



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:06 AM UTC

PDB ID : 6JLL / pdb_00006jll
Title : XFEL structure of cyanobacterial photosystem II (2F state, dataset1)
Authors : Suga, M.; Shen, J.R.
Deposited on : 2019-03-06
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

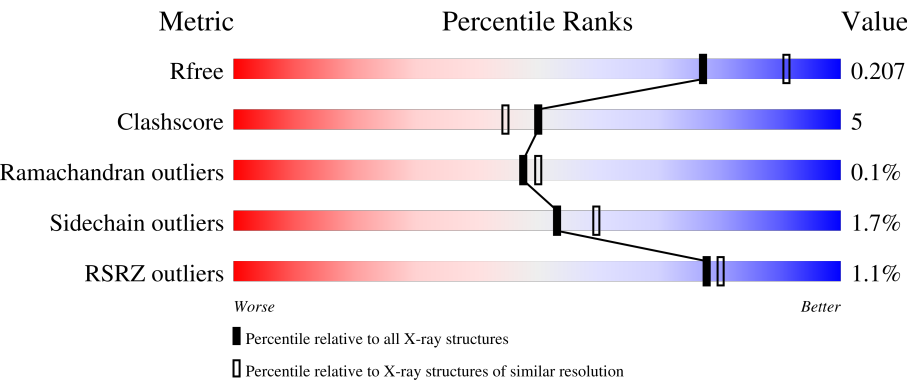
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



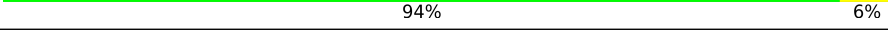
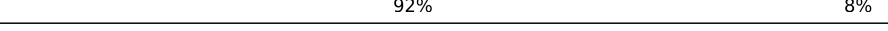
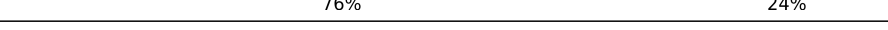
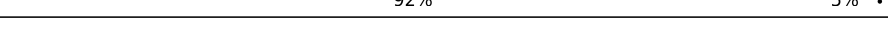
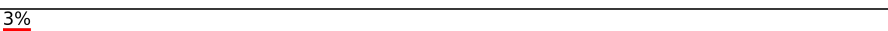
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	90%7%
1	a	344	2% 88%9%
2	B	505	89%10%
2	b	505	2% 90%10%
3	C	455	91%8%

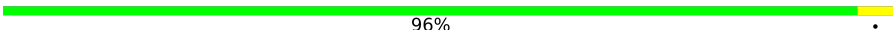
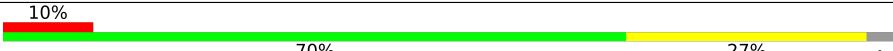
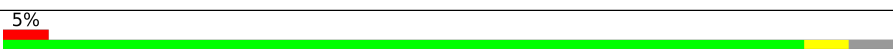
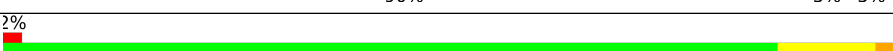
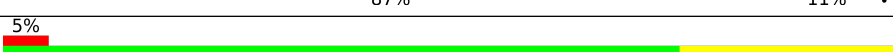
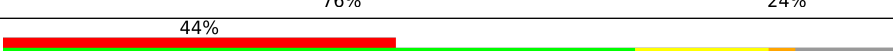
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 86% 14%
17	Y	30	 10% 70% 27% .
17	y	30	 63% 33% .
18	X	40	 90% 8% .
18	x	40	 5% 90% 5% 5%
19	Z	62	 2% 87% 11% .
19	z	62	 5% 76% 24%
20	R	34	 44% 71% 15% . 12%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	A	405	X	-	-	-
24	CLA	A	406	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	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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
24	CLA	D	402	X	-	-	-
24	CLA	D	403	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	617	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	b	626	X	-	-	-
24	CLA	c	505	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	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	d	401	X	-	-	-
24	CLA	d	402	X	-	-	-
24	CLA	d	403	X	-	-	-

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 55675 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	54	0
			3014	1963	496	537	18			
1	a	334	Total	C	N	O	S	0	56	0
			3010	1964	494	534	18			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	13			

- 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	14	0
			3553	2322	592	626	13			
3	c	455	Total	C	N	O	S	0	20	0
			3641	2382	606	639	14			

There are 8 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

- 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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	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	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			280	187	43	48	2			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	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	1	0
			274	184	40	49	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	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	0	0
			215	142	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O		0	0	0
			287	191	46	50				
18	x	38	Total	C	N	O		0	0	0
			281	188	45	48				

- 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 a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O		98	0	0
			239	163	41	35				

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	1
			2	2		
21	a	1	Total	Fe	0	1
			1	1		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

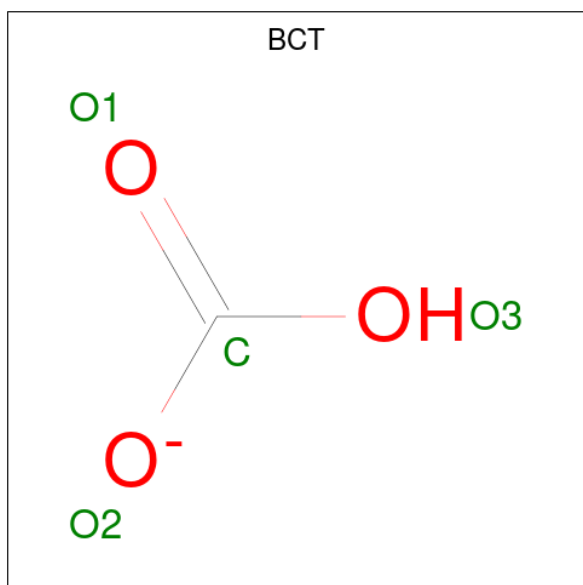
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

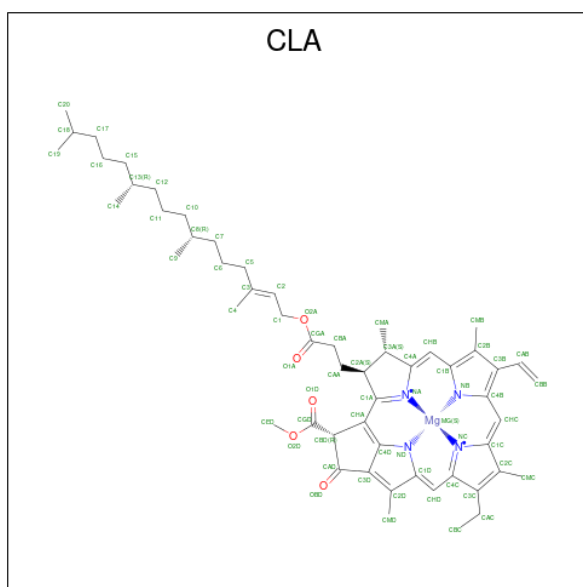
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	a	2	Total	Cl	0	2
			4	4		
22	v	1	Total	Cl	0	0
			1	1		

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3^-).



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

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $\text{C}_{55}\text{H}_{72}\text{MgN}_4\text{O}_5$).

[illegible]

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

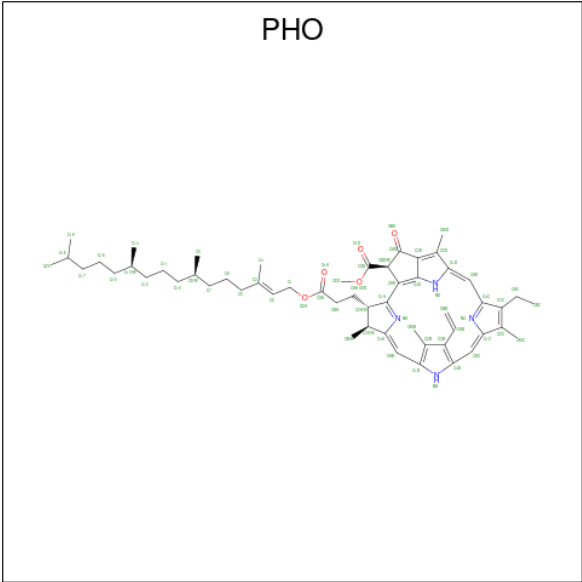
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	b	1	Total 65	C 55	Mg 1	N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

Continued on next page...

Continued from previous page...

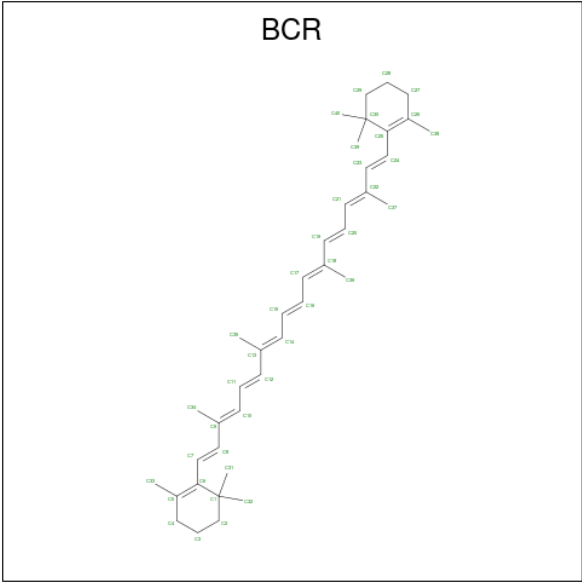
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
24	c	1	Total 65	C 55	Mg 1	N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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



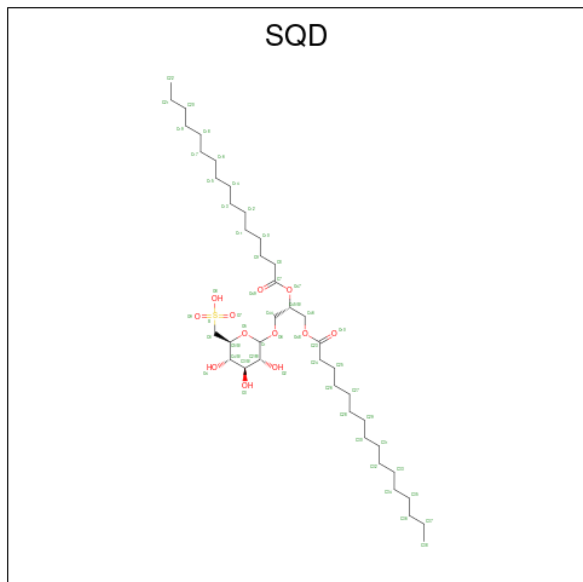
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	A	1	Total	C	N	O	0	1
			128	110	8	10		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



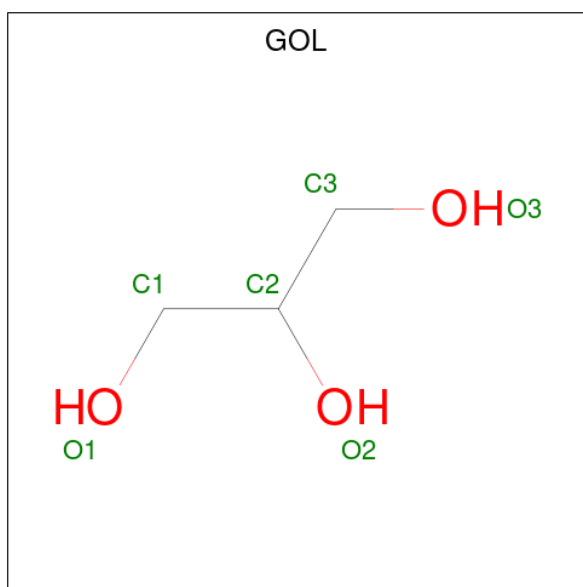
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

- Molecule 27 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



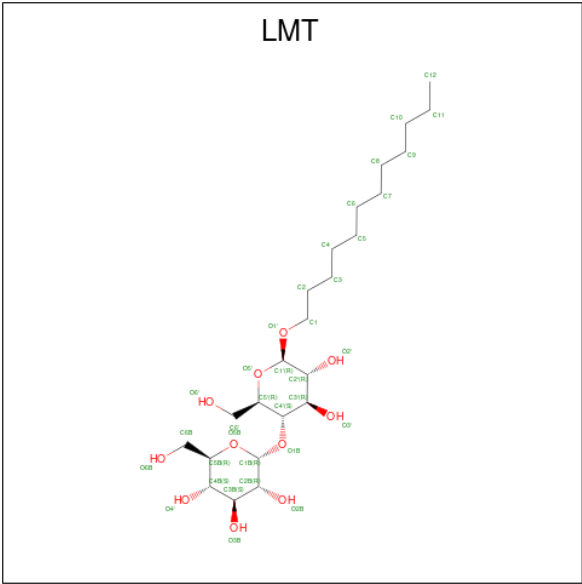
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	A	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28	B	1	Total	C	O	0	0
			6	3	3		
28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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	V	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	a	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	b	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	c	1	Total 6	C 3	O 3	0	0
28	f	1	Total 6	C 3	O 3	0	0
28	o	1	Total 6	C 3	O 3	0	0
28	t	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0
28	v	1	Total 6	C 3	O 3	0	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



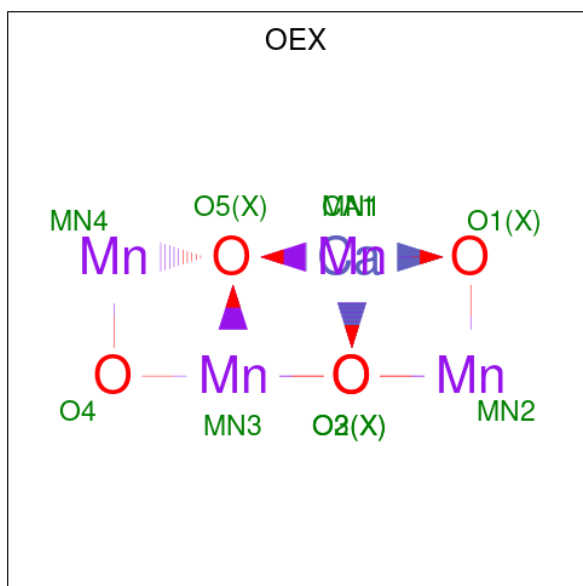
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			35	24	11		
29	B	1	Total	C	O	0	0
			25	19	6		
29	C	1	Total	C	O	0	0
			35	24	11		
29	D	1	Total	C	O	0	0
			35	24	11		
29	F	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	M	1	Total	C	O	0	0
			35	24	11		
29	T	1	Total	C	O	0	0
			25	19	6		
29	a	1	Total	C	O	0	0
			35	24	11		
29	a	1	Total	C	O	0	0
			35	24	11		
29	b	1	Total	C	O	0	0
			25	19	6		
29	f	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

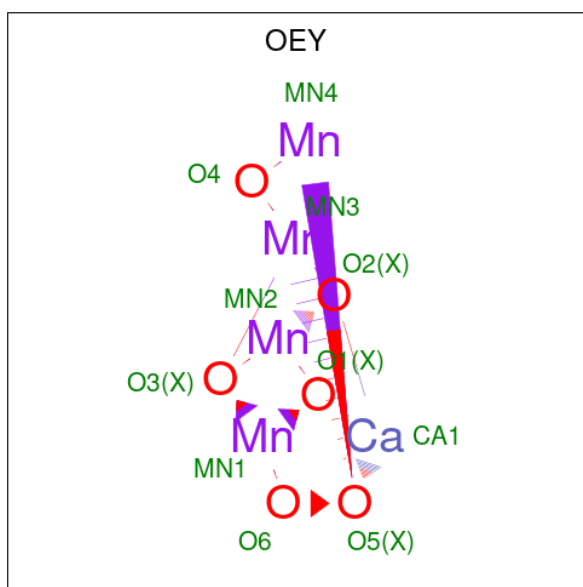
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	m	1	Total	C	O	0	0
			35	24	11		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).



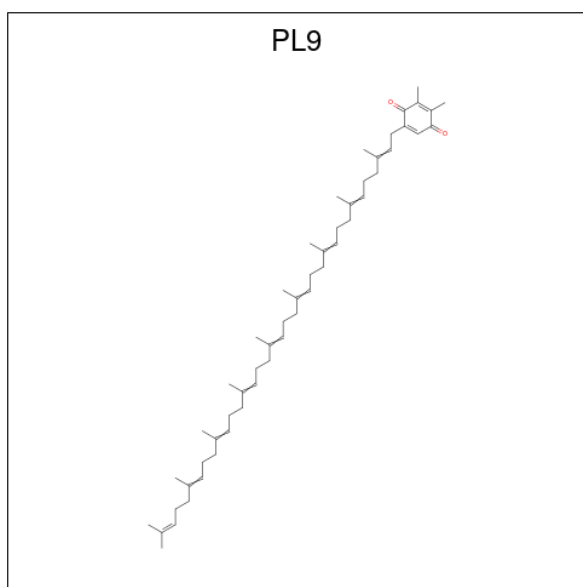
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 31 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
31	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 32 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	1
			110	106	4		

Continued on next page...

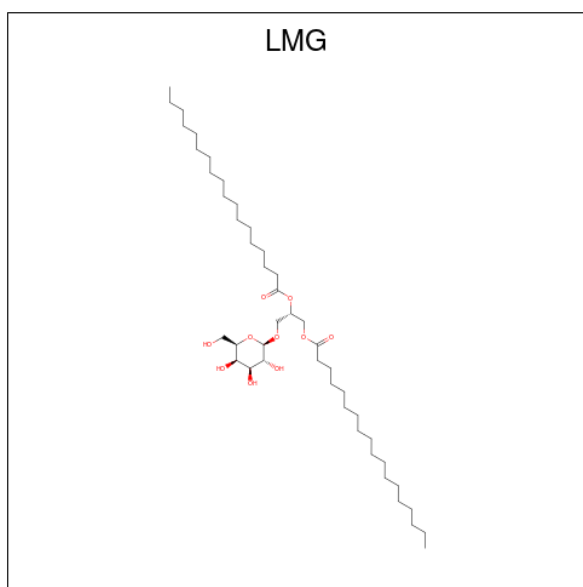
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	D	1	Total	C	O	0	1
			110	106	4		
32	a	1	Total	C	O	0	1
			110	106	4		
32	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 33 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			28	23	5		
33	B	1	Total	C	O	0	0
			33	28	5		
33	C	1	Total	C	O	0	0
			34	29	5		
33	D	2	Total	C	O	0	0
			57	51	6		
33	I	1	Total	C	O	0	0
			40	35	5		
33	J	1	Total	C		0	0
			10	10			
33	M	1	Total	C		0	0
			10	10			
33	X	1	Total	C	O	0	0
			18	16	2		
33	a	1	Total	C	O	0	0
			30	25	5		
33	b	1	Total	C	O	0	0
			33	28	5		
33	c	1	Total	C	O	0	0
			32	27	5		
33	d	3	Total	C	O	0	0
			71	63	8		
33	i	1	Total	C	O	0	0
			40	35	5		
33	j	1	Total	C		0	0
			10	10			
33	m	1	Total	C		0	0
			10	10			

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

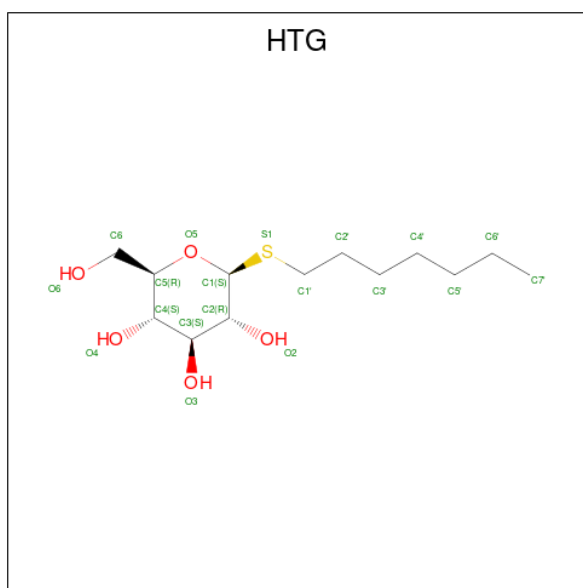


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	A	1	Total	C	O	0	0
			51	41	10		
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	Z	1	Total	C	O	0	0
			37	27	10		
34	a	1	Total	C	O	0	0
			51	41	10		
34	b	1	Total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

- Molecule 35 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total Ca 1 1	0	0
35	C	1	Total Ca 1 1	0	0
35	F	1	Total Ca 1 1	0	0
35	O	1	Total Ca 1 1	0	0
35	b	1	Total Ca 1 1	0	0
35	c	2	Total Ca 2 2	0	0
35	f	1	Total Ca 1 1	0	0
35	o	1	Total Ca 1 1	0	0

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



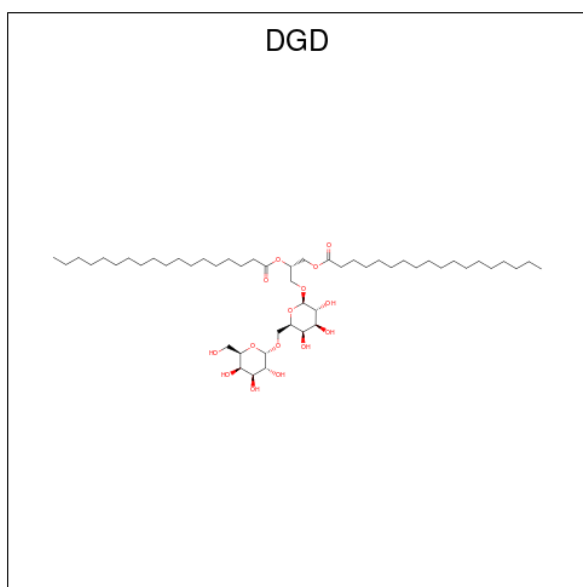
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0
36	B	1	Total C O S 19 13 5 1	0	0

Continued on next page...

Continued from previous page...

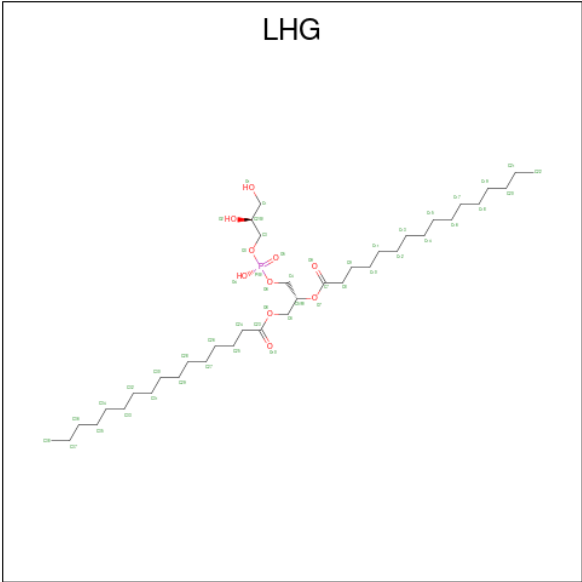
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	B	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	C	1	Total	C	O	S	0	0
			19	13	5	1		
36	H	1	Total	C	O	S	0	0
			16	10	5	1		
36	V	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	b	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	c	1	Total	C	O	S	0	0
			19	13	5	1		
36	d	1	Total	C	O	S	0	0
			16	10	5	1		

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



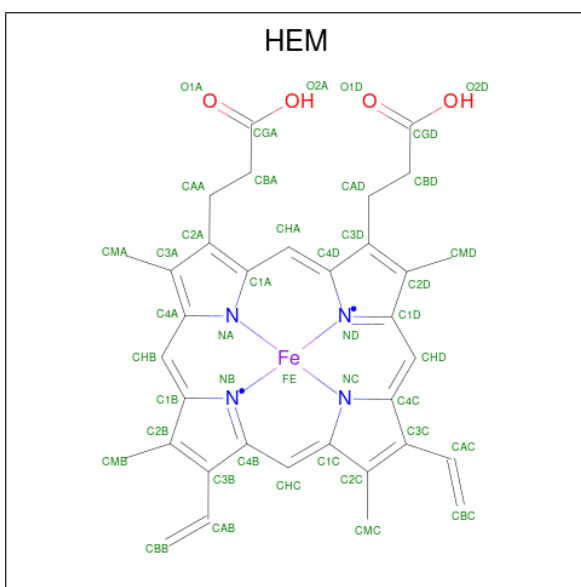
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	C	1	Total	C	O	0	0
			62	47	15		
37	D	1	Total	C	O	0	0
			52	42	10		
37	H	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total	C	O	0	0
			62	47	15		
37	c	1	Total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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	D	1	Total	C	O	P	0	0
			49	38	10	1		
38	E	1	Total	C	O	P	0	0
			42	31	10	1		
38	L	1	Total	C	O	P	0	0
			49	38	10	1		
38	a	1	Total	C	O	P	0	0
			42	31	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	d	1	Total	C	O	P	0	0
			49	38	10	1		
38	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

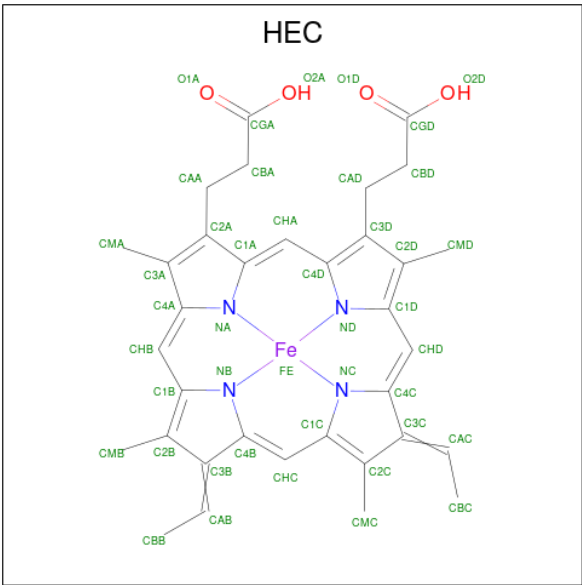


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
39	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
39	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 40 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 41 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	161	Total	O	0	14
			173	173		
42	B	290	Total	O	0	4
			294	294		
42	C	228	Total	O	0	4
			232	232		
42	D	146	Total	O	0	5
			150	150		
42	E	30	Total	O	0	0
			30	30		
42	F	9	Total	O	0	0
			9	9		
42	H	48	Total	O	0	1
			49	49		
42	I	5	Total	O	0	0
			5	5		
42	J	10	Total	O	0	0
			10	10		
42	K	9	Total	O	0	0
			9	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	L	13	Total O 14 14	0	1
42	M	23	Total O 23 23	0	0
42	O	178	Total O 180 180	0	2
42	T	17	Total O 18 18	0	1
42	U	77	Total O 77 77	0	0
42	V	117	Total O 119 119	0	2
42	Y	4	Total O 4 4	0	0
42	X	6	Total O 6 6	0	0
42	Z	1	Total O 1 1	0	0
42	a	153	Total O 162 162	0	12
42	b	266	Total O 269 269	0	3
42	c	200	Total O 205 205	0	5
42	d	129	Total O 132 132	0	3
42	e	19	Total O 19 19	0	0
42	f	8	Total O 8 8	0	0
42	h	44	Total O 44 44	0	0
42	i	5	Total O 5 5	0	0
42	j	6	Total O 6 6	0	0
42	k	7	Total O 7 7	0	0
42	l	9	Total O 9 9	0	0
42	m	11	Total O 11 11	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	o	155	Total 155	O 155	0	0
42	t	11	Total 11	O 11	0	0
42	u	93	Total 93	O 93	0	0
42	v	81	Total 82	O 82	0	1
42	y	2	Total 2	O 2	0	0
42	x	6	Total 6	O 6	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.

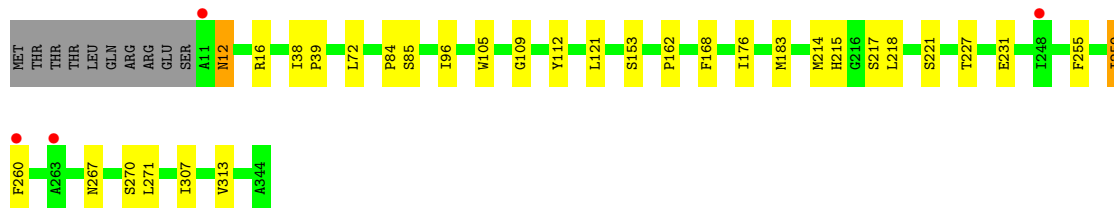
• Molecule 1: Photosystem II protein D1

Chain A: 



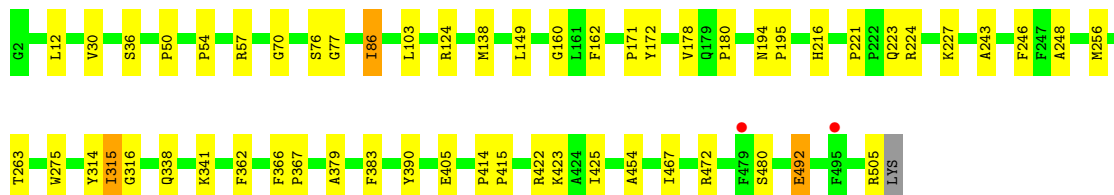
• Molecule 1: Photosystem II protein D1

Chain a: 



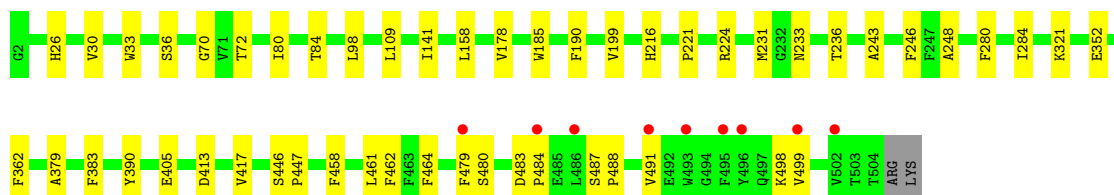
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B: 

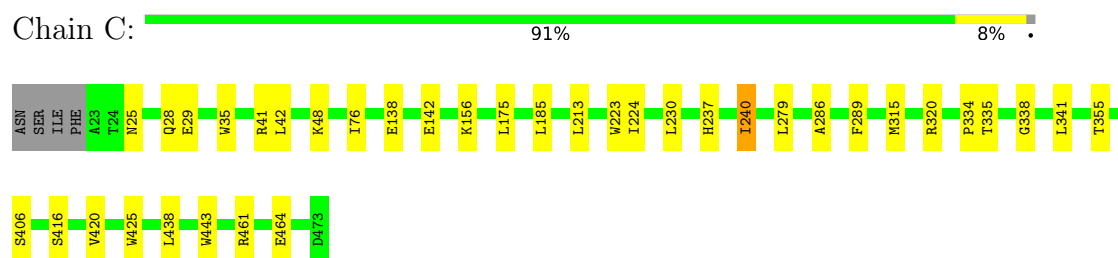


• Molecule 2: Photosystem II CP47 reaction center protein

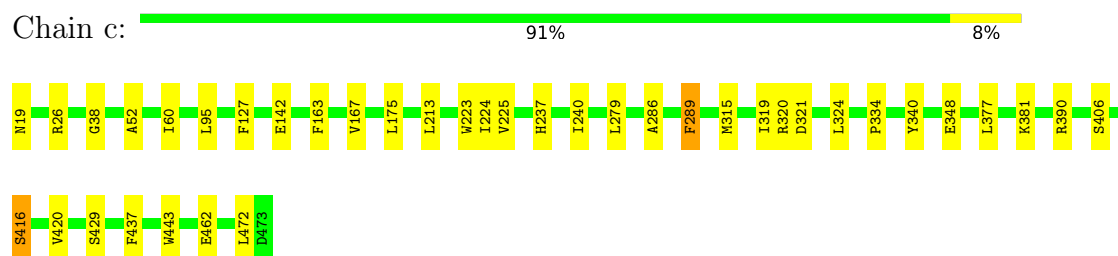
Chain b: 



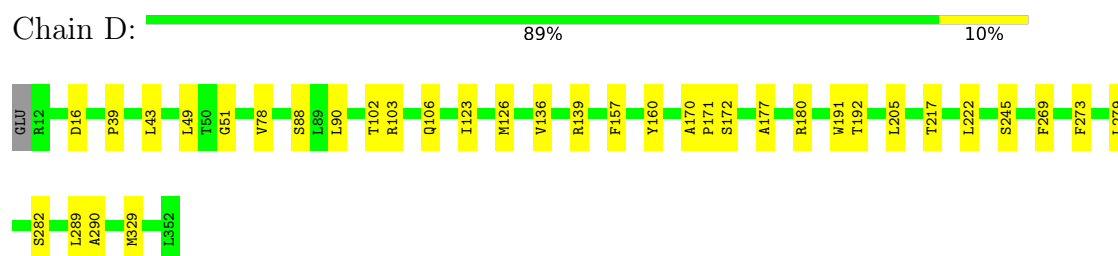
- Molecule 3: Photosystem II CP43 reaction center protein



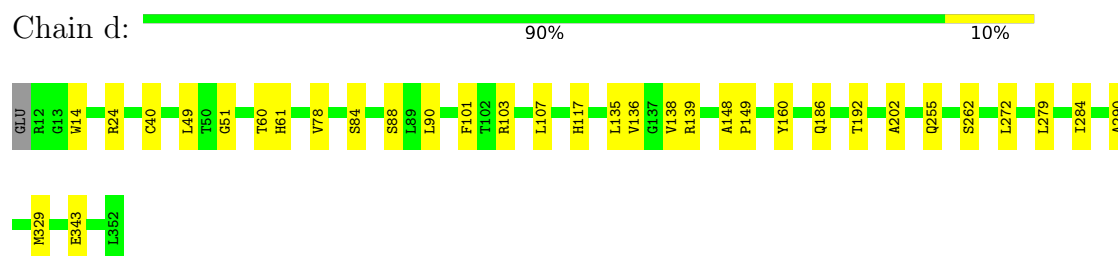
- Molecule 3: Photosystem II CP43 reaction center protein



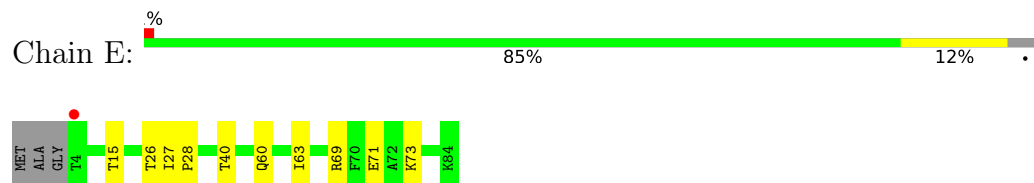
- Molecule 4: Photosystem II D2 protein



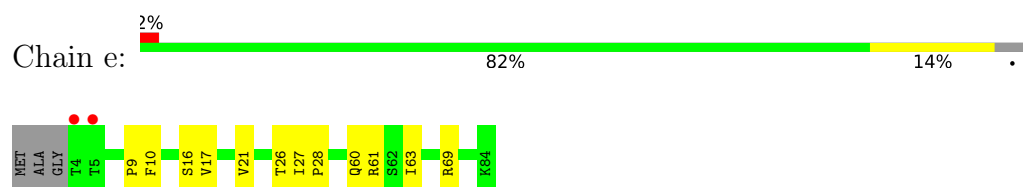
- Molecule 4: Photosystem II D2 protein



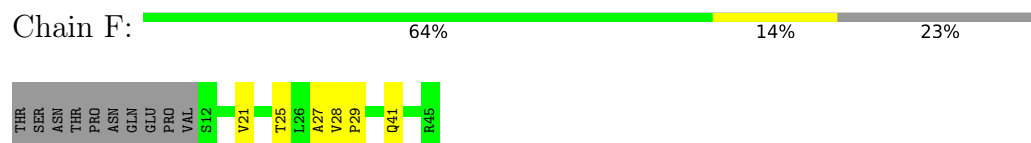
- Molecule 5: Cytochrome b559 subunit alpha



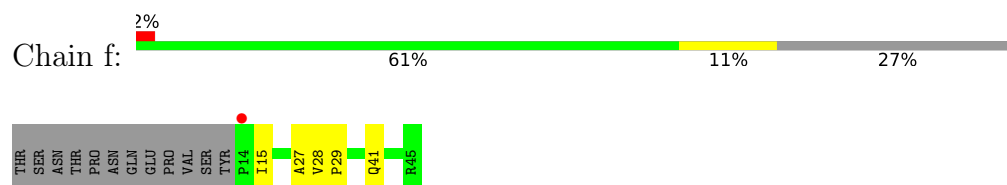
- Molecule 5: Cytochrome b559 subunit alpha



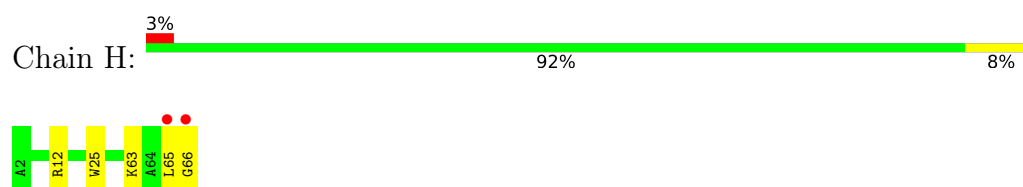
- Molecule 6: Cytochrome b559 subunit beta



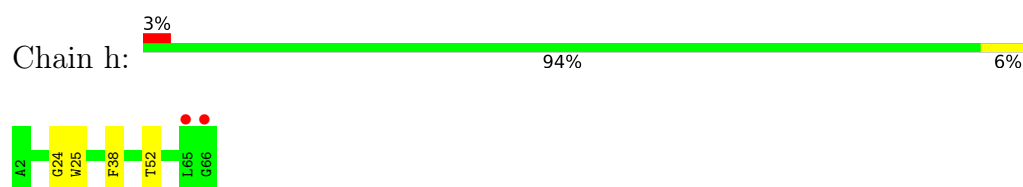
- Molecule 6: Cytochrome b559 subunit beta



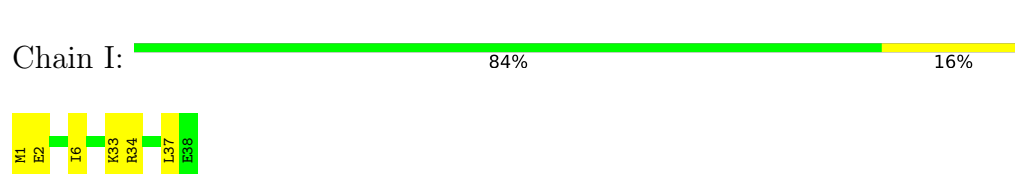
- Molecule 7: Photosystem II reaction center protein H



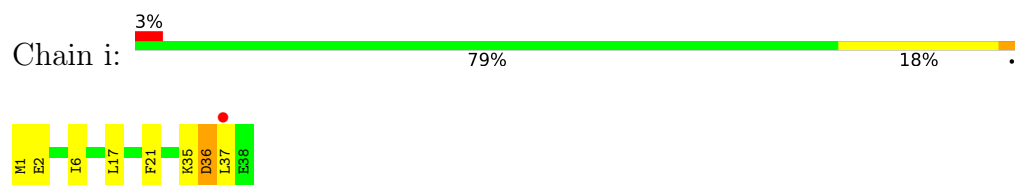
- Molecule 7: Photosystem II reaction center protein H



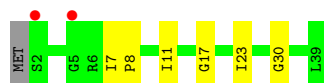
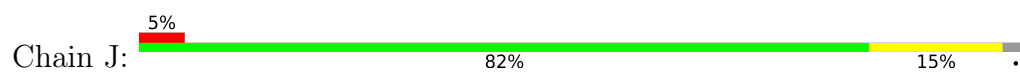
- Molecule 8: Photosystem II reaction center protein I



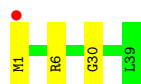
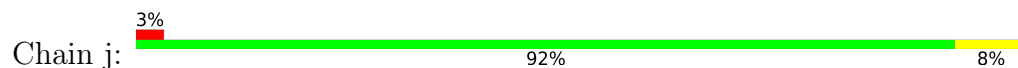
- Molecule 8: Photosystem II reaction center protein I



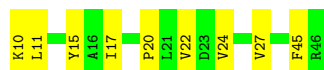
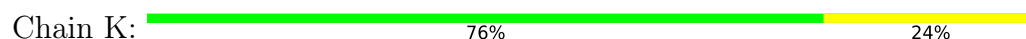
- Molecule 9: Photosystem II reaction center protein J



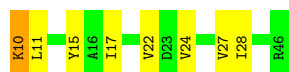
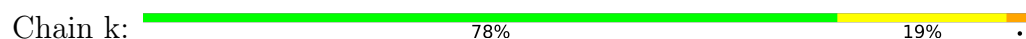
- Molecule 9: Photosystem II reaction center protein J



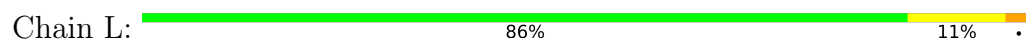
- Molecule 10: Photosystem II reaction center protein K



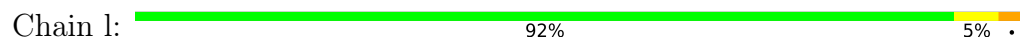
- Molecule 10: Photosystem II reaction center protein K



- Molecule 11: Photosystem II reaction center protein L



- Molecule 11: Photosystem II reaction center protein L



- Molecule 12: Photosystem II reaction center protein M

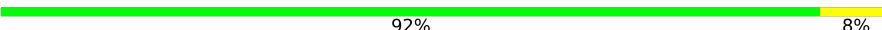


- Molecule 12: Photosystem II reaction center protein M

Chain m:  75% 17% 6%



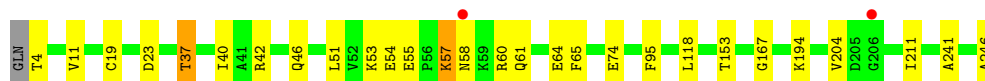
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  92% 8%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  88% 11% 1%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 3% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  81% 12% 3% 6%



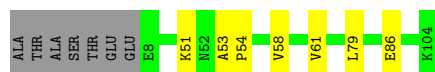
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 9% 7%

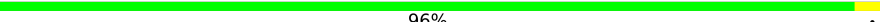


- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 7% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96%



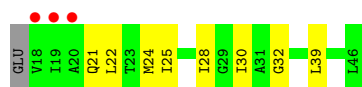
- Molecule 16: Cytochrome c-550

Chain v:  86% 14%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:  10% 70% 27%



- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:  63% 33%



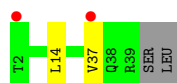
- Molecule 18: Photosystem II reaction center protein X

Chain X:  90% 8%



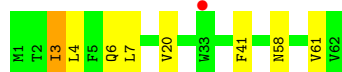
- Molecule 18: Photosystem II reaction center protein X

Chain x:  5% 90% 5% 5%



- Molecule 19: Photosystem II reaction center protein Z

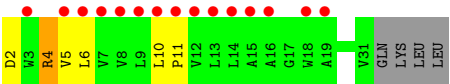
Chain Z:  2% 87% 11%



- Molecule 19: Photosystem II reaction center protein Z



● Molecule 20: Photosystem II protein Y



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	121.97Å 228.72Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.15 19.99 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.15) 99.8 (19.99-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.156 , 0.203 0.163 , 0.207	Depositor DCC
R_{free} test set	26822 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	55675	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% 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: BCR, OEX, CL, FE2, GOL, FME, UNL, CLA, PHO, HEC, OEY, CA, LMT, SQD, PL9, LHG, HEM, MG, LMG, DGD, BCT, HTG

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	0.54	0/3115	0.82	0/4242
1	a	0.56	0/3117	0.79	1/4245 (0.0%)
2	B	0.54	0/4191	0.81	1/5709 (0.0%)
2	b	0.53	0/4198	0.82	1/5720 (0.0%)
3	C	0.48	0/3678	0.79	2/5007 (0.0%)
3	c	0.47	0/3774	0.78	0/5135
4	D	0.59	0/2952	0.81	2/4021 (0.0%)
4	d	0.54	0/2952	0.80	1/4021 (0.0%)
5	E	0.44	0/693	0.79	0/944
5	e	0.44	0/695	0.80	0/948
6	F	0.54	0/284	0.77	0/387
6	f	0.53	0/265	0.80	0/360
7	H	0.44	0/535	0.88	0/728
7	h	0.42	0/524	0.77	0/713
8	I	0.44	0/311	0.77	0/419
8	i	0.45	0/311	0.77	0/419
9	J	0.43	0/278	0.75	0/376
9	j	0.44	0/286	0.76	0/386
10	K	0.45	0/303	0.81	0/416
10	k	0.49	0/303	0.85	0/416
11	L	0.56	0/319	0.72	0/433
11	l	0.52	0/319	0.74	0/433
12	M	0.59	0/270	0.85	0/368
12	m	0.59	0/262	0.88	0/357
13	O	0.45	0/1958	0.78	1/2654 (0.0%)
13	o	0.45	0/1937	0.80	2/2625 (0.1%)
14	T	0.57	0/266	0.72	0/362
14	t	0.57	0/266	0.74	0/362
15	U	0.47	0/785	0.76	0/1064
15	u	0.47	0/785	0.74	0/1064
16	V	0.51	0/1109	0.72	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.46	0/1098	0.77	0/1488
17	Y	0.48	0/216	0.83	0/289
17	y	0.42	0/216	0.74	0/289
18	X	0.43	0/290	0.76	0/392
18	x	0.42	0/284	0.76	0/384
19	Z	0.41	0/490	0.80	0/669
19	z	0.35	0/490	0.80	0/669
20	R	0.35	0/245	0.69	0/338
All	All	0.51	0/44370	0.79	11/60354 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	170	ALA	CA-C-N	-6.09	113.67	119.76
4	D	170	ALA	C-N-CA	-6.09	113.67	119.76
3	C	76	ILE	CA-C-N	5.76	125.62	119.28
3	C	76	ILE	C-N-CA	5.76	125.62	119.28
2	b	221	PRO	O-C-N	5.67	123.81	121.15
13	o	55	GLU	CA-C-N	5.27	125.56	119.92
13	o	55	GLU	C-N-CA	5.27	125.56	119.92
4	d	262	SER	N-CA-C	-5.24	107.90	114.56
13	O	121	THR	N-CA-C	5.13	116.63	108.79
1	a	176	ILE	N-CA-C	5.12	115.23	110.42
2	B	77	GLY	N-CA-C	5.11	121.79	114.64

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3014	0	2870	23	0
1	a	3010	0	2876	28	0
2	B	4021	0	3898	45	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	b	4022	0	3908	42	0
3	C	3553	0	3473	25	0
3	c	3641	0	3569	27	0
4	D	2849	0	2741	30	0
4	d	2849	0	2741	27	0
5	E	668	0	658	9	0
5	e	670	0	664	10	0
6	F	275	0	282	4	0
6	f	257	0	269	3	0
7	H	519	0	545	7	0
7	h	511	0	532	6	0
8	I	314	0	328	3	0
8	i	314	0	328	3	0
9	J	272	0	279	5	0
9	j	280	0	291	2	0
10	K	293	0	305	5	0
10	k	293	0	305	6	0
11	L	309	0	327	6	0
11	l	309	0	327	4	0
12	M	274	0	299	9	0
12	m	269	0	288	6	0
13	O	1903	0	1886	9	0
13	o	1891	0	1870	15	0
14	T	264	0	267	4	0
14	t	264	0	267	2	0
15	U	774	0	773	4	0
15	u	774	0	773	3	0
16	V	1085	0	1095	3	0
16	v	1077	0	1082	14	0
17	Y	215	0	246	6	0
17	y	215	0	246	6	0
18	X	287	0	317	2	0
18	x	281	0	312	2	0
19	Z	479	0	516	3	0
19	z	479	0	516	8	0
20	R	239	0	262	4	0
21	A	2	0	0	0	0
21	a	1	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	1	0
22	a	4	0	0	0	0
22	v	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	A	8	0	0	0	0
23	a	8	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	30	0
24	C	845	0	936	29	0
24	D	130	0	144	4	0
24	a	195	0	216	6	0
24	b	1040	0	1152	29	0
24	c	845	0	936	34	0
24	d	195	0	216	7	0
25	A	192	0	222	7	0
25	a	192	0	222	5	0
26	A	40	0	56	1	0
26	B	120	0	168	8	0
26	C	80	0	112	4	0
26	D	40	0	56	2	0
26	H	40	0	56	3	0
26	K	40	0	56	2	0
26	T	40	0	56	4	0
26	Y	40	0	56	4	0
26	a	40	0	56	0	0
26	b	120	0	168	7	0
26	c	80	0	112	3	0
26	d	40	0	56	3	0
26	h	40	0	56	4	0
26	k	40	0	56	2	0
26	t	40	0	56	6	0
26	y	40	0	56	1	0
27	A	108	0	156	6	0
27	B	54	0	78	3	0
27	F	43	0	53	2	0
27	a	108	0	156	3	0
27	b	54	0	78	2	0
27	f	43	0	53	3	0
28	A	18	0	24	2	0
28	B	42	0	56	1	0
28	C	12	0	16	1	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	30	0	40	0	0
28	a	12	0	16	1	0
28	b	30	0	40	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	c	12	0	16	2	0
28	f	6	0	7	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	18	0	24	1	0
29	A	35	0	46	3	0
29	B	25	0	35	0	0
29	C	35	0	46	1	0
29	D	35	0	46	1	0
29	F	35	0	46	1	0
29	M	105	0	138	7	0
29	T	25	0	35	0	0
29	a	70	0	92	2	0
29	b	25	0	35	2	0
29	f	35	0	46	1	0
29	m	35	0	46	2	0
30	A	10	0	0	0	0
30	a	10	0	0	0	0
31	A	11	0	0	1	0
31	a	11	0	0	1	0
32	A	110	0	160	10	0
32	D	110	0	160	3	0
32	a	110	0	160	17	0
32	d	110	0	160	1	0
33	A	28	0	0	0	0
33	B	33	0	0	0	0
33	C	34	0	0	0	0
33	D	57	0	0	0	0
33	I	40	0	0	0	0
33	J	10	0	0	0	0
33	M	10	0	0	0	0
33	X	18	0	0	0	0
33	a	30	0	0	0	0
33	b	33	0	0	0	0
33	c	32	0	0	0	0
33	d	71	0	0	0	0
33	i	40	0	0	0	0
33	j	10	0	0	0	0
33	m	10	0	0	0	0
34	A	51	0	72	5	0
34	B	51	0	72	1	0
34	C	102	0	144	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D	51	0	72	1	0
34	Z	37	0	44	2	0
34	a	51	0	72	3	0
34	b	51	0	72	2	0
34	c	102	0	144	3	0
34	j	51	0	72	2	0
34	z	39	0	48	4	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	F	1	0	0	0	0
35	O	1	0	0	0	0
35	b	1	0	0	0	0
35	c	2	0	0	0	0
35	f	1	0	0	0	0
35	o	1	0	0	0	0
36	B	95	0	130	2	0
36	C	38	0	52	0	0
36	H	16	0	17	2	0
36	V	19	0	26	3	0
36	b	95	0	130	3	0
36	c	38	0	52	0	0
36	d	16	0	17	3	0
37	C	186	0	246	7	0
37	D	52	0	71	3	0
37	H	62	0	82	1	0
37	c	186	0	246	3	0
37	e	62	0	82	6	0
37	h	62	0	82	1	0
38	D	147	0	222	9	0
38	E	42	0	57	2	0
38	L	49	0	74	3	0
38	a	42	0	57	5	0
38	d	147	0	222	7	0
38	l	49	0	74	2	0
39	F	43	0	30	3	0
39	e	43	0	30	3	0
40	J	1	0	0	0	0
40	j	1	0	0	0	0
41	V	43	0	30	0	0
41	v	43	0	30	0	0
42	A	173	0	0	2	0
42	B	294	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	C	232	0	0	4	0
42	D	150	0	0	0	0
42	E	30	0	0	0	0
42	F	9	0	0	0	0
42	H	49	0	0	0	0
42	I	5	0	0	1	0
42	J	10	0	0	0	0
42	K	9	0	0	1	0
42	L	14	0	0	0	0
42	M	23	0	0	0	0
42	O	180	0	0	2	0
42	T	18	0	0	2	0
42	U	77	0	0	1	0
42	V	119	0	0	2	0
42	X	6	0	0	0	0
42	Y	4	0	0	0	0
42	Z	1	0	0	0	0
42	a	162	0	0	0	0
42	b	269	0	0	3	0
42	c	205	0	0	2	0
42	d	132	0	0	1	0
42	e	19	0	0	0	0
42	f	8	0	0	0	0
42	h	44	0	0	0	0
42	i	5	0	0	0	0
42	j	6	0	0	0	0
42	k	7	0	0	0	0
42	l	9	0	0	1	0
42	m	11	0	0	0	0
42	o	155	0	0	2	0
42	t	11	0	0	0	0
42	u	93	0	0	0	0
42	v	82	0	0	3	0
42	x	6	0	0	0	0
42	y	2	0	0	0	0
All	All	55675	0	54222	563	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (563) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214[A]:MET:HG2	32:A:420[A]:PL9:H102	1.48	0.93
31:a:418[B]:OEY:O6	31:a:418[B]:OEY:O5	1.89	0.90
24:B:616:CLA:H71	24:B:617:CLA:H192	1.53	0.89
31:A:419[B]:OEY:O6	31:A:419[B]:OEY:O5	1.90	0.88
24:c:517:CLA:HHC	24:c:517:CLA:HBB1	1.56	0.87
4:d:192:THR:HG23	24:d:402:CLA:HBC2	1.61	0.82
1:A:214[B]:MET:HG2	32:A:420[B]:PL9:H102	1.60	0.81
24:c:505:CLA:H202	24:c:511:CLA:HBB1	1.64	0.80
24:c:507:CLA:HBB1	34:c:523:LMG:H231	1.64	0.79
22:U:201:CL:CL	42:V:411:HOH:O	2.38	0.78
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.70	0.73
16:v:71:GLY:HA2	28:v:201:GOL:H31	1.69	0.73
38:d:408:LHG:H342	38:d:408:LHG:H151	1.71	0.72
32:a:416[A]:PL9:H28	38:a:422:LHG:H222	1.72	0.72
24:a:410:CLA:H203	34:j:101:LMG:H412	1.71	0.71
24:D:403:CLA:H171	18:X:15:LEU:HD13	1.72	0.71
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.73	0.71
24:c:512:CLA:H191	34:c:522:LMG:H232	1.74	0.70
1:a:215[A]:HIS:ND1	32:a:416[A]:PL9:O1	2.24	0.69
1:a:214[A]:MET:HG2	32:a:416[A]:PL9:H102	1.73	0.68
32:a:416[B]:PL9:H28	38:a:422:LHG:H222	1.75	0.68
16:v:35:TYR:OH	42:v:301:HOH:O	2.10	0.68
3:c:320:ARG:HB2	28:c:502:GOL:H32	1.75	0.68
26:T:103:BCR:H321	26:T:103:BCR:HC8	1.77	0.67
2:B:248:ALA:HA	24:B:604:CLA:H42	1.77	0.67
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.75	0.67
26:t:101:BCR:H321	26:t:101:BCR:HC8	1.76	0.67
34:a:415:LMG:H221	37:c:519:DGD:HA81	1.76	0.66
8:I:37:LEU:O	42:I:201:HOH:O	2.13	0.66
28:T:102:GOL:O1	42:T:201:HOH:O	2.13	0.66
13:O:74[A]:GLU:OE2	42:O:401:HOH:O	2.12	0.66
4:D:157:PHE:CE2	4:D:171:PRO:HG2	2.32	0.65
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.28	0.65
24:C:505:CLA:CMD	24:C:507:CLA:HAB	2.26	0.64
3:C:286:ALA:HB2	24:C:502:CLA:HMD1	1.79	0.64
24:c:508:CLA:H201	38:d:408:LHG:H352	1.78	0.64
24:c:506:CLA:H61	24:c:516:CLA:H42	1.79	0.64
12:m:6:LEU:HD11	29:m:102:LMT:H11	1.79	0.64
13:o:74[B]:GLU:OE1	42:o:401:HOH:O	2.15	0.64
38:D:409:LHG:H132	38:D:409:LHG:H372	1.80	0.63
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.79	0.63
1:a:221[B]:SER:HB2	4:d:139:ARG:O	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.81	0.62
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.81	0.62
24:C:513:CLA:H171	26:C:514:BCR:H373	1.81	0.61
42:C:602:HOH:O	15:U:51:LYS:NZ	2.33	0.61
1:a:72:LEU:HD11	29:a:404:LMT:H52	1.81	0.60
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.82	0.60
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.84	0.59
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.84	0.59
27:A:412:SQD:H251	38:D:409:LHG:H131	1.83	0.59
24:b:625:CLA:H2	24:b:626:CLA:HBB2	1.83	0.59
2:b:224:ARG:HH11	29:b:631:LMT:H1'	1.67	0.59
24:c:509:CLA:HHC	24:c:509:CLA:HBB1	1.84	0.59
11:L:13:ASN:ND2	11:L:16:SER:H	1.99	0.59
1:A:257:ARG:NH2	2:B:492:GLU:O	2.35	0.59
24:C:502:CLA:H61	24:C:512:CLA:H42	1.85	0.59
27:A:412:SQD:H192	38:D:409:LHG:H201	1.84	0.58
24:B:616:CLA:H2	24:B:617:CLA:HBB2	1.84	0.58
4:D:192:THR:HG23	24:D:402:CLA:HBC2	1.85	0.58
25:A:409[B]:PHO:HBC3	4:D:279:LEU:HD22	1.86	0.58
4:D:103:ARG:HG3	5:E:73:LYS:HE2	1.86	0.57
38:D:409:LHG:H352	38:D:409:LHG:H151	1.86	0.57
34:c:522:LMG:H181	10:k:27:VAL:HG11	1.85	0.57
1:a:214[B]:MET:HG2	32:a:416[B]:PL9:H102	1.87	0.57
24:b:621:CLA:H142	38:l:101:LHG:H362	1.85	0.57
4:d:24:ARG:HD3	18:x:37:VAL:HG22	1.87	0.57
26:d:404:BCR:H313	37:e:101:DGD:HA91	1.86	0.57
37:e:101:DGD:HE3	37:e:101:DGD:HD4	1.85	0.57
32:a:416[B]:PL9:H512	27:f:102:SQD:H302	1.87	0.57
38:a:422:LHG:HC31	5:e:9:PRO:HA	1.85	0.56
24:c:510:CLA:HMC2	24:c:511:CLA:H102	1.86	0.56
6:F:21:VAL:O	6:F:25:THR:HG23	2.05	0.56
17:Y:28:ILE:HG23	26:Y:101:BCR:H10C	1.86	0.56
1:a:271:LEU:HD11	32:a:416[A]:PL9:HC8	1.88	0.56
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.18	0.56
24:b:611:CLA:H193	26:h:101:BCR:H353	1.87	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.40	0.56
24:c:516:CLA:O2D	24:c:517:CLA:HBB2	2.05	0.56
4:D:123:ILE:HD11	37:H:103:DGD:HAE1	1.88	0.56
2:b:248:ALA:HA	24:b:613:CLA:H42	1.88	0.56
13:o:40:ILE:HD12	13:o:95:PHE:CD1	2.41	0.56
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.88	0.55
27:a:414:SQD:H271	38:d:408:LHG:H141	1.87	0.55
32:a:416[B]:PL9:HC2	32:a:416[B]:PL9:H103	1.88	0.55
24:B:607:CLA:H191	26:B:620:BCR:H363	1.88	0.55
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.88	0.55
26:B:619:BCR:H363	26:t:101:BCR:H19C	1.89	0.55
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.88	0.55
1:a:183:MET:HA	24:a:409:CLA:HMD1	1.89	0.55
24:C:513:CLA:HHC	24:C:513:CLA:HBB1	1.89	0.54
24:B:615:CLA:H93	29:M:104:LMT:H112	1.90	0.54
4:D:16:ASP:OD2	29:D:401:LMT:O6'	2.25	0.54
28:f:101:GOL:H11	16:v:27:LEU:HD21	1.89	0.54
3:c:26:ARG:NH2	17:y:46:LEU:OXT	2.39	0.54
2:B:472:ARG:NH2	42:B:709:HOH:O	2.41	0.54
1:A:63:ILE:HB	3:C:335:THR:HG21	1.89	0.54
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.90	0.54
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.90	0.54
1:A:238[B]:LYS:NZ	42:A:502:HOH:O	2.34	0.54
13:O:27:ARG:NH1	13:O:202:ALA:O	2.41	0.54
2:b:216:HIS:HE1	24:b:619:CLA:C1A	2.21	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.90	0.53
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.53
29:M:101:LMT:H6D	11:l:9:PRO:HA	1.90	0.53
27:b:601:SQD:H101	26:b:627:BCR:H383	1.90	0.53
38:d:407:LHG:HC62	11:l:15:THR:HG23	1.90	0.53
26:B:620:BCR:H331	26:B:620:BCR:C8	2.38	0.53
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.39	0.53
26:H:102:BCR:H331	26:H:102:BCR:C8	2.38	0.53
24:c:505:CLA:C4D	24:c:507:CLA:H2	2.38	0.53
11:L:13:ASN:C	11:L:13:ASN:HD22	2.17	0.53
27:b:601:SQD:H1	27:b:601:SQD:H462	1.91	0.53
26:B:618:BCR:H383	27:B:621:SQD:H101	1.89	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
32:a:416[A]:PL9:HC2	32:a:416[A]:PL9:H103	1.91	0.53
2:b:190:PHE:HZ	24:b:612:CLA:HBB1	1.73	0.53
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.91	0.53
3:C:338:GLY:HA3	3:C:341:LEU:O	2.09	0.53
2:b:224:ARG:NH1	29:b:631:LMT:H1'	2.24	0.53
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.07	0.53
13:o:37:THR:HG22	13:o:246:ALA:HB3	1.90	0.52
28:T:102:GOL:H12	29:m:102:LMT:H12	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:GLN:HA	13:o:57:LYS:HE3	1.89	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.44	0.52
3:C:438:LEU:HD11	24:C:505:CLA:HBB1	1.91	0.52
24:C:510:CLA:H43	38:D:409:LHG:H383	1.91	0.52
11:L:13:ASN:HD22	11:L:16:SER:H	1.58	0.52
1:a:153:SER:HB2	24:a:409:CLA:H43	1.92	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.45	0.52
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.92	0.52
24:B:615:CLA:H42	29:M:104:LMT:H61	1.90	0.52
3:C:443:TRP:CZ2	24:C:508:CLA:HMD1	2.44	0.52
26:H:102:BCR:H331	26:H:102:BCR:HC8	1.92	0.52
24:C:505:CLA:HMD3	24:C:507:CLA:HAB	1.91	0.52
24:d:403:CLA:H2	18:x:14:LEU:HA	1.91	0.52
7:H:25:TRP:CD1	36:H:101:HTG:H1	2.45	0.51
2:b:498:LYS:HA	4:d:24:ARG:HA	1.93	0.51
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.75	0.51
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.92	0.51
19:z:47:TRP:CE2	34:z:101:LMG:H241	2.45	0.51
3:c:279:LEU:HD22	24:c:513:CLA:HED2	1.92	0.51
4:d:136:VAL:HG12	4:d:138:VAL:HG13	1.92	0.51
37:D:406:DGD:O1B	37:D:406:DGD:O2D	2.28	0.51
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.45	0.51
24:c:517:CLA:HBB1	24:c:517:CLA:CHC	2.37	0.51
13:O:39:ARG:HB2	13:O:246:ALA:HB2	1.92	0.51
24:b:625:CLA:H2	24:b:626:CLA:CBB	2.41	0.51
24:c:517:CLA:H171	26:c:527:BCR:H373	1.93	0.51
2:B:480[B]:SER:OG	42:B:701:HOH:O	2.19	0.51
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.39	0.51
38:D:409:LHG:H112	38:D:409:LHG:H382	1.92	0.51
16:V:26:TYR:O	42:V:301:HOH:O	2.19	0.51
2:b:405:GLU:OE1	42:b:701:HOH:O	2.19	0.51
29:C:521:LMT:O3B	42:C:601:HOH:O	2.19	0.51
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.92	0.51
3:c:38:GLY:HA3	24:c:515:CLA:HMD2	1.92	0.51
37:e:101:DGD:HAW1	27:f:102:SQD:H382	1.91	0.51
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.92	0.51
34:A:422:LMG:H211	37:C:516:DGD:HA62	1.93	0.51
24:c:513:CLA:HBB1	24:c:513:CLA:HMB1	1.92	0.51
16:V:96:ARG:HH21	36:V:207:HTG:H6'1	1.75	0.50
3:c:286:ALA:HB2	24:c:506:CLA:HMD1	1.93	0.50
24:d:401:CLA:HMB1	24:d:401:CLA:HBB1	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:202:ALA:HB2	32:d:405[B]:PL9:H353	1.92	0.50
32:A:420[A]:PL9:H261	38:E:101:LHG:H223	1.92	0.50
24:B:607:CLA:H151	24:B:617:CLA:H122	1.93	0.50
36:d:411:HTG:H1	7:h:25:TRP:CD1	2.46	0.50
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.93	0.50
24:A:405:CLA:HMB3	24:A:405:CLA:HBB1	1.92	0.50
24:a:410:CLA:HMB2	24:d:402:CLA:H122	1.93	0.50
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.47	0.50
27:A:416:SQD:H272	2:b:109:LEU:HD13	1.94	0.50
27:a:405:SQD:H141	26:t:101:BCR:HC41	1.94	0.50
5:E:40:THR:HB	20:R:4:ARG:HG2	1.94	0.50
1:a:214[A]:MET:HE2	1:a:255:PHE:CE1	2.47	0.50
1:a:227:THR:HB	1:a:231:GLU:HG3	1.93	0.50
24:A:406:CLA:HED1	32:D:405[B]:PL9:H362	1.93	0.50
1:a:162:PRO:HB3	1:a:168[A]:PHE:HA	1.94	0.50
8:I:2:GLU:O	8:I:6:ILE:HG12	2.11	0.50
27:A:412:SQD:H171	38:D:409:LHG:H181	1.94	0.49
4:D:269:PHE:CD2	38:D:407:LHG:HC11	2.47	0.49
15:U:16:LYS:NZ	42:U:303:HOH:O	2.42	0.49
3:C:213:LEU:HD21	26:C:515:BCR:C20	2.43	0.49
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.94	0.49
7:H:25:TRP:CD2	36:H:101:HTG:H1'2	2.48	0.49
2:B:405[B]:GLU:OE1	13:o:60:ARG:HD3	2.13	0.49
24:C:503:CLA:HBB1	24:C:512:CLA:H41	1.93	0.49
12:M:34:LYS:HG2	29:M:101:LMT:O3B	2.13	0.49
26:T:103:BCR:H19C	26:b:628:BCR:H363	1.94	0.49
24:b:615:CLA:HHC	24:b:615:CLA:HBB1	1.94	0.49
3:c:223:TRP:CG	3:c:224:ILE:H	2.31	0.49
25:A:408:PHO:HAB	4:D:205:LEU:HD13	1.95	0.49
3:C:464:GLU:OE2	4:D:245:SER:OG	2.22	0.49
34:D:412:LMG:H152	34:D:412:LMG:H292	1.95	0.49
3:c:443:TRP:CZ2	24:c:512:CLA:HMD1	2.47	0.49
32:a:416[A]:PL9:H512	27:f:102:SQD:H302	1.95	0.49
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.48	0.49
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.95	0.49
2:b:190:PHE:CZ	24:b:612:CLA:HBB1	2.47	0.49
1:A:50:ILE:HG12	29:A:417:LMT:H102	1.95	0.48
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
25:A:409[B]:PHO:HMA2	32:A:420[B]:PL9:H221	1.94	0.48
32:A:420[A]:PL9:H512	27:F:103:SQD:H301	1.95	0.48
25:A:409[A]:PHO:HBC3	4:D:279:LEU:HD22	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:26:THR:HB	39:F:102:HEM:HAB	1.95	0.48
28:b:605:GOL:H11	16:v:51:SER:HA	1.95	0.48
25:a:420[B]:PHO:HBC3	4:d:279:LEU:HD22	1.95	0.48
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.95	0.48
26:b:627:BCR:H12C	34:b:630:LMG:C43	2.44	0.48
3:c:213[A]:LEU:HG	24:c:510:CLA:H202	1.94	0.48
8:i:35:LYS:O	8:i:37:LEU:N	2.46	0.48
20:R:6:LEU:O	20:R:10:LEU:HB2	2.13	0.48
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.13	0.48
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.94	0.48
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.14	0.48
2:b:72:THR:HG22	2:b:80:ILE:HD11	1.95	0.48
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.46	0.48
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.48	0.48
24:A:407:CLA:H122	32:A:420[B]:PL9:H252	1.94	0.48
25:A:409[A]:PHO:HMA2	32:A:420[A]:PL9:H221	1.96	0.48
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.95	0.48
11:L:9:PRO:HA	29:M:104:LMT:H6D	1.94	0.48
3:c:334:PRO:HA	13:o:153:THR:OG1	2.14	0.48
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.96	0.48
4:d:343:GLU:HG2	16:v:135:VAL:HG11	1.96	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.47
34:A:422:LMG:C25	24:C:505:CLA:HBB2	2.44	0.47
4:D:273:PHE:CZ	38:L:101:LHG:H112	2.49	0.47
2:B:256:MET:HA	2:B:263:THR:HG21	1.95	0.47
29:M:101:LMT:H6'2	11:l:9:PRO:HB3	1.95	0.47
13:o:42:ARG:O	13:o:241:ALA:HA	2.14	0.47
2:B:162:PHE:O	24:B:607:CLA:HHD	2.14	0.47
24:C:511:CLA:H41	17:Y:39:LEU:HD13	1.96	0.47
2:B:422:ARG:O	2:B:425:ILE:HG12	2.14	0.47
13:O:54:GLU:O	13:O:56:PRO:HD3	2.14	0.47
1:a:85:SER:HA	1:a:109:GLY:HA3	1.97	0.47
24:a:412:CLA:H102	24:a:412:CLA:H61	1.67	0.47
34:a:415:LMG:H182	34:a:415:LMG:H152	1.67	0.47
29:f:103:LMT:O3'	29:f:103:LMT:O2B	2.26	0.47
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.96	0.47
26:T:103:BCR:H11C	26:T:103:BCR:H341	1.78	0.47
24:b:615:CLA:HBD	24:b:615:CLA:HAA1	1.96	0.47
27:A:412:SQD:O7	3:C:28:GLN:NE2	2.41	0.47
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.45	0.47
3:C:25:ASN:O	3:C:41:ARG:HD3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.50	0.47
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.97	0.47
3:c:406:SER:HA	3:c:420:VAL:HG23	1.97	0.47
24:c:514:CLA:H41	38:d:408:LHG:H383	1.97	0.47
3:C:461:ARG:NH2	42:C:610:HOH:O	2.44	0.46
4:D:102:THR:OG1	37:D:406:DGD:HG31	2.16	0.46
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.50	0.46
34:a:415:LMG:H242	24:c:509:CLA:H92	1.97	0.46
2:b:30:VAL:HG12	24:b:615:CLA:HHD	1.96	0.46
32:A:420[B]:PL9:H261	38:E:101:LHG:H223	1.95	0.46
1:a:271:LEU:HD11	32:a:416[B]:PL9:HC8	1.96	0.46
16:v:41:HIS:HA	16:v:45:ILE:O	2.15	0.46
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.50	0.46
24:C:512:CLA:O2D	24:C:513:CLA:HBB2	2.15	0.46
26:D:404:BCR:HC22	37:D:406:DGD:HA92	1.98	0.46
1:a:217[B]:SER:HB3	4:d:272:LEU:HD12	1.97	0.46
26:t:101:BCR:HC7	26:t:101:BCR:H331	1.58	0.46
19:z:37:LYS:NZ	34:z:101:LMG:HC4	2.31	0.46
1:A:221[B]:SER:HB2	4:D:139:ARG:O	2.15	0.46
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.51	0.46
3:C:223:TRP:CG	3:C:224:ILE:H	2.34	0.46
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.98	0.46
17:Y:32:GLY:HA3	26:Y:101:BCR:C15	2.46	0.46
3:c:429:SER:HA	37:c:520:DGD:HBW1	1.97	0.46
17:y:23:THR:O	17:y:27:MET:HG3	2.16	0.46
2:B:149:LEU:HD22	24:B:605:CLA:H152	1.97	0.46
26:H:102:BCR:H24C	26:H:102:BCR:H371	1.70	0.46
12:M:27:VAL:HG12	12:m:28:GLN:HB3	1.98	0.46
4:d:49:LEU:HD13	26:d:404:BCR:C15	2.46	0.46
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.46	0.46
3:C:48:LYS:HG3	3:C:138:GLU:HG3	1.97	0.46
2:b:231:MET:HE2	24:b:620:CLA:HMC2	1.98	0.46
2:b:461:LEU:HD21	4:d:284:ILE:HD11	1.96	0.46
1:A:162:PRO:HB3	1:A:168[B]:PHE:HA	1.98	0.46
24:B:616:CLA:H2	24:B:617:CLA:CBB	2.45	0.46
3:C:406:SER:HA	3:C:420:VAL:HG23	1.98	0.46
3:c:60:ILE:HG22	24:c:507:CLA:HHD	1.97	0.46
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.82	0.46
4:d:139:ARG:NH2	42:d:505:HOH:O	2.48	0.46
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.97	0.46
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:604:CLA:H3A	24:B:604:CLA:CGA	2.45	0.46
42:c:602:HOH:O	15:u:51:LYS:NZ	2.48	0.46
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.98	0.46
2:B:454:ALA:HB2	34:B:622:LMG:H172	1.98	0.46
26:B:620:BCR:H331	26:B:620:BCR:HC8	1.98	0.46
1:a:162:PRO:HB3	1:a:168[B]:PHE:HA	1.97	0.46
24:b:625:CLA:H92	24:b:625:CLA:H61	1.80	0.46
4:d:186:GLN:HB2	24:d:402:CLA:HBC1	1.97	0.46
1:A:221[A]:SER:HB2	4:D:139:ARG:O	2.16	0.45
34:A:422:LMG:H212	34:A:422:LMG:H242	1.78	0.45
2:b:224:ARG:HG3	7:h:24:GLY:O	2.16	0.45
19:z:37:LYS:HZ2	34:z:101:LMG:HC4	1.80	0.45
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.84	0.45
26:b:629:BCR:C8	26:b:629:BCR:H331	2.46	0.45
3:c:52:ALA:HB2	24:c:515:CLA:HMA2	1.97	0.45
24:c:512:CLA:HBC3	24:c:514:CLA:H71	1.97	0.45
1:A:72:LEU:HD13	29:A:417:LMT:H11	1.99	0.45
1:a:215[B]:HIS:HA	32:a:416[B]:PL9:HC71	1.98	0.45
3:c:95:LEU:HD21	24:c:505:CLA:OBD	2.15	0.45
37:c:520:DGD:HB32	37:c:520:DGD:HB61	1.65	0.45
4:d:14:TRP:CD1	36:d:411:HTG:H61	2.51	0.45
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.46	0.45
24:A:407:CLA:H122	32:A:420[A]:PL9:H252	1.97	0.45
2:B:76[B]:SER:HB2	36:B:623:HTG:HO6	1.80	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.52	0.45
24:c:512:CLA:H141	24:c:514:CLA:H203	1.97	0.45
26:k:101:BCR:H371	26:k:101:BCR:H24C	1.66	0.45
2:b:446:SER:HB2	2:b:447:PRO:HD2	1.99	0.45
4:d:51:GLY:HA3	4:d:78:VAL:HG22	1.98	0.45
24:d:401:CLA:H203	24:d:401:CLA:H162	1.66	0.45
5:e:26:THR:HB	39:e:102:HEM:HAB	1.97	0.45
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.98	0.45
2:b:36:SER:OG	26:b:628:BCR:H362	2.17	0.45
2:b:98:LEU:HB2	36:b:602:HTG:H7'1	1.98	0.45
3:C:156:LYS:HE3	42:C:782:HOH:O	2.16	0.44
16:V:12:LEU:HD12	16:V:69:ILE:HB	1.98	0.44
16:v:55:ARG:NH1	42:v:304:HOH:O	2.32	0.44
2:b:26:HIS:CE1	24:b:622:CLA:HMA2	2.53	0.44
2:b:413:ASP:O	2:b:417:VAL:HG23	2.17	0.44
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.82	0.44
24:B:615:CLA:H41	24:B:615:CLA:H62	1.72	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:377:LEU:HG	3:c:381:LYS:HE3	2.00	0.44
24:c:516:CLA:H192	24:c:516:CLA:H161	1.84	0.44
2:B:223:GLN:NE2	2:B:227:LYS:HD3	2.33	0.44
24:C:510:CLA:HED2	24:C:510:CLA:H2	1.99	0.44
2:b:464:PHE:CZ	38:d:406:LHG:H252	2.53	0.44
24:b:625:CLA:H91	24:b:625:CLA:H112	1.79	0.44
36:d:411:HTG:H1	7:h:25:TRP:CG	2.52	0.44
16:v:57:GLU:H	16:v:57:GLU:CD	2.25	0.44
24:B:615:CLA:H61	24:B:615:CLA:H92	1.71	0.44
36:B:623:HTG:H7'3	29:a:404:LMT:H102	1.99	0.44
37:C:517:DGD:HA61	37:C:518:DGD:HB71	2.00	0.44
15:U:27:LEU:HD21	15:U:82:PHE:CG	2.53	0.44
3:c:315:MET:O	3:c:319:ILE:HG13	2.17	0.44
37:e:101:DGD:HB71	37:e:101:DGD:HBW2	1.98	0.44
13:o:51:LEU:HB3	13:o:65:PHE:HB3	1.99	0.44
1:A:217[B]:SER:O	1:A:221[B]:SER:HB3	2.18	0.44
34:Z:101:LMG:HC8	34:Z:101:LMG:H111	1.63	0.44
24:b:612:CLA:H171	37:h:102:DGD:HAT2	2.00	0.44
24:c:509:CLA:HAA1	24:c:509:CLA:HBD	2.00	0.44
5:e:17:VAL:O	5:e:21:VAL:HG23	2.18	0.44
5:e:27:ILE:HB	5:e:28:PRO:HD3	2.00	0.44
38:a:422:LHG:H241	38:a:422:LHG:HC61	1.85	0.44
11:l:2:GLU:HB2	42:l:208:HOH:O	2.17	0.44
13:o:54:GLU:HG2	13:o:64:GLU:O	2.18	0.44
24:C:511:CLA:HMB1	26:K:101:BCR:H382	2.00	0.44
5:E:27:ILE:CD1	39:F:102:HEM:HBC2	2.48	0.44
1:a:121[A]:LEU:HD11	24:c:509:CLA:H152	1.99	0.44
26:h:101:BCR:H24C	26:h:101:BCR:H371	1.80	0.44
4:D:39:PRO:O	4:D:43:LEU:HG	2.18	0.44
20:R:10:LEU:HB3	20:R:11:PRO:HD3	2.00	0.44
3:c:127:PHE:CE1	34:z:101:LMG:H152	2.52	0.44
3:c:348:GLU:OE1	13:o:11:VAL:HA	2.18	0.44
26:h:101:BCR:H331	26:h:101:BCR:C8	2.47	0.44
24:A:407:CLA:HED1	37:C:518:DGD:HAE2	2.00	0.43
2:B:54:PRO:HD2	2:B:57:ARG:HG3	1.99	0.43
29:F:101:LMT:H112	9:J:23:ILE:HD13	2.00	0.43
1:a:214[B]:MET:HE2	1:a:255:PHE:CE1	2.53	0.43
24:b:612:CLA:H143	24:b:612:CLA:H161	1.84	0.43
3:c:390:ARG:HD3	16:v:100:ILE:HD12	1.99	0.43
24:c:517:CLA:H61	26:c:527:BCR:H281	1.99	0.43
10:k:10:LYS:HD2	10:k:10:LYS:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:19:CYS:SG	13:o:46:GLN:HB2	2.58	0.43
13:o:53:LYS:NZ	42:o:420:HOH:O	2.51	0.43
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.53	0.43
4:d:101:PHE:HB3	37:e:101:DGD:HG2	2.01	0.43
29:A:417:LMT:H62	36:b:602:HTG:H5'1	2.01	0.43
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.00	0.43
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.82	0.43
2:b:280:PHE:O	2:b:284:ILE:HG13	2.18	0.43
24:b:614:CLA:H43	24:b:615:CLA:H2	1.99	0.43
24:b:624:CLA:H62	24:b:624:CLA:H41	1.61	0.43
24:c:512:CLA:H122	24:c:512:CLA:H162	1.69	0.43
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.84	0.43
1:a:267[B]:ASN:HB3	1:a:270[B]:SER:OG	2.18	0.43
32:a:416[A]:PL9:H171	32:a:416[A]:PL9:H151	1.70	0.43
10:k:28:ILE:HD11	17:y:28:ILE:HD13	2.00	0.43
16:v:87:GLU:CD	16:v:96:ARG:HH12	2.26	0.43
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.01	0.43
32:A:420[B]:PL9:H512	27:F:103:SQD:H301	2.00	0.43
34:A:422:LMG:H221	37:C:516:DGD:HAE1	2.01	0.43
24:B:614:CLA:H121	24:B:614:CLA:H162	1.86	0.43
4:D:282:SER:OG	24:D:402:CLA:HED3	2.18	0.43
26:b:628:BCR:H24C	26:b:628:BCR:H371	1.81	0.43
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.01	0.43
24:B:602:CLA:H91	24:B:602:CLA:H111	1.77	0.43
24:B:607:CLA:H201	27:a:405:SQD:H282	1.99	0.43
1:a:215[A]:HIS:HA	32:a:416[A]:PL9:HC71	2.00	0.43
2:b:185:TRP:CZ2	36:b:633:HTG:H2'1	2.54	0.43
28:c:502:GOL:H2	42:c:754:HOH:O	2.18	0.43
26:c:518:BCR:H15C	26:c:518:BCR:H351	1.84	0.43
4:d:60:THR:OG1	4:d:61:HIS:HD2	2.01	0.43
28:A:414:GOL:H11	12:M:1:FME:HG2	2.01	0.43
4:D:160:TYR:HA	4:D:290:ALA:HB2	2.01	0.43
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.46	0.43
1:a:259:ILE:HG22	1:a:260:PHE:CD1	2.54	0.43
7:h:38:PHE:HB2	26:h:101:BCR:C10	2.48	0.43
2:B:50:PRO:HB2	28:B:630:GOL:H12	2.01	0.43
27:B:621:SQD:O8	11:L:7:ARG:HD3	2.19	0.43
13:O:53:LYS:HE2	13:O:63:ALA:HB3	1.99	0.43
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	2.00	0.43
18:X:29:ILE:O	18:X:33:GLN:HG2	2.19	0.43
4:d:40:CYS:HB3	4:d:117:HIS:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:e:102:HEM:CAC	6:f:27:ALA:HB1	2.49	0.43
19:z:15:LEU:O	19:z:19:MET:HG2	2.19	0.43
3:C:35:TRP:CD1	10:K:45:PHE:HB3	2.54	0.42
26:C:515:BCR:H15C	26:C:515:BCR:H351	1.89	0.42
19:Z:41:PHE:CZ	34:Z:101:LMG:HC91	2.54	0.42
16:v:23:GLU:OE1	42:v:302:HOH:O	2.21	0.42
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	2.00	0.42
3:C:175:LEU:HD23	3:C:237:HIS:CG	2.54	0.42
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.00	0.42
24:A:406:CLA:HBA1	24:A:406:CLA:C4A	2.48	0.42
24:C:503:CLA:HBB1	24:C:503:CLA:HHC	2.02	0.42
12:M:6:LEU:HD11	29:M:103:LMT:H32	2.01	0.42
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.01	0.42
25:a:420[A]:PHO:ND	25:a:420[A]:PHO:NC	2.67	0.42
34:b:630:LMG:O2	42:b:702:HOH:O	2.21	0.42
3:c:225:VAL:HG13	3:c:289:PHE:HA	2.00	0.42
5:e:60:GLN:HG2	5:e:61:ARG:N	2.34	0.42
2:B:221:PRO:HA	24:B:610:CLA:HED3	2.00	0.42
3:C:425:TRP:CD1	24:C:504:CLA:HMA3	2.54	0.42
24:b:615:CLA:H41	24:b:615:CLA:H62	1.80	0.42
1:A:283:VAL:HG21	25:A:408:PHO:HBC3	2.00	0.42
2:B:227:LYS:HB3	2:B:227:LYS:HE2	1.86	0.42
6:F:27:ALA:HB1	39:F:102:HEM:HAC	2.02	0.42
36:V:207:HTG:H3'2	36:V:207:HTG:H6'2	1.83	0.42
26:k:101:BCR:H15C	26:k:101:BCR:H351	1.89	0.42
4:D:49:LEU:HD13	26:D:404:BCR:C15	2.49	0.42
8:I:33:LYS:HB3	8:I:34:ARG:H	1.54	0.42
19:Z:3:ILE:O	19:Z:7:LEU:HB2	2.19	0.42
26:b:629:BCR:H15C	26:b:629:BCR:H351	1.92	0.42
2:B:138:MET:HE3	24:B:616:CLA:CHD	2.50	0.42
36:V:207:HTG:H4'1	36:V:207:HTG:H1'1	1.88	0.42
1:a:218[B]:LEU:HD12	32:a:416[B]:PL9:C3	2.50	0.42
2:b:499:VAL:HG12	4:d:135:LEU:HB3	2.02	0.42
37:e:101:DGD:HG2	37:e:101:DGD:HB21	1.88	0.42
26:t:101:BCR:H11C	26:t:101:BCR:H341	1.94	0.42
24:C:513:CLA:H202	34:C:520:LMG:H402	2.01	0.42
5:E:15:THR:HB	9:J:7:ILE:O	2.20	0.42
2:b:233:ASN:O	2:b:236:THR:HG22	2.20	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.42
1:A:143:ILE:HD11	4:D:217:THR:HA	2.02	0.42
1:A:214[A]:MET:HE2	1:A:255:PHE:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:LEU:HD21	24:B:606:CLA:HMC3	2.00	0.42
42:B:907:HOH:O	12:M:5:GLN:HG3	2.20	0.42
3:C:320:ARG:HB2	28:C:524:GOL:H32	2.02	0.42
24:C:505:CLA:HMD2	24:C:507:CLA:HAB	2.01	0.42
13:O:180:GLU:CD	13:O:180:GLU:H	2.27	0.42
28:T:101:GOL:H12	42:T:209[B]:HOH:O	2.20	0.42
2:b:352:GLU:HB3	42:b:719:HOH:O	2.19	0.42
24:b:611:CLA:H93	24:b:611:CLA:H111	1.73	0.42
25:a:411:PHO:H61	25:a:411:PHO:H2	1.90	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.75	0.41
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.55	0.41
37:C:517:DGD:HB1	37:C:517:DGD:HBE2	1.81	0.41
26:T:103:BCR:H24C	26:T:103:BCR:H371	1.86	0.41
2:b:321:LYS:HE3	2:b:321:LYS:HB3	1.81	0.41
24:c:510:CLA:HBB1	24:c:510:CLA:HMB3	2.02	0.41
8:i:2:GLU:O	8:i:6:ILE:HG12	2.20	0.41
24:A:407:CLA:HBB1	4:D:157:PHE:CZ	2.56	0.41
28:A:415:GOL:H32	5:E:63:ILE:HD11	2.02	0.41
34:C:520:LMG:H411	34:C:520:LMG:H381	1.72	0.41
25:a:420[B]:PHO:HMC3	4:d:279:LEU:HD11	2.01	0.41
3:c:321:ASP:OD2	3:c:340:TYR:OH	2.34	0.41
24:d:401:CLA:C4A	24:d:401:CLA:HBA1	2.50	0.41
9:j:6:ARG:HA	9:j:6:ARG:NH2	2.36	0.41
24:D:402:CLA:HAA2	24:D:402:CLA:HBD	2.02	0.41
9:J:8:PRO:HD2	9:J:11:ILE:HD12	2.03	0.41
25:a:420[B]:PHO:ND	25:a:420[B]:PHO:NC	2.68	0.41
2:b:458:PHE:HB3	24:b:614:CLA:HBC2	2.02	0.41
3:c:163:PHE:O	3:c:167:VAL:HG23	2.21	0.41
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.49	0.41
24:A:406:CLA:H203	24:A:406:CLA:H162	1.72	0.41
9:J:17:GLY:HA3	26:Y:101:BCR:H371	2.03	0.41
3:c:437:PHE:CE1	24:c:514:CLA:HMB2	2.56	0.41
1:A:162:PRO:HB3	1:A:168[A]:PHE:HA	2.03	0.41
2:B:216:HIS:CE1	24:B:610:CLA:C1A	3.01	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.41
34:C:519:LMG:H161	34:C:519:LMG:H292	2.03	0.41
1:a:38:ILE:HB	1:a:39:PRO:HD3	2.03	0.41
2:b:216:HIS:CE1	24:b:619:CLA:C1A	3.03	0.41
24:c:512:CLA:HBC2	38:d:408:LHG:H362	2.01	0.41
5:e:10:PHE:HE2	39:e:102:HEM:HBD2	1.85	0.41
34:A:422:LMG:H382	37:C:516:DGD:HB51	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:B:621:SQD:H462	27:B:621:SQD:H1	2.02	0.41
24:C:503:CLA:CBB	24:C:512:CLA:H41	2.49	0.41
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	2.02	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.55	0.41
12:M:3:VAL:HG11	14:T:2:GLU:HG2	2.02	0.41
2:b:483:ASP:HA	2:b:484:PRO:HD3	1.96	0.41
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.03	0.41
26:B:619:BCR:H371	26:B:619:BCR:H24C	1.80	0.41
1:a:12:ASN:O	1:a:16:ARG:HG3	2.20	0.41
24:a:409:CLA:HAA2	24:a:409:CLA:HBD	2.03	0.41
4:d:103:ARG:O	4:d:107:LEU:HG	2.20	0.41
24:A:410:CLA:H162	24:A:410:CLA:H122	1.81	0.41
2:B:480[A]:SER:OG	42:B:702:HOH:O	2.22	0.41
4:D:273:PHE:CE2	38:L:101:LHG:H112	2.55	0.41
2:b:33:TRP:CH2	24:b:614:CLA:HMB1	2.56	0.41
2:b:487:SER:HA	2:b:488:PRO:HD3	1.78	0.41
24:b:621:CLA:H71	38:l:101:LHG:H311	2.03	0.41
4:d:84:SER:O	5:e:69:ARG:HB2	2.21	0.41
17:y:27:MET:HE2	17:y:27:MET:HB3	1.97	0.41
1:A:269:ARG:NE	4:D:222:LEU:HD22	2.35	0.41
25:A:409[B]:PHO:H72	25:A:409[B]:PHO:H112	1.90	0.41
2:B:172:TYR:OH	7:H:63:LYS:HE3	2.20	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.21	0.41
10:K:10:LYS:N	42:K:204:HOH:O	2.54	0.41
28:a:402:GOL:H2	5:e:63[A]:ILE:HD11	2.03	0.41
32:a:416[B]:PL9:H171	32:a:416[B]:PL9:H151	1.62	0.41
10:k:24:VAL:HG13	17:y:25:ILE:HD13	2.02	0.41
15:u:53:ALA:HB1	15:u:54:PRO:HA	2.02	0.41
17:y:34:MET:O	17:y:38:LEU:HG	2.21	0.41
26:A:411:BCR:H371	26:A:411:BCR:H24C	1.75	0.40
24:B:605:CLA:H141	24:B:605:CLA:H161	1.83	0.40
32:D:405[B]:PL9:H201	38:L:101:LHG:H202	2.02	0.40
26:K:101:BCR:H351	26:K:101:BCR:H15C	1.80	0.40
24:c:506:CLA:H141	24:c:506:CLA:H162	1.82	0.40
2:B:423:LYS:HE2	42:O:428:HOH:O	2.21	0.40
26:B:620:BCR:H24C	26:B:620:BCR:H371	1.93	0.40
24:C:512:CLA:H101	24:C:513:CLA:H141	2.03	0.40
32:D:405[A]:PL9:H471	32:D:405[A]:PL9:H43	1.89	0.40
12:M:28:GLN:HB3	12:m:27:VAL:HG12	2.02	0.40
13:O:204:VAL:HG22	13:O:211:ILE:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.02	0.40
2:B:275:TRP:CE2	2:B:315:ILE:HG13	2.57	0.40
2:B:467:ILE:HG13	4:D:126:MET:HE1	2.03	0.40
24:B:616:CLA:H112	24:B:616:CLA:H152	1.41	0.40
24:C:513:CLA:CBB	26:C:514:BCR:H24C	2.52	0.40
15:U:42:TYR:HA	15:U:43:PRO:HA	1.82	0.40
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	2.03	0.40
17:Y:30:ILE:HD12	17:Y:30:ILE:HA	2.00	0.40
2:b:216:HIS:CE1	24:b:619:CLA:NA	2.88	0.40
3:c:324:LEU:HD23	3:c:324:LEU:HA	1.92	0.40
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.03	0.40
14:t:18:PHE:CD1	26:t:101:BCR:H343	2.56	0.40
19:z:39:LEU:HD23	19:z:39:LEU:HA	1.83	0.40
2:B:194:ASN:HA	2:B:195:PRO:HD2	1.97	0.40
37:C:517:DGD:HB51	34:C:519:LMG:H392	2.04	0.40
38:D:408:LHG:H141	11:L:22:LEU:HD21	2.03	0.40
32:a:416[A]:PL9:H262	38:a:422:LHG:H171	2.03	0.40
24:b:613:CLA:CGA	24:b:613:CLA:H3A	2.52	0.40
26:d:404:BCR:H15C	26:d:404:BCR:H351	1.99	0.40
1:A:238[A]:LYS:HG2	14:T:30:THR:HG21	2.04	0.40
1:A:238[A]:LYS:NZ	42:A:510:HOH:O	2.52	0.40
27:A:412:SQD:H291	24:C:508:CLA:H71	2.03	0.40
4:D:43:LEU:HD23	4:D:43:LEU:HA	1.83	0.40
14:T:20:ALA:O	14:T:24:ARG:HB3	2.21	0.40
2:b:141:ILE:HG21	24:b:625:CLA:HBB1	2.03	0.40
2:b:462:PHE:CE1	24:b:623:CLA:HMB3	2.57	0.40
34:j:101:LMG:H392	34:j:101:LMG:H362	1.91	0.40

There are no symmetry-related clashes.

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	384/344 (112%)	380 (99%)	3 (1%)	1 (0%)	36	34
1	a	384/344 (112%)	378 (98%)	5 (1%)	1 (0%)	36	34
2	B	512/505 (101%)	506 (99%)	6 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	461/455 (101%)	450 (98%)	9 (2%)	2 (0%)	30	26
3	c	473/455 (104%)	459 (97%)	12 (2%)	2 (0%)	30	26
4	D	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
4	d	355/342 (104%)	345 (97%)	10 (3%)	0	100	100
5	E	81/84 (96%)	81 (100%)	0	0	100	100
5	e	81/84 (96%)	81 (100%)	0	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	61 (95%)	3 (5%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	1
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	245 (98%)	4 (2%)	0	100	100
13	o	246/244 (101%)	240 (98%)	6 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	131 (96%)	5 (4%)	0	100	100
16	v	135/137 (98%)	129 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	X	37/40 (92%)	37 (100%)	0	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
19	z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	2
20	R	28/34 (82%)	27 (96%)	1 (4%)	0	100	100
All	All	5429/5384 (101%)	5309 (98%)	111 (2%)	9 (0%)	48	44

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
8	i	36	ASP
19	z	30	PRO
1	a	259	ILE
1	A	259	ILE
19	Z	61	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	311/279 (112%)	311 (100%)	0	100	100
1	a	311/279 (112%)	310 (100%)	1 (0%)	86	91
2	B	412/403 (102%)	407 (99%)	5 (1%)	63	70
2	b	413/403 (102%)	409 (99%)	4 (1%)	68	75
3	C	361/356 (101%)	355 (98%)	6 (2%)	53	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	c	371/356 (104%)	364 (98%)	7 (2%)	50	56
4	D	290/277 (105%)	287 (99%)	3 (1%)	68	75
4	d	290/277 (105%)	288 (99%)	2 (1%)	76	82
5	E	74/73 (101%)	73 (99%)	1 (1%)	59	66
5	e	74/73 (101%)	73 (99%)	1 (1%)	59	66
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	25 (96%)	1 (4%)	29	29
7	H	55/54 (102%)	54 (98%)	1 (2%)	51	58
7	h	54/54 (100%)	53 (98%)	1 (2%)	50	56
8	I	34/34 (100%)	34 (100%)	0	100	100
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	39
9	J	26/27 (96%)	26 (100%)	0	100	100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30	30
10	K	30/30 (100%)	27 (90%)	3 (10%)	7	3
10	k	30/30 (100%)	28 (93%)	2 (7%)	15	10
11	L	36/35 (103%)	35 (97%)	1 (3%)	38	40
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	40
12	M	31/32 (97%)	31 (100%)	0	100	100
12	m	30/32 (94%)	29 (97%)	1 (3%)	33	34
13	O	214/207 (103%)	209 (98%)	5 (2%)	44	49
13	o	211/207 (102%)	205 (97%)	6 (3%)	38	40
14	T	27/28 (96%)	25 (93%)	2 (7%)	13	8
14	t	27/28 (96%)	25 (93%)	2 (7%)	13	8
15	U	84/89 (94%)	81 (96%)	3 (4%)	31	31
15	u	84/89 (94%)	82 (98%)	2 (2%)	43	47
16	V	119/117 (102%)	118 (99%)	1 (1%)	73	79
16	v	118/117 (101%)	117 (99%)	1 (1%)	73	79
17	Y	22/23 (96%)	21 (96%)	1 (4%)	24	22
17	y	22/23 (96%)	19 (86%)	3 (14%)	3	1
18	X	32/33 (97%)	32 (100%)	0	100	100
18	x	31/33 (94%)	31 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Z	52/52 (100%)	48 (92%)	4 (8%)	12 7
19	z	52/52 (100%)	48 (92%)	4 (8%)	12 7
20	R	25/29 (86%)	24 (96%)	1 (4%)	28 27
All	All	4504/4403 (102%)	4426 (98%)	78 (2%)	53 60

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	B	315	ILE
2	B	362	PHE
2	B	492	GLU
2	B	505	ARG
3	C	29	GLU
3	C	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315	MET
3	C	355	THR
4	D	90	LEU
4	D	136	VAL
4	D	329	MET
5	E	71	GLU
7	H	65	LEU
10	K	17	ILE
10	K	24	VAL
10	K	27	VAL
11	L	13	ASN
13	O	4	THR
13	O	34	SER
13	O	69	LYS
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	58	VAL
15	U	59	GLU
15	U	70	ARG
16	V	42	VAL
17	Y	24	MET
19	Z	3	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Z	4	LEU
19	Z	6	GLN
19	Z	20	VAL
20	R	4	ARG
1	a	12	ASN
2	b	84	THR
2	b	362	PHE
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	142	GLU
3	c	289	PHE
3	c	416[A]	SER
3	c	416[B]	SER
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	90	LEU
4	d	329	MET
5	e	16	SER
6	f	15	ILE
7	h	52	THR
8	i	36	ASP
9	j	1	MET
10	k	10	LYS
10	k	17	ILE
11	l	15	THR
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	37	THR
13	o	57	LYS
13	o	118	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	61	VAL
15	u	86	GLU
16	v	42	VAL
17	y	18	VAL
17	y	24	MET
17	y	30	ILE
19	z	7	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	z	29	SER
19	z	32	ASP
19	z	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	234	ASN
2	B	53	ASN
3	C	201	ASN
4	D	61	HIS
4	D	83	ASN
4	D	186	GLN
4	D	255	GLN
4	D	301	GLN
4	D	332	GLN
11	L	13	ASN
13	O	61	GLN
13	O	124	ASN
13	O	147	ASN
13	O	231	HIS
19	Z	31	GLN
19	Z	38	GLN
19	Z	58	ASN
1	a	12	ASN
1	a	165	GLN
1	a	315	ASN
2	b	53	ASN
2	b	281	GLN
2	b	394	GLN
3	c	28	GLN
3	c	373	ASN
3	c	418	ASN
4	d	61	HIS
4	d	83	ASN
4	d	186	GLN
4	d	301	GLN
4	d	332	GLN
5	e	74	GLN
5	e	82	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	k	40	GLN
11	l	8	GLN
13	o	130	GLN
13	o	155	ASN
15	u	78	ASN
15	u	81	HIS
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 ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	FME	t	1	14	8,9,10	0.81	0	8,9,11	2.19	4 (50%)
12	FME	M	1	12	8,9,10	0.71	0	8,9,11	1.33	2 (25%)
8	FME	i	1	8	8,9,10	0.64	0	8,9,11	1.15	1 (12%)
8	FME	I	1	8	8,9,10	0.66	0	8,9,11	1.19	1 (12%)
12	FME	m	1	12	8,9,10	0.69	0	8,9,11	1.25	1 (12%)
14	FME	T	1	14	8,9,10	0.74	0	8,9,11	1.24	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FME	t	1	14	-	1/7/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	1/7/9/11	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	CA-N-CN	-3.87	116.87	122.82
14	t	1	FME	C-CA-N	2.79	114.89	109.50
14	T	1	FME	O-C-CA	-2.55	118.22	124.77
14	t	1	FME	O-C-CA	-2.48	118.40	124.77
14	t	1	FME	O1-CN-N	-2.40	119.13	125.32
12	m	1	FME	O-C-CA	-2.34	118.76	124.77
8	I	1	FME	O-C-CA	-2.32	118.79	124.77
12	M	1	FME	CA-N-CN	-2.28	119.31	122.82
12	M	1	FME	O-C-CA	-2.10	119.36	124.77
8	i	1	FME	O-C-CA	-2.08	119.43	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 266 ligands modelled in this entry, 24 are monoatomic and 18 are unknown - leaving 224 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
38	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.12	6 (11%)
32	PL9	D	405[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.71	19 (27%)
24	CLA	C	503	-	69,73,73	2.04	19 (27%)	82,113,113	2.60	29 (35%)
37	DGD	h	102	-	63,63,67	0.92	3 (4%)	77,77,81	0.97	4 (5%)
24	CLA	B	602	42	69,73,73	2.04	19 (27%)	82,113,113	2.67	29 (35%)
24	CLA	b	619	-	69,73,73	2.01	19 (27%)	82,113,113	2.66	31 (37%)
24	CLA	B	616	-	69,73,73	1.99	19 (27%)	82,113,113	2.70	32 (39%)
25	PHO	a	411	-	58,69,69	2.76	14 (24%)	55,99,99	2.79	15 (27%)
26	BCR	h	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	8 (14%)
32	PL9	D	405[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.67	19 (27%)
25	PHO	A	409[B]	-	58,69,69	2.82	14 (24%)	55,99,99	2.89	15 (27%)
37	DGD	c	519	-	63,63,67	0.83	2 (3%)	77,77,81	1.10	5 (6%)
29	LMT	M	101	-	36,36,36	0.41	0	47,47,47	0.95	1 (2%)
24	CLA	B	610	-	69,73,73	2.05	19 (27%)	82,113,113	2.63	30 (36%)
32	PL9	a	416[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.87	21 (30%)
36	HTG	b	609	-	19,19,19	0.98	2 (10%)	23,24,24	1.13	3 (13%)
41	HEC	v	205	16	46,50,50	1.72	10 (21%)	58,82,82	1.65	13 (22%)
27	SQD	a	414	-	52,54,54	0.92	2 (3%)	62,65,65	1.50	12 (19%)
28	GOL	v	202	-	5,5,5	0.35	0	5,5,5	0.28	0
24	CLA	A	410	-	69,73,73	2.05	20 (28%)	82,113,113	2.65	35 (42%)
24	CLA	C	511	3	69,73,73	2.03	19 (27%)	82,113,113	2.63	31 (37%)
37	DGD	H	103	-	63,63,67	0.89	3 (4%)	77,77,81	1.05	7 (9%)
29	LMT	a	404	-	36,36,36	0.49	1 (2%)	47,47,47	1.23	3 (6%)
24	CLA	B	614	-	69,73,73	1.98	18 (26%)	82,113,113	2.53	33 (40%)
28	GOL	A	415	-	5,5,5	0.42	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	M	104	-	36,36,36	0.46	0	47,47,47	0.88	2 (4%)
26	BCR	Y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.63	9 (16%)
29	LMT	T	104	-	25,25,36	0.50	0	30,30,47	0.94	1 (3%)
28	GOL	V	202	-	5,5,5	0.38	0	5,5,5	0.29	0
36	HTG	b	602	-	19,19,19	0.85	1 (5%)	23,24,24	1.07	2 (8%)
34	LMG	z	101	-	39,39,55	1.07	2 (5%)	47,47,63	1.14	4 (8%)
24	CLA	c	517	-	69,73,73	2.02	19 (27%)	82,113,113	2.69	33 (40%)
28	GOL	O	301	-	5,5,5	0.38	0	5,5,5	0.44	0
24	CLA	d	402	-	69,73,73	1.99	18 (26%)	82,113,113	2.66	31 (37%)
24	CLA	d	403	-	69,73,73	2.02	21 (30%)	82,113,113	2.71	31 (37%)
37	DGD	c	521	-	63,63,67	0.88	2 (3%)	77,77,81	1.09	6 (7%)
28	GOL	b	605	-	5,5,5	0.38	0	5,5,5	0.33	0
34	LMG	j	101	40	51,51,55	0.93	2 (3%)	59,59,63	0.94	4 (6%)
37	DGD	c	520	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	2 (2%)
28	GOL	V	203	-	5,5,5	0.36	0	5,5,5	0.46	0
28	GOL	B	627	-	5,5,5	0.34	0	5,5,5	0.50	0
24	CLA	B	608	42	69,73,73	2.00	20 (28%)	82,113,113	2.63	33 (40%)
24	CLA	c	511	42	69,73,73	2.00	19 (27%)	82,113,113	2.63	28 (34%)
24	CLA	b	620	42	69,73,73	2.05	20 (28%)	82,113,113	2.65	30 (36%)
32	PL9	d	405[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.61	17 (25%)
24	CLA	C	507	42	69,73,73	2.01	20 (28%)	82,113,113	2.63	31 (37%)
24	CLA	A	405	-	69,73,73	2.01	20 (28%)	82,113,113	2.62	30 (36%)
24	CLA	C	505	-	69,73,73	2.01	20 (28%)	82,113,113	2.61	29 (35%)
32	PL9	d	405[A]	-	55,55,55	0.67	2 (3%)	68,69,69	1.55	13 (19%)
34	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.18	4 (6%)
38	LHG	L	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	4 (7%)
24	CLA	a	412	-	69,73,73	2.03	19 (27%)	82,113,113	2.72	34 (41%)
24	CLA	C	504	42	69,73,73	2.00	19 (27%)	82,113,113	2.73	32 (39%)
26	BCR	b	628	-	41,41,41	0.98	1 (2%)	56,56,56	1.34	9 (16%)
36	HTG	B	623	-	19,19,19	0.95	1 (5%)	23,24,24	1.14	1 (4%)
24	CLA	b	617	42	69,73,73	1.96	18 (26%)	82,113,113	2.73	29 (35%)
24	CLA	c	507	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	30 (36%)
26	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.47	11 (19%)
24	CLA	c	515	3	69,73,73	1.99	19 (27%)	82,113,113	2.59	29 (35%)
24	CLA	B	617	-	69,73,73	1.99	19 (27%)	82,113,113	2.63	30 (36%)
27	SQD	A	412	-	52,54,54	0.91	2 (3%)	62,65,65	1.50	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	GOL	a	402	-	5,5,5	0.37	0	5,5,5	0.30	0
32	PL9	A	420[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.79	21 (30%)
36	HTG	B	633	-	19,19,19	0.93	1 (5%)	23,24,24	1.29	2 (8%)
24	CLA	b	612	-	69,73,73	2.03	21 (30%)	82,113,113	2.72	31 (37%)
24	CLA	C	508	-	69,73,73	2.05	20 (28%)	82,113,113	2.67	31 (37%)
24	CLA	b	624	-	69,73,73	1.97	18 (26%)	82,113,113	2.77	32 (39%)
24	CLA	B	605	-	69,73,73	1.96	19 (27%)	82,113,113	2.75	31 (37%)
26	BCR	b	629	-	41,41,41	1.10	1 (2%)	56,56,56	1.24	7 (12%)
26	BCR	d	404	-	41,41,41	1.14	1 (2%)	56,56,56	1.59	12 (21%)
26	BCR	a	413	-	41,41,41	1.05	1 (2%)	56,56,56	1.16	6 (10%)
37	DGD	D	406	-	52,52,67	1.01	3 (5%)	60,60,81	1.17	4 (6%)
25	PHO	A	409[A]	-	58,69,69	2.78	15 (25%)	55,99,99	2.92	15 (27%)
28	GOL	b	604	-	5,5,5	0.37	0	5,5,5	0.26	0
28	GOL	T	102	-	5,5,5	0.39	0	5,5,5	0.30	0
32	PL9	a	416[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.94	21 (30%)
31	OEY	a	418[B]	3,42,1	0,16,16	-	-	-	-	-
28	GOL	A	413	-	5,5,5	0.35	0	5,5,5	0.26	0
24	CLA	b	618	-	69,73,73	2.09	20 (28%)	82,113,113	2.56	34 (41%)
36	HTG	b	608	-	19,19,19	0.94	2 (10%)	23,24,24	1.35	2 (8%)
28	GOL	c	502	-	5,5,5	0.42	0	5,5,5	0.54	0
24	CLA	b	622	-	69,73,73	2.02	19 (27%)	82,113,113	2.60	33 (40%)
24	CLA	c	506	-	69,73,73	2.02	21 (30%)	82,113,113	2.60	27 (32%)
26	BCR	A	411	-	41,41,41	1.05	1 (2%)	56,56,56	1.21	7 (12%)
24	CLA	C	509	-	69,73,73	2.08	20 (28%)	82,113,113	2.66	31 (37%)
27	SQD	a	405	-	52,54,54	1.00	2 (3%)	62,65,65	1.18	4 (6%)
34	LMG	b	630	-	51,51,55	0.91	2 (3%)	59,59,63	1.04	4 (6%)
26	BCR	B	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	8 (14%)
41	HEC	V	206	16	46,50,50	1.78	11 (23%)	58,82,82	1.56	10 (17%)
38	LHG	D	409	-	48,48,48	0.95	2 (4%)	51,54,54	1.08	4 (7%)
28	GOL	B	631	-	5,5,5	0.38	0	5,5,5	0.34	0
24	CLA	d	401	42	69,73,73	2.03	20 (28%)	82,113,113	2.69	34 (41%)
28	GOL	C	524	-	5,5,5	0.39	0	5,5,5	0.81	0
34	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
24	CLA	C	510	-	69,73,73	2.05	20 (28%)	82,113,113	2.58	30 (36%)
29	LMT	f	103	-	36,36,36	0.47	0	47,47,47	0.84	1 (2%)
29	LMT	M	103	-	36,36,36	0.53	1 (2%)	47,47,47	1.00	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCT	a	419[B]	21	3,3,3	0.53	0	2,3,3	0.73	0
36	HTG	H	101	-	16,16,19	1.03	2 (12%)	20,21,24	1.07	1 (5%)
24	CLA	A	406	42	69,73,73	1.98	18 (26%)	82,113,113	2.80	33 (40%)
37	DGD	e	101	-	63,63,67	0.93	2 (3%)	77,77,81	1.24	7 (9%)
28	GOL	B	630	-	5,5,5	0.40	0	5,5,5	0.13	0
24	CLA	c	514	-	69,73,73	2.03	19 (27%)	82,113,113	2.67	32 (39%)
24	CLA	B	612	-	69,73,73	1.97	20 (28%)	82,113,113	2.74	31 (37%)
26	BCR	B	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.48	9 (16%)
26	BCR	D	404	-	41,41,41	1.03	1 (2%)	56,56,56	1.82	11 (19%)
26	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.57	10 (17%)
28	GOL	T	101	-	5,5,5	0.51	0	5,5,5	0.22	0
24	CLA	C	512	-	69,73,73	2.01	20 (28%)	82,113,113	2.68	31 (37%)
26	BCR	b	627	-	41,41,41	1.04	1 (2%)	56,56,56	1.35	6 (10%)
28	GOL	c	501	-	5,5,5	0.33	0	5,5,5	0.34	0
38	LHG	a	422	-	41,41,48	1.03	2 (4%)	44,47,54	0.96	3 (6%)
38	LHG	d	406	-	48,48,48	0.89	3 (6%)	51,54,54	1.07	5 (9%)
36	HTG	c	524	-	19,19,19	0.95	2 (10%)	23,24,24	1.37	1 (4%)
24	CLA	C	506	-	69,73,73	2.02	19 (27%)	82,113,113	2.59	31 (37%)
25	PHO	A	408	-	58,69,69	2.73	13 (22%)	55,99,99	3.00	15 (27%)
26	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.56	13 (23%)
24	CLA	C	513	-	69,73,73	2.03	20 (28%)	82,113,113	2.63	31 (37%)
28	GOL	B	628	-	5,5,5	0.36	0	5,5,5	0.59	0
28	GOL	V	205	-	5,5,5	0.35	0	5,5,5	0.41	0
39	HEM	F	102	6,5	50,50,50	1.53	7 (14%)	67,82,82	1.71	12 (17%)
24	CLA	D	402	-	69,73,73	1.94	19 (27%)	82,113,113	2.74	32 (39%)
24	CLA	D	403	-	69,73,73	2.02	21 (30%)	82,113,113	2.68	31 (37%)
30	OEX	a	417[A]	3,42,1	0,15,15	-	-	-	-	-
37	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.09	6 (7%)
38	LHG	D	407	-	48,48,48	0.87	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	t	102	-	5,5,5	0.48	0	5,5,5	0.16	0
24	CLA	b	616	-	69,73,73	2.02	20 (28%)	82,113,113	2.68	29 (35%)
25	PHO	a	420[B]	-	58,69,69	2.79	13 (22%)	55,99,99	2.87	13 (23%)
26	BCR	T	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.76	16 (28%)
26	BCR	C	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.50	9 (16%)
36	HTG	b	633	-	19,19,19	1.06	2 (10%)	23,24,24	1.75	4 (17%)
24	CLA	b	625	-	69,73,73	2.01	20 (28%)	82,113,113	2.67	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMT	F	101	-	36,36,36	0.48	0	47,47,47	0.93	1 (2%)
38	LHG	d	408	-	48,48,48	0.94	2 (4%)	51,54,54	0.99	2 (3%)
24	CLA	c	513	-	69,73,73	2.06	20 (28%)	82,113,113	2.64	30 (36%)
24	CLA	b	623	-	69,73,73	2.03	20 (28%)	82,113,113	2.60	30 (36%)
29	LMT	C	521	-	36,36,36	0.48	0	47,47,47	1.15	3 (6%)
29	LMT	a	421	-	36,36,36	0.46	0	47,47,47	0.84	1 (2%)
23	BCT	A	404[B]	21	3,3,3	0.51	0	2,3,3	1.01	0
24	CLA	a	409	-	69,73,73	2.02	19 (27%)	82,113,113	2.68	34 (41%)
36	HTG	B	625	-	19,19,19	0.99	1 (5%)	23,24,24	1.72	4 (17%)
36	HTG	B	632	-	19,19,19	1.00	2 (10%)	23,24,24	1.25	2 (8%)
24	CLA	b	614	-	69,73,73	2.01	19 (27%)	82,113,113	2.66	30 (36%)
27	SQD	B	621	-	52,54,54	0.97	2 (3%)	62,65,65	1.41	8 (12%)
26	BCR	B	620	-	41,41,41	1.07	1 (2%)	56,56,56	1.54	9 (16%)
29	LMT	A	417	-	36,36,36	0.62	1 (2%)	47,47,47	1.27	3 (6%)
29	LMT	m	102	-	36,36,36	0.45	0	47,47,47	1.03	3 (6%)
34	LMG	B	622	-	51,51,55	0.94	2 (3%)	59,59,63	1.08	4 (6%)
34	LMG	c	523	-	51,51,55	0.96	3 (5%)	59,59,63	1.23	8 (13%)
36	HTG	b	632	-	19,19,19	0.71	1 (5%)	23,24,24	1.17	2 (8%)
24	CLA	c	510	-	69,73,73	2.00	20 (28%)	82,113,113	2.63	29 (35%)
28	GOL	o	301	-	5,5,5	0.38	0	5,5,5	0.29	0
24	CLA	C	502	-	69,73,73	2.00	20 (28%)	82,113,113	2.62	30 (36%)
34	LMG	c	522	-	51,51,55	0.91	2 (3%)	59,59,63	1.14	5 (8%)
28	GOL	B	629	-	5,5,5	0.36	0	5,5,5	0.37	0
26	BCR	C	514	-	41,41,41	1.05	1 (2%)	56,56,56	1.56	10 (17%)
24	CLA	B	607	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	31 (37%)
39	HEM	e	102	6,5	50,50,50	1.54	8 (16%)	67,82,82	1.61	15 (22%)
28	GOL	b	603	-	5,5,5	0.43	0	5,5,5	0.53	0
24	CLA	c	516	-	69,73,73	2.02	20 (28%)	82,113,113	2.75	33 (40%)
23	BCT	a	419[A]	-	3,3,3	0.53	0	2,3,3	0.85	0
29	LMT	D	401	-	36,36,36	0.43	0	47,47,47	1.01	1 (2%)
24	CLA	b	615	-	69,73,73	2.00	19 (27%)	82,113,113	2.77	28 (34%)
36	HTG	c	525	-	19,19,19	0.93	2 (10%)	23,24,24	1.33	2 (8%)
31	OXY	A	419[B]	3,42,1	0,16,16	-	-	-	-	-
38	LHG	d	407	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	4 (7%)
28	GOL	f	101	35	5,5,5	0.33	0	5,5,5	0.39	0
26	BCR	H	102	-	41,41,41	1.12	1 (2%)	56,56,56	1.44	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	609	-	69,73,73	2.02	20 (28%)	82,113,113	2.63	32 (39%)
24	CLA	B	615	-	69,73,73	1.98	19 (27%)	82,113,113	2.75	31 (37%)
24	CLA	c	508	42	69,73,73	2.02	19 (27%)	82,113,113	2.74	34 (41%)
37	DGD	C	517	-	63,63,67	0.89	3 (4%)	77,77,81	0.99	5 (6%)
34	LMG	C	519	-	51,51,55	0.97	2 (3%)	59,59,63	0.99	3 (5%)
24	CLA	b	613	-	69,73,73	1.97	20 (28%)	82,113,113	2.67	32 (39%)
28	GOL	v	201	-	5,5,5	0.35	0	5,5,5	0.26	0
28	GOL	B	626	-	5,5,5	0.44	0	5,5,5	0.37	0
24	CLA	A	407	42	69,73,73	2.00	20 (28%)	82,113,113	2.68	34 (41%)
28	GOL	C	525	-	5,5,5	0.40	0	5,5,5	0.72	0
28	GOL	b	606	-	5,5,5	0.39	0	5,5,5	0.30	0
38	LHG	D	408	-	48,48,48	0.90	2 (4%)	51,54,54	0.86	3 (5%)
24	CLA	b	621	-	69,73,73	1.95	19 (27%)	82,113,113	2.67	31 (37%)
24	CLA	c	512	-	69,73,73	2.02	20 (28%)	82,113,113	2.61	32 (39%)
24	CLA	a	410	42	69,73,73	2.01	20 (28%)	82,113,113	2.69	33 (40%)
37	DGD	C	518	-	63,63,67	0.86	2 (3%)	77,77,81	0.92	4 (5%)
36	HTG	B	624	-	19,19,19	0.76	1 (5%)	23,24,24	1.38	2 (8%)
29	LMT	b	631	-	25,25,36	0.53	0	30,30,47	0.67	0
24	CLA	C	501	-	69,73,73	2.01	19 (27%)	82,113,113	2.65	29 (35%)
38	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.09	3 (6%)
34	LMG	D	412	40	51,51,55	0.90	2 (3%)	59,59,63	1.00	3 (5%)
25	PHO	a	420[A]	-	58,69,69	2.77	13 (22%)	55,99,99	3.03	15 (27%)
24	CLA	B	604	-	69,73,73	2.06	19 (27%)	82,113,113	2.69	29 (35%)
27	SQD	F	103	-	41,43,54	1.09	2 (4%)	51,54,65	1.61	11 (21%)
24	CLA	b	626	-	69,73,73	2.00	20 (28%)	82,113,113	2.66	31 (37%)
28	GOL	V	204	-	5,5,5	0.39	0	5,5,5	0.28	0
28	GOL	a	401	-	5,5,5	0.49	0	5,5,5	0.54	0
36	HTG	C	523	-	19,19,19	0.95	1 (5%)	23,24,24	1.70	4 (17%)
24	CLA	b	611	42	69,73,73	2.04	19 (27%)	82,113,113	2.67	27 (32%)
24	CLA	B	613	-	69,73,73	1.98	18 (26%)	82,113,113	2.75	31 (37%)
24	CLA	B	603	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	33 (40%)
36	HTG	C	522	-	19,19,19	0.92	2 (10%)	23,24,24	1.39	2 (8%)
34	LMG	Z	101	-	37,37,55	0.96	2 (5%)	45,45,63	1.39	6 (13%)
28	GOL	b	607	-	5,5,5	0.37	0	5,5,5	0.33	0
28	GOL	A	414	-	5,5,5	0.47	0	5,5,5	0.59	0
27	SQD	f	102	-	41,43,54	1.11	2 (4%)	51,54,65	1.40	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	611	42	69,73,73	2.09	19 (27%)	82,113,113	2.64	34 (41%)
36	HTG	V	207	-	19,19,19	0.96	2 (10%)	23,24,24	1.16	2 (8%)
23	BCT	A	404[A]	21	3,3,3	0.50	0	2,3,3	1.09	0
26	BCR	c	527	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	7 (12%)
28	GOL	B	636	-	5,5,5	0.41	0	5,5,5	0.56	0
24	CLA	c	509	-	69,73,73	1.99	20 (28%)	82,113,113	2.58	30 (36%)
26	BCR	t	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.64	12 (21%)
24	CLA	B	606	-	69,73,73	1.99	18 (26%)	82,113,113	2.76	30 (36%)
30	OEX	A	418[A]	3,42,1	0,15,15	-	-	-	-	-
28	GOL	V	201	35	5,5,5	0.37	0	5,5,5	0.27	0
27	SQD	A	416	-	52,54,54	0.96	2 (3%)	62,65,65	1.16	5 (8%)
27	SQD	b	601	-	52,54,54	0.98	2 (3%)	62,65,65	1.53	9 (14%)
36	HTG	d	411	-	16,16,19	1.04	2 (12%)	20,21,24	1.70	2 (10%)
29	LMT	B	635	-	25,25,36	0.52	0	30,30,47	0.88	1 (3%)
28	GOL	v	203	-	5,5,5	0.41	0	5,5,5	0.26	0
32	PL9	A	420[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.78	22 (32%)
26	BCR	c	518	-	41,41,41	1.06	1 (2%)	56,56,56	1.51	10 (17%)
34	LMG	A	422	-	51,51,55	0.94	2 (3%)	59,59,63	1.14	5 (8%)
24	CLA	c	505	-	69,73,73	2.00	19 (27%)	82,113,113	2.58	30 (36%)

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
38	LHG	l	101	-	-	15/53/53/53	-
32	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
24	CLA	C	503	-	1/1/15/20	1/39/115/115	-
37	DGD	h	102	-	-	11/51/91/95	0/2/2/2
24	CLA	B	602	42	1/1/15/20	13/39/115/115	-
24	CLA	b	619	-	1/1/15/20	5/39/115/115	-
24	CLA	B	616	-	1/1/15/20	12/39/115/115	-
25	PHO	a	411	-	-	3/37/103/103	0/5/6/6
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
32	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1
25	PHO	A	409[B]	-	-	1/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	c	519	-	-	14/51/91/95	0/2/2/2
29	LMT	M	101	-	-	4/21/61/61	0/2/2/2
24	CLA	B	610	-	1/1/15/20	6/39/115/115	-
32	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
36	HTG	b	609	-	-	0/10/30/30	0/1/1/1
41	HEC	v	205	16	-	6/14/54/54	-
27	SQD	a	414	-	-	14/49/69/69	0/1/1/1
28	GOL	v	202	-	-	2/4/4/4	-
24	CLA	A	410	-	1/1/15/20	9/39/115/115	-
24	CLA	C	511	3	1/1/15/20	3/39/115/115	-
37	DGD	H	103	-	-	14/51/91/95	0/2/2/2
29	LMT	a	404	-	-	9/21/61/61	0/2/2/2
24	CLA	B	614	-	1/1/15/20	3/39/115/115	-
28	GOL	A	415	-	-	2/4/4/4	-
29	LMT	M	104	-	-	8/21/61/61	0/2/2/2
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
29	LMT	T	104	-	-	7/17/37/61	0/1/1/2
28	GOL	V	202	-	-	2/4/4/4	-
36	HTG	b	602	-	-	3/10/30/30	0/1/1/1
34	LMG	z	101	-	-	15/34/54/70	0/1/1/1
24	CLA	c	517	-	-	4/39/115/115	-
28	GOL	O	301	-	-	2/4/4/4	-
24	CLA	d	402	-	1/1/15/20	4/39/115/115	-
24	CLA	d	403	-	1/1/15/20	4/39/115/115	-
37	DGD	c	521	-	-	16/51/91/95	0/2/2/2
28	GOL	b	605	-	-	1/4/4/4	-
34	LMG	j	101	40	-	11/46/66/70	0/1/1/1
37	DGD	c	520	-	-	17/51/91/95	0/2/2/2
28	GOL	V	203	-	-	2/4/4/4	-
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	B	608	42	1/1/15/20	7/39/115/115	-
24	CLA	c	511	42	1/1/15/20	6/39/115/115	-
24	CLA	b	620	42	1/1/15/20	5/39/115/115	-
32	PL9	d	405[B]	-	-	5/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	C	507	42	1/1/15/20	8/39/115/115	-
24	CLA	A	405	-	1/1/15/20	7/39/115/115	-
24	CLA	C	505	-	1/1/15/20	4/39/115/115	-
32	PL9	d	405[A]	-	-	8/53/73/73	0/1/1/1
34	LMG	a	415	-	-	16/46/66/70	0/1/1/1
38	LHG	L	101	-	-	16/53/53/53	-
24	CLA	a	412	-	1/1/15/20	9/39/115/115	-
24	CLA	C	504	42	1/1/15/20	5/39/115/115	-
26	BCR	b	628	-	-	0/29/63/63	0/2/2/2
36	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	b	617	42	1/1/15/20	2/39/115/115	-
24	CLA	c	507	-	-	3/39/115/115	-
26	BCR	k	101	-	-	2/29/63/63	0/2/2/2
24	CLA	c	515	3	1/1/15/20	5/39/115/115	-
24	CLA	B	617	-	1/1/15/20	6/39/115/115	-
27	SQD	A	412	-	-	9/49/69/69	0/1/1/1
28	GOL	a	402	-	-	2/4/4/4	-
32	PL9	A	420[A]	-	-	10/53/73/73	0/1/1/1
36	HTG	B	633	-	-	0/10/30/30	0/1/1/1
24	CLA	b	612	-	1/1/15/20	5/39/115/115	-
24	CLA	C	508	-	1/1/15/20	3/39/115/115	-
24	CLA	b	624	-	1/1/15/20	17/39/115/115	-
24	CLA	B	605	-	1/1/15/20	5/39/115/115	-
26	BCR	b	629	-	-	0/29/63/63	0/2/2/2
26	BCR	d	404	-	-	3/29/63/63	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
37	DGD	D	406	-	-	22/47/67/95	0/1/1/2
25	PHO	A	409[A]	-	-	0/37/103/103	0/5/6/6
28	GOL	b	604	-	-	0/4/4/4	-
28	GOL	T	102	-	-	2/4/4/4	-
32	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
28	GOL	A	413	-	-	1/4/4/4	-
24	CLA	b	618	-	-	1/39/115/115	-
36	HTG	b	608	-	-	1/10/30/30	0/1/1/1
28	GOL	c	502	-	-	1/4/4/4	-
24	CLA	b	622	-	1/1/15/20	1/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	c	506	-	-	6/39/115/115	-
26	BCR	A	411	-	-	0/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/15/20	14/39/115/115	-
27	SQD	a	405	-	-	17/49/69/69	0/1/1/1
34	LMG	b	630	-	-	10/46/66/70	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
41	HEC	V	206	16	-	6/14/54/54	-
38	LHG	D	409	-	-	11/53/53/53	-
28	GOL	B	631	-	-	1/4/4/4	-
24	CLA	d	401	42	1/1/15/20	4/39/115/115	-
28	GOL	C	524	-	-	2/4/4/4	-
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
24	CLA	C	510	-	1/1/15/20	6/39/115/115	-
29	LMT	f	103	-	-	9/21/61/61	0/2/2/2
29	LMT	M	103	-	-	9/21/61/61	0/2/2/2
36	HTG	H	101	-	-	0/7/27/30	0/1/1/1
24	CLA	A	406	42	1/1/15/20	4/39/115/115	-
37	DGD	e	101	-	-	27/51/91/95	0/2/2/2
28	GOL	B	630	-	-	4/4/4/4	-
24	CLA	c	514	-	1/1/15/20	9/39/115/115	-
24	CLA	B	612	-	1/1/15/20	0/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	BCR	D	404	-	-	8/29/63/63	0/2/2/2
26	BCR	y	101	-	-	4/29/63/63	0/2/2/2
28	GOL	T	101	-	-	1/4/4/4	-
24	CLA	C	512	-	1/1/15/20	9/39/115/115	-
26	BCR	b	627	-	-	2/29/63/63	0/2/2/2
28	GOL	c	501	-	-	0/4/4/4	-
38	LHG	a	422	-	-	18/46/46/53	-
38	LHG	d	406	-	-	10/53/53/53	-
36	HTG	c	524	-	-	3/10/30/30	0/1/1/1
24	CLA	C	506	-	1/1/15/20	8/39/115/115	-
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
26	BCR	K	101	-	-	1/29/63/63	0/2/2/2
24	CLA	C	513	-	1/1/15/20	7/39/115/115	-
28	GOL	B	628	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	V	205	-	-	2/4/4/4	-
39	HEM	F	102	6,5	-	8/14/54/54	-
24	CLA	D	402	-	1/1/15/20	3/39/115/115	-
24	CLA	D	403	-	1/1/15/20	3/39/115/115	-
37	DGD	C	516	-	-	16/51/91/95	0/2/2/2
38	LHG	D	407	-	-	13/53/53/53	-
28	GOL	t	102	-	-	0/4/4/4	-
24	CLA	b	616	-	1/1/15/20	5/39/115/115	-
25	PHO	a	420[B]	-	-	3/37/103/103	0/5/6/6
26	BCR	T	103	-	-	3/29/63/63	0/2/2/2
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
36	HTG	b	633	-	-	5/10/30/30	0/1/1/1
24	CLA	b	625	-	1/1/15/20	5/39/115/115	-
29	LMT	F	101	-	-	3/21/61/61	0/2/2/2
38	LHG	d	408	-	-	11/53/53/53	-
24	CLA	c	513	-	1/1/15/20	13/39/115/115	-
24	CLA	b	623	-	1/1/15/20	3/39/115/115	-
29	LMT	C	521	-	-	11/21/61/61	0/2/2/2
29	LMT	a	421	-	-	4/21/61/61	0/2/2/2
24	CLA	a	409	-	1/1/15/20	4/39/115/115	-
36	HTG	B	625	-	-	4/10/30/30	0/1/1/1
36	HTG	B	632	-	-	3/10/30/30	0/1/1/1
24	CLA	b	614	-	1/1/15/20	5/39/115/115	-
27	SQD	B	621	-	-	20/49/69/69	0/1/1/1
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
29	LMT	A	417	-	-	5/21/61/61	0/2/2/2
29	LMT	m	102	-	-	7/21/61/61	0/2/2/2
34	LMG	B	622	-	-	9/46/66/70	0/1/1/1
34	LMG	c	523	-	-	3/46/66/70	0/1/1/1
36	HTG	b	632	-	-	3/10/30/30	0/1/1/1
24	CLA	c	510	-	1/1/15/20	14/39/115/115	-
28	GOL	o	301	-	-	0/4/4/4	-
24	CLA	C	502	-	1/1/15/20	7/39/115/115	-
34	LMG	c	522	-	-	14/46/66/70	0/1/1/1
28	GOL	B	629	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	C	514	-	-	2/29/63/63	0/2/2/2
24	CLA	B	607	-	1/1/15/20	3/39/115/115	-
39	HEM	e	102	6,5	-	9/14/54/54	-
28	GOL	b	603	-	-	1/4/4/4	-
24	CLA	c	516	-	1/1/15/20	10/39/115/115	-
29	LMT	D	401	-	-	8/21/61/61	0/2/2/2
36	HTG	c	525	-	-	0/10/30/30	0/1/1/1
24	CLA	b	615	-	1/1/15/20	4/39/115/115	-
38	LHG	d	407	-	-	10/53/53/53	-
28	GOL	f	101	35	-	3/4/4/4	-
26	BCR	H	102	-	-	1/29/63/63	0/2/2/2
24	CLA	B	615	-	1/1/15/20	14/39/115/115	-
24	CLA	B	609	-	-	1/39/115/115	-
24	CLA	c	508	42	1/1/15/20	4/39/115/115	-
37	DGD	C	517	-	-	16/51/91/95	0/2/2/2
34	LMG	C	519	-	-	13/46/66/70	0/1/1/1
24	CLA	b	613	-	1/1/15/20	4/39/115/115	-
28	GOL	v	201	-	-	2/4/4/4	-
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	A	407	42	-	2/39/115/115	-
28	GOL	C	525	-	-	0/4/4/4	-
28	GOL	b	606	-	-	2/4/4/4	-
38	LHG	D	408	-	-	11/53/53/53	-
24	CLA	b	621	-	-	3/39/115/115	-
24	CLA	c	512	-	1/1/15/20	2/39/115/115	-
24	CLA	a	410	42	-	6/39/115/115	-
37	DGD	C	518	-	-	11/51/91/95	0/2/2/2
36	HTG	B	624	-	-	2/10/30/30	0/1/1/1
29	LMT	b	631	-	-	4/17/37/61	0/1/1/2
24	CLA	C	501	-	1/1/15/20	3/39/115/115	-
38	LHG	E	101	-	-	19/46/46/53	-
34	LMG	D	412	40	-	6/46/66/70	0/1/1/1
25	PHO	a	420[A]	-	-	1/37/103/103	0/5/6/6
24	CLA	B	604	-	1/1/15/20	7/39/115/115	-
27	SQD	F	103	-	-	16/38/58/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	626	-	1/1/15/20	8/39/115/115	-
28	GOL	V	204	-	-	1/4/4/4	-
28	GOL	a	401	-	-	0/4/4/4	-
36	HTG	C	523	-	-	3/10/30/30	0/1/1/1
24	CLA	b	611	42	1/1/15/20	15/39/115/115	-
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
24	CLA	B	603	-	1/1/15/20	3/39/115/115	-
36	HTG	C	522	-	-	0/10/30/30	0/1/1/1
34	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
28	GOL	b	607	-	-	3/4/4/4	-
28	GOL	A	414	-	-	2/4/4/4	-
27	SQD	f	102	-	-	14/38/58/69	0/1/1/1
24	CLA	B	611	42	1/1/15/20	3/39/115/115	-
36	HTG	V	207	-	-	1/10/30/30	0/1/1/1
26	BCR	c	527	-	-	0/29/63/63	0/2/2/2
28	GOL	B	636	-	-	0/4/4/4	-
24	CLA	c	509	-	1/1/15/20	1/39/115/115	-
26	BCR	t	101	-	-	2/29/63/63	0/2/2/2
24	CLA	B	606	-	1/1/15/20	5/39/115/115	-
28	GOL	V	201	35	-	2/4/4/4	-
27	SQD	A	416	-	-	15/49/69/69	0/1/1/1
27	SQD	b	601	-	-	22/49/69/69	0/1/1/1
36	HTG	d	411	-	-	1/7/27/30	0/1/1/1
29	LMT	B	635	-	-	7/17/37/61	0/1/1/2
28	GOL	v	203	-	-	2/4/4/4	-
32	PL9	A	420[B]	-	-	11/53/73/73	0/1/1/1
26	BCR	c	518	-	-	2/29/63/63	0/2/2/2
34	LMG	A	422	-	-	19/46/66/70	0/1/1/1
24	CLA	c	505	-	1/1/15/20	4/39/115/115	-

