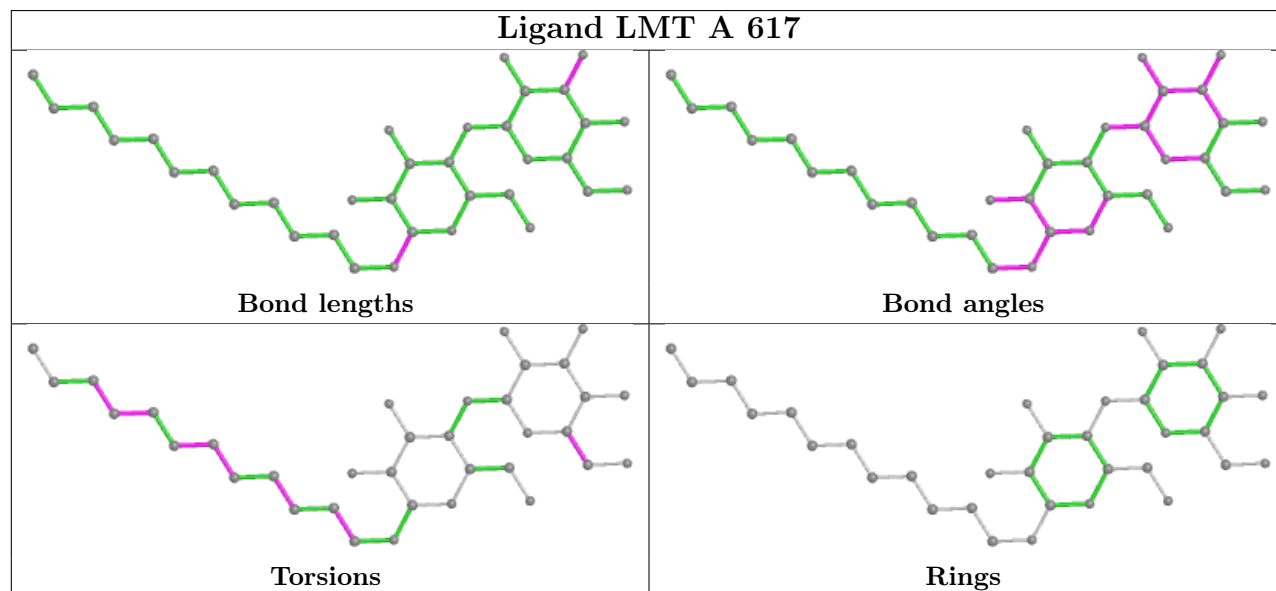
Ligand CLA B 609



Ligand CLA C 511



Ligand LMT A 617



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	334/344 (97%)	-0.86	2 (0%) 89 90	16, 22, 46, 78	0
1	a	334/344 (97%)	-0.83	3 (0%) 84 85	17, 24, 52, 89	0
2	B	504/506 (99%)	-0.63	17 (3%) 45 48	17, 26, 57, 92	0
2	b	506/506 (100%)	-0.49	29 (5%) 23 26	19, 29, 71, 129	0
3	C	451/458 (98%)	-0.75	4 (0%) 84 85	19, 31, 46, 87	0
3	c	458/458 (100%)	-0.62	12 (2%) 56 58	24, 35, 51, 108	0
4	D	341/342 (99%)	-0.88	4 (1%) 79 81	16, 23, 40, 114	0
4	d	341/342 (99%)	-0.82	5 (1%) 73 76	18, 26, 44, 110	0
5	E	81/83 (97%)	-0.23	5 (6%) 20 23	26, 41, 66, 92	0
5	e	81/83 (97%)	0.25	8 (9%) 7 8	32, 46, 75, 118	0
6	F	34/44 (77%)	-0.37	3 (8%) 10 11	26, 33, 63, 82	0
6	f	32/44 (72%)	-0.22	2 (6%) 20 22	30, 38, 78, 117	0
7	H	65/65 (100%)	-0.43	4 (6%) 20 23	23, 33, 47, 123	0
7	h	65/65 (100%)	-0.22	3 (4%) 32 35	26, 38, 56, 116	0
8	I	37/38 (97%)	-0.35	3 (8%) 12 13	28, 35, 75, 91	0
8	i	37/38 (97%)	-0.38	2 (5%) 25 29	27, 34, 67, 89	0
9	J	39/40 (97%)	-0.30	6 (15%) 2 2	24, 36, 108, 130	0
9	j	39/40 (97%)	-0.26	5 (12%) 3 4	29, 43, 75, 89	0
10	K	37/37 (100%)	-0.54	0 100 100	31, 37, 56, 70	0
10	k	37/37 (100%)	-0.48	0 100 100	36, 44, 64, 75	0
11	L	37/37 (100%)	-0.45	3 (8%) 12 13	15, 21, 70, 92	0
11	l	37/37 (100%)	-0.33	4 (10%) 5 6	18, 22, 70, 95	0
12	M	33/36 (91%)	-0.59	2 (6%) 21 24	19, 22, 44, 88	0
12	m	34/36 (94%)	-0.49	3 (8%) 10 11	20, 24, 75, 98	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	245/245 (100%)	-0.11	15 (6%) 21 24	18, 33, 69, 128	0
13	o	245/245 (100%)	0.04	25 (10%) 6 8	21, 34, 84, 136	0
14	T	29/32 (90%)	-0.66	2 (6%) 16 19	18, 23, 47, 101	0
14	t	29/32 (90%)	-0.81	1 (3%) 45 48	19, 23, 44, 81	0
15	U	97/104 (93%)	-0.53	2 (2%) 63 66	21, 31, 58, 95	0
15	u	97/104 (93%)	-0.58	1 (1%) 82 84	24, 31, 47, 84	0
16	V	137/137 (100%)	-0.76	0 100 100	20, 29, 46, 66	0
16	v	137/137 (100%)	-0.49	4 (2%) 51 54	26, 38, 58, 73	0
17	Y	29/30 (96%)	1.34	6 (20%) 1 1	36, 49, 76, 109	0
17	y	29/30 (96%)	1.18	6 (20%) 1 1	46, 60, 81, 92	0
18	X	40/41 (97%)	0.24	5 (12%) 3 4	30, 40, 100, 118	0
18	x	40/41 (97%)	0.28	6 (15%) 2 2	36, 43, 112, 132	0
19	Z	62/62 (100%)	0.22	8 (12%) 3 3	37, 47, 86, 94	0
19	z	62/62 (100%)	0.82	14 (22%) 0 0	50, 62, 101, 117	0
All	All	5272/5362 (98%)	-0.52	224 (4%) 36 39	15, 30, 65, 136	0

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	o	2	ALA	13.7
7	h	66	GLY	13.4
13	o	3	ALA	13.1
13	O	2	ALA	12.7
17	Y	19	ILE	12.0
13	O	3	ALA	10.6
17	Y	18	VAL	10.4
18	x	40	SER	9.4
18	X	1	MET	9.2
12	m	35	SER	9.0
17	y	18	VAL	8.1
19	z	3	ILE	8.0
7	H	65	LEU	7.9
2	b	507	ASP	7.9
17	y	19	ILE	7.8
18	X	40	SER	7.8
18	x	1	MET	7.8
13	O	58	ASN	7.7

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Mol	Chain	Res	Type	RSRZ
3	c	17	ALA	7.6
5	e	5	THR	7.5
5	e	4	THR	7.3
2	b	495	PHE	7.2
13	o	25	THR	6.9
19	Z	3	ILE	6.8
7	h	65	LEU	6.7
2	b	506	SER	6.6
6	f	14	PRO	6.6
13	o	60	ARG	6.6
3	c	18	ALA	6.5
2	b	505	ARG	6.4
4	d	11	GLU	6.4
14	T	30	THR	6.4
9	J	2	GLU	6.2
2	b	485	GLU	6.2
5	E	84	LYS	6.0
18	X	38	GLN	6.0
2	b	488	PRO	6.0
19	z	60	PHE	5.9
12	M	34	LYS	5.9
13	o	246	ALA	5.8
17	y	20	ALA	5.8
2	B	485	GLU	5.7
13	O	62	GLU	5.7
17	Y	22	LEU	5.5
13	o	62	GLU	5.5
2	b	502	VAL	5.5
19	z	62	VAL	5.5
13	O	56	PRO	5.3
12	M	33	GLN	5.3
19	z	31	GLN	5.3
13	o	4	THR	5.3
19	Z	31	GLN	5.2
2	b	503	THR	5.2
18	x	38	GLN	5.2
13	O	4	THR	5.1
13	o	35	SER	5.1
2	b	489	GLU	5.1
5	e	84	LYS	5.0
11	L	1	MET	5.0
5	E	4	THR	4.9

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Mol	Chain	Res	Type	RSRZ
3	C	23	ALA	4.8
19	z	1	MET	4.8
13	O	61	GLN	4.7
18	X	2	THR	4.6
17	Y	20	ALA	4.6
19	z	32	ASP	4.6
9	j	6	GLY	4.6
11	L	2	GLU	4.6
2	B	495	PHE	4.5
2	B	494	GLY	4.5
11	l	3	PRO	4.5
1	a	11	ALA	4.5
11	l	1	MET	4.5
5	e	6	GLY	4.5
4	D	11	GLU	4.4
2	b	127	ARG	4.4
2	B	502	VAL	4.4
13	o	59	LYS	4.3
5	e	61	ARG	4.3
19	z	4	LEU	4.3
2	b	486	LEU	4.3
13	o	27	ARG	4.3
12	m	34	LYS	4.2
3	c	21	ILE	4.2
11	l	2	GLU	4.2
16	v	15	GLU	4.2
1	A	11	ALA	4.2
18	x	2	THR	4.1
3	c	19	ASN	4.1
6	f	16	PHE	4.1
17	Y	43	ARG	4.1
15	u	8	GLU	4.1
9	J	6	GLY	4.1
4	D	238	THR	4.1
13	O	25	THR	4.1
2	b	484	PRO	4.1
4	d	238	THR	4.0
15	U	8	GLU	4.0
7	H	64	ALA	4.0
19	Z	30	PRO	3.9
19	z	34	ASP	3.9
5	e	25	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
13	o	36	GLN	3.9
3	C	24	THR	3.9
13	O	60	ARG	3.9
17	y	22	LEU	3.9
13	O	89	SER	3.9
2	b	487	SER	3.9
4	D	12	ARG	3.8
8	i	36	ASP	3.8
8	I	36	ASP	3.7
19	Z	32	ASP	3.6
13	o	26	ALA	3.6
13	o	61	GLN	3.6
9	J	3	SER	3.6
6	F	12	SER	3.6
13	o	58	ASN	3.6
17	y	41	VAL	3.6
2	B	505	ARG	3.5
13	o	23	ASP	3.5
2	b	86	ILE	3.5
3	c	207	ARG	3.5
2	b	85	GLY	3.5
8	I	34	ARG	3.5
4	D	240	ALA	3.4
12	m	33	GLN	3.4
7	H	66	GLY	3.4
9	j	5	GLY	3.4
13	O	207	ARG	3.4
2	B	503	THR	3.3
18	x	37	VAL	3.3
7	h	64	ALA	3.3
2	B	489	GLU	3.3
17	y	43	ARG	3.3
2	b	494	GLY	3.3
9	j	4	GLU	3.3
19	z	61	VAL	3.3
1	a	262	TYR	3.3
2	B	487	SER	3.3
13	o	56	PRO	3.3
2	b	496	TYR	3.2
6	F	16	PHE	3.2
6	F	13	TYR	3.2
14	t	30	THR	3.1

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Mol	Chain	Res	Type	RSRZ
19	Z	35	ARG	3.1
2	b	293	ALA	3.1
16	v	106	ASN	3.1
11	L	3	PRO	3.1
9	J	4	GLU	3.0
4	d	237	PRO	3.0
9	J	5	GLY	2.9
2	b	294	SER	2.9
19	z	35	ARG	2.9
9	J	7[A]	ARG	2.9
18	x	39	ARG	2.9
2	b	497	GLN	2.8
2	B	492	GLU	2.8
2	b	492	GLU	2.8
4	d	236	ASN	2.8
13	o	24	ASP	2.8
19	z	30	PRO	2.8
13	O	59	LYS	2.8
19	z	33	TRP	2.7
3	C	191	PRO	2.7
13	O	24	ASP	2.7
13	o	207	ARG	2.7
2	b	295	GLY	2.7
19	z	7	LEU	2.6
13	o	34	SER	2.6
13	o	211	ILE	2.6
5	E	6	GLY	2.6
2	B	295	GLY	2.6
19	z	42	LEU	2.6
13	o	132	ASN	2.6
5	E	81	GLU	2.5
2	b	504	THR	2.5
19	Z	1	MET	2.5
2	b	84	THR	2.5
2	B	488	PRO	2.5
3	c	191	PRO	2.5
19	Z	34	ASP	2.5
3	c	106	VAL	2.4
3	c	22	PHE	2.4
2	B	484	PRO	2.4
19	Z	38	GLN	2.4
15	U	65	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLY	2.4
1	a	12	ASN	2.4
2	B	501	ASP	2.4
13	o	57	LYS	2.4
2	B	504	THR	2.4
2	b	128	THR	2.4
8	i	34	ARG	2.3
13	O	63	ALA	2.3
13	O	23	ASP	2.3
1	A	243	GLU	2.3
2	b	499	VAL	2.3
16	v	17	LYS	2.3
2	b	374	ASN	2.3
2	b	373	LYS	2.3
9	j	7	ARG	2.3
5	e	62[A]	SER	2.3
3	C	207	ARG	2.3
5	e	81	GLU	2.2
2	B	293	ALA	2.2
8	I	38	GLU	2.2
13	o	33	ASP	2.2
4	d	240	ALA	2.2
16	v	16	GLY	2.2
3	c	16	GLU	2.2
9	j	2	GLU	2.2
13	o	89	SER	2.2
17	Y	21	GLN	2.2
2	b	130[A]	GLU	2.1
3	c	20	SER	2.1
7	H	6	TRP	2.1
3	c	142	GLU	2.1
2	B	486	LEU	2.1
13	o	28	GLY	2.1
5	E	21	VAL	2.0
14	T	29	ILE	2.0
3	c	462[A]	GLU	2.0
11	l	5	PRO	2.0
18	X	3	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	FME	m	1[A]	10/11	0.97	0.10	24,30,61,84	7
12	FME	m	1[B]	10/11	0.97	0.10	30,33,55,66	7
12	FME	M	1	10/11	0.98	0.07	27,32,64,68	0
4	MHS	D	336	11/12	0.98	0.07	23,28,37,38	0
8	FME	I	1	10/11	0.98	0.05	26,32,40,44	0
14	FME	t	1[A]	10/11	0.98	0.07	20,24,39,42	7
14	FME	t	1[B]	10/11	0.98	0.07	20,24,31,36	7
14	FME	T	1[A]	10/11	0.99	0.07	21,25,47,47	7
14	FME	T	1[B]	10/11	0.99	0.07	21,25,32,35	7
4	MHS	d	336	11/12	0.99	0.05	27,32,44,44	0
8	FME	i	1	10/11	0.99	0.06	30,33,36,37	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	GOL	O	307	6/6	0.35	0.78	116,117,120,123	0
31	LMT	Y	101	35/35	0.38	0.39	61,118,170,188	0
31	LMT	j	103	35/35	0.40	0.44	68,114,162,168	0
39	1PE	B	653	16/16	0.41	0.61	103,121,137,148	0
34	PGE	f	105	10/10	0.43	0.55	91,98,114,127	0
38	HTG	C	529	19/19	0.46	0.27	70,102,136,144	0
28	SQD	h	105	54/54	0.51	0.45	76,100,195,214	0
31	LMT	C	533	35/35	0.52	0.56	72,121,170,191	0
34	PGE	i	106	10/10	0.52	0.52	78,95,100,103	0
34	PGE	c	536	10/10	0.54	0.58	87,105,124,125	0
30	GOL	v	205	6/6	0.54	0.70	102,122,135,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	PG4	e	103	13/13	0.54	0.40	72,107,125,136	0
34	PGE	E	107	10/10	0.54	0.59	73,106,142,143	0
34	PGE	E	108	10/10	0.54	0.41	52,65,68,73	10
34	PGE	b	646	10/10	0.56	0.46	70,102,120,121	0
33	PG4	C	534	13/13	0.56	0.54	81,103,119,119	0
35	P6G	D	418	19/19	0.59	0.39	68,99,126,131	0
34	PGE	J	106	10/10	0.61	0.39	85,121,129,138	0
34	PGE	o	307	10/10	0.62	0.55	90,112,130,142	0
34	PGE	D	415	10/10	0.63	0.60	86,105,110,122	0
36	EDO	E	111	4/4	0.63	0.24	66,83,90,97	0
38	HTG	H	101	19/19	0.65	0.24	50,94,122,122	0
34	PGE	h	110	10/10	0.65	0.26	71,99,111,117	0
34	PGE	c	540	10/10	0.66	0.42	82,92,110,113	0
33	PG4	X	103	13/13	0.66	0.38	78,99,111,115	0
39	1PE	j	107	16/16	0.66	0.29	74,106,155,159	0
38	HTG	h	101	19/19	0.67	0.28	62,86,123,141	0
33	PG4	B	636	13/13	0.67	0.35	71,98,116,121	0
33	PG4	c	533	13/13	0.67	0.38	77,90,105,109	0
40	DGD	D	408	66/66	0.67	0.29	56,88,142,175	0
34	PGE	J	107	10/10	0.68	0.26	87,137,168,170	0
34	PGE	E	105	10/10	0.68	0.60	90,96,116,118	0
34	PGE	B	650	10/10	0.68	0.51	88,109,126,128	0
38	HTG	c	530	19/19	0.68	0.31	66,104,128,145	0
38	HTG	c	531	19/19	0.69	0.31	59,99,122,124	0
34	PGE	b	644	10/10	0.69	0.47	83,100,113,125	0
30	GOL	y	101	6/6	0.69	0.30	82,90,98,101	0
39	1PE	V	217	16/16	0.69	0.55	63,93,120,133	0
35	P6G	C	541	19/19	0.69	0.49	79,103,127,142	0
33	PG4	J	104	13/13	0.69	0.36	74,82,107,108	0
30	GOL	o	303	6/6	0.70	0.47	79,96,110,126	0
36	EDO	V	218	4/4	0.70	0.46	87,88,88,96	0
33	PG4	J	105	13/13	0.70	0.37	75,88,110,115	0
38	HTG	C	530	19/19	0.70	0.48	98,124,143,150	0
34	PGE	E	106	10/10	0.70	0.35	85,95,111,116	0
34	PGE	b	647	10/10	0.70	0.59	77,97,109,109	0
33	PG4	b	637	13/13	0.71	0.52	74,97,124,130	0
33	PG4	K	102	13/13	0.71	0.25	56,70,102,109	0
33	PG4	C	536	13/13	0.71	0.24	66,72,93,103	0
34	PGE	B	646	10/10	0.71	0.45	83,95,114,119	0
33	PG4	b	634	13/13	0.71	0.29	78,90,111,123	0
31	LMT	J	103	35/35	0.72	0.27	47,78,115,134	0
33	PG4	B	640	13/13	0.72	0.21	66,86,95,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
31	LMT	u	203	35/35	0.72	0.39	42,77,115,137	0
38	HTG	C	532	19/19	0.72	0.32	57,85,128,156	0
34	PGE	h	108	10/10	0.73	0.31	70,75,101,105	0
29	LMG	d	412	55/55	0.73	0.25	47,77,119,137	0
38	HTG	C	531	19/19	0.73	0.44	72,109,139,142	0
33	PG4	H	106	13/13	0.74	0.31	38,53,67,74	13
33	PG4	B	643	13/13	0.74	0.45	75,92,114,118	0
38	HTG	B	624	19/19	0.74	0.28	47,103,125,143	0
33	PG4	E	103	13/13	0.74	0.24	59,76,89,105	0
35	P6G	I	106	19/19	0.74	0.26	56,81,119,121	0
36	EDO	A	625	4/4	0.75	0.16	70,71,80,80	0
33	PG4	e	104	13/13	0.75	0.50	78,94,120,120	0
34	PGE	H	111	10/10	0.75	0.36	82,100,121,127	0
34	PGE	c	539	10/10	0.75	0.48	80,90,104,104	0
33	PG4	B	642	13/13	0.76	0.47	66,86,115,120	0
38	HTG	a	418	19/19	0.76	0.28	53,84,123,124	0
36	EDO	c	542	4/4	0.76	0.68	88,91,102,107	0
36	EDO	o	311	4/4	0.76	0.35	81,83,83,86	0
33	PG4	j	104	13/13	0.76	0.24	78,97,113,116	0
33	PG4	C	538	13/13	0.76	0.34	65,93,115,123	0
34	PGE	b	639	10/10	0.76	0.44	79,97,111,119	0
36	EDO	D	419	4/4	0.76	0.33	66,70,78,97	0
39	1PE	x	104	16/16	0.76	0.35	85,105,130,136	0
34	PGE	H	110	10/10	0.76	0.53	91,103,116,118	0
44	2PE	V	216	28/28	0.76	0.36	44,91,110,123	0
28	SQD	A	622	54/54	0.77	0.27	63,85,136,187	0
34	PGE	H	109	10/10	0.77	0.38	84,95,102,105	0
38	HTG	b	624	19/19	0.77	0.23	54,91,117,133	0
34	PGE	O	309	10/10	0.77	0.48	62,86,111,111	0
34	PGE	V	215	10/10	0.77	0.50	66,90,103,111	0
36	EDO	B	657	4/4	0.77	0.34	93,95,100,102	0
34	PGE	I	105	10/10	0.78	0.20	60,83,95,99	0
33	PG4	V	212	13/13	0.78	0.29	82,96,120,123	0
36	EDO	X	104	4/4	0.78	0.25	73,80,83,88	0
35	P6G	c	541	19/19	0.78	0.32	43,61,68,72	19
33	PG4	c	535	13/13	0.78	0.35	69,89,109,115	0
34	PGE	b	645	10/10	0.78	0.44	106,110,126,134	0
38	HTG	b	632	19/19	0.78	0.20	49,79,119,135	0
33	PG4	B	637	13/13	0.78	0.18	68,82,106,106	0
33	PG4	E	102	13/13	0.79	0.35	62,81,106,120	0
33	PG4	X	102	13/13	0.79	0.27	77,95,113,114	0
34	PGE	h	109	10/10	0.79	0.49	84,97,111,113	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	EDO	B	656	4/4	0.79	0.43	78,87,100,107	0
30	GOL	e	102	6/6	0.79	0.36	79,91,112,117	0
36	EDO	C	542	4/4	0.79	0.48	77,84,88,96	0
38	HTG	B	631	19/19	0.79	0.21	46,90,129,147	0
40	DGD	d	408	66/66	0.79	0.35	57,89,155,184	0
35	P6G	E	110	19/19	0.79	0.46	49,95,111,122	0
33	PG4	V	211	13/13	0.80	0.38	54,89,114,120	0
28	SQD	a	424	54/54	0.80	0.26	63,83,134,198	0
31	LMT	m	101	35/35	0.80	0.20	45,62,75,92	0
31	LMT	t	103	35/35	0.80	0.22	32,75,110,117	0
35	P6G	b	649	19/19	0.80	0.26	71,103,125,128	0
33	PG4	B	638	13/13	0.80	0.34	66,84,114,130	0
34	PGE	B	649	10/10	0.81	0.24	66,82,101,105	0
34	PGE	Y	102	10/10	0.81	0.17	61,84,103,104	0
33	PG4	B	641	13/13	0.81	0.34	74,97,107,115	0
29	LMG	B	634	55/55	0.81	0.19	39,69,141,167	0
33	PG4	i	103	13/13	0.81	0.37	74,85,98,105	0
30	GOL	C	527	6/6	0.81	0.49	96,108,112,135	0
34	PGE	B	645	10/10	0.81	0.36	68,81,89,93	0
34	PGE	o	306	10/10	0.81	0.46	70,92,102,103	0
29	LMG	C	526	55/55	0.81	0.23	47,83,115,124	0
34	PGE	V	214	10/10	0.82	0.43	50,86,96,98	0
29	LMG	z	101	55/55	0.82	0.21	49,95,120,160	0
36	EDO	e	106	4/4	0.82	0.11	72,76,79,89	0
32	LHG	e	101	42/49	0.82	0.27	60,105,123,171	0
33	PG4	V	210	13/13	0.82	0.38	53,84,115,120	0
31	LMT	F	102	35/35	0.82	0.28	43,81,105,126	0
33	PG4	H	107	13/13	0.82	0.20	68,83,105,110	0
33	PG4	V	213	13/13	0.82	0.48	68,80,103,112	0
33	PG4	I	103	13/13	0.82	0.23	73,97,121,129	0
31	LMT	b	622	35/35	0.82	0.22	49,76,124,132	0
34	PGE	c	537	10/10	0.82	0.28	96,106,120,123	0
34	PGE	c	538	10/10	0.82	0.29	68,102,115,129	0
33	PG4	A	619	13/13	0.83	0.22	83,96,112,112	0
33	PG4	H	104	13/13	0.83	0.39	83,98,117,119	0
34	PGE	A	621	10/10	0.83	0.20	66,116,120,129	0
34	PGE	H	108	10/10	0.83	0.29	66,86,129,136	0
33	PG4	C	535	13/13	0.84	0.33	66,74,108,121	0
34	PGE	i	105	10/10	0.84	0.23	70,81,89,92	0
33	PG4	B	639	13/13	0.84	0.21	64,79,104,115	0
33	PG4	X	101	13/13	0.84	0.35	63,89,105,108	0
35	P6G	d	416	19/19	0.84	0.17	43,61,100,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	GOL	v	203	6/6	0.84	0.17	66,79,82,98	0
35	P6G	A	623	19/19	0.84	0.18	48,60,95,96	0
33	PG4	H	105	13/13	0.84	0.25	72,87,126,147	0
33	PG4	a	420	13/13	0.84	0.18	79,94,105,106	0
34	PGE	b	641	10/10	0.85	0.21	99,104,114,125	0
38	HTG	c	523	19/19	0.85	0.31	65,86,104,106	0
32	LHG	A	618	42/49	0.85	0.22	49,90,145,167	0
33	PG4	x	102	13/13	0.85	0.48	79,95,107,108	0
38	HTG	C	522	19/19	0.85	0.24	50,83,100,110	0
29	LMG	c	520	51/55	0.85	0.22	47,76,100,124	0
33	PG4	d	414	13/13	0.85	0.26	65,79,85,87	0
39	1PE	e	105	16/16	0.85	0.21	77,93,116,121	0
29	LMG	C	520	51/55	0.85	0.20	38,79,108,121	0
30	GOL	f	104	6/6	0.85	0.31	94,115,135,150	0
31	LMT	f	101	35/35	0.85	0.28	54,85,110,119	0
33	PG4	i	104	13/13	0.85	0.15	56,71,90,91	0
36	EDO	o	310	4/4	0.85	0.32	60,65,77,90	0
36	EDO	H	112	4/4	0.86	0.26	70,85,94,95	0
33	PG4	U	202	13/13	0.86	0.32	52,80,100,102	0
34	PGE	A	620	7/10	0.86	0.11	68,77,83,87	0
31	LMT	M	101	35/35	0.86	0.14	34,51,70,73	0
34	PGE	a	423	10/10	0.86	0.26	78,91,107,107	0
31	LMT	M	102	35/35	0.86	0.17	43,59,82,96	0
31	LMT	B	622	35/35	0.86	0.16	46,73,107,123	0
33	PG4	i	101	13/13	0.86	0.17	71,84,95,98	0
33	PG4	i	102	13/13	0.86	0.25	65,71,81,82	0
33	PG4	b	636	13/13	0.86	0.21	71,79,90,93	0
31	LMT	a	401	35/35	0.86	0.16	37,52,75,83	0
28	SQD	F	104	54/54	0.86	0.26	55,80,110,135	0
34	PGE	x	103	10/10	0.86	0.58	81,98,110,112	0
34	PGE	O	310	10/10	0.86	0.57	58,81,122,137	0
36	EDO	E	112	4/4	0.86	0.17	84,94,96,100	0
36	EDO	I	107	4/4	0.87	0.16	84,89,91,96	0
34	PGE	o	308	10/10	0.87	0.22	48,87,100,104	0
33	PG4	C	537	13/13	0.87	0.23	67,76,92,108	0
33	PG4	b	635	13/13	0.87	0.15	58,76,103,109	0
34	PGE	E	109	10/10	0.87	0.32	51,93,103,106	0
28	SQD	l	102	54/54	0.87	0.14	46,71,104,172	0
33	PG4	I	104	13/13	0.87	0.15	65,73,90,93	0
34	PGE	j	105	10/10	0.87	0.22	73,109,124,125	0
33	PG4	D	414	13/13	0.87	0.33	86,95,105,110	0
30	GOL	B	633	6/6	0.87	0.16	69,71,84,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	PGE	B	648	10/10	0.88	0.21	55,75,82,93	0
34	PGE	o	309	10/10	0.88	0.36	53,78,92,97	0
34	PGE	J	108	10/10	0.88	0.29	80,98,116,120	0
30	GOL	O	302	6/6	0.88	0.12	51,55,67,70	0
34	PGE	b	638	10/10	0.88	0.18	55,77,90,93	0
30	GOL	B	635	6/6	0.88	0.28	46,67,79,83	0
34	PGE	C	540	10/10	0.88	0.25	74,83,102,111	0
28	SQD	b	633	54/54	0.89	0.13	46,66,104,116	0
32	LHG	a	419	41/49	0.89	0.20	52,85,176,193	0
28	SQD	x	101	54/54	0.89	0.20	62,84,132,147	0
33	PG4	c	534	13/13	0.89	0.28	69,85,99,112	0
30	GOL	O	305	6/6	0.89	0.34	55,65,71,77	0
34	PGE	b	643	10/10	0.89	0.21	70,85,103,116	0
39	1PE	B	654	16/16	0.89	0.21	46,68,92,105	0
29	LMG	A	613	51/55	0.90	0.13	45,60,82,95	0
35	P6G	B	652	19/19	0.90	0.28	42,84,105,109	0
31	LMT	m	102	35/35	0.90	0.12	28,50,66,82	0
30	GOL	O	304	6/6	0.90	0.36	60,69,79,88	0
28	SQD	A	616	54/54	0.90	0.13	39,65,102,107	0
30	GOL	u	201	6/6	0.90	0.24	43,70,71,77	0
32	LHG	E	101	42/49	0.90	0.18	54,80,100,127	0
29	LMG	a	414	51/55	0.90	0.13	42,64,80,90	0
34	PGE	b	640	10/10	0.90	0.20	61,88,103,118	0
34	PGE	B	647	10/10	0.90	0.31	78,92,122,122	0
30	GOL	d	413	6/6	0.90	0.17	74,88,114,116	0
34	PGE	h	107	10/10	0.90	0.17	67,78,92,95	0
45	PE8	i	107	25/25	0.90	0.14	44,66,104,122	0
30	GOL	u	202	6/6	0.91	0.22	50,56,61,63	0
35	P6G	A	624	19/19	0.91	0.10	70,85,105,113	0
33	PG4	c	532	13/13	0.91	0.19	70,78,98,101	0
31	LMT	I	101	35/35	0.91	0.15	57,83,111,113	0
30	GOL	b	626	6/6	0.91	0.10	42,46,50,54	0
27	PL9	A	611	55/55	0.91	0.13	39,63,96,107	0
38	HTG	c	522	19/19	0.91	0.23	60,74,96,106	0
28	SQD	a	417	54/54	0.92	0.10	40,64,93,101	0
31	LMT	A	617	35/35	0.92	0.15	37,55,92,105	0
39	1PE	L	101	16/16	0.92	0.12	56,72,99,100	0
33	PG4	V	209	13/13	0.92	0.26	51,84,95,101	0
24	CLA	C	513	65/65	0.92	0.11	33,44,73,92	0
30	GOL	v	207	6/6	0.92	0.31	63,73,86,86	0
35	P6G	d	415	19/19	0.92	0.12	51,64,88,97	0
34	PGE	E	104	10/10	0.92	0.12	67,76,99,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	PG4	a	421	13/13	0.92	0.09	76,89,99,102	0
31	LMT	c	521	35/35	0.92	0.26	54,77,95,101	0
36	EDO	a	425	4/4	0.92	0.24	74,78,96,120	0
30	GOL	c	529	6/6	0.93	0.33	27,31,39,40	6
34	PGE	t	104	10/10	0.93	0.09	60,79,99,100	0
35	P6G	b	648	19/19	0.93	0.11	59,66,80,84	0
34	PGE	a	422	10/10	0.93	0.14	72,75,85,92	0
33	PG4	h	106	13/13	0.93	0.22	67,76,106,108	0
37	CA	h	102	1/1	0.93	0.12	97,97,97,97	0
38	HTG	b	631	19/19	0.93	0.11	41,48,77,98	0
30	GOL	A	615	6/6	0.93	0.11	34,54,62,66	0
38	HTG	B	630	19/19	0.93	0.11	38,50,78,82	0
27	PL9	a	412	55/55	0.93	0.12	46,69,101,108	0
30	GOL	T	103	6/6	0.93	0.14	62,79,91,111	0
24	CLA	b	602	65/65	0.93	0.13	28,47,99,111	0
30	GOL	B	626	6/6	0.94	0.12	34,41,49,61	0
30	GOL	m	103	6/6	0.94	0.15	47,69,88,116	0
29	LMG	c	519	51/55	0.94	0.12	34,67,104,112	0
24	CLA	c	513	65/65	0.94	0.10	37,51,89,99	0
34	PGE	B	644	10/10	0.94	0.09	58,71,117,137	0
35	P6G	j	106	19/19	0.94	0.09	50,74,98,112	0
34	PGE	O	308	10/10	0.94	0.29	31,62,83,96	0
30	GOL	U	201	6/6	0.94	0.24	40,67,78,98	0
26	BCR	C	514	40/40	0.94	0.10	31,41,50,57	0
30	GOL	D	412	6/6	0.94	0.13	55,80,95,102	0
33	PG4	I	102	13/13	0.94	0.19	62,73,97,112	0
26	BCR	c	514	40/40	0.94	0.12	39,51,58,60	0
26	BCR	d	406	40/40	0.94	0.08	28,36,70,82	0
34	PGE	t	105	7/10	0.95	0.12	58,79,84,87	0
36	EDO	B	658	4/4	0.95	0.25	82,84,89,110	0
24	CLA	c	512	65/65	0.95	0.09	30,44,74,79	0
30	GOL	v	206	6/6	0.95	0.09	50,54,66,75	0
38	HTG	V	204	19/19	0.95	0.27	36,52,89,102	0
24	CLA	B	602	65/65	0.95	0.10	27,39,92,115	0
35	P6G	B	651	19/19	0.95	0.07	49,63,77,81	0
30	GOL	C	523	6/6	0.95	0.17	35,46,56,62	0
24	CLA	b	617	60/65	0.95	0.10	26,31,82,92	0
36	EDO	J	109	4/4	0.95	0.10	78,79,85,96	0
30	GOL	C	528	6/6	0.95	0.27	24,27,36,38	6
26	BCR	D	406	40/40	0.95	0.07	23,28,60,65	0
34	PGE	C	539	10/10	0.95	0.23	56,73,94,96	0
35	P6G	T	105	19/19	0.95	0.10	42,59,85,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	PGE	b	642	10/10	0.95	0.09	51,65,87,92	0
36	EDO	i	108	4/4	0.95	0.21	70,71,76,87	0
30	GOL	o	305	6/6	0.95	0.08	51,56,61,62	0
30	GOL	t	101	6/6	0.95	0.15	44,49,56,62	0
33	PG4	l	103	13/13	0.95	0.09	48,64,71,74	0
30	GOL	a	416	6/6	0.95	0.12	39,57,72,77	0
30	GOL	D	413	6/6	0.95	0.21	58,67,76,84	0
34	PGE	T	104	7/10	0.95	0.10	76,77,96,103	0
38	HTG	C	521	19/19	0.95	0.14	53,65,84,85	0
36	EDO	B	655	4/4	0.95	0.31	45,50,57,88	0
30	GOL	c	528	6/6	0.95	0.22	78,79,88,89	0
26	BCR	H	102	40/40	0.96	0.08	23,33,52,55	0
24	CLA	C	512	65/65	0.96	0.08	31,39,74,85	0
29	LMG	C	519	51/55	0.96	0.10	29,59,104,117	0
30	GOL	O	306	6/6	0.96	0.13	39,45,55,97	0
26	BCR	C	525	40/40	0.96	0.10	26,33,39,41	0
26	BCR	k	101	40/40	0.96	0.08	34,40,51,54	0
24	CLA	c	506	65/65	0.96	0.08	26,37,83,95	0
38	HTG	B	623	19/19	0.96	0.09	28,40,74,88	0
30	GOL	V	207	6/6	0.96	0.13	44,49,52,55	0
30	GOL	B	627	6/6	0.96	0.08	35,44,48,48	0
30	GOL	F	101	6/6	0.96	0.11	43,48,50,54	0
40	DGD	h	104	62/66	0.96	0.08	25,35,49,55	0
30	GOL	b	629	6/6	0.96	0.14	36,42,45,50	0
35	P6G	D	417	19/19	0.96	0.09	35,56,89,111	0
24	CLA	a	410	65/65	0.97	0.09	20,25,98,113	0
30	GOL	A	614	6/6	0.97	0.09	33,37,38,44	0
36	EDO	d	417	4/4	0.97	0.09	46,49,52,58	0
30	GOL	f	103	6/6	0.97	0.11	50,53,56,56	0
24	CLA	d	405	65/65	0.97	0.08	25,33,91,101	0
30	GOL	B	625	6/6	0.97	0.07	32,36,38,50	0
28	SQD	A	612	54/54	0.97	0.07	31,55,78,87	0
37	CA	b	601	1/1	0.97	0.19	72,72,72,72	0
30	GOL	o	304	6/6	0.97	0.08	45,53,55,62	0
26	BCR	B	619	40/40	0.97	0.07	20,26,50,62	0
30	GOL	B	629	6/6	0.97	0.09	31,39,60,64	0
24	CLA	C	506	65/65	0.97	0.08	28,39,97,106	0
26	BCR	C	515	40/40	0.97	0.09	28,33,52,59	0
24	CLA	C	510	65/65	0.97	0.07	22,29,41,48	0
24	CLA	c	503	65/65	0.97	0.07	26,35,42,52	0
35	P6G	D	416	19/19	0.97	0.06	38,60,84,87	0
24	CLA	c	504	60/65	0.97	0.06	25,31,67,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
30	GOL	D	402	6/6	0.97	0.12	31,37,43,44	0
26	BCR	K	101	40/40	0.97	0.08	27,36,45,47	0
26	BCR	T	102	40/40	0.97	0.07	20,29,45,60	0
38	HTG	O	303	19/19	0.97	0.07	27,31,50,65	0
26	BCR	a	411	40/40	0.97	0.06	20,25,31,32	0
26	BCR	b	619	40/40	0.97	0.07	21,28,47,57	0
38	HTG	b	623	19/19	0.97	0.09	26,42,77,81	0
29	LMG	B	621	51/55	0.97	0.07	27,39,54,88	0
26	BCR	b	620	40/40	0.97	0.07	24,32,45,48	0
22	CL	V	202	1/1	0.97	0.05	68,68,68,68	0
26	BCR	c	515	40/40	0.97	0.08	26,35,47,55	0
30	GOL	T	101	6/6	0.97	0.12	52,52,56,59	0
26	BCR	c	527	40/40	0.97	0.09	34,42,53,59	0
29	LMG	J	101	47/55	0.97	0.07	23,29,74,83	0
30	GOL	V	201	6/6	0.97	0.06	28,30,35,39	0
38	HTG	o	301	19/19	0.97	0.08	25,32,41,63	0
24	CLA	c	511	65/65	0.97	0.08	28,36,47,52	0
30	GOL	V	208	6/6	0.97	0.07	65,70,82,83	0
30	GOL	a	415	6/6	0.97	0.07	29,39,45,45	0
29	LMG	b	621	51/55	0.97	0.08	28,39,53,103	0
26	BCR	h	103	40/40	0.97	0.06	25,35,50,53	0
30	GOL	b	627	6/6	0.97	0.07	40,47,52,54	0
24	CLA	B	617	60/65	0.97	0.07	21,27,90,107	0
30	GOL	b	630	6/6	0.97	0.08	30,39,52,53	0
40	DGD	H	103	62/66	0.97	0.08	21,31,45,54	0
40	DGD	c	516	62/66	0.97	0.08	23,35,77,86	0
40	DGD	c	517	57/66	0.97	0.07	27,34,75,108	0
26	BCR	t	102	40/40	0.97	0.07	21,29,48,53	0
36	EDO	O	311	4/4	0.97	0.22	42,54,57,72	0
41	HEM	e	107	43/43	0.97	0.10	40,47,74,103	0
29	LMG	j	101	47/55	0.97	0.09	26,35,80,91	0
30	GOL	d	402	6/6	0.97	0.08	35,39,45,48	0
23	BCT	A	605	4/4	0.98	0.06	27,31,35,52	0
32	LHG	d	410	49/49	0.98	0.08	21,27,42,51	0
32	LHG	d	411	49/49	0.98	0.09	26,31,79,84	0
24	CLA	C	501	65/65	0.98	0.06	25,30,48,57	0
24	CLA	C	502	65/65	0.98	0.06	21,27,37,54	0
24	CLA	C	503	65/65	0.98	0.06	26,30,38,43	0
24	CLA	C	504	60/65	0.98	0.06	20,26,70,81	0
24	CLA	C	505	65/65	0.98	0.06	23,29,47,52	0
26	BCR	b	618	40/40	0.98	0.07	19,26,33,37	0
23	BCT	a	406	4/4	0.98	0.05	27,28,31,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	C	507	65/65	0.98	0.06	27,33,48,64	0
24	CLA	C	508	60/65	0.98	0.07	23,29,51,61	0
24	CLA	C	509	65/65	0.98	0.09	27,33,50,57	0
30	GOL	V	205	6/6	0.98	0.09	26,34,37,43	0
30	GOL	V	206	6/6	0.98	0.17	33,35,42,42	0
23	BCT	m	104[A]	4/4	0.98	0.11	18,34,38,38	4
24	CLA	C	511	65/65	0.98	0.08	26,33,40,45	0
23	BCT	m	104[B]	4/4	0.98	0.11	7,13,18,19	4
24	CLA	A	607	60/65	0.98	0.06	17,20,66,78	0
30	GOL	b	625	6/6	0.98	0.07	34,39,44,54	0
24	CLA	D	404	65/65	0.98	0.06	13,18,35,40	0
24	CLA	D	405	65/65	0.98	0.06	22,29,91,98	0
30	GOL	b	628	6/6	0.98	0.06	32,34,35,44	0
27	PL9	D	407	55/55	0.98	0.07	17,22,33,48	0
24	CLA	a	407	65/65	0.98	0.07	17,20,27,41	0
30	GOL	c	525	6/6	0.98	0.20	47,49,64,80	0
30	GOL	c	526	6/6	0.98	0.07	24,28,29,32	0
37	CA	B	601	1/1	0.98	0.21	82,82,82,82	0
37	CA	O	301	1/1	0.98	0.08	53,53,53,53	0
27	PL9	d	407	55/55	0.98	0.07	19,24,31,39	0
24	CLA	a	408	60/65	0.98	0.07	18,25,73,85	0
37	CA	o	302	1/1	0.98	0.08	55,55,55,55	0
24	CLA	A	609	65/65	0.98	0.07	19,24,109,130	0
22	CL	v	201	1/1	0.98	0.07	72,72,72,72	0
24	CLA	b	603	65/65	0.98	0.07	21,28,39,43	0
28	SQD	a	413	54/54	0.98	0.07	33,54,92,96	0
24	CLA	b	605	65/65	0.98	0.06	17,23,53,59	0
24	CLA	b	606	65/65	0.98	0.06	20,25,33,39	0
24	CLA	b	607	55/65	0.98	0.07	22,27,36,49	0
24	CLA	b	608	65/65	0.98	0.06	17,22,31,37	0
24	CLA	b	610	65/65	0.98	0.07	23,30,35,44	0
24	CLA	b	611	65/65	0.98	0.05	23,28,38,44	0
24	CLA	b	613	65/65	0.98	0.07	20,25,32,41	0
24	CLA	b	614	65/65	0.98	0.06	19,23,48,54	0
24	CLA	b	615	65/65	0.98	0.06	18,26,94,117	0
24	CLA	b	616	65/65	0.98	0.05	22,29,47,56	0
24	CLA	B	603	65/65	0.98	0.06	21,26,33,38	0
24	CLA	c	501	65/65	0.98	0.06	27,35,49,53	0
24	CLA	B	605	65/65	0.98	0.06	17,21,55,58	0
24	CLA	B	606	65/65	0.98	0.07	18,22,34,38	0
24	CLA	c	505	65/65	0.98	0.06	25,29,44,50	0
24	CLA	B	607	55/65	0.98	0.06	19,25,33,49	0

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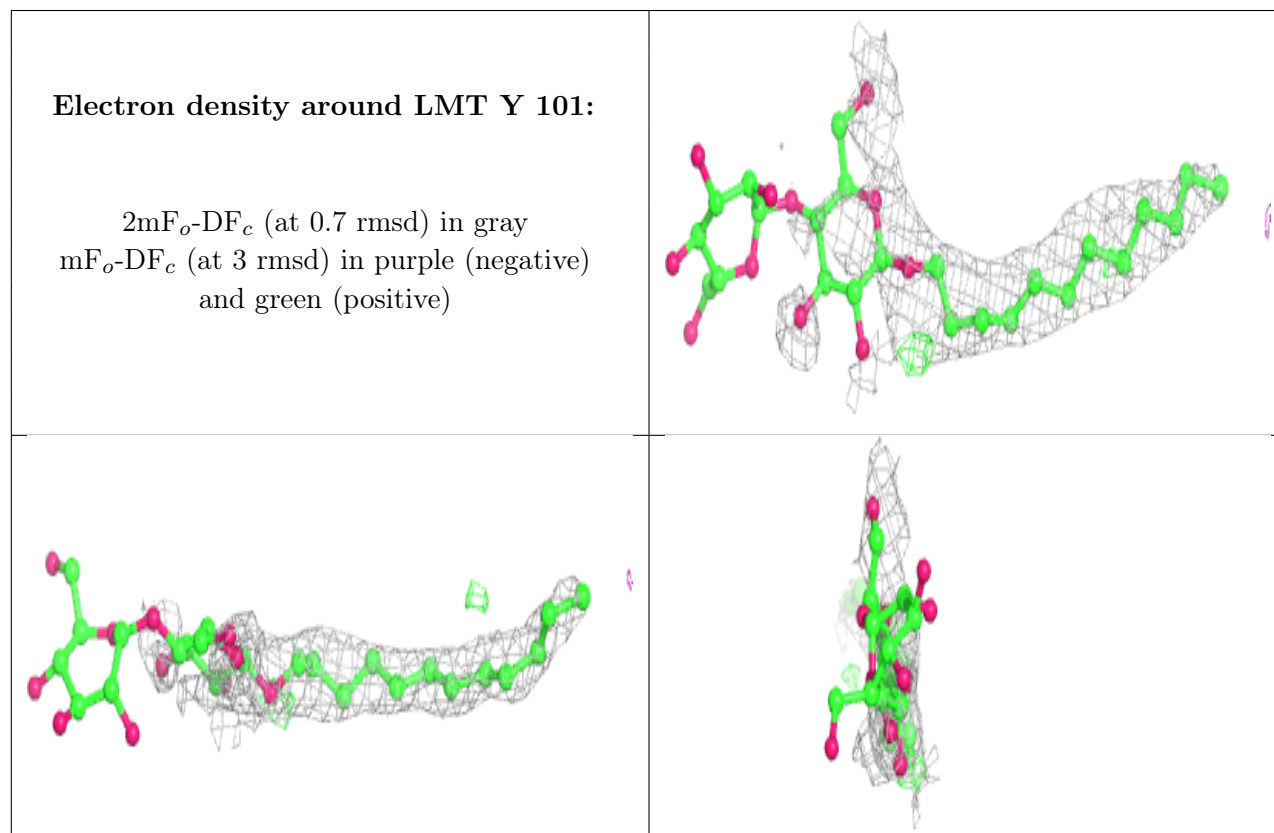
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
24	CLA	c	507	65/65	0.98	0.07	28,34,50,59	0
24	CLA	c	508	60/65	0.98	0.06	23,29,52,62	0
24	CLA	c	510	65/65	0.98	0.06	26,32,41,48	0
24	CLA	B	608	65/65	0.98	0.06	16,20,32,38	0
24	CLA	B	610	65/65	0.98	0.07	22,27,33,37	0
24	CLA	B	611	65/65	0.98	0.06	20,24,38,51	0
24	CLA	B	613	65/65	0.98	0.06	17,23,30,39	0
25	PHO	A	608	64/64	0.98	0.06	17,19,26,26	0
25	PHO	D	401	64/64	0.98	0.06	17,23,31,41	0
25	PHO	a	409	64/64	0.98	0.07	17,21,26,32	0
25	PHO	d	401	64/64	0.98	0.07	20,25,31,41	0
40	DGD	C	516	62/66	0.98	0.07	20,31,90,104	0
40	DGD	C	517	56/66	0.98	0.07	21,31,74,88	0
40	DGD	C	518	62/66	0.98	0.07	20,30,71,80	0
26	BCR	A	610	40/40	0.98	0.07	20,25,32,35	0
26	BCR	B	618	40/40	0.98	0.07	21,25,33,34	0
24	CLA	B	614	65/65	0.98	0.06	17,21,48,64	0
26	BCR	B	620	40/40	0.98	0.06	22,31,46,50	0
40	DGD	c	518	62/66	0.98	0.06	25,36,65,81	0
24	CLA	B	615	55/65	0.98	0.06	17,23,55,82	0
32	LHG	B	632	49/49	0.98	0.08	20,30,52,61	0
41	HEM	E	113	43/43	0.98	0.07	35,42,61,68	0
32	LHG	D	409	49/49	0.98	0.07	25,35,45,55	0
42	MG	F	103	1/1	0.98	0.09	32,32,32,32	0
43	HEC	v	202	43/43	0.98	0.08	26,31,34,38	0
32	LHG	D	411	49/49	0.98	0.08	23,31,81,89	0
24	CLA	B	616	65/65	0.98	0.06	21,27,48,56	0
30	GOL	v	204	6/6	0.99	0.06	30,36,41,50	0
24	CLA	B	612	65/65	0.99	0.05	16,21,35,39	0
32	LHG	l	101	49/49	0.99	0.07	23,30,49,62	0
24	CLA	c	502	65/65	0.99	0.07	24,30,41,50	0
24	CLA	b	604	65/65	0.99	0.05	22,28,38,45	0
24	CLA	d	403	65/65	0.99	0.05	17,20,29,38	0
24	CLA	d	404	65/65	0.99	0.07	17,21,37,43	0
24	CLA	b	612	65/65	0.99	0.06	18,24,37,42	0
30	GOL	B	628	6/6	0.99	0.07	34,40,48,49	0
24	CLA	B	609	65/65	0.99	0.06	19,24,33,40	0
24	CLA	A	606	65/65	0.99	0.08	14,18,27,44	0
24	CLA	D	403	65/65	0.99	0.06	14,18,28,44	0
32	LHG	D	410	49/49	0.99	0.08	21,27,41,48	0
24	CLA	B	604	65/65	0.99	0.05	19,23,34,41	0
30	GOL	C	524	6/6	0.99	0.07	21,22,24,26	0

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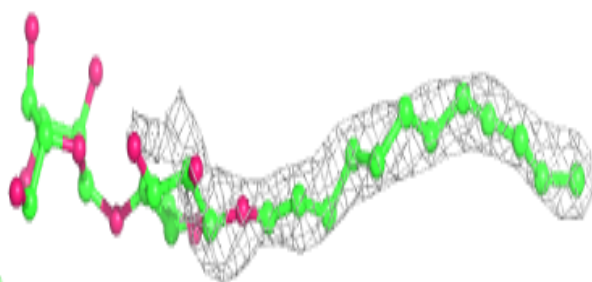
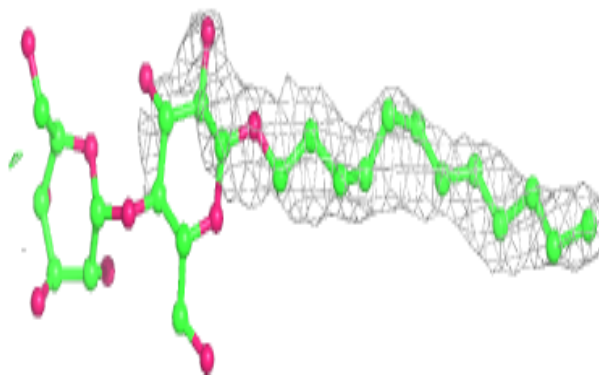
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
42	MG	J	102	1/1	0.99	0.04	27,27,27,27	0
42	MG	f	102	1/1	0.99	0.07	45,45,45,45	0
42	MG	j	102	1/1	0.99	0.05	35,35,35,35	0
43	HEC	V	203	43/43	0.99	0.06	20,24,27,29	0
24	CLA	c	509	65/65	0.99	0.07	25,33,52,53	0
32	LHG	d	409	49/49	0.99	0.08	27,37,48,52	0
24	CLA	b	609	65/65	0.99	0.05	22,27,37,44	0
37	CA	c	524	1/1	1.00	0.08	45,45,45,45	0
20	OEX	a	402	10/10	1.00	0.02	23,24,26,27	0
21	FE2	A	602	1/1	1.00	0.02	25,25,25,25	0
21	FE2	a	403	1/1	1.00	0.02	25,25,25,25	0
22	CL	A	603	1/1	1.00	0.01	23,23,23,23	0
22	CL	A	604	1/1	1.00	0.04	21,21,21,21	0
20	OEX	A	601	10/10	1.00	0.02	20,21,24,26	0
22	CL	a	404	1/1	1.00	0.02	28,28,28,28	0
22	CL	a	405	1/1	1.00	0.02	25,25,25,25	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.