All (1634) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	408	PHO	C1B-C2B	9.39	1.49	1.39
25	a	411	PHO	C1D-C2D	9.35	1.49	1.39
25	a	420[B]	PHO	C1B-C2B	9.28	1.49	1.39
25	A	409[B]	PHO	C1B-C2B	9.16	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	420[A]	PHO	C1D-C2D	8.87	1.49	1.39
25	a	420[B]	PHO	C1D-C2D	8.83	1.49	1.39
25	A	408	PHO	C1D-C2D	8.78	1.49	1.39
25	a	420[A]	PHO	C1B-C2B	8.77	1.49	1.39
25	A	409[B]	PHO	C1D-C2D	8.75	1.49	1.39
25	A	409[A]	PHO	C1D-C2D	8.63	1.49	1.39
25	a	411	PHO	C1B-C2B	8.47	1.48	1.39
25	A	409[A]	PHO	C1B-C2B	8.44	1.48	1.39
25	A	409[A]	PHO	C3B-C4B	8.12	1.49	1.41
25	a	420[A]	PHO	C3B-C4B	7.99	1.49	1.41
25	a	411	PHO	C3B-C4B	7.93	1.49	1.41
25	A	409[B]	PHO	C3B-C4B	7.88	1.49	1.41
25	a	420[B]	PHO	C3B-C4B	7.78	1.49	1.41
25	A	408	PHO	C4D-CHA	6.96	1.49	1.39
25	A	409[B]	PHO	C4D-CHA	6.94	1.49	1.39
25	A	409[A]	PHO	C4D-CHA	6.93	1.49	1.39
25	a	420[A]	PHO	C4D-CHA	6.81	1.49	1.39
25	A	408	PHO	C3B-C4B	6.79	1.48	1.41
25	a	420[B]	PHO	C4D-CHA	6.73	1.49	1.39
25	A	409[A]	PHO	C3B-C2B	6.61	1.49	1.40
25	A	409[B]	PHO	C3B-C2B	6.61	1.49	1.40
25	a	420[B]	PHO	C3B-C2B	6.30	1.48	1.40
25	a	411	PHO	C4D-CHA	6.26	1.48	1.39
25	a	420[A]	PHO	C3B-C2B	6.24	1.48	1.40
25	A	409[B]	PHO	C3D-C2D	5.85	1.49	1.39
25	A	408	PHO	C3B-C2B	5.74	1.48	1.40
25	a	420[A]	PHO	C3D-C2D	5.73	1.49	1.39
25	a	411	PHO	C3D-C2D	5.72	1.49	1.39
24	b	611	CLA	C3C-C2C	5.71	1.49	1.36
25	a	411	PHO	C3B-C2B	5.69	1.48	1.40
24	B	604	CLA	C3C-C2C	5.63	1.48	1.36
24	b	623	CLA	C3C-C2C	5.58	1.48	1.36
25	A	409[A]	PHO	C3D-C2D	5.51	1.49	1.39
24	b	620	CLA	C3C-C2C	5.51	1.48	1.36
24	b	615	CLA	C3C-C2C	5.50	1.48	1.36
24	B	605	CLA	C1D-ND	5.46	1.45	1.37
25	a	420[B]	PHO	C3D-C2D	5.45	1.48	1.39
24	B	603	CLA	C3C-C2C	5.45	1.48	1.36
24	B	611	CLA	C3C-C2C	5.45	1.48	1.36
24	c	514	CLA	C3C-C2C	5.41	1.48	1.36
24	B	602	CLA	C3C-C2C	5.39	1.48	1.36
24	b	623	CLA	O2D-CGD	5.38	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3C-C2C	5.35	1.48	1.36
25	a	411	PHO	OBD-CAD	5.32	1.29	1.22
24	C	510	CLA	C3C-C2C	5.31	1.48	1.36
24	c	517	CLA	C3C-C2C	5.31	1.48	1.36
24	B	606	CLA	O2D-CGD	5.30	1.46	1.33
25	A	408	PHO	C3D-C2D	5.30	1.48	1.39
25	A	408	PHO	OBD-CAD	5.30	1.29	1.22
24	b	612	CLA	C3C-C2C	5.29	1.48	1.36
24	C	507	CLA	C3C-C2C	5.27	1.48	1.36
24	b	618	CLA	C3C-C2C	5.26	1.48	1.36
24	d	401	CLA	C3C-C2C	5.25	1.48	1.36
24	b	616	CLA	C3C-C2C	5.25	1.48	1.36
24	C	509	CLA	C3C-C2C	5.25	1.48	1.36
24	a	410	CLA	CHC-C1C	5.24	1.49	1.38
24	c	516	CLA	C3C-C2C	5.23	1.48	1.36
26	b	629	BCR	C23-C22	-5.21	1.34	1.46
24	c	508	CLA	O2D-CGD	5.20	1.46	1.33
24	A	406	CLA	C3C-C2C	5.18	1.48	1.36
24	D	403	CLA	C1D-ND	5.18	1.44	1.37
24	a	412	CLA	O2D-CGD	5.17	1.45	1.33
24	B	610	CLA	C3C-C2C	5.17	1.47	1.36
24	c	510	CLA	C3C-C2C	5.17	1.47	1.36
24	B	608	CLA	C3C-C2C	5.17	1.47	1.36
24	C	512	CLA	C3C-C2C	5.16	1.47	1.36
24	C	513	CLA	C3C-C2C	5.16	1.47	1.36
24	C	503	CLA	C3C-C2C	5.16	1.47	1.36
24	B	616	CLA	O2D-CGD	5.16	1.45	1.33
39	e	102	HEM	FE-NB	5.16	2.10	1.94
24	C	502	CLA	C3C-C2C	5.16	1.47	1.36
24	B	614	CLA	O2D-CGD	5.13	1.45	1.33
24	c	512	CLA	C3C-C2C	5.13	1.47	1.36
24	c	506	CLA	C3C-C2C	5.12	1.47	1.36
24	c	506	CLA	O2D-CGD	5.12	1.45	1.33
26	B	620	BCR	C23-C22	-5.12	1.35	1.46
24	A	407	CLA	C3C-C2C	5.12	1.47	1.36
24	C	505	CLA	C3C-C2C	5.11	1.47	1.36
24	a	409	CLA	C3C-C2C	5.11	1.47	1.36
24	D	403	CLA	C3C-C2C	5.11	1.47	1.36
25	A	409[B]	PHO	O2D-CGD	5.10	1.45	1.33
24	B	609	CLA	C3C-C2C	5.10	1.47	1.36
24	a	412	CLA	C3C-C2C	5.09	1.47	1.36
24	c	511	CLA	C3C-C2C	5.07	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	626	CLA	O2D-CGD	5.06	1.45	1.33
24	b	622	CLA	O2D-CGD	5.06	1.45	1.33
24	C	511	CLA	C3C-C2C	5.06	1.47	1.36
24	C	508	CLA	O2D-CGD	5.06	1.45	1.33
25	A	409[A]	PHO	O2D-CGD	5.06	1.45	1.33
24	a	409	CLA	C1D-ND	5.06	1.44	1.37
24	B	616	CLA	CHC-C1C	5.06	1.48	1.38
24	c	515	CLA	C3C-C2C	5.06	1.47	1.36
24	b	619	CLA	O2D-CGD	5.05	1.45	1.33
24	B	612	CLA	O2D-CGD	5.05	1.45	1.33
24	A	405	CLA	CHC-C1C	5.05	1.48	1.38
24	d	403	CLA	C3C-C2C	5.05	1.47	1.36
24	C	509	CLA	C1D-ND	5.05	1.44	1.37
25	a	411	PHO	O2D-CGD	5.05	1.45	1.33
24	c	513	CLA	C3C-C2C	5.04	1.47	1.36
24	A	406	CLA	C1D-ND	5.04	1.44	1.37
24	C	503	CLA	CHC-C1C	5.04	1.48	1.38
24	C	503	CLA	C1D-ND	5.04	1.44	1.37
24	b	623	CLA	C1D-ND	5.04	1.44	1.37
24	C	504	CLA	C3C-C2C	5.03	1.47	1.36
24	c	507	CLA	C3C-C2C	5.03	1.47	1.36
24	A	410	CLA	O2D-CGD	5.03	1.45	1.33
24	B	607	CLA	O2D-CGD	5.03	1.45	1.33
24	c	507	CLA	CHC-C1C	5.03	1.48	1.38
24	c	508	CLA	C3C-C2C	5.02	1.47	1.36
24	C	501	CLA	CHC-C1C	5.02	1.48	1.38
24	B	611	CLA	C1D-ND	5.02	1.44	1.37
24	c	513	CLA	O2D-CGD	5.01	1.45	1.33
24	d	403	CLA	O2D-CGD	5.01	1.45	1.33
24	A	405	CLA	C3C-C2C	5.01	1.47	1.36
24	d	401	CLA	O2D-CGD	5.01	1.45	1.33
24	B	607	CLA	C3C-C2C	5.01	1.47	1.36
24	b	615	CLA	O2D-CGD	5.01	1.45	1.33
24	b	614	CLA	C3C-C2C	5.01	1.47	1.36
24	b	624	CLA	O2D-CGD	5.00	1.45	1.33
24	b	618	CLA	O2D-CGD	5.00	1.45	1.33
24	B	612	CLA	C3C-C2C	5.00	1.47	1.36
24	b	622	CLA	C3C-C2C	5.00	1.47	1.36
24	B	617	CLA	O2D-CGD	5.00	1.45	1.33
24	b	625	CLA	C1D-ND	4.99	1.44	1.37
24	b	621	CLA	C3C-C2C	4.99	1.47	1.36
24	b	624	CLA	C3C-C2C	4.99	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	O2D-CGD	4.99	1.45	1.33
24	c	513	CLA	C1D-ND	4.99	1.44	1.37
24	B	615	CLA	C3C-C2C	4.99	1.47	1.36
24	B	610	CLA	CHC-C1C	4.98	1.48	1.38
24	C	505	CLA	O2D-CGD	4.98	1.45	1.33
26	C	514	BCR	C23-C22	-4.98	1.35	1.46
24	B	606	CLA	C3C-C2C	4.98	1.47	1.36
25	a	420[B]	PHO	O2D-CGD	4.97	1.45	1.33
24	b	619	CLA	C3C-C2C	4.97	1.47	1.36
24	b	617	CLA	C3C-C2C	4.97	1.47	1.36
24	B	605	CLA	C3C-C2C	4.97	1.47	1.36
24	c	516	CLA	CHC-C1C	4.96	1.48	1.38
24	c	516	CLA	O2D-CGD	4.95	1.45	1.33
24	C	505	CLA	CHC-C1C	4.95	1.48	1.38
24	b	620	CLA	O2D-CGD	4.95	1.45	1.33
26	k	101	BCR	C23-C22	-4.94	1.35	1.46
39	F	102	HEM	FE-NB	4.94	2.10	1.94
24	c	512	CLA	O2D-CGD	4.94	1.45	1.33
25	a	420[A]	PHO	O2D-CGD	4.94	1.45	1.33
24	A	407	CLA	CHC-C1C	4.93	1.48	1.38
24	B	604	CLA	CHC-C1C	4.93	1.48	1.38
24	C	502	CLA	C1D-ND	4.92	1.44	1.37
24	c	505	CLA	O2D-CGD	4.92	1.45	1.33
24	C	506	CLA	C1D-ND	4.92	1.44	1.37
24	C	513	CLA	O2D-CGD	4.91	1.45	1.33
24	b	621	CLA	O2D-CGD	4.91	1.45	1.33
24	C	510	CLA	C1D-ND	4.91	1.44	1.37
25	A	408	PHO	O2D-CGD	4.91	1.45	1.33
24	d	401	CLA	C1D-ND	4.91	1.44	1.37
24	c	509	CLA	C3C-C2C	4.91	1.47	1.36
24	C	501	CLA	C3C-C2C	4.90	1.47	1.36
26	d	404	BCR	C23-C22	-4.90	1.35	1.46
24	C	506	CLA	O2D-CGD	4.90	1.45	1.33
24	b	618	CLA	C1D-ND	4.90	1.44	1.37
24	B	602	CLA	CHC-C1C	4.90	1.48	1.38
26	T	103	BCR	C23-C22	-4.90	1.35	1.46
24	b	625	CLA	C3C-C2C	4.90	1.47	1.36
24	B	602	CLA	C1D-ND	4.89	1.44	1.37
24	C	511	CLA	O2D-CGD	4.88	1.45	1.33
24	d	402	CLA	C3C-C2C	4.88	1.47	1.36
24	B	617	CLA	C3C-C2C	4.88	1.47	1.36
24	C	510	CLA	O2D-CGD	4.88	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	O2D-CGD	4.88	1.45	1.33
24	A	410	CLA	C3C-C2C	4.86	1.47	1.36
24	D	402	CLA	C3C-C2C	4.85	1.47	1.36
24	c	505	CLA	C3C-C2C	4.84	1.47	1.36
24	b	616	CLA	C1D-ND	4.84	1.44	1.37
24	C	501	CLA	C1D-ND	4.84	1.44	1.37
24	B	603	CLA	O2D-CGD	4.84	1.45	1.33
24	C	506	CLA	C3C-C2C	4.83	1.47	1.36
24	b	612	CLA	CHC-C1C	4.83	1.48	1.38
24	c	506	CLA	CHC-C1C	4.83	1.48	1.38
26	y	101	BCR	C23-C22	-4.83	1.35	1.46
24	C	507	CLA	CHC-C1C	4.83	1.48	1.38
26	K	101	BCR	C23-C22	-4.82	1.35	1.46
24	B	603	CLA	CHC-C1C	4.82	1.48	1.38
24	C	512	CLA	CHC-C1C	4.82	1.48	1.38
24	b	613	CLA	C3C-C2C	4.82	1.47	1.36
26	c	527	BCR	C23-C22	-4.81	1.35	1.46
24	a	410	CLA	O2D-CGD	4.81	1.45	1.33
24	c	511	CLA	O2D-CGD	4.80	1.45	1.33
24	b	618	CLA	CHC-C1C	4.80	1.48	1.38
24	D	403	CLA	O2D-CGD	4.80	1.45	1.33
24	c	514	CLA	C1D-ND	4.79	1.44	1.37
24	B	614	CLA	C3C-C2C	4.79	1.47	1.36
24	c	517	CLA	C1D-ND	4.79	1.44	1.37
24	c	514	CLA	O2D-CGD	4.79	1.45	1.33
24	B	610	CLA	O2D-CGD	4.78	1.45	1.33
24	B	606	CLA	C1D-ND	4.78	1.44	1.37
24	b	613	CLA	O2D-CGD	4.78	1.45	1.33
24	B	602	CLA	O2D-CGD	4.78	1.45	1.33
24	c	517	CLA	O2D-CGD	4.78	1.45	1.33
24	c	509	CLA	CHC-C1C	4.78	1.48	1.38
24	b	611	CLA	C1D-ND	4.77	1.44	1.37
26	h	101	BCR	C23-C22	-4.77	1.35	1.46
24	C	502	CLA	CHC-C1C	4.77	1.48	1.38
24	c	517	CLA	CHC-C1C	4.77	1.48	1.38
24	b	611	CLA	CHC-C1C	4.76	1.48	1.38
24	b	620	CLA	CHC-C1C	4.76	1.48	1.38
24	C	501	CLA	O2D-CGD	4.76	1.44	1.33
24	C	502	CLA	O2D-CGD	4.76	1.44	1.33
24	b	614	CLA	O2D-CGD	4.76	1.44	1.33
24	b	619	CLA	CHC-C1C	4.75	1.48	1.38
24	B	613	CLA	O2D-CGD	4.75	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	616	CLA	C3C-C2C	4.75	1.47	1.36
24	c	510	CLA	O2D-CGD	4.75	1.44	1.33
24	c	510	CLA	C1D-ND	4.75	1.44	1.37
25	a	420[B]	PHO	OBD-CAD	4.75	1.28	1.22
26	t	101	BCR	C23-C22	-4.74	1.35	1.46
24	B	611	CLA	O2D-CGD	4.74	1.44	1.33
24	a	410	CLA	C3C-C2C	4.73	1.47	1.36
24	a	409	CLA	O2D-CGD	4.73	1.44	1.33
24	b	615	CLA	CHC-C1C	4.73	1.48	1.38
24	B	608	CLA	O2D-CGD	4.73	1.44	1.33
24	A	410	CLA	CHC-C1C	4.73	1.48	1.38
24	c	507	CLA	O2D-CGD	4.73	1.44	1.33
24	C	504	CLA	C1D-ND	4.73	1.44	1.37
24	b	626	CLA	C3C-C2C	4.72	1.47	1.36
24	B	602	CLA	O2A-CGA	4.72	1.47	1.33
24	a	412	CLA	C1D-ND	4.72	1.44	1.37
24	C	509	CLA	CHC-C1C	4.71	1.47	1.38
24	C	513	CLA	C1D-ND	4.71	1.44	1.37
24	c	512	CLA	C1D-ND	4.71	1.44	1.37
24	c	505	CLA	C1D-ND	4.71	1.44	1.37
24	A	410	CLA	C1D-ND	4.70	1.44	1.37
24	C	513	CLA	CHC-C1C	4.70	1.47	1.38
24	C	510	CLA	CHC-C1C	4.69	1.47	1.38
24	B	613	CLA	CHC-C1C	4.69	1.47	1.38
24	B	609	CLA	O2D-CGD	4.69	1.44	1.33
24	d	402	CLA	CHC-C1C	4.69	1.47	1.38
24	B	616	CLA	C1D-ND	4.69	1.44	1.37
24	C	507	CLA	C1D-ND	4.69	1.44	1.37
24	B	606	CLA	CHC-C1C	4.68	1.47	1.38
24	B	609	CLA	C1D-ND	4.68	1.44	1.37
24	C	512	CLA	O2D-CGD	4.67	1.44	1.33
26	H	102	BCR	C23-C22	-4.67	1.35	1.46
24	B	617	CLA	CHC-C1C	4.67	1.47	1.38
24	c	509	CLA	O2D-CGD	4.67	1.44	1.33
24	C	504	CLA	O2D-CGD	4.66	1.44	1.33
24	c	512	CLA	CHC-C1C	4.66	1.47	1.38
26	Y	101	BCR	C23-C22	-4.66	1.36	1.46
24	c	508	CLA	C1D-ND	4.66	1.44	1.37
24	B	614	CLA	C1D-ND	4.66	1.44	1.37
24	A	407	CLA	O2D-CGD	4.66	1.44	1.33
24	B	612	CLA	CHC-C1C	4.65	1.47	1.38
24	C	504	CLA	CHC-C1C	4.65	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	612	CLA	O2D-CGD	4.65	1.44	1.33
24	b	622	CLA	C1D-ND	4.65	1.44	1.37
24	c	513	CLA	CHC-C1C	4.65	1.47	1.38
24	D	403	CLA	CHC-C1C	4.65	1.47	1.38
24	b	614	CLA	C1D-ND	4.64	1.44	1.37
24	b	625	CLA	O2D-CGD	4.64	1.44	1.33
24	b	620	CLA	C1D-ND	4.64	1.44	1.37
24	B	608	CLA	CHC-C1C	4.64	1.47	1.38
24	b	618	CLA	CHD-C1D	4.64	1.47	1.38
24	B	604	CLA	O2D-CGD	4.63	1.44	1.33
24	b	617	CLA	O2D-CGD	4.63	1.44	1.33
24	B	608	CLA	C1D-ND	4.63	1.43	1.37
24	c	515	CLA	CHC-C1C	4.62	1.47	1.38
24	C	512	CLA	C1D-ND	4.62	1.43	1.37
24	B	607	CLA	CHC-C1C	4.62	1.47	1.38
24	C	507	CLA	O2D-CGD	4.62	1.44	1.33
24	B	605	CLA	O2D-CGD	4.61	1.44	1.33
26	A	411	BCR	C23-C22	-4.61	1.36	1.46
27	a	405	SQD	O48-C23	4.61	1.46	1.33
24	A	407	CLA	CHD-C1D	4.61	1.47	1.38
24	d	403	CLA	C1D-ND	4.60	1.43	1.37
24	b	624	CLA	C1D-ND	4.60	1.43	1.37
24	c	510	CLA	CHC-C1C	4.60	1.47	1.38
24	C	508	CLA	CHC-C1C	4.60	1.47	1.38
24	A	405	CLA	O2D-CGD	4.59	1.44	1.33
25	A	409[B]	PHO	OBD-CAD	4.59	1.28	1.22
24	a	412	CLA	CHC-C1C	4.59	1.47	1.38
24	d	402	CLA	O2D-CGD	4.59	1.44	1.33
26	C	515	BCR	C23-C22	-4.58	1.36	1.46
24	d	403	CLA	CHC-C1C	4.58	1.47	1.38
24	b	617	CLA	CHC-C1C	4.57	1.47	1.38
24	b	612	CLA	CHD-C1D	4.57	1.47	1.38
27	A	416	SQD	O48-C23	4.57	1.46	1.33
24	c	515	CLA	O2D-CGD	4.57	1.44	1.33
24	c	514	CLA	CHC-C1C	4.56	1.47	1.38
24	b	616	CLA	O2D-CGD	4.55	1.44	1.33
24	c	515	CLA	C1D-ND	4.55	1.43	1.37
24	a	409	CLA	CHD-C1D	4.55	1.47	1.38
24	B	611	CLA	CHD-C1D	4.55	1.47	1.38
26	c	518	BCR	C23-C22	-4.54	1.36	1.46
24	c	512	CLA	O2A-CGA	4.54	1.46	1.33
24	B	610	CLA	O2A-CGA	4.54	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C1D-ND	4.54	1.43	1.37
24	b	616	CLA	CHC-C1C	4.54	1.47	1.38
37	D	406	DGD	O1G-C1A	4.53	1.46	1.33
24	b	619	CLA	C1D-ND	4.53	1.43	1.37
24	b	624	CLA	CHC-C1C	4.53	1.47	1.38
24	C	510	CLA	CHD-C1D	4.53	1.47	1.38
24	B	613	CLA	C3C-C2C	4.53	1.46	1.36
26	a	413	BCR	C23-C22	-4.52	1.36	1.46
24	c	511	CLA	CHC-C1C	4.52	1.47	1.38
24	C	511	CLA	C1D-ND	4.51	1.43	1.37
24	C	506	CLA	CHC-C1C	4.51	1.47	1.38
25	A	409[A]	PHO	OBD-CAD	4.50	1.28	1.22
24	C	506	CLA	CHD-C1D	4.50	1.47	1.38
27	f	102	SQD	O47-C7	4.49	1.47	1.34
24	c	516	CLA	C1D-ND	4.49	1.43	1.37
24	B	615	CLA	O2D-CGD	4.49	1.44	1.33
24	c	507	CLA	C1D-ND	4.49	1.43	1.37
24	b	612	CLA	C1D-ND	4.48	1.43	1.37
24	b	613	CLA	CHC-C1C	4.48	1.47	1.38
24	b	623	CLA	CHC-C1C	4.48	1.47	1.38
24	c	508	CLA	CHC-C1C	4.48	1.47	1.38
24	B	617	CLA	C1D-ND	4.47	1.43	1.37
24	c	511	CLA	O2A-CGA	4.46	1.46	1.33
24	b	625	CLA	O2A-CGA	4.46	1.46	1.33
24	C	509	CLA	O2A-CGA	4.46	1.46	1.33
34	z	101	LMG	O8-C28	4.46	1.46	1.33
24	C	503	CLA	O2D-CGD	4.46	1.44	1.33
24	c	505	CLA	CHC-C1C	4.46	1.47	1.38
24	b	625	CLA	CHC-C1C	4.45	1.47	1.38
24	b	621	CLA	CHC-C1C	4.45	1.47	1.38
24	a	410	CLA	C1D-ND	4.45	1.43	1.37
24	b	626	CLA	C1D-ND	4.45	1.43	1.37
27	F	103	SQD	O47-C7	4.44	1.46	1.34
24	B	609	CLA	O2A-CGA	4.44	1.46	1.33
26	B	619	BCR	C23-C22	-4.44	1.36	1.46
34	C	519	LMG	O8-C28	4.43	1.46	1.33
24	c	509	CLA	C1D-ND	4.43	1.43	1.37
24	B	615	CLA	C1D-ND	4.43	1.43	1.37
24	b	619	CLA	CHD-C1D	4.43	1.47	1.38
34	C	520	LMG	O7-C10	4.43	1.46	1.34
24	B	615	CLA	CHC-C1C	4.42	1.47	1.38
26	D	404	BCR	C23-C22	-4.42	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	CHD-C1D	4.42	1.47	1.38
24	b	611	CLA	O2A-CGA	4.42	1.46	1.33
24	B	610	CLA	C1D-ND	4.41	1.43	1.37
24	c	513	CLA	O2A-CGA	4.41	1.46	1.33
25	a	420[A]	PHO	OBD-CAD	4.41	1.28	1.22
24	D	402	CLA	O2D-CGD	4.41	1.44	1.33
24	A	406	CLA	O2D-CGD	4.40	1.44	1.33
24	c	507	CLA	CHD-C1D	4.40	1.47	1.38
24	C	508	CLA	CHD-C1D	4.40	1.47	1.38
24	B	609	CLA	CHD-C1D	4.39	1.47	1.38
24	B	606	CLA	O2A-CGA	4.39	1.46	1.33
37	e	101	DGD	O2G-C1B	4.39	1.46	1.34
41	V	206	HEC	CAB-C3B	4.38	1.49	1.35
24	B	607	CLA	C1D-ND	4.38	1.43	1.37
26	b	627	BCR	C23-C22	-4.38	1.36	1.46
24	b	616	CLA	CHD-C1D	4.38	1.47	1.38
24	c	515	CLA	CHD-C1D	4.37	1.46	1.38
24	c	511	CLA	C1D-ND	4.37	1.43	1.37
27	a	405	SQD	O47-C7	4.37	1.46	1.34
24	c	513	CLA	CHD-C1D	4.36	1.46	1.38
38	E	101	LHG	O8-C23	4.36	1.46	1.33
24	C	511	CLA	CHC-C1C	4.36	1.47	1.38
41	V	206	HEC	CAC-C3C	4.36	1.49	1.35
24	A	405	CLA	C1D-ND	4.35	1.43	1.37
24	A	406	CLA	O2A-CGA	4.35	1.46	1.33
24	B	605	CLA	CHC-C1C	4.35	1.47	1.38
24	C	507	CLA	O2A-CGA	4.35	1.46	1.33
27	B	621	SQD	O47-C7	4.35	1.46	1.34
41	v	205	HEC	CAC-C3C	4.35	1.49	1.35
24	b	626	CLA	O2A-CGA	4.34	1.46	1.33
24	c	516	CLA	O2A-CGA	4.34	1.46	1.33
24	A	407	CLA	C1D-ND	4.33	1.43	1.37
24	b	625	CLA	CHD-C1D	4.33	1.46	1.38
24	c	512	CLA	CHD-C1D	4.33	1.46	1.38
26	B	618	BCR	C23-C22	-4.33	1.36	1.46
24	b	621	CLA	C1D-ND	4.33	1.43	1.37
24	b	626	CLA	CHC-C1C	4.33	1.47	1.38
24	B	603	CLA	C1D-ND	4.32	1.43	1.37
24	c	509	CLA	CHD-C1D	4.32	1.46	1.38
39	e	102	HEM	FE-NC	4.32	2.09	1.95
37	D	406	DGD	O2G-C1B	4.32	1.46	1.34
24	C	506	CLA	O2A-CGA	4.32	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	611	CLA	OBD-CAD	4.32	1.29	1.22
24	C	512	CLA	O2A-CGA	4.31	1.45	1.33
24	B	610	CLA	CHD-C1D	4.31	1.46	1.38
39	F	102	HEM	FE-NC	4.31	2.09	1.95
24	C	511	CLA	CHD-C1D	4.31	1.46	1.38
24	c	514	CLA	CHD-C1D	4.31	1.46	1.38
24	B	617	CLA	O2A-CGA	4.30	1.45	1.33
24	b	611	CLA	CHD-C1D	4.30	1.46	1.38
24	B	617	CLA	CHD-C1D	4.30	1.46	1.38
24	B	609	CLA	CHC-C1C	4.30	1.47	1.38
37	e	101	DGD	O1G-C1A	4.30	1.45	1.33
24	b	614	CLA	CHC-C1C	4.30	1.47	1.38
34	A	422	LMG	O7-C10	4.29	1.46	1.34
24	b	622	CLA	CHD-C1D	4.29	1.46	1.38
34	A	422	LMG	O8-C28	4.29	1.45	1.33
24	B	604	CLA	C1D-ND	4.29	1.43	1.37
24	b	622	CLA	CHC-C1C	4.29	1.47	1.38
24	d	401	CLA	O2A-CGA	4.29	1.45	1.33
24	b	621	CLA	O2A-CGA	4.29	1.45	1.33
27	f	102	SQD	O48-C23	4.29	1.45	1.33
41	v	205	HEC	CBC-CAC	-4.28	1.33	1.49
24	C	511	CLA	O2A-CGA	4.28	1.45	1.33
24	B	612	CLA	C1D-ND	4.28	1.43	1.37
24	C	503	CLA	CHD-C1D	4.28	1.46	1.38
24	C	508	CLA	O2A-CGA	4.28	1.45	1.33
24	C	513	CLA	CHD-C1D	4.28	1.46	1.38
24	B	614	CLA	C3D-C2D	4.28	1.50	1.39
24	B	608	CLA	O2A-CGA	4.27	1.45	1.33
24	A	410	CLA	CHD-C1D	4.27	1.46	1.38
24	c	506	CLA	C1D-ND	4.27	1.43	1.37
24	d	402	CLA	CHD-C1D	4.26	1.46	1.38
24	a	409	CLA	CHD-C4C	4.26	1.48	1.39
24	b	615	CLA	C1D-ND	4.26	1.43	1.37
24	b	613	CLA	O2A-CGA	4.26	1.45	1.33
24	c	510	CLA	CHD-C1D	4.26	1.46	1.38
41	v	205	HEC	CAB-C3B	4.26	1.48	1.35
38	a	422	LHG	O8-C23	4.25	1.45	1.33
24	c	515	CLA	O2A-CGA	4.25	1.45	1.33
34	a	415	LMG	O8-C28	4.25	1.45	1.33
24	C	513	CLA	O2A-CGA	4.25	1.45	1.33
24	a	410	CLA	O2A-CGA	4.25	1.45	1.33
25	a	420[A]	PHO	O2A-CGA	4.25	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	D	409	LHG	O7-C7	4.24	1.46	1.34
24	B	611	CLA	CHC-C1C	4.23	1.47	1.38
24	c	506	CLA	O2A-CGA	4.23	1.45	1.33
34	c	523	LMG	O7-C10	4.23	1.46	1.34
24	d	402	CLA	O2A-CGA	4.23	1.45	1.33
24	D	403	CLA	CHD-C1D	4.22	1.46	1.38
24	C	511	CLA	C3D-C2D	4.22	1.50	1.39
37	h	102	DGD	O1G-C1A	4.22	1.45	1.33
24	C	503	CLA	O2A-CGA	4.22	1.45	1.33
24	c	517	CLA	O2A-CGA	4.22	1.45	1.33
37	c	521	DGD	O1G-C1A	4.22	1.45	1.33
24	C	501	CLA	CHD-C1D	4.22	1.46	1.38
37	C	517	DGD	O1G-C1A	4.22	1.45	1.33
34	c	523	LMG	O8-C28	4.21	1.45	1.33
38	d	408	LHG	O8-C23	4.21	1.45	1.33
27	b	601	SQD	O48-C23	4.21	1.45	1.33
26	b	628	BCR	C23-C22	-4.21	1.36	1.46
24	C	501	CLA	O2A-CGA	4.21	1.45	1.33
24	b	620	CLA	CHD-C1D	4.21	1.46	1.38
24	d	401	CLA	CHD-C1D	4.21	1.46	1.38
24	b	618	CLA	CHD-C4C	4.20	1.48	1.39
24	b	616	CLA	CHD-C4C	4.20	1.48	1.39
27	b	601	SQD	O47-C7	4.20	1.46	1.34
24	c	505	CLA	CHD-C1D	4.20	1.46	1.38
24	C	510	CLA	CHD-C4C	4.20	1.48	1.39
24	B	607	CLA	O2A-CGA	4.20	1.45	1.33
24	B	616	CLA	CHC-C4B	4.20	1.48	1.39
24	C	512	CLA	CHD-C1D	4.19	1.46	1.38
34	j	101	LMG	O7-C10	4.19	1.46	1.34
38	d	408	LHG	O7-C7	4.19	1.46	1.34
37	H	103	DGD	O1G-C1A	4.19	1.45	1.33
24	b	624	CLA	O2A-CGA	4.19	1.45	1.33
24	a	409	CLA	CHC-C1C	4.19	1.46	1.38
24	c	507	CLA	O2A-CGA	4.19	1.45	1.33
34	B	622	LMG	O8-C28	4.18	1.45	1.33
41	V	206	HEC	CBC-CAC	-4.18	1.34	1.49
24	d	401	CLA	CHC-C1C	4.18	1.46	1.38
24	C	505	CLA	C1D-ND	4.18	1.43	1.37
34	b	630	LMG	O8-C28	4.18	1.45	1.33
24	b	615	CLA	CHD-C1D	4.17	1.46	1.38
24	B	610	CLA	C3D-C2D	4.17	1.50	1.39
24	A	410	CLA	CHC-C4B	4.17	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	a	414	SQD	O48-C23	4.17	1.45	1.33
34	C	520	LMG	O8-C28	4.17	1.45	1.33
24	a	412	CLA	CHD-C1D	4.16	1.46	1.38
24	B	608	CLA	CHD-C1D	4.15	1.46	1.38
38	l	101	LHG	O8-C23	4.15	1.45	1.33
24	b	612	CLA	O2A-CGA	4.15	1.45	1.33
24	a	410	CLA	CHD-C1D	4.15	1.46	1.38
24	b	618	CLA	O2A-CGA	4.15	1.45	1.33
24	C	510	CLA	O2A-CGA	4.15	1.45	1.33
24	b	614	CLA	CHB-C1B	4.15	1.48	1.39
24	c	505	CLA	O2A-CGA	4.14	1.45	1.33
24	C	507	CLA	CHD-C1D	4.14	1.46	1.38
24	B	611	CLA	C3D-C2D	4.14	1.50	1.39
34	c	522	LMG	O8-C28	4.14	1.45	1.33
24	B	613	CLA	C1B-NB	-4.14	1.32	1.37
24	d	403	CLA	O2A-CGA	4.13	1.45	1.33
38	E	101	LHG	O7-C7	4.13	1.46	1.34
24	c	507	CLA	OBD-CAD	4.13	1.29	1.22
24	C	503	CLA	CHD-C4C	4.13	1.48	1.39
24	C	502	CLA	CHD-C1D	4.13	1.46	1.38
24	B	613	CLA	O2A-CGA	4.12	1.45	1.33
25	A	409[A]	PHO	O2A-CGA	4.12	1.45	1.33
37	c	520	DGD	O1G-C1A	4.12	1.45	1.33
25	A	408	PHO	O2A-CGA	4.12	1.45	1.33
24	B	602	CLA	CHD-C1D	4.12	1.46	1.38
27	F	103	SQD	O48-C23	4.12	1.45	1.33
24	b	613	CLA	CHD-C1D	4.12	1.46	1.38
27	B	621	SQD	O48-C23	4.12	1.45	1.33
24	C	509	CLA	CHD-C1D	4.11	1.46	1.38
24	d	401	CLA	CHB-C1B	4.11	1.48	1.39
38	L	101	LHG	O8-C23	4.11	1.45	1.33
24	c	512	CLA	C3D-C2D	4.11	1.50	1.39
24	B	611	CLA	CHD-C4C	4.11	1.48	1.39
24	C	505	CLA	CHD-C4C	4.11	1.48	1.39
24	b	617	CLA	CHC-C4B	4.11	1.48	1.39
38	a	422	LHG	O7-C7	4.11	1.45	1.34
24	B	616	CLA	O2A-CGA	4.11	1.45	1.33
34	Z	101	LMG	O7-C10	4.10	1.45	1.34
24	C	509	CLA	CHD-C4C	4.10	1.48	1.39
24	C	505	CLA	CHD-C1D	4.10	1.46	1.38
24	c	508	CLA	CHD-C1D	4.10	1.46	1.38
24	B	608	CLA	CHC-C4B	4.10	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	CHD-C1D	4.10	1.46	1.38
24	C	511	CLA	CHD-C4C	4.09	1.48	1.39
24	b	623	CLA	CHD-C4C	4.09	1.48	1.39
24	b	616	CLA	O2A-CGA	4.09	1.45	1.33
37	C	516	DGD	O1G-C1A	4.09	1.45	1.33
24	B	603	CLA	OBD-CAD	4.09	1.29	1.22
24	c	505	CLA	C3D-C2D	4.08	1.50	1.39
24	b	618	CLA	CHB-C1B	4.08	1.48	1.39
24	B	604	CLA	CHD-C1D	4.08	1.46	1.38
24	c	511	CLA	CHD-C1D	4.07	1.46	1.38
24	b	626	CLA	CHD-C1D	4.07	1.46	1.38
24	c	516	CLA	CHD-C1D	4.07	1.46	1.38
25	a	420[B]	PHO	O2A-CGA	4.07	1.45	1.33
24	C	504	CLA	CHD-C1D	4.07	1.46	1.38
24	A	410	CLA	O2A-CGA	4.07	1.45	1.33
24	C	506	CLA	CHD-C4C	4.07	1.48	1.39
24	B	604	CLA	O2A-CGA	4.06	1.45	1.33
24	b	626	CLA	C3D-C2D	4.06	1.50	1.39
24	c	517	CLA	CHD-C1D	4.06	1.46	1.38
24	D	402	CLA	CHC-C1C	4.06	1.46	1.38
24	c	506	CLA	C3D-C2D	4.06	1.50	1.39
24	C	504	CLA	O2A-CGA	4.06	1.45	1.33
24	B	614	CLA	CHC-C1C	4.06	1.46	1.38
24	C	510	CLA	CHB-C1B	4.06	1.48	1.39
37	C	518	DGD	O1G-C1A	4.06	1.45	1.33
24	b	611	CLA	C3D-C2D	4.05	1.50	1.39
24	A	406	CLA	C3D-C2D	4.05	1.50	1.39
24	b	619	CLA	O2A-CGA	4.05	1.45	1.33
34	c	522	LMG	O7-C10	4.05	1.45	1.34
24	C	512	CLA	C3D-C2D	4.05	1.50	1.39
24	b	619	CLA	CHD-C4C	4.05	1.48	1.39
24	A	410	CLA	CHB-C1B	4.05	1.48	1.39
24	b	614	CLA	O2A-CGA	4.05	1.45	1.33
34	D	412	LMG	O8-C28	4.05	1.45	1.33
24	B	608	CLA	CHD-C4C	4.05	1.48	1.39
24	c	517	CLA	CHD-C4C	4.05	1.48	1.39
24	D	402	CLA	C1D-ND	4.04	1.43	1.37
24	A	405	CLA	CHD-C4C	4.04	1.48	1.39
24	c	514	CLA	CHD-C4C	4.04	1.48	1.39
24	B	615	CLA	CHB-C1B	4.04	1.48	1.39
37	h	102	DGD	O2G-C1B	4.04	1.45	1.34
24	c	510	CLA	CHD-C4C	4.03	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	519	LMG	O7-C10	4.03	1.45	1.34
25	A	409[B]	PHO	O2A-CGA	4.03	1.45	1.33
24	b	622	CLA	C3D-C2D	4.03	1.50	1.39
24	d	403	CLA	CHC-C4B	4.03	1.48	1.39
37	C	516	DGD	O2G-C1B	4.03	1.45	1.34
24	c	513	CLA	CHB-C1B	4.03	1.48	1.39
24	B	603	CLA	O2A-CGA	4.03	1.45	1.33
24	c	516	CLA	C3D-C2D	4.03	1.50	1.39
34	j	101	LMG	O8-C28	4.03	1.45	1.33
24	C	513	CLA	CHD-C4C	4.02	1.48	1.39
24	b	617	CLA	C1D-ND	4.02	1.43	1.37
24	C	504	CLA	C3D-C2D	4.02	1.50	1.39
24	C	503	CLA	CHC-C4B	4.02	1.48	1.39
24	b	618	CLA	OBD-CAD	4.02	1.29	1.22
34	B	622	LMG	O7-C10	4.01	1.45	1.34
24	b	620	CLA	O2A-CGA	4.01	1.45	1.33
37	c	521	DGD	O2G-C1B	4.01	1.45	1.34
24	c	513	CLA	CHD-C4C	4.01	1.48	1.39
24	b	626	CLA	CHB-C1B	4.01	1.48	1.39
24	a	412	CLA	O2A-CGA	4.01	1.45	1.33
24	C	501	CLA	CHD-C4C	4.01	1.48	1.39
24	C	506	CLA	C3D-C2D	4.00	1.49	1.39
24	D	402	CLA	O2A-CGA	4.00	1.45	1.33
24	c	514	CLA	CHB-C1B	4.00	1.48	1.39
24	b	620	CLA	OBD-CAD	4.00	1.29	1.22
24	B	614	CLA	CHD-C1D	4.00	1.46	1.38
24	C	509	CLA	CHB-C1B	4.00	1.48	1.39
24	B	607	CLA	CHD-C4C	3.99	1.48	1.39
24	c	506	CLA	CHD-C1D	3.99	1.46	1.38
34	z	101	LMG	O7-C10	3.99	1.45	1.34
24	c	510	CLA	O2A-CGA	3.99	1.45	1.33
41	v	205	HEC	CBB-CAB	-3.99	1.34	1.49
24	B	613	CLA	CHD-C1D	3.99	1.46	1.38
24	c	511	CLA	C3D-C2D	3.99	1.49	1.39
24	B	612	CLA	CHD-C1D	3.98	1.46	1.38
24	b	614	CLA	CHD-C1D	3.98	1.46	1.38
24	D	402	CLA	CHD-C1D	3.98	1.46	1.38
27	A	416	SQD	O47-C7	3.98	1.45	1.34
24	C	512	CLA	CHD-C4C	3.97	1.48	1.39
24	C	504	CLA	CHD-C4C	3.97	1.48	1.39
37	C	518	DGD	O2G-C1B	3.97	1.45	1.34
24	c	509	CLA	CHB-C1B	3.97	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	D	409	LHG	O8-C23	3.97	1.44	1.33
24	B	613	CLA	CHC-C4B	3.97	1.48	1.39
24	D	403	CLA	O2A-CGA	3.97	1.44	1.33
24	C	505	CLA	O2A-CGA	3.97	1.44	1.33
24	c	508	CLA	CHD-C4C	3.97	1.48	1.39
24	a	410	CLA	OBD-CAD	3.96	1.29	1.22
27	a	414	SQD	O47-C7	3.96	1.45	1.34
24	b	625	CLA	C3D-C2D	3.96	1.49	1.39
24	B	612	CLA	CHC-C4B	3.96	1.48	1.39
27	A	412	SQD	O48-C23	3.96	1.44	1.33
24	B	606	CLA	CHC-C4B	3.96	1.48	1.39
24	B	603	CLA	CHD-C1D	3.95	1.46	1.38
24	D	403	CLA	CHD-C4C	3.95	1.48	1.39
24	A	406	CLA	CHC-C1C	3.95	1.46	1.38
24	A	405	CLA	C3D-C2D	3.95	1.49	1.39
41	V	206	HEC	CBB-CAB	-3.94	1.34	1.49
24	b	624	CLA	C3D-C2D	3.94	1.49	1.39
24	a	412	CLA	OBD-CAD	3.94	1.29	1.22
24	b	624	CLA	CHD-C4C	3.94	1.48	1.39
24	C	509	CLA	C3D-C2D	3.94	1.49	1.39
24	A	407	CLA	O2A-CGA	3.93	1.44	1.33
24	B	610	CLA	OBD-CAD	3.93	1.29	1.22
24	C	507	CLA	C3D-C2D	3.93	1.49	1.39
24	a	412	CLA	CHD-C4C	3.93	1.48	1.39
38	d	407	LHG	O7-C7	3.93	1.45	1.34
24	B	609	CLA	C3D-C2D	3.93	1.49	1.39
34	b	630	LMG	O7-C10	3.93	1.45	1.34
24	B	613	CLA	C1D-ND	3.93	1.43	1.37
24	C	509	CLA	OBD-CAD	3.93	1.29	1.22
24	d	402	CLA	C1D-ND	3.93	1.43	1.37
24	B	606	CLA	C3D-C2D	3.93	1.49	1.39
24	C	503	CLA	C3D-C2D	3.93	1.49	1.39
24	b	615	CLA	O2A-CGA	3.92	1.44	1.33
24	d	402	CLA	CHD-C4C	3.92	1.48	1.39
24	C	502	CLA	C3D-C2D	3.92	1.49	1.39
24	C	508	CLA	CHD-C4C	3.92	1.48	1.39
38	D	408	LHG	O7-C7	3.92	1.45	1.34
24	c	508	CLA	O2A-CGA	3.92	1.44	1.33
24	c	514	CLA	OBD-CAD	3.92	1.29	1.22
24	b	618	CLA	CHC-C4B	3.92	1.48	1.39
38	d	407	LHG	O8-C23	3.92	1.44	1.33
24	d	401	CLA	CHD-C4C	3.92	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	l	101	LHG	O7-C7	3.92	1.45	1.34
24	B	602	CLA	C3D-C2D	3.91	1.49	1.39
34	a	415	LMG	O7-C10	3.91	1.45	1.34
24	B	605	CLA	CHB-C1B	3.91	1.48	1.39
24	A	407	CLA	CHD-C4C	3.91	1.48	1.39
24	B	615	CLA	O2A-CGA	3.91	1.44	1.33
24	d	403	CLA	CHB-C1B	3.91	1.48	1.39
24	d	401	CLA	C3D-C2D	3.91	1.49	1.39
24	b	623	CLA	CHD-C1D	3.90	1.46	1.38
24	b	611	CLA	CHD-C4C	3.90	1.48	1.39
24	b	621	CLA	CHD-C1D	3.90	1.46	1.38
24	c	507	CLA	CHC-C4B	3.90	1.48	1.39
24	C	506	CLA	CHB-C1B	3.90	1.48	1.39
34	D	412	LMG	O7-C10	3.90	1.45	1.34
24	b	622	CLA	CHB-C1B	3.90	1.48	1.39
37	H	103	DGD	O2G-C1B	3.90	1.45	1.34
24	c	508	CLA	C3D-C2D	3.90	1.49	1.39
24	b	612	CLA	OBD-CAD	3.89	1.29	1.22
24	B	613	CLA	CHB-C1B	3.89	1.48	1.39
24	A	405	CLA	O2A-CGA	3.89	1.44	1.33
24	c	517	CLA	CHC-C4B	3.89	1.48	1.39
24	B	604	CLA	CHD-C4C	3.89	1.48	1.39
24	b	613	CLA	C1D-ND	3.89	1.43	1.37
24	c	509	CLA	CHD-C4C	3.89	1.48	1.39
24	a	412	CLA	CHB-C1B	3.89	1.48	1.39
24	B	612	CLA	CHB-C1B	3.88	1.48	1.39
24	c	513	CLA	C3D-C2D	3.88	1.49	1.39
24	C	505	CLA	CHC-C4B	3.88	1.48	1.39
24	b	620	CLA	C3D-C2D	3.88	1.49	1.39
24	C	513	CLA	C3D-C2D	3.88	1.49	1.39
24	B	609	CLA	CHD-C4C	3.88	1.48	1.39
24	b	619	CLA	C3D-C2D	3.88	1.49	1.39
24	c	516	CLA	CHD-C4C	3.88	1.48	1.39
24	C	501	CLA	CHC-C4B	3.88	1.48	1.39
24	B	604	CLA	CHC-C4B	3.88	1.48	1.39
24	c	514	CLA	O2A-CGA	3.87	1.44	1.33
24	b	625	CLA	CHD-C4C	3.87	1.48	1.39
37	c	520	DGD	O2G-C1B	3.87	1.45	1.34
24	b	615	CLA	CHB-C1B	3.87	1.48	1.39
24	b	612	CLA	CHD-C4C	3.87	1.48	1.39
24	C	508	CLA	C3D-C2D	3.87	1.49	1.39
24	C	511	CLA	CHB-C1B	3.86	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	L	101	LHG	O7-C7	3.86	1.45	1.34
24	b	612	CLA	C3D-C2D	3.86	1.49	1.39
24	b	620	CLA	CHD-C4C	3.86	1.48	1.39
24	A	407	CLA	CHC-C4B	3.86	1.48	1.39
24	d	402	CLA	CHB-C1B	3.86	1.48	1.39
24	B	610	CLA	CHD-C4C	3.86	1.48	1.39
38	D	407	LHG	O8-C23	3.86	1.44	1.33
24	C	502	CLA	O2A-CGA	3.85	1.44	1.33
24	b	619	CLA	CHB-C1B	3.85	1.48	1.39
24	b	621	CLA	CHB-C1B	3.85	1.48	1.39
24	d	402	CLA	C3D-C2D	3.85	1.49	1.39
24	B	615	CLA	CHD-C1D	3.85	1.45	1.38
24	B	603	CLA	CHD-C4C	3.84	1.48	1.39
24	B	602	CLA	CHB-C1B	3.84	1.48	1.39
24	c	515	CLA	CHD-C4C	3.84	1.47	1.39
24	C	502	CLA	CHD-C4C	3.84	1.47	1.39
24	C	513	CLA	CHC-C4B	3.84	1.48	1.39
24	b	618	CLA	C3D-C2D	3.84	1.49	1.39
24	b	623	CLA	CHB-C1B	3.84	1.48	1.39
24	c	508	CLA	CHB-C1B	3.83	1.48	1.39
24	a	412	CLA	C3D-C2D	3.83	1.49	1.39
24	B	604	CLA	C3D-C2D	3.83	1.49	1.39
24	C	509	CLA	CHC-C4B	3.83	1.48	1.39
24	c	516	CLA	CHC-C4B	3.83	1.48	1.39
24	C	507	CLA	CHC-C4B	3.83	1.48	1.39
24	C	511	CLA	OBD-CAD	3.83	1.29	1.22
24	c	509	CLA	O2A-CGA	3.83	1.44	1.33
24	b	617	CLA	CHD-C1D	3.83	1.45	1.38
27	A	412	SQD	O47-C7	3.82	1.45	1.34
24	c	506	CLA	CHD-C4C	3.82	1.47	1.39
37	c	519	DGD	O1G-C1A	3.82	1.44	1.33
24	D	403	CLA	CHB-C1B	3.81	1.48	1.39
24	d	401	CLA	OBD-CAD	3.81	1.29	1.22
24	C	510	CLA	C3D-C2D	3.81	1.49	1.39
24	a	410	CLA	CHD-C4C	3.81	1.47	1.39
24	c	505	CLA	CHD-C4C	3.81	1.47	1.39
24	B	605	CLA	CHD-C1D	3.81	1.45	1.38
24	B	614	CLA	O2A-CGA	3.81	1.44	1.33
24	b	619	CLA	OBD-CAD	3.81	1.29	1.22
24	B	612	CLA	C3D-C2D	3.81	1.49	1.39
24	C	501	CLA	C3D-C2D	3.81	1.49	1.39
24	C	505	CLA	CHB-C1B	3.80	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	CHD-C1D	3.80	1.45	1.38
24	A	406	CLA	CHD-C4C	3.80	1.47	1.39
24	c	513	CLA	OBD-CAD	3.80	1.29	1.22
24	B	606	CLA	CHD-C1D	3.80	1.45	1.38
24	B	615	CLA	C3D-C2D	3.80	1.49	1.39
24	B	615	CLA	CHD-C4C	3.80	1.47	1.39
24	b	623	CLA	O2A-CGA	3.80	1.44	1.33
24	C	507	CLA	CHD-C4C	3.80	1.47	1.39
24	C	504	CLA	CHB-C1B	3.80	1.47	1.39
24	b	624	CLA	CHD-C1D	3.80	1.45	1.38
24	B	604	CLA	C1B-NB	-3.79	1.32	1.37
24	D	402	CLA	CHB-C1B	3.79	1.47	1.39
24	c	511	CLA	CHD-C4C	3.79	1.47	1.39
24	c	505	CLA	CHB-C1B	3.79	1.47	1.39
24	b	622	CLA	O2A-CGA	3.79	1.44	1.33
24	c	515	CLA	C3D-C2D	3.79	1.49	1.39
24	b	615	CLA	C3D-C2D	3.79	1.49	1.39
24	b	623	CLA	C3D-C2D	3.79	1.49	1.39
24	B	606	CLA	OBD-CAD	3.79	1.29	1.22
24	b	626	CLA	CHD-C4C	3.79	1.47	1.39
24	b	617	CLA	CHD-C4C	3.79	1.47	1.39
24	A	410	CLA	C3D-C2D	3.79	1.49	1.39
24	A	410	CLA	OBD-CAD	3.78	1.29	1.22
24	D	403	CLA	C3D-C2D	3.78	1.49	1.39
24	b	616	CLA	C3D-C2D	3.78	1.49	1.39
24	c	507	CLA	CHD-C4C	3.78	1.47	1.39
24	b	620	CLA	CHC-C4B	3.78	1.47	1.39
24	a	409	CLA	OBD-CAD	3.78	1.29	1.22
24	B	603	CLA	C3D-C2D	3.78	1.49	1.39
24	c	517	CLA	C3D-C2D	3.77	1.49	1.39
24	C	512	CLA	CHB-C1B	3.77	1.47	1.39
24	c	512	CLA	CHD-C4C	3.77	1.47	1.39
24	B	602	CLA	CHD-C4C	3.76	1.47	1.39
24	B	617	CLA	C3D-C2D	3.76	1.49	1.39
24	B	606	CLA	CHD-C4C	3.76	1.47	1.39
24	B	617	CLA	CHC-C4B	3.76	1.47	1.39
38	d	406	LHG	O8-C23	3.76	1.44	1.33
24	D	402	CLA	CHD-C4C	3.75	1.47	1.39
24	c	511	CLA	CHB-C1B	3.75	1.47	1.39
24	B	610	CLA	CHB-C1B	3.75	1.47	1.39
24	c	516	CLA	OBD-CAD	3.75	1.28	1.22
24	A	410	CLA	CHD-C4C	3.75	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	CHC-C4B	3.75	1.47	1.39
24	b	615	CLA	CHC-C4B	3.75	1.47	1.39
24	C	508	CLA	OBD-CAD	3.74	1.28	1.22
24	b	615	CLA	CHD-C4C	3.74	1.47	1.39
24	B	613	CLA	OBD-CAD	3.73	1.28	1.22
24	B	611	CLA	O2A-CGA	3.73	1.44	1.33
38	D	408	LHG	O8-C23	3.73	1.44	1.33
24	c	515	CLA	CHB-C1B	3.73	1.47	1.39
24	C	504	CLA	OBD-CAD	3.73	1.28	1.22
37	c	519	DGD	O2G-C1B	3.73	1.44	1.34
24	c	510	CLA	C3D-C2D	3.73	1.49	1.39
24	b	625	CLA	OBD-CAD	3.73	1.28	1.22
24	B	611	CLA	CHB-C1B	3.72	1.47	1.39
24	A	406	CLA	CHD-C1D	3.72	1.45	1.38
37	C	517	DGD	O2G-C1B	3.72	1.44	1.34
24	B	609	CLA	CHB-C1B	3.72	1.47	1.39
36	b	633	HTG	C1'-S1	-3.72	1.76	1.81
24	b	616	CLA	CHB-C1B	3.72	1.47	1.39
24	C	512	CLA	OBD-CAD	3.72	1.28	1.22
24	B	617	CLA	CHB-C1B	3.71	1.47	1.39
24	b	617	CLA	O2A-CGA	3.71	1.44	1.33
24	B	616	CLA	CHD-C1D	3.71	1.45	1.38
24	B	602	CLA	OBD-CAD	3.71	1.28	1.22
24	b	613	CLA	C3D-C2D	3.71	1.49	1.39
24	b	622	CLA	CHD-C4C	3.70	1.47	1.39
24	c	509	CLA	OBD-CAD	3.70	1.28	1.22
24	B	616	CLA	OBD-CAD	3.70	1.28	1.22
24	b	614	CLA	CHC-C4B	3.70	1.47	1.39
24	b	613	CLA	CHC-C4B	3.69	1.47	1.39
24	B	609	CLA	C4B-NB	-3.69	1.33	1.37
24	a	412	CLA	CHC-C4B	3.69	1.47	1.39
24	c	507	CLA	C3D-C2D	3.69	1.49	1.39
24	C	502	CLA	CHB-C1B	3.69	1.47	1.39
24	c	509	CLA	C3D-C2D	3.69	1.49	1.39
24	c	512	CLA	CHB-C1B	3.69	1.47	1.39
24	B	615	CLA	CHC-C4B	3.69	1.47	1.39
24	b	613	CLA	OBD-CAD	3.68	1.28	1.22
24	b	617	CLA	CHB-C1B	3.68	1.47	1.39
24	B	604	CLA	OBD-CAD	3.68	1.28	1.22
24	b	620	CLA	CHB-C1B	3.68	1.47	1.39
24	d	403	CLA	CHD-C4C	3.68	1.47	1.39
24	c	510	CLA	CHB-C1B	3.67	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	CHC-C4B	3.67	1.47	1.39
24	A	407	CLA	C3D-C2D	3.67	1.49	1.39
24	d	403	CLA	C3D-C2D	3.67	1.49	1.39
24	C	512	CLA	CHC-C4B	3.67	1.47	1.39
24	B	611	CLA	CHC-C4B	3.67	1.47	1.39
24	b	611	CLA	CHC-C4B	3.66	1.47	1.39
24	b	614	CLA	C3D-C2D	3.66	1.49	1.39
24	b	621	CLA	C3D-C2D	3.66	1.49	1.39
24	D	402	CLA	C3D-C2D	3.66	1.49	1.39
24	b	624	CLA	CHB-C1B	3.66	1.47	1.39
24	d	403	CLA	OBD-CAD	3.66	1.28	1.22
24	B	604	CLA	CHB-C1B	3.66	1.47	1.39
24	B	615	CLA	OBD-CAD	3.66	1.28	1.22
24	b	626	CLA	OBD-CAD	3.65	1.28	1.22
24	D	403	CLA	OBD-CAD	3.64	1.28	1.22
24	B	609	CLA	OBD-CAD	3.64	1.28	1.22
24	b	625	CLA	CHB-C1B	3.64	1.47	1.39
24	b	621	CLA	CHD-C4C	3.64	1.47	1.39
24	B	614	CLA	OBD-CAD	3.63	1.28	1.22
24	b	624	CLA	OBD-CAD	3.63	1.28	1.22
24	a	410	CLA	C3D-C2D	3.63	1.48	1.39
24	c	514	CLA	C3D-C2D	3.63	1.48	1.39
24	b	621	CLA	CHC-C4B	3.63	1.47	1.39
24	c	515	CLA	OBD-CAD	3.62	1.28	1.22
24	C	502	CLA	CHC-C4B	3.62	1.47	1.39
24	d	402	CLA	C1B-NB	-3.62	1.33	1.37
24	B	605	CLA	O2A-CGA	3.62	1.43	1.33
24	b	613	CLA	CHD-C4C	3.61	1.47	1.39
24	c	506	CLA	CHC-C4B	3.61	1.47	1.39
24	B	612	CLA	O2A-CGA	3.61	1.43	1.33
24	C	501	CLA	OBD-CAD	3.61	1.28	1.22
24	C	510	CLA	CHC-C4B	3.61	1.47	1.39
24	B	610	CLA	CHC-C4B	3.61	1.47	1.39
24	B	614	CLA	CHB-C1B	3.61	1.47	1.39
24	b	622	CLA	CHC-C4B	3.61	1.47	1.39
24	b	615	CLA	OBD-CAD	3.61	1.28	1.22
24	d	402	CLA	OBD-CAD	3.61	1.28	1.22
24	a	410	CLA	CHB-C1B	3.60	1.47	1.39
24	b	617	CLA	C3D-C2D	3.59	1.48	1.39
24	B	612	CLA	CHD-C4C	3.59	1.47	1.39
24	A	405	CLA	CHC-C4B	3.59	1.47	1.39
24	c	506	CLA	CHB-C1B	3.59	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	507	CLA	CHB-C1B	3.59	1.47	1.39
24	c	511	CLA	OBD-CAD	3.59	1.28	1.22
24	B	607	CLA	C1B-NB	-3.59	1.33	1.37
24	B	608	CLA	CHB-C1B	3.59	1.47	1.39
24	a	409	CLA	CHB-C1B	3.58	1.47	1.39
24	B	607	CLA	C3D-C2D	3.58	1.48	1.39
24	B	608	CLA	C3D-C2D	3.58	1.48	1.39
24	b	617	CLA	C1B-NB	-3.58	1.33	1.37
24	B	603	CLA	CHC-C4B	3.58	1.47	1.39
24	B	613	CLA	C3D-C2D	3.58	1.48	1.39
24	b	611	CLA	OBD-CAD	3.57	1.28	1.22
24	b	616	CLA	OBD-CAD	3.57	1.28	1.22
24	c	509	CLA	CHC-C4B	3.56	1.47	1.39
24	B	616	CLA	CHD-C4C	3.55	1.47	1.39
24	A	406	CLA	CHB-C1B	3.55	1.47	1.39
36	B	632	HTG	C1'-S1	-3.55	1.76	1.81
24	c	512	CLA	OBD-CAD	3.54	1.28	1.22
24	b	613	CLA	CHB-C1B	3.54	1.47	1.39
24	B	614	CLA	CHD-C4C	3.53	1.47	1.39
24	c	513	CLA	CHC-C4B	3.53	1.47	1.39
24	d	402	CLA	CHC-C4B	3.53	1.47	1.39
24	c	508	CLA	CHC-C4B	3.52	1.47	1.39
24	b	612	CLA	CHC-C4B	3.52	1.47	1.39
24	B	616	CLA	CHB-C1B	3.52	1.47	1.39
38	D	407	LHG	O7-C7	3.52	1.44	1.34
24	B	617	CLA	OBD-CAD	3.52	1.28	1.22
24	a	409	CLA	CHC-C4B	3.52	1.47	1.39
24	b	619	CLA	CHC-C4B	3.52	1.47	1.39
24	C	501	CLA	CHB-C1B	3.52	1.47	1.39
24	B	617	CLA	CHD-C4C	3.52	1.47	1.39
24	B	607	CLA	CHB-C1B	3.51	1.47	1.39
24	b	614	CLA	CHD-C4C	3.51	1.47	1.39
24	D	402	CLA	CHC-C4B	3.51	1.47	1.39
38	d	406	LHG	O7-C7	3.51	1.44	1.34
24	C	504	CLA	C1B-NB	-3.50	1.33	1.37
24	D	403	CLA	CHC-C4B	3.50	1.47	1.39
24	B	605	CLA	CHC-C4B	3.50	1.47	1.39
24	C	507	CLA	CHB-C1B	3.50	1.47	1.39
24	C	503	CLA	OBD-CAD	3.50	1.28	1.22
24	B	605	CLA	CHD-C4C	3.50	1.47	1.39
24	A	407	CLA	OBD-CAD	3.50	1.28	1.22
24	b	626	CLA	CHC-C4B	3.50	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	OBD-CAD	3.49	1.28	1.22
24	B	616	CLA	C3D-C2D	3.49	1.48	1.39
24	c	506	CLA	OBD-CAD	3.49	1.28	1.22
24	b	622	CLA	OBD-CAD	3.49	1.28	1.22
24	a	409	CLA	O2A-CGA	3.49	1.43	1.33
36	B	623	HTG	C1'-S1	-3.48	1.76	1.81
24	B	603	CLA	CHB-C1B	3.48	1.47	1.39
24	B	607	CLA	CHC-C4B	3.47	1.47	1.39
24	b	625	CLA	CHC-C4B	3.47	1.47	1.39
24	C	503	CLA	CHB-C1B	3.46	1.47	1.39
24	C	510	CLA	OBD-CAD	3.46	1.28	1.22
24	c	508	CLA	C1B-NB	-3.46	1.33	1.37
24	b	611	CLA	CHB-C1B	3.46	1.47	1.39
24	c	510	CLA	CHC-C4B	3.46	1.47	1.39
24	b	612	CLA	CHB-C1B	3.46	1.47	1.39
24	C	513	CLA	CHB-C1B	3.46	1.47	1.39
24	C	505	CLA	C3D-C2D	3.45	1.48	1.39
39	e	102	HEM	C4D-ND	-3.44	1.34	1.40
24	a	409	CLA	C3D-C2D	3.44	1.48	1.39
24	b	621	CLA	OBD-CAD	3.43	1.28	1.22
24	D	402	CLA	C1B-NB	-3.43	1.33	1.37
24	b	616	CLA	CHC-C4B	3.43	1.47	1.39
24	B	612	CLA	OBD-CAD	3.41	1.28	1.22
24	c	517	CLA	OBD-CAD	3.40	1.28	1.22
24	b	614	CLA	OBD-CAD	3.40	1.28	1.22
36	B	625	HTG	C1'-S1	-3.40	1.76	1.81
24	C	508	CLA	CHB-C1B	3.40	1.47	1.39
24	B	614	CLA	CHC-C4B	3.39	1.47	1.39
25	a	411	PHO	O2A-CGA	3.39	1.43	1.33
24	C	513	CLA	OBD-CAD	3.39	1.28	1.22
24	B	611	CLA	C4B-NB	-3.38	1.33	1.37
24	c	512	CLA	CHC-C4B	3.38	1.47	1.39
24	d	401	CLA	CHC-C4B	3.37	1.47	1.39
39	F	102	HEM	C4D-ND	-3.37	1.34	1.40
24	A	406	CLA	C1B-NB	-3.37	1.33	1.37
24	c	510	CLA	C1B-NB	-3.37	1.33	1.37
24	b	614	CLA	C1B-NB	-3.36	1.33	1.37
36	V	207	HTG	C1'-S1	-3.36	1.76	1.81
24	c	517	CLA	CHB-C1B	3.36	1.47	1.39
24	B	607	CLA	OBD-CAD	3.36	1.28	1.22
36	b	609	HTG	C1'-S1	-3.36	1.76	1.81
24	C	504	CLA	CHC-C4B	3.36	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	C1B-NB	-3.35	1.33	1.37
24	C	508	CLA	CHC-C4B	3.35	1.46	1.39
24	B	606	CLA	CHB-C1B	3.35	1.46	1.39
24	c	505	CLA	C1B-NB	-3.34	1.33	1.37
24	c	516	CLA	CHB-C1B	3.34	1.46	1.39
36	b	608	HTG	C1'-S1	-3.34	1.76	1.81
24	a	412	CLA	C4B-NB	-3.33	1.33	1.37
24	c	505	CLA	OBD-CAD	3.33	1.28	1.22
24	c	510	CLA	OBD-CAD	3.33	1.28	1.22
24	b	624	CLA	C1B-NB	-3.33	1.33	1.37
24	c	514	CLA	CHC-C4B	3.31	1.46	1.39
24	C	506	CLA	CHC-C4B	3.31	1.46	1.39
24	c	508	CLA	OBD-CAD	3.30	1.28	1.22
24	b	624	CLA	CHC-C4B	3.30	1.46	1.39
24	A	406	CLA	CHC-C4B	3.30	1.46	1.39
36	d	411	HTG	C1'-S1	-3.29	1.76	1.81
24	D	402	CLA	OBD-CAD	3.29	1.28	1.22
24	B	605	CLA	C1B-NB	-3.28	1.33	1.37
24	b	622	CLA	C1B-NB	-3.28	1.33	1.37
24	B	613	CLA	C1C-C2C	3.28	1.51	1.44
24	b	617	CLA	OBD-CAD	3.27	1.28	1.22
41	V	206	HEC	C4D-ND	-3.26	1.33	1.39
24	B	613	CLA	CHD-C4C	3.25	1.46	1.39
36	c	524	HTG	C1'-S1	-3.25	1.76	1.81
36	C	523	HTG	C1'-S1	-3.25	1.76	1.81
24	A	406	CLA	OBD-CAD	3.25	1.28	1.22
24	B	609	CLA	CHC-C4B	3.24	1.46	1.39
24	A	407	CLA	CHB-C1B	3.24	1.46	1.39
36	B	633	HTG	C1'-S1	-3.24	1.76	1.81
24	a	410	CLA	C1B-NB	-3.23	1.33	1.37
24	b	623	CLA	CHC-C4B	3.23	1.46	1.39
24	C	507	CLA	OBD-CAD	3.23	1.28	1.22
24	B	608	CLA	OBD-CAD	3.22	1.28	1.22
24	c	505	CLA	CHC-C4B	3.22	1.46	1.39
24	B	605	CLA	C3D-C2D	3.22	1.47	1.39
24	C	502	CLA	OBD-CAD	3.22	1.28	1.22
24	c	515	CLA	CHC-C4B	3.21	1.46	1.39
24	B	616	CLA	C1B-NB	-3.21	1.33	1.37
24	b	616	CLA	C1B-NB	-3.21	1.33	1.37
36	c	525	HTG	C1'-S1	-3.20	1.76	1.81
24	C	508	CLA	C1B-NB	-3.20	1.33	1.37
24	C	505	CLA	C1B-NB	-3.20	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	623	CLA	OBD-CAD	3.20	1.28	1.22
36	H	101	HTG	C1'-S1	-3.19	1.76	1.81
24	C	506	CLA	OBD-CAD	3.19	1.28	1.22
24	b	615	CLA	C1B-NB	-3.18	1.33	1.37
39	e	102	HEM	C1B-NB	-3.18	1.34	1.40
24	a	410	CLA	CHC-C4B	3.17	1.46	1.39
24	B	603	CLA	C1B-NB	-3.17	1.33	1.37
24	D	402	CLA	C4C-C3C	3.17	1.50	1.45
24	C	511	CLA	C1B-C2B	3.17	1.50	1.43
24	A	405	CLA	C1B-NB	-3.16	1.33	1.37
24	B	614	CLA	C4B-NB	-3.16	1.33	1.37
24	b	617	CLA	C1B-C2B	3.16	1.50	1.43
24	C	505	CLA	OBD-CAD	3.15	1.27	1.22
24	c	508	CLA	C4B-NB	-3.15	1.33	1.37
24	b	623	CLA	C1B-C2B	3.15	1.50	1.43
24	B	605	CLA	C1B-C2B	3.14	1.50	1.43
24	A	406	CLA	C4B-NB	-3.13	1.33	1.37
24	b	619	CLA	C1B-NB	-3.13	1.33	1.37
24	d	401	CLA	C1B-C2B	3.13	1.50	1.43
24	b	611	CLA	C1B-NB	-3.13	1.33	1.37
24	b	626	CLA	C4B-NB	-3.11	1.33	1.37
24	c	511	CLA	C4D-CHA	3.11	1.49	1.38
24	A	405	CLA	CHB-C1B	3.10	1.46	1.39
36	C	522	HTG	C1'-S1	-3.10	1.77	1.81
24	b	614	CLA	C1B-C2B	3.09	1.50	1.43
24	B	611	CLA	C1B-NB	-3.09	1.33	1.37
36	b	602	HTG	C1'-S1	-3.09	1.77	1.81
24	c	514	CLA	C4B-NB	-3.09	1.33	1.37
24	B	609	CLA	C1B-NB	-3.08	1.33	1.37
24	B	615	CLA	C4B-NB	-3.08	1.33	1.37
24	B	610	CLA	C1B-C2B	3.07	1.50	1.43
24	A	405	CLA	C4B-NB	-3.07	1.33	1.37
24	A	407	CLA	C1B-NB	-3.06	1.33	1.37
24	c	513	CLA	C1B-C2B	3.06	1.50	1.43
24	b	620	CLA	C1B-NB	-3.06	1.33	1.37
24	c	516	CLA	C4B-NB	-3.06	1.33	1.37
24	C	513	CLA	C1B-NB	-3.05	1.33	1.37
24	d	401	CLA	C4B-NB	-3.05	1.33	1.37
24	b	623	CLA	C1B-NB	-3.05	1.33	1.37
24	c	514	CLA	C1B-NB	-3.05	1.33	1.37
24	C	506	CLA	C1B-NB	-3.05	1.33	1.37
24	C	512	CLA	C1B-C2B	3.04	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	402	CLA	C1B-C2B	3.04	1.50	1.43
24	C	505	CLA	C1B-C2B	3.04	1.50	1.43
39	F	102	HEM	C1B-NB	-3.04	1.35	1.40
24	c	513	CLA	C1B-NB	-3.04	1.33	1.37
24	C	509	CLA	C1B-C2B	3.03	1.50	1.43
24	c	513	CLA	C4B-NB	-3.03	1.33	1.37
24	B	614	CLA	C4C-C3C	3.02	1.50	1.45
24	C	506	CLA	C4B-NB	-3.02	1.33	1.37
24	C	501	CLA	C1B-NB	-3.01	1.33	1.37
24	B	608	CLA	C1B-NB	-3.01	1.33	1.37
24	b	626	CLA	C1B-C2B	3.01	1.50	1.43
24	c	515	CLA	C1B-NB	-3.01	1.33	1.37
24	b	621	CLA	C1B-NB	-3.00	1.33	1.37
24	C	507	CLA	C4D-CHA	2.99	1.48	1.38
24	c	506	CLA	C4B-NB	-2.99	1.33	1.37
24	c	507	CLA	C1C-C2C	2.99	1.50	1.44
24	C	511	CLA	CHC-C4B	2.99	1.46	1.39
24	c	515	CLA	C4B-NB	-2.98	1.33	1.37
24	d	403	CLA	C1B-NB	-2.98	1.33	1.37
24	c	509	CLA	C1B-C2B	2.98	1.50	1.43
24	b	625	CLA	C1B-NB	-2.98	1.33	1.37
24	b	625	CLA	C1B-C2B	2.97	1.50	1.43
24	c	505	CLA	C4B-NB	-2.97	1.34	1.37
24	C	509	CLA	C1B-NB	-2.97	1.34	1.37
24	b	622	CLA	C4D-CHA	2.96	1.48	1.38
24	b	622	CLA	C4B-NB	-2.96	1.34	1.37
24	b	614	CLA	C4D-CHA	2.96	1.48	1.38
24	c	516	CLA	C1B-NB	-2.96	1.34	1.37
24	D	403	CLA	C4B-NB	-2.95	1.34	1.37
41	V	206	HEC	C1B-NB	-2.95	1.34	1.39
24	c	512	CLA	C1B-C2B	2.95	1.50	1.43
39	F	102	HEM	C1C-C2C	-2.94	1.39	1.45
24	C	507	CLA	C1B-NB	-2.94	1.34	1.37
24	c	517	CLA	C4B-NB	-2.93	1.34	1.37
24	C	510	CLA	C1B-NB	-2.93	1.34	1.37
24	b	625	CLA	C4D-CHA	2.93	1.48	1.38
24	C	509	CLA	C4B-NB	-2.92	1.34	1.37
24	c	512	CLA	C1B-NB	-2.92	1.34	1.37
24	c	505	CLA	C4D-CHA	2.92	1.48	1.38
24	D	403	CLA	C1B-C2B	2.91	1.50	1.43
24	C	505	CLA	C4B-NB	-2.91	1.34	1.37
24	B	608	CLA	C1B-C2B	2.91	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409[B]	PHO	CHA-CBD	-2.91	1.48	1.51
24	B	612	CLA	C1B-NB	-2.90	1.34	1.37
24	C	503	CLA	C1B-NB	-2.90	1.34	1.37
24	c	511	CLA	C4B-NB	-2.90	1.34	1.37
24	d	403	CLA	C4B-NB	-2.90	1.34	1.37
24	c	517	CLA	C1B-NB	-2.89	1.34	1.37
24	A	406	CLA	C1B-C2B	2.89	1.49	1.43
24	B	604	CLA	C1C-C2C	2.89	1.50	1.44
24	A	406	CLA	C4D-CHA	2.88	1.48	1.38
24	b	618	CLA	C1B-C2B	2.88	1.49	1.43
24	b	626	CLA	C4D-CHA	2.88	1.48	1.38
24	C	512	CLA	C1B-NB	-2.88	1.34	1.37
24	B	611	CLA	C4D-CHA	2.88	1.48	1.38
24	C	502	CLA	C1B-NB	-2.88	1.34	1.37
24	B	605	CLA	C4D-CHA	2.88	1.48	1.38
24	C	511	CLA	C4B-NB	-2.88	1.34	1.37
24	b	618	CLA	C4D-CHA	2.87	1.48	1.38
24	B	614	CLA	C4D-CHA	2.87	1.48	1.38
24	C	508	CLA	C4C-C3C	2.87	1.49	1.45
24	B	606	CLA	C1C-C2C	2.87	1.50	1.44
24	c	506	CLA	C4D-CHA	2.87	1.48	1.38
24	A	405	CLA	C4C-C3C	2.86	1.49	1.45
24	C	510	CLA	C4D-CHA	2.86	1.48	1.38
24	b	626	CLA	C1B-NB	-2.86	1.34	1.37
24	c	514	CLA	C1B-C2B	2.86	1.49	1.43
36	B	624	HTG	C1'-S1	-2.86	1.77	1.81
24	b	612	CLA	C1B-NB	-2.86	1.34	1.37
24	b	612	CLA	C4B-NB	-2.85	1.34	1.37
24	C	502	CLA	C4B-NB	-2.85	1.34	1.37
41	V	206	HEC	C1D-ND	-2.85	1.34	1.39
24	A	410	CLA	C1C-C2C	2.84	1.50	1.44
24	B	617	CLA	C4D-CHA	2.84	1.48	1.38
24	C	510	CLA	C1B-C2B	2.84	1.49	1.43
24	C	513	CLA	C4B-NB	-2.84	1.34	1.37
24	C	503	CLA	C1C-C2C	2.83	1.50	1.44
24	b	616	CLA	C1B-C2B	2.83	1.49	1.43
24	C	504	CLA	C4B-NB	-2.83	1.34	1.37
24	b	613	CLA	C1B-NB	-2.83	1.34	1.37
24	B	617	CLA	C1B-C2B	2.83	1.49	1.43
24	c	513	CLA	C4D-CHA	2.82	1.48	1.38
24	a	409	CLA	C4C-C3C	2.82	1.49	1.45
24	b	622	CLA	C1B-C2B	2.82	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C1B-NB	-2.82	1.34	1.37
24	C	504	CLA	C4D-CHA	2.81	1.48	1.38
24	A	410	CLA	C4B-NB	-2.81	1.34	1.37
24	b	618	CLA	C4B-NB	-2.81	1.34	1.37
24	c	505	CLA	C1B-C2B	2.81	1.49	1.43
24	B	614	CLA	C1C-C2C	2.80	1.50	1.44
24	C	511	CLA	C4D-CHA	2.80	1.48	1.38
24	B	609	CLA	C1B-C2B	2.80	1.49	1.43
24	C	511	CLA	C4C-C3C	2.80	1.49	1.45
24	B	602	CLA	C4B-NB	-2.80	1.34	1.37
24	B	607	CLA	C4B-NB	-2.80	1.34	1.37
24	C	509	CLA	C4C-C3C	2.79	1.49	1.45
24	B	612	CLA	C1B-C2B	2.79	1.49	1.43
24	C	511	CLA	C1B-NB	-2.78	1.34	1.37
24	a	409	CLA	C1B-NB	-2.78	1.34	1.37
24	C	502	CLA	C1B-C2B	2.78	1.49	1.43
24	A	405	CLA	C4D-CHA	2.78	1.47	1.38
24	b	621	CLA	C4D-CHA	2.78	1.47	1.38
24	C	509	CLA	C4D-CHA	2.78	1.47	1.38
24	a	409	CLA	C1C-C2C	2.78	1.50	1.44
29	A	417	LMT	O1'-C1'	2.77	1.44	1.40
24	c	515	CLA	C1B-C2B	2.77	1.49	1.43
24	b	617	CLA	C4D-CHA	2.77	1.47	1.38
24	D	403	CLA	C1B-NB	-2.77	1.34	1.37
24	C	513	CLA	C4D-CHA	2.76	1.47	1.38
24	c	506	CLA	C1B-C2B	2.76	1.49	1.43
24	b	612	CLA	C4C-C3C	2.76	1.49	1.45
24	b	620	CLA	C4B-NB	-2.76	1.34	1.37
32	A	420[B]	PL9	C6-C5	2.75	1.48	1.35
32	a	416[A]	PL9	C6-C5	2.75	1.48	1.35
24	B	616	CLA	C1B-C2B	2.75	1.49	1.43
24	B	607	CLA	C4C-C3C	2.75	1.49	1.45
24	a	409	CLA	C4B-NB	-2.75	1.34	1.37
24	B	617	CLA	C1B-NB	-2.75	1.34	1.37
24	B	611	CLA	C4C-C3C	2.74	1.49	1.45
32	a	416[B]	PL9	C6-C5	2.74	1.48	1.35
24	a	412	CLA	C1B-C2B	2.74	1.49	1.43
24	a	412	CLA	C1B-NB	-2.74	1.34	1.37
24	C	506	CLA	C4D-CHA	2.74	1.47	1.38
41	v	205	HEC	C1B-NB	-2.74	1.34	1.39
24	C	508	CLA	C4B-NB	-2.74	1.34	1.37
24	B	614	CLA	C1B-C2B	2.73	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C4D-CHA	2.73	1.47	1.38
24	C	504	CLA	C1B-C2B	2.73	1.49	1.43
24	B	607	CLA	C4D-CHA	2.73	1.47	1.38
24	b	620	CLA	C1B-C2B	2.73	1.49	1.43
24	A	410	CLA	C1B-NB	-2.73	1.34	1.37
32	D	405[A]	PL9	C6-C5	2.73	1.48	1.35
24	b	617	CLA	C3D-C4D	-2.72	1.38	1.44
24	B	607	CLA	C1B-C2B	2.72	1.49	1.43
25	a	420[B]	PHO	C3A-C2A	-2.72	1.52	1.54
24	B	602	CLA	C1B-C2B	2.72	1.49	1.43
24	c	511	CLA	C1B-C2B	2.72	1.49	1.43
32	A	420[A]	PL9	C6-C5	2.72	1.48	1.35
24	A	410	CLA	C1B-C2B	2.71	1.49	1.43
24	C	512	CLA	C4D-CHA	2.71	1.47	1.38
24	C	507	CLA	C1C-C2C	2.71	1.50	1.44
24	C	508	CLA	C4D-CHA	2.71	1.47	1.38
25	a	411	PHO	CHA-CBD	-2.71	1.48	1.51
24	B	605	CLA	C4B-NB	-2.71	1.34	1.37
24	c	507	CLA	C4B-NB	-2.71	1.34	1.37
24	d	401	CLA	C1B-NB	-2.70	1.34	1.37
24	c	509	CLA	C4C-C3C	2.70	1.49	1.45
24	c	508	CLA	C1C-C2C	2.70	1.50	1.44
24	c	516	CLA	C4D-CHA	2.70	1.47	1.38
24	B	608	CLA	C4D-CHA	2.70	1.47	1.38
24	B	613	CLA	C1B-C2B	2.70	1.49	1.43
25	A	409[A]	PHO	CHA-CBD	-2.70	1.48	1.51
24	C	506	CLA	C4C-C3C	2.70	1.49	1.45
24	A	410	CLA	C4D-CHA	2.70	1.47	1.38
24	b	623	CLA	C4C-C3C	2.70	1.49	1.45
24	C	508	CLA	C1B-C2B	2.70	1.49	1.43
32	d	405[A]	PL9	C6-C5	2.70	1.48	1.35
24	B	613	CLA	C4B-NB	-2.70	1.34	1.37
24	C	505	CLA	C4D-CHA	2.69	1.47	1.38
24	d	402	CLA	C4C-C3C	2.69	1.49	1.45
24	b	613	CLA	C1B-C2B	2.69	1.49	1.43
24	b	619	CLA	C4D-CHA	2.69	1.47	1.38
24	B	615	CLA	C1C-C2C	2.68	1.50	1.44
24	b	618	CLA	C1B-NB	-2.68	1.34	1.37
24	B	615	CLA	C4C-C3C	2.68	1.49	1.45
24	c	506	CLA	C1B-NB	-2.68	1.34	1.37
24	C	507	CLA	C1B-C2B	2.68	1.49	1.43
24	b	612	CLA	C1B-C2B	2.68	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C4D-CHA	2.68	1.47	1.38
24	b	613	CLA	C1C-C2C	2.68	1.50	1.44
24	B	611	CLA	C1B-C2B	2.68	1.49	1.43
24	c	510	CLA	C1B-C2B	2.67	1.49	1.43
32	D	405[B]	PL9	C6-C5	2.67	1.48	1.35
24	B	603	CLA	C4C-C3C	2.67	1.49	1.45
34	Z	101	LMG	O8-C28	2.67	1.46	1.33
24	B	612	CLA	C4D-CHA	2.67	1.47	1.38
24	d	403	CLA	C1C-C2C	2.67	1.49	1.44
32	d	405[B]	PL9	C6-C5	2.67	1.48	1.35
24	C	502	CLA	C4D-CHA	2.66	1.47	1.38
24	B	610	CLA	C4D-CHA	2.66	1.47	1.38
24	A	407	CLA	C4B-NB	-2.66	1.34	1.37
24	B	616	CLA	C4D-CHA	2.66	1.47	1.38
24	c	514	CLA	C4D-CHA	2.65	1.47	1.38
24	B	615	CLA	C1B-C2B	2.65	1.49	1.43
24	b	624	CLA	C1B-C2B	2.65	1.49	1.43
24	a	412	CLA	C4D-CHA	2.65	1.47	1.38
25	a	420[B]	PHO	C4B-NB	-2.65	1.33	1.38
24	B	612	CLA	C1C-C2C	2.65	1.49	1.44
24	c	508	CLA	C4D-CHA	2.65	1.47	1.38
24	B	609	CLA	C4D-CHA	2.65	1.47	1.38
24	B	602	CLA	C4D-CHA	2.64	1.47	1.38
24	b	614	CLA	C1C-C2C	2.64	1.49	1.44
24	a	409	CLA	C1B-C2B	2.64	1.49	1.43
24	c	515	CLA	C4D-CHA	2.64	1.47	1.38
24	B	606	CLA	C1B-C2B	2.64	1.49	1.43
24	d	402	CLA	C1B-C2B	2.64	1.49	1.43
24	c	514	CLA	C4C-C3C	2.64	1.49	1.45
24	c	509	CLA	C1B-NB	-2.64	1.34	1.37
24	B	606	CLA	C4B-NB	-2.64	1.34	1.37
24	b	613	CLA	C4B-NB	-2.63	1.34	1.37
24	c	517	CLA	C1C-C2C	2.63	1.49	1.44
24	C	506	CLA	C1B-C2B	2.63	1.49	1.43
24	B	612	CLA	C4B-NB	-2.63	1.34	1.37
24	C	513	CLA	C3B-C4B	2.63	1.50	1.42
24	b	611	CLA	C3B-C4B	2.63	1.50	1.42
25	a	420[B]	PHO	CHA-CBD	-2.63	1.48	1.51
24	B	604	CLA	C1B-C2B	2.62	1.49	1.43
24	C	501	CLA	C4D-CHA	2.62	1.47	1.38
24	b	616	CLA	C4B-NB	-2.62	1.34	1.37
24	a	410	CLA	C3B-C4B	2.62	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	v	205	HEC	C1D-ND	-2.62	1.34	1.39
41	V	206	HEC	C4B-NB	-2.61	1.34	1.39
24	b	621	CLA	C1B-C2B	2.61	1.49	1.43
24	b	611	CLA	C4D-CHA	2.61	1.47	1.38
24	b	614	CLA	C4B-NB	-2.61	1.34	1.37
24	b	623	CLA	C4D-CHA	2.60	1.47	1.38
24	d	403	CLA	C1B-C2B	2.60	1.49	1.43
24	B	604	CLA	C4D-CHA	2.60	1.47	1.38
24	b	615	CLA	C4D-CHA	2.60	1.47	1.38
24	b	613	CLA	C4D-CHA	2.60	1.47	1.38
24	D	402	CLA	C3D-C4D	-2.60	1.38	1.44
24	d	402	CLA	C4D-CHA	2.60	1.47	1.38
24	c	510	CLA	C4B-NB	-2.59	1.34	1.37
24	b	622	CLA	C4C-C3C	2.59	1.49	1.45
24	a	410	CLA	C1C-C2C	2.59	1.49	1.44
24	B	608	CLA	C4C-C3C	2.59	1.49	1.45
24	c	505	CLA	C4C-C3C	2.59	1.49	1.45
24	C	507	CLA	C4B-NB	-2.59	1.34	1.37
24	c	507	CLA	C4C-C3C	2.58	1.49	1.45
24	A	410	CLA	C4C-C3C	2.58	1.49	1.45
24	c	517	CLA	C4D-CHA	2.58	1.47	1.38
24	c	517	CLA	C3B-C4B	2.57	1.50	1.42
24	c	512	CLA	C4D-CHA	2.57	1.47	1.38
24	C	501	CLA	C3B-C4B	2.57	1.50	1.42
24	B	617	CLA	C3D-C4D	-2.57	1.38	1.44
24	A	407	CLA	C4D-CHA	2.57	1.47	1.38
24	C	503	CLA	C3B-C4B	2.57	1.50	1.42
24	B	613	CLA	C4D-CHA	2.56	1.47	1.38
24	a	410	CLA	C4D-CHA	2.56	1.47	1.38
24	C	505	CLA	C3D-C4D	-2.56	1.38	1.44
24	b	611	CLA	C1B-C2B	2.56	1.49	1.43
24	b	616	CLA	C1C-C2C	2.56	1.49	1.44
24	A	405	CLA	C1B-C2B	2.55	1.49	1.43
24	B	617	CLA	C4B-NB	-2.55	1.34	1.37
24	c	511	CLA	C1C-C2C	2.55	1.49	1.44
24	b	612	CLA	C4D-CHA	2.55	1.47	1.38
24	b	621	CLA	C4B-NB	-2.54	1.34	1.37
24	d	403	CLA	C4D-CHA	2.54	1.47	1.38
24	b	620	CLA	C4C-C3C	2.54	1.49	1.45
24	B	603	CLA	C4D-CHA	2.54	1.47	1.38
24	c	507	CLA	C4D-CHA	2.54	1.47	1.38
24	c	511	CLA	C1B-NB	-2.53	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C3D-C4D	-2.53	1.38	1.44
24	B	610	CLA	C3D-C4D	-2.53	1.38	1.44
24	c	511	CLA	C4C-C3C	2.53	1.49	1.45
24	a	410	CLA	C4B-NB	-2.53	1.34	1.37
24	c	506	CLA	C1C-C2C	2.53	1.49	1.44
24	d	403	CLA	C4C-C3C	2.52	1.49	1.45
41	v	205	HEC	C4D-ND	-2.52	1.34	1.39
24	c	509	CLA	C4D-CHA	2.52	1.47	1.38
24	d	402	CLA	C4B-NB	-2.52	1.34	1.37
24	A	407	CLA	C3B-C4B	2.52	1.50	1.42
24	c	509	CLA	C3B-C4B	2.52	1.50	1.42
25	a	420[A]	PHO	C4B-NB	-2.51	1.34	1.38
24	B	605	CLA	OBD-CAD	2.51	1.26	1.22
24	b	612	CLA	C3B-C4B	2.51	1.50	1.42
36	b	632	HTG	C1'-S1	-2.51	1.77	1.81
24	b	622	CLA	C3B-C2B	2.51	1.49	1.41
24	C	510	CLA	C4B-NB	-2.51	1.34	1.37
24	C	508	CLA	C1C-C2C	2.51	1.49	1.44
24	c	516	CLA	C1C-C2C	2.50	1.49	1.44
24	c	513	CLA	C1C-C2C	2.50	1.49	1.44
24	C	503	CLA	C4D-CHA	2.50	1.47	1.38
24	B	603	CLA	C1B-C2B	2.50	1.49	1.43
25	a	411	PHO	C3A-C2A	-2.50	1.52	1.54
24	D	403	CLA	C4D-CHA	2.50	1.47	1.38
24	a	409	CLA	C4D-CHA	2.50	1.47	1.38
24	b	614	CLA	C4C-C3C	2.50	1.49	1.45
24	B	605	CLA	C1C-C2C	2.50	1.49	1.44
24	c	510	CLA	C4D-CHA	2.49	1.47	1.38
25	A	409[A]	PHO	C3A-C2A	-2.49	1.52	1.54
24	c	507	CLA	C1B-NB	-2.49	1.34	1.37
24	c	508	CLA	C1B-C2B	2.49	1.49	1.43
24	C	513	CLA	C4C-C3C	2.48	1.49	1.45
24	B	606	CLA	C4D-CHA	2.48	1.46	1.38
24	b	620	CLA	C4D-CHA	2.48	1.46	1.38
25	a	420[A]	PHO	C3A-C2A	-2.48	1.52	1.54
24	c	510	CLA	C3D-C4D	-2.48	1.38	1.44
25	A	409[B]	PHO	C4B-NB	-2.47	1.34	1.38
24	b	612	CLA	C1C-C2C	2.47	1.49	1.44
24	C	501	CLA	C1B-C2B	2.47	1.48	1.43
24	D	403	CLA	C1C-C2C	2.47	1.49	1.44
24	C	502	CLA	C4C-C3C	2.47	1.49	1.45
24	B	613	CLA	C3B-C2B	2.45	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	512	CLA	C1C-C2C	2.45	1.49	1.44
24	B	616	CLA	C1C-C2C	2.45	1.49	1.44
24	A	405	CLA	C3D-C4D	-2.45	1.38	1.44
24	d	402	CLA	C3D-C4D	-2.45	1.38	1.44
24	b	619	CLA	C1B-C2B	2.45	1.48	1.43
24	b	617	CLA	C3B-C4B	2.44	1.49	1.42
24	C	505	CLA	C1C-C2C	2.44	1.49	1.44
24	C	509	CLA	C3B-C2B	2.44	1.49	1.41
25	A	408	PHO	C1B-NB	-2.44	1.34	1.38
24	c	516	CLA	C3B-C4B	2.44	1.49	1.42
24	b	615	CLA	C1C-C2C	2.44	1.49	1.44
24	b	622	CLA	C1C-C2C	2.44	1.49	1.44
24	c	507	CLA	C1B-C2B	2.43	1.48	1.43
24	C	501	CLA	C1C-C2C	2.43	1.49	1.44
24	B	602	CLA	C3B-C4B	2.43	1.49	1.42
24	C	506	CLA	C3D-C4D	-2.43	1.38	1.44
24	C	513	CLA	C1C-C2C	2.43	1.49	1.44
24	B	603	CLA	C3B-C2B	2.42	1.49	1.41
24	B	604	CLA	C4B-NB	-2.42	1.34	1.37
24	A	405	CLA	C1C-C2C	2.42	1.49	1.44
24	b	624	CLA	C1C-C2C	2.42	1.49	1.44
24	B	610	CLA	C3B-C4B	2.42	1.49	1.42
24	B	606	CLA	C1B-NB	-2.41	1.34	1.37
24	C	508	CLA	C3D-C4D	-2.41	1.38	1.44
39	e	102	HEM	C1C-C2C	-2.41	1.40	1.45
24	C	507	CLA	C3B-C4B	2.41	1.49	1.42
24	c	507	CLA	C3D-C4D	-2.41	1.38	1.44
24	B	605	CLA	C4C-C3C	2.40	1.49	1.45
24	b	615	CLA	C3B-C4B	2.40	1.49	1.42
24	C	504	CLA	C3B-C2B	2.40	1.49	1.41
24	B	615	CLA	C3D-C4D	-2.40	1.38	1.44
24	B	613	CLA	C4C-C3C	2.40	1.49	1.45
24	A	407	CLA	C1C-C2C	2.40	1.49	1.44
24	B	607	CLA	C1C-C2C	2.40	1.49	1.44
24	b	615	CLA	C4B-NB	-2.39	1.34	1.37
24	c	512	CLA	C4B-NB	-2.39	1.34	1.37
24	b	620	CLA	C3B-C4B	2.39	1.49	1.42
24	C	501	CLA	C4B-NB	-2.39	1.34	1.37
24	C	509	CLA	C1C-C2C	2.39	1.49	1.44
24	B	609	CLA	C4C-C3C	2.39	1.49	1.45
24	B	616	CLA	C4B-NB	-2.38	1.34	1.37
24	c	507	CLA	C3B-C4B	2.38	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C3B-C4B	2.38	1.49	1.42
24	a	412	CLA	C3B-C4B	2.38	1.49	1.42
24	C	503	CLA	C1B-C2B	2.38	1.48	1.43
24	B	614	CLA	C1B-NB	-2.38	1.34	1.37
37	h	102	DGD	O5D-C1E	2.38	1.44	1.40
24	b	614	CLA	C3B-C2B	2.38	1.49	1.41
24	a	412	CLA	C1C-C2C	2.38	1.49	1.44
24	B	611	CLA	C3B-C4B	2.38	1.49	1.42
24	b	615	CLA	C3D-C4D	-2.38	1.38	1.44
24	d	401	CLA	C4D-CHA	2.37	1.46	1.38
24	A	410	CLA	C3B-C4B	2.37	1.49	1.42
24	b	623	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	517	CLA	C3D-C4D	-2.37	1.38	1.44
24	C	503	CLA	C4C-C3C	2.37	1.49	1.45
24	a	409	CLA	C3D-C4D	-2.37	1.38	1.44
24	A	407	CLA	C1B-C2B	2.37	1.48	1.43
24	b	619	CLA	C3D-C4D	-2.37	1.38	1.44
24	B	616	CLA	C3B-C4B	2.37	1.49	1.42
24	b	618	CLA	C3B-C4B	2.36	1.49	1.42
24	D	402	CLA	C4D-CHA	2.36	1.46	1.38
24	C	513	CLA	C3D-C4D	-2.36	1.38	1.44
24	C	505	CLA	C4C-C3C	2.36	1.49	1.45
25	a	411	PHO	CBD-CGD	-2.36	1.49	1.52
24	c	506	CLA	C3D-C4D	-2.36	1.38	1.44
25	a	411	PHO	C4B-NB	-2.36	1.34	1.38
24	c	508	CLA	C4C-C3C	2.36	1.49	1.45
24	B	603	CLA	C4B-NB	-2.36	1.34	1.37
24	B	604	CLA	C4C-C3C	2.36	1.49	1.45
24	C	508	CLA	C3B-C4B	2.36	1.49	1.42
24	C	502	CLA	C3B-C4B	2.35	1.49	1.42
25	A	409[B]	PHO	C1B-NB	-2.35	1.34	1.38
24	a	412	CLA	C4C-C3C	2.35	1.49	1.45
24	B	616	CLA	C3D-C4D	-2.35	1.38	1.44
39	F	102	HEM	C3C-C4C	-2.35	1.41	1.46
24	b	624	CLA	C4D-CHA	2.35	1.46	1.38
24	c	512	CLA	C3D-C4D	-2.35	1.38	1.44
24	B	614	CLA	C3B-C2B	2.35	1.49	1.41
24	b	624	CLA	C4B-NB	-2.35	1.34	1.37
24	c	512	CLA	C3B-C2B	2.35	1.49	1.41
24	D	402	CLA	C1C-C2C	2.35	1.49	1.44
24	c	513	CLA	C3B-C2B	2.34	1.49	1.41
24	B	604	CLA	C3D-C4D	-2.34	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	C1B-NB	-2.34	1.34	1.37
24	c	513	CLA	C4C-C3C	2.34	1.49	1.45
25	A	409[A]	PHO	C1B-NB	-2.34	1.34	1.38
24	C	504	CLA	C1C-C2C	2.34	1.49	1.44
24	B	617	CLA	C3B-C2B	2.34	1.49	1.41
24	d	401	CLA	C3D-C4D	-2.34	1.38	1.44
24	C	511	CLA	C1C-C2C	2.34	1.49	1.44
36	H	101	HTG	C1-S1	-2.34	1.76	1.80
24	B	603	CLA	C3D-C4D	-2.34	1.38	1.44
24	C	502	CLA	C1C-C2C	2.34	1.49	1.44
24	D	403	CLA	C4C-C3C	2.33	1.49	1.45
24	B	605	CLA	C3B-C2B	2.33	1.49	1.41
24	b	615	CLA	C1B-C2B	2.33	1.48	1.43
24	b	624	CLA	C3B-C2B	2.33	1.49	1.41
24	a	410	CLA	C1B-C2B	2.33	1.48	1.43
24	C	513	CLA	C1B-C2B	2.33	1.48	1.43
24	c	516	CLA	C1B-C2B	2.33	1.48	1.43
24	B	610	CLA	C4C-C3C	2.32	1.49	1.45
24	B	612	CLA	C4C-C3C	2.32	1.49	1.45
24	c	515	CLA	C3B-C2B	2.32	1.49	1.41
25	A	408	PHO	C3A-C2A	-2.32	1.52	1.54
24	C	508	CLA	C3B-C2B	2.32	1.49	1.41
24	c	510	CLA	C3B-C2B	2.32	1.49	1.41
24	B	608	CLA	C1C-C2C	2.32	1.49	1.44
24	b	616	CLA	C3B-C2B	2.32	1.49	1.41
24	B	607	CLA	C3D-C4D	-2.32	1.39	1.44
24	b	616	CLA	C3B-C4B	2.32	1.49	1.42
25	A	409[A]	PHO	C4B-NB	-2.32	1.34	1.38
25	a	411	PHO	C1B-NB	-2.32	1.34	1.38
24	A	406	CLA	C3B-C2B	2.32	1.49	1.41
25	A	409[B]	PHO	C3A-C2A	-2.32	1.52	1.54
24	b	618	CLA	C3D-C4D	-2.31	1.39	1.44
24	c	509	CLA	C1C-C2C	2.31	1.49	1.44
24	D	402	CLA	C4B-NB	-2.31	1.34	1.37
24	B	609	CLA	C1C-C2C	2.31	1.49	1.44
24	c	508	CLA	C3B-C2B	2.31	1.48	1.41
24	C	510	CLA	C3B-C2B	2.30	1.48	1.41
24	B	603	CLA	C1C-C2C	2.30	1.49	1.44
24	C	512	CLA	C3B-C4B	2.30	1.49	1.42
24	b	618	CLA	C4C-C3C	2.30	1.48	1.45
24	b	621	CLA	C3B-C2B	2.30	1.48	1.41
24	c	508	CLA	C3D-C4D	-2.30	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	406	DGD	O3G-C1D	2.30	1.44	1.40
24	b	621	CLA	C4C-C3C	2.29	1.48	1.45
24	d	401	CLA	C3B-C2B	2.29	1.48	1.41
24	b	617	CLA	C1C-C2C	2.29	1.49	1.44
24	A	410	CLA	C3D-C4D	-2.29	1.39	1.44
24	c	513	CLA	C3D-C4D	-2.29	1.39	1.44
24	B	606	CLA	C3B-C4B	2.29	1.49	1.42
24	c	517	CLA	C1B-C2B	2.29	1.48	1.43
24	b	625	CLA	C4B-NB	-2.28	1.34	1.37
24	C	512	CLA	C4B-NB	-2.28	1.34	1.37
25	A	408	PHO	C4B-NB	-2.28	1.34	1.38
24	C	503	CLA	C3D-C4D	-2.28	1.39	1.44
24	b	623	CLA	C1C-C2C	2.28	1.49	1.44
24	B	606	CLA	C3D-C4D	-2.28	1.39	1.44
24	b	625	CLA	C3B-C4B	2.27	1.49	1.42
24	B	611	CLA	C3D-C4D	-2.27	1.39	1.44
24	b	623	CLA	C3B-C2B	2.27	1.48	1.41
24	C	510	CLA	C4C-C3C	2.27	1.48	1.45
24	b	611	CLA	C3B-C2B	2.27	1.48	1.41
24	b	626	CLA	C3B-C2B	2.27	1.48	1.41
41	v	205	HEC	C1D-C2D	2.26	1.48	1.43
24	c	517	CLA	C4C-C3C	2.26	1.48	1.45
24	c	514	CLA	C3D-C4D	-2.26	1.39	1.44
24	d	401	CLA	C1C-C2C	2.26	1.49	1.44
24	B	607	CLA	C3B-C2B	2.26	1.48	1.41
24	c	506	CLA	C3B-C4B	2.25	1.49	1.42
24	b	611	CLA	C4B-NB	-2.25	1.34	1.37
24	b	613	CLA	C4C-C3C	2.25	1.48	1.45
24	C	501	CLA	C3D-C4D	-2.25	1.39	1.44
25	a	420[A]	PHO	CHA-CBD	-2.24	1.49	1.51
24	c	514	CLA	C3B-C2B	2.24	1.48	1.41
39	e	102	HEM	C3B-C4B	2.24	1.49	1.44
25	A	408	PHO	CHA-CBD	-2.24	1.49	1.51
24	b	619	CLA	C4B-NB	-2.24	1.34	1.37
24	D	402	CLA	C3B-C2B	2.24	1.48	1.41
24	C	501	CLA	C4C-C3C	2.23	1.48	1.45
24	b	618	CLA	C1C-C2C	2.23	1.49	1.44
24	B	609	CLA	C3D-C4D	-2.23	1.39	1.44
24	b	612	CLA	C3D-C4D	-2.23	1.39	1.44
24	B	602	CLA	C1C-C2C	2.23	1.49	1.44
24	B	608	CLA	C4B-NB	-2.23	1.34	1.37
36	c	524	HTG	C1-S1	-2.23	1.77	1.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C3B-C4B	2.23	1.49	1.42
24	A	407	CLA	C4C-C3C	2.23	1.48	1.45
36	b	633	HTG	C1-S1	-2.22	1.77	1.80
24	C	511	CLA	C3B-C2B	2.22	1.48	1.41
24	C	510	CLA	C1C-C2C	2.22	1.49	1.44
24	a	409	CLA	C3B-C2B	2.22	1.48	1.41
24	C	510	CLA	C3B-C4B	2.22	1.49	1.42
32	D	405[B]	PL9	C2-C3	2.22	1.40	1.34
24	b	613	CLA	C3D-C4D	-2.22	1.39	1.44
24	c	511	CLA	C3D-C4D	-2.21	1.39	1.44
24	b	616	CLA	C4C-C3C	2.21	1.48	1.45
24	c	509	CLA	C4B-NB	-2.21	1.35	1.37
25	a	420[B]	PHO	C1B-NB	-2.21	1.34	1.38
24	c	511	CLA	C3B-C2B	2.21	1.48	1.41
24	C	502	CLA	C3D-C4D	-2.21	1.39	1.44
24	B	609	CLA	C3B-C4B	2.21	1.49	1.42
25	a	420[A]	PHO	C1B-NB	-2.20	1.34	1.38
24	b	626	CLA	C1C-NC	-2.20	1.34	1.37
24	b	620	CLA	C3B-C2B	2.20	1.48	1.41
24	b	624	CLA	C3D-C4D	-2.20	1.39	1.44
24	b	625	CLA	C3D-C4D	-2.20	1.39	1.44
24	C	512	CLA	C4C-C3C	2.20	1.48	1.45
24	A	405	CLA	C3B-C4B	2.20	1.49	1.42
24	B	605	CLA	C1A-CHA	2.20	1.52	1.43
36	V	207	HTG	C1-S1	-2.19	1.77	1.80
24	B	603	CLA	C3B-C4B	2.19	1.49	1.42
24	B	610	CLA	C1C-C2C	2.19	1.49	1.44
24	d	403	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	614	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	626	CLA	C4C-C3C	2.18	1.48	1.45
24	c	506	CLA	C3B-C2B	2.18	1.48	1.41
24	b	611	CLA	C3D-C4D	-2.18	1.39	1.44
24	A	410	CLA	C3B-C2B	2.18	1.48	1.41
24	d	402	CLA	C3B-C2B	2.18	1.48	1.41
24	B	615	CLA	C3B-C2B	2.18	1.48	1.41
24	b	623	CLA	C4B-NB	-2.18	1.35	1.37
24	A	407	CLA	C3D-C4D	-2.18	1.39	1.44
39	e	102	HEM	C3C-C4C	-2.18	1.42	1.46
24	C	505	CLA	C3B-C2B	2.18	1.48	1.41
41	V	206	HEC	C3B-C4B	2.18	1.49	1.46
24	B	612	CLA	C3B-C4B	2.17	1.49	1.42
38	d	406	LHG	O7-C5	-2.17	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	C3B-C4B	2.17	1.49	1.42
24	A	406	CLA	C4C-C3C	2.17	1.48	1.45
29	a	404	LMT	O1'-C1'	2.17	1.43	1.40
25	A	409[A]	PHO	C3D-C4D	-2.17	1.38	1.41
24	C	504	CLA	C4C-C3C	2.17	1.48	1.45
24	C	505	CLA	C3B-C4B	2.17	1.49	1.42
24	c	510	CLA	C3B-C4B	2.17	1.49	1.42
24	c	505	CLA	C3D-C4D	-2.16	1.39	1.44
32	D	405[A]	PL9	C2-C3	2.16	1.40	1.34
24	c	516	CLA	C3D-C4D	-2.16	1.39	1.44
39	F	102	HEM	C1A-C2A	-2.16	1.40	1.44
36	b	608	HTG	C1-S1	-2.16	1.77	1.80
24	D	403	CLA	C3B-C4B	2.16	1.49	1.42
24	D	403	CLA	C3B-C2B	2.16	1.48	1.41
24	c	505	CLA	C3B-C2B	2.15	1.48	1.41
32	d	405[B]	PL9	C2-C3	2.15	1.40	1.34
32	d	405[A]	PL9	C2-C3	2.15	1.40	1.34
24	B	602	CLA	C3B-C2B	2.15	1.48	1.41
24	d	403	CLA	C3B-C2B	2.15	1.48	1.41
24	b	623	CLA	C3B-C4B	2.15	1.49	1.42
24	D	403	CLA	C3D-C4D	-2.15	1.39	1.44
24	b	619	CLA	C1C-C2C	2.14	1.48	1.44
24	B	617	CLA	C4C-C3C	2.14	1.48	1.45
24	c	512	CLA	C4C-C3C	2.14	1.48	1.45
24	b	621	CLA	C3B-C4B	2.14	1.49	1.42
24	b	613	CLA	C3B-C2B	2.14	1.48	1.41
32	a	416[B]	PL9	C2-C3	2.14	1.40	1.34
37	H	103	DGD	O5D-C1E	2.13	1.43	1.40
32	a	416[A]	PL9	C2-C3	2.13	1.40	1.34
36	d	411	HTG	C1-S1	-2.13	1.77	1.80
24	B	612	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	607	CLA	C3B-C4B	2.13	1.48	1.42
24	b	625	CLA	C4C-C3C	2.13	1.48	1.45
24	b	616	CLA	C3D-C4D	-2.13	1.39	1.44
24	b	618	CLA	C3B-C2B	2.13	1.48	1.41
24	C	513	CLA	C3B-C2B	2.12	1.48	1.41
41	v	205	HEC	C4B-NB	-2.12	1.35	1.39
36	B	632	HTG	C1-S1	-2.12	1.77	1.80
24	b	620	CLA	C1C-C2C	2.12	1.48	1.44
24	d	403	CLA	C3B-C4B	2.12	1.48	1.42
32	A	420[B]	PL9	C2-C3	2.11	1.39	1.34
24	c	505	CLA	C1C-C2C	2.11	1.48	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	CLA	C3B-C4B	2.10	1.48	1.42
24	A	405	CLA	C3B-C2B	2.10	1.48	1.41
24	C	507	CLA	C4C-C3C	2.10	1.48	1.45
36	c	525	HTG	C1-S1	-2.10	1.77	1.80
24	c	512	CLA	C1C-C2C	2.09	1.48	1.44
24	C	512	CLA	C3B-C2B	2.09	1.48	1.41
24	B	608	CLA	C3B-C4B	2.09	1.48	1.42
24	b	625	CLA	C3B-C2B	2.09	1.48	1.41
24	c	506	CLA	C1C-NC	-2.09	1.34	1.37
24	a	410	CLA	C3D-C4D	-2.09	1.39	1.44
36	b	609	HTG	C1-S1	-2.09	1.77	1.80
24	B	608	CLA	C3B-C2B	2.09	1.48	1.41
29	M	103	LMT	O1'-C1'	2.09	1.43	1.40
24	b	622	CLA	C1C-NC	-2.09	1.34	1.37
24	B	610	CLA	C4B-NB	-2.09	1.35	1.37
24	d	401	CLA	C1C-NC	-2.08	1.34	1.37
25	A	409[B]	PHO	C1D-ND	-2.08	1.34	1.38
24	c	516	CLA	C4C-C3C	2.08	1.48	1.45
24	C	504	CLA	C3D-C4D	-2.08	1.39	1.44
24	C	509	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	604	CLA	C3B-C2B	2.08	1.48	1.41
24	d	401	CLA	C4C-C3C	2.08	1.48	1.45
32	A	420[A]	PL9	C2-C3	2.07	1.39	1.34
24	b	611	CLA	C1C-C2C	2.07	1.48	1.44
24	b	620	CLA	C3D-C4D	-2.07	1.39	1.44
24	C	512	CLA	C3D-C4D	-2.07	1.39	1.44
24	c	514	CLA	C1C-C2C	2.07	1.48	1.44
24	b	619	CLA	C3B-C4B	2.07	1.48	1.42
24	C	502	CLA	C3B-C2B	2.07	1.48	1.41
24	c	506	CLA	C4C-C3C	2.07	1.48	1.45
24	b	626	CLA	C3D-C4D	-2.07	1.39	1.44
24	c	507	CLA	C3B-C2B	2.06	1.48	1.41
24	B	608	CLA	C1D-C2D	2.06	1.49	1.45
24	b	612	CLA	C1D-C2D	2.06	1.49	1.45
41	v	205	HEC	C4A-C3A	-2.06	1.41	1.45
24	c	515	CLA	C3D-C4D	-2.06	1.39	1.44
24	b	626	CLA	C1D-C2D	2.06	1.49	1.45
24	a	410	CLA	C3B-C2B	2.06	1.48	1.41
24	B	611	CLA	C3B-C2B	2.05	1.48	1.41
24	c	510	CLA	C1C-C2C	2.05	1.48	1.44
24	A	407	CLA	C3B-C2B	2.05	1.48	1.41
24	C	503	CLA	C4B-NB	-2.05	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	410	CLA	C4C-C3C	2.05	1.48	1.45
24	b	621	CLA	C3D-C4D	-2.05	1.39	1.44
24	b	612	CLA	C3B-C2B	2.05	1.48	1.41
24	a	412	CLA	C3B-C2B	2.04	1.48	1.41
24	c	512	CLA	C3B-C4B	2.04	1.48	1.42
39	e	102	HEM	C4B-NB	-2.04	1.34	1.38
24	d	403	CLA	C1D-C2D	2.04	1.49	1.45
24	B	612	CLA	C3B-C2B	2.04	1.48	1.41
24	B	616	CLA	C4C-C3C	2.04	1.48	1.45
24	c	515	CLA	C4C-C3C	2.04	1.48	1.45
24	c	510	CLA	C4C-C3C	2.04	1.48	1.45
36	C	522	HTG	C1-S1	-2.04	1.77	1.80
24	B	609	CLA	C3B-C2B	2.04	1.48	1.41
24	b	625	CLA	C1C-C2C	2.04	1.48	1.44
41	V	206	HEC	C1D-C2D	2.03	1.47	1.43
24	c	516	CLA	C3B-C2B	2.03	1.48	1.41
24	C	506	CLA	C1C-C2C	2.03	1.48	1.44
25	A	409[A]	PHO	C1D-ND	-2.03	1.34	1.38
24	c	509	CLA	C3B-C2B	2.03	1.48	1.41
37	C	517	DGD	O5D-C1E	2.03	1.43	1.40
24	b	615	CLA	C3B-C2B	2.03	1.48	1.41
24	C	511	CLA	C3D-C4D	-2.03	1.39	1.44
24	b	617	CLA	C3B-C2B	2.02	1.48	1.41
24	b	619	CLA	C4C-C3C	2.02	1.48	1.45
24	C	507	CLA	C3B-C2B	2.02	1.48	1.41
24	D	403	CLA	C1D-C2D	2.02	1.49	1.45
24	c	513	CLA	C3B-C4B	2.02	1.48	1.42
24	C	506	CLA	C3B-C2B	2.01	1.48	1.41
41	V	206	HEC	C1A-C2A	-2.01	1.41	1.45
24	c	509	CLA	C3D-C4D	-2.01	1.39	1.44
24	A	406	CLA	C1C-C2C	2.01	1.48	1.44
34	c	523	LMG	O1-C1	2.01	1.43	1.40
24	C	507	CLA	C3D-C4D	-2.01	1.39	1.44
24	B	602	CLA	C3D-C4D	-2.00	1.39	1.44

All (2945) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	408	PHO	C2D-C1D-ND	11.62	117.83	109.43
25	A	409[B]	PHO	C2D-C1D-ND	11.53	117.76	109.43
25	A	409[A]	PHO	C2D-C1D-ND	11.23	117.55	109.43
25	a	420[B]	PHO	C2D-C1D-ND	10.95	117.34	109.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	420[A]	PHO	C2D-C1D-ND	10.80	117.24	109.43
25	a	411	PHO	C2D-C1D-ND	10.52	117.03	109.43
24	b	615	CLA	C1D-ND-C4D	-10.50	98.94	106.31
24	a	410	CLA	C1D-ND-C4D	-10.34	99.06	106.31
24	B	613	CLA	C1D-ND-C4D	-10.21	99.15	106.31
24	B	606	CLA	C1D-ND-C4D	-10.05	99.26	106.31
24	C	503	CLA	C1D-ND-C4D	-9.95	99.33	106.31
24	A	407	CLA	C1D-ND-C4D	-9.83	99.41	106.31
24	d	403	CLA	C1D-ND-C4D	-9.83	99.41	106.31
24	B	616	CLA	C1D-ND-C4D	-9.82	99.42	106.31
24	a	412	CLA	C1D-ND-C4D	-9.80	99.44	106.31
24	B	612	CLA	C1D-ND-C4D	-9.75	99.47	106.31
24	c	507	CLA	C1D-ND-C4D	-9.73	99.49	106.31
24	B	608	CLA	C1D-ND-C4D	-9.67	99.52	106.31
24	D	403	CLA	C1D-ND-C4D	-9.65	99.54	106.31
24	b	621	CLA	C1D-ND-C4D	-9.63	99.55	106.31
24	B	602	CLA	C1D-ND-C4D	-9.63	99.56	106.31
24	b	619	CLA	C1D-ND-C4D	-9.58	99.59	106.31
24	B	603	CLA	C1D-ND-C4D	-9.56	99.61	106.31
24	c	515	CLA	C1D-ND-C4D	-9.53	99.62	106.31
24	c	517	CLA	C1D-ND-C4D	-9.50	99.64	106.31
24	b	617	CLA	C1D-ND-C4D	-9.48	99.66	106.31
24	C	509	CLA	C1D-ND-C4D	-9.47	99.67	106.31
24	b	620	CLA	C1D-ND-C4D	-9.47	99.67	106.31
24	A	406	CLA	C1D-ND-C4D	-9.46	99.67	106.31
24	C	501	CLA	C1D-ND-C4D	-9.46	99.67	106.31
24	C	512	CLA	C1D-ND-C4D	-9.41	99.71	106.31
24	D	402	CLA	C1D-ND-C4D	-9.34	99.76	106.31
24	d	401	CLA	C1D-ND-C4D	-9.32	99.77	106.31
24	b	624	CLA	C1D-ND-C4D	-9.32	99.77	106.31
24	c	514	CLA	C1D-ND-C4D	-9.27	99.81	106.31
24	b	613	CLA	C1D-ND-C4D	-9.26	99.81	106.31
24	C	511	CLA	C1D-ND-C4D	-9.25	99.83	106.31
24	c	508	CLA	C1D-ND-C4D	-9.21	99.85	106.31
24	B	604	CLA	C1D-ND-C4D	-9.20	99.86	106.31
24	A	410	CLA	C1D-ND-C4D	-9.18	99.87	106.31
24	B	615	CLA	C1D-ND-C4D	-9.17	99.88	106.31
24	C	513	CLA	C1D-ND-C4D	-9.13	99.91	106.31
24	c	510	CLA	C1D-ND-C4D	-9.12	99.91	106.31
24	B	607	CLA	C1D-ND-C4D	-9.12	99.92	106.31
24	c	513	CLA	C1D-ND-C4D	-9.09	99.93	106.31
24	b	612	CLA	C1D-ND-C4D	-9.09	99.94	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	605	CLA	C1D-ND-C4D	-9.08	99.94	106.31
24	a	409	CLA	C1D-ND-C4D	-9.07	99.95	106.31
24	C	507	CLA	C1D-ND-C4D	-9.04	99.97	106.31
24	c	516	CLA	C1D-ND-C4D	-9.01	99.99	106.31
24	b	625	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	b	616	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	b	611	CLA	C1D-ND-C4D	-8.99	100.00	106.31
24	C	504	CLA	C1D-ND-C4D	-8.99	100.00	106.31
25	A	408	PHO	C3B-C4B-NB	8.97	113.31	107.46
24	c	506	CLA	C1D-ND-C4D	-8.95	100.03	106.31
24	c	509	CLA	C1D-ND-C4D	-8.94	100.04	106.31
24	C	502	CLA	C1D-ND-C4D	-8.93	100.05	106.31
25	a	420[A]	PHO	O2D-CGD-CBD	8.91	120.74	110.95
24	b	618	CLA	C1D-ND-C4D	-8.84	100.11	106.31
24	b	626	CLA	C1D-ND-C4D	-8.80	100.14	106.31
24	d	402	CLA	C1D-ND-C4D	-8.76	100.17	106.31
24	B	609	CLA	C1D-ND-C4D	-8.75	100.17	106.31
24	B	610	CLA	C1D-ND-C4D	-8.65	100.24	106.31
24	b	623	CLA	C1D-ND-C4D	-8.61	100.27	106.31
24	C	505	CLA	C1D-ND-C4D	-8.59	100.28	106.31
24	C	506	CLA	C1D-ND-C4D	-8.58	100.29	106.31
24	C	508	CLA	C1D-ND-C4D	-8.56	100.31	106.31
24	b	622	CLA	C1D-ND-C4D	-8.53	100.33	106.31
24	B	611	CLA	C1D-ND-C4D	-8.43	100.39	106.31
24	c	512	CLA	C1D-ND-C4D	-8.42	100.41	106.31
24	c	505	CLA	C1D-ND-C4D	-8.39	100.43	106.31
24	B	617	CLA	C1D-ND-C4D	-8.36	100.44	106.31
24	c	511	CLA	C1D-ND-C4D	-8.34	100.46	106.31
24	C	510	CLA	C1D-ND-C4D	-8.32	100.47	106.31
25	A	408	PHO	O2D-CGD-CBD	8.19	119.95	110.95
24	b	614	CLA	C1D-ND-C4D	-8.16	100.59	106.31
24	A	405	CLA	C1D-ND-C4D	-8.15	100.59	106.31
25	a	411	PHO	O2D-CGD-CBD	7.98	119.72	110.95
25	a	420[B]	PHO	O2D-CGD-CBD	7.75	119.47	110.95
25	a	420[A]	PHO	C3B-C4B-NB	7.74	112.51	107.46
24	B	605	CLA	CMD-C2D-C1D	7.73	138.34	124.73
25	A	409[A]	PHO	O2D-CGD-CBD	7.53	119.22	110.95
25	A	409[B]	PHO	C3B-C4B-NB	7.45	112.32	107.46
24	B	614	CLA	C1D-ND-C4D	-7.39	101.12	106.31
25	a	420[B]	PHO	C3B-C4B-NB	7.35	112.25	107.46
25	a	411	PHO	C3B-C4B-NB	7.32	112.24	107.46
24	a	409	CLA	CMD-C2D-C1D	7.32	137.61	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	CHD-C4C-C3C	-7.32	114.11	124.77
25	A	409[B]	PHO	O2D-CGD-CBD	7.25	118.92	110.95
25	a	420[A]	PHO	C2B-C1B-NB	7.21	114.64	109.43
25	A	409[A]	PHO	C3B-C4B-NB	7.20	112.16	107.46
24	b	615	CLA	CHD-C4C-C3C	-7.19	114.29	124.77
24	b	617	CLA	CMD-C2D-C1D	7.04	137.13	124.73
24	c	511	CLA	O2D-CGD-CBD	7.01	123.48	111.23
24	A	406	CLA	C2D-C1D-ND	6.98	117.03	110.13
24	d	403	CLA	CMD-C2D-C1D	6.97	137.01	124.73
24	b	612	CLA	C4A-NA-C1A	-6.97	103.50	106.68
24	B	616	CLA	CMD-C2D-C1D	6.95	136.96	124.73
24	B	613	CLA	C2D-C1D-ND	6.93	116.98	110.13
24	b	611	CLA	O2D-CGD-CBD	6.84	123.19	111.23
24	D	402	CLA	CMD-C2D-C1D	6.78	136.68	124.73
24	b	625	CLA	CMD-C2D-C1D	6.74	136.60	124.73
24	c	517	CLA	CMD-C2D-C1D	6.74	136.60	124.73
24	c	510	CLA	CMD-C2D-C1D	6.73	136.59	124.73
25	A	409[A]	PHO	C2B-C1B-NB	6.71	114.28	109.43
24	B	613	CLA	CHD-C4C-C3C	-6.70	115.00	124.77
24	B	616	CLA	CHD-C4C-C3C	-6.70	115.01	124.77
24	C	510	CLA	CMD-C2D-C1D	6.69	136.51	124.73
24	c	514	CLA	CMD-C2D-C1D	6.68	136.49	124.73
24	C	505	CLA	C4A-NA-C1A	-6.68	103.63	106.68
24	d	402	CLA	C4A-NA-C1A	-6.67	103.64	106.68
24	B	606	CLA	C2D-C1D-ND	6.64	116.70	110.13
24	C	501	CLA	O2D-CGD-CBD	6.64	122.83	111.23
24	C	504	CLA	CMD-C2D-C1D	6.63	136.40	124.73
24	B	612	CLA	CHD-C4C-C3C	-6.62	115.12	124.77
26	D	404	BCR	C7-C8-C9	-6.59	116.48	126.23
24	B	605	CLA	C2D-C1D-ND	6.59	116.65	110.13
24	B	603	CLA	CMD-C2D-C1D	6.56	136.29	124.73
24	C	513	CLA	CMD-C2D-C1D	6.56	136.28	124.73
24	C	507	CLA	C2D-C1D-ND	6.53	116.59	110.13
24	b	612	CLA	CMD-C2D-C1D	6.52	136.21	124.73
24	c	508	CLA	CMD-C2D-C1D	6.51	136.18	124.73
24	c	507	CLA	CMD-C2D-C1D	6.48	136.15	124.73
24	d	402	CLA	CMD-C2D-C1D	6.48	136.13	124.73
24	B	605	CLA	CHD-C4C-C3C	-6.45	115.36	124.77
24	b	615	CLA	CMD-C2D-C1D	6.45	136.09	124.73
24	b	615	CLA	C2D-C1D-ND	6.44	116.50	110.13
24	D	403	CLA	CMD-C2D-C1D	6.43	136.06	124.73
24	b	624	CLA	C2D-C1D-ND	6.42	116.48	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	C2D-C1D-ND	6.41	116.47	110.13
24	b	621	CLA	C2D-C1D-ND	6.41	116.47	110.13
24	b	617	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
24	b	614	CLA	CMD-C2D-C1D	6.41	136.01	124.73
24	B	602	CLA	CHD-C4C-C3C	-6.39	115.46	124.77
24	a	412	CLA	C2D-C1D-ND	6.37	116.43	110.13
24	b	611	CLA	CHD-C4C-C3C	-6.36	115.49	124.77
24	C	507	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
24	b	625	CLA	C4A-NA-C1A	-6.34	103.79	106.68
24	C	504	CLA	C2D-C1D-ND	6.33	116.39	110.13
24	B	610	CLA	CMD-C2D-C1D	6.33	135.88	124.73
24	C	506	CLA	CMD-C2D-C1D	6.32	135.86	124.73
24	B	615	CLA	CMD-C2D-C1D	6.32	135.85	124.73
25	a	411	PHO	C2B-C1B-NB	6.31	113.99	109.43
24	d	401	CLA	CMD-C2D-C1D	6.31	135.85	124.73
24	a	410	CLA	C2D-C1D-ND	6.31	116.37	110.13
24	B	602	CLA	O2D-CGD-CBD	6.30	122.24	111.23
24	c	516	CLA	C4A-NA-C1A	-6.28	103.81	106.68
24	C	512	CLA	C2D-C1D-ND	6.28	116.34	110.13
24	C	509	CLA	CMD-C2D-C1D	6.27	135.77	124.73
24	b	624	CLA	CMD-C2D-C1D	6.27	135.77	124.73
24	b	626	CLA	O2D-CGD-CBD	6.27	122.19	111.23
24	b	620	CLA	CMD-C2D-C1D	6.26	135.76	124.73
24	d	403	CLA	C2D-C1D-ND	6.26	116.32	110.13
24	c	516	CLA	CHD-C4C-C3C	-6.26	115.65	124.77
24	C	503	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
24	B	617	CLA	CHD-C4C-C3C	-6.25	115.66	124.77
24	A	405	CLA	CMD-C2D-C1D	6.24	135.72	124.73
25	A	409[B]	PHO	C2B-C1B-NB	6.24	113.94	109.43
24	C	508	CLA	CMD-C2D-C1D	6.23	135.70	124.73
24	b	611	CLA	CMD-C2D-C1D	6.22	135.68	124.73
24	b	624	CLA	O2D-CGD-CBD	6.21	122.08	111.23
24	A	405	CLA	C4A-NA-C1A	-6.21	103.85	106.68
24	B	607	CLA	CMD-C2D-C1D	6.20	135.65	124.73
24	C	512	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
24	B	604	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
24	B	615	CLA	C2D-C1D-ND	6.18	116.25	110.13
24	B	617	CLA	O2D-CGD-CBD	6.17	122.02	111.23
24	b	621	CLA	CMD-C2D-C1D	6.17	135.59	124.73
24	B	604	CLA	O2D-CGD-CBD	6.15	121.98	111.23
24	B	608	CLA	C2D-C1D-ND	6.15	116.21	110.13
24	c	516	CLA	C2D-C1D-ND	6.15	116.21	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	624	CLA	CHD-C4C-C3C	-6.14	115.81	124.77
24	C	507	CLA	CMD-C2D-C1D	6.14	135.54	124.73
24	c	516	CLA	O2D-CGD-CBD	6.12	121.93	111.23
24	D	402	CLA	C2C-C1C-NC	6.12	116.41	109.98
24	c	507	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
24	c	511	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
24	b	619	CLA	CMD-C2D-C1D	6.11	135.49	124.73
24	c	507	CLA	C2D-C1D-ND	6.11	116.17	110.13
24	b	616	CLA	CMD-C2D-C1D	6.10	135.47	124.73
24	d	403	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
24	b	616	CLA	C4A-NA-C1A	-6.10	103.90	106.68
24	c	513	CLA	CMD-C2D-C1D	6.09	135.45	124.73
24	B	611	CLA	CMD-C2D-C1D	6.09	135.44	124.73
24	C	501	CLA	CMD-C2D-C1D	6.08	135.44	124.73
24	b	614	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
24	a	410	CLA	CMD-C2D-C1D	6.08	135.43	124.73
24	b	614	CLA	O2D-CGD-CBD	6.07	121.85	111.23
25	A	408	PHO	C4D-ND-C1D	-6.07	101.60	108.87
24	B	610	CLA	C4A-NA-C1A	-6.07	103.91	106.68
24	C	505	CLA	CMD-C2D-C1D	6.07	135.41	124.73
24	c	509	CLA	C4A-NA-C1A	-6.06	103.91	106.68
24	c	506	CLA	CHD-C4C-C3C	-6.06	115.93	124.77
24	B	608	CLA	CMD-C2D-C1D	6.06	135.40	124.73
25	a	420[B]	PHO	C2B-C1B-NB	6.06	113.81	109.43
24	a	410	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
24	C	512	CLA	O2D-CGD-CBD	6.04	121.79	111.23
24	C	503	CLA	CMD-C2D-C1D	6.04	135.36	124.73
24	C	509	CLA	C2D-C1D-ND	6.03	116.09	110.13
24	B	616	CLA	C2D-C1D-ND	6.03	116.09	110.13
24	B	609	CLA	CMD-C2D-C1D	6.03	135.35	124.73
24	B	602	CLA	C2D-C1D-ND	6.03	116.09	110.13
24	A	407	CLA	C2D-C1D-ND	6.03	116.09	110.13
24	b	625	CLA	CHD-C4C-C3C	-6.02	115.99	124.77
24	D	403	CLA	C2D-C1D-ND	6.01	116.08	110.13
24	b	618	CLA	C4A-NA-C1A	-6.01	103.94	106.68
24	B	607	CLA	C2D-C1D-ND	6.00	116.06	110.13
24	C	502	CLA	CHD-C4C-C3C	-5.99	116.03	124.77
24	b	619	CLA	C4A-NA-C1A	-5.99	103.95	106.68
24	c	506	CLA	C2D-C1D-ND	5.99	116.05	110.13
24	C	511	CLA	C2D-C1D-ND	5.99	116.05	110.13
24	b	616	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
24	d	401	CLA	CHD-C4C-C3C	-5.97	116.06	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	603	CLA	C4A-NA-C1A	-5.97	103.95	106.68
24	b	620	CLA	C2D-C1D-ND	5.97	116.03	110.13
24	b	622	CLA	C2D-C1D-ND	5.96	116.03	110.13
24	b	613	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
24	C	503	CLA	C2D-C1D-ND	5.96	116.02	110.13
24	b	617	CLA	C2D-C1D-ND	5.96	116.02	110.13
24	B	617	CLA	CMD-C2D-C1D	5.95	135.21	124.73
24	c	517	CLA	CHD-C4C-C3C	-5.95	116.09	124.77
24	b	626	CLA	CMD-C2D-C1D	5.95	135.21	124.73
24	c	506	CLA	C4A-NA-C1A	-5.95	103.97	106.68
24	b	615	CLA	C4A-NA-C1A	-5.95	103.97	106.68
24	C	505	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
24	c	508	CLA	C2D-C1D-ND	5.93	116.00	110.13
24	c	513	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
24	D	402	CLA	C4A-NA-C1A	-5.91	103.98	106.68
24	C	504	CLA	O2D-CGD-CBD	5.91	121.56	111.23
24	d	402	CLA	C2C-C1C-NC	5.91	116.19	109.98
36	d	411	HTG	C1'-S1-C1	5.90	113.20	100.45
24	B	610	CLA	CHD-C4C-C3C	-5.90	116.16	124.77
24	A	410	CLA	CMD-C2D-C1D	5.90	135.12	124.73
25	A	408	PHO	C2B-C1B-NB	5.90	113.69	109.43
24	B	602	CLA	CMD-C2D-C1D	5.90	135.12	124.73
24	C	501	CLA	CHD-C4C-C3C	-5.90	116.18	124.77
25	A	409[A]	PHO	C4D-ND-C1D	-5.89	101.82	108.87
24	a	412	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
24	c	511	CLA	C2D-C1D-ND	5.88	115.95	110.13
24	d	401	CLA	C2D-C1D-ND	5.88	115.95	110.13
24	B	615	CLA	O2D-CGD-CBD	5.88	121.51	111.23
24	b	619	CLA	C2D-C1D-ND	5.88	115.94	110.13
24	C	502	CLA	C2D-C1D-ND	5.87	115.93	110.13
24	c	505	CLA	C2D-C1D-ND	5.86	115.93	110.13
25	A	409[B]	PHO	C4D-ND-C1D	-5.86	101.85	108.87
24	b	619	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
24	C	502	CLA	CMD-C2D-C1D	5.86	135.04	124.73
24	C	510	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
24	b	614	CLA	C2C-C1C-NC	5.85	116.13	109.98
24	c	508	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
24	A	406	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
24	C	501	CLA	C2D-C1D-ND	5.84	115.91	110.13
24	b	614	CLA	C2D-C1D-ND	5.84	115.91	110.13
24	c	507	CLA	C4A-NA-C1A	-5.84	104.02	106.68
24	b	621	CLA	CHD-C4C-C3C	-5.84	116.26	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	420[A]	PHO	C4D-ND-C1D	-5.83	101.89	108.87
24	A	410	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
24	B	614	CLA	C2C-C1C-NC	5.83	116.10	109.98
24	b	618	CLA	CMD-C2D-C1D	5.82	134.98	124.73
24	b	622	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
24	C	508	CLA	O2D-CGD-CBD	5.81	121.39	111.23
26	Y	101	BCR	C33-C5-C6	-5.81	118.14	124.48
24	c	508	CLA	O2D-CGD-CBD	5.81	121.39	111.23
24	B	613	CLA	O2D-CGD-CBD	5.81	121.38	111.23
24	B	612	CLA	CMD-C2D-C1D	5.81	134.95	124.73
24	A	407	CLA	CMD-C2D-C1D	5.80	134.95	124.73
24	B	603	CLA	C2D-C1D-ND	5.80	115.86	110.13
24	b	623	CLA	C2D-C1D-ND	5.79	115.85	110.13
25	a	420[B]	PHO	C4D-ND-C1D	-5.78	101.94	108.87
24	B	616	CLA	C4A-NA-C1A	-5.78	104.04	106.68
24	C	513	CLA	C2D-C1D-ND	5.77	115.84	110.13
24	B	603	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
24	B	614	CLA	C2D-C1D-ND	5.77	115.84	110.13
24	a	412	CLA	CMD-C2D-C1D	5.75	134.86	124.73
24	c	505	CLA	CMD-C2D-C1D	5.75	134.85	124.73
24	c	515	CLA	C2D-C1D-ND	5.75	115.81	110.13
24	B	615	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
24	B	605	CLA	C2C-C1C-NC	5.75	116.02	109.98
24	b	625	CLA	C2D-C1D-ND	5.74	115.81	110.13
24	c	513	CLA	C2D-C1D-ND	5.74	115.81	110.13
24	c	505	CLA	O2D-CGD-CBD	5.73	121.24	111.23
24	c	509	CLA	O2D-CGD-CBD	5.73	121.24	111.23
24	c	517	CLA	C2D-C1D-ND	5.72	115.79	110.13
24	B	609	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
24	b	611	CLA	C2D-C1D-ND	5.70	115.77	110.13
24	A	410	CLA	C2D-C1D-ND	5.70	115.77	110.13
24	b	623	CLA	CMD-C2D-C1D	5.69	134.75	124.73
24	c	515	CLA	CHD-C4C-C3C	-5.69	116.48	124.77
24	D	402	CLA	C2D-C1D-ND	5.68	115.75	110.13
24	B	609	CLA	C2D-C1D-ND	5.68	115.75	110.13
24	C	507	CLA	O2D-CGD-CBD	5.68	121.16	111.23
24	b	626	CLA	CHD-C4C-C3C	-5.68	116.50	124.77
24	b	626	CLA	C2D-C1D-ND	5.67	115.74	110.13
24	c	512	CLA	CHD-C4C-C3C	-5.67	116.50	124.77
24	B	614	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
24	b	616	CLA	C2D-C1D-ND	5.65	115.72	110.13
24	c	512	CLA	C4A-NA-C1A	-5.65	104.10	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CMD-C2D-C1D	5.65	134.68	124.73
24	B	604	CLA	CMD-C2D-C1D	5.65	134.67	124.73
24	B	614	CLA	CMD-C2D-C1D	5.65	134.67	124.73
24	b	618	CLA	CHD-C4C-C3C	-5.64	116.56	124.77
24	C	508	CLA	C2D-C1D-ND	5.63	115.70	110.13
24	B	617	CLA	C2D-C1D-ND	5.63	115.70	110.13
24	c	509	CLA	CHD-C4C-C3C	-5.63	116.57	124.77
24	C	509	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
24	B	606	CLA	CMD-C2D-C1D	5.61	134.61	124.73
24	C	503	CLA	C4A-NA-C1A	-5.61	104.12	106.68
24	B	610	CLA	C2D-C1D-ND	5.60	115.67	110.13
24	A	406	CLA	C2C-C1C-NC	5.60	115.86	109.98
24	b	620	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
24	d	403	CLA	C4A-NA-C1A	-5.58	104.13	106.68
24	b	623	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
24	c	510	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
24	A	407	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
24	c	515	CLA	CMD-C2D-C1D	5.56	134.52	124.73
24	C	511	CLA	CHD-C4C-C3C	-5.56	116.67	124.77
24	B	604	CLA	C4A-NA-C1A	-5.54	104.15	106.68
24	c	516	CLA	CMD-C2D-C1D	5.54	134.49	124.73
24	A	406	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	C	511	CLA	CMD-C2D-C1D	5.53	134.47	124.73
24	d	401	CLA	C2C-C1C-NC	5.53	115.79	109.98
24	b	613	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	c	516	CLA	C2B-C1B-NB	5.52	116.05	110.33
24	c	510	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	B	604	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	c	512	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	c	511	CLA	C2C-C1C-NC	5.50	115.76	109.98
25	A	408	PHO	C3D-C4D-ND	5.50	114.76	107.71
24	c	505	CLA	C2C-C1C-NC	5.50	115.76	109.98
24	c	511	CLA	CMD-C2D-C1D	5.50	134.41	124.73
24	c	514	CLA	CHD-C4C-C3C	-5.50	116.76	124.77
24	c	505	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
24	A	406	CLA	C3D-C2D-C1D	-5.49	98.34	105.83
24	B	613	CLA	CMD-C2D-C1D	5.49	134.39	124.73
25	a	411	PHO	C4D-ND-C1D	-5.48	102.30	108.87
24	B	607	CLA	O2D-CGD-CBD	5.47	120.79	111.23
24	b	612	CLA	C2D-C1D-ND	5.47	115.54	110.13
24	B	605	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
24	b	612	CLA	O2D-CGD-CBD	5.45	120.76	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	CMD-C2D-C1D	5.44	134.31	124.73
39	F	102	HEM	CHC-C4B-NB	5.44	130.27	124.42
24	c	516	CLA	C3B-C2B-C1B	-5.43	100.76	107.17
25	a	420[A]	PHO	C3D-C4D-ND	5.43	114.67	107.71
24	c	514	CLA	C2D-C1D-ND	5.43	115.50	110.13
24	B	615	CLA	C4A-NA-C1A	-5.42	104.20	106.68
24	C	504	CLA	CHD-C4C-C3C	-5.42	116.87	124.77
24	C	506	CLA	CHD-C4C-C3C	-5.42	116.87	124.77
24	B	611	CLA	C2C-C1C-NC	5.42	115.67	109.98
24	C	513	CLA	CHD-C4C-C3C	-5.41	116.88	124.77
24	c	509	CLA	C2C-C1C-NC	5.41	115.66	109.98
24	b	613	CLA	O2D-CGD-CBD	5.40	120.68	111.23
24	C	506	CLA	C2D-C1D-ND	5.39	115.46	110.13
24	D	403	CLA	CHD-C4C-C3C	-5.39	116.91	124.77
24	C	508	CLA	CHD-C4C-C3C	-5.39	116.92	124.77
25	a	411	PHO	C3D-C4D-ND	5.39	114.61	107.71
25	A	409[B]	PHO	C3D-C4D-ND	5.38	114.60	107.71
24	A	407	CLA	C4A-NA-C1A	-5.37	104.23	106.68
24	c	509	CLA	CMD-C2D-C1D	5.37	134.18	124.73
24	B	609	CLA	O2D-CGD-CBD	5.37	120.61	111.23
24	B	607	CLA	C4A-NA-C1A	-5.36	104.23	106.68
24	C	508	CLA	C4A-NA-C1A	-5.36	104.23	106.68
24	B	617	CLA	C4A-NA-C1A	-5.36	104.23	106.68
24	c	517	CLA	C4A-NA-C1A	-5.34	104.24	106.68
25	A	409[A]	PHO	C1-C2-C3	-5.34	117.45	126.20
24	C	513	CLA	C4A-NA-C1A	-5.33	104.25	106.68
24	D	402	CLA	CHD-C4C-C3C	-5.32	117.02	124.77
24	C	506	CLA	C2C-C1C-NC	5.30	115.55	109.98
24	B	609	CLA	C2C-C1C-NC	5.30	115.55	109.98
27	b	601	SQD	O6-C1-C2	5.29	116.30	108.27
27	f	102	SQD	O47-C7-C8	5.29	122.92	111.48
24	B	611	CLA	C2D-C1D-ND	5.28	115.35	110.13
25	a	420[B]	PHO	C3D-C4D-ND	5.27	114.47	107.71
24	b	612	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
24	d	402	CLA	C2D-C1D-ND	5.27	115.34	110.13
24	B	608	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
25	a	420[B]	PHO	C1-C2-C3	-5.26	117.57	126.20
24	b	623	CLA	C2C-C1C-NC	5.26	115.51	109.98
24	B	607	CLA	CHD-C4C-C3C	-5.25	117.11	124.77
24	B	605	CLA	O2D-CGD-CBD	5.25	120.41	111.23
24	B	607	CLA	C2C-C1C-NC	5.23	115.48	109.98
36	C	522	HTG	C1'-S1-C1	5.23	111.75	100.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	O2D-CGD-CBD	5.23	120.37	111.23
24	a	410	CLA	C4A-NA-C1A	-5.23	104.30	106.68
25	A	409[A]	PHO	C3D-C4D-ND	5.23	114.41	107.71
24	b	620	CLA	O2D-CGD-CBD	5.22	120.36	111.23
24	a	409	CLA	CHD-C4C-C3C	-5.22	117.17	124.77
24	C	511	CLA	C2C-C1C-NC	5.22	115.46	109.98
24	C	505	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
24	A	405	CLA	C2B-C1B-NB	5.21	115.73	110.33
24	b	611	CLA	C4A-NA-C1A	-5.21	104.30	106.68
24	b	618	CLA	C2D-C1D-ND	5.20	115.27	110.13
24	A	405	CLA	C2D-C1D-ND	5.20	115.27	110.13
24	b	621	CLA	C2C-C1C-NC	5.20	115.44	109.98
26	t	101	BCR	C33-C5-C6	-5.19	118.82	124.48
24	b	626	CLA	C4A-NA-C1A	-5.19	104.31	106.68
24	a	409	CLA	C4A-NA-C1A	-5.18	104.31	106.68
24	b	624	CLA	C2C-C1C-NC	5.18	115.43	109.98
24	c	508	CLA	C2C-C1C-NC	5.18	115.42	109.98
24	B	611	CLA	O2D-CGD-CBD	5.18	120.29	111.23
24	B	608	CLA	O2D-CGD-CBD	5.17	120.27	111.23
24	c	506	CLA	C3B-C2B-C1B	-5.16	101.08	107.17
24	C	512	CLA	CMD-C2D-C1D	5.15	133.80	124.73
24	A	405	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
24	c	512	CLA	O2D-CGD-CBD	5.15	120.23	111.23
25	a	420[A]	PHO	C1-C2-C3	-5.14	117.78	126.20
24	D	403	CLA	C4A-NA-C1A	-5.14	104.34	106.68
24	c	514	CLA	C2C-C1C-NC	5.13	115.37	109.98
24	b	617	CLA	O2D-CGD-CBD	5.12	120.17	111.23
24	B	612	CLA	C2C-C1C-NC	5.12	115.36	109.98
24	C	504	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
24	C	509	CLA	C1-C2-C3	-5.11	117.82	126.20
24	a	412	CLA	C2C-C1C-NC	5.11	115.35	109.98
24	c	517	CLA	C2B-C1B-NB	5.11	115.62	110.33
24	C	508	CLA	C2B-C1B-NB	5.10	115.62	110.33
24	C	513	CLA	C2B-C1B-NB	5.10	115.61	110.33
24	B	615	CLA	C2C-C1C-NC	5.09	115.33	109.98
24	C	510	CLA	C2D-C1D-ND	5.08	115.16	110.13
24	C	507	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
24	B	612	CLA	C4A-NA-C1A	-5.08	104.36	106.68
24	B	611	CLA	C3B-C2B-C1B	-5.08	101.19	107.17
24	a	409	CLA	C2D-C1D-ND	5.07	115.14	110.13
24	A	405	CLA	C2C-C1C-NC	5.07	115.30	109.98
24	c	509	CLA	C2D-C1D-ND	5.06	115.14	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	609	CLA	C3B-C2B-C1B	-5.06	101.20	107.17
24	b	624	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
24	A	410	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
24	B	611	CLA	C2B-C1B-NB	5.06	115.57	110.33
24	b	622	CLA	C2C-C1C-NC	5.05	115.29	109.98
24	C	509	CLA	C2C-C1C-NC	5.04	115.28	109.98
24	a	409	CLA	C2C-C1C-NC	5.04	115.28	109.98
24	c	511	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
24	c	512	CLA	C2C-C1C-NC	5.04	115.27	109.98
24	B	607	CLA	C2B-C1B-NB	5.04	115.55	110.33
24	b	619	CLA	C2C-C1C-NC	5.03	115.27	109.98
24	a	409	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
24	C	508	CLA	C2C-C1C-NC	5.03	115.26	109.98
24	C	502	CLA	C4A-NA-C1A	-5.02	104.39	106.68
24	c	517	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
24	c	508	CLA	C4A-NA-C1A	-5.02	104.39	106.68
27	B	621	SQD	O6-C1-C2	5.02	115.89	108.27
25	A	409[B]	PHO	C1-C2-C3	-5.02	117.97	126.20
24	b	615	CLA	C3D-C4D-ND	5.02	118.14	109.99
27	F	103	SQD	O47-C7-C8	5.01	122.33	111.48
24	c	515	CLA	C3B-C2B-C1B	-5.01	101.26	107.17
24	b	616	CLA	C2B-C1B-NB	5.01	115.52	110.33
24	B	606	CLA	O2D-CGD-CBD	5.00	119.97	111.23
24	A	406	CLA	O2D-CGD-CBD	5.00	119.97	111.23
24	c	507	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	A	407	CLA	C2B-C1B-NB	4.98	115.49	110.33
24	B	607	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
24	C	513	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
26	B	620	BCR	C15-C14-C13	-4.96	120.32	127.28
24	C	505	CLA	C2D-C1D-ND	4.96	115.03	110.13
24	C	507	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
24	b	612	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
24	C	504	CLA	C2C-C1C-NC	4.95	115.18	109.98
24	C	510	CLA	O2D-CGD-CBD	4.95	119.88	111.23
24	B	615	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
24	c	506	CLA	CMD-C2D-C1D	4.94	133.42	124.73
24	B	606	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
24	C	505	CLA	C2C-C1C-NC	4.93	115.16	109.98
27	A	412	SQD	O47-C7-C8	4.93	122.15	111.48
24	b	614	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
24	c	513	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	b	616	CLA	C3B-C2B-C1B	-4.92	101.37	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	O2D-CGD-CBD	4.92	119.83	111.23
24	A	406	CLA	C1C-C2C-C3C	-4.92	101.81	106.98
27	a	414	SQD	O6-C1-C2	4.91	115.73	108.27
24	B	611	CLA	CHD-C4C-C3C	-4.91	117.62	124.77
24	C	506	CLA	O2D-CGD-CBD	4.91	119.81	111.23
24	b	620	CLA	C4A-NA-C1A	-4.91	104.44	106.68
24	D	403	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
24	a	412	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
24	A	407	CLA	C3D-C4D-ND	4.89	117.94	109.99
24	c	513	CLA	O2D-CGD-CBD	4.89	119.78	111.23
24	d	403	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	A	407	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
24	c	513	CLA	C2C-C1C-NC	4.89	115.11	109.98
24	b	625	CLA	C2C-C1C-NC	4.88	115.11	109.98
24	b	621	CLA	C4A-NA-C1A	-4.88	104.45	106.68
41	v	205	HEC	CBB-CAB-C3B	-4.87	117.69	127.43
24	a	410	CLA	C3D-C4D-ND	4.87	117.91	109.99
36	C	523	HTG	C1-O5-C5	4.87	121.30	112.56
24	B	613	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
24	B	603	CLA	C2C-C1C-NC	4.85	115.07	109.98
24	c	514	CLA	O2D-CGD-CBD	4.84	119.69	111.23
24	C	510	CLA	C4A-NA-C1A	-4.84	104.47	106.68
24	b	623	CLA	C3B-C4B-NB	4.84	114.85	110.53
24	C	509	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
24	B	615	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
24	A	406	CLA	C3B-C4B-NB	4.84	114.85	110.53
36	c	524	HTG	C1'-S1-C1	4.83	110.89	100.45
24	D	403	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
24	b	618	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
24	B	604	CLA	C2C-C1C-NC	4.83	115.06	109.98
24	C	512	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
27	B	621	SQD	O47-C7-C8	4.83	121.94	111.48
36	B	625	HTG	O5-C1-C2	4.83	116.97	110.32
24	B	614	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
24	b	623	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
24	b	613	CLA	C2C-C1C-NC	4.82	115.05	109.98
24	B	606	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	c	506	CLA	C2B-C1B-NB	4.82	115.33	110.33
24	b	624	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
24	b	611	CLA	C2B-C1B-NB	4.82	115.32	110.33
24	b	616	CLA	C2C-C1C-NC	4.82	115.04	109.98
24	b	612	CLA	C2B-C1B-NB	4.81	115.32	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	406	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
24	C	510	CLA	C2C-C1C-NC	4.81	115.03	109.98
24	C	503	CLA	C2B-C1B-NB	4.81	115.31	110.33
24	a	410	CLA	O2D-CGD-CBD	4.80	119.62	111.23
24	B	613	CLA	C3C-C4C-NC	4.80	116.58	110.43
24	b	614	CLA	C4A-NA-C1A	-4.80	104.49	106.68
24	b	617	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	A	407	CLA	O2D-CGD-CBD	4.78	119.59	111.23
24	C	508	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
24	c	505	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
24	C	511	CLA	C3B-C4B-NB	4.77	114.79	110.53
24	b	622	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
24	c	515	CLA	C3D-C4D-ND	4.77	117.74	109.99
24	d	401	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	C	511	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
24	A	405	CLA	CHD-C4C-C3C	-4.77	117.82	124.77
24	B	607	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
24	B	616	CLA	C3B-C2B-C1B	-4.76	101.55	107.17
24	c	506	CLA	O2D-CGD-CBD	4.76	119.55	111.23
24	B	612	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
24	b	624	CLA	C4A-NA-C1A	-4.76	104.51	106.68
24	B	603	CLA	O2D-CGD-CBD	4.76	119.54	111.23
24	B	608	CLA	C2C-C1C-NC	4.75	114.97	109.98
37	e	101	DGD	O6E-C5E-C4E	4.75	118.27	109.70
24	C	502	CLA	C2C-C1C-NC	4.75	114.97	109.98
24	B	617	CLA	C2C-C1C-NC	4.75	114.97	109.98
26	T	103	BCR	C33-C5-C6	-4.74	119.31	124.48
24	C	508	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
24	a	412	CLA	O2D-CGD-CBD	4.74	119.52	111.23
24	C	503	CLA	C3D-C4D-ND	4.73	117.68	109.99
36	b	633	HTG	C1'-S1-C1	4.73	110.67	100.45
24	b	620	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	b	618	CLA	C2C-C1C-NC	4.73	114.95	109.98
24	b	622	CLA	O2D-CGD-CBD	4.73	119.49	111.23
24	B	603	CLA	C2B-C1B-NB	4.73	115.23	110.33
24	b	623	CLA	C4A-NA-C1A	-4.72	104.53	106.68
24	C	504	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
27	b	601	SQD	O47-C7-C8	4.72	121.69	111.48
24	B	616	CLA	C2B-C1B-NB	4.72	115.22	110.33
24	c	507	CLA	O2D-CGD-CBD	4.72	119.47	111.23
24	A	410	CLA	C2B-C1B-NB	4.72	115.22	110.33
24	C	502	CLA	C3D-C2D-C1D	-4.71	99.40	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	505	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
24	B	614	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
24	B	609	CLA	C2B-C1B-NB	4.71	115.21	110.33
24	A	406	CLA	C2B-C1B-NB	4.70	115.20	110.33
24	c	508	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
24	C	512	CLA	C4A-NA-C1A	-4.69	104.54	106.68
24	B	606	CLA	C1D-CHD-C4C	-4.69	116.05	126.02
24	B	603	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
24	c	515	CLA	C2B-C1B-NB	4.69	115.19	110.33
24	B	608	CLA	C3D-C2D-C1D	-4.69	99.44	105.83
24	c	510	CLA	C2C-C1C-NC	4.68	114.90	109.98
24	C	506	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	b	620	CLA	C3D-C4D-ND	4.68	117.59	109.99
24	b	617	CLA	C2C-C1C-NC	4.67	114.89	109.98
24	b	621	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	c	514	CLA	C3B-C2B-C1B	-4.67	101.67	107.17
24	b	619	CLA	C3D-C4D-ND	4.67	117.58	109.99
24	b	612	CLA	C3D-C4D-ND	4.67	117.57	109.99
24	C	513	CLA	C2C-C1C-NC	4.67	114.88	109.98
24	c	511	CLA	C3D-C2D-C1D	-4.66	99.46	105.83
24	C	513	CLA	C3D-C2D-C1D	-4.66	99.46	105.83
24	D	403	CLA	O2D-CGD-CBD	4.66	119.38	111.23
24	B	616	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
24	d	402	CLA	C3D-C4D-ND	4.66	117.56	109.99
24	c	507	CLA	C2B-C1B-NB	4.66	115.16	110.33
24	d	402	CLA	CHD-C4C-C3C	-4.66	117.98	124.77
24	a	410	CLA	C2B-C1B-NB	4.66	115.15	110.33
24	b	613	CLA	C4A-NA-C1A	-4.66	104.56	106.68
24	a	412	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
24	b	625	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	610	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
24	B	603	CLA	C3D-C4D-ND	4.64	117.53	109.99
24	B	617	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	C	502	CLA	C1-C2-C3	-4.63	118.61	126.20
24	C	511	CLA	O2D-CGD-CBD	4.63	119.33	111.23
24	D	402	CLA	C3D-C4D-ND	4.63	117.51	109.99
24	b	613	CLA	C3D-C4D-ND	4.63	117.51	109.99
24	C	512	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	c	510	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
24	c	510	CLA	C4A-NA-C1A	-4.62	104.57	106.68
24	C	512	CLA	C2B-C1B-NB	4.62	115.12	110.33
24	D	402	CLA	C1C-C2C-C3C	-4.62	102.12	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	d	403	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
24	b	615	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
36	B	633	HTG	C1'-S1-C1	4.61	110.41	100.45
24	B	617	CLA	C3B-C2B-C1B	-4.61	101.73	107.17
24	b	620	CLA	C2B-C1B-NB	4.61	115.10	110.33
34	a	415	LMG	O7-C10-C11	4.61	121.44	111.48
37	C	516	DGD	O2G-C1B-C2B	4.61	121.44	111.48
24	B	602	CLA	C3D-C4D-ND	4.60	117.47	109.99
24	c	507	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
24	c	514	CLA	C3D-C4D-ND	4.60	117.47	109.99
24	c	517	CLA	C3D-C4D-ND	4.60	117.46	109.99
24	C	501	CLA	C4A-NA-C1A	-4.60	104.58	106.68
24	C	501	CLA	C2C-C1C-NC	4.60	114.81	109.98
24	c	509	CLA	C3D-C4D-ND	4.60	117.46	109.99
24	B	612	CLA	C3B-C2B-C1B	-4.59	101.75	107.17
24	B	606	CLA	C3D-C4D-ND	4.59	117.45	109.99
24	B	604	CLA	C3D-C4D-ND	4.59	117.45	109.99
24	c	507	CLA	C3D-C4D-ND	4.59	117.45	109.99
24	a	412	CLA	C2B-C1B-NB	4.59	115.08	110.33
36	b	633	HTG	O5-C1-C2	4.58	116.64	110.32
24	D	403	CLA	C2B-C1B-NB	4.58	115.08	110.33
34	A	422	LMG	O7-C10-C11	4.57	121.38	111.48
24	C	502	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
36	C	523	HTG	C1'-S1-C1	4.57	110.33	100.45
24	b	619	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
24	C	509	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	c	516	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
24	b	624	CLA	C1-C2-C3	-4.56	118.72	126.20
24	D	403	CLA	C2C-C1C-NC	4.56	114.77	109.98
34	c	523	LMG	O7-C10-C11	4.56	121.35	111.48
24	b	626	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
24	d	401	CLA	C1C-C2C-C3C	-4.55	102.19	106.98
24	C	502	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	B	605	CLA	C3B-C4B-NB	4.55	114.59	110.53
24	B	606	CLA	C2B-C1B-NB	4.55	115.04	110.33
24	b	617	CLA	CHD-C1D-ND	-4.54	118.41	124.80
24	B	602	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
24	d	403	CLA	C3D-C4D-ND	4.54	117.37	109.99
24	b	615	CLA	CHD-C1D-ND	-4.54	118.42	124.80
24	B	613	CLA	C3D-C4D-ND	4.54	117.36	109.99
24	C	503	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	C	501	CLA	C3D-C4D-ND	4.53	117.36	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	409	CLA	C2B-C1B-NB	4.53	115.03	110.33
24	C	501	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	608	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	d	403	CLA	O2D-CGD-CBD	4.53	119.15	111.23
24	b	620	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	B	602	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	c	515	CLA	C2C-C1C-NC	4.53	114.74	109.98
24	c	506	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
24	D	403	CLA	C3D-C4D-ND	4.52	117.34	109.99
24	A	410	CLA	C4A-NA-C1A	-4.52	104.62	106.68
24	C	511	CLA	C3D-C4D-ND	4.52	117.33	109.99
24	d	401	CLA	C3D-C4D-ND	4.52	117.33	109.99
24	d	401	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
24	B	613	CLA	C3B-C2B-C1B	-4.52	101.85	107.17
36	B	625	HTG	C1'-S1-C1	4.51	110.20	100.45
24	b	617	CLA	C3D-C4D-ND	4.51	117.31	109.99
26	b	627	BCR	C33-C5-C6	-4.51	119.57	124.48
24	b	618	CLA	C2B-C1B-NB	4.51	115.00	110.33
24	b	614	CLA	C1C-C2C-C3C	-4.50	102.25	106.98
24	A	407	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	a	412	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	a	410	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
37	e	101	DGD	O2G-C1B-C2B	4.49	121.20	111.48
24	b	611	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
24	A	407	CLA	CHD-C1D-ND	-4.49	118.48	124.80
24	c	514	CLA	C3B-C4B-NB	4.49	114.54	110.53
24	B	604	CLA	C3B-C2B-C1B	-4.49	101.88	107.17
24	B	614	CLA	C3C-C4C-NC	4.49	116.18	110.43
24	b	620	CLA	C2C-C1C-NC	4.49	114.69	109.98
24	C	507	CLA	C2B-C1B-NB	4.48	114.98	110.33
24	a	412	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
24	b	616	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
34	C	520	LMG	O7-C10-C11	4.48	121.17	111.48
24	c	512	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
24	B	608	CLA	C3D-C4D-ND	4.47	117.25	109.99
24	B	612	CLA	C3D-C4D-ND	4.47	117.25	109.99
24	c	512	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
24	C	512	CLA	C2C-C1C-NC	4.47	114.67	109.98
24	B	611	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
24	d	401	CLA	C3B-C4B-NB	4.46	114.52	110.53
26	B	618	BCR	C33-C5-C6	-4.46	119.62	124.48
24	c	513	CLA	C3D-C2D-C1D	-4.46	99.74	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	611	CLA	C3D-C4D-ND	4.46	117.24	109.99
24	C	512	CLA	C3D-C4D-ND	4.46	117.23	109.99
36	c	525	HTG	C1'-S1-C1	4.46	110.07	100.45
24	c	508	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	c	514	CLA	C2B-C1B-NB	4.45	114.94	110.33
24	B	615	CLA	O2D-CGD-O1D	-4.45	115.18	123.85
24	c	510	CLA	C3D-C4D-ND	4.45	117.22	109.99
26	D	404	BCR	C33-C5-C6	-4.45	119.63	124.48
24	C	513	CLA	CHD-C1D-ND	-4.45	118.54	124.80
24	c	517	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	C	505	CLA	C2B-C1B-NB	4.45	114.94	110.33
24	B	616	CLA	C3D-C4D-ND	4.45	117.21	109.99
36	b	608	HTG	C1'-S1-C1	4.44	110.05	100.45
24	B	609	CLA	C3D-C2D-C1D	-4.44	99.78	105.83
24	a	409	CLA	C3D-C4D-ND	4.44	117.20	109.99
24	c	510	CLA	CHD-C1D-ND	-4.43	118.56	124.80
24	b	619	CLA	O2D-CGD-CBD	4.43	118.98	111.23
24	B	603	CLA	CHD-C1D-ND	-4.43	118.56	124.80
24	A	410	CLA	O2D-CGD-CBD	4.43	118.98	111.23
24	D	402	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
24	b	613	CLA	C2B-C1B-NB	4.43	114.92	110.33
24	C	509	CLA	O2D-CGD-CBD	4.43	118.98	111.23
24	A	410	CLA	C3D-C4D-ND	4.43	117.19	109.99
24	B	609	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
24	C	503	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
24	b	617	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
24	b	615	CLA	O2D-CGD-CBD	4.42	118.96	111.23
24	A	410	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
24	b	613	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
24	b	626	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
24	c	509	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
24	B	604	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
24	C	504	CLA	CHD-C1D-ND	-4.40	118.61	124.80
24	C	509	CLA	C3D-C4D-ND	4.40	117.14	109.99
24	b	626	CLA	C3B-C4B-NB	4.40	114.46	110.53
24	B	608	CLA	CHD-C1D-ND	-4.39	118.62	124.80
24	c	513	CLA	C4A-NA-C1A	-4.39	104.67	106.68
24	C	511	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	b	621	CLA	C3D-C4D-ND	4.39	117.12	109.99
24	c	517	CLA	O2D-CGD-CBD	4.39	118.90	111.23
24	B	610	CLA	C3D-C4D-ND	4.39	117.12	109.99
24	b	626	CLA	C3D-C4D-ND	4.39	117.12	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	513	CLA	C2B-C1B-NB	4.39	114.88	110.33
37	c	521	DGD	O2G-C1B-C2B	4.39	120.97	111.48
24	D	402	CLA	CHD-C1D-ND	-4.39	118.63	124.80
24	c	508	CLA	C3D-C4D-ND	4.39	117.12	109.99
24	B	610	CLA	C2C-C1C-NC	4.38	114.59	109.98
29	A	417	LMT	C1'-O5'-C5'	4.38	122.28	113.72
24	b	612	CLA	C2C-C1C-NC	4.38	114.58	109.98
24	b	622	CLA	C4A-NA-C1A	-4.38	104.68	106.68
24	b	621	CLA	O2D-CGD-CBD	4.38	118.88	111.23
24	c	516	CLA	C2C-C1C-NC	4.38	114.58	109.98
24	b	614	CLA	C3C-C4C-NC	4.37	116.02	110.43
24	b	626	CLA	C2C-C1C-NC	4.36	114.56	109.98
24	B	610	CLA	C2B-C1B-NB	4.36	114.85	110.33
24	b	618	CLA	C3D-C4D-ND	4.36	117.07	109.99
24	c	506	CLA	C2C-C1C-NC	4.36	114.56	109.98
24	C	510	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
24	A	410	CLA	C2C-C1C-NC	4.35	114.56	109.98
41	v	205	HEC	CHC-C4B-NB	4.35	129.19	124.45
27	A	412	SQD	O6-C1-C2	4.35	114.88	108.27
24	C	513	CLA	C3D-C4D-ND	4.35	117.06	109.99
24	B	616	CLA	CHD-C1D-ND	-4.35	118.68	124.80
24	C	507	CLA	C4A-NA-C1A	-4.35	104.69	106.68
24	d	401	CLA	O2D-CGD-CBD	4.35	118.83	111.23
24	d	402	CLA	C1C-C2C-C3C	-4.35	102.41	106.98
24	C	501	CLA	C2B-C1B-NB	4.34	114.83	110.33
24	d	402	CLA	CHD-C1D-ND	-4.34	118.69	124.80
24	B	603	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
24	A	407	CLA	C2C-C1C-NC	4.34	114.54	109.98
24	b	615	CLA	C3C-C4C-NC	4.34	115.99	110.43
24	a	409	CLA	CHD-C1D-ND	-4.34	118.69	124.80
24	C	502	CLA	C2B-C1B-NB	4.33	114.82	110.33
24	B	602	CLA	C2B-C1B-NB	4.33	114.82	110.33
24	b	625	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
24	C	510	CLA	C1-C2-C3	-4.33	119.11	126.20
24	c	514	CLA	C1-C2-C3	-4.33	119.11	126.20
24	b	622	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
24	B	611	CLA	C4A-NA-C1A	-4.33	104.70	106.68
24	A	405	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
24	d	403	CLA	C2C-C1C-NC	4.32	114.52	109.98
24	b	612	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
24	a	410	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
32	d	405[B]	PL9	C42-C43-C44	-4.32	117.75	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	504	CLA	C2B-C1B-NB	4.31	114.80	110.33
24	B	604	CLA	O2D-CGD-O1D	-4.31	115.45	123.85
26	y	101	BCR	C33-C5-C6	-4.31	119.78	124.48
24	A	405	CLA	C3D-C4D-ND	4.31	116.99	109.99
24	C	503	CLA	C2C-C1C-NC	4.31	114.50	109.98
24	b	611	CLA	C3B-C2B-C1B	-4.30	102.09	107.17
24	a	410	CLA	CHD-C1D-ND	-4.30	118.75	124.80
24	B	611	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	c	506	CLA	C3D-C4D-ND	4.30	116.98	109.99
24	B	602	CLA	C2C-C1C-NC	4.30	114.50	109.98
24	a	409	CLA	C1C-C2C-C3C	-4.30	102.46	106.98
24	B	612	CLA	C3C-C4C-NC	4.30	115.94	110.43
24	B	610	CLA	O2D-CGD-CBD	4.30	118.75	111.23
24	B	613	CLA	C2C-C1C-NC	4.30	114.50	109.98
24	D	403	CLA	CHD-C1D-ND	-4.30	118.75	124.80
24	C	507	CLA	C2C-C1C-NC	4.30	114.50	109.98
24	C	506	CLA	C3D-C4D-ND	4.30	116.97	109.99
24	B	614	CLA	C3B-C4B-NB	4.30	114.36	110.53
24	b	624	CLA	C3D-C4D-ND	4.29	116.96	109.99
24	b	625	CLA	C2B-C1B-NB	4.29	114.78	110.33
24	B	605	CLA	C1D-CHD-C4C	-4.29	116.91	126.02
24	b	622	CLA	C3C-C4C-NC	4.29	115.92	110.43
24	B	610	CLA	CMB-C2B-C1B	4.29	131.95	125.42
24	c	513	CLA	C3D-C4D-ND	4.29	116.95	109.99
24	b	612	CLA	CHD-C1D-ND	-4.28	118.78	124.80
24	B	605	CLA	C3C-C4C-NC	4.28	115.91	110.43
24	B	612	CLA	C2B-C1B-NB	4.28	114.76	110.33
24	B	606	CLA	C4A-NA-C1A	-4.28	104.73	106.68
24	C	504	CLA	C4A-NA-C1A	-4.27	104.73	106.68
24	B	605	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
24	C	509	CLA	C2B-C1B-NB	4.27	114.75	110.33
24	b	615	CLA	C2B-C1B-NB	4.27	114.75	110.33
24	c	510	CLA	O2D-CGD-CBD	4.27	118.69	111.23
24	C	504	CLA	CBC-CAC-C3C	-4.27	100.86	112.42
24	d	403	CLA	CHD-C1D-ND	-4.26	118.80	124.80
24	A	406	CLA	CBC-CAC-C3C	-4.26	100.86	112.42
24	C	504	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
24	C	506	CLA	C4A-NA-C1A	-4.26	104.73	106.68
24	b	625	CLA	C3D-C4D-ND	4.26	116.92	109.99
24	c	514	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
24	b	615	CLA	C2C-C1C-NC	4.26	114.45	109.98
24	c	511	CLA	C1C-C2C-C3C	-4.26	102.50	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	C2C-C1C-NC	4.26	114.45	109.98
24	c	508	CLA	CHD-C1D-ND	-4.26	118.81	124.80
24	b	621	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
24	c	510	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
24	B	612	CLA	O2D-CGD-CBD	4.25	118.66	111.23
24	B	617	CLA	C2B-C1B-NB	4.25	114.73	110.33
24	c	512	CLA	C3D-C4D-ND	4.25	116.89	109.99
39	e	102	HEM	CHC-C4B-NB	4.25	128.99	124.42
24	b	618	CLA	O2D-CGD-CBD	4.25	118.65	111.23
24	B	607	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
24	c	515	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
26	H	102	BCR	C38-C26-C25	-4.24	119.86	124.48
26	c	527	BCR	C15-C14-C13	-4.24	121.33	127.28
24	C	511	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
24	b	625	CLA	CHD-C1D-ND	-4.24	118.84	124.80
24	b	622	CLA	C2B-C1B-NB	4.24	114.72	110.33
24	B	609	CLA	C3D-C4D-ND	4.23	116.86	109.99
24	b	622	CLA	CMD-C2D-C1D	4.23	132.18	124.73
24	b	624	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
27	a	405	SQD	O47-C7-C8	4.23	120.62	111.48
24	C	502	CLA	C3D-C4D-ND	4.22	116.85	109.99
24	c	517	CLA	C2C-C1C-NC	4.22	114.42	109.98
24	C	501	CLA	C1D-CHD-C4C	-4.22	117.05	126.02
24	c	516	CLA	C3D-C4D-ND	4.22	116.85	109.99
24	b	619	CLA	CHD-C1D-ND	-4.22	118.87	124.80
26	d	404	BCR	C24-C23-C22	-4.21	120.00	126.23
24	b	613	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
26	T	103	BCR	C11-C10-C9	-4.21	121.37	127.28
24	c	517	CLA	CHD-C1D-ND	-4.21	118.88	124.80
24	a	409	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
24	D	402	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	b	614	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	b	616	CLA	C3D-C4D-ND	4.21	116.83	109.99
24	b	613	CLA	C3C-C4C-NC	4.21	115.82	110.43
24	B	610	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	b	613	CLA	C1D-CHD-C4C	-4.19	117.11	126.02
24	c	508	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
24	C	506	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
24	C	501	CLA	C3B-C2B-C1B	-4.19	102.24	107.17
24	c	511	CLA	C4A-NA-C1A	-4.18	104.77	106.68
24	B	615	CLA	C3D-C4D-ND	4.18	116.79	109.99
24	B	617	CLA	C1D-CHD-C4C	-4.18	117.13	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	616	CLA	C1D-CHD-C4C	-4.18	117.14	126.02
24	A	405	CLA	C1C-C2C-C3C	-4.18	102.59	106.98
24	B	608	CLA	C4A-NA-C1A	-4.18	104.77	106.68
24	c	515	CLA	C4A-NA-C1A	-4.18	104.77	106.68
24	C	503	CLA	CHD-C1D-ND	-4.17	118.93	124.80
24	B	608	CLA	C2B-C1B-NB	4.17	114.65	110.33
24	c	517	CLA	C1D-CHD-C4C	-4.16	117.17	126.02
24	b	623	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	d	403	CLA	C2B-C1B-NB	4.16	114.64	110.33
24	C	510	CLA	C3D-C4D-ND	4.16	116.74	109.99
37	D	406	DGD	O2G-C1B-C2B	4.16	120.47	111.48
24	B	614	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
24	B	615	CLA	C2B-C1B-NB	4.15	114.63	110.33
38	D	409	LHG	O7-C7-C8	4.15	120.45	111.48
24	b	622	CLA	C1D-CHD-C4C	-4.15	117.21	126.02
24	c	511	CLA	C3C-C4C-NC	4.14	115.74	110.43
24	b	615	CLA	C1D-CHD-C4C	-4.14	117.22	126.02
24	B	606	CLA	CMC-C2C-C1C	4.14	131.50	125.03
24	c	507	CLA	C3C-C4C-NC	4.14	115.73	110.43
24	c	510	CLA	C2B-C1B-NB	4.14	114.62	110.33
24	C	505	CLA	C3D-C4D-ND	4.14	116.71	109.99
24	c	512	CLA	C2B-C1B-NB	4.13	114.61	110.33
24	B	610	CLA	CHD-C1D-ND	-4.13	118.98	124.80
24	B	614	CLA	C2B-C1B-NB	4.13	114.61	110.33
24	C	508	CLA	C3D-C4D-ND	4.13	116.70	109.99
24	c	507	CLA	C1D-CHD-C4C	-4.13	117.24	126.02
24	A	406	CLA	C3D-C4D-ND	4.13	116.70	109.99
24	B	607	CLA	C3D-C4D-ND	4.13	116.70	109.99
24	d	402	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
41	V	206	HEC	CBB-CAB-C3B	-4.12	119.19	127.43
24	b	611	CLA	C2C-C1C-NC	4.12	114.31	109.98
24	B	604	CLA	C2B-C1B-NB	4.12	114.60	110.33
24	C	503	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
24	c	508	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
24	c	513	CLA	C1D-CHD-C4C	-4.12	117.27	126.02
24	b	624	CLA	C2B-C1B-NB	4.11	114.59	110.33
24	c	513	CLA	C3B-C4B-NB	4.11	114.20	110.53
24	d	402	CLA	C1-C2-C3	-4.11	119.46	126.20
24	B	613	CLA	C4A-NA-C1A	-4.11	104.81	106.68
24	c	510	CLA	C1-C2-C3	-4.10	119.47	126.20
24	B	602	CLA	CHD-C1D-ND	-4.10	119.03	124.80
24	a	412	CLA	C1-C2-C3	-4.10	119.48	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
24	b	626	CLA	CAC-C3C-C4C	4.10	130.12	124.79
24	C	504	CLA	C3D-C4D-ND	4.10	116.65	109.99
24	b	619	CLA	C1C-C2C-C3C	-4.09	102.67	106.98
24	c	505	CLA	C2B-C1B-NB	4.09	114.57	110.33
24	B	606	CLA	C3C-C4C-NC	4.09	115.67	110.43
24	D	402	CLA	C3B-C4B-NB	4.09	114.18	110.53
24	B	602	CLA	C4A-NA-C1A	-4.09	104.81	106.68
24	b	617	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
24	C	505	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
24	b	615	CLA	C3B-C2B-C1B	-4.09	102.35	107.17
24	c	509	CLA	C3C-C4C-NC	4.08	115.66	110.43
32	D	405[B]	PL9	C42-C43-C44	-4.08	118.29	127.62
24	b	611	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
24	b	625	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
24	b	624	CLA	CHD-C1D-ND	-4.07	119.07	124.80
39	F	102	HEM	CAD-CBD-CGD	4.07	124.46	113.67
24	c	509	CLA	C2B-C1B-NB	4.07	114.55	110.33
24	C	508	CLA	C3B-C4B-NB	4.07	114.16	110.53
24	B	607	CLA	CHD-C1D-ND	-4.07	119.08	124.80
24	c	514	CLA	CHD-C1D-ND	-4.07	119.08	124.80
24	B	616	CLA	C2C-C1C-NC	4.07	114.25	109.98
24	b	617	CLA	C2B-C1B-NB	4.07	114.54	110.33
24	b	623	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
24	B	611	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
24	b	611	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	C	505	CLA	C3C-C4C-NC	4.06	115.63	110.43
24	b	620	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	B	602	CLA	O2D-CGD-O1D	-4.06	115.95	123.85
24	c	506	CLA	C3C-C4C-NC	4.06	115.63	110.43
24	c	516	CLA	C1D-CHD-C4C	-4.06	117.40	126.02
24	b	622	CLA	C3B-C4B-NB	4.05	114.15	110.53
24	c	510	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
24	C	503	CLA	C3C-C4C-NC	4.05	115.62	110.43
29	A	417	LMT	O5'-C5'-C4'	4.05	118.10	109.72
24	C	510	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
24	b	621	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
24	c	515	CLA	C1D-CHD-C4C	-4.05	117.42	126.02
27	a	414	SQD	O47-C7-C8	4.05	120.23	111.48
24	B	616	CLA	C1D-CHD-C4C	-4.05	117.42	126.02
24	B	604	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
24	B	602	CLA	C1D-CHD-C4C	-4.04	117.43	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	416[A]	PL9	C22-C23-C24	-4.03	118.39	127.62
24	d	402	CLA	O2D-CGD-CBD	4.03	118.28	111.23
24	d	402	CLA	C3B-C4B-NB	4.03	114.13	110.53
24	C	507	CLA	CHD-C1D-ND	-4.03	119.13	124.80
24	b	618	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
24	B	616	CLA	CMB-C2B-C1B	4.03	131.55	125.42
24	C	509	CLA	CHD-C1D-ND	-4.02	119.14	124.80
29	a	404	LMT	O5'-C5'-C4'	4.02	118.04	109.72
24	B	605	CLA	C3B-C2B-C1B	-4.02	102.43	107.17
24	B	617	CLA	C3C-C4C-NC	4.02	115.58	110.43
39	e	102	HEM	CHD-C1D-ND	4.02	128.75	124.42
24	C	509	CLA	C1C-C2C-C3C	-4.02	102.76	106.98
29	a	404	LMT	C1'-O5'-C5'	4.01	121.56	113.72
24	b	621	CLA	C2B-C1B-NB	4.01	114.49	110.33
24	a	409	CLA	C1D-CHD-C4C	-4.01	117.50	126.02
24	b	611	CLA	O2D-CGD-O1D	-4.01	116.05	123.85
32	a	416[A]	PL9	C32-C33-C34	-4.01	118.45	127.62
24	B	606	CLA	C2C-C1C-NC	4.00	114.19	109.98
24	B	616	CLA	C3C-C4C-NC	4.00	115.56	110.43
24	B	611	CLA	CAA-C2A-C3A	-4.00	102.19	113.00
36	H	101	HTG	C1'-S1-C1	4.00	109.08	100.45
24	b	624	CLA	C3C-C4C-NC	3.99	115.54	110.43
24	b	626	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
24	B	615	CLA	C1C-C2C-C3C	-3.99	102.79	106.98
24	B	604	CLA	CAA-C2A-C3A	-3.99	102.23	113.00
24	c	505	CLA	C3D-C4D-ND	3.98	116.46	109.99
24	B	615	CLA	CHD-C1D-ND	-3.98	119.20	124.80
29	D	401	LMT	O1B-C4'-C3'	3.98	117.34	107.23
24	B	606	CLA	CMB-C2B-C1B	3.98	131.47	125.42
24	b	622	CLA	C1-C2-C3	-3.98	119.68	126.20
24	d	401	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
24	c	505	CLA	C3C-C4C-NC	3.97	115.52	110.43
24	b	626	CLA	C2B-C1B-NB	3.97	114.44	110.33
24	a	409	CLA	C1-C2-C3	-3.96	119.70	126.20
24	C	513	CLA	O2D-CGD-CBD	3.96	118.16	111.23
36	B	624	HTG	C1'-S1-C1	3.96	109.01	100.45
27	A	416	SQD	O48-C23-C24	3.96	123.91	111.83
24	C	502	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
24	B	607	CLA	C1D-CHD-C4C	-3.95	117.61	126.02
24	c	511	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
24	b	616	CLA	CHD-C1D-ND	-3.95	119.24	124.80
24	C	508	CLA	C3C-C4C-NC	3.95	115.49	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	515	CLA	CHD-C1D-ND	-3.95	119.24	124.80
24	B	612	CLA	C1C-C2C-C3C	-3.95	102.82	106.98
24	C	511	CLA	CHD-C1D-ND	-3.95	119.24	124.80
24	c	509	CLA	CMB-C2B-C1B	3.95	131.43	125.42
24	C	510	CLA	C3B-C4B-NB	3.94	114.05	110.53
36	b	632	HTG	C1'-S1-C1	3.94	108.97	100.45
24	a	412	CLA	CHD-C1D-ND	-3.94	119.25	124.80
25	a	411	PHO	O1D-CGD-CBD	-3.94	118.75	124.72
24	C	507	CLA	C3C-C4C-NC	3.94	115.48	110.43
37	c	520	DGD	O2G-C1B-C2B	3.94	120.01	111.48
24	b	623	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	C	510	CLA	C2B-C1B-NB	3.94	114.41	110.33
24	c	512	CLA	C3B-C4B-NB	3.94	114.05	110.53
24	B	604	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
24	c	509	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
38	D	407	LHG	O7-C7-C8	3.93	119.99	111.48
24	c	508	CLA	C3C-C4C-NC	3.93	115.47	110.43
26	T	103	BCR	C15-C16-C17	-3.93	115.48	123.52
24	B	617	CLA	C3D-C4D-ND	3.93	116.37	109.99
24	A	406	CLA	C1D-CHD-C4C	-3.93	117.68	126.02
24	C	511	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
26	y	101	BCR	C15-C14-C13	-3.92	121.78	127.28
24	c	505	CLA	CAC-C3C-C4C	3.92	129.89	124.79
24	b	622	CLA	C3D-C4D-ND	3.92	116.36	109.99
24	C	507	CLA	C3D-C4D-ND	3.91	116.34	109.99
24	C	506	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
24	A	405	CLA	CHD-C1D-ND	-3.91	119.30	124.80
24	c	514	CLA	C1C-C2C-C3C	-3.90	102.87	106.98
34	Z	101	LMG	O7-C10-C11	3.90	119.92	111.48
24	B	603	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
24	c	507	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	C	506	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	c	511	CLA	C3D-C4D-ND	3.89	116.32	109.99
24	A	410	CLA	C3C-C4C-NC	3.89	115.42	110.43
24	b	614	CLA	C3B-C4B-NB	3.89	114.00	110.53
24	d	401	CLA	CHD-C1D-ND	-3.89	119.33	124.80
24	c	513	CLA	C1-C2-C3	-3.89	119.82	126.20
24	C	508	CLA	CHD-C1D-ND	-3.89	119.33	124.80
37	e	101	DGD	C3E-C4E-C5E	3.89	117.28	110.23
24	C	504	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
25	A	408	PHO	C1A-C2A-C3A	-3.88	99.15	102.84
24	B	612	CLA	C1D-CHD-C4C	-3.88	117.78	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	519	DGD	O2G-C1B-C2B	3.87	119.86	111.48
24	B	612	CLA	C1-C2-C3	-3.87	119.85	126.20
24	B	612	CLA	CHD-C1D-ND	-3.87	119.36	124.80
24	C	512	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
24	d	402	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
24	B	606	CLA	CHD-C4C-NC	3.86	130.22	124.23
24	B	615	CLA	C3C-C4C-NC	3.86	115.38	110.43
25	A	408	PHO	CBC-CAC-C3C	-3.86	107.35	112.87
24	b	623	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
24	B	612	CLA	CMC-C2C-C1C	3.85	131.05	125.03
24	b	626	CLA	CHD-C1D-ND	-3.85	119.39	124.80
24	c	508	CLA	C2B-C1B-NB	3.85	114.31	110.33
24	c	505	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
26	C	515	BCR	C33-C5-C6	-3.84	120.29	124.48
24	B	611	CLA	CHD-C1D-ND	-3.84	119.39	124.80
24	b	621	CLA	CHD-C1D-ND	-3.84	119.39	124.80
24	B	603	CLA	C1-C2-C3	-3.84	119.90	126.20
24	b	613	CLA	CHD-C1D-ND	-3.84	119.40	124.80
24	B	609	CLA	C4A-NA-C1A	-3.84	104.93	106.68
24	B	607	CLA	C3B-C4B-NB	3.84	113.95	110.53
24	C	513	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
24	b	623	CLA	C1D-CHD-C4C	-3.83	117.87	126.02
24	C	511	CLA	CAC-C3C-C4C	3.83	129.78	124.79
24	c	505	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
24	b	613	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
24	C	502	CLA	C3C-C4C-NC	3.83	115.33	110.43
24	d	403	CLA	C3C-C4C-NC	3.83	115.33	110.43
24	C	501	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
24	b	616	CLA	C3C-C4C-NC	3.82	115.33	110.43
24	D	402	CLA	C1-C2-C3	-3.82	119.94	126.20
24	B	615	CLA	CAC-C3C-C4C	3.82	129.76	124.79
24	c	512	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
24	c	515	CLA	O2D-CGD-CBD	3.82	117.90	111.23
24	C	512	CLA	C3C-C4C-NC	3.81	115.32	110.43
24	b	619	CLA	C3B-C2B-C1B	-3.81	102.67	107.17
24	B	609	CLA	C3B-C4B-NB	3.81	113.94	110.53
24	C	511	CLA	C4A-NA-C1A	-3.81	104.94	106.68
24	c	512	CLA	C3C-C4C-NC	3.81	115.31	110.43
24	D	403	CLA	C3B-C4B-NB	3.81	113.93	110.53
24	b	625	CLA	C3B-C4B-NB	3.81	113.93	110.53
24	a	409	CLA	CAA-C2A-C3A	-3.81	102.71	113.00
24	b	616	CLA	C3B-C4B-NB	3.81	113.93	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
24	b	618	CLA	C1D-CHD-C4C	-3.80	117.93	126.02
24	c	506	CLA	CHD-C1D-ND	-3.80	119.45	124.80
27	a	405	SQD	O48-C23-C24	3.80	123.43	111.83
39	F	102	HEM	CHD-C4C-NC	3.80	128.59	124.45
26	b	628	BCR	C29-C30-C25	3.80	115.96	110.44
24	b	624	CLA	O2D-CGD-O1D	-3.80	116.45	123.85
38	E	101	LHG	O7-C7-C8	3.80	119.69	111.48
24	C	505	CLA	CMB-C2B-C1B	3.79	131.19	125.42
24	A	407	CLA	C1C-C2C-C3C	-3.79	103.00	106.98
24	b	623	CLA	C3C-C4C-NC	3.79	115.28	110.43
24	D	402	CLA	CMC-C2C-C1C	3.78	130.95	125.03
24	B	610	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
24	b	612	CLA	CAC-C3C-C4C	3.78	129.70	124.79
26	C	514	BCR	C7-C8-C9	-3.78	120.65	126.23
24	A	406	CLA	CHD-C1D-ND	-3.78	119.49	124.80
32	a	416[B]	PL9	C7-C8-C9	-3.77	120.33	126.83
24	C	512	CLA	CHD-C1D-ND	-3.77	119.50	124.80
27	b	601	SQD	C3-C4-C5	3.77	117.06	110.23
24	d	403	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
24	c	509	CLA	C1C-C2C-C3C	-3.77	103.02	106.98
24	D	402	CLA	CAC-C3C-C4C	3.76	129.68	124.79
24	B	609	CLA	CHD-C1D-ND	-3.76	119.52	124.80
24	c	510	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
24	b	614	CLA	CMC-C2C-C1C	3.75	130.90	125.03
24	b	624	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
24	b	616	CLA	C1C-C2C-C3C	-3.75	103.03	106.98
24	b	620	CLA	C1-C2-C3	-3.75	120.05	126.20
24	B	609	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
26	C	515	BCR	C7-C8-C9	-3.75	120.69	126.23
24	c	506	CLA	C1D-CHD-C4C	-3.75	118.05	126.02
24	a	410	CLA	C2C-C1C-NC	3.75	113.92	109.98
24	c	515	CLA	C1-C2-C3	-3.75	120.06	126.20
24	b	622	CLA	CAC-C3C-C4C	3.75	129.66	124.79
24	B	604	CLA	C3C-C4C-NC	3.75	115.23	110.43
24	d	402	CLA	C2B-C1B-NB	3.74	114.21	110.33
24	C	506	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
24	c	511	CLA	CHD-C1D-ND	-3.74	119.54	124.80
24	C	506	CLA	CAC-C3C-C4C	3.74	129.66	124.79
24	b	612	CLA	CAA-C2A-C3A	-3.74	102.89	113.00
24	c	516	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
24	b	623	CLA	C1-C2-C3	-3.73	120.09	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	501	CLA	CHD-C1D-ND	-3.73	119.56	124.80
24	B	605	CLA	CHD-C1D-ND	-3.72	119.56	124.80
24	C	505	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
27	A	416	SQD	O47-C7-C8	3.72	119.53	111.48
24	C	507	CLA	CMB-C2B-C1B	3.72	131.08	125.42
26	H	102	BCR	C16-C17-C18	-3.72	122.06	127.28
26	c	527	BCR	C16-C17-C18	-3.72	122.06	127.28
34	C	519	LMG	O7-C10-C11	3.72	119.52	111.48
24	c	511	CLA	C2B-C1B-NB	3.71	114.18	110.33
34	c	522	LMG	O8-C28-C29	3.71	123.15	111.83
24	b	617	CLA	C3C-C4C-NC	3.71	115.18	110.43
24	b	618	CLA	CHD-C1D-ND	-3.71	119.58	124.80
37	C	517	DGD	O2G-C1B-C2B	3.71	119.50	111.48
24	D	402	CLA	O2D-CGD-CBD	3.70	117.71	111.23
24	B	613	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
24	b	623	CLA	C4B-C3B-C2B	-3.70	102.70	107.30
24	B	608	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	c	513	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	C	513	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	c	510	CLA	C3B-C4B-NB	3.70	113.83	110.53
24	B	613	CLA	CMC-C2C-C1C	3.70	130.81	125.03
24	c	510	CLA	CBC-CAC-C3C	-3.70	102.40	112.42
24	C	504	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
24	C	501	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	C	507	CLA	C1D-CHD-C4C	-3.70	118.17	126.02
24	c	512	CLA	C1D-CHD-C4C	-3.70	118.17	126.02
24	b	621	CLA	C3C-C4C-NC	3.69	115.16	110.43
24	A	410	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
38	l	101	LHG	O7-C7-C8	3.69	119.47	111.48
24	b	619	CLA	C2B-C1B-NB	3.69	114.15	110.33
24	c	513	CLA	CHD-C1D-ND	-3.69	119.61	124.80
24	B	613	CLA	C2B-C1B-NB	3.68	114.15	110.33
24	c	512	CLA	CHD-C1D-ND	-3.68	119.62	124.80
24	c	516	CLA	C3C-C4C-NC	3.68	115.15	110.43
24	A	405	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
24	B	602	CLA	C3C-C4C-NC	3.68	115.14	110.43
38	d	407	LHG	O7-C7-C8	3.68	119.44	111.48
26	c	518	BCR	C7-C8-C9	-3.67	120.80	126.23
24	a	410	CLA	C3C-C4C-NC	3.67	115.14	110.43
24	c	515	CLA	C3B-C4B-NB	3.67	113.81	110.53
24	D	402	CLA	C2B-C1B-NB	3.67	114.13	110.33
24	c	505	CLA	CHD-C1D-ND	-3.67	119.64	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C2B-C1B-NB	3.67	114.13	110.33
24	C	511	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
24	C	502	CLA	CHD-C1D-ND	-3.67	119.64	124.80
24	b	613	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
24	B	604	CLA	CHD-C1D-ND	-3.66	119.65	124.80
24	B	603	CLA	C3C-C4C-NC	3.66	115.12	110.43
24	C	504	CLA	C3B-C4B-NB	3.66	113.80	110.53
24	C	508	CLA	C1D-CHD-C4C	-3.66	118.25	126.02
32	a	416[A]	PL9	C7-C3-C4	3.66	119.92	116.91
24	b	626	CLA	C3C-C4C-NC	3.65	115.11	110.43
24	b	625	CLA	C3C-C4C-NC	3.65	115.10	110.43
24	c	513	CLA	C3C-C4C-NC	3.65	115.10	110.43
24	C	512	CLA	C1-C2-C3	-3.64	120.23	126.20
24	b	618	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
24	A	405	CLA	O2D-CGD-CBD	3.64	117.60	111.23
26	d	404	BCR	C33-C5-C6	-3.64	120.51	124.48
32	a	416[B]	PL9	C32-C33-C34	-3.64	119.29	127.62
24	C	505	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
24	D	403	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
27	F	103	SQD	O5-C5-C4	3.64	116.26	109.70
24	a	412	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
24	a	410	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
26	D	404	BCR	C24-C23-C22	-3.64	120.85	126.23
26	b	627	BCR	C7-C8-C9	-3.64	120.86	126.23
24	c	516	CLA	CHD-C1D-ND	-3.64	119.69	124.80
24	b	617	CLA	CAA-C2A-C3A	-3.64	103.17	113.00
32	A	420[A]	PL9	C7-C3-C4	3.63	119.90	116.91
32	a	416[B]	PL9	C7-C3-C4	3.63	119.90	116.91
24	d	401	CLA	C3C-C4C-NC	3.63	115.08	110.43
34	b	630	LMG	O7-C10-C11	3.63	119.33	111.48
24	C	507	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	b	617	CLA	C4A-NA-C1A	-3.63	105.03	106.68
24	A	405	CLA	C3B-C4B-NB	3.62	113.77	110.53
27	a	414	SQD	C1-C2-C3	-3.62	102.39	110.01
36	B	632	HTG	C1'-S1-C1	3.62	108.27	100.45
24	d	402	CLA	C4B-C3B-C2B	-3.62	102.80	107.30
27	A	412	SQD	C45-O47-C7	-3.62	109.13	117.80
24	C	503	CLA	CMB-C2B-C1B	3.62	130.93	125.42
24	b	619	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
24	C	503	CLA	O2D-CGD-CBD	3.62	117.55	111.23
24	C	510	CLA	C3C-C4C-NC	3.61	115.06	110.43
26	h	101	BCR	C16-C17-C18	-3.61	122.21	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	C3B-C4B-NB	3.61	113.75	110.53
24	C	509	CLA	C3B-C4B-NB	3.61	113.75	110.53
24	B	614	CLA	C1-C2-C3	-3.61	120.29	126.20
24	B	605	CLA	CMB-C2B-C1B	3.60	130.90	125.42
24	B	613	CLA	CHD-C1D-ND	-3.60	119.73	124.80
24	b	612	CLA	C3C-C4C-NC	3.59	115.03	110.43
24	b	619	CLA	C3C-C4C-NC	3.59	115.03	110.43
24	b	620	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
24	A	410	CLA	CHD-C1D-ND	-3.59	119.75	124.80
24	C	510	CLA	CHD-C1D-ND	-3.59	119.75	124.80
24	d	401	CLA	C2B-C1B-NB	3.58	114.04	110.33
26	C	514	BCR	C15-C14-C13	-3.58	122.25	127.28
24	B	605	CLA	C4B-C3B-C2B	-3.58	102.85	107.30
37	D	406	DGD	C1D-C2D-C3D	3.58	117.55	110.01
24	c	505	CLA	C3B-C4B-NB	3.58	113.73	110.53
32	a	416[B]	PL9	C7-C3-C2	-3.58	119.17	123.39
24	B	610	CLA	C3B-C4B-NB	3.58	113.72	110.53
26	c	518	BCR	C33-C5-C6	-3.58	120.58	124.48
24	C	510	CLA	C1C-C2C-C3C	-3.58	103.22	106.98
24	b	622	CLA	C4C-C3C-C2C	-3.57	101.69	106.89
32	a	416[B]	PL9	C22-C23-C24	-3.57	119.44	127.62
24	c	515	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
24	B	611	CLA	C3B-C4B-NB	3.57	113.72	110.53
24	D	402	CLA	C3C-C4C-NC	3.57	115.00	110.43
24	A	405	CLA	CAA-C2A-C3A	-3.57	103.36	113.00
32	A	420[A]	PL9	C32-C33-C34	-3.57	119.46	127.62
24	b	625	CLA	CMB-C2B-C1B	3.57	130.85	125.42
24	B	603	CLA	C1D-CHD-C4C	-3.56	118.44	126.02
24	b	617	CLA	C1D-CHD-C4C	-3.56	118.44	126.02
26	d	404	BCR	C38-C26-C25	-3.56	120.59	124.48
37	h	102	DGD	O2G-C1B-C2B	3.56	119.18	111.48
24	C	509	CLA	C3C-C4C-NC	3.56	114.99	110.43
26	K	101	BCR	C15-C14-C13	-3.56	122.28	127.28
32	A	420[B]	PL9	C37-C38-C39	-3.56	119.47	127.62
24	C	501	CLA	C3C-C4C-NC	3.56	114.99	110.43
36	B	623	HTG	C1'-S1-C1	3.56	108.13	100.45
24	b	619	CLA	CMB-C2B-C1B	3.56	130.84	125.42
24	d	403	CLA	CAC-C3C-C4C	3.56	129.42	124.79
24	b	620	CLA	C3C-C4C-NC	3.55	114.98	110.43
24	A	410	CLA	CAC-C3C-C4C	3.55	129.41	124.79
24	b	611	CLA	C3C-C4C-NC	3.55	114.98	110.43
24	c	514	CLA	C1D-CHD-C4C	-3.55	118.47	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	F	103	SQD	O6-C1-C2	3.55	113.66	108.27
32	a	416[A]	PL9	C15-C14-C16	3.55	121.39	115.23
24	b	621	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
24	C	513	CLA	C3C-C4C-NC	3.55	114.97	110.43
32	A	420[B]	PL9	C32-C33-C34	-3.54	119.51	127.62
24	B	602	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
34	c	522	LMG	O7-C10-C11	3.54	119.14	111.48
24	c	516	CLA	C1-C2-C3	-3.54	120.39	126.20
24	b	612	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
24	b	613	CLA	C3B-C4B-NB	3.54	113.69	110.53
24	b	618	CLA	C3C-C4C-NC	3.54	114.96	110.43
24	B	614	CLA	C4A-NA-C1A	-3.54	105.06	106.68
24	a	412	CLA	C4A-NA-C1A	-3.54	105.07	106.68
24	b	615	CLA	CHD-C4C-NC	3.53	129.71	124.23
24	B	611	CLA	C1D-CHD-C4C	-3.53	118.52	126.02
24	d	402	CLA	C3C-C4C-NC	3.53	114.95	110.43
24	c	517	CLA	C1-C2-C3	-3.53	120.41	126.20
32	a	416[A]	PL9	C7-C8-C9	-3.53	120.75	126.83
24	B	608	CLA	CAA-C2A-C3A	-3.52	103.47	113.00
24	c	505	CLA	C4A-NA-C1A	-3.52	105.07	106.68
24	B	607	CLA	C3C-C4C-NC	3.52	114.94	110.43
34	a	415	LMG	C8-O7-C10	-3.52	109.36	117.80
34	z	101	LMG	O7-C10-C11	3.52	119.10	111.48
24	c	517	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
24	A	410	CLA	C1-C2-C3	-3.52	120.44	126.20
24	b	614	CLA	C3D-C4D-ND	3.51	115.70	109.99
24	B	615	CLA	CMC-C2C-C1C	3.51	130.52	125.03
24	B	615	CLA	C1D-CHD-C4C	-3.51	118.55	126.02
24	B	613	CLA	C4-C3-C5	3.51	121.33	115.23
24	c	508	CLA	C3B-C4B-NB	3.51	113.66	110.53
24	B	615	CLA	O2A-CGA-O1A	-3.51	114.85	123.63
29	C	521	LMT	O1B-C4'-C3'	3.51	116.15	107.23
24	B	617	CLA	C3B-C4B-NB	3.51	113.66	110.53
25	A	409[A]	PHO	C1A-C2A-C3A	-3.51	99.50	102.84
32	a	416[A]	PL9	C7-C3-C2	-3.51	119.26	123.39
24	C	508	CLA	C1C-C2C-C3C	-3.51	103.29	106.98
41	V	206	HEC	CHC-C4B-NB	3.50	128.27	124.45
24	c	505	CLA	C1D-CHD-C4C	-3.50	118.57	126.02
24	b	623	CLA	O2D-CGD-CBD	3.50	117.36	111.23
24	c	509	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
26	k	101	BCR	C24-C23-C22	-3.50	121.05	126.23
32	A	420[A]	PL9	C7-C3-C2	-3.50	119.26	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	626	CLA	C4C-C3C-C2C	-3.49	101.81	106.89
32	d	405[A]	PL9	C42-C43-C44	-3.49	119.63	127.62
24	b	617	CLA	CMB-C2B-C1B	3.49	130.73	125.42
24	B	609	CLA	C3C-C4C-NC	3.49	114.90	110.43
26	t	101	BCR	C15-C16-C17	-3.49	116.39	123.52
24	C	506	CLA	C3C-C4C-NC	3.48	114.89	110.43
24	D	403	CLA	C1D-CHD-C4C	-3.48	118.62	126.02
24	C	508	CLA	C1-C2-C3	-3.48	120.50	126.20
24	c	508	CLA	C1-C2-C3	-3.48	120.50	126.20
25	a	420[A]	PHO	C1A-C2A-C3A	-3.48	99.53	102.84
24	D	403	CLA	CAC-C3C-C4C	3.48	129.31	124.79
24	B	613	CLA	C1D-CHD-C4C	-3.48	118.63	126.02
24	A	407	CLA	C4-C3-C5	3.48	121.26	115.23
24	a	412	CLA	C3C-C4C-NC	3.48	114.88	110.43
24	C	509	CLA	C4A-NA-C1A	-3.48	105.09	106.68
27	a	405	SQD	O8-S-C6	3.48	112.68	105.97
24	A	405	CLA	C3C-C4C-NC	3.48	114.88	110.43
25	a	420[A]	PHO	O2D-CGD-O1D	-3.47	117.09	123.85
24	C	502	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
38	L	101	LHG	O7-C7-C8	3.47	118.99	111.48
24	c	517	CLA	C3C-C4C-NC	3.47	114.88	110.43
24	B	607	CLA	C1-C2-C3	-3.47	120.52	126.20
24	B	603	CLA	CAA-C2A-C3A	-3.46	103.64	113.00
32	a	416[A]	PL9	C17-C18-C19	-3.46	119.69	127.62
24	C	512	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
24	C	504	CLA	C3C-C4C-NC	3.46	114.87	110.43
24	b	625	CLA	O2D-CGD-CBD	3.46	117.28	111.23
24	C	509	CLA	C1D-CHD-C4C	-3.45	118.68	126.02
26	d	404	BCR	C7-C8-C9	-3.45	121.12	126.23
32	d	405[B]	PL9	C27-C28-C29	-3.45	119.72	127.62
24	d	402	CLA	CAC-C3C-C4C	3.45	129.28	124.79
24	C	511	CLA	C3C-C4C-NC	3.45	114.85	110.43
24	D	403	CLA	C3C-C4C-NC	3.45	114.85	110.43
24	B	608	CLA	C1D-CHD-C4C	-3.45	118.69	126.02
32	D	405[B]	PL9	C37-C38-C39	-3.45	119.74	127.62
24	B	613	CLA	C4C-C3C-C2C	-3.44	101.88	106.89
24	B	607	CLA	CAC-C3C-C4C	3.44	129.27	124.79
24	C	507	CLA	CMC-C2C-C1C	3.44	130.41	125.03
24	A	405	CLA	CAC-C3C-C4C	3.44	129.26	124.79
24	b	615	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
24	B	608	CLA	C3C-C4C-NC	3.44	114.83	110.43
24	a	412	CLA	CMB-C2B-C1B	3.44	130.65	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C33-C5-C6	-3.43	120.74	124.48
36	b	602	HTG	C1'-S1-C1	3.43	107.86	100.45
24	C	502	CLA	CMB-C2B-C1B	3.43	130.65	125.42
34	D	412	LMG	O7-C10-C11	3.43	118.90	111.48
24	a	409	CLA	C3B-C4B-NB	3.43	113.59	110.53
24	C	510	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
26	C	514	BCR	C33-C5-C6	-3.43	120.75	124.48
24	C	512	CLA	CMB-C2B-C1B	3.42	130.63	125.42
26	B	619	BCR	C29-C30-C25	3.42	115.41	110.44
24	b	621	CLA	C3B-C4B-NB	3.42	113.59	110.53
24	b	625	CLA	C1C-C2C-C3C	-3.42	103.38	106.98
24	B	614	CLA	C1D-CHD-C4C	-3.42	118.75	126.02
24	B	606	CLA	CHD-C1D-ND	-3.42	119.99	124.80
24	C	508	CLA	CAC-C3C-C4C	3.42	129.24	124.79
39	F	102	HEM	C1B-NB-C4B	3.42	109.25	105.21
24	b	611	CLA	CHD-C4C-NC	3.41	129.53	124.23
24	A	406	CLA	C4B-C3B-C2B	-3.41	103.07	107.30
24	b	612	CLA	O2D-CGD-O1D	-3.41	117.22	123.85
24	D	403	CLA	C4-C3-C5	3.40	121.13	115.23
24	A	406	CLA	CHC-C1C-C2C	-3.40	117.29	126.95
29	C	521	LMT	C1'-O5'-C5'	3.40	120.36	113.72
24	b	614	CLA	CHD-C1D-ND	-3.40	120.02	124.80
24	c	514	CLA	C4-C3-C5	3.39	121.12	115.23
24	b	611	CLA	C1C-C2C-C3C	-3.39	103.41	106.98
34	c	523	LMG	O6-C5-C4	3.39	115.81	109.70
26	K	101	BCR	C7-C8-C9	-3.39	121.22	126.23
25	a	420[B]	PHO	C1A-C2A-C3A	-3.39	99.61	102.84
24	b	611	CLA	C3B-C4B-NB	3.39	113.56	110.53
25	A	408	PHO	O1D-CGD-CBD	-3.39	119.58	124.72
24	B	614	CLA	C3D-C4D-ND	3.38	115.49	109.99
32	A	420[B]	PL9	C7-C3-C2	-3.38	119.40	123.39
24	c	510	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
24	c	507	CLA	CMB-C2B-C1B	3.38	130.56	125.42
24	b	617	CLA	CBC-CAC-C3C	-3.38	103.26	112.42
24	C	506	CLA	CBC-CAC-C3C	-3.37	103.27	112.42
24	A	407	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
24	B	611	CLA	CHC-C1C-C2C	-3.37	117.37	126.95
24	c	511	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
24	c	514	CLA	C3C-C4C-NC	3.37	114.75	110.43
24	B	610	CLA	C3C-C4C-NC	3.37	114.75	110.43
39	e	102	HEM	CHD-C4C-NC	3.37	128.12	124.45
24	B	617	CLA	C4C-C3C-C2C	-3.37	101.99	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	608	CLA	C3B-C4B-NB	3.37	113.53	110.53
24	d	401	CLA	C4A-NA-C1A	-3.36	105.14	106.68
24	b	622	CLA	O2A-CGA-O1A	-3.36	115.22	123.63
26	Y	101	BCR	C15-C14-C13	-3.36	122.56	127.28
24	B	610	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
24	C	508	CLA	C4C-C3C-C2C	-3.36	102.00	106.89
24	B	616	CLA	CHD-C4C-NC	3.36	129.44	124.23
24	b	614	CLA	C1-C2-C3	-3.36	120.70	126.20
32	D	405[A]	PL9	C42-C43-C44	-3.36	119.94	127.62
24	c	509	CLA	CHD-C1D-ND	-3.35	120.09	124.80
24	b	622	CLA	O2A-CGA-CBA	3.35	122.04	111.83
26	D	404	BCR	C29-C30-C25	3.34	115.30	110.44
32	a	416[A]	PL9	C37-C38-C39	-3.34	119.98	127.62
24	D	402	CLA	C1D-CHD-C4C	-3.34	118.93	126.02
26	D	404	BCR	C38-C26-C25	-3.34	120.84	124.48
24	B	611	CLA	O2A-CGA-CBA	3.34	122.00	111.83
24	c	506	CLA	C4C-C3C-C2C	-3.33	102.04	106.89
24	B	602	CLA	O2A-CGA-CBA	3.33	122.00	111.83
32	A	420[B]	PL9	C7-C3-C4	3.33	119.65	116.91
24	b	617	CLA	C3B-C4B-NB	3.33	113.50	110.53
24	b	611	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
24	B	602	CLA	CHD-C4C-NC	3.33	129.39	124.23
24	C	512	CLA	C3B-C4B-NB	3.33	113.50	110.53
24	b	617	CLA	CHD-C4C-NC	3.33	129.39	124.23
24	b	615	CLA	C4C-C3C-C2C	-3.32	102.05	106.89
24	c	506	CLA	C1C-C2C-C3C	-3.32	103.48	106.98
24	B	602	CLA	C3B-C4B-NB	3.32	113.49	110.53
24	C	505	CLA	CHD-C1D-ND	-3.32	120.13	124.80
24	A	407	CLA	CBC-CAC-C3C	-3.32	103.42	112.42
34	B	622	LMG	O8-C28-C29	3.32	121.95	111.83
32	a	416[A]	PL9	C27-C28-C29	-3.32	120.03	127.62
24	c	508	CLA	C4-C3-C5	3.31	120.98	115.23
32	d	405[A]	PL9	C37-C38-C39	-3.31	120.04	127.62
24	B	605	CLA	C2B-C1B-NB	3.31	113.76	110.33
39	e	102	HEM	C1B-NB-C4B	3.31	109.13	105.21
24	B	612	CLA	CMB-C2B-C1B	3.31	130.46	125.42
24	B	604	CLA	CMC-C2C-C1C	3.31	130.21	125.03
24	c	507	CLA	CAC-C3C-C4C	3.31	129.09	124.79
26	y	101	BCR	C16-C17-C18	-3.31	122.64	127.28
24	b	623	CLA	CHD-C1D-ND	-3.30	120.15	124.80
24	c	515	CLA	C3C-C4C-NC	3.30	114.66	110.43
26	B	619	BCR	C2-C1-C6	3.30	115.24	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	420[A]	PL9	C37-C38-C39	-3.30	120.06	127.62
24	a	412	CLA	C3B-C4B-NB	3.30	113.48	110.53
24	b	613	CLA	CMC-C2C-C1C	3.30	130.19	125.03
26	B	620	BCR	C38-C26-C25	-3.30	120.89	124.48
36	B	624	HTG	C1-O5-C5	3.30	118.47	112.56
24	A	407	CLA	C3C-C4C-NC	3.29	114.65	110.43
32	a	416[B]	PL9	C37-C38-C39	-3.29	120.09	127.62
32	D	405[A]	PL9	C37-C38-C39	-3.29	120.10	127.62
24	C	513	CLA	C1-C2-C3	-3.29	120.81	126.20
24	B	605	CLA	C4A-NA-C1A	-3.28	105.18	106.68
24	B	603	CLA	C3B-C4B-NB	3.28	113.46	110.53
24	b	621	CLA	C1-C2-C3	-3.28	120.82	126.20
24	B	606	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
24	B	603	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
27	f	102	SQD	C1-O5-C5	3.28	120.13	113.72
24	B	612	CLA	C3B-C4B-NB	3.28	113.46	110.53
26	k	101	BCR	C7-C8-C9	-3.28	121.39	126.23
24	C	502	CLA	C3B-C4B-NB	3.28	113.46	110.53
32	a	416[B]	PL9	C17-C18-C19	-3.28	120.12	127.62
26	Y	101	BCR	C10-C11-C12	-3.28	113.71	123.20
24	B	614	CLA	O2D-CGD-CBD	3.27	116.95	111.23
26	C	514	BCR	C16-C17-C18	-3.27	122.69	127.28
24	C	508	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
24	B	617	CLA	C1-O2A-CGA	3.27	124.56	116.65
24	B	605	CLA	C3D-C4D-ND	3.27	115.30	109.99
26	D	404	BCR	C28-C27-C26	-3.26	108.23	114.06
26	k	101	BCR	C20-C21-C22	-3.26	122.71	127.28
24	D	402	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
24	c	507	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
24	A	410	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
24	b	612	CLA	CMB-C2B-C1B	3.25	130.37	125.42
24	B	607	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
24	c	514	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
32	A	420[B]	PL9	C22-C23-C24	-3.25	120.19	127.62
24	B	613	CLA	C1-C2-C3	-3.25	120.88	126.20
24	A	406	CLA	CHD-C4C-NC	3.24	129.26	124.23
24	b	620	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
24	b	614	CLA	C2B-C1B-NB	3.24	113.69	110.33
24	d	401	CLA	CMB-C2B-C1B	3.24	130.35	125.42
24	d	403	CLA	C1C-C2C-C3C	-3.24	103.57	106.98
32	D	405[B]	PL9	C7-C8-C9	-3.24	121.25	126.83
24	b	614	CLA	C4B-C3B-C2B	-3.24	103.28	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	618	CLA	C3B-C4B-NB	3.23	113.42	110.53
24	c	506	CLA	C3B-C4B-NB	3.23	113.42	110.53
32	a	416[B]	PL9	C15-C14-C16	3.23	120.84	115.23
24	B	614	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
24	B	617	CLA	CHD-C1D-ND	-3.23	120.26	124.80
24	B	613	CLA	C3B-C4B-NB	3.23	113.41	110.53
24	c	515	CLA	CAC-C3C-C4C	3.22	128.99	124.79
24	c	506	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
34	C	519	LMG	O8-C28-C29	3.22	121.67	111.83
24	b	620	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
24	C	501	CLA	CMC-C2C-C1C	3.22	130.06	125.03
24	c	514	CLA	C4A-NA-C1A	-3.22	105.21	106.68
24	B	615	CLA	C3B-C4B-NB	3.22	113.40	110.53
32	a	416[A]	PL9	C42-C43-C44	-3.22	120.26	127.62
24	b	612	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
24	A	407	CLA	CMB-C2B-C1B	3.22	130.31	125.42
38	d	406	LHG	O8-C23-O10	-3.21	115.59	123.63
24	d	402	CLA	CHC-C1C-C2C	-3.21	117.83	126.95
24	C	509	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
24	B	606	CLA	O2A-CGA-CBA	3.21	121.62	111.83
24	C	511	CLA	CHC-C1C-C2C	-3.21	117.83	126.95
24	c	516	CLA	CHD-C4C-NC	3.21	129.20	124.23
26	c	518	BCR	C15-C14-C13	-3.21	122.78	127.28
32	d	405[A]	PL9	C27-C28-C29	-3.20	120.29	127.62
32	a	416[B]	PL9	C27-C28-C29	-3.20	120.29	127.62
24	C	506	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
38	l	101	LHG	O8-C23-C24	3.20	121.59	111.83
24	b	622	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
37	H	103	DGD	O2G-C1B-C2B	3.20	118.40	111.48
24	b	617	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
24	c	509	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
37	e	101	DGD	O5D-C1E-C2E	3.20	113.13	108.27
24	d	401	CLA	C2A-C1A-CHA	-3.20	118.32	123.87
24	c	508	CLA	CMC-C2C-C1C	3.20	130.03	125.03
24	d	401	CLA	CAA-C2A-C3A	-3.20	104.36	113.00
41	V	206	HEC	CHA-C1A-NA	3.20	127.93	124.45
24	b	620	CLA	C3B-C4B-NB	3.20	113.38	110.53
24	B	611	CLA	CAC-C3C-C4C	3.20	128.95	124.79
24	B	613	CLA	C1C-C2C-C3C	-3.19	103.62	106.98
24	D	402	CLA	CHC-C1C-C2C	-3.19	117.88	126.95
24	B	615	CLA	C4-C3-C5	3.19	120.77	115.23
24	C	503	CLA	C1C-C2C-C3C	-3.19	103.63	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	606	CLA	C4-C3-C5	3.18	120.76	115.23
24	a	409	CLA	C3C-C4C-NC	3.18	114.51	110.43
24	b	625	CLA	CAC-C3C-C4C	3.18	128.93	124.79
37	c	519	DGD	C2G-O2G-C1B	-3.18	110.19	117.80
41	v	205	HEC	CBC-CAC-C3C	-3.18	121.08	127.43
32	a	416[B]	PL9	C42-C43-C44	-3.18	120.35	127.62
32	D	405[B]	PL9	C40-C39-C41	3.18	120.74	115.23
24	C	512	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
24	B	617	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
24	b	626	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
24	b	616	CLA	CMC-C2C-C1C	3.17	129.99	125.03
24	d	403	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
24	b	623	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
27	B	621	SQD	O7-S-C6	3.17	111.49	106.76
24	b	612	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
24	c	511	CLA	CMB-C2B-C1B	3.17	130.24	125.42
25	A	409[A]	PHO	C4-C3-C5	3.16	120.72	115.23
24	b	622	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
24	A	410	CLA	CMC-C2C-C1C	3.16	129.98	125.03
24	B	616	CLA	O2D-CGD-CBD	3.16	116.76	111.23
24	C	502	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
34	B	622	LMG	O7-C10-C11	3.16	118.31	111.48
24	b	624	CLA	CMC-C2C-C1C	3.16	129.97	125.03
25	A	409[B]	PHO	C1A-C2A-C3A	-3.16	99.84	102.84
24	B	613	CLA	CAC-C3C-C4C	3.16	128.90	124.79
24	C	501	CLA	CMB-C2B-C1B	3.15	130.22	125.42
24	A	406	CLA	C3C-C4C-NC	3.15	114.47	110.43
38	D	409	LHG	O8-C23-C24	3.15	121.44	111.83
24	b	624	CLA	C3B-C4B-NB	3.15	113.34	110.53
24	b	617	CLA	CMC-C2C-C1C	3.15	129.95	125.03
24	B	617	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
24	b	623	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
24	b	621	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
24	b	613	CLA	CAC-C3C-C4C	3.14	128.88	124.79
24	c	505	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
37	h	102	DGD	O1G-C1A-C2A	3.14	121.41	111.83
24	b	615	CLA	C2A-C1A-CHA	-3.14	118.42	123.87
24	C	503	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
24	a	409	CLA	O2D-CGD-CBD	3.14	116.71	111.23
26	A	411	BCR	C33-C5-C6	-3.14	121.06	124.48
24	B	612	CLA	CAC-C3C-C4C	3.13	128.87	124.79
26	t	101	BCR	C15-C14-C13	3.13	131.67	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	607	CLA	CMC-C2C-C1C	3.13	129.93	125.03
24	B	610	CLA	CHD-C4C-NC	3.13	129.09	124.23
24	A	406	CLA	C4A-NA-C1A	-3.13	105.25	106.68
25	a	420[A]	PHO	C4-C3-C5	3.13	120.66	115.23
24	B	616	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
41	v	205	HEC	CHA-C1A-NA	3.13	127.86	124.45
39	e	102	HEM	CHB-C1B-NB	3.13	128.24	124.37
24	b	626	CLA	O2A-CGA-CBA	3.13	121.37	111.83
32	A	420[A]	PL9	C20-C19-C21	3.13	120.66	115.23
24	C	506	CLA	C4-C3-C5	3.12	120.65	115.23
26	B	619	BCR	C28-C27-C26	-3.12	108.48	114.06
24	a	410	CLA	C1C-C2C-C3C	-3.12	103.69	106.98
24	d	402	CLA	O2A-CGA-CBA	3.12	121.36	111.83
24	c	512	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
24	B	610	CLA	CAC-C3C-C4C	3.12	128.85	124.79
24	c	508	CLA	C4B-C3B-C2B	-3.12	103.43	107.30
24	C	505	CLA	C4C-C3C-C2C	-3.12	102.36	106.89
38	d	408	LHG	O7-C7-C8	3.12	118.22	111.48
24	b	626	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
24	C	511	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
24	b	621	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
24	b	625	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
24	C	508	CLA	CHC-C1C-C2C	-3.11	118.10	126.95
24	c	510	CLA	C3C-C4C-NC	3.11	114.42	110.43
24	d	401	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
32	D	405[A]	PL9	C7-C8-C9	-3.11	121.47	126.83
26	B	620	BCR	C32-C1-C6	-3.11	105.37	110.24
26	K	101	BCR	C20-C21-C22	-3.11	122.92	127.28
24	b	620	CLA	CAC-C3C-C4C	3.11	128.83	124.79
24	c	514	CLA	CHC-C1C-C2C	-3.11	118.12	126.95
24	D	403	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
25	A	409[A]	PHO	CMB-C2B-C3B	3.11	130.89	124.68
24	C	511	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
24	b	611	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
34	Z	101	LMG	O6-C5-C4	3.11	115.30	109.70
32	a	416[A]	PL9	C10-C9-C11	3.11	120.62	115.23
24	A	410	CLA	CMB-C2B-C1B	3.10	130.14	125.42
24	B	616	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
24	A	406	CLA	CAA-C2A-C3A	-3.10	104.62	113.00
24	d	401	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
24	c	505	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
37	h	102	DGD	O1G-C1A-O1A	-3.10	115.87	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	506	CLA	CMB-C2B-C1B	3.10	130.14	125.42
26	C	514	BCR	C20-C21-C22	-3.10	122.93	127.28
32	A	420[A]	PL9	C22-C23-C24	-3.10	120.53	127.62
24	A	410	CLA	C4C-C3C-C2C	-3.10	102.39	106.89
24	c	517	CLA	CHD-C4C-NC	3.10	129.03	124.23
24	B	607	CLA	CHC-C1C-C2C	-3.10	118.15	126.95
24	B	616	CLA	CMC-C2C-C1C	3.10	129.87	125.03
24	B	614	CLA	CMB-C2B-C1B	3.09	130.13	125.42
38	E	101	LHG	O8-C23-C24	3.09	121.26	111.83
24	C	504	CLA	CAC-C3C-C4C	3.09	128.81	124.79
36	b	609	HTG	C1'-S1-C1	3.09	107.12	100.45
24	B	604	CLA	CHD-C4C-NC	3.09	129.02	124.23
24	b	616	CLA	O2A-CGA-CBA	3.09	121.25	111.83
38	D	407	LHG	O8-C23-C24	3.09	121.25	111.83
24	B	608	CLA	CAC-C3C-C4C	3.09	128.80	124.79
24	b	614	CLA	CAC-C3C-C4C	3.09	128.80	124.79
26	K	101	BCR	C24-C23-C22	-3.08	121.67	126.23
26	B	620	BCR	C10-C11-C12	-3.08	114.27	123.20
32	a	416[A]	PL9	C20-C19-C21	3.08	120.58	115.23
37	H	103	DGD	O1G-C1A-C2A	3.08	121.24	111.83
37	C	518	DGD	O2G-C1B-C2B	3.08	118.15	111.48
27	A	412	SQD	C1-O5-C5	-3.08	107.70	113.72
24	B	613	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
24	b	613	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
24	b	613	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
24	C	504	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
24	B	614	CLA	CHD-C1D-ND	-3.08	120.47	124.80
24	C	507	CLA	CHD-C4C-NC	3.07	129.00	124.23
24	B	605	CLA	CHC-C1C-C2C	-3.07	118.21	126.95
26	B	618	BCR	C7-C8-C9	-3.07	121.69	126.23
24	A	405	CLA	O2A-CGA-CBA	3.07	121.20	111.83
24	a	412	CLA	CAA-C2A-C3A	-3.07	104.70	113.00
36	C	523	HTG	O5-C5-C4	3.07	115.23	109.70
26	B	619	BCR	C31-C1-C6	-3.07	105.43	110.24
24	B	613	CLA	C2A-C1A-CHA	-3.07	118.54	123.87
32	A	420[B]	PL9	C7-C8-C9	-3.07	121.55	126.83
24	b	625	CLA	CHC-C1C-C2C	-3.07	118.24	126.95
24	D	403	CLA	CMB-C2B-C1B	3.07	130.09	125.42
24	B	615	CLA	O2A-CGA-CBA	3.06	121.17	111.83
29	T	104	LMT	C1'-O5'-C5'	3.06	119.70	113.72
24	B	607	CLA	CBC-CAC-C3C	-3.06	104.12	112.42
24	B	610	CLA	C4B-C3B-C2B	-3.06	103.50	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	510	CLA	C4-C3-C5	3.06	120.54	115.23
24	d	403	CLA	C3B-C4B-NB	3.06	113.26	110.53
24	C	504	CLA	CMC-C2C-C1C	3.06	129.81	125.03
24	c	509	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
32	A	420[B]	PL9	C20-C19-C21	3.06	120.53	115.23
24	b	615	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
32	A	420[A]	PL9	C7-C8-C9	-3.05	121.57	126.83
24	b	621	CLA	CAC-C3C-C4C	3.05	128.76	124.79
24	C	505	CLA	C1-O2A-CGA	3.05	124.04	116.65
24	B	614	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
24	b	611	CLA	CHC-C1C-C2C	-3.05	118.28	126.95
32	A	420[A]	PL9	C27-C28-C29	-3.05	120.64	127.62
24	C	506	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
24	b	618	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
32	D	405[A]	PL9	C10-C9-C11	3.05	120.52	115.23
39	e	102	HEM	CHA-C4D-ND	3.05	128.13	124.37
24	c	517	CLA	CMC-C2C-C1C	3.05	129.79	125.03
24	c	510	CLA	CHD-C4C-NC	3.04	128.95	124.23
24	C	502	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
24	C	512	CLA	CHD-C4C-NC	3.04	128.95	124.23
24	c	513	CLA	O2A-CGA-CBA	3.04	121.11	111.83
24	b	614	CLA	O2A-CGA-CBA	3.04	121.11	111.83
38	d	406	LHG	O8-C23-C24	3.04	121.11	111.83
24	B	609	CLA	CBC-CAC-C3C	-3.04	104.18	112.42
24	A	410	CLA	CAA-C2A-C3A	-3.04	104.79	113.00
24	b	617	CLA	CHC-C1C-C2C	-3.04	118.31	126.95
24	A	410	CLA	C4-C3-C5	3.04	120.50	115.23
37	c	521	DGD	O1G-C1A-C2A	3.04	121.10	111.83
24	b	616	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
24	B	612	CLA	CHD-C4C-NC	3.04	128.94	124.23
24	B	607	CLA	C4-C3-C5	3.04	120.50	115.23
24	b	615	CLA	C4-C3-C5	3.03	120.50	115.23
24	C	508	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
24	c	507	CLA	CMC-C2C-C1C	3.03	129.77	125.03
24	B	603	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
24	B	602	CLA	CMB-C2B-C1B	3.03	130.03	125.42
24	B	606	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
24	B	607	CLA	C4B-C3B-C2B	-3.03	103.54	107.30
24	c	509	CLA	CAC-C3C-C4C	3.03	128.73	124.79
24	a	412	CLA	CHD-C4C-NC	3.03	128.93	124.23
24	b	626	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
24	C	513	CLA	CAC-C3C-C4C	3.03	128.73	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	610	CLA	CHC-C1C-C2C	-3.03	118.35	126.95
32	A	420[A]	PL9	C42-C43-C44	-3.02	120.70	127.62
24	B	611	CLA	C3C-C4C-NC	3.02	114.30	110.43
24	b	623	CLA	O2A-CGA-CBA	3.02	121.05	111.83
24	C	503	CLA	O2A-CGA-CBA	3.02	121.05	111.83
32	a	416[B]	PL9	C20-C19-C21	3.02	120.47	115.23
24	B	604	CLA	C2A-C1A-CHA	-3.02	118.63	123.87
24	B	602	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
24	b	621	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
24	B	605	CLA	C1-C2-C3	-3.01	121.26	126.20
24	b	625	CLA	C4C-C3C-C2C	-3.01	102.50	106.89
24	B	604	CLA	O2A-CGA-O1A	-3.01	116.10	123.63
24	b	625	CLA	CHD-C4C-NC	3.01	128.90	124.23
24	c	507	CLA	C1C-C2C-C3C	-3.01	103.81	106.98
24	d	402	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
24	a	410	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
24	c	507	CLA	C1-C2-C3	-3.01	121.27	126.20
24	C	512	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
27	F	103	SQD	O48-C23-C24	3.01	121.00	111.83
24	d	402	CLA	C1D-CHD-C4C	-3.01	119.63	126.02
24	a	410	CLA	C1-C2-C3	-3.00	121.28	126.20
24	b	623	CLA	CAC-C3C-C4C	3.00	128.70	124.79
24	a	410	CLA	CHD-C4C-NC	3.00	128.89	124.23
24	B	609	CLA	O2A-CGA-CBA	3.00	120.99	111.83
41	V	206	HEC	CHD-C4C-NC	3.00	127.72	124.45
24	a	410	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
26	B	618	BCR	C16-C17-C18	-3.00	123.08	127.28
24	C	510	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
32	D	405[B]	PL9	C22-C23-C24	-2.99	120.77	127.62
25	a	420[A]	PHO	CMB-C2B-C3B	2.99	130.66	124.68
24	c	510	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
26	c	518	BCR	C16-C17-C18	-2.99	123.08	127.28
24	b	613	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
34	c	523	LMG	C3-C4-C5	2.99	115.65	110.23
32	d	405[B]	PL9	C37-C38-C39	-2.99	120.79	127.62
24	c	515	CLA	O2A-CGA-CBA	2.99	120.94	111.83
24	b	616	CLA	C4-C3-C5	2.99	120.41	115.23
24	b	619	CLA	C3B-C4B-NB	2.99	113.19	110.53
24	B	603	CLA	C4B-C3B-C2B	-2.98	103.59	107.30
24	C	509	CLA	O2A-CGA-CBA	2.98	120.93	111.83
24	a	409	CLA	CAA-C2A-C1A	-2.98	102.20	111.97
24	d	401	CLA	CHD-C4C-NC	2.98	128.85	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	613	CLA	O2A-CGA-CBA	2.98	120.93	111.83
24	c	515	CLA	CHD-C4C-NC	2.98	128.85	124.23
24	c	512	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
24	a	412	CLA	C4-C3-C5	2.98	120.40	115.23
41	V	206	HEC	CBC-CAC-C3C	-2.98	121.48	127.43
24	d	402	CLA	C4-C3-C5	2.98	120.40	115.23
26	d	404	BCR	C29-C30-C25	2.98	114.76	110.44
24	b	619	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
24	c	513	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
24	B	612	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
24	A	405	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
24	C	506	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	C	501	CLA	CHD-C4C-NC	2.97	128.83	124.23
24	a	409	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
24	c	512	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
24	a	412	CLA	CMC-C2C-C1C	2.96	129.66	125.03
24	B	610	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
37	D	406	DGD	O1G-C1A-C2A	2.96	120.86	111.83
24	B	614	CLA	C4-C3-C5	2.96	120.36	115.23
24	B	608	CLA	CMC-C2C-C1C	2.96	129.65	125.03
24	c	509	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
24	B	617	CLA	CHC-C1C-C2C	-2.95	118.55	126.95
32	a	416[B]	PL9	C10-C9-C11	2.95	120.36	115.23
27	a	414	SQD	C44-O6-C1	-2.95	107.46	113.80
24	b	622	CLA	C4-C3-C5	2.95	120.36	115.23
24	B	609	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
24	C	511	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
24	C	510	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
24	a	409	CLA	C2A-C1A-CHA	-2.94	118.76	123.87
24	C	509	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
24	C	504	CLA	C4-C3-C5	2.94	120.33	115.23
24	C	506	CLA	C1-C2-C3	-2.94	121.38	126.20
24	C	504	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
24	B	608	CLA	C1-C2-C3	-2.94	121.38	126.20
24	B	605	CLA	C4C-C3C-C2C	-2.94	102.62	106.89
24	d	403	CLA	CHD-C4C-NC	2.93	128.78	124.23
24	A	410	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
24	B	609	CLA	CHC-C1C-C2C	-2.93	118.61	126.95
24	c	516	CLA	CMC-C2C-C1C	2.93	129.61	125.03
24	a	412	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
24	C	501	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
26	T	103	BCR	C36-C18-C19	2.93	122.56	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	618	BCR	C15-C14-C13	-2.92	123.18	127.28
24	B	614	CLA	CAC-C3C-C4C	2.92	128.59	124.79
24	C	501	CLA	CBC-CAC-C3C	-2.92	104.49	112.42
24	b	623	CLA	C4-C3-C5	2.92	120.30	115.23
32	A	420[B]	PL9	C27-C28-C29	-2.92	120.94	127.62
24	D	402	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
24	B	609	CLA	CMA-C3A-C4A	-2.92	103.92	111.77
32	D	405[A]	PL9	C22-C23-C24	-2.92	120.94	127.62
24	B	617	CLA	CHD-C4C-NC	2.92	128.76	124.23
24	c	513	CLA	CHD-C4C-NC	2.92	128.76	124.23
24	c	517	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
26	c	527	BCR	C33-C5-C6	-2.92	121.30	124.48
32	D	405[B]	PL9	C17-C18-C19	-2.92	120.94	127.62
24	B	605	CLA	C4-C3-C5	2.92	120.29	115.23
32	d	405[B]	PL9	C40-C39-C41	2.92	120.29	115.23
24	D	402	CLA	CMB-C2B-C1B	2.91	129.86	125.42
25	a	420[B]	PHO	O2D-CGD-O1D	-2.91	118.18	123.85
27	A	412	SQD	O48-C23-C24	2.91	120.72	111.83
27	f	102	SQD	O5-C5-C4	2.91	114.95	109.70
26	H	102	BCR	C24-C23-C22	-2.91	121.93	126.23
24	b	611	CLA	C4-C3-C5	2.91	120.28	115.23
24	C	502	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
24	c	515	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
32	D	405[A]	PL9	C27-C28-C29	-2.91	120.96	127.62
24	d	401	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
24	b	616	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
24	b	619	CLA	CHD-C4C-NC	2.91	128.74	124.23
24	B	617	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
24	c	512	CLA	CHC-C1C-C2C	-2.91	118.69	126.95
24	b	619	CLA	CHC-C1C-C2C	-2.90	118.69	126.95
24	C	513	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	c	511	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	B	603	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
26	c	527	BCR	C11-C10-C9	-2.90	123.21	127.28
24	C	506	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	C	503	CLA	CMC-C2C-C1C	2.90	129.56	125.03
24	B	605	CLA	CHD-C4C-NC	2.89	128.72	124.23
24	A	407	CLA	CHD-C4C-NC	2.89	128.71	124.23
24	d	402	CLA	C2A-C1A-CHA	-2.89	118.85	123.87
24	b	622	CLA	CHD-C1D-ND	-2.89	120.73	124.80
26	c	518	BCR	C3-C4-C5	-2.89	108.90	114.06
24	C	503	CLA	CHD-C4C-NC	2.89	128.71	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	614	CLA	CHC-C1C-C2C	-2.89	118.75	126.95
24	c	514	CLA	C4C-C3C-C2C	-2.88	102.69	106.89
36	V	207	HTG	C1'-S1-C1	2.88	106.68	100.45
24	a	409	CLA	O2A-CGA-CBA	2.88	120.62	111.83
34	z	101	LMG	O8-C28-C29	2.88	120.62	111.83
24	C	510	CLA	CHD-C4C-NC	2.88	128.70	124.23
24	C	510	CLA	CAC-C3C-C4C	2.88	128.54	124.79
32	A	420[B]	PL9	C42-C43-C44	-2.88	121.03	127.62
25	A	409[B]	PHO	C4-C3-C5	2.88	120.23	115.23
24	c	516	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
36	V	207	HTG	C1-C2-C3	-2.88	104.92	110.55
24	b	618	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
24	b	615	CLA	CMB-C2B-C1B	2.88	129.80	125.42
25	a	411	PHO	CMA-C3A-C4A	-2.88	108.41	114.61
24	B	615	CLA	CHC-C1C-C2C	-2.88	118.78	126.95
24	b	620	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
24	c	514	CLA	CBC-CAC-C3C	-2.87	104.63	112.42
24	B	617	CLA	CBC-CAC-C3C	-2.87	104.63	112.42
24	C	507	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
24	c	516	CLA	CMB-C2B-C1B	2.87	129.79	125.42
24	C	509	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
24	C	502	CLA	CHC-C1C-C2C	-2.87	118.80	126.95
24	C	511	CLA	O2A-CGA-CBA	2.87	120.57	111.83
24	c	515	CLA	CMC-C2C-C1C	2.86	129.51	125.03
25	a	411	PHO	C1-O2A-CGA	2.86	123.58	116.65
26	C	514	BCR	C38-C26-C25	-2.86	121.36	124.48
24	C	506	CLA	CMB-C2B-C1B	2.86	129.78	125.42
24	b	620	CLA	O2A-CGA-CBA	2.86	120.56	111.83
24	c	511	CLA	CMC-C2C-C1C	2.86	129.50	125.03
24	C	505	CLA	C3B-C4B-NB	2.86	113.08	110.53
24	b	618	CLA	CHC-C1C-C2C	-2.86	118.82	126.95
38	a	422	LHG	O7-C7-C8	2.86	117.67	111.48
32	d	405[A]	PL9	C40-C39-C41	2.86	120.19	115.23
38	d	406	LHG	O7-C7-C8	2.86	117.66	111.48
24	D	403	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
24	b	612	CLA	C1-C2-C3	-2.86	121.52	126.20
24	B	606	CLA	C2A-C1A-CHA	-2.86	118.91	123.87
24	b	616	CLA	CAC-C3C-C4C	2.86	128.50	124.79
27	A	416	SQD	O48-C23-O10	-2.85	116.49	123.63
24	c	512	CLA	C1-C2-C3	-2.85	121.52	126.20
24	c	512	CLA	CAC-C3C-C4C	2.85	128.50	124.79
24	C	511	CLA	C4-C3-C5	2.85	120.18	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	620	CLA	C4B-C3B-C2B	-2.85	103.75	107.30
24	c	511	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
26	k	101	BCR	C10-C11-C12	-2.85	114.94	123.20
38	D	409	LHG	O8-C23-O10	-2.85	116.50	123.63
27	b	601	SQD	O48-C23-C24	2.85	120.53	111.83
24	b	612	CLA	C4-C3-C5	2.85	120.17	115.23
32	D	405[B]	PL9	C10-C9-C11	2.85	120.17	115.23
24	c	513	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	b	624	CLA	CHD-C4C-NC	2.85	128.65	124.23
27	F	103	SQD	C3-C4-C5	2.85	115.39	110.23
26	h	101	BCR	C38-C26-C25	-2.85	121.38	124.48
24	B	610	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
24	a	410	CLA	CAA-C2A-C3A	-2.85	105.31	113.00
24	c	506	CLA	CAC-C3C-C4C	2.85	128.49	124.79
24	b	622	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
24	B	614	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
24	B	609	CLA	CHD-C4C-NC	2.85	128.64	124.23
24	c	517	CLA	CAA-C2A-C3A	-2.84	105.31	113.00
32	D	405[B]	PL9	C27-C28-C29	-2.84	121.11	127.62
24	a	410	CLA	O2A-CGA-O1A	-2.84	116.51	123.63
24	D	402	CLA	O2A-CGA-CBA	2.84	120.50	111.83
25	a	420[B]	PHO	C4-C3-C5	2.84	120.16	115.23
25	a	411	PHO	C1A-C2A-C3A	-2.84	100.14	102.84
26	k	101	BCR	C11-C10-C9	-2.84	123.29	127.28
24	B	612	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
24	B	605	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
24	C	502	CLA	CHD-C4C-NC	2.84	128.63	124.23
32	D	405[B]	PL9	C12-C13-C14	-2.84	121.12	127.62
24	C	505	CLA	CAC-C3C-C4C	2.84	128.48	124.79
24	b	614	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
34	b	630	LMG	O8-C28-C29	2.83	120.47	111.83
24	B	604	CLA	C3B-C4B-NB	2.83	113.06	110.53
24	C	512	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	D	402	CLA	C4-C3-C5	2.83	120.14	115.23
38	L	101	LHG	O8-C23-C24	2.83	120.46	111.83
24	c	507	CLA	O2A-CGA-CBA	2.83	120.45	111.83
24	C	502	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
25	a	420[A]	PHO	CMA-C3A-C4A	-2.82	108.53	114.61
41	v	205	HEC	CHD-C4C-NC	2.82	127.53	124.45
26	t	101	BCR	C7-C6-C5	-2.82	115.05	121.56
24	C	509	CLA	CAC-C3C-C4C	2.82	128.46	124.79
24	B	614	CLA	O2A-CGA-O1A	-2.82	116.57	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	508	CLA	CBC-CAC-C3C	-2.82	104.77	112.42
24	b	624	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
24	b	616	CLA	CHD-C4C-NC	2.82	128.60	124.23
24	A	407	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
24	b	616	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
24	d	403	CLA	C2A-C1A-CHA	-2.82	118.97	123.87
24	c	505	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
24	C	511	CLA	CBC-CAC-C3C	-2.82	104.78	112.42
24	b	615	CLA	C3B-C4B-NB	2.82	113.05	110.53
24	b	615	CLA	O2A-CGA-O1A	-2.82	116.58	123.63
24	b	618	CLA	O2A-CGA-CBA	2.82	120.42	111.83
24	c	508	CLA	CHC-C1C-C2C	-2.82	118.95	126.95
24	c	515	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
26	T	103	BCR	C12-C13-C14	-2.82	114.58	119.01
36	d	411	HTG	C1-O5-C5	2.81	117.61	112.56
24	B	602	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
24	B	611	CLA	CMB-C2B-C1B	2.81	129.70	125.42
24	c	516	CLA	O2A-CGA-CBA	2.81	120.41	111.83
39	F	102	HEM	CHB-C1B-NB	2.81	127.84	124.37
24	B	615	CLA	C2A-C1A-CHA	-2.81	119.00	123.87
26	Y	101	BCR	C16-C17-C18	-2.80	123.34	127.28
36	b	633	HTG	C1-O5-C5	2.80	117.59	112.56
24	b	621	CLA	CHD-C4C-NC	2.80	128.58	124.23
24	b	616	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
24	C	513	CLA	O2A-CGA-CBA	2.80	120.38	111.83
24	A	405	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
26	t	101	BCR	C1-C6-C7	2.80	123.24	115.65
24	C	501	CLA	C1-O2A-CGA	2.80	123.43	116.65
24	B	609	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
24	B	608	CLA	CMB-C2B-C1B	2.80	129.68	125.42
24	C	509	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
32	a	416[A]	PL9	C35-C34-C36	2.80	120.08	115.23
24	B	604	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
26	T	103	BCR	C35-C13-C12	2.79	122.36	118.09
24	A	407	CLA	C1-C2-C3	-2.79	121.62	126.20
24	b	625	CLA	C4-C3-C5	2.79	120.07	115.23
24	B	610	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
24	c	513	CLA	CHC-C1C-C2C	-2.79	119.03	126.95
24	A	410	CLA	C3B-C4B-NB	2.79	113.02	110.53
24	A	407	CLA	C2A-C1A-CHA	-2.79	119.03	123.87
24	b	616	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
24	c	510	CLA	C4-C3-C5	2.78	120.06	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	C3B-C4B-NB	2.78	113.02	110.53
24	B	602	CLA	CHC-C1C-C2C	-2.78	119.03	126.95
24	B	611	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
24	B	604	CLA	O2A-CGA-CBA	2.78	120.32	111.83
24	C	507	CLA	C1-C2-C3	-2.78	121.64	126.20
32	a	416[A]	PL9	C25-C24-C26	2.78	120.05	115.23
24	C	505	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
32	D	405[A]	PL9	C40-C39-C41	2.77	120.04	115.23
24	B	611	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	B	615	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	c	508	CLA	CAC-C3C-C4C	2.77	128.40	124.79
24	C	513	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
24	c	516	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	c	508	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
24	C	509	CLA	C1-O2A-CGA	2.77	123.35	116.65
24	B	608	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
24	B	606	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
24	B	603	CLA	CHD-C4C-NC	2.77	128.52	124.23
34	a	415	LMG	O8-C28-C29	2.77	120.27	111.83
24	c	508	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	b	624	CLA	C2A-C1A-CHA	-2.77	119.07	123.87
24	b	619	CLA	CMC-C2C-C1C	2.77	129.36	125.03
24	D	403	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
24	b	613	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
24	b	621	CLA	CMB-C2B-C1B	2.76	129.63	125.42
24	b	619	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
24	a	412	CLA	CBC-CAC-C3C	-2.76	104.93	112.42
24	b	612	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
24	b	617	CLA	C4-C3-C5	2.76	120.02	115.23
27	F	103	SQD	C44-O6-C1	-2.76	107.88	113.80
24	D	403	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
24	c	506	CLA	C1-C2-C3	-2.76	121.68	126.20
24	C	508	CLA	C4-C3-C5	2.75	120.01	115.23
24	C	510	CLA	O2A-CGA-CBA	2.75	120.23	111.83
27	a	414	SQD	O48-C23-C24	2.75	120.23	111.83
24	a	410	CLA	C4-C3-C5	2.75	120.01	115.23
24	b	621	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	B	608	CLA	CHC-C1C-C2C	-2.75	119.13	126.95
24	C	508	CLA	O2A-CGA-CBA	2.75	120.22	111.83
24	b	617	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
24	b	612	CLA	C3B-C4B-NB	2.75	112.99	110.53
26	t	101	BCR	C28-C27-C26	-2.75	109.15	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	h	101	BCR	C10-C11-C12	-2.75	115.23	123.20
24	C	507	CLA	O2A-CGA-CBA	2.75	120.22	111.83
24	c	513	CLA	CAC-C3C-C4C	2.75	128.37	124.79
24	c	505	CLA	CMC-C2C-C1C	2.75	129.33	125.03
24	A	405	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
24	d	403	CLA	CAA-C2A-C3A	-2.75	105.58	113.00
24	a	409	CLA	O2A-CGA-O1A	-2.75	116.76	123.63
24	B	616	CLA	CAC-C3C-C4C	2.75	128.36	124.79
24	c	514	CLA	CHD-C4C-NC	2.75	128.49	124.23
24	b	624	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
24	b	618	CLA	CHD-C4C-NC	2.74	128.48	124.23
36	B	625	HTG	C1-O5-C5	2.74	117.48	112.56
24	C	511	CLA	CHD-C4C-NC	2.74	128.48	124.23
27	F	103	SQD	O7-S-C6	2.74	110.84	106.76
24	b	625	CLA	CBC-CAC-C3C	-2.74	105.00	112.42
24	b	618	CLA	C2A-C1A-CHA	-2.74	119.12	123.87
26	t	101	BCR	C7-C8-C9	-2.74	122.19	126.23
24	b	621	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
26	b	629	BCR	C2-C1-C6	2.74	114.41	110.44
24	B	611	CLA	CMA-C3A-C4A	-2.74	104.42	111.77
26	b	629	BCR	C38-C26-C25	-2.74	121.50	124.48
39	e	102	HEM	CAD-CBD-CGD	2.73	120.92	113.67
24	A	406	CLA	O2A-CGA-O1A	-2.73	116.79	123.63
24	b	619	CLA	O2A-CGA-CBA	2.73	120.17	111.83
32	A	420[B]	PL9	C12-C13-C14	-2.73	121.37	127.62
24	B	608	CLA	C4C-C3C-C2C	-2.73	102.91	106.89
24	b	615	CLA	CAC-C3C-C2C	2.73	132.58	127.56
24	D	402	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
24	C	511	CLA	CMB-C2B-C1B	2.73	129.58	125.42
24	b	616	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
24	B	617	CLA	CMB-C2B-C1B	2.73	129.57	125.42
24	A	406	CLA	CAA-CBA-CGA	2.73	120.96	113.21
24	c	517	CLA	O2A-CGA-CBA	2.73	120.15	111.83
24	B	606	CLA	CED-O2D-CGD	2.73	122.10	115.92
24	C	502	CLA	O2A-CGA-CBA	2.73	120.15	111.83
32	A	420[B]	PL9	C15-C14-C16	2.73	119.96	115.23
27	B	621	SQD	O48-C23-C24	2.73	120.15	111.83
32	d	405[A]	PL9	C12-C13-C14	-2.73	121.38	127.62
24	B	612	CLA	CHC-C1C-C2C	-2.72	119.20	126.95
24	c	509	CLA	C3B-C4B-NB	2.72	112.96	110.53
24	D	403	CLA	CMC-C2C-C1C	2.72	129.29	125.03
24	A	410	CLA	C2A-C1A-CHA	-2.72	119.14	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	512	CLA	CAA-C2A-C3A	-2.72	105.65	113.00
25	a	411	PHO	CBC-CAC-C3C	-2.72	108.98	112.87
24	c	513	CLA	CMC-C2C-C1C	2.72	129.28	125.03
24	d	403	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
24	b	621	CLA	CMC-C2C-C1C	2.72	129.28	125.03
24	d	403	CLA	CHC-C1C-C2C	-2.72	119.22	126.95
24	C	512	CLA	O2A-CGA-CBA	2.72	120.12	111.83
34	C	520	LMG	O8-C28-C29	2.71	120.11	111.83
24	B	612	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
24	c	506	CLA	CHD-C4C-NC	2.71	128.44	124.23
37	C	517	DGD	O1G-C1A-C2A	2.71	120.10	111.83
24	C	509	CLA	CHD-C4C-NC	2.71	128.43	124.23
24	c	513	CLA	CMB-C2B-C1B	2.71	129.54	125.42
24	c	514	CLA	O2A-CGA-CBA	2.71	120.09	111.83
24	A	406	CLA	CMA-C3A-C4A	-2.71	104.50	111.77
39	F	102	HEM	CHD-C1D-ND	2.71	127.34	124.42
32	A	420[A]	PL9	C12-C13-C14	-2.71	121.43	127.62
27	b	601	SQD	O47-C7-O49	-2.71	117.38	123.70
24	B	612	CLA	CBC-CAC-C3C	-2.71	105.09	112.42
24	D	403	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
26	b	627	BCR	C15-C14-C13	-2.70	123.48	127.28
26	d	404	BCR	C28-C27-C26	-2.70	109.23	114.06
24	b	624	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
32	a	416[A]	PL9	C53-C6-C1	2.70	120.81	115.28
24	B	613	CLA	CHD-C4C-NC	2.70	128.42	124.23
32	a	416[B]	PL9	C53-C6-C1	2.70	120.81	115.28
24	b	614	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
32	D	405[A]	PL9	C25-C24-C26	2.70	119.91	115.23
24	c	506	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
29	B	635	LMT	C1'-O5'-C5'	2.70	118.99	113.72
24	B	612	CLA	CMA-C3A-C4A	-2.70	104.52	111.77
26	h	101	BCR	C7-C8-C9	-2.70	122.25	126.23
32	A	420[A]	PL9	C53-C6-C1	2.70	120.80	115.28
24	B	614	CLA	O2A-CGA-CBA	2.70	120.05	111.83
24	c	515	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
36	b	609	HTG	C1-O5-C5	2.69	117.39	112.56
34	c	523	LMG	C8-O7-C10	-2.69	111.35	117.80
24	d	403	CLA	CMC-C2C-C1C	2.69	129.24	125.03
32	d	405[A]	PL9	C15-C14-C16	2.69	119.90	115.23
24	a	409	CLA	CMC-C2C-C1C	2.69	129.24	125.03
32	a	416[B]	PL9	C25-C24-C26	2.69	119.90	115.23
24	b	614	CLA	CMB-C2B-C1B	2.69	129.52	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	507	CLA	CHD-C4C-NC	2.69	128.40	124.23
24	c	511	CLA	O1D-CGD-CBD	-2.69	119.21	124.52
24	c	505	CLA	CBC-CAC-C3C	-2.69	105.13	112.42
24	a	410	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
24	C	502	CLA	CAC-C3C-C4C	2.69	128.29	124.79
24	b	624	CLA	O2A-CGA-CBA	2.69	120.03	111.83
32	d	405[B]	PL9	C7-C8-C9	-2.69	122.20	126.83
38	d	407	LHG	C6-C5-C4	-2.69	105.52	111.78
24	b	620	CLA	CHD-C4C-NC	2.69	128.40	124.23
24	C	506	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
32	a	416[A]	PL9	C40-C39-C41	2.69	119.89	115.23
24	C	501	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
24	A	407	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
24	b	615	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
26	K	101	BCR	C38-C26-C25	-2.69	121.55	124.48
27	a	414	SQD	O9-S-C6	2.69	110.77	106.76
24	c	517	CLA	CMB-C2B-C1B	2.68	129.51	125.42
26	h	101	BCR	C11-C10-C9	-2.68	123.52	127.28
24	b	626	CLA	CHD-C4C-NC	2.68	128.39	124.23
32	a	416[B]	PL9	C40-C39-C41	2.68	119.88	115.23
32	d	405[B]	PL9	C25-C24-C26	2.68	119.88	115.23
25	a	420[A]	PHO	C4D-CHA-CBD	2.68	109.74	108.45
27	b	601	SQD	C44-O6-C1	-2.68	108.05	113.80
34	Z	101	LMG	C1-O6-C5	2.68	118.95	113.72
26	B	619	BCR	C37-C22-C21	-2.68	118.48	122.82
24	A	405	CLA	CAA-C2A-C1A	-2.68	103.20	111.97
27	f	102	SQD	O48-C23-C24	2.68	120.00	111.83
24	c	515	CLA	C4-C3-C5	2.67	119.87	115.23
24	b	613	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
24	b	615	CLA	C1-C2-C3	-2.67	121.82	126.20
24	c	511	CLA	CHD-C4C-NC	2.67	128.38	124.23
26	y	101	BCR	C21-C20-C19	-2.67	115.45	123.20
24	d	401	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
24	C	513	CLA	CBC-CAC-C3C	-2.67	105.17	112.42
38	D	407	LHG	O8-C23-O10	-2.67	116.94	123.63
25	A	409[A]	PHO	O2D-CGD-O1D	-2.67	118.65	123.85
26	y	101	BCR	C38-C26-C25	-2.67	121.57	124.48
24	B	605	CLA	OBD-CAD-C3D	-2.67	122.17	128.42
37	C	518	DGD	O1G-C1A-C2A	2.67	119.98	111.83
24	B	607	CLA	O2A-CGA-CBA	2.67	119.97	111.83
24	b	613	CLA	CBC-CAC-C3C	-2.67	105.18	112.42
24	b	619	CLA	O2A-CGA-O1A	-2.67	116.95	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	412	CLA	CMA-C3A-C2A	-2.67	103.67	113.98
24	C	501	CLA	C3B-C4B-NB	2.67	112.91	110.53
24	B	615	CLA	C1-C2-C3	-2.67	121.83	126.20
24	a	412	CLA	O2A-CGA-CBA	2.67	119.96	111.83
24	c	511	CLA	C4-C3-C5	2.66	119.85	115.23
24	a	410	CLA	C3B-C4B-NB	2.66	112.91	110.53
24	B	610	CLA	CMC-C2C-C1C	2.66	129.19	125.03
37	H	103	DGD	O1G-C1A-O1A	-2.66	116.97	123.63
26	C	515	BCR	C24-C23-C22	-2.66	122.30	126.23
26	C	515	BCR	C21-C20-C19	-2.66	115.49	123.20
24	c	515	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
26	c	527	BCR	C29-C30-C25	2.66	114.30	110.44
24	A	407	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
24	c	513	CLA	C4-C3-C5	2.66	119.85	115.23
24	C	503	CLA	CAC-C3C-C4C	2.66	128.25	124.79
24	d	403	CLA	C4-C3-C5	2.66	119.84	115.23
24	D	403	CLA	CAA-C2A-C3A	-2.66	105.82	113.00
24	b	615	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
24	b	626	CLA	C1-C2-C3	-2.66	121.84	126.20
24	a	412	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
38	a	422	LHG	O8-C23-C24	2.66	119.93	111.83
32	A	420[B]	PL9	C53-C6-C1	2.65	120.71	115.28
32	A	420[A]	PL9	C45-C44-C46	2.65	119.83	115.23
24	c	516	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
24	a	410	CLA	C2A-C1A-CHA	-2.65	119.26	123.87
32	A	420[A]	PL9	C17-C18-C19	-2.65	121.56	127.62
24	d	402	CLA	C4C-C3C-C2C	-2.65	103.04	106.89
32	A	420[A]	PL9	C15-C14-C16	2.65	119.82	115.23
24	b	621	CLA	CMA-C3A-C4A	-2.65	104.66	111.77
24	c	517	CLA	C4-C3-C5	2.65	119.82	115.23
24	c	516	CLA	C4-C3-C5	2.64	119.82	115.23
32	d	405[A]	PL9	C20-C19-C21	2.64	119.82	115.23
24	C	511	CLA	CMC-C2C-C1C	2.64	129.16	125.03
32	A	420[B]	PL9	C25-C24-C26	2.64	119.82	115.23
24	B	611	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
24	c	506	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	c	514	CLA	CMA-C3A-C4A	-2.64	104.67	111.77
24	B	615	CLA	CMB-C2B-C1B	2.64	129.44	125.42
26	B	620	BCR	C2-C1-C6	2.64	114.28	110.44
32	a	416[A]	PL9	C30-C29-C31	2.64	119.81	115.23
24	b	619	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
34	c	523	LMG	O8-C28-C29	2.64	119.88	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	420[A]	PL9	C25-C24-C26	2.64	119.81	115.23
34	A	422	LMG	C8-O7-C10	-2.64	111.49	117.80
24	B	604	CLA	CMB-C2B-C1B	2.64	129.43	125.42
24	a	409	CLA	CHD-C4C-NC	2.63	128.32	124.23
24	b	618	CLA	C1-C2-C3	-2.63	121.88	126.20
29	M	103	LMT	O5'-C5'-C4'	2.63	115.17	109.72
24	a	412	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
24	c	511	CLA	O2A-CGA-CBA	2.63	119.86	111.83
24	A	410	CLA	CHD-C4C-NC	2.63	128.31	124.23
24	C	509	CLA	C4-C3-C5	2.63	119.79	115.23
37	C	517	DGD	C2G-O2G-C1B	-2.63	111.51	117.80
24	b	623	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
25	A	408	PHO	CMA-C3A-C4A	-2.63	108.95	114.61
26	T	103	BCR	C21-C20-C19	-2.62	115.59	123.20
24	b	620	CLA	CMB-C2B-C1B	2.62	129.41	125.42
37	C	516	DGD	O3G-C3G-C2G	-2.62	104.44	110.82
26	c	527	BCR	C28-C27-C26	-2.62	109.38	114.06
24	b	626	CLA	CBC-CAC-C3C	-2.62	105.31	112.42
24	C	501	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
24	b	620	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
24	B	608	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
24	C	513	CLA	CMC-C2C-C1C	2.62	129.13	125.03
27	A	412	SQD	O47-C7-O49	-2.62	117.58	123.70
24	b	618	CLA	C4B-C3B-C2B	-2.62	104.05	107.30
26	t	101	BCR	C11-C10-C9	-2.62	123.61	127.28
26	K	101	BCR	C10-C11-C12	-2.62	115.61	123.20
24	A	406	CLA	C4-C3-C5	2.62	119.77	115.23
32	d	405[A]	PL9	C53-C6-C1	2.62	120.64	115.28
24	c	508	CLA	CHD-C4C-NC	2.61	128.29	124.23
26	t	101	BCR	C21-C20-C19	-2.61	115.63	123.20
32	d	405[A]	PL9	C10-C9-C11	2.61	119.76	115.23
34	j	101	LMG	O7-C10-C11	2.61	117.13	111.48
24	c	516	CLA	CHC-C1C-C2C	-2.61	119.53	126.95
24	B	615	CLA	CBC-CAC-C3C	-2.61	105.34	112.42
32	a	416[B]	PL9	C35-C34-C36	2.61	119.76	115.23
36	c	525	HTG	C1-O5-C5	2.61	117.24	112.56
37	c	519	DGD	O2G-C1B-O1B	-2.61	117.61	123.70
24	d	401	CLA	CMA-C3A-C2A	-2.61	103.90	113.98
24	c	517	CLA	CAC-C3C-C4C	2.60	128.18	124.79
24	A	410	CLA	CHB-C4A-NA	2.60	128.16	124.40
26	b	629	BCR	C24-C23-C22	-2.60	122.38	126.23
24	B	616	CLA	CBC-CAC-C3C	-2.60	105.36	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	k	101	BCR	C15-C14-C13	-2.60	123.63	127.28
32	D	405[B]	PL9	C53-C6-C1	2.60	120.61	115.28
36	B	625	HTG	C1-C2-C3	2.60	115.63	110.55
24	c	512	CLA	C2A-C1A-CHA	-2.60	119.36	123.87
24	C	504	CLA	CHD-C4C-NC	2.60	128.26	124.23
24	c	517	CLA	C2A-C1A-CHA	-2.60	119.36	123.87
24	A	406	CLA	CED-O2D-CGD	2.60	121.81	115.92
24	C	512	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
24	B	611	CLA	CAA-CBA-CGA	-2.60	105.84	113.21
32	d	405[B]	PL9	C20-C19-C21	2.60	119.73	115.23
24	c	509	CLA	C4B-C3B-C2B	-2.60	104.08	107.30
24	C	505	CLA	CHD-C4C-NC	2.59	128.25	124.23
27	f	102	SQD	O47-C7-O49	-2.59	117.64	123.70
34	c	522	LMG	O8-C28-O10	-2.59	117.14	123.63
24	C	512	CLA	C4-C3-C5	2.59	119.72	115.23
24	c	508	CLA	C2A-C1A-CHA	-2.59	119.37	123.87
24	B	606	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
26	h	101	BCR	C16-C15-C14	-2.59	118.22	123.52
39	F	102	HEM	CBD-CAD-C3D	-2.59	105.38	112.53
24	A	407	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
24	B	611	CLA	CHB-C4A-NA	2.59	128.13	124.40
27	A	412	SQD	O9-S-C6	2.59	110.62	106.76
27	A	412	SQD	O8-S-C6	2.59	110.97	105.97
24	c	510	CLA	CAA-C2A-C3A	-2.59	106.01	113.00
24	A	410	CLA	O2A-CGA-CBA	2.59	119.72	111.83
24	D	403	CLA	CHD-C4C-NC	2.59	128.24	124.23
24	b	619	CLA	C4C-C3C-C2C	-2.58	103.13	106.89
24	C	507	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
24	B	609	CLA	C4C-C3C-C2C	-2.58	103.13	106.89
24	B	608	CLA	C2A-C1A-CHA	-2.58	119.39	123.87
24	B	604	CLA	CMA-C3A-C2A	-2.58	104.00	113.98
24	C	506	CLA	CHD-C4C-NC	2.58	128.23	124.23
27	F	103	SQD	O9-S-C6	2.58	110.60	106.76
24	C	509	CLA	CMC-C2C-C1C	2.58	129.06	125.03
24	b	614	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
24	B	616	CLA	O2A-CGA-O1A	-2.57	117.19	123.63
24	c	505	CLA	O2A-CGA-CBA	2.57	119.67	111.83
24	d	402	CLA	CMB-C2B-C1B	2.57	129.33	125.42
24	B	609	CLA	CMC-C2C-C1C	2.57	129.05	125.03
24	B	612	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
24	b	624	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
24	B	615	CLA	CHD-C4C-NC	2.57	128.21	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	616	CLA	CHC-C1C-C2C	-2.57	119.65	126.95
24	C	513	CLA	C4-C3-C5	2.56	119.68	115.23
32	A	420[B]	PL9	C45-C44-C46	2.56	119.68	115.23
24	b	625	CLA	C11-C10-C8	-2.56	107.44	115.97
27	a	414	SQD	O8-S-C6	2.56	110.92	105.97
37	e	101	DGD	O1G-C1A-C2A	2.56	119.65	111.83
24	a	410	CLA	CMC-C2C-C1C	2.56	129.04	125.03
24	c	512	CLA	CMC-C2C-C1C	2.56	129.04	125.03
26	H	102	BCR	C29-C30-C25	2.56	114.16	110.44
41	V	206	HEC	C4B-NB-C1B	2.56	110.00	105.82
32	D	405[B]	PL9	C45-C44-C46	2.56	119.67	115.23
24	c	508	CLA	CMB-C2B-C1B	2.56	129.32	125.42
32	d	405[B]	PL9	C45-C44-C46	2.56	119.67	115.23
24	d	402	CLA	CMC-C2C-C1C	2.56	129.03	125.03
32	A	420[B]	PL9	C17-C18-C19	-2.56	121.77	127.62
24	A	407	CLA	CMC-C2C-C1C	2.56	129.03	125.03
34	Z	101	LMG	C8-O7-C10	-2.56	111.67	117.80
24	B	604	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
24	B	607	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
24	b	622	CLA	CMC-C2C-C1C	2.56	129.03	125.03
24	B	607	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
24	d	403	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
32	A	420[A]	PL9	C30-C29-C31	2.55	119.66	115.23
24	a	410	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
24	B	611	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
24	c	512	CLA	CHD-C4C-NC	2.55	128.19	124.23
24	A	407	CLA	CAC-C3C-C4C	2.55	128.11	124.79
24	C	513	CLA	CMB-C2B-C1B	2.55	129.30	125.42
24	B	602	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
24	b	621	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
24	C	501	CLA	C4-C3-C5	2.55	119.65	115.23
24	A	405	CLA	O2A-CGA-O1A	-2.55	117.26	123.63
39	F	102	HEM	CHA-C1A-NA	2.54	128.47	123.86
32	D	405[B]	PL9	C51-C49-C50	2.54	120.44	114.59
24	C	501	CLA	C1-C2-C3	-2.54	122.03	126.20
32	A	420[B]	PL9	C10-C9-C11	2.54	119.64	115.23
24	c	512	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	A	405	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	b	619	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	C	501	CLA	CAC-C3C-C4C	2.54	128.09	124.79
24	c	511	CLA	C3B-C4B-NB	2.54	112.80	110.53
24	C	507	CLA	CHC-C1C-C2C	-2.54	119.74	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	SQD	C1-O5-C5	-2.54	108.77	113.72
24	b	624	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
38	L	101	LHG	O8-C23-O10	-2.53	117.29	123.63
24	D	403	CLA	CBC-CAC-C3C	-2.53	105.55	112.42
24	A	407	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
32	D	405[B]	PL9	C25-C24-C26	2.53	119.63	115.23
24	c	517	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
24	B	604	CLA	CHC-C1C-C2C	-2.53	119.75	126.95
24	c	516	CLA	C3B-C4B-NB	2.53	112.79	110.53
37	H	103	DGD	C3G-O3G-C1D	-2.53	108.38	113.80
39	e	102	HEM	CBD-CAD-C3D	-2.53	105.54	112.53
24	b	626	CLA	CMB-C2B-C1B	2.53	129.27	125.42
24	d	403	CLA	CMB-C2B-C1B	2.53	129.27	125.42
24	B	605	CLA	O2A-CGA-CBA	2.53	119.53	111.83
38	d	408	LHG	O8-C23-C24	2.52	119.53	111.83
24	B	617	CLA	CAC-C3C-C4C	2.52	128.07	124.79
24	C	503	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
24	b	624	CLA	CBC-CAC-C3C	-2.52	105.58	112.42
32	D	405[A]	PL9	C12-C13-C14	-2.52	121.85	127.62
32	D	405[B]	PL9	C20-C19-C21	2.52	119.61	115.23
24	C	513	CLA	CHD-C4C-NC	2.52	128.14	124.23
24	b	619	CLA	C4-C3-C5	2.52	119.60	115.23
24	C	505	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	B	605	CLA	CMC-C2C-C1C	2.52	128.97	125.03
24	D	402	CLA	C4C-C3C-C2C	-2.52	103.22	106.89
38	D	408	LHG	O8-C23-O10	-2.52	117.33	123.63
24	B	607	CLA	CAA-C2A-C3A	-2.51	106.21	113.00
37	C	516	DGD	O1G-C1A-O1A	-2.51	117.35	123.63
24	a	409	CLA	CMB-C2B-C1B	2.51	129.24	125.42
24	C	502	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
39	e	102	HEM	C4D-ND-C1D	2.51	108.18	105.21
27	a	414	SQD	C45-O47-C7	-2.51	111.79	117.80
24	C	513	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
24	d	403	CLA	O2A-CGA-CBA	2.51	119.47	111.83
24	a	410	CLA	CAC-C3C-C4C	2.50	128.05	124.79
26	b	628	BCR	C8-C7-C6	-2.50	120.31	127.00
24	b	626	CLA	C2A-C1A-CHA	-2.50	119.52	123.87
26	C	515	BCR	C15-C14-C13	-2.50	123.77	127.28
25	A	409[A]	PHO	C4D-CHA-CBD	2.50	109.66	108.45
24	a	412	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
27	F	103	SQD	O47-C7-O49	-2.50	117.86	123.70
29	M	103	LMT	O1B-C1B-C2B	2.50	114.24	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	410	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
25	a	420[B]	PHO	CMB-C2B-C3B	2.50	129.67	124.68
27	a	405	SQD	O48-C23-O10	-2.50	117.39	123.63
24	c	505	CLA	CMB-C2B-C1B	2.49	129.22	125.42
24	c	508	CLA	O2A-CGA-O1A	-2.49	117.39	123.63
24	b	613	CLA	CHD-C4C-NC	2.49	128.10	124.23
24	a	409	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
24	b	626	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
24	A	410	CLA	CED-O2D-CGD	2.49	121.56	115.92
24	b	623	CLA	CHD-C4C-NC	2.49	128.09	124.23
24	B	612	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
37	C	516	DGD	C2G-O2G-C1B	-2.49	111.84	117.80
24	C	512	CLA	CMC-C2C-C1C	2.49	128.92	125.03
24	b	620	CLA	C4-C3-C5	2.49	119.55	115.23
24	D	402	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
24	B	611	CLA	CHD-C4C-NC	2.48	128.08	124.23
37	h	102	DGD	C2G-O2G-C1B	-2.48	111.86	117.80
41	V	206	HEC	CHB-C1B-NB	2.48	128.36	123.86
27	b	601	SQD	C1-C2-C3	-2.48	104.79	110.01
32	D	405[A]	PL9	C17-C18-C19	-2.48	121.95	127.62
24	B	616	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
26	c	518	BCR	C38-C26-C25	-2.48	121.78	124.48
32	d	405[B]	PL9	C15-C14-C16	2.48	119.53	115.23
32	D	405[A]	PL9	C20-C19-C21	2.48	119.53	115.23
41	v	205	HEC	C2A-C1A-NA	-2.48	107.93	110.32
24	B	608	CLA	CHD-C4C-NC	2.48	128.07	124.23
24	c	510	CLA	C4C-C3C-C2C	-2.48	103.29	106.89
26	a	413	BCR	C15-C14-C13	-2.47	123.81	127.28
29	m	102	LMT	O5'-C5'-C4'	2.47	114.84	109.72
25	A	409[B]	PHO	O2D-CGD-O1D	-2.47	119.03	123.85
24	A	407	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
24	b	612	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
24	b	614	CLA	CHD-C4C-NC	2.47	128.07	124.23
24	b	614	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
24	A	410	CLA	CMA-C3A-C2A	-2.47	104.43	113.98
24	C	503	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
34	Z	101	LMG	C9-O8-C28	2.47	123.17	117.08
26	C	514	BCR	C11-C10-C9	-2.47	123.82	127.28
24	B	617	CLA	O2A-CGA-CBA	2.47	119.36	111.83
24	b	624	CLA	CMB-C2B-C1B	2.47	129.17	125.42
32	d	405[B]	PL9	C12-C13-C14	-2.46	121.98	127.62
24	b	623	CLA	CMA-C3A-C4A	-2.46	105.15	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	420[B]	PL9	C8-C7-C3	2.46	118.40	112.03
24	B	609	CLA	C1-C2-C3	-2.46	122.16	126.20
24	b	625	CLA	CMC-C2C-C1C	2.46	128.88	125.03
24	C	513	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
24	c	517	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
24	C	507	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
24	c	508	CLA	O2A-CGA-CBA	2.46	119.34	111.83
24	b	611	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
24	c	507	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
24	C	505	CLA	CMC-C2C-C1C	2.46	128.88	125.03
24	C	502	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
24	b	615	CLA	O2A-CGA-CBA	2.46	119.33	111.83
24	B	609	CLA	CMB-C2B-C1B	2.46	129.16	125.42
26	k	101	BCR	C2-C1-C6	2.46	114.01	110.44
41	V	206	HEC	O2D-CGD-CBD	2.46	121.76	114.00
24	C	503	CLA	C4B-C3B-C2B	-2.46	104.25	107.30
26	A	411	BCR	C24-C23-C22	-2.46	122.60	126.23
24	b	617	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
26	b	628	BCR	C37-C22-C21	-2.45	118.84	122.82
24	A	410	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
24	c	509	CLA	C4-C3-C5	2.45	119.49	115.23
24	c	517	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
32	d	405[B]	PL9	C10-C9-C11	2.45	119.49	115.23
26	y	101	BCR	C10-C11-C12	-2.45	116.09	123.20
24	C	504	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
32	a	416[A]	PL9	C51-C49-C50	2.45	120.23	114.59
24	B	610	CLA	C1-C2-C3	-2.45	122.18	126.20
24	a	410	CLA	CAA-CBA-CGA	2.45	120.17	113.21
24	c	506	CLA	C4B-C3B-C2B	-2.45	104.26	107.30
26	Y	101	BCR	C28-C27-C26	-2.45	109.69	114.06
24	b	612	CLA	CMC-C2C-C1C	2.45	128.86	125.03
25	A	409[B]	PHO	CMB-C2B-C3B	2.44	129.57	124.68
24	B	609	CLA	CHB-C4A-NA	2.44	127.92	124.40
24	B	614	CLA	CHB-C4A-NA	2.44	127.92	124.40
34	z	101	LMG	C8-O7-C10	-2.44	111.95	117.80
34	j	101	LMG	O6-C5-C4	2.44	114.10	109.70
24	B	615	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	b	619	CLA	C1-O2A-CGA	2.44	122.55	116.65
24	b	623	CLA	CED-O2D-CGD	2.44	121.44	115.92
24	B	605	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
32	a	416[B]	PL9	C30-C29-C31	2.44	119.46	115.23
24	a	412	CLA	C2A-C1A-CHA	-2.43	119.64	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	612	CLA	O2A-CGA-CBA	2.43	119.25	111.83
24	c	507	CLA	CHC-C1C-C2C	-2.43	120.03	126.95
24	C	504	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
27	F	103	SQD	C1-C2-C3	-2.43	104.89	110.01
24	c	510	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
24	c	509	CLA	C1-C2-C3	-2.43	122.21	126.20
24	C	506	CLA	CMC-C2C-C1C	2.43	128.83	125.03
32	a	416[B]	PL9	C12-C13-C14	-2.43	122.06	127.62
37	C	516	DGD	C3G-C2G-C1G	-2.43	106.12	111.78
24	B	606	CLA	C3B-C4B-NB	2.43	112.70	110.53
32	A	420[B]	PL9	C30-C29-C31	2.43	119.44	115.23
32	A	420[A]	PL9	C8-C7-C3	2.43	118.31	112.03
34	c	522	LMG	C8-O7-C10	-2.43	111.99	117.80
24	c	515	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
38	d	406	LHG	O7-C7-O9	-2.42	118.04	123.70
24	b	625	CLA	CHA-C1A-NA	-2.42	120.90	126.39
24	c	512	CLA	C4-C3-C5	2.42	119.44	115.23
26	t	101	BCR	C12-C13-C14	-2.42	115.20	119.01
24	C	510	CLA	CMC-C2C-C1C	2.42	128.82	125.03
24	c	507	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
24	b	612	CLA	C2A-C1A-CHA	-2.42	119.67	123.87
27	A	412	SQD	O48-C23-O10	-2.42	117.57	123.63
34	D	412	LMG	C9-C8-C7	-2.42	106.14	111.78
24	b	623	CLA	CMB-C2B-C1B	2.42	129.10	125.42
24	B	604	CLA	C1-O2A-CGA	2.42	122.51	116.65
24	B	614	CLA	OBD-CAD-C3D	-2.42	122.76	128.42
24	B	616	CLA	C1-C2-C3	-2.42	122.23	126.20
24	D	402	CLA	CHD-C4C-NC	2.42	127.98	124.23
41	v	205	HEC	CHA-C4D-ND	2.42	128.24	123.86
26	c	518	BCR	C21-C20-C19	-2.42	116.20	123.20
34	A	422	LMG	O8-C28-C29	2.42	119.20	111.83
24	B	613	CLA	O2A-CGA-CBA	2.42	119.20	111.83
34	B	622	LMG	O1-C7-C8	-2.41	104.95	110.82
32	D	405[A]	PL9	C53-C6-C1	2.41	120.22	115.28
24	c	513	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
37	c	521	DGD	C2G-O2G-C1B	-2.41	112.03	117.80
24	b	619	CLA	CED-O2D-CGD	2.41	121.38	115.92
24	a	410	CLA	O2A-CGA-CBA	2.41	119.17	111.83
24	b	617	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
24	C	512	CLA	CAC-C3C-C4C	2.41	127.92	124.79
32	a	416[B]	PL9	C51-C49-C50	2.40	120.12	114.59
26	Y	101	BCR	C37-C22-C23	2.40	121.75	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	407	CLA	CAA-CBA-CGA	2.40	120.02	113.21
26	b	628	BCR	C24-C23-C22	-2.40	122.69	126.23
24	d	402	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
24	c	510	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
24	A	405	CLA	CMB-C2B-C1B	2.40	129.07	125.42
24	C	504	CLA	C1-O2A-CGA	2.40	122.45	116.65
32	D	405[A]	PL9	C32-C33-C34	-2.40	122.14	127.62
24	b	621	CLA	O2A-CGA-CBA	2.40	119.14	111.83
24	A	407	CLA	C3B-C4B-NB	2.39	112.67	110.53
27	A	412	SQD	C1-C2-C3	-2.39	104.97	110.01
26	D	404	BCR	C21-C20-C19	-2.39	116.27	123.20
24	B	603	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
24	c	510	CLA	CMC-C2C-C1C	2.39	128.77	125.03
24	B	603	CLA	CAC-C3C-C4C	2.39	127.90	124.79
24	c	513	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
24	B	607	CLA	CHD-C4C-NC	2.39	127.94	124.23
24	d	403	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
24	b	616	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
24	A	410	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
24	C	505	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
24	A	405	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
36	C	523	HTG	O5-C1-C2	2.39	113.61	110.32
24	C	513	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
24	c	507	CLA	C4-C3-C5	2.39	119.37	115.23
32	A	420[B]	PL9	C40-C39-C41	2.39	119.37	115.23
24	A	406	CLA	CHB-C4A-NA	2.38	127.84	124.40
26	K	101	BCR	C16-C17-C18	-2.38	123.93	127.28
38	D	408	LHG	O7-C7-C8	2.38	116.64	111.48
26	C	515	BCR	C28-C27-C26	-2.38	109.81	114.06
24	B	602	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
24	a	409	CLA	C4C-C3C-C2C	-2.38	103.42	106.89
26	K	101	BCR	C2-C1-C6	2.38	113.90	110.44
24	B	603	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
24	c	516	CLA	CBA-CAA-C2A	-2.38	106.71	113.79
24	B	611	CLA	CGD-CBD-CAD	-2.38	103.14	110.85
26	b	628	BCR	C28-C27-C26	-2.38	109.81	114.06
24	c	516	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
37	D	406	DGD	O6D-C5D-C6D	2.38	111.41	106.69
24	b	626	CLA	C4-C3-C5	2.38	119.35	115.23
32	A	420[A]	PL9	C10-C9-C11	2.38	119.35	115.23
24	B	614	CLA	CED-O2D-CGD	2.38	121.30	115.92
39	e	102	HEM	CHA-C1A-NA	2.37	128.17	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	611	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
38	D	407	LHG	C5-O7-C7	-2.37	112.11	117.80
24	a	412	CLA	CHB-C4A-NA	2.37	127.82	124.40
37	e	101	DGD	C1E-O6E-C5E	2.37	118.35	113.72
24	d	401	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
26	d	404	BCR	C39-C30-C25	-2.37	106.53	110.24
26	C	515	BCR	C37-C22-C23	2.37	121.71	118.09
24	c	513	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
26	D	404	BCR	C10-C11-C12	-2.37	116.34	123.20
24	A	406	CLA	C2A-C1A-CHA	-2.37	119.76	123.87
24	C	510	CLA	C4-C3-C2	-2.37	117.55	123.63
24	B	613	CLA	CMA-C3A-C2A	-2.37	104.83	113.98
24	b	626	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
24	b	625	CLA	O2A-CGA-CBA	2.36	119.05	111.83
24	d	401	CLA	C1-O2A-CGA	2.36	122.37	116.65
26	d	404	BCR	C21-C20-C19	-2.36	116.35	123.20
24	b	618	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
29	a	404	LMT	C1B-O1B-C4'	-2.36	112.38	117.98
32	D	405[A]	PL9	C2-C1-C6	2.36	121.81	119.00
24	B	610	CLA	C1-O2A-CGA	2.36	122.36	116.65
24	c	512	CLA	CMB-C2B-C1B	2.36	129.01	125.42
26	K	101	BCR	C33-C5-C6	-2.36	121.91	124.48
26	a	413	BCR	C38-C26-C25	-2.36	121.91	124.48
25	A	408	PHO	C4-C3-C5	2.36	119.32	115.23
32	d	405[B]	PL9	C53-C6-C1	2.36	120.11	115.28
24	B	608	CLA	CBC-CAC-C3C	-2.36	106.03	112.42
24	a	409	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
24	B	611	CLA	C4-C3-C5	2.36	119.32	115.23
25	A	409[B]	PHO	O2A-CGA-CBA	2.35	119.01	111.83
26	b	628	BCR	C33-C5-C6	-2.35	121.92	124.48
24	b	617	CLA	CAA-CBA-CGA	2.35	119.89	113.21
24	b	612	CLA	CHD-C4C-NC	2.35	127.88	124.23
32	D	405[A]	PL9	C15-C14-C16	2.35	119.31	115.23
26	a	413	BCR	C40-C30-C25	-2.35	106.56	110.24
25	A	409[A]	PHO	O2A-CGA-CBA	2.35	119.00	111.83
37	C	517	DGD	O2G-C1B-O1B	-2.35	118.22	123.70
24	b	612	CLA	O2A-CGA-CBA	2.34	118.98	111.83
24	B	614	CLA	CMC-C2C-C1C	2.34	128.69	125.03
24	d	403	CLA	CGD-CBD-CAD	-2.34	103.27	110.85
39	e	102	HEM	C3B-C4B-NB	-2.34	107.79	109.47
24	C	502	CLA	C4-C3-C5	2.34	119.29	115.23
26	b	627	BCR	C29-C30-C25	2.34	113.83	110.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	520	DGD	O1G-C1A-C2A	2.34	118.96	111.83
24	c	509	CLA	C1-O2A-CGA	2.34	122.31	116.65
27	a	414	SQD	O9-S-O7	-2.34	106.23	113.82
26	H	102	BCR	C10-C11-C12	-2.34	116.43	123.20
24	b	618	CLA	CAC-C3C-C4C	2.33	127.83	124.79
24	a	409	CLA	CAC-C3C-C4C	2.33	127.82	124.79
24	B	603	CLA	C1-O2A-CGA	2.33	122.29	116.65
24	c	509	CLA	CBC-CAC-C3C	-2.33	106.11	112.42
24	c	505	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
26	H	102	BCR	C7-C8-C9	-2.33	122.79	126.23
24	B	606	CLA	C1-C2-C3	-2.33	122.38	126.20
26	C	515	BCR	C11-C10-C9	-2.33	124.02	127.28
32	D	405[B]	PL9	C7-C3-C2	-2.33	120.65	123.39
29	A	417	LMT	C6'-C5'-C4'	-2.33	106.84	113.38
32	D	405[A]	PL9	C45-C44-C46	2.33	119.26	115.23
24	c	514	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
24	D	402	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
26	T	103	BCR	C1-C6-C7	2.32	121.95	115.65
24	b	617	CLA	C4C-C3C-C2C	-2.32	103.51	106.89
24	A	410	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
34	Z	101	LMG	C1-C2-C3	2.32	114.89	110.01
26	y	101	BCR	C24-C23-C22	-2.32	122.80	126.23
24	a	412	CLA	CAC-C3C-C4C	2.32	127.81	124.79
36	b	633	HTG	C1-C2-C3	2.32	115.08	110.55
24	C	513	CLA	C3B-C4B-NB	2.32	112.60	110.53
26	B	620	BCR	C28-C27-C26	-2.32	109.92	114.06
26	Y	101	BCR	C21-C20-C19	-2.32	116.49	123.20
24	c	507	CLA	CBC-CAC-C3C	-2.32	106.14	112.42
32	D	405[A]	PL9	C7-C3-C2	-2.31	120.66	123.39
24	B	608	CLA	O2A-CGA-CBA	2.31	118.89	111.83
25	a	411	PHO	CBA-CAA-C2A	-2.31	106.97	113.78
24	D	403	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
24	A	405	CLA	CMA-C3A-C4A	-2.31	105.56	111.77
32	D	405[B]	PL9	C32-C33-C34	-2.31	122.34	127.62
26	d	404	BCR	C29-C28-C27	-2.31	106.20	111.28
26	H	102	BCR	C31-C1-C6	-2.31	106.62	110.24
37	C	518	DGD	O3G-C3G-C2G	-2.31	105.21	110.82
37	H	103	DGD	C3E-C4E-C5E	-2.31	106.05	110.23
24	b	618	CLA	CMB-C2B-C1B	2.31	128.93	125.42
32	d	405[A]	PL9	C22-C23-C24	-2.31	122.35	127.62
27	b	601	SQD	O8-S-C6	2.31	110.42	105.97
26	c	518	BCR	C11-C10-C9	-2.30	124.05	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	505	CLA	C4B-C3B-C2B	-2.30	104.44	107.30
24	b	618	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
26	B	618	BCR	C11-C10-C9	-2.30	124.05	127.28
39	F	102	HEM	O2A-CGA-CBA	2.30	121.27	114.00
24	b	613	CLA	CMB-C2B-C1B	2.30	128.92	125.42
24	c	509	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
34	b	630	LMG	O8-C28-O10	-2.30	117.88	123.63
25	a	420[A]	PHO	O2A-CGA-CBA	2.30	118.84	111.83
26	K	101	BCR	C3-C4-C5	-2.30	109.96	114.06
24	d	402	CLA	CBC-CAC-C3C	-2.30	106.19	112.42
24	B	615	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
24	b	622	CLA	CED-O2D-CGD	2.30	121.12	115.92
38	D	408	LHG	O8-C23-C24	2.29	118.83	111.83
24	d	401	CLA	O2A-CGA-CBA	2.29	118.83	111.83
24	c	511	CLA	CAC-C3C-C4C	2.29	127.77	124.79
29	a	421	LMT	C1B-O1B-C4'	-2.29	112.54	117.98
24	b	622	CLA	CHD-C4C-NC	2.29	127.78	124.23
32	a	416[A]	PL9	C45-C44-C46	2.29	119.20	115.23
24	b	614	CLA	CHA-C1A-NA	-2.29	121.21	126.39
38	d	407	LHG	O8-C23-C24	2.29	118.81	111.83
24	c	509	CLA	CHD-C4C-NC	2.29	127.78	124.23
24	d	402	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
24	C	507	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
24	C	511	CLA	C1-C2-C3	-2.29	122.45	126.20
24	C	503	CLA	C2A-C1A-CHA	-2.28	119.90	123.87
26	T	103	BCR	C10-C11-C12	-2.28	116.58	123.20
24	B	606	CLA	CHC-C1C-C2C	-2.28	120.46	126.95
37	c	521	DGD	O2G-C1B-O1B	-2.28	118.37	123.70
24	a	410	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
24	C	507	CLA	CAC-C3C-C4C	2.28	127.76	124.79
24	b	620	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
32	A	420[A]	PL9	C40-C39-C41	2.28	119.19	115.23
32	D	405[A]	PL9	C35-C34-C36	2.28	119.19	115.23
37	C	516	DGD	O1G-C1A-C2A	2.28	118.79	111.83
24	C	511	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
29	M	103	LMT	O5B-C5B-C4B	2.28	113.80	109.70
26	K	101	BCR	C29-C30-C25	2.27	113.74	110.44
25	a	420[B]	PHO	O2A-CGA-CBA	2.27	118.77	111.83
24	A	406	CLA	O1D-CGD-CBD	-2.27	120.03	124.52
41	v	205	HEC	O2A-CGA-CBA	2.27	121.18	114.00
26	b	628	BCR	C38-C26-C25	-2.27	122.00	124.48
24	c	517	CLA	C4B-C3B-C2B	-2.27	104.48	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	508	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
24	A	405	CLA	CHB-C4A-NA	2.27	127.68	124.40
37	c	519	DGD	O3G-C3G-C2G	-2.27	105.30	110.82
36	b	609	HTG	O5-C1-C2	2.27	113.44	110.32
36	b	632	HTG	C1-C2-C3	2.27	114.98	110.55
24	A	406	CLA	CMA-C3A-C2A	-2.27	105.21	113.98
24	c	506	CLA	CMC-C2C-C1C	2.27	128.58	125.03
24	B	616	CLA	O2A-CGA-CBA	2.27	118.74	111.83
24	C	504	CLA	C2A-C1A-CHA	-2.27	119.94	123.87
24	B	610	CLA	O2A-CGA-CBA	2.26	118.74	111.83
24	A	406	CLA	C4C-C3C-C2C	-2.26	103.60	106.89
32	d	405[A]	PL9	C45-C44-C46	2.26	119.16	115.23
27	B	621	SQD	O47-C7-O49	-2.26	118.42	123.70
24	C	511	CLA	C1-O2A-CGA	2.26	122.12	116.65
24	d	401	CLA	C1-C2-C3	-2.26	122.50	126.20
25	a	411	PHO	CMC-C2C-C1C	2.26	128.80	124.73
24	B	614	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
24	A	407	CLA	CMA-C3A-C2A	-2.26	105.26	113.98
24	d	403	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
24	c	505	CLA	OBD-CAD-C3D	-2.25	123.15	128.42
24	C	506	CLA	O2A-CGA-CBA	2.25	118.70	111.83
24	c	505	CLA	CHD-C4C-NC	2.25	127.72	124.23
24	B	616	CLA	C4-C3-C5	2.25	119.14	115.23
24	c	506	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
29	m	102	LMT	C1B-O5B-C5B	2.25	118.11	113.72
27	B	621	SQD	C1-C2-C3	-2.25	105.28	110.01
24	c	512	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
24	A	410	CLA	CBC-CAC-C3C	-2.25	106.33	112.42
26	T	103	BCR	C29-C28-C27	-2.25	106.34	111.28
24	b	618	CLA	C4-C3-C5	2.25	119.12	115.23
26	Y	101	BCR	C24-C23-C22	-2.24	122.92	126.23
26	y	101	BCR	C37-C22-C23	2.24	121.51	118.09
24	C	503	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
24	A	406	CLA	O2A-CGA-CBA	2.24	118.67	111.83
24	B	613	CLA	CBC-CAC-C3C	-2.24	106.35	112.42
24	B	614	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
24	b	625	CLA	C1-O2A-CGA	2.24	122.07	116.65
26	T	103	BCR	C16-C17-C18	-2.24	124.14	127.28
24	b	619	CLA	CAC-C3C-C4C	2.24	127.70	124.79
24	D	402	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
24	b	611	CLA	O2A-CGA-CBA	2.24	118.65	111.83
24	B	603	CLA	C4-C3-C5	2.24	119.11	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	515	BCR	C15-C16-C17	-2.23	118.95	123.52
37	C	518	DGD	C3G-C2G-C1G	-2.23	106.58	111.78
27	a	414	SQD	O47-C7-O49	-2.23	118.49	123.70
24	B	616	CLA	CED-O2D-CGD	2.23	120.97	115.92
26	C	514	BCR	C37-C22-C23	2.23	121.49	118.09
24	B	616	CLA	C2A-C1A-CHA	-2.23	120.00	123.87
41	v	205	HEC	CHD-C1D-ND	2.22	127.89	123.86
32	a	416[B]	PL9	C45-C44-C46	2.22	119.09	115.23
24	b	621	CLA	C2A-C1A-CHA	-2.22	120.01	123.87
27	b	601	SQD	O7-S-C6	2.22	110.08	106.76
24	B	603	CLA	CMC-C2C-C1C	2.22	128.51	125.03
24	c	517	CLA	CHB-C4A-NA	2.22	127.61	124.40
24	c	517	CLA	C3B-C4B-NB	2.22	112.51	110.53
24	b	613	CLA	CMA-C3A-C2A	-2.22	105.39	113.98
24	C	503	CLA	C3B-C4B-NB	2.22	112.51	110.53
24	d	402	CLA	CMA-C3A-C2A	-2.22	105.40	113.98
24	B	606	CLA	CAC-C3C-C4C	2.22	127.68	124.79
26	y	101	BCR	C40-C30-C25	-2.22	106.76	110.24
24	C	512	CLA	CBC-CAC-C3C	-2.22	106.41	112.42
24	c	509	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	b	624	CLA	C4-C3-C2	-2.22	117.94	123.63
27	a	414	SQD	O48-C23-O10	-2.22	118.09	123.63
24	B	613	CLA	CHC-C1C-C2C	-2.22	120.65	126.95
24	c	508	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
32	A	420[B]	PL9	C35-C34-C36	2.21	119.07	115.23
36	C	522	HTG	C1-O5-C5	2.21	116.53	112.56
34	c	523	LMG	O8-C28-O10	-2.21	118.09	123.63
26	B	619	BCR	C37-C22-C23	2.21	121.47	118.09
38	D	407	LHG	O7-C7-O9	-2.21	118.54	123.70
26	a	413	BCR	C33-C5-C6	-2.21	122.07	124.48
24	c	514	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
34	c	523	LMG	O7-C10-O9	-2.21	118.55	123.70
34	j	101	LMG	O8-C28-C29	2.20	118.55	111.83
24	b	625	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
24	c	511	CLA	C1-C2-C3	-2.20	122.59	126.20
24	c	508	CLA	C11-C10-C8	-2.20	108.65	115.97
24	B	605	CLA	CAC-C3C-C4C	2.20	127.65	124.79
24	B	602	CLA	CHB-C4A-NA	2.20	127.57	124.40
24	b	623	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
24	B	613	CLA	CMB-C2B-C1B	2.20	128.77	125.42
24	b	613	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
32	a	416[A]	PL9	C12-C13-C14	-2.20	122.59	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	510	CLA	O2A-CGA-CBA	2.20	118.53	111.83
24	C	508	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
24	C	508	CLA	OBD-CAD-C3D	-2.19	123.29	128.42
24	c	514	CLA	CMB-C2B-C1B	2.19	128.76	125.42
24	c	517	CLA	CHB-C1B-C2B	-2.19	121.06	127.43
27	A	412	SQD	C44-O6-C1	-2.19	109.10	113.80
24	b	626	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
38	L	101	LHG	C5-O7-C7	-2.19	112.56	117.80
32	d	405[B]	PL9	C30-C29-C31	2.19	119.03	115.23
24	B	611	CLA	C1-C2-C3	-2.19	122.61	126.20
24	C	509	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
26	b	627	BCR	C16-C17-C18	-2.19	124.21	127.28
39	F	102	HEM	CBA-CAA-C2A	-2.19	106.49	112.53
25	a	420[B]	PHO	CMA-C3A-C4A	-2.19	109.90	114.61
24	c	516	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
24	b	624	CLA	C4-C3-C5	2.18	119.02	115.23
24	b	622	CLA	O2D-CGD-O1D	-2.18	119.60	123.85
24	a	410	CLA	CMB-C2B-C1B	2.18	128.75	125.42
26	K	101	BCR	C36-C18-C19	2.18	121.42	118.09
34	B	622	LMG	O8-C28-O10	-2.18	118.17	123.63
24	b	612	CLA	CMA-C3A-C2A	-2.18	105.55	113.98
26	D	404	BCR	C16-C17-C18	-2.18	124.22	127.28
26	b	628	BCR	C15-C14-C13	-2.18	124.22	127.28
24	b	618	CLA	CMC-C2C-C1C	2.18	128.44	125.03
24	c	507	CLA	C3B-C4B-NB	2.18	112.47	110.53
24	C	510	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
24	c	514	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
24	c	514	CLA	CHB-C4A-NA	2.18	127.54	124.40
24	C	513	CLA	C2A-C1A-CHA	-2.18	120.09	123.87
24	b	612	CLA	C1-O2A-CGA	2.18	121.92	116.65
26	B	618	BCR	C24-C23-C22	-2.17	123.02	126.23
24	c	514	CLA	CAC-C3C-C4C	2.17	127.62	124.79
24	B	605	CLA	CHA-C1A-NA	-2.17	121.47	126.39
37	H	103	DGD	O6E-C5E-C6E	2.17	111.83	106.44
25	a	420[A]	PHO	C4A-C3A-C2A	-2.17	100.77	102.84
26	T	103	BCR	C34-C9-C10	-2.17	119.30	122.82
24	C	510	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
24	b	620	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
32	D	405[A]	PL9	C51-C49-C50	2.17	119.58	114.59
26	B	620	BCR	C37-C22-C23	2.17	121.40	118.09
24	B	603	CLA	CMA-C3A-C2A	-2.17	105.60	113.98
37	C	517	DGD	O1G-C1A-O1A	-2.17	118.21	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	630	LMG	O7-C10-O9	-2.17	118.64	123.70
24	B	617	CLA	C2A-C1A-CHA	-2.17	120.11	123.87
24	C	513	CLA	O2A-CGA-O1A	-2.17	118.21	123.63
26	T	103	BCR	C7-C6-C5	-2.17	116.57	121.56
24	C	510	CLA	O1D-CGD-CBD	-2.17	120.25	124.52
32	A	420[A]	PL9	C35-C34-C36	2.16	118.98	115.23
24	C	508	CLA	CHD-C4C-NC	2.16	127.58	124.23
24	B	607	CLA	C2A-C1A-CHA	-2.16	120.11	123.87
24	b	611	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
24	B	608	CLA	C1-O2A-CGA	2.16	121.88	116.65
39	F	102	HEM	CHA-C4D-ND	2.16	127.04	124.37
26	h	101	BCR	C20-C21-C22	-2.16	124.25	127.28
32	D	405[B]	PL9	C7-C3-C4	2.16	118.69	116.91
24	B	609	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
32	a	416[B]	PL9	C8-C7-C3	2.16	117.60	112.03
27	A	416	SQD	O8-S-C6	2.16	110.14	105.97
25	A	409[A]	PHO	C4A-C3A-C2A	-2.16	100.79	102.84
37	H	103	DGD	C2G-O2G-C1B	-2.16	112.64	117.80
24	b	625	CLA	C6-C7-C8	-2.15	108.81	115.97
24	b	624	CLA	CHB-C4A-NA	2.15	127.51	124.40
24	C	507	CLA	C4B-C3B-C2B	-2.15	104.62	107.30
24	c	512	CLA	C1-O2A-CGA	2.15	121.86	116.65
41	v	205	HEC	C4C-NC-C1C	2.15	109.33	105.82
26	B	619	BCR	C30-C25-C26	-2.15	119.70	122.64
24	b	611	CLA	C1-O2A-CGA	2.15	121.85	116.65
32	D	405[B]	PL9	C15-C14-C16	2.15	118.95	115.23
24	C	509	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
24	c	508	CLA	CMA-C3A-C2A	-2.14	105.69	113.98
24	c	516	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
36	B	633	HTG	C1-O5-C5	2.14	116.41	112.56
26	b	628	BCR	C39-C30-C25	-2.14	106.88	110.24
34	D	412	LMG	O8-C28-C29	2.14	118.37	111.83
26	t	101	BCR	C29-C28-C27	-2.14	106.57	111.28
26	k	101	BCR	C39-C30-C25	-2.14	106.89	110.24
25	a	411	PHO	C4A-C3A-C2A	-2.14	100.80	102.84
24	a	409	CLA	C7-C6-C5	-2.14	107.56	113.26
37	c	521	DGD	O1G-C1A-O1A	-2.14	118.28	123.63
24	C	506	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
34	a	415	LMG	O7-C10-O9	-2.14	118.71	123.70
24	B	617	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
24	b	614	CLA	C6-C7-C8	-2.14	108.86	115.97
24	a	409	CLA	CBC-CAC-C3C	-2.14	106.63	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	509	CLA	CMB-C2B-C1B	2.14	128.67	125.42
24	c	505	CLA	C4-C3-C5	2.14	118.93	115.23
24	B	610	CLA	C2A-C1A-CHA	-2.13	120.16	123.87
24	B	609	CLA	CAA-C2A-C3A	-2.13	107.23	113.00
24	C	508	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
24	D	403	CLA	C1-O2A-CGA	2.13	121.81	116.65
37	c	521	DGD	C1D-O6D-C5D	2.13	117.88	113.72
25	A	408	PHO	CMC-C2C-C1C	2.13	128.57	124.73
37	c	519	DGD	O1G-C1A-C2A	2.13	118.33	111.83
26	b	629	BCR	C21-C20-C19	-2.13	117.03	123.20
24	C	507	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
29	C	521	LMT	O5'-C5'-C4'	2.13	114.13	109.72
24	C	503	CLA	C4-C3-C5	2.13	118.92	115.23
25	A	409[B]	PHO	C6-C5-C3	-2.13	108.28	113.47
24	B	608	CLA	C4-C3-C5	2.13	118.92	115.23
24	B	617	CLA	C4-C3-C5	2.13	118.92	115.23
24	A	407	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
24	d	401	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
24	B	602	CLA	CMC-C2C-C1C	2.13	128.35	125.03
36	b	602	HTG	C1-O5-C5	2.12	116.37	112.56
24	A	407	CLA	O2A-CGA-CBA	2.12	118.31	111.83
38	a	422	LHG	C6-C5-C4	-2.12	106.83	111.78
26	k	101	BCR	C38-C26-C25	-2.12	122.17	124.48
32	d	405[A]	PL9	C25-C24-C26	2.12	118.91	115.23
24	c	517	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
25	A	408	PHO	CBA-CAA-C2A	-2.12	107.53	113.78
24	c	516	CLA	C1-O2A-CGA	2.12	121.78	116.65
34	A	422	LMG	O7-C10-O9	-2.12	118.75	123.70
24	B	612	CLA	CHB-C4A-NA	2.12	127.46	124.40
24	c	508	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
24	B	606	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
26	a	413	BCR	C8-C7-C6	-2.12	121.35	127.00
34	c	523	LMG	O1-C1-C2	2.12	111.48	108.27
24	d	401	CLA	CMC-C2C-C1C	2.11	128.34	125.03
24	a	409	CLA	CHB-C4A-NA	2.11	127.45	124.40
24	d	401	CLA	CAA-CBA-CGA	2.11	119.21	113.21
24	A	405	CLA	C1-C2-C3	-2.11	122.74	126.20
41	v	205	HEC	O2D-CGD-CBD	2.11	120.67	114.00
24	b	621	CLA	CHB-C4A-NA	2.11	127.45	124.40
41	V	206	HEC	CHA-C4D-ND	2.11	127.69	123.86
24	C	504	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
24	C	502	CLA	CMC-C2C-C1C	2.11	128.33	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	101	BCR	C35-C13-C12	2.11	121.31	118.09
32	A	420[B]	PL9	C51-C49-C50	2.11	119.44	114.59
24	B	608	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
24	C	509	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
25	A	408	PHO	O2A-CGA-CBA	2.11	118.27	111.83
29	M	101	LMT	O6'-C6'-C5'	-2.11	104.15	111.33
29	M	104	LMT	C1B-O5B-C5B	2.11	117.83	113.72
39	e	102	HEM	C4C-CHD-C1D	-2.11	121.54	126.02
26	A	411	BCR	C21-C20-C19	-2.11	117.10	123.20
25	A	409[A]	PHO	CMA-C3A-C4A	-2.11	110.07	114.61
26	D	404	BCR	C30-C25-C24	2.10	121.36	115.65
24	C	504	CLA	C1-C2-C3	-2.10	122.75	126.20
32	d	405[B]	PL9	C17-C18-C19	-2.10	122.81	127.62
24	c	507	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
29	m	102	LMT	C1B-O1B-C4'	-2.10	113.00	117.98
24	B	603	CLA	CMB-C2B-C1B	2.10	128.62	125.42
24	d	401	CLA	CED-O2D-CGD	2.10	120.68	115.92
39	e	102	HEM	C4C-NC-C1C	2.10	109.24	105.82
24	b	618	CLA	CMA-C3A-C2A	-2.10	105.87	113.98
24	C	504	CLA	C11-C10-C8	-2.10	108.99	115.97
24	C	507	CLA	C3B-C4B-NB	2.10	112.40	110.53
32	a	416[A]	PL9	C8-C7-C3	2.10	117.45	112.03
37	e	101	DGD	O2G-C1B-O1B	-2.10	118.81	123.70
41	v	205	HEC	C4B-NB-C1B	2.09	109.24	105.82
27	f	102	SQD	O48-C23-O10	-2.09	118.39	123.63
24	b	616	CLA	C2A-C1A-CHA	-2.09	120.23	123.87
36	b	608	HTG	O5-C5-C4	2.09	113.47	109.70
24	d	401	CLA	CAC-C3C-C4C	2.09	127.51	124.79
24	b	613	CLA	C7-C6-C5	-2.09	107.69	113.26
26	t	101	BCR	C37-C22-C23	2.09	121.28	118.09
24	C	512	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
26	C	514	BCR	C23-C24-C25	-2.09	121.42	127.00
24	D	403	CLA	CHB-C4A-NA	2.08	127.41	124.40
24	B	613	CLA	CMA-C3A-C4A	-2.08	106.18	111.77
38	d	407	LHG	O8-C23-O10	-2.08	118.42	123.63
24	B	605	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
24	B	603	CLA	CHB-C4A-NA	2.08	127.40	124.40
24	B	611	CLA	C11-C12-C13	-2.08	109.05	115.97
26	A	411	BCR	C37-C22-C23	2.08	121.26	118.09
24	C	511	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
24	b	618	CLA	C11-C12-C13	-2.08	109.06	115.97
29	f	103	LMT	C1B-O5B-C5B	2.08	117.78	113.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	519	LMG	O8-C28-O10	-2.08	118.43	123.63
26	T	103	BCR	C2-C1-C6	2.08	113.46	110.44
38	l	101	LHG	O4-P-O5	2.08	122.10	112.44
26	d	404	BCR	C10-C11-C12	-2.07	117.19	123.20
39	e	102	HEM	CHD-C1D-C2D	-2.07	121.75	125.03
24	b	622	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	b	620	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
26	B	620	BCR	C23-C24-C25	-2.07	121.46	127.00
26	T	103	BCR	C7-C8-C9	-2.07	123.17	126.23
32	d	405[B]	PL9	C51-C49-C50	2.07	119.36	114.59
24	C	501	CLA	C2A-C1A-CHA	-2.07	120.27	123.87
24	c	510	CLA	CAC-C3C-C4C	2.07	127.48	124.79
24	c	512	CLA	CED-O2D-CGD	2.07	120.61	115.92
24	c	505	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
26	A	411	BCR	C8-C7-C6	-2.07	121.47	127.00
38	l	101	LHG	O8-C23-O10	-2.07	118.45	123.63
41	v	205	HEC	CHB-C1B-NB	2.07	127.61	123.86
32	D	405[B]	PL9	C2-C1-C6	2.06	121.45	119.00
26	B	618	BCR	C21-C20-C19	-2.06	117.22	123.20
38	E	101	LHG	O8-C23-O10	-2.06	118.47	123.63
26	b	627	BCR	C21-C20-C19	-2.06	117.22	123.20
27	B	621	SQD	O48-C23-O10	-2.06	118.47	123.63
26	d	404	BCR	C2-C1-C6	2.06	113.44	110.44
34	j	101	LMG	O8-C28-O10	-2.06	118.47	123.63
29	M	104	LMT	O1B-C1B-C2B	2.06	113.16	108.09
27	F	103	SQD	O48-C23-O10	-2.06	118.47	123.63
24	B	614	CLA	CHB-C1B-NB	-2.06	120.96	124.05
26	c	518	BCR	C37-C22-C23	2.06	121.24	118.09
26	a	413	BCR	C3-C4-C5	-2.06	110.38	114.06
24	C	507	CLA	C4-C3-C5	2.06	118.80	115.23
24	a	412	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
41	V	206	HEC	CAD-CBD-CGD	2.06	119.12	113.67
26	A	411	BCR	C2-C1-C6	2.06	113.43	110.44
38	l	101	LHG	O7-C7-O9	-2.06	118.89	123.70
25	a	411	PHO	C4-C3-C5	2.06	118.80	115.23
38	D	409	LHG	O7-C7-O9	-2.06	118.90	123.70
24	B	616	CLA	C11-C10-C8	-2.06	109.13	115.97
24	c	513	CLA	C2A-C1A-CHA	-2.06	120.30	123.87
24	b	618	CLA	OBD-CAD-C3D	-2.05	123.61	128.42
24	b	611	CLA	CHC-C1C-NC	2.05	127.41	124.31
24	B	609	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
24	B	609	CLA	C2A-C1A-CHA	-2.05	120.30	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	CLA	CED-O2D-CGD	2.05	120.57	115.92
25	A	409[B]	PHO	CMA-C3A-C4A	-2.05	110.19	114.61
34	C	520	LMG	O7-C10-O9	-2.05	118.91	123.70
34	z	101	LMG	C7-O1-C1	-2.05	109.40	113.80
26	A	411	BCR	C20-C21-C22	-2.05	124.40	127.28
26	b	629	BCR	C16-C17-C18	-2.05	124.40	127.28
24	c	515	CLA	CMB-C2B-C1B	2.05	128.54	125.42
24	b	620	CLA	C2A-C1A-CHA	-2.05	120.31	123.87
32	d	405[B]	PL9	C22-C23-C24	-2.05	122.93	127.62
26	c	518	BCR	C32-C1-C6	-2.05	107.03	110.24
24	a	412	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
24	a	409	CLA	O2D-CGD-O1D	-2.05	119.86	123.85
39	e	102	HEM	C2A-C1A-NA	-2.05	107.88	110.15
26	D	404	BCR	C3-C4-C5	-2.04	110.41	114.06
24	C	510	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
38	l	101	LHG	C6-C5-C4	-2.04	107.02	111.78
32	A	420[A]	PL9	C51-C49-C50	2.04	119.29	114.59
26	H	102	BCR	C39-C30-C25	-2.04	107.04	110.24
26	h	101	BCR	C29-C30-C25	2.04	113.41	110.44
26	T	103	BCR	C20-C21-C22	-2.04	124.41	127.28
24	b	622	CLA	CMB-C2B-C1B	2.04	128.53	125.42
29	F	101	LMT	C1B-O5B-C5B	2.04	117.71	113.72
24	c	514	CLA	C4-C3-C2	-2.04	118.39	123.63
24	B	617	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
24	C	507	CLA	CHA-C1A-NA	-2.04	121.78	126.39
32	A	420[B]	PL9	C47-C48-C49	-2.04	120.85	127.64
24	b	622	CLA	CMA-C3A-C4A	-2.03	106.30	111.77
27	B	621	SQD	C44-O6-C1	-2.03	109.43	113.80
24	D	402	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
24	B	608	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
24	c	515	CLA	C1-O2A-CGA	2.03	121.57	116.65
24	B	610	CLA	CHA-C1A-NA	-2.03	121.79	126.39
24	b	613	CLA	CHB-C4A-NA	2.03	127.33	124.40
24	a	410	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
24	B	602	CLA	C1-C2-C3	-2.03	122.87	126.20
32	d	405[B]	PL9	C35-C34-C36	2.03	118.75	115.23
26	C	514	BCR	C28-C27-C26	-2.02	110.44	114.06
26	B	620	BCR	C7-C8-C9	-2.02	123.24	126.23
24	B	616	CLA	CHA-C1A-NA	-2.02	121.81	126.39
25	A	408	PHO	C1-C2-C3	-2.02	122.88	126.20
24	b	618	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
24	C	504	CLA	O2A-CGA-O1A	-2.02	118.57	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	512	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
24	c	509	CLA	CED-O2D-CGD	2.02	120.50	115.92
38	d	406	LHG	O4-P-O5	2.02	121.85	112.44
26	Y	101	BCR	C29-C30-C25	2.02	113.38	110.44
24	C	512	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	C	505	CLA	O2A-CGA-CBA	2.02	118.00	111.83
24	C	505	CLA	CHA-C1A-NA	-2.02	121.81	126.39
26	K	101	BCR	C15-C16-C17	-2.02	119.38	123.52
34	c	522	LMG	C30-C29-C28	-2.02	106.29	113.69
32	d	405[A]	PL9	C35-C34-C36	2.02	118.73	115.23
24	b	622	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
24	B	614	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
24	c	516	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
34	C	520	LMG	C8-O7-C10	-2.02	112.97	117.80
24	A	406	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
26	b	629	BCR	C15-C14-C13	-2.02	124.45	127.28
26	k	101	BCR	C3-C4-C5	-2.02	110.46	114.06
26	k	101	BCR	C33-C5-C6	-2.02	122.28	124.48
24	B	603	CLA	O2A-CGA-CBA	2.01	117.98	111.83
24	C	508	CLA	CHB-C4A-NA	2.01	127.31	124.40
24	b	622	CLA	OBD-CAD-C3D	-2.01	123.71	128.42
34	A	422	LMG	C7-O1-C1	-2.01	109.48	113.80
24	B	607	CLA	CHB-C4A-NA	2.01	127.30	124.40
26	c	527	BCR	C7-C8-C9	-2.01	123.26	126.23
25	A	409[B]	PHO	CED-O2D-CGD	2.01	120.48	115.92
24	b	626	CLA	CHC-C1C-NC	2.01	127.34	124.31
39	F	102	HEM	O2D-CGD-CBD	2.01	120.36	114.00
24	C	505	CLA	C4-C3-C5	2.01	118.72	115.23
26	d	404	BCR	C40-C30-C25	-2.01	107.09	110.24
27	A	416	SQD	O6-C44-C45	-2.01	105.93	110.82
24	C	508	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
24	C	503	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
24	B	602	CLA	C4-C3-C5	2.01	118.72	115.23
26	b	629	BCR	C3-C4-C5	-2.01	110.47	114.06
24	b	625	CLA	O2D-CGD-O1D	-2.01	119.94	123.85
24	b	623	CLA	CHA-C1A-NA	-2.01	121.84	126.39
26	B	618	BCR	C10-C11-C12	-2.01	117.39	123.20
24	c	511	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
26	H	102	BCR	C20-C21-C22	-2.00	124.47	127.28
36	B	632	HTG	C3-C4-C5	2.00	113.86	110.23
24	c	516	CLA	CHA-C1A-NA	-2.00	121.86	126.39
24	c	507	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	619	BCR	C20-C21-C22	-2.00	124.47	127.28