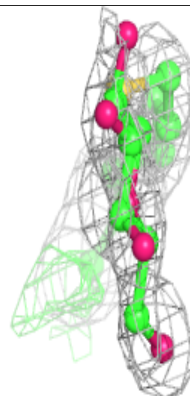
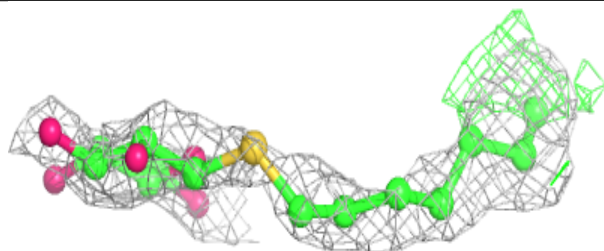
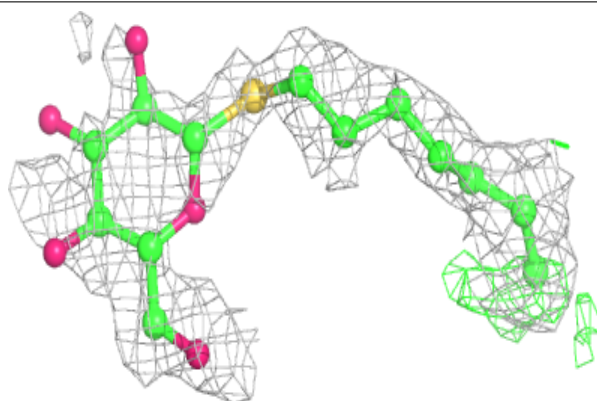


Electron density around LMT j 103:

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

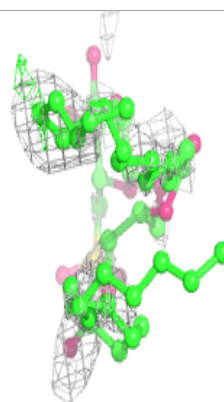
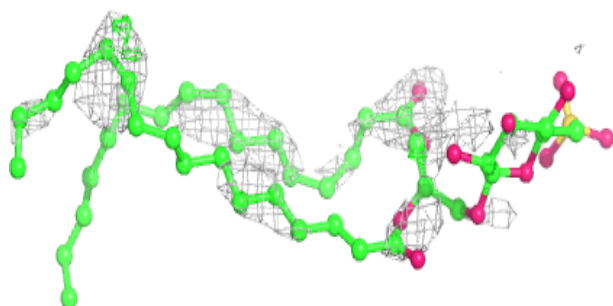
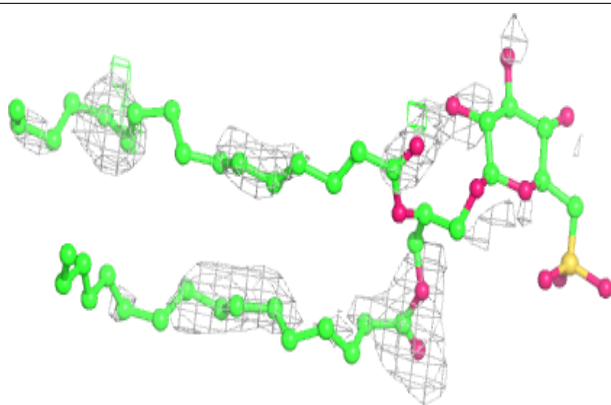
**Electron density around HTG C 529:**

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

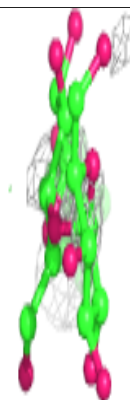
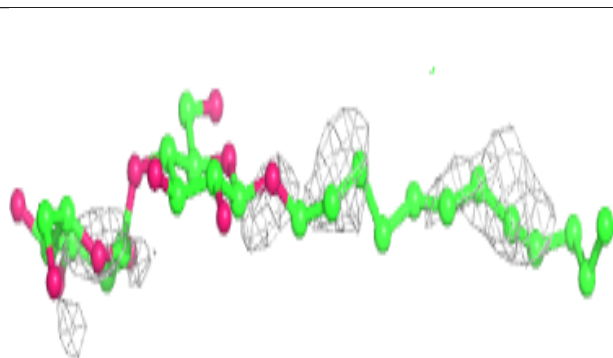
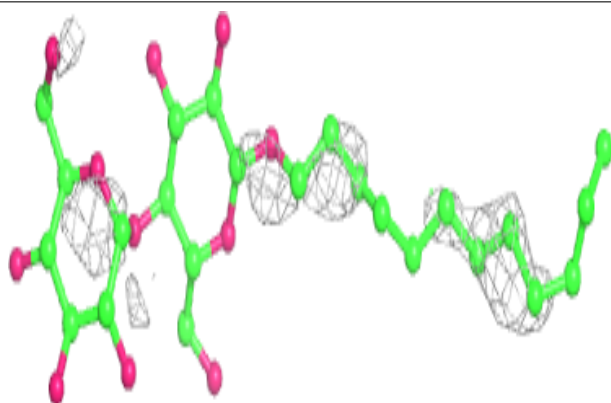


Electron density around SQD h 105:

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

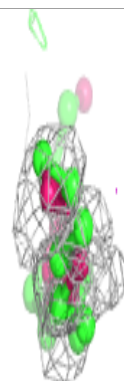
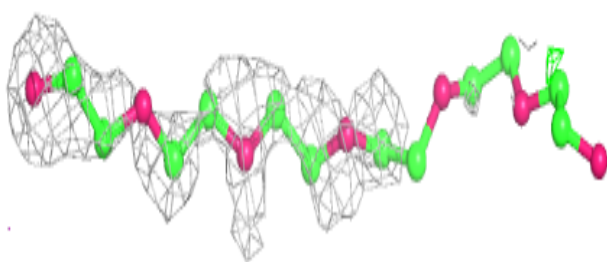
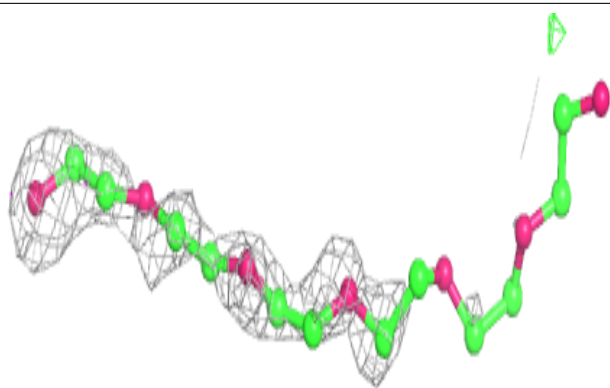
**Electron density around LMT C 533:**

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

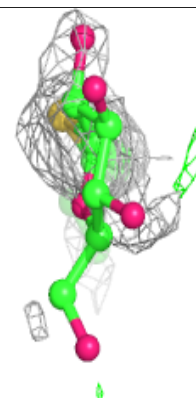
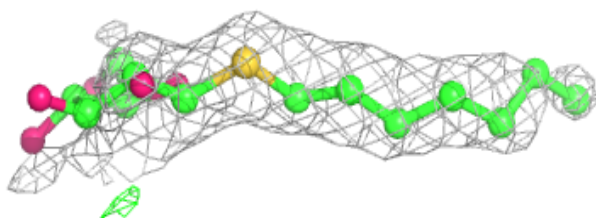
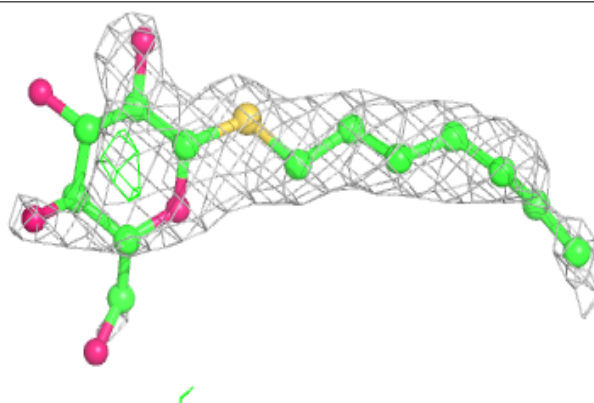


Electron density around P6G D 418:

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

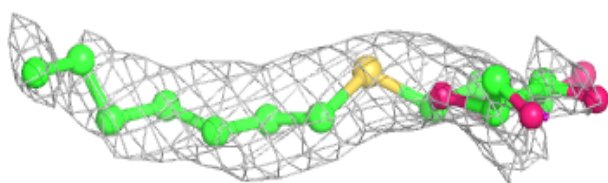
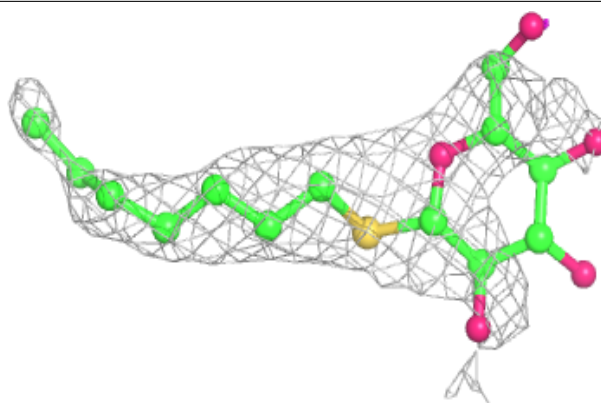
**Electron density around HTG H 101:**

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

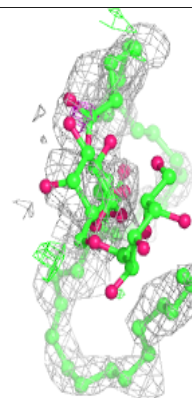
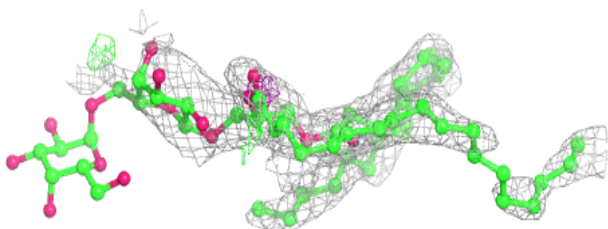
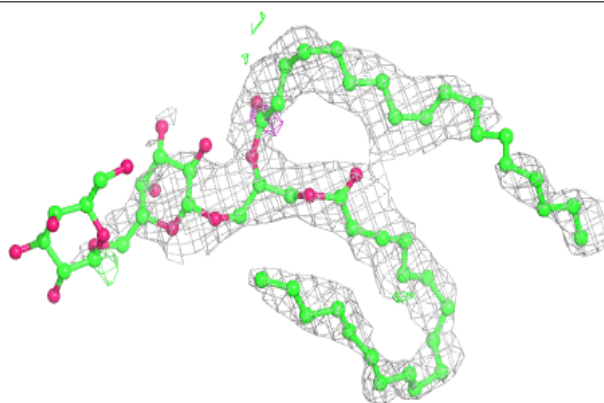


Electron density around HTG h 101:

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

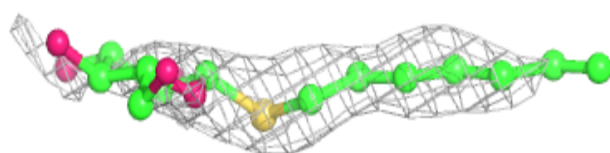
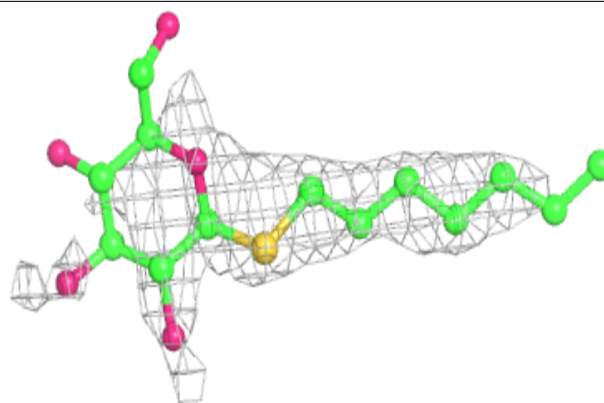
**Electron density around DGD D 408:**

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

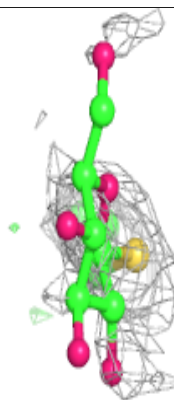
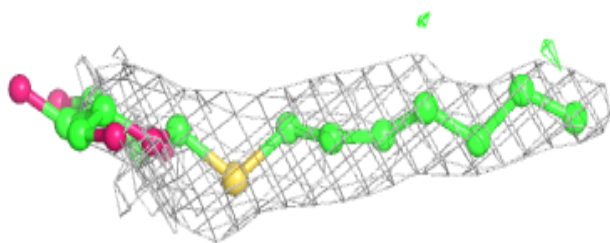
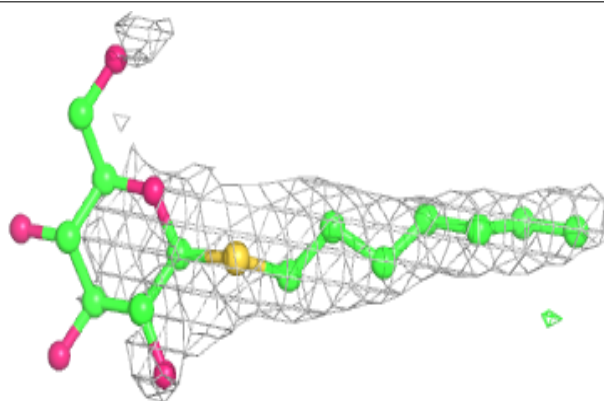


Electron density around HTG c 530:

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

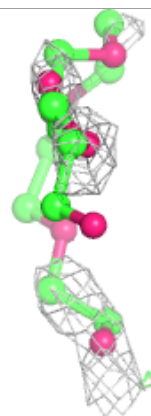
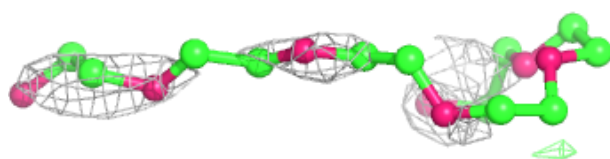
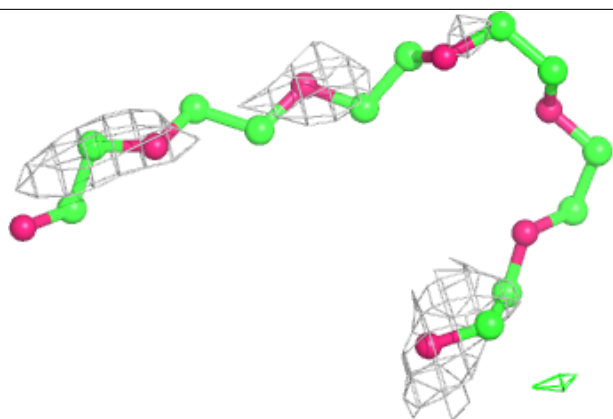
**Electron density around HTG c 531:**

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

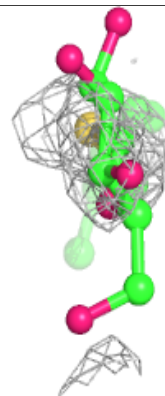
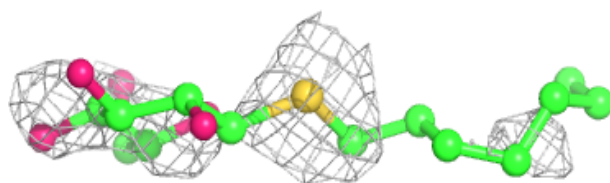
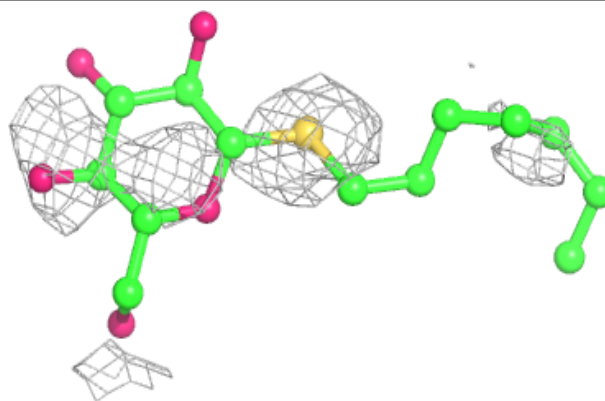


Electron density around P6G C 541:

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

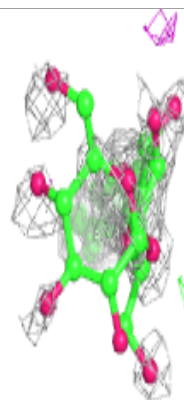
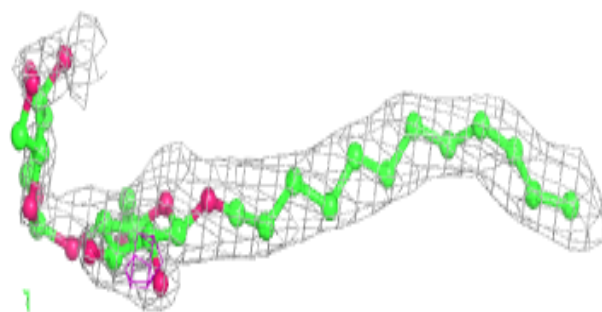
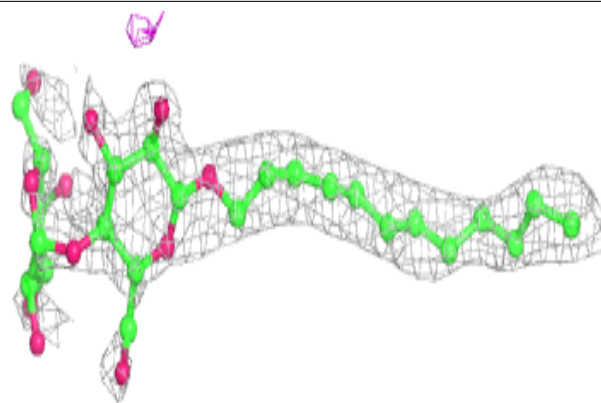
**Electron density around HTG C 530:**

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

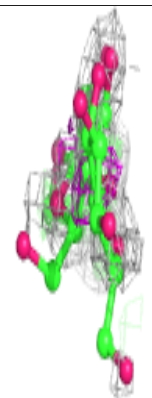
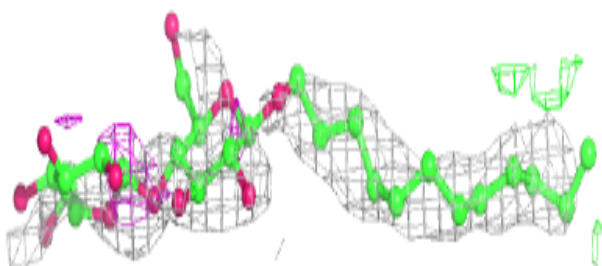
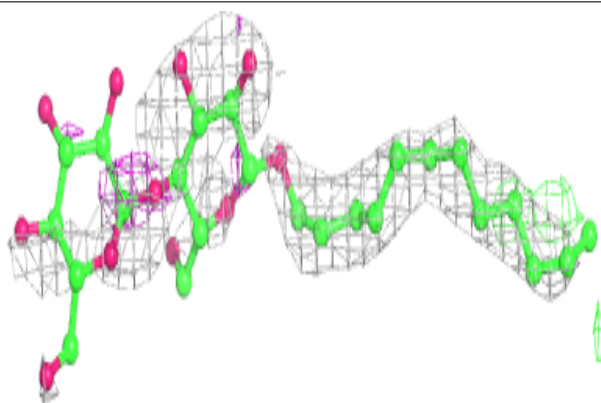


Electron density around LMT J 103:

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

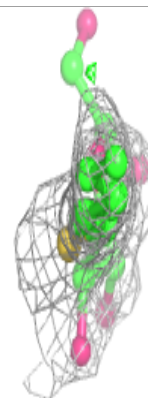
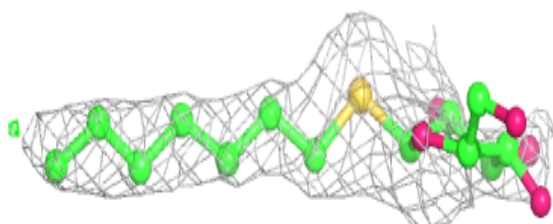
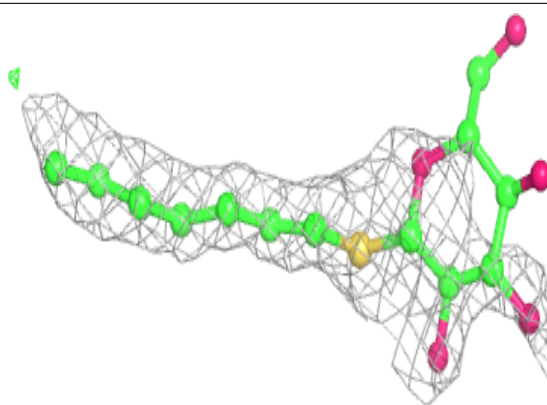
**Electron density around LMT u 203:**

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

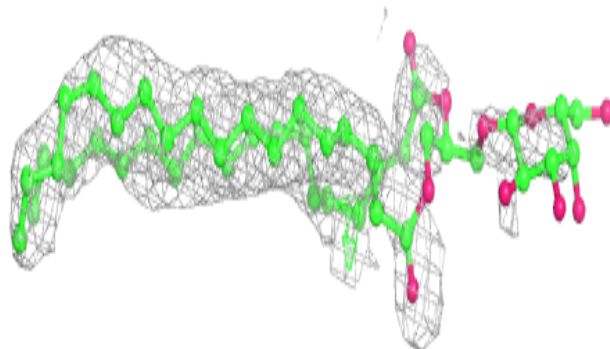
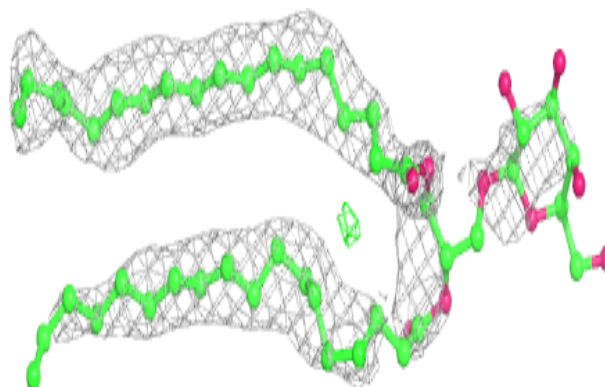


Electron density around HTG C 532:

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

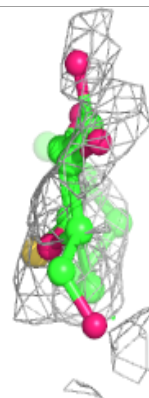
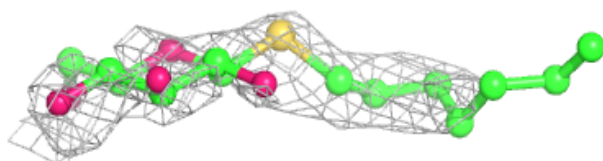
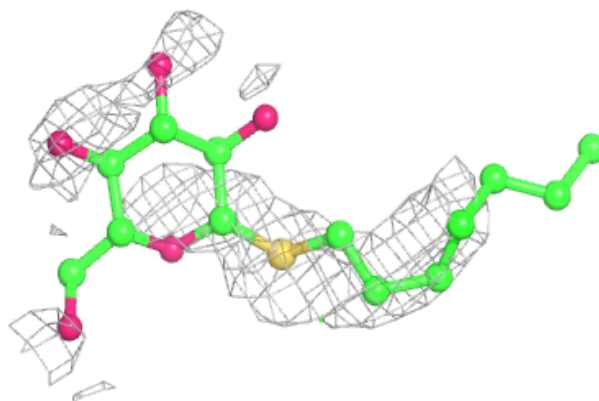
**Electron density around LMG d 412:**

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

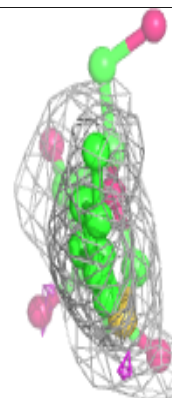
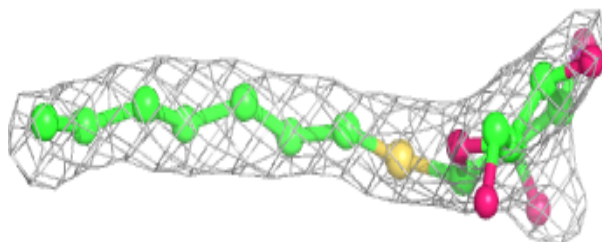
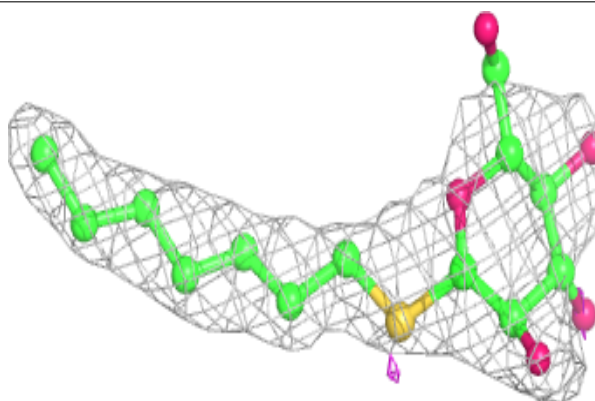


Electron density around HTG C 531:

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

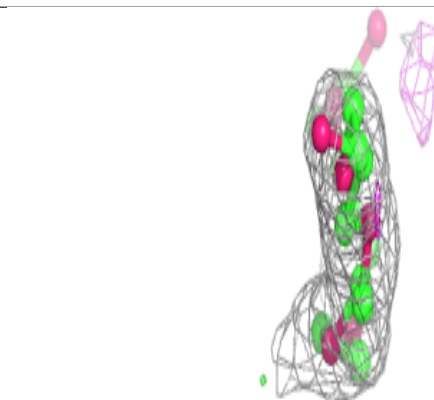
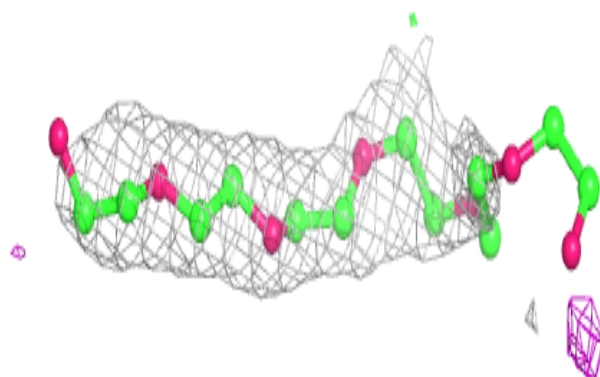
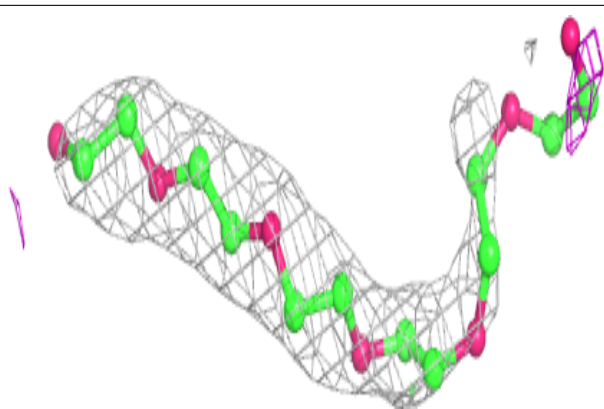
**Electron density around HTG B 624:**

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

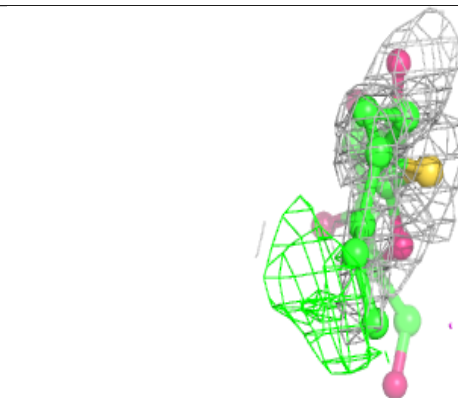
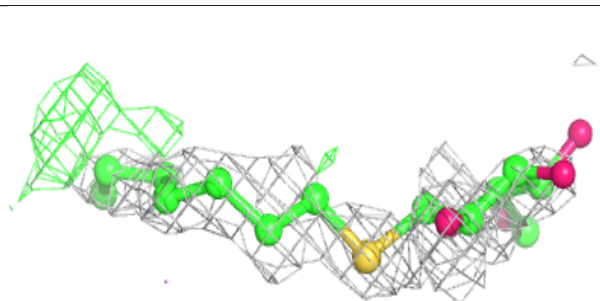
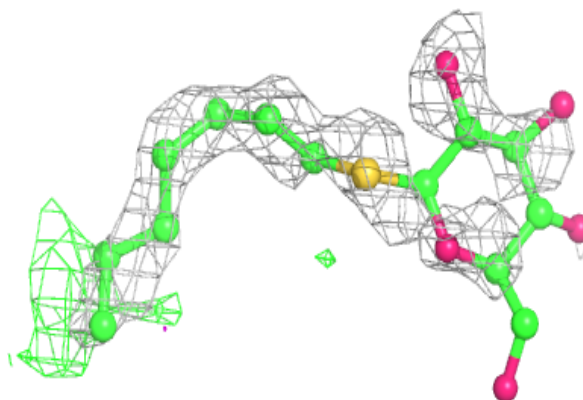


Electron density around P6G I 106:

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

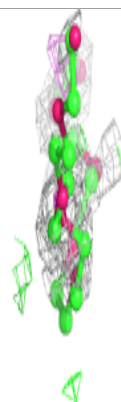
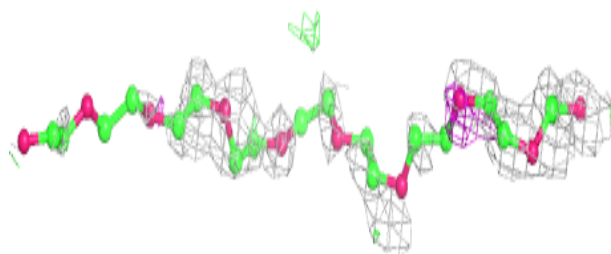
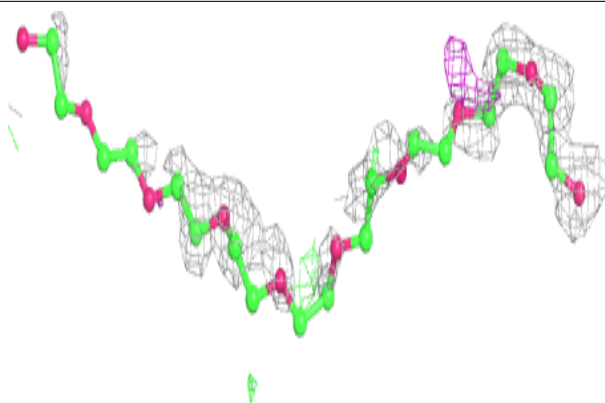
**Electron density around HTG a 418:**

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



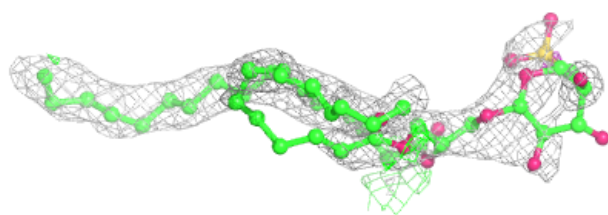
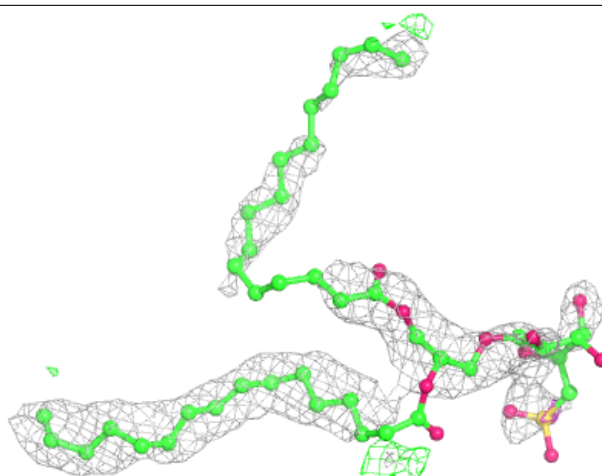
Electron density around 2PE V 216:

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



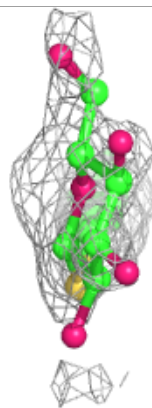
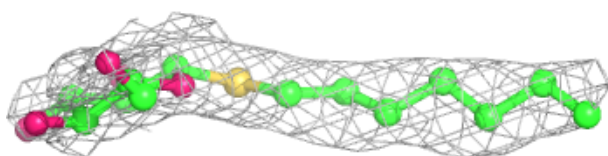
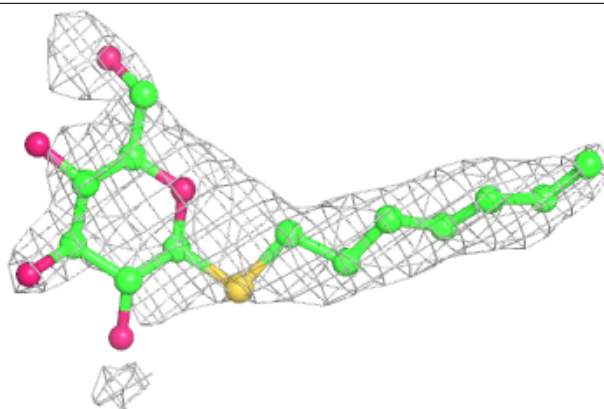
Electron density around SQD A 622:

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

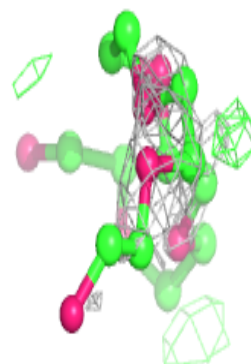
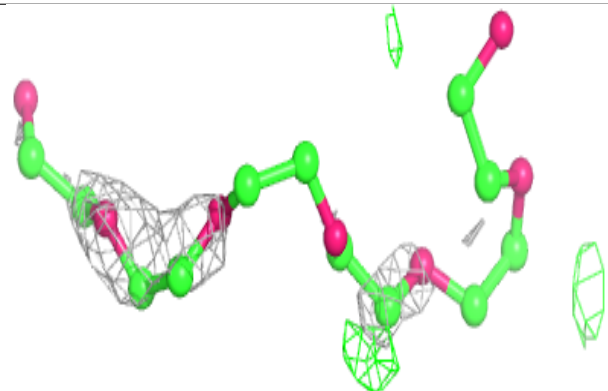
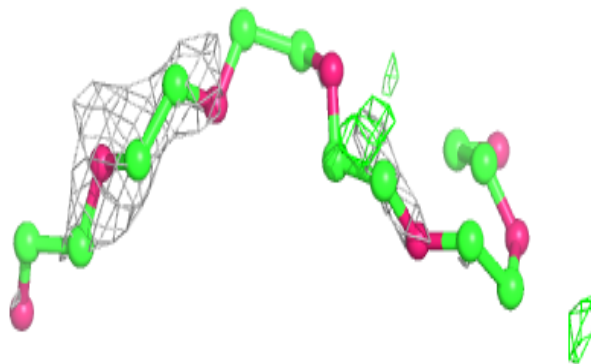


Electron density around HTG b 624:

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

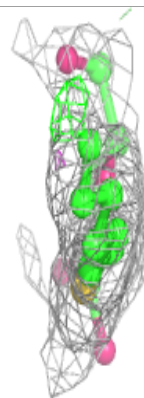
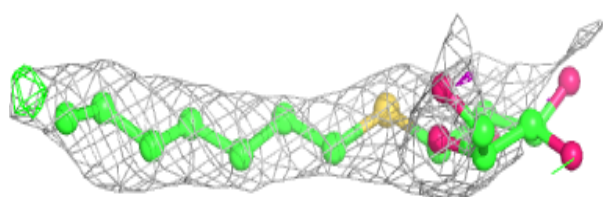
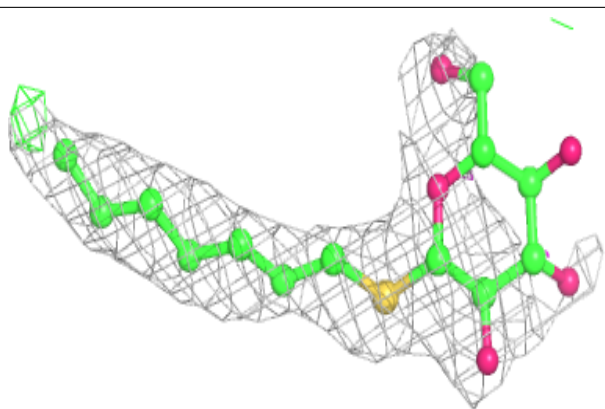
**Electron density around P6G c 541:**

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

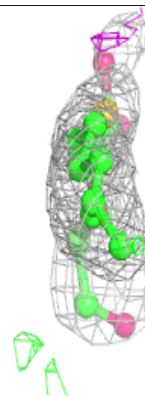
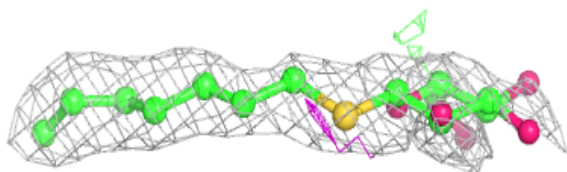
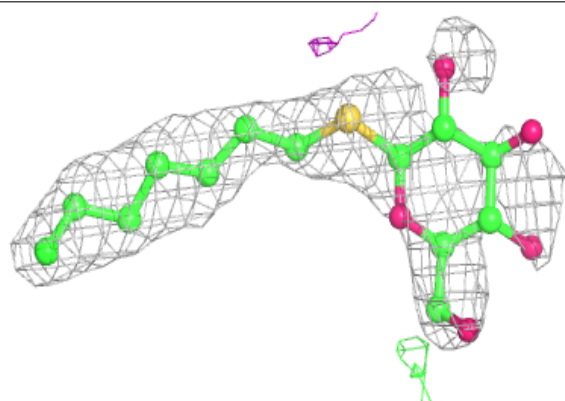


Electron density around HTG b 632:

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

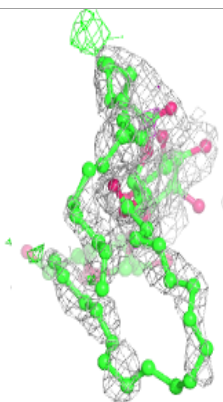
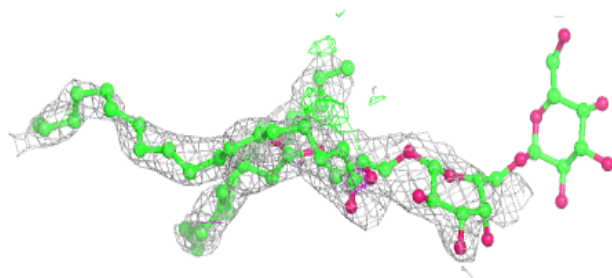
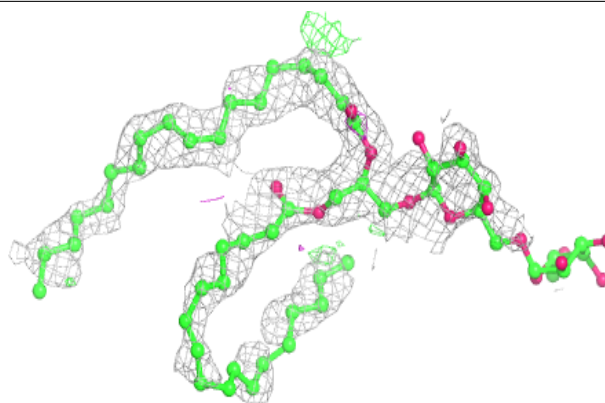
**Electron density around HTG B 631:**

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

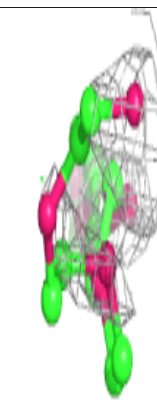
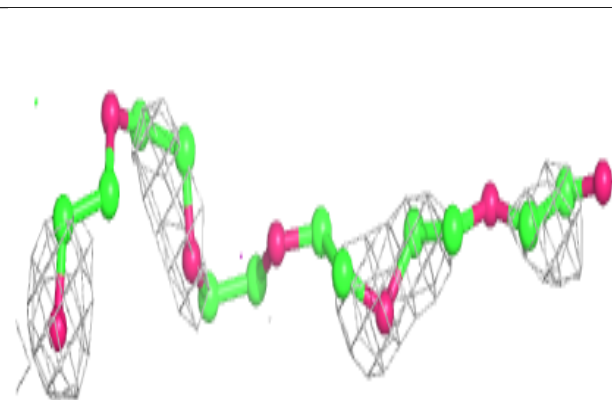
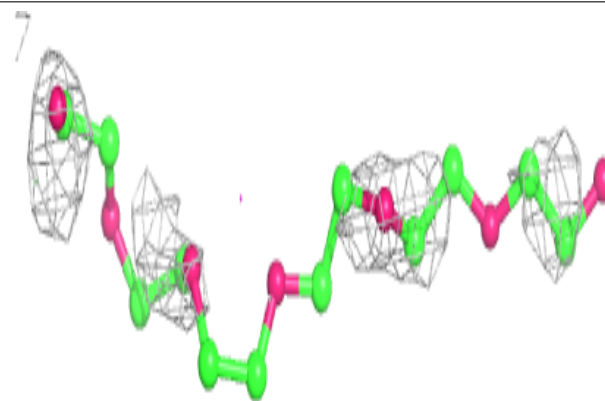


Electron density around DGD d 408:

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

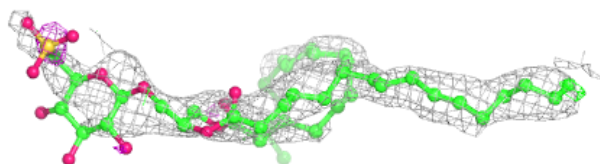
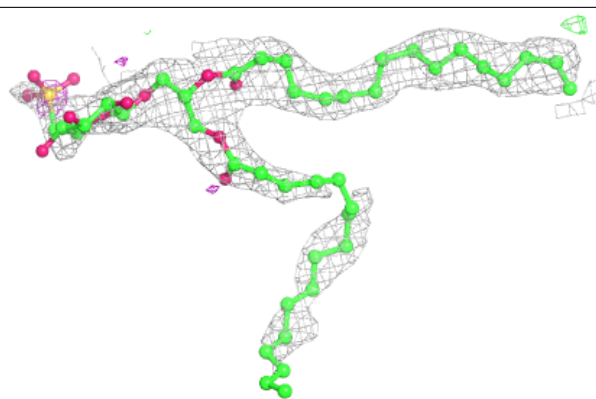
**Electron density around P6G E 110:**

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

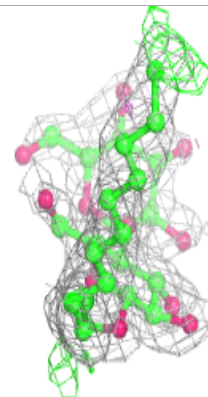
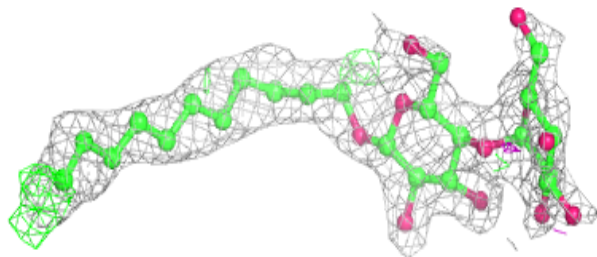
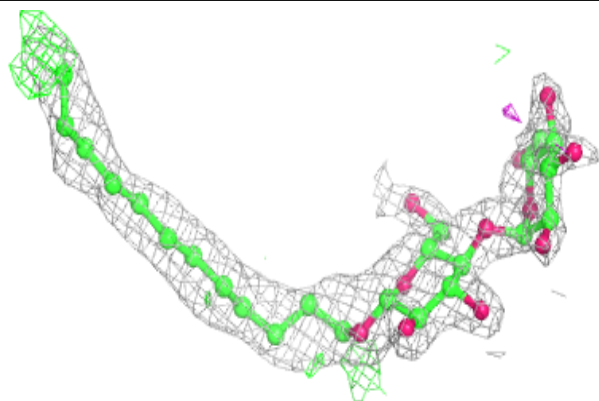


Electron density around SQD a 424:

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

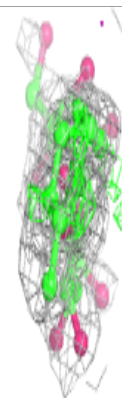
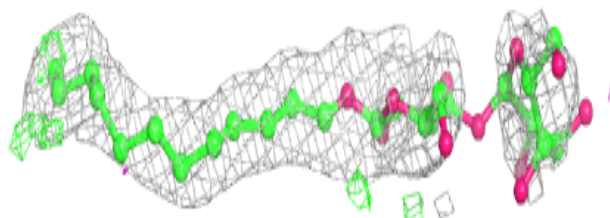
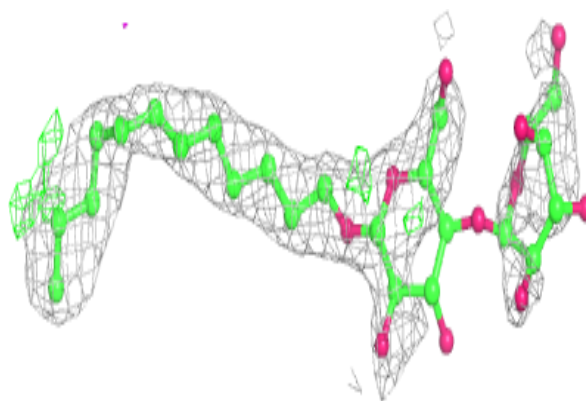
**Electron density around LMT m 101:**

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

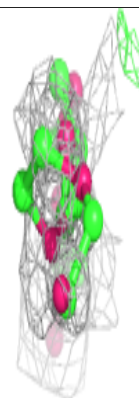
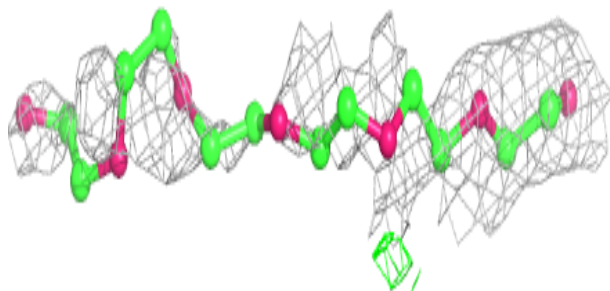
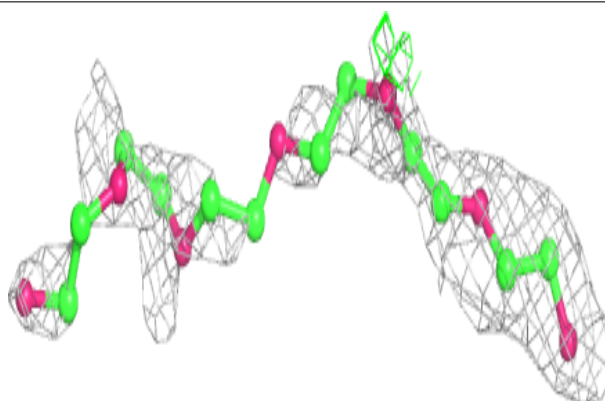


Electron density around LMT t 103:

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

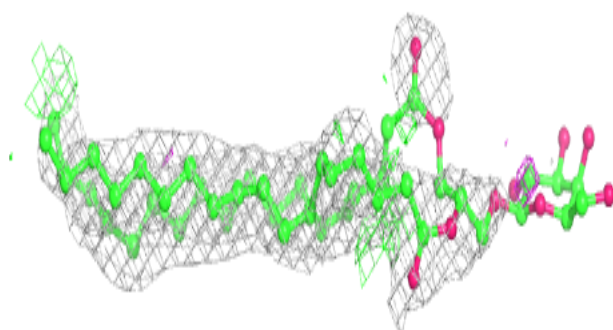
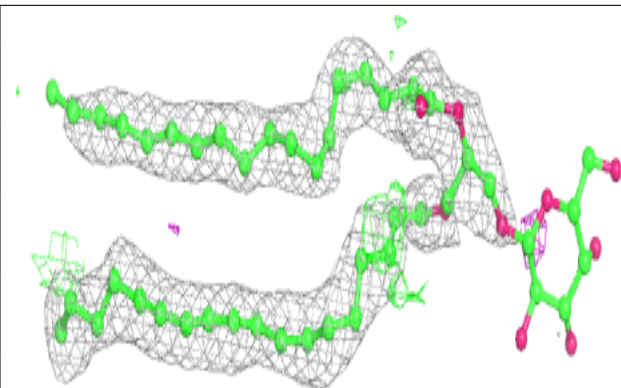
**Electron density around P6G b 649:**

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

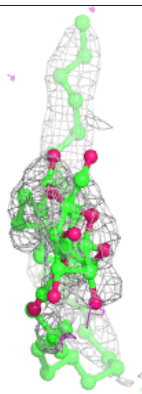
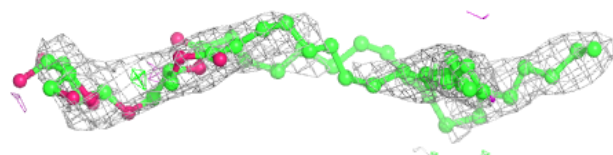
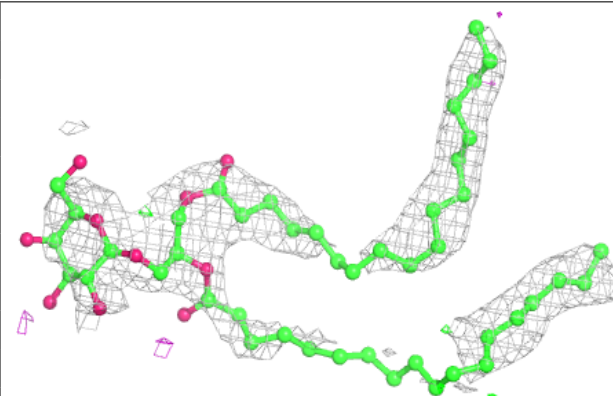


Electron density around LMG B 634:

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

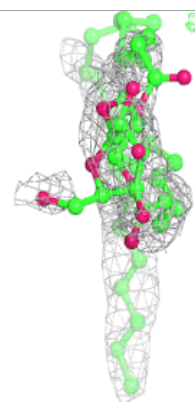
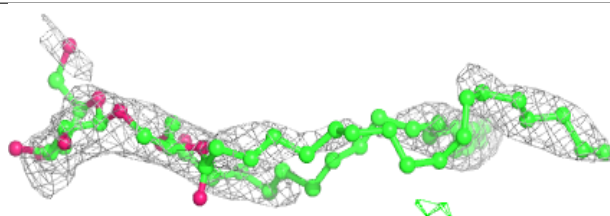
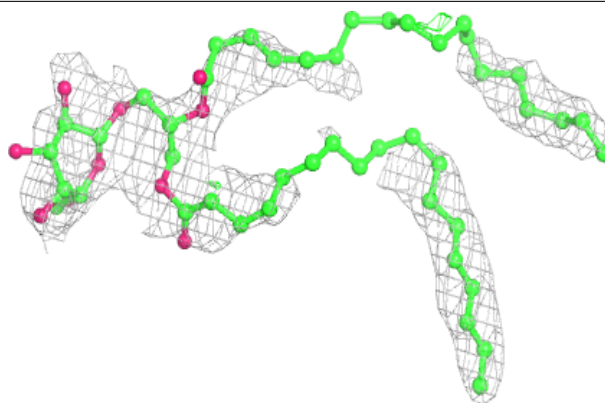
**Electron density around LMG C 526:**