All (62) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	A	410	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	501	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	511	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	402	CLA	ND
24	D	403	CLA	ND
24	a	409	CLA	ND
24	a	412	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	617	CLA	ND
24	b	619	CLA	ND
24	b	620	CLA	ND
24	b	622	CLA	ND
24	b	623	CLA	ND
24	b	624	CLA	ND
24	b	625	CLA	ND
24	b	626	CLA	ND
24	c	505	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	c	515	CLA	ND
24	c	516	CLA	ND
24	d	401	CLA	ND
24	d	402	CLA	ND
24	d	403	CLA	ND

All (1298) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	B	615	CLA	C4-C3-C5-C6
24	C	502	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C2-C1-O2A-CGA
24	b	612	CLA	C4B-C3B-CAB-CBB
24	b	615	CLA	C2-C3-C5-C6
24	b	624	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	624	CLA	CAD-CBD-CGD-O2D
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D
24	c	513	CLA	CHA-CBD-CGD-O2D
24	c	516	CLA	C2B-C3B-CAB-CBB
24	c	516	CLA	C4B-C3B-CAB-CBB
26	D	404	BCR	C7-C8-C9-C10
26	D	404	BCR	C21-C22-C23-C24
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	d	404	BCR	C21-C22-C23-C24
26	d	404	BCR	C37-C22-C23-C24
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
26	y	101	BCR	C21-C22-C23-C24
27	A	416	SQD	O6-C44-C45-O47
27	B	621	SQD	O49-C7-O47-C45
27	B	621	SQD	C8-C7-O47-C45
27	B	621	SQD	C5-C6-S-O7
27	B	621	SQD	C5-C6-S-O8
27	B	621	SQD	C5-C6-S-O9
27	F	103	SQD	O49-C7-O47-C45
27	F	103	SQD	C8-C7-O47-C45
27	F	103	SQD	C5-C6-S-O7
27	F	103	SQD	C5-C6-S-O9
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
27	b	601	SQD	O5-C1-O6-C44
27	b	601	SQD	O49-C7-O47-C45
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
28	A	414	GOL	C1-C2-C3-O3
28	A	415	GOL	C1-C2-C3-O3
28	B	627	GOL	O1-C1-C2-O2
28	B	627	GOL	O1-C1-C2-C3
28	B	628	GOL	O1-C1-C2-C3
28	B	630	GOL	O1-C1-C2-C3
28	B	630	GOL	C1-C2-C3-O3
28	B	630	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	C	524	GOL	O1-C1-C2-C3
28	O	301	GOL	O1-C1-C2-C3
28	T	102	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-C3
28	V	201	GOL	O1-C1-C2-C3
28	a	402	GOL	O1-C1-C2-C3
28	f	101	GOL	O1-C1-C2-C3
28	v	202	GOL	O1-C1-C2-C3
29	A	417	LMT	C2'-C1'-O1'-C1
29	A	417	LMT	O5'-C1'-O1'-C1
29	M	103	LMT	O5'-C1'-O1'-C1
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
29	b	631	LMT	C2'-C1'-O1'-C1
29	b	631	LMT	O5'-C1'-O1'-C1
32	a	416[A]	PL9	C12-C11-C9-C10
32	a	416[B]	PL9	C12-C11-C9-C10
34	C	520	LMG	O9-C10-O7-C8
34	C	520	LMG	C11-C10-O7-C8
34	Z	101	LMG	O6-C1-O1-C7
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	O9-C10-O7-C8
36	B	624	HTG	C2'-C1'-S1-C1
36	B	625	HTG	O5-C1-S1-C1'
37	D	406	DGD	C2B-C1B-O2G-C2G
37	D	406	DGD	O1B-C1B-O2G-C2G
37	e	101	DGD	C2B-C1B-O2G-C2G
37	e	101	DGD	O1B-C1B-O2G-C2G
37	e	101	DGD	O6E-C1E-O5D-C6D
38	D	408	LHG	C4-O6-P-O3
38	D	408	LHG	C4-O6-P-O4
38	D	409	LHG	C4-O6-P-O4
38	E	101	LHG	C3-O3-P-O4
38	E	101	LHG	C3-O3-P-O5
38	E	101	LHG	C3-O3-P-O6
38	E	101	LHG	C4-O6-P-O5
38	L	101	LHG	C3-O3-P-O4
38	L	101	LHG	C4-O6-P-O3
38	L	101	LHG	C4-O6-P-O4
38	a	422	LHG	C3-O3-P-O5
38	a	422	LHG	C3-O3-P-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	d	407	LHG	O2-C2-C3-O3
38	d	407	LHG	C3-O3-P-O4
38	d	407	LHG	C3-O3-P-O6
38	l	101	LHG	C4-O6-P-O3
38	l	101	LHG	C4-O6-P-O4
38	l	101	LHG	C4-O6-P-O5
39	F	102	HEM	C2B-C3B-CAB-CBB
39	F	102	HEM	C2C-C3C-CAC-CBC
41	V	206	HEC	C2B-C3B-CAB-CBB
41	V	206	HEC	C4B-C3B-CAB-CBB
41	V	206	HEC	C2C-C3C-CAC-CBC
41	V	206	HEC	C4C-C3C-CAC-CBC
41	v	205	HEC	C2B-C3B-CAB-CBB
41	v	205	HEC	C4B-C3B-CAB-CBB
41	v	205	HEC	C2C-C3C-CAC-CBC
41	v	205	HEC	C4C-C3C-CAC-CBC
29	D	401	LMT	C3'-C4'-O1B-C1B
38	a	422	LHG	O10-C23-O8-C6
29	C	521	LMT	C3'-C4'-O1B-C1B
38	a	422	LHG	C24-C23-O8-C6
38	E	101	LHG	O10-C23-O8-C6
24	D	403	CLA	C3-C5-C6-C7
24	b	624	CLA	C3-C5-C6-C7
24	c	510	CLA	C3-C5-C6-C7
38	E	101	LHG	C24-C23-O8-C6
24	c	515	CLA	CBD-CGD-O2D-CED
27	b	601	SQD	C8-C7-O47-C45
34	z	101	LMG	C11-C10-O7-C8
24	B	606	CLA	C4-C3-C5-C6
24	b	615	CLA	C4-C3-C5-C6
24	b	624	CLA	C4-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
32	a	416[A]	PL9	C20-C19-C21-C22
24	B	606	CLA	C2-C3-C5-C6
24	b	624	CLA	C2-C3-C5-C6
24	c	508	CLA	C2-C3-C5-C6
32	a	416[A]	PL9	C18-C19-C21-C22
24	A	410	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
34	z	101	LMG	O6-C5-C6-O5
24	B	615	CLA	C3-C5-C6-C7
29	M	103	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	A	422	LMG	C11-C10-O7-C8
29	f	103	LMT	C4'-C5'-C6'-O6'
24	c	513	CLA	C3-C5-C6-C7
32	A	420[A]	PL9	C25-C24-C26-C27
32	A	420[B]	PL9	C25-C24-C26-C27
32	a	416[A]	PL9	C15-C14-C16-C17
32	a	416[A]	PL9	C25-C24-C26-C27
32	a	416[B]	PL9	C15-C14-C16-C17
32	a	416[B]	PL9	C20-C19-C21-C22
32	A	420[A]	PL9	C23-C24-C26-C27
32	A	420[B]	PL9	C23-C24-C26-C27
32	a	416[A]	PL9	C13-C14-C16-C17
32	a	416[A]	PL9	C23-C24-C26-C27
32	a	416[B]	PL9	C13-C14-C16-C17
32	a	416[B]	PL9	C18-C19-C21-C22
32	a	416[B]	PL9	C23-C24-C26-C27
34	A	422	LMG	O9-C10-O7-C8
34	C	520	LMG	O6-C5-C6-O5
32	d	405[A]	PL9	C39-C41-C42-C43
29	C	521	LMT	O5'-C5'-C6'-O6'
36	B	625	HTG	O5-C5-C6-O6
34	z	101	LMG	C4-C5-C6-O5
24	C	509	CLA	O1A-CGA-O2A-C1
27	B	621	SQD	O5-C1-O6-C44
29	B	635	LMT	O5'-C1'-O1'-C1
29	C	521	LMT	O5'-C1'-O1'-C1
29	F	101	LMT	O5'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
29	a	421	LMT	O5'-C1'-O1'-C1
29	f	103	LMT	O5'-C1'-O1'-C1
34	z	101	LMG	O6-C1-O1-C7
37	D	406	DGD	O6D-C1D-O3G-C3G
24	C	509	CLA	CBA-CGA-O2A-C1
24	b	614	CLA	CBD-CGD-O2D-CED
29	M	101	LMT	O5B-C5B-C6B-O6B
29	M	103	LMT	C4'-C5'-C6'-O6'
24	B	605	CLA	CBD-CGD-O2D-CED
29	M	101	LMT	C4B-C5B-C6B-O6B
37	e	101	DGD	C4E-C5E-C6E-O5E
32	a	416[B]	PL9	C25-C24-C26-C27
24	C	507	CLA	CBD-CGD-O2D-CED
24	B	602	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	603	CLA	C14-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C9
24	c	510	CLA	C6-C7-C8-C9
24	c	515	CLA	O1D-CGD-O2D-CED
29	B	635	LMT	C2'-C1'-O1'-C1
29	C	521	LMT	C2'-C1'-O1'-C1
29	D	401	LMT	C2'-C1'-O1'-C1
29	F	101	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	C2'-C1'-O1'-C1
29	a	421	LMT	C2'-C1'-O1'-C1
29	f	103	LMT	C2'-C1'-O1'-C1
37	D	406	DGD	C2D-C1D-O3G-C3G
37	C	516	DGD	C4A-C5A-C6A-C7A
38	D	408	LHG	O2-C2-C3-O3
38	E	101	LHG	O2-C2-C3-O3
26	D	404	BCR	C7-C8-C9-C34
26	D	404	BCR	C37-C22-C23-C24
26	y	101	BCR	C37-C22-C23-C24
36	b	633	HTG	S1-C1'-C2'-C3'
29	f	103	LMT	O5'-C5'-C6'-O6'
34	Z	101	LMG	C10-C11-C12-C13
24	B	602	CLA	C3-C5-C6-C7
34	c	522	LMG	C11-C10-O7-C8
24	C	512	CLA	CBA-CGA-O2A-C1
34	C	520	LMG	C28-C29-C30-C31
24	B	617	CLA	C2-C1-O2A-CGA
24	b	611	CLA	C2-C1-O2A-CGA
29	m	102	LMT	O5'-C5'-C6'-O6'
28	B	630	GOL	O1-C1-C2-O2
28	b	606	GOL	O1-C1-C2-O2
28	f	101	GOL	O1-C1-C2-O2
28	v	201	GOL	O1-C1-C2-O2
24	C	508	CLA	C10-C11-C12-C13
24	B	616	CLA	C11-C12-C13-C15
24	b	616	CLA	C12-C13-C15-C16
27	b	601	SQD	C24-C23-O48-C46
36	b	633	HTG	O5-C5-C6-O6
34	a	415	LMG	C17-C18-C19-C20
24	B	602	CLA	C10-C11-C12-C13
26	T	103	BCR	C13-C14-C15-C16
32	D	405[B]	PL9	C39-C41-C42-C43
32	d	405[B]	PL9	C39-C41-C42-C43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	A	416	SQD	C23-C24-C25-C26
34	a	415	LMG	C10-C11-C12-C13
24	B	615	CLA	C10-C11-C12-C13
24	B	615	CLA	C5-C6-C7-C8
24	B	615	CLA	C8-C10-C11-C12
24	C	501	CLA	C15-C16-C17-C18
24	c	507	CLA	CBD-CGD-O2D-CED
36	C	523	HTG	S1-C1'-C2'-C3'
29	D	401	LMT	O5'-C1'-O1'-C1
34	C	520	LMG	C4-C5-C6-O5
24	B	616	CLA	C8-C10-C11-C12
24	b	624	CLA	C5-C6-C7-C8
24	b	625	CLA	C10-C11-C12-C13
29	T	104	LMT	O1'-C1-C2-C3
29	A	417	LMT	O5B-C5B-C6B-O6B
34	c	522	LMG	O9-C10-O7-C8
24	c	512	CLA	C15-C16-C17-C18
27	b	601	SQD	O10-C23-O48-C46
36	c	524	HTG	S1-C1'-C2'-C3'
37	e	101	DGD	O6D-C5D-C6D-O5D
24	C	506	CLA	C5-C6-C7-C8
24	C	512	CLA	O1A-CGA-O2A-C1
38	E	101	LHG	C1-C2-C3-O3
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	616	CLA	C2A-CAA-CBA-CGA
34	B	622	LMG	C15-C16-C17-C18
24	B	616	CLA	C5-C6-C7-C8
24	A	410	CLA	C13-C15-C16-C17
24	a	412	CLA	C15-C16-C17-C18
24	c	517	CLA	C10-C11-C12-C13
24	B	617	CLA	C10-C11-C12-C13
24	b	616	CLA	C13-C15-C16-C17
24	c	508	CLA	C15-C16-C17-C18
29	D	401	LMT	O5B-C5B-C6B-O6B
34	j	101	LMG	O6-C5-C6-O5
29	C	521	LMT	O5B-C1B-O1B-C4'
37	C	517	DGD	C2E-C1E-O5D-C6D
37	c	520	DGD	C2E-C1E-O5D-C6D
37	e	101	DGD	C2D-C1D-O3G-C3G
37	e	101	DGD	C2E-C1E-O5D-C6D
24	C	508	CLA	C5-C6-C7-C8
32	a	416[A]	PL9	C9-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	416[B]	PL9	C9-C11-C12-C13
32	a	416[B]	PL9	C14-C16-C17-C18
24	C	511	CLA	CBA-CGA-O2A-C1
24	b	611	CLA	C8-C10-C11-C12
26	Y	101	BCR	C37-C22-C23-C24
24	B	604	CLA	C5-C6-C7-C8
24	C	506	CLA	C13-C15-C16-C17
24	b	624	CLA	C13-C15-C16-C17
28	B	626	GOL	C1-C2-C3-O3
28	B	631	GOL	O1-C1-C2-C3
28	V	202	GOL	C1-C2-C3-O3
28	V	203	GOL	O1-C1-C2-C3
28	V	205	GOL	C1-C2-C3-O3
28	b	605	GOL	O1-C1-C2-C3
28	b	606	GOL	O1-C1-C2-C3
28	v	201	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
38	D	407	LHG	O1-C1-C2-C3
38	a	422	LHG	O1-C1-C2-C3
26	t	101	BCR	C13-C14-C15-C16
24	b	621	CLA	C16-C17-C18-C19
27	F	103	SQD	C26-C27-C28-C29
37	C	517	DGD	O6E-C1E-O5D-C6D
37	c	520	DGD	O6E-C1E-O5D-C6D
37	e	101	DGD	O6D-C1D-O3G-C3G
36	b	602	HTG	C1'-C2'-C3'-C4'
37	e	101	DGD	C4D-C5D-C6D-O5D
24	c	516	CLA	CBA-CGA-O2A-C1
38	a	422	LHG	C11-C12-C13-C14
37	c	519	DGD	O6D-C5D-C6D-O5D
24	c	513	CLA	C2-C1-O2A-CGA
24	C	502	CLA	C16-C17-C18-C20
24	A	410	CLA	C10-C11-C12-C13
36	C	523	HTG	O5-C5-C6-O6
38	l	101	LHG	C33-C34-C35-C36
29	T	104	LMT	C1-C2-C3-C4
29	T	104	LMT	C4-C5-C6-C7
37	C	517	DGD	C9A-CAA-CBA-CCA
37	D	406	DGD	C7A-C8A-C9A-CAA
37	c	519	DGD	C9A-CAA-CBA-CCA
37	c	519	DGD	CAB-CBB-CCB-CDB
38	L	101	LHG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	e	101	DGD	CAA-CBA-CCA-CDA
37	C	516	DGD	O6D-C5D-C6D-O5D
37	c	521	DGD	C6A-C7A-C8A-C9A
28	A	414	GOL	O2-C2-C3-O3
28	A	415	GOL	O2-C2-C3-O3
28	B	628	GOL	O1-C1-C2-O2
28	O	301	GOL	O1-C1-C2-O2
28	V	203	GOL	O1-C1-C2-O2
28	a	402	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
24	C	509	CLA	C3-C5-C6-C7
27	A	412	SQD	C9-C10-C11-C12
27	a	414	SQD	C11-C12-C13-C14
34	B	622	LMG	C29-C30-C31-C32
36	b	632	HTG	C2'-C3'-C4'-C5'
24	a	412	CLA	C10-C11-C12-C13
24	C	505	CLA	C4B-C3B-CAB-CBB
24	b	617	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB
29	a	421	LMT	C6-C7-C8-C9
34	D	412	LMG	O6-C5-C6-O5
37	c	521	DGD	C7B-C8B-C9B-CAB
37	e	101	DGD	C8B-C9B-CAB-CBB
24	B	615	CLA	C12-C13-C15-C16
24	b	611	CLA	C6-C7-C8-C10
38	D	407	LHG	C23-C24-C25-C26
34	B	622	LMG	C36-C37-C38-C39
29	T	104	LMT	C11-C10-C9-C8
37	C	516	DGD	C4B-C5B-C6B-C7B
37	C	518	DGD	CAA-CBA-CCA-CDA
37	c	521	DGD	CBB-CCB-CDB-CEB
27	A	412	SQD	C14-C15-C16-C17
24	D	403	CLA	C8-C10-C11-C12
24	c	514	CLA	C8-C10-C11-C12
34	A	422	LMG	C30-C31-C32-C33
24	B	616	CLA	C16-C17-C18-C20
24	a	412	CLA	C16-C17-C18-C19
24	a	412	CLA	C16-C17-C18-C20
24	C	511	CLA	O1A-CGA-O2A-C1
24	C	509	CLA	CBD-CGD-O2D-CED
38	a	422	LHG	C24-C25-C26-C27
38	d	406	LHG	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	d	407	LHG	C1-C2-C3-O3
34	c	522	LMG	C7-C8-C9-O8
34	z	101	LMG	O1-C7-C8-C9
27	b	601	SQD	C12-C13-C14-C15
34	A	422	LMG	C11-C12-C13-C14
38	d	408	LHG	C29-C30-C31-C32
36	B	625	HTG	C4-C5-C6-O6
29	A	417	LMT	C6-C7-C8-C9
37	C	516	DGD	C3B-C4B-C5B-C6B
37	C	518	DGD	C8A-C9A-CAA-CBA
37	c	520	DGD	C4A-C5A-C6A-C7A
34	C	519	LMG	C11-C12-C13-C14
37	c	519	DGD	C8B-C9B-CAB-CBB
29	M	104	LMT	O5'-C5'-C6'-O6'
24	C	505	CLA	C2B-C3B-CAB-CBB
24	C	507	CLA	C2B-C3B-CAB-CBB
24	b	612	CLA	C2B-C3B-CAB-CBB
27	A	416	SQD	C26-C27-C28-C29
34	D	412	LMG	C19-C20-C21-C22
37	c	520	DGD	C9A-CAA-CBA-CCA
24	c	516	CLA	C15-C16-C17-C18
34	a	415	LMG	C14-C15-C16-C17
34	c	522	LMG	C34-C35-C36-C37
24	c	516	CLA	O1A-CGA-O2A-C1
27	b	601	SQD	C29-C30-C31-C32
34	A	422	LMG	C14-C15-C16-C17
34	j	101	LMG	C19-C20-C21-C22
36	b	602	HTG	C3'-C4'-C5'-C6'
32	a	416[A]	PL9	C12-C11-C9-C8
32	a	416[B]	PL9	C12-C11-C9-C8
29	B	635	LMT	C3-C4-C5-C6
36	b	633	HTG	C1'-C2'-C3'-C4'
24	a	412	CLA	CBA-CGA-O2A-C1
24	C	501	CLA	C11-C12-C13-C14
24	a	410	CLA	C14-C13-C15-C16
24	b	620	CLA	C11-C12-C13-C14
24	a	412	CLA	C8-C10-C11-C12
34	z	101	LMG	C12-C13-C14-C15
27	A	416	SQD	C11-C12-C13-C14
37	D	406	DGD	C6A-C7A-C8A-C9A
38	D	407	LHG	C24-C25-C26-C27
36	B	632	HTG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	b	632	HTG	C3'-C4'-C5'-C6'
37	c	521	DGD	C6B-C7B-C8B-C9B
37	c	521	DGD	C1A-C2A-C3A-C4A
27	a	405	SQD	C31-C32-C33-C34
38	d	407	LHG	C34-C35-C36-C37
34	C	520	LMG	C13-C14-C15-C16
34	b	630	LMG	C38-C39-C40-C41
24	b	612	CLA	C16-C17-C18-C19
36	B	624	HTG	C2'-C3'-C4'-C5'
34	j	101	LMG	C38-C39-C40-C41
34	B	622	LMG	C34-C35-C36-C37
37	C	516	DGD	C2A-C3A-C4A-C5A
29	M	103	LMT	C2-C3-C4-C5
37	D	406	DGD	C1B-C2B-C3B-C4B
38	a	422	LHG	C23-C24-C25-C26
27	a	414	SQD	C29-C30-C31-C32
34	A	422	LMG	C32-C33-C34-C35
37	c	521	DGD	C7A-C8A-C9A-CAA
32	D	405[B]	PL9	C15-C14-C16-C17
32	d	405[A]	PL9	C13-C14-C16-C17
29	a	404	LMT	C2-C3-C4-C5
36	B	625	HTG	C3'-C4'-C5'-C6'
37	H	103	DGD	CBB-CCB-CDB-CEB
38	l	101	LHG	C27-C28-C29-C30
27	B	621	SQD	C7-C8-C9-C10
38	d	406	LHG	C25-C26-C27-C28
29	M	103	LMT	O5B-C5B-C6B-O6B
29	B	635	LMT	C7-C8-C9-C10
34	a	415	LMG	C11-C10-O7-C8
39	F	102	HEM	C4B-C3B-CAB-CBB
39	F	102	HEM	C4C-C3C-CAC-CBC
24	B	616	CLA	C16-C17-C18-C19
24	C	502	CLA	C16-C17-C18-C19
24	a	412	CLA	O1A-CGA-O2A-C1
34	Z	101	LMG	O6-C5-C6-O5
34	j	101	LMG	C35-C36-C37-C38
27	b	601	SQD	C7-C8-C9-C10
37	D	406	DGD	C2A-C3A-C4A-C5A
37	H	103	DGD	C7A-C8A-C9A-CAA
29	b	631	LMT	C3'-C4'-O1B-C1B
37	C	516	DGD	C5B-C6B-C7B-C8B
37	C	518	DGD	C2A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	e	101	DGD	C2A-C1A-O1G-C1G
27	a	414	SQD	C9-C10-C11-C12
38	D	409	LHG	C29-C30-C31-C32
37	c	519	DGD	O6E-C5E-C6E-O5E
34	Z	101	LMG	C19-C20-C21-C22
37	C	516	DGD	C4D-C5D-C6D-O5D
27	b	601	SQD	C35-C36-C37-C38
32	d	405[B]	PL9	C45-C44-C46-C47
32	d	405[A]	PL9	C43-C44-C46-C47
29	T	104	LMT	C7-C8-C9-C10
38	d	407	LHG	C24-C23-O8-C6
29	B	635	LMT	C4-C5-C6-C7
37	c	519	DGD	C4D-C5D-C6D-O5D
34	A	422	LMG	C10-C11-C12-C13
27	b	601	SQD	C32-C33-C34-C35
36	B	623	HTG	C3'-C4'-C5'-C6'
28	C	524	GOL	O1-C1-C2-O2
28	V	201	GOL	O1-C1-C2-O2
28	V	202	GOL	O2-C2-C3-O3
28	v	202	GOL	O1-C1-C2-O2
34	z	101	LMG	C15-C16-C17-C18
37	C	517	DGD	CBB-CCB-CDB-CEB
24	C	506	CLA	C1A-C2A-CAA-CBA
27	A	416	SQD	C30-C31-C32-C33
37	C	518	DGD	O1A-C1A-O1G-C1G
37	C	516	DGD	O6E-C5E-C6E-O5E
34	a	415	LMG	O9-C10-O7-C8
37	D	406	DGD	C8B-C9B-CAB-CBB
24	B	616	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	b	624	CLA	C11-C12-C13-C15
24	b	624	CLA	C12-C13-C15-C16
24	c	513	CLA	C6-C7-C8-C10
24	C	504	CLA	C15-C16-C17-C18
24	c	511	CLA	C5-C6-C7-C8
37	e	101	DGD	C5A-C6A-C7A-C8A
32	D	405[A]	PL9	C15-C14-C16-C17
37	e	101	DGD	O6E-C5E-C6E-O5E
34	a	415	LMG	C29-C30-C31-C32
37	D	406	DGD	C3B-C4B-C5B-C6B
37	e	101	DGD	C2A-C3A-C4A-C5A
24	d	401	CLA	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	615	CLA	C14-C13-C15-C16
24	B	616	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C9
24	b	611	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C10-C8-C9
38	l	101	LHG	C10-C11-C12-C13
34	j	101	LMG	C14-C15-C16-C17
34	C	520	LMG	C10-C11-C12-C13
27	A	416	SQD	O6-C44-C45-C46
27	B	621	SQD	C44-C45-C46-O48
27	F	103	SQD	C44-C45-C46-O48
27	a	405	SQD	O6-C44-C45-C46
27	a	414	SQD	O6-C44-C45-C46
34	a	415	LMG	C7-C8-C9-O8
34	c	522	LMG	O1-C7-C8-C9
37	D	406	DGD	O1G-C1G-C2G-C3G
38	a	422	LHG	C4-C5-C6-O8
37	h	102	DGD	C4E-C5E-C6E-O5E
27	a	405	SQD	C25-C26-C27-C28
27	A	412	SQD	C16-C17-C18-C19
34	C	520	LMG	C14-C15-C16-C17
37	C	517	DGD	C5A-C6A-C7A-C8A
24	c	515	CLA	CBA-CGA-O2A-C1
27	A	416	SQD	C24-C23-O48-C46
24	b	612	CLA	C16-C17-C18-C20
37	C	517	DGD	C8A-C9A-CAA-CBA
34	z	101	LMG	C13-C14-C15-C16
27	a	405	SQD	C23-C24-C25-C26
38	d	407	LHG	O10-C23-O8-C6
32	d	405[B]	PL9	C13-C14-C16-C17
34	b	630	LMG	C32-C33-C34-C35
37	e	101	DGD	C9B-CAB-CBB-CCB
38	D	409	LHG	C28-C29-C30-C31
29	C	521	LMT	O5B-C5B-C6B-O6B
26	Y	101	BCR	C21-C22-C23-C24
24	c	515	CLA	O1A-CGA-O2A-C1
37	e	101	DGD	O1A-C1A-O1G-C1G
24	c	510	CLA	C15-C16-C17-C18
34	B	622	LMG	C31-C32-C33-C34
34	j	101	LMG	C36-C37-C38-C39
37	c	519	DGD	C7B-C8B-C9B-CAB
38	d	408	LHG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C11-C10-C9-C8
37	h	102	DGD	CAA-CBA-CCA-CDA
27	b	601	SQD	C27-C28-C29-C30
27	b	601	SQD	C28-C29-C30-C31
34	b	630	LMG	C33-C34-C35-C36
34	j	101	LMG	C17-C18-C19-C20
24	b	611	CLA	CBA-CGA-O2A-C1
38	D	409	LHG	C24-C23-O8-C6
36	b	602	HTG	C2'-C3'-C4'-C5'
32	d	405[A]	PL9	C15-C14-C16-C17
34	b	630	LMG	C40-C41-C42-C43
36	b	608	HTG	C4'-C5'-C6'-C7'
38	L	101	LHG	C13-C14-C15-C16
38	d	408	LHG	C28-C29-C30-C31
27	a	414	SQD	O6-C44-C45-O47
27	f	102	SQD	O6-C44-C45-O47
34	j	101	LMG	C16-C17-C18-C19
37	e	101	DGD	C4A-C5A-C6A-C7A
38	D	407	LHG	C17-C18-C19-C20
37	c	521	DGD	CBA-CCA-CDA-CEA
27	a	414	SQD	C27-C28-C29-C30
29	B	635	LMT	C11-C10-C9-C8
29	D	401	LMT	O1'-C1-C2-C3
34	A	422	LMG	C13-C14-C15-C16
34	b	630	LMG	C37-C38-C39-C40
24	B	602	CLA	CBA-CGA-O2A-C1
37	c	520	DGD	C2B-C3B-C4B-C5B
24	B	614	CLA	C13-C15-C16-C17
24	C	509	CLA	C10-C11-C12-C13
24	C	507	CLA	O1D-CGD-O2D-CED
24	C	510	CLA	CBA-CGA-O2A-C1
29	C	521	LMT	O1'-C1-C2-C3
37	c	520	DGD	C3B-C4B-C5B-C6B
27	a	414	SQD	C15-C16-C17-C18
29	m	102	LMT	C11-C10-C9-C8
37	c	521	DGD	C5B-C6B-C7B-C8B
38	D	407	LHG	C25-C26-C27-C28
38	E	101	LHG	C24-C25-C26-C27
28	V	205	GOL	O2-C2-C3-O3
38	D	407	LHG	O1-C1-C2-O2
24	A	410	CLA	C6-C7-C8-C9
24	b	611	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	616	CLA	C14-C13-C15-C16
24	b	624	CLA	C11-C12-C13-C14
24	c	513	CLA	C6-C7-C8-C9
24	c	513	CLA	C14-C13-C15-C16
24	A	410	CLA	C4B-C3B-CAB-CBB
24	B	608	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
24	c	511	CLA	C4B-C3B-CAB-CBB
24	d	402	CLA	C4B-C3B-CAB-CBB
24	B	605	CLA	O1D-CGD-O2D-CED
24	C	509	CLA	C8-C10-C11-C12
27	a	414	SQD	C19-C20-C21-C22
34	a	415	LMG	C33-C34-C35-C36
27	F	103	SQD	C2-C1-O6-C44
24	b	626	CLA	C10-C11-C12-C13
27	f	102	SQD	C31-C32-C33-C34
24	c	507	CLA	O1D-CGD-O2D-CED
24	A	410	CLA	C6-C7-C8-C10
24	B	617	CLA	C6-C7-C8-C10
24	c	513	CLA	C12-C13-C15-C16
24	C	503	CLA	C8-C10-C11-C12
34	a	415	LMG	C21-C22-C23-C24
34	b	630	LMG	C16-C17-C18-C19
37	C	518	DGD	C2A-C3A-C4A-C5A
38	D	409	LHG	C12-C13-C14-C15
34	c	523	LMG	O6-C5-C6-O5
24	c	506	CLA	C16-C17-C18-C19
27	F	103	SQD	C32-C33-C34-C35
24	b	613	CLA	C5-C6-C7-C8
32	d	405[B]	PL9	C43-C44-C46-C47
29	M	104	LMT	O5'-C1'-O1'-C1
38	d	408	LHG	C33-C34-C35-C36
29	a	404	LMT	C6-C7-C8-C9
36	V	207	HTG	S1-C1'-C2'-C3'
38	D	409	LHG	O10-C23-O8-C6
38	l	101	LHG	C11-C12-C13-C14
24	A	410	CLA	C8-C10-C11-C12
37	h	102	DGD	C5B-C6B-C7B-C8B
34	c	523	LMG	C32-C33-C34-C35
38	D	408	LHG	C32-C33-C34-C35
27	b	601	SQD	C44-C45-C46-O48
34	Z	101	LMG	C7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	e	101	DGD	O1G-C1G-C2G-C3G
38	E	101	LHG	C4-C5-C6-O8
37	C	517	DGD	C4A-C5A-C6A-C7A
27	f	102	SQD	C24-C25-C26-C27
32	d	405[A]	PL9	C45-C44-C46-C47
34	b	630	LMG	C39-C40-C41-C42
24	b	619	CLA	C2-C3-C5-C6
24	C	510	CLA	O1A-CGA-O2A-C1
24	B	611	CLA	C16-C17-C18-C19
24	B	611	CLA	C16-C17-C18-C20
24	B	614	CLA	C15-C16-C17-C18
26	B	618	BCR	C1-C6-C7-C8
26	D	404	BCR	C1-C6-C7-C8
26	b	627	BCR	C1-C6-C7-C8
34	a	415	LMG	C12-C13-C14-C15
27	A	416	SQD	O10-C23-O48-C46
37	c	521	DGD	C4A-C5A-C6A-C7A
34	a	415	LMG	C35-C36-C37-C38
37	c	520	DGD	C1A-C2A-C3A-C4A
38	d	406	LHG	C7-C8-C9-C10
29	F	101	LMT	O1'-C1-C2-C3
27	F	103	SQD	O47-C45-C46-O48
34	Z	101	LMG	O1-C7-C8-O7
34	Z	101	LMG	O7-C8-C9-O8
34	z	101	LMG	O1-C7-C8-O7
27	a	414	SQD	C35-C36-C37-C38
32	A	420[A]	PL9	C4-C3-C7-C8
32	A	420[B]	PL9	C4-C3-C7-C8
32	a	416[A]	PL9	C4-C3-C7-C8
32	a	416[B]	PL9	C4-C3-C7-C8
38	D	407	LHG	C34-C35-C36-C37
24	C	510	CLA	C4-C3-C5-C6
24	b	619	CLA	C4-C3-C5-C6
25	a	411	PHO	C4-C3-C5-C6
24	C	505	CLA	C2-C3-C5-C6
24	C	510	CLA	C2-C3-C5-C6
32	D	405[A]	PL9	C13-C14-C16-C17
32	D	405[B]	PL9	C13-C14-C16-C17
38	L	101	LHG	C33-C34-C35-C36
24	b	611	CLA	O1A-CGA-O2A-C1
24	b	614	CLA	O1D-CGD-O2D-CED
24	A	405	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	c	513	CLA	C10-C11-C12-C13
27	F	103	SQD	C31-C32-C33-C34
24	B	607	CLA	C10-C11-C12-C13
27	a	405	SQD	C19-C20-C21-C22
24	b	621	CLA	C16-C17-C18-C20
34	Z	101	LMG	C2-C1-O1-C7
32	D	405[A]	PL9	C9-C11-C12-C13
37	C	517	DGD	CAB-CBB-CCB-CDB
27	b	601	SQD	C31-C32-C33-C34
28	c	502	GOL	O1-C1-C2-O2
28	f	101	GOL	O2-C2-C3-O3
38	a	422	LHG	O1-C1-C2-O2
24	b	611	CLA	CAA-CBA-CGA-O2A
25	a	411	PHO	C2-C3-C5-C6
32	D	405[A]	PL9	C28-C29-C31-C32
37	e	101	DGD	C2B-C3B-C4B-C5B
24	A	406	CLA	C2C-C3C-CAC-CBC
24	b	611	CLA	C13-C15-C16-C17
38	d	406	LHG	C11-C10-C9-C8
37	H	103	DGD	CDB-CEB-CFB-CGB
34	A	422	LMG	C12-C13-C14-C15
27	b	601	SQD	C11-C12-C13-C14
24	B	602	CLA	C8-C10-C11-C12
24	b	611	CLA	C10-C11-C12-C13
24	c	513	CLA	C15-C16-C17-C18
37	H	103	DGD	CDA-CEA-CFA-CGA
24	B	602	CLA	C11-C10-C8-C7
24	c	510	CLA	C11-C10-C8-C7
24	c	516	CLA	C11-C10-C8-C7
34	c	522	LMG	C10-C11-C12-C13
37	C	517	DGD	C1A-C2A-C3A-C4A
37	H	103	DGD	CCA-CDA-CEA-CFA
38	D	408	LHG	C33-C34-C35-C36
34	C	519	LMG	C30-C31-C32-C33
37	D	406	DGD	C2B-C3B-C4B-C5B
27	F	103	SQD	C5-C6-S-O8
34	C	520	LMG	C8-C7-O1-C1
37	c	520	DGD	C2G-C3G-O3G-C1D
37	c	520	DGD	C5D-C6D-O5D-C1E
24	b	621	CLA	C8-C10-C11-C12
24	c	506	CLA	C16-C17-C18-C20
27	A	412	SQD	C15-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	B	602	CLA	O1A-CGA-O2A-C1
24	c	514	CLA	C2-C3-C5-C6
39	e	102	HEM	C2B-C3B-CAB-CBB
39	e	102	HEM	C2C-C3C-CAC-CBC
24	b	622	CLA	C8-C10-C11-C12
37	h	102	DGD	C6A-C7A-C8A-C9A
28	b	607	GOL	C1-C2-C3-O3
36	b	633	HTG	C4-C5-C6-O6
34	C	519	LMG	C14-C15-C16-C17
34	C	519	LMG	C29-C30-C31-C32
34	D	412	LMG	C13-C14-C15-C16
24	C	509	CLA	C16-C17-C18-C19
27	b	601	SQD	C30-C31-C32-C33
29	B	635	LMT	C2-C3-C4-C5
29	a	404	LMT	C4B-C5B-C6B-O6B
37	C	517	DGD	C4B-C5B-C6B-C7B
24	b	618	CLA	C13-C15-C16-C17
38	a	422	LHG	O6-C4-C5-O7
27	F	103	SQD	O5-C1-O6-C44
29	M	101	LMT	O5'-C1'-O1'-C1
37	e	101	DGD	C6A-C7A-C8A-C9A
32	D	405[A]	PL9	C39-C41-C42-C43
34	A	422	LMG	O1-C7-C8-C9
34	A	422	LMG	C7-C8-C9-O8
34	C	520	LMG	C7-C8-C9-O8
24	A	405	CLA	C16-C17-C18-C19
37	H	103	DGD	C9B-CAB-CBB-CCB
24	C	505	CLA	C4-C3-C5-C6
24	c	514	CLA	C4-C3-C5-C6
32	A	420[A]	PL9	C15-C14-C16-C17
32	D	405[A]	PL9	C45-C44-C46-C47
24	b	620	CLA	C15-C16-C17-C18
27	B	621	SQD	C31-C32-C33-C34
34	c	522	LMG	C39-C40-C41-C42
27	B	621	SQD	O47-C45-C46-O48
27	b	601	SQD	O47-C45-C46-O48
34	a	415	LMG	O7-C8-C9-O8
37	D	406	DGD	O1G-C1G-C2G-O2G
37	e	101	DGD	O1G-C1G-C2G-O2G
24	b	624	CLA	C11-C10-C8-C9
37	c	519	DGD	CBA-CCA-CDA-CEA
34	C	520	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	a	422	LHG	C13-C14-C15-C16
29	M	104	LMT	C1-C2-C3-C4
29	f	103	LMT	C4-C5-C6-C7
37	C	516	DGD	C6A-C7A-C8A-C9A
38	D	407	LHG	C11-C10-C9-C8
24	b	624	CLA	C15-C16-C17-C18
37	c	519	DGD	C2A-C3A-C4A-C5A
34	C	519	LMG	C31-C32-C33-C34
34	C	519	LMG	C12-C13-C14-C15
37	c	520	DGD	C9B-CAB-CBB-CCB
24	b	626	CLA	C4-C3-C5-C6
24	b	620	CLA	C2A-CAA-CBA-CGA
24	b	624	CLA	C16-C17-C18-C19
37	c	521	DGD	C2A-C1A-O1G-C1G
36	B	632	HTG	O5-C5-C6-O6
27	a	414	SQD	C17-C18-C19-C20
28	b	607	GOL	O1-C1-C2-O2
27	a	405	SQD	C27-C28-C29-C30
24	B	602	CLA	C4B-C3B-CAB-CBB
24	B	610	CLA	C4B-C3B-CAB-CBB
24	B	616	CLA	C4B-C3B-CAB-CBB
24	b	619	CLA	C4B-C3B-CAB-CBB
24	c	512	CLA	C1A-C2A-CAA-CBA
32	A	420[B]	PL9	C15-C14-C16-C17
24	b	625	CLA	C16-C17-C18-C19
38	d	406	LHG	C30-C31-C32-C33
38	l	101	LHG	C7-C8-C9-C10
38	l	101	LHG	O6-C4-C5-C6
27	B	621	SQD	C19-C20-C21-C22
27	a	405	SQD	C35-C36-C37-C38
24	B	604	CLA	C11-C10-C8-C7
24	C	504	CLA	C12-C13-C15-C16
24	d	402	CLA	C11-C12-C13-C15
27	B	621	SQD	C24-C23-O48-C46
37	c	520	DGD	C6A-C7A-C8A-C9A
29	C	521	LMT	C5'-C4'-O1B-C1B
34	A	422	LMG	C18-C19-C20-C21
24	C	509	CLA	O1D-CGD-O2D-CED
38	D	409	LHG	C2-C3-O3-P
38	d	408	LHG	C2-C3-O3-P
24	b	624	CLA	C16-C17-C18-C20
38	l	101	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	c	510	CLA	C11-C10-C8-C9
24	c	513	CLA	C11-C12-C13-C14
27	F	103	SQD	C34-C35-C36-C37
37	h	102	DGD	CBB-CCB-CDB-CEB
38	D	408	LHG	C26-C27-C28-C29
24	C	512	CLA	C3-C5-C6-C7
27	B	621	SQD	C33-C34-C35-C36
34	A	422	LMG	O1-C7-C8-O7
34	c	522	LMG	O1-C7-C8-O7
34	c	522	LMG	O7-C8-C9-O8
38	E	101	LHG	O7-C5-C6-O8
34	Z	101	LMG	O1-C7-C8-C9
24	B	605	CLA	C4-C3-C5-C6
27	f	102	SQD	C25-C26-C27-C28
24	b	626	CLA	C2-C3-C5-C6
32	D	405[B]	PL9	C43-C44-C46-C47
38	E	101	LHG	C15-C16-C17-C18
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	608	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	b	611	CLA	CAD-CBD-CGD-O2D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	O1A-CGA-O2A-C1
36	B	623	HTG	C4'-C5'-C6'-C7'
34	C	519	LMG	O10-C28-O8-C9
27	a	405	SQD	C24-C25-C26-C27
29	f	103	LMT	C5-C6-C7-C8
24	d	401	CLA	C4C-C3C-CAC-CBC
38	D	408	LHG	C13-C14-C15-C16
24	B	602	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
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	506	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	611	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	615	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	c	513	CLA	CHA-CBD-CGD-O1D
38	D	408	LHG	C4-O6-P-O5
38	L	101	LHG	C3-O3-P-O6
38	L	101	LHG	C4-O6-P-O5
38	a	422	LHG	C4-O6-P-O5
24	C	502	CLA	C3-C5-C6-C7
24	C	513	CLA	C3-C5-C6-C7
27	a	414	SQD	C30-C31-C32-C33
38	a	422	LHG	C14-C15-C16-C17
38	l	101	LHG	C28-C29-C30-C31
24	C	506	CLA	C4-C3-C5-C6
24	a	412	CLA	C4-C3-C5-C6
32	D	405[B]	PL9	C35-C34-C36-C37
32	D	405[B]	PL9	C45-C44-C46-C47
32	a	416[A]	PL9	C45-C44-C46-C47
24	B	608	CLA	C2B-C3B-CAB-CBB
24	b	617	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	d	402	CLA	C2B-C3B-CAB-CBB
34	a	415	LMG	C34-C35-C36-C37
27	F	103	SQD	C7-C8-C9-C10
37	c	520	DGD	C2A-C3A-C4A-C5A
27	B	621	SQD	C35-C36-C37-C38
37	C	518	DGD	CDA-CEA-CFA-CGA
28	V	204	GOL	O2-C2-C3-O3
34	z	101	LMG	C16-C17-C18-C19
27	B	621	SQD	C46-C45-O47-C7
27	b	601	SQD	C46-C45-O47-C7
27	F	103	SQD	C30-C31-C32-C33
37	C	518	DGD	C9A-CAA-CBA-CCA
37	h	102	DGD	O2G-C1B-C2B-C3B
24	C	501	CLA	C13-C15-C16-C17
37	h	102	DGD	O6E-C5E-C6E-O5E
29	D	401	LMT	O5B-C1B-O1B-C4'
37	c	521	DGD	O1A-C1A-O1G-C1G
24	B	616	CLA	C11-C12-C13-C14
38	E	101	LHG	C23-C24-C25-C26
27	B	621	SQD	O10-C23-O48-C46
38	D	408	LHG	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	j	101	LMG	C15-C16-C17-C18
24	b	625	CLA	C16-C17-C18-C20
37	C	517	DGD	C6B-C7B-C8B-C9B
24	A	405	CLA	C15-C16-C17-C18
29	M	104	LMT	C2'-C1'-O1'-C1
27	b	601	SQD	C11-C10-C9-C8
38	D	408	LHG	C31-C32-C33-C34
37	H	103	DGD	C5B-C6B-C7B-C8B
37	c	519	DGD	CBB-CCB-CDB-CEB
37	c	520	DGD	C3A-C4A-C5A-C6A
38	d	408	LHG	C11-C10-C9-C8
38	a	422	LHG	O7-C5-C6-O8
37	H	103	DGD	O2G-C1B-C2B-C3B
24	C	513	CLA	CBA-CGA-O2A-C1
37	D	406	DGD	C4A-C5A-C6A-C7A
24	c	513	CLA	C13-C15-C16-C17
24	B	616	CLA	C4-C3-C5-C6
32	A	420[A]	PL9	C13-C14-C16-C17
37	C	518	DGD	CBA-CCA-CDA-CEA
27	f	102	SQD	O6-C44-C45-C46
32	D	405[B]	PL9	C9-C11-C12-C13
32	a	416[A]	PL9	C14-C16-C17-C18
38	L	101	LHG	C16-C17-C18-C19
36	c	524	HTG	C1'-C2'-C3'-C4'
27	a	405	SQD	C18-C19-C20-C21
27	a	414	SQD	C34-C35-C36-C37
29	C	521	LMT	C4'-C5'-C6'-O6'
24	A	405	CLA	C2C-C3C-CAC-CBC
37	h	102	DGD	CDB-CEB-CFB-CGB
34	Z	101	LMG	C8-C7-O1-C1
37	C	517	DGD	C5D-C6D-O5D-C1E
34	a	415	LMG	C30-C31-C32-C33
38	E	101	LHG	C16-C17-C18-C19
32	a	416[B]	PL9	C45-C44-C46-C47
24	B	616	CLA	C2-C3-C5-C6
32	a	416[A]	PL9	C43-C44-C46-C47
34	C	519	LMG	C29-C28-O8-C9
29	M	103	LMT	C2-C1-O1'-C1'
24	b	620	CLA	C16-C17-C18-C19
24	b	626	CLA	C16-C17-C18-C19
27	F	103	SQD	C33-C34-C35-C36
24	B	604	CLA	C11-C10-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	A	422	LMG	C17-C18-C19-C20
25	a	411	PHO	C2C-C3C-CAC-CBC
24	B	604	CLA	C4B-C3B-CAB-CBB
34	C	519	LMG	C35-C36-C37-C38
34	B	622	LMG	C16-C17-C18-C19
34	C	519	LMG	C28-C29-C30-C31
37	H	103	DGD	C4E-C5E-C6E-O5E
41	V	206	HEC	CAD-CBD-CGD-O2D
24	c	517	CLA	C4-C3-C5-C6
27	a	405	SQD	C28-C29-C30-C31
32	A	420[B]	PL9	C43-C44-C46-C47
32	a	416[B]	PL9	C43-C44-C46-C47
24	b	614	CLA	C3-C5-C6-C7
27	A	416	SQD	C24-C25-C26-C27
24	c	514	CLA	O1A-CGA-O2A-C1
39	e	102	HEM	C4C-C3C-CAC-CBC
24	b	620	CLA	C16-C17-C18-C20
38	d	406	LHG	C33-C34-C35-C36
37	c	519	DGD	CDA-CEA-CFA-CGA
24	c	514	CLA	C12-C13-C15-C16
38	L	101	LHG	C10-C11-C12-C13
24	c	514	CLA	CBA-CGA-O2A-C1
27	f	102	SQD	C26-C27-C28-C29
38	E	101	LHG	C14-C15-C16-C17
34	c	523	LMG	O7-C8-C9-O8
38	d	406	LHG	C29-C30-C31-C32
24	B	608	CLA	C3A-C2A-CAA-CBA
25	A	408	PHO	C2-C3-C5-C6
32	A	420[A]	PL9	C43-C44-C46-C47
29	M	104	LMT	C5-C6-C7-C8
37	C	518	DGD	C8B-C9B-CAB-CBB
37	D	406	DGD	CBA-CCA-CDA-CEA
27	B	621	SQD	C17-C18-C19-C20
38	d	406	LHG	C26-C27-C28-C29
27	B	621	SQD	C14-C15-C16-C17
34	D	412	LMG	C20-C21-C22-C23
38	D	408	LHG	C34-C35-C36-C37
24	B	609	CLA	C13-C15-C16-C17
27	b	601	SQD	C33-C34-C35-C36
24	c	515	CLA	C2-C1-O2A-CGA
24	c	516	CLA	C2-C1-O2A-CGA
26	H	102	BCR	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
37	c	520	DGD	C8B-C9B-CAB-CBB
24	B	605	CLA	C13-C15-C16-C17
24	a	412	CLA	C2-C3-C5-C6
32	A	420[B]	PL9	C13-C14-C16-C17
32	d	405[A]	PL9	C28-C29-C31-C32
27	B	621	SQD	C12-C13-C14-C15
27	A	412	SQD	C18-C19-C20-C21
27	A	416	SQD	C12-C13-C14-C15
29	a	404	LMT	C3-C4-C5-C6
34	C	519	LMG	C21-C22-C23-C24
27	a	414	SQD	C33-C34-C35-C36
24	C	504	CLA	C14-C13-C15-C16
24	D	403	CLA	C6-C7-C8-C9
24	a	410	CLA	C11-C12-C13-C14
24	b	613	CLA	C6-C7-C8-C9
24	c	514	CLA	C11-C12-C13-C14
24	d	402	CLA	C11-C12-C13-C14
34	a	415	LMG	C31-C32-C33-C34
28	A	413	GOL	C1-C2-C3-O3
28	B	629	GOL	O1-C1-C2-C3
38	d	408	LHG	O1-C1-C2-C3
24	B	608	CLA	C16-C17-C18-C19
34	A	422	LMG	C36-C37-C38-C39
26	h	101	BCR	C9-C10-C11-C12
26	k	101	BCR	C9-C10-C11-C12
32	A	420[B]	PL9	C30-C29-C31-C32
24	B	602	CLA	CAA-CBA-CGA-O2A
38	d	408	LHG	C35-C36-C37-C38
29	M	103	LMT	C2B-C1B-O1B-C4'
41	V	206	HEC	CAD-CBD-CGD-O1D
24	b	612	CLA	C2A-CAA-CBA-CGA
24	c	505	CLA	C2A-CAA-CBA-CGA
37	C	516	DGD	CAA-CBA-CCA-CDA
24	A	405	CLA	C16-C17-C18-C20
24	B	615	CLA	C16-C17-C18-C19
27	b	601	SQD	C14-C15-C16-C17
37	H	103	DGD	C4B-C5B-C6B-C7B
24	B	602	CLA	C2B-C3B-CAB-CBB
24	B	604	CLA	C2B-C3B-CAB-CBB
24	B	610	CLA	C2B-C3B-CAB-CBB
24	B	616	CLA	C2B-C3B-CAB-CBB
24	C	512	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	D	402	CLA	C2B-C3B-CAB-CBB
24	b	619	CLA	C2B-C3B-CAB-CBB
24	c	511	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C5-C6-C7-C8
26	C	514	BCR	C1-C6-C7-C8
26	C	515	BCR	C1-C6-C7-C8
26	D	404	BCR	C5-C6-C7-C8
26	b	627	BCR	C5-C6-C7-C8
26	d	404	BCR	C23-C24-C25-C30
34	b	630	LMG	C29-C28-O8-C9
24	B	613	CLA	C8-C10-C11-C12
29	C	521	LMT	C3-C4-C5-C6
24	b	611	CLA	C3-C5-C6-C7
36	B	632	HTG	C4'-C5'-C6'-C7'
29	f	103	LMT	C2B-C1B-O1B-C4'
34	j	101	LMG	C13-C14-C15-C16
32	d	405[B]	PL9	C15-C14-C16-C17
27	a	405	SQD	C34-C35-C36-C37
27	a	414	SQD	C10-C11-C12-C13
38	a	422	LHG	O6-C4-C5-C6
29	D	401	LMT	C2B-C1B-O1B-C4'
39	e	102	HEM	C3D-CAD-CBD-CGD
24	A	407	CLA	C11-C10-C8-C7
24	c	510	CLA	C6-C7-C8-C10
37	H	103	DGD	C5A-C6A-C7A-C8A
24	B	611	CLA	C2A-CAA-CBA-CGA
38	E	101	LHG	C17-C18-C19-C20
37	D	406	DGD	O2G-C2G-C3G-O3G
29	M	104	LMT	C11-C10-C9-C8
38	D	409	LHG	C10-C11-C12-C13
24	B	610	CLA	C16-C17-C18-C19
34	D	412	LMG	C16-C17-C18-C19
24	b	614	CLA	C13-C15-C16-C17
37	C	516	DGD	C1B-C2B-C3B-C4B
32	A	420[A]	PL9	C30-C29-C31-C32
34	B	622	LMG	C22-C23-C24-C25
24	C	513	CLA	C5-C6-C7-C8
24	c	517	CLA	C2-C3-C5-C6
38	d	408	LHG	C9-C10-C11-C12
29	f	103	LMT	C9-C10-C11-C12
34	C	520	LMG	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	c	522	LMG	C36-C37-C38-C39
24	c	517	CLA	C2-C1-O2A-CGA
24	A	406	CLA	C15-C16-C17-C18
39	F	102	HEM	CAD-CBD-CGD-O1D
36	C	523	HTG	C1'-C2'-C3'-C4'
37	H	103	DGD	C3B-C4B-C5B-C6B
24	B	604	CLA	C6-C7-C8-C9
24	b	626	CLA	C11-C12-C13-C14
38	L	101	LHG	C12-C13-C14-C15
24	d	401	CLA	C15-C16-C17-C18
24	d	403	CLA	C15-C16-C17-C18
37	c	521	DGD	C3A-C4A-C5A-C6A
29	A	417	LMT	O1'-C1-C2-C3
27	b	601	SQD	C10-C11-C12-C13
24	b	611	CLA	C4-C3-C5-C6
32	A	420[A]	PL9	C45-C44-C46-C47
32	A	420[B]	PL9	C45-C44-C46-C47
32	D	405[A]	PL9	C35-C34-C36-C37
29	C	521	LMT	C1-C2-C3-C4
24	B	605	CLA	C2-C3-C5-C6
41	v	205	HEC	CAD-CBD-CGD-O2D
37	D	406	DGD	C4B-C5B-C6B-C7B
29	M	101	LMT	C2'-C1'-O1'-C1
24	C	509	CLA	C13-C15-C16-C17
34	B	622	LMG	O8-C28-C29-C30
34	a	415	LMG	C15-C16-C17-C18
32	A	420[A]	PL9	C19-C21-C22-C23
37	h	102	DGD	O1G-C1G-C2G-C3G
24	a	409	CLA	C2A-CAA-CBA-CGA
24	c	510	CLA	C13-C15-C16-C17
25	a	420[B]	PHO	C8-C10-C11-C12
24	A	410	CLA	C15-C16-C17-C18
24	C	510	CLA	C8-C10-C11-C12
25	A	408	PHO	C4-C3-C5-C6
32	A	420[A]	PL9	C20-C19-C21-C22
24	C	512	CLA	C4B-C3B-CAB-CBB
24	D	402	CLA	C4B-C3B-CAB-CBB
24	d	403	CLA	C4B-C3B-CAB-CBB
24	a	410	CLA	C10-C11-C12-C13
27	a	405	SQD	O10-C23-O48-C46
34	b	630	LMG	O10-C28-O8-C9
38	d	407	LHG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	F	102	HEM	CAD-CBD-CGD-O2D
34	A	422	LMG	O8-C28-C29-C30
25	A	409[B]	PHO	CHA-CBD-CGD-O2D
25	a	420[B]	PHO	CHA-CBD-CGD-O1D
25	a	420[B]	PHO	CHA-CBD-CGD-O2D
27	a	405	SQD	C24-C23-O48-C46
29	m	102	LMT	C4-C5-C6-C7
37	C	516	DGD	C8B-C9B-CAB-CBB
38	D	407	LHG	C33-C34-C35-C36
36	B	623	HTG	C4-C5-C6-O6
24	c	511	CLA	C4-C3-C5-C6
38	d	407	LHG	O7-C5-C6-O8
38	E	101	LHG	C12-C13-C14-C15
37	C	516	DGD	O6E-C1E-O5D-C6D
24	b	616	CLA	C8-C10-C11-C12
24	B	604	CLA	C6-C7-C8-C10
24	b	626	CLA	C11-C12-C13-C15
38	d	408	LHG	C10-C11-C12-C13
24	B	615	CLA	C6-C7-C8-C9
24	C	506	CLA	C6-C7-C8-C9
27	A	412	SQD	C45-C44-O6-C1
34	z	101	LMG	C8-C7-O1-C1
37	C	516	DGD	C5D-C6D-O5D-C1E
37	D	406	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
34	D	412	LMG	C30-C31-C32-C33
24	C	513	CLA	C2-C1-O2A-CGA
24	b	623	CLA	C2-C1-O2A-CGA
24	b	624	CLA	C2-C1-O2A-CGA
29	m	102	LMT	C4'-C5'-C6'-O6'
29	m	102	LMT	C7-C8-C9-C10
24	C	513	CLA	C3A-C2A-CAA-CBA
24	b	619	CLA	C3A-C2A-CAA-CBA
37	c	520	DGD	C7A-C8A-C9A-CAA
28	b	607	GOL	O1-C1-C2-C3
41	v	205	HEC	CAD-CBD-CGD-O1D
34	c	522	LMG	C2-C1-O1-C7
37	C	516	DGD	C2E-C1E-O5D-C6D
24	A	406	CLA	C4C-C3C-CAC-CBC
37	C	517	DGD	C1B-C2B-C3B-C4B
24	C	506	CLA	C2-C3-C5-C6
27	a	405	SQD	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
39	e	102	HEM	CAD-CBD-CGD-O1D
24	c	507	CLA	C8-C10-C11-C12
29	M	103	LMT	O1'-C1-C2-C3
34	A	422	LMG	C33-C34-C35-C36
37	c	519	DGD	O6E-C1E-O5D-C6D
32	a	416[A]	PL9	C39-C41-C42-C43
37	H	103	DGD	C1G-C2G-C3G-O3G
39	e	102	HEM	C4B-C3B-CAB-CBB
28	T	101	GOL	O1-C1-C2-O2
34	C	519	LMG	C16-C17-C18-C19
24	d	403	CLA	C4-C3-C5-C6
34	A	422	LMG	C16-C17-C18-C19
37	c	519	DGD	C5A-C6A-C7A-C8A
29	b	631	LMT	C6-C7-C8-C9
37	h	102	DGD	CDA-CEA-CFA-CGA
38	E	101	LHG	C25-C26-C27-C28
34	c	522	LMG	C17-C18-C19-C20
29	m	102	LMT	C5-C6-C7-C8
38	l	101	LHG	C17-C18-C19-C20
24	C	512	CLA	CAA-CBA-CGA-O2A
34	Z	101	LMG	O7-C10-C11-C12
34	z	101	LMG	O7-C10-C11-C12
38	a	422	LHG	O8-C23-C24-C25
37	c	521	DGD	O6E-C5E-C6E-O5E
24	c	510	CLA	C4-C3-C5-C6
24	a	410	CLA	C11-C10-C8-C7
24	a	410	CLA	C11-C12-C13-C15
24	b	613	CLA	C6-C7-C8-C10
24	b	611	CLA	CAA-CBA-CGA-O1A
27	A	416	SQD	C15-C16-C17-C18
29	D	401	LMT	C5-C6-C7-C8
24	A	410	CLA	C2B-C3B-CAB-CBB
24	C	509	CLA	C2B-C3B-CAB-CBB
24	c	505	CLA	C2B-C3B-CAB-CBB
26	C	514	BCR	C5-C6-C7-C8
26	C	515	BCR	C5-C6-C7-C8
26	D	404	BCR	C23-C24-C25-C26
26	D	404	BCR	C23-C24-C25-C30
26	T	103	BCR	C1-C6-C7-C8
26	T	103	BCR	C5-C6-C7-C8
26	c	518	BCR	C1-C6-C7-C8
26	c	518	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	t	101	BCR	C5-C6-C7-C8
24	A	406	CLA	C13-C15-C16-C17
37	C	518	DGD	O1G-C1A-C2A-C3A
27	f	102	SQD	C33-C34-C35-C36
29	a	421	LMT	C5-C6-C7-C8
37	e	101	DGD	C7B-C8B-C9B-CAB
36	d	411	HTG	C1'-C2'-C3'-C4'
24	c	510	CLA	C16-C17-C18-C19
38	L	101	LHG	C30-C31-C32-C33
27	f	102	SQD	O47-C7-C8-C9
24	c	510	CLA	O1A-CGA-O2A-C1
36	b	633	HTG	C2'-C1'-S1-C1
36	c	524	HTG	C2'-C1'-S1-C1
24	b	624	CLA	C2A-CAA-CBA-CGA
27	A	412	SQD	C8-C7-O47-C45
37	C	516	DGD	O2G-C1B-C2B-C3B
37	e	101	DGD	O2G-C1B-C2B-C3B
37	c	520	DGD	C8A-C9A-CAA-CBA
39	F	102	HEM	CAA-CBA-CGA-O2A
24	b	624	CLA	C10-C11-C12-C13
38	D	407	LHG	C28-C29-C30-C31
37	c	521	DGD	O1G-C1A-C2A-C3A
38	D	407	LHG	C26-C27-C28-C29
24	A	405	CLA	C4C-C3C-CAC-CBC
37	D	406	DGD	O1G-C1A-C2A-C3A
32	d	405[A]	PL9	C18-C19-C21-C22
39	e	102	HEM	CAD-CBD-CGD-O2D
27	A	416	SQD	C18-C19-C20-C21
38	D	409	LHG	C33-C34-C35-C36
24	C	509	CLA	C16-C17-C18-C20
34	j	101	LMG	C29-C30-C31-C32
38	d	406	LHG	O8-C23-C24-C25
34	C	519	LMG	C40-C41-C42-C43
39	F	102	HEM	CAA-CBA-CGA-O1A
39	e	102	HEM	CAA-CBA-CGA-O1A
24	C	507	CLA	C11-C10-C8-C9
24	c	516	CLA	C11-C10-C8-C9
38	D	409	LHG	C9-C10-C11-C12
24	C	510	CLA	CAA-CBA-CGA-O2A
37	e	101	DGD	C3A-C4A-C5A-C6A
37	D	406	DGD	C1G-C2G-C3G-O3G
24	b	625	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	c	505	CLA	C1A-C2A-CAA-CBA
24	c	505	CLA	C4B-C3B-CAB-CBB
32	A	420[B]	PL9	C20-C19-C21-C22
27	A	416	SQD	O5-C1-O6-C44
34	A	422	LMG	O6-C1-O1-C7
34	c	522	LMG	O6-C1-O1-C7
38	L	101	LHG	O7-C7-C8-C9
27	A	412	SQD	O6-C44-C45-O47
32	a	416[B]	PL9	C11-C12-C13-C14
26	K	101	BCR	C7-C8-C9-C10
26	k	101	BCR	C19-C20-C21-C22
24	c	516	CLA	CAA-CBA-CGA-O2A
38	L	101	LHG	C26-C27-C28-C29
37	C	517	DGD	C3A-C4A-C5A-C6A
27	A	416	SQD	C2-C1-O6-C44
24	a	409	CLA	C13-C15-C16-C17
38	l	101	LHG	C9-C10-C11-C12
38	l	101	LHG	O7-C7-C8-C9
28	b	603	GOL	C1-C2-C3-O3
32	d	405[A]	PL9	C30-C29-C31-C32
24	B	602	CLA	C2-C1-O2A-CGA
24	C	511	CLA	C2-C1-O2A-CGA
24	D	402	CLA	C2-C1-O2A-CGA
24	B	603	CLA	C12-C13-C15-C16
24	B	615	CLA	C11-C10-C8-C7
24	C	506	CLA	C6-C7-C8-C10
24	C	507	CLA	C11-C10-C8-C7
24	a	410	CLA	C12-C13-C15-C16
24	b	614	CLA	C6-C7-C8-C10
24	b	626	CLA	C12-C13-C15-C16
32	A	420[B]	PL9	C28-C29-C31-C32
34	c	522	LMG	C40-C41-C42-C43
24	B	613	CLA	C13-C15-C16-C17
24	B	608	CLA	C16-C17-C18-C20
34	B	622	LMG	C9-C8-O7-C10
38	a	422	LHG	O10-C23-C24-C25
29	a	404	LMT	C7-C8-C9-C10
38	D	407	LHG	C7-C8-C9-C10
24	c	514	CLA	CAA-CBA-CGA-O2A
25	a	420[A]	PHO	C2C-C3C-CAC-CBC
24	B	603	CLA	C2A-CAA-CBA-CGA
24	b	613	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	A	412	SQD	O49-C7-O47-C45
39	e	102	HEM	CAA-CBA-CGA-O2A
24	C	512	CLA	CAA-CBA-CGA-O1A
38	d	407	LHG	C32-C33-C34-C35
24	B	607	CLA	C4-C3-C5-C6
34	Z	101	LMG	O9-C10-C11-C12
24	a	409	CLA	C2C-C3C-CAC-CBC
24	B	606	CLA	O1A-CGA-O2A-C1
24	b	625	CLA	C13-C15-C16-C17
24	d	401	CLA	C16-C17-C18-C20
34	z	101	LMG	O9-C10-C11-C12
38	D	409	LHG	C30-C31-C32-C33
37	c	520	DGD	O2G-C1B-C2B-C3B
36	b	632	HTG	S1-C1'-C2'-C3'
24	A	405	CLA	C2A-CAA-CBA-CGA
24	B	615	CLA	C2A-CAA-CBA-CGA
24	c	510	CLA	CBA-CGA-O2A-C1
24	A	407	CLA	C11-C10-C8-C9
24	b	626	CLA	C14-C13-C15-C16
24	b	623	CLA	CAA-CBA-CGA-O2A
27	A	416	SQD	C29-C30-C31-C32
34	z	101	LMG	C11-C12-C13-C14
38	D	407	LHG	C27-C28-C29-C30
37	c	521	DGD	O1A-C1A-C2A-C3A
37	e	101	DGD	O1B-C1B-C2B-C3B
27	a	405	SQD	C32-C33-C34-C35
29	m	102	LMT	C9-C10-C11-C12
24	B	614	CLA	CAA-CBA-CGA-O2A
29	f	103	LMT	C1-C2-C3-C4
38	L	101	LHG	C9-C10-C11-C12
28	B	626	GOL	O2-C2-C3-O3
37	C	518	DGD	O1A-C1A-C2A-C3A
37	D	406	DGD	O1A-C1A-C2A-C3A
38	d	406	LHG	O10-C23-C24-C25
37	C	517	DGD	C2G-C3G-O3G-C1D
37	h	102	DGD	C2G-C3G-O3G-C1D
37	H	103	DGD	O1G-C1G-C2G-O2G
29	M	104	LMT	C4'-C5'-C6'-O6'
37	D	406	DGD	C9B-CAB-CBB-CCB
24	c	514	CLA	CAA-CBA-CGA-O1A
38	d	408	LHG	C30-C31-C32-C33
29	a	404	LMT	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	420[B]	PL9	C19-C21-C22-C23
27	f	102	SQD	O49-C7-C8-C9
29	a	404	LMT	O5B-C5B-C6B-O6B
24	C	508	CLA	C13-C15-C16-C17
38	E	101	LHG	O8-C23-C24-C25
32	D	405[B]	PL9	C33-C34-C36-C37
24	c	516	CLA	CAA-CBA-CGA-O1A
29	M	104	LMT	C9-C10-C11-C12
24	B	610	CLA	CAD-CBD-CGD-O2D
24	B	617	CLA	CAD-CBD-CGD-O2D
24	C	513	CLA	CAD-CBD-CGD-O2D
24	c	508	CLA	CAD-CBD-CGD-O2D
38	l	101	LHG	O9-C7-C8-C9
37	c	521	DGD	O6D-C5D-C6D-O5D
24	c	510	CLA	C2-C1-O2A-CGA
24	B	610	CLA	C10-C11-C12-C13
24	B	613	CLA	CAA-CBA-CGA-O2A
24	c	509	CLA	CAA-CBA-CGA-O2A
34	b	630	LMG	O8-C28-C29-C30
37	C	517	DGD	O2G-C1B-C2B-C3B
37	e	101	DGD	CAB-CBB-CCB-CDB
24	a	409	CLA	C4C-C3C-CAC-CBC
29	M	103	LMT	C9-C10-C11-C12
24	b	623	CLA	C5-C6-C7-C8
38	L	101	LHG	O9-C7-C8-C9

There are no ring outliers.

169 monomers are involved in 335 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	l	101	LHG	2	0
32	D	405[B]	PL9	2	0
24	C	503	CLA	4	0
37	h	102	DGD	1	0
24	B	602	CLA	1	0
24	b	619	CLA	3	0
24	B	616	CLA	5	0
25	a	411	PHO	1	0
26	h	101	BCR	4	0
32	D	405[A]	PL9	1	0
25	A	409[B]	PHO	3	0
37	c	519	DGD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	M	101	LMT	3	0
24	B	610	CLA	4	0
32	a	416[B]	PL9	8	0
27	a	414	SQD	1	0
24	A	410	CLA	1	0
24	C	511	CLA	3	0
37	H	103	DGD	1	0
29	a	404	LMT	2	0
24	B	614	CLA	2	0
28	A	415	GOL	1	0
29	M	104	LMT	3	0
26	Y	101	BCR	4	0
36	b	602	HTG	2	0
34	z	101	LMG	4	0
24	c	517	CLA	5	0
24	d	402	CLA	3	0
24	d	403	CLA	1	0
28	b	605	GOL	1	0
34	j	101	LMG	2	0
37	c	520	DGD	2	0
24	B	608	CLA	1	0
24	c	511	CLA	2	0
24	b	620	CLA	1	0
32	d	405[B]	PL9	1	0
24	C	507	CLA	4	0
24	A	405	CLA	3	0
24	C	505	CLA	6	0
34	a	415	LMG	3	0
38	L	101	LHG	3	0
24	a	412	CLA	1	0
24	C	504	CLA	1	0
26	b	628	BCR	3	0
36	B	623	HTG	2	0
24	c	507	CLA	3	0
26	k	101	BCR	2	0
24	c	515	CLA	2	0
24	B	617	CLA	5	0
27	A	412	SQD	5	0
28	a	402	GOL	1	0
32	A	420[A]	PL9	5	0
24	b	612	CLA	4	0
24	C	508	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	624	CLA	1	0
24	B	605	CLA	2	0
26	b	629	BCR	2	0
26	d	404	BCR	3	0
37	D	406	DGD	3	0
25	A	409[A]	PHO	2	0
28	T	102	GOL	2	0
32	a	416[A]	PL9	9	0
31	a	418[B]	OEY	1	0
28	c	502	GOL	2	0
24	b	622	CLA	1	0
24	c	506	CLA	3	0
26	A	411	BCR	1	0
24	C	509	CLA	2	0
27	a	405	SQD	2	0
34	b	630	LMG	2	0
26	B	618	BCR	1	0
38	D	409	LHG	7	0
24	d	401	CLA	3	0
28	C	524	GOL	1	0
34	C	520	LMG	2	0
24	C	510	CLA	2	0
29	f	103	LMT	1	0
29	M	103	LMT	1	0
36	H	101	HTG	2	0
24	A	406	CLA	4	0
37	e	101	DGD	6	0
28	B	630	GOL	1	0
24	c	514	CLA	4	0
26	B	619	BCR	3	0
26	D	404	BCR	2	0
26	y	101	BCR	1	0
28	T	101	GOL	2	0
24	C	512	CLA	5	0
26	b	627	BCR	2	0
38	a	422	LHG	5	0
38	d	406	LHG	1	0
24	C	506	CLA	1	0
25	A	408	PHO	2	0
26	K	101	BCR	2	0
24	C	513	CLA	6	0
39	F	102	HEM	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	D	402	CLA	3	0
24	D	403	CLA	1	0
37	C	516	DGD	3	0
38	D	407	LHG	1	0
25	a	420[B]	PHO	3	0
26	T	103	BCR	4	0
26	C	515	BCR	2	0
36	b	633	HTG	1	0
24	b	625	CLA	5	0
29	F	101	LMT	1	0
38	d	408	LHG	5	0
24	c	513	CLA	2	0
24	b	623	CLA	1	0
29	C	521	LMT	1	0
24	a	409	CLA	3	0
24	b	614	CLA	3	0
27	B	621	SQD	3	0
26	B	620	BCR	4	0
29	A	417	LMT	3	0
29	m	102	LMT	2	0
34	B	622	LMG	1	0
34	c	523	LMG	1	0
24	c	510	CLA	3	0
24	C	502	CLA	2	0
34	c	522	LMG	2	0
26	C	514	BCR	2	0
24	B	607	CLA	4	0
39	e	102	HEM	3	0
24	c	516	CLA	3	0
29	D	401	LMT	1	0
24	b	615	CLA	5	0
31	A	419[B]	OEY	1	0
38	d	407	LHG	1	0
28	f	101	GOL	1	0
26	H	102	BCR	3	0
24	B	615	CLA	4	0
24	c	508	CLA	1	0
37	C	517	DGD	3	0
34	C	519	LMG	2	0
24	b	613	CLA	2	0
28	v	201	GOL	1	0
24	A	407	CLA	4	0

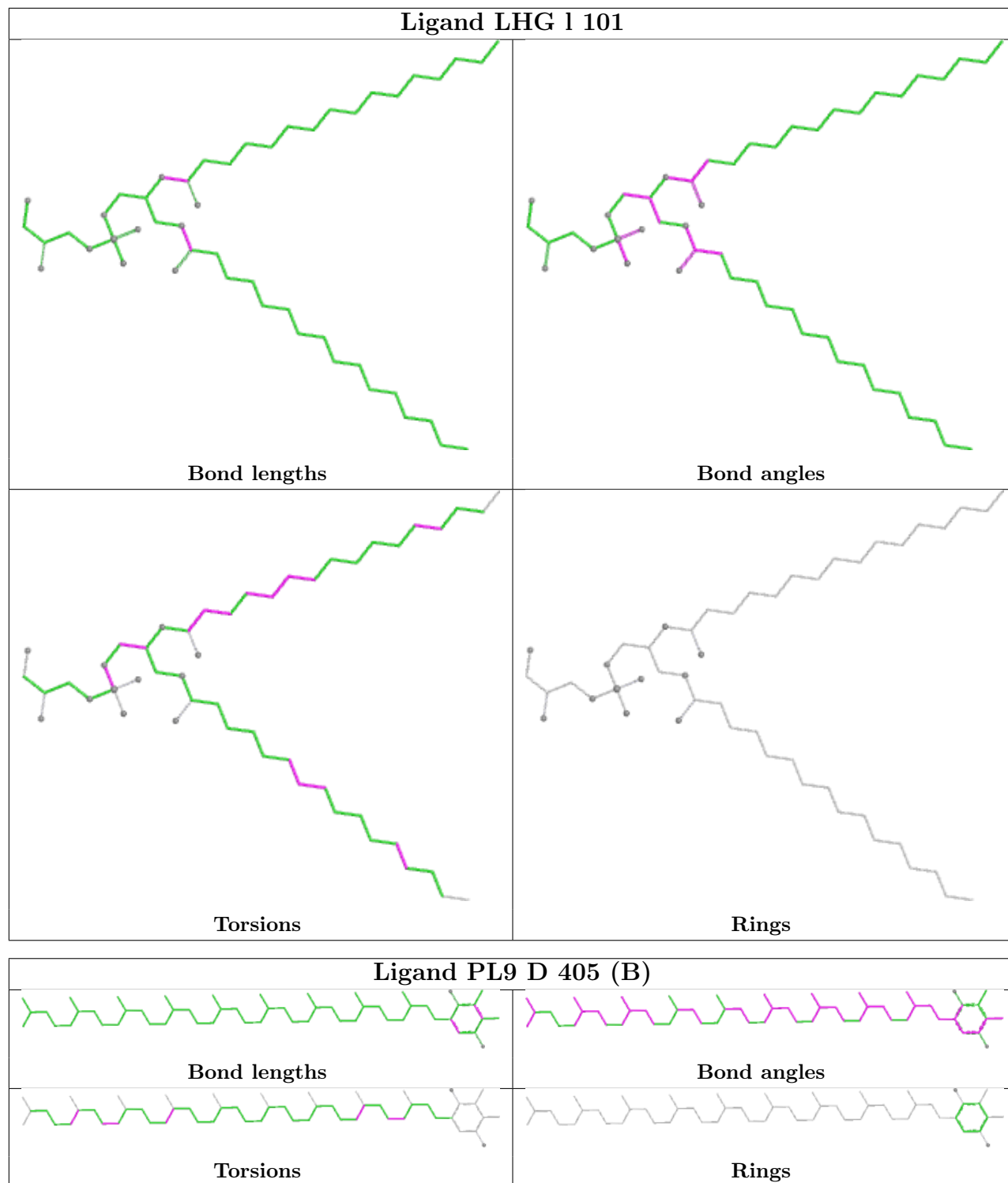
Continued on next page...

Continued from previous page...

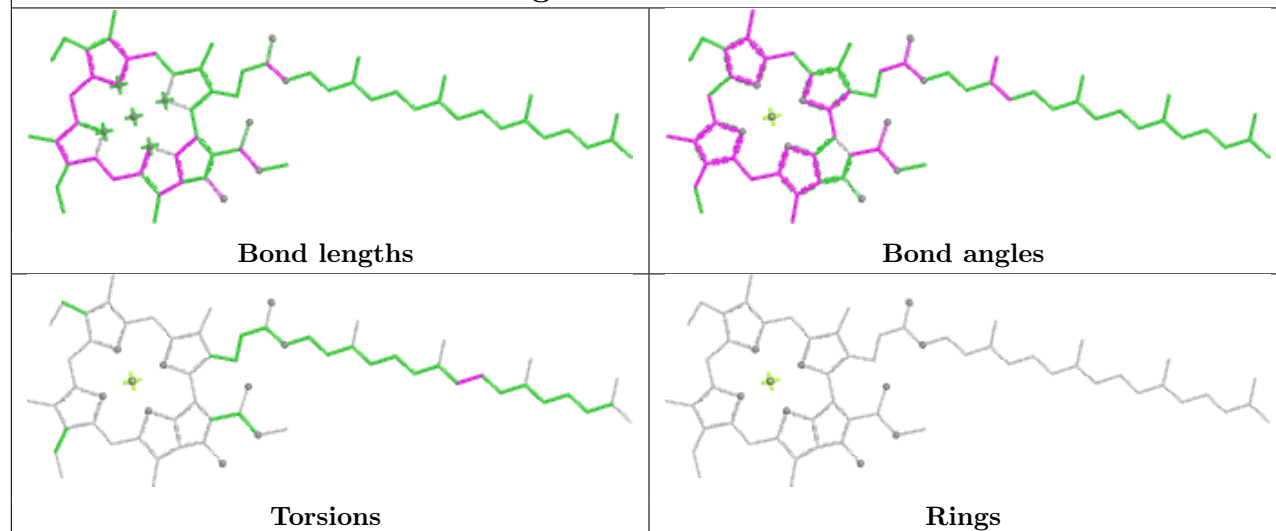
Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	D	408	LHG	1	0
24	b	621	CLA	2	0
24	c	512	CLA	6	0
24	a	410	CLA	2	0
37	C	518	DGD	2	0
29	b	631	LMT	2	0
24	C	501	CLA	1	0
38	E	101	LHG	2	0
34	D	412	LMG	1	0
25	a	420[A]	PHO	1	0
24	B	604	CLA	2	0
27	F	103	SQD	2	0
24	b	626	CLA	2	0
24	b	611	CLA	2	0
24	B	613	CLA	1	0
34	Z	101	LMG	2	0
28	A	414	GOL	1	0
27	f	102	SQD	3	0
24	B	611	CLA	1	0
36	V	207	HTG	3	0
26	c	527	BCR	2	0
24	c	509	CLA	4	0
26	t	101	BCR	6	0
24	B	606	CLA	2	0
27	A	416	SQD	1	0
27	b	601	SQD	2	0
36	d	411	HTG	3	0
32	A	420[B]	PL9	5	0
26	c	518	BCR	1	0
34	A	422	LMG	5	0
24	c	505	CLA	3	0

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

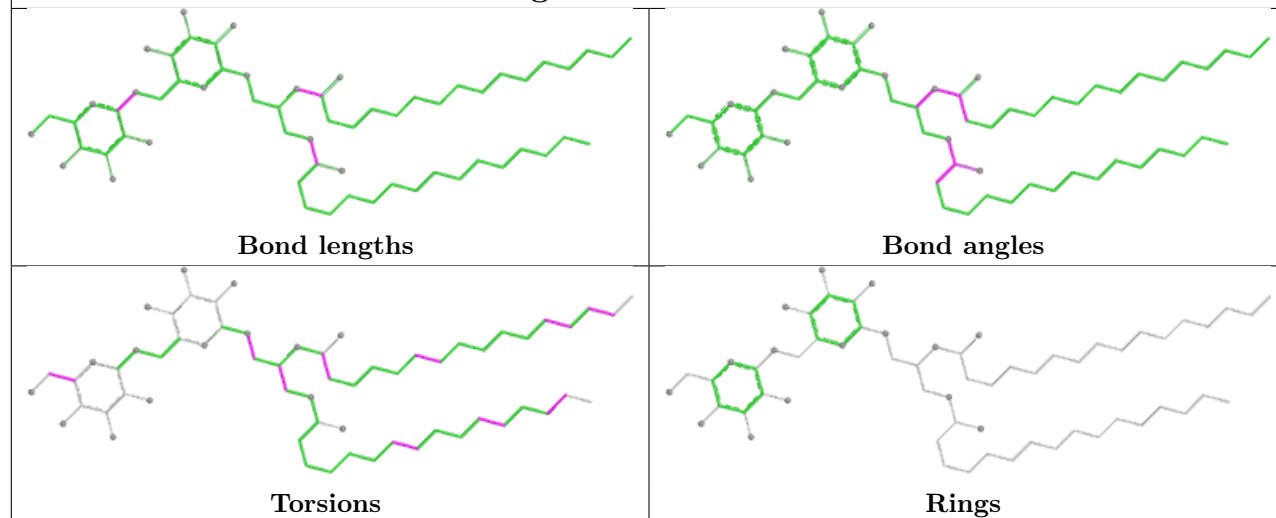
equivalents in the CSD to analyse the geometry.