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

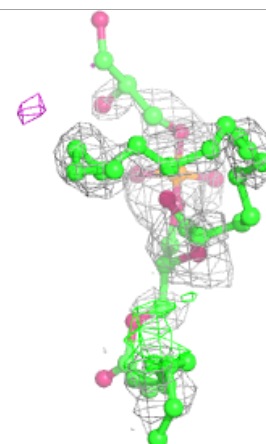
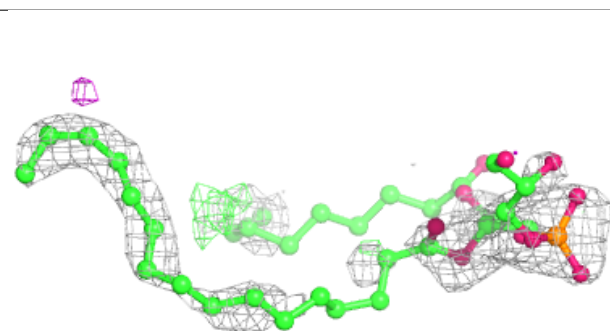
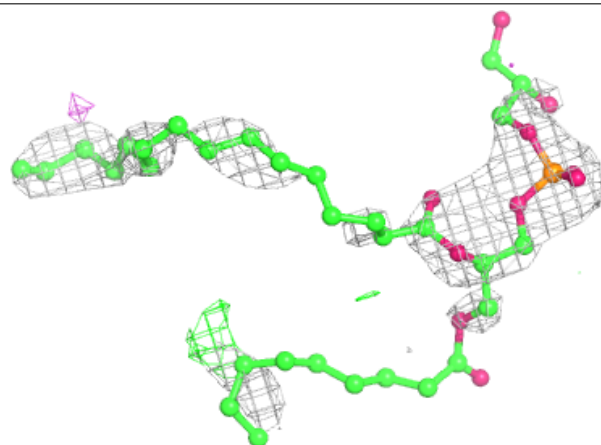


Electron density around LMG z 101:

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

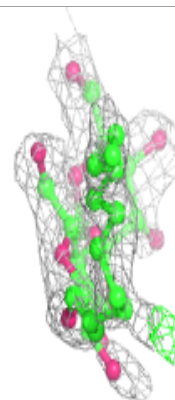
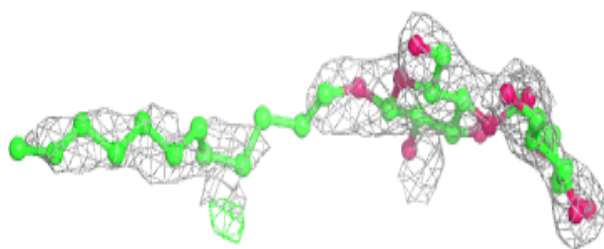
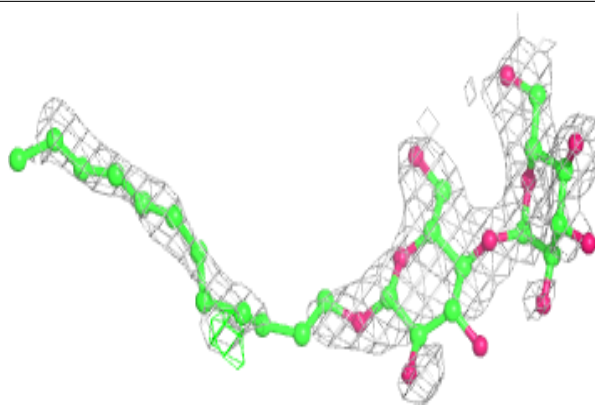
**Electron density around LHG e 101:**

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

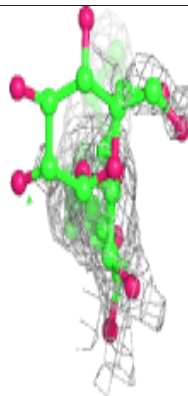
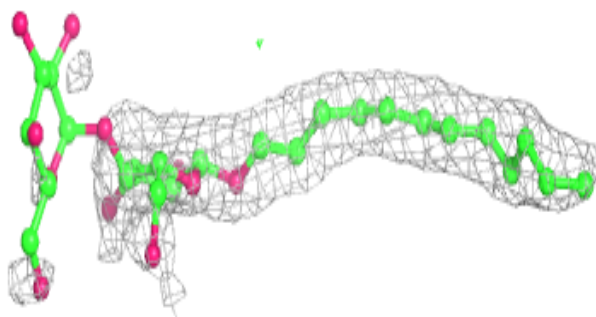
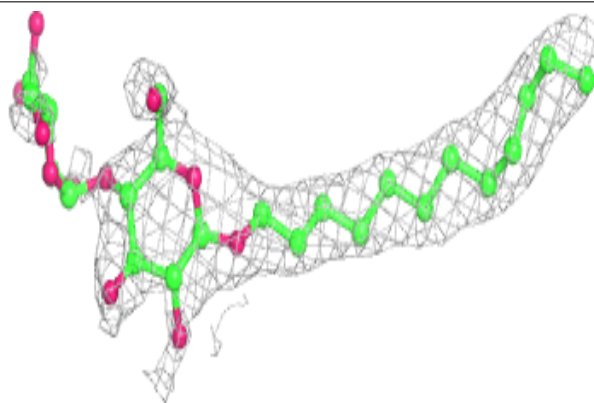


Electron density around LMT F 102:

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

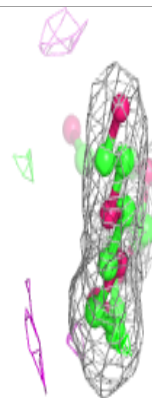
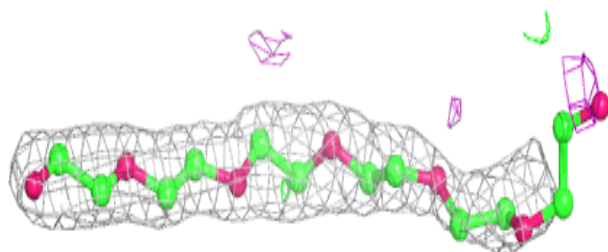
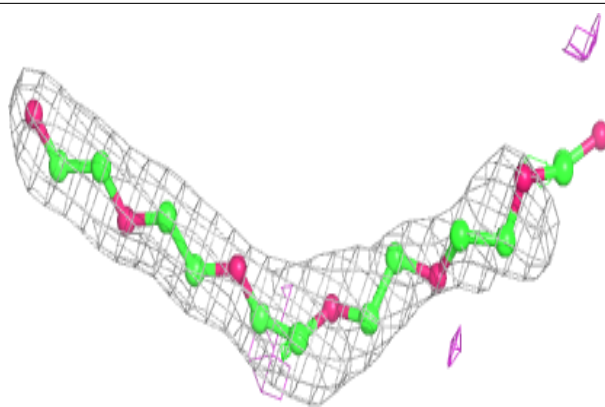
**Electron density around LMT b 622:**

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

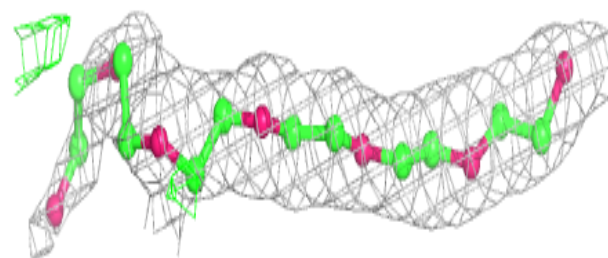
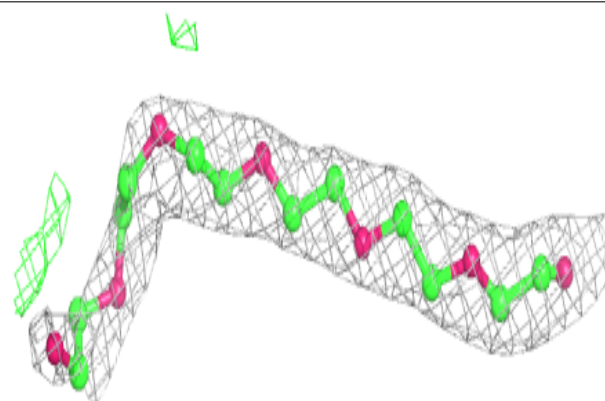


Electron density around P6G d 416:

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

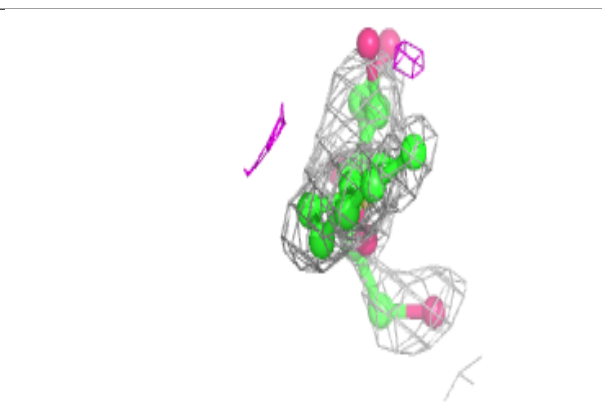
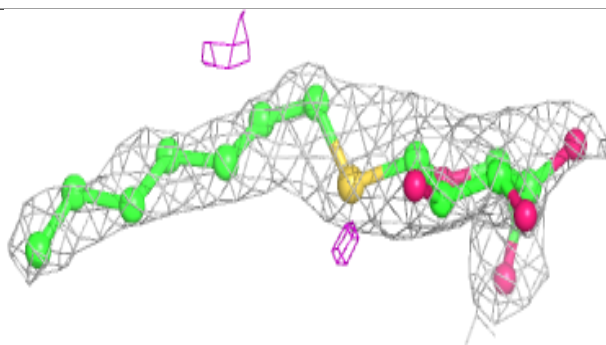
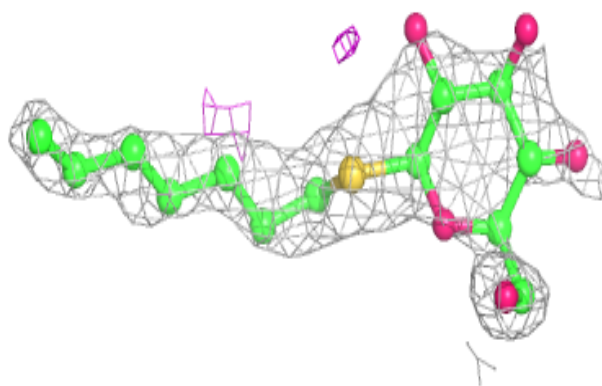
**Electron density around P6G A 623:**

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

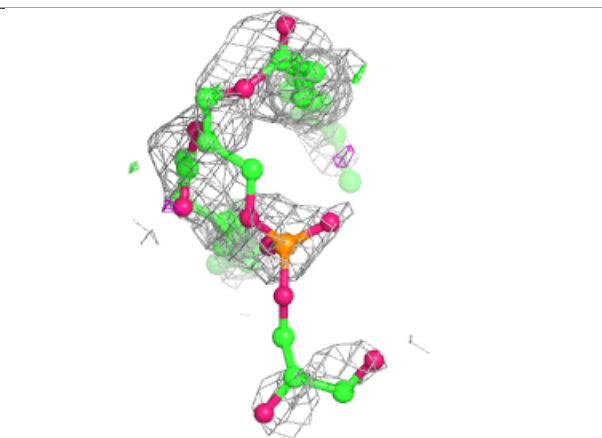
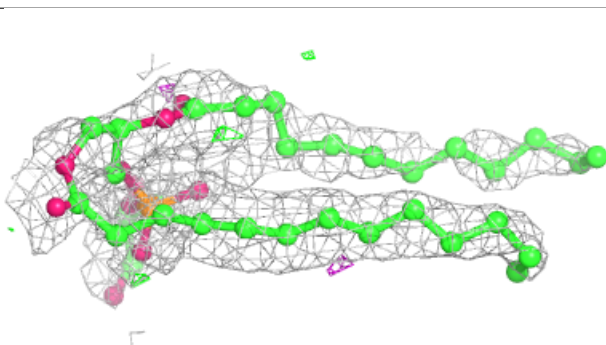
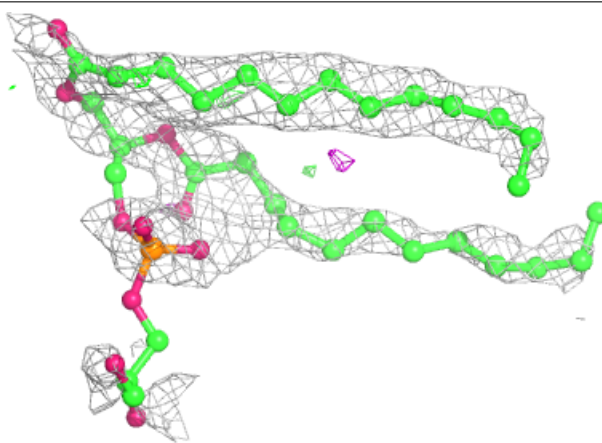


Electron density around HTG c 523:

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

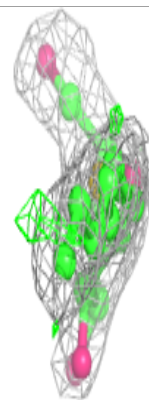
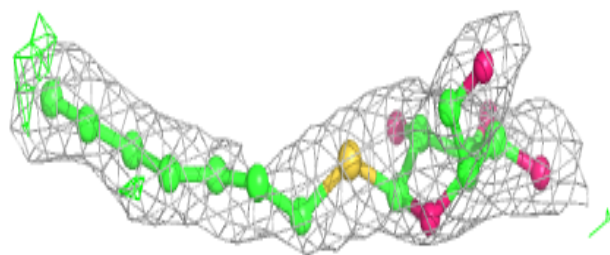
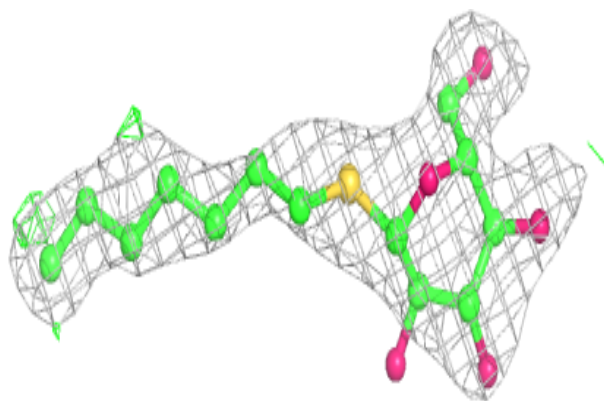
**Electron density around LHG A 618:**

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

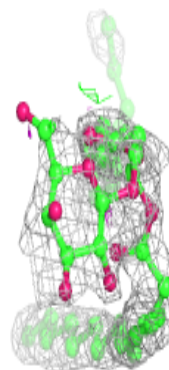
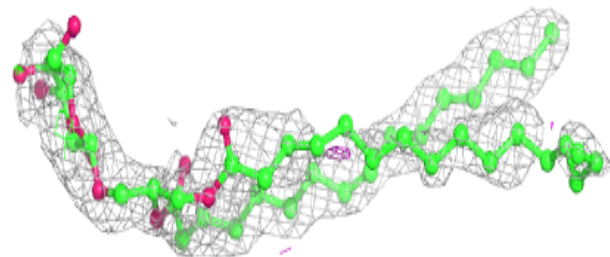
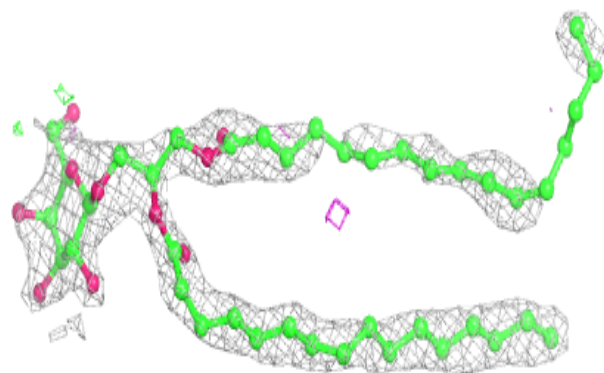


Electron density around HTG C 522:

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

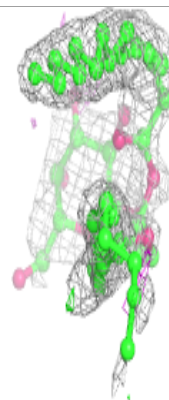
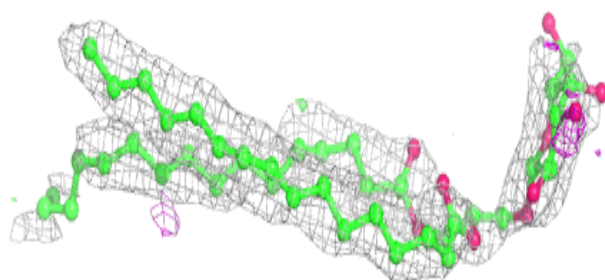
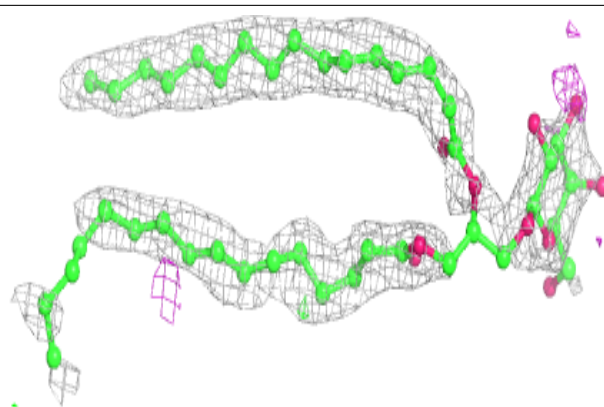
**Electron density around LMG c 520:**

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

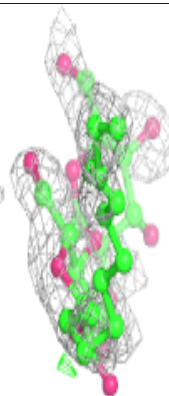
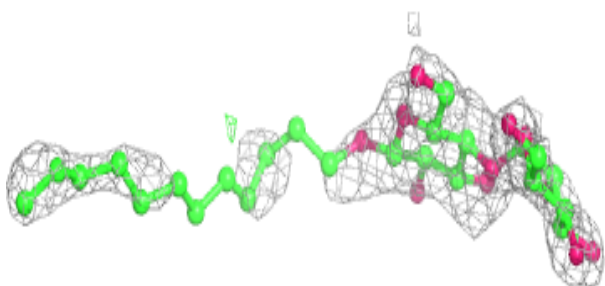
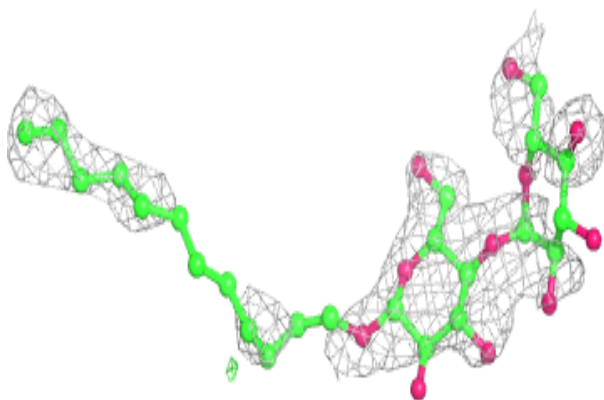


Electron density around LMG C 520:

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

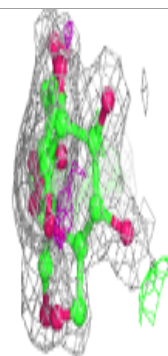
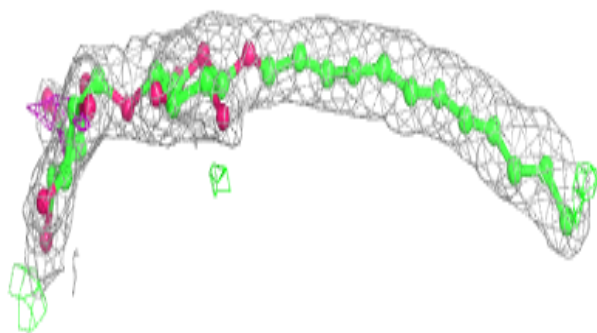
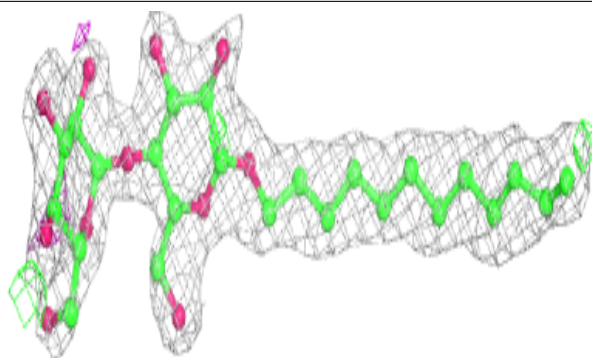
**Electron density around LMT f 101:**

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

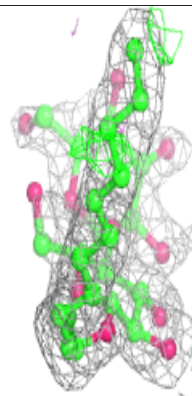
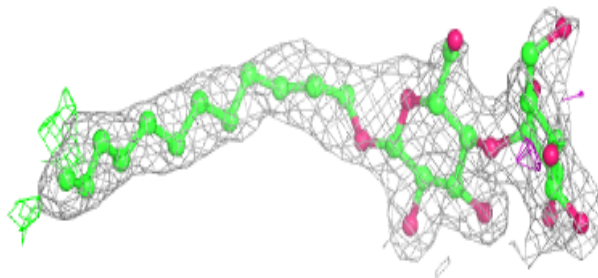
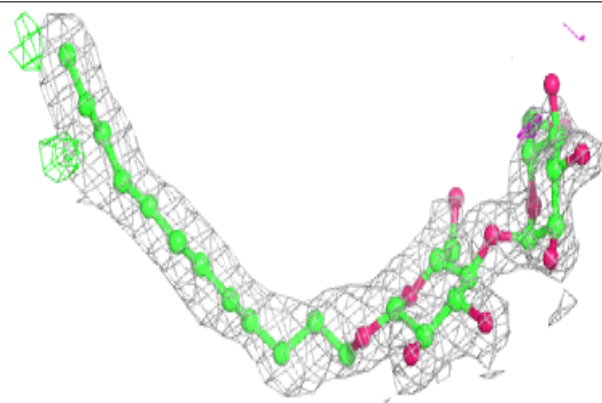


Electron density around LMT M 101:

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

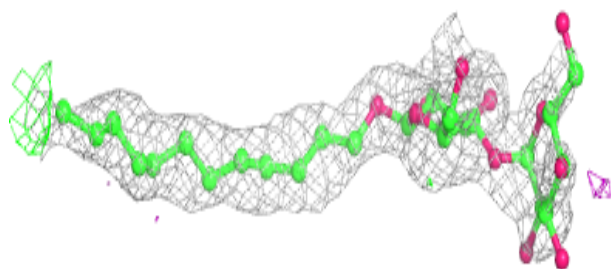
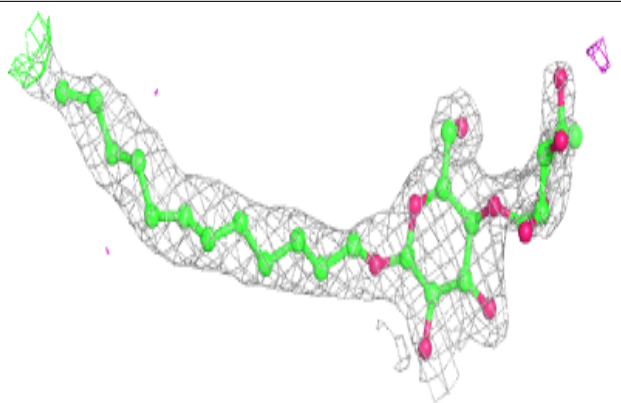
**Electron density around LMT M 102:**

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

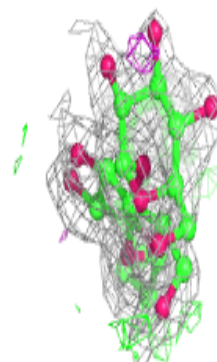
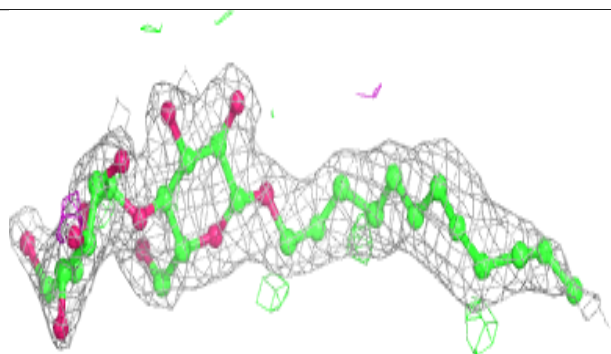
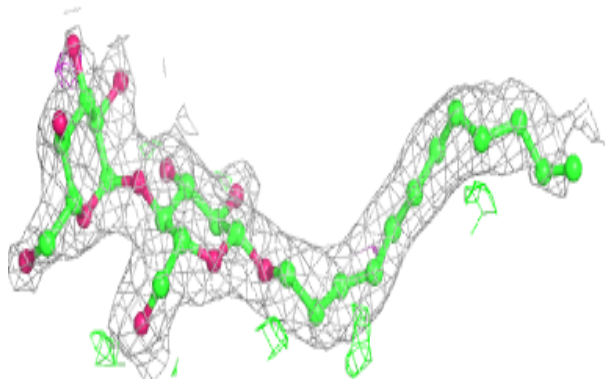


Electron density around LMT B 622:

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

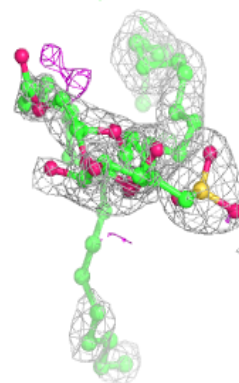
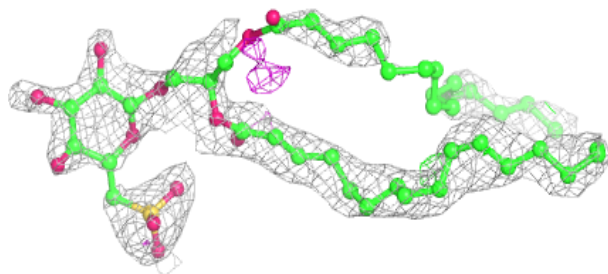
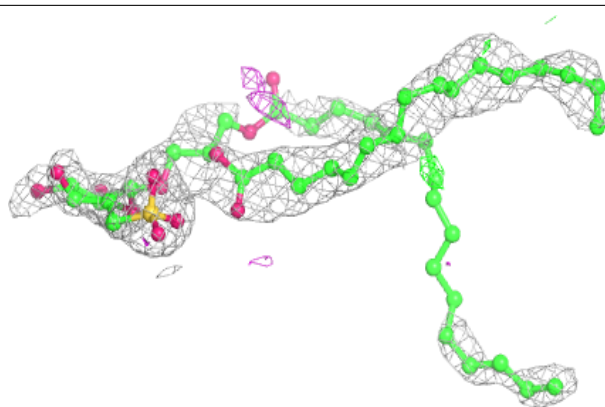
**Electron density around LMT a 401:**

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

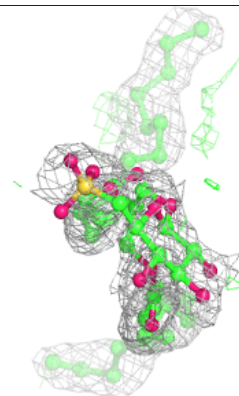
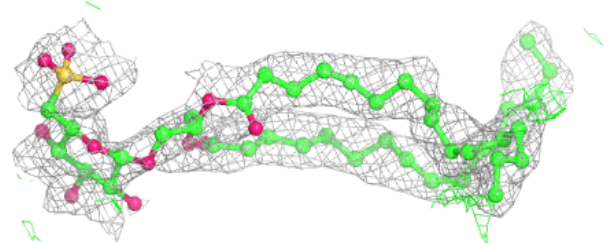
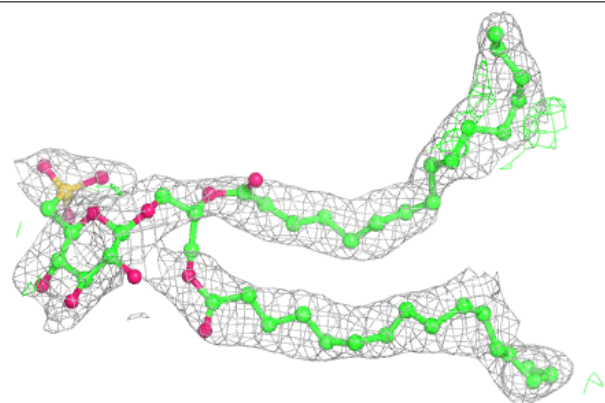


Electron density around SQD F 104:

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

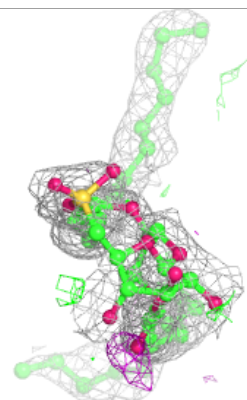
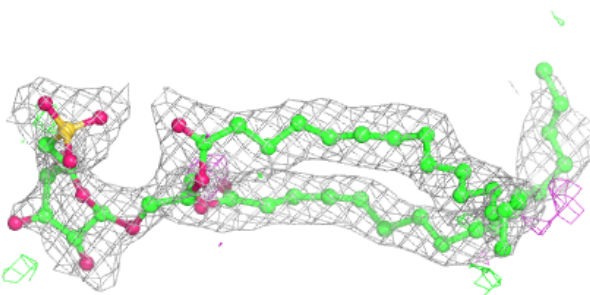
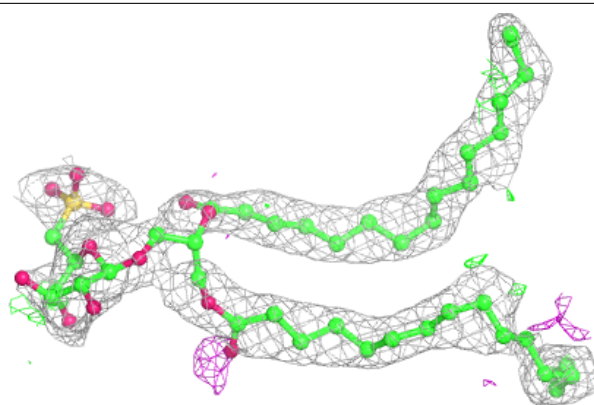
**Electron density around SQD I 102:**

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

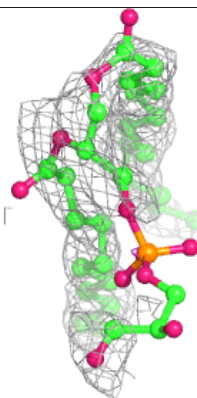
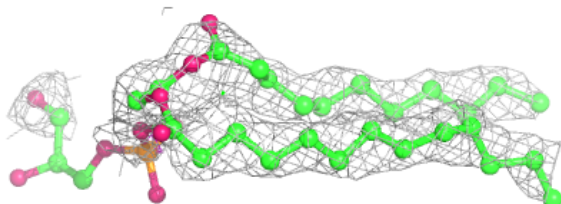
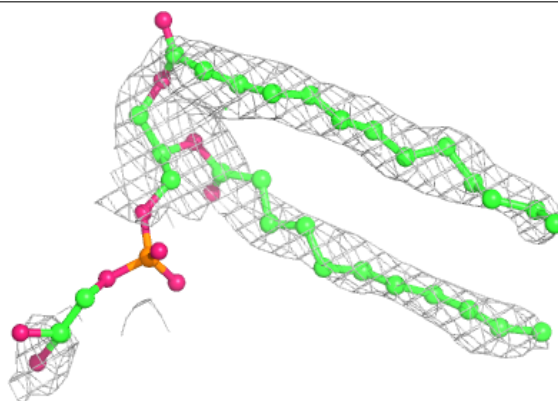


Electron density around SQD b 633:

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

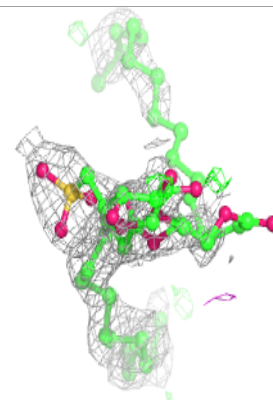
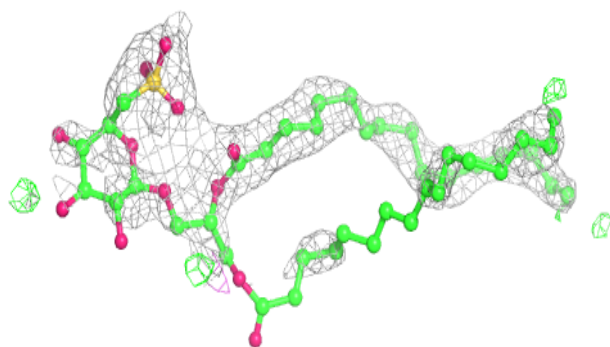
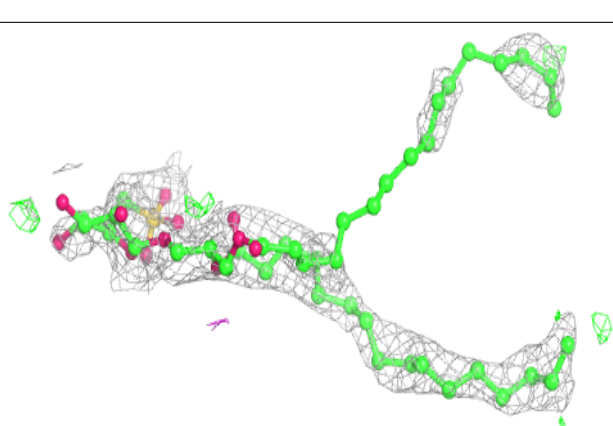
**Electron density around LHG a 419:**

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

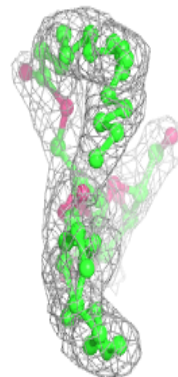
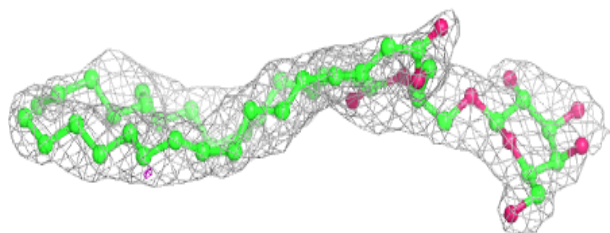
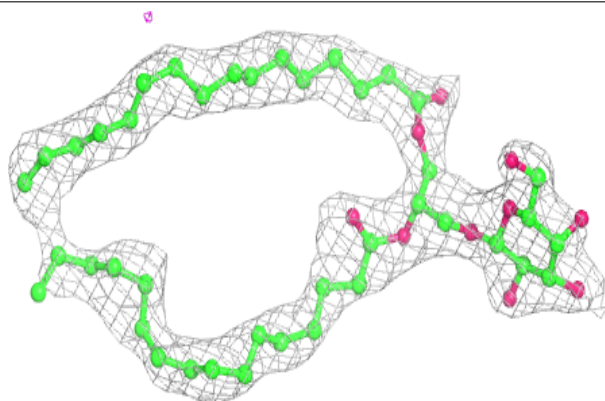


Electron density around SQD x 101:

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

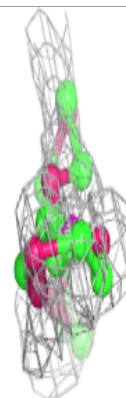
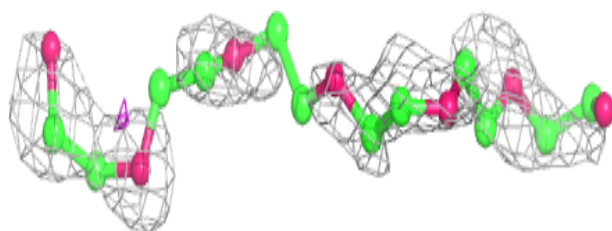
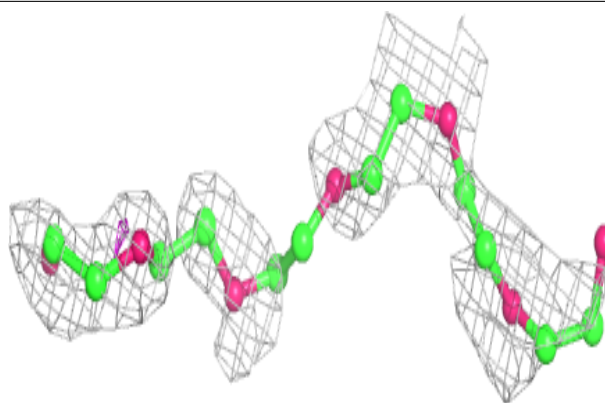
**Electron density around LMG A 613:**

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

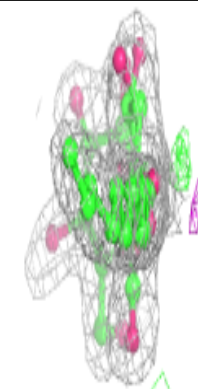
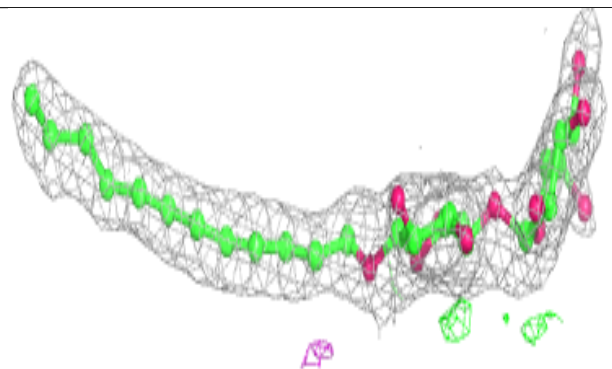
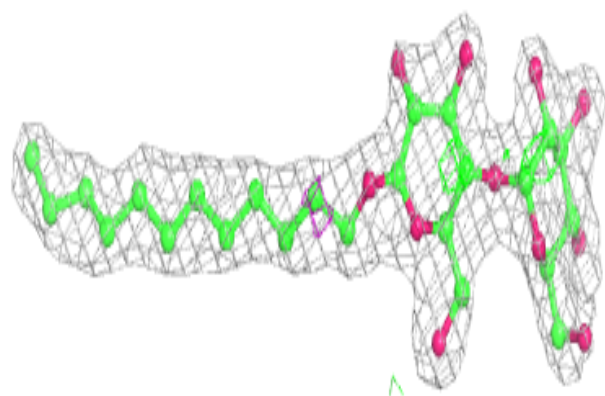


Electron density around P6G B 652:

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

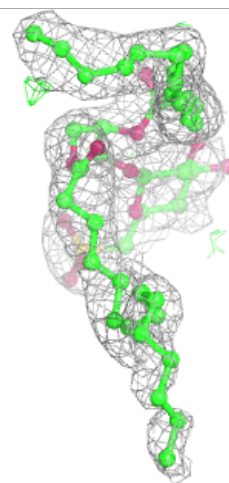
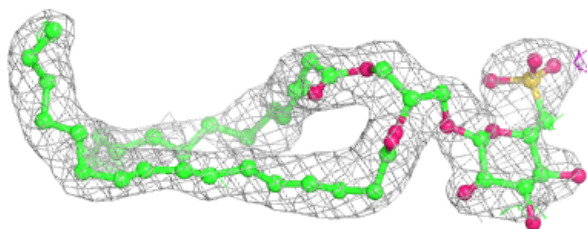
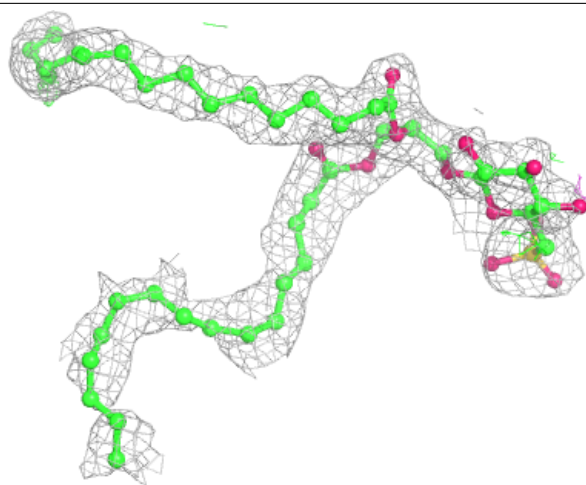
**Electron density around LMT m 102:**

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



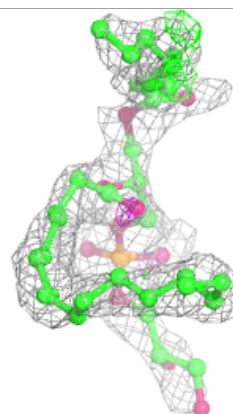
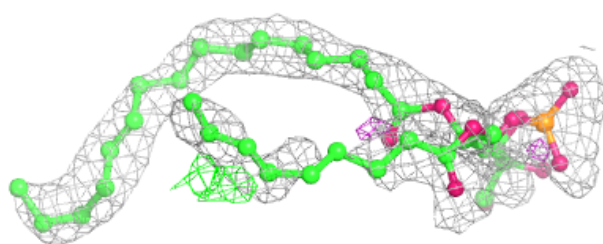
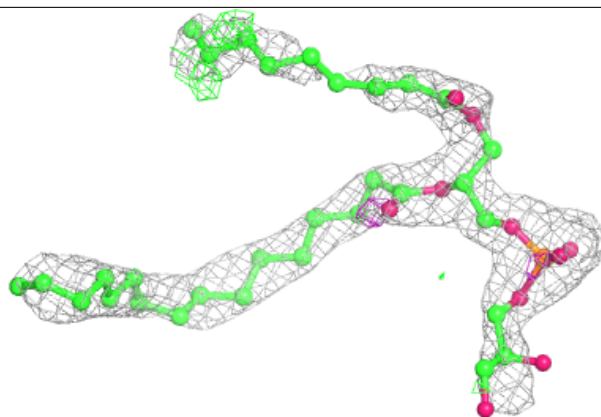
Electron density around SQD A 616:

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

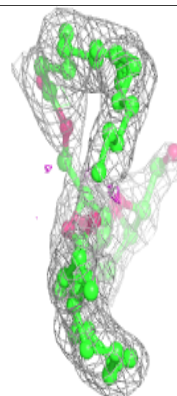
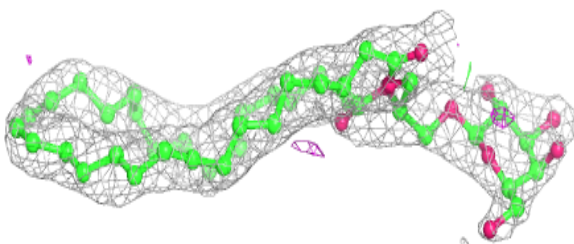
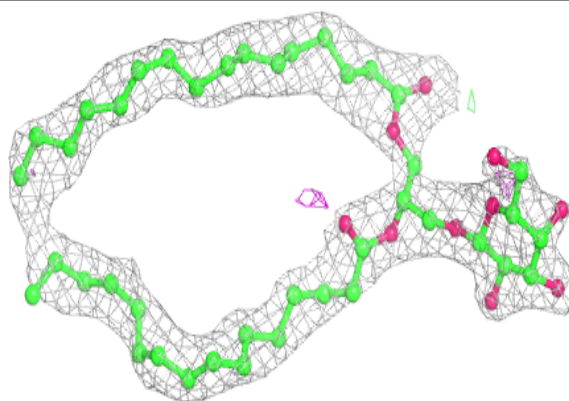


Electron density around LHG E 101:

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

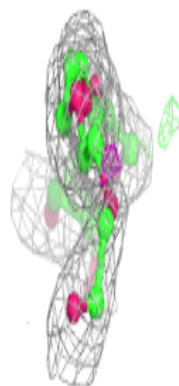
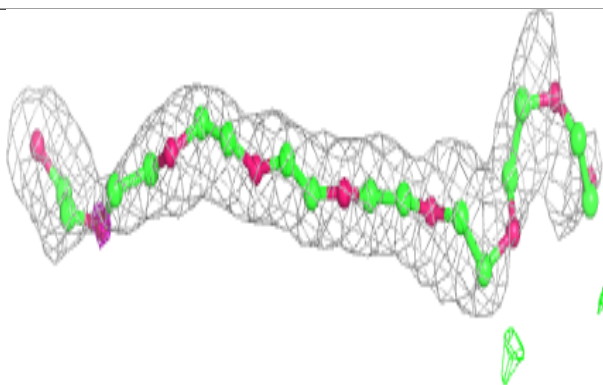
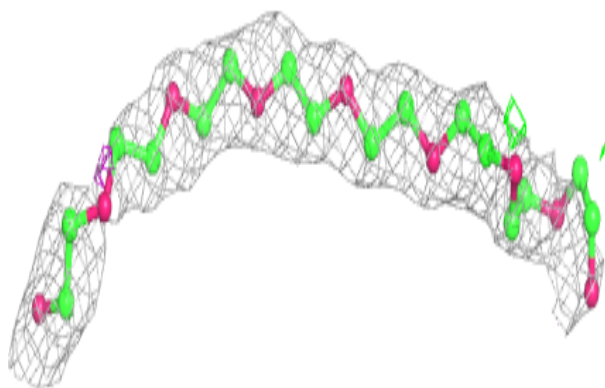
**Electron density around LMG a 414:**

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

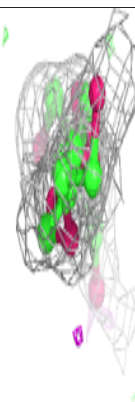
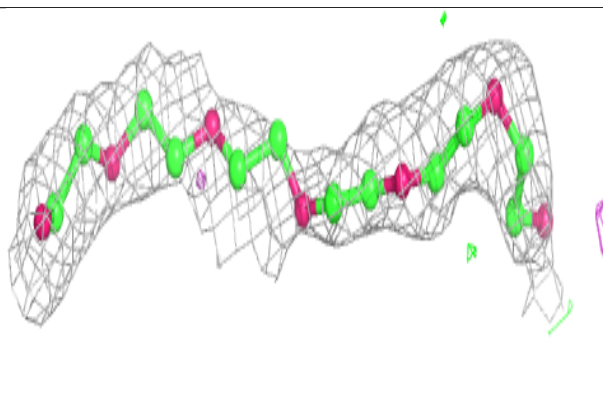
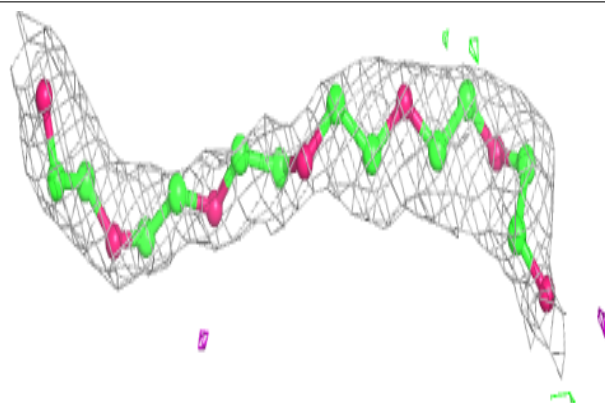


Electron density around PE8 i 107:

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

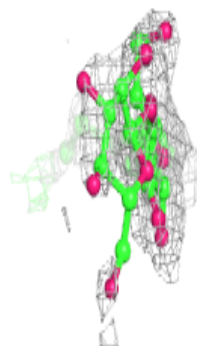
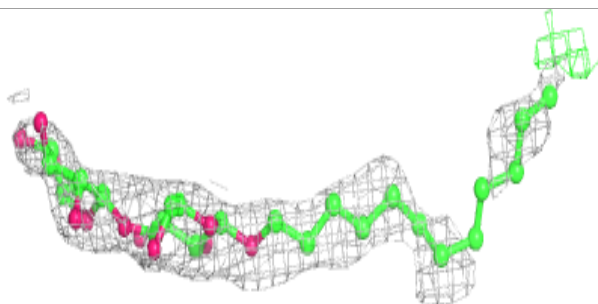
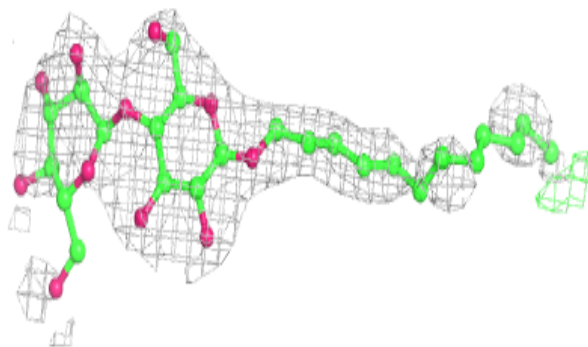
**Electron density around P6G A 624:**

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

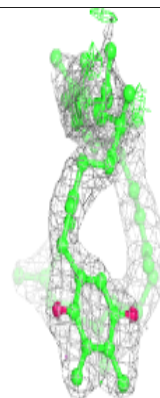
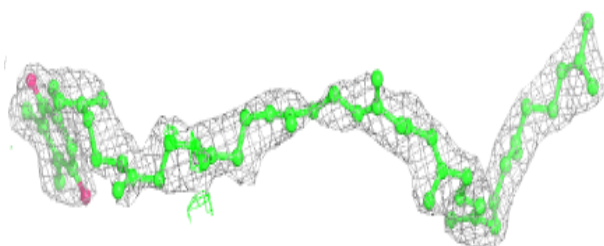
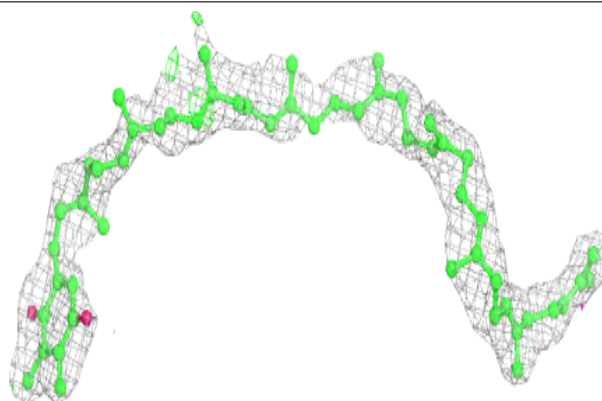


Electron density around LMT I 101:

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

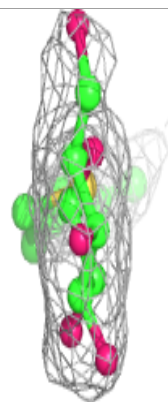
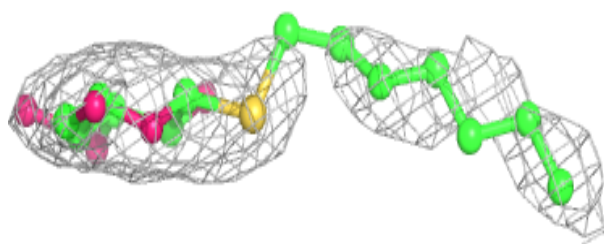
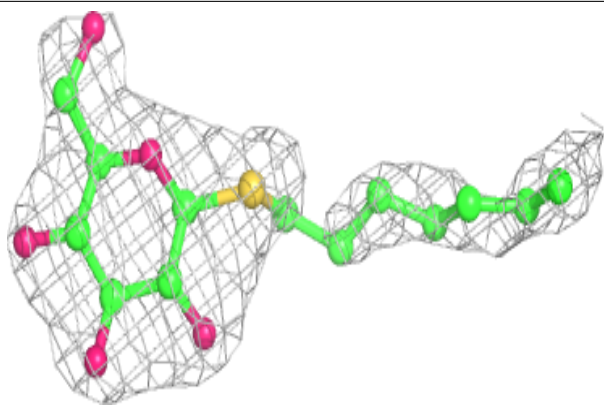
**Electron density around PL9 A 611:**