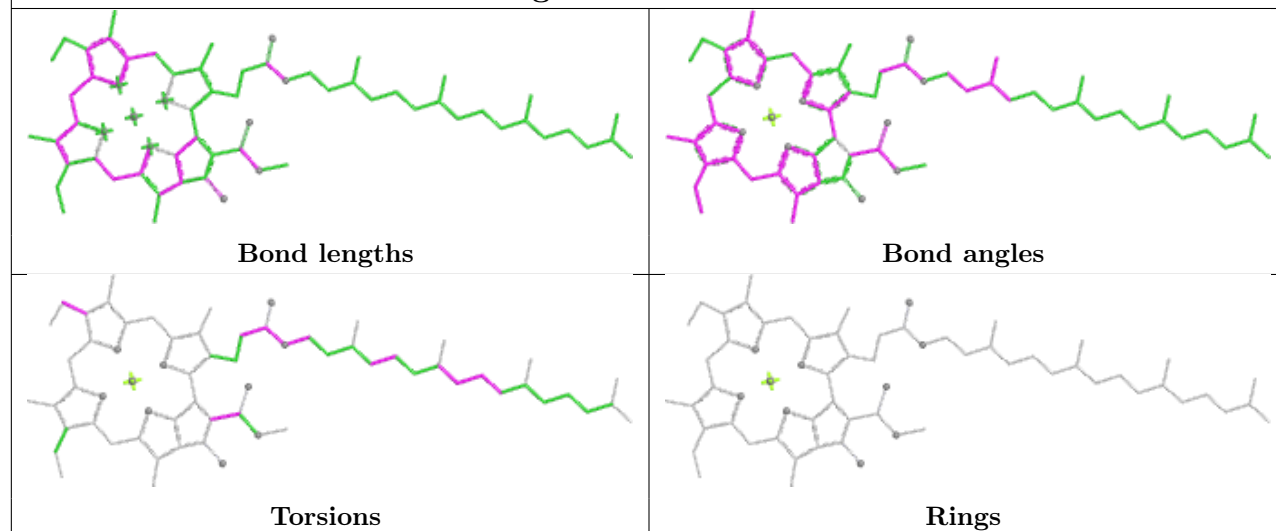
Ligand CLA C 503

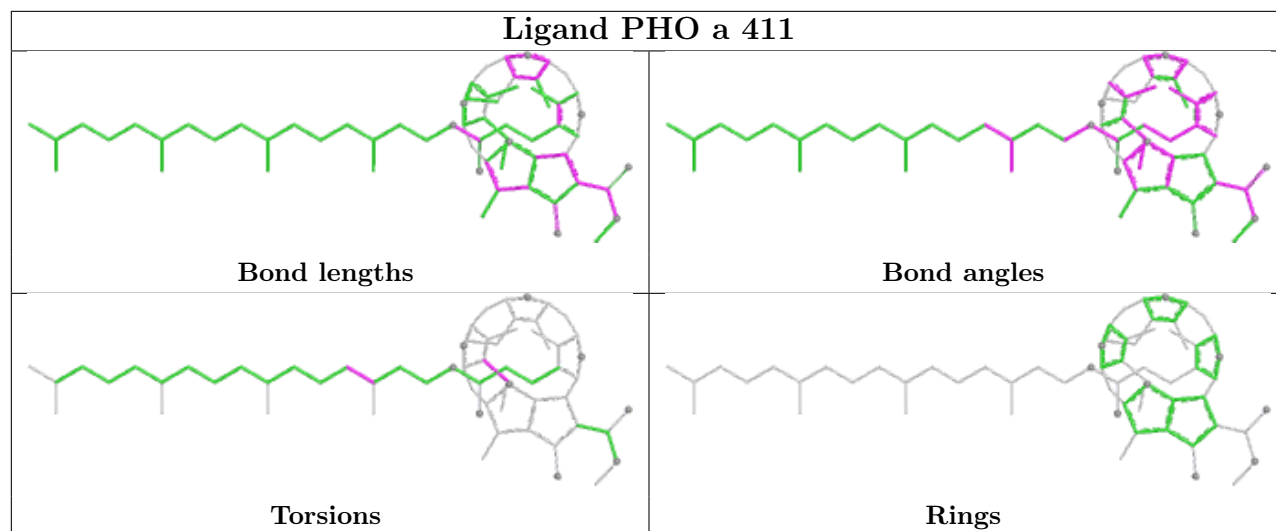
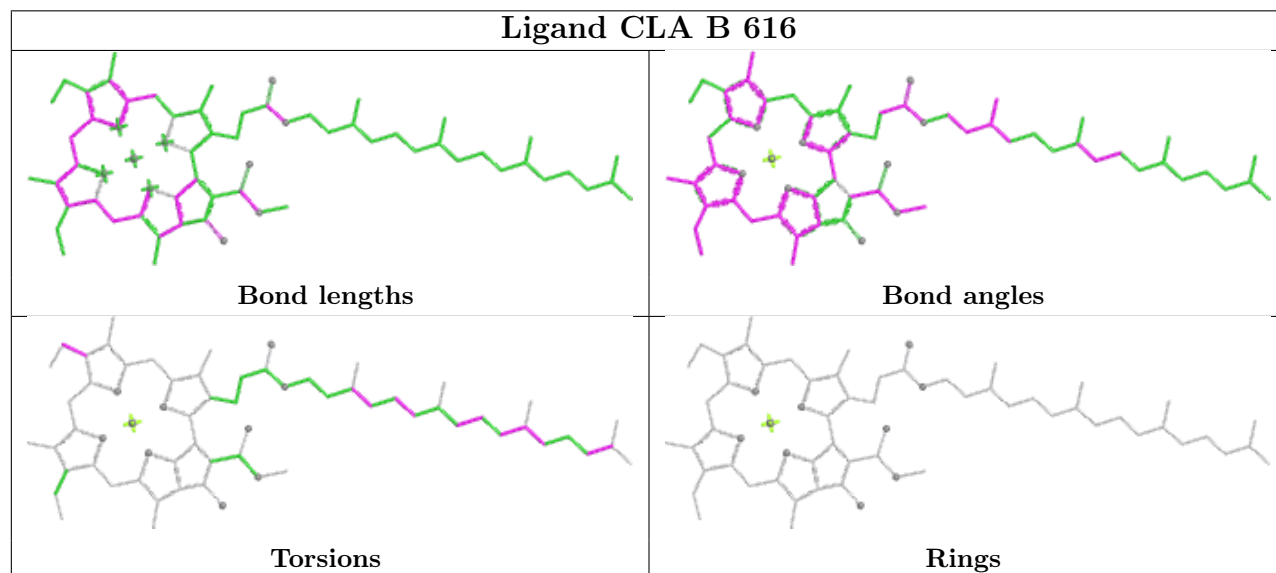
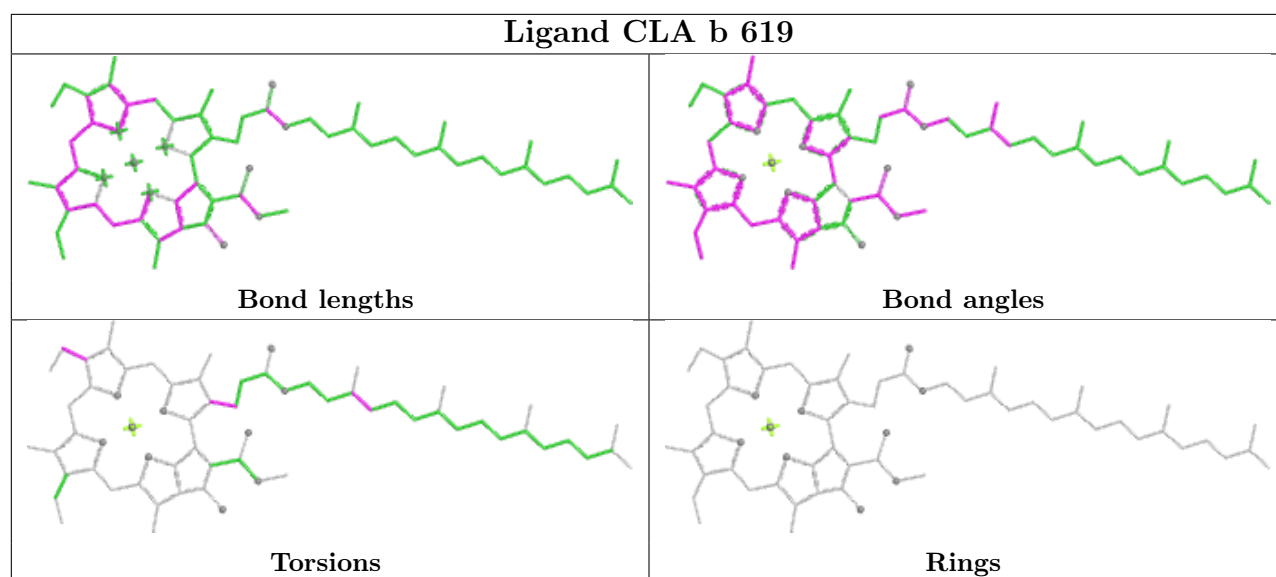


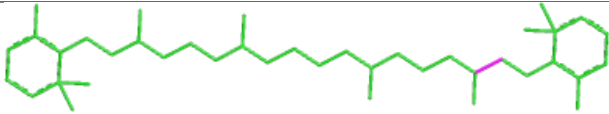
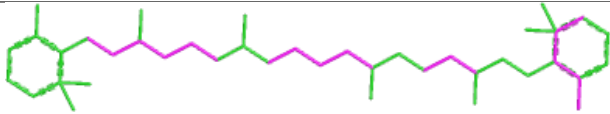
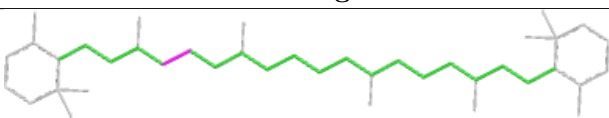
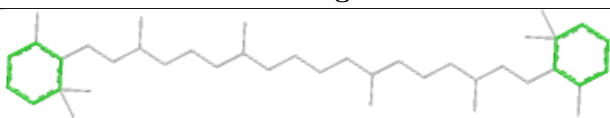
Ligand DGD h 102



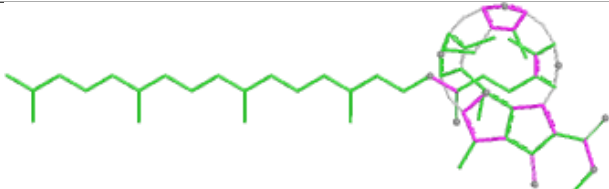
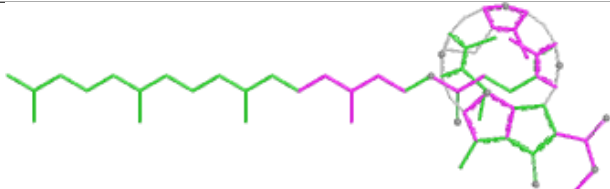
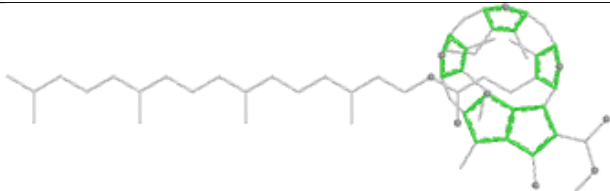
Ligand CLA B 602

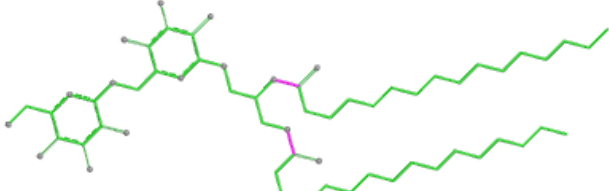
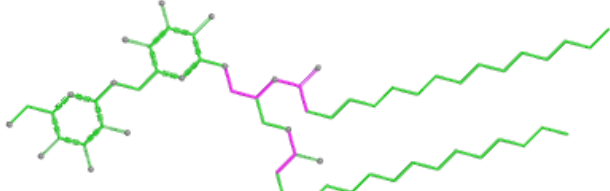
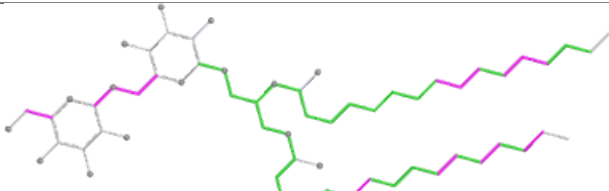
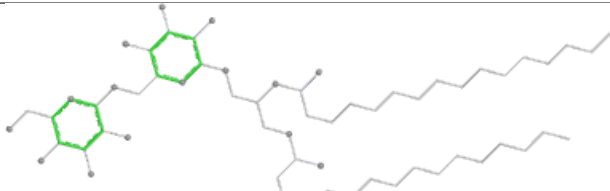


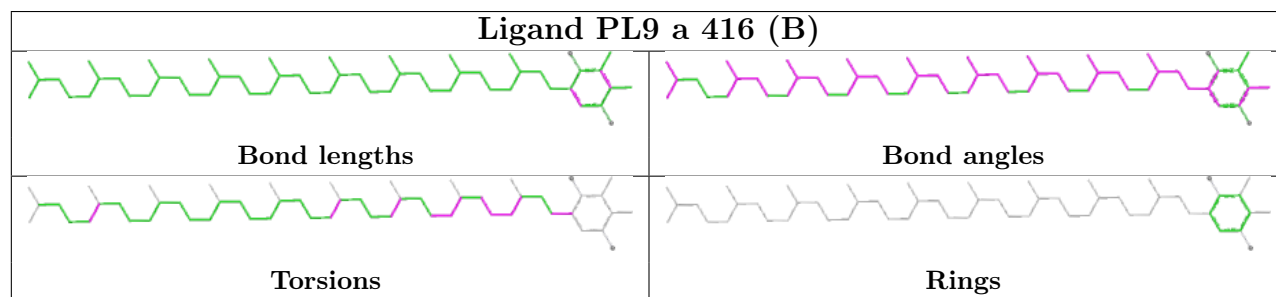
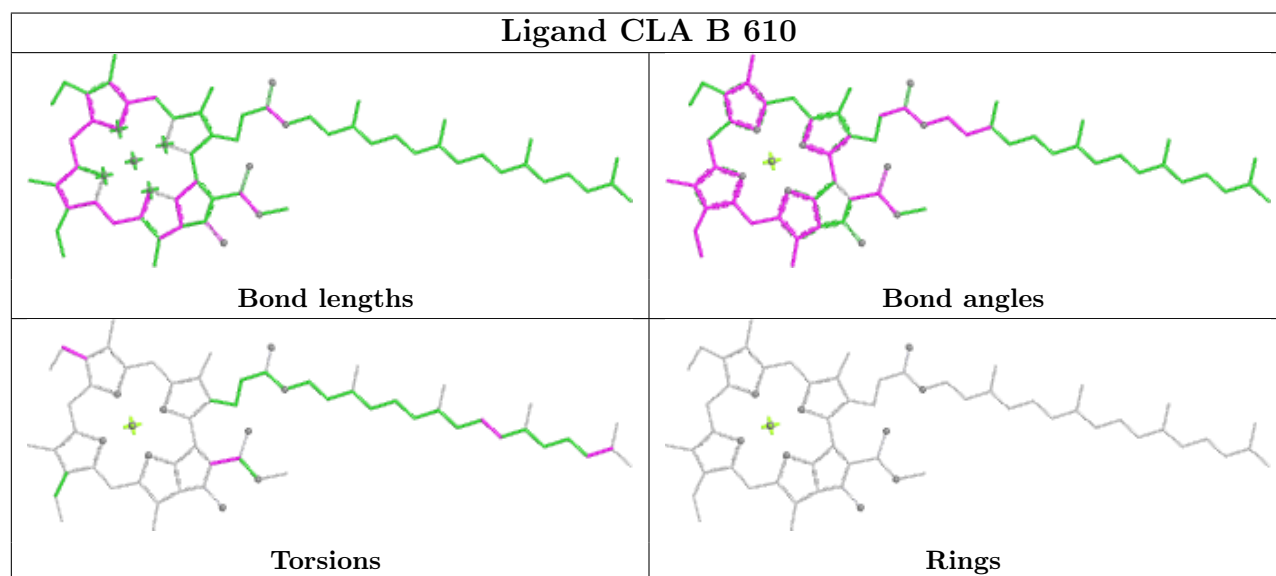
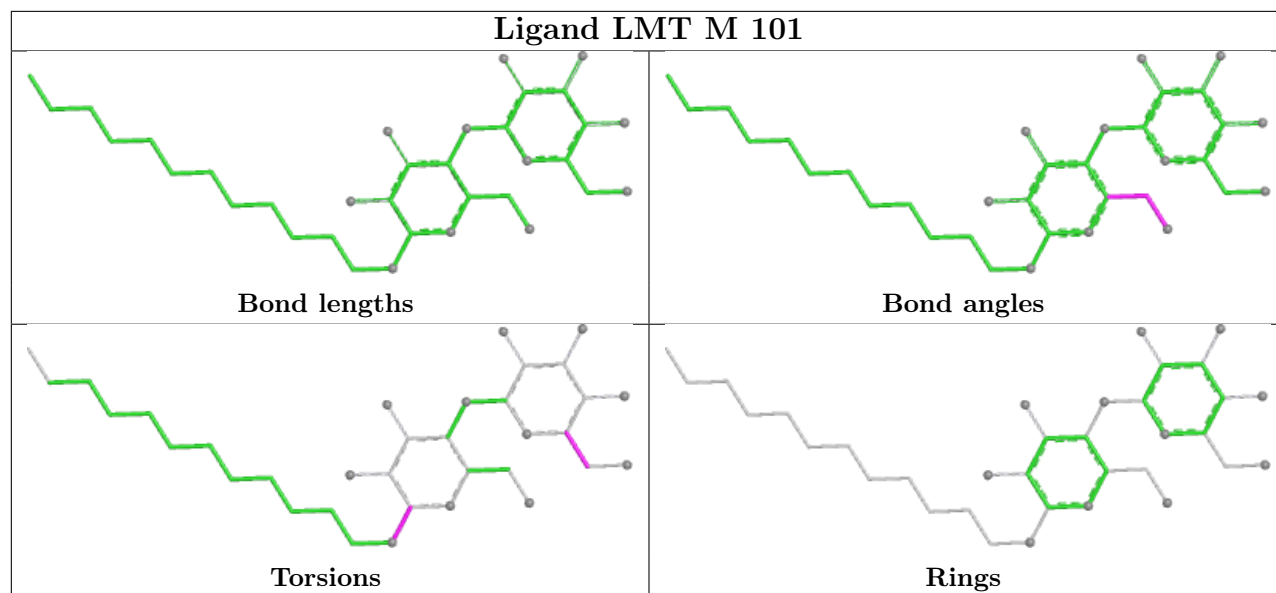


Ligand BCR h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

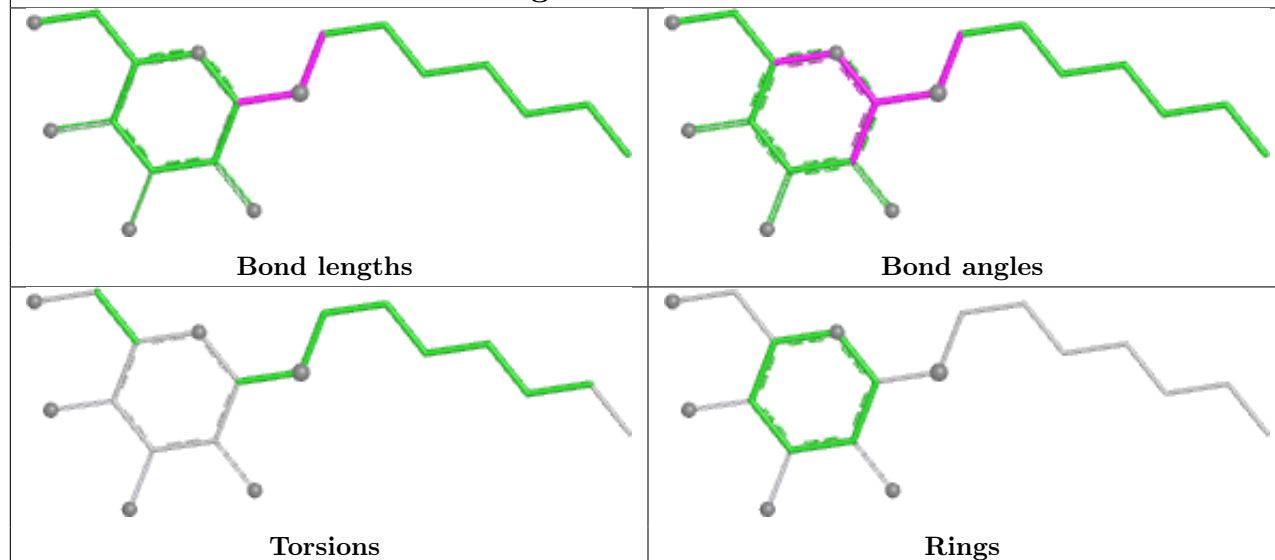
Ligand PL9 D 405 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand PHO A 409 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

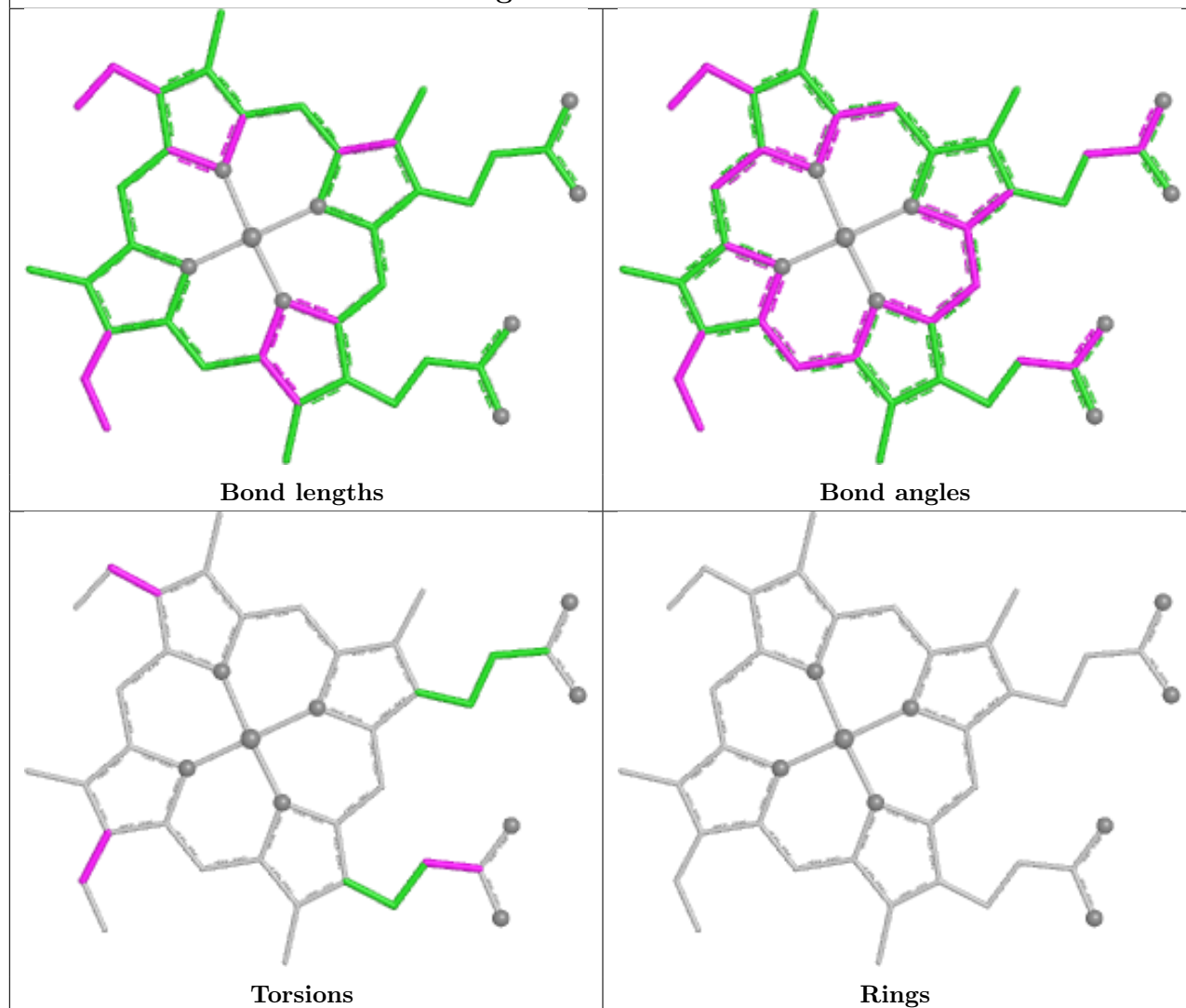
Ligand DGD c 519	
	
Bond lengths	Bond angles
	
Torsions	Rings

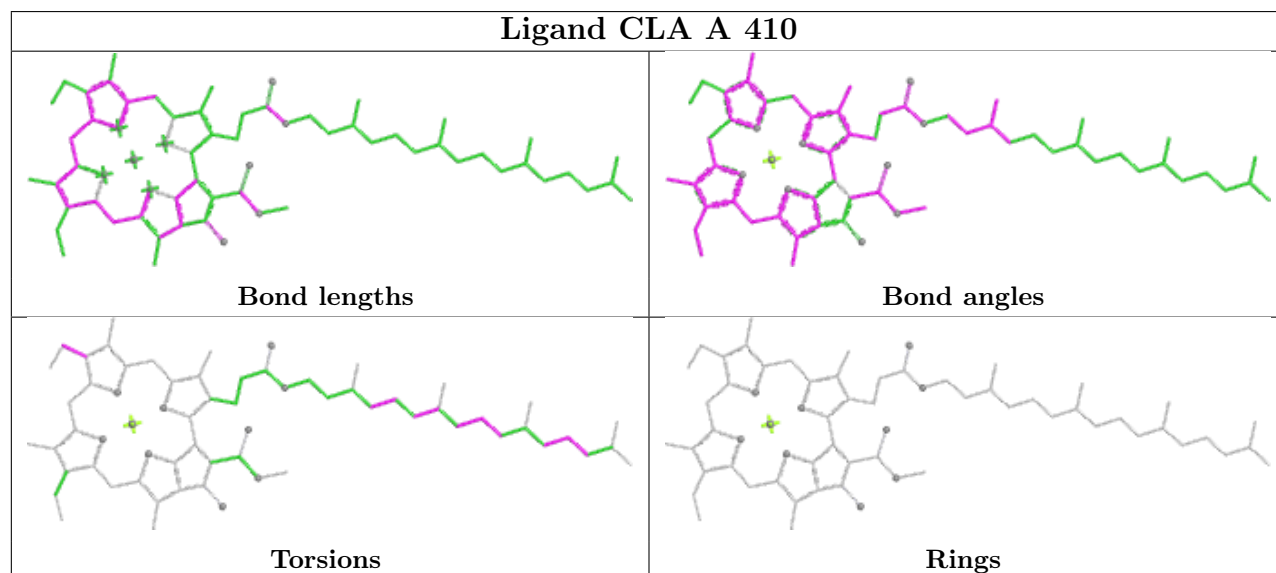
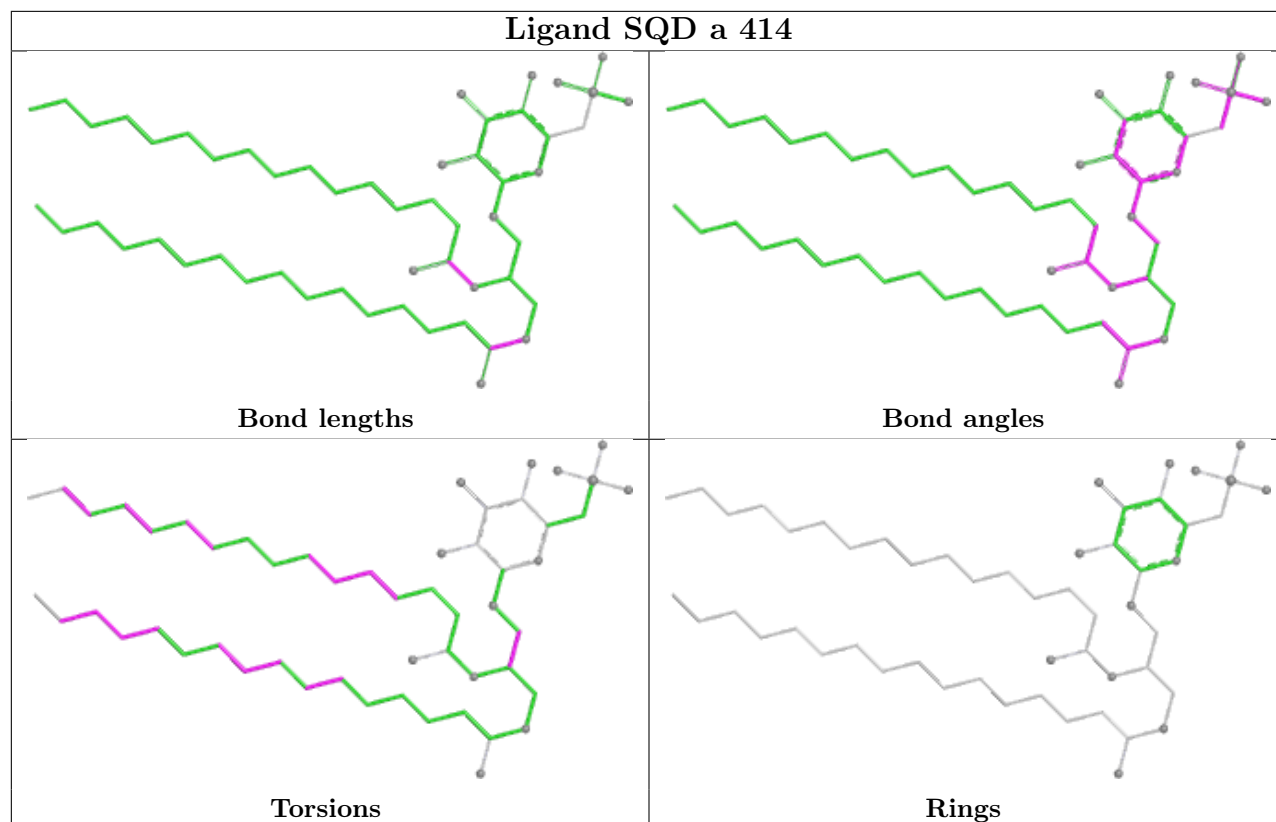


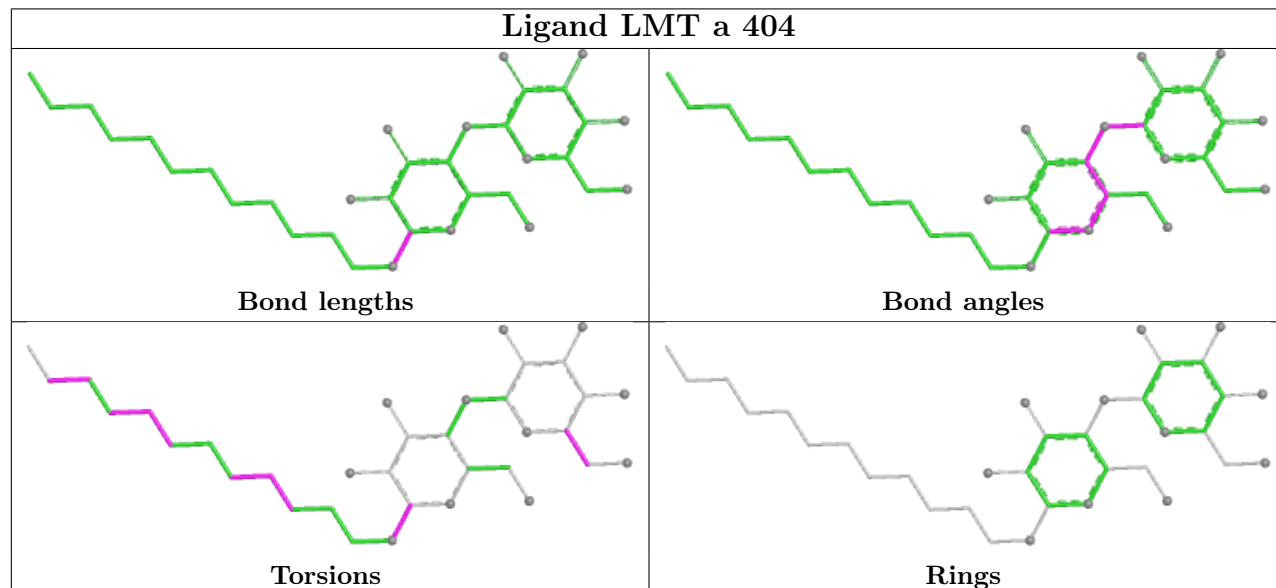
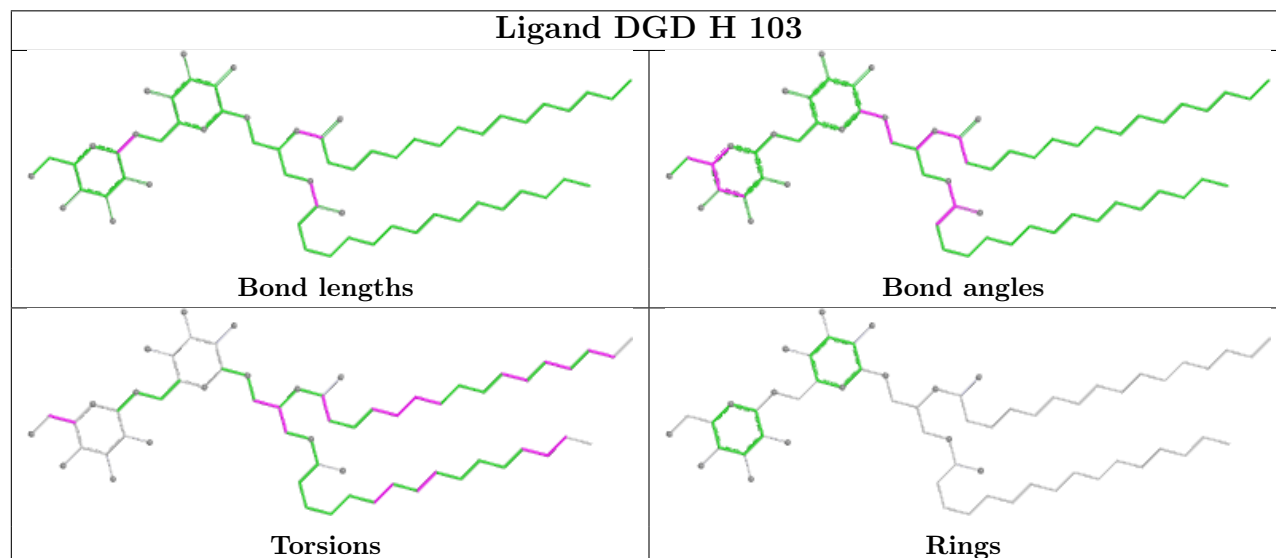
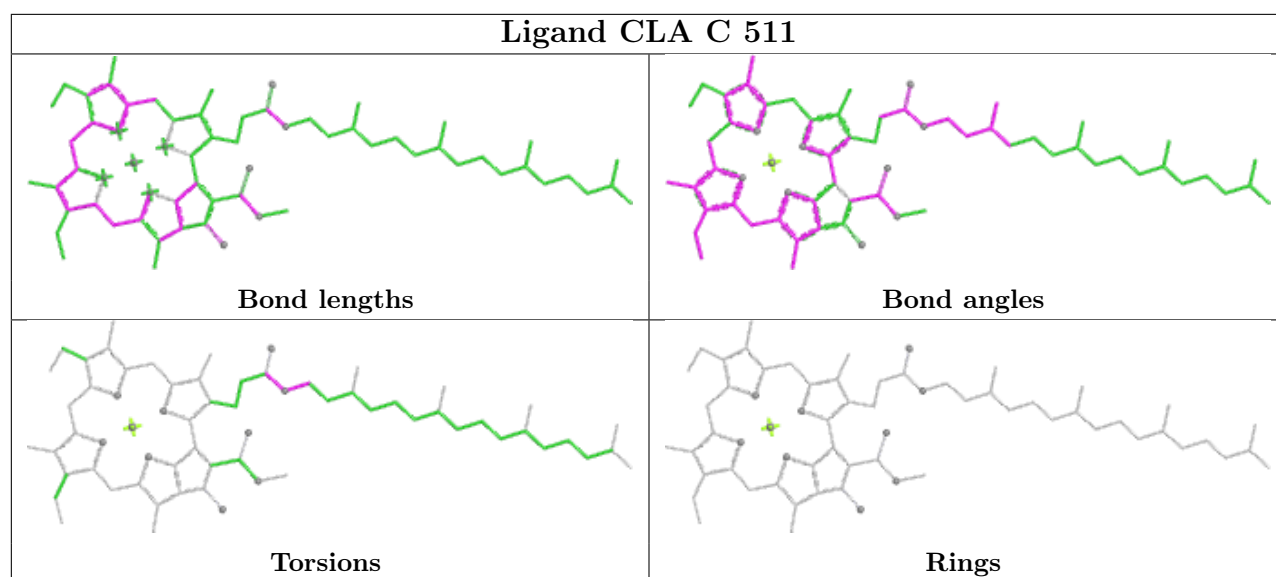
Ligand HTG b 609

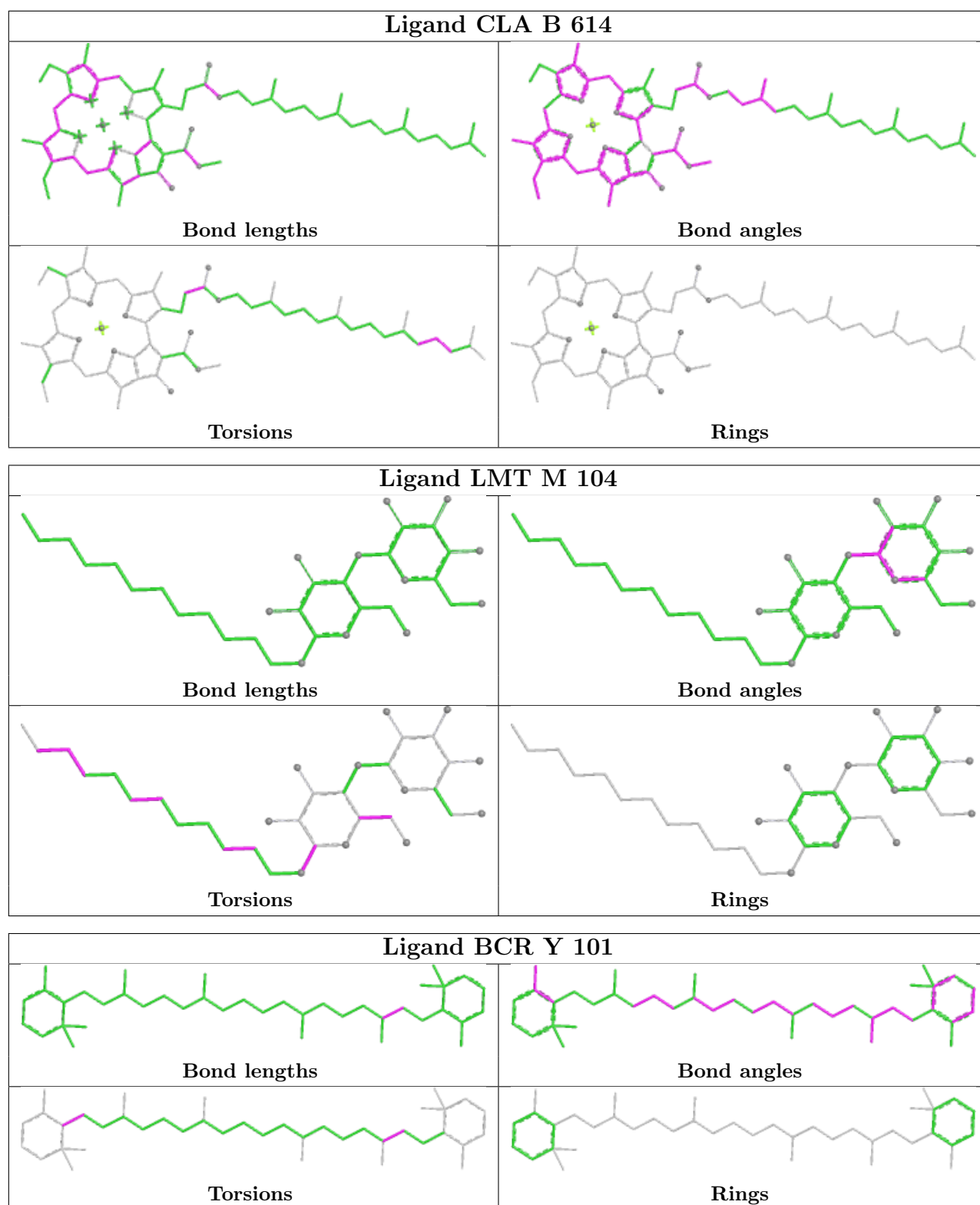


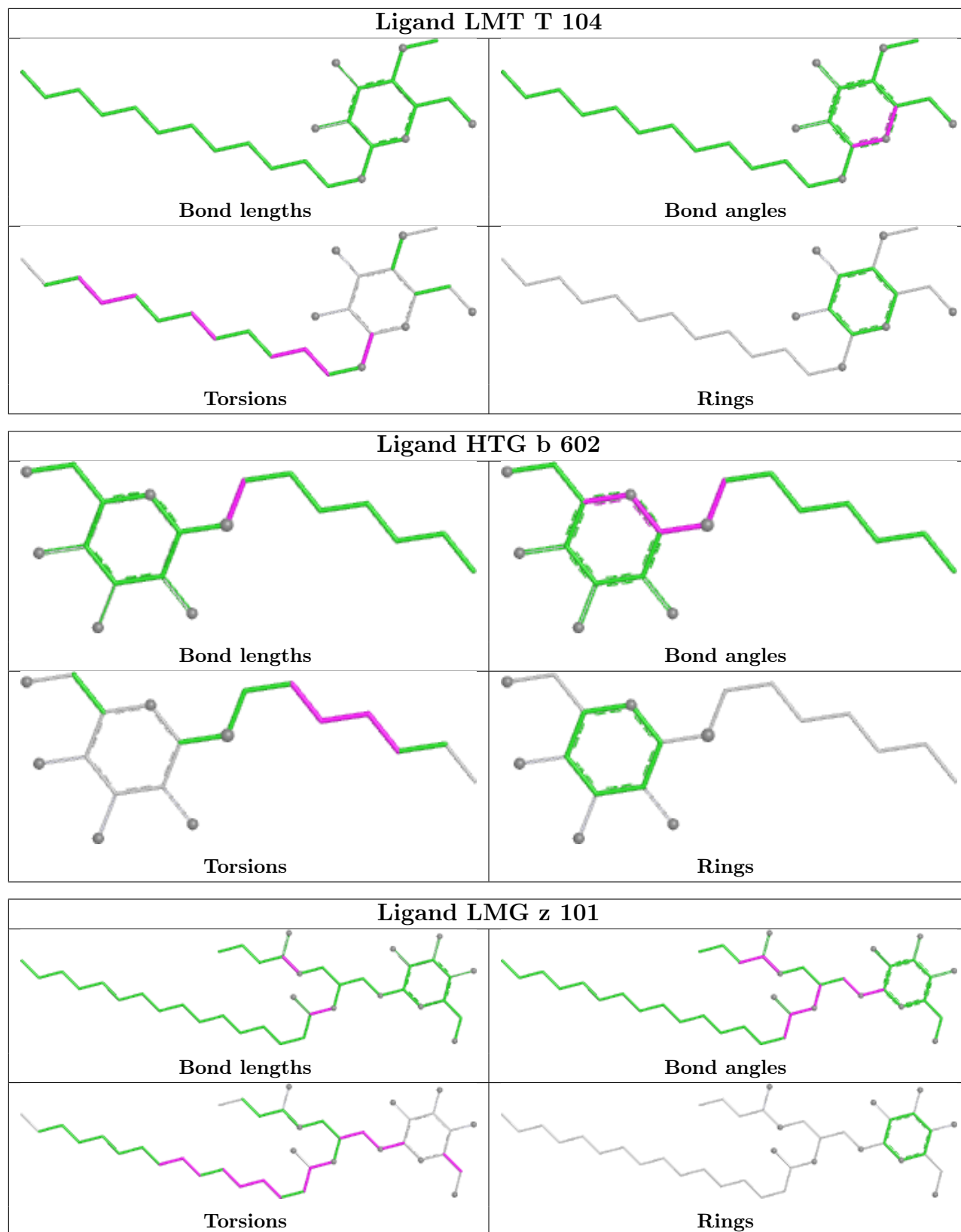
Ligand HEC v 205



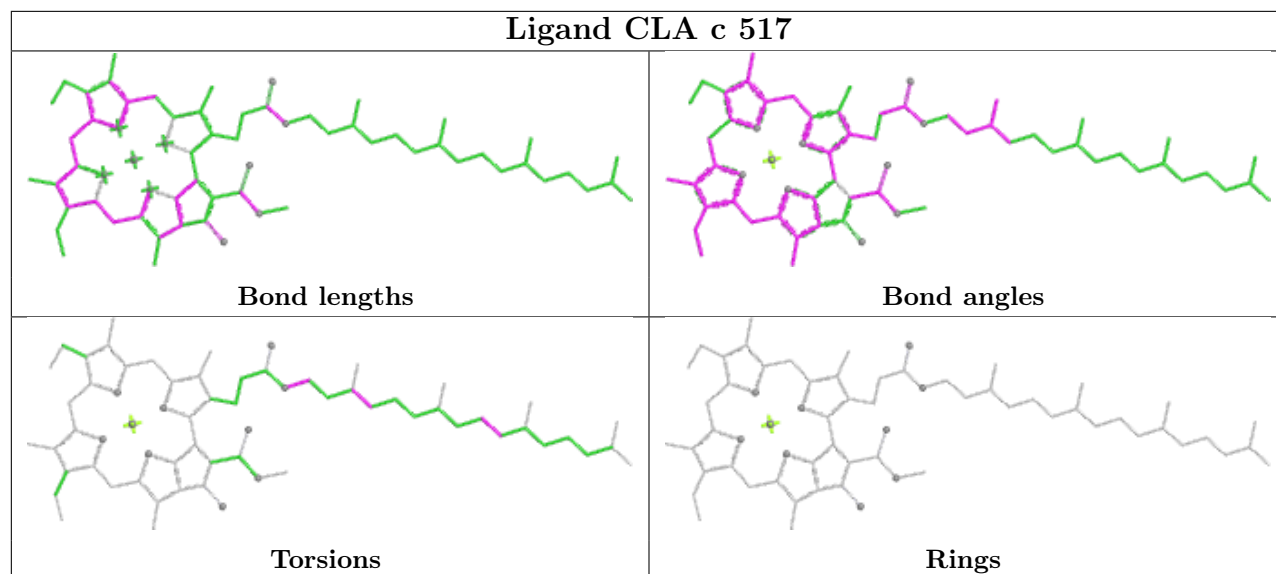




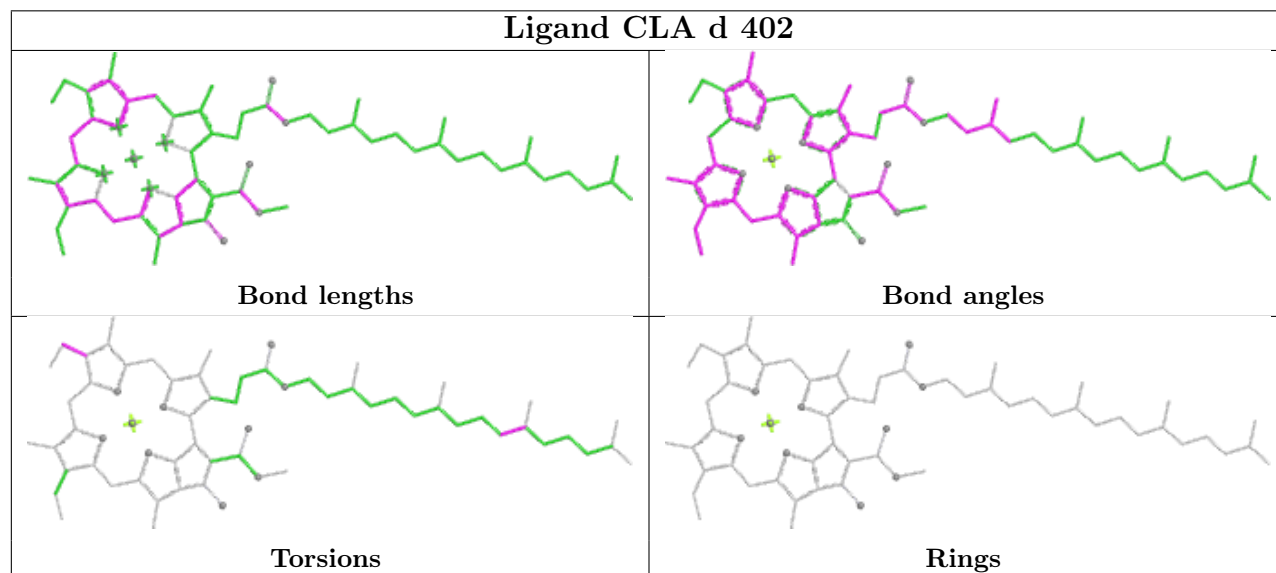




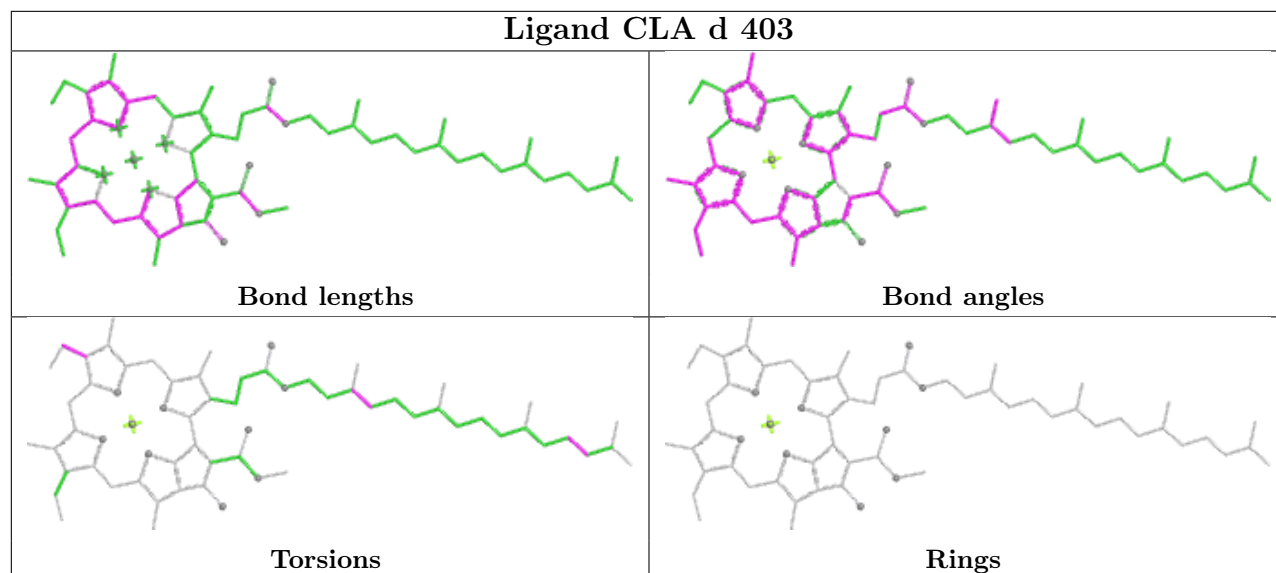
Ligand CLA c 517

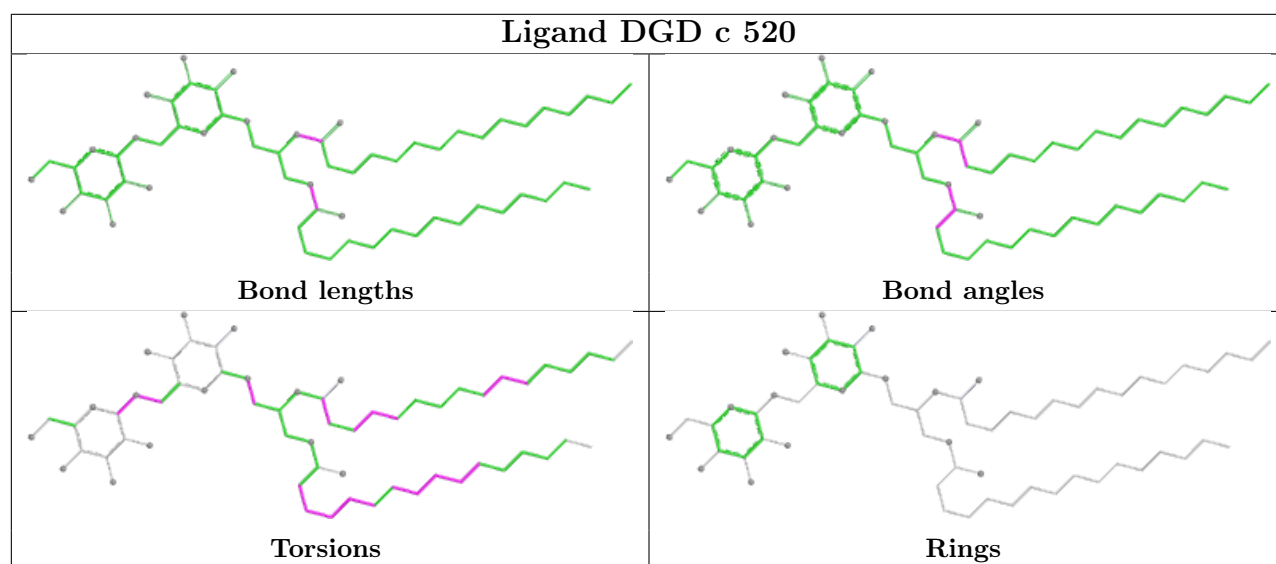
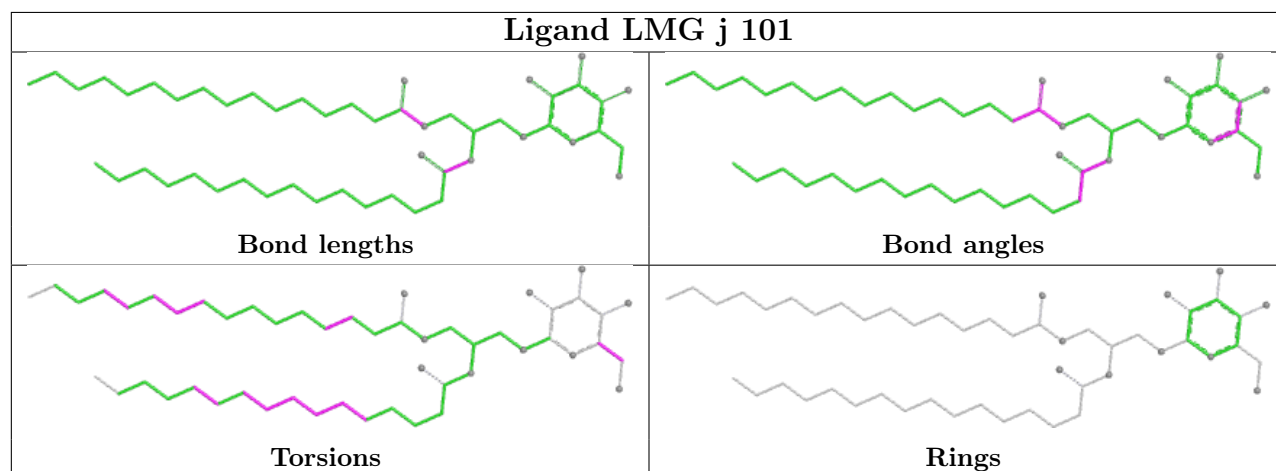
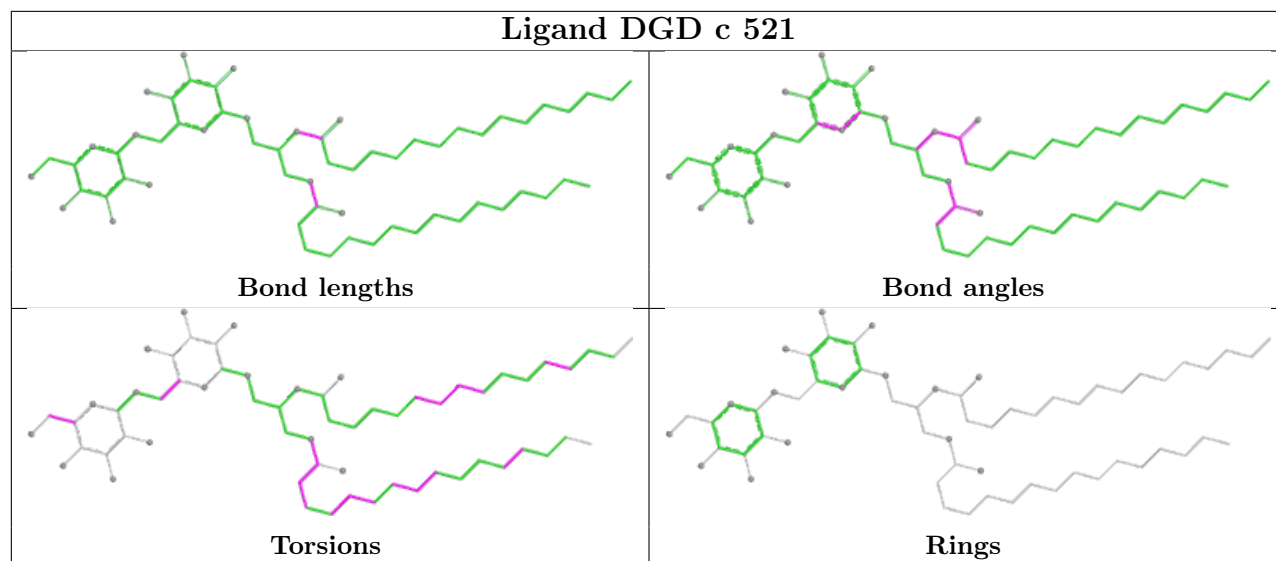


Ligand CLA d 402

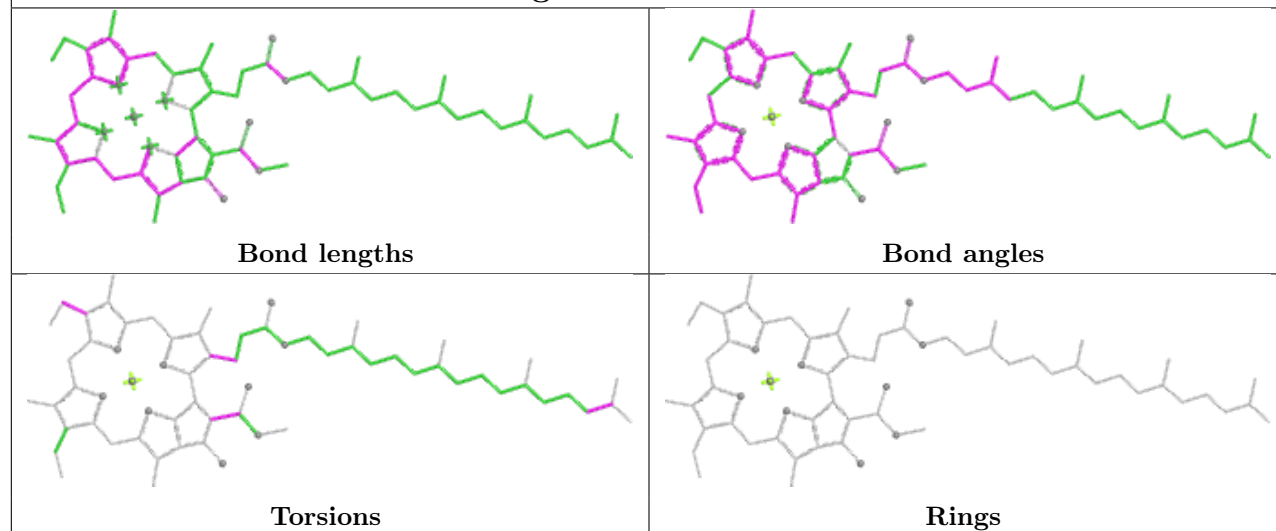


Ligand CLA d 403

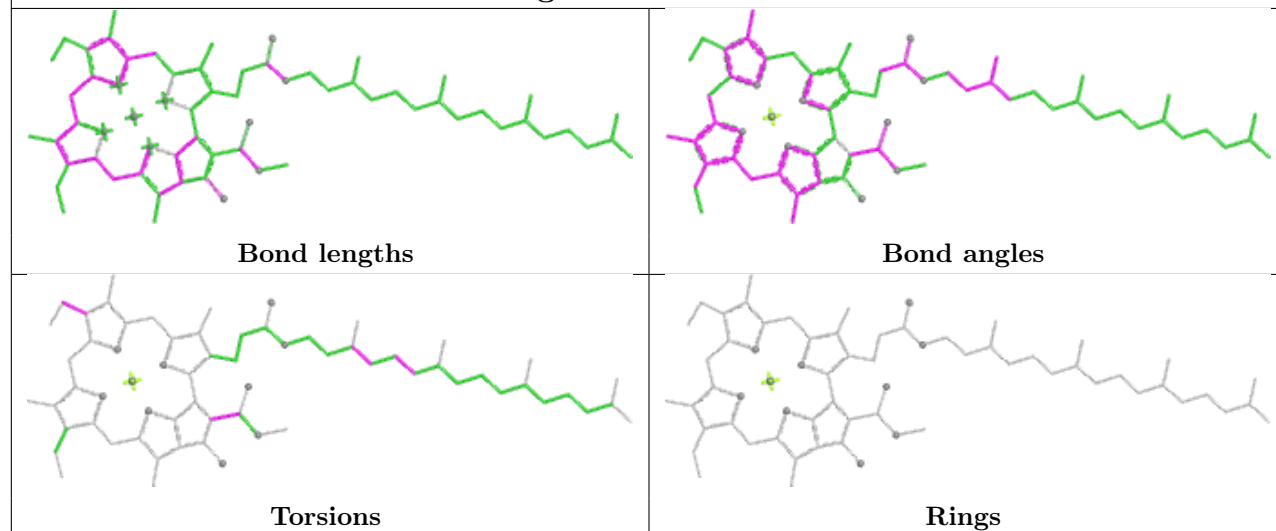




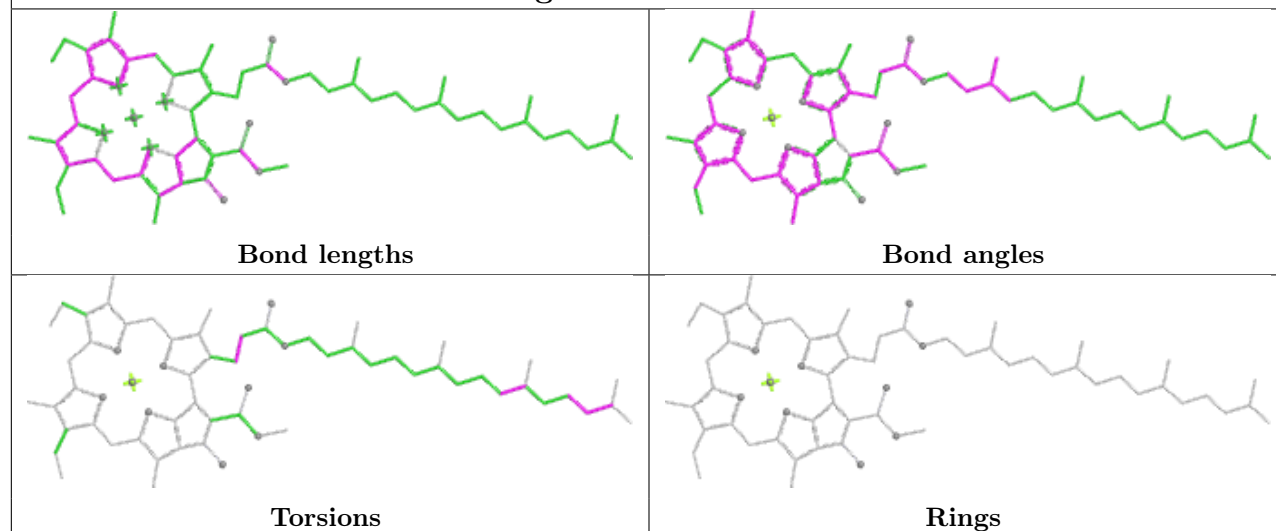
Ligand CLA B 608

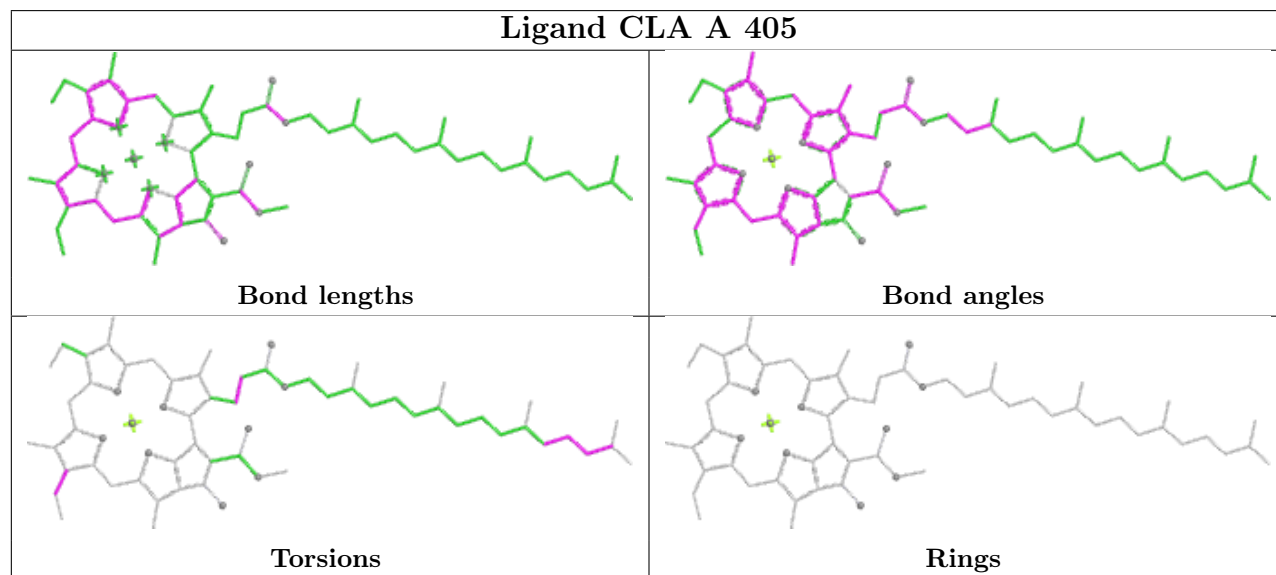
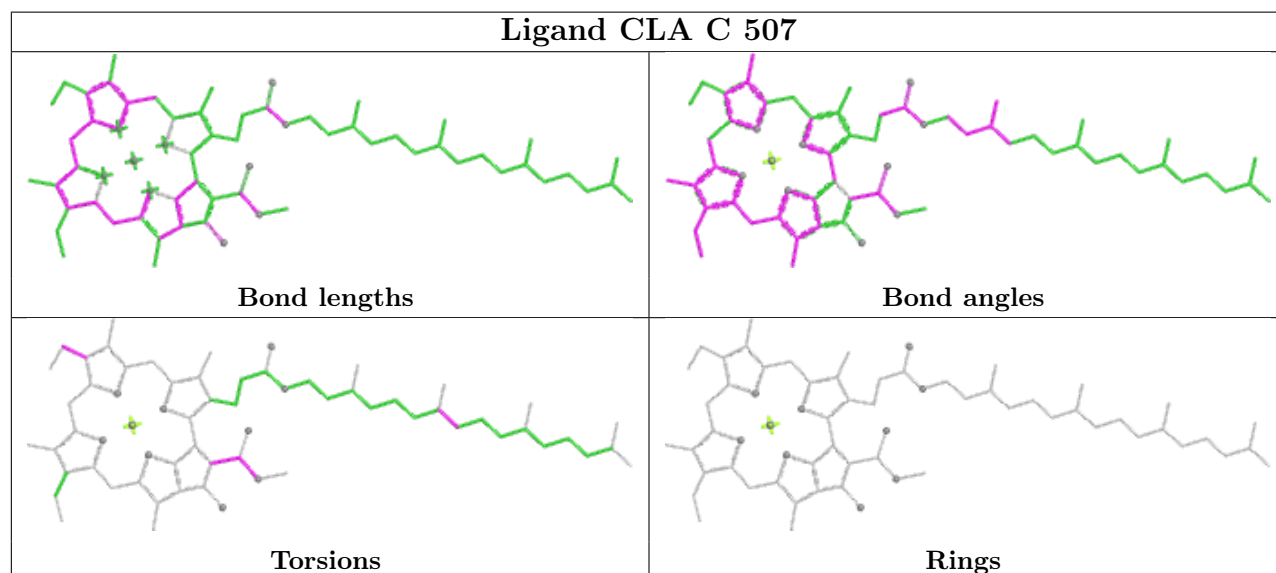
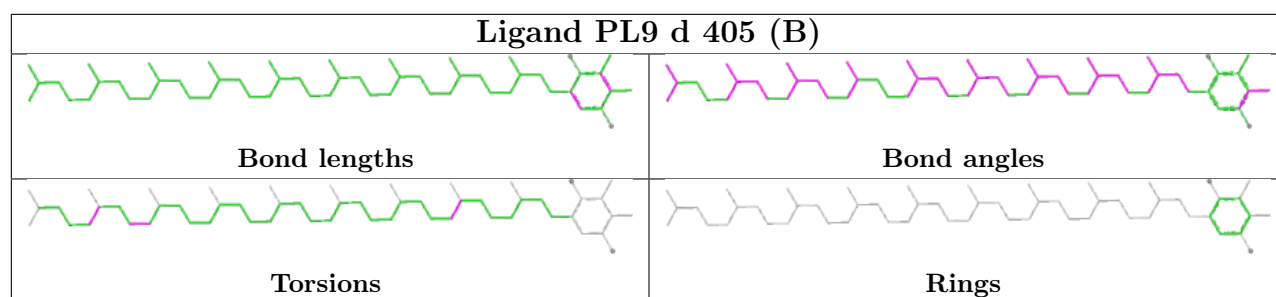


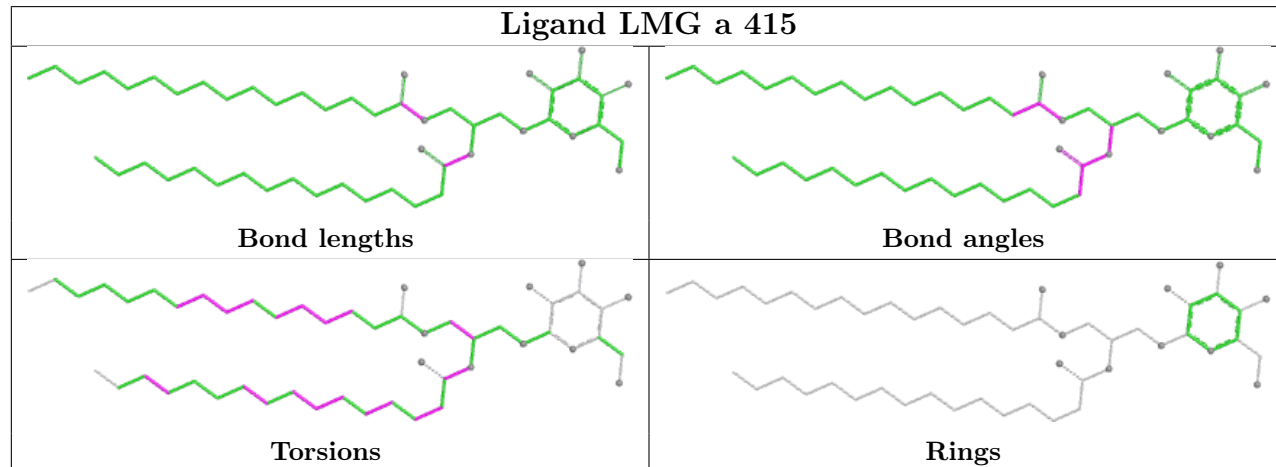
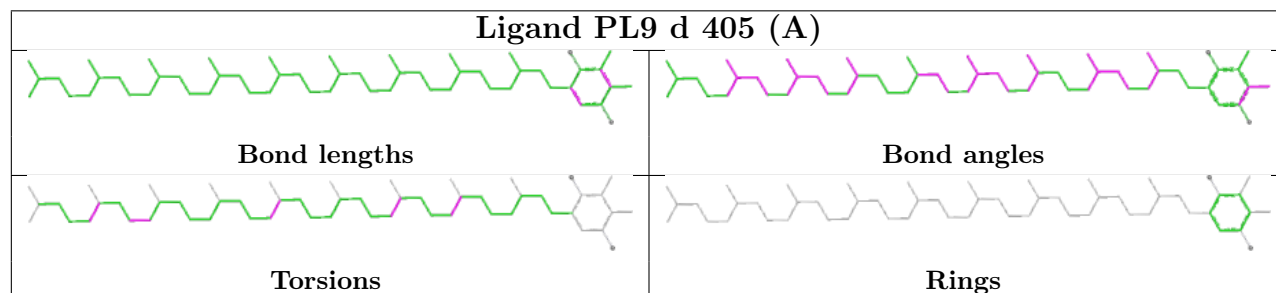
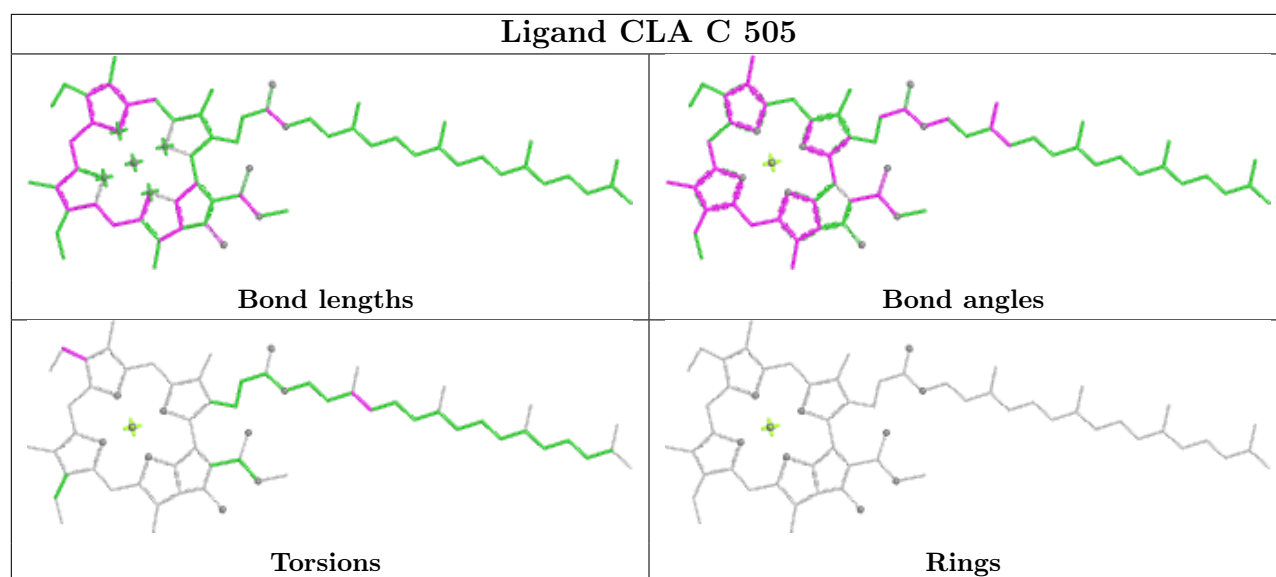
Ligand CLA c 511

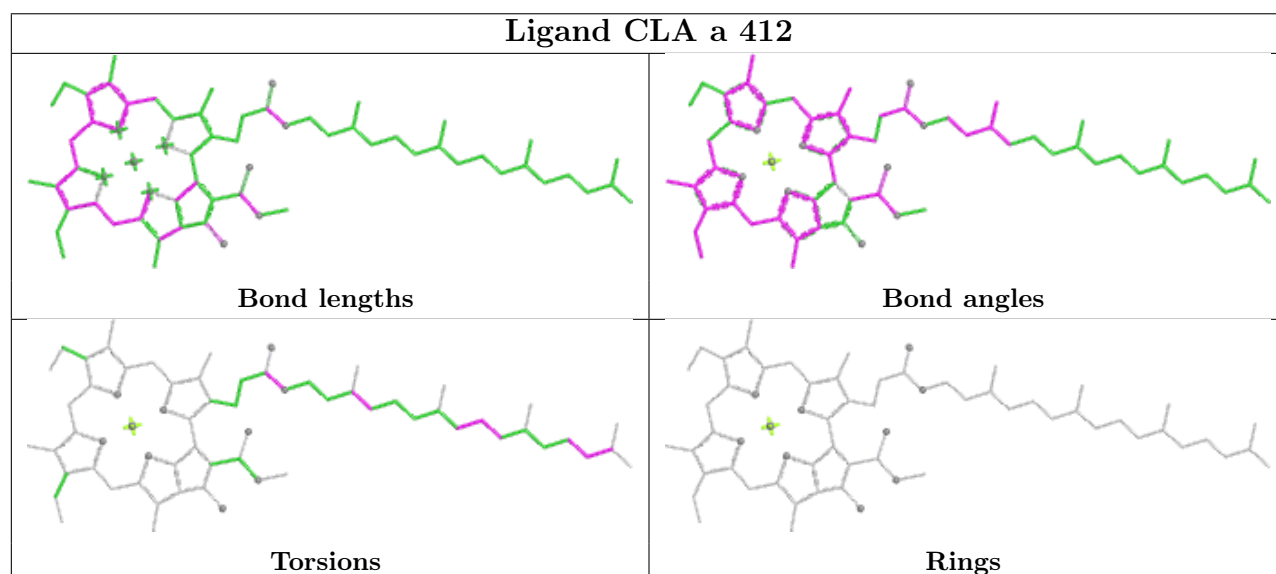
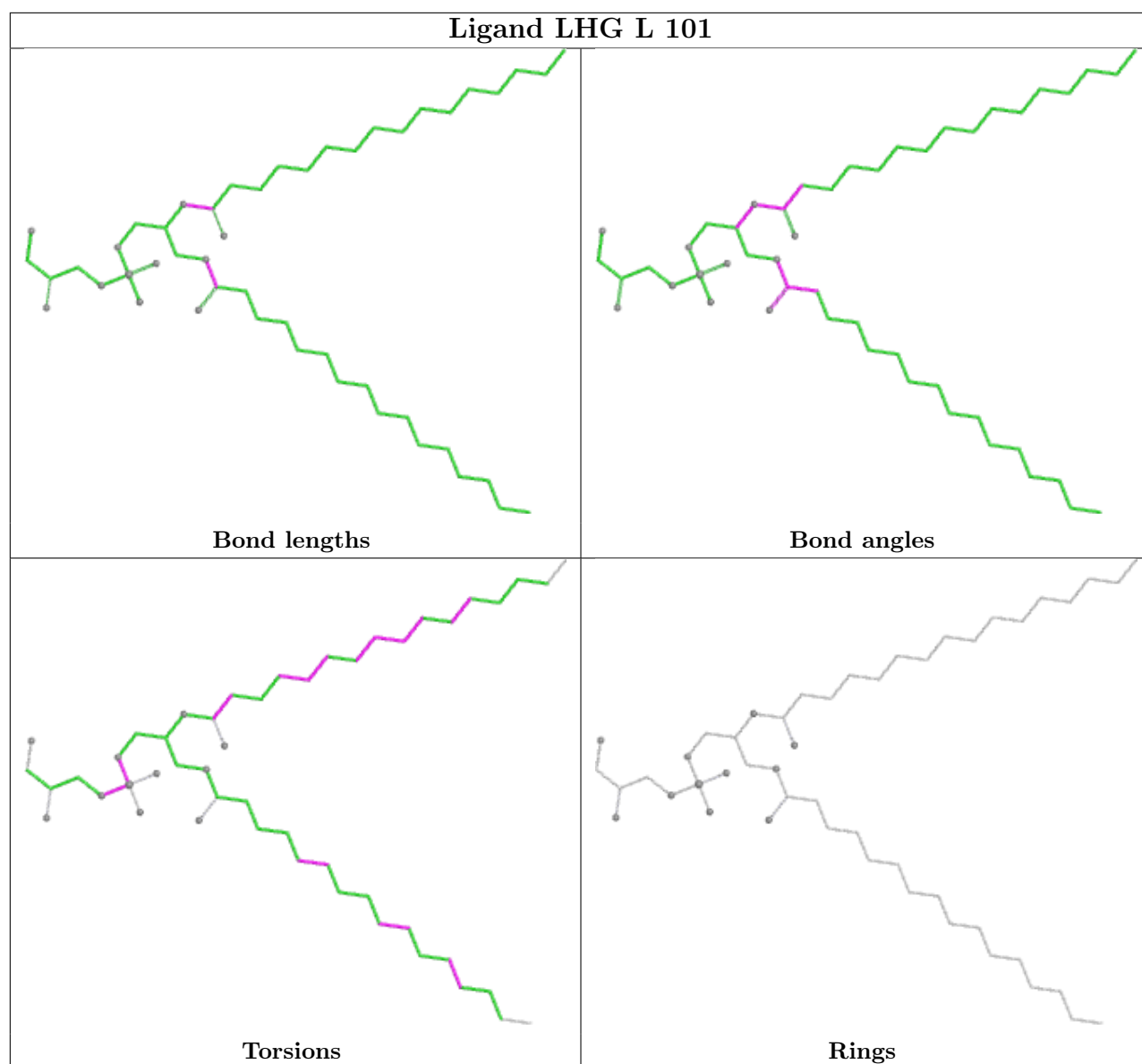


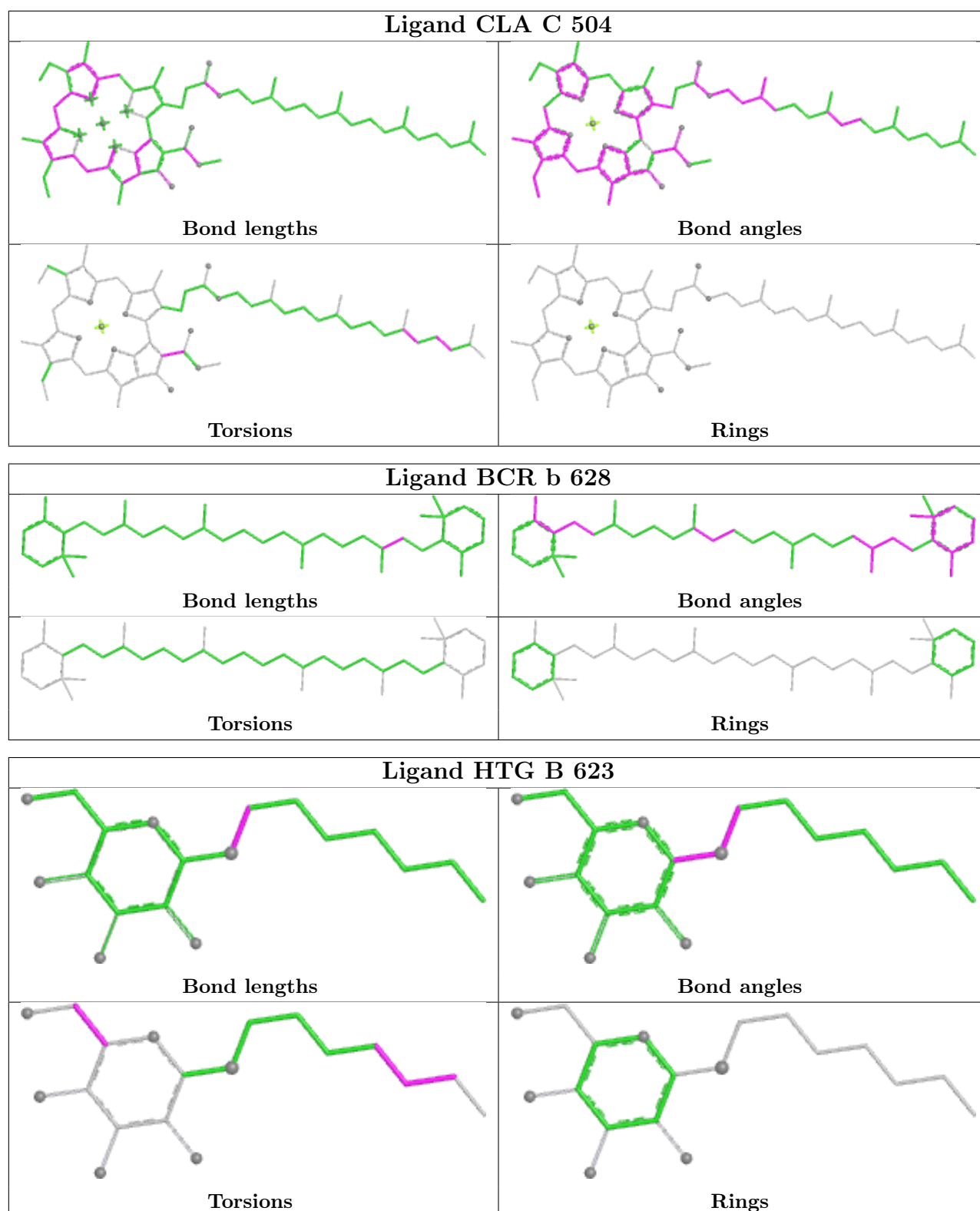
Ligand CLA b 620

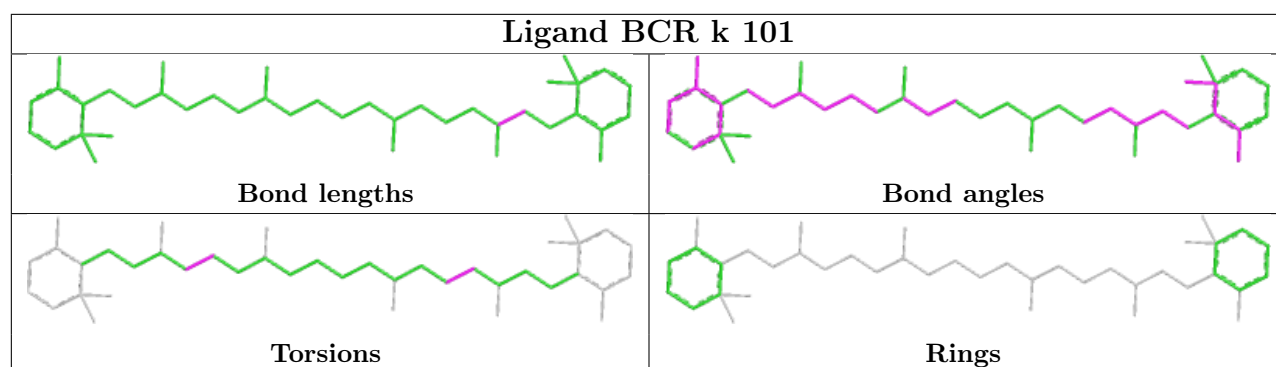
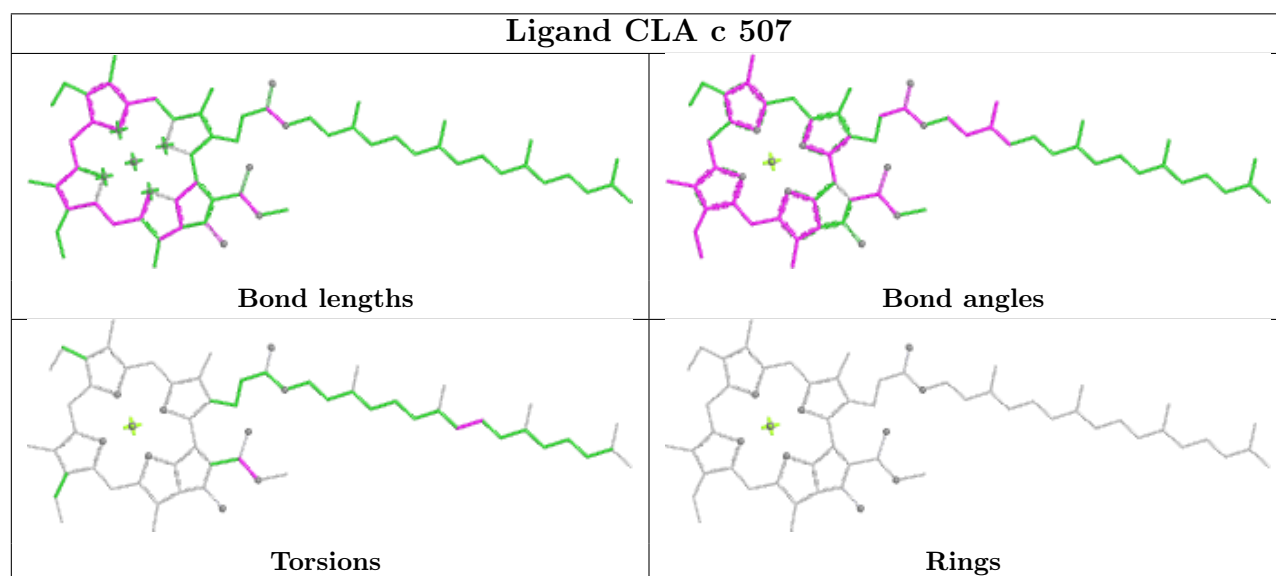
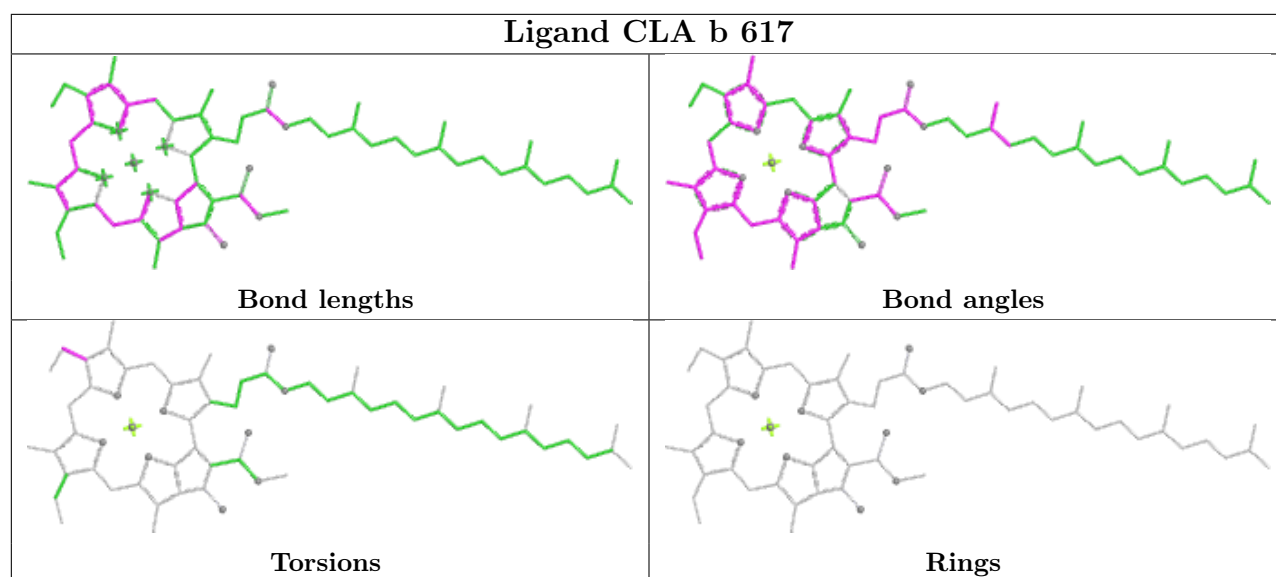




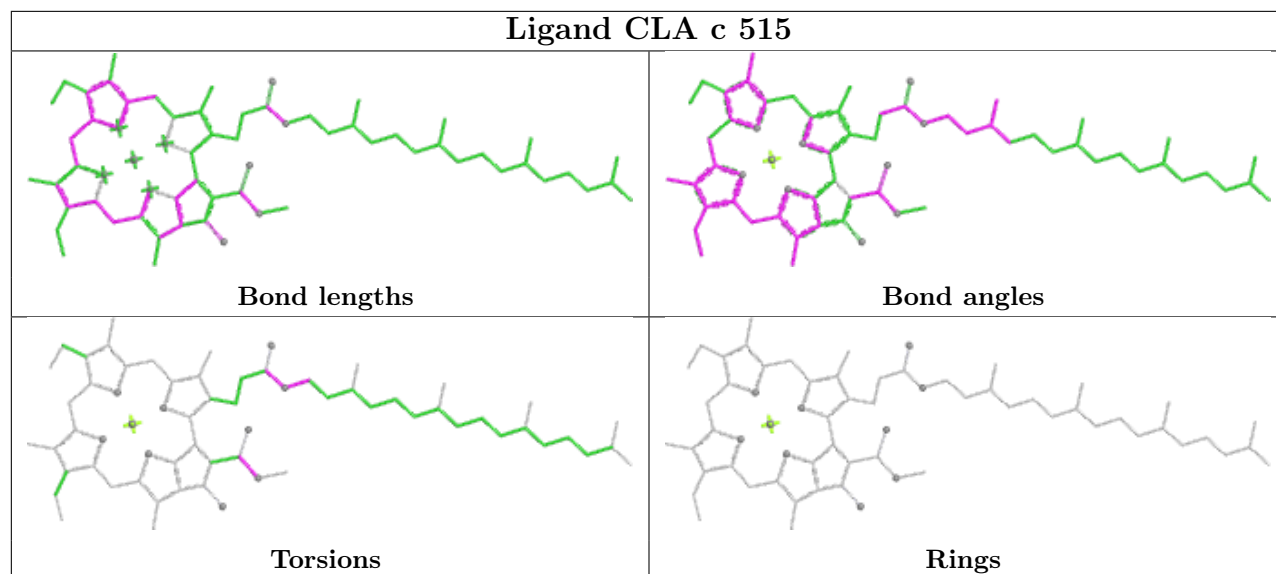




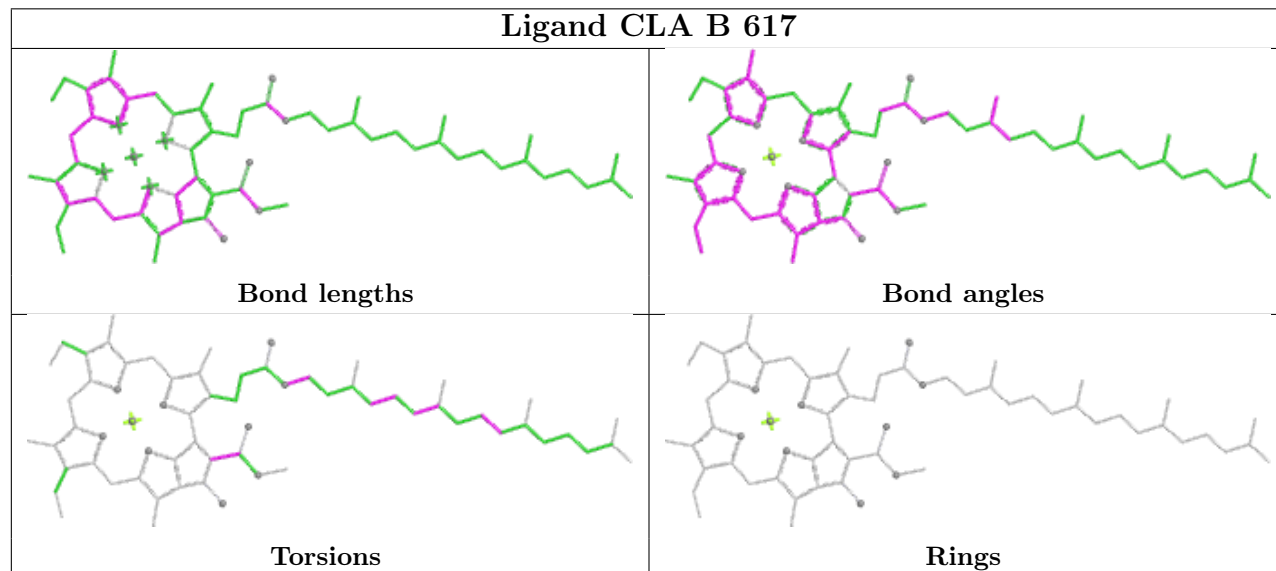


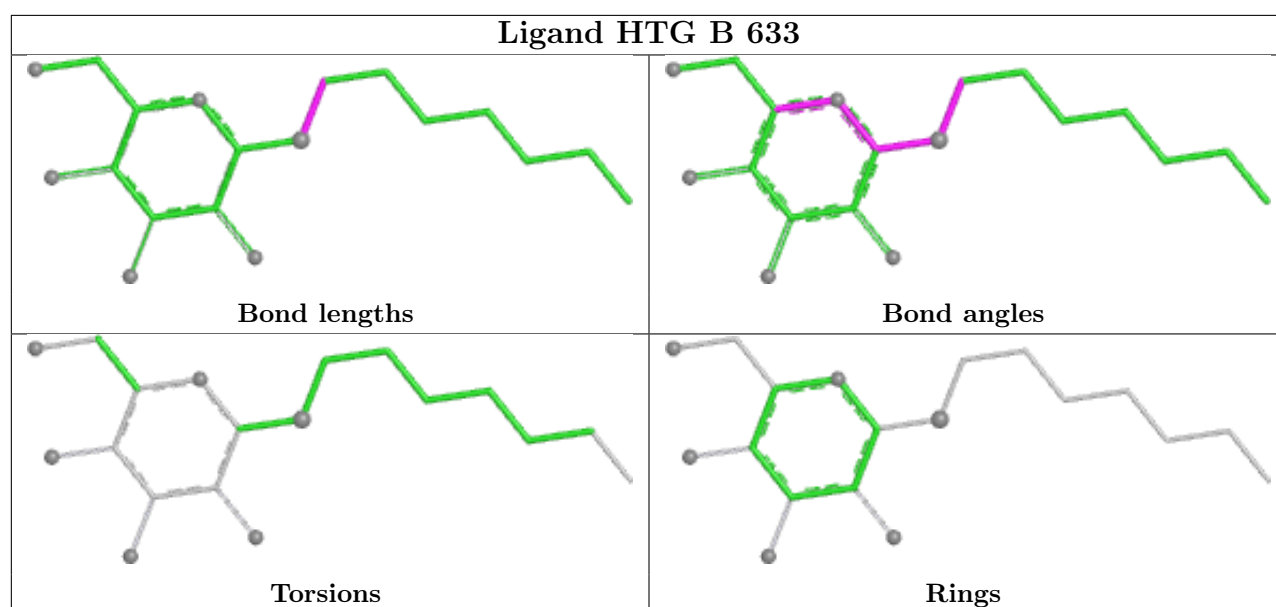
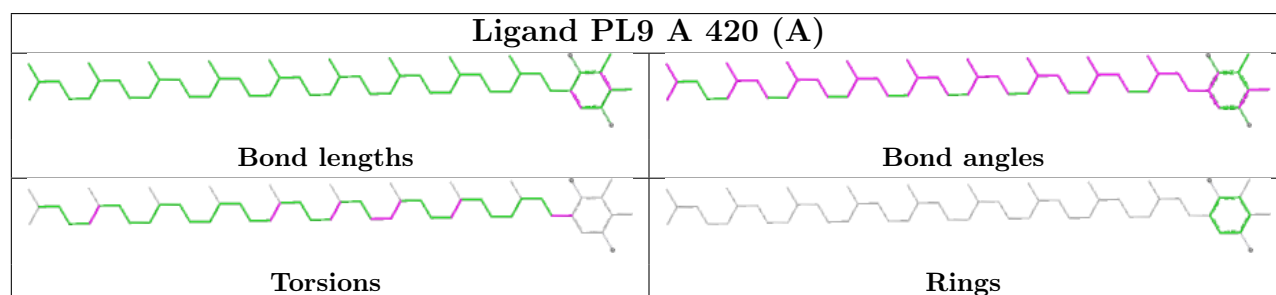
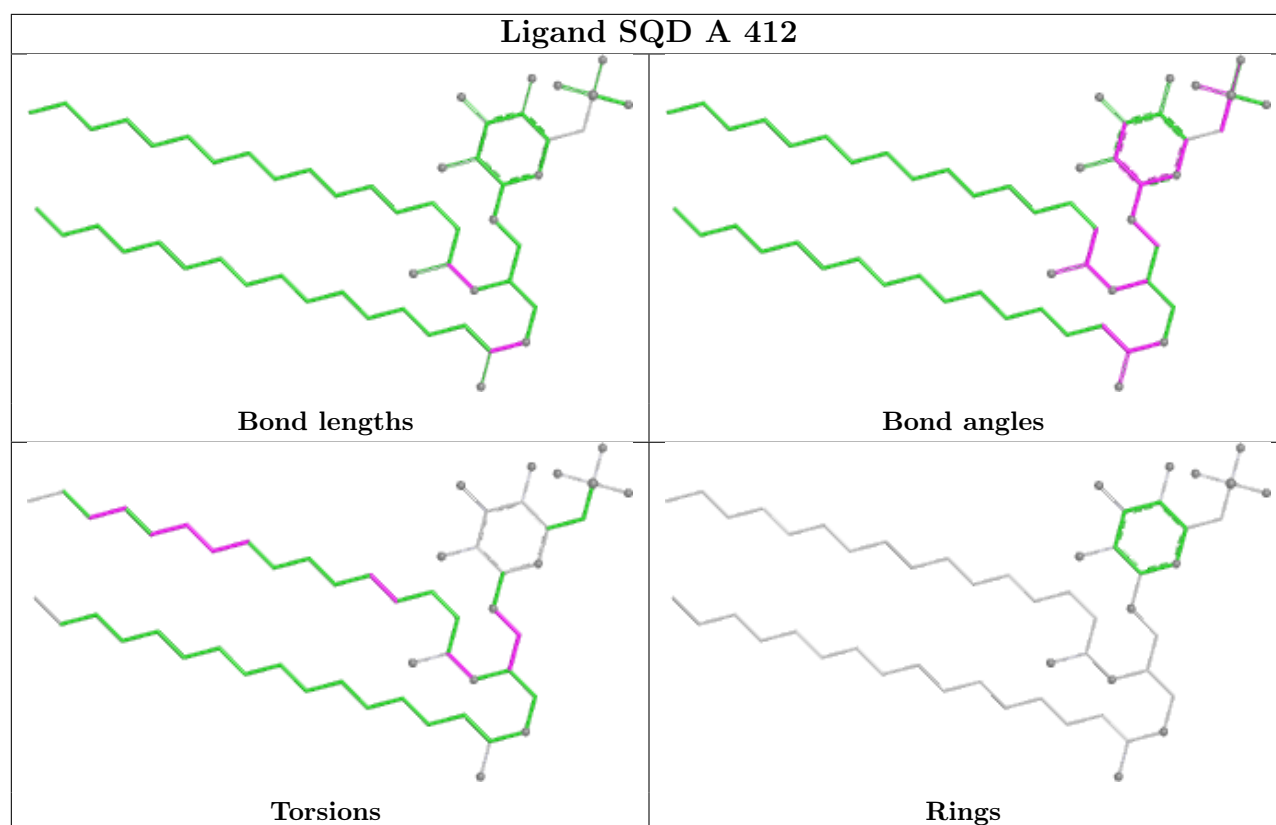


Ligand CLA c 515

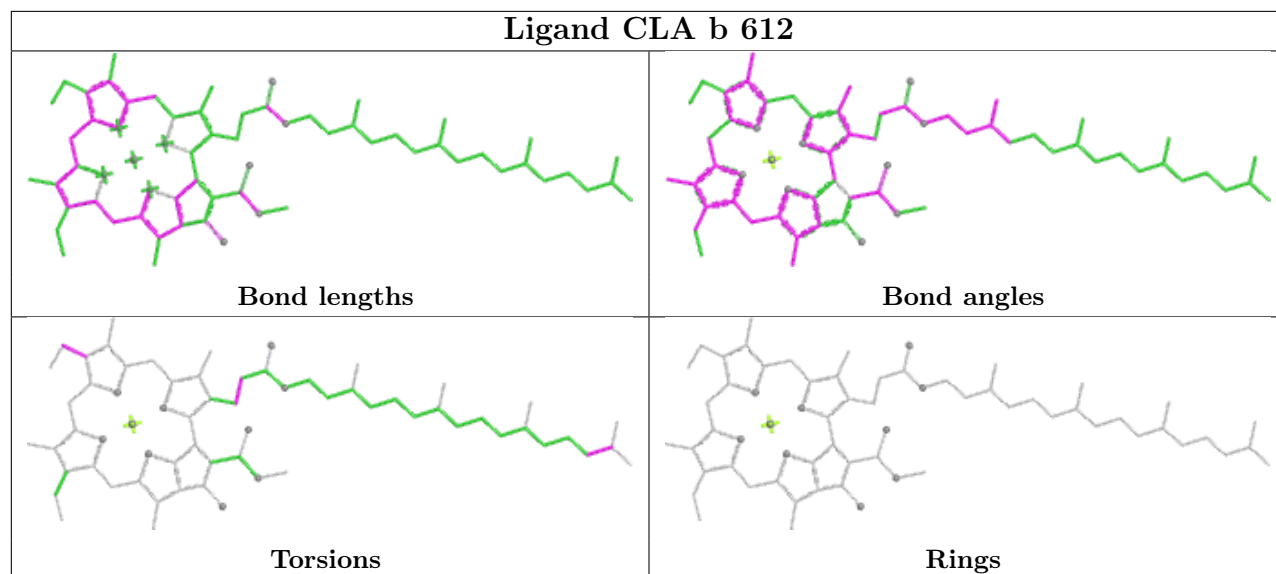


Ligand CLA B 617

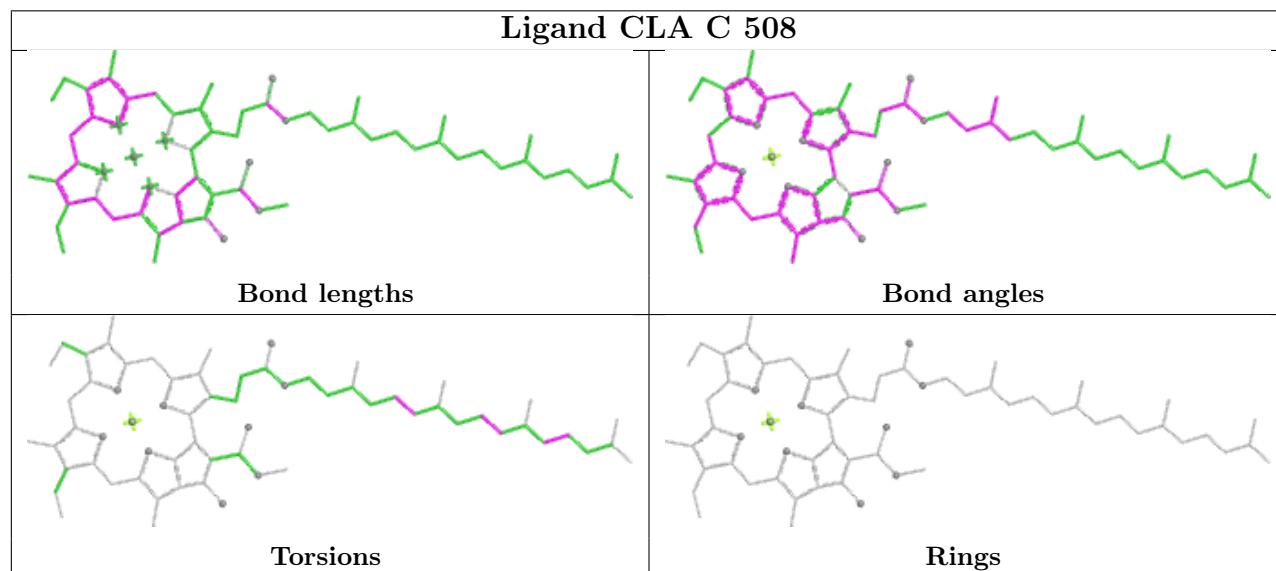




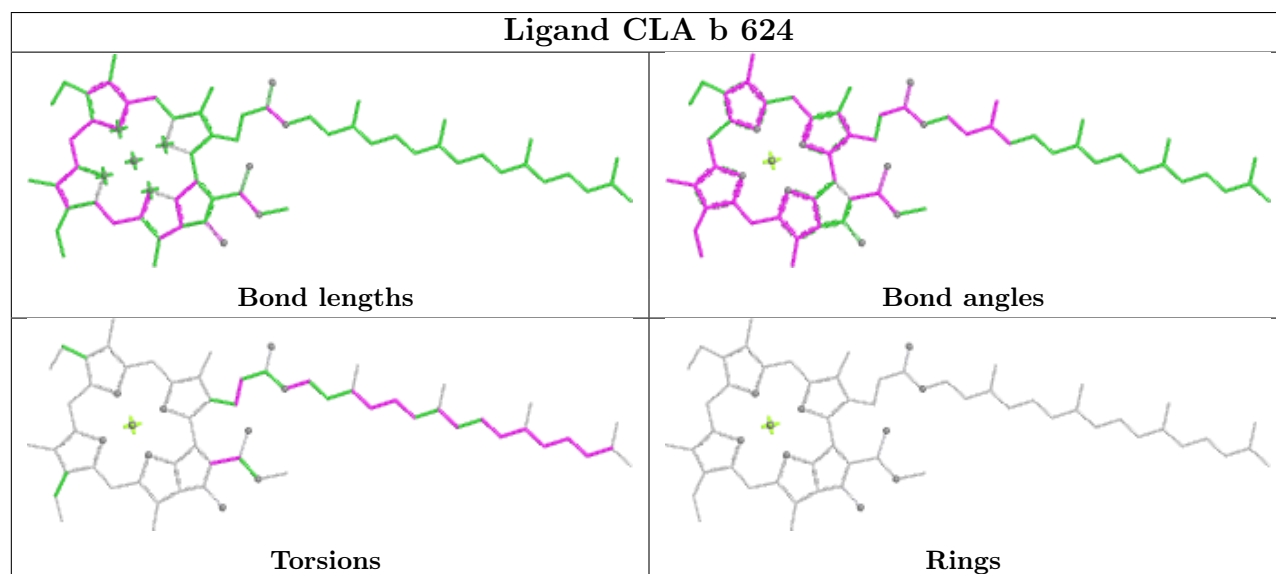
Ligand CLA b 612

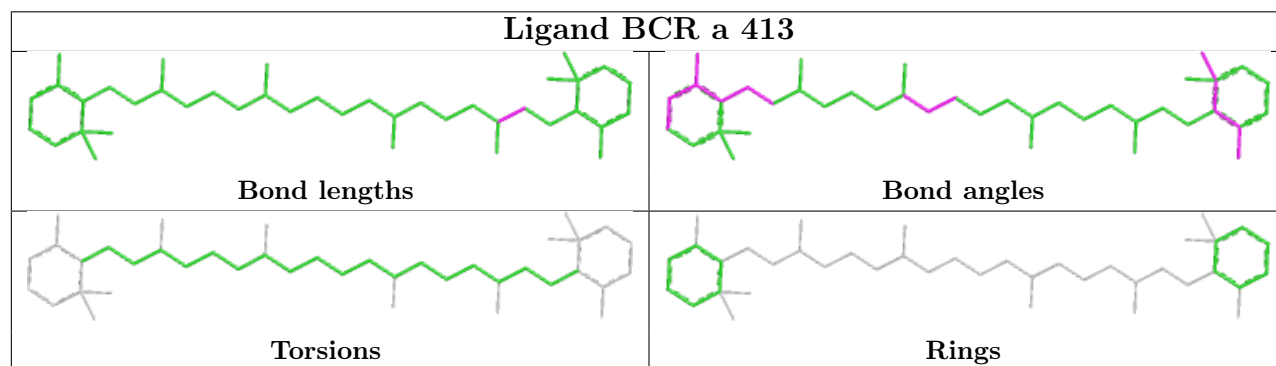
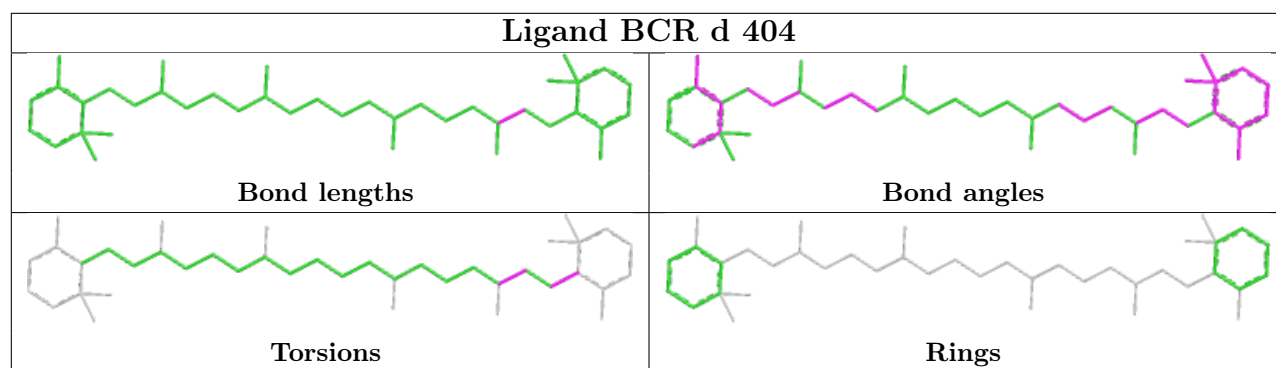
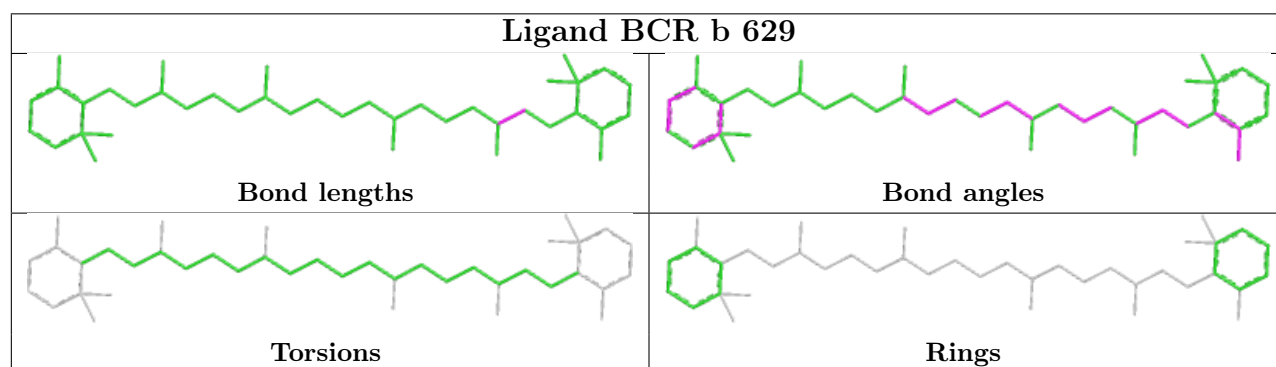
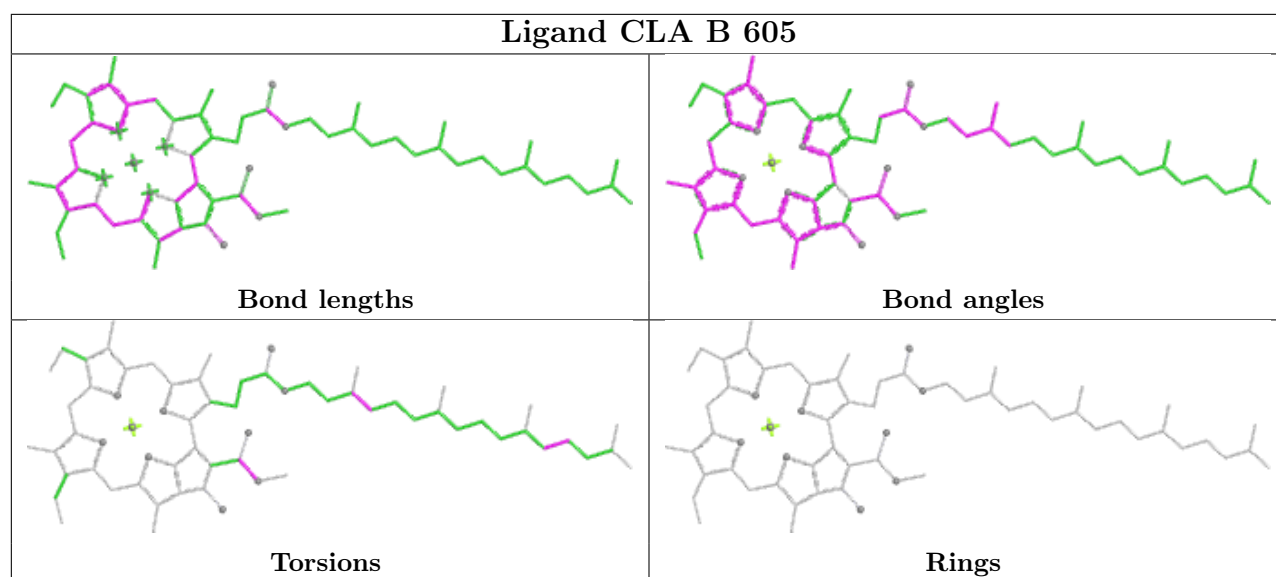


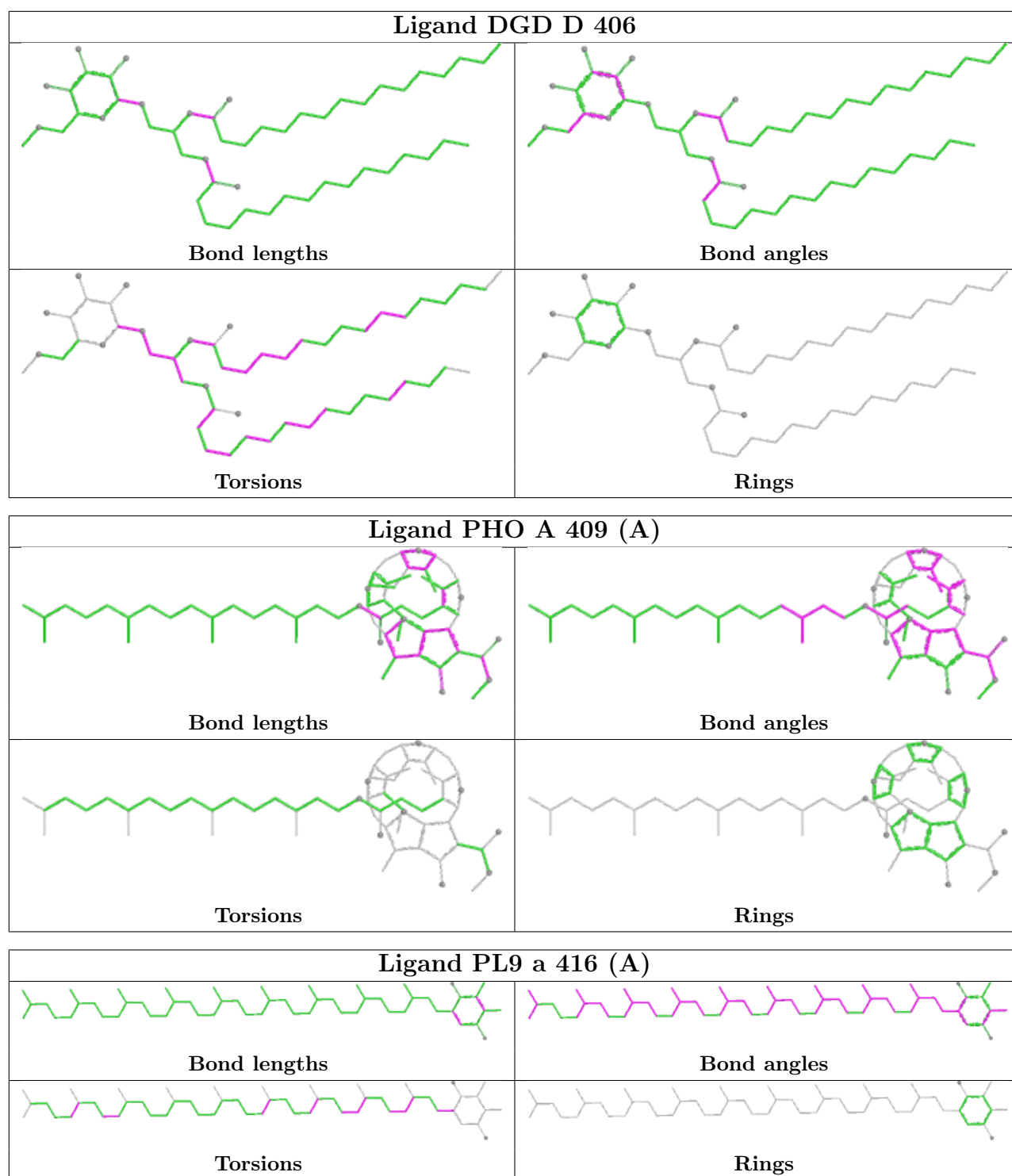
Ligand CLA C 508

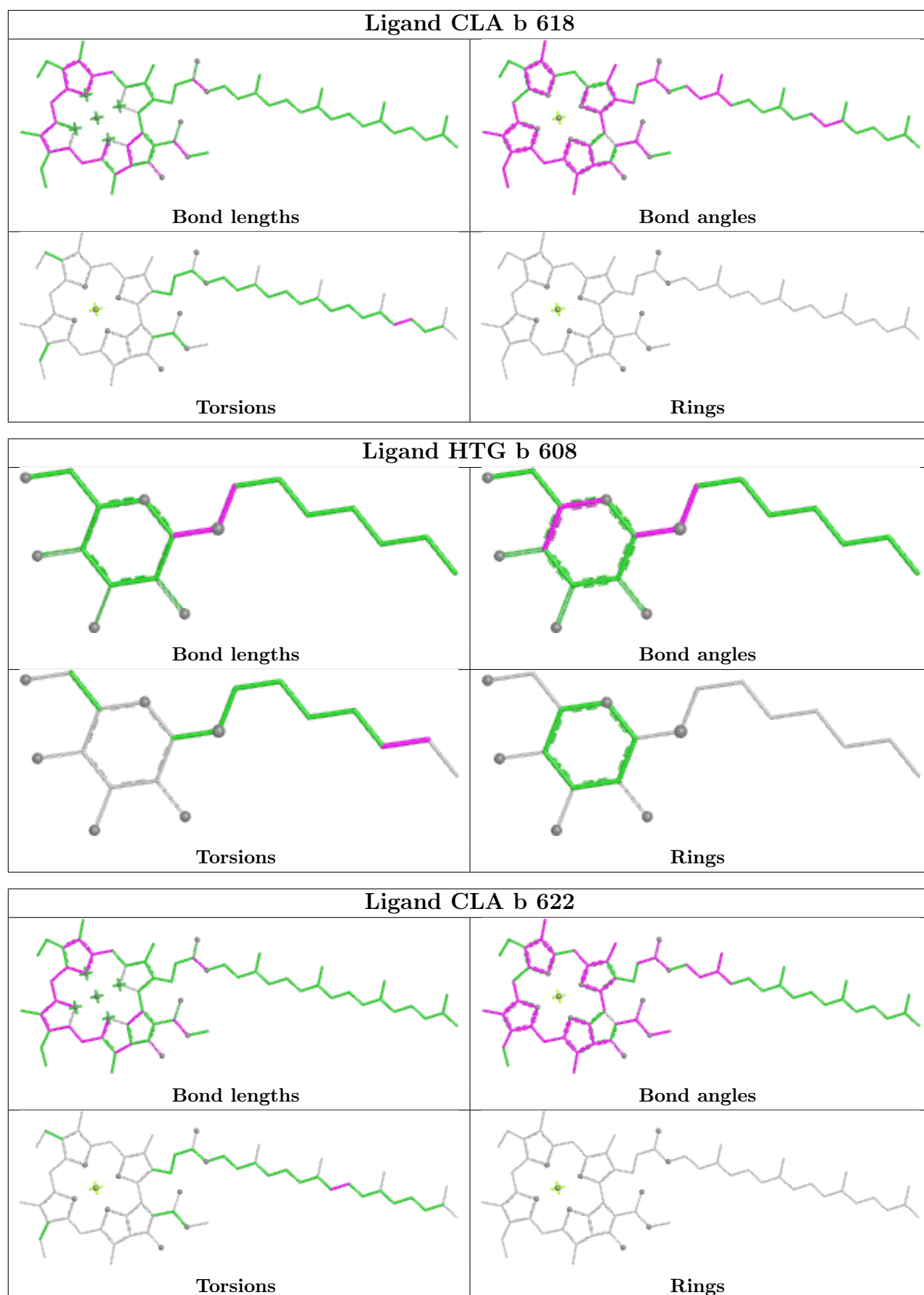


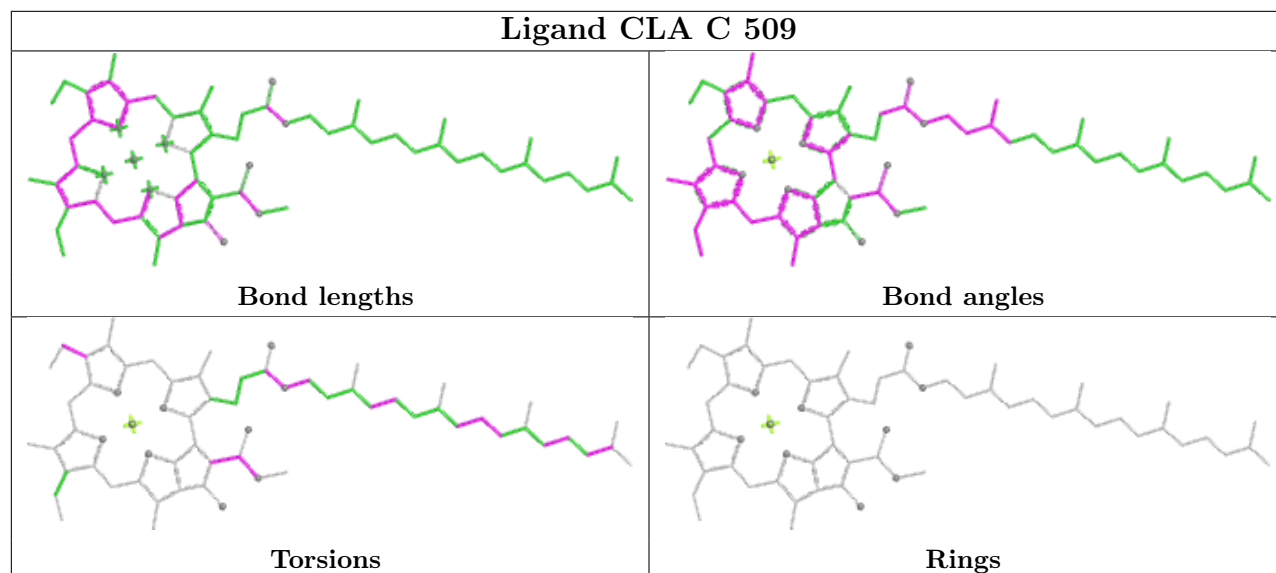
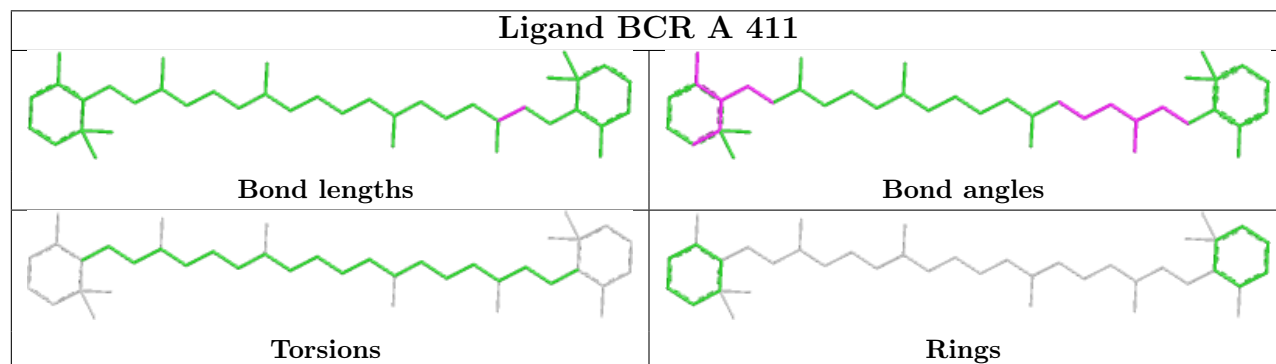
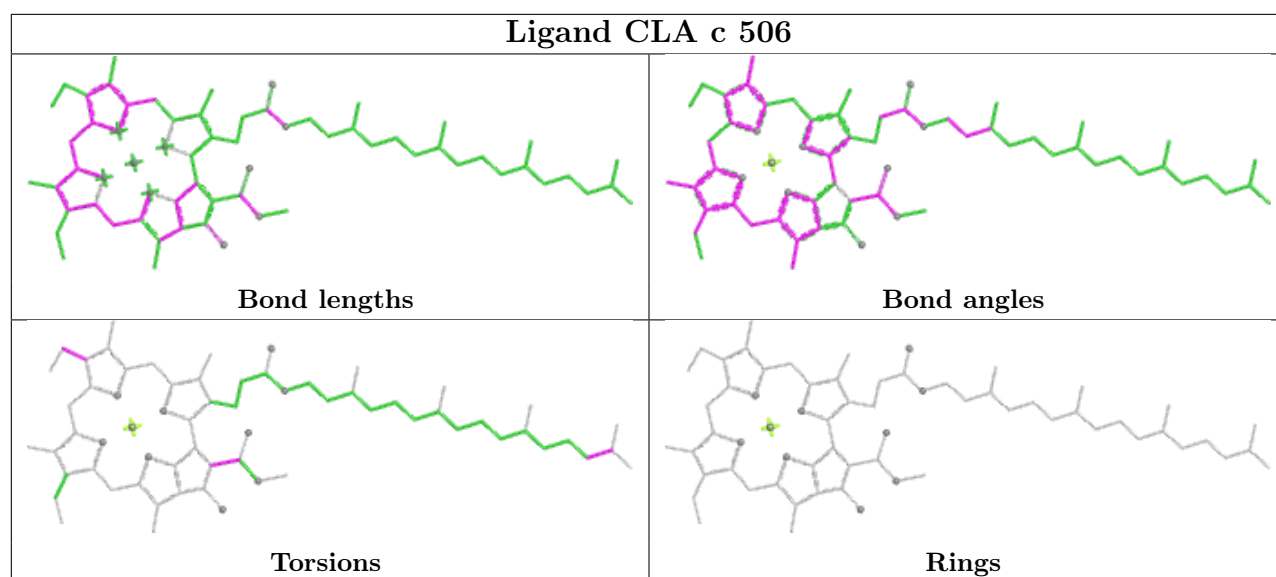
Ligand CLA b 624

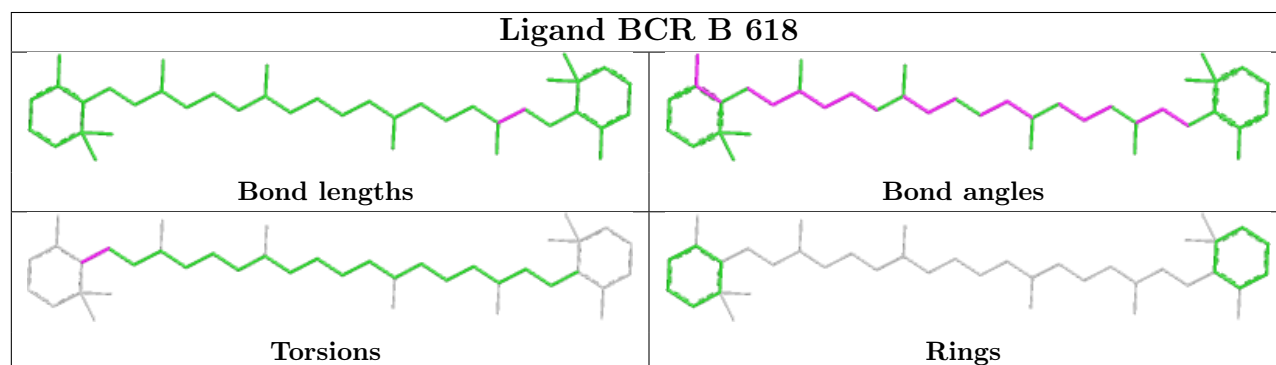
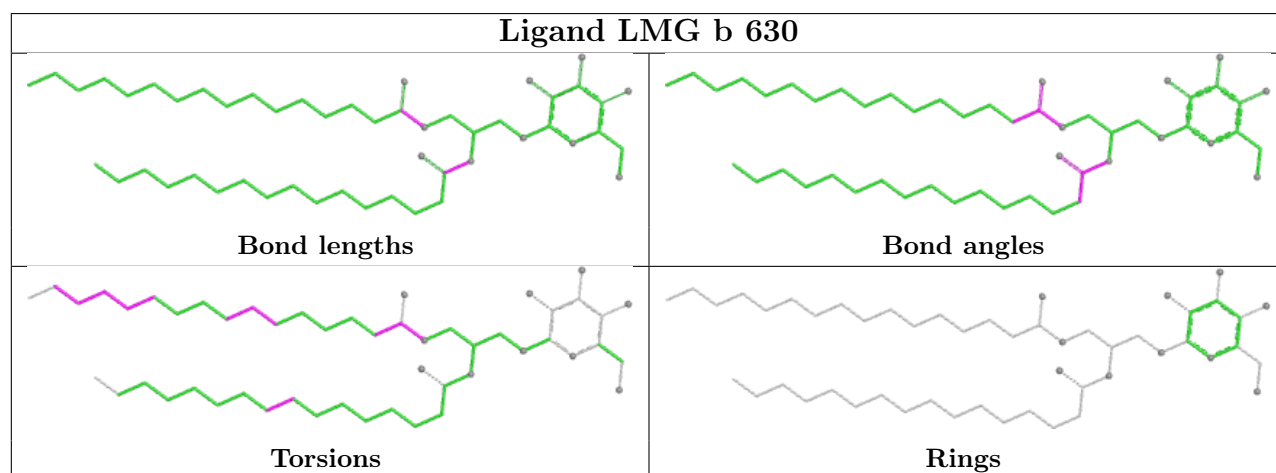
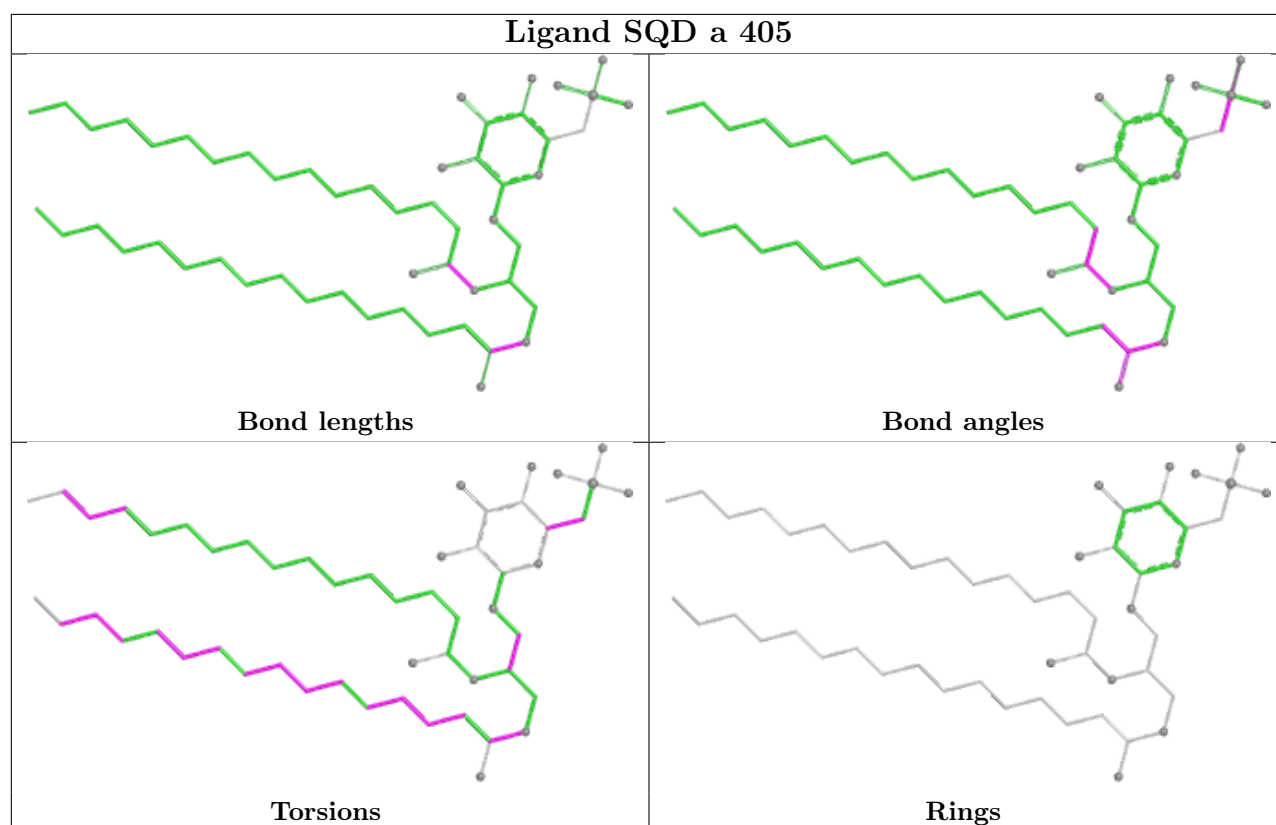




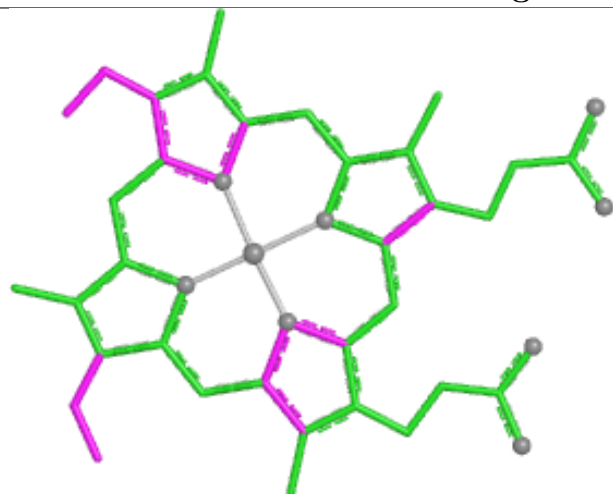




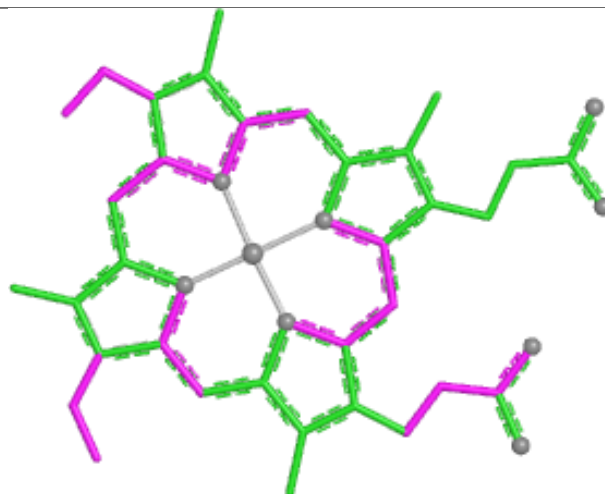




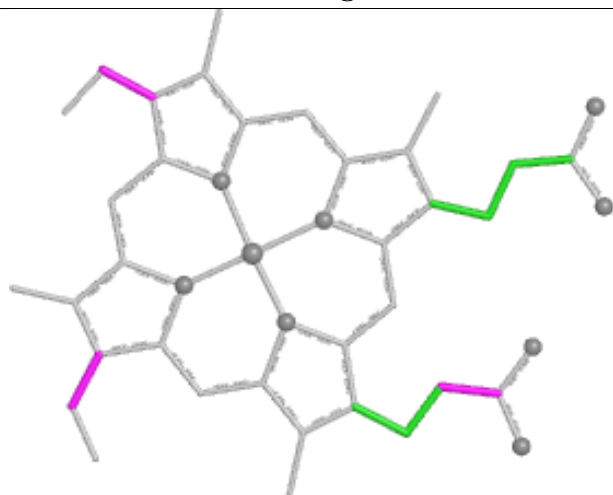
Ligand HEC V 206



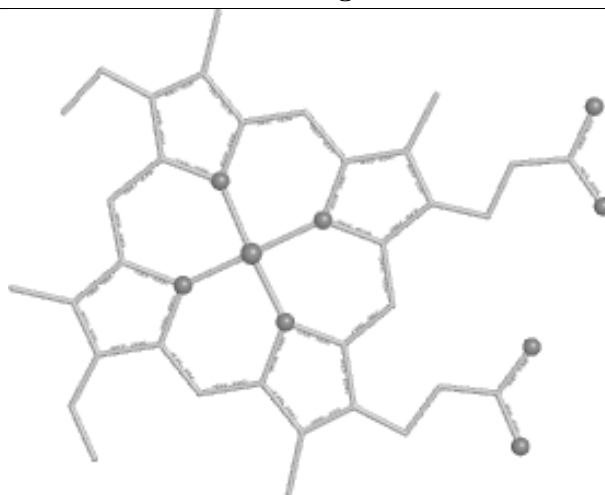
Bond lengths



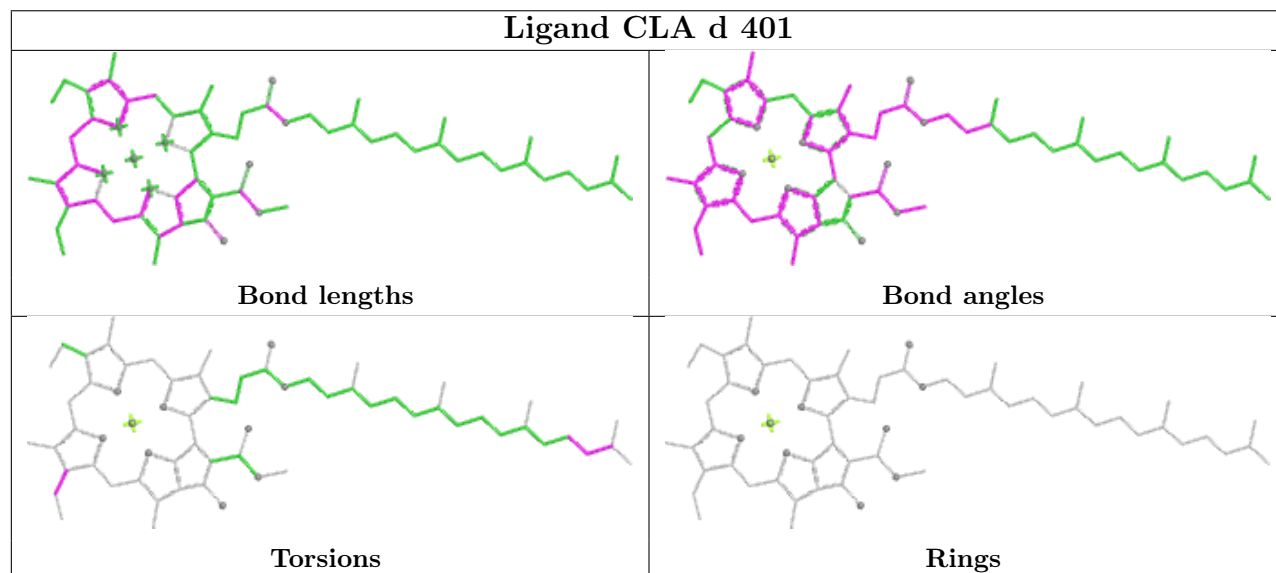
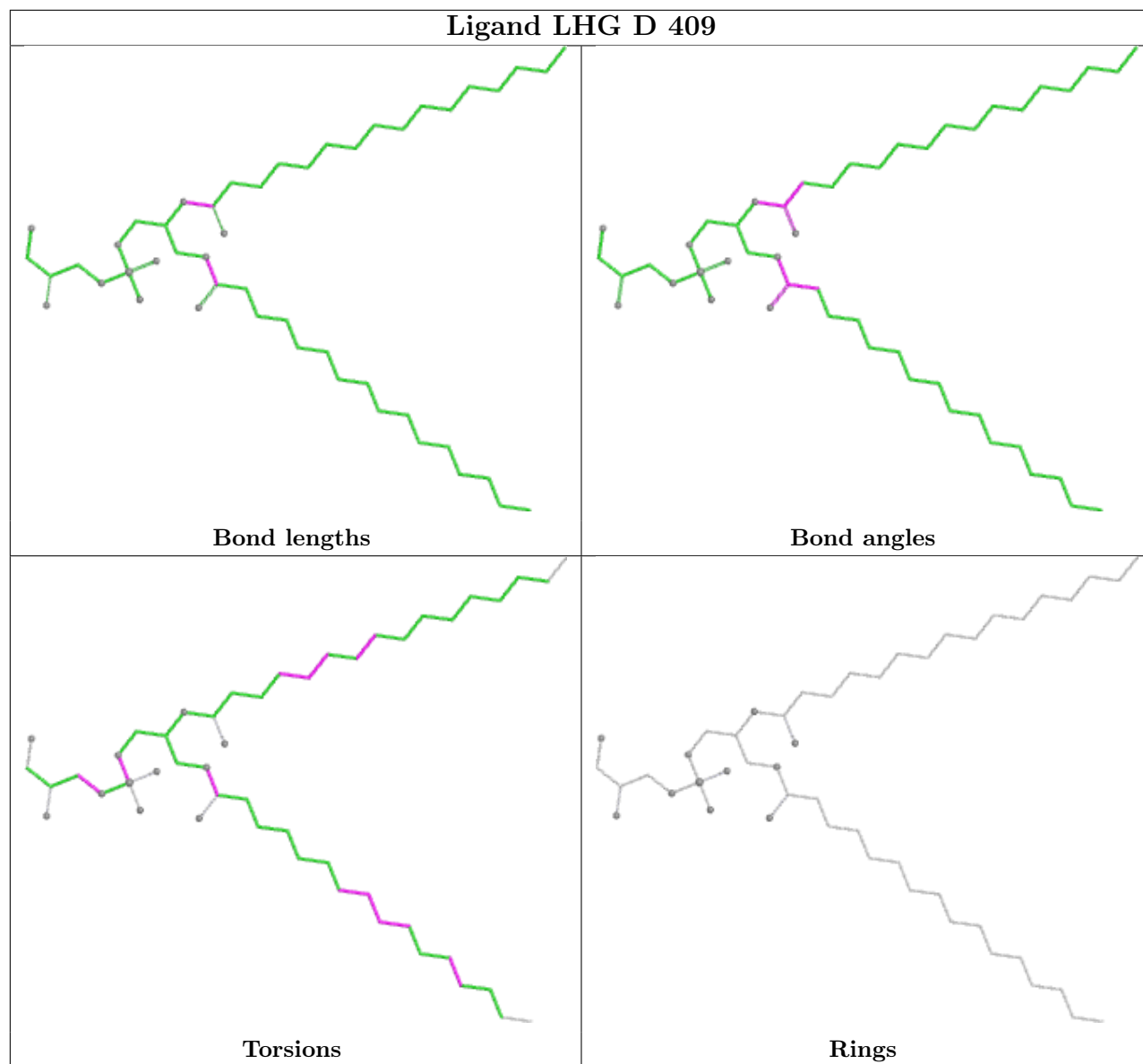
Bond angles

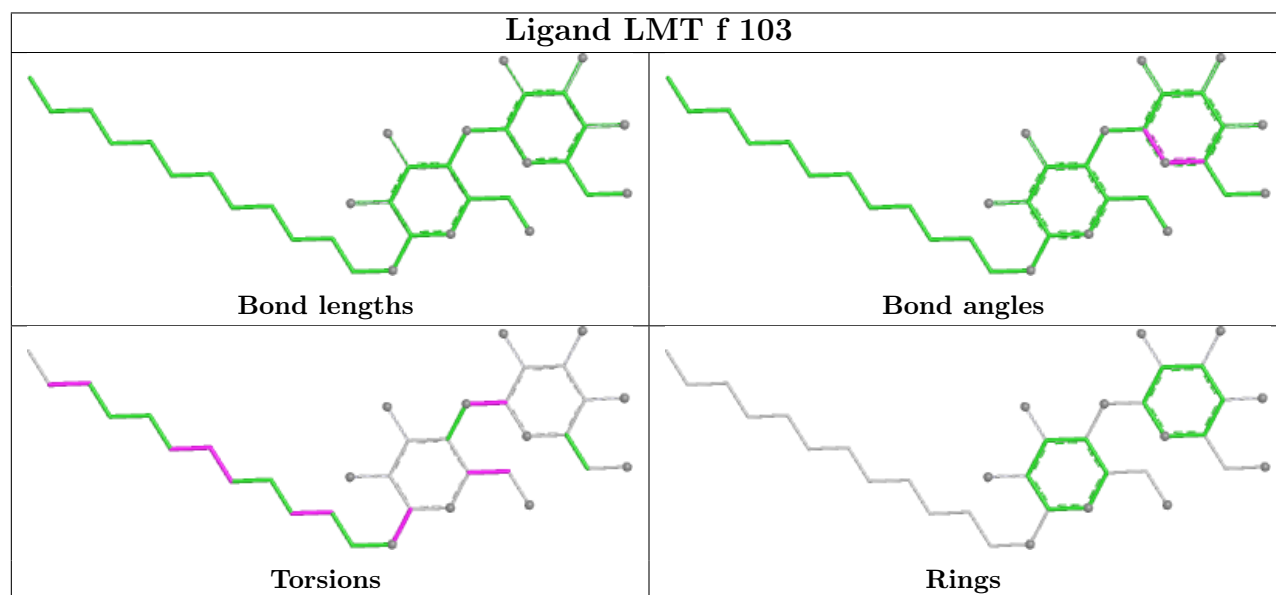
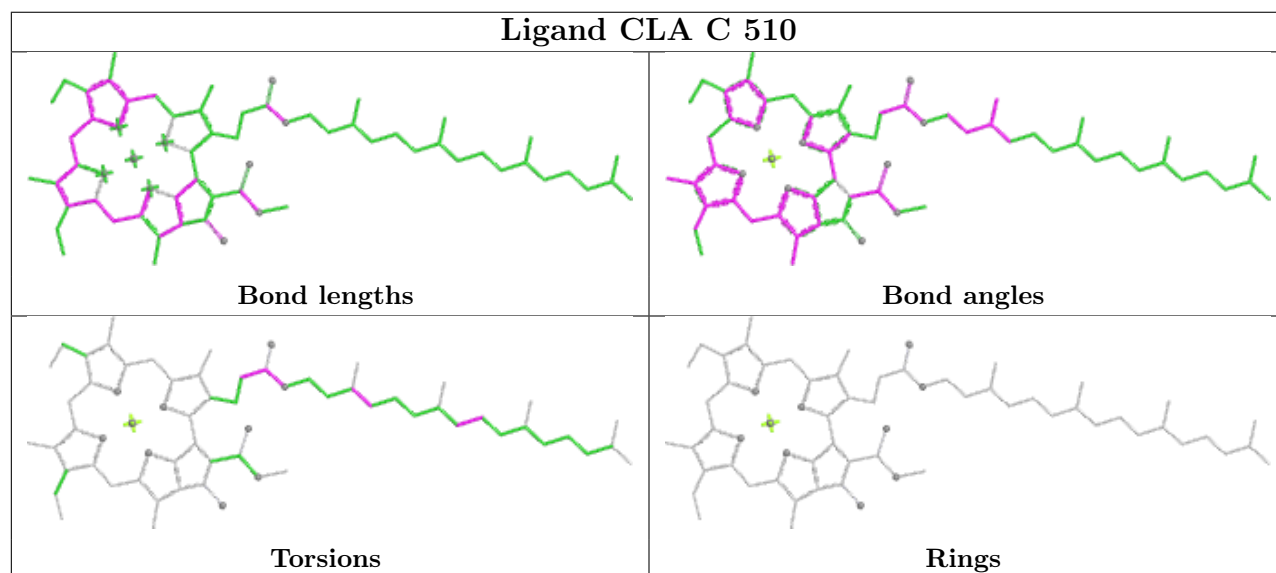
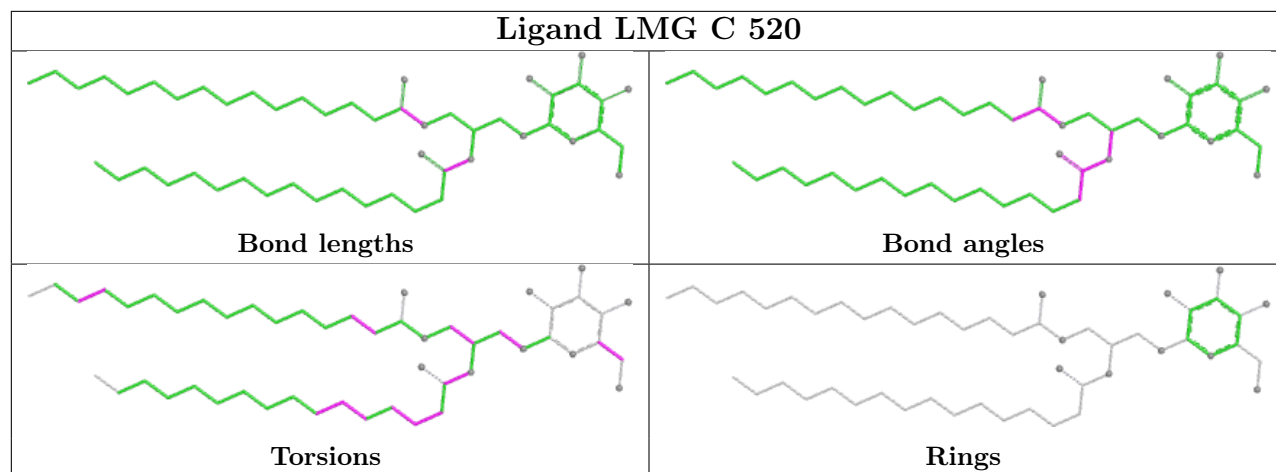


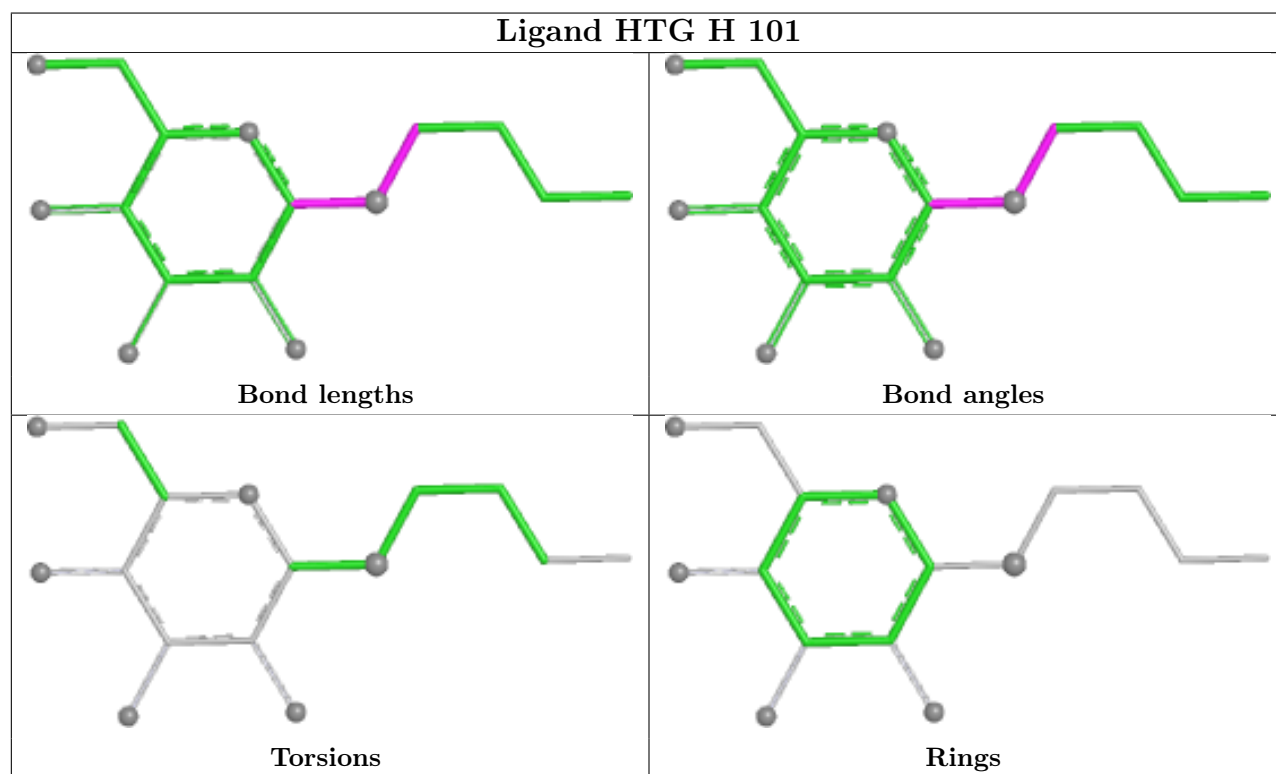
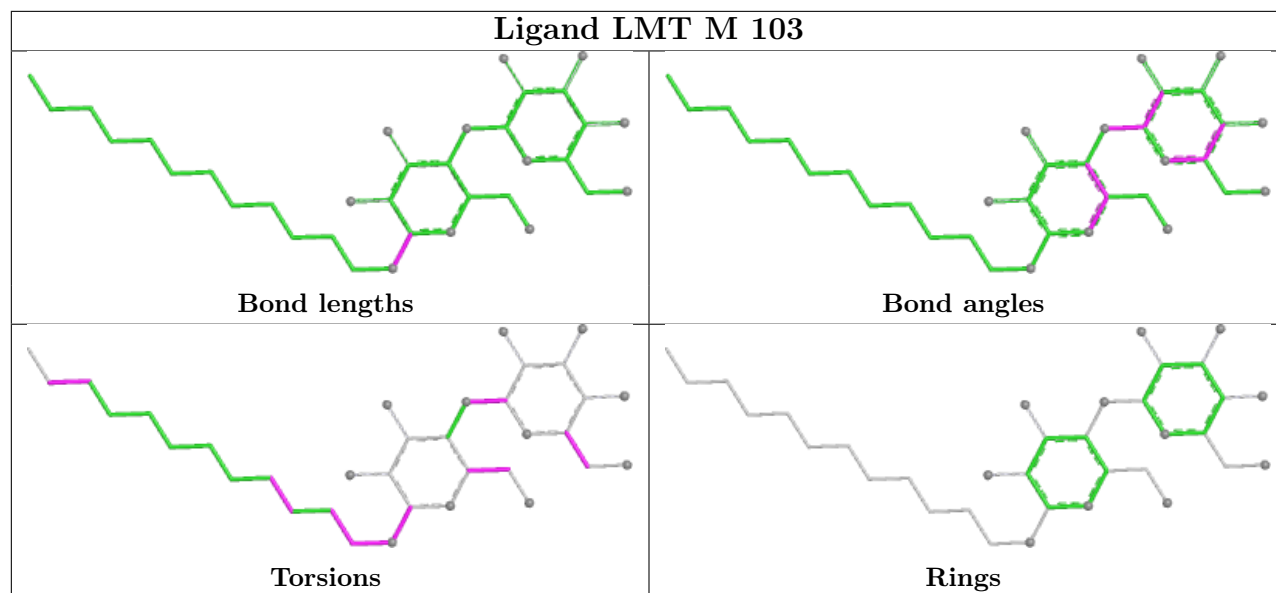
Torsions



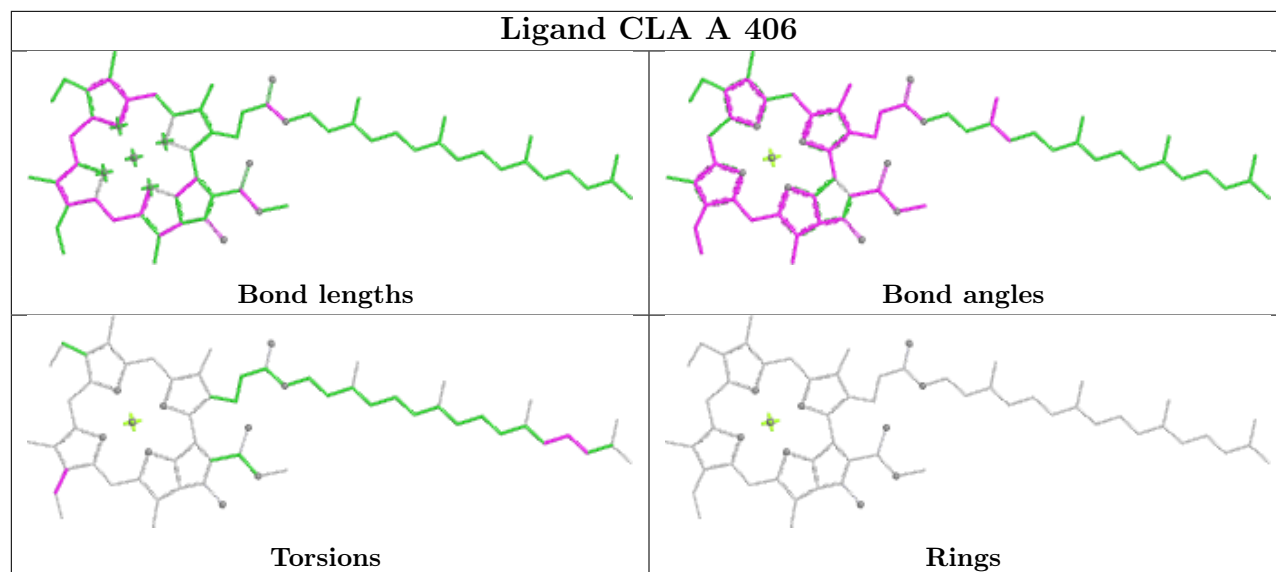
Rings



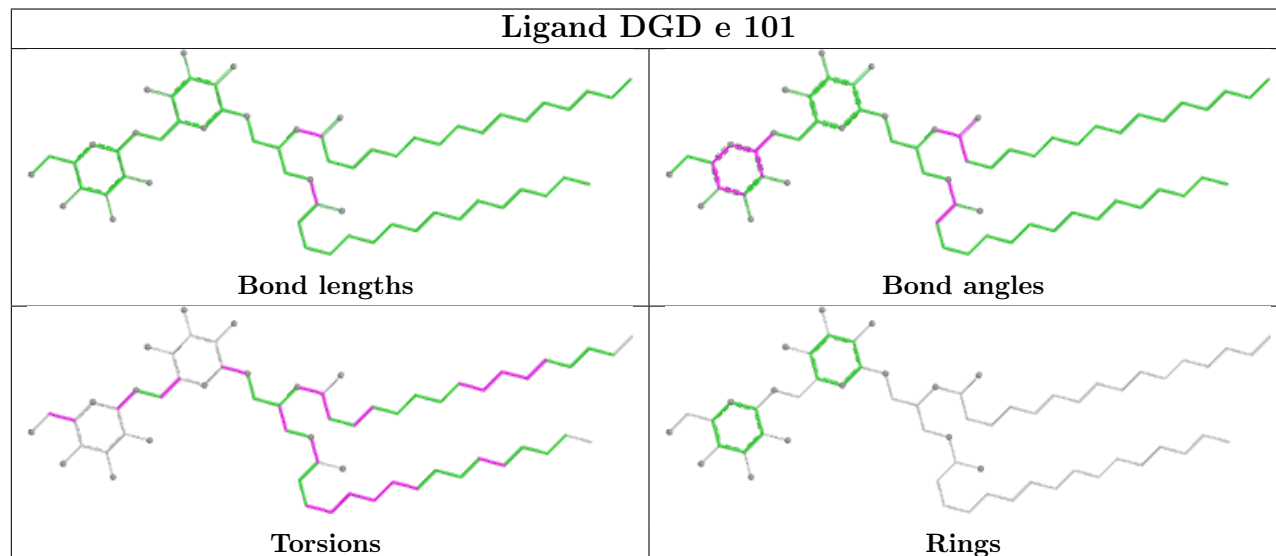




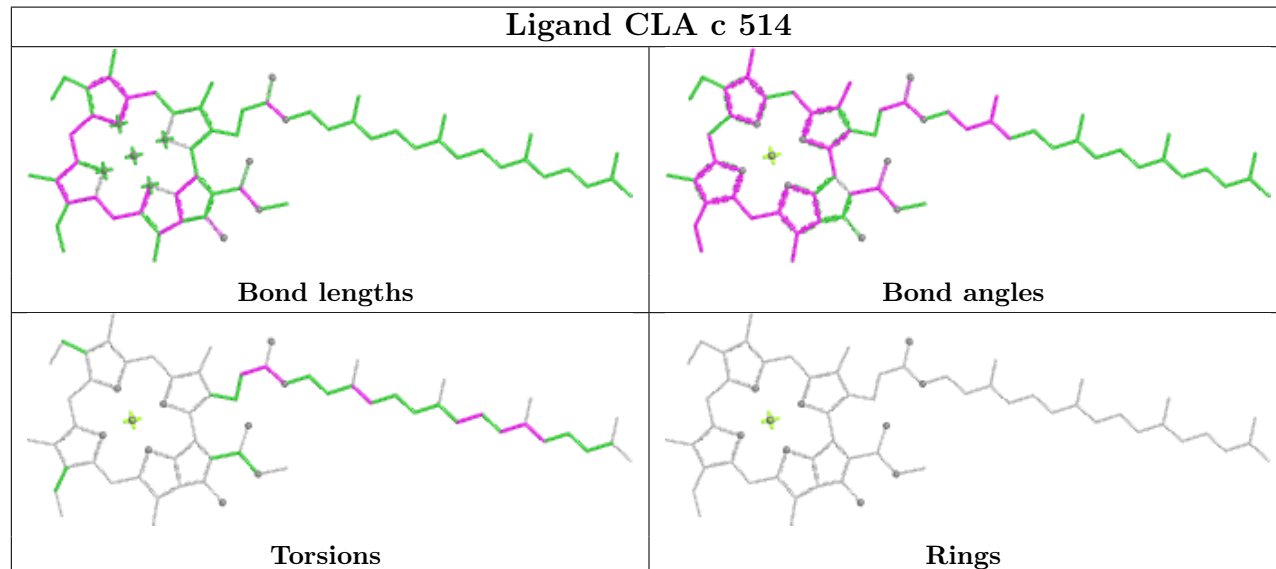
Ligand CLA A 406

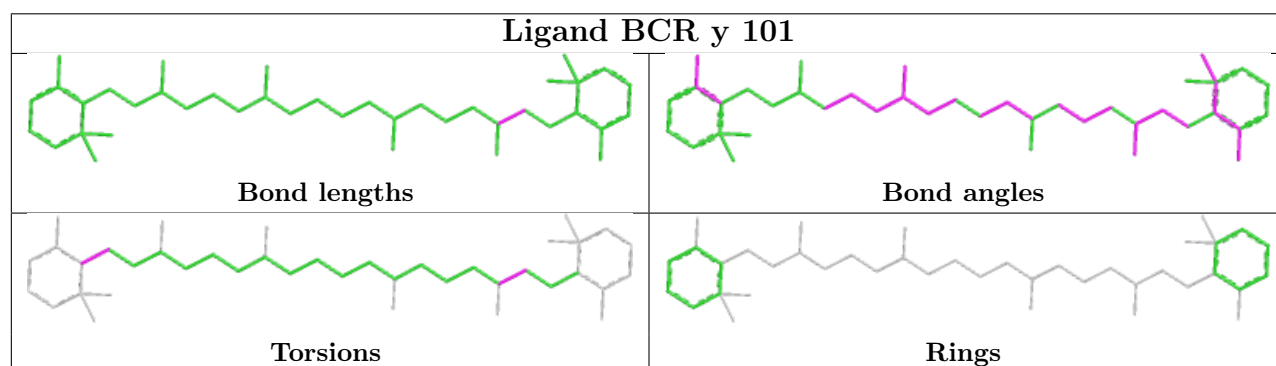
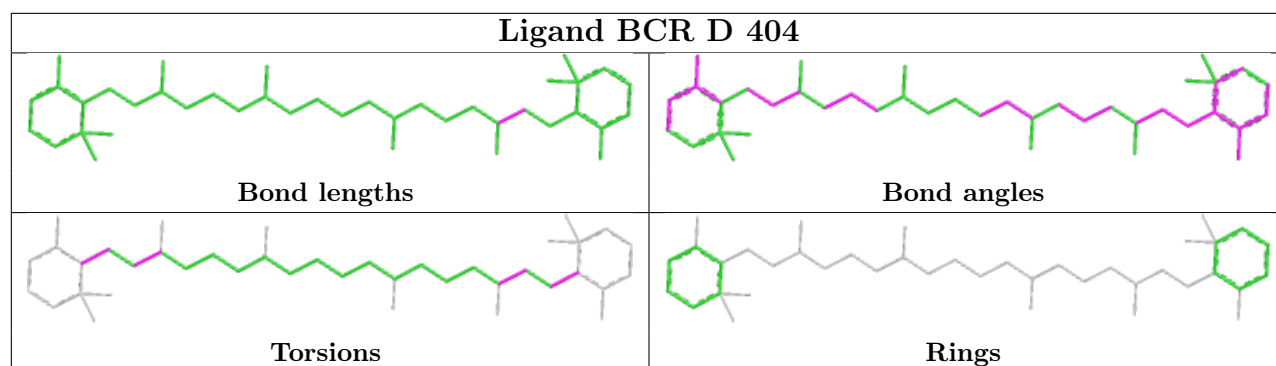
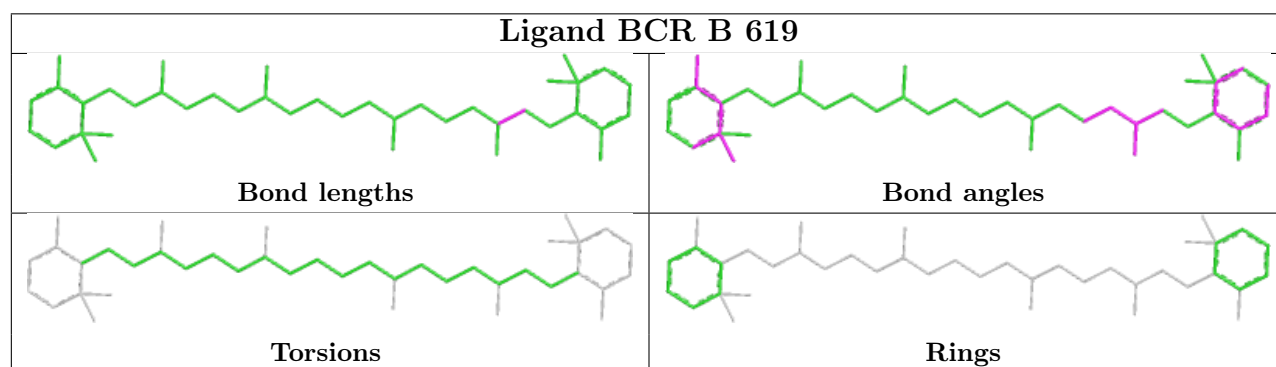
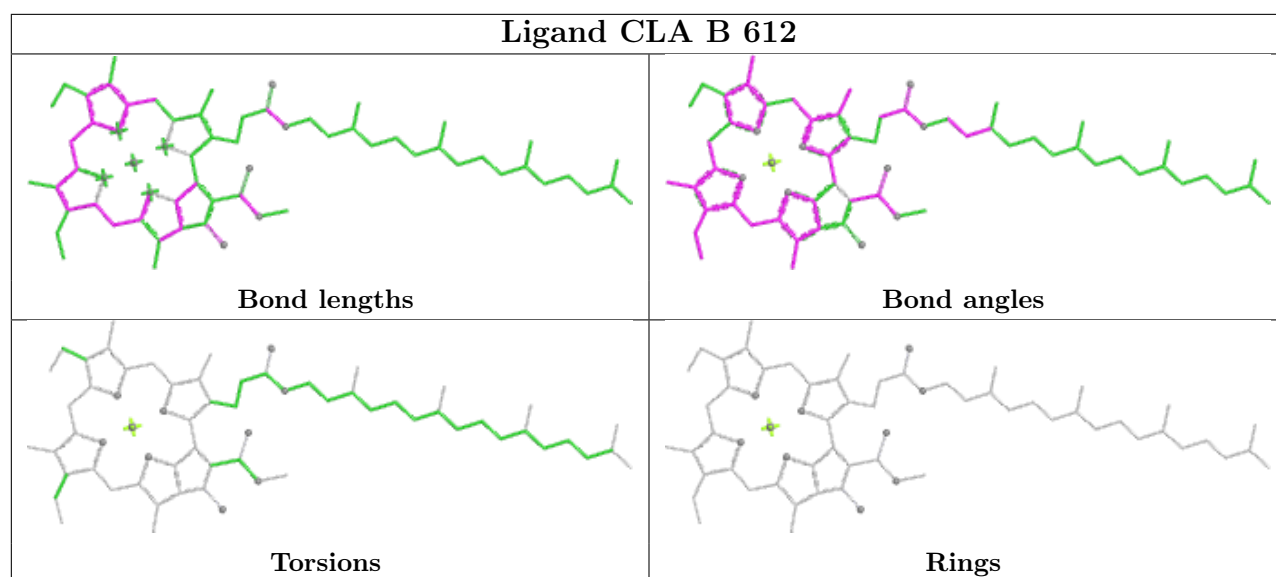


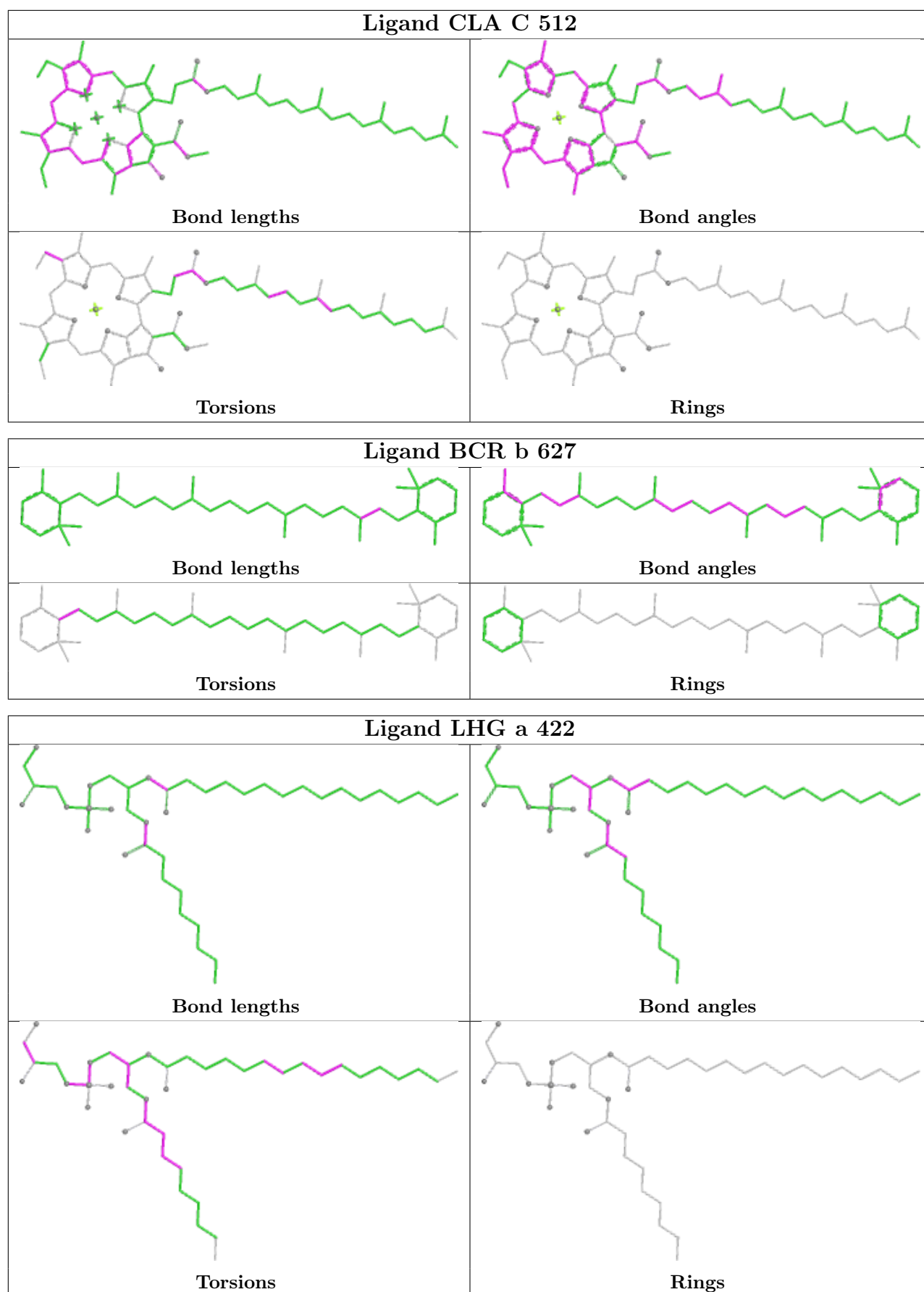
Ligand DGD e 101

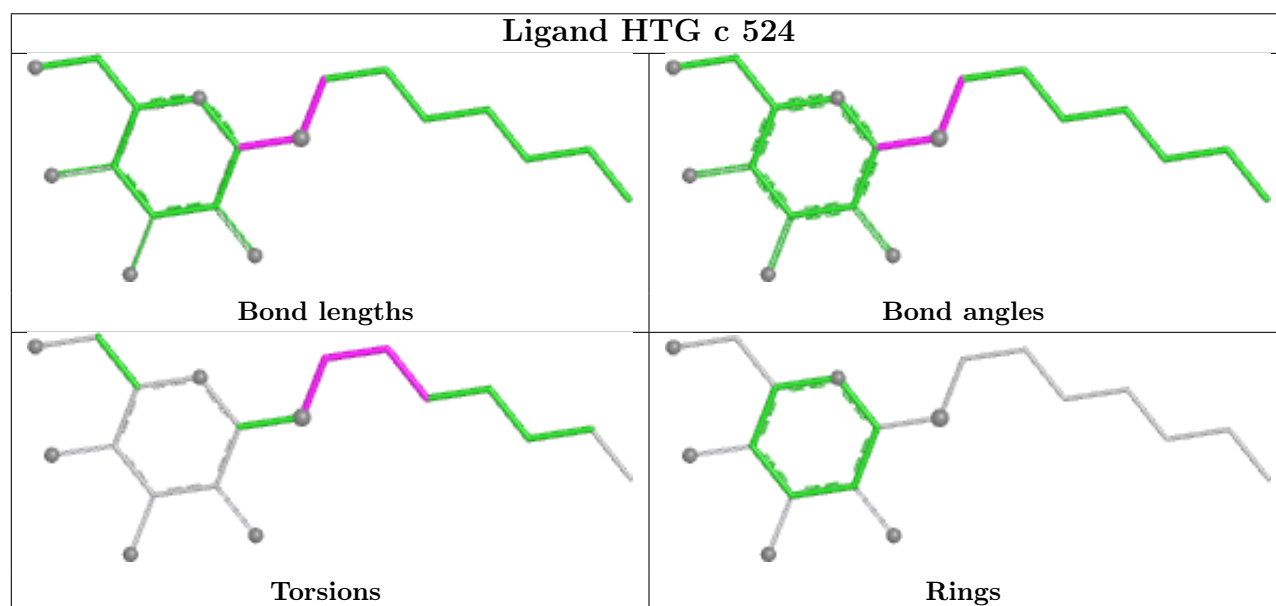
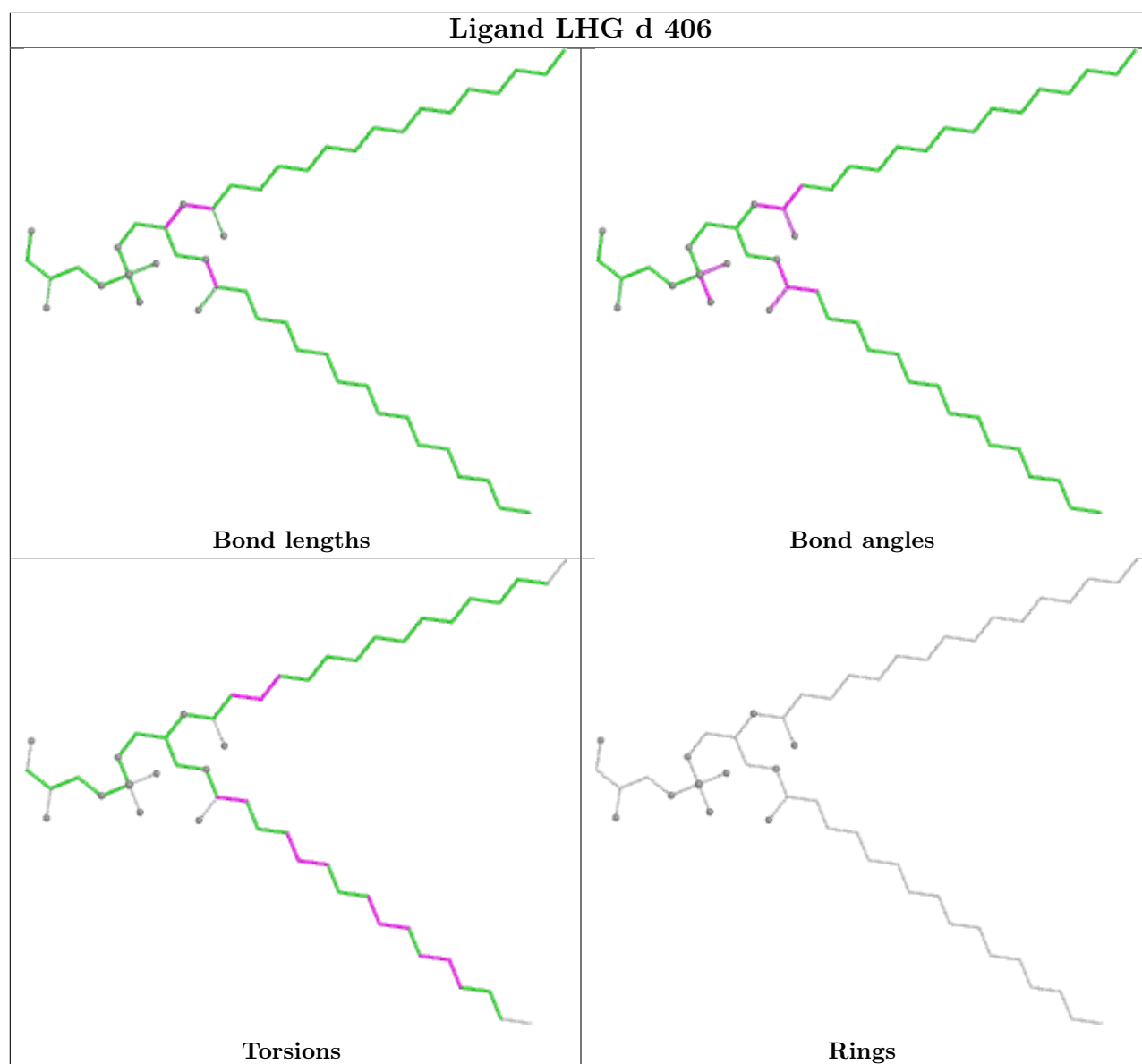


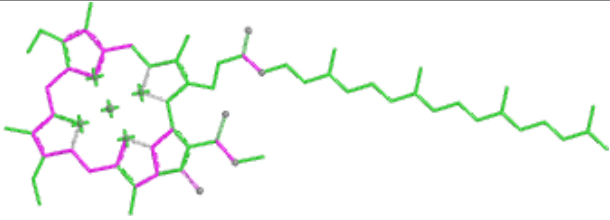
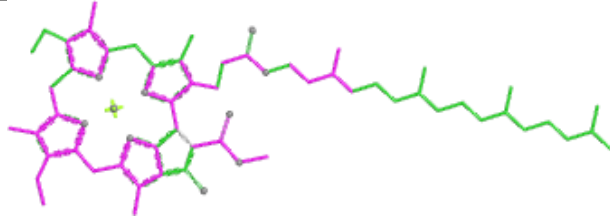
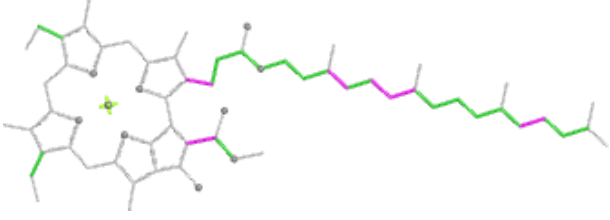
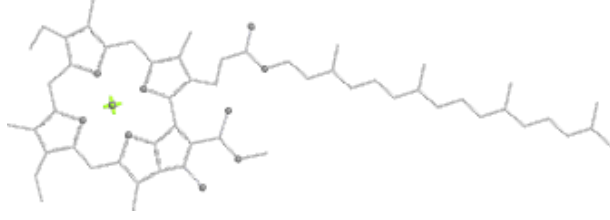
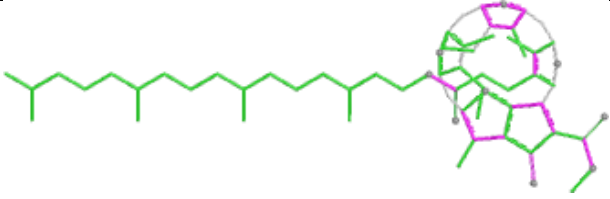
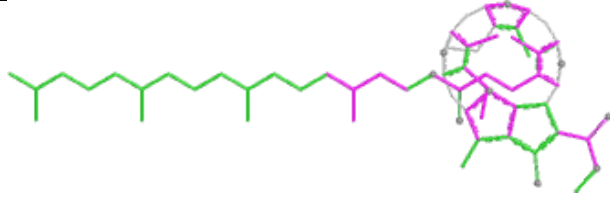
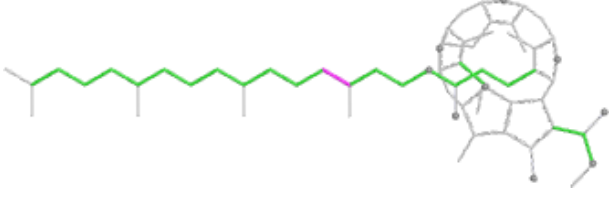
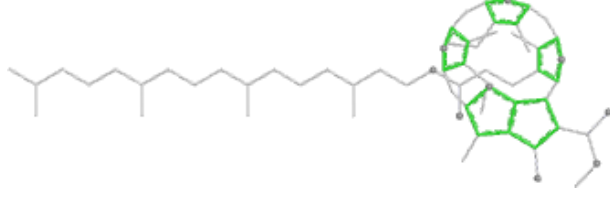
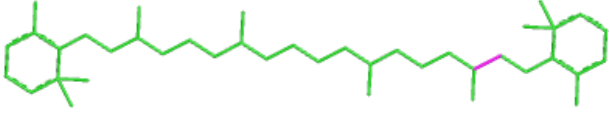
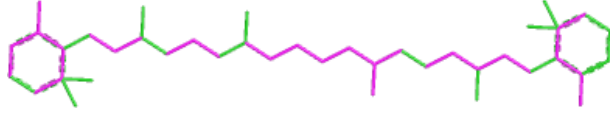
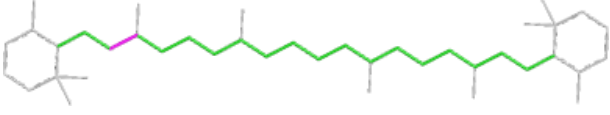
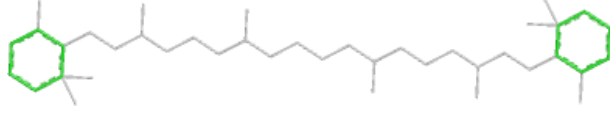
Ligand CLA c 514



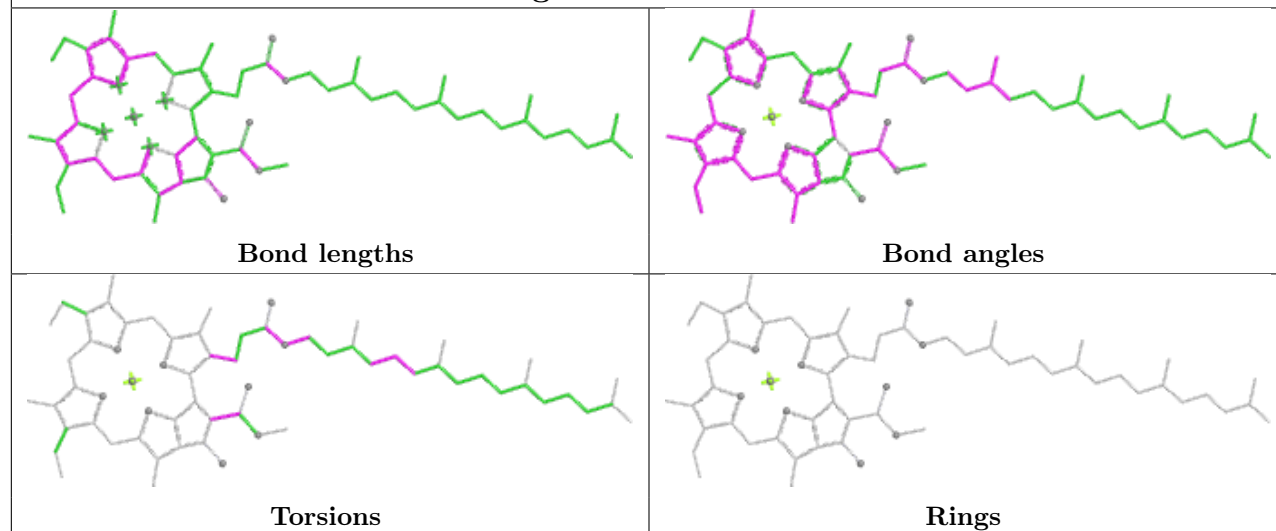




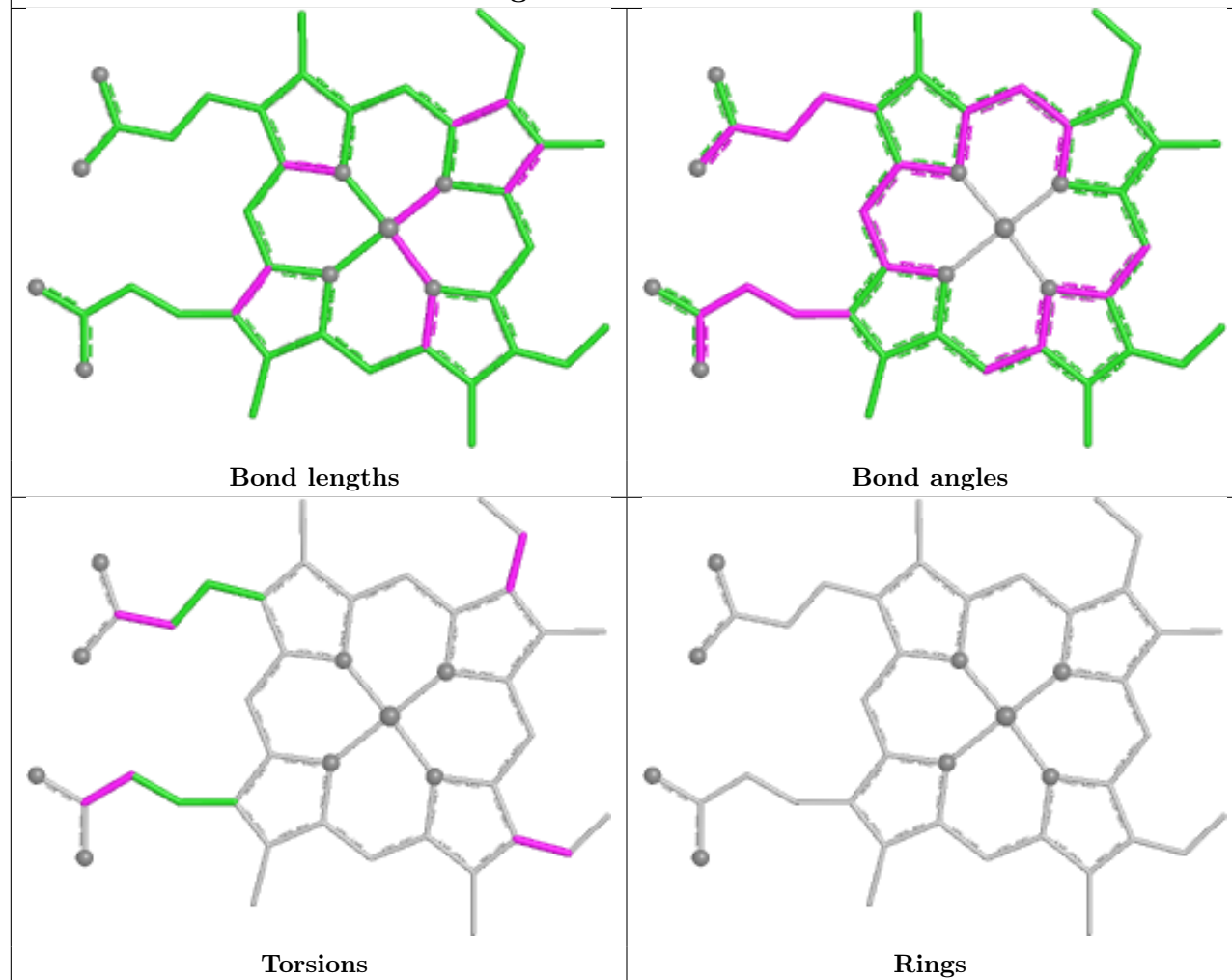


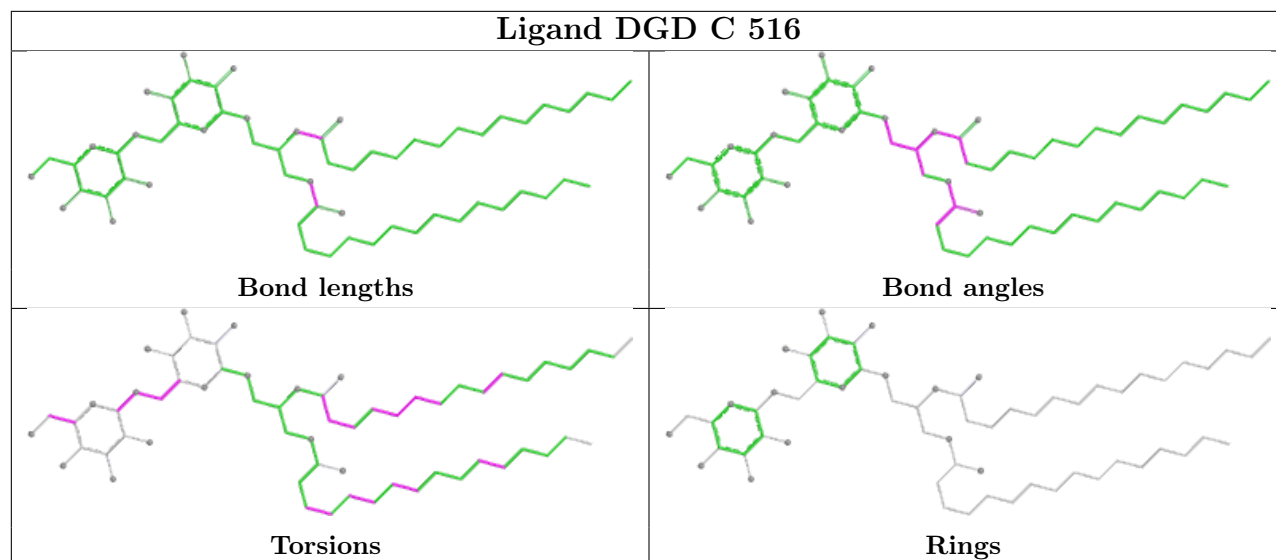
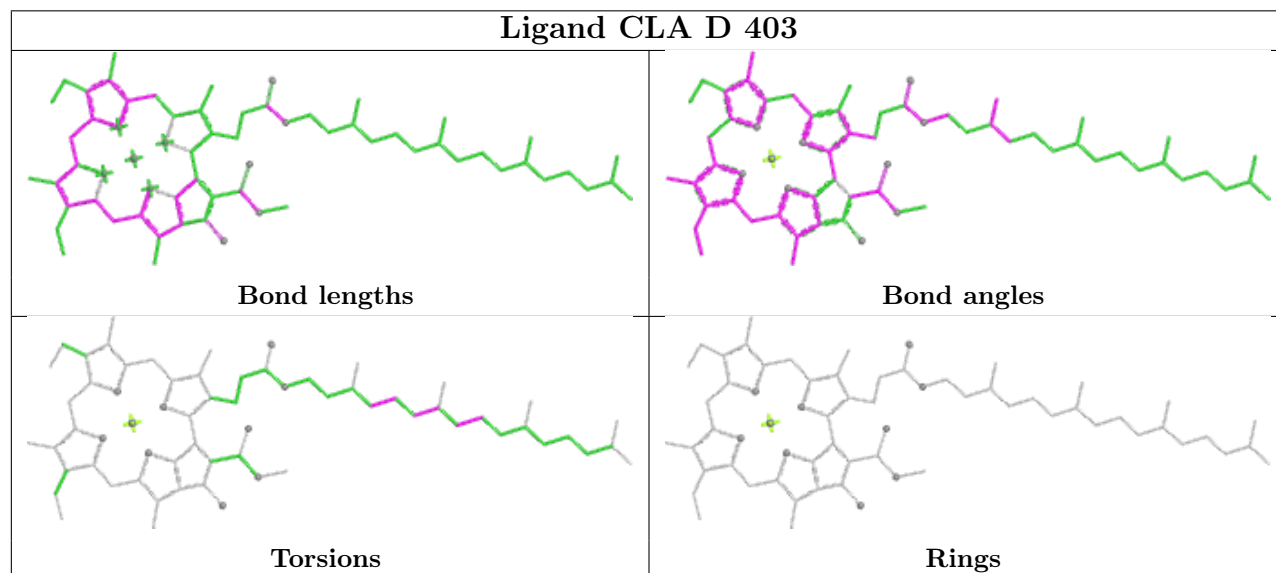
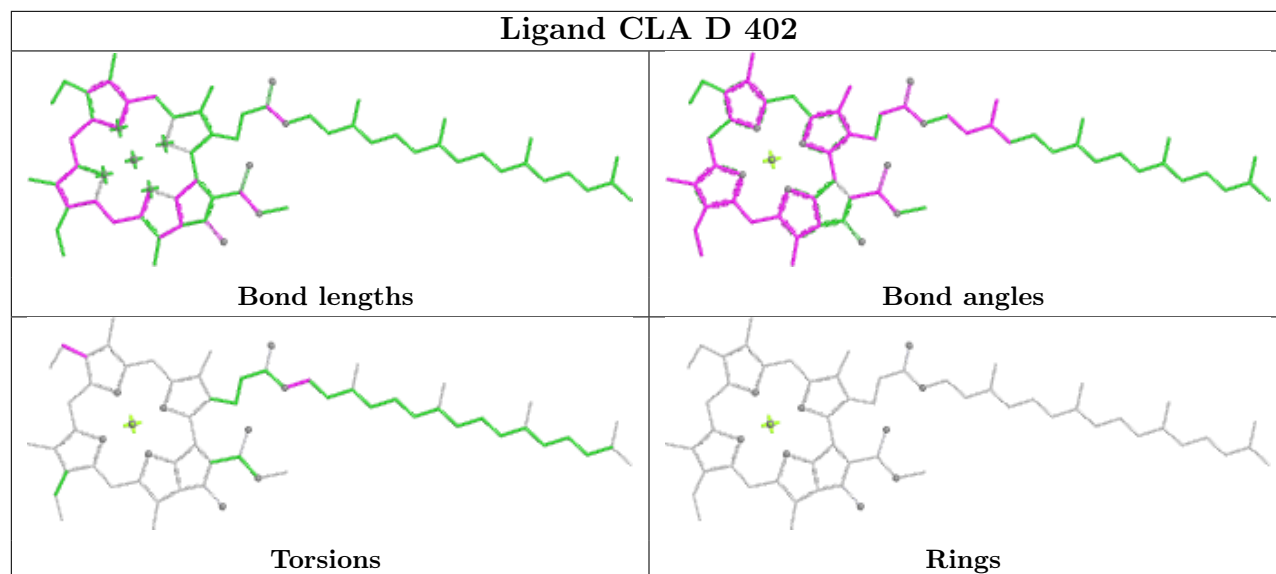
Ligand CLA C 506	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PHO A 408	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

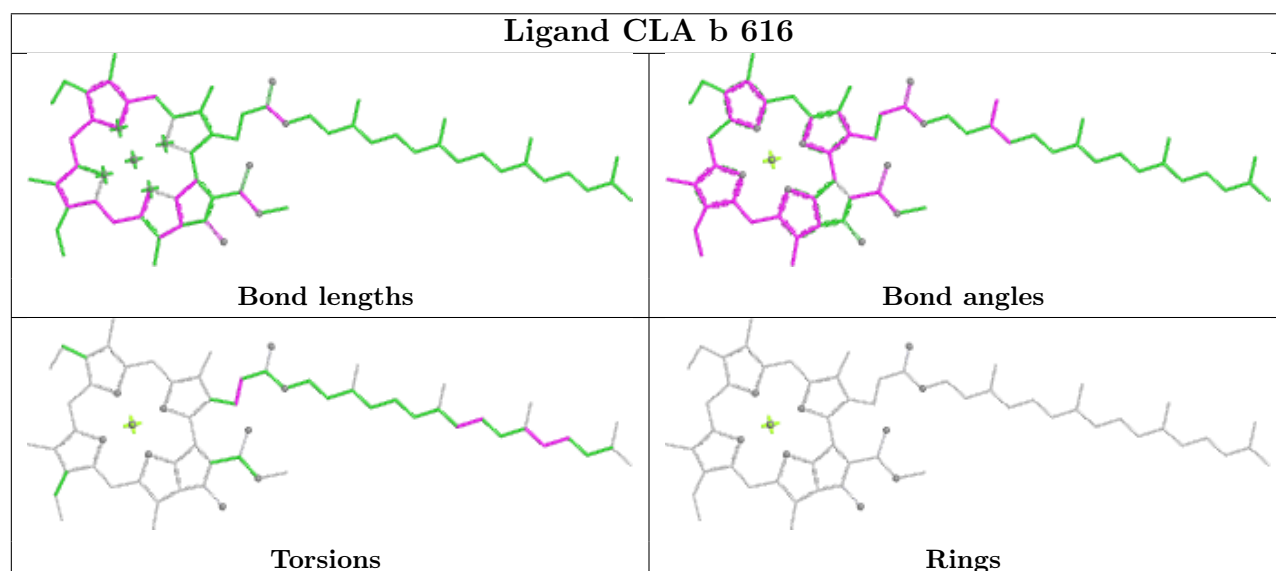
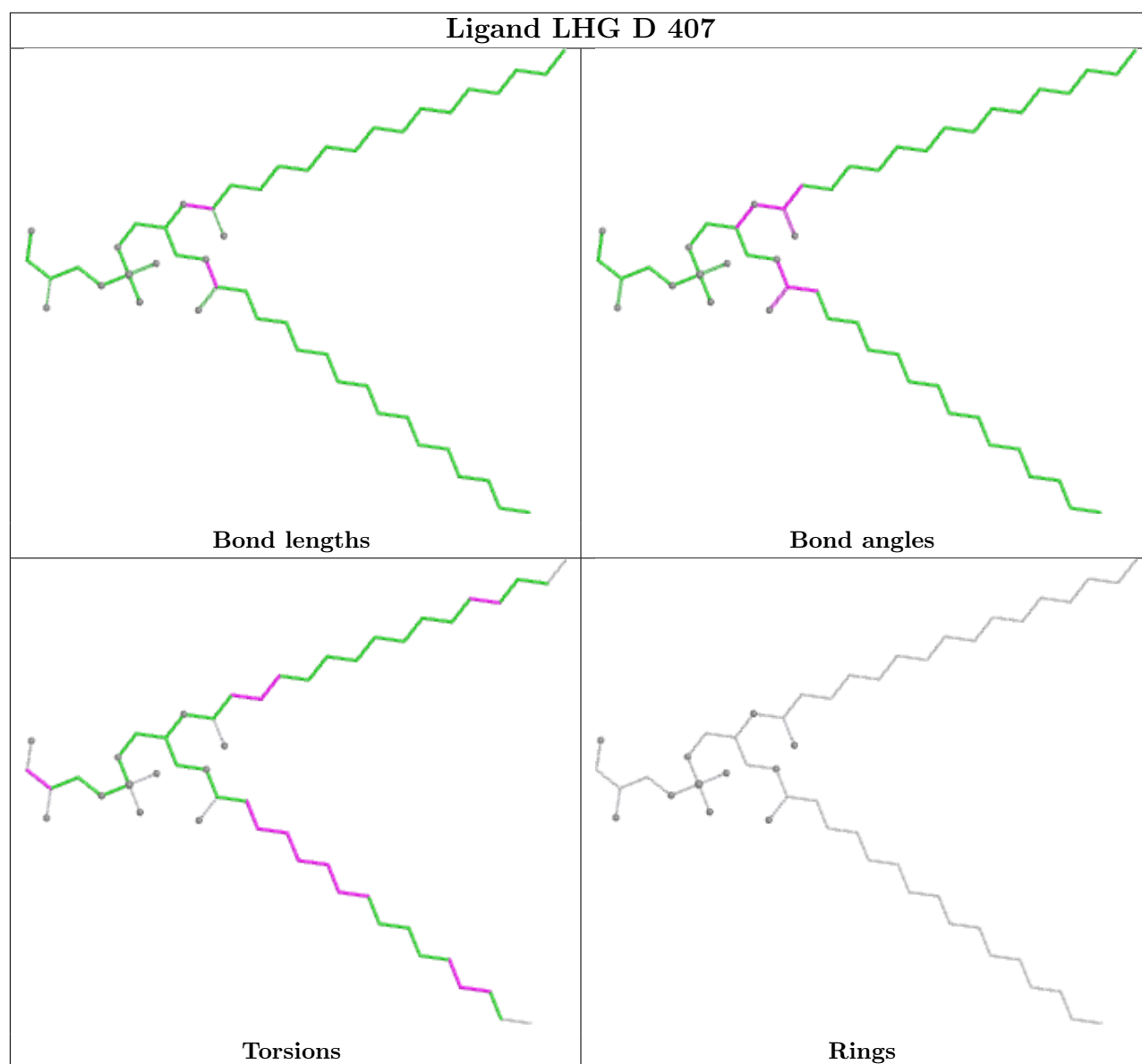
Ligand CLA C 513

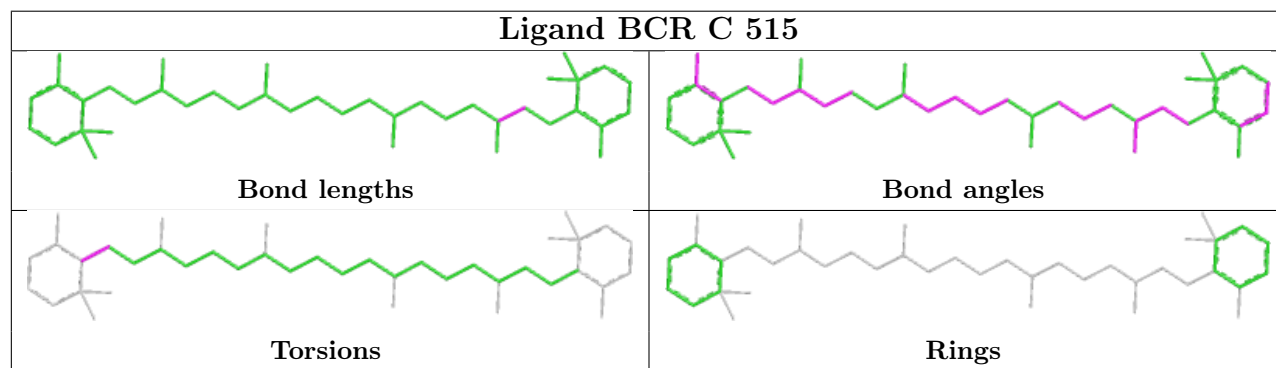
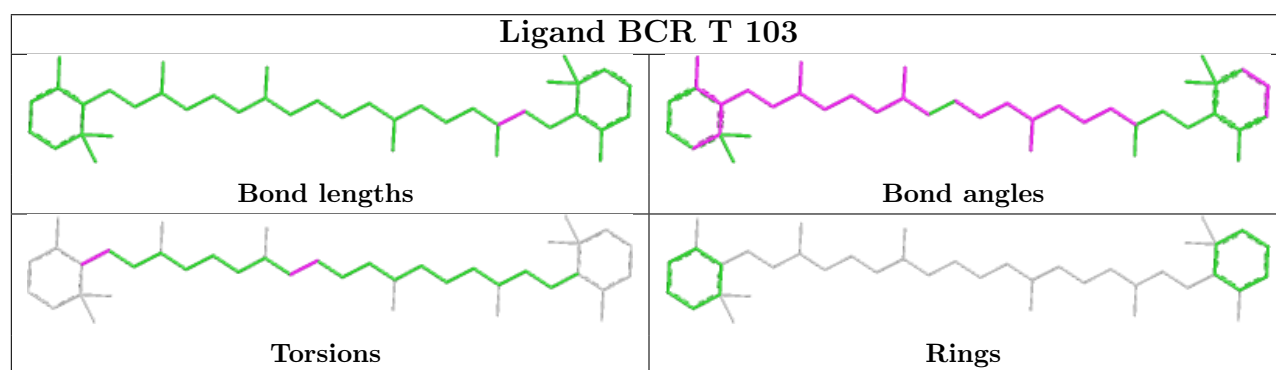
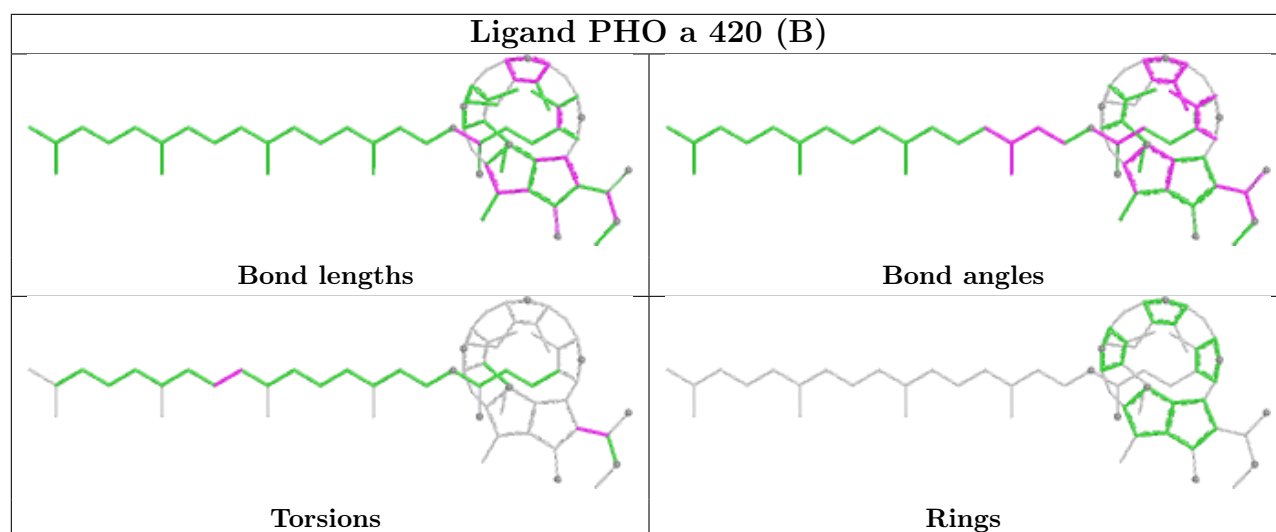


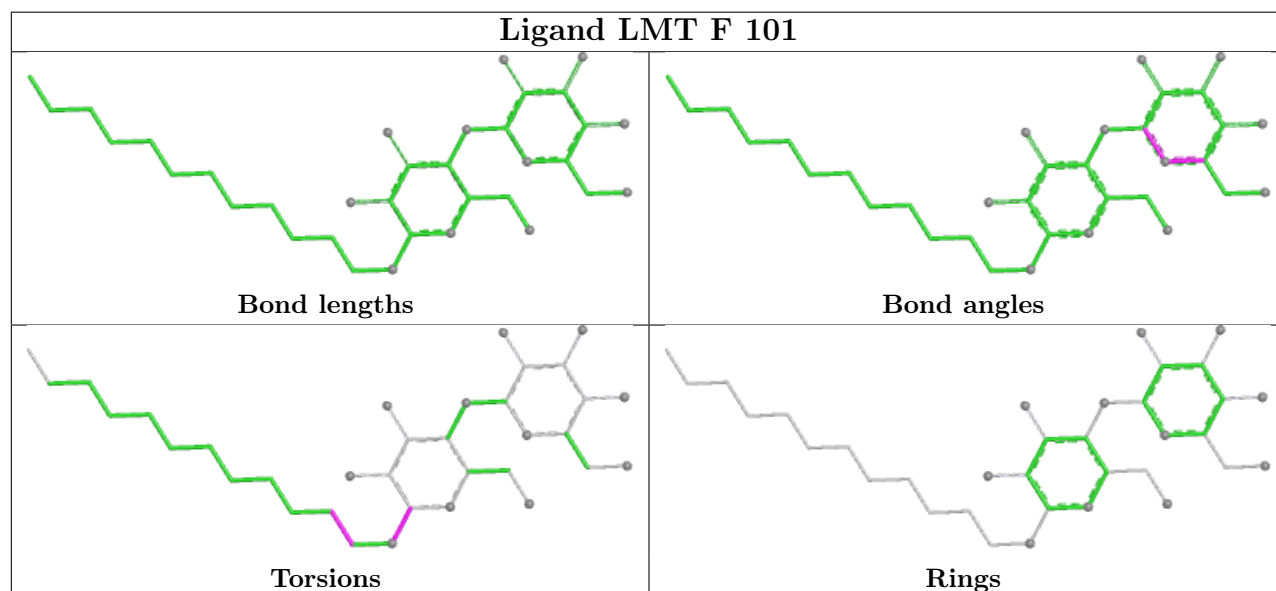
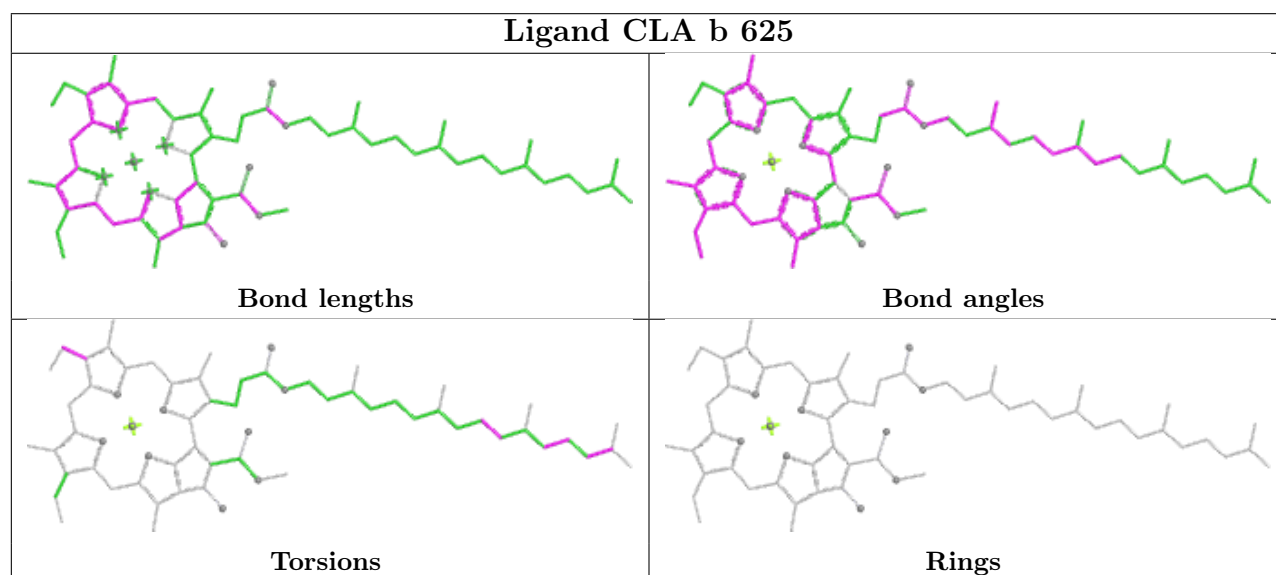
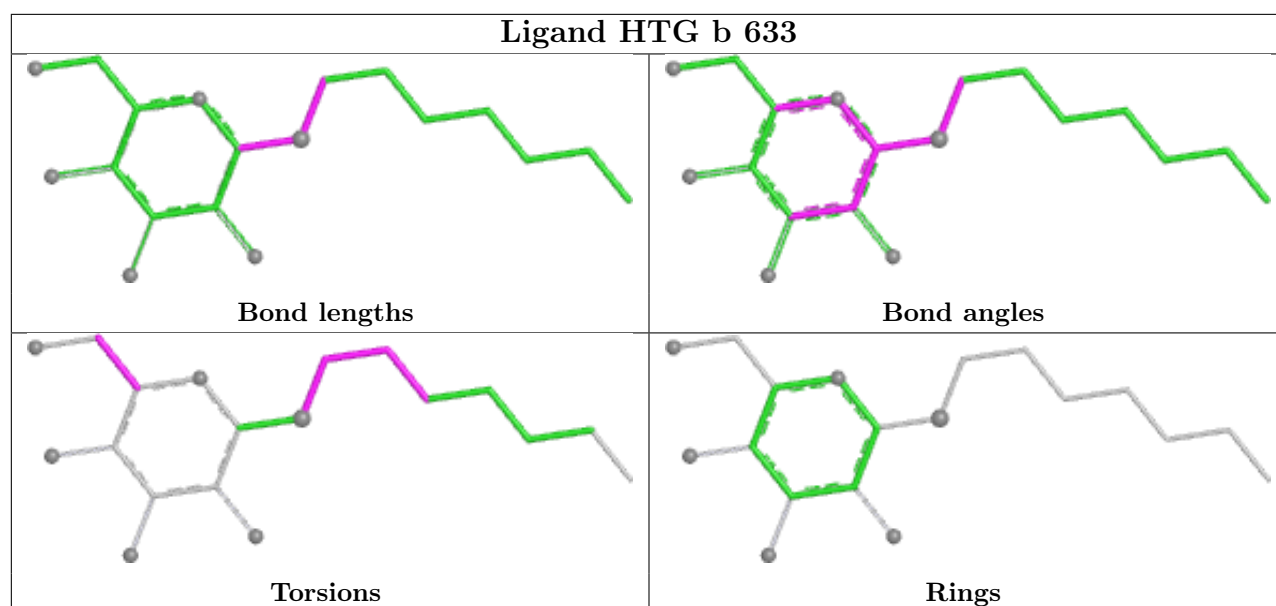
Ligand HEM F 102

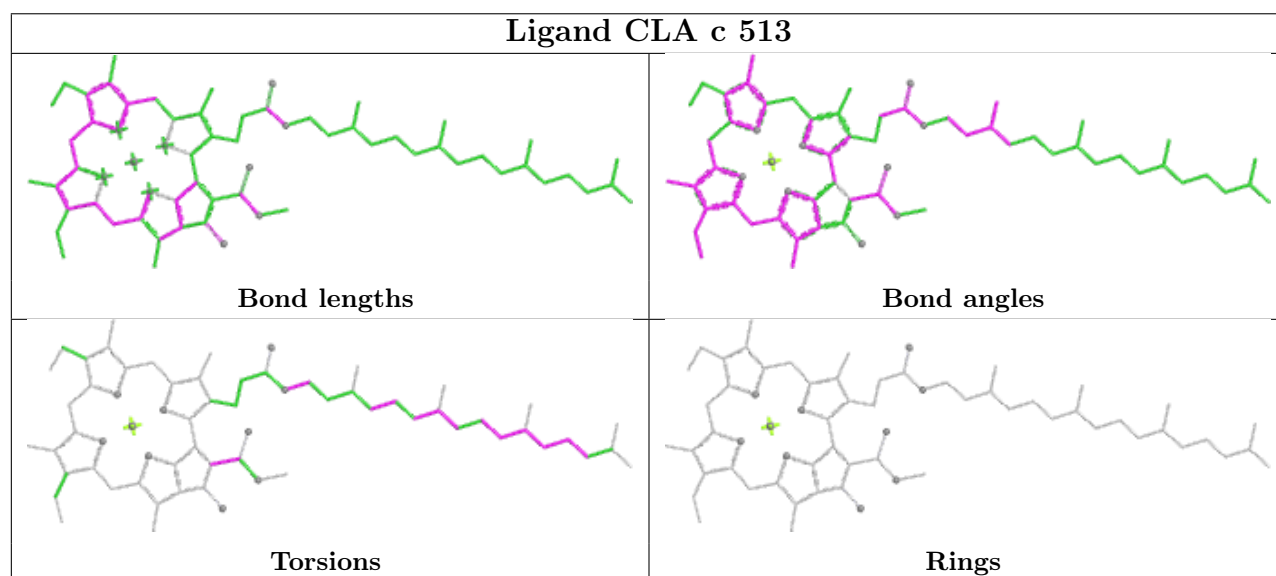
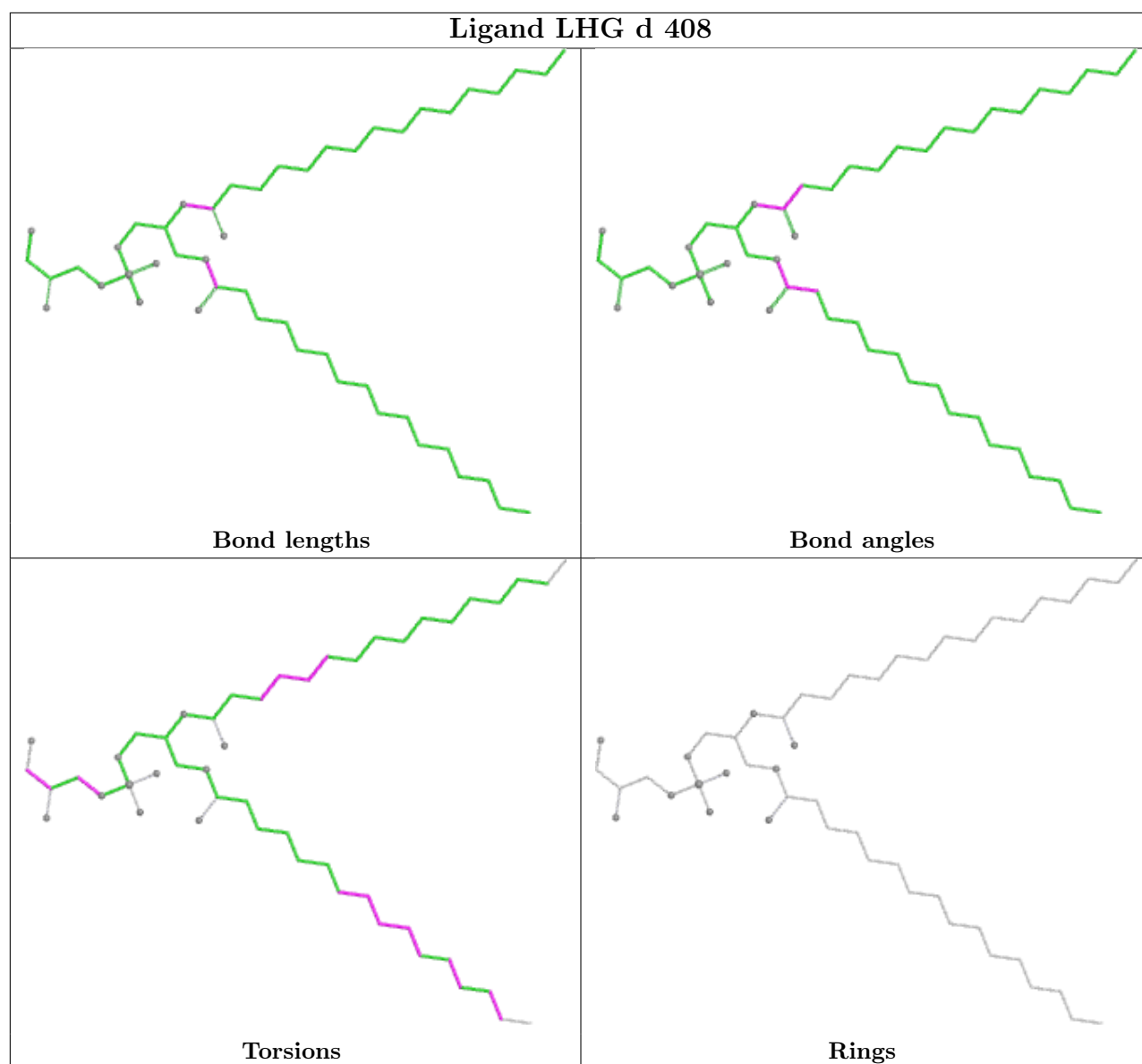


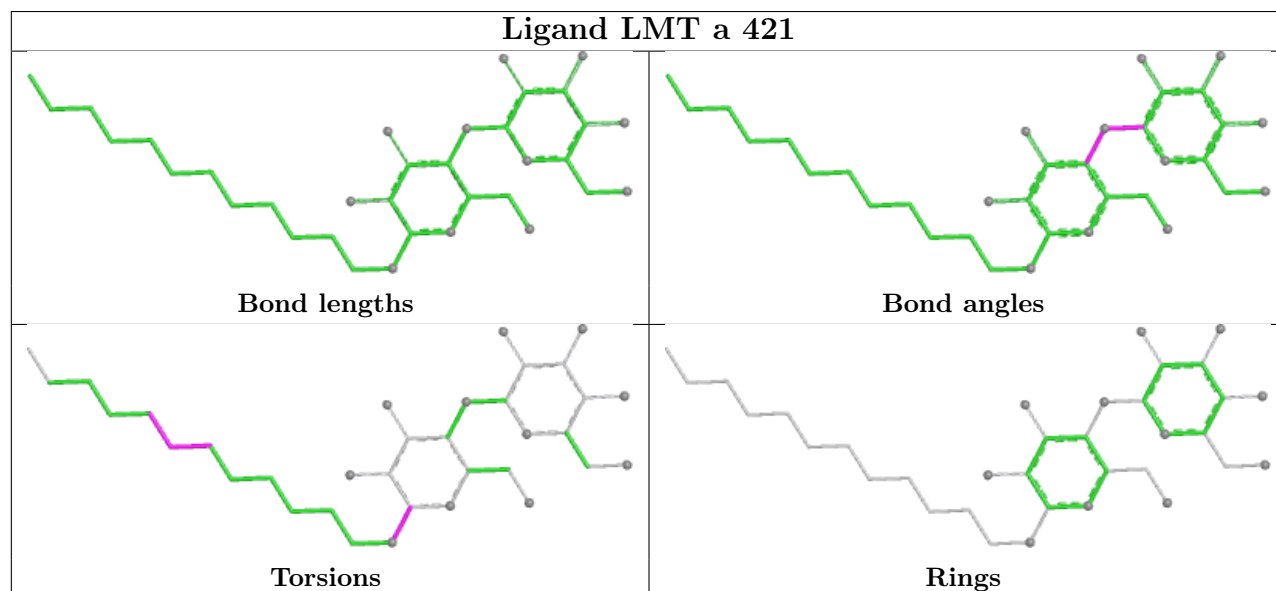
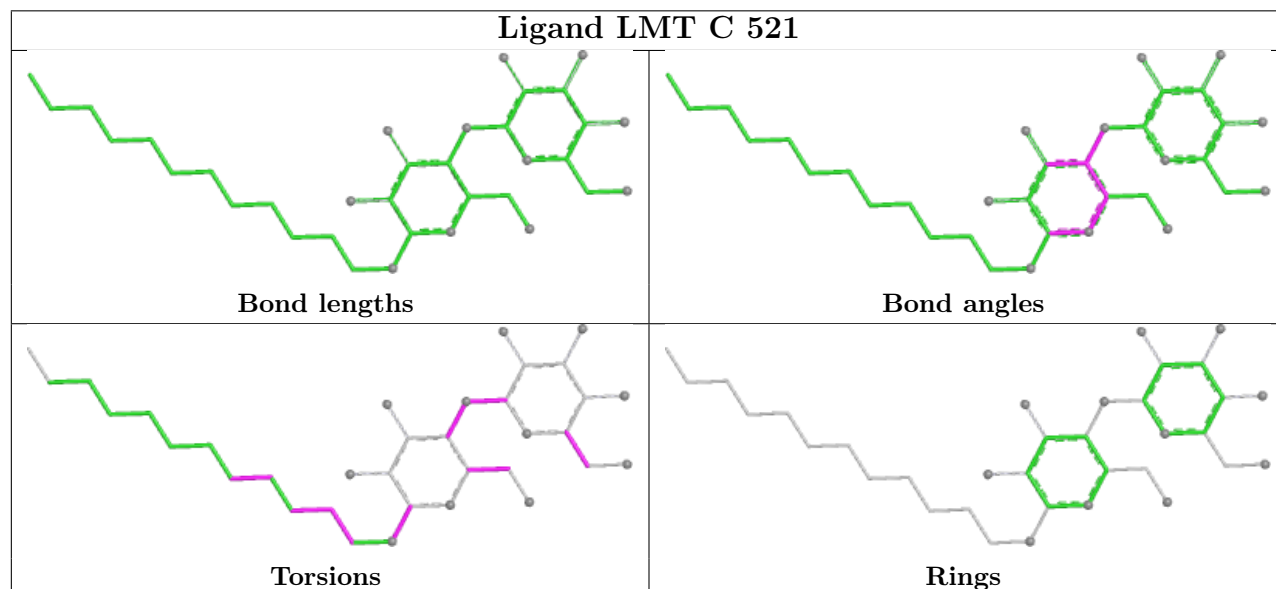
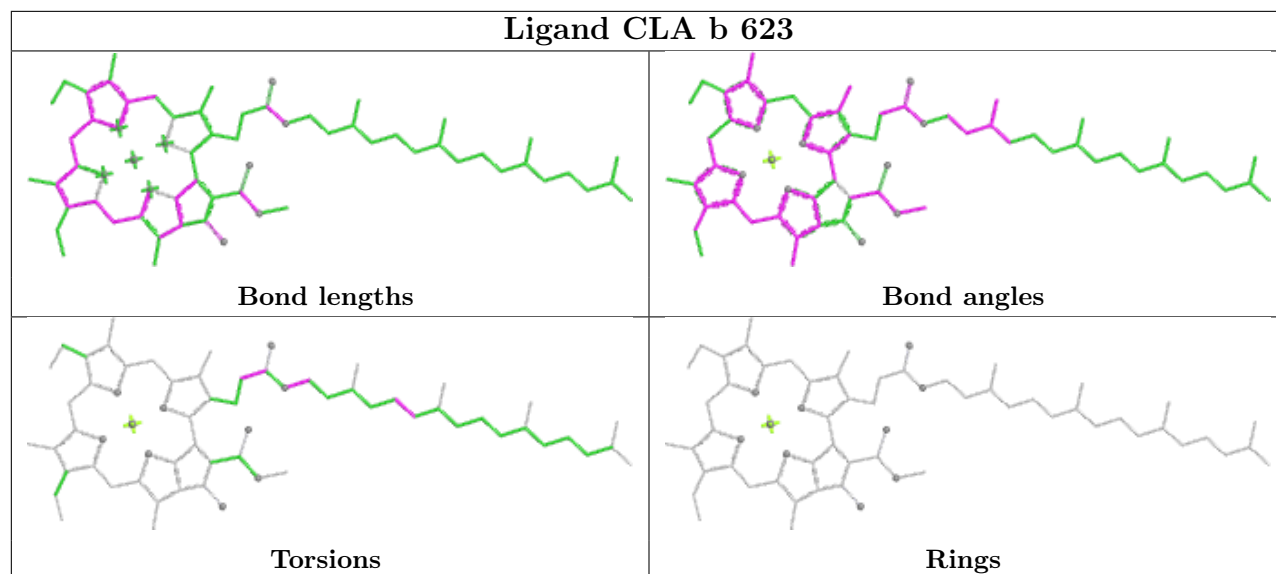




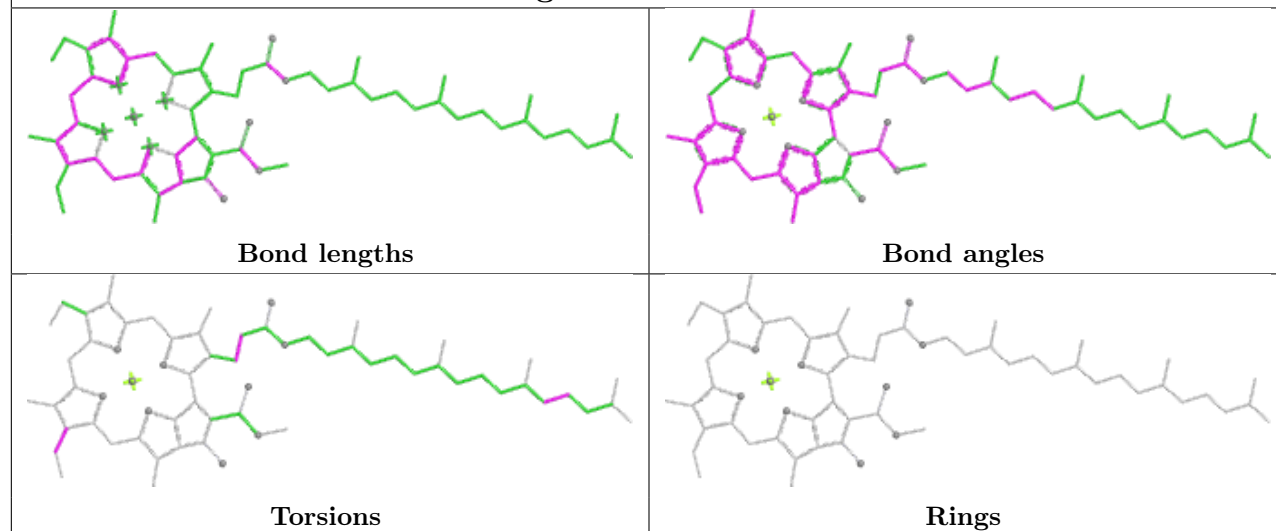




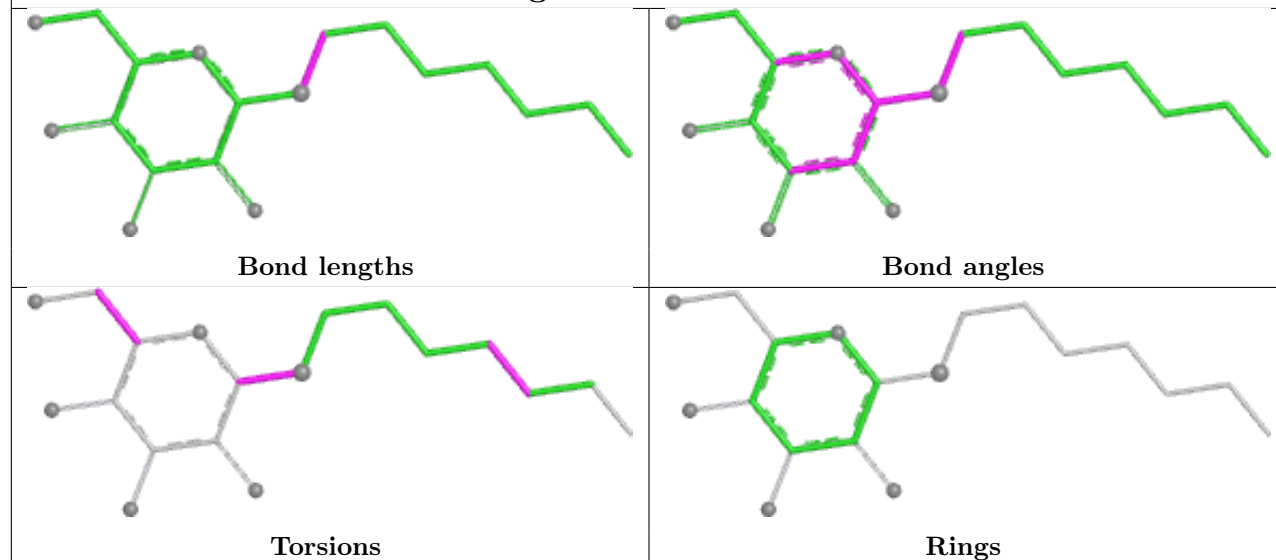




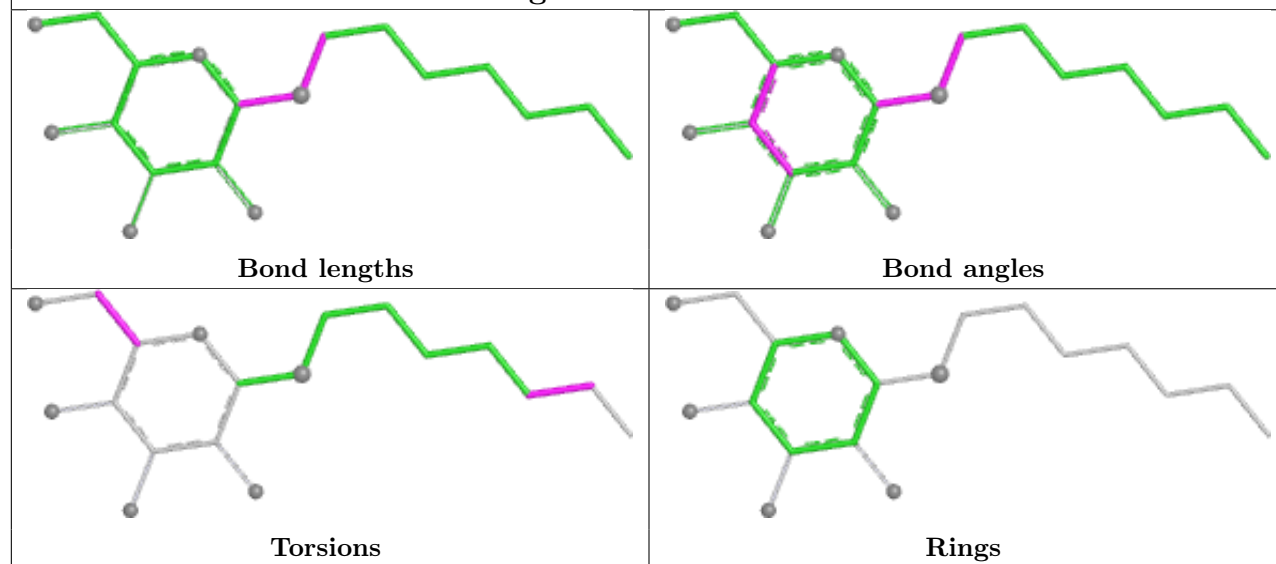
Ligand CLA a 409

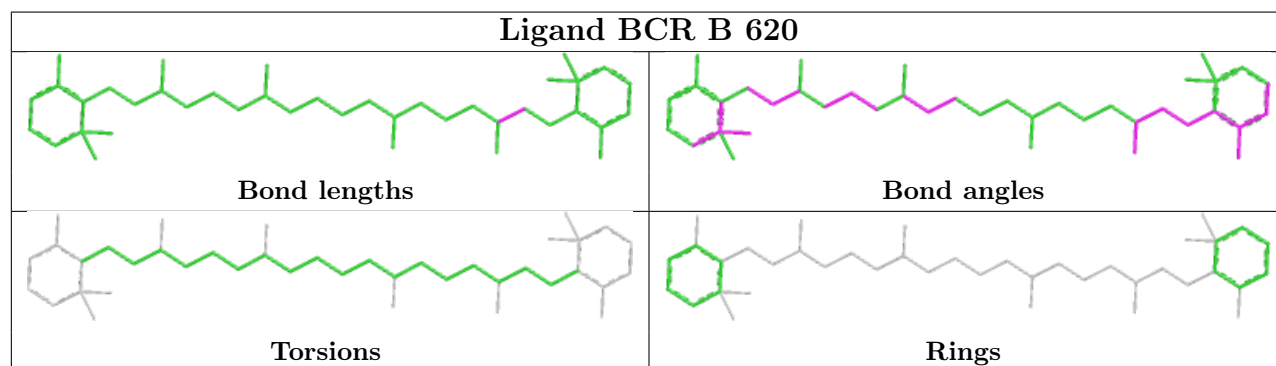
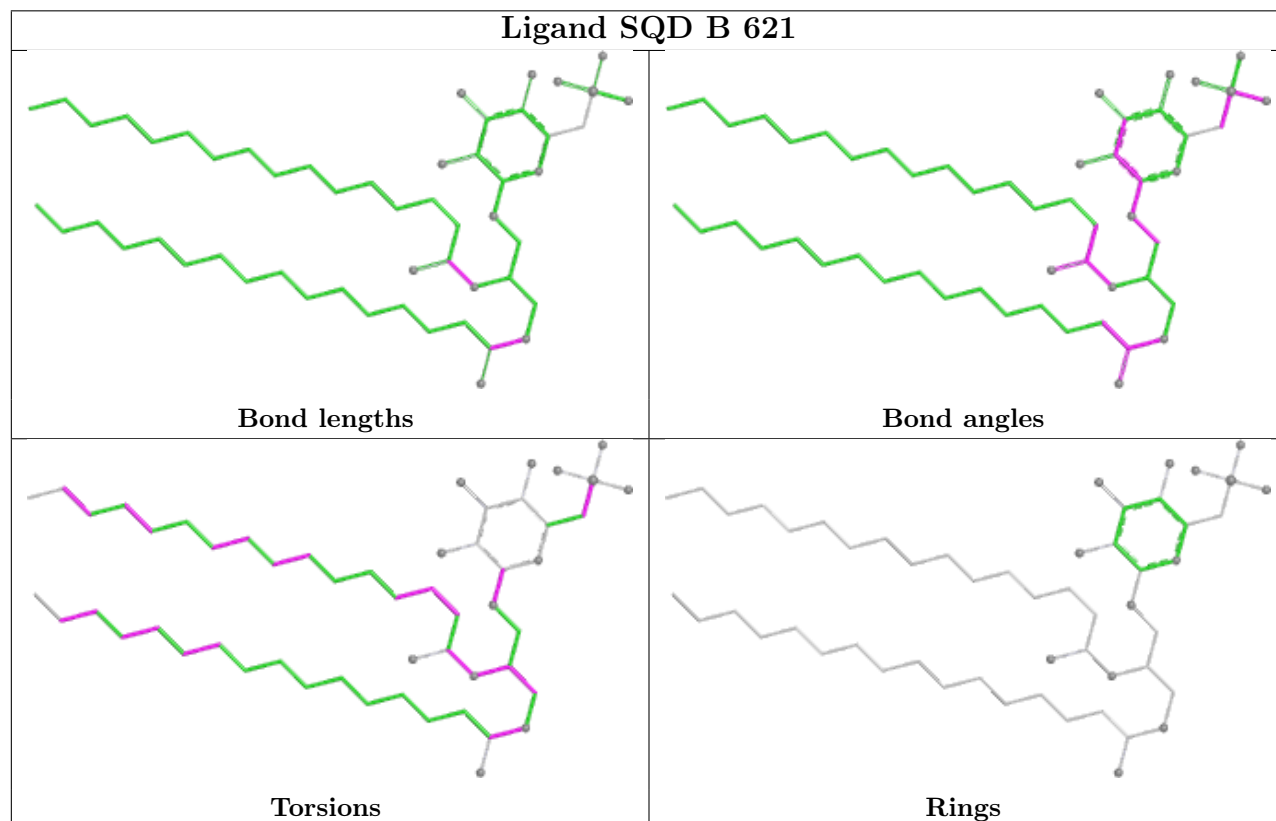
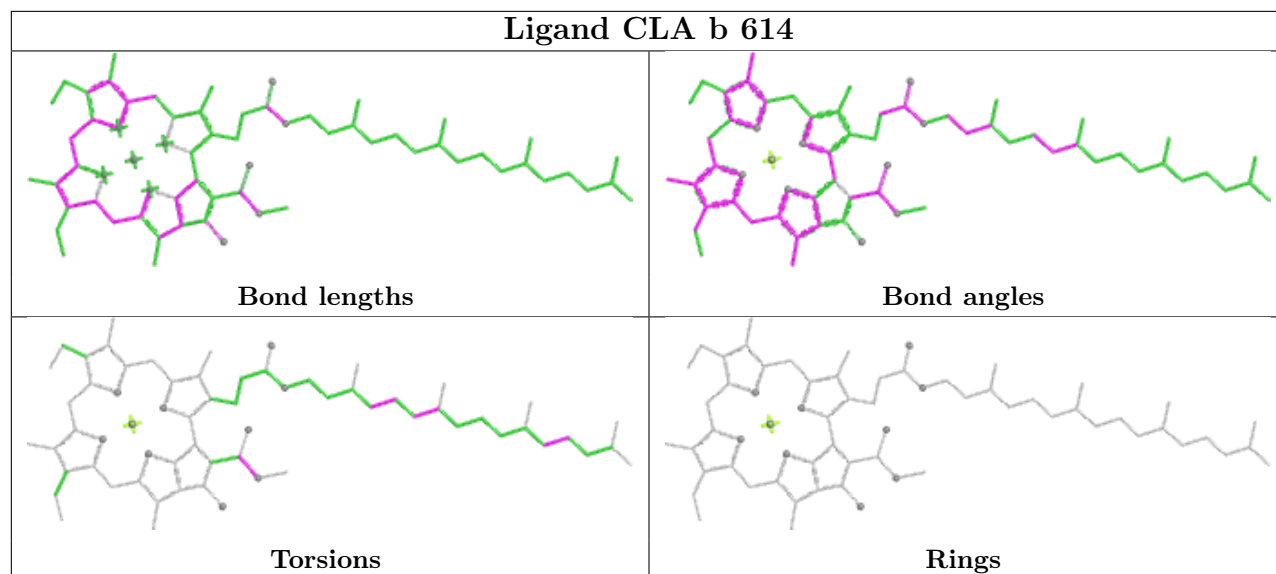


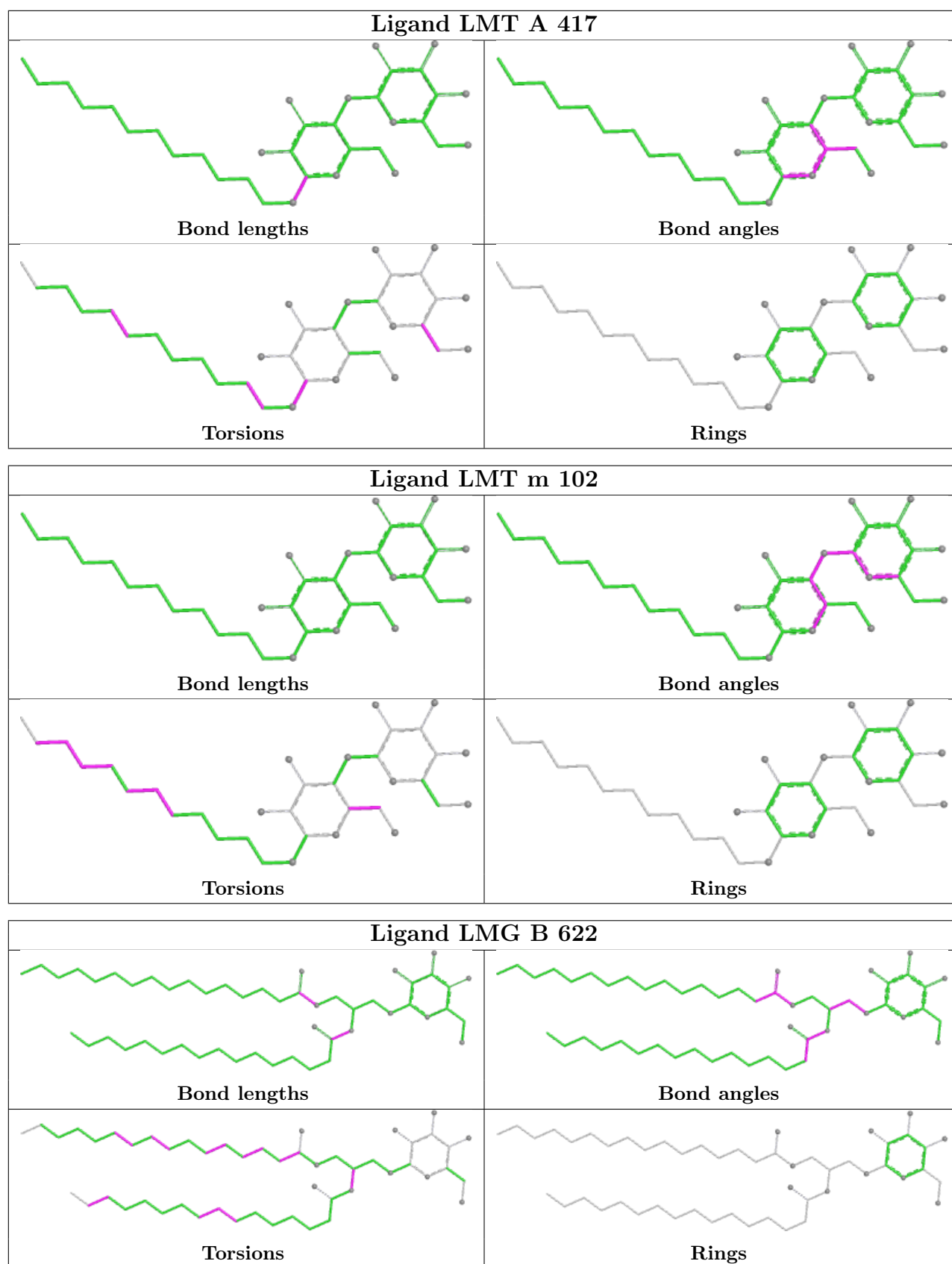
Ligand HTG B 625

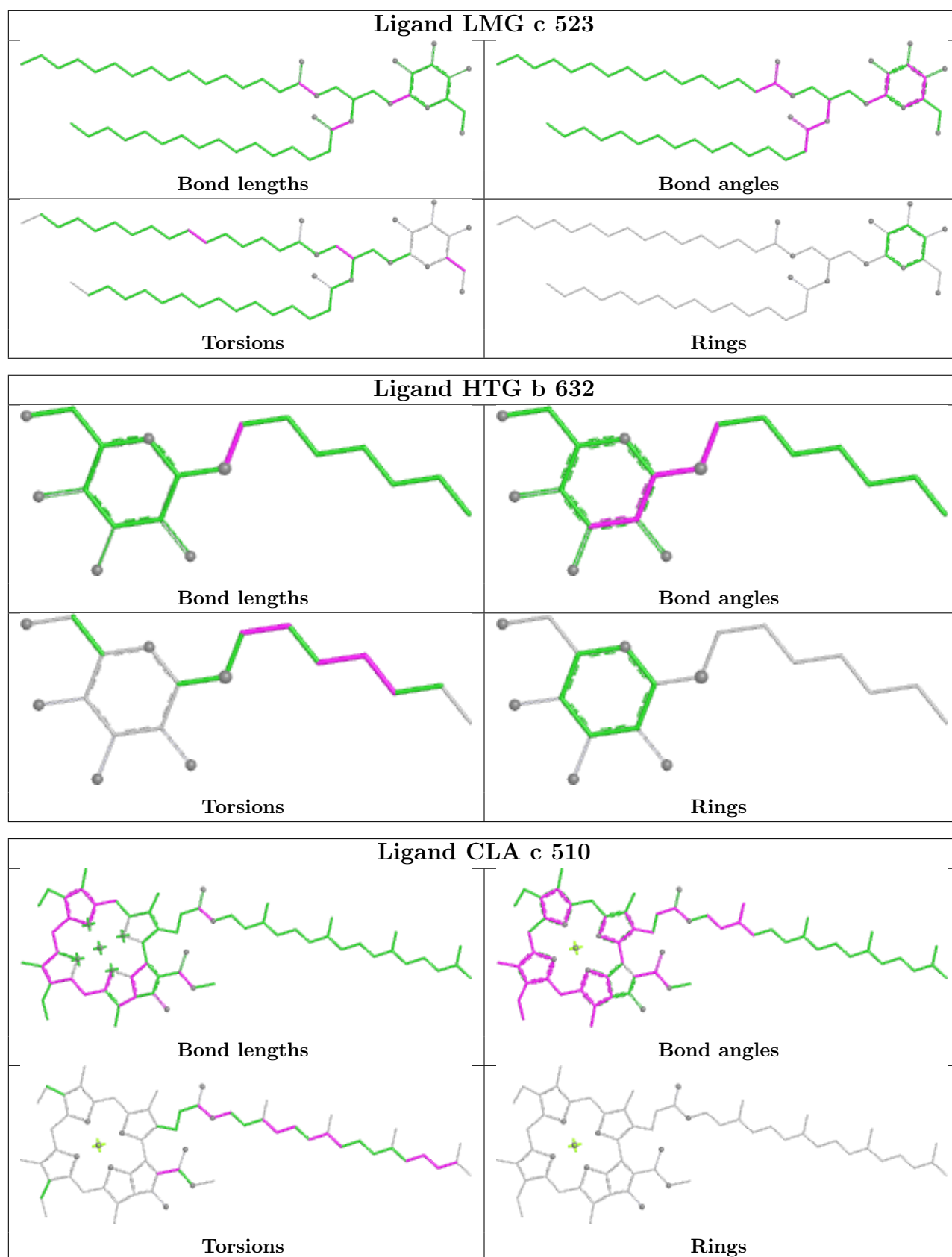


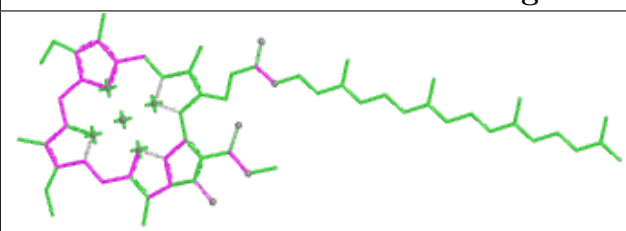
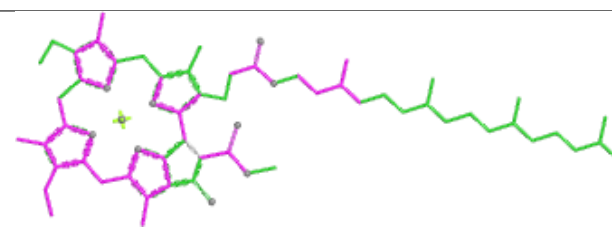
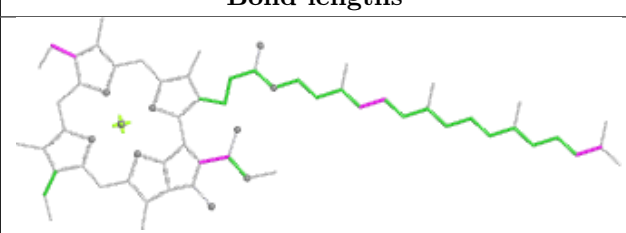
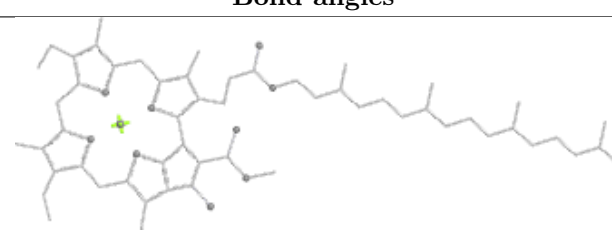
Ligand HTG B 632

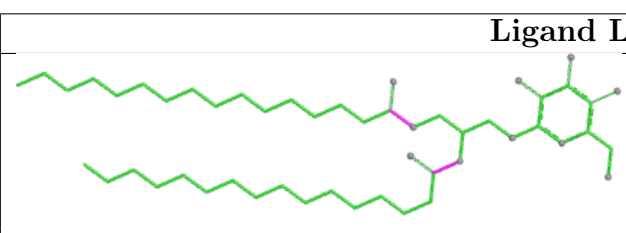
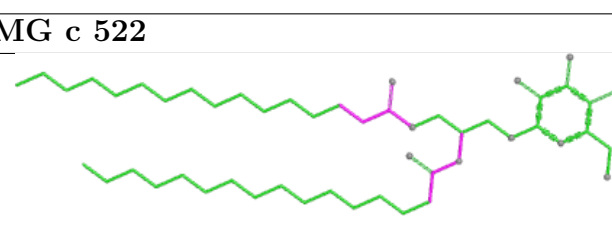
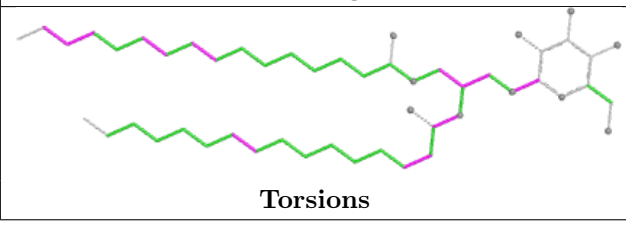
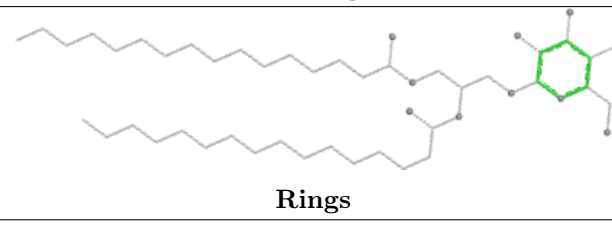


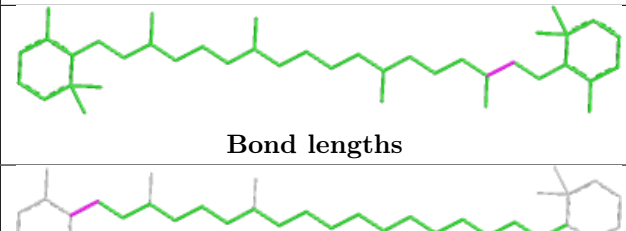
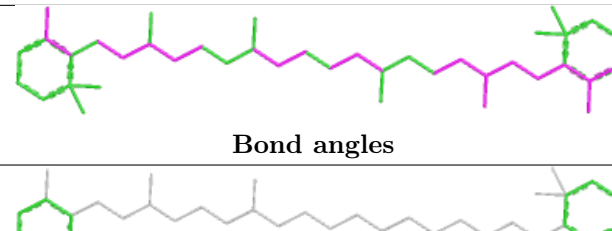




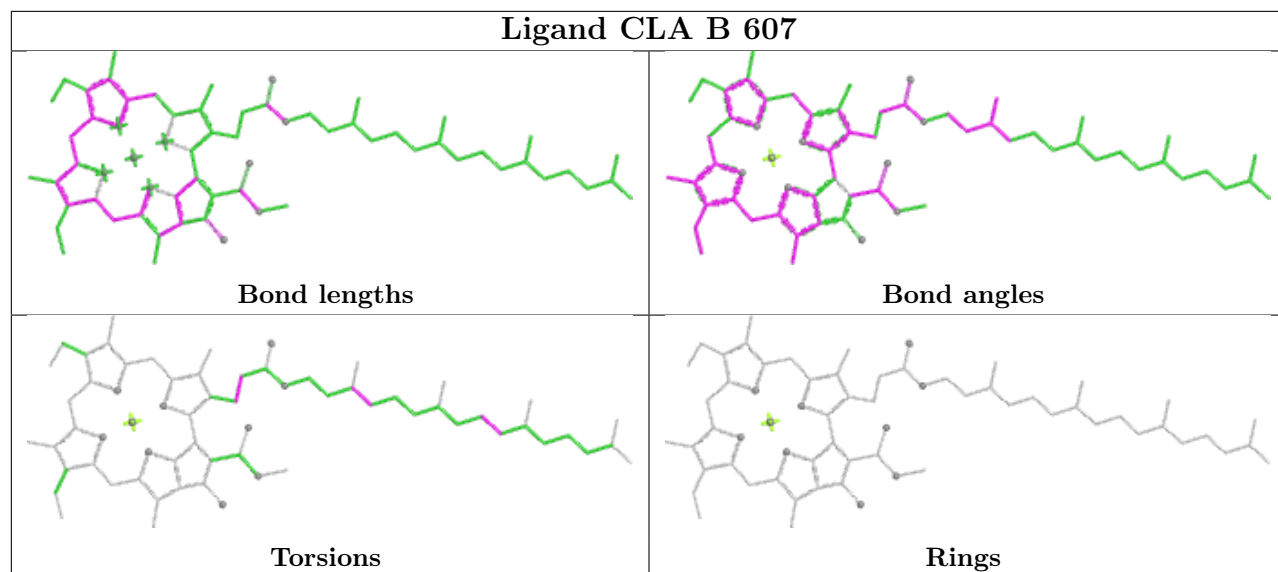


Ligand CLA C 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

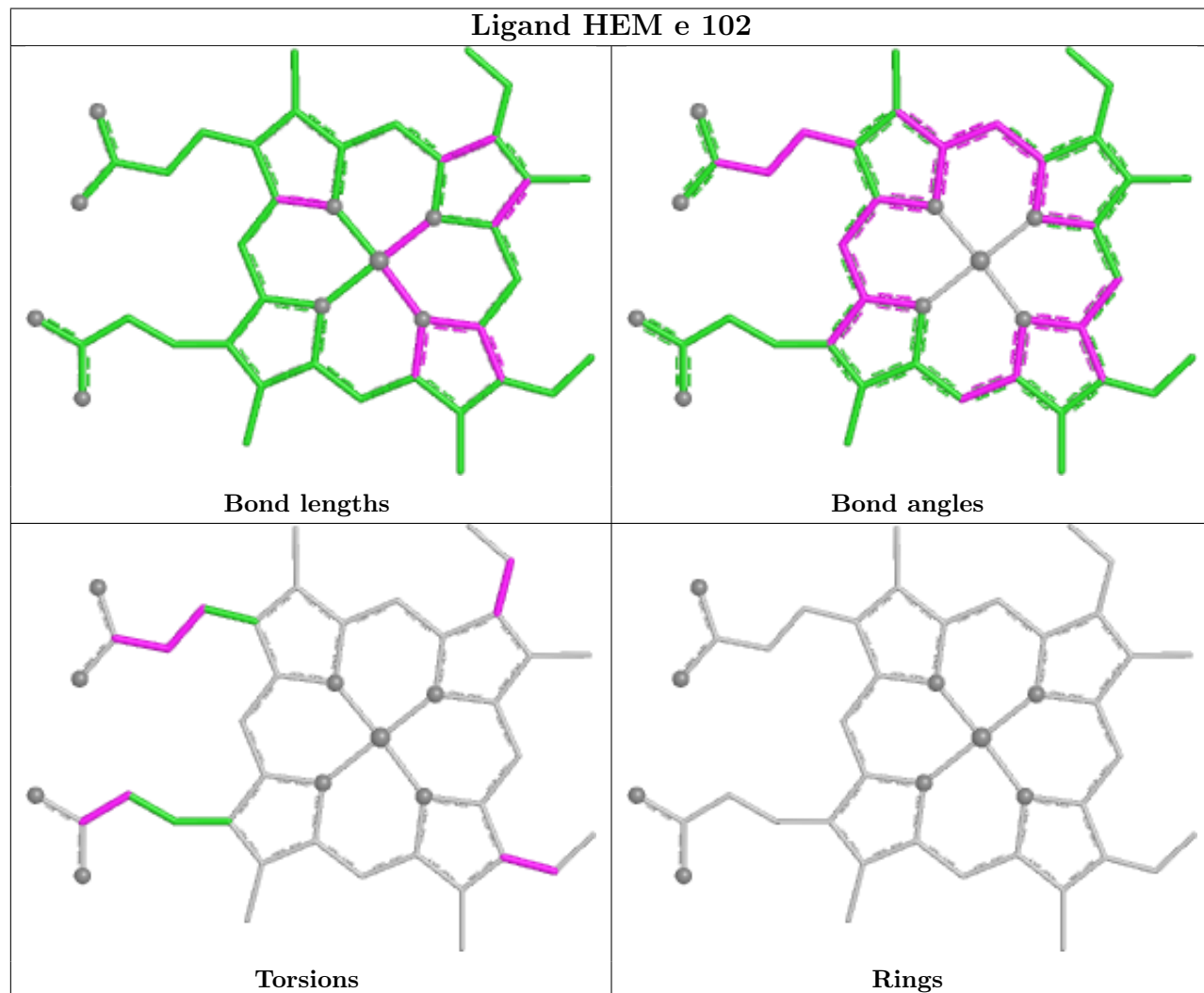
Ligand LMG c 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR C 514	
	
Bond lengths	Bond angles
	
Torsions	Rings

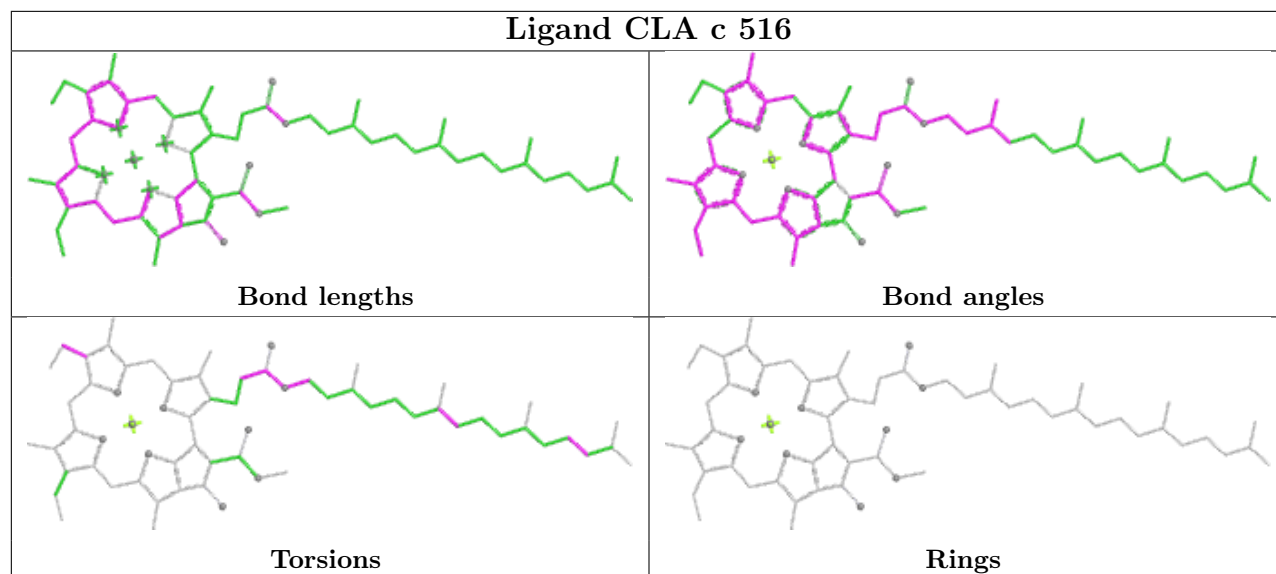
Ligand CLA B 607



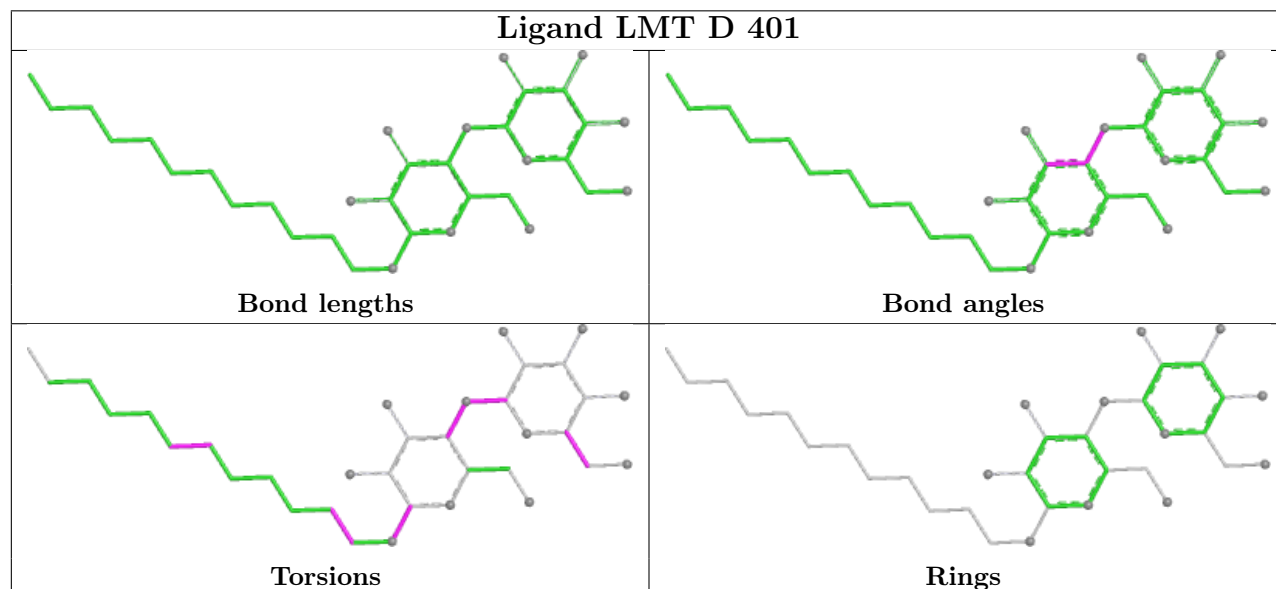
Ligand HEM e 102



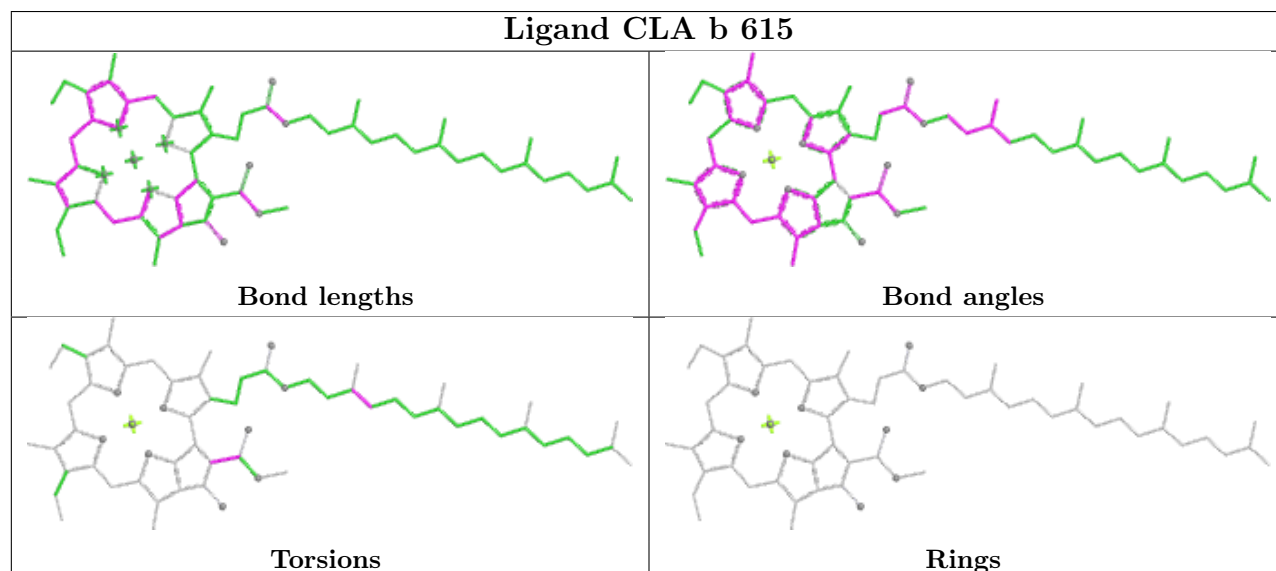
Ligand CLA c 516

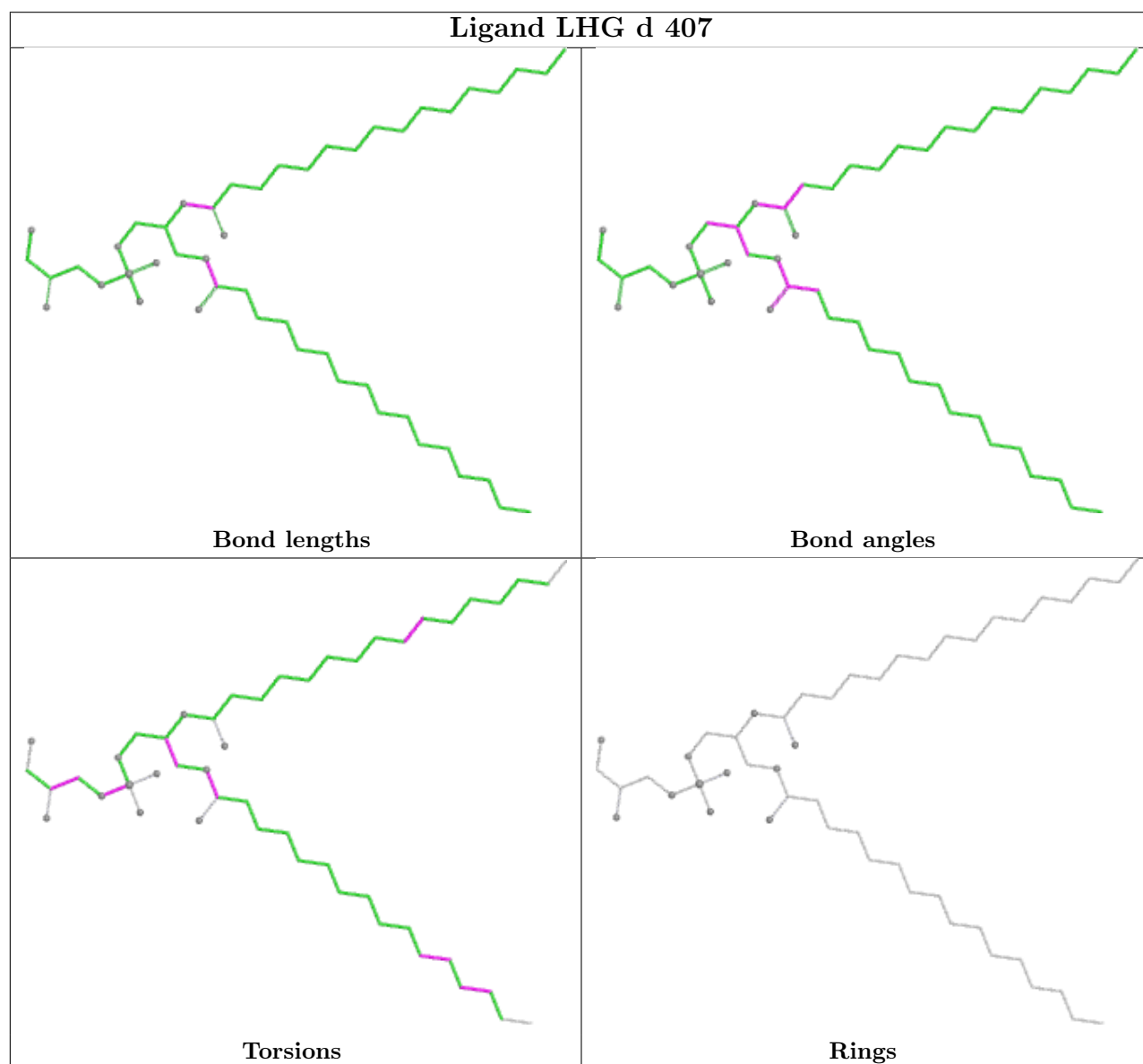
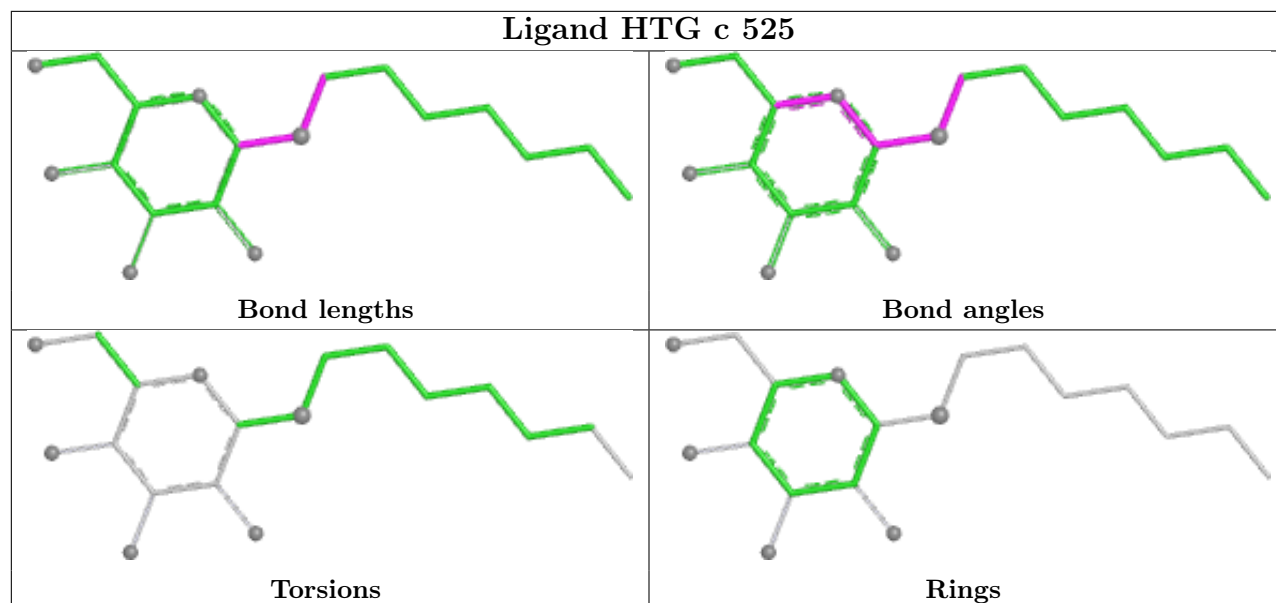


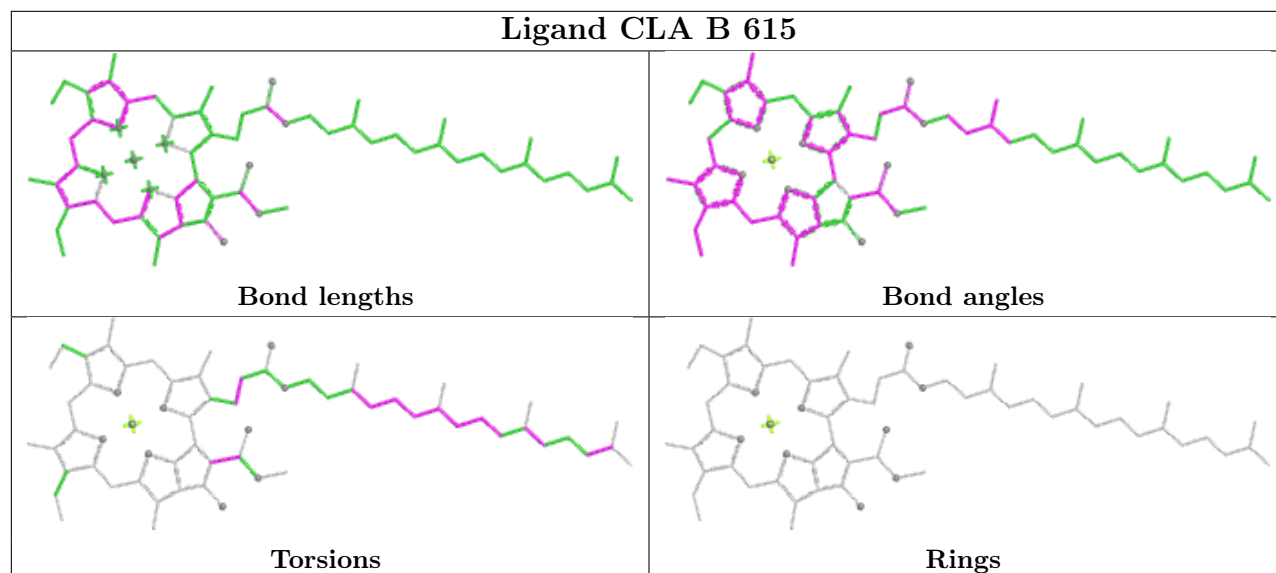
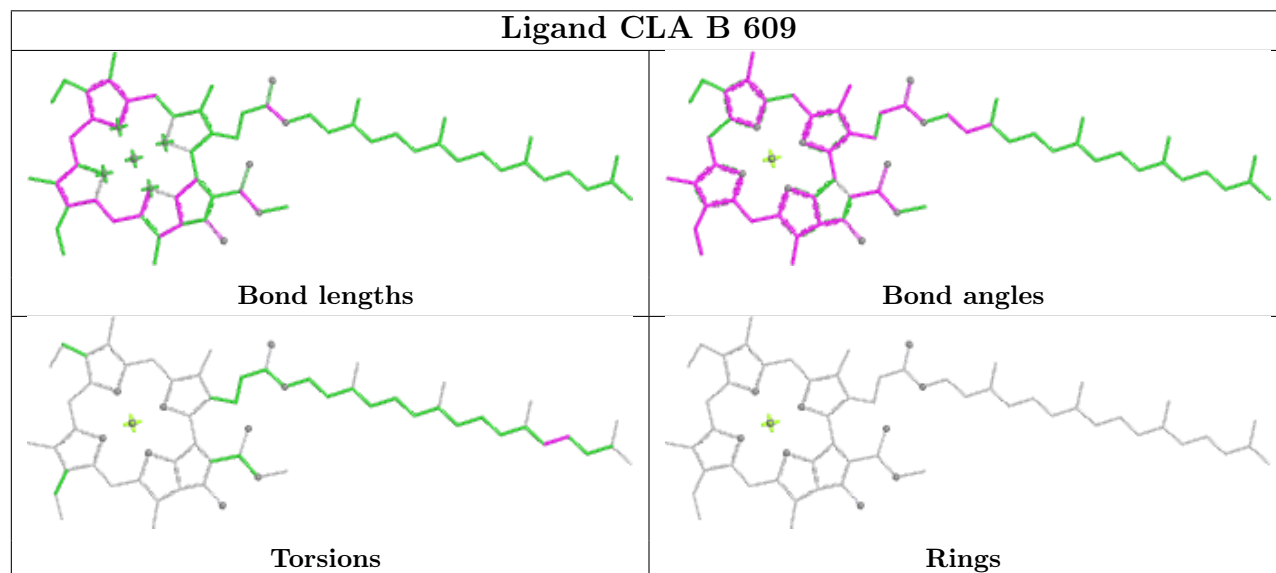
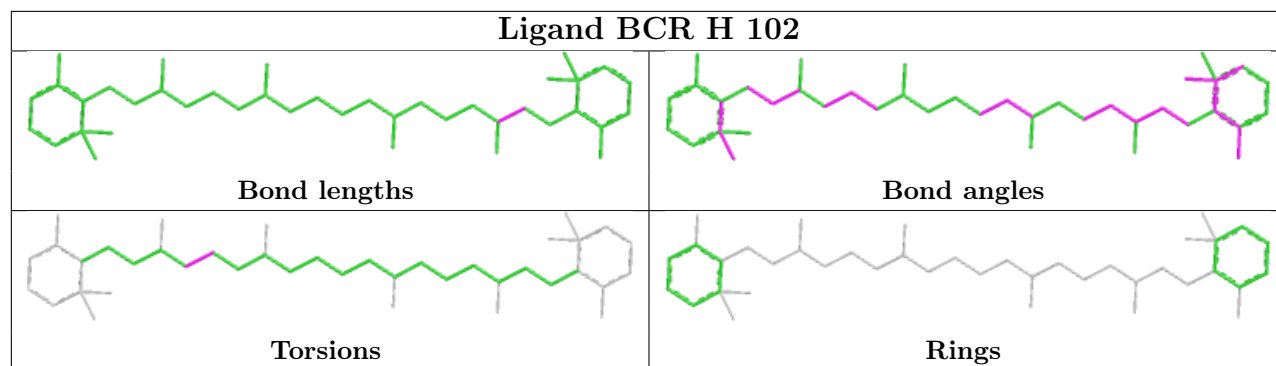
Ligand LMT D 401

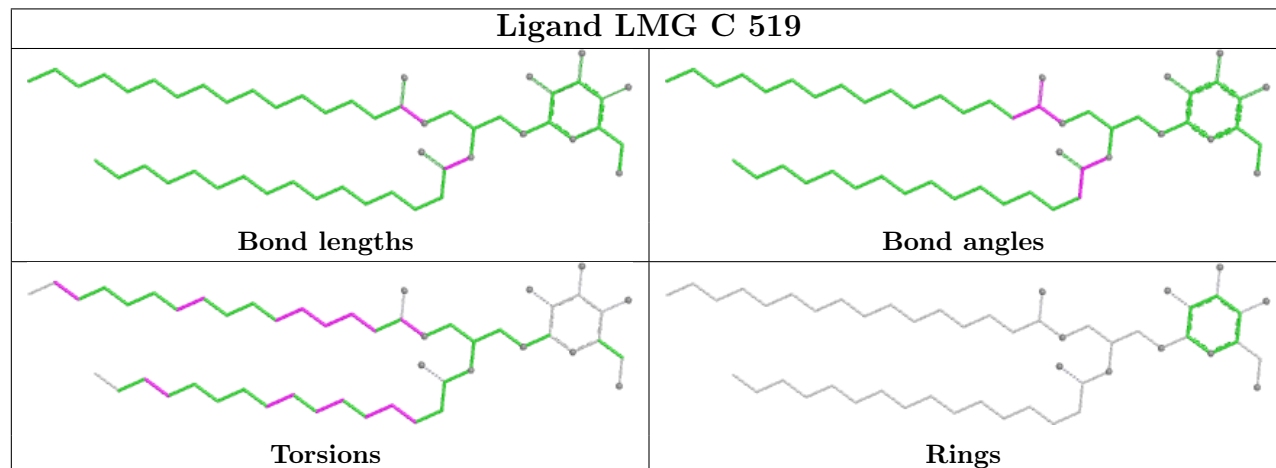
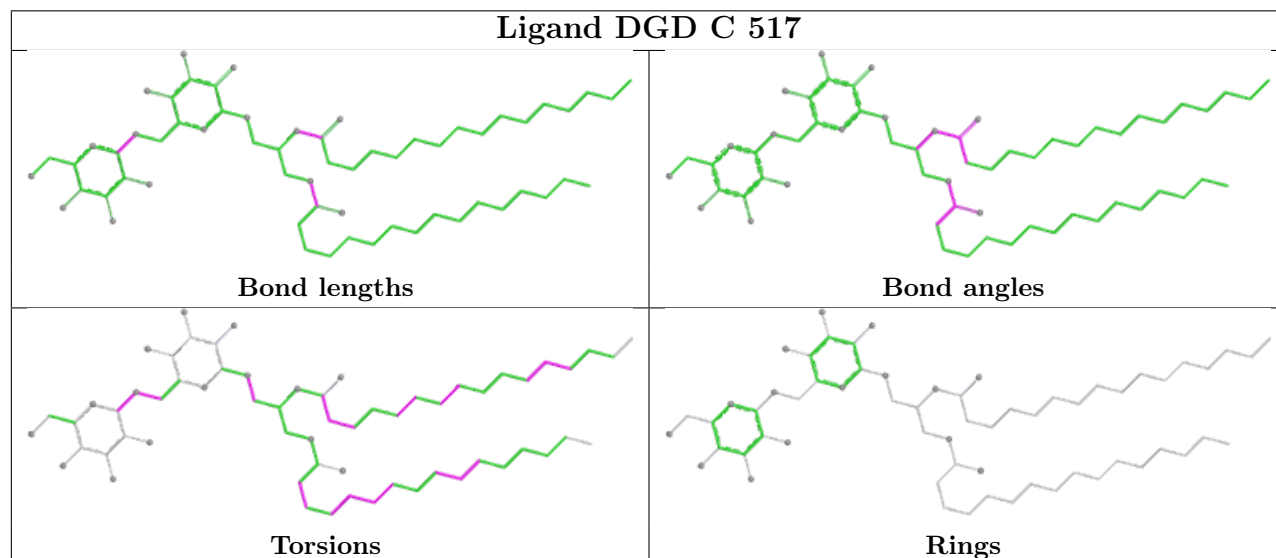
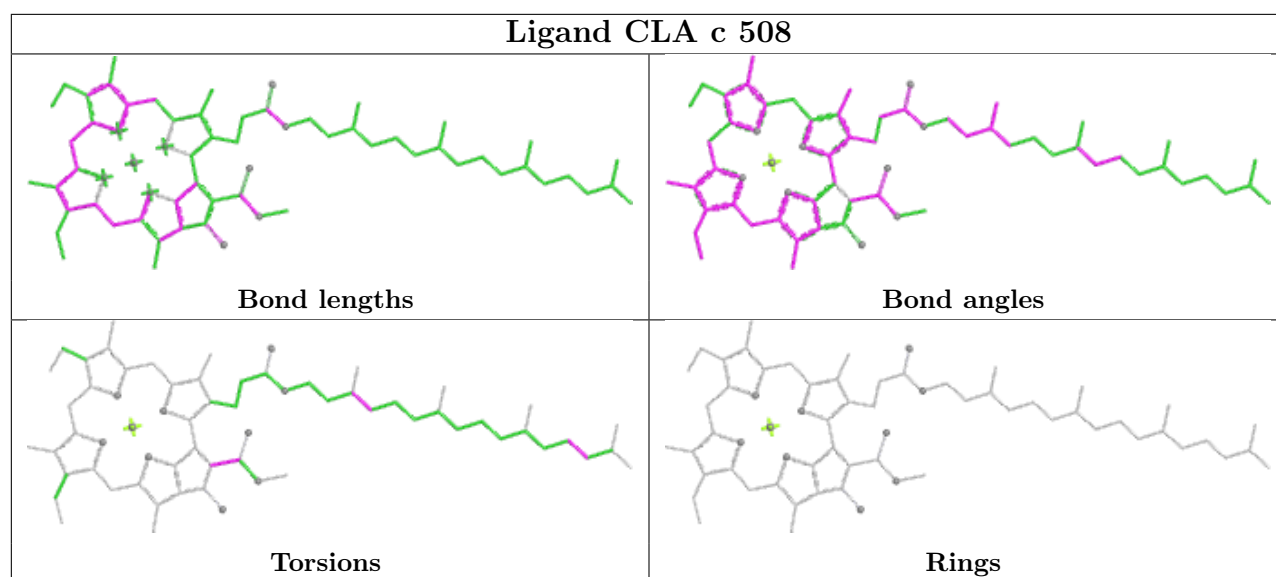


Ligand CLA b 615

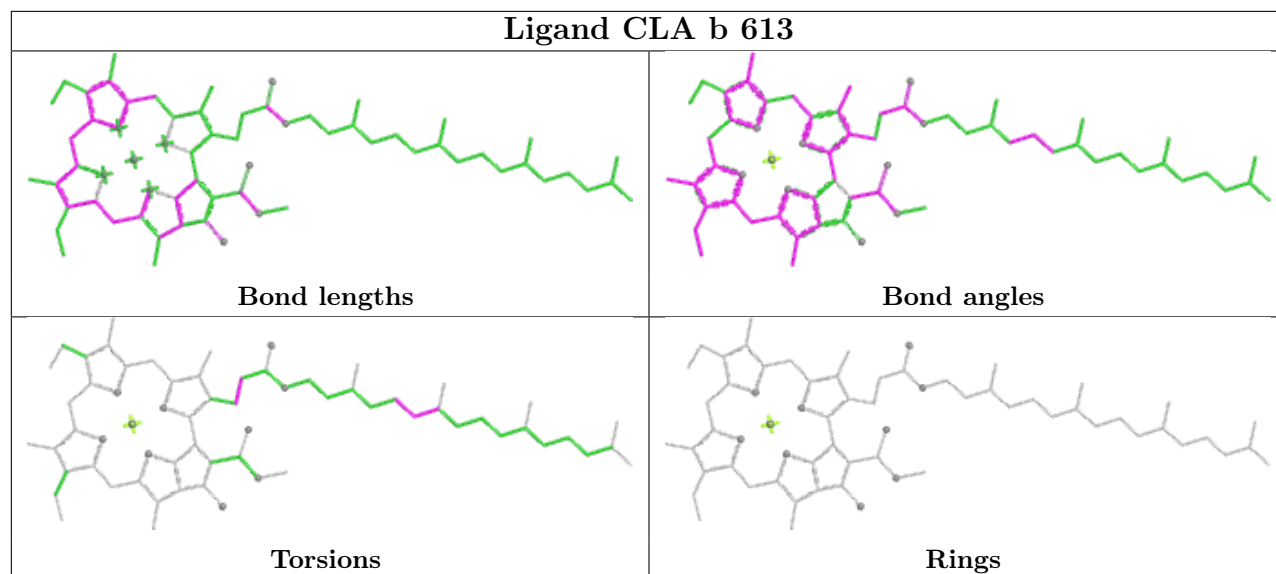




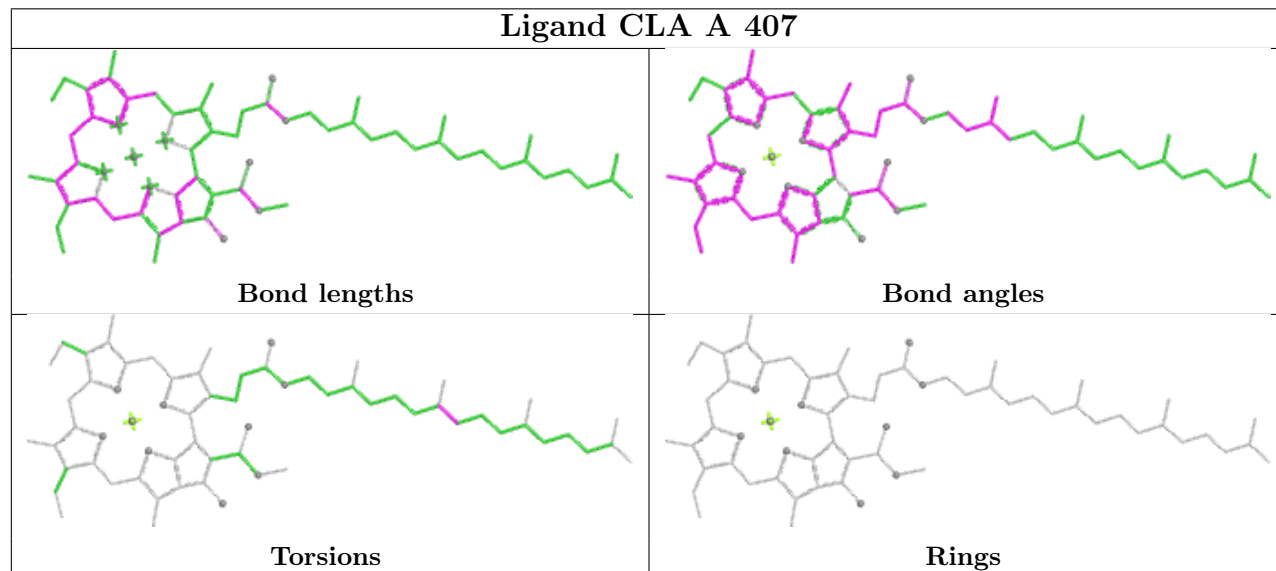


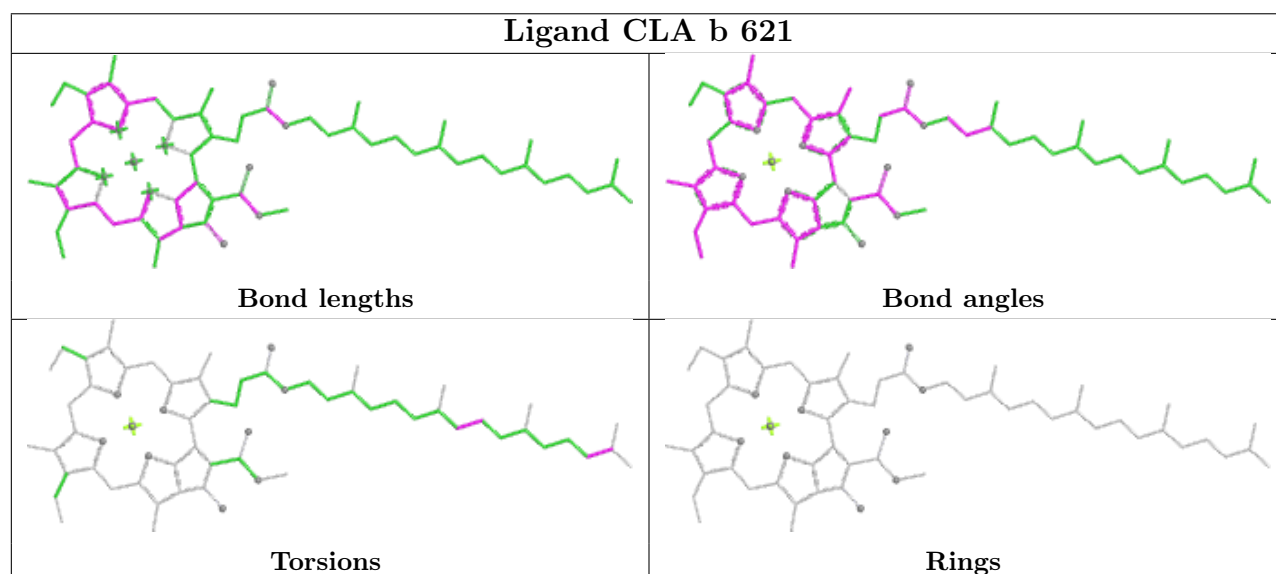
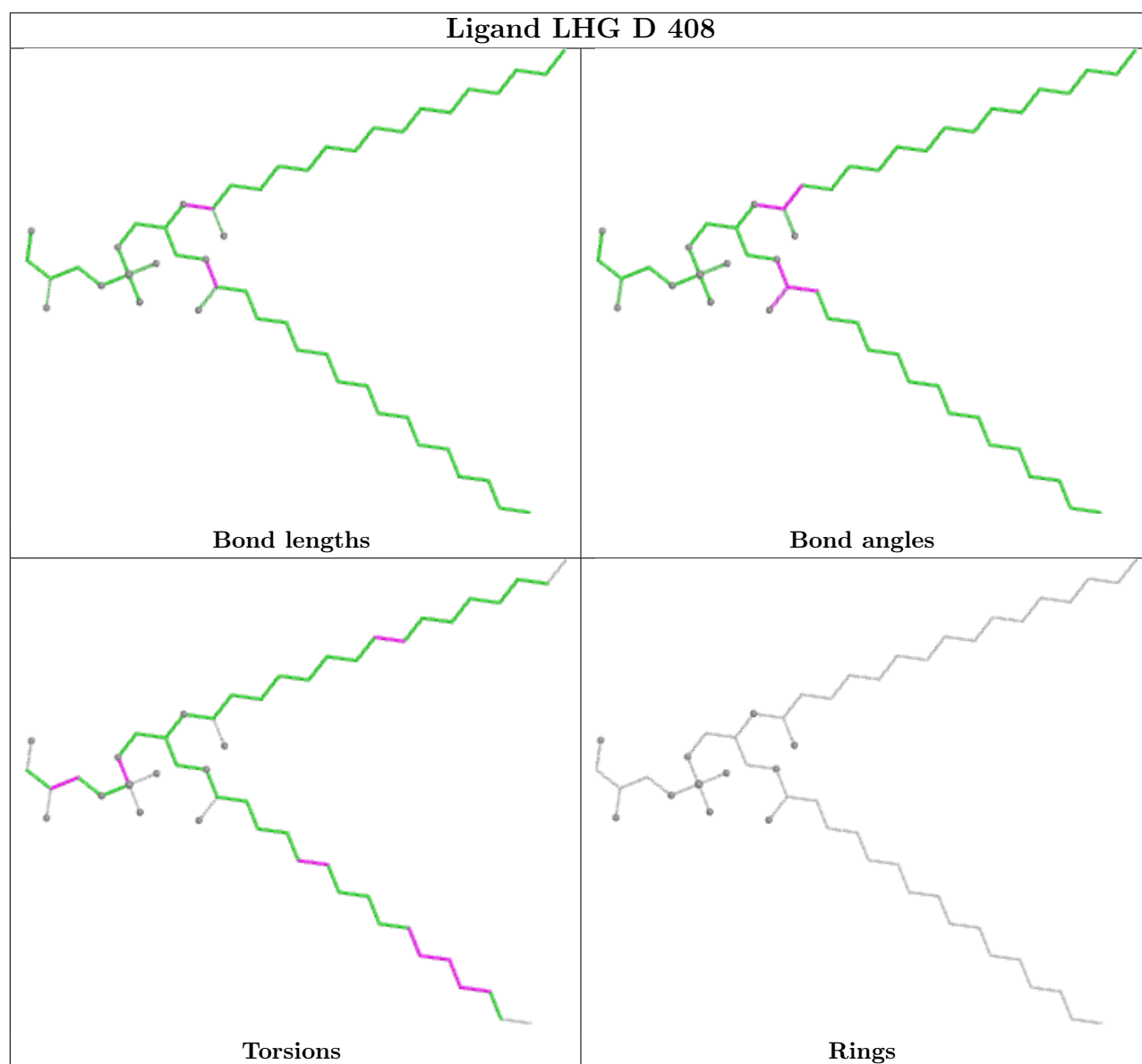