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

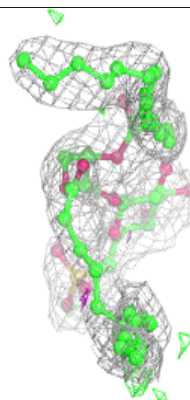
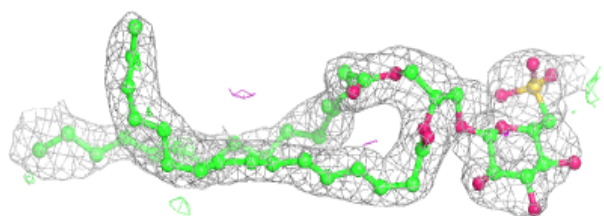
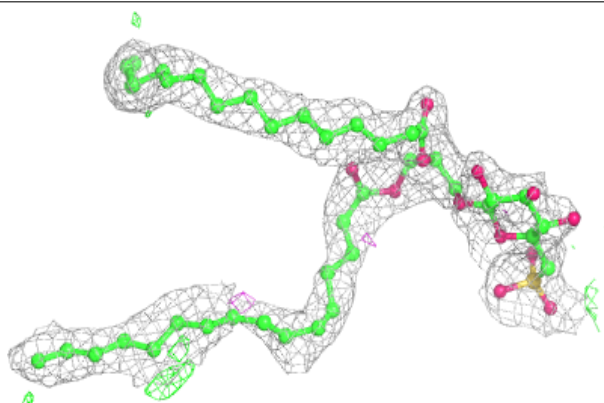


Electron density around HTG c 522:

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

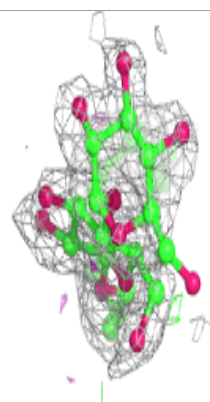
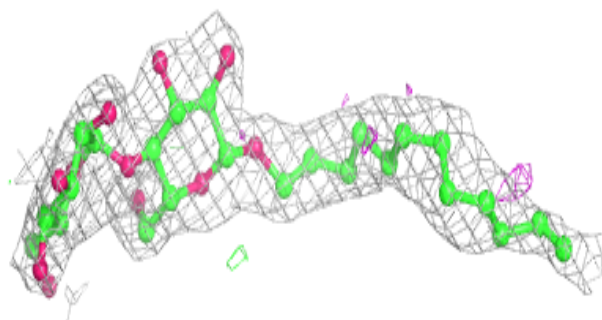
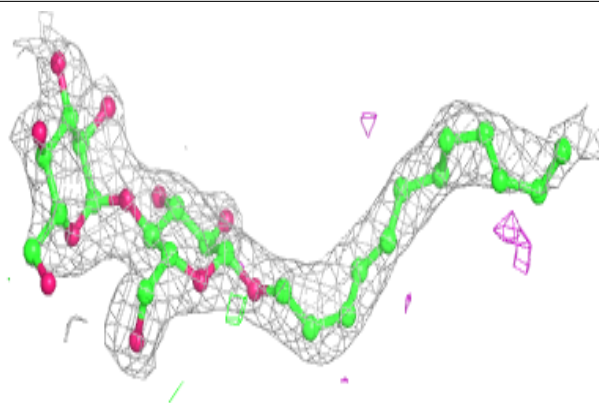
**Electron density around SQD a 417:**

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

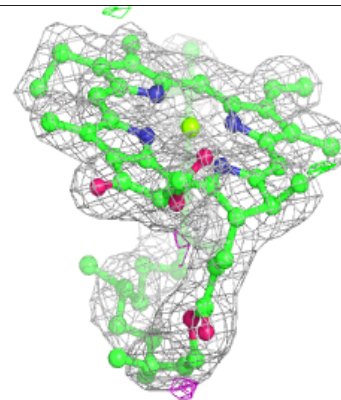
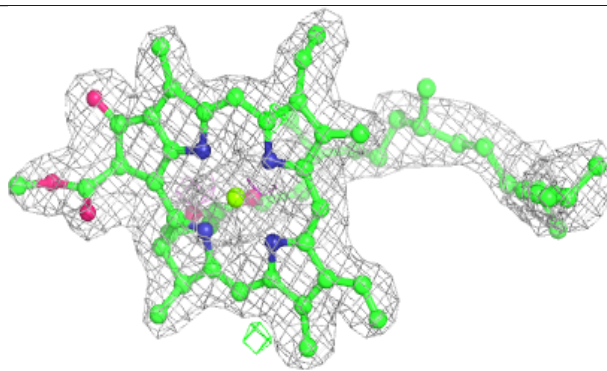
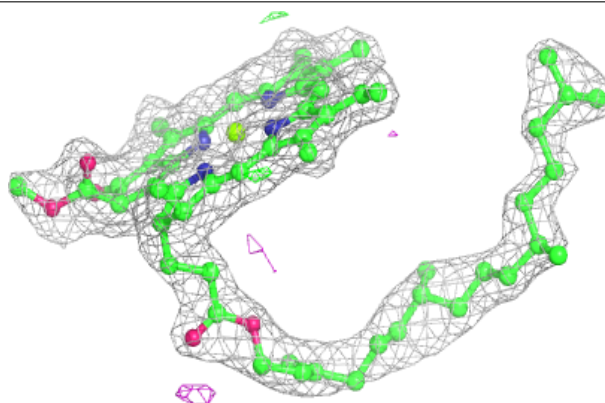


Electron density around LMT A 617:

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

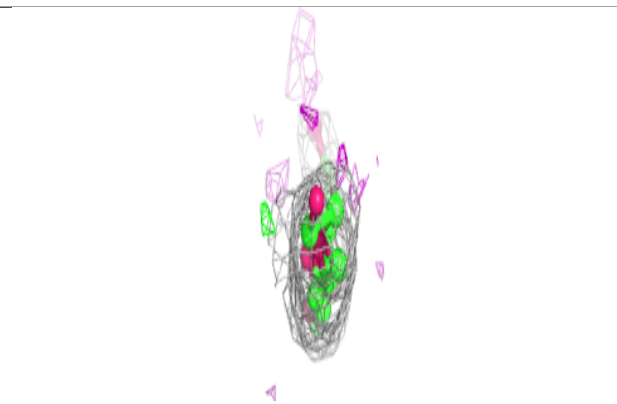
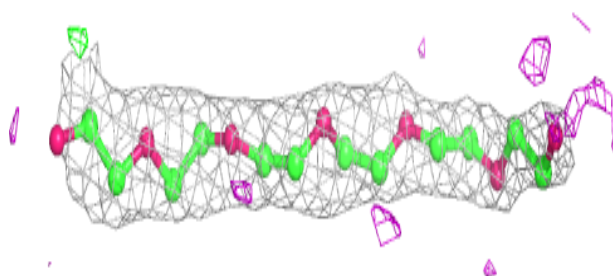
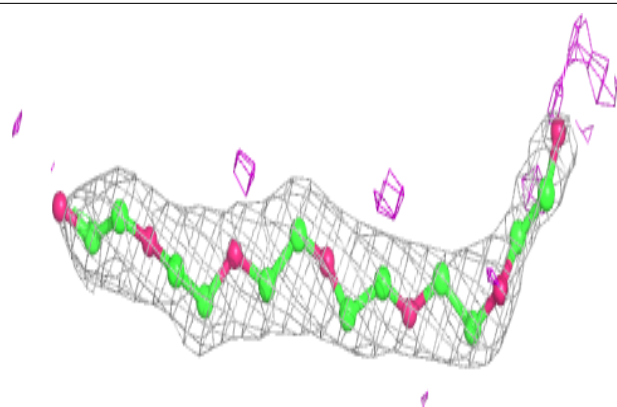
**Electron density around CLA C 513:**

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

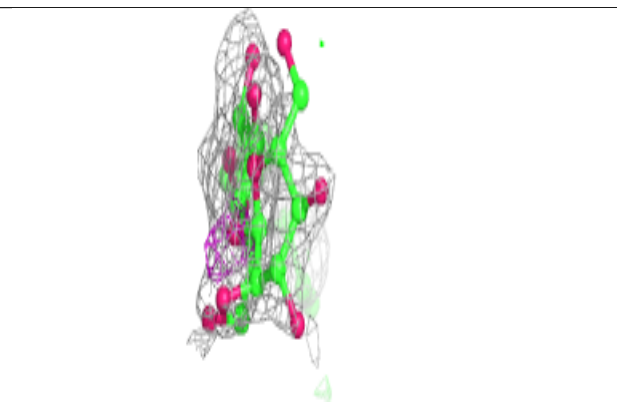
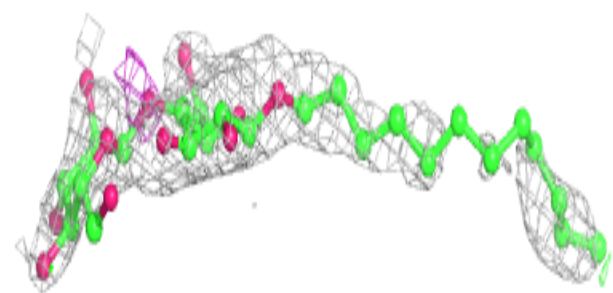
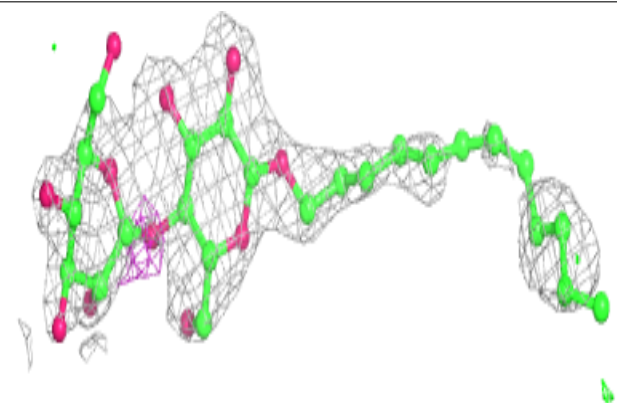


Electron density around P6G d 415:

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

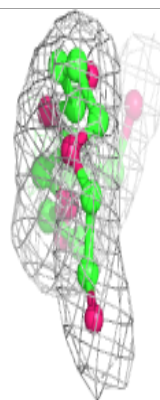
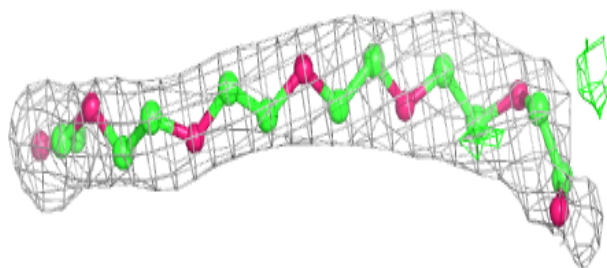
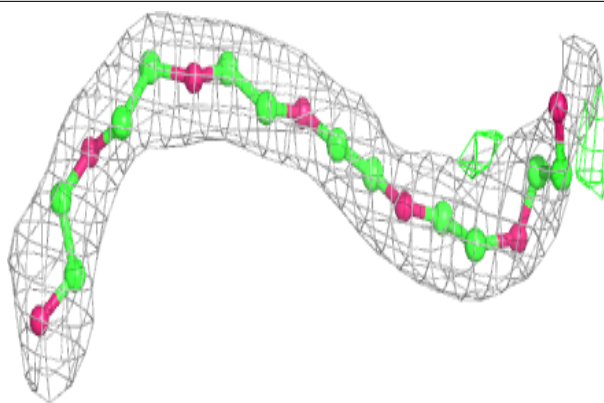
**Electron density around LMT c 521:**

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

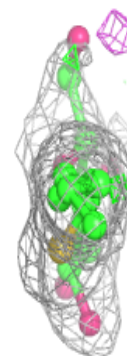
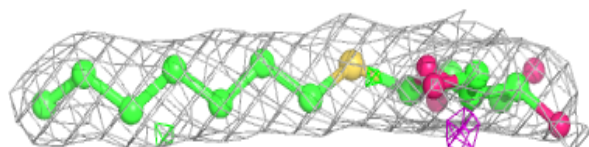
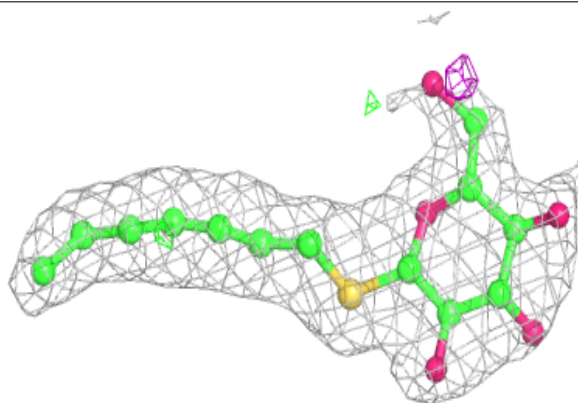


Electron density around P6G b 648:

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

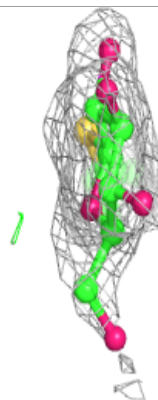
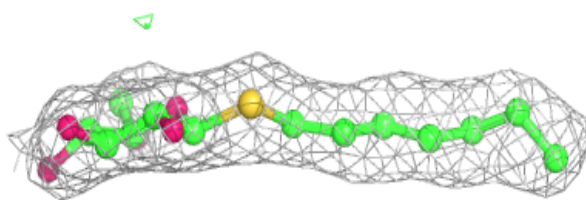
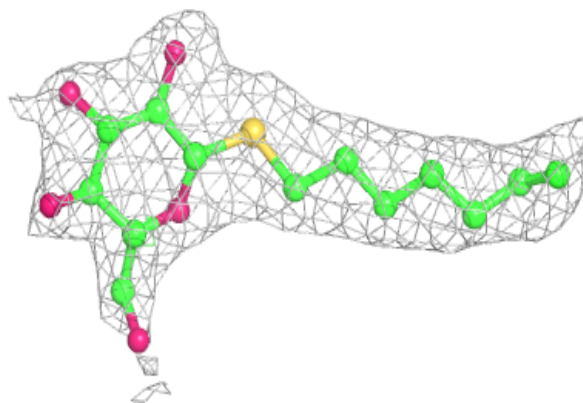
**Electron density around HTG b 631:**

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

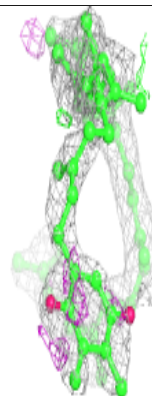
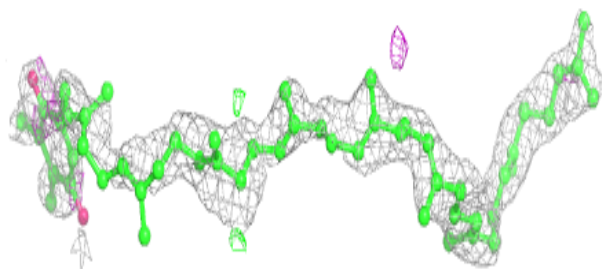
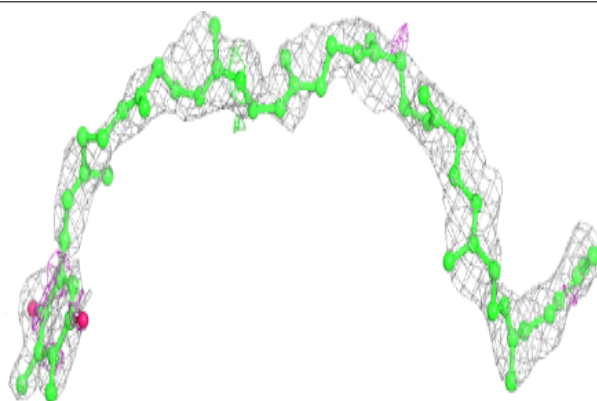


Electron density around HTG B 630:

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

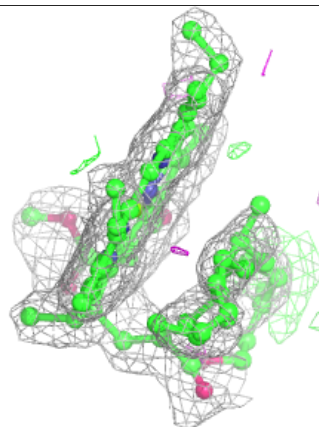
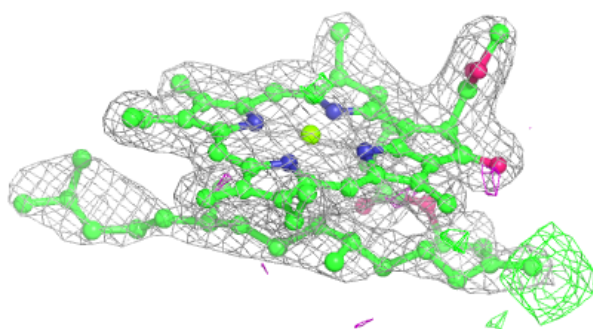
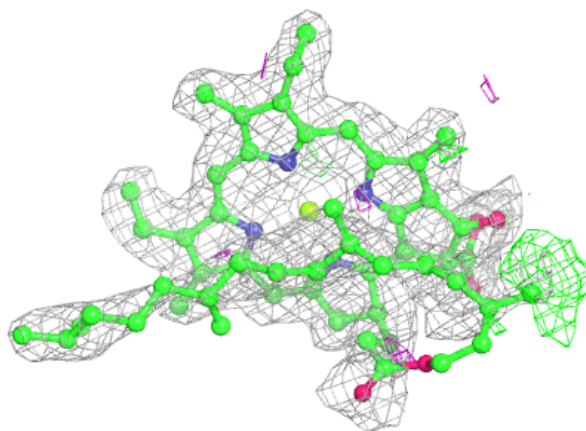
**Electron density around PL9 a 412:**

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



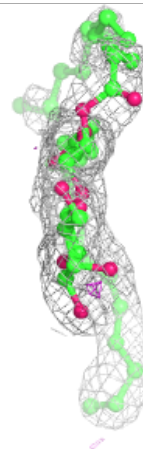
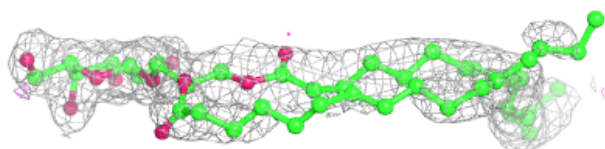
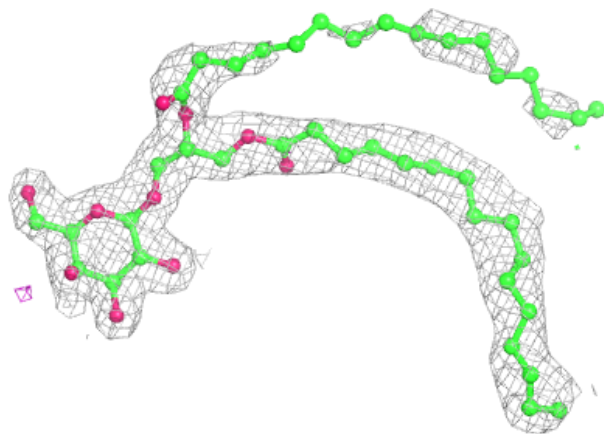
Electron density around CLA b 602:

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

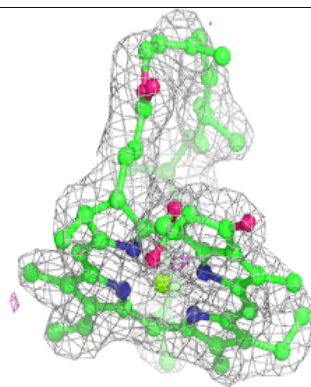
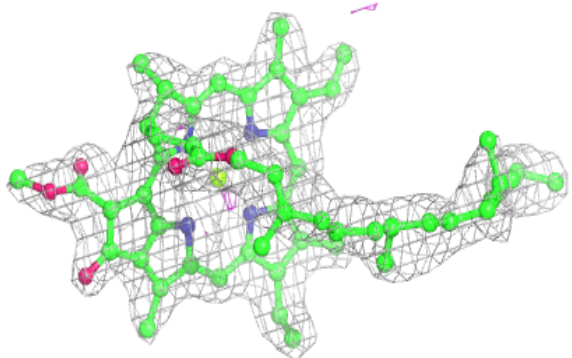
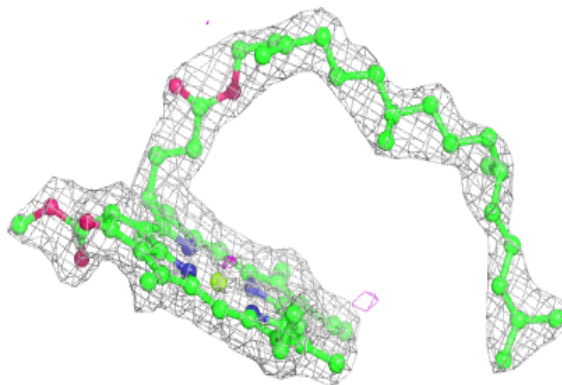


Electron density around LMG c 519:

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

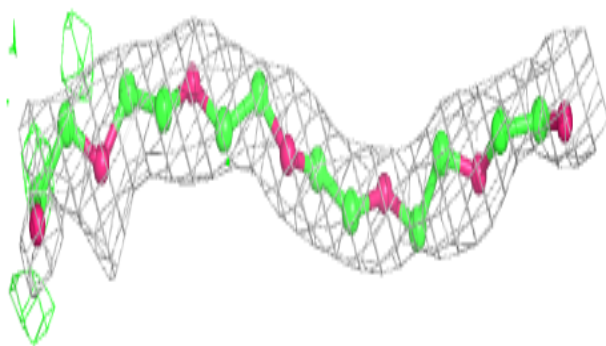
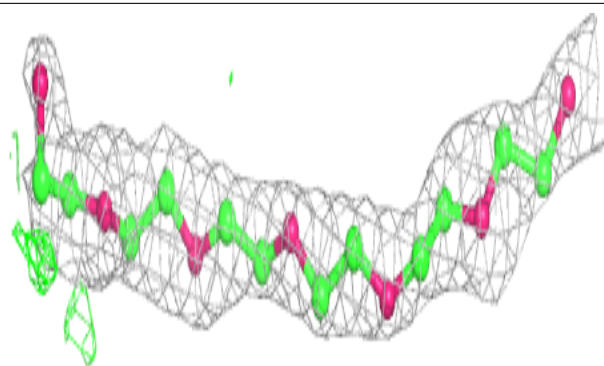
**Electron density around CLA c 513:**

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

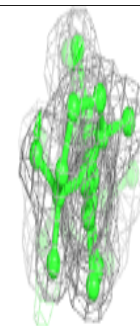
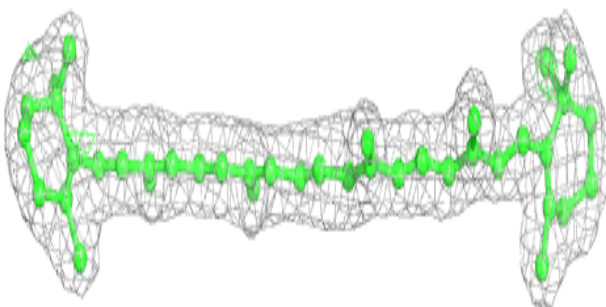
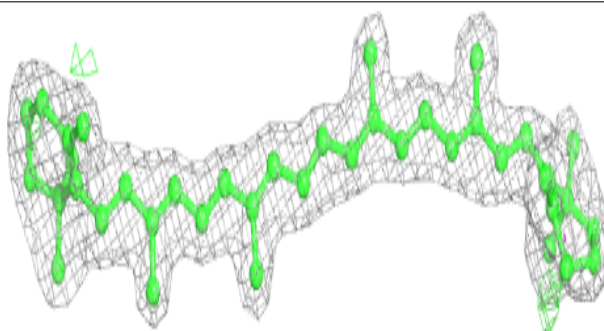


Electron density around P6G j 106:

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

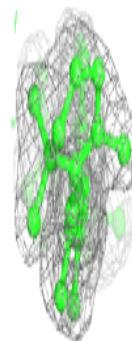
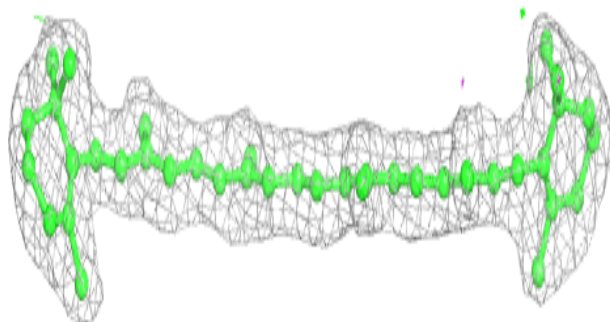
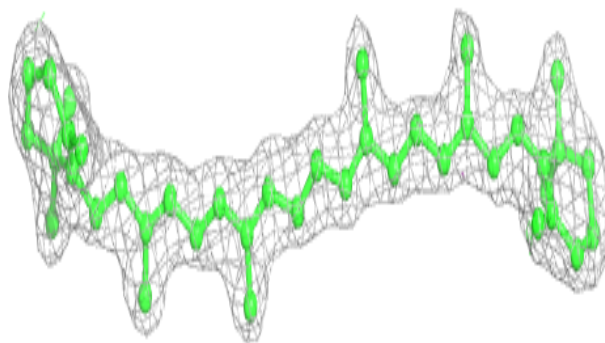
**Electron density around BCR C 514:**

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

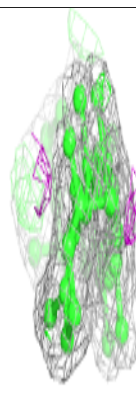
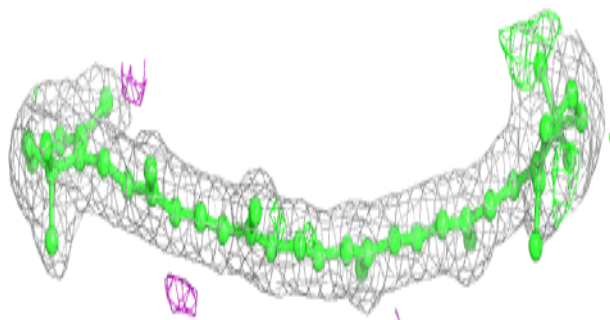
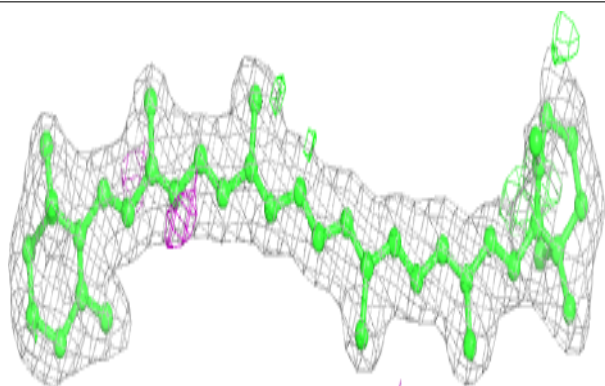


Electron density around BCR c 514:

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

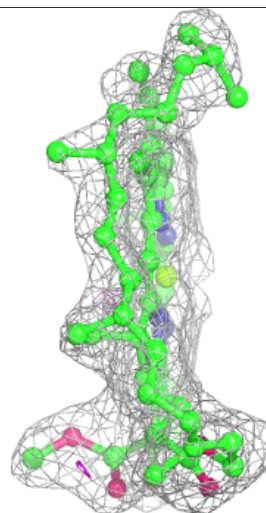
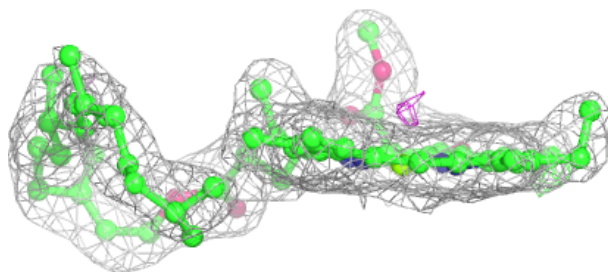
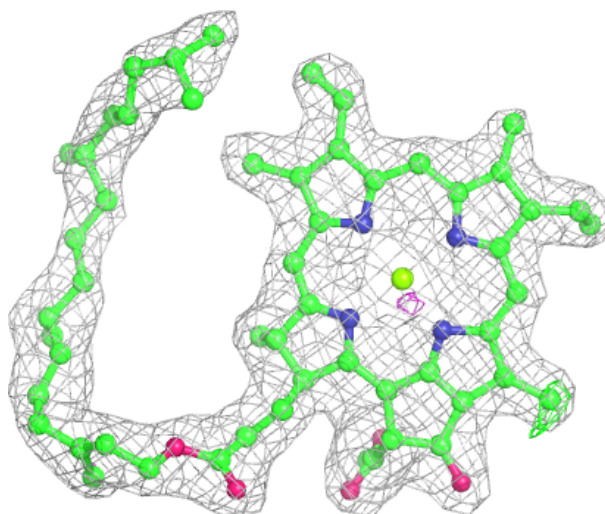
**Electron density around BCR d 406:**

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



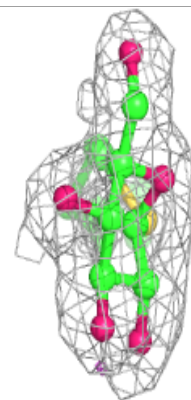
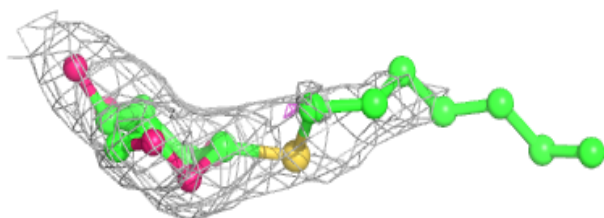
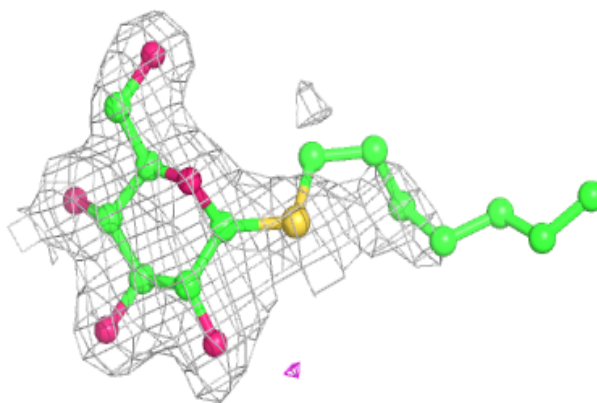
Electron density around CLA c 512:

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

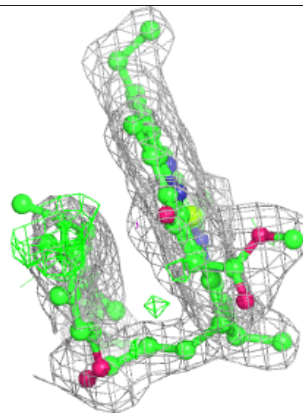
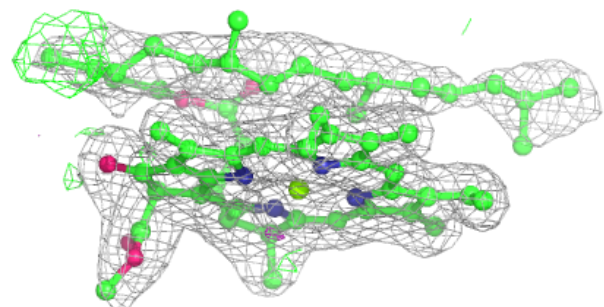
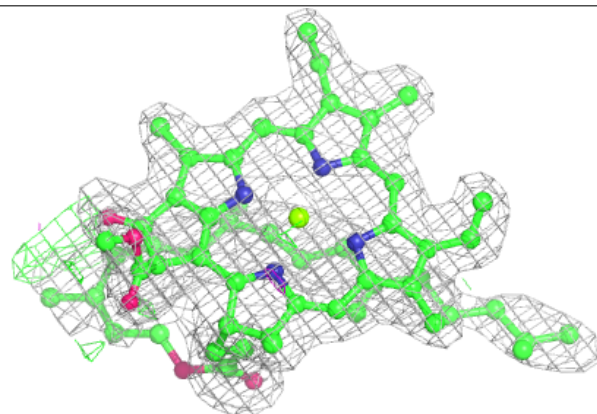


Electron density around HTG V 204:

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

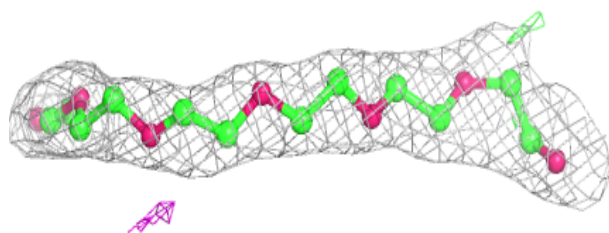
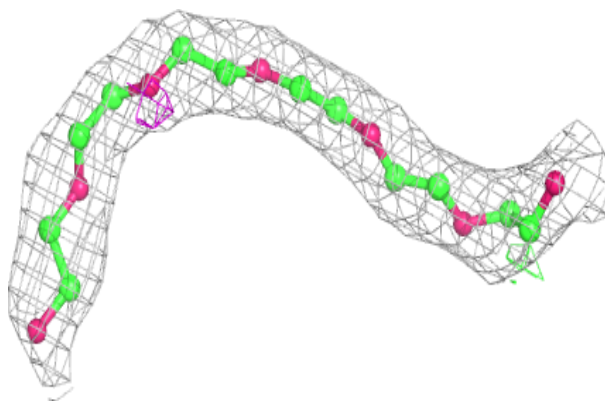
**Electron density around CLA B 602:**

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



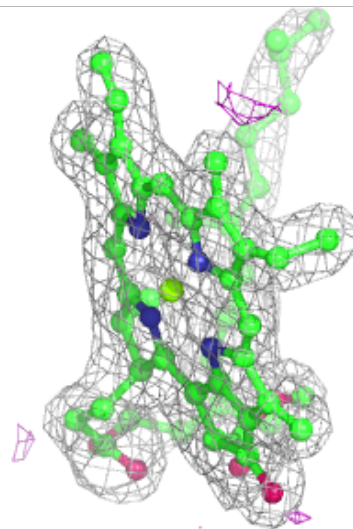
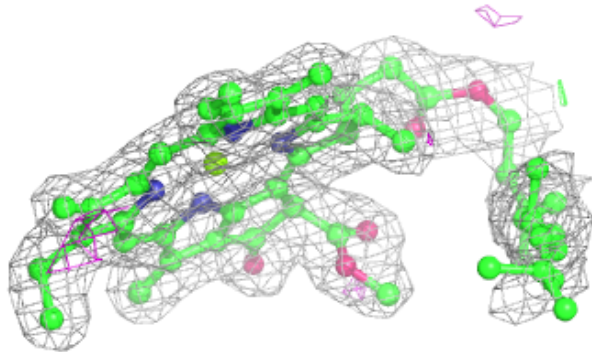
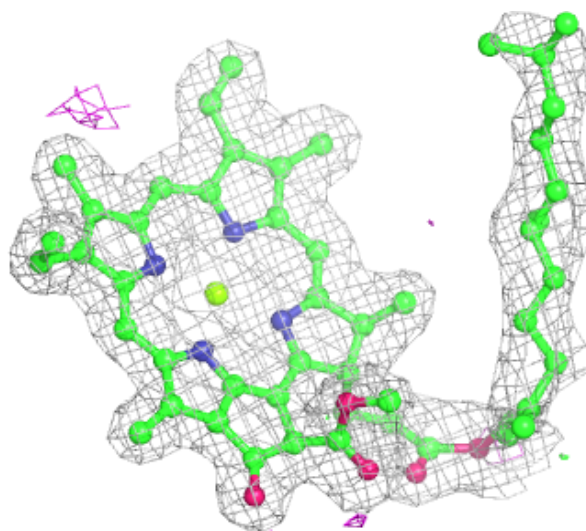
Electron density around P6G B 651:

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



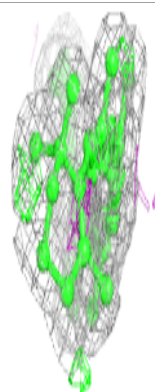
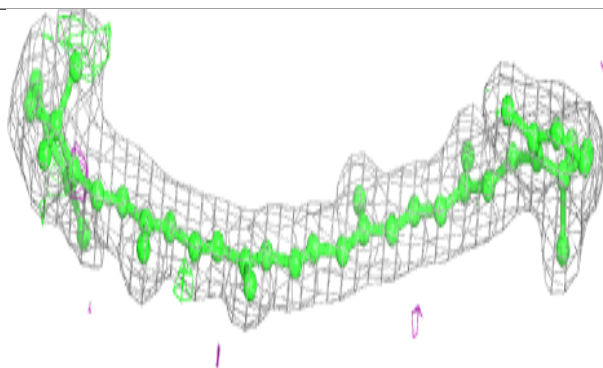
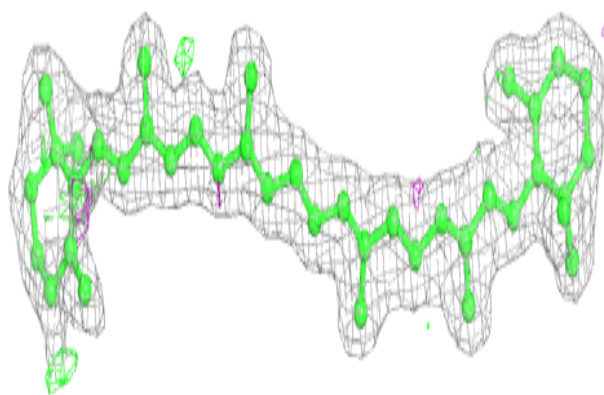
Electron density around CLA b 617:

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

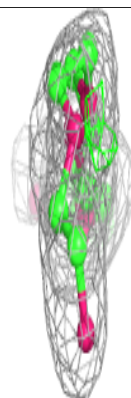
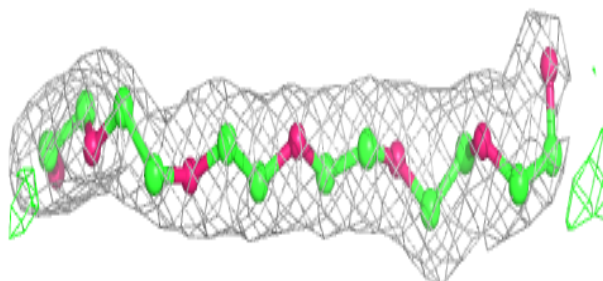
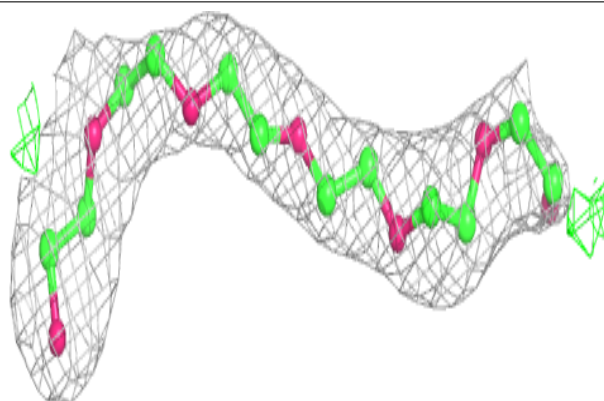


Electron density around BCR D 406:

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

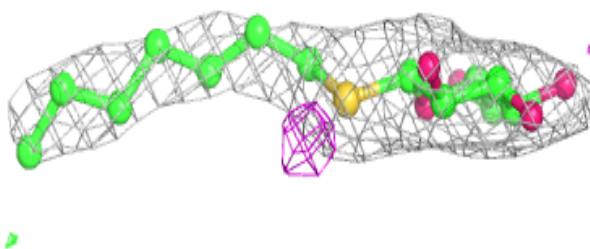
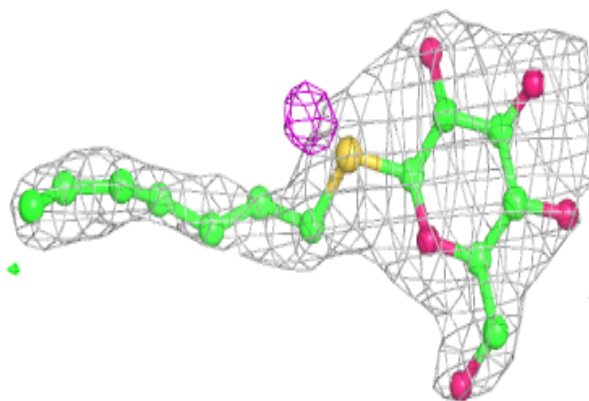
**Electron density around P6G T 105:**

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

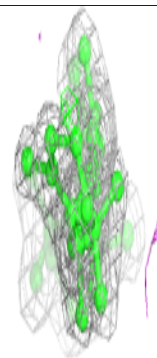
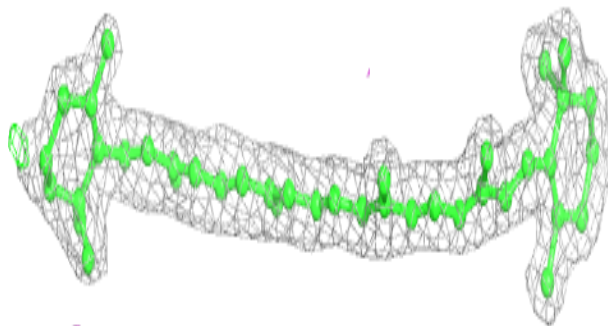
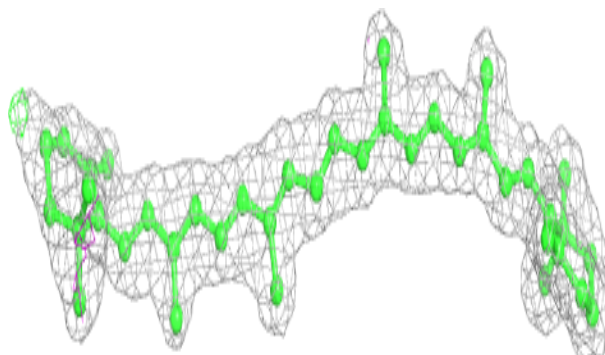


Electron density around HTG C 521:

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

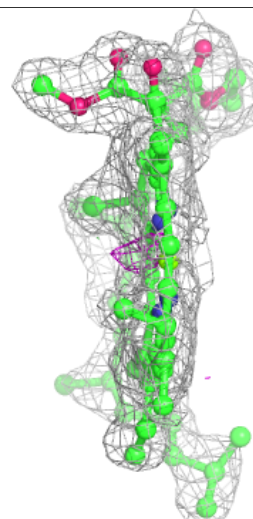
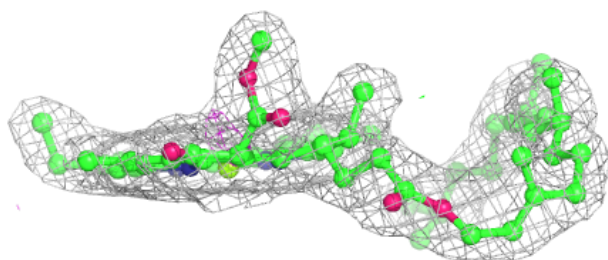
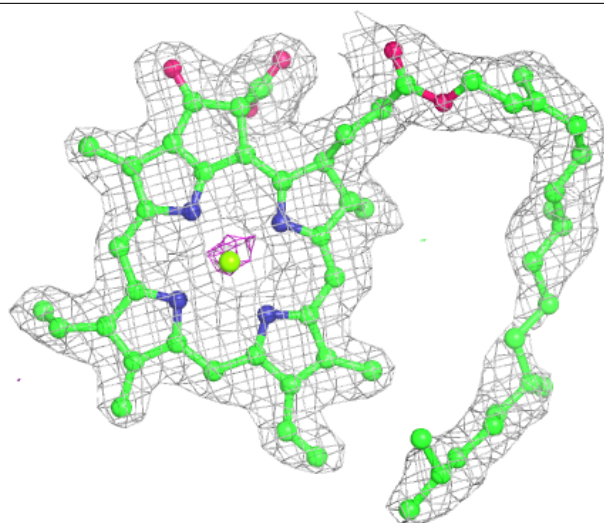
**Electron density around BCR H 102:**

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



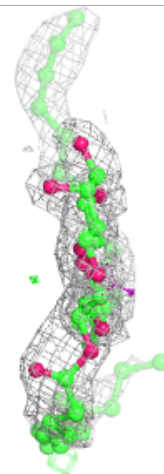
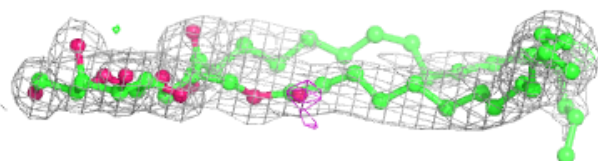
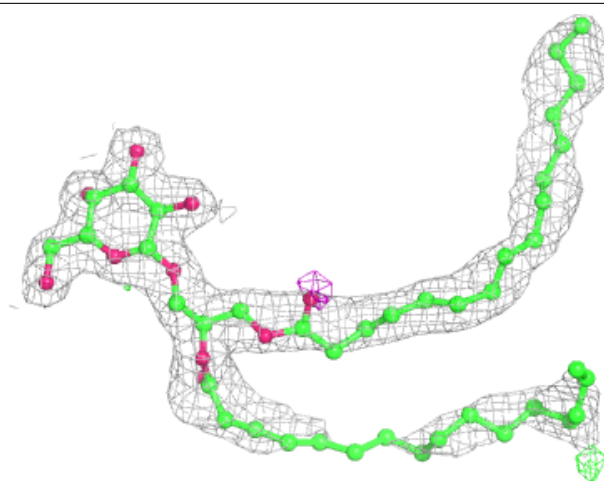
Electron density around CLA C 512:

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



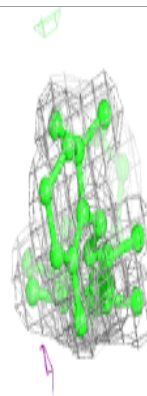
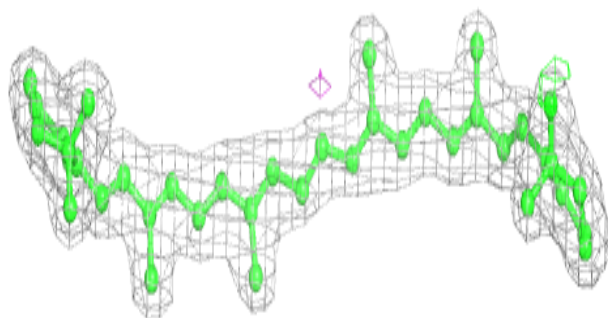
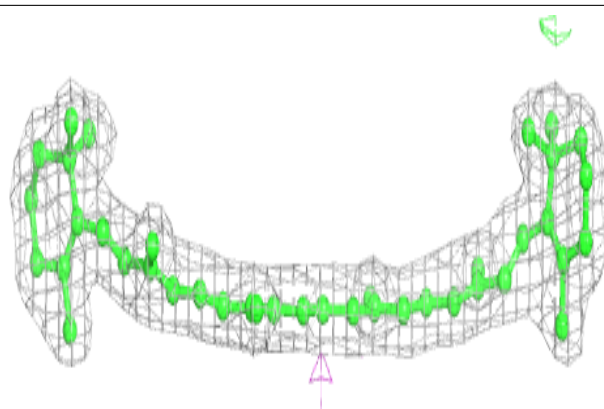
Electron density around LMG C 519:

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

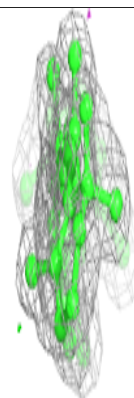
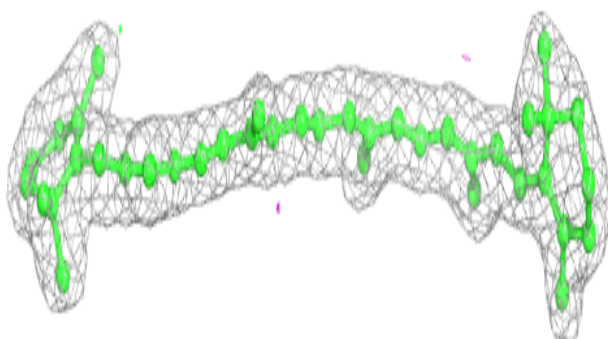
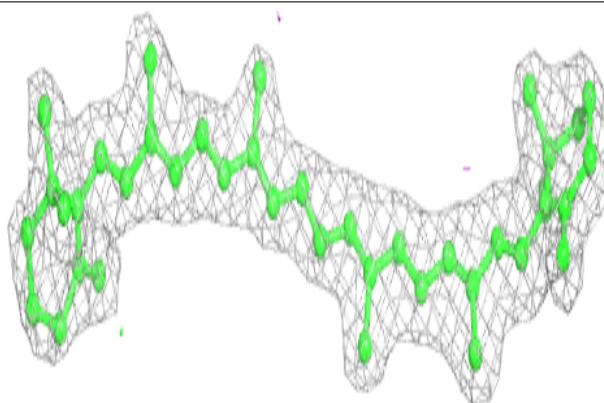


Electron density around BCR C 525:

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

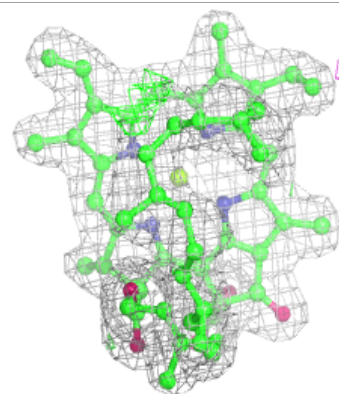
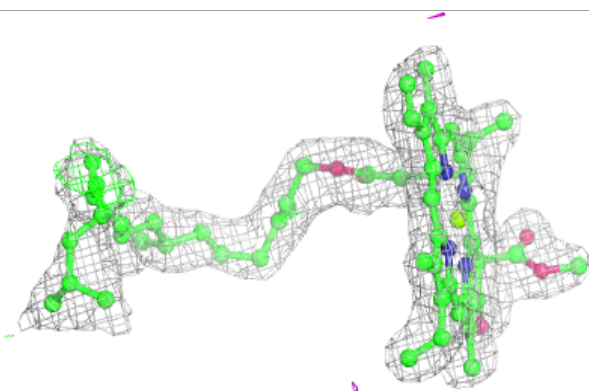
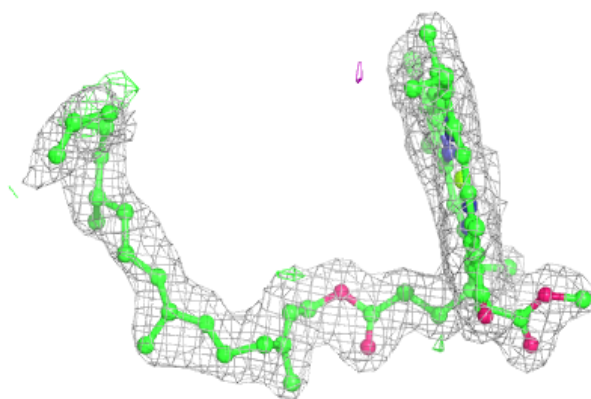
**Electron density around BCR k 101:**

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

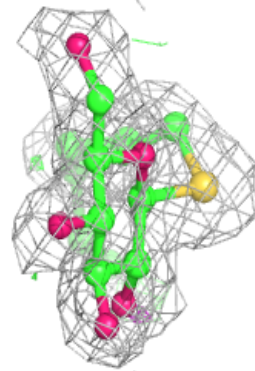
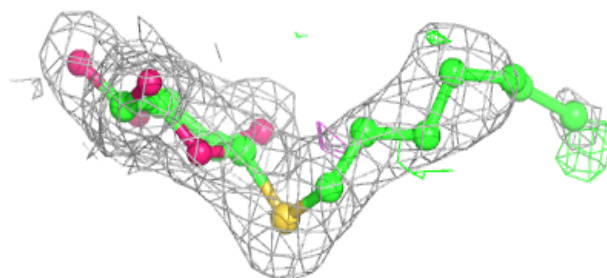
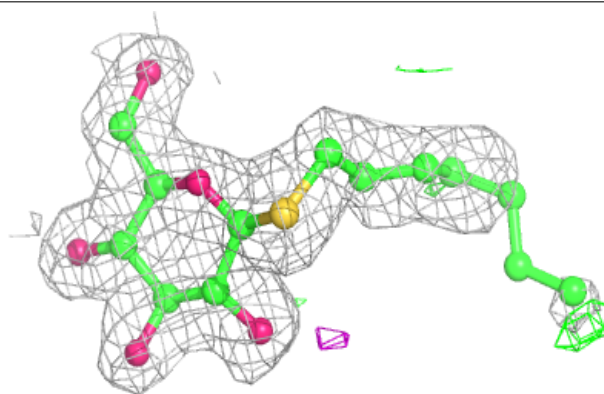


Electron density around CLA c 506:

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

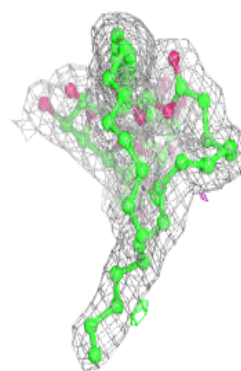
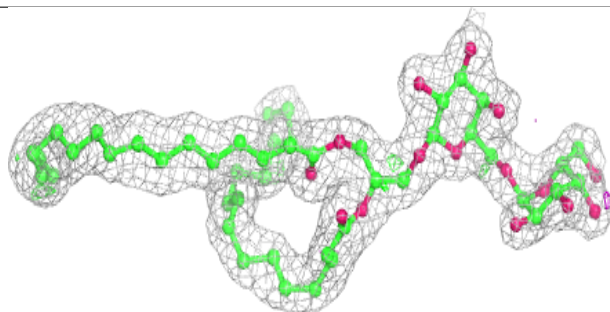
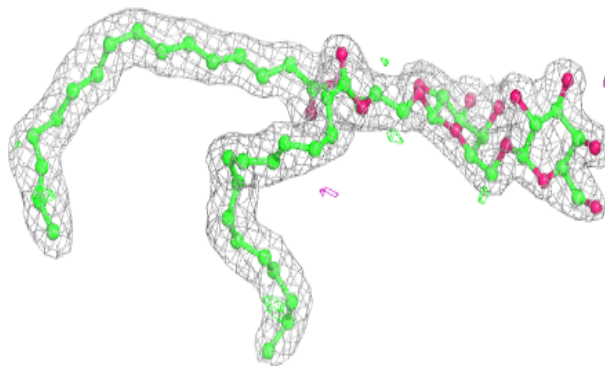
**Electron density around HTG B 623:**

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

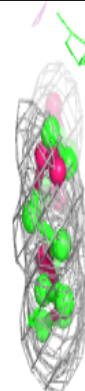
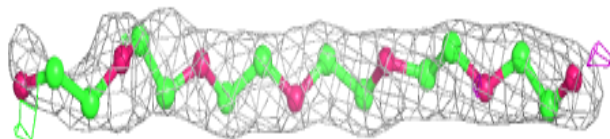
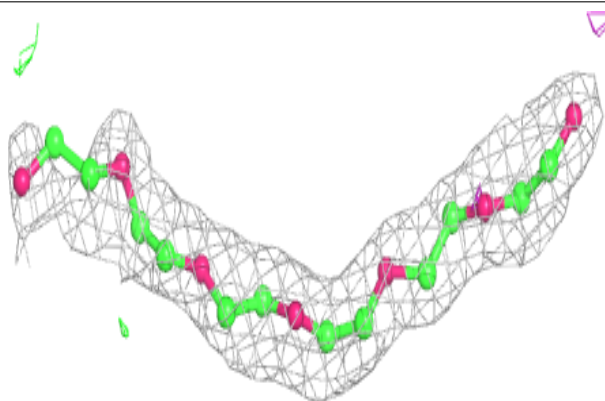


Electron density around DGD h 104:

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

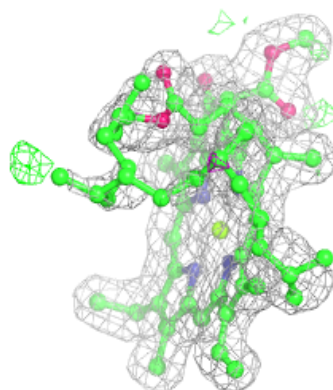
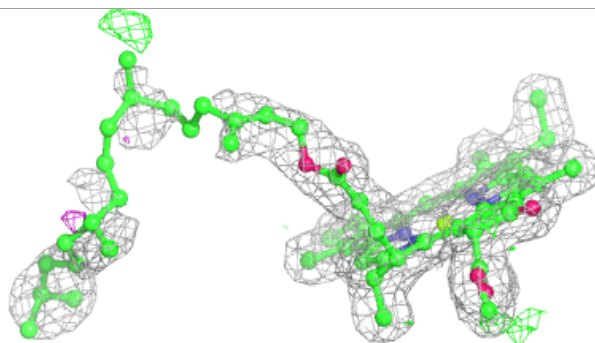
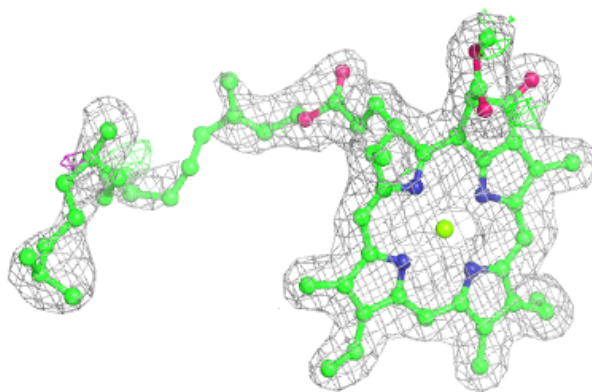
**Electron density around P6G D 417:**

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

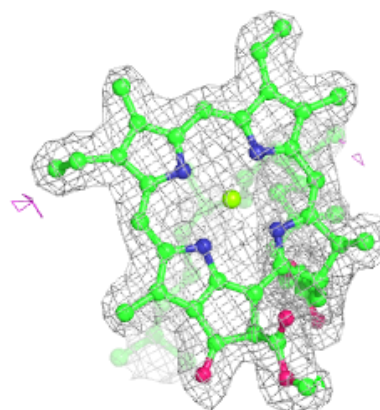
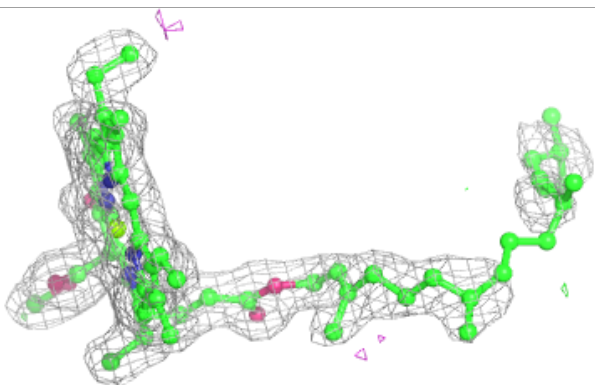
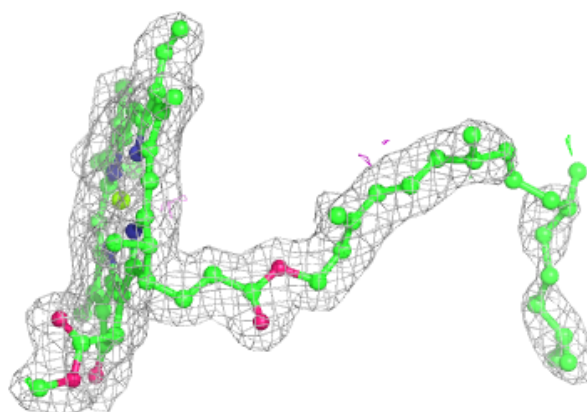


Electron density around CLA a 410:

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

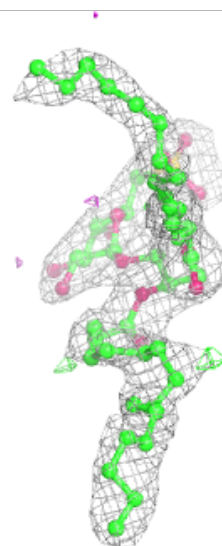
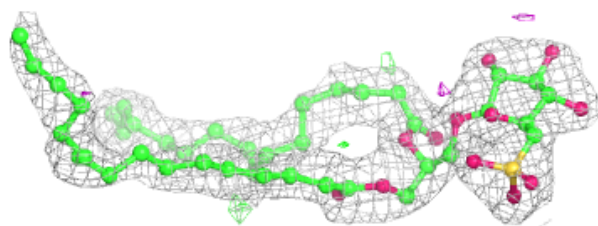
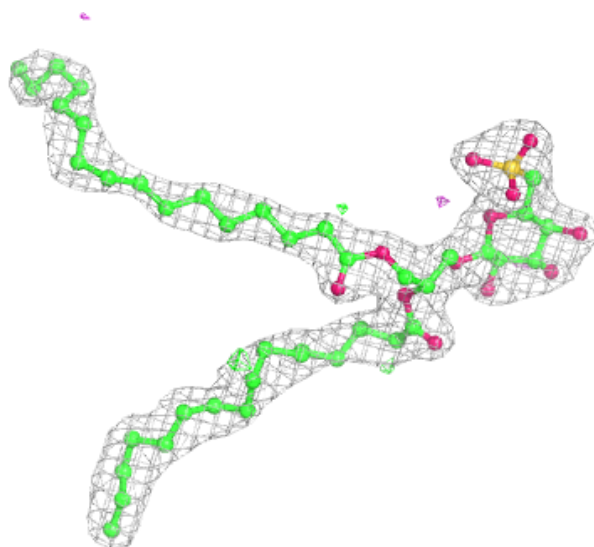
**Electron density around CLA d 405:**

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



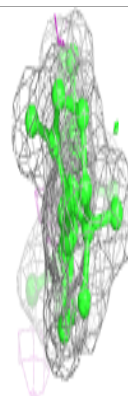
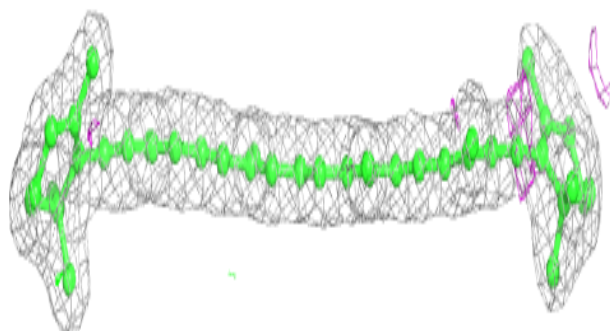
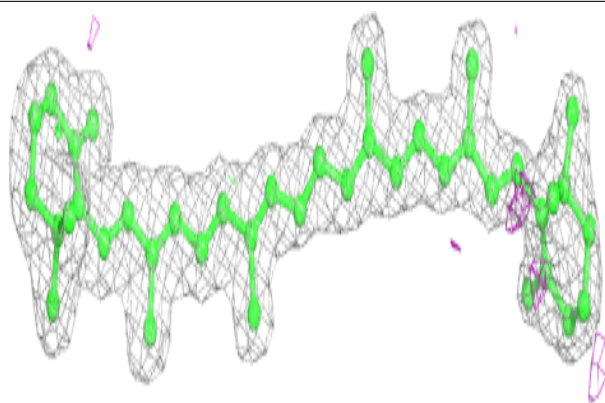
Electron density around SQD A 612:

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

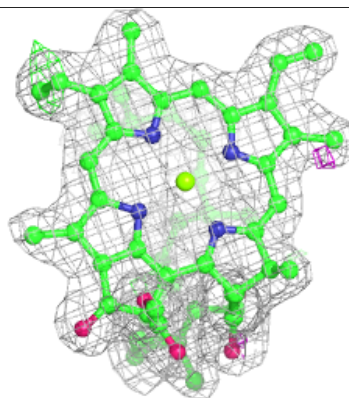
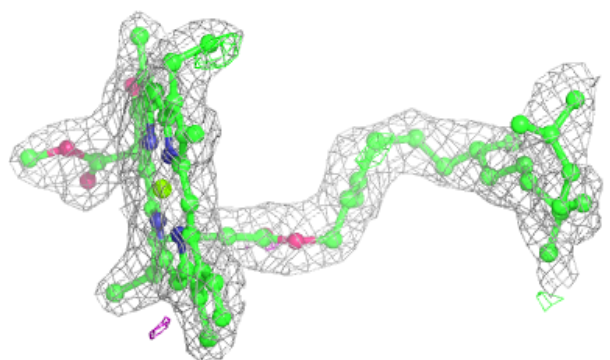
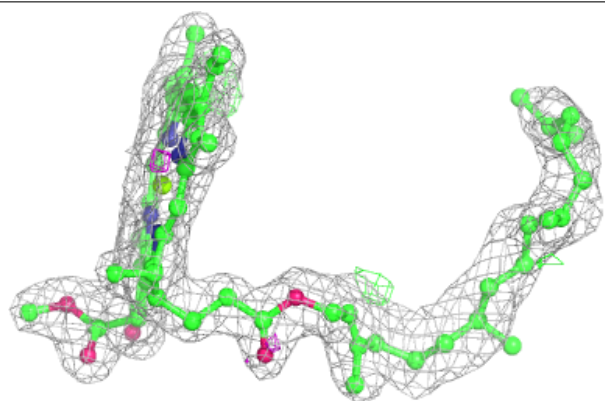


Electron density around BCR B 619:

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

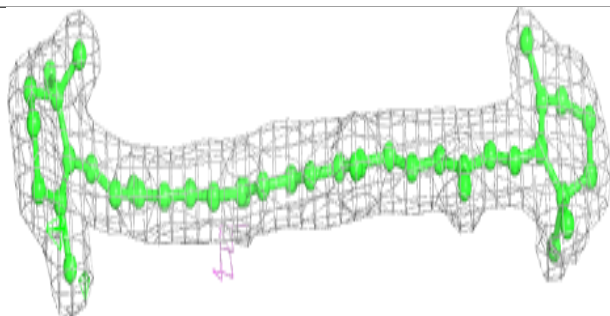
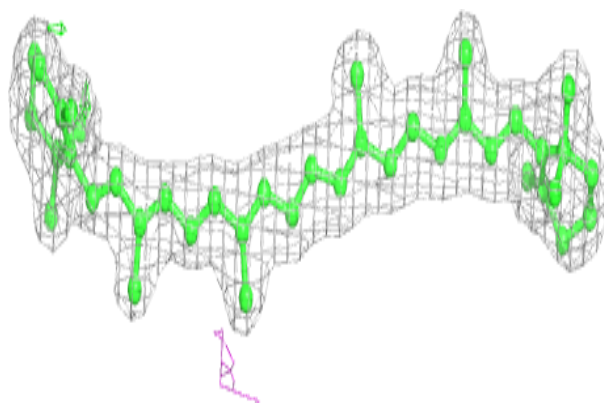
**Electron density around CLA C 506:**

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



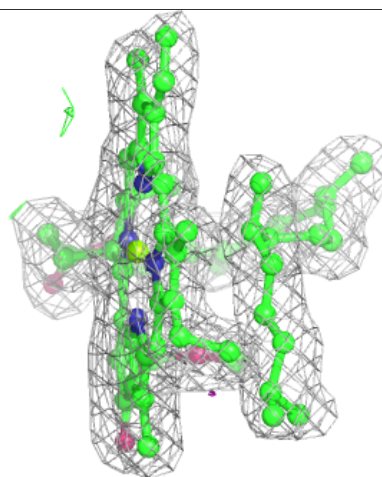
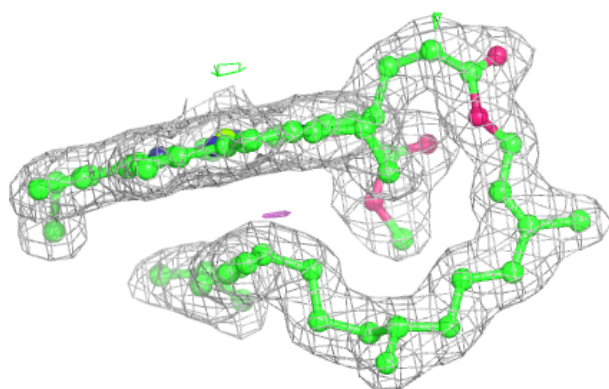
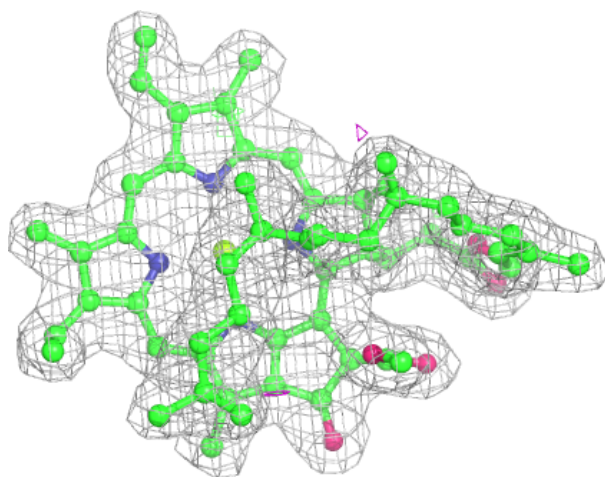
Electron density around BCR C 515:

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



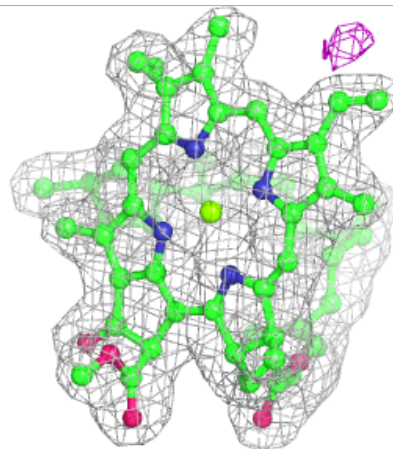
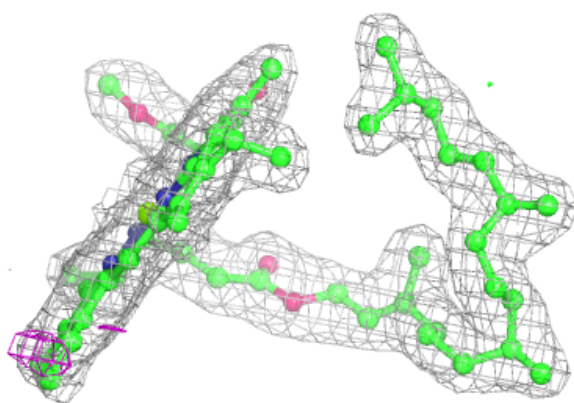
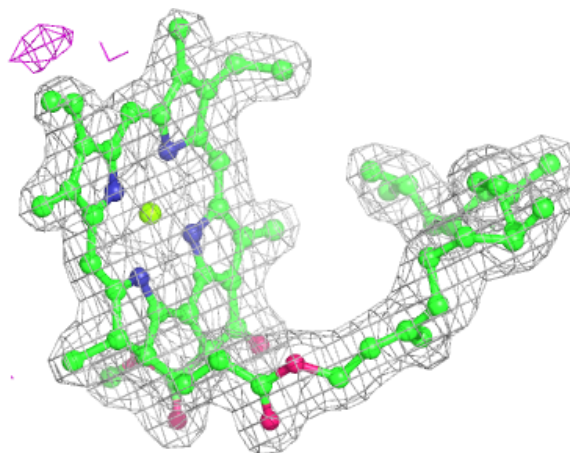
Electron density around CLA C 510:

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



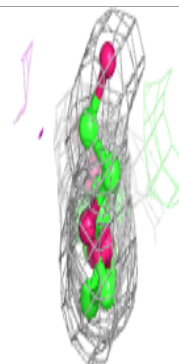
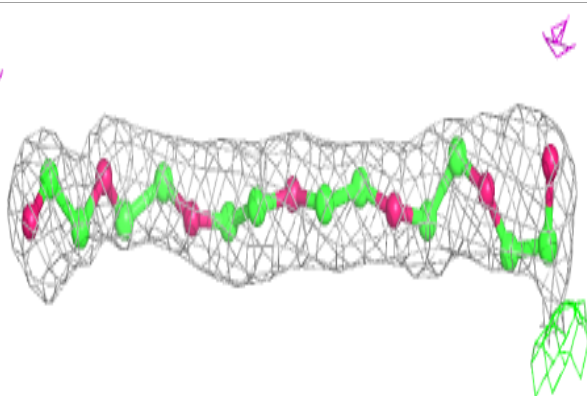
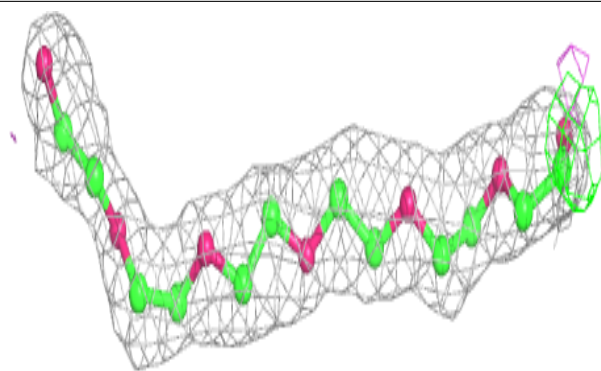
Electron density around CLA c 503:

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

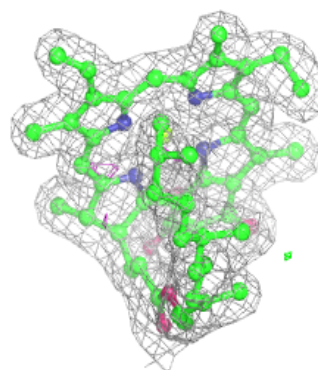
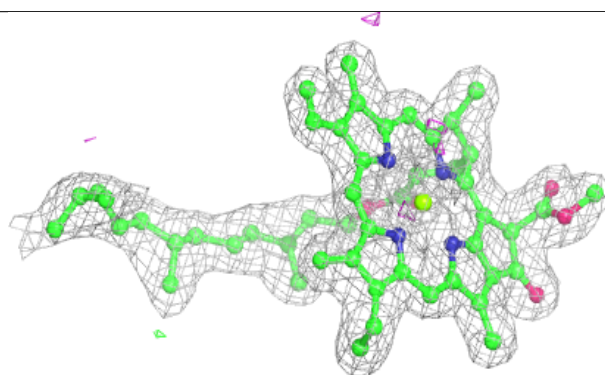
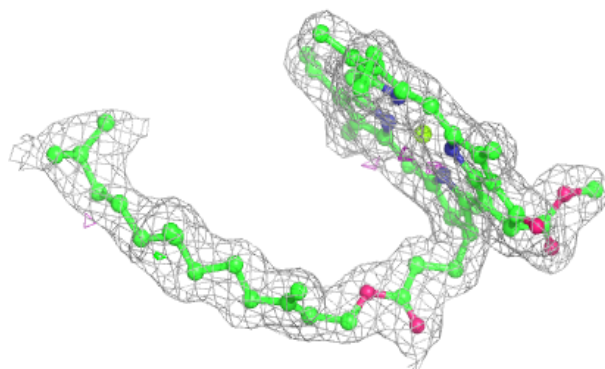


Electron density around P6G D 416:

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

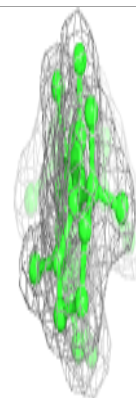
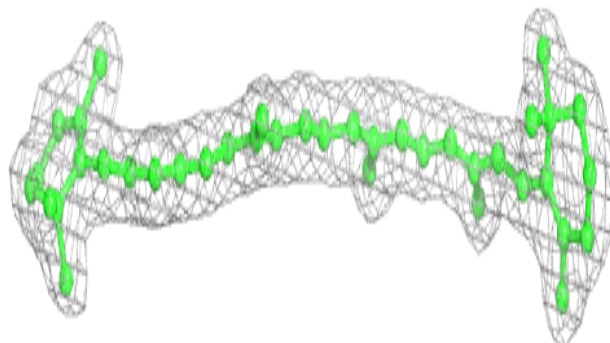
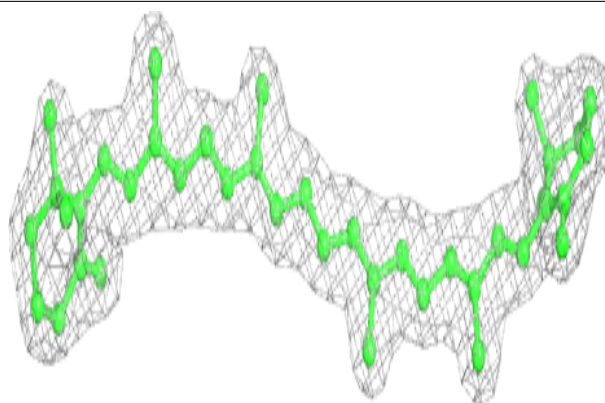
**Electron density around CLA c 504:**

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

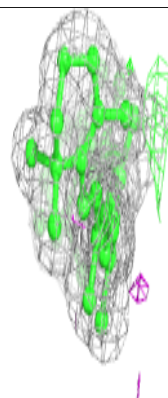
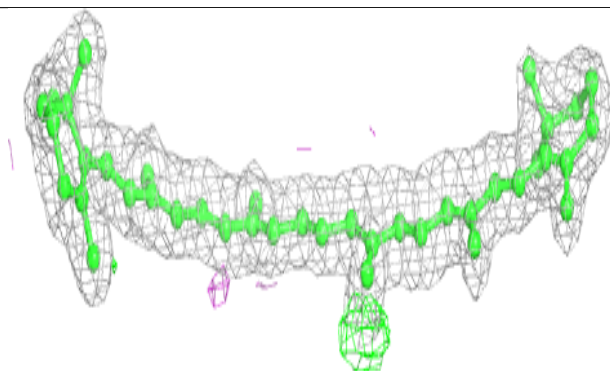
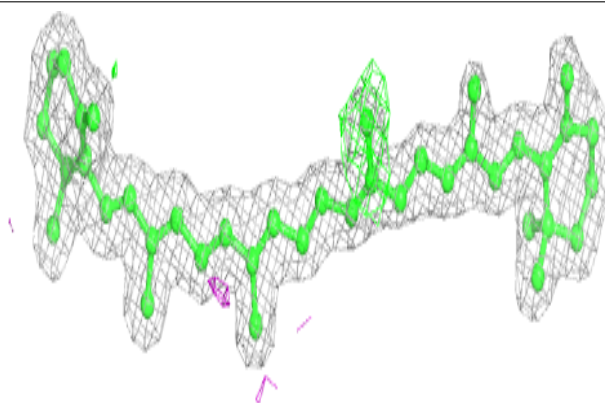


Electron density around BCR K 101:

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

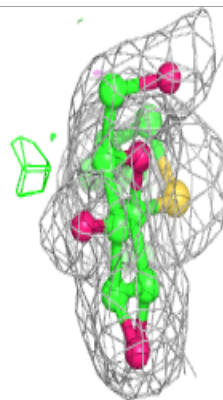
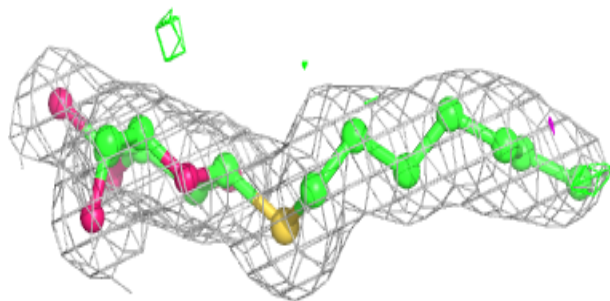
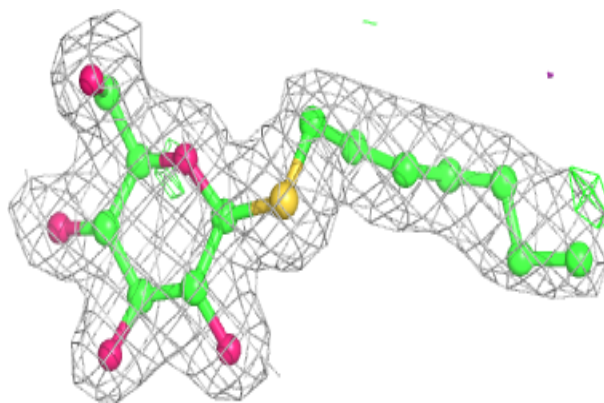
**Electron density around BCR T 102:**

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

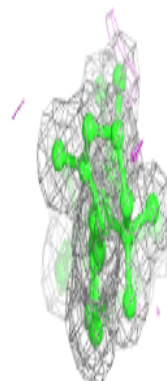
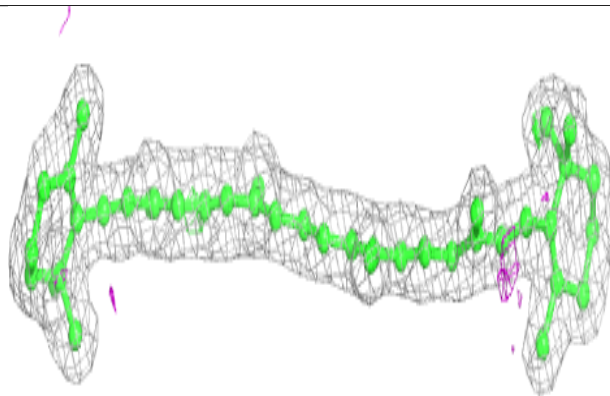
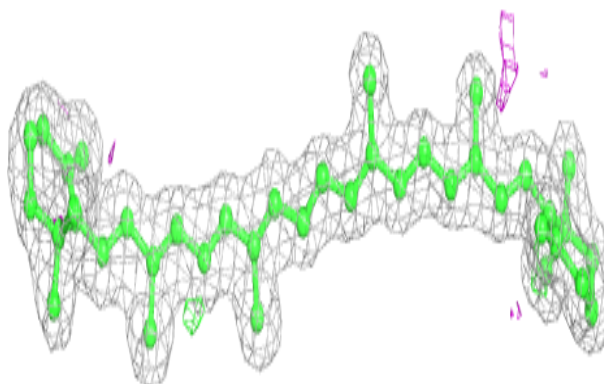


Electron density around HTG O 303:

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

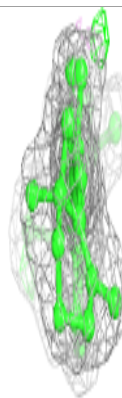
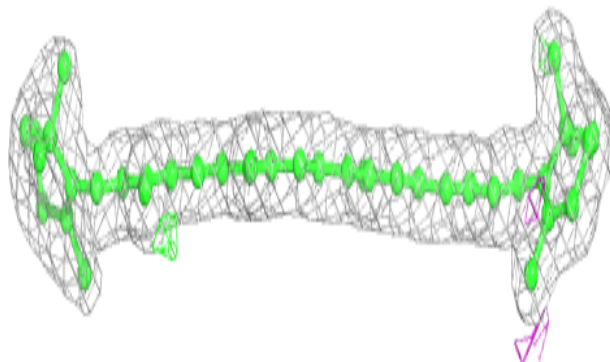
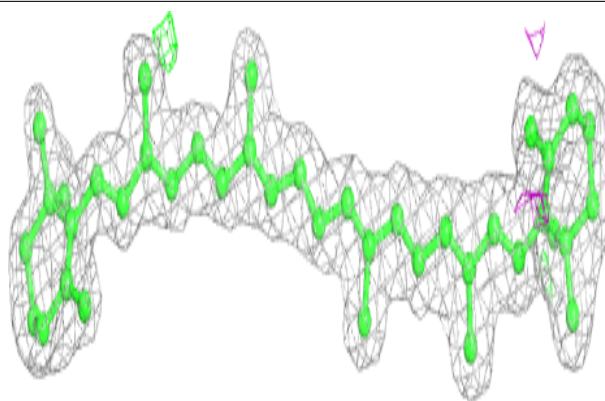
**Electron density around BCR a 411:**

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

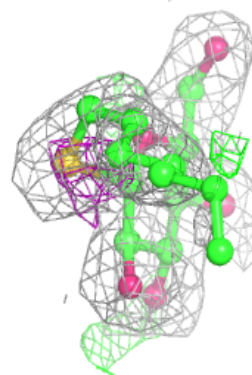
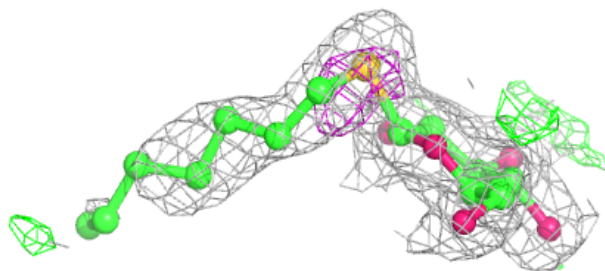
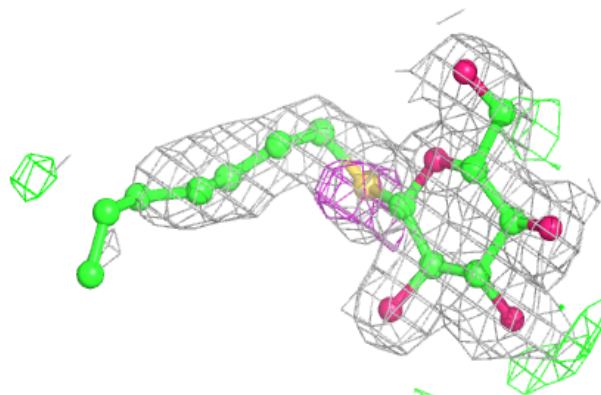


Electron density around BCR b 619:

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

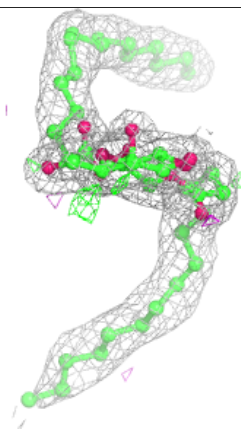
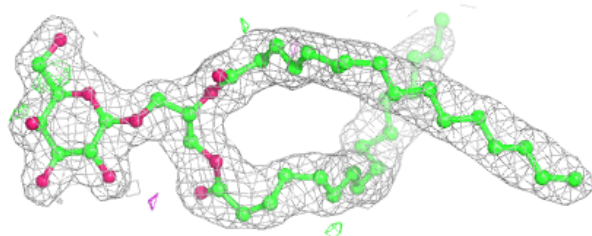
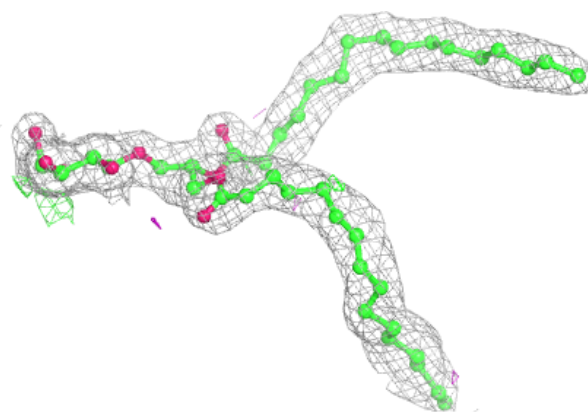
**Electron density around HTG b 623:**

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

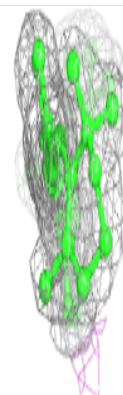
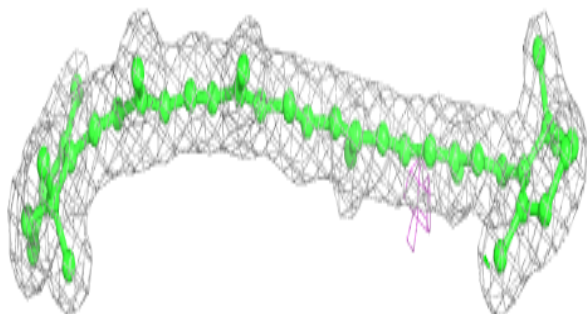
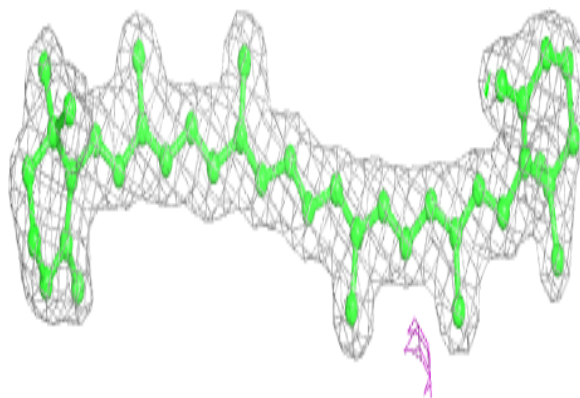


Electron density around LMG B 621:

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

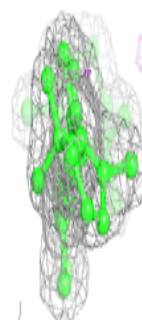
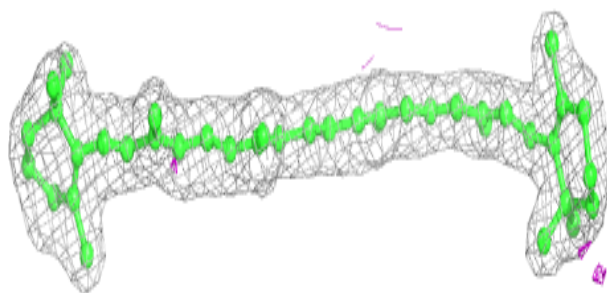
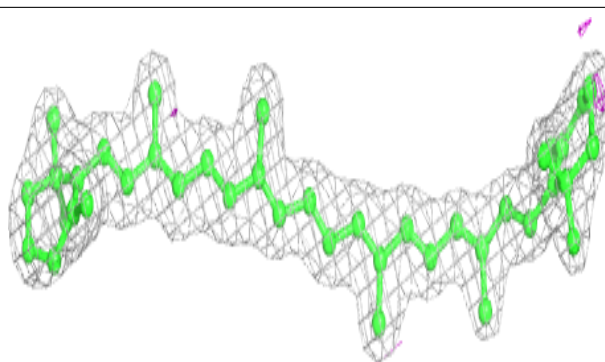
**Electron density around BCR b 620:**

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

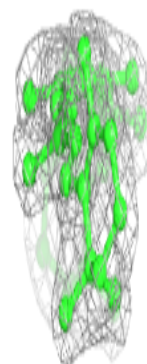
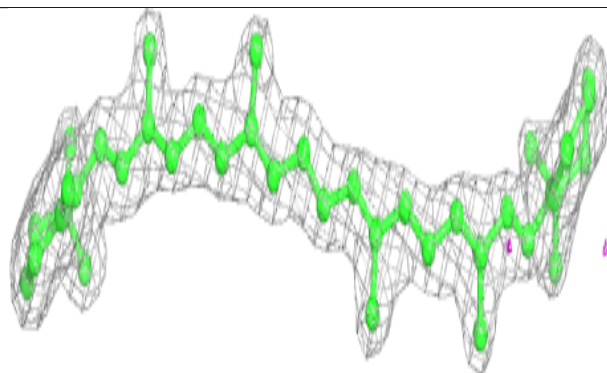
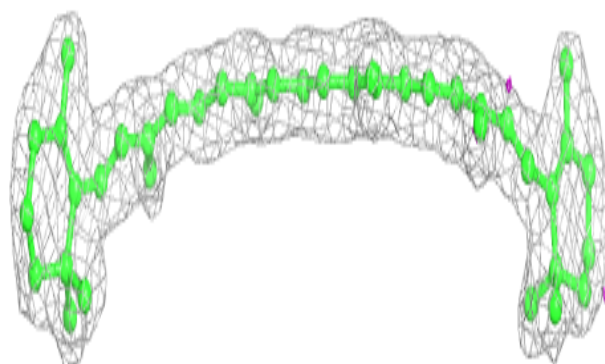


Electron density around BCR c 515:

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

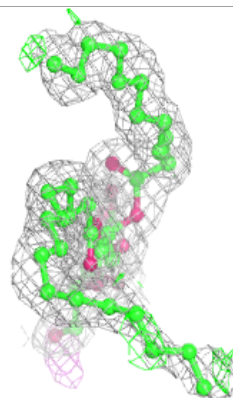
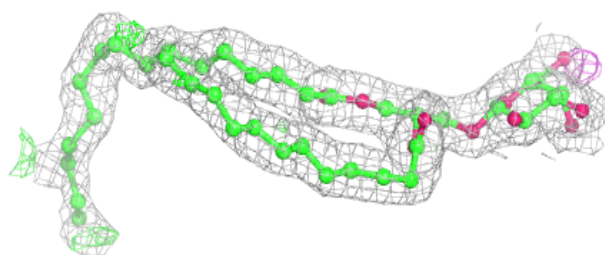
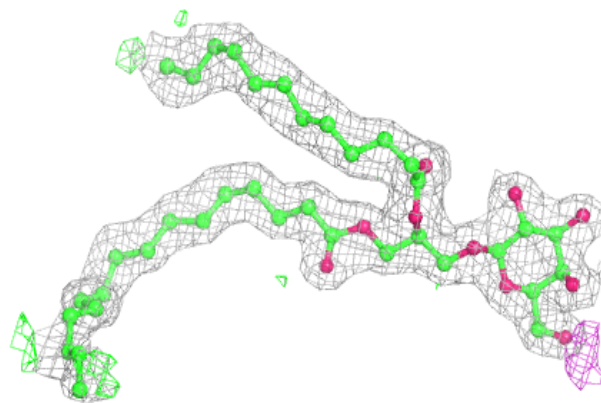
**Electron density around BCR c 527:**

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

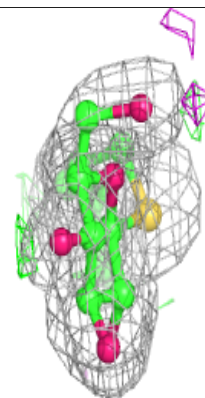
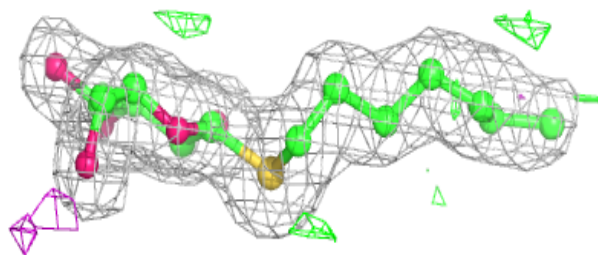
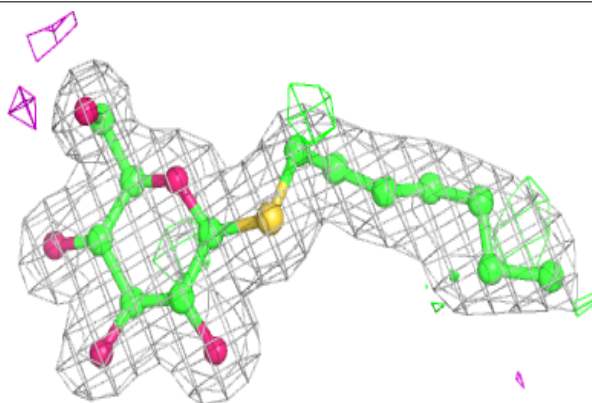


Electron density around LMG J 101:

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

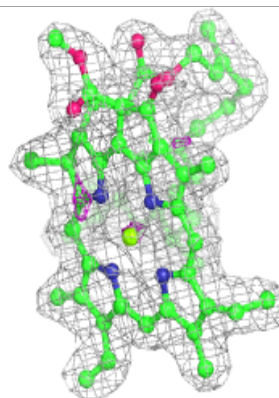
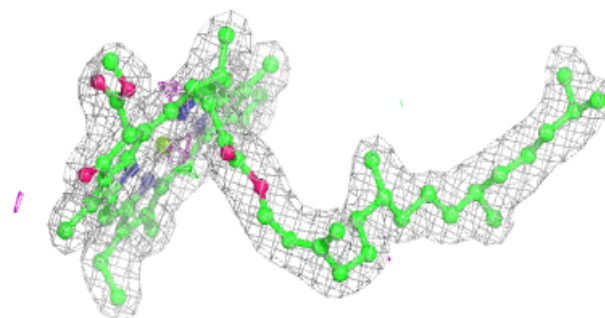
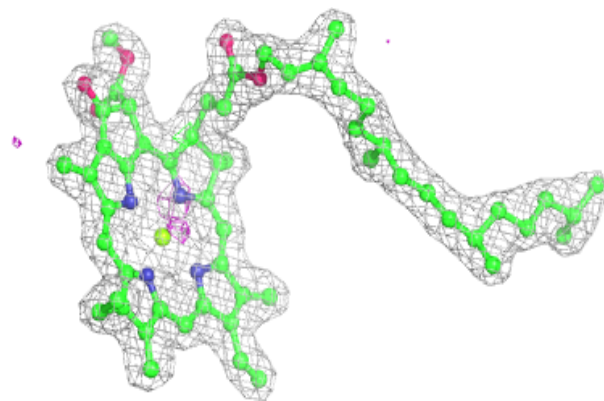
**Electron density around HTG o 301:**

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

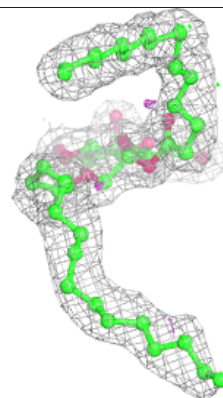
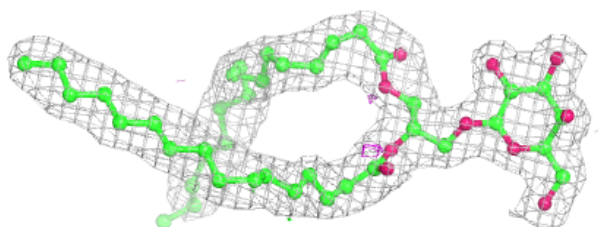
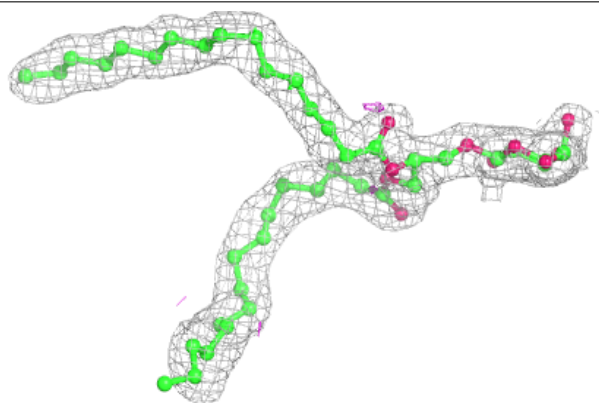


Electron density around CLA c 511:

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

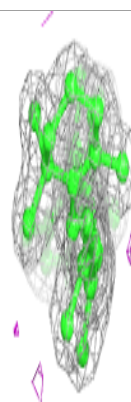
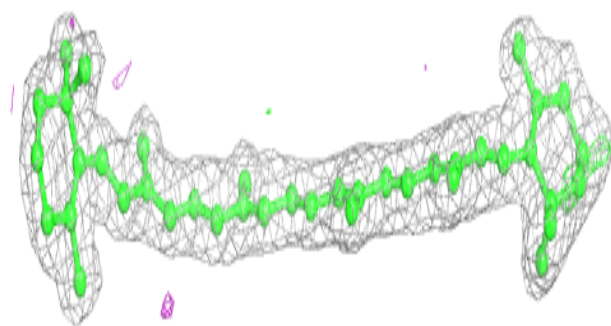
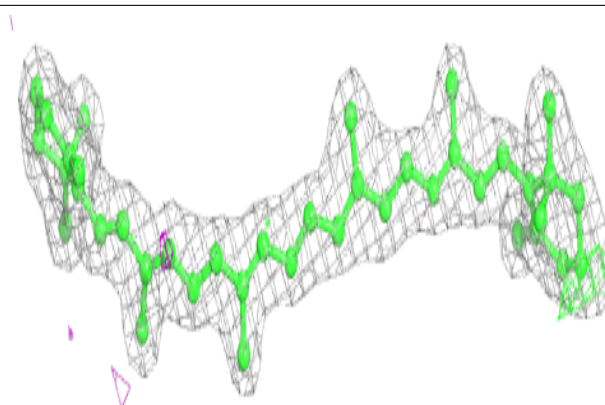
**Electron density around LMG b 621:**

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



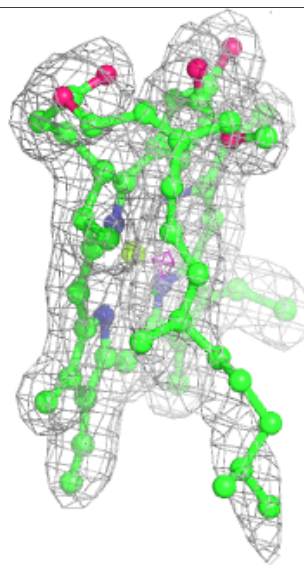
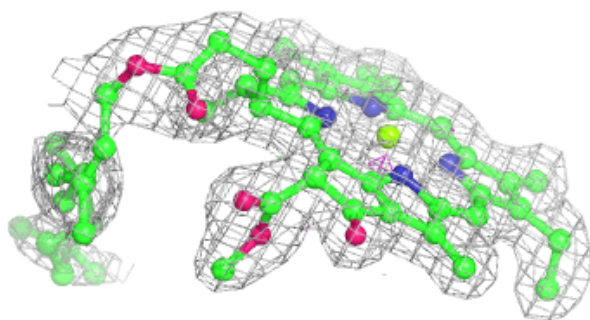
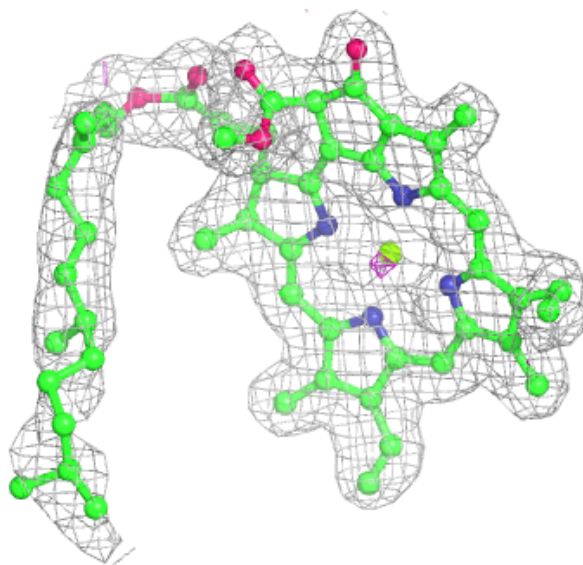
Electron density around BCR h 103:

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



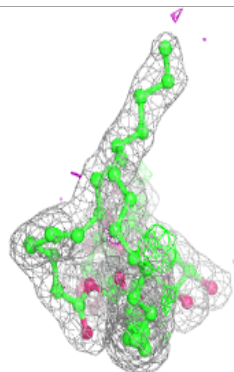
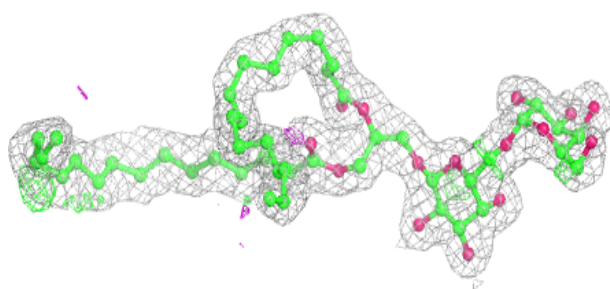
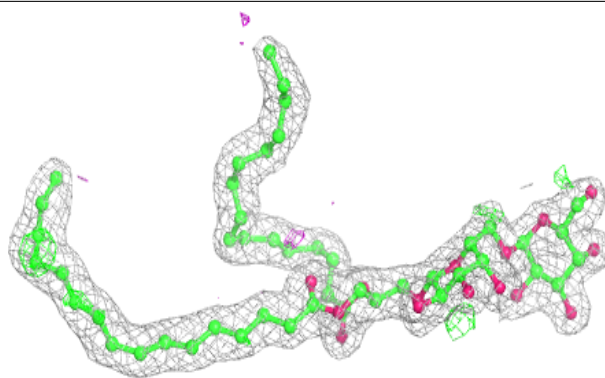
Electron density around CLA B 617:

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

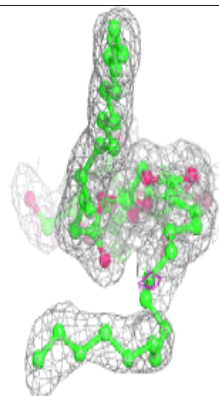
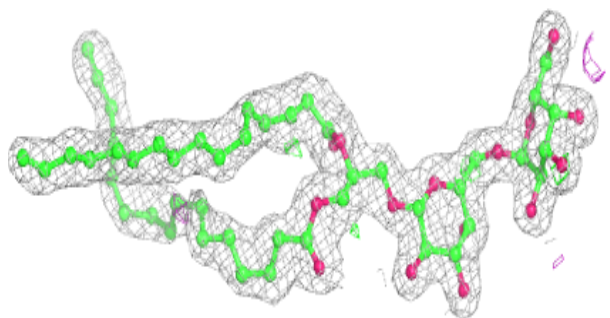
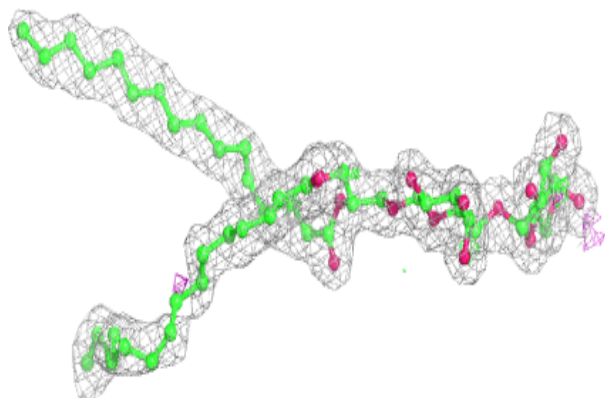


Electron density around DGD H 103:

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

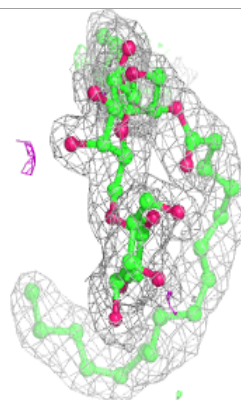
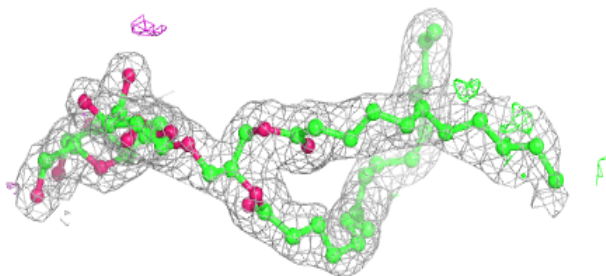
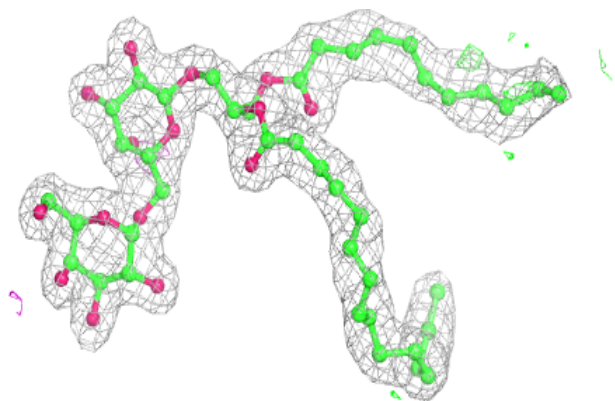
**Electron density around DGD c 516:**

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

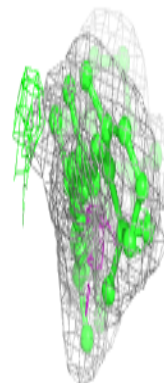
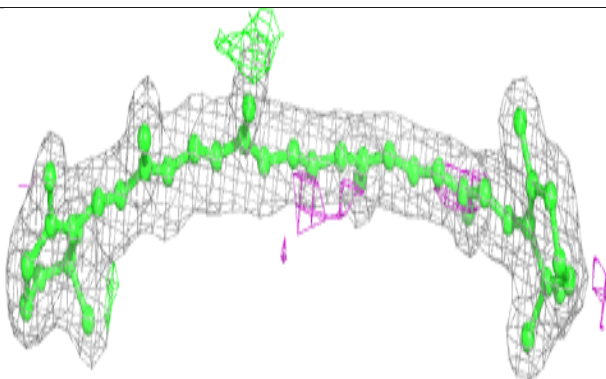
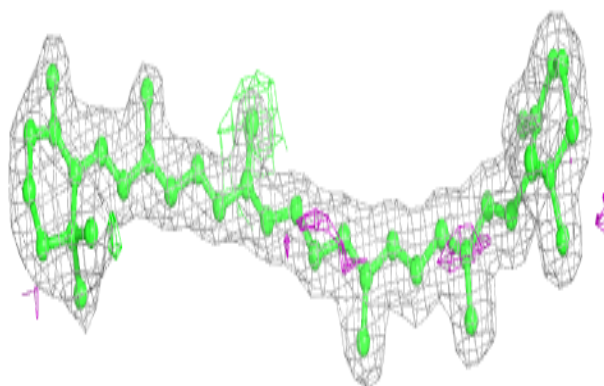


Electron density around DGD c 517:

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

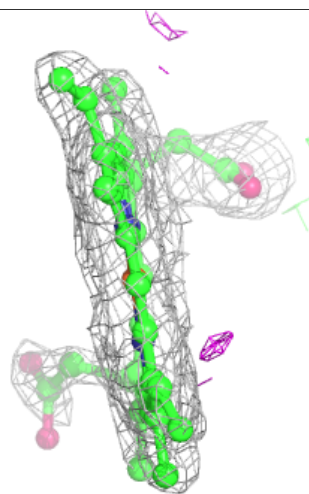
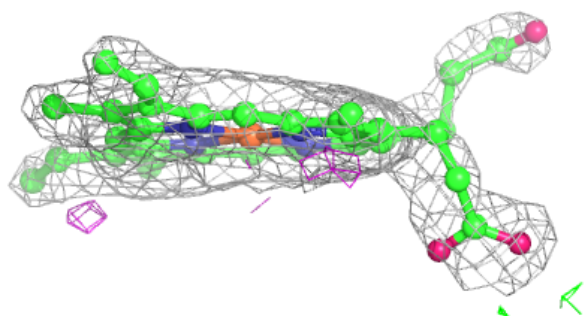
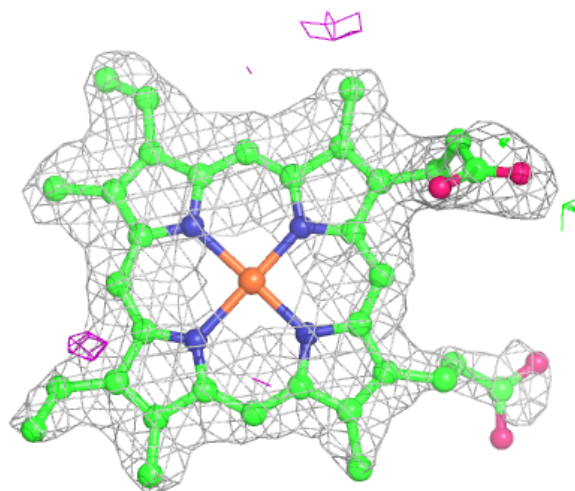
**Electron density around BCR t 102:**

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



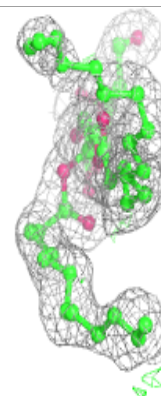
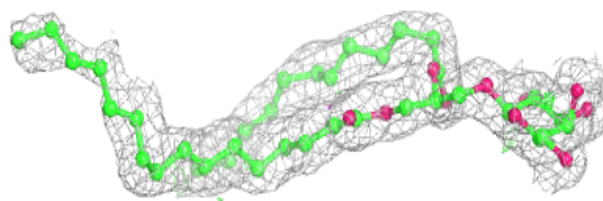
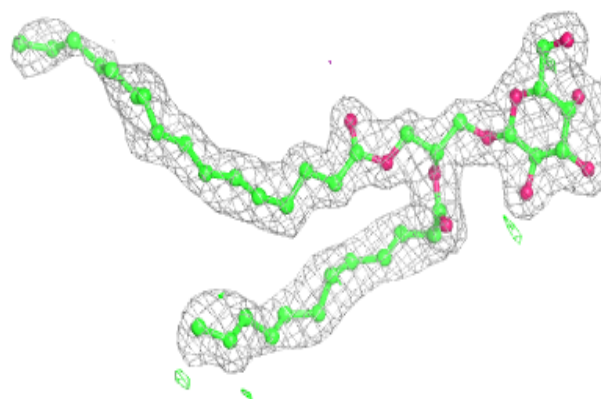
Electron density around HEM e 107:

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

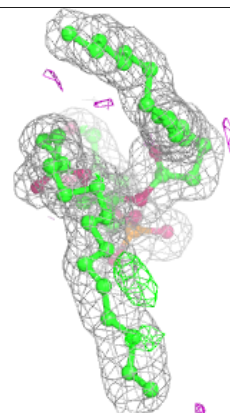
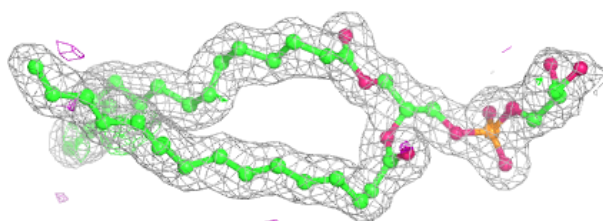
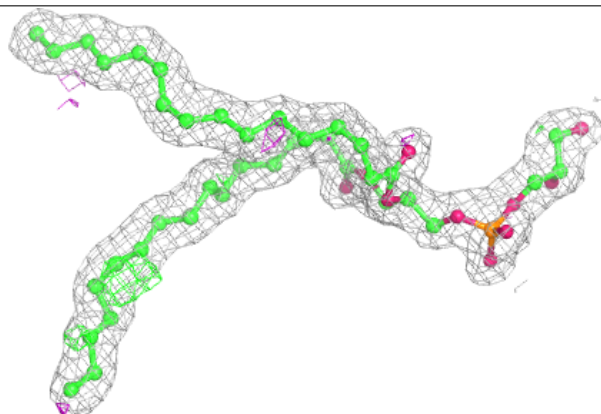


Electron density around LMG j 101:

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

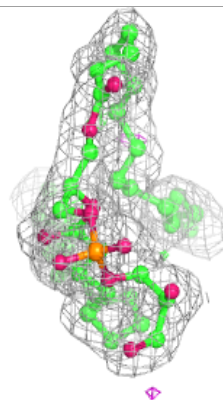
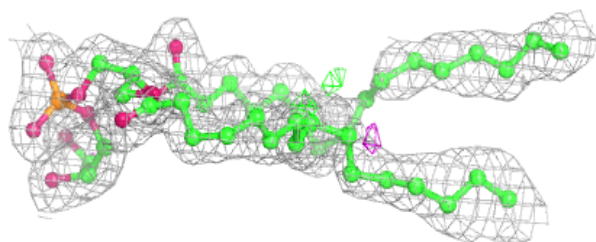
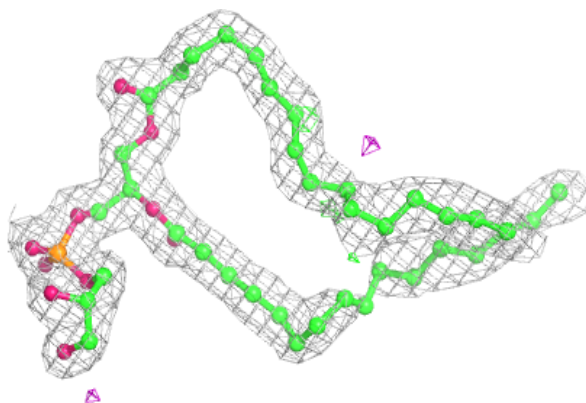
**Electron density around LHG d 410:**

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

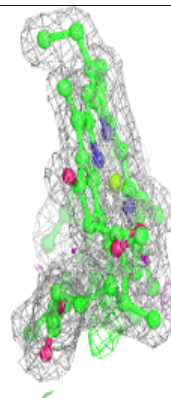
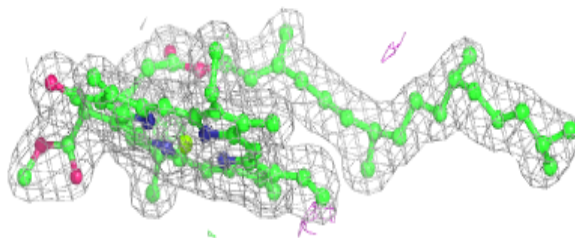
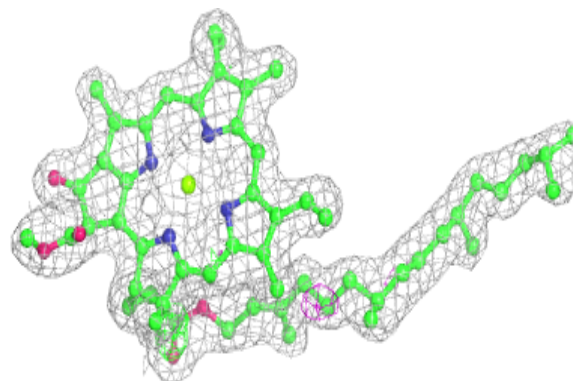


Electron density around LHG d 411:

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

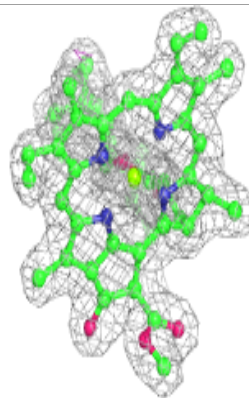
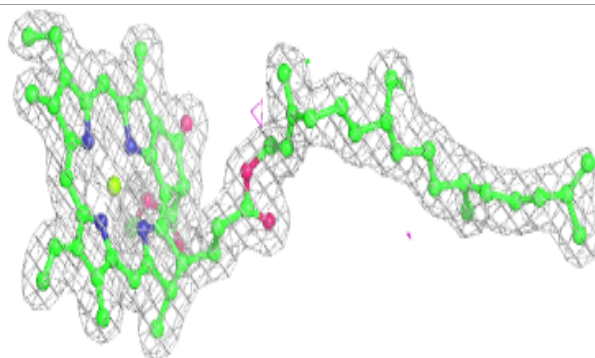
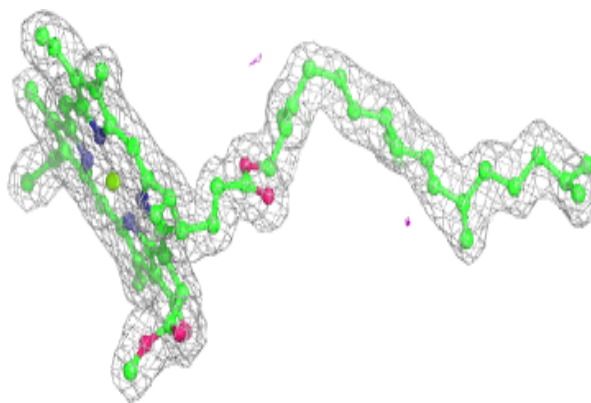
**Electron density around CLA C 501:**

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



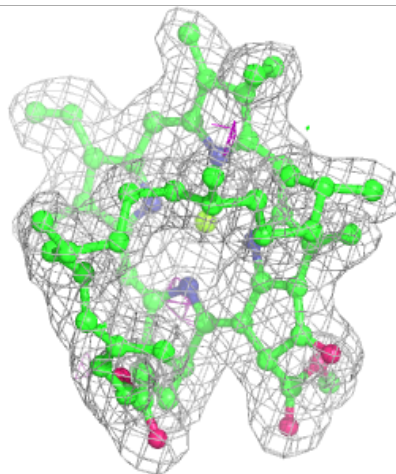
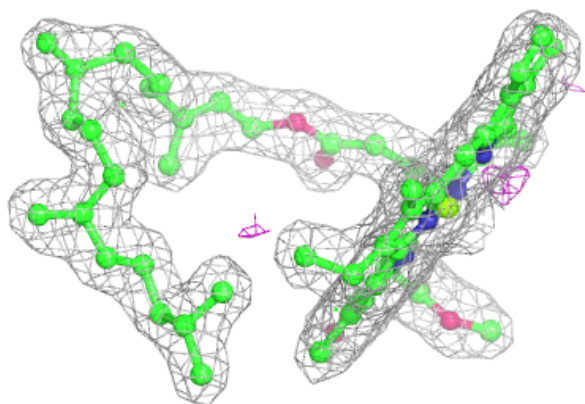
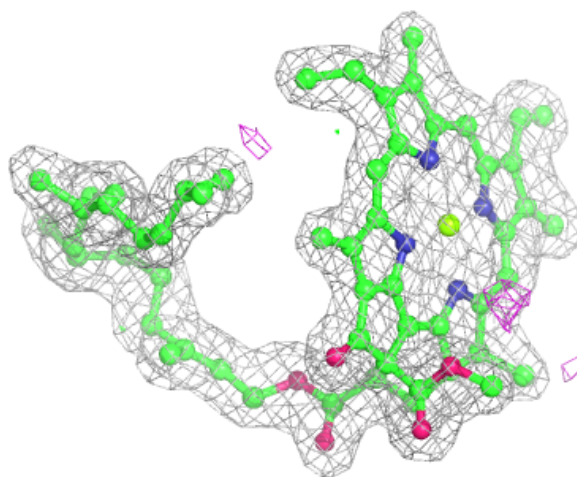
Electron density around CLA C 502:

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



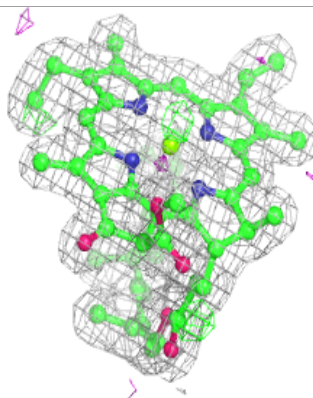
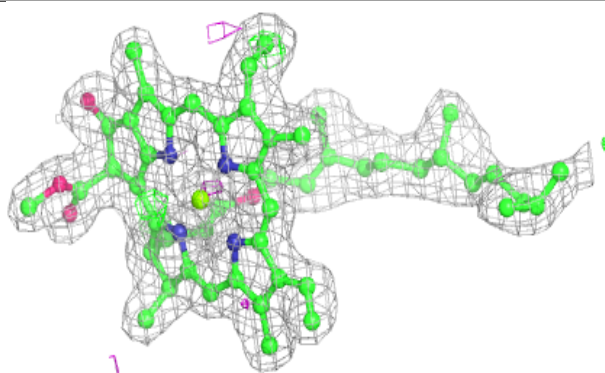
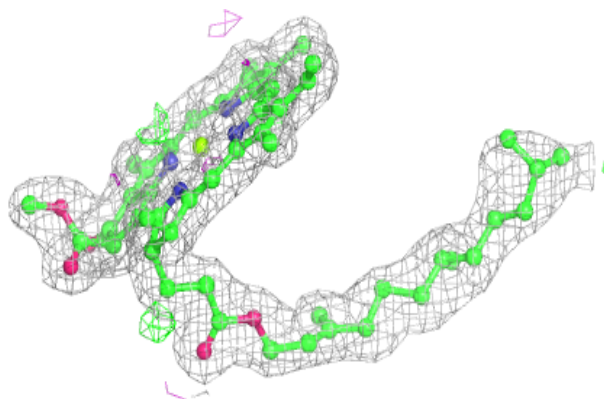
Electron density around CLA C 503:

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

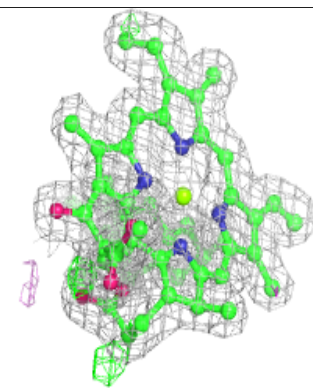
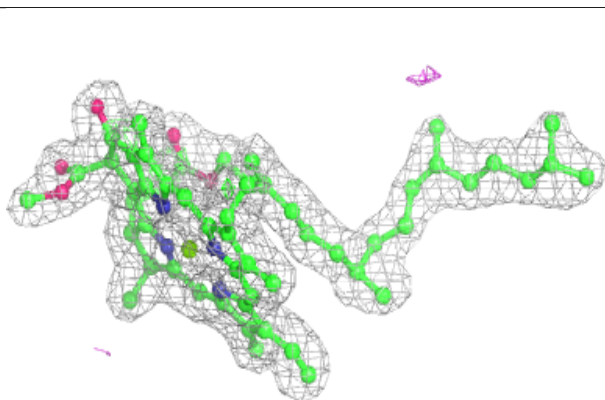
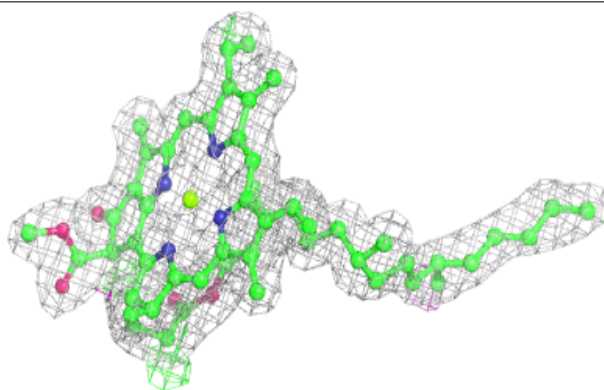


Electron density around CLA C 504:

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

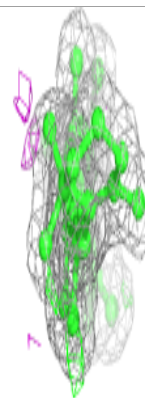
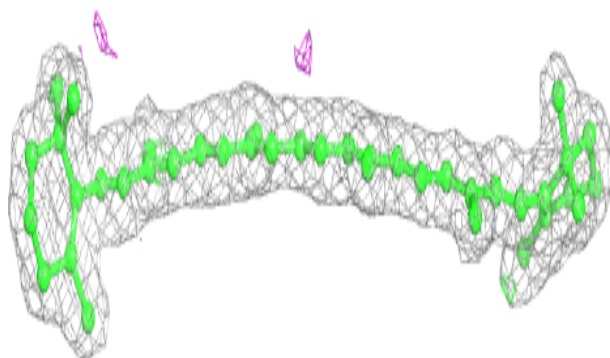
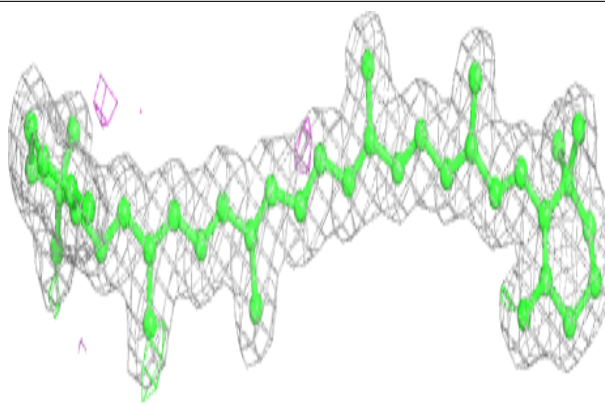
**Electron density around CLA C 505:**

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



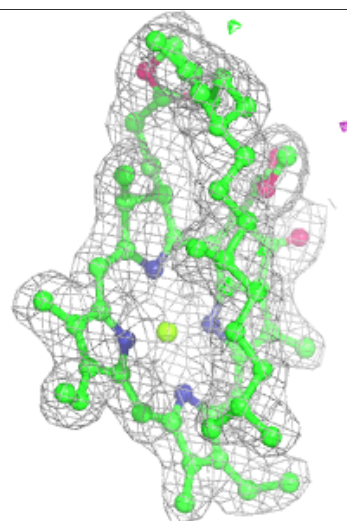
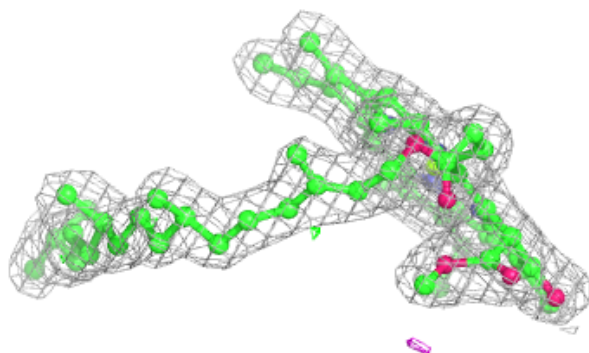
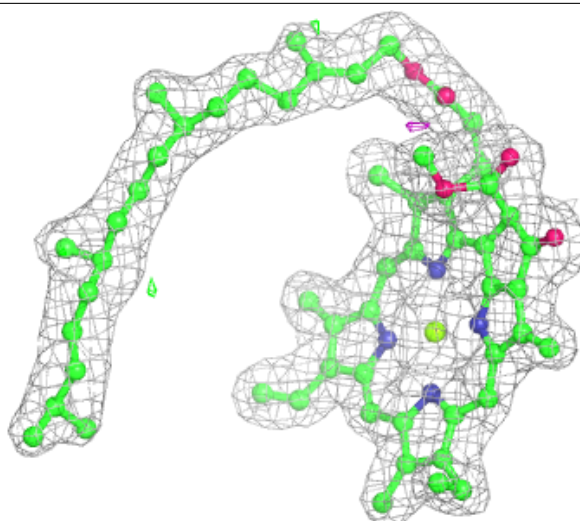
Electron density around BCR b 618:

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



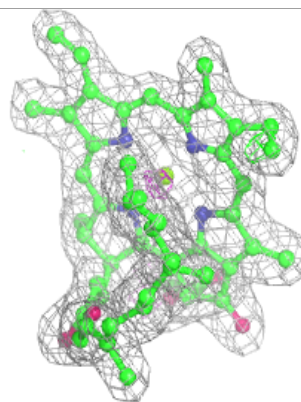
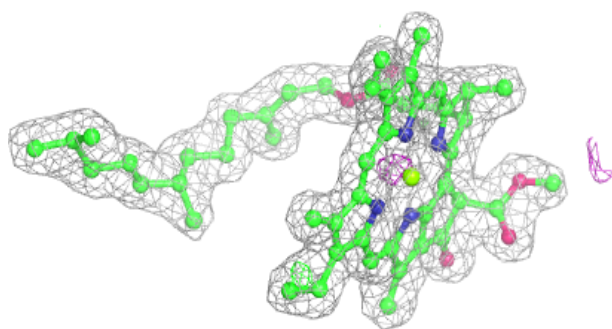
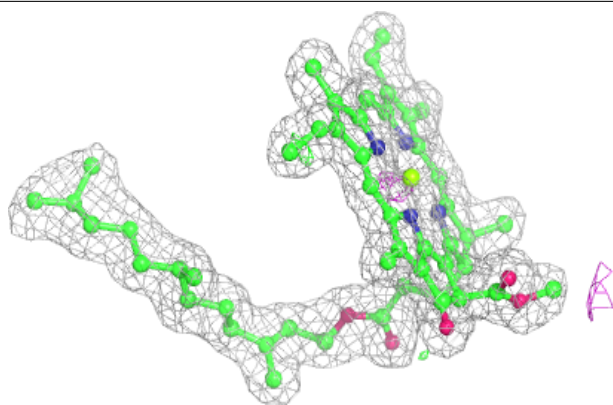
Electron density around CLA C 507:

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



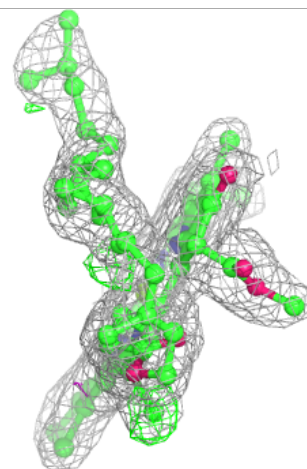
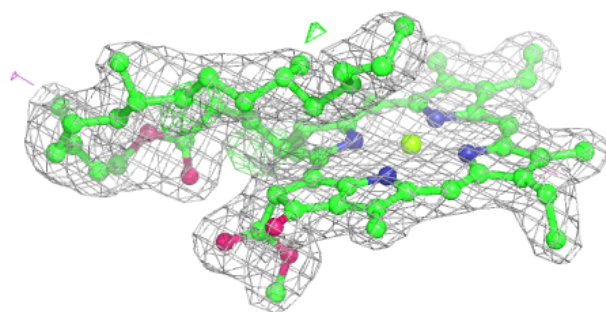
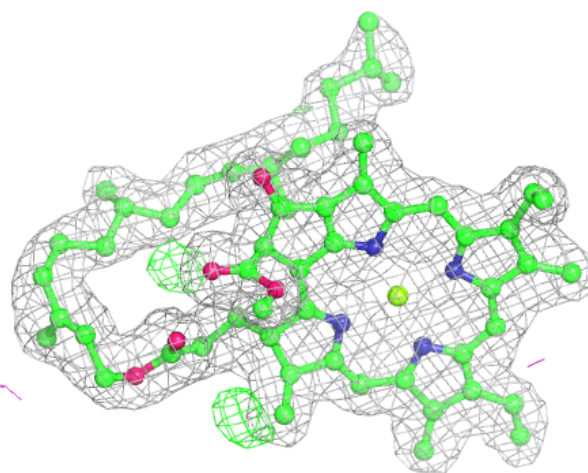
Electron density around CLA C 508:

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



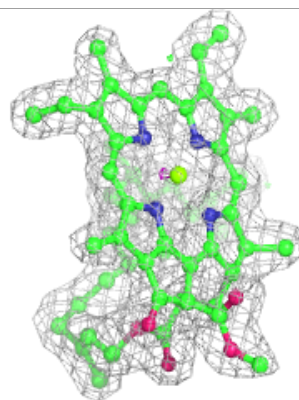
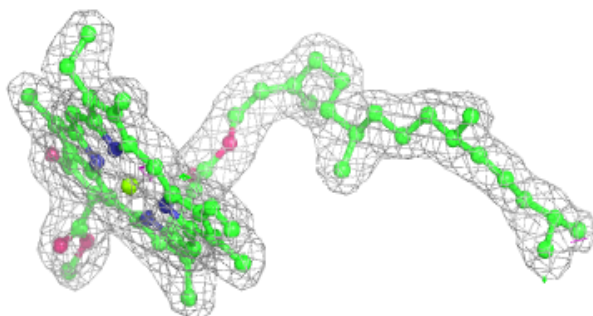
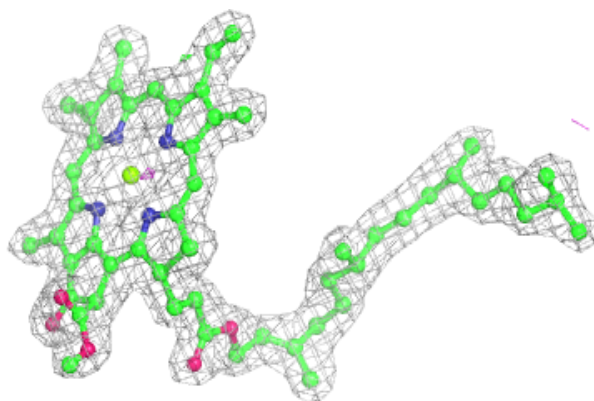
Electron density around CLA C 509:

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

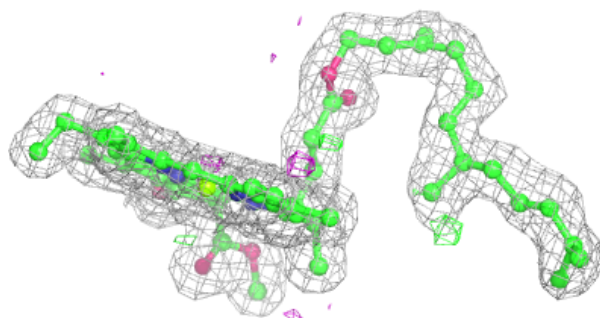
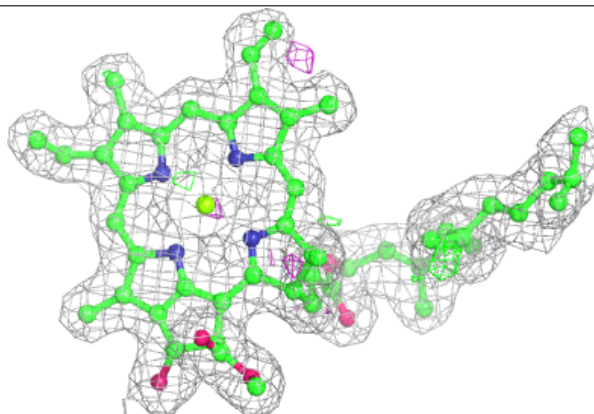


Electron density around CLA C 511:

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

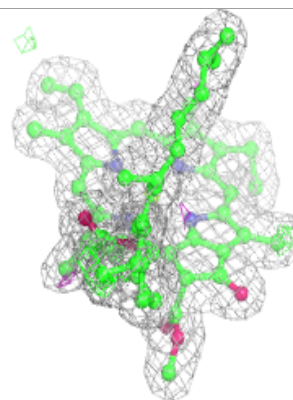
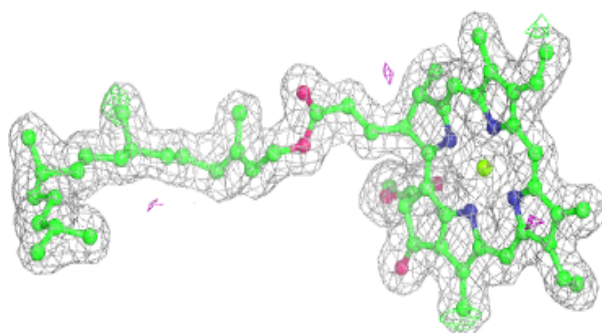
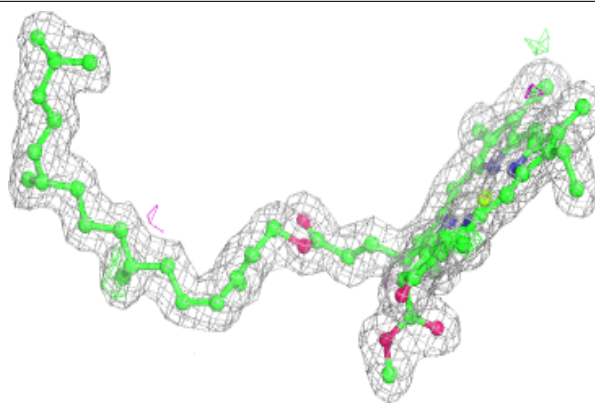
**Electron density around CLA A 607:**

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

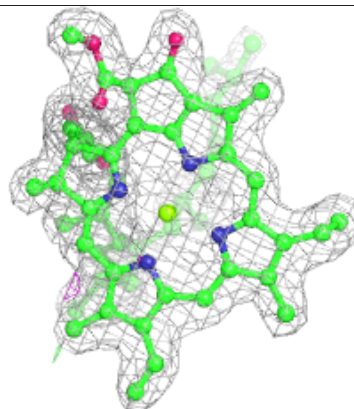
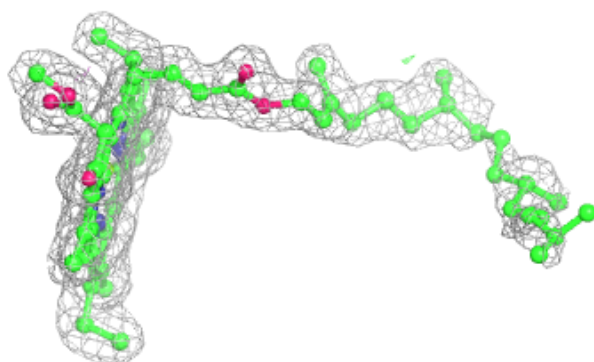
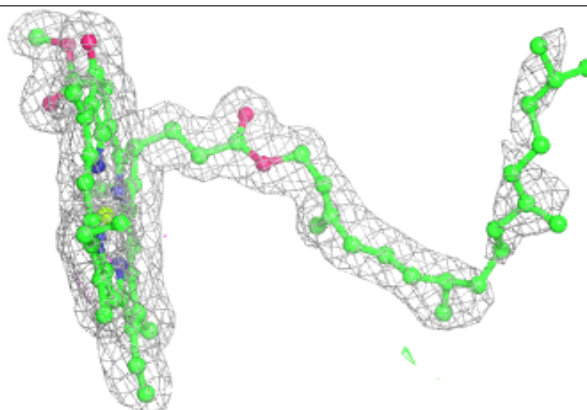


Electron density around CLA D 404:

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

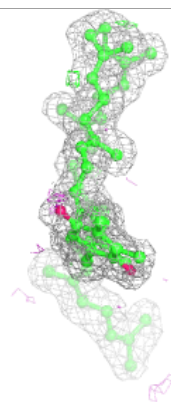
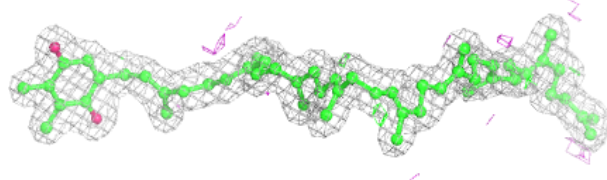
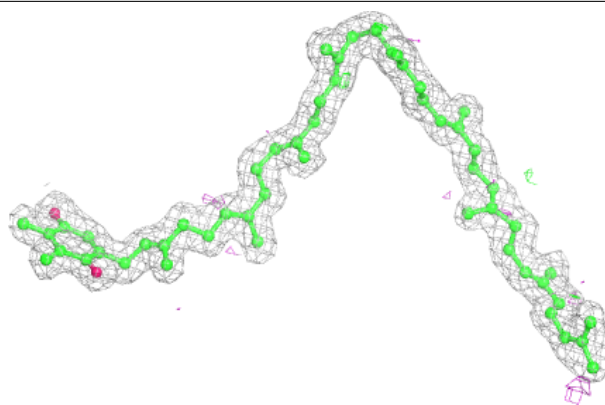
**Electron density around CLA D 405:**

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

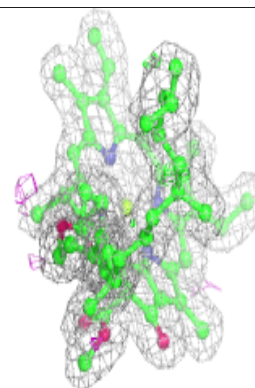
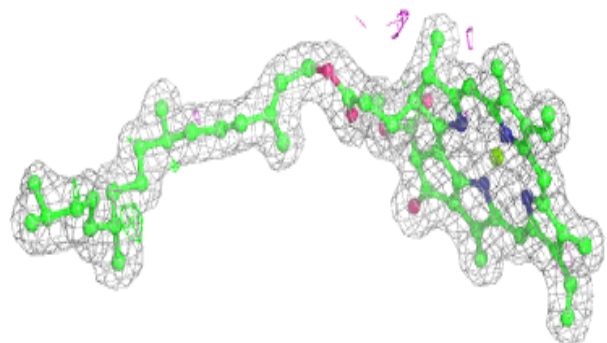
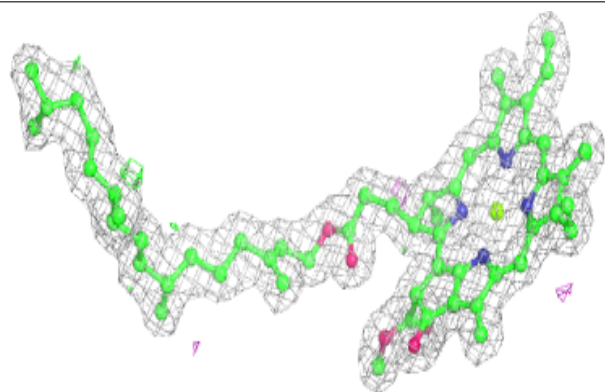


Electron density around PL9 D 407:

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

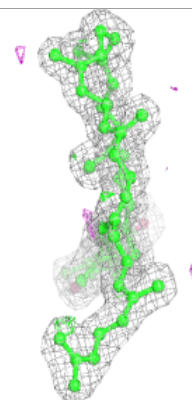
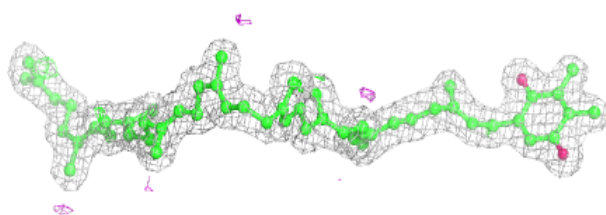
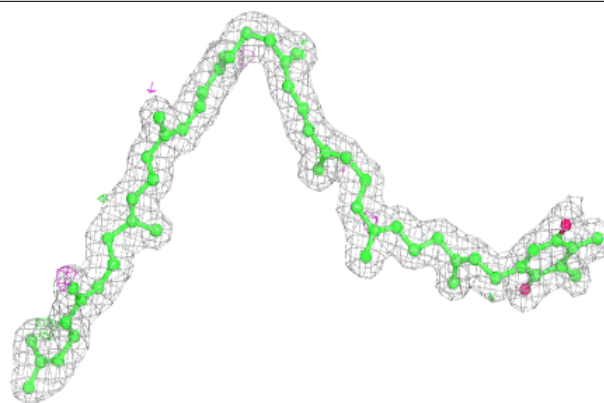
**Electron density around CLA a 407:**

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

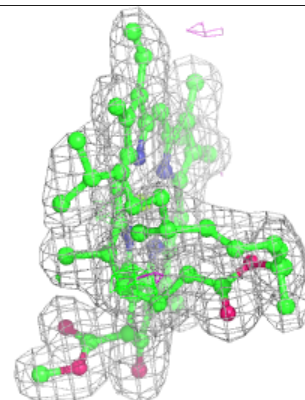
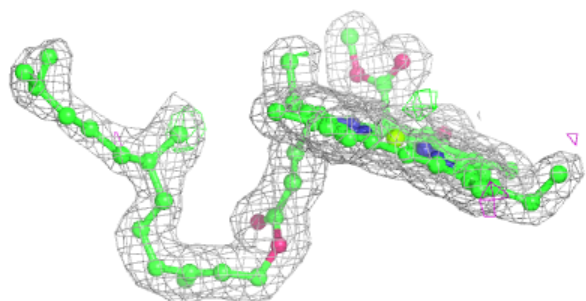
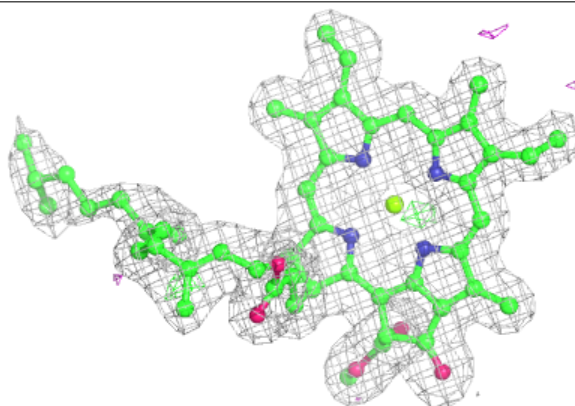


Electron density around PL9 d 407:

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

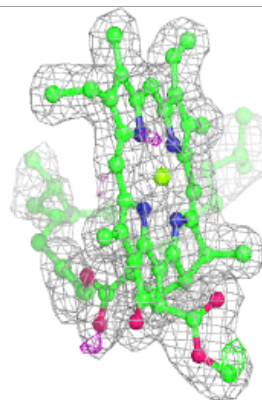
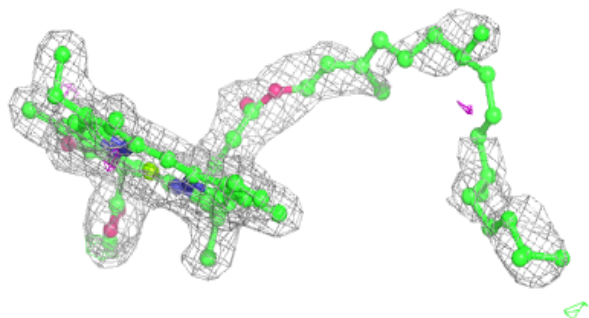
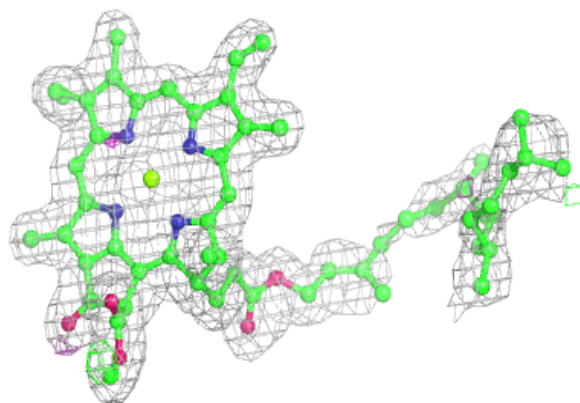
**Electron density around CLA a 408:**

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

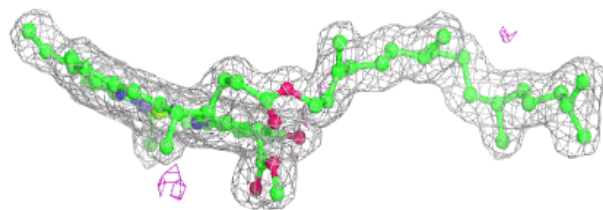
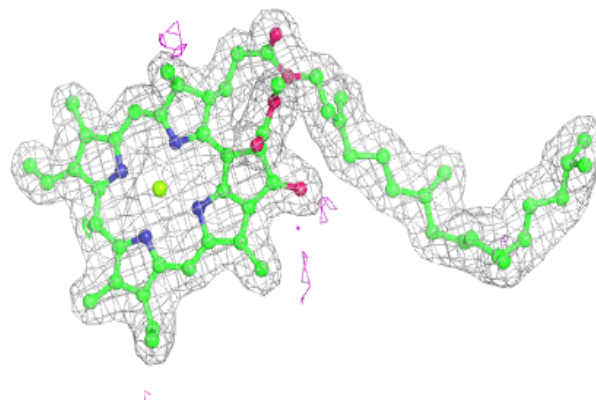


Electron density around CLA A 609:

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

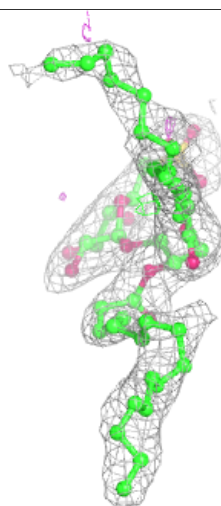
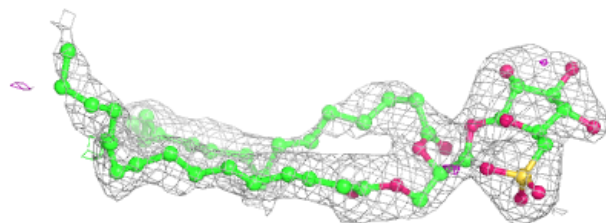
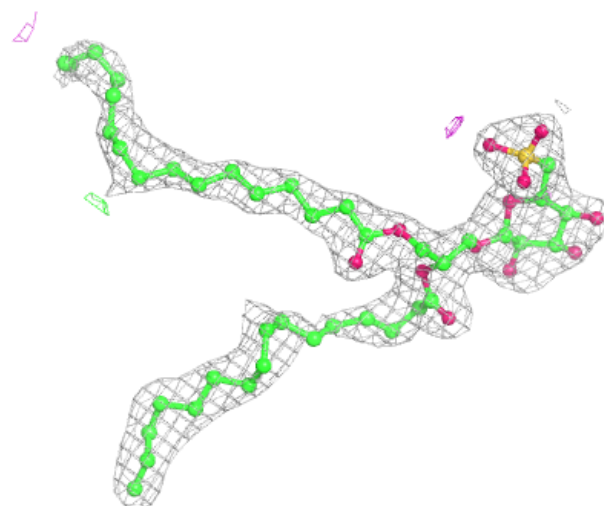
**Electron density around CLA b 603:**

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



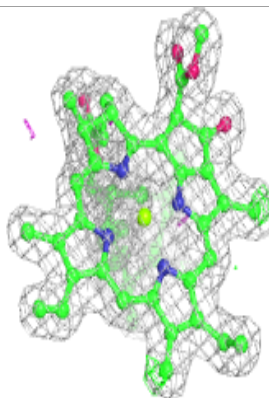
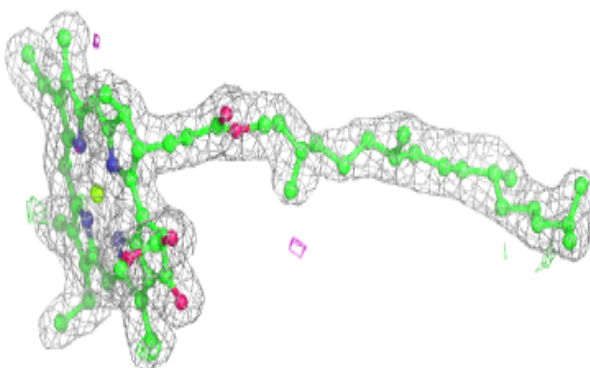
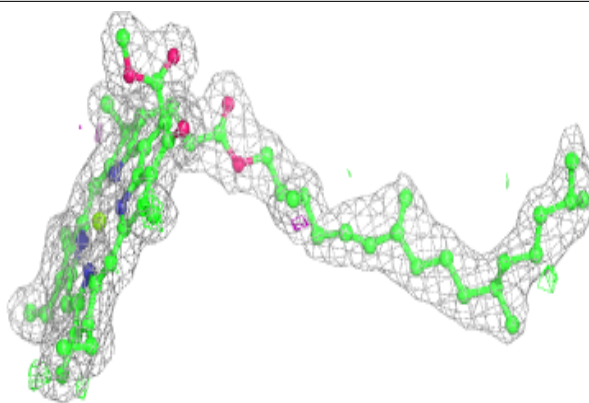
Electron density around SQD a 413:

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

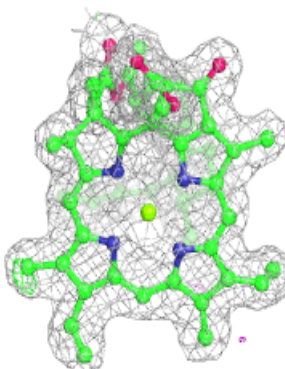
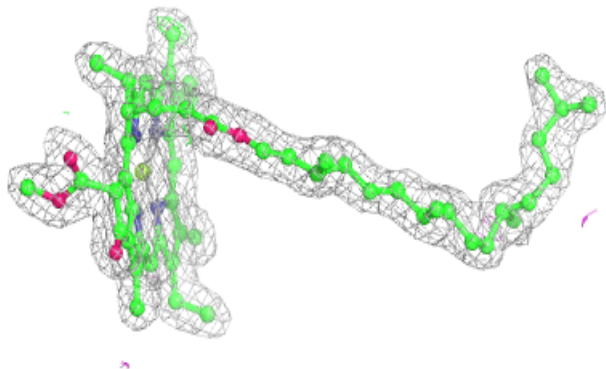
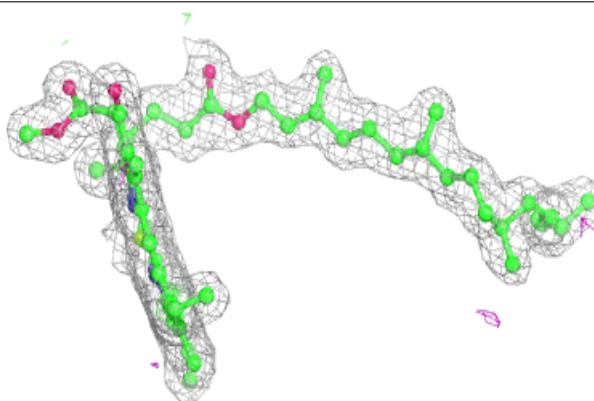


Electron density around CLA b 605:

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

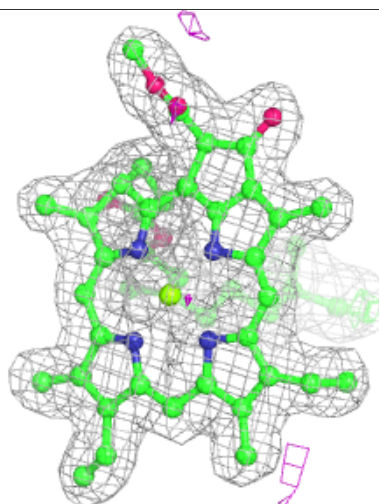
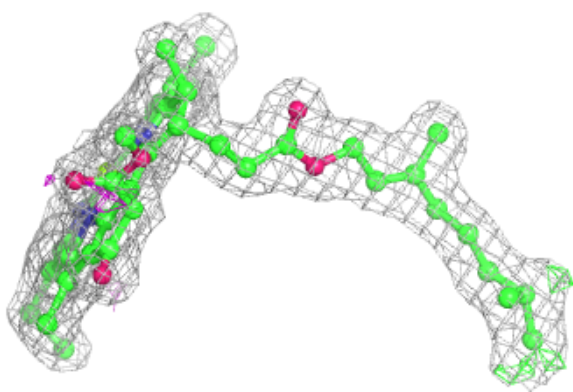
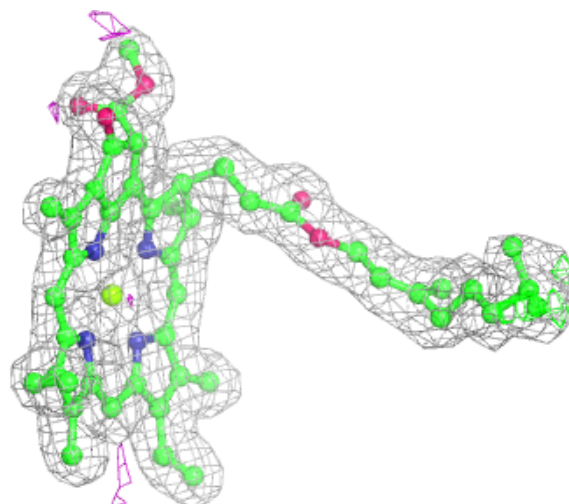
**Electron density around CLA b 606:**