Ligand CLA b 613

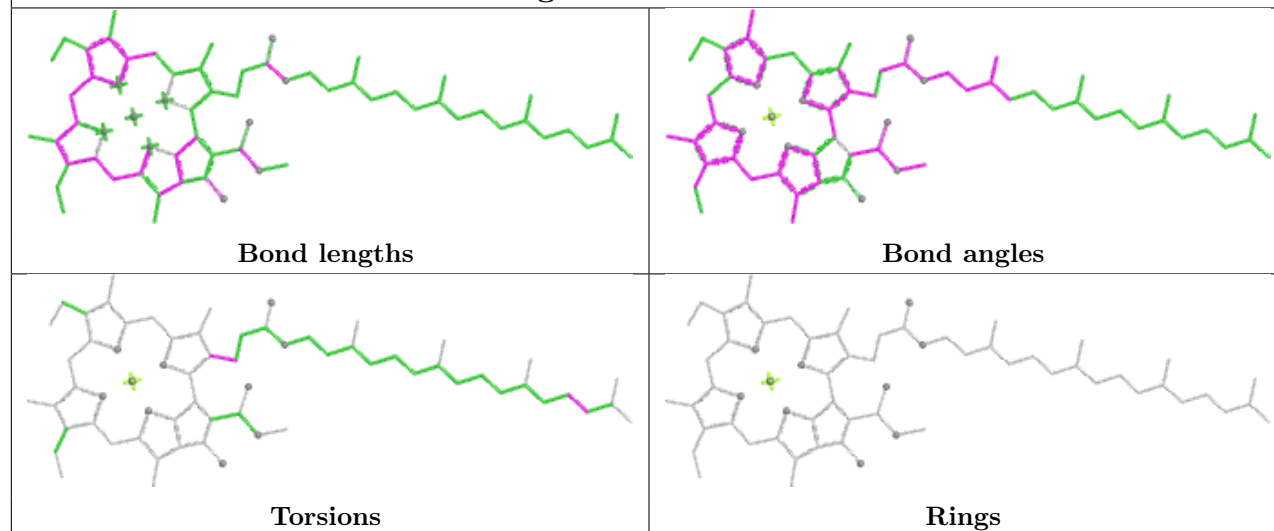


Ligand CLA A 407

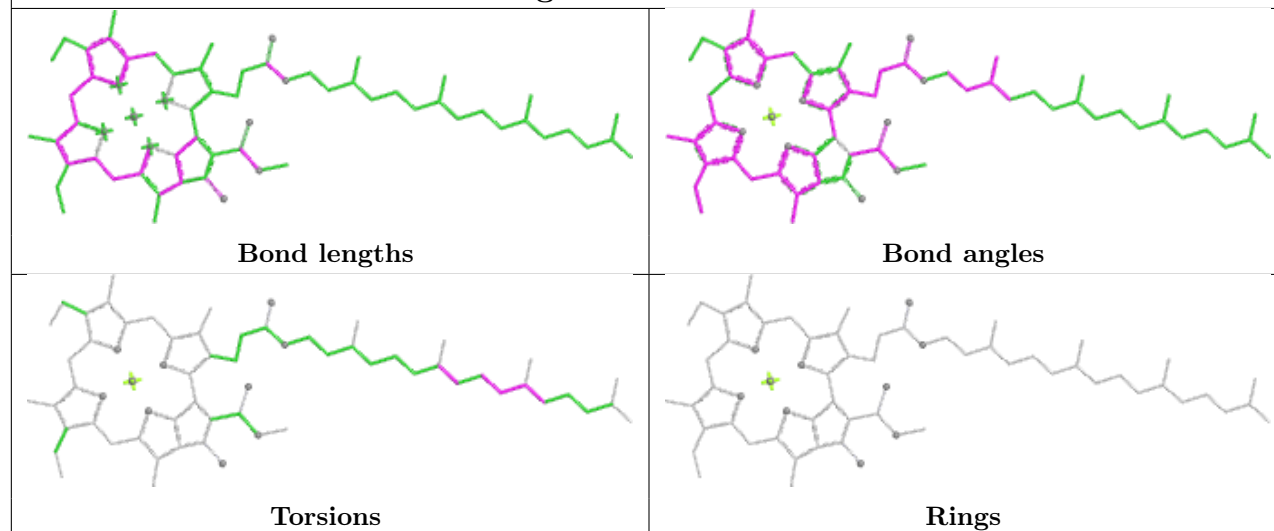




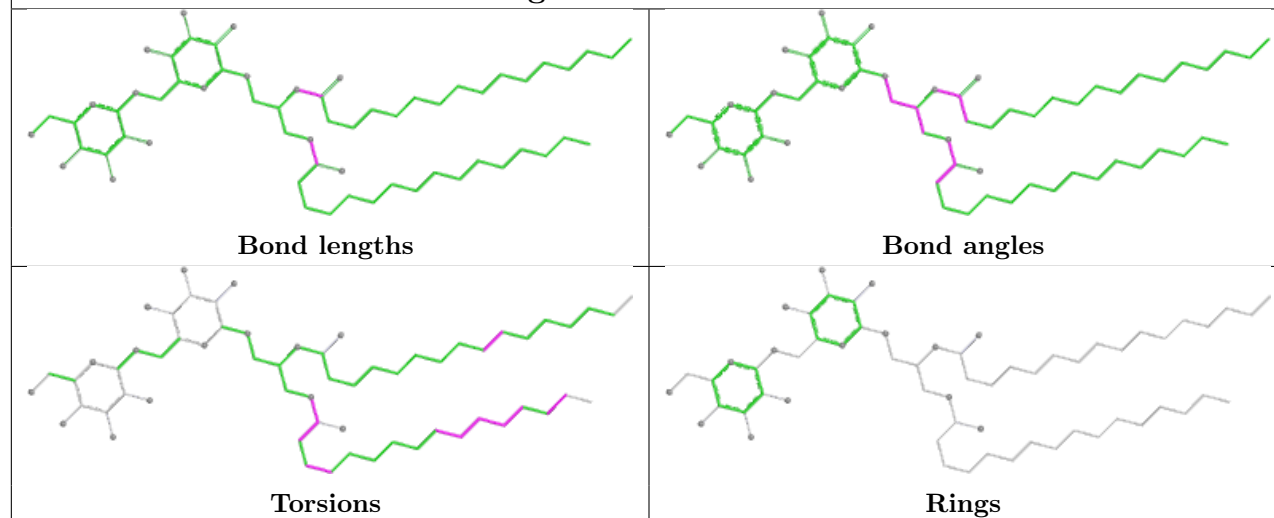
Ligand CLA c 512

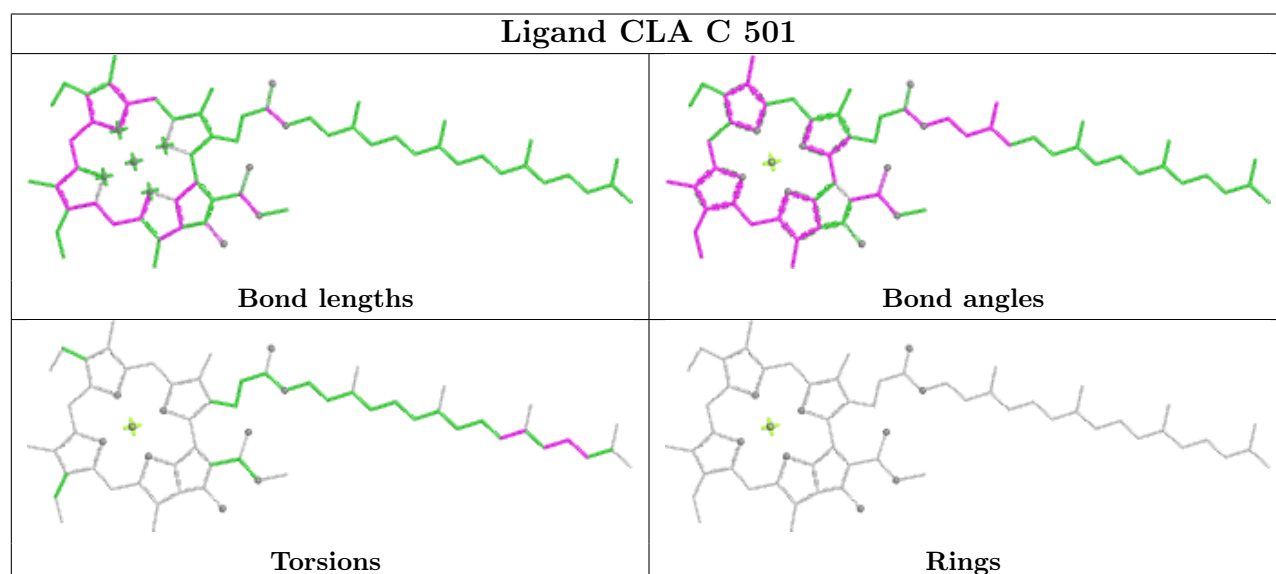
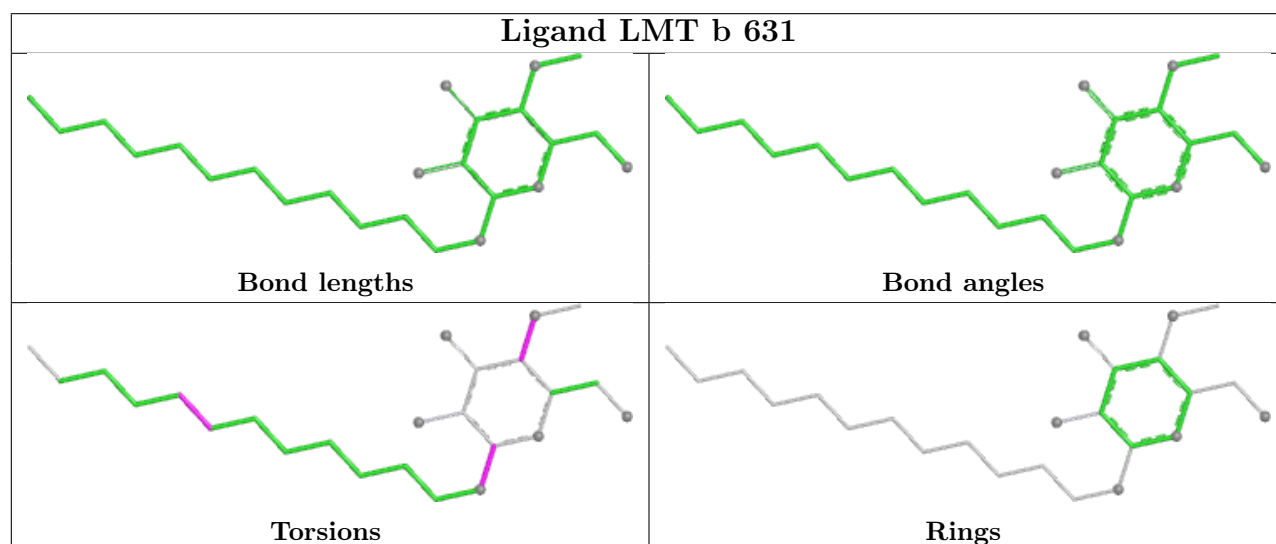
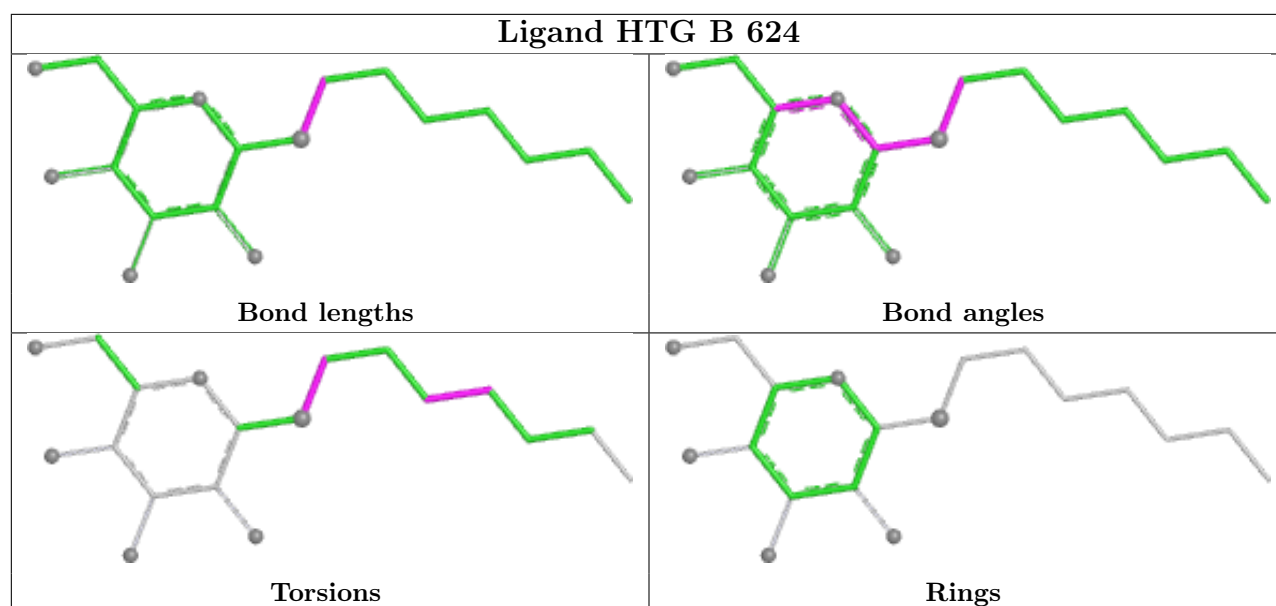


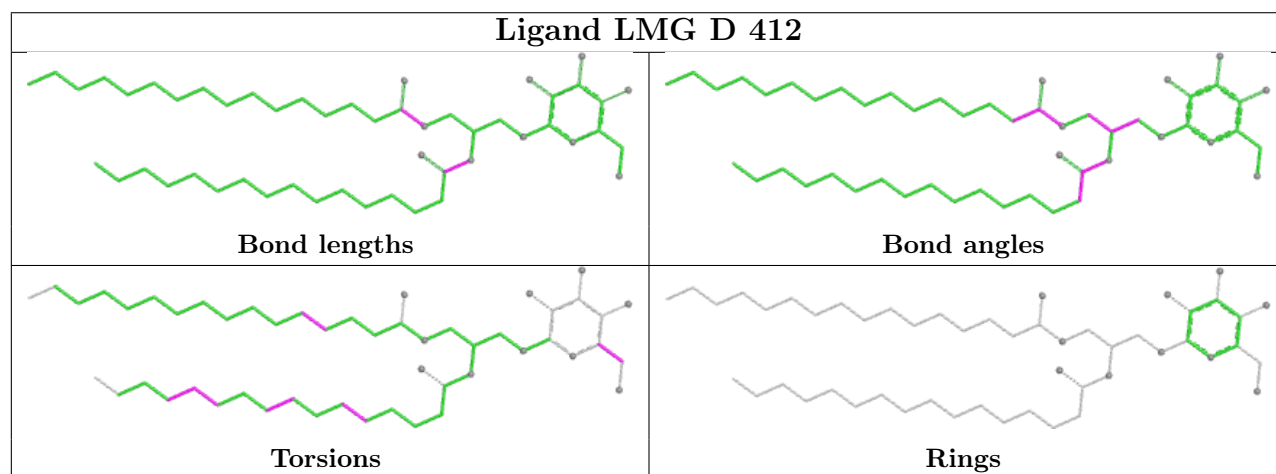
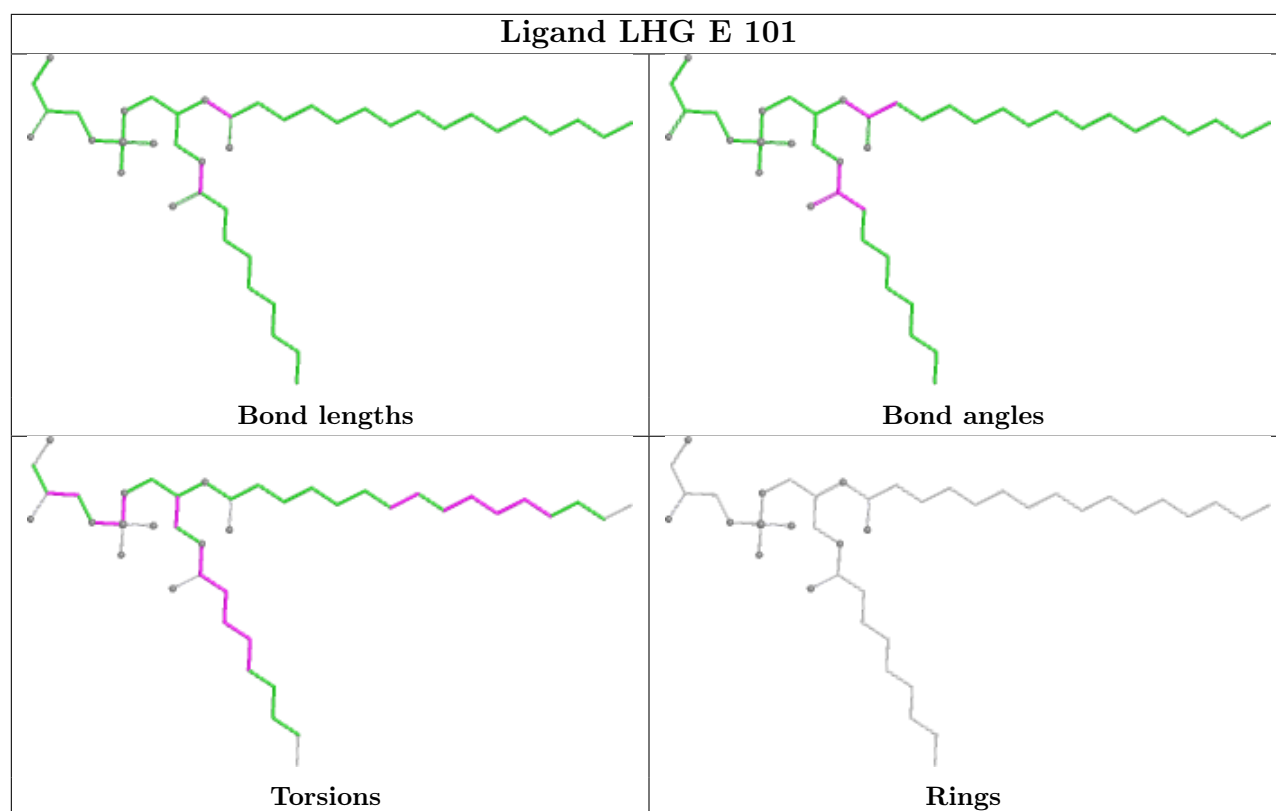
Ligand CLA a 410

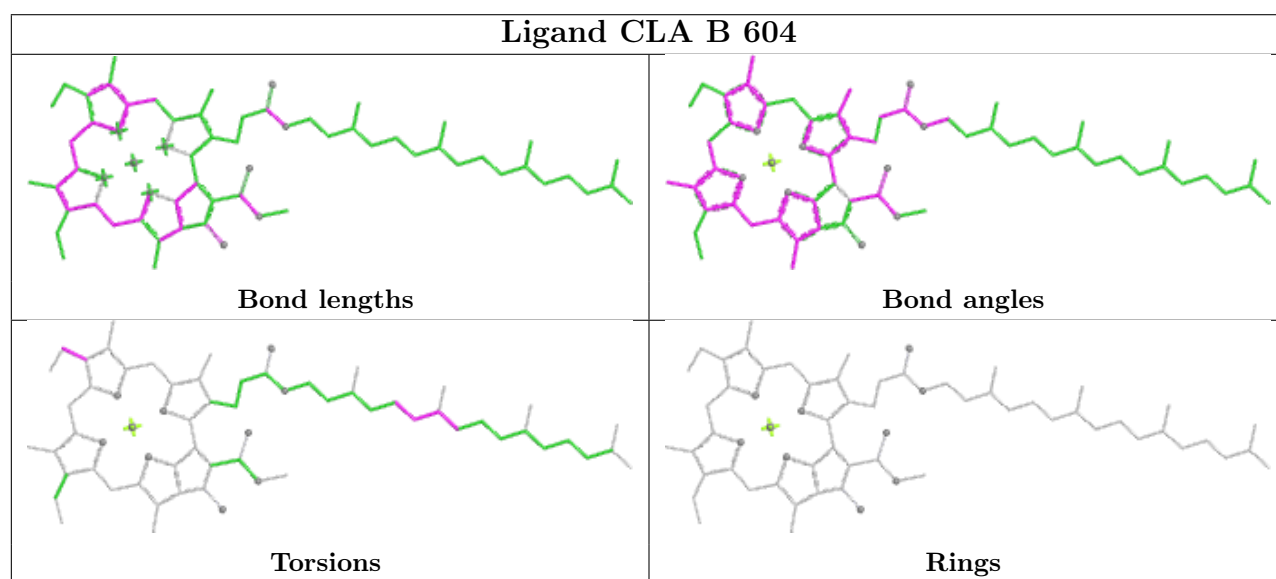
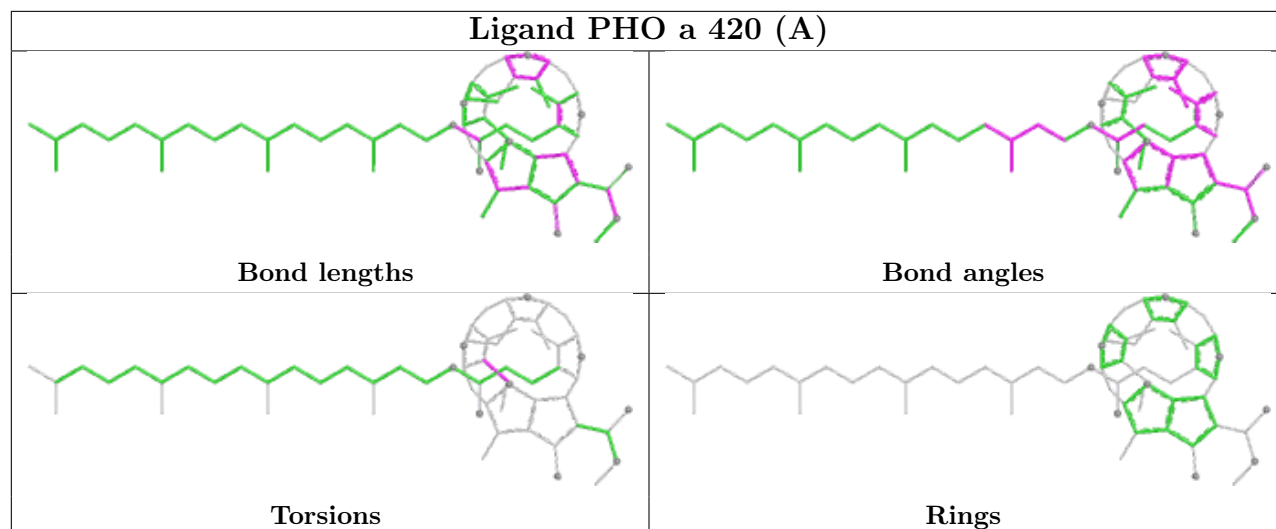


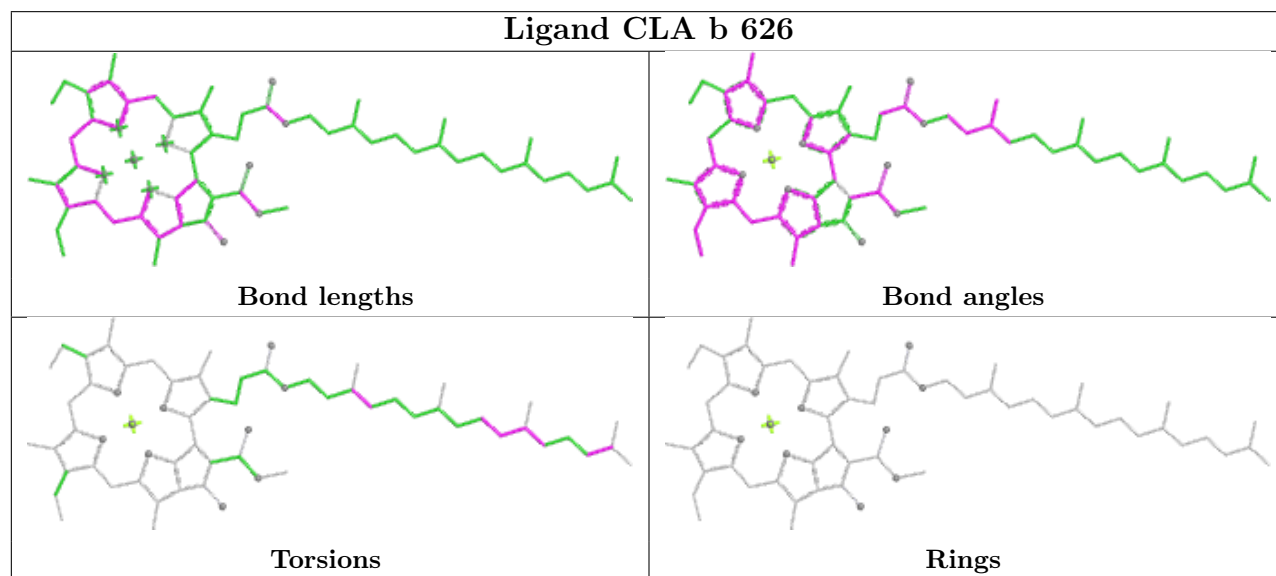
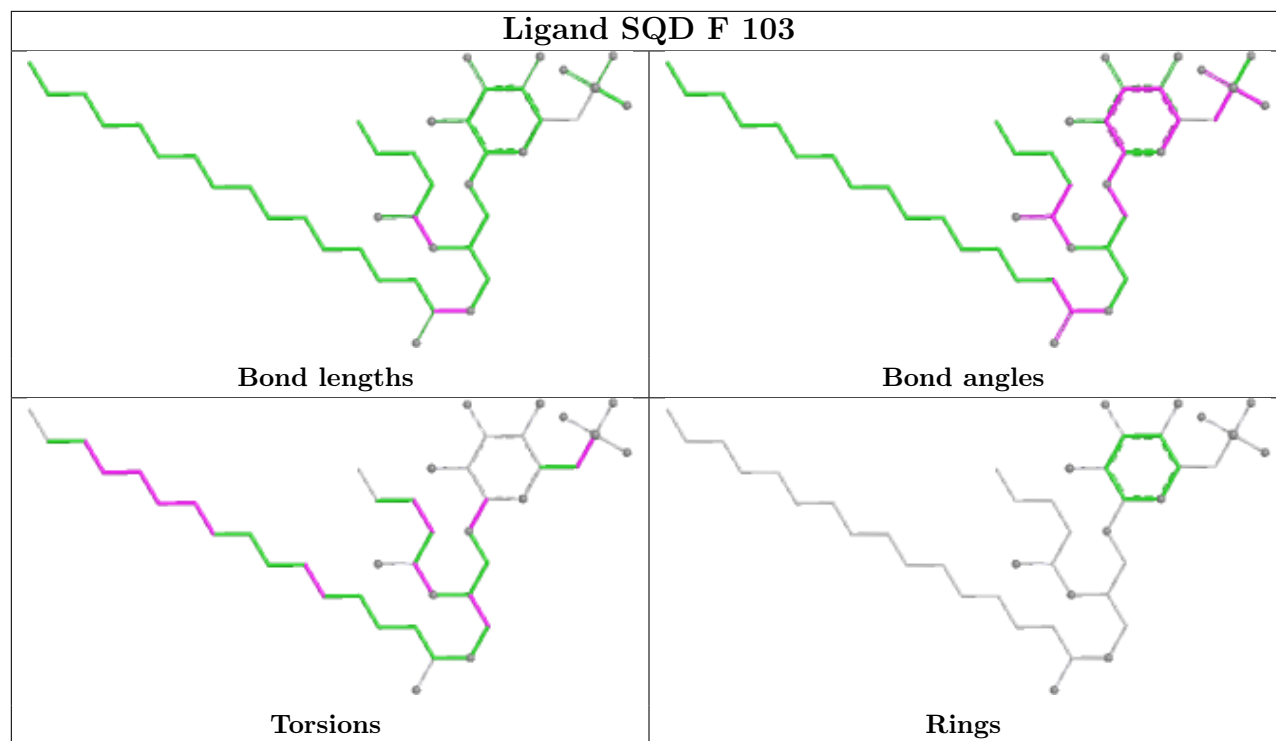
Ligand DGD C 518

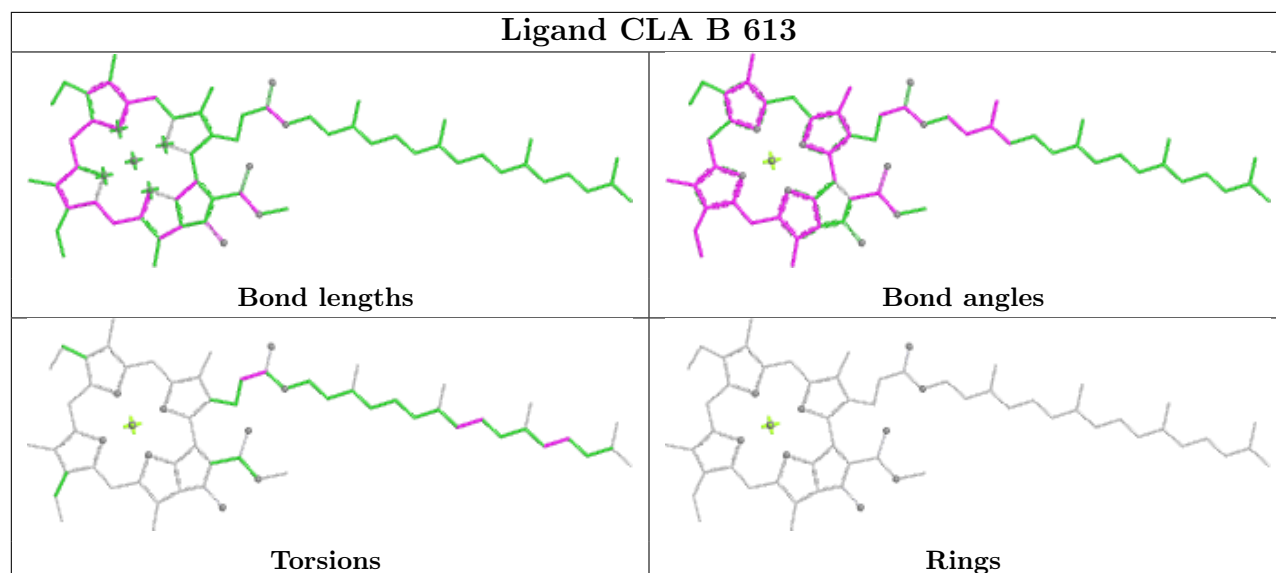
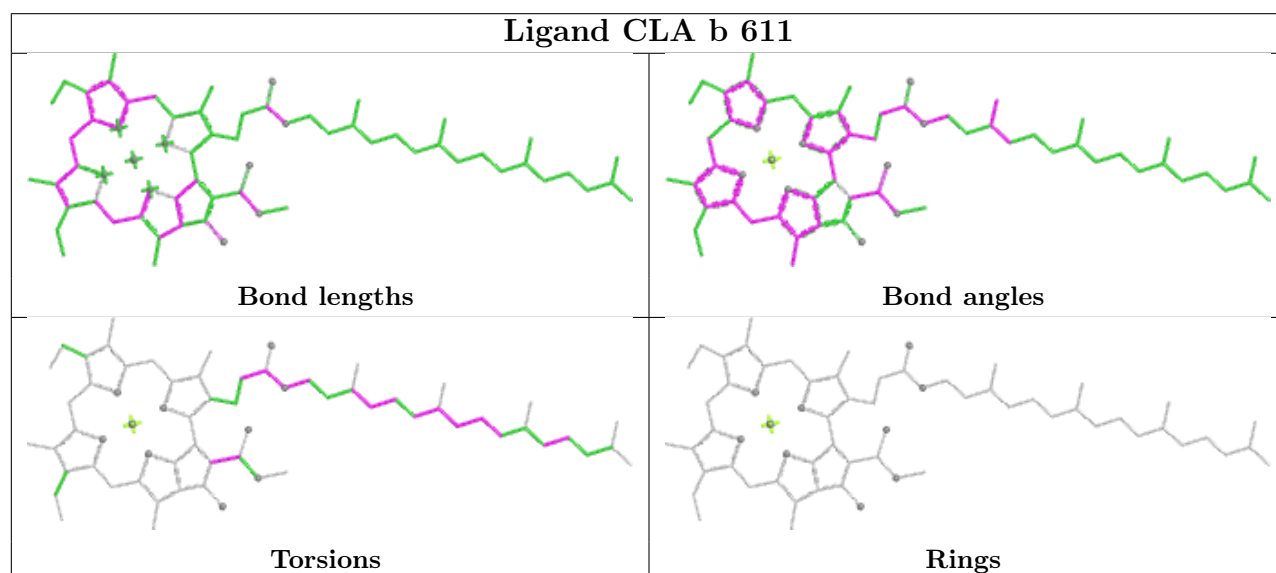
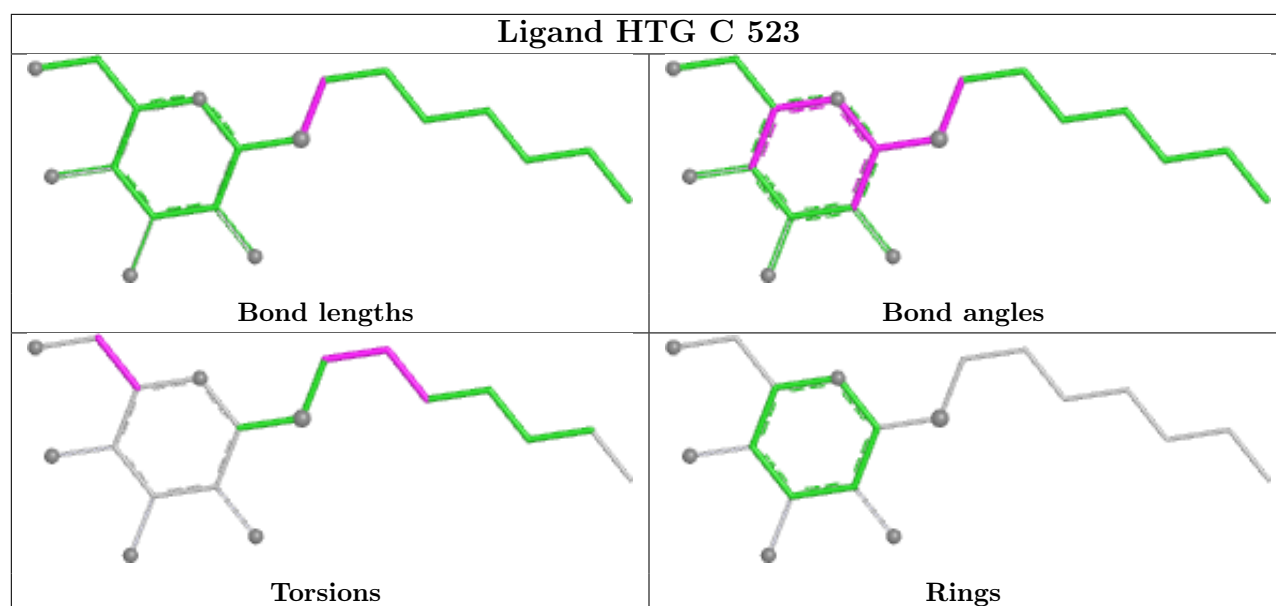




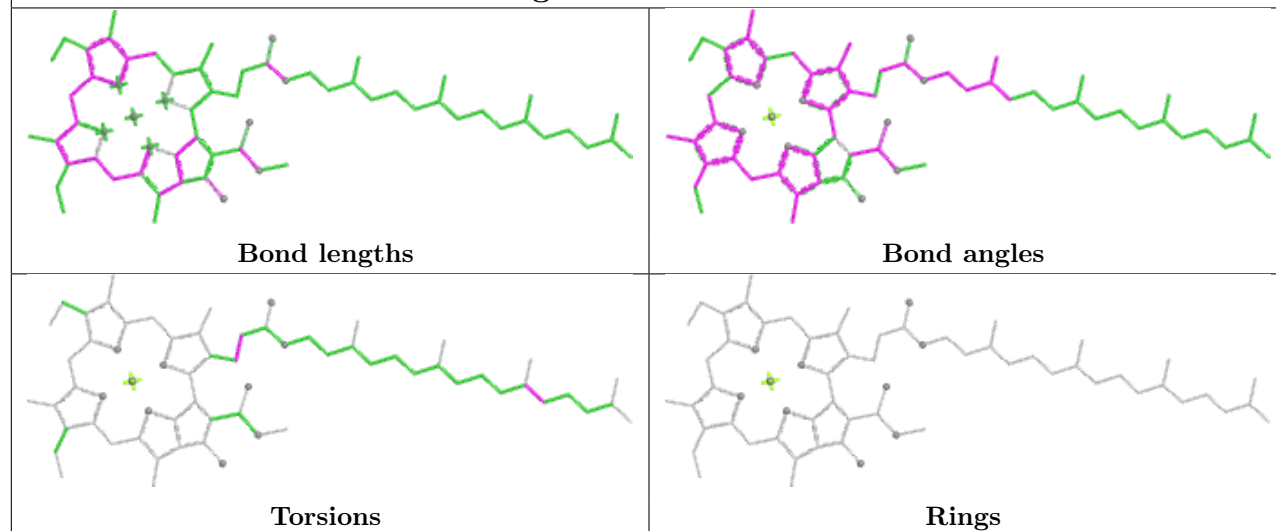




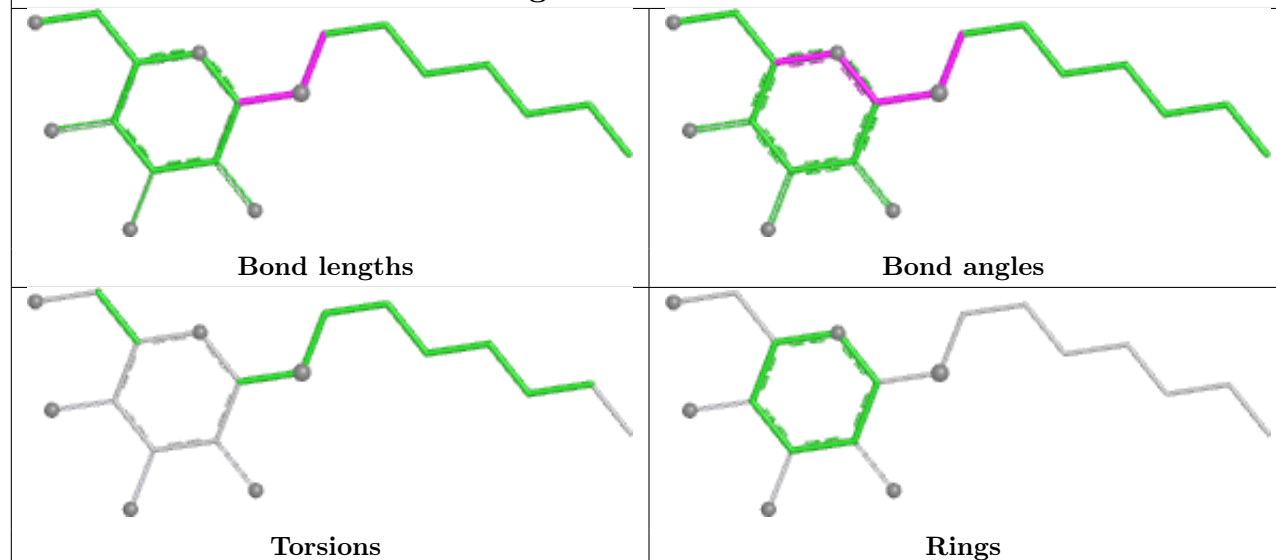




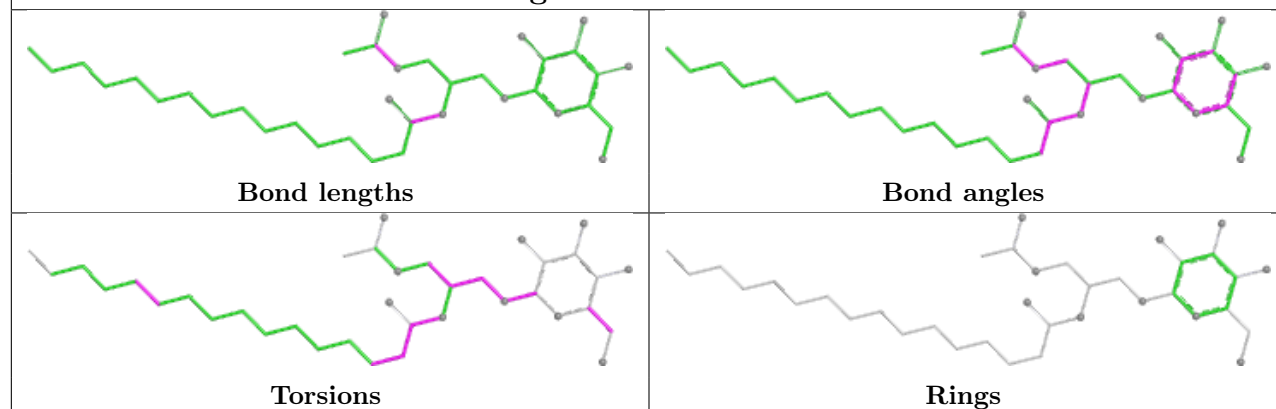
Ligand CLA B 603

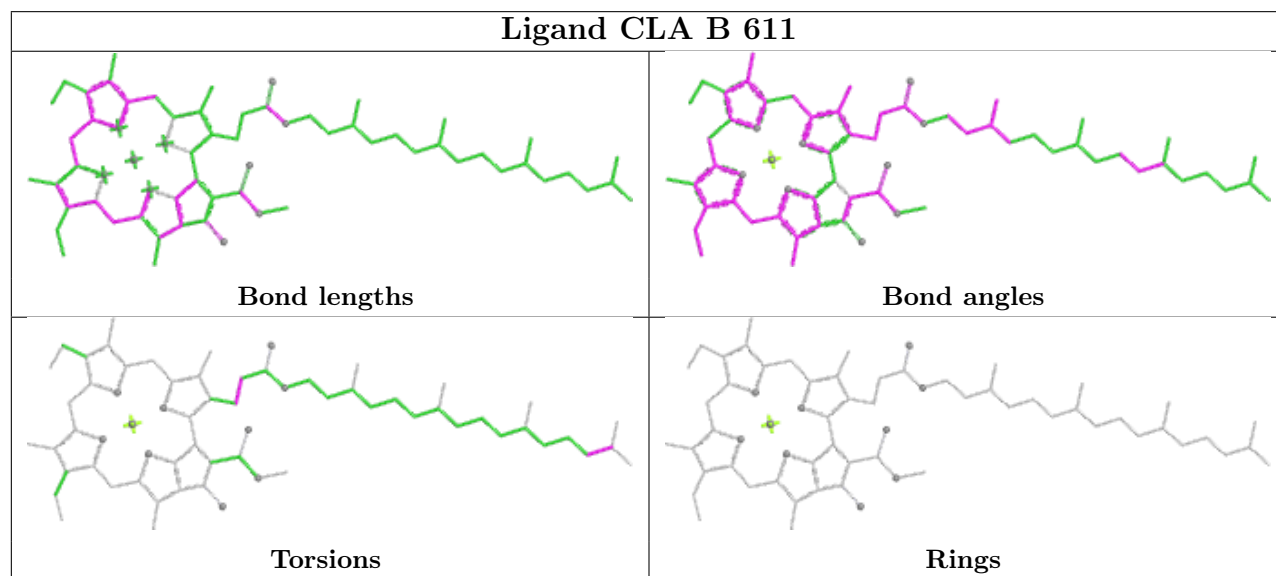
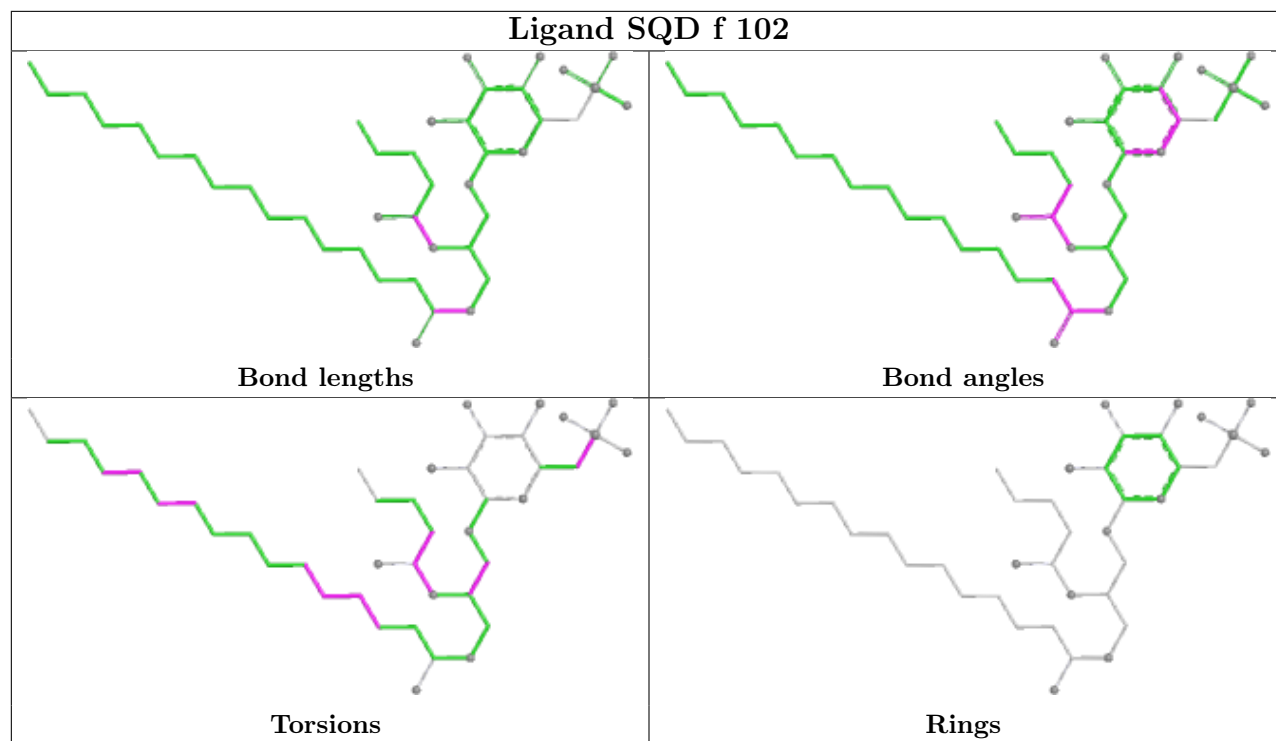


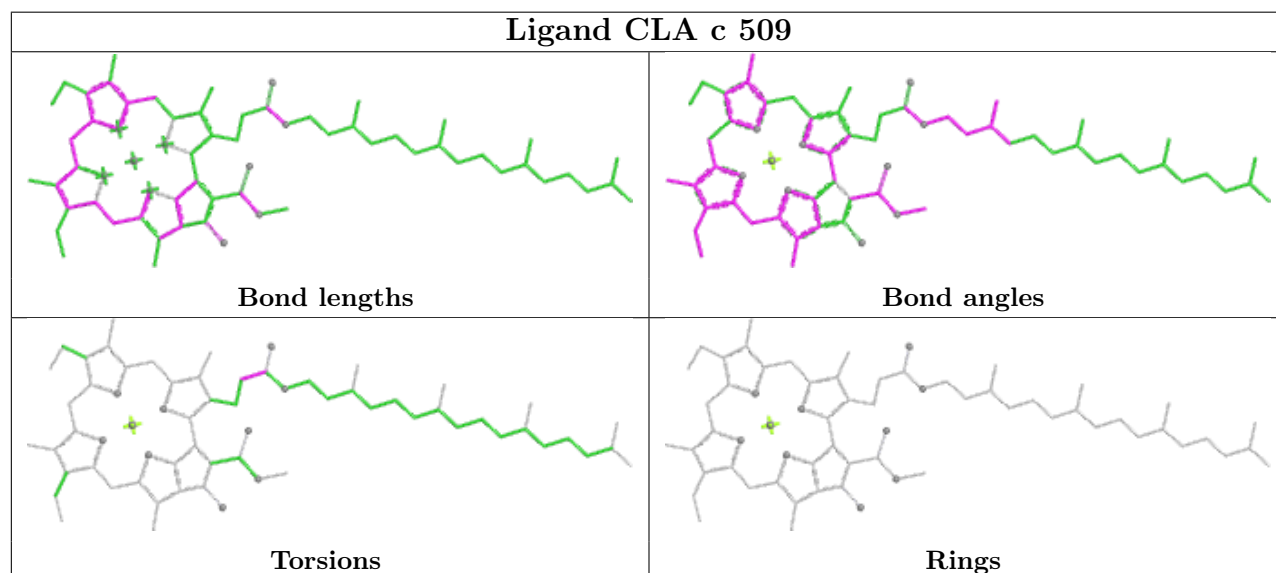
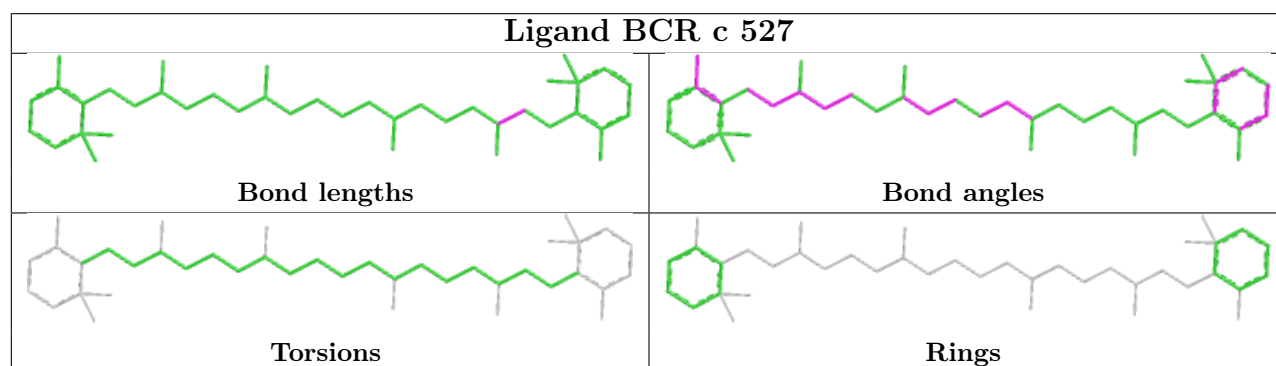
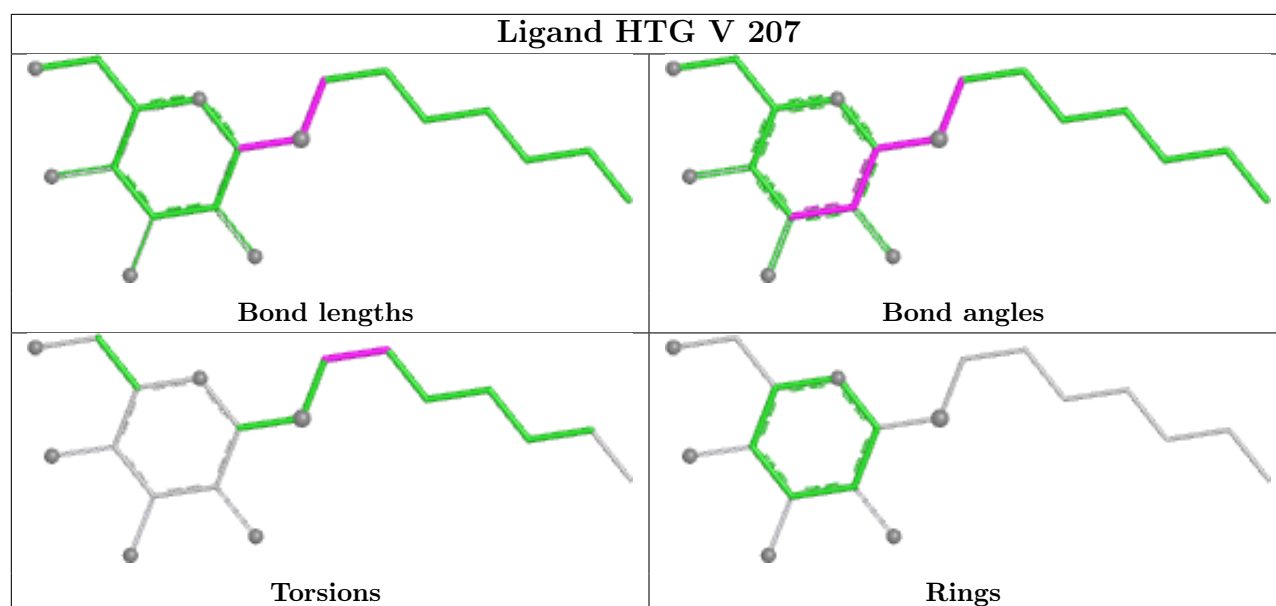
Ligand HTG C 522

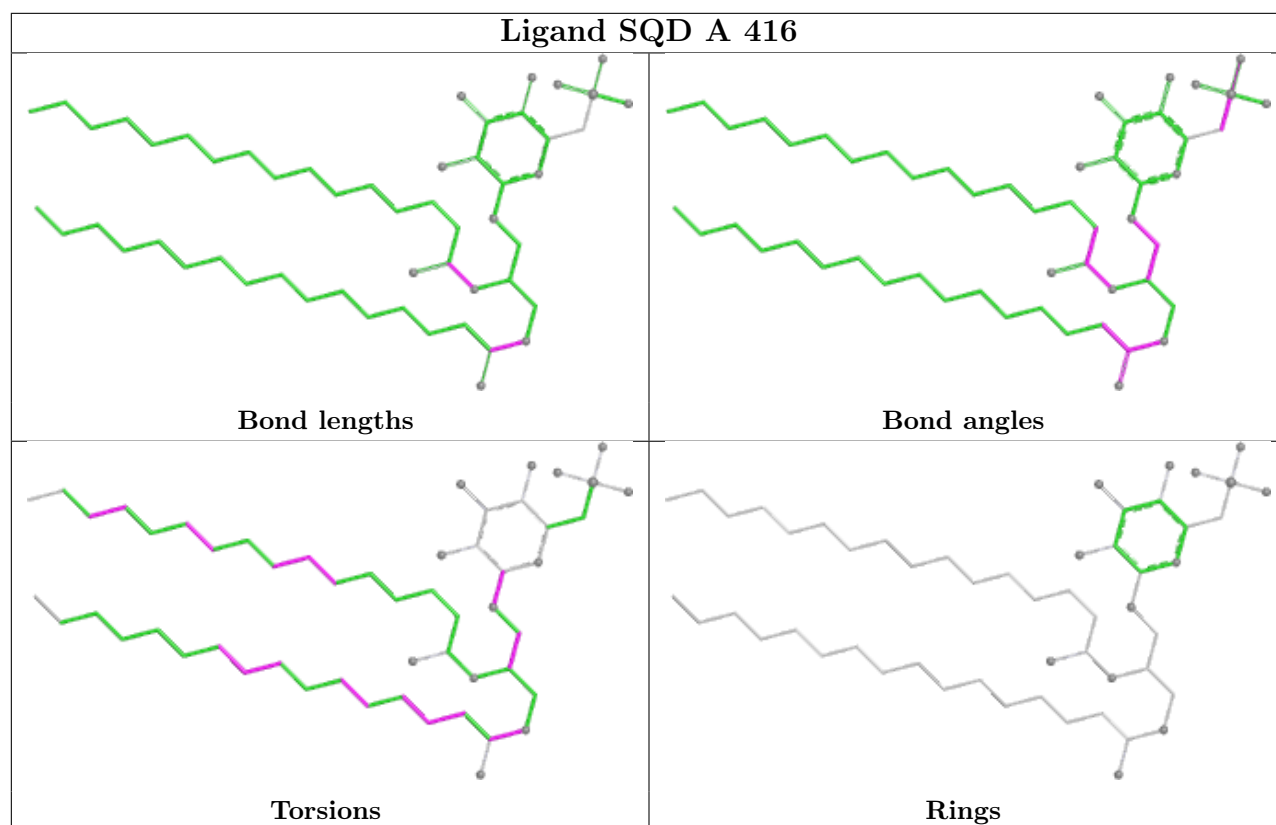
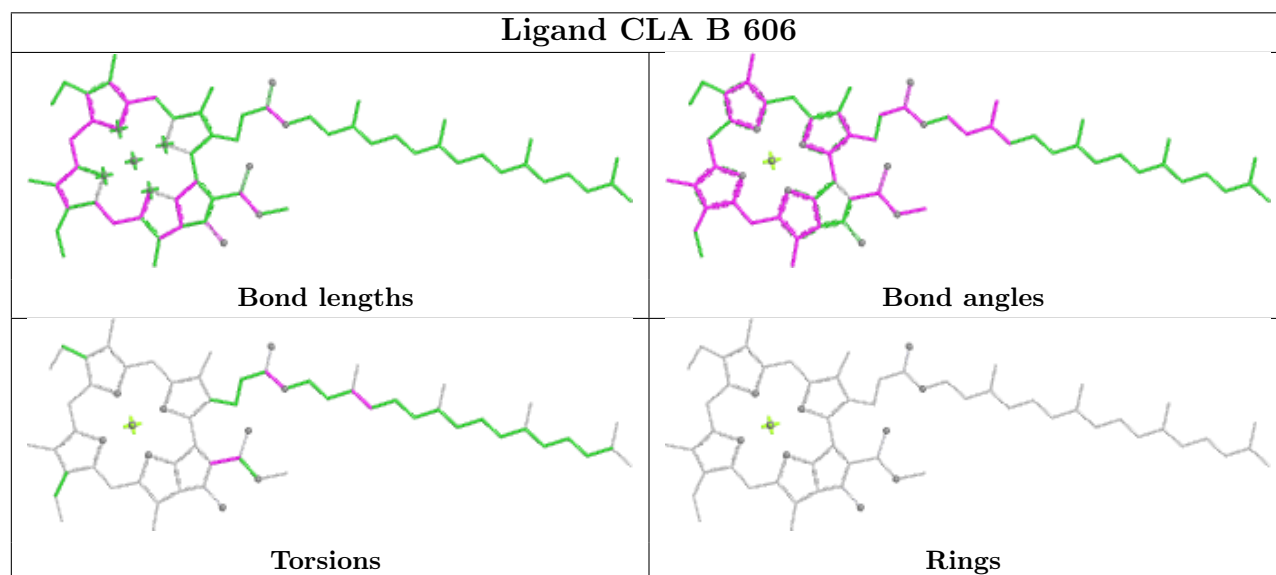
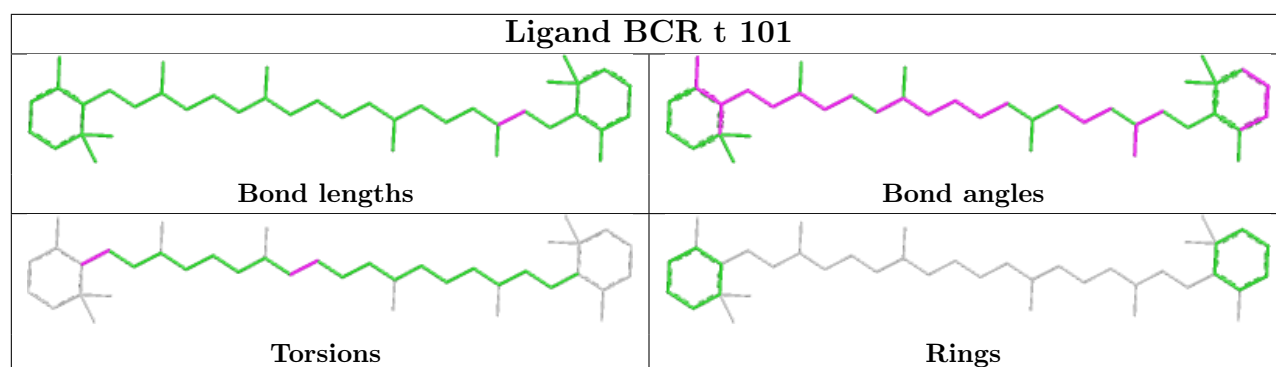


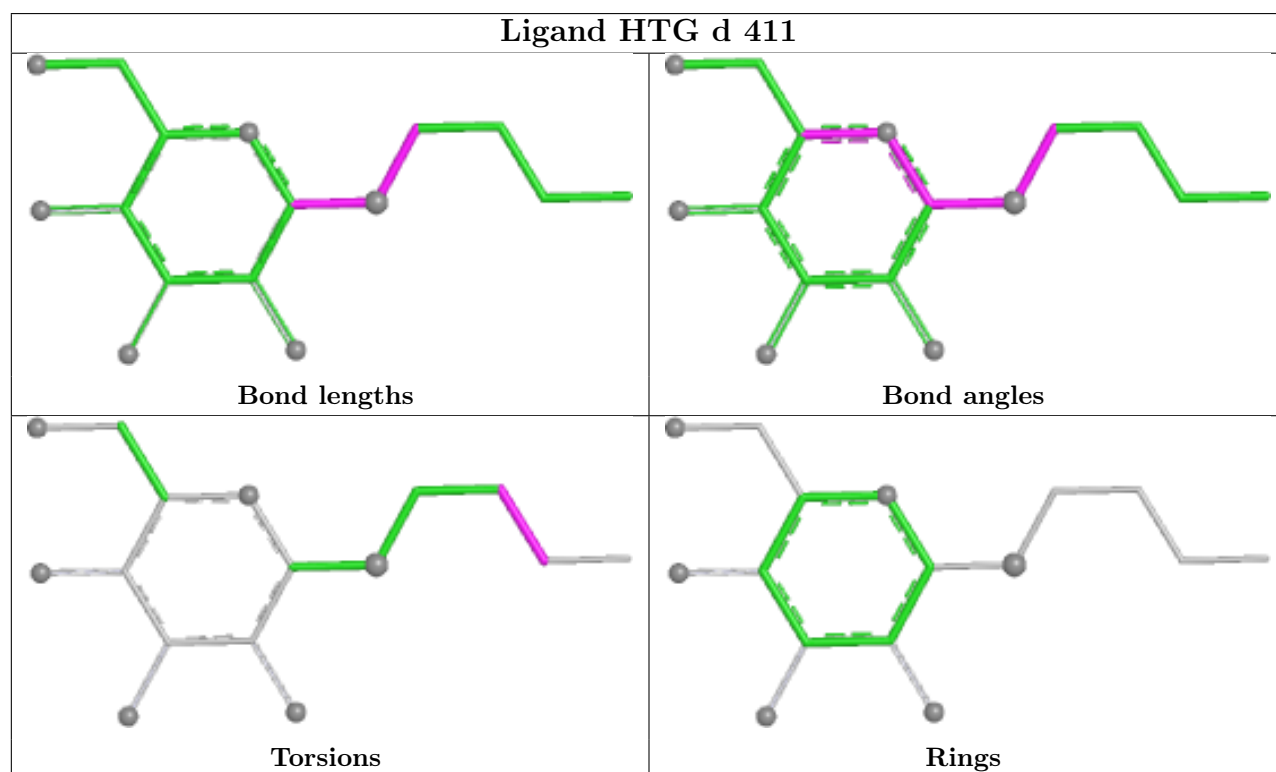
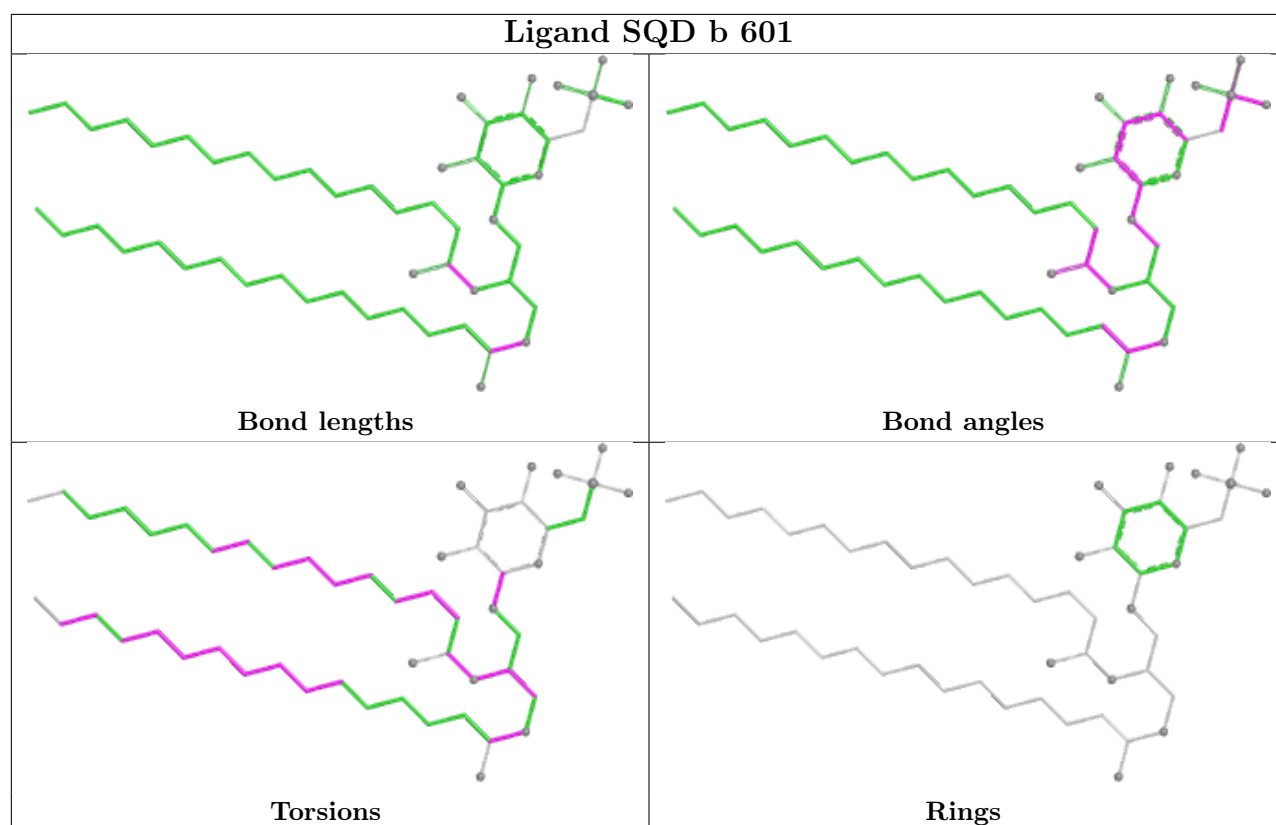
Ligand LMG Z 101

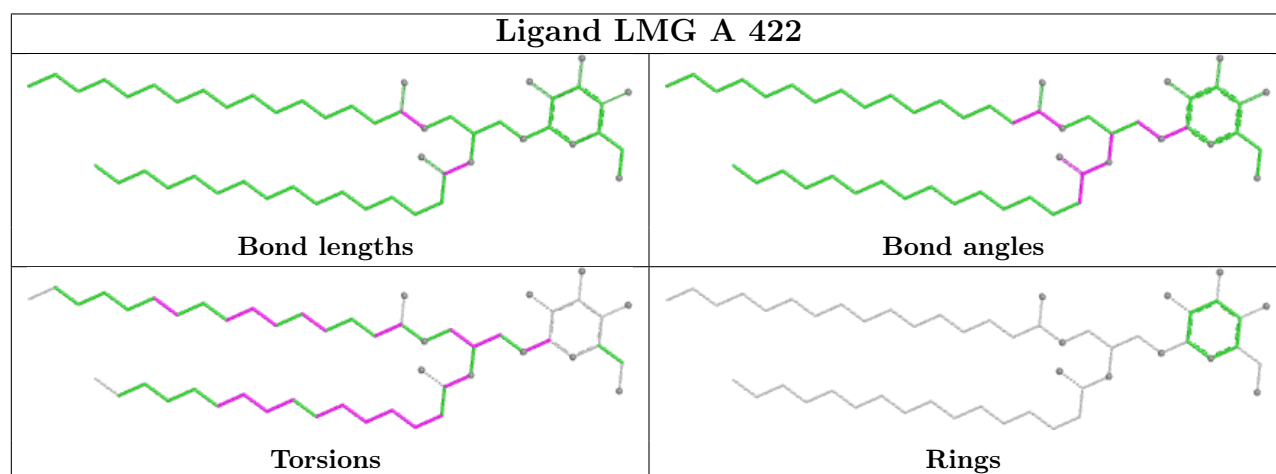
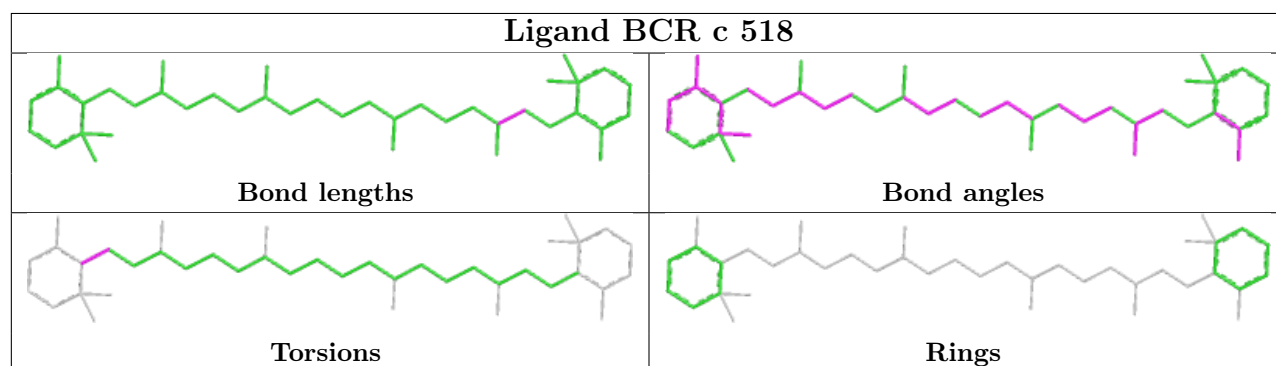
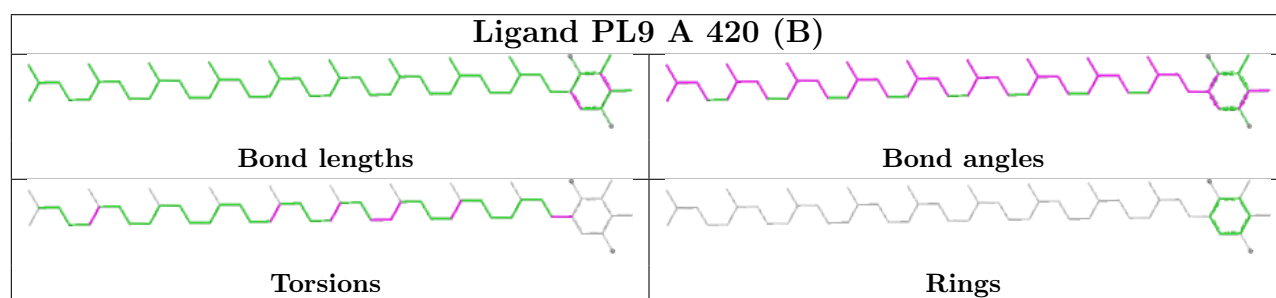
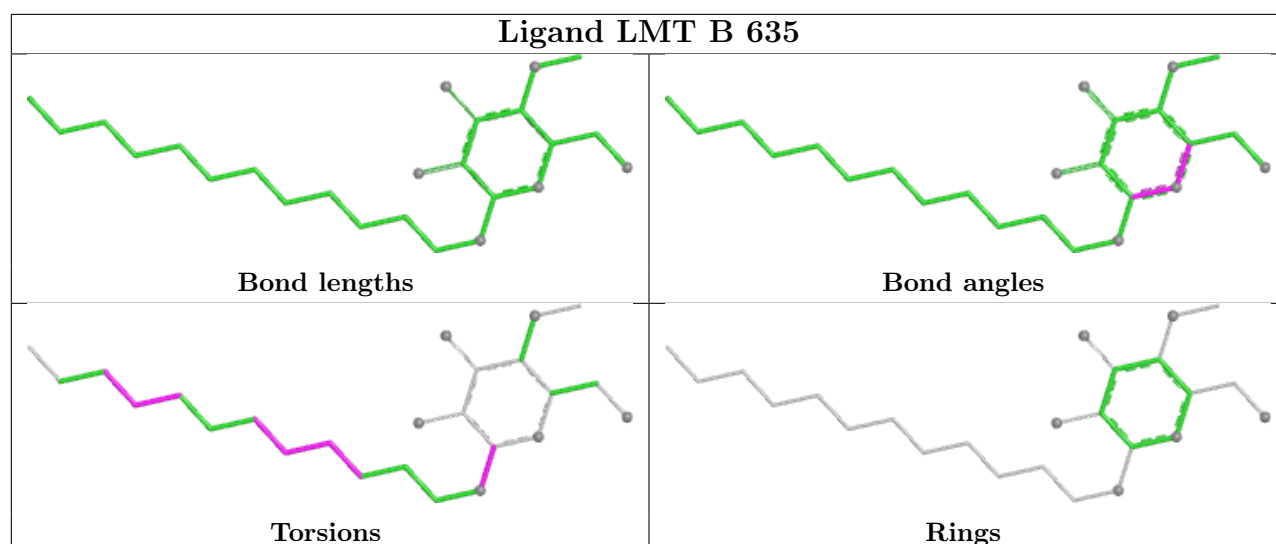


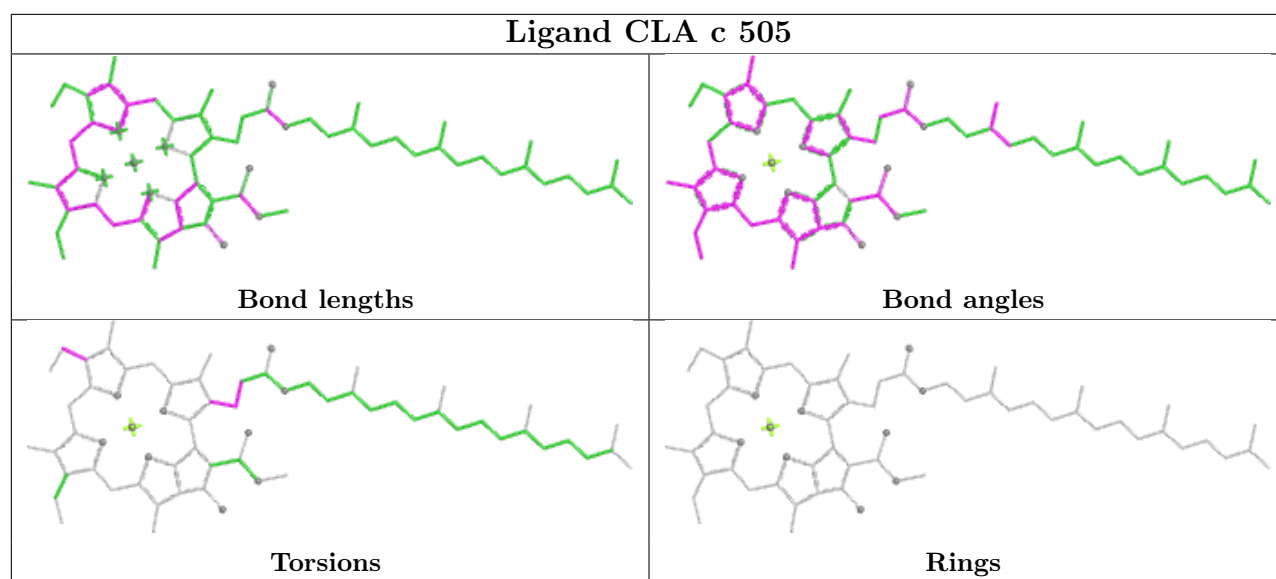












5.7 Other polymers [i](#)

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%)	-0.67	0 100 100	16, 36, 59, 107	53 (15%)
1	a	334/344 (97%)	-0.63	4 (1%) 76 79	16, 37, 71, 150	53 (15%)
2	B	504/505 (99%)	-0.61	2 (0%) 88 90	21, 42, 76, 120	10 (1%)
2	b	503/505 (99%)	-0.49	9 (1%) 67 71	26, 43, 75, 162	12 (2%)
3	C	451/455 (99%)	-0.55	0 100 100	18, 49, 68, 110	12 (2%)
3	c	455/455 (100%)	-0.51	0 100 100	18, 52, 70, 121	20 (4%)
4	D	341/342 (99%)	-0.73	0 100 100	18, 38, 59, 134	16 (4%)
4	d	341/342 (99%)	-0.71	0 100 100	19, 40, 58, 112	16 (4%)
5	E	81/84 (96%)	-0.09	1 (1%) 76 79	30, 62, 92, 139	2 (2%)
5	e	81/84 (96%)	-0.00	2 (2%) 58 62	36, 64, 110, 167	2 (2%)
6	F	34/44 (77%)	-0.25	0 100 100	45, 54, 92, 96	0
6	f	32/44 (72%)	-0.16	1 (3%) 51 55	45, 54, 112, 130	0
7	H	65/65 (100%)	-0.37	2 (3%) 51 55	33, 52, 68, 144	1 (1%)
7	h	65/65 (100%)	-0.37	2 (3%) 51 55	40, 54, 74, 162	0
8	I	37/38 (97%)	-0.21	0 100 100	44, 52, 104, 148	0
8	i	37/38 (97%)	-0.27	1 (2%) 56 60	41, 50, 97, 126	0
9	J	38/39 (97%)	-0.02	2 (5%) 32 36	42, 58, 135, 165	0
9	j	39/39 (100%)	-0.09	1 (2%) 57 61	46, 59, 130, 162	0
10	K	37/37 (100%)	-0.38	0 100 100	50, 58, 72, 91	0
10	k	37/37 (100%)	-0.27	0 100 100	50, 63, 79, 98	0
11	L	37/37 (100%)	-0.68	0 100 100	18, 34, 94, 106	1 (2%)
11	l	37/37 (100%)	-0.63	0 100 100	22, 35, 90, 121	1 (2%)
12	M	33/36 (91%)	-0.73	0 100 100	22, 36, 61, 112	1 (3%)
12	m	33/36 (91%)	-0.64	0 100 100	30, 37, 66, 108	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	243/244 (99%)	-0.60	1 (0%) 88 90	24, 47, 91, 130	8 (3%)
13	o	243/244 (99%)	-0.44	2 (0%) 82 84	26, 49, 103, 167	5 (2%)
14	T	29/32 (90%)	-0.74	1 (3%) 48 52	30, 36, 62, 135	1 (3%)
14	t	29/32 (90%)	-0.64	1 (3%) 48 52	27, 36, 64, 128	1 (3%)
15	U	97/104 (93%)	-0.63	0 100 100	35, 46, 75, 109	0
15	u	97/104 (93%)	-0.60	0 100 100	37, 49, 68, 117	0
16	V	137/137 (100%)	-0.67	0 100 100	19, 45, 65, 84	2 (1%)
16	v	137/137 (100%)	-0.51	0 100 100	22, 56, 82, 129	1 (0%)
17	Y	29/30 (96%)	0.60	3 (10%) 12 13	60, 71, 151, 153	0
17	y	29/30 (96%)	0.36	0 100 100	68, 80, 106, 124	0
18	X	39/40 (97%)	-0.04	0 100 100	47, 60, 112, 132	0
18	x	38/40 (95%)	0.18	2 (5%) 32 36	52, 61, 113, 134	0
19	Z	62/62 (100%)	0.09	1 (1%) 70 74	56, 72, 108, 126	0
19	z	62/62 (100%)	0.43	3 (4%) 35 40	70, 83, 128, 175	0
20	R	18/34 (52%)	3.00	15 (83%) 0 0	111, 142, 168, 174	0
All	All	5275/5384 (97%)	-0.50	56 (1%) 78 80	16, 46, 88, 175	218 (4%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	5.2
20	R	13	LEU	4.6
20	R	3	TRP	4.1
20	R	9	LEU	4.0
2	b	486	LEU	3.8
7	h	65	LEU	3.8
5	e	4	THR	3.8
2	B	479	PHE	3.8
20	R	5	VAL	3.8
19	z	3	ILE	3.7
5	e	5	THR	3.7
2	b	499	VAL	3.6
20	R	16	ALA	3.6
7	H	65	LEU	3.5
13	o	58	ASN	3.4
20	R	6	LEU	3.4
2	b	495	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	R	12	VAL	3.3
17	Y	20	ALA	3.3
17	Y	18	VAL	3.2
20	R	14	LEU	3.2
18	x	37	VAL	3.2
20	R	10	LEU	3.2
14	t	30	THR	3.0
20	R	18	TRP	3.0
18	x	2	THR	3.0
2	B	495	PHE	2.9
7	h	66	GLY	2.9
5	E	4	THR	2.9
9	j	1	MET	2.9
7	H	66	GLY	2.9
2	b	502	VAL	2.9
9	J	2	SER	2.8
20	R	7	VAL	2.8
1	a	263	ALA	2.8
2	b	493	TRP	2.8
20	R	11	PRO	2.7
17	Y	19	ILE	2.6
6	f	14	PRO	2.6
19	z	62	VAL	2.6
13	O	4	THR	2.6
9	J	5	GLY	2.5
1	a	260	PHE	2.5
14	T	30	THR	2.4
2	b	479	PHE	2.4
1	a	248[A]	ILE	2.4
2	b	496	TYR	2.3
8	i	37	LEU	2.3
1	a	11	ALA	2.2
2	b	484	PRO	2.2
2	b	491	VAL	2.2
20	R	19	ALA	2.2
19	Z	33	TRP	2.2
13	o	206	GLY	2.1
19	z	61	VAL	2.1
20	R	8	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	37,40,54,78	0
12	FME	m	1	10/11	0.96	0.07	34,45,87,98	0
8	FME	i	1	10/11	0.97	0.07	39,48,57,57	0
12	FME	M	1	10/11	0.97	0.07	26,45,71,76	0
14	FME	t	1	10/11	0.97	0.05	28,35,39,84	0
8	FME	I	1	10/11	0.98	0.06	36,46,51,55	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
37	DGD	e	101	62/66	0.66	0.17	66,114,163,166	0
37	DGD	D	406	52/66	0.69	0.15	67,101,132,138	0
38	LHG	a	422	42/49	0.70	0.13	78,125,159,162	0
33	UNL	m	101	10/-	0.71	0.16	50,57,79,81	0
29	LMT	F	101	35/35	0.73	0.16	97,128,145,146	0
29	LMT	b	631	25/35	0.73	0.15	72,95,139,144	0
28	GOL	V	202	6/6	0.74	0.15	62,77,81,82	0
33	UNL	a	403	30/-	0.74	0.15	77,91,116,118	0
33	UNL	M	102	10/-	0.75	0.12	50,64,69,73	0
29	LMT	a	421	35/35	0.75	0.15	94,110,132,135	0
36	HTG	c	525	19/19	0.76	0.13	68,104,113,143	0
33	UNL	j	102	10/-	0.76	0.14	70,80,90,91	0
29	LMT	C	521	35/35	0.77	0.14	94,119,146,148	0
27	SQD	f	102	43/54	0.77	0.15	97,116,146,147	0
33	UNL	C	527	34/-	0.78	0.14	76,103,111,117	0
33	UNL	A	421	28/-	0.79	0.14	68,84,98,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	LMT	A	417	35/35	0.79	0.12	41,79,99,112	0
36	HTG	B	625	19/19	0.79	0.12	64,120,133,158	0
36	HTG	H	101	16/19	0.79	0.13	70,131,138,139	0
33	UNL	I	101	40/-	0.79	0.15	43,83,129,135	0
29	LMT	M	103	35/35	0.79	0.14	45,92,128,137	0
29	LMT	f	103	35/35	0.79	0.12	72,117,137,137	0
33	UNL	i	101	40/-	0.79	0.14	50,74,125,128	0
29	LMT	D	401	35/35	0.80	0.13	75,118,137,137	0
35	CA	b	610	1/1	0.80	0.13	130,130,130,130	0
38	LHG	E	101	42/49	0.81	0.12	69,98,119,122	0
33	UNL	D	411	40/-	0.81	0.12	57,79,113,123	0
29	LMT	a	404	35/35	0.82	0.12	47,86,111,123	0
34	LMG	C	520	51/55	0.82	0.12	53,105,116,119	0
36	HTG	B	633	19/19	0.82	0.12	53,110,132,175	0
34	LMG	z	101	39/55	0.82	0.14	69,112,127,136	0
36	HTG	b	609	19/19	0.82	0.12	62,113,140,141	0
33	UNL	d	410	36/-	0.83	0.12	53,77,122,126	0
33	UNL	J	101	10/-	0.83	0.13	46,70,80,85	0
36	HTG	d	411	16/19	0.83	0.12	70,111,121,126	0
33	UNL	B	634	33/-	0.83	0.14	54,88,123,126	0
27	SQD	F	103	43/54	0.83	0.12	74,97,116,118	0
33	UNL	c	526	32/-	0.83	0.13	77,98,122,128	0
36	HTG	V	207	19/19	0.83	0.12	63,87,104,205	0
33	UNL	b	634	33/-	0.84	0.14	48,98,141,142	0
27	SQD	B	621	54/54	0.84	0.12	48,81,143,146	0
28	GOL	C	524	6/6	0.84	0.14	63,65,79,82	0
28	GOL	O	301	6/6	0.84	0.09	68,76,77,77	0
32	PL9	A	420[B]	55/55	0.85	0.14	71,87,101,101	55
36	HTG	b	633	19/19	0.85	0.12	70,120,135,135	0
27	SQD	a	405	54/54	0.85	0.10	45,76,111,114	0
29	LMT	B	635	25/35	0.85	0.13	38,73,124,127	0
32	PL9	A	420[A]	55/55	0.85	0.14	70,87,101,101	55
36	HTG	C	523	19/19	0.85	0.10	75,95,121,124	0
34	LMG	Z	101	37/55	0.85	0.14	57,108,124,127	0
34	LMG	c	523	51/55	0.85	0.11	49,106,118,120	0
29	LMT	m	102	35/35	0.86	0.11	47,95,121,125	0
27	SQD	b	601	54/54	0.86	0.10	52,72,120,129	0
28	GOL	c	502	6/6	0.86	0.15	70,79,91,98	0
32	PL9	a	416[A]	55/55	0.86	0.14	83,102,111,114	55
32	PL9	a	416[B]	55/55	0.86	0.14	84,102,111,114	55
27	SQD	A	416	54/54	0.86	0.10	47,73,104,112	0
36	HTG	b	632	19/19	0.86	0.13	51,67,77,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	HTG	B	624	19/19	0.88	0.11	54,64,74,81	0
29	LMT	M	104	35/35	0.88	0.10	46,79,89,95	0
36	HTG	c	524	19/19	0.88	0.10	81,89,96,118	0
29	LMT	T	104	25/35	0.88	0.13	38,71,116,121	0
36	HTG	C	522	19/19	0.88	0.09	72,80,91,95	0
28	GOL	T	102	6/6	0.88	0.13	103,114,116,120	0
28	GOL	v	201	6/6	0.88	0.13	78,85,89,90	0
28	GOL	A	415	6/6	0.88	0.11	54,73,76,79	0
28	GOL	b	607	6/6	0.88	0.11	64,77,80,80	0
34	LMG	c	522	51/55	0.89	0.10	52,86,107,110	0
28	GOL	T	101	6/6	0.89	0.14	55,69,88,96	0
28	GOL	t	102	6/6	0.89	0.14	49,76,86,89	0
34	LMG	C	519	51/55	0.90	0.10	50,78,102,103	0
28	GOL	b	606	6/6	0.90	0.15	75,79,94,95	0
28	GOL	B	630	6/6	0.90	0.11	50,66,68,71	0
28	GOL	a	402	6/6	0.90	0.11	76,90,92,92	0
33	UNL	X	101	18/-	0.91	0.10	58,70,93,100	0
33	UNL	d	412	18/-	0.91	0.11	61,68,102,107	0
34	LMG	a	415	51/55	0.91	0.09	58,75,96,97	0
28	GOL	B	636	6/6	0.91	0.09	48,51,55,55	0
29	LMT	M	101	35/35	0.91	0.09	39,82,98,103	0
28	GOL	o	301	6/6	0.91	0.10	64,70,80,88	0
34	LMG	A	422	51/55	0.91	0.09	56,79,99,104	0
33	UNL	d	409	17/-	0.91	0.10	46,63,91,92	0
24	CLA	b	611	65/65	0.92	0.09	46,69,101,116	0
28	GOL	B	626	6/6	0.92	0.10	39,52,57,71	0
28	GOL	v	202	6/6	0.92	0.10	72,79,89,99	0
28	GOL	B	628	6/6	0.92	0.10	52,70,78,85	0
28	GOL	f	101	6/6	0.93	0.08	74,84,86,89	0
23	BCT	a	419[A]	4/4	0.93	0.07	53,54,57,63	4
36	HTG	B	632	19/19	0.93	0.07	41,75,91,92	0
33	UNL	D	410	17/-	0.93	0.08	39,67,83,87	0
23	BCT	a	419[B]	4/4	0.93	0.07	53,53,57,64	4
24	CLA	B	602	65/65	0.93	0.09	44,61,94,111	0
24	CLA	C	506	65/65	0.93	0.08	44,60,101,105	0
24	CLA	C	513	65/65	0.93	0.08	50,64,93,98	0
22	CL	U	201	1/1	0.93	0.11	93,93,93,93	0
28	GOL	A	414	6/6	0.93	0.13	52,54,57,60	0
34	LMG	b	630	51/55	0.93	0.08	39,48,68,82	0
24	CLA	c	517	65/65	0.93	0.08	61,77,92,94	0
26	BCR	y	101	40/40	0.93	0.07	43,60,68,76	0
34	LMG	j	101	51/55	0.93	0.08	46,56,92,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
28	GOL	B	627	6/6	0.93	0.11	56,65,80,92	0
35	CA	B	601	1/1	0.93	0.06	118,118,118,118	0
38	LHG	D	409	49/49	0.93	0.10	37,54,105,113	0
27	SQD	A	412	54/54	0.93	0.09	43,76,91,94	0
35	CA	f	104	1/1	0.93	0.06	97,97,97,97	0
32	PL9	D	405[B]	55/55	0.94	0.06	27,35,43,47	55
26	BCR	K	101	40/40	0.94	0.08	43,55,62,63	0
27	SQD	a	414	54/54	0.94	0.09	54,77,98,101	0
26	BCR	T	103	40/40	0.94	0.06	28,45,55,58	0
26	BCR	b	628	40/40	0.94	0.07	31,43,54,61	0
34	LMG	B	622	51/55	0.94	0.07	32,49,69,85	0
26	BCR	c	527	40/40	0.94	0.08	56,72,78,81	0
28	GOL	b	603	6/6	0.94	0.09	53,57,64,80	0
36	HTG	b	608	19/19	0.94	0.07	48,68,78,79	0
34	LMG	D	412	51/55	0.94	0.09	35,55,100,106	0
26	BCR	d	404	40/40	0.94	0.07	38,50,73,79	0
26	BCR	k	101	40/40	0.94	0.07	44,60,70,74	0
24	CLA	b	616	65/65	0.94	0.08	30,43,84,96	0
24	CLA	b	626	65/65	0.94	0.08	35,50,97,100	0
28	GOL	B	629	6/6	0.94	0.10	43,47,50,52	0
37	DGD	C	517	62/66	0.94	0.07	37,52,86,94	0
24	CLA	C	504	65/65	0.94	0.07	35,46,77,83	0
26	BCR	C	514	40/40	0.94	0.07	49,65,73,78	0
26	BCR	D	404	40/40	0.94	0.07	36,49,79,88	0
28	GOL	C	525	6/6	0.94	0.08	39,48,50,51	0
32	PL9	D	405[A]	55/55	0.94	0.06	28,35,45,49	55
24	CLA	C	512	65/65	0.95	0.07	46,64,76,80	0
24	CLA	B	615	65/65	0.95	0.07	27,38,82,86	0
26	BCR	Y	101	40/40	0.95	0.07	48,59,67,72	0
24	CLA	a	412	65/65	0.95	0.09	32,45,111,115	0
24	CLA	B	617	65/65	0.95	0.09	31,50,107,110	0
24	CLA	C	501	65/65	0.95	0.07	38,47,69,78	0
28	GOL	V	201	6/6	0.95	0.07	68,75,76,79	0
26	BCR	h	101	40/40	0.95	0.06	39,54,64,66	0
28	GOL	V	203	6/6	0.95	0.09	39,50,64,67	0
28	GOL	V	205	6/6	0.95	0.08	71,75,81,91	0
28	GOL	a	401	6/6	0.95	0.10	50,61,66,76	0
24	CLA	b	619	65/65	0.95	0.07	35,49,56,65	0
26	BCR	t	101	40/40	0.95	0.06	30,43,60,68	0
24	CLA	b	624	65/65	0.95	0.07	27,39,83,97	0
23	BCT	A	404[B]	4/4	0.95	0.07	51,52,57,63	4
24	CLA	c	505	65/65	0.95	0.07	40,54,62,66	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	c	507	65/65	0.95	0.07	41,51,60,77	0
24	CLA	c	508	65/65	0.95	0.06	38,50,71,75	0
24	CLA	c	510	65/65	0.95	0.07	44,62,87,95	0
24	CLA	c	511	65/65	0.95	0.07	43,54,62,67	0
24	CLA	c	516	65/65	0.95	0.07	51,62,77,83	0
28	GOL	v	203	6/6	0.95	0.10	46,50,57,61	0
24	CLA	C	505	65/65	0.95	0.07	32,47,66,74	0
28	GOL	A	413	6/6	0.95	0.07	43,44,56,59	0
25	PHO	a	420[A]	64/64	0.95	0.06	31,41,46,49	64
25	PHO	a	420[B]	64/64	0.95	0.06	31,40,46,50	64
26	BCR	A	411	40/40	0.95	0.06	29,37,44,45	0
37	DGD	C	518	62/66	0.95	0.06	37,47,75,87	0
26	BCR	B	620	40/40	0.95	0.06	31,43,57,59	0
37	DGD	H	103	62/66	0.95	0.07	32,47,70,74	0
37	DGD	c	520	62/66	0.95	0.07	38,51,100,112	0
37	DGD	c	521	62/66	0.95	0.07	39,51,82,89	0
23	BCT	A	404[A]	4/4	0.95	0.07	51,52,57,63	4
37	DGD	h	102	62/66	0.95	0.07	35,48,63,73	0
38	LHG	D	407	49/49	0.95	0.07	35,47,59,64	0
24	CLA	C	507	65/65	0.95	0.07	40,52,67,72	0
26	BCR	H	102	40/40	0.95	0.06	36,52,65,68	0
28	GOL	B	631	6/6	0.95	0.15	48,62,69,70	0
38	LHG	d	406	49/49	0.95	0.07	41,49,58,63	0
38	LHG	d	408	49/49	0.95	0.09	34,52,103,105	0
24	CLA	b	620	65/65	0.96	0.06	33,44,51,57	0
24	CLA	b	621	65/65	0.96	0.06	26,38,48,55	0
24	CLA	b	622	65/65	0.96	0.06	29,39,47,49	0
24	CLA	b	623	65/65	0.96	0.05	28,39,55,57	0
26	BCR	b	627	40/40	0.96	0.05	30,39,47,47	0
24	CLA	A	410	65/65	0.96	0.07	29,47,108,113	0
26	BCR	c	518	40/40	0.96	0.06	39,55,64,64	0
24	CLA	b	625	65/65	0.96	0.05	34,44,62,67	0
32	PL9	d	405[A]	55/55	0.96	0.06	25,35,44,49	55
32	PL9	d	405[B]	55/55	0.96	0.06	25,35,43,49	55
24	CLA	C	508	65/65	0.96	0.07	35,48,107,117	0
24	CLA	C	509	65/65	0.96	0.07	41,52,73,76	0
24	CLA	c	506	65/65	0.96	0.07	38,50,63,69	0
28	GOL	b	604	6/6	0.96	0.08	41,56,70,75	0
28	GOL	b	605	6/6	0.96	0.07	53,64,74,84	0
36	HTG	b	602	19/19	0.96	0.07	35,49,65,66	0
24	CLA	C	510	65/65	0.96	0.06	39,51,60,69	0
24	CLA	C	511	65/65	0.96	0.07	42,56,67,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	CLA	A	407	65/65	0.96	0.06	27,37,90,96	0
24	CLA	B	603	65/65	0.96	0.05	33,42,47,53	0
24	CLA	c	512	65/65	0.96	0.07	36,46,109,121	0
24	CLA	c	513	65/65	0.96	0.07	43,54,67,82	0
24	CLA	c	514	65/65	0.96	0.06	38,50,60,68	0
37	DGD	C	516	62/66	0.96	0.06	33,44,85,86	0
24	CLA	c	515	65/65	0.96	0.07	43,55,73,80	0
24	CLA	D	403	65/65	0.96	0.07	39,49,99,104	0
24	CLA	a	410	65/65	0.96	0.07	29,40,99,105	0
24	CLA	d	403	65/65	0.96	0.07	39,49,98,106	0
37	DGD	c	519	62/66	0.96	0.07	37,46,91,95	0
25	PHO	A	409[A]	64/64	0.96	0.05	29,40,44,47	64
25	PHO	A	409[B]	64/64	0.96	0.05	30,39,44,49	64
24	CLA	C	503	65/65	0.96	0.06	39,50,59,65	0
24	CLA	B	607	65/65	0.96	0.07	31,43,85,91	0
24	CLA	B	611	65/65	0.96	0.06	35,44,50,57	0
26	BCR	B	619	40/40	0.96	0.05	26,36,55,58	0
24	CLA	b	617	65/65	0.96	0.05	26,34,42,50	0
24	CLA	b	618	65/65	0.96	0.05	32,42,51,56	0
26	BCR	C	515	40/40	0.96	0.06	39,53,60,63	0
24	CLA	B	614	65/65	0.96	0.06	25,35,63,75	0
39	HEM	e	102	43/43	0.96	0.10	53,76,114,130	0
25	PHO	a	411	64/64	0.97	0.05	26,34,40,45	0
28	GOL	V	204	6/6	0.97	0.07	55,61,65,65	0
24	CLA	B	605	65/65	0.97	0.05	25,35,67,69	0
24	CLA	B	606	65/65	0.97	0.05	28,37,50,52	0
24	CLA	a	409	65/65	0.97	0.05	27,32,48,57	0
26	BCR	B	618	40/40	0.97	0.04	28,37,45,45	0
24	CLA	C	502	65/65	0.97	0.05	36,44,55,70	0
24	CLA	A	405	65/65	0.97	0.05	25,32,41,57	0
24	CLA	B	608	65/65	0.97	0.05	24,33,44,53	0
24	CLA	b	612	65/65	0.97	0.06	33,44,51,57	0
24	CLA	c	509	65/65	0.97	0.06	34,45,64,72	0
24	CLA	b	613	65/65	0.97	0.06	34,43,52,58	0
24	CLA	b	614	65/65	0.97	0.06	26,39,70,74	0
24	CLA	b	615	65/65	0.97	0.06	28,38,50,52	0
24	CLA	B	609	65/65	0.97	0.05	32,42,52,54	0
26	BCR	a	413	40/40	0.97	0.04	28,38,46,47	0
24	CLA	B	610	65/65	0.97	0.05	35,46,55,71	0
24	CLA	A	406	65/65	0.97	0.05	24,32,38,45	0
26	BCR	b	629	40/40	0.97	0.05	37,48,60,64	0
24	CLA	B	612	65/65	0.97	0.05	26,35,47,53	0

Continued on next page...

Continued from previous page...

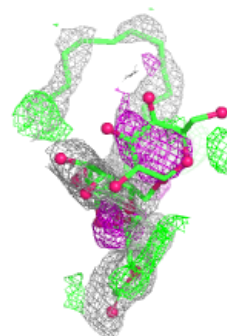
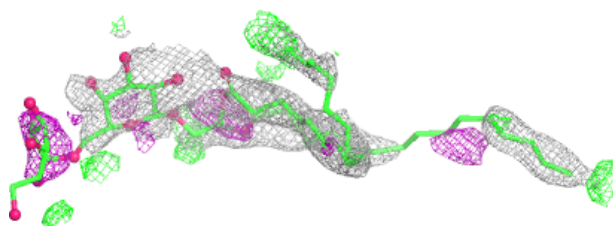
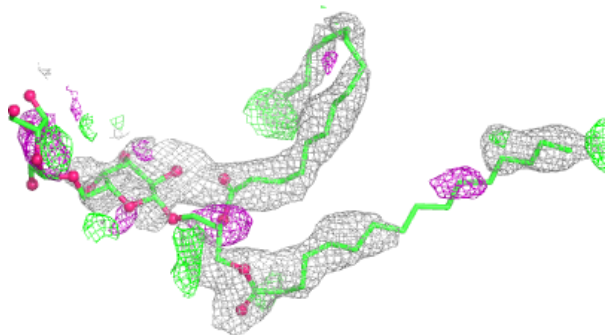
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	HTG	B	623	19/19	0.97	0.06	37,51,65,70	0
38	LHG	D	408	49/49	0.97	0.06	30,41,62,74	0
24	CLA	B	613	65/65	0.97	0.05	27,36,45,47	0
24	CLA	d	401	65/65	0.97	0.04	26,32,41,51	0
38	LHG	L	101	49/49	0.97	0.05	31,43,54,61	0
22	CL	v	204	1/1	0.97	0.07	88,88,88,88	0
25	PHO	A	408	64/64	0.97	0.04	26,32,38,43	0
38	LHG	d	407	49/49	0.97	0.06	30,39,57,75	0
24	CLA	B	604	65/65	0.97	0.05	33,43,50,53	0
38	LHG	l	101	49/49	0.97	0.06	33,44,53,59	0
24	CLA	B	616	65/65	0.97	0.06	33,44,60,68	0
40	MG	j	103	1/1	0.97	0.07	55,55,55,55	0
22	CL	A	403[B]	1/1	0.98	0.08	33,33,33,33	1
28	GOL	c	501	6/6	0.98	0.07	43,46,52,53	0
22	CL	A	403[A]	1/1	0.98	0.08	33,33,33,33	1
24	CLA	d	402	65/65	0.98	0.05	26,35,54,64	0
24	CLA	D	402	65/65	0.98	0.05	24,33,52,57	0
22	CL	a	408[A]	1/1	0.98	0.03	40,40,40,40	1
39	HEM	F	102	43/43	0.98	0.06	46,64,75,83	0
35	CA	F	104	1/1	0.98	0.04	82,82,82,82	0
40	MG	J	102	1/1	0.98	0.04	50,50,50,50	0
22	CL	a	408[B]	1/1	0.98	0.03	38,38,38,38	1
41	HEC	V	206	43/43	0.98	0.05	34,39,47,50	0
41	HEC	v	205	43/43	0.98	0.05	41,49,55,57	0
22	CL	a	407[B]	1/1	0.99	0.04	33,33,33,33	1
35	CA	c	503	1/1	0.99	0.09	63,63,63,63	0
35	CA	c	504	1/1	0.99	0.03	73,73,73,73	0
31	OEY	A	419[B]	11/11	0.99	0.03	31,36,42,47	11
35	CA	o	302	1/1	0.99	0.03	86,86,86,86	0
35	CA	C	526	1/1	0.99	0.06	67,67,67,67	0
22	CL	a	407[A]	1/1	0.99	0.04	34,34,34,34	1
35	CA	O	302	1/1	0.99	0.02	80,80,80,80	0
21	FE2	A	401[A]	1/1	1.00	0.01	45,45,45,45	1
21	FE2	A	401[B]	1/1	1.00	0.01	47,47,47,47	1
30	OEX	A	418[A]	10/10	1.00	0.02	31,35,38,46	10
30	OEX	a	417[A]	10/10	1.00	0.02	31,37,39,45	10
21	FE2	a	406[B]	1/1	1.00	0.01	46,46,46,46	0
31	OEY	a	418[B]	11/11	1.00	0.02	32,37,44,57	11
22	CL	A	402[A]	1/1	1.00	0.02	30,30,30,30	1
22	CL	A	402[B]	1/1	1.00	0.02	31,31,31,31	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

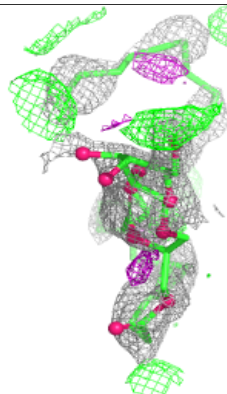
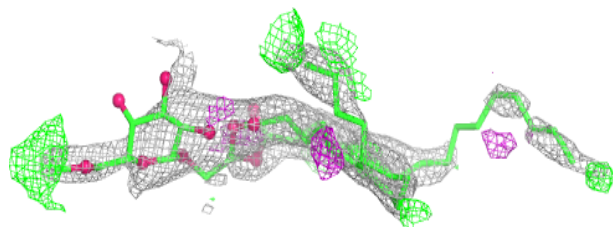
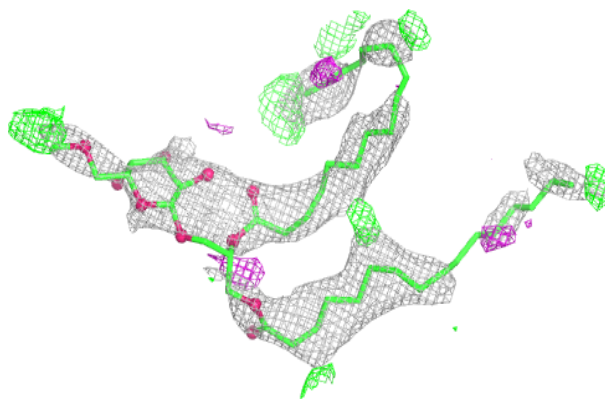
Electron density around DGD e 101:

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



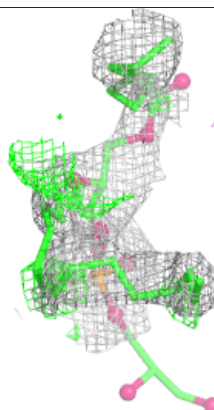
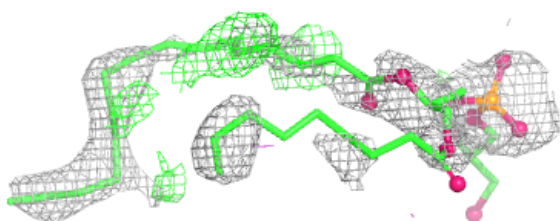
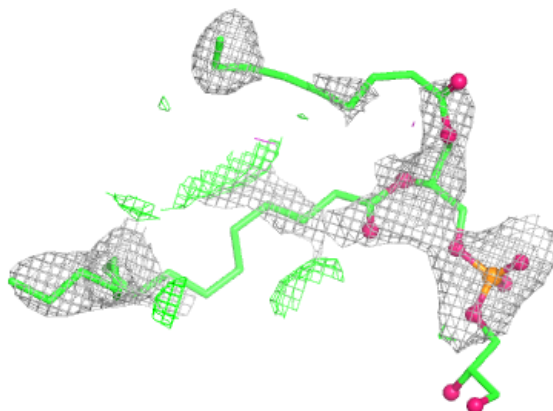
Electron density around DGD D 406:

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

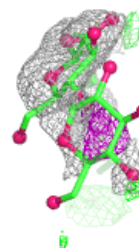
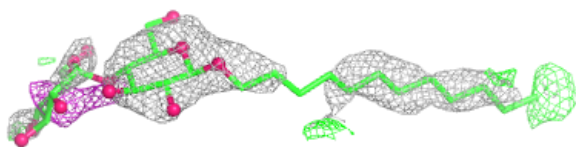
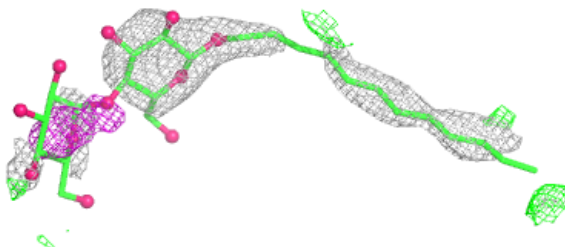


Electron density around LHG a 422:

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

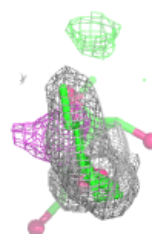
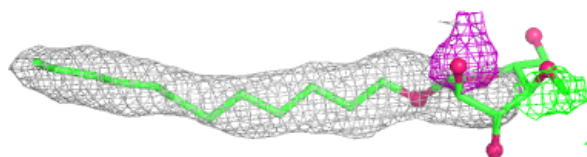
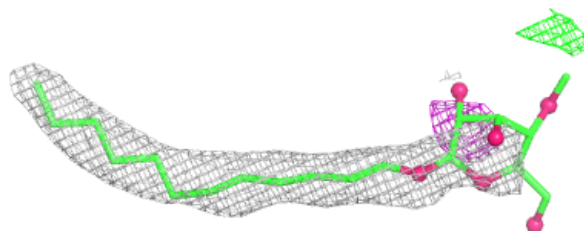
**Electron density around LMT F 101:**

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

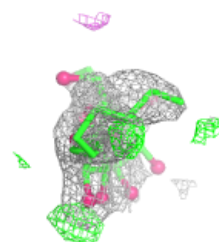
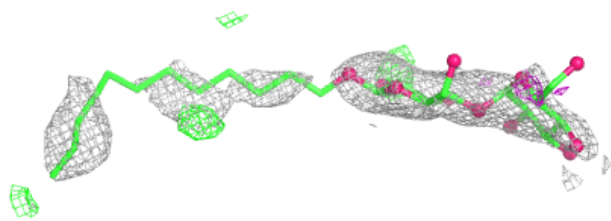
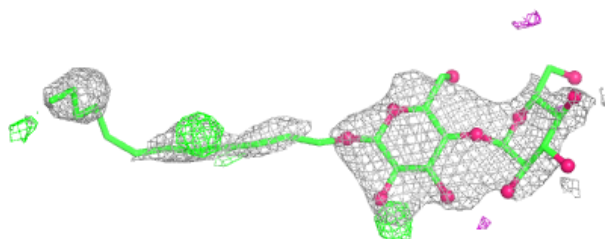


Electron density around LMT b 631:

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

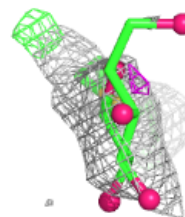
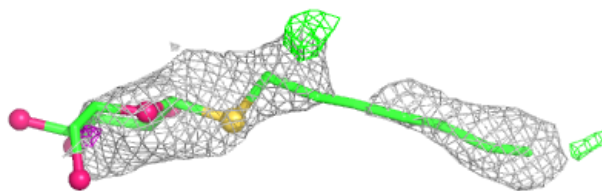
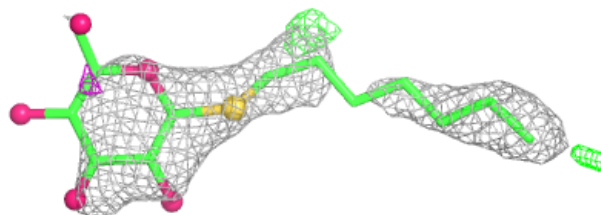
**Electron density around LMT a 421:**

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

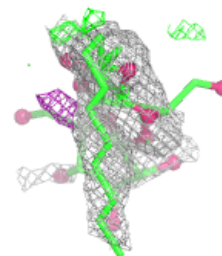
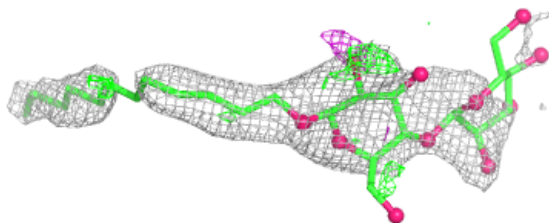
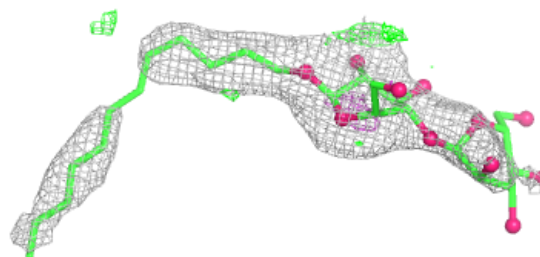


Electron density around HTG c 525:

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

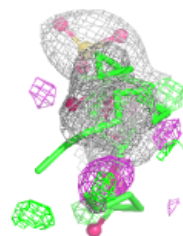
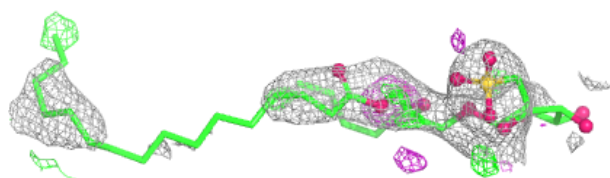
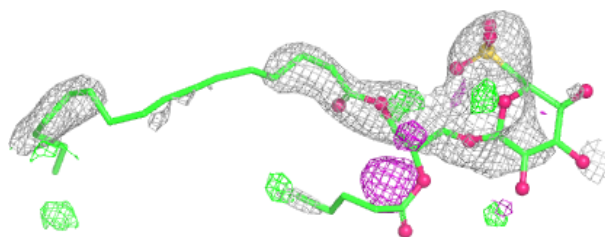
**Electron density around LMT C 521:**

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

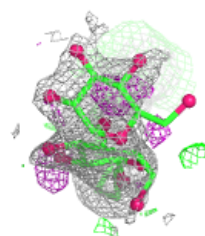
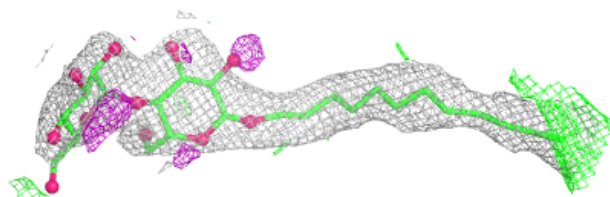
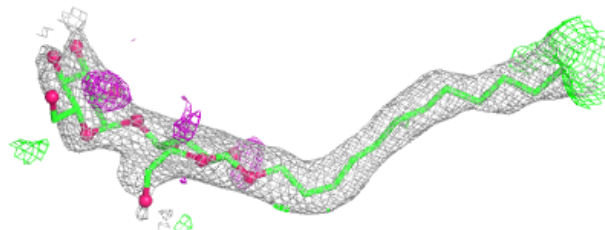


Electron density around SQD f 102:

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

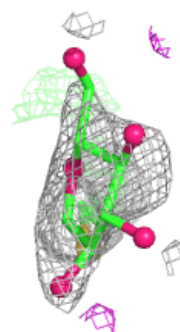
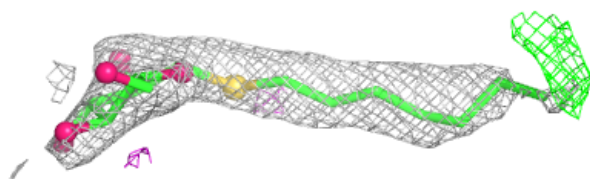
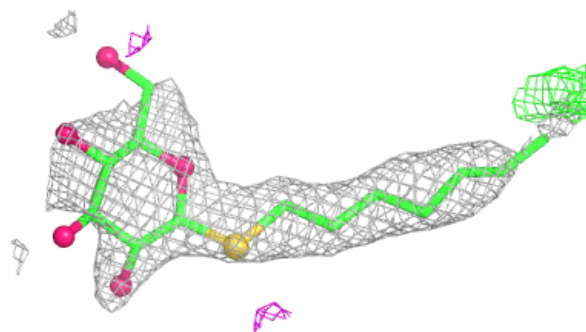
**Electron density around LMT A 417:**

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

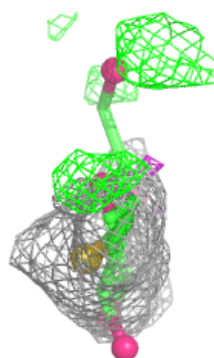
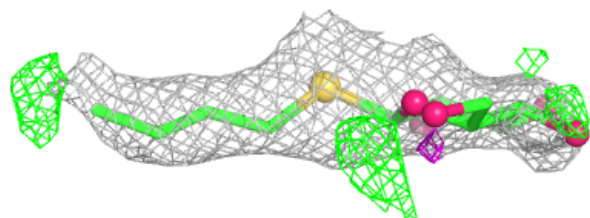
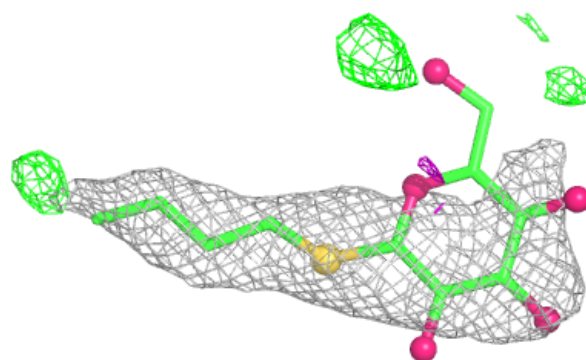


Electron density around HTG B 625:

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

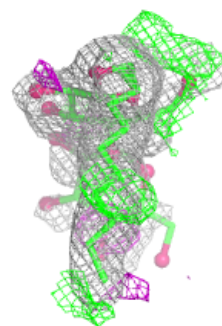
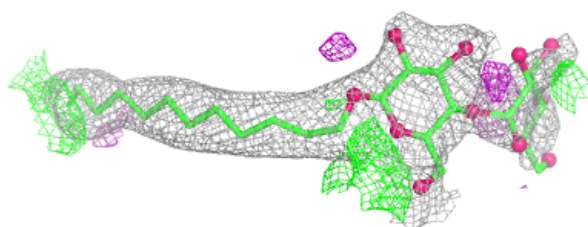
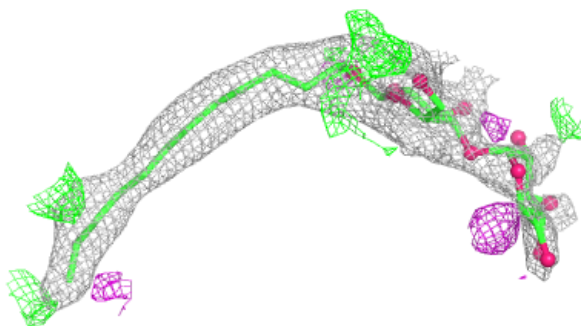
**Electron density around HTG H 101:**

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

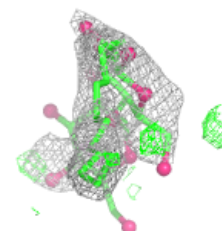
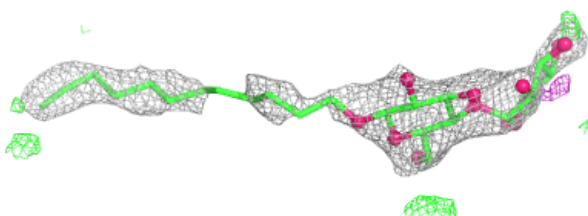
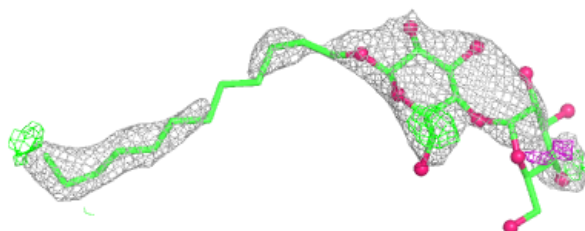


Electron density around LMT M 103:

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

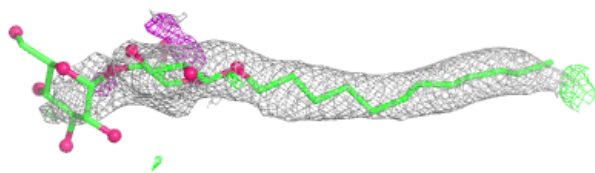
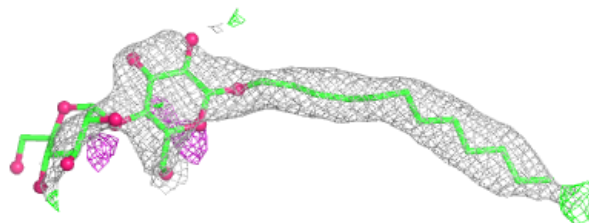
**Electron density around LMT f 103:**

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



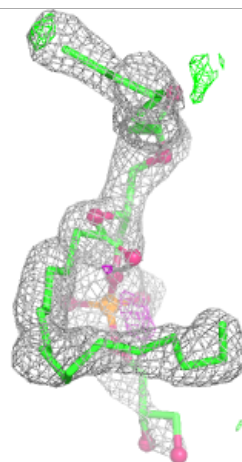
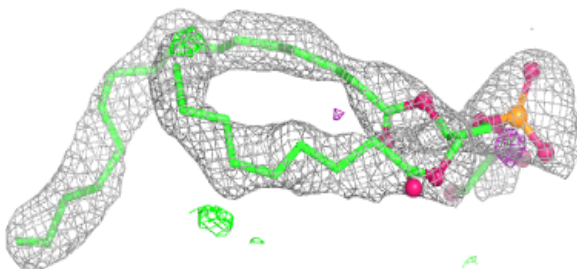
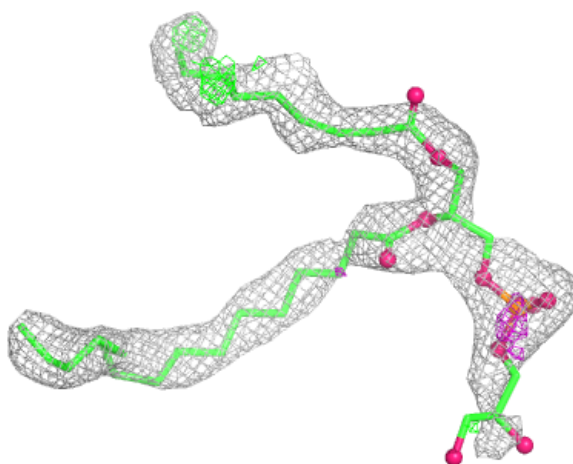
Electron density around LMT D 401:

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



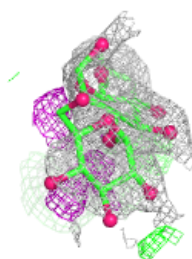
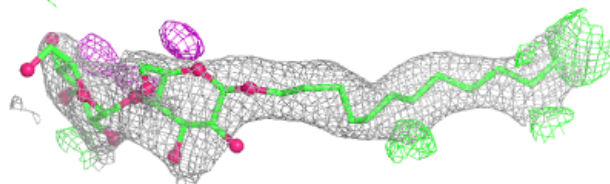
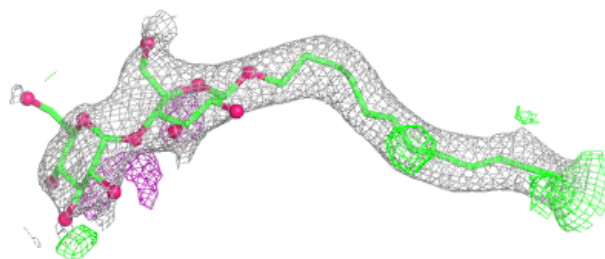
Electron density around LHG E 101:

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

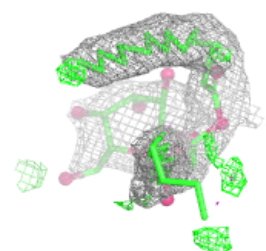
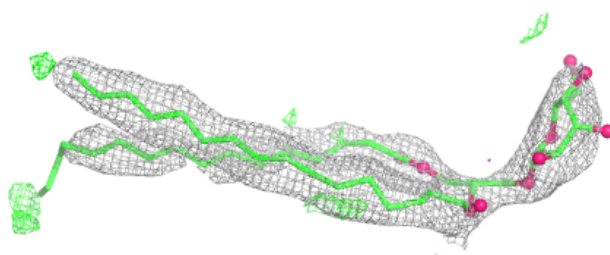
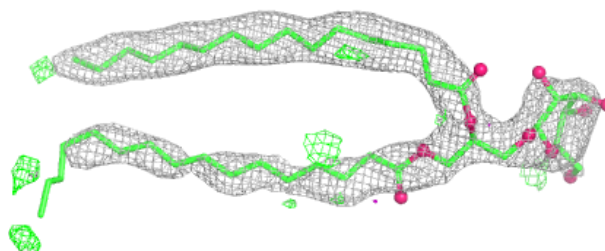


Electron density around LMT a 404:

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

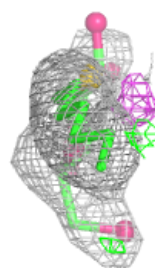
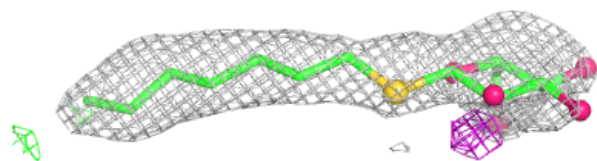
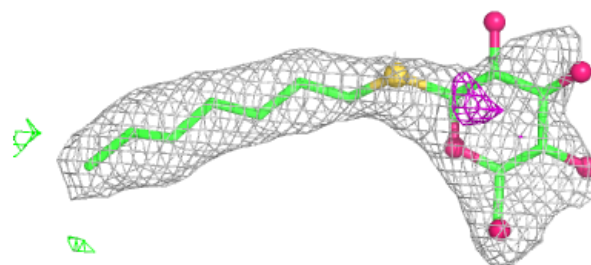
**Electron density around LMG C 520:**

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

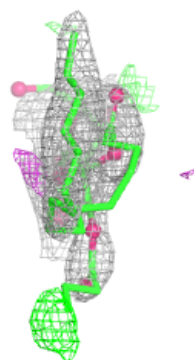
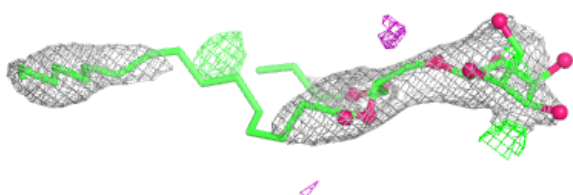
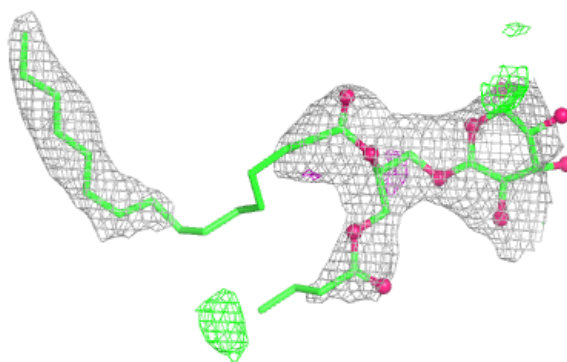


Electron density around HTG B 633:

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

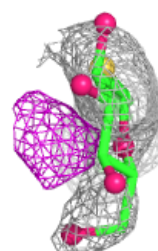
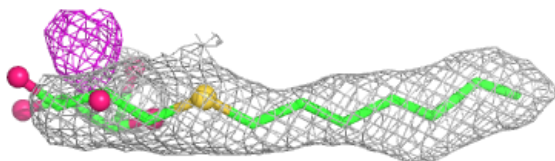
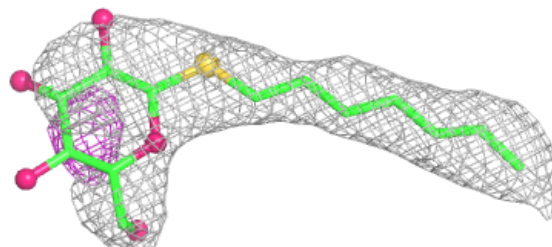
**Electron density around LMG z 101:**

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

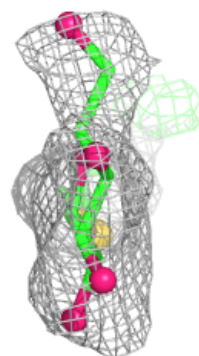
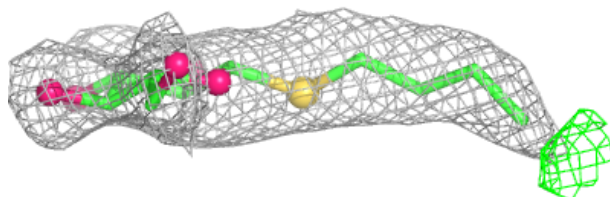
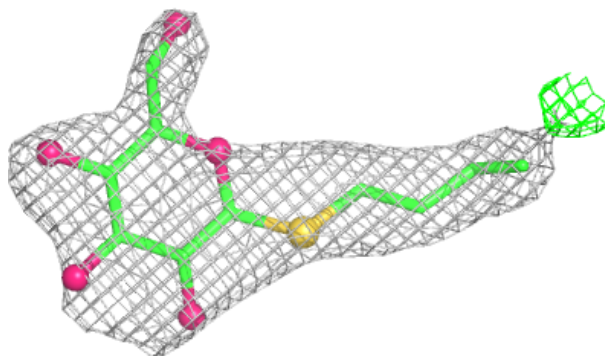


Electron density around HTG b 609:

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

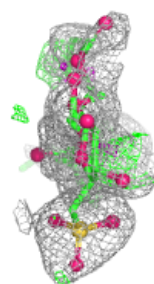
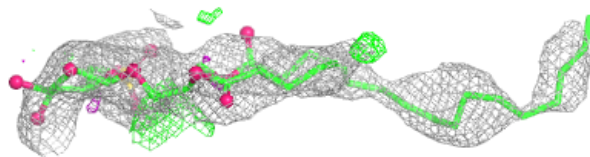
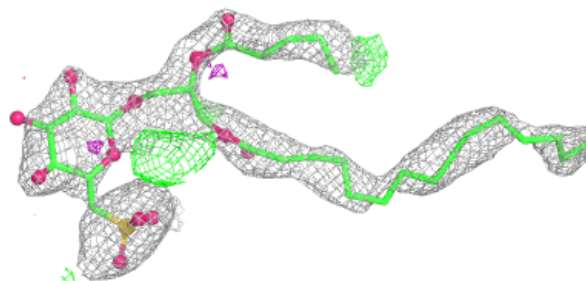
**Electron density around HTG d 411:**

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

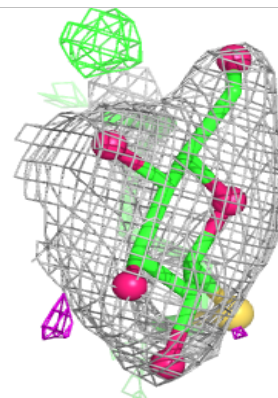
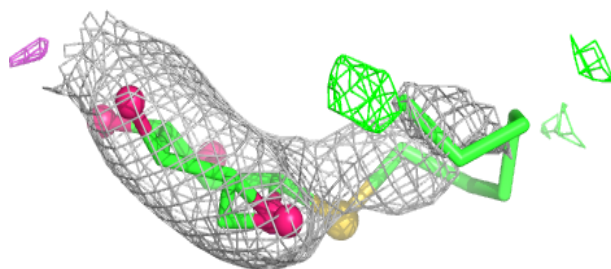
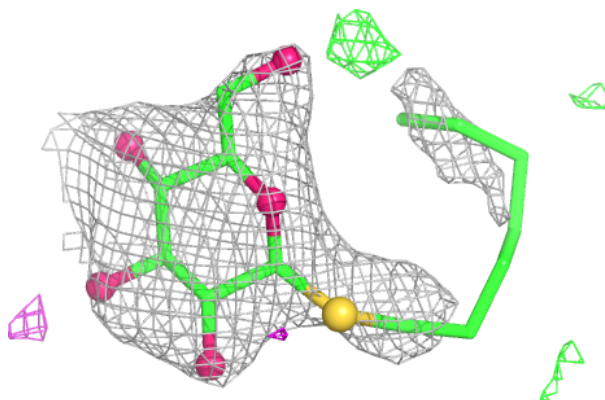


Electron density around SQD F 103:

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

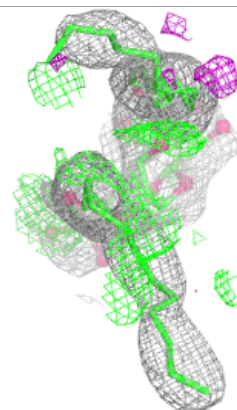
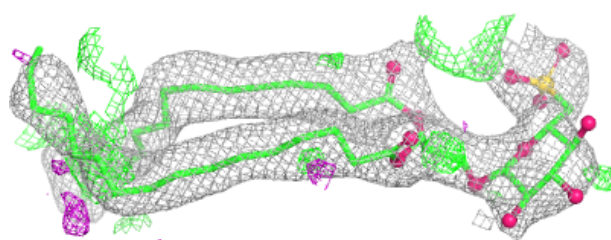
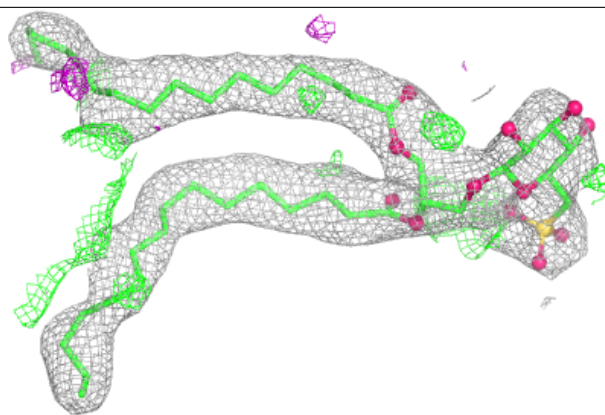
**Electron density around HTG V 207:**