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



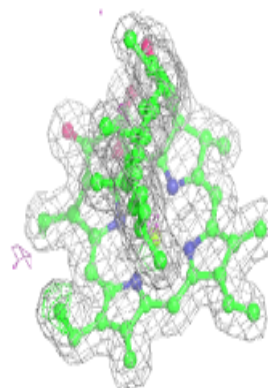
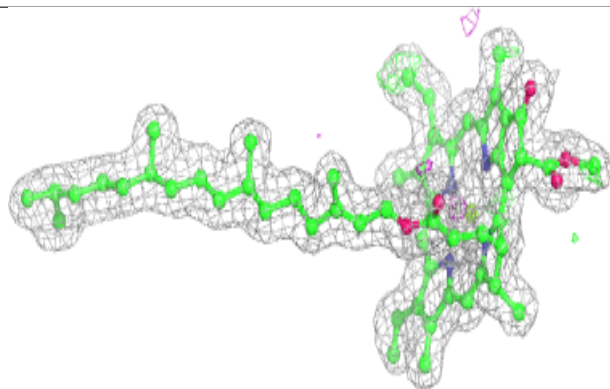
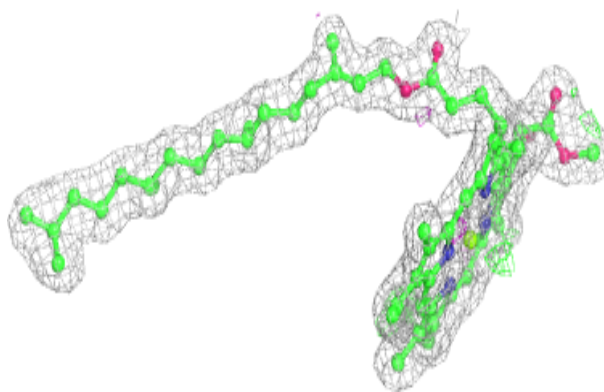
Electron density around CLA b 607:

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

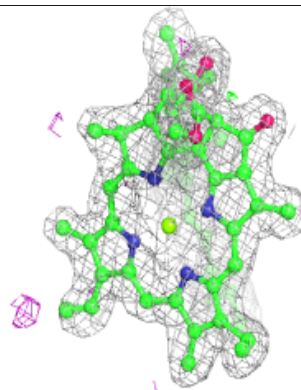
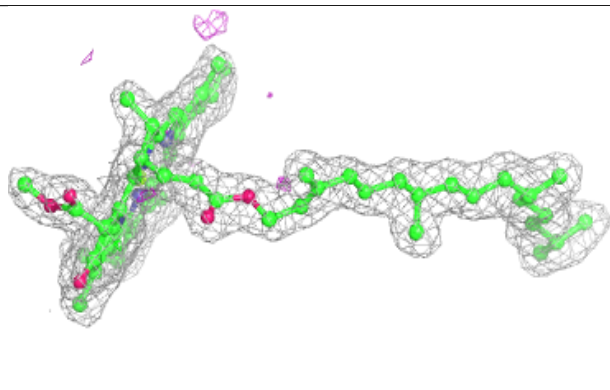
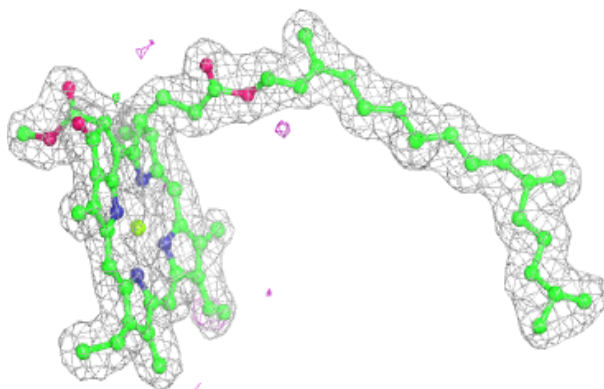


Electron density around CLA b 608:

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

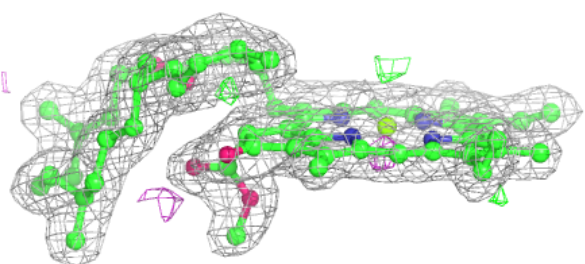
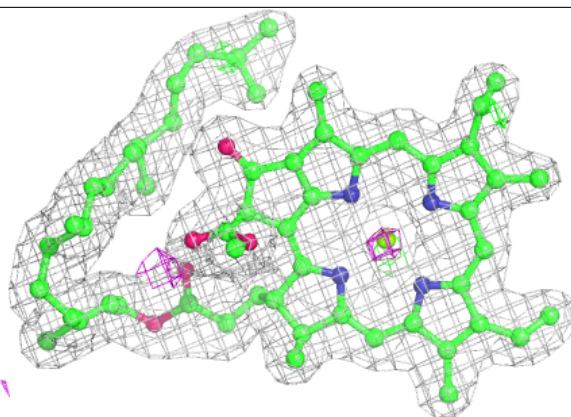
**Electron density around CLA b 610:**

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

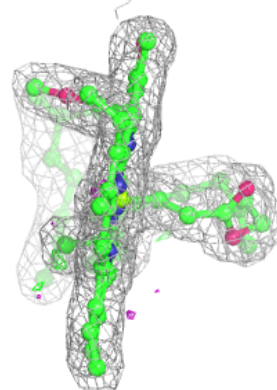
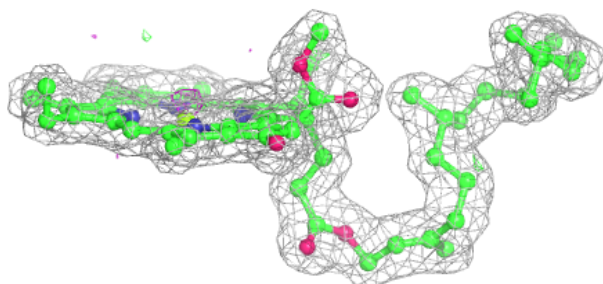
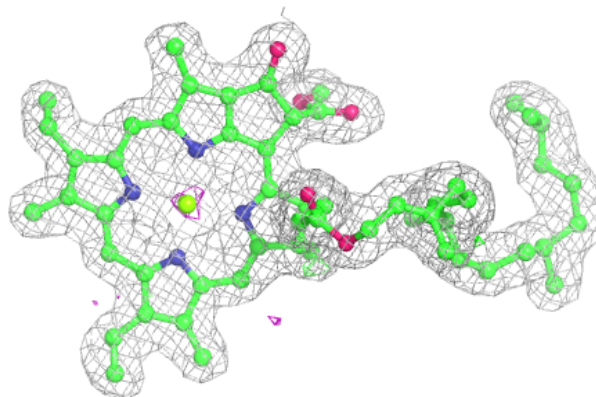


Electron density around CLA b 611:

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

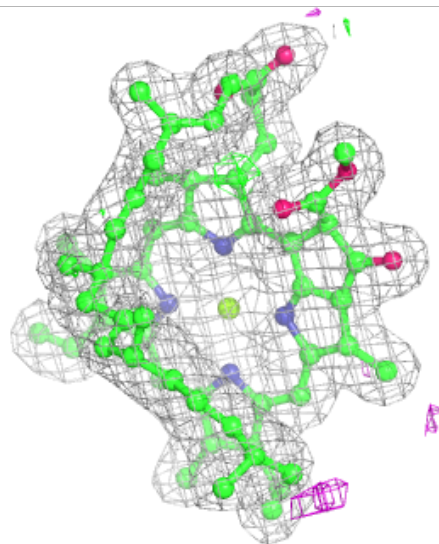
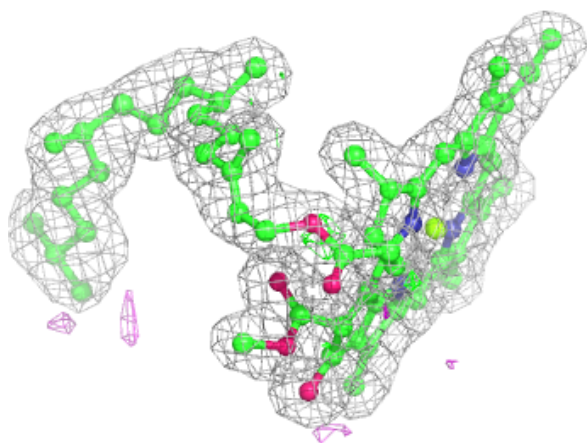
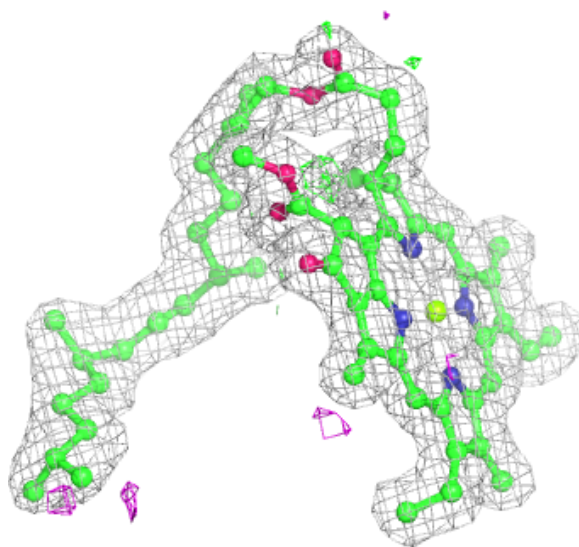
**Electron density around CLA b 613:**

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



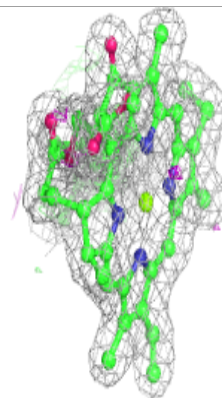
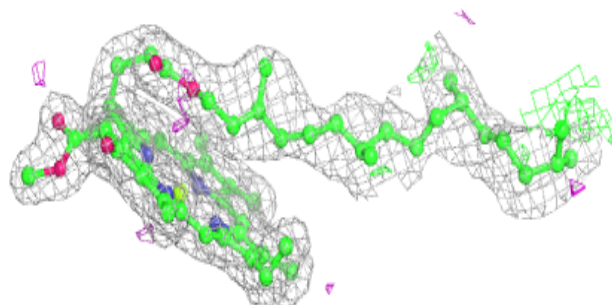
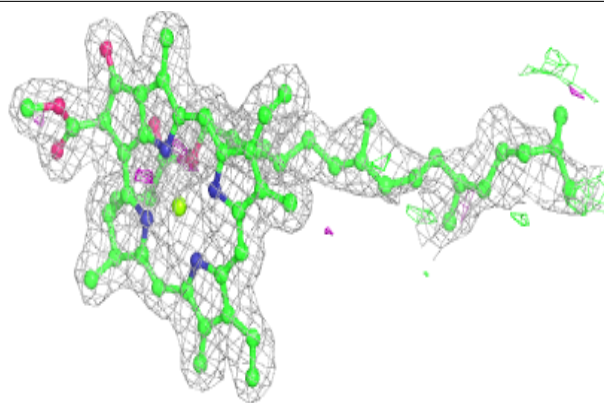
Electron density around CLA b 614:

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



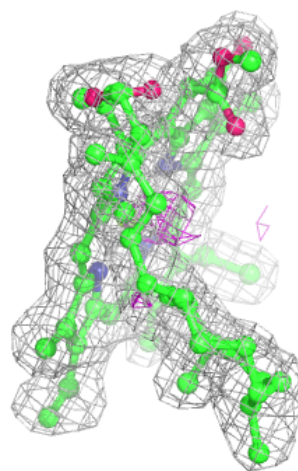
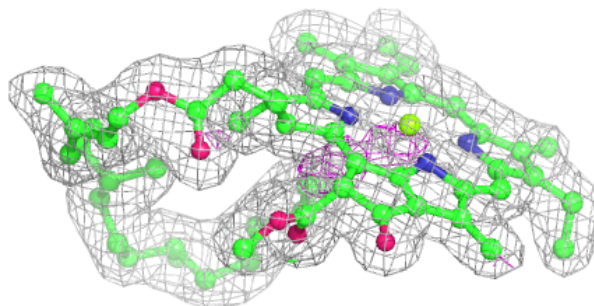
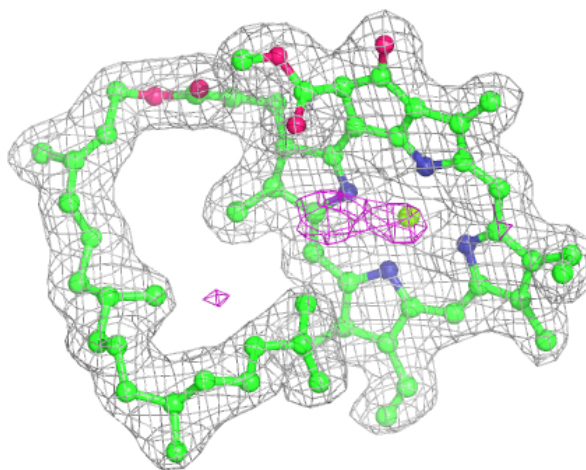
Electron density around CLA b 615:

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



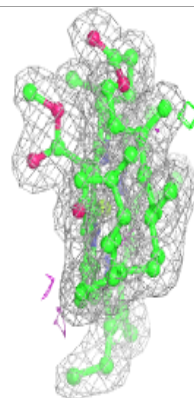
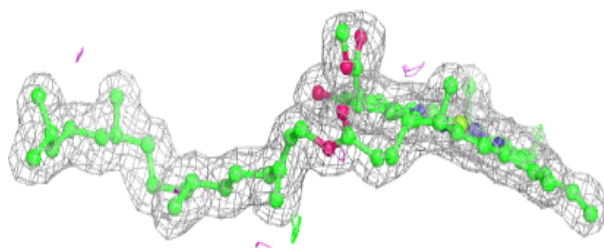
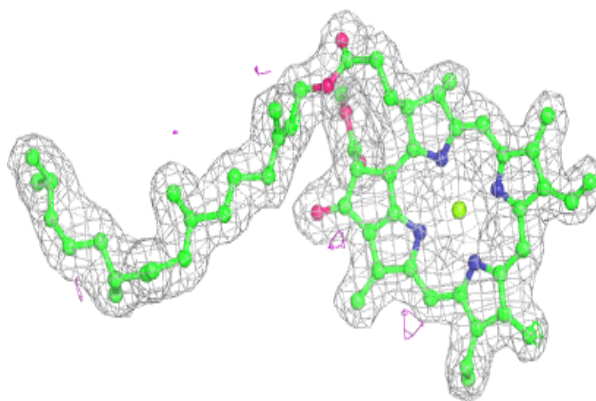
Electron density around CLA b 616:

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

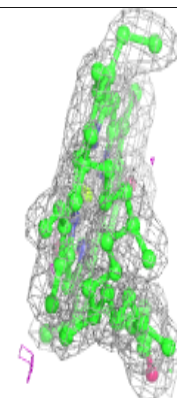
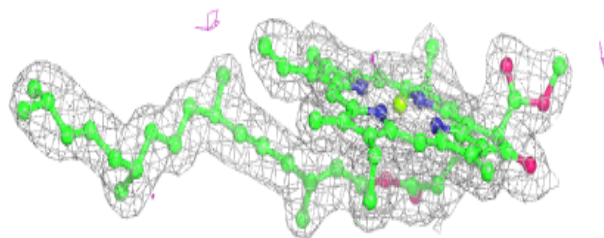
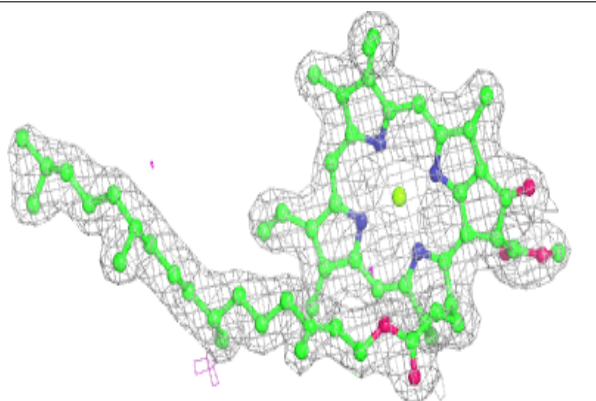


Electron density around CLA B 603:

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

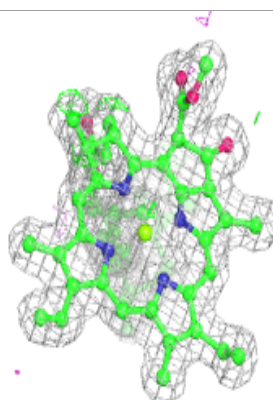
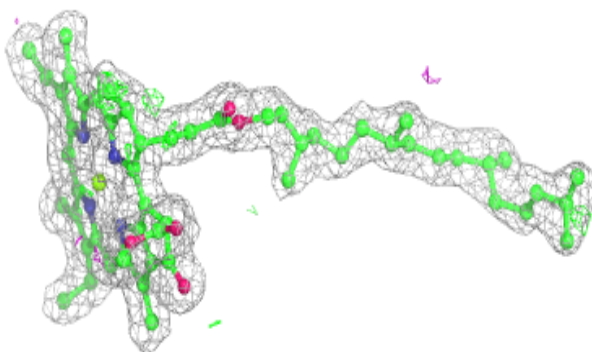
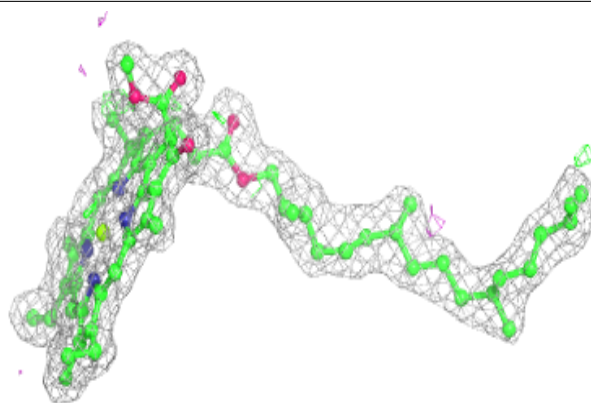
**Electron density around CLA c 501:**

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

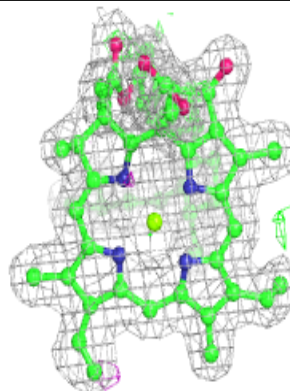
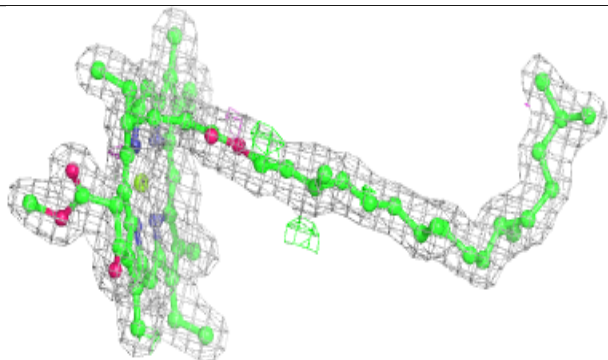
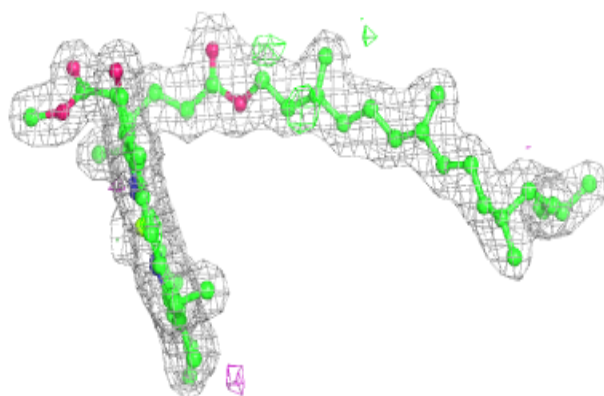


Electron density around CLA B 605:

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

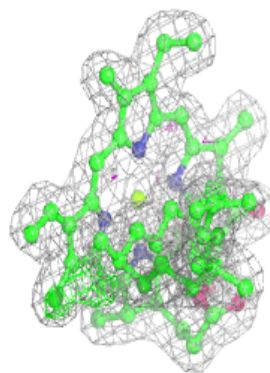
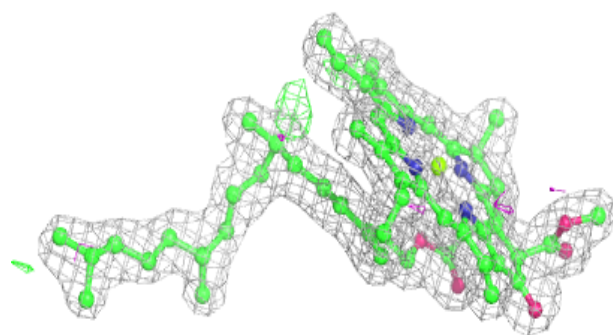
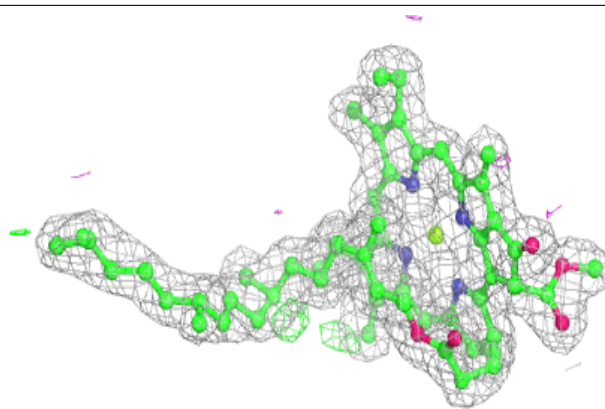
**Electron density around CLA B 606:**

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



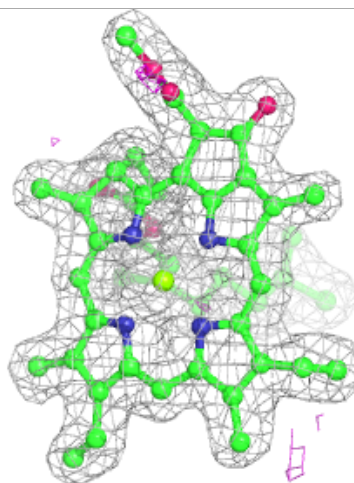
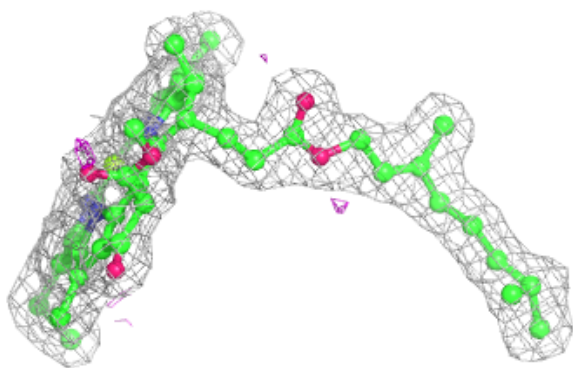
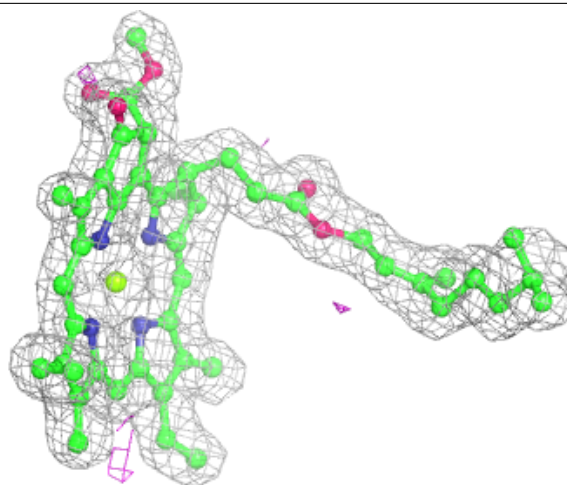
Electron density around CLA c 505:

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



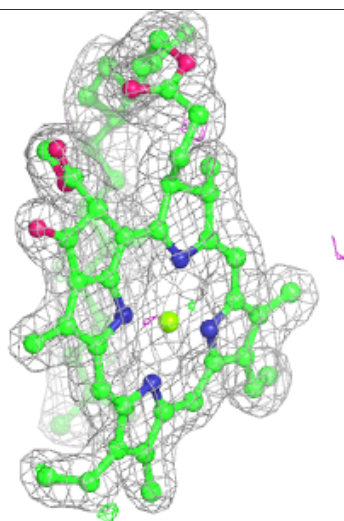
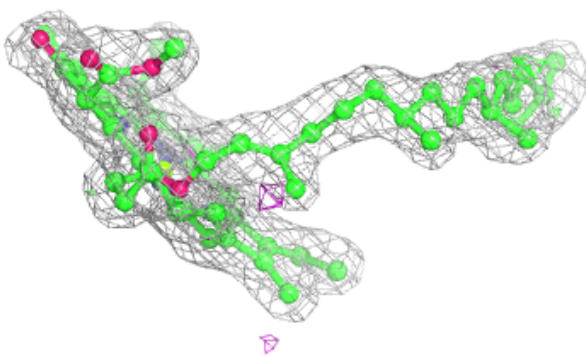
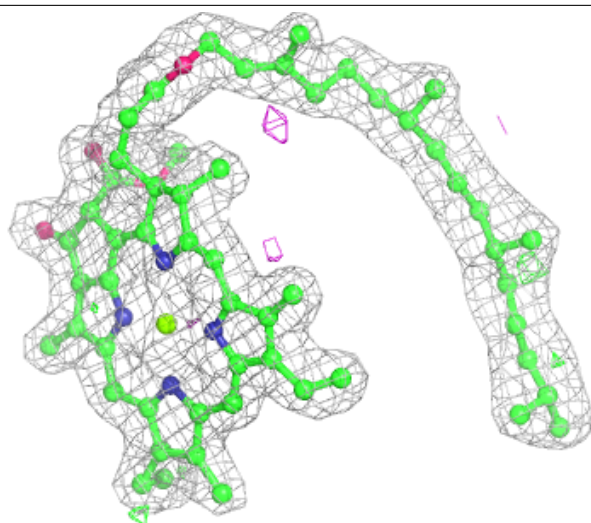
Electron density around CLA B 607:

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



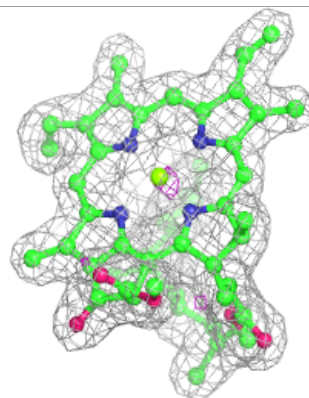
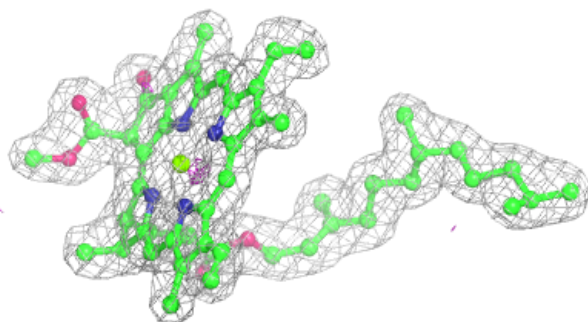
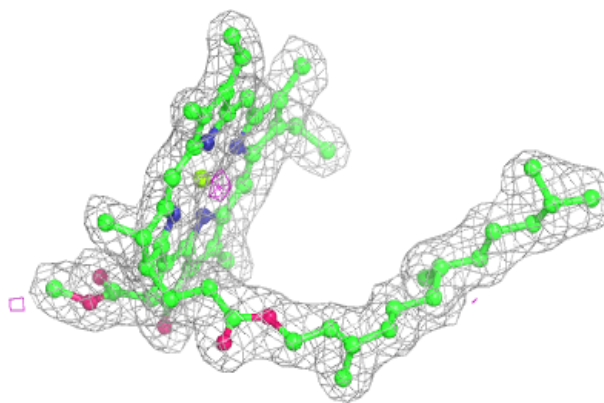
Electron density around CLA c 507:

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



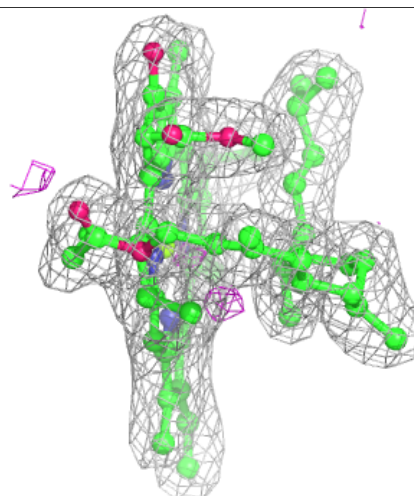
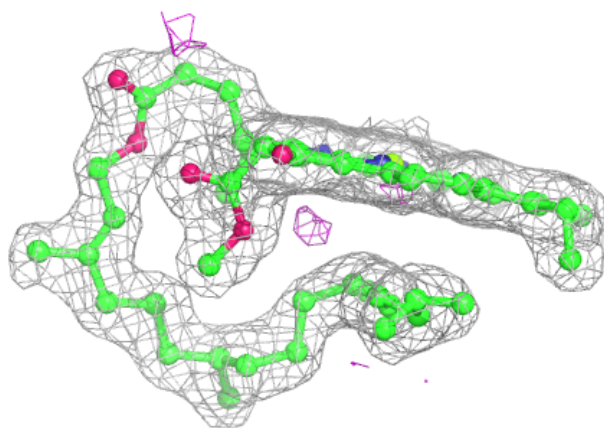
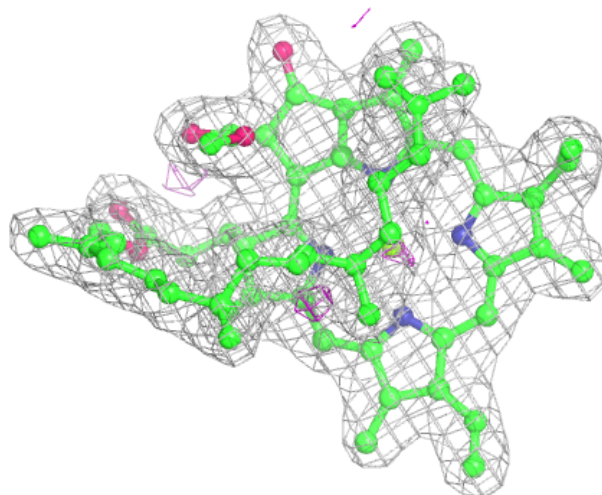
Electron density around CLA c 508:

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



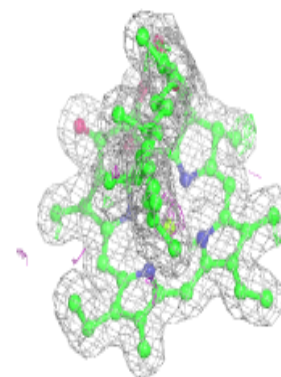
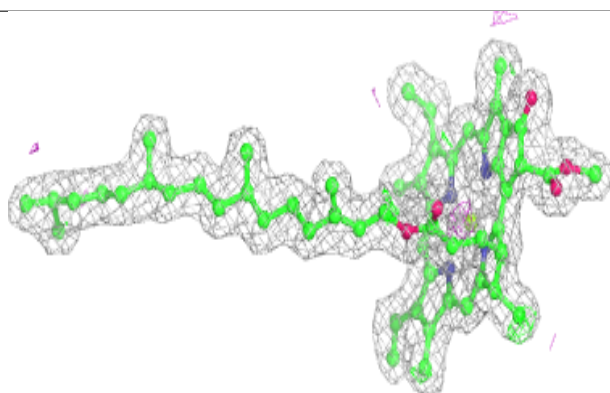
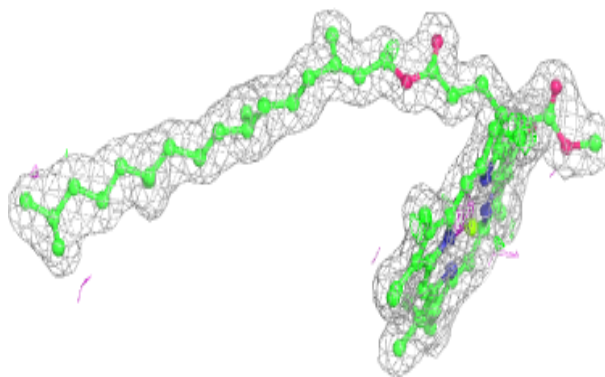
Electron density around CLA c 510:

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

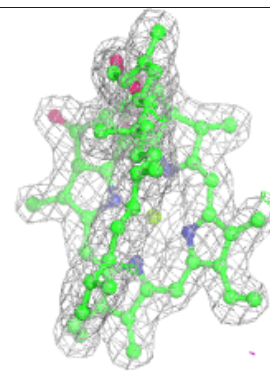
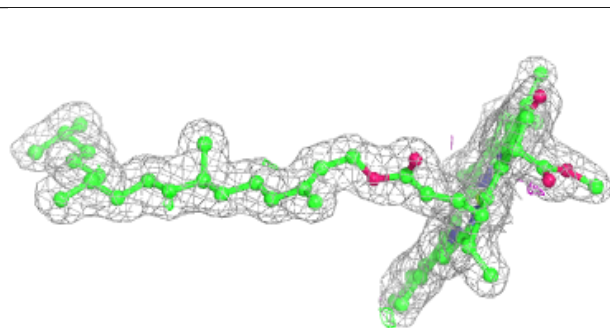
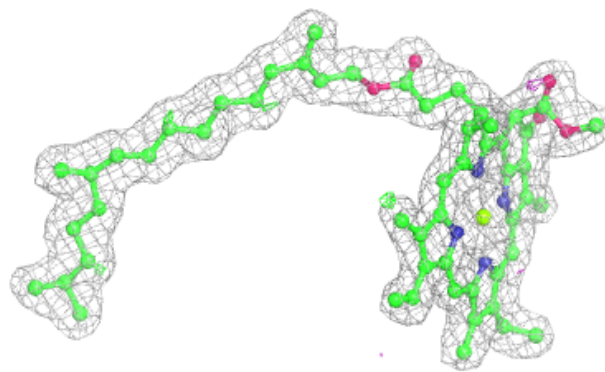


Electron density around CLA B 608:

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

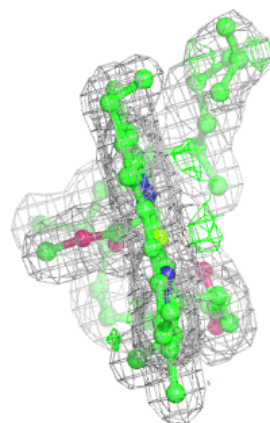
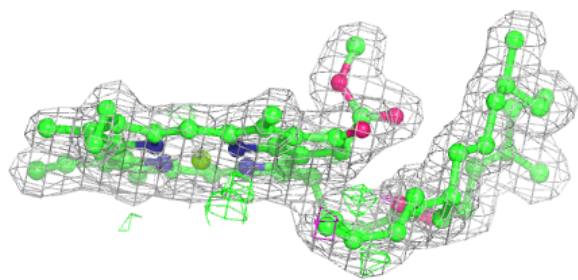
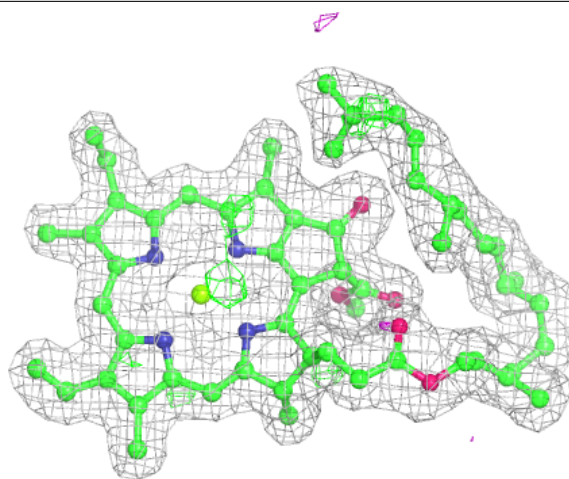
**Electron density around CLA B 610:**

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



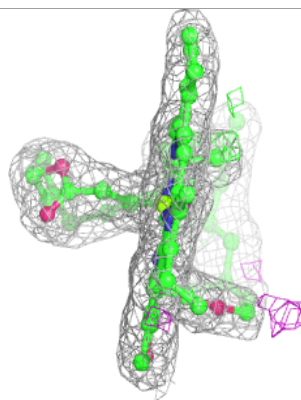
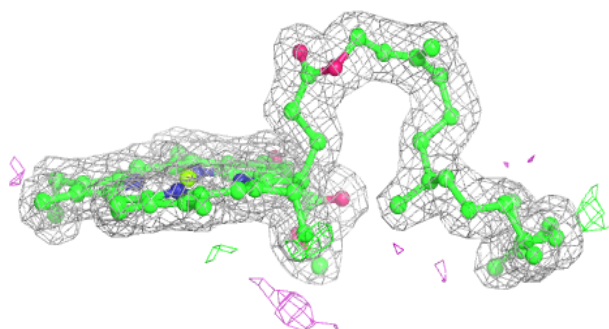
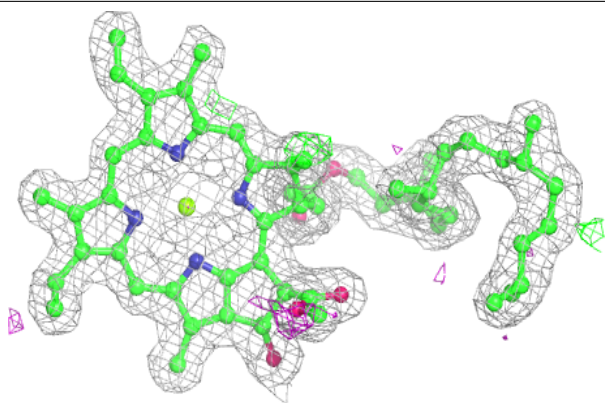
Electron density around CLA B 611:

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



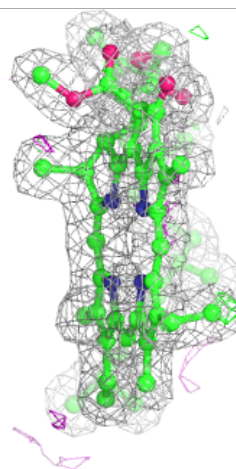
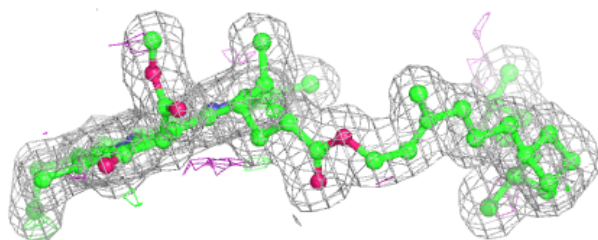
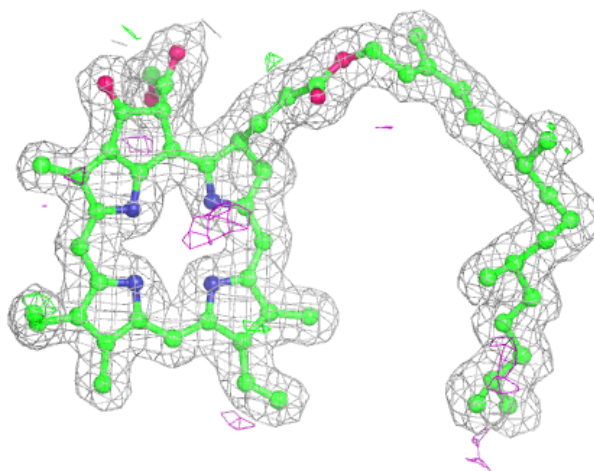
Electron density around CLA B 613:

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



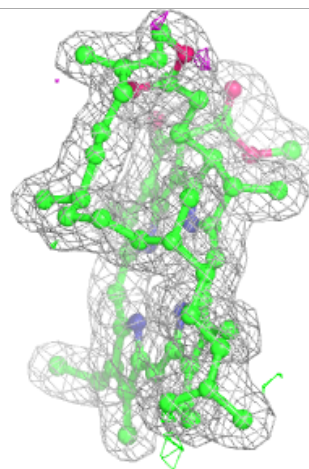
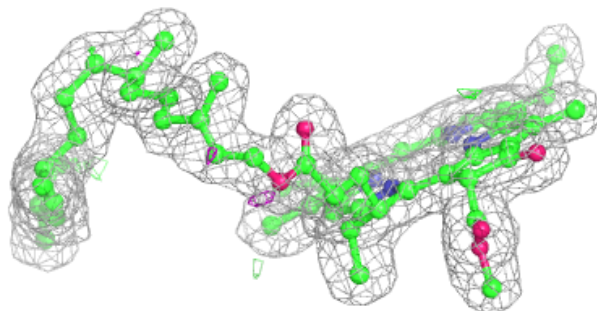
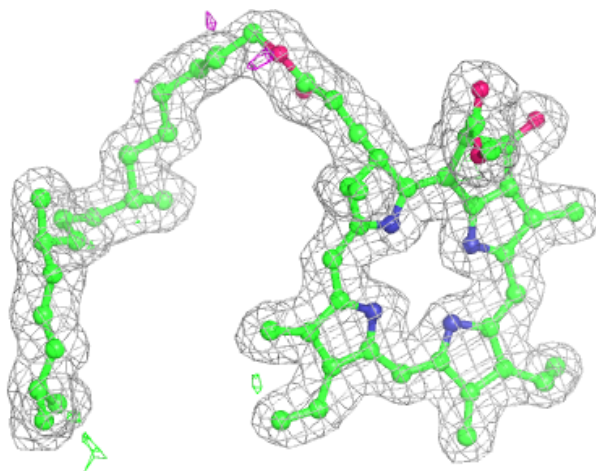
Electron density around PHO A 608:

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



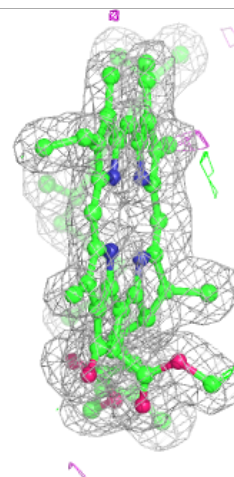
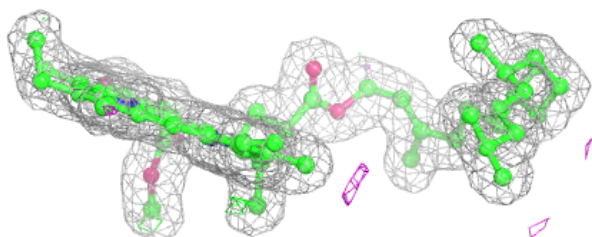
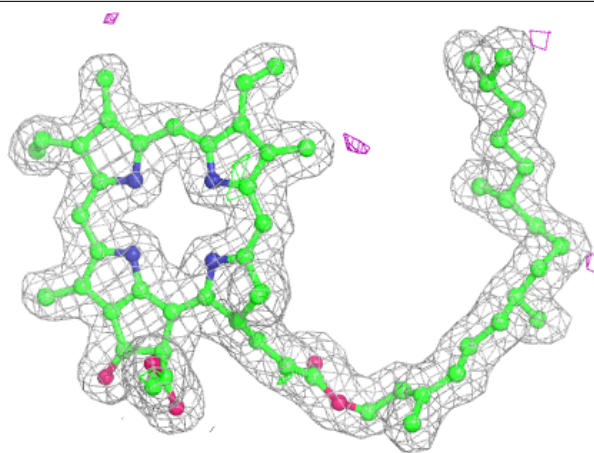
Electron density around PHO D 401:

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



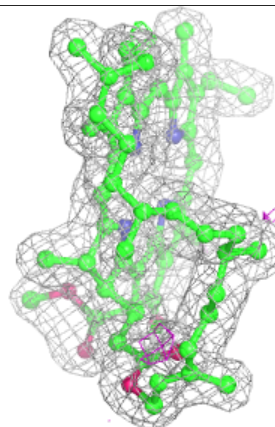
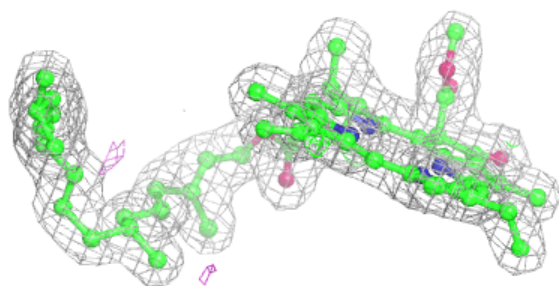
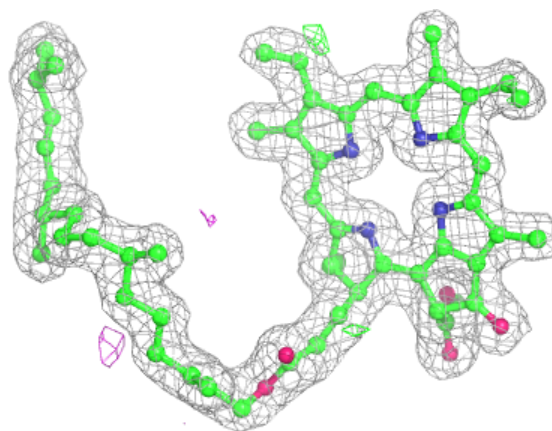
Electron density around PHO a 409:

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

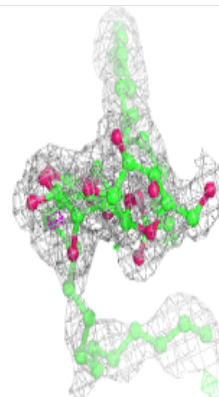
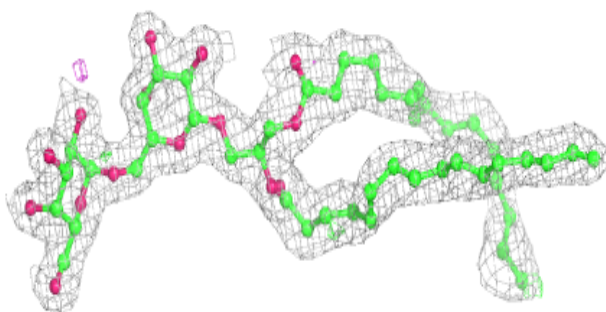
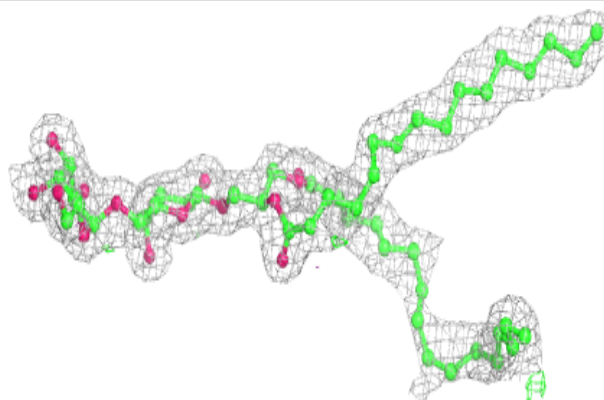


Electron density around PHO d 401:

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

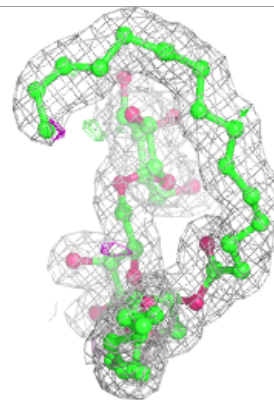
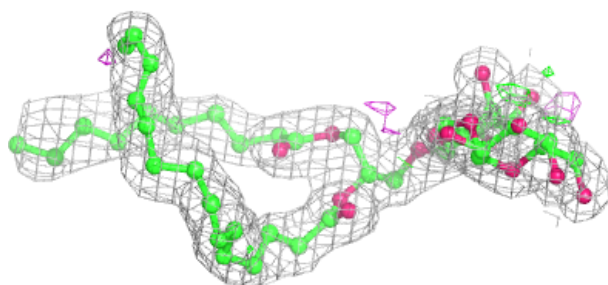
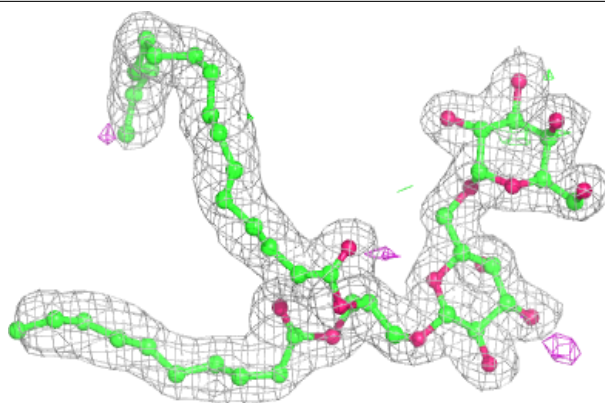
**Electron density around DGD C 516:**

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

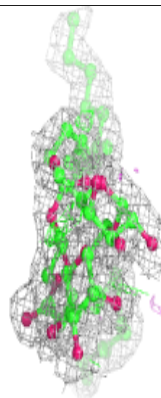
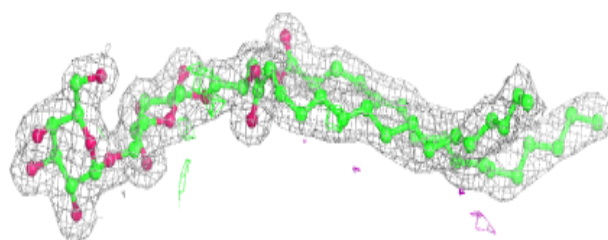
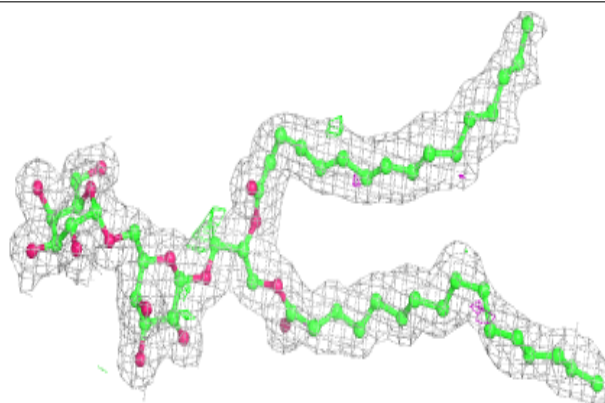


Electron density around DGD C 517:

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

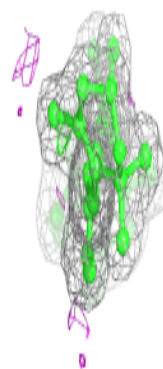
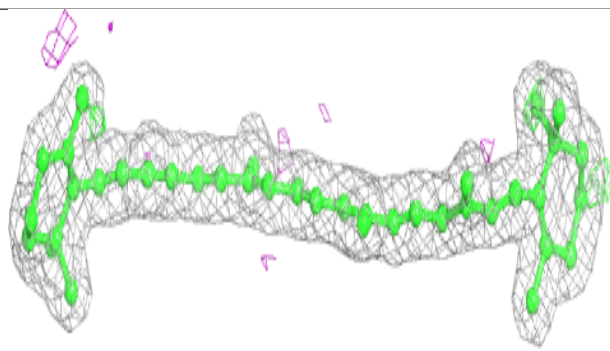
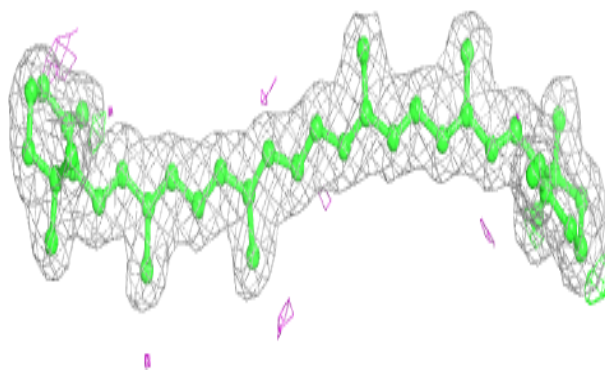
**Electron density around DGD C 518:**

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

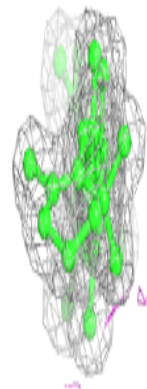
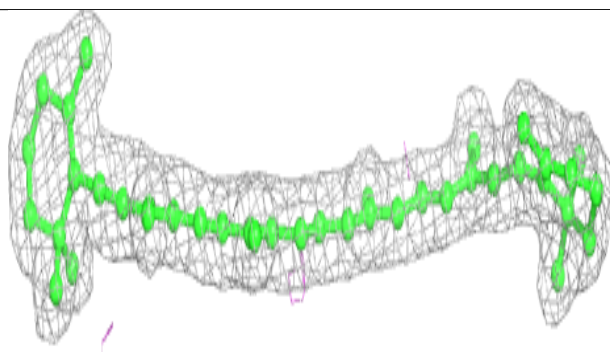
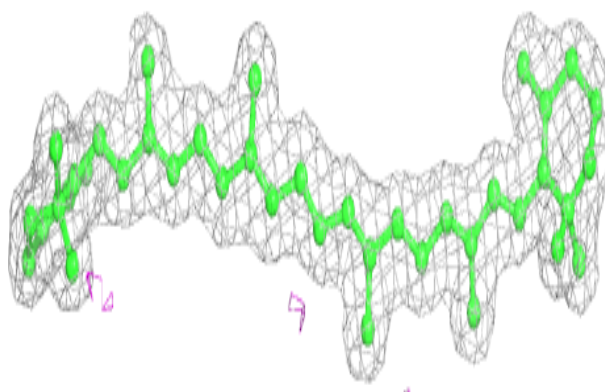


Electron density around BCR A 610:

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

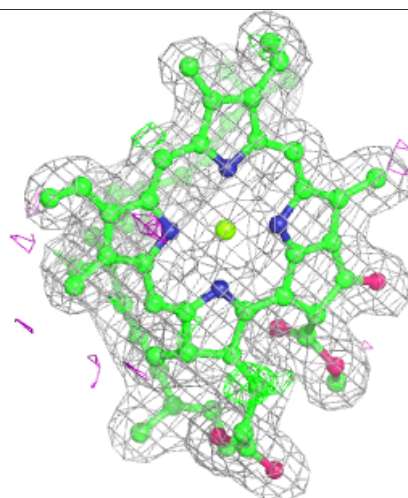
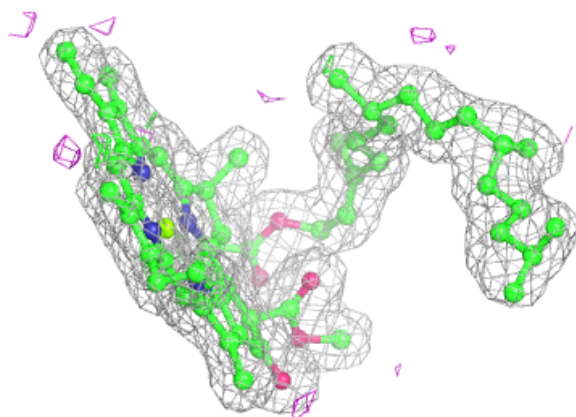
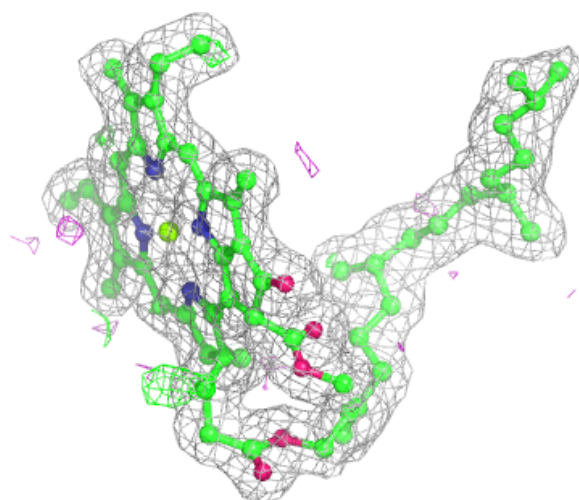
**Electron density around BCR B 618:**

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



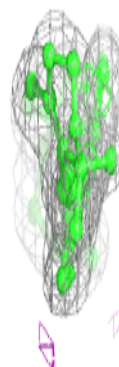
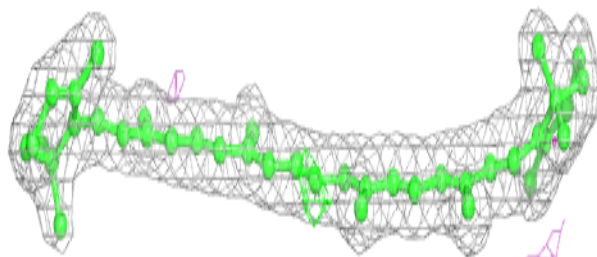
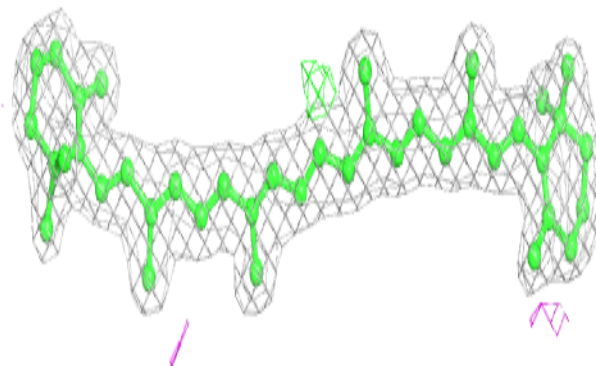
Electron density around CLA B 614:

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

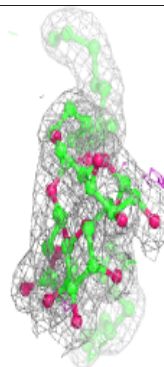
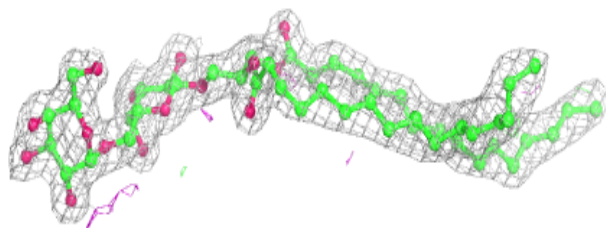
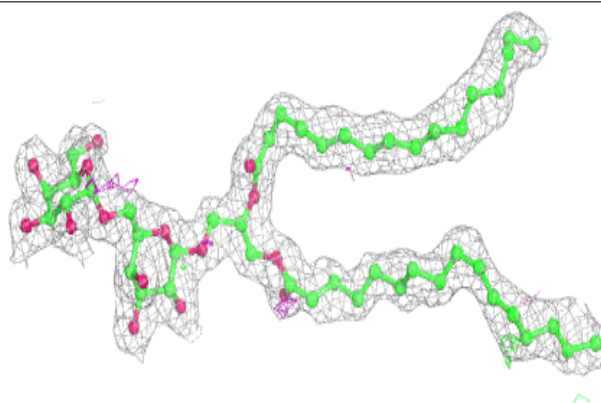


Electron density around BCR B 620:

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

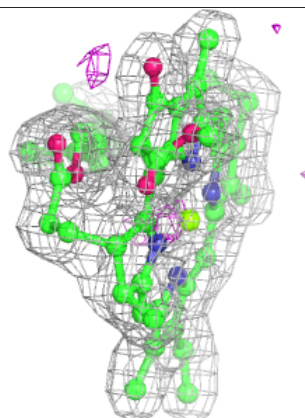
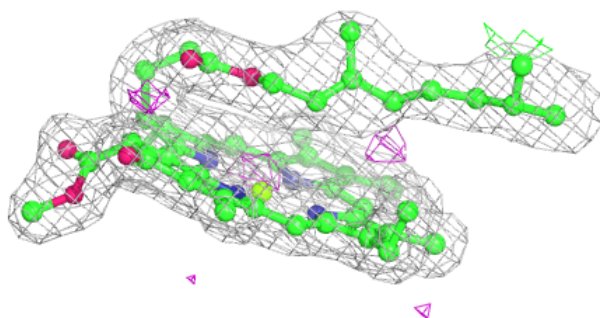
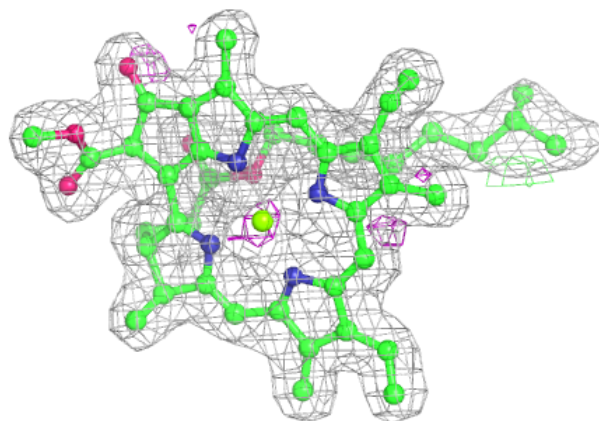
**Electron density around DGD c 518:**

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



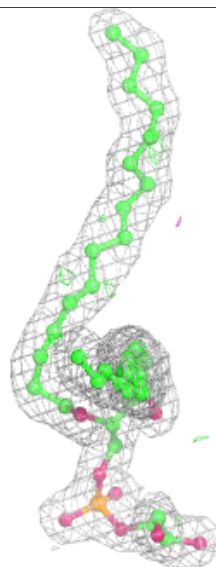
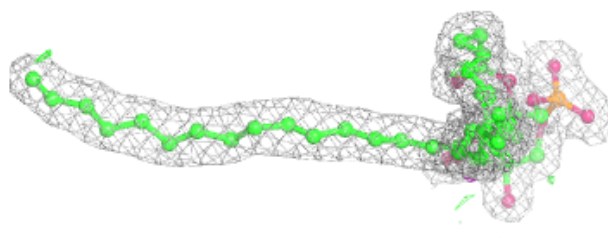
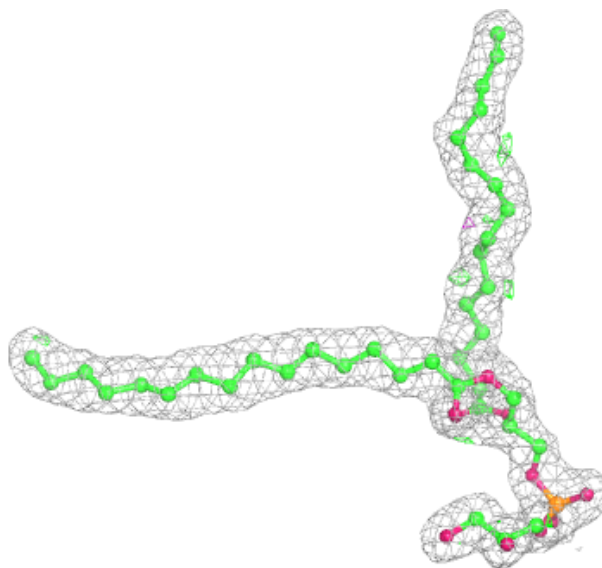
Electron density around CLA B 615:

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



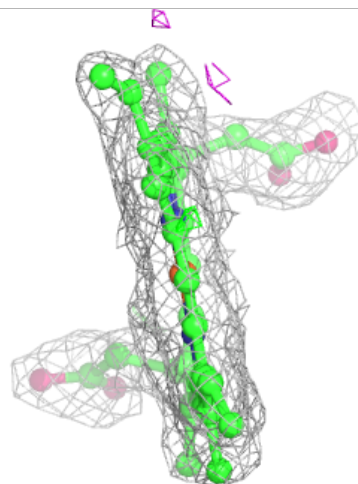
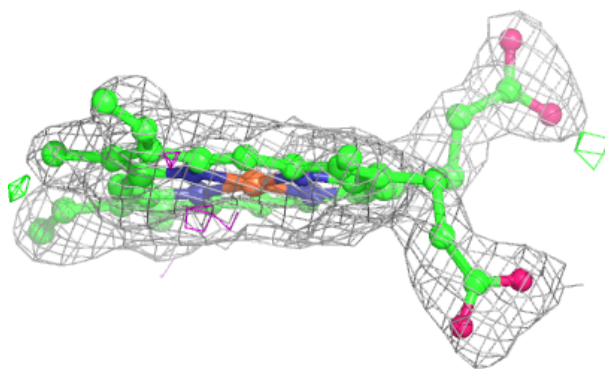
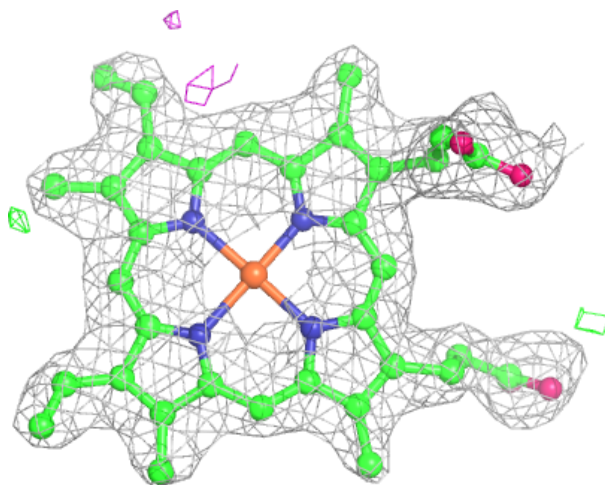
Electron density around LHG B 632:

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



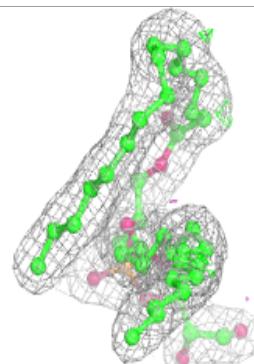
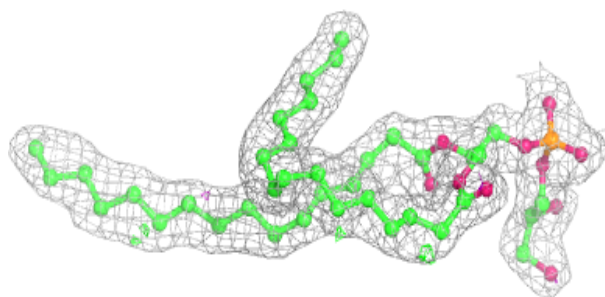
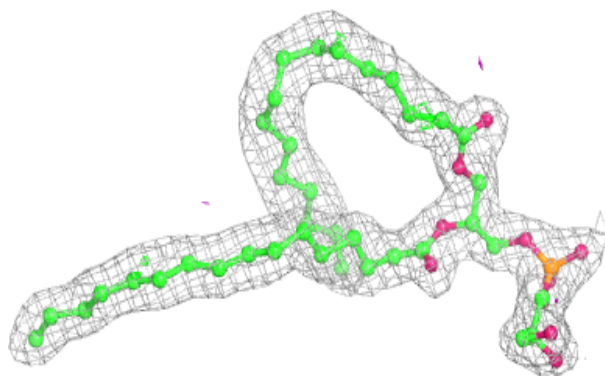
Electron density around HEM E 113:

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



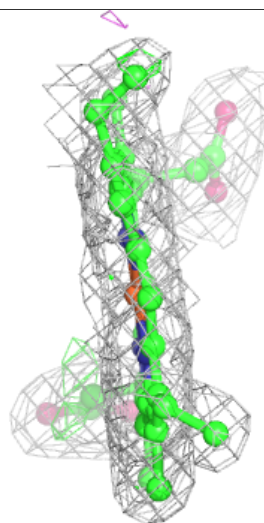
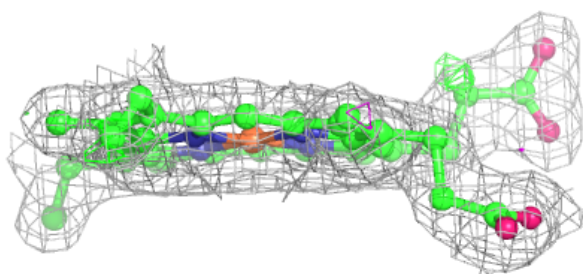
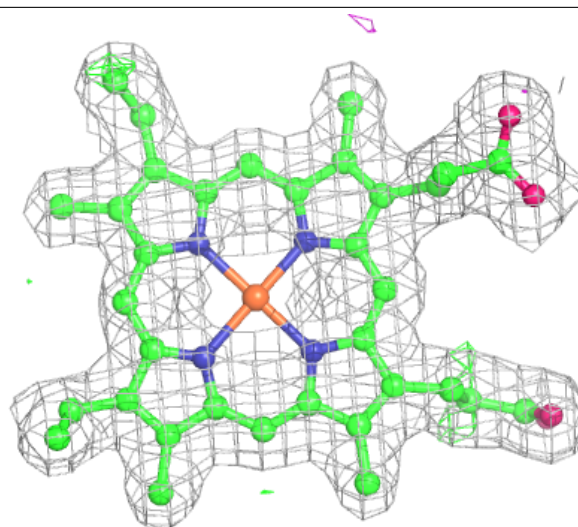
Electron density around LHG D 409:

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



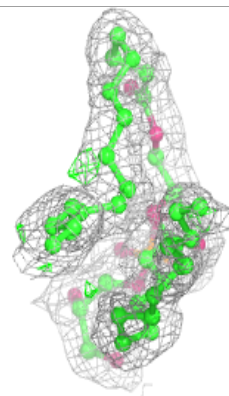
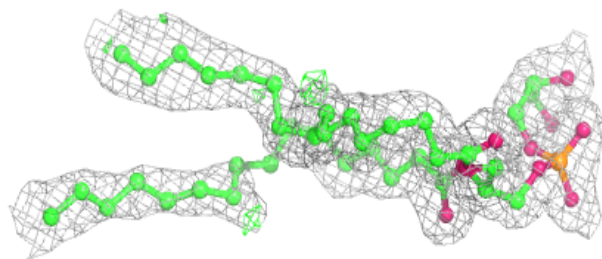
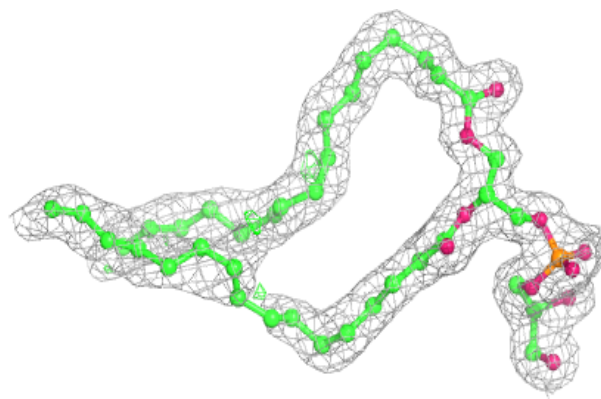
Electron density around HEC v 202:

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



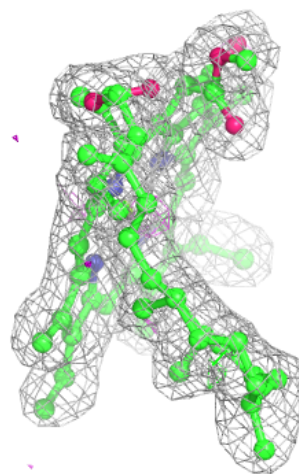
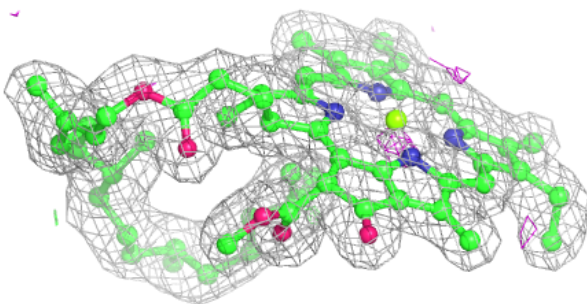
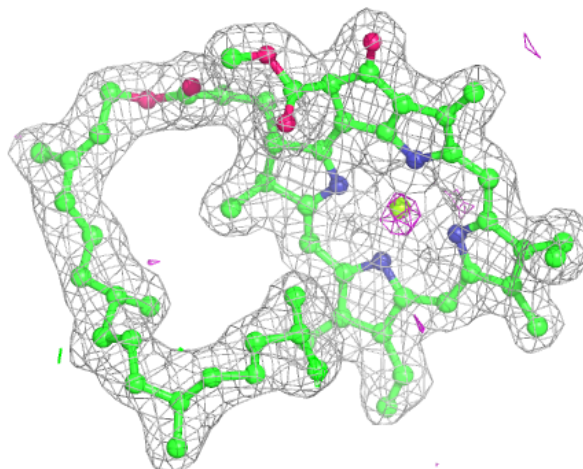
Electron density around LHG D 411:

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



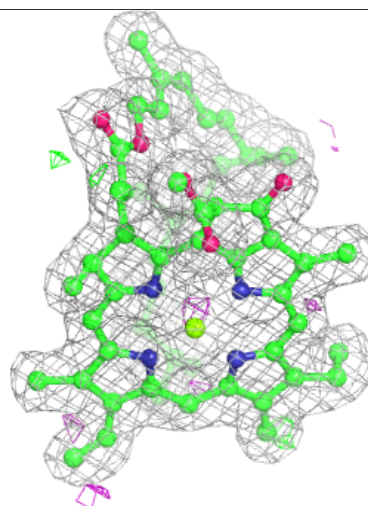
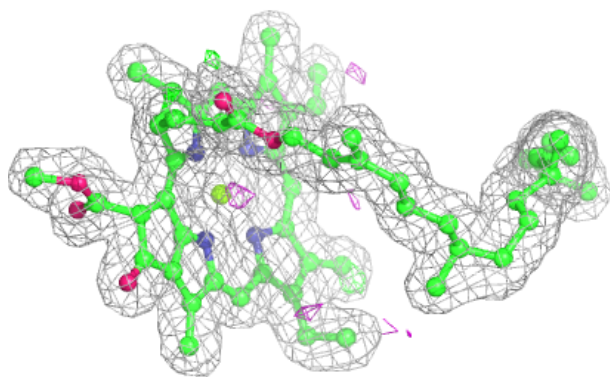
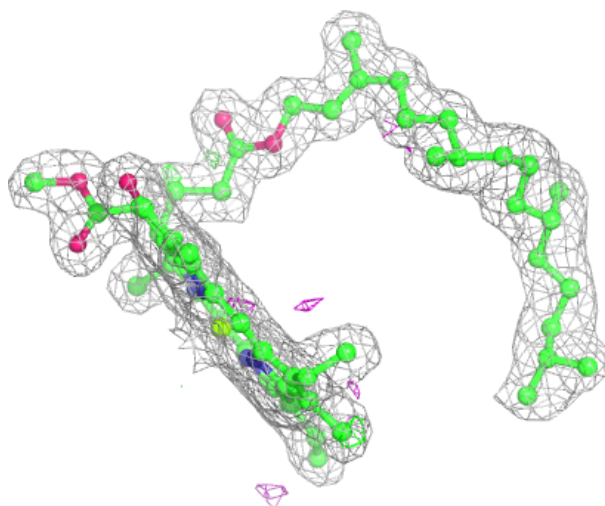
Electron density around CLA B 616:

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



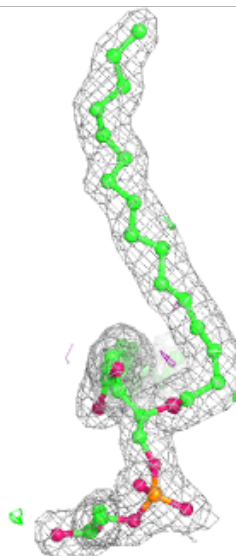
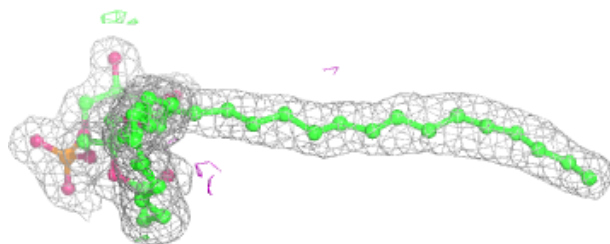
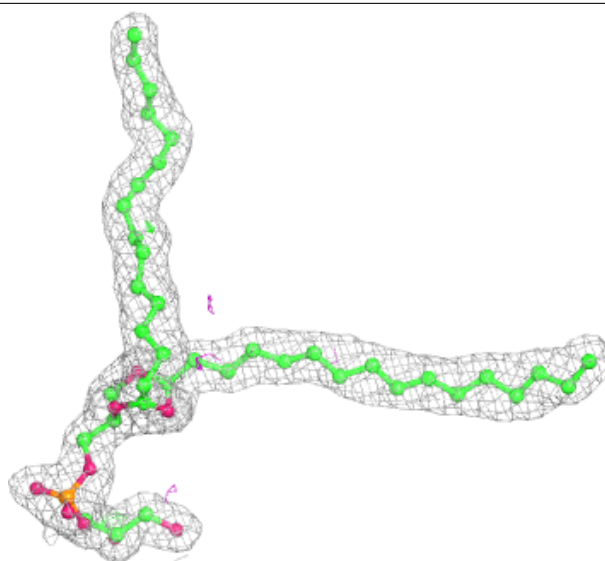
Electron density around CLA B 612:

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



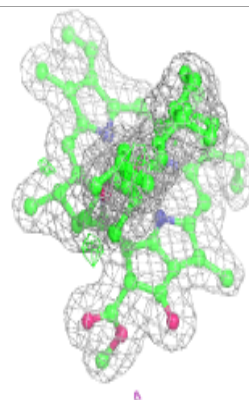
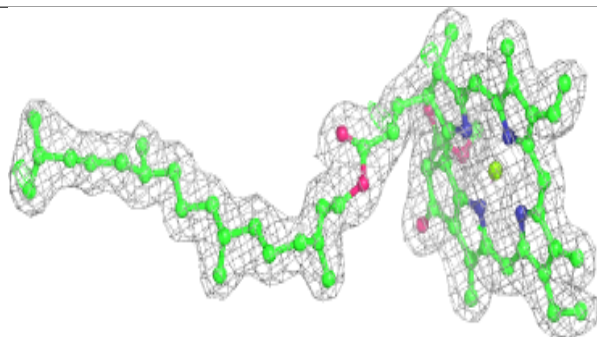
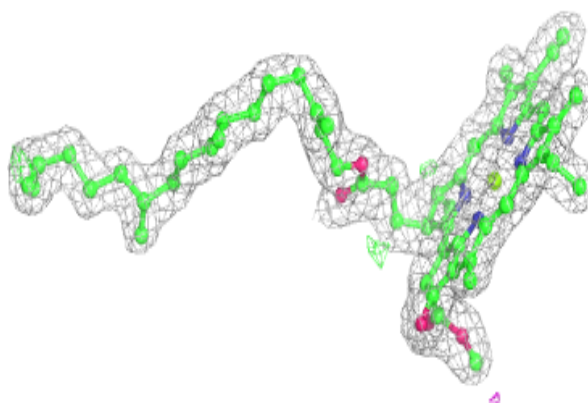
Electron density around LHG 1 101:

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

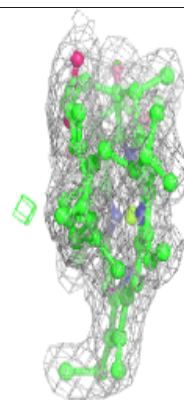
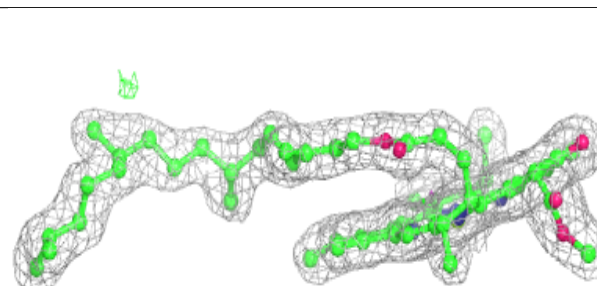
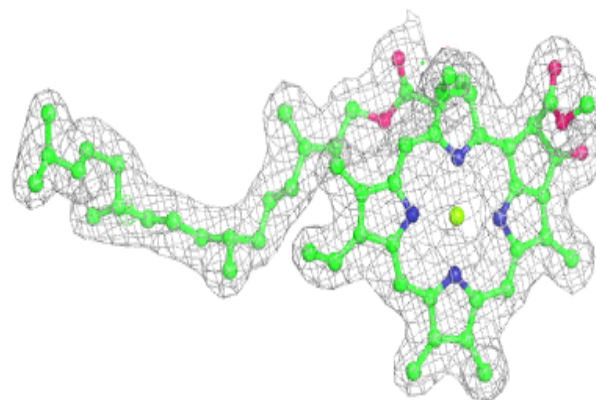


Electron density around CLA c 502:

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

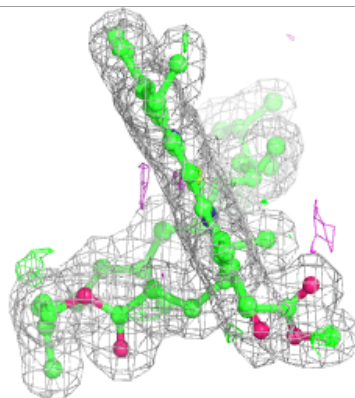
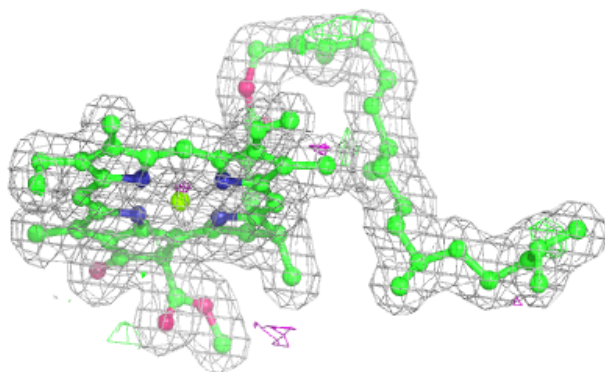
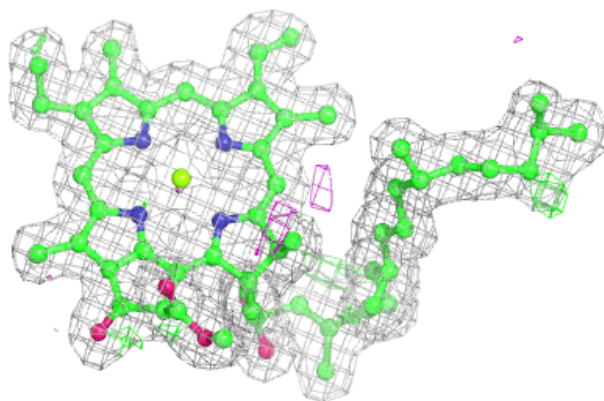
**Electron density around CLA b 604:**

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

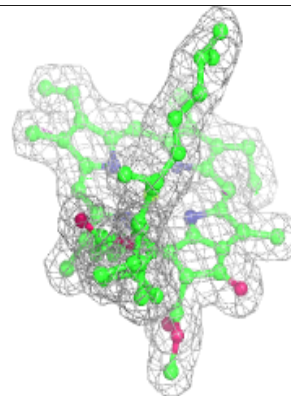
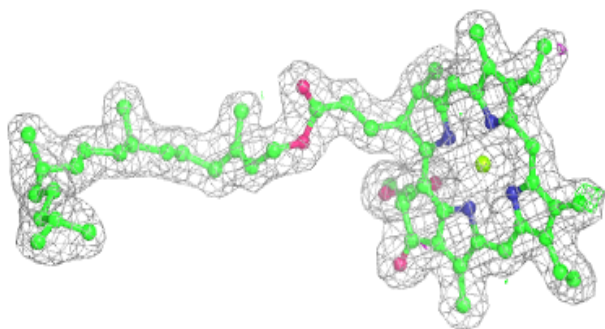
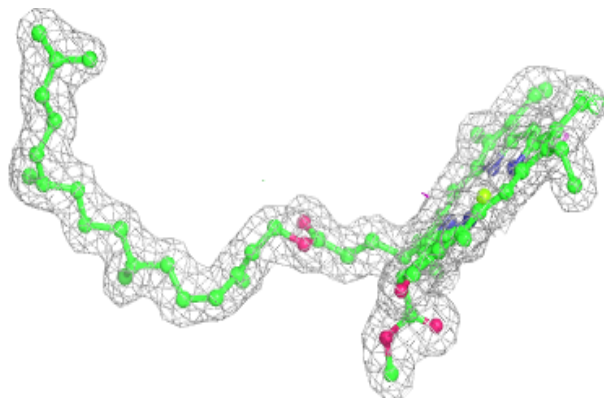


Electron density around CLA d 403:

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

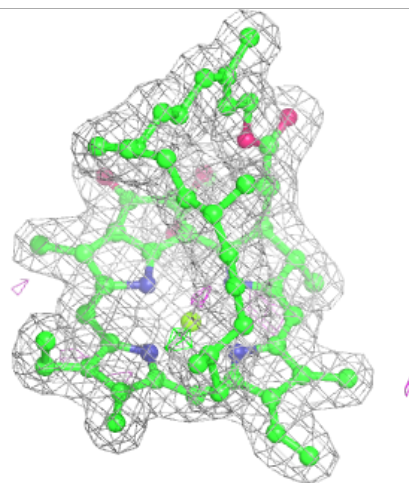
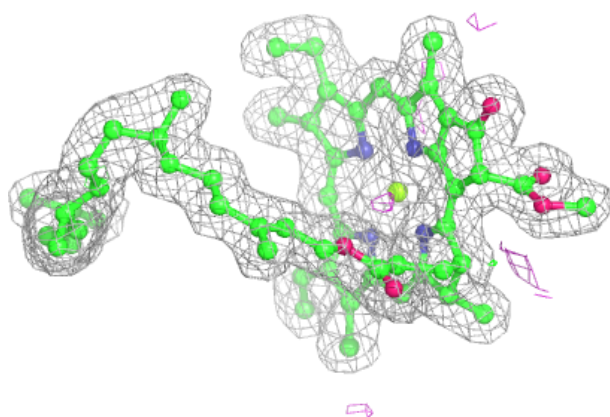
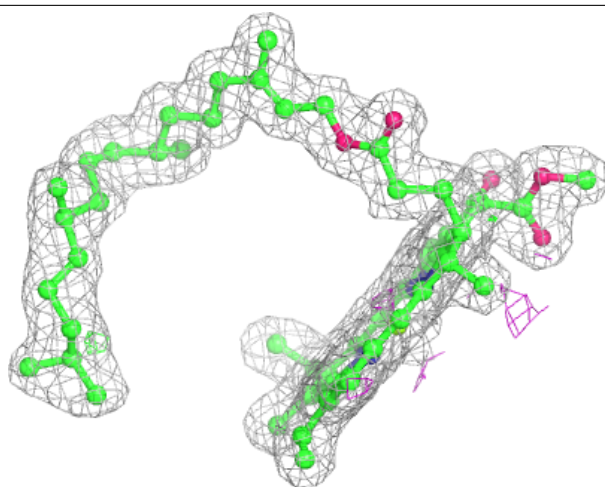
**Electron density around CLA d 404:**

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



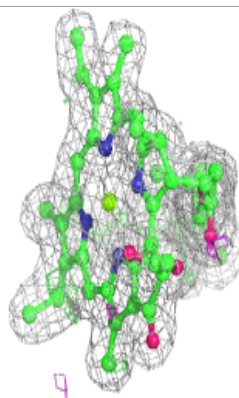
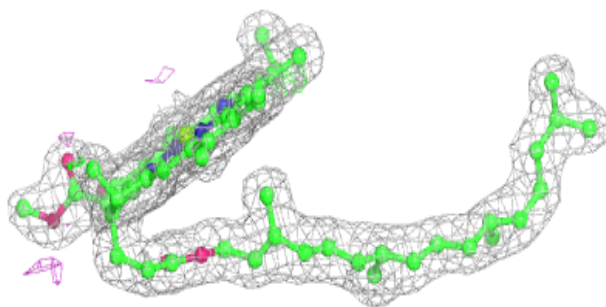
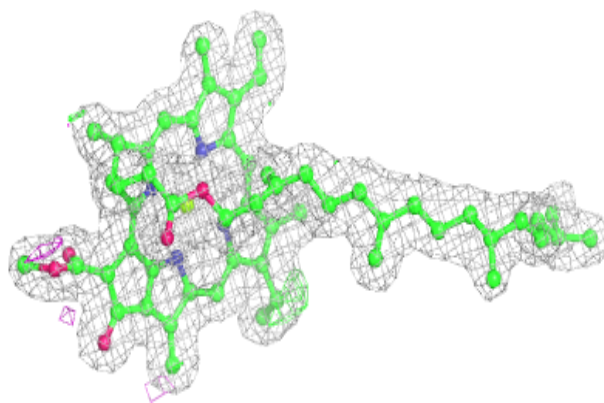
Electron density around CLA b 612:

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

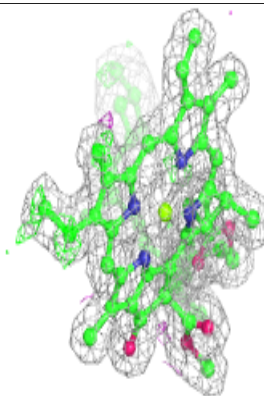
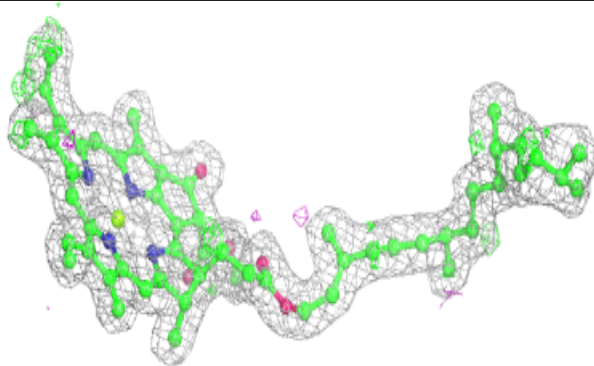
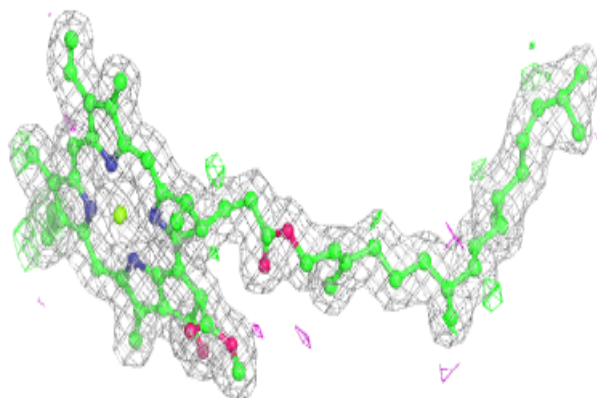


Electron density around CLA B 609:

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

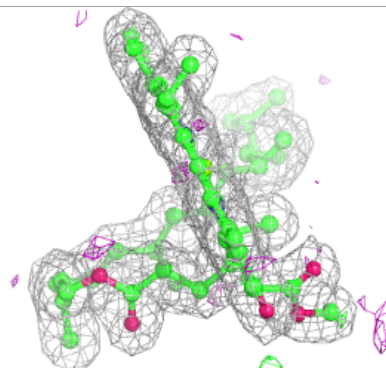
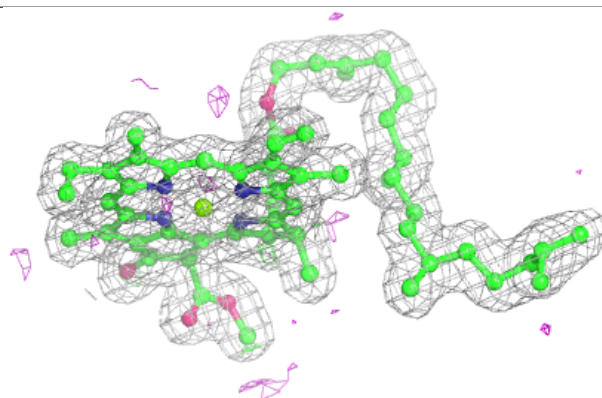
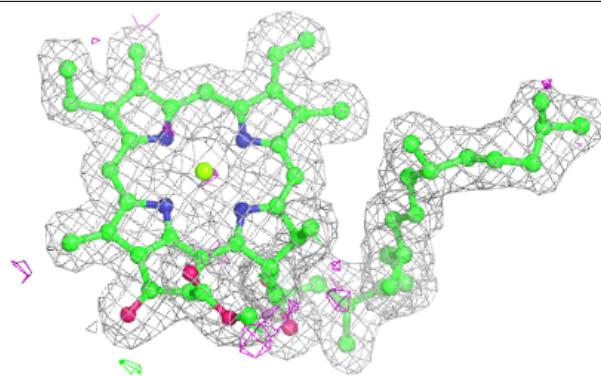
**Electron density around CLA A 606:**

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

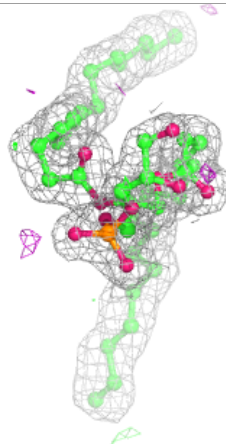
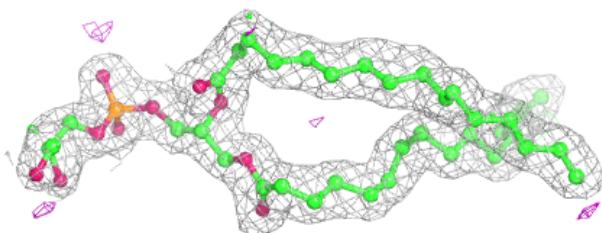
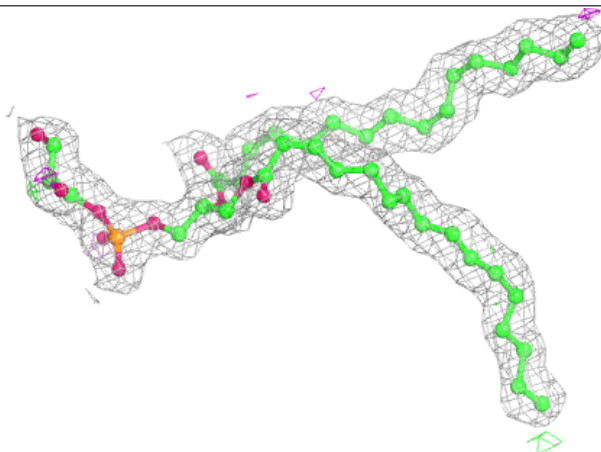


Electron density around CLA D 403:

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

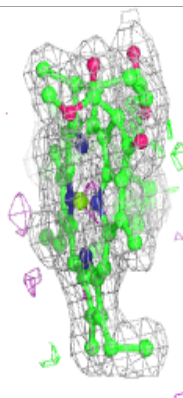
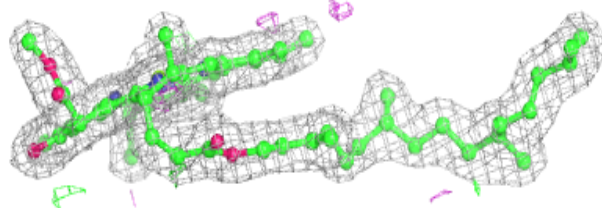
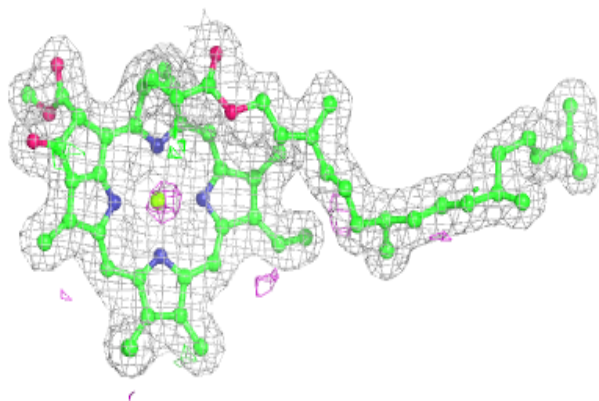
**Electron density around LHG D 410:**

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



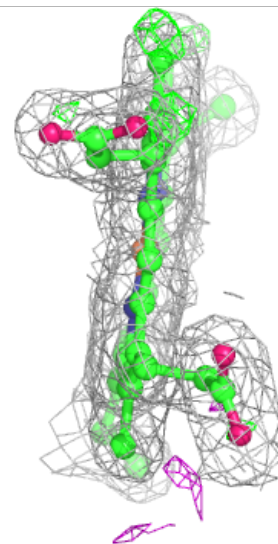
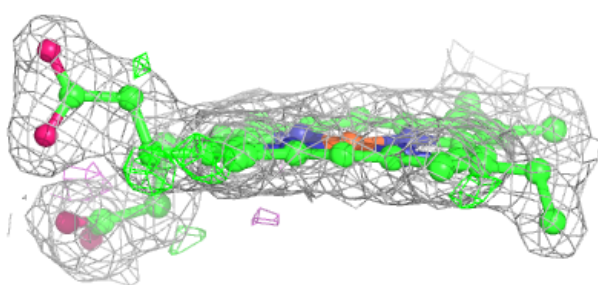
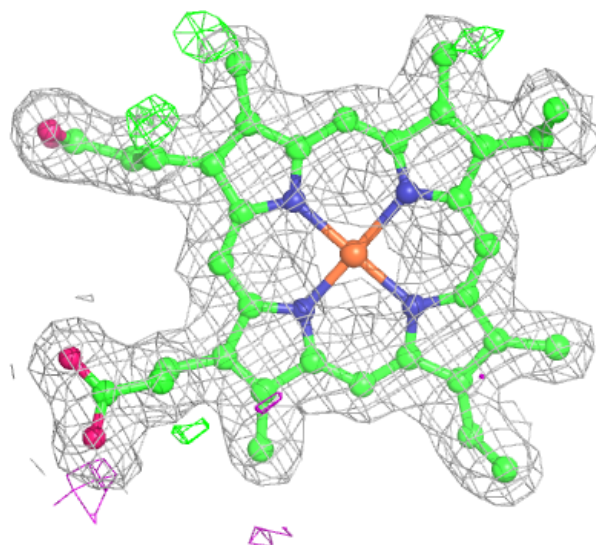
Electron density around CLA B 604:

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



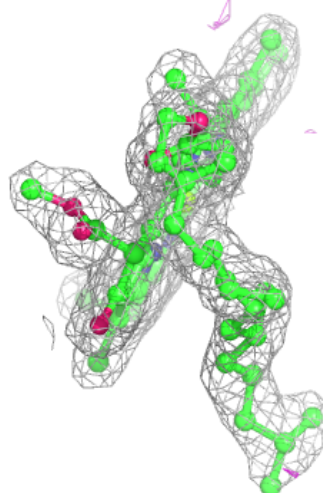
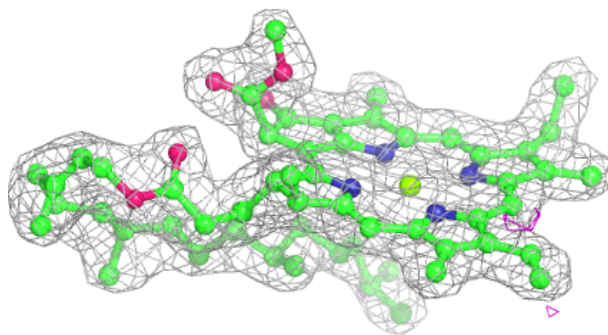
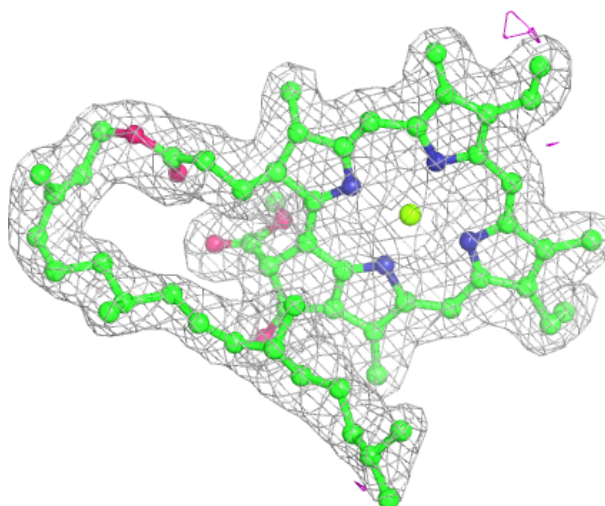
Electron density around HEC V 203:

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



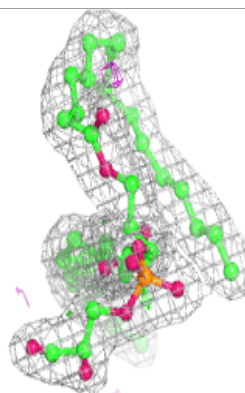
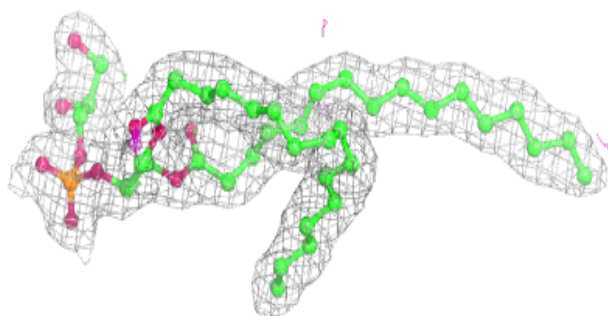
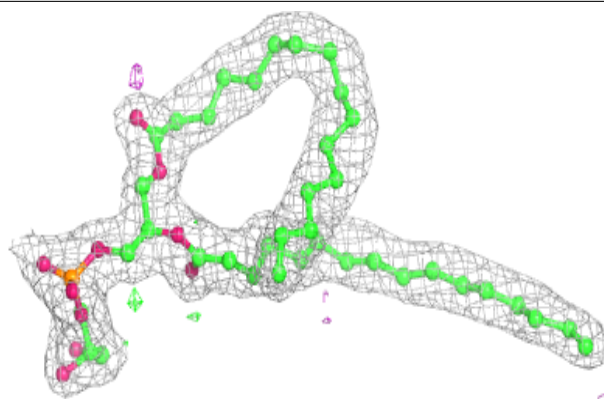
Electron density around CLA c 509:

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

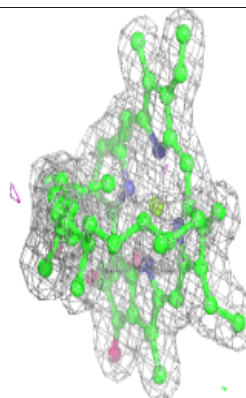
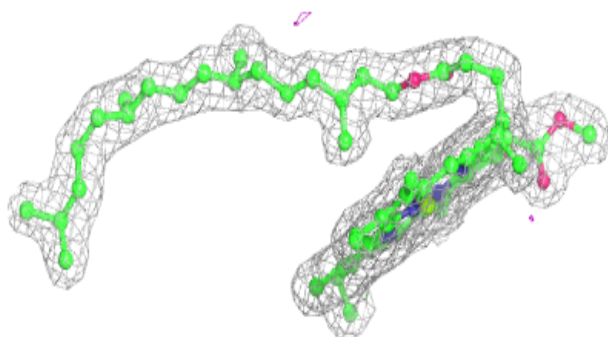
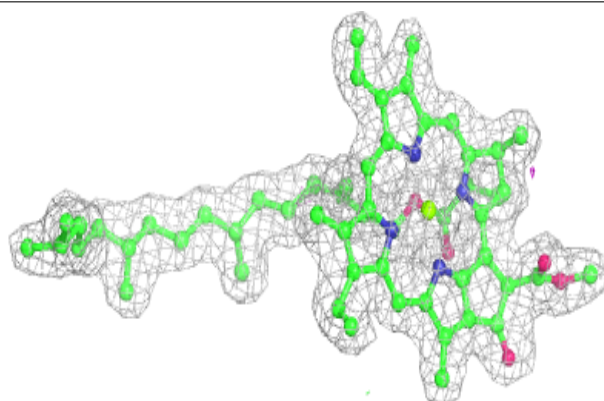


Electron density around LHG d 409:

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

**Electron density around CLA b 609:**

$2mF_o-DF_c$ (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.