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

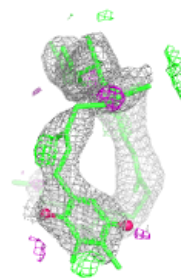
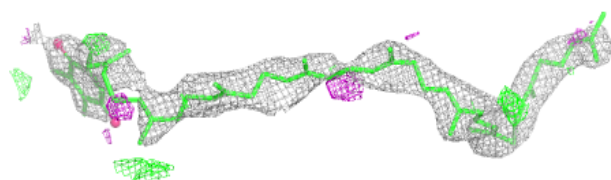
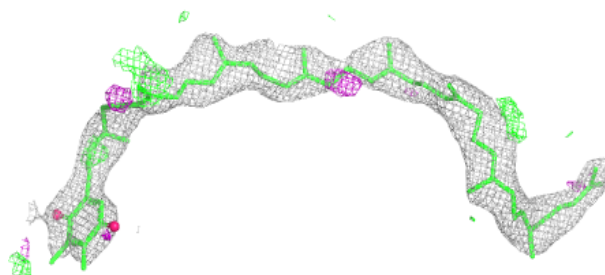


Electron density around SQD B 621:

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

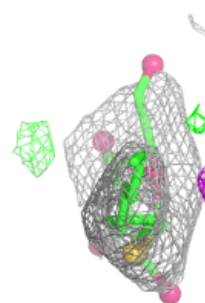
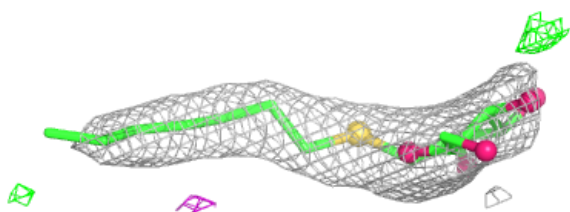
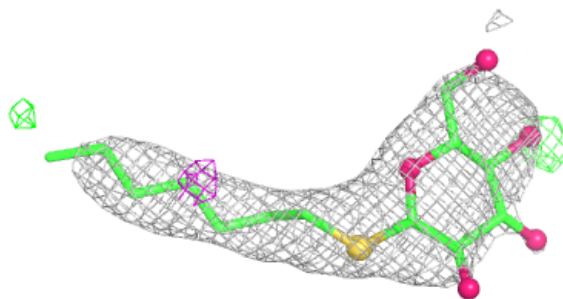
**Electron density around PL9 A 420 (B):**

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

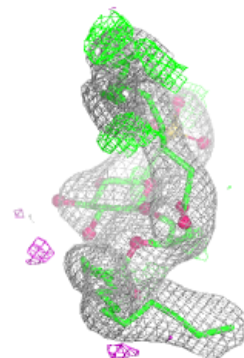
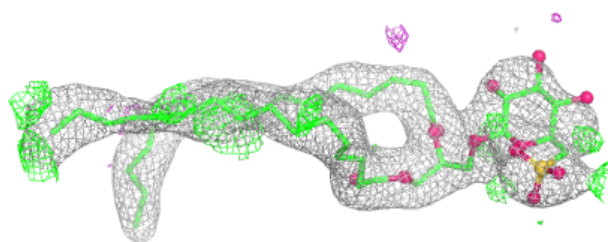
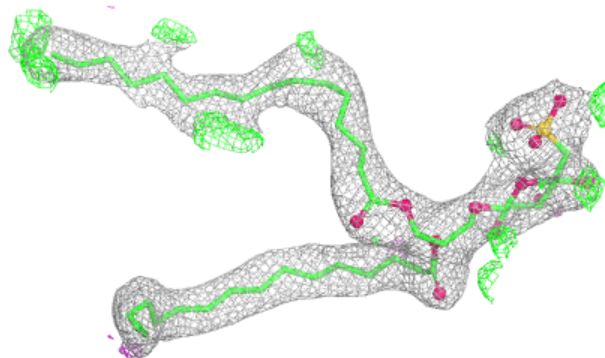


Electron density around HTG b 633:

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

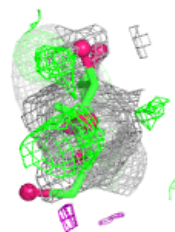
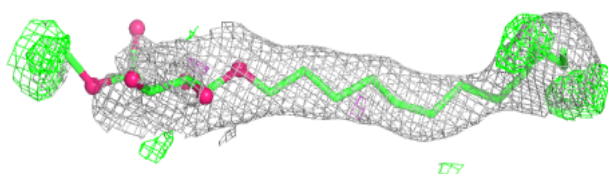
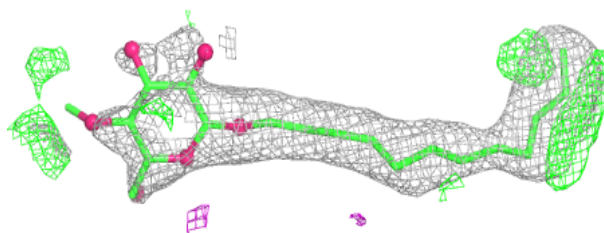
**Electron density around SQD a 405:**

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

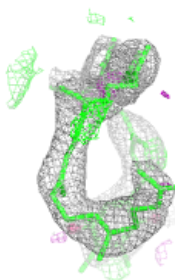
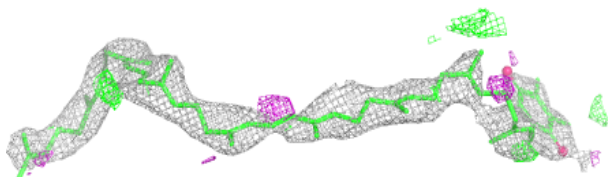
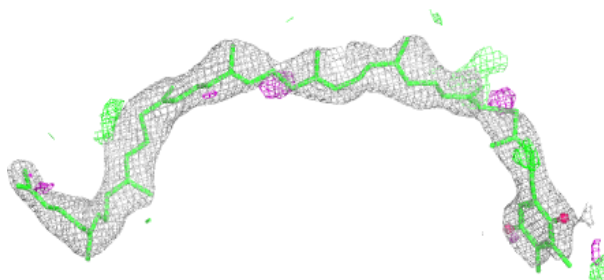


Electron density around LMT B 635:

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

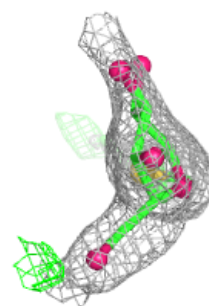
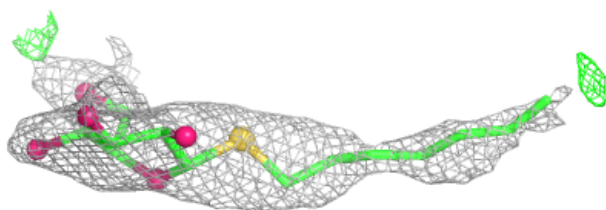
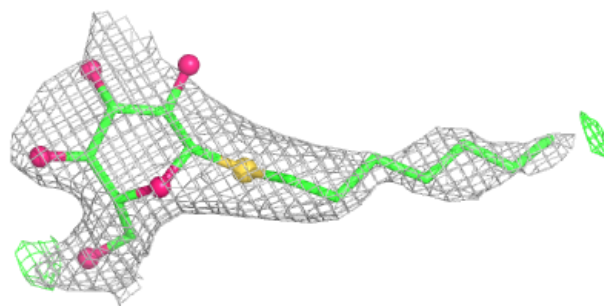
**Electron density around PL9 A 420 (A):**

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

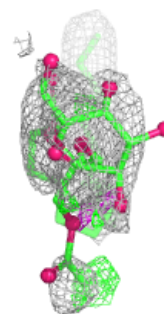
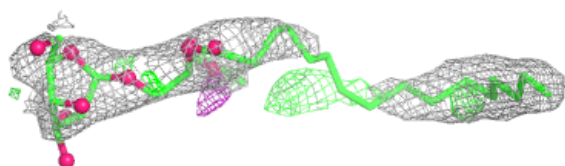
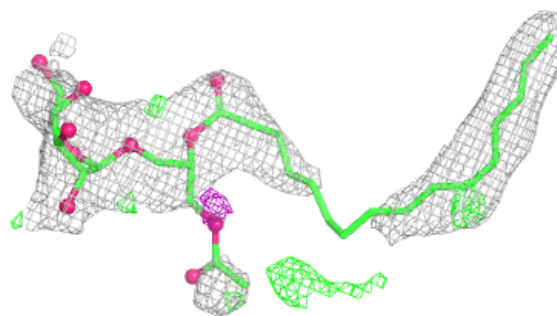


Electron density around HTG C 523:

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

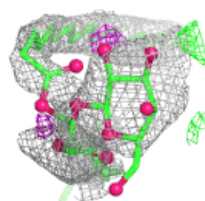
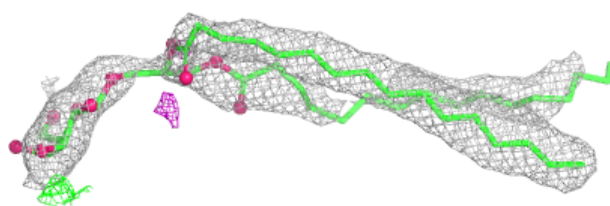
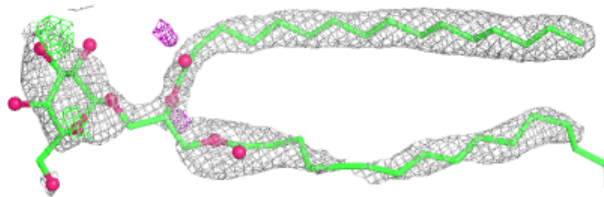
**Electron density around LMG Z 101:**

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

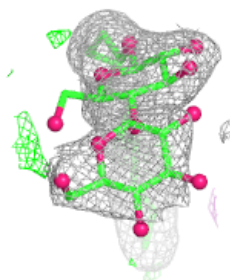
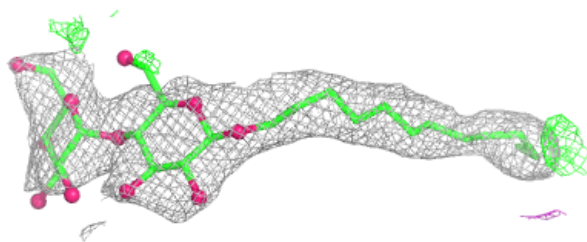
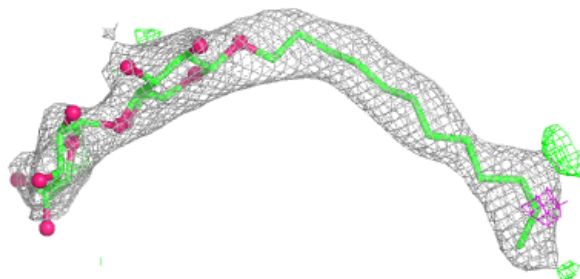


Electron density around LMG c 523:

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

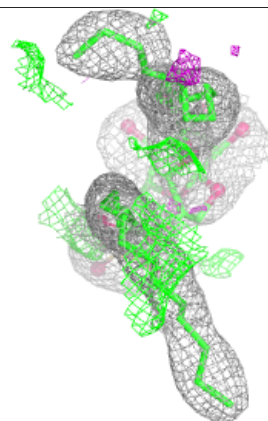
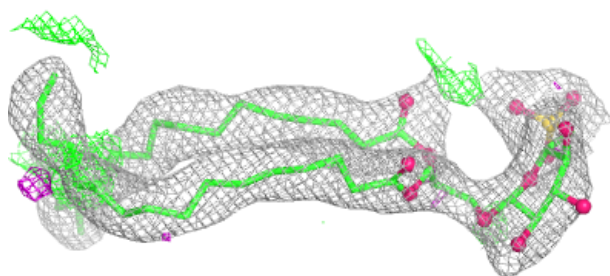
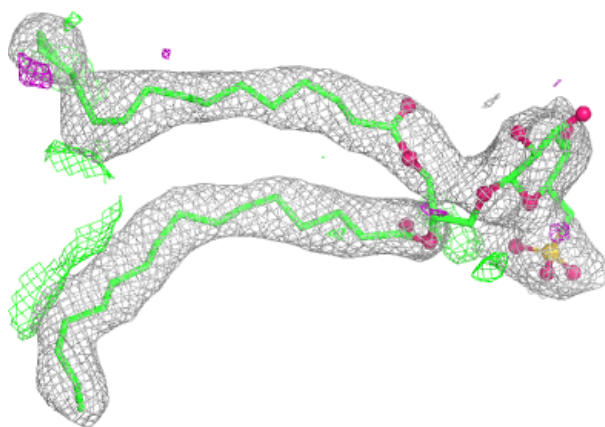
**Electron density around LMT m 102:**

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

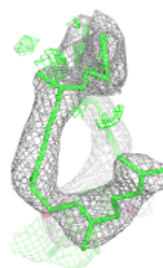
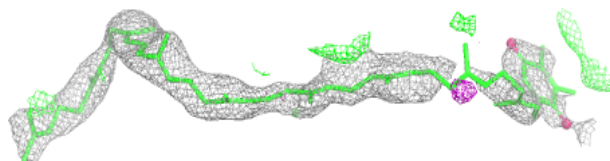
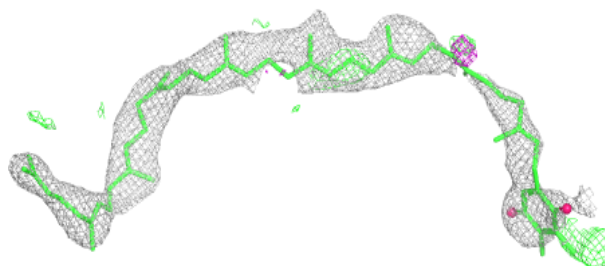


Electron density around SQD b 601:

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

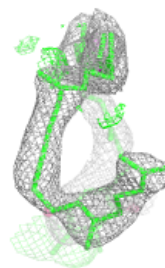
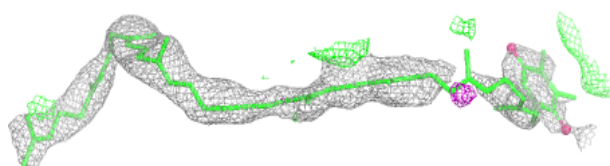
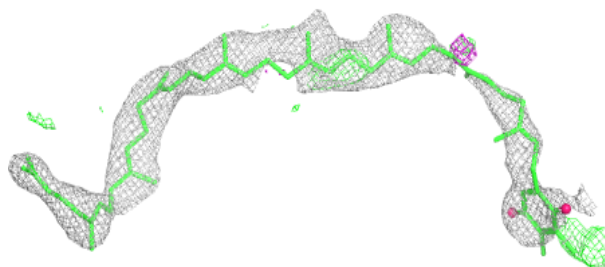
**Electron density around PL9 a 416 (A):**

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

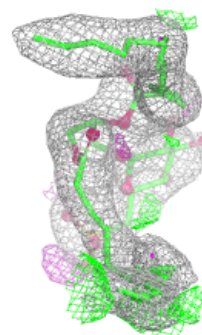
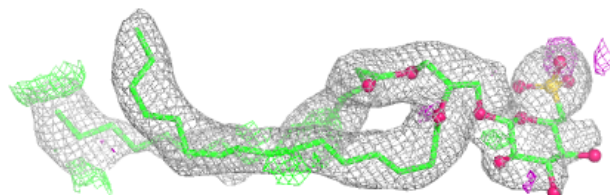
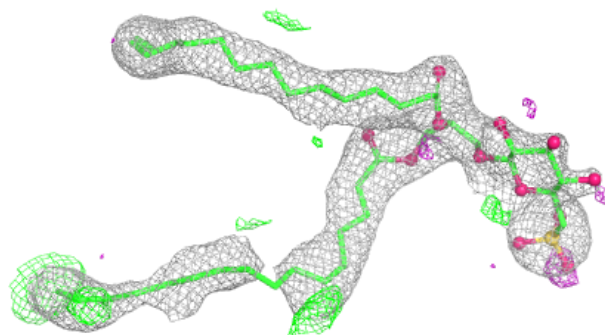


Electron density around PL9 a 416 (B):

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

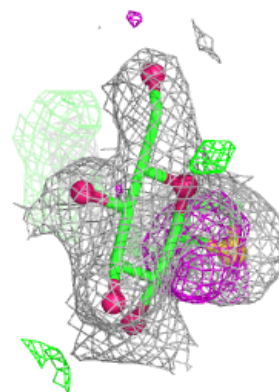
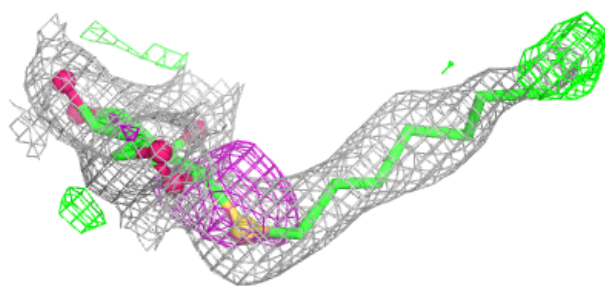
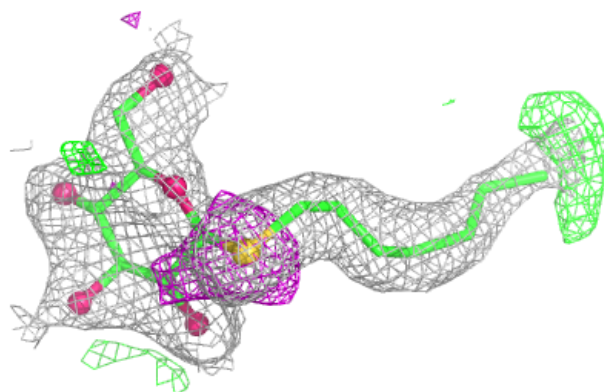
**Electron density around SQD A 416:**

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

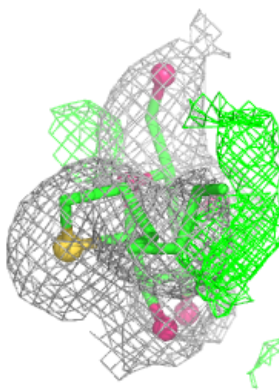
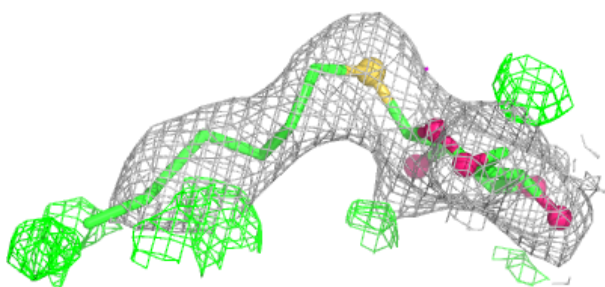
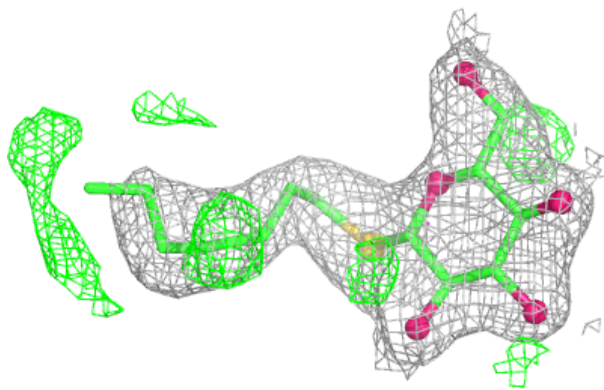


Electron density around HTG b 632:

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

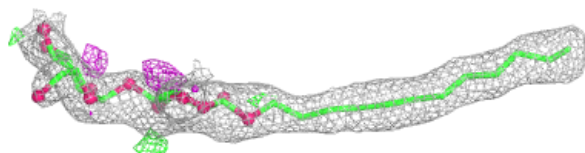
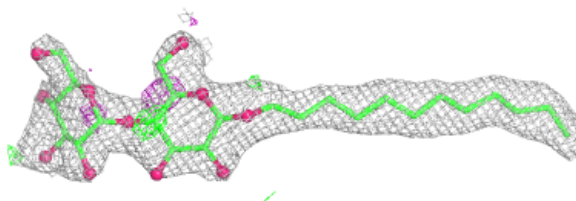
**Electron density around HTG B 624:**

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

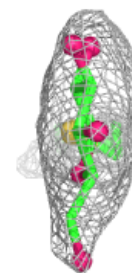
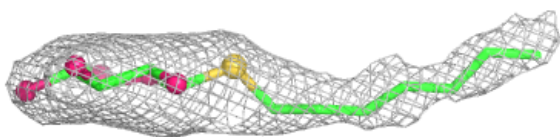
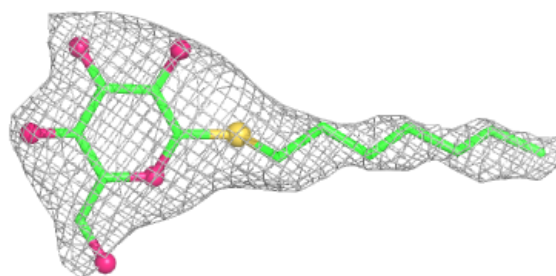


Electron density around LMT M 104:

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

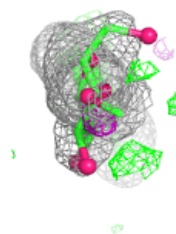
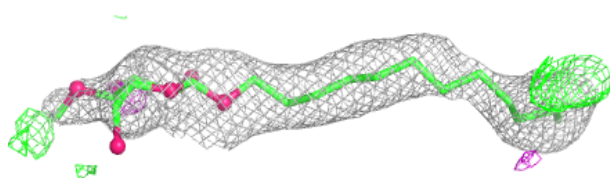
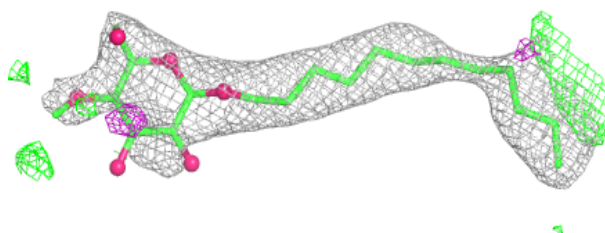
**Electron density around HTG c 524:**

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

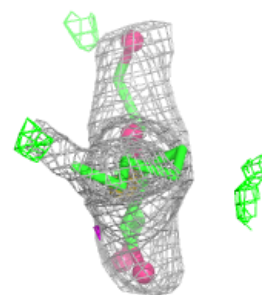
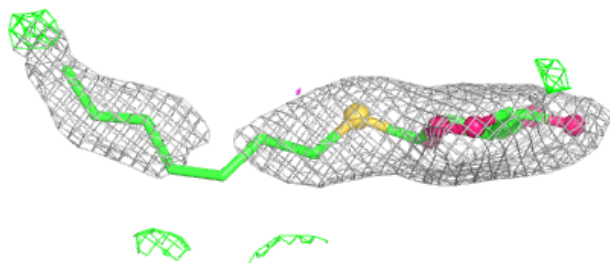
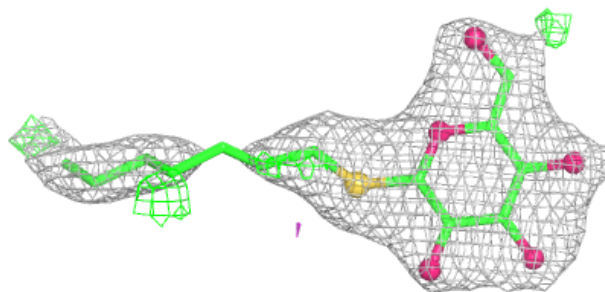


Electron density around LMT T 104:

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

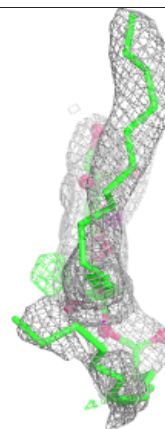
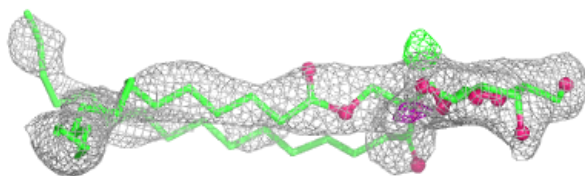
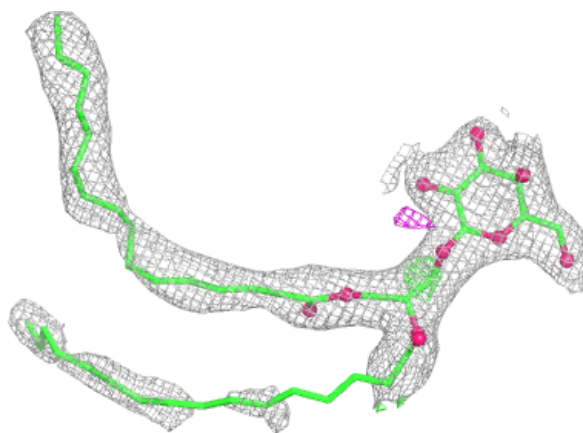
**Electron density around HTG C 522:**

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

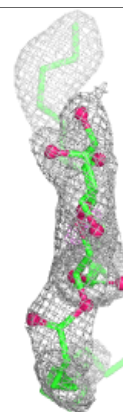
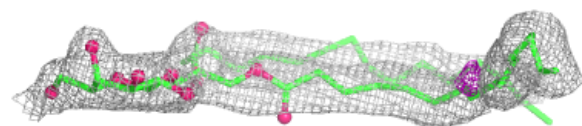
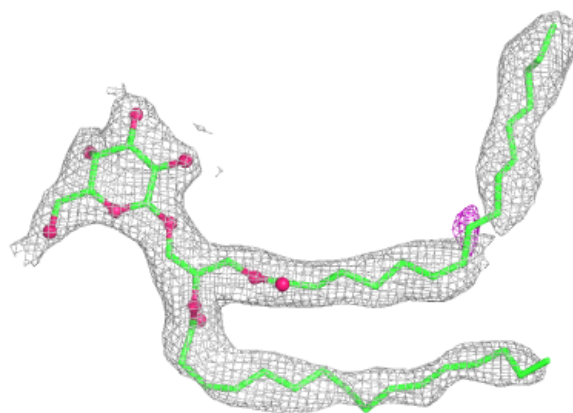


Electron density around LMG c 522:

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

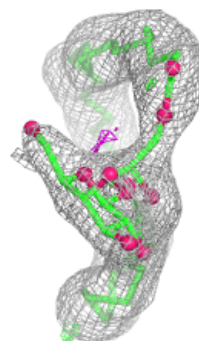
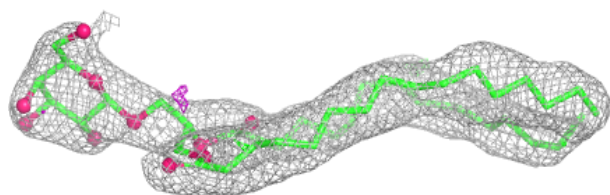
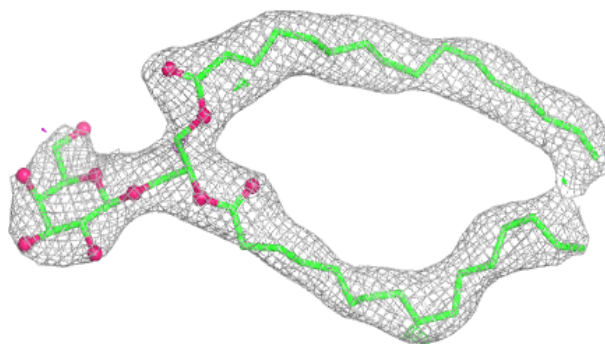
**Electron density around LMG C 519:**

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

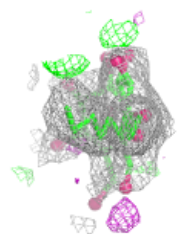
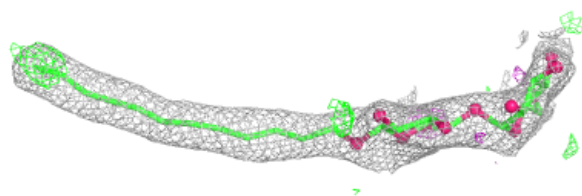
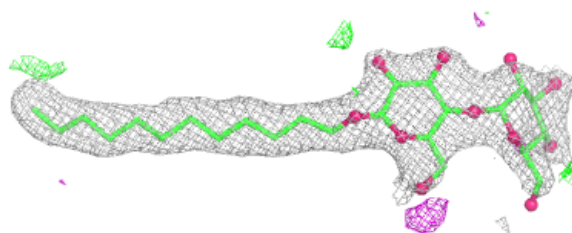


Electron density around LMG a 415:

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

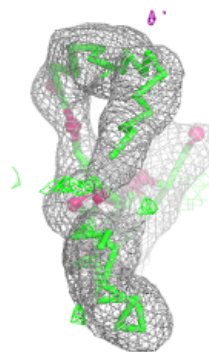
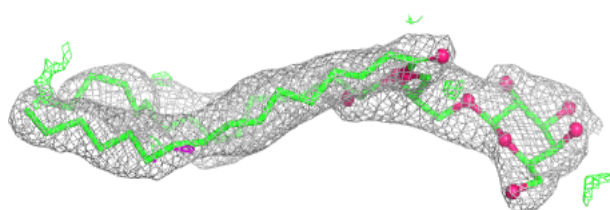
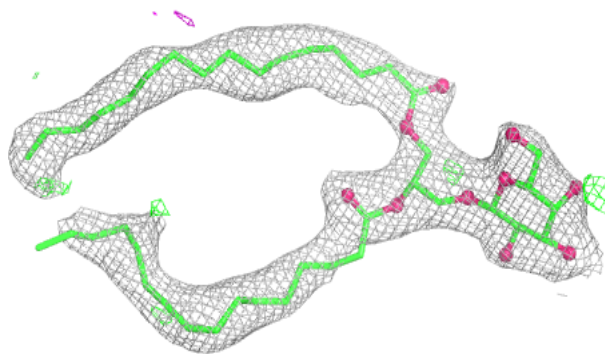
**Electron density around LMT M 101:**

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

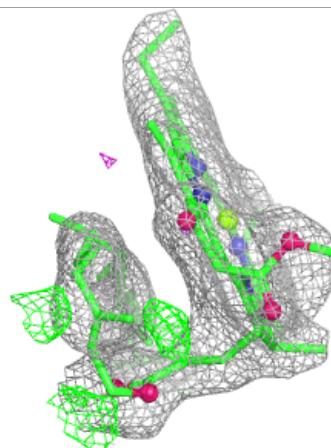
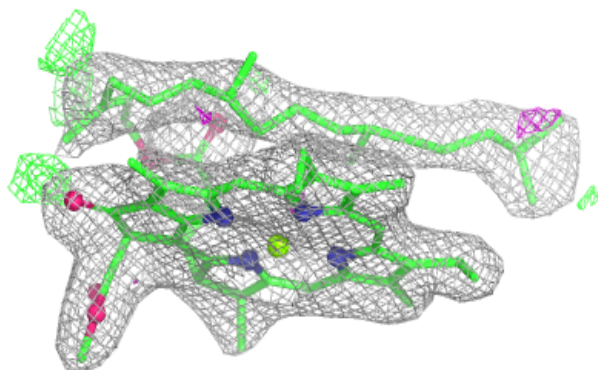
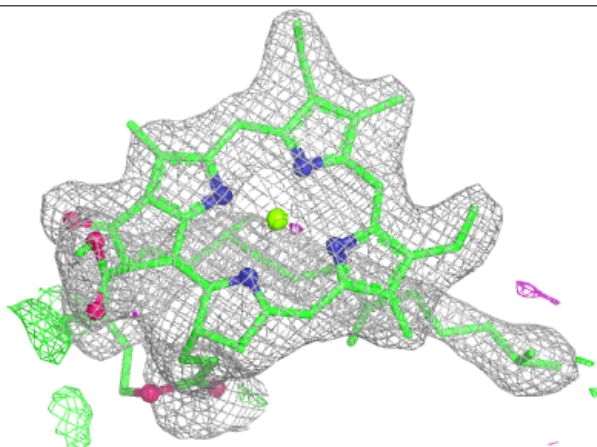


Electron density around LMG A 422:

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

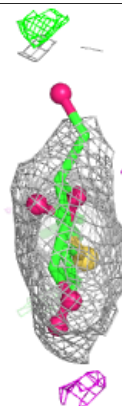
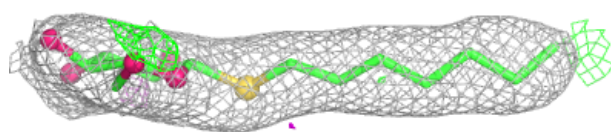
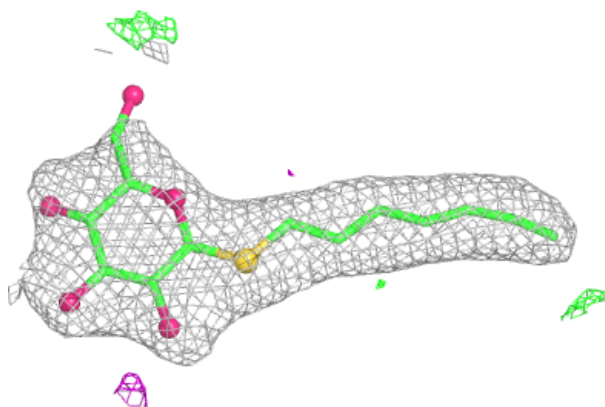
**Electron density around CLA b 611:**

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

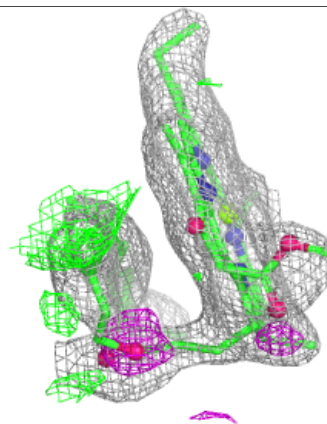
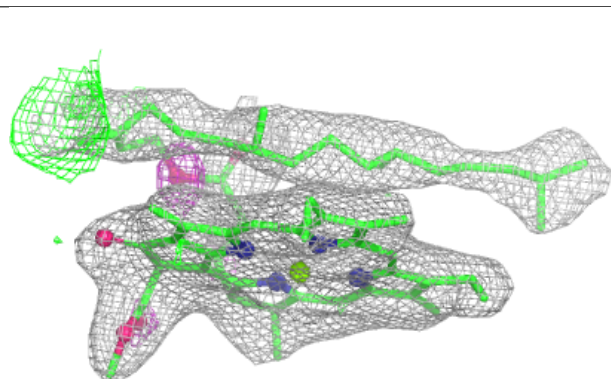
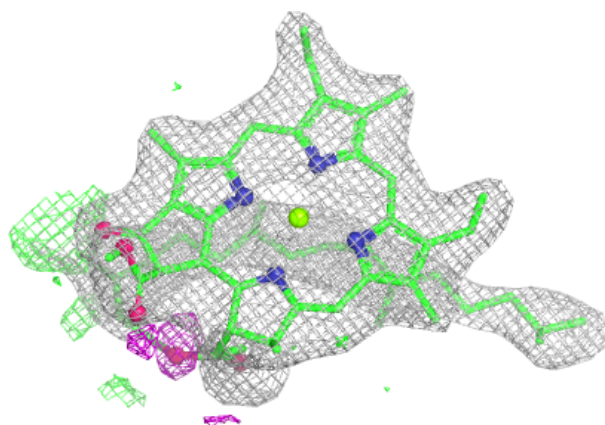


Electron density around HTG B 632:

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

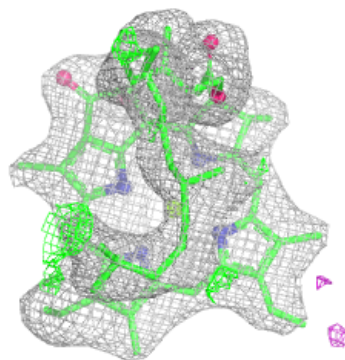
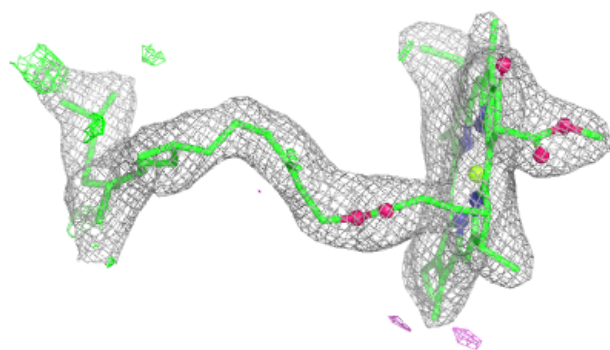
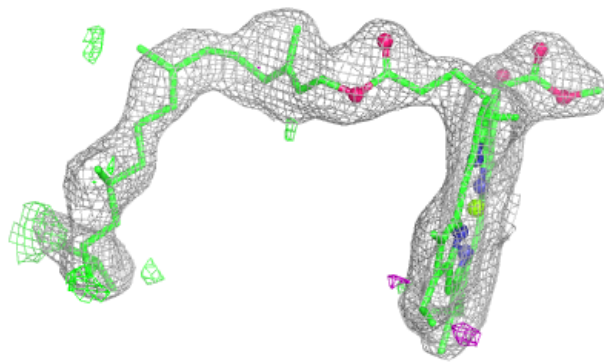
**Electron density around CLA B 602:**

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

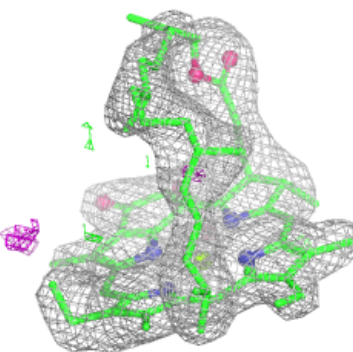
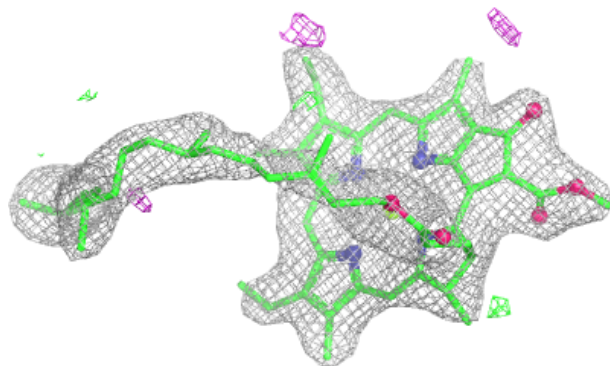
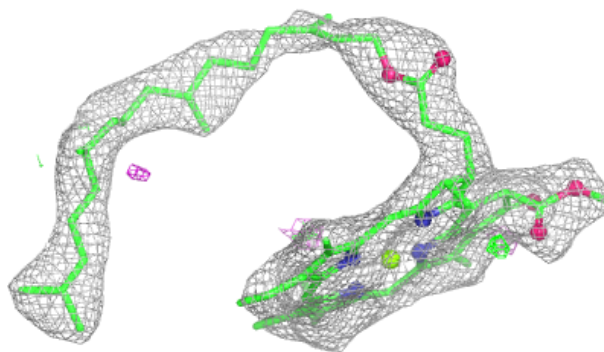


Electron density around CLA C 506:

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

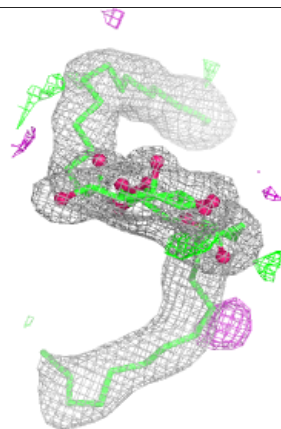
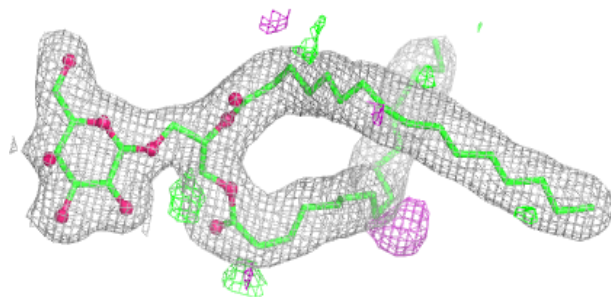
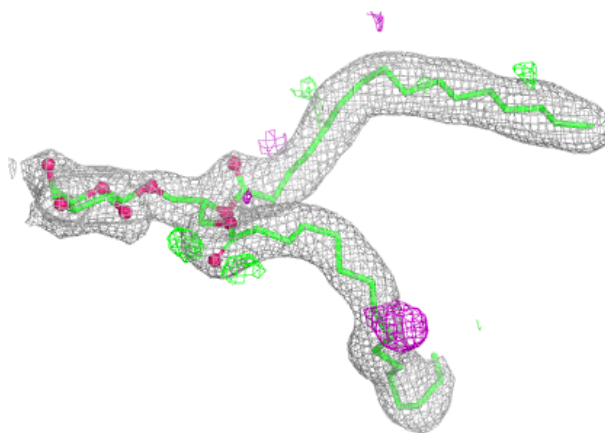
**Electron density around CLA C 513:**

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

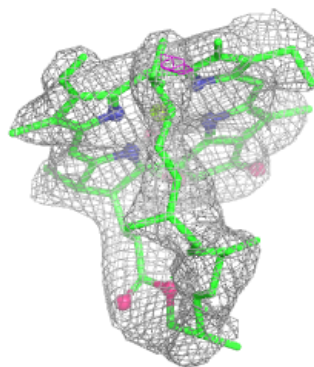
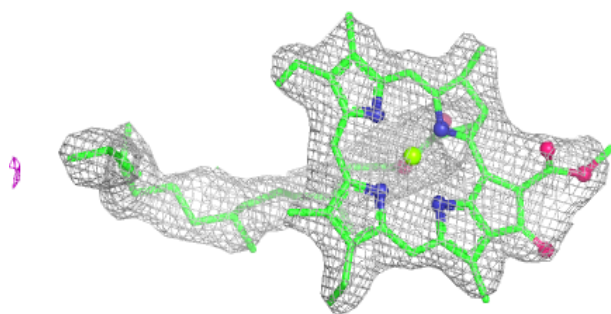
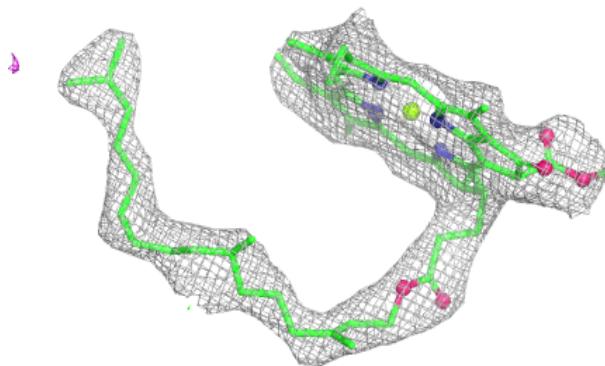


Electron density around LMG b 630:

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

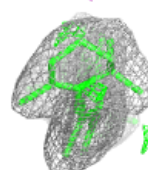
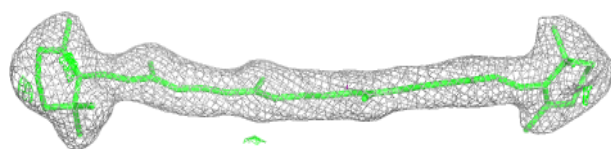
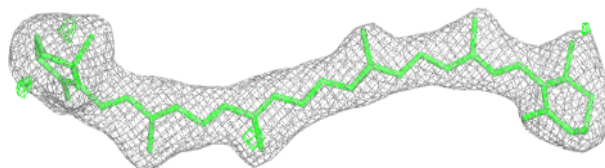
**Electron density around CLA c 517:**

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

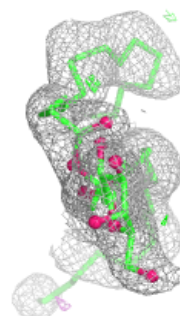
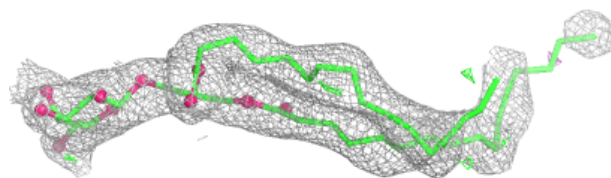
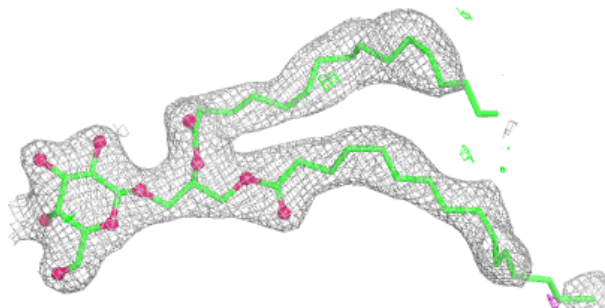


Electron density around BCR y 101:

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

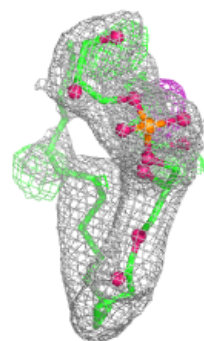
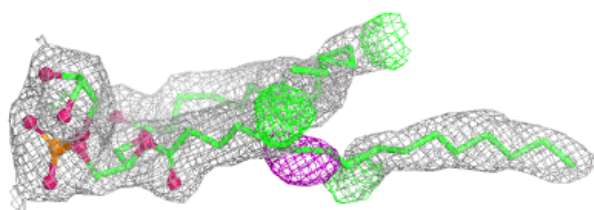
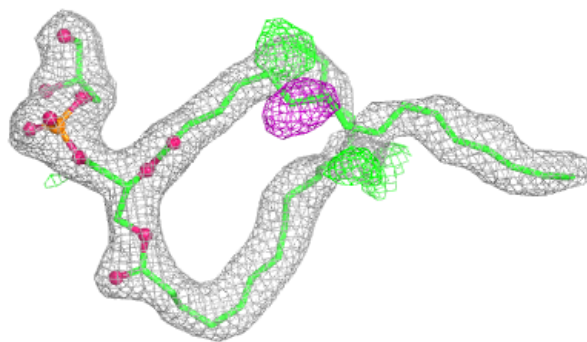
**Electron density around LMG j 101:**

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



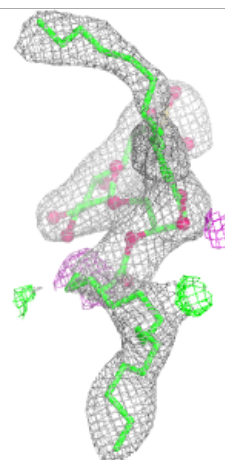
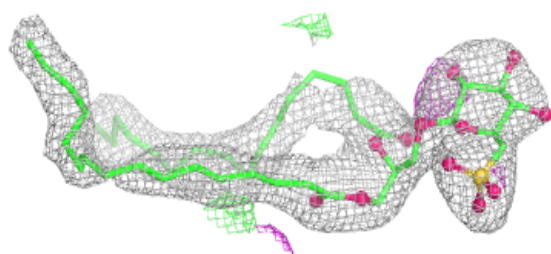
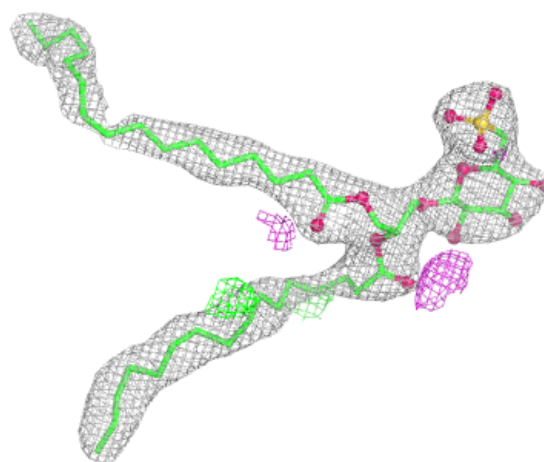
Electron density around LHG D 409:

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



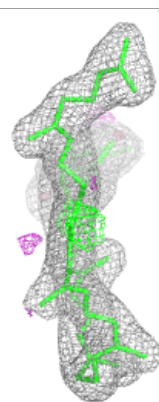
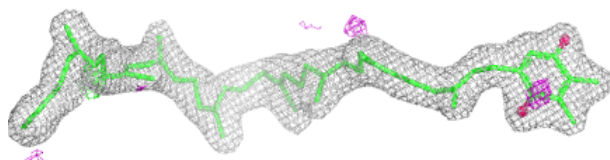
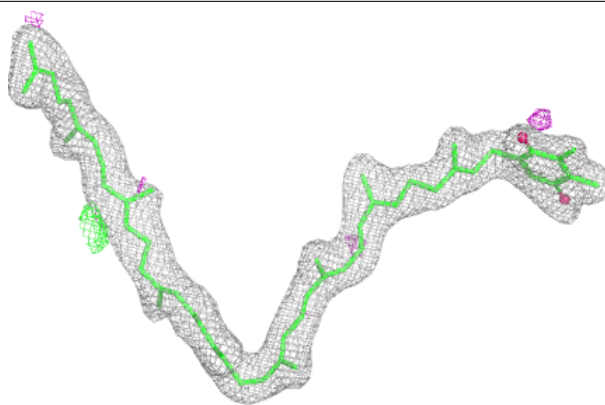
Electron density around SQD A 412:

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

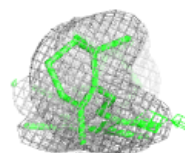
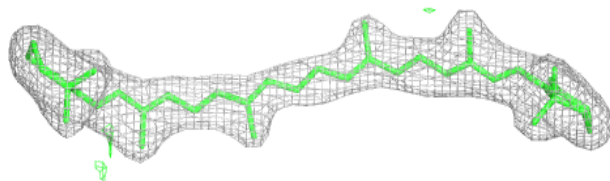
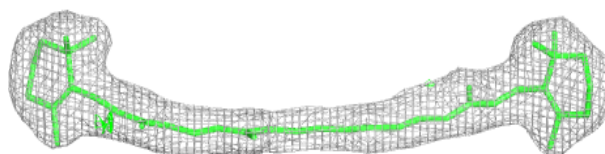


Electron density around PL9 D 405 (B):

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

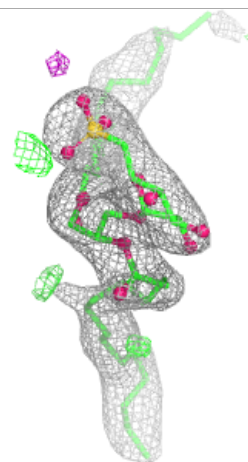
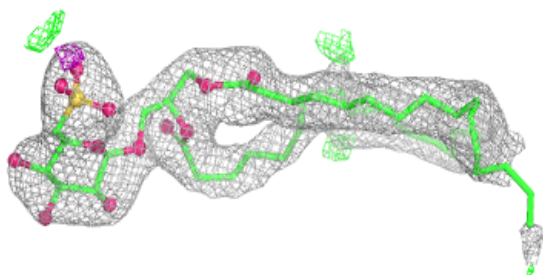
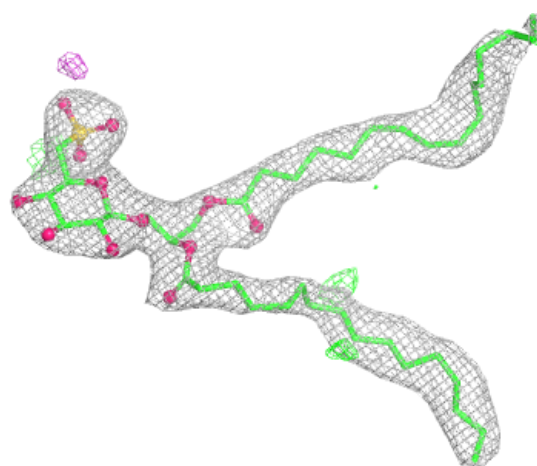
**Electron density around BCR K 101:**

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



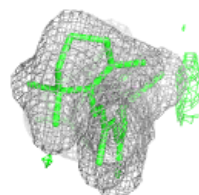
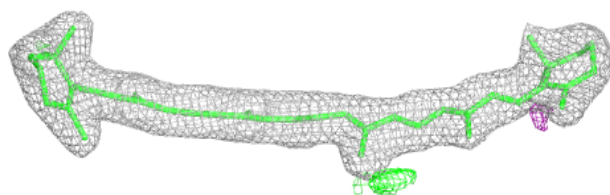
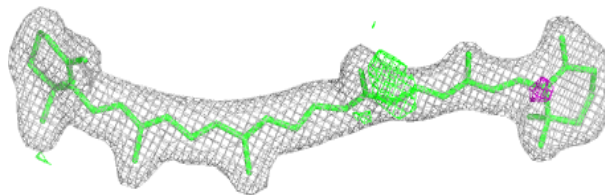
Electron density around SQD a 414:

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

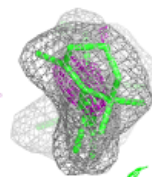
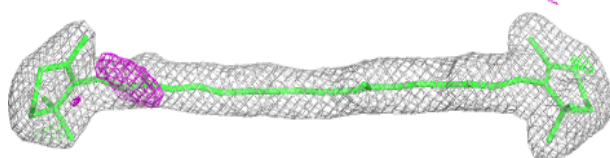
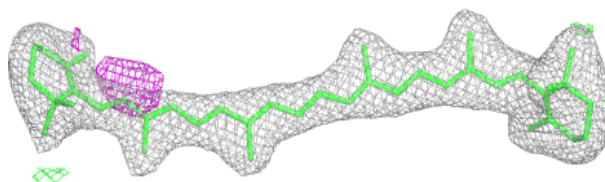


Electron density around BCR T 103:

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

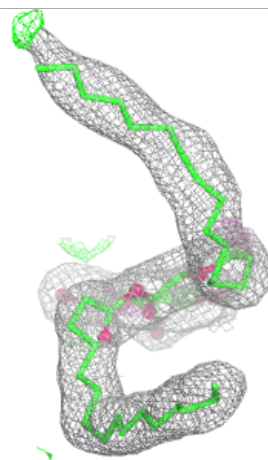
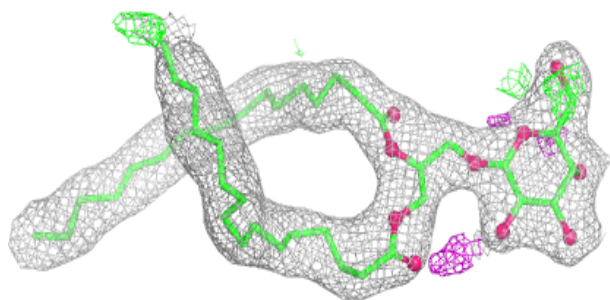
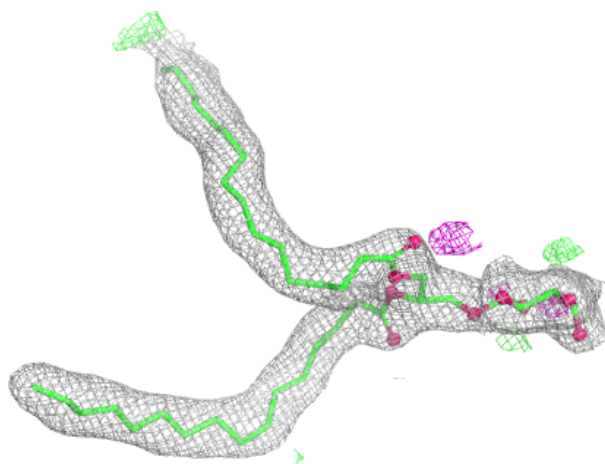
**Electron density around BCR b 628:**

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



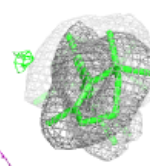
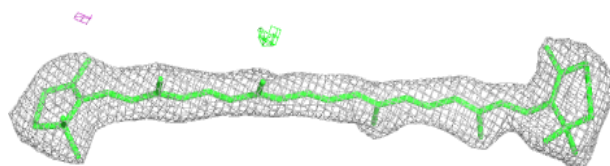
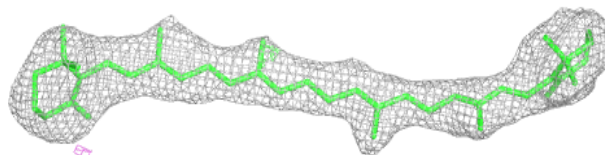
Electron density around LMG B 622:

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

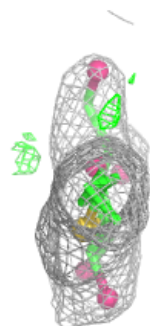
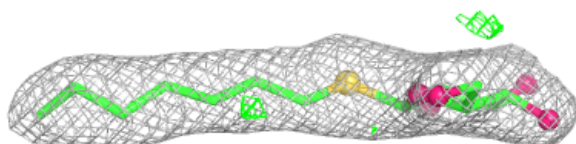
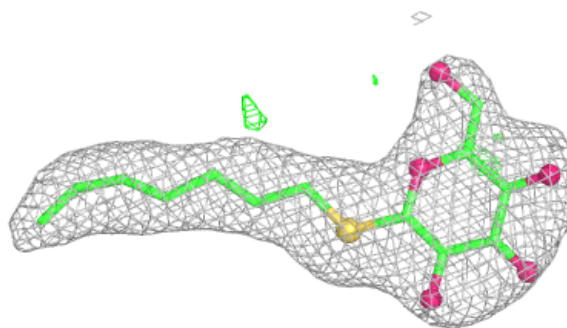


Electron density around BCR c 527:

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

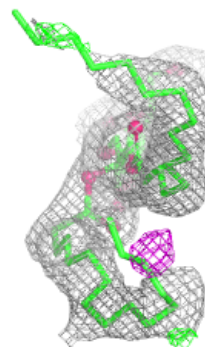
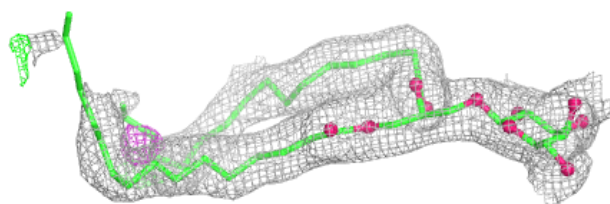
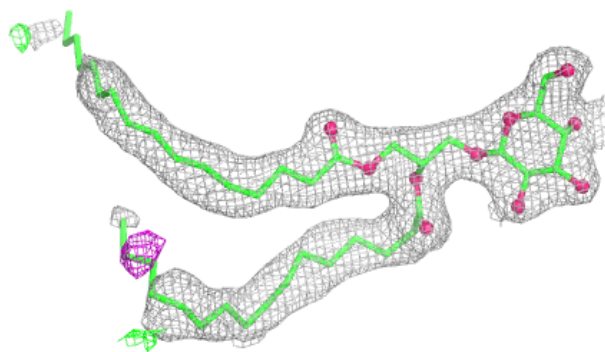
**Electron density around HTG b 608:**

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

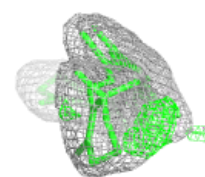
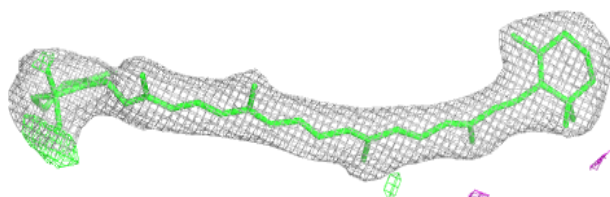
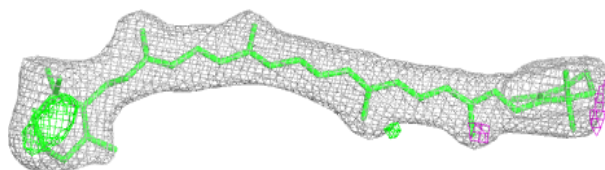


Electron density around LMG D 412:

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

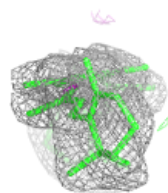
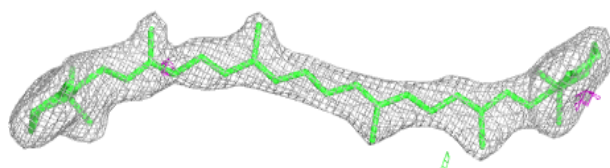
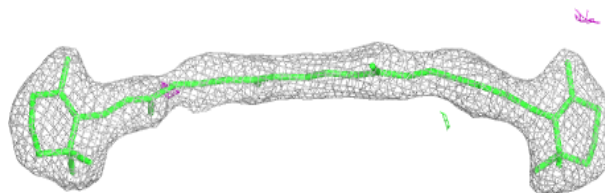
**Electron density around BCR d 404:**

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

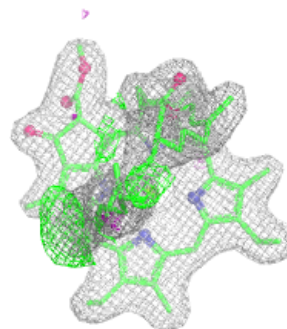
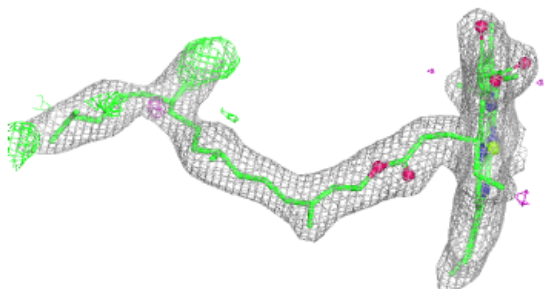
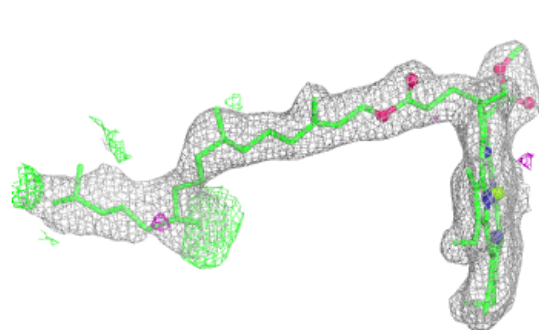


Electron density around BCR k 101:

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

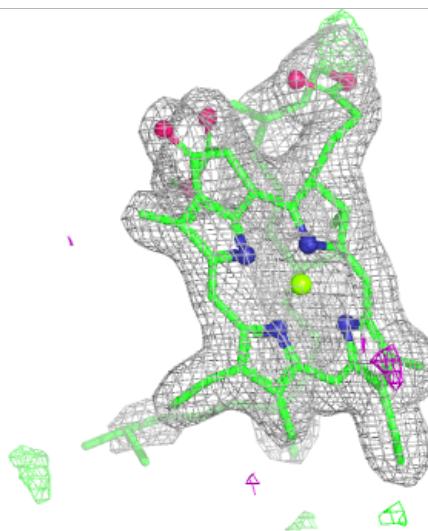
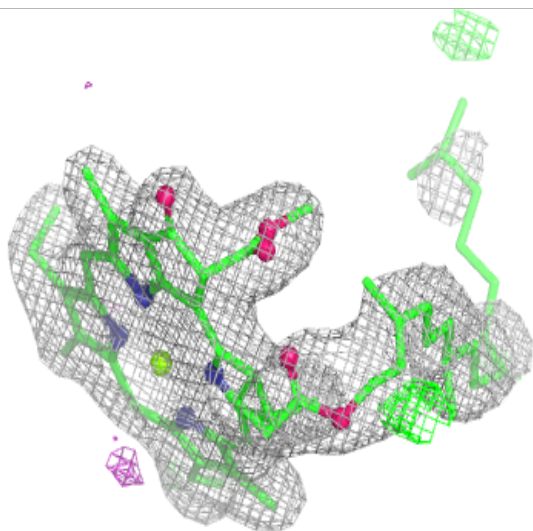
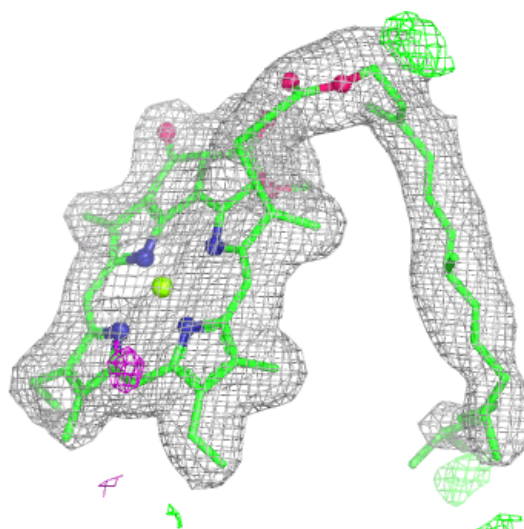
**Electron density around CLA b 616:**

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



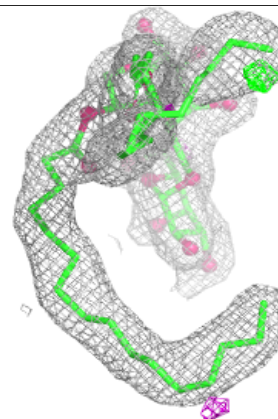
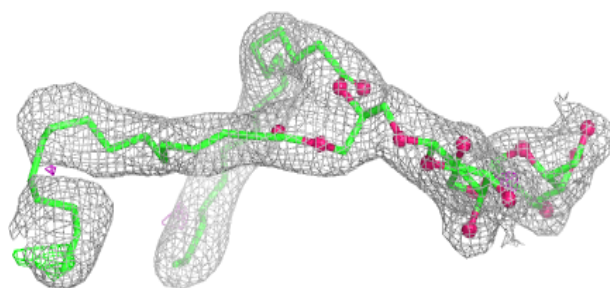
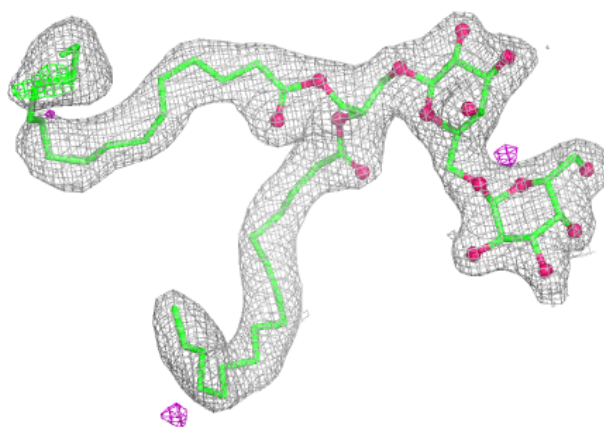
Electron density around CLA b 626:

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

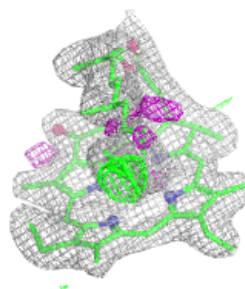
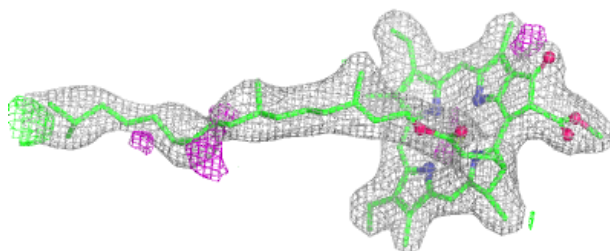
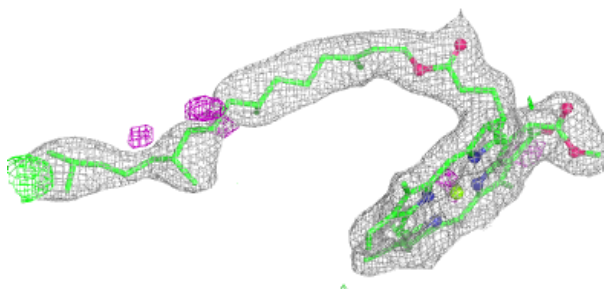


Electron density around DGD C 517:

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

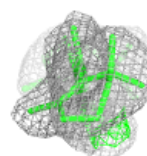
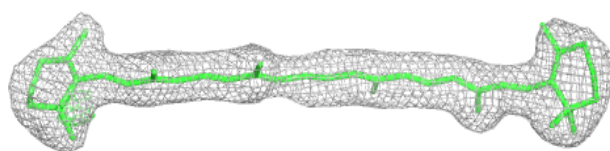
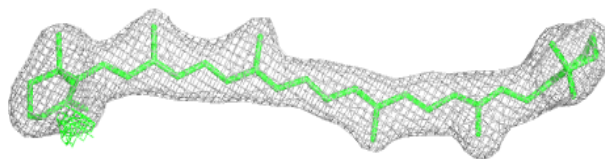
**Electron density around CLA C 504:**

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

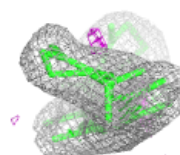
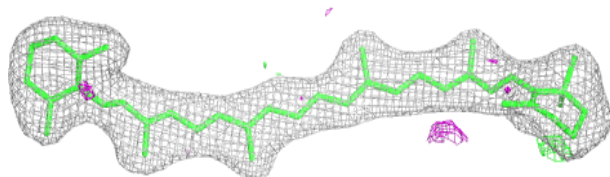
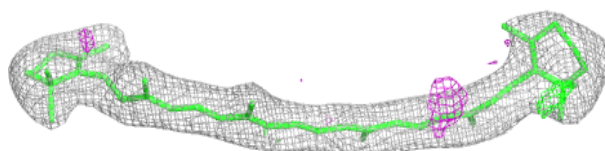


Electron density around BCR C 514:

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

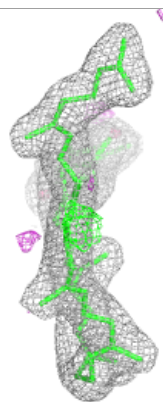
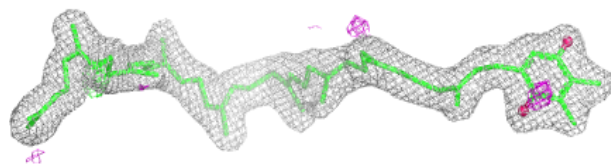
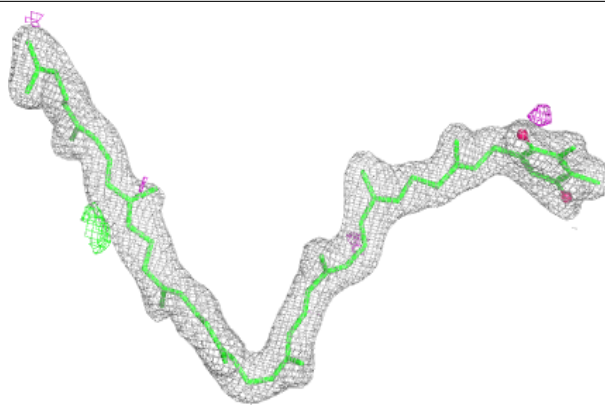
**Electron density around BCR D 404:**

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



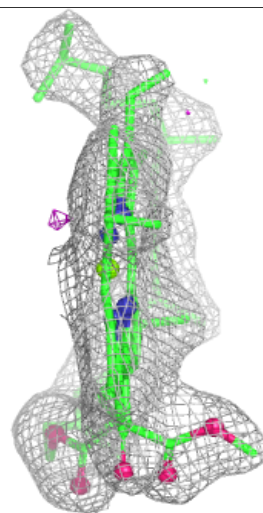
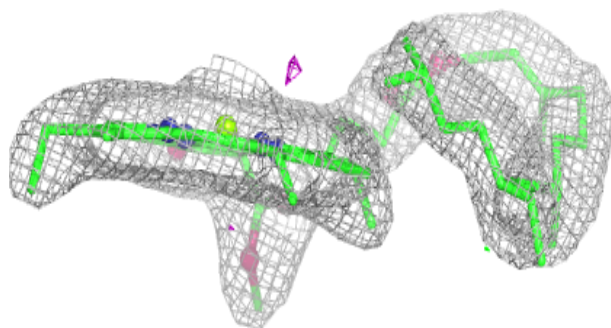
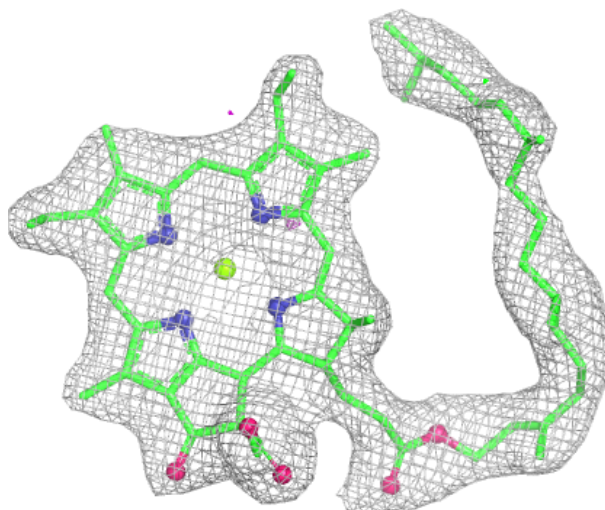
Electron density around PL9 D 405 (A):

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



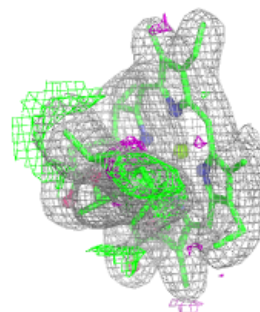
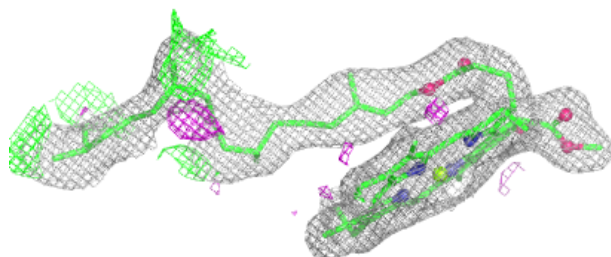
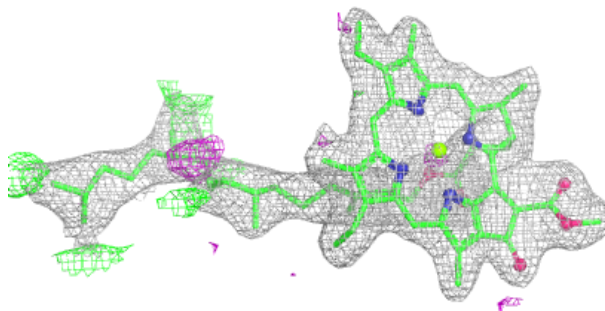
Electron density around CLA C 512:

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

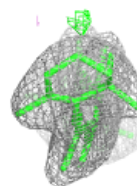
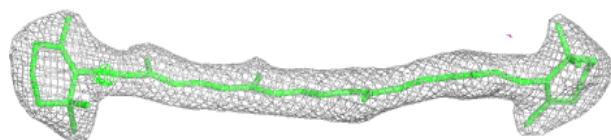
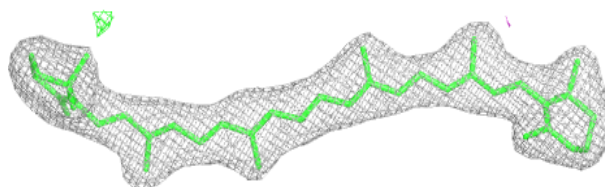


Electron density around CLA B 615:

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

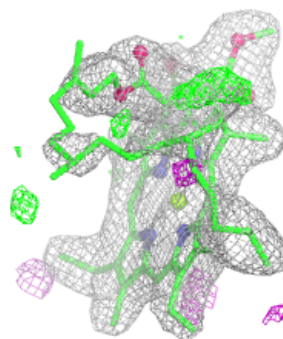
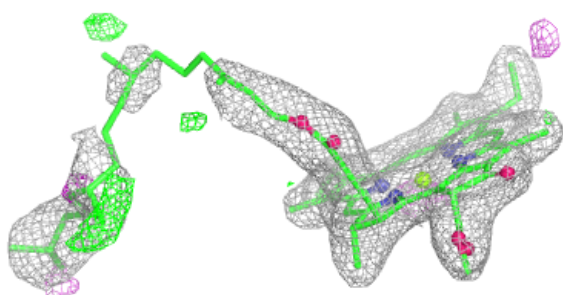
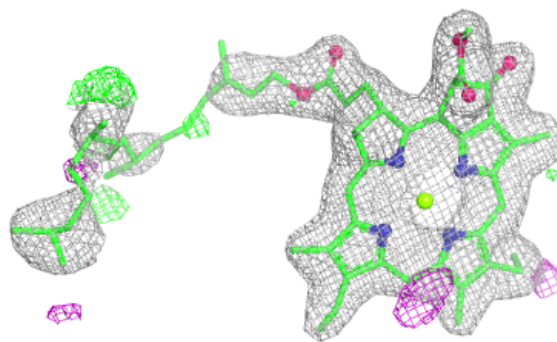
**Electron density around BCR Y 101:**

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



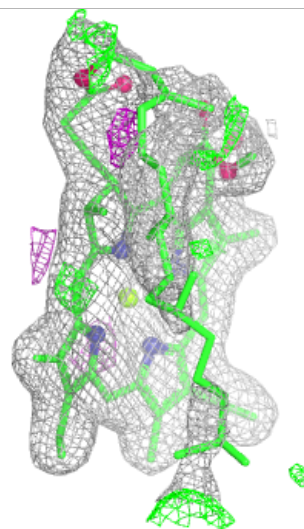
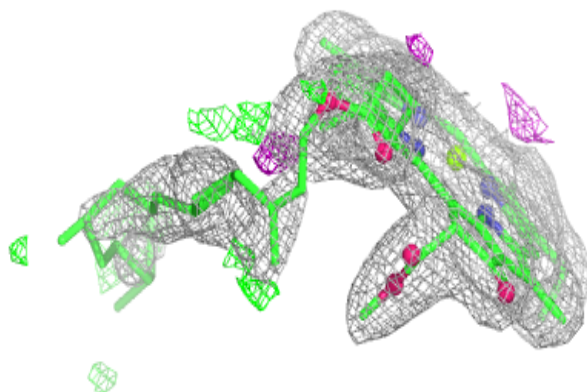
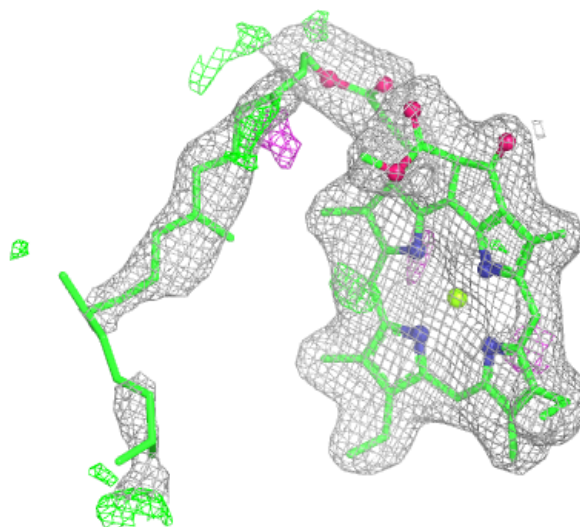
Electron density around CLA a 412:

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



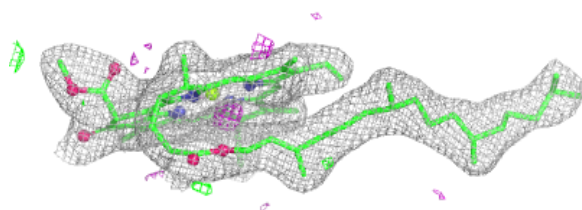
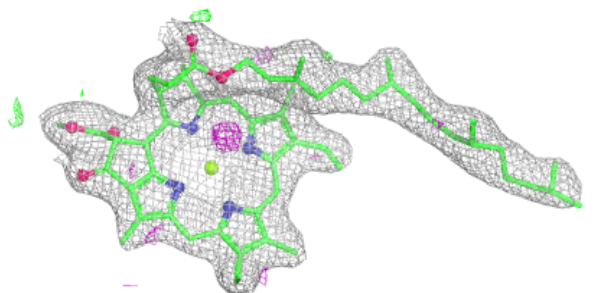
Electron density around CLA B 617:

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

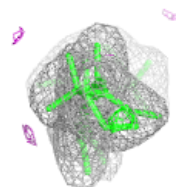
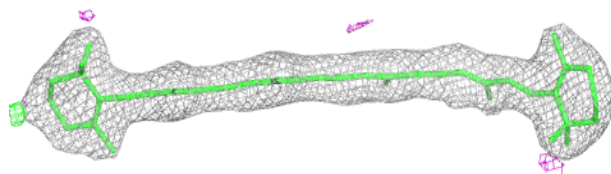
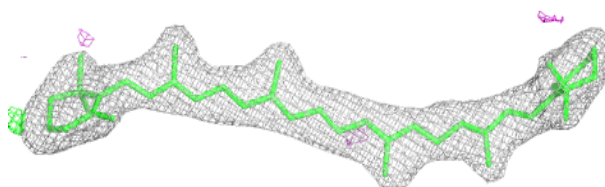


Electron density around CLA C 501:

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

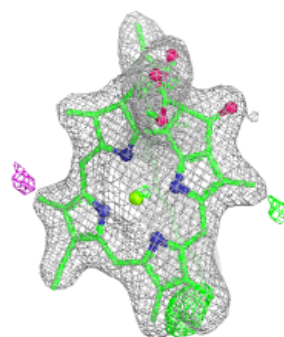
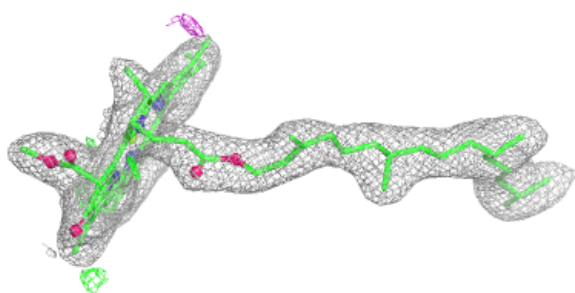
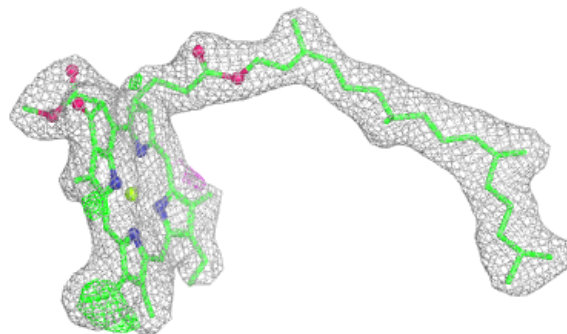
**Electron density around BCR h 101:**

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

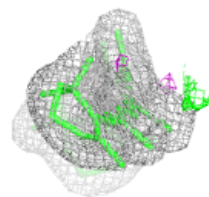
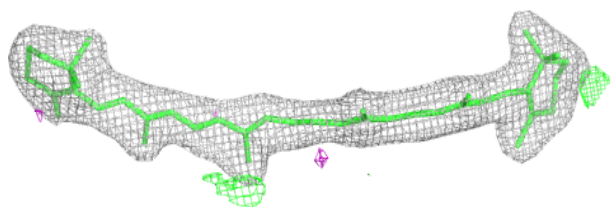
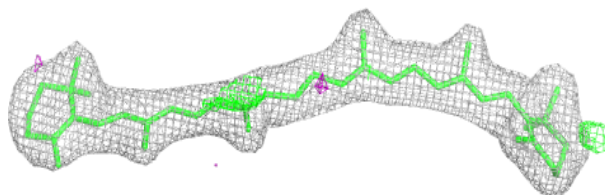


Electron density around CLA b 619:

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

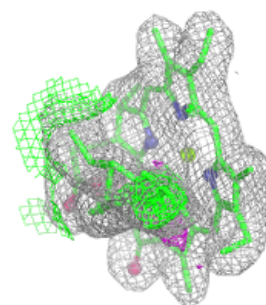
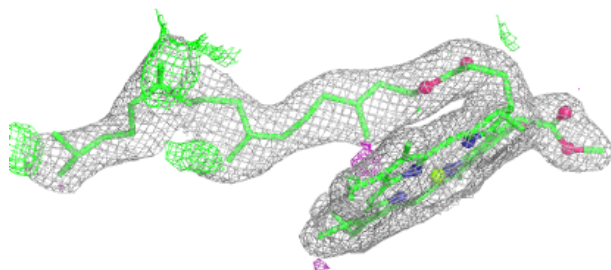
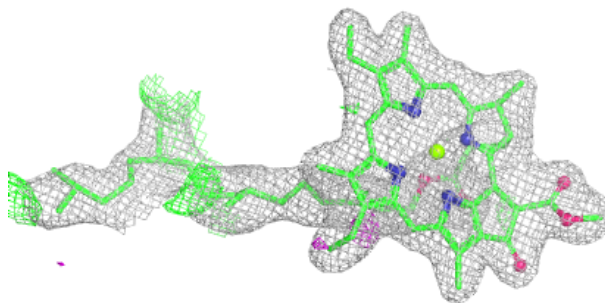
**Electron density around BCR t 101:**

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

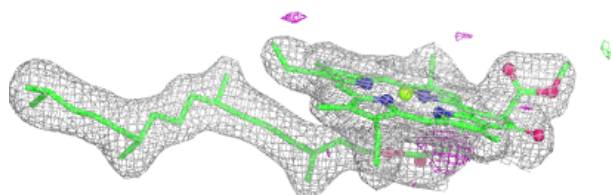
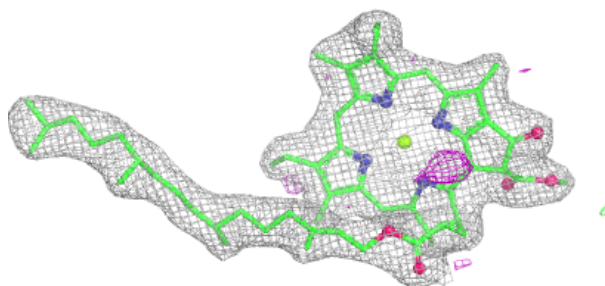


Electron density around CLA b 624:

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

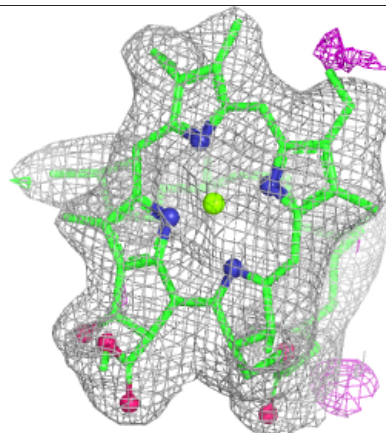
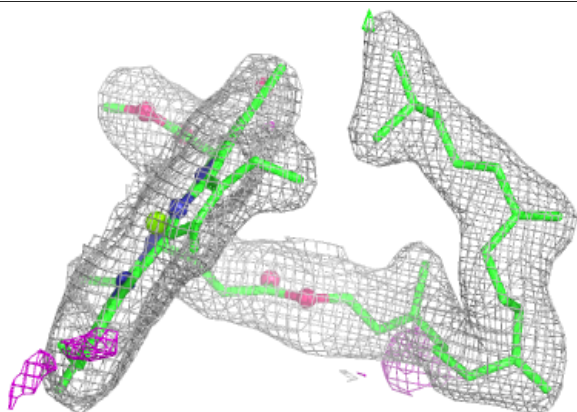
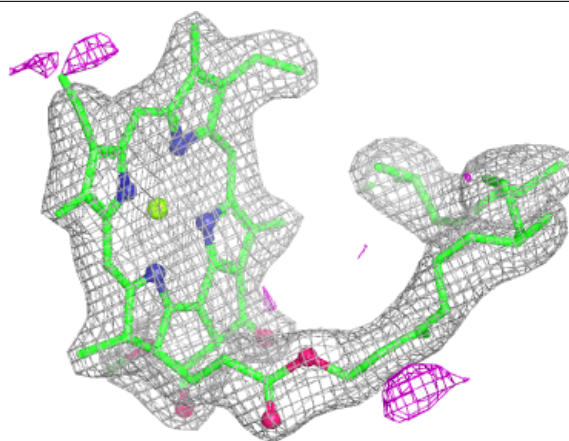
**Electron density around CLA c 505:**

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

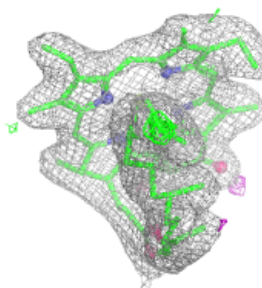
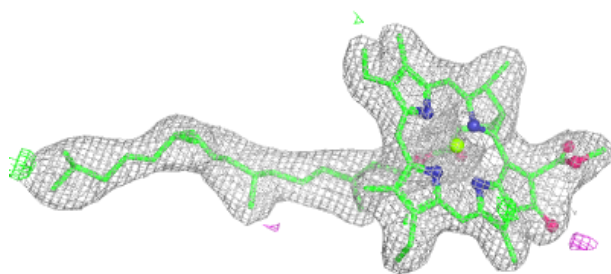
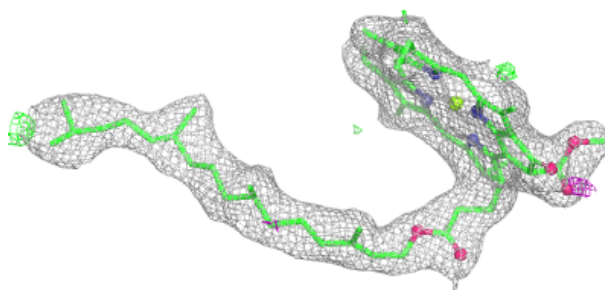


Electron density around CLA c 507:

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

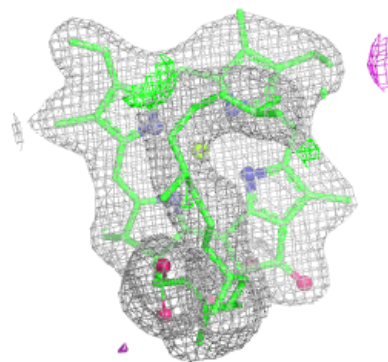
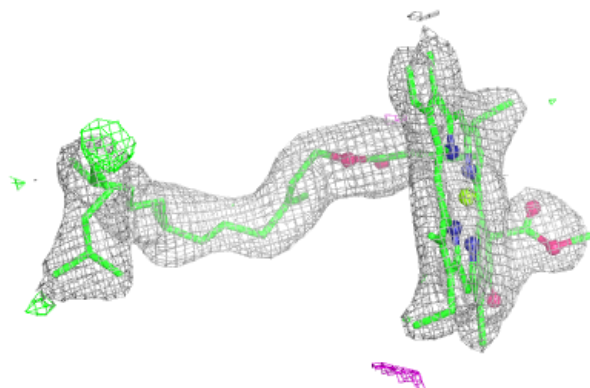
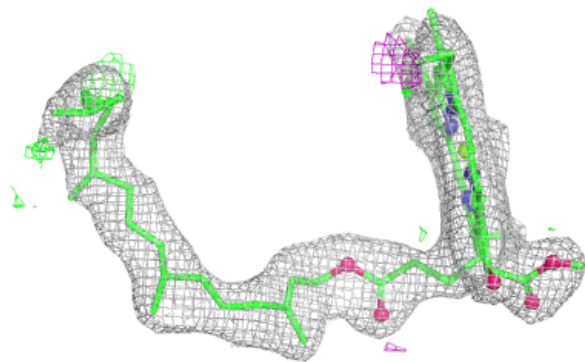
**Electron density around CLA c 508:**

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



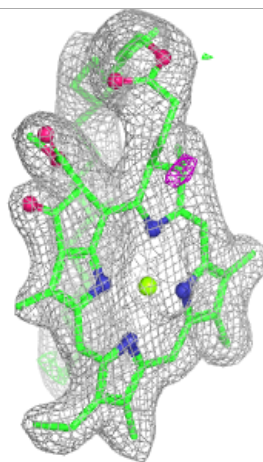
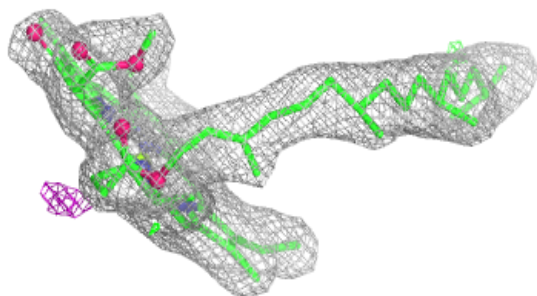
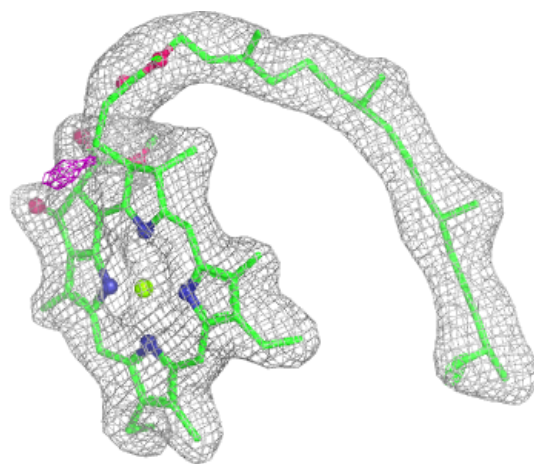
Electron density around CLA c 510:

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



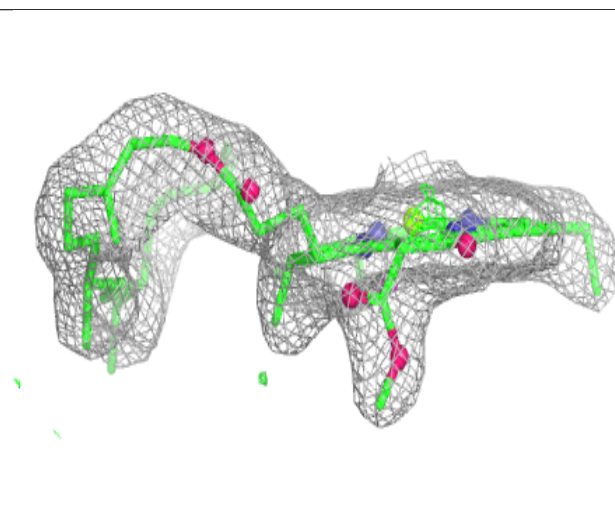
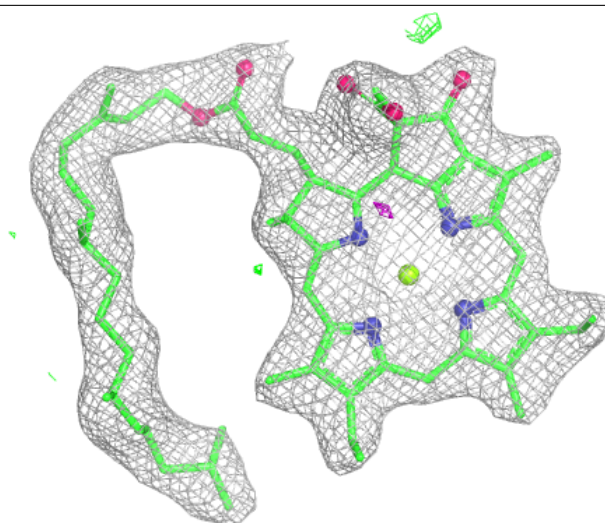
Electron density around CLA c 511:

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



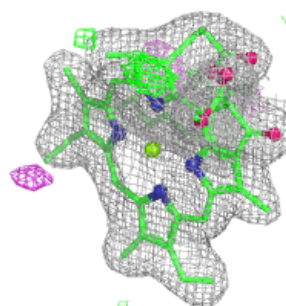
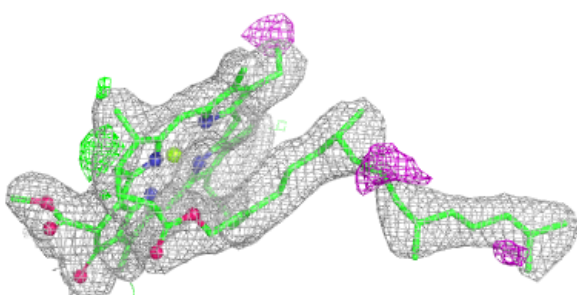
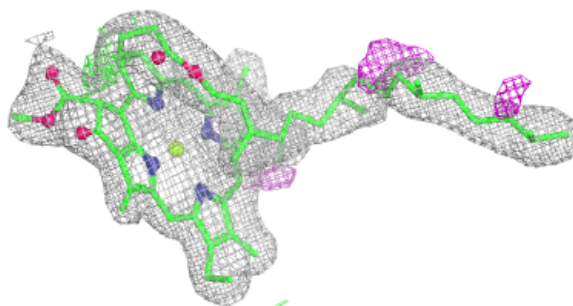
Electron density around CLA c 516:

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



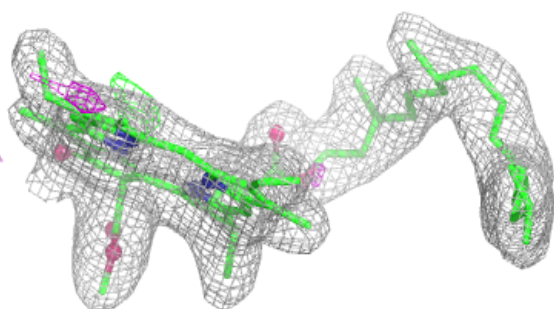
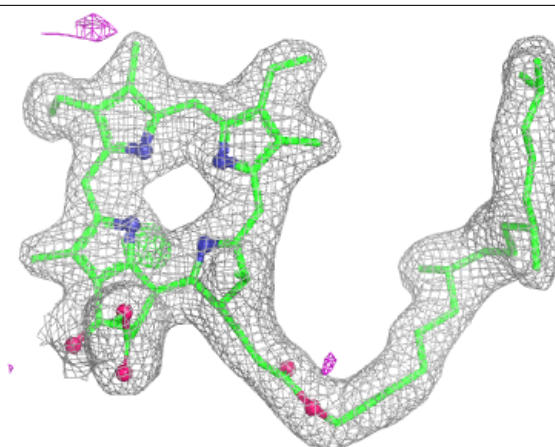
Electron density around CLA C 505:

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



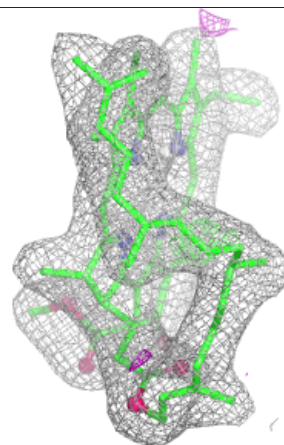
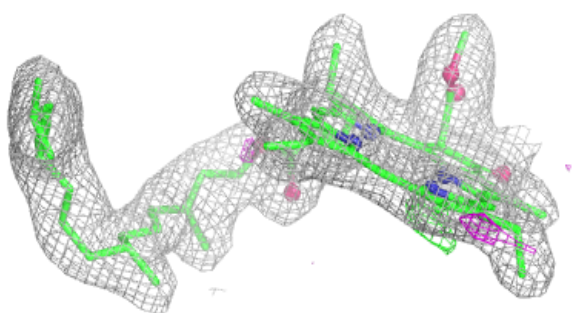
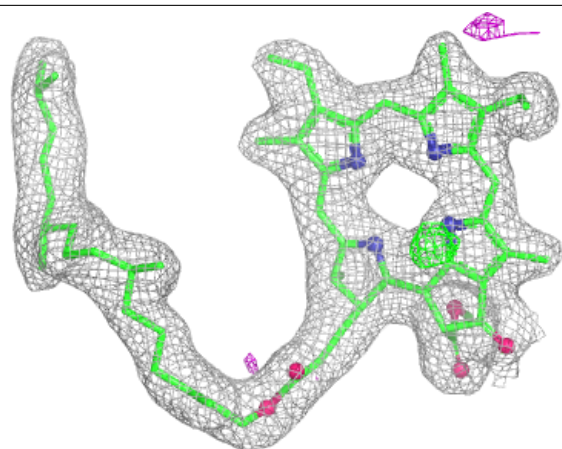
Electron density around PHO a 420 (A):

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

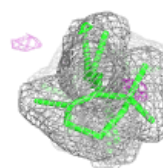
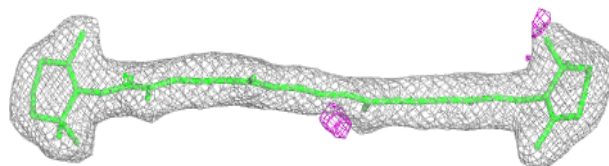
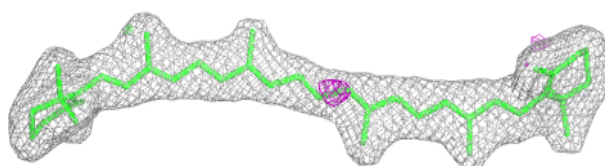


Electron density around PHO a 420 (B):

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

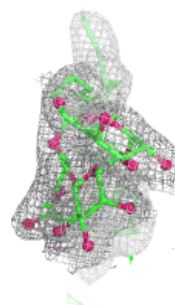
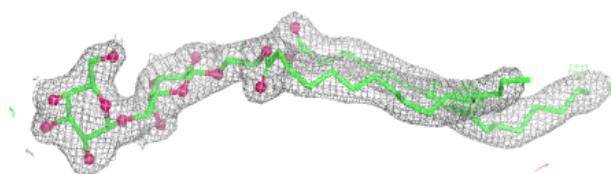
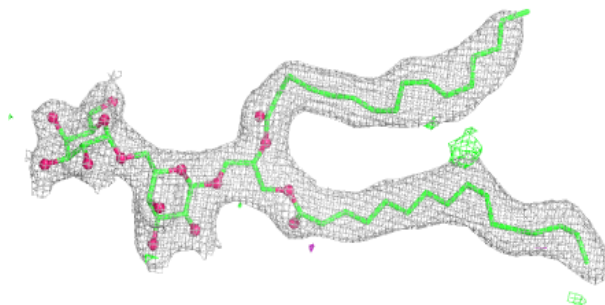
**Electron density around BCR A 411:**

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

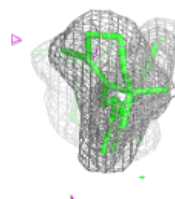
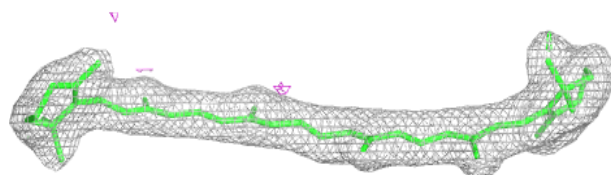
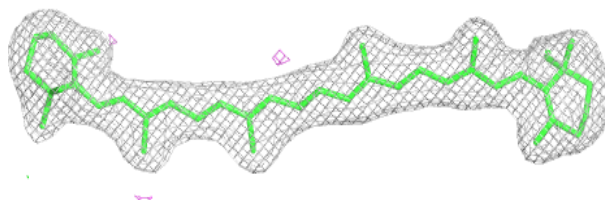


Electron density around DGD C 518:

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

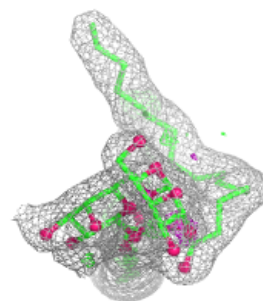
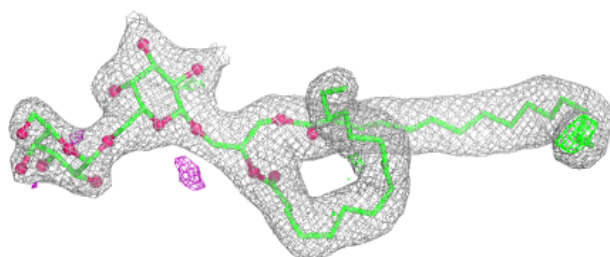
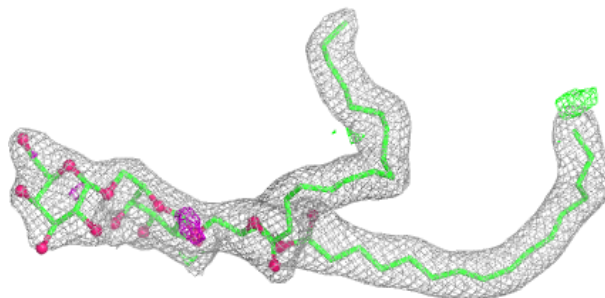
**Electron density around BCR B 620:**

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

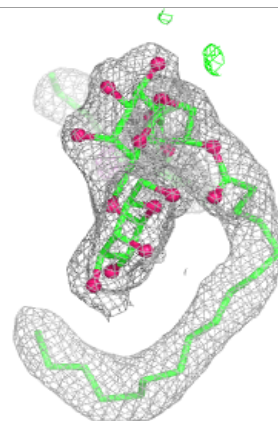
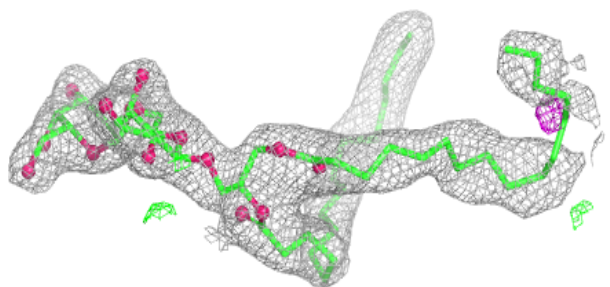
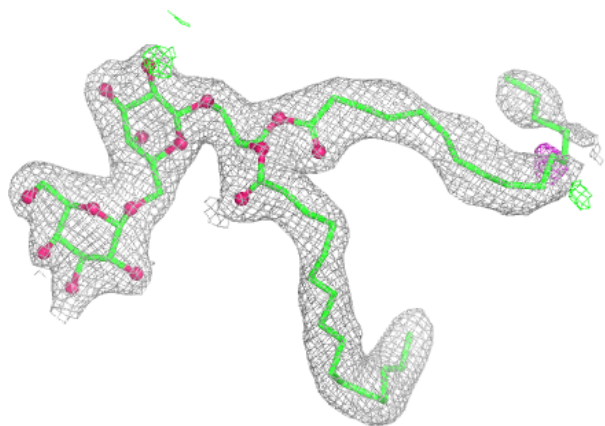


Electron density around DGD H 103:

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

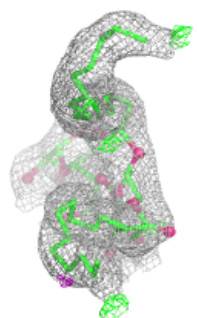
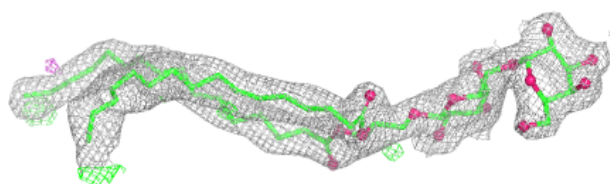
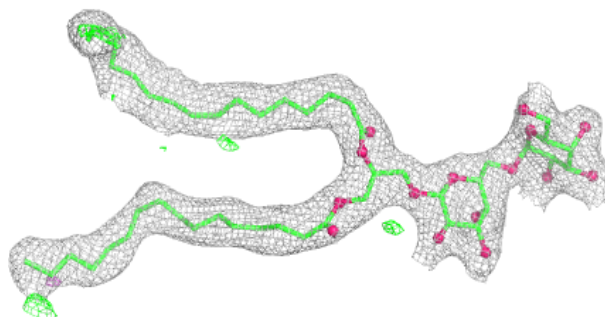
**Electron density around DGD c 520:**

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

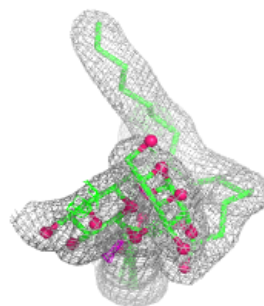
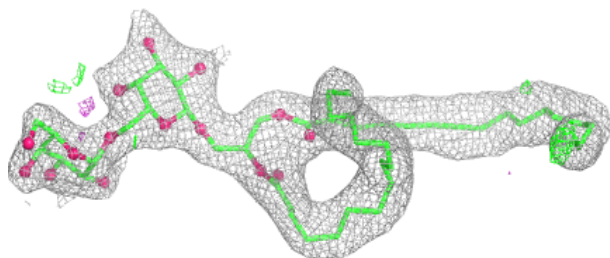
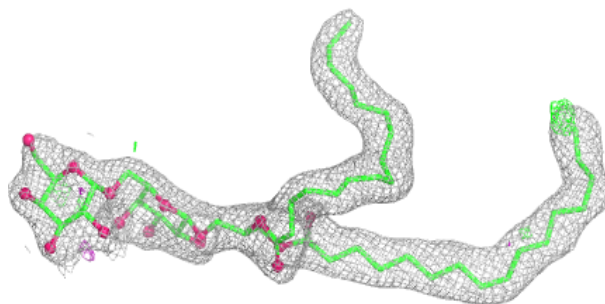


Electron density around DGD c 521:

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

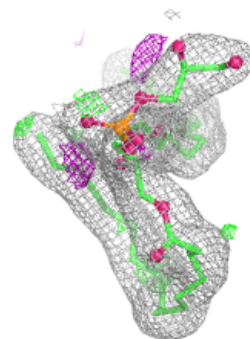
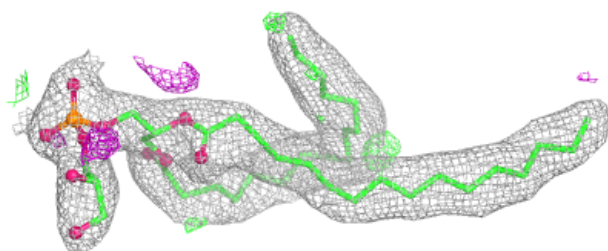
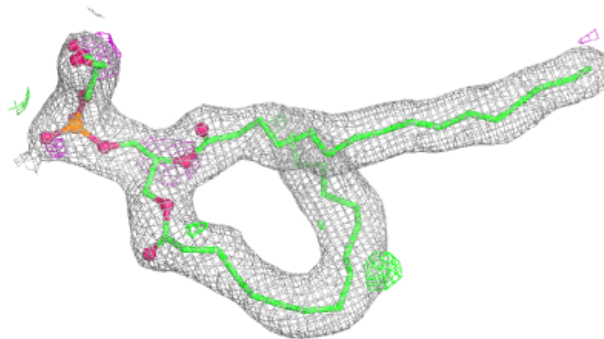
**Electron density around DGD h 102:**

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



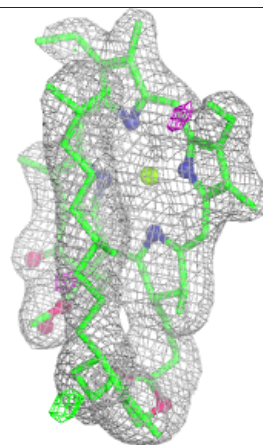
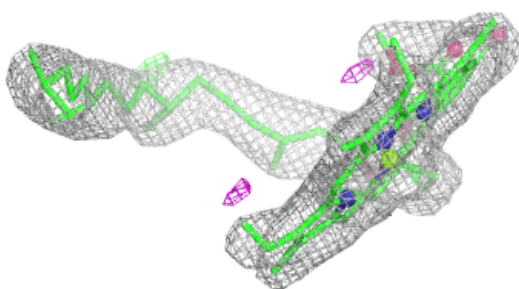
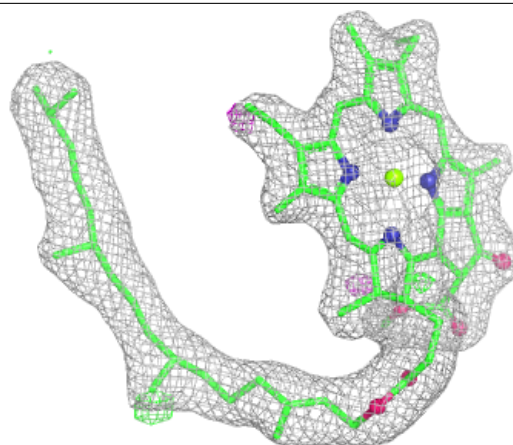
Electron density around LHG D 407:

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

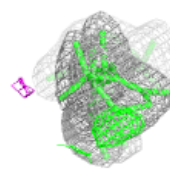
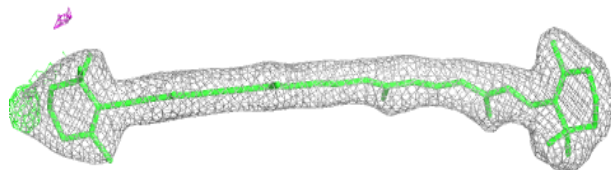
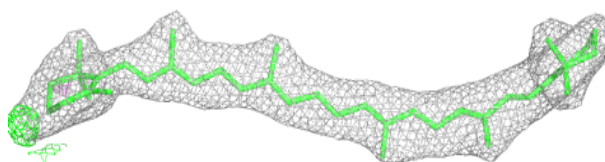


Electron density around CLA C 507:

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

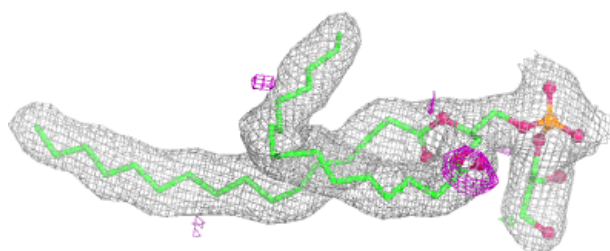
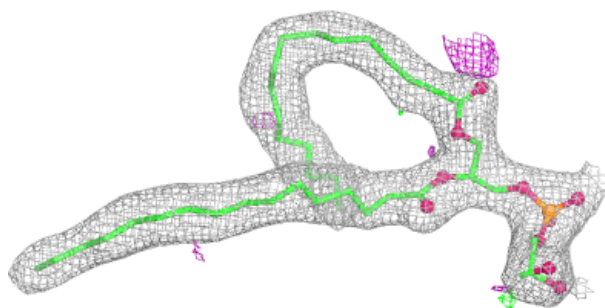
**Electron density around BCR H 102:**

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

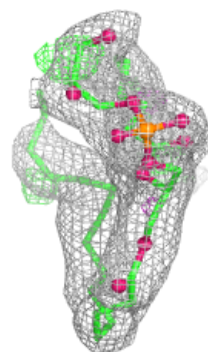
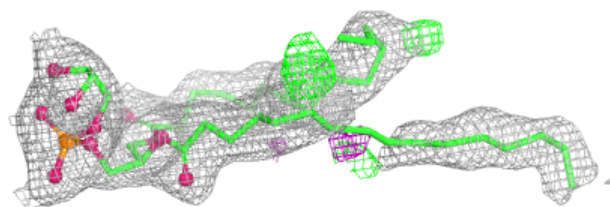
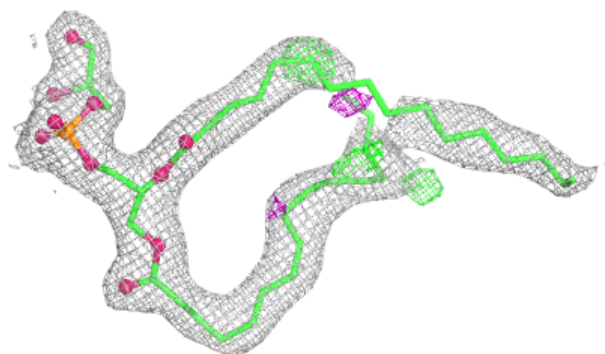


Electron density around LHG d 406:

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

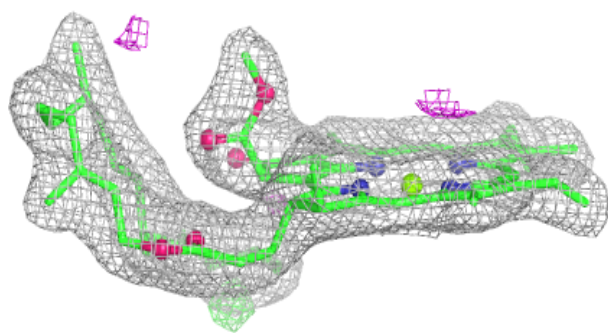
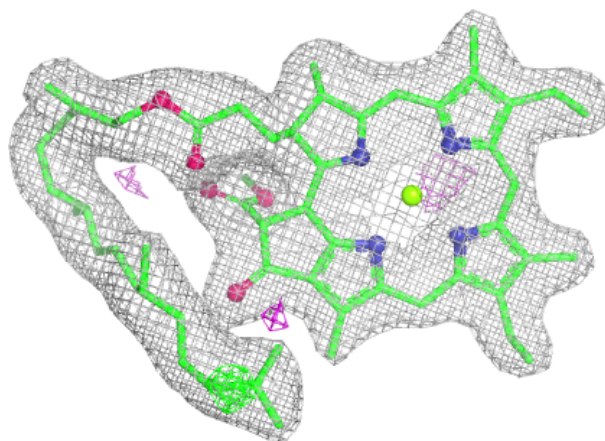
**Electron density around LHG d 408:**

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



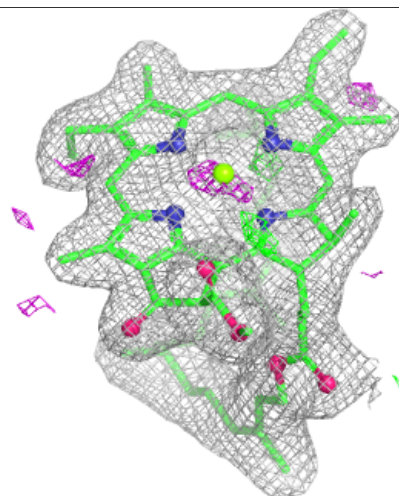
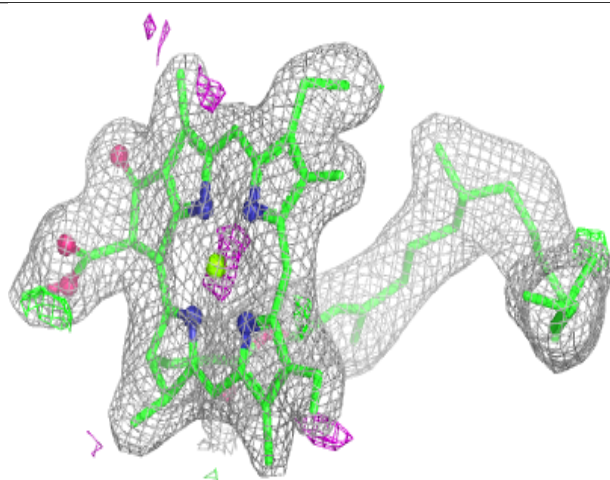
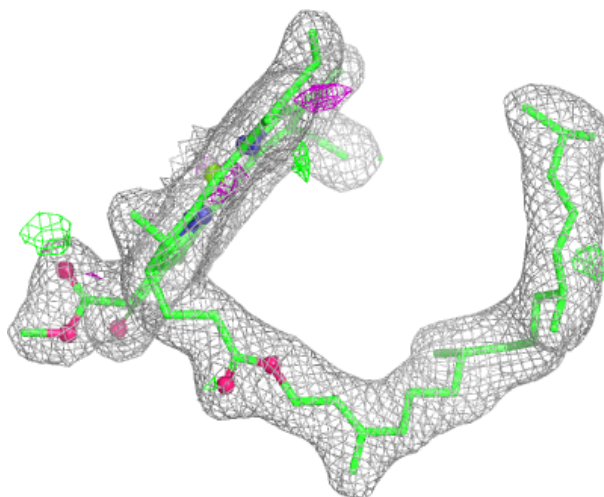
Electron density around CLA b 620:

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



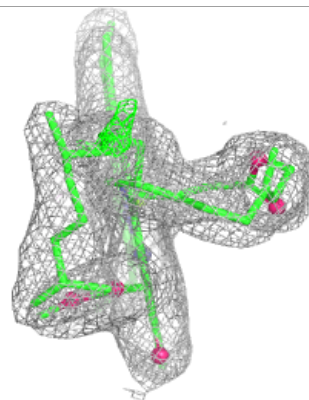
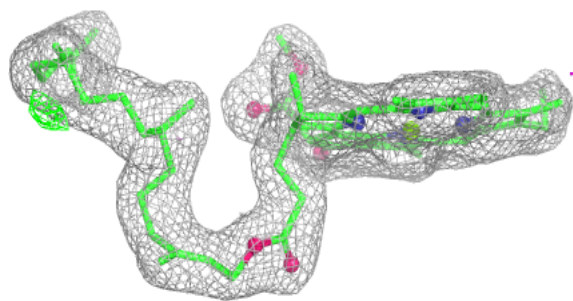
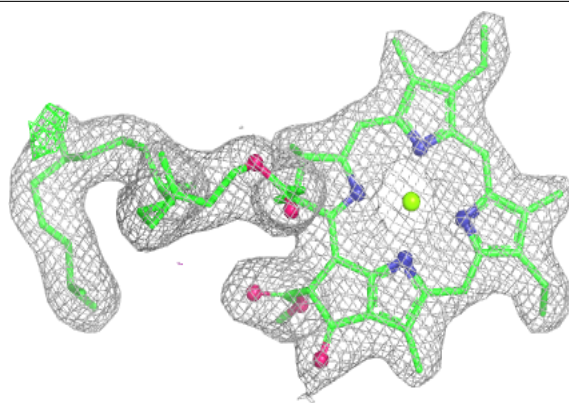
Electron density around CLA b 621:

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



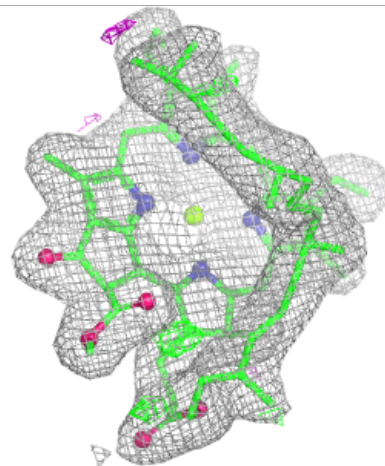
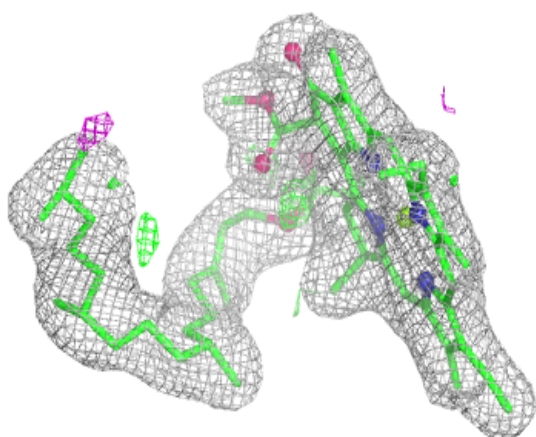
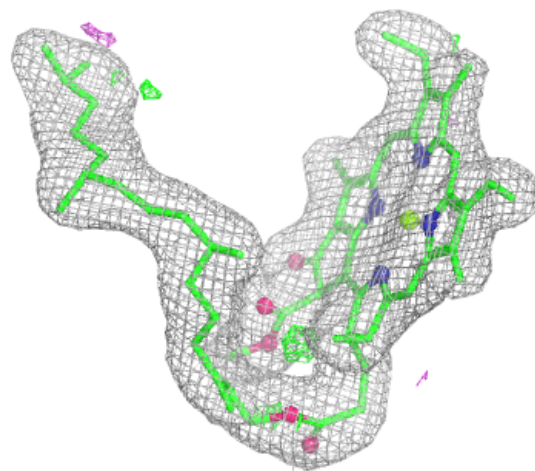
Electron density around CLA b 622:

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



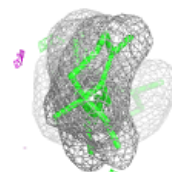
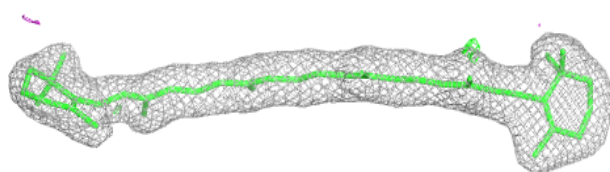
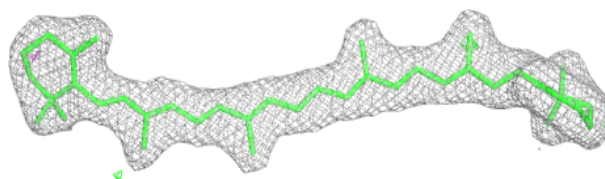
Electron density around CLA b 623:

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

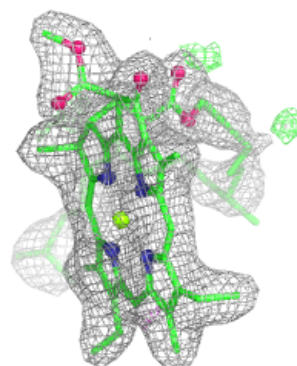
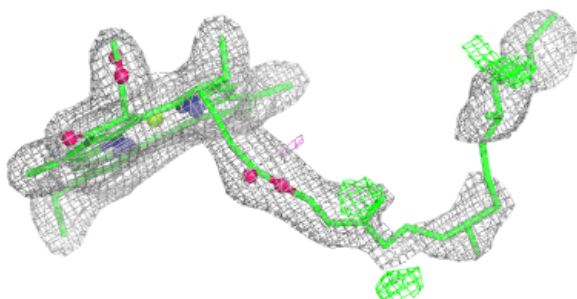
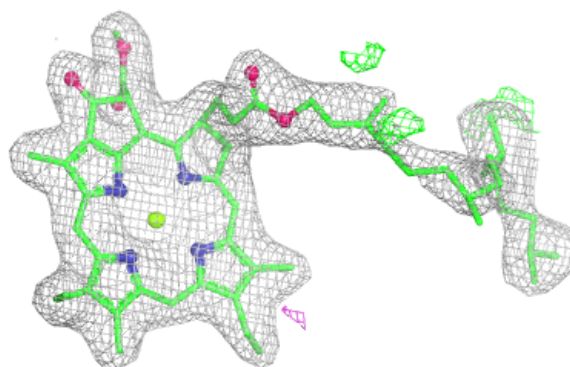


Electron density around BCR b 627:

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

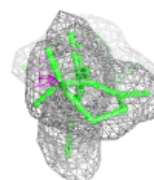
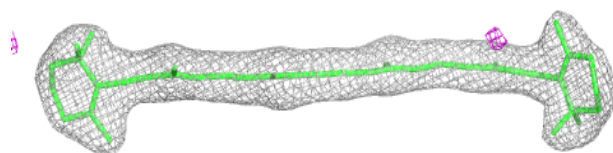
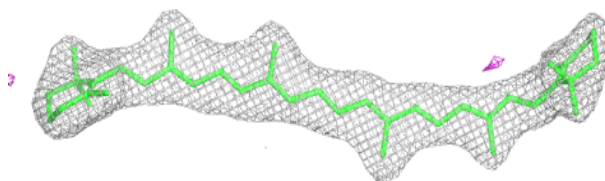
**Electron density around CLA A 410:**

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



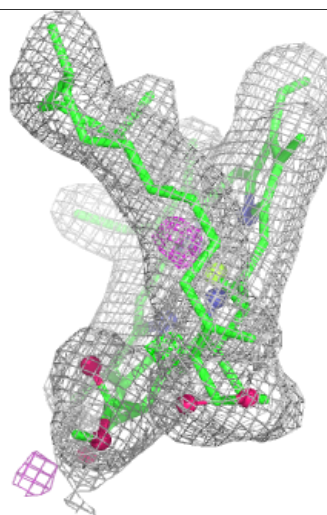
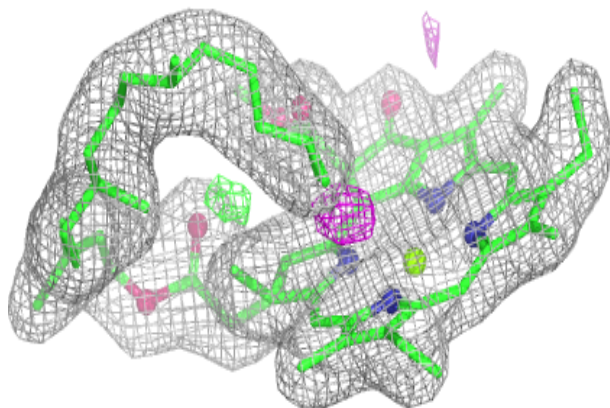
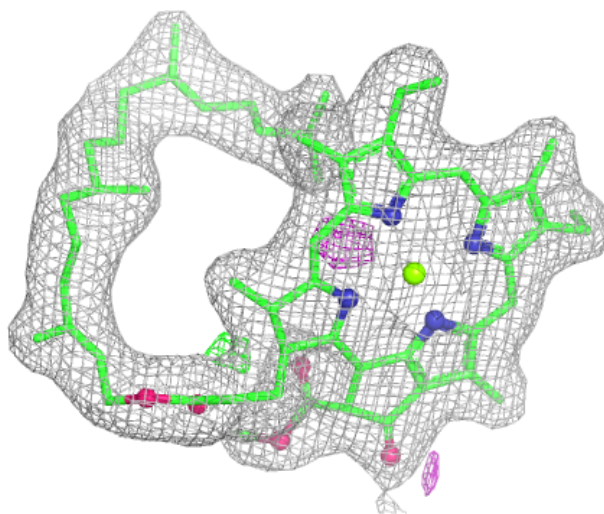
Electron density around BCR c 518:

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



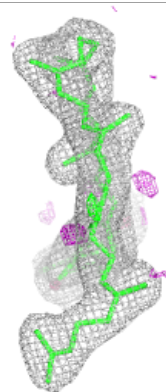
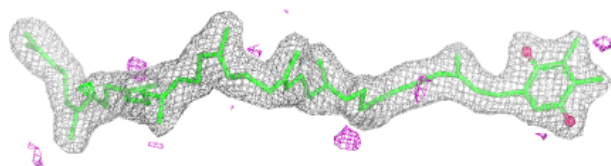
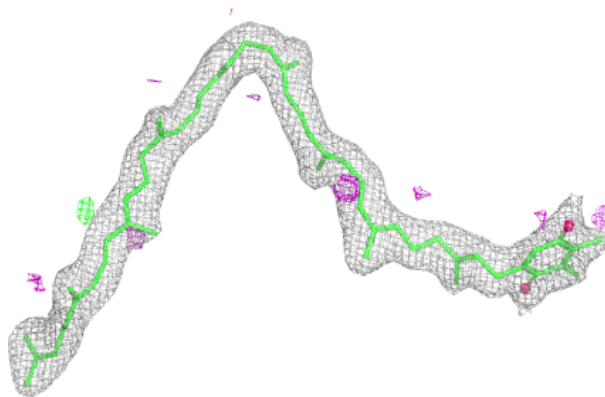
Electron density around CLA b 625:

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

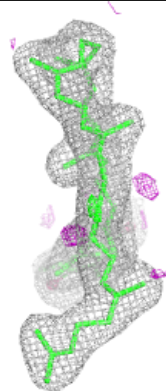
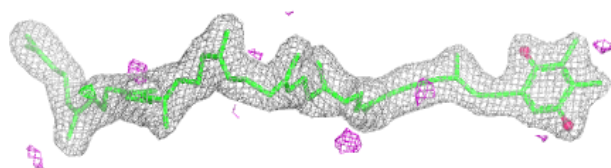
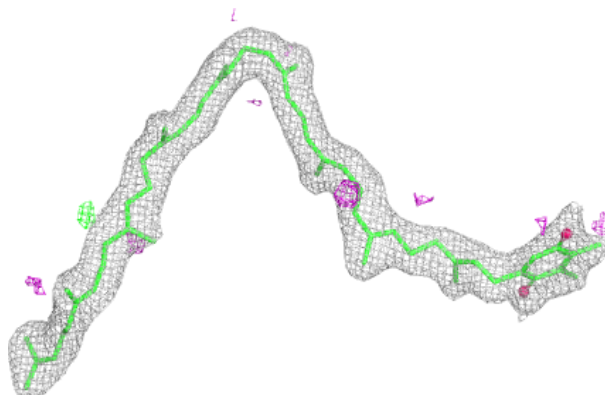


Electron density around PL9 d 405 (A):

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

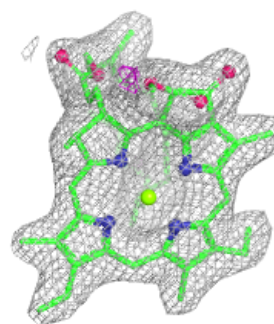
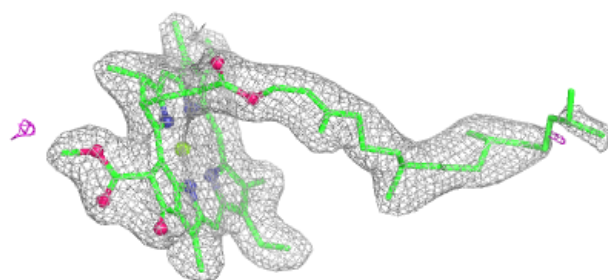
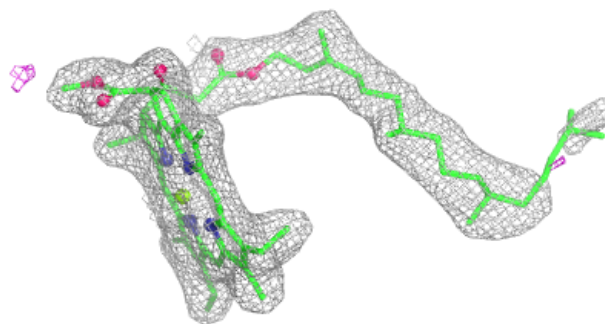
**Electron density around PL9 d 405 (B):**

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



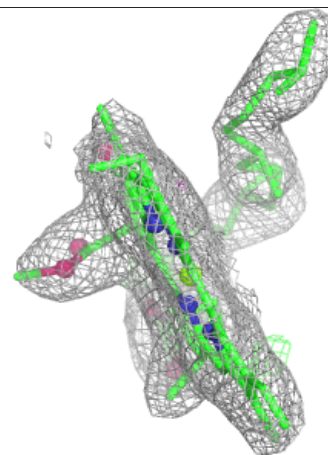
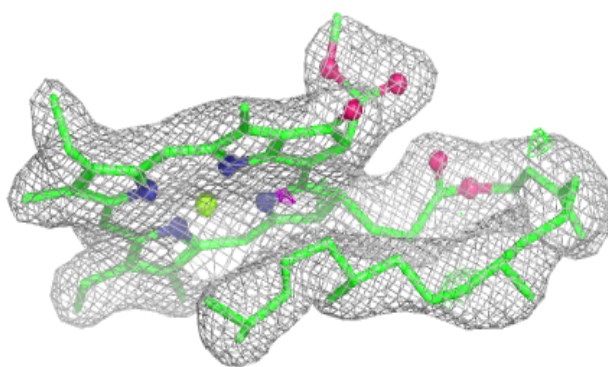
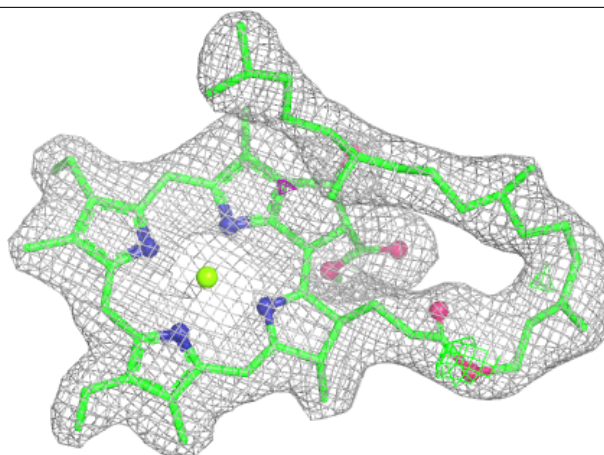
Electron density around CLA C 508:

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



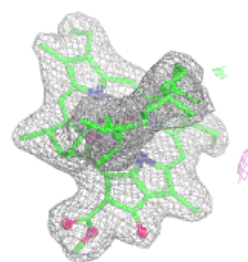
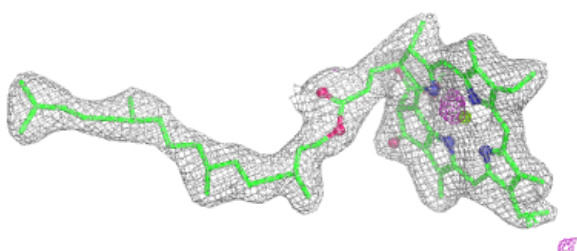
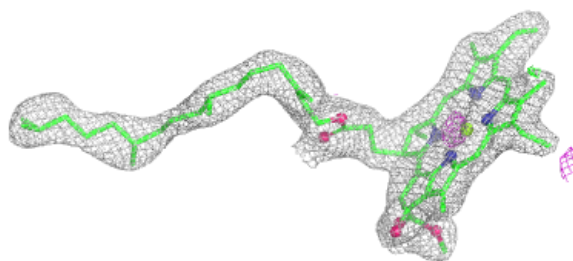
Electron density around CLA C 509:

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

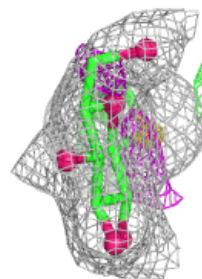
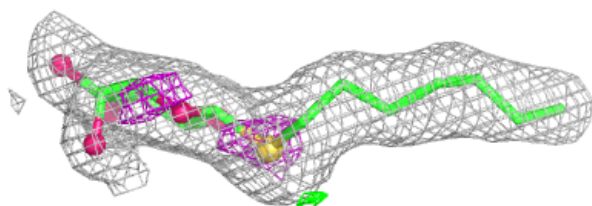
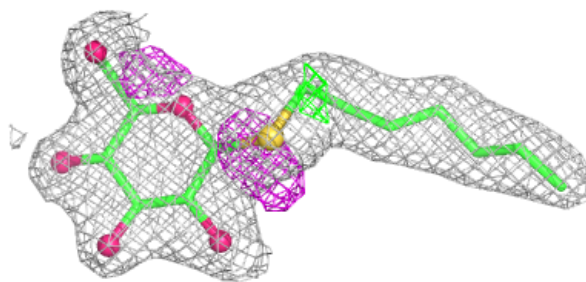


Electron density around CLA c 506:

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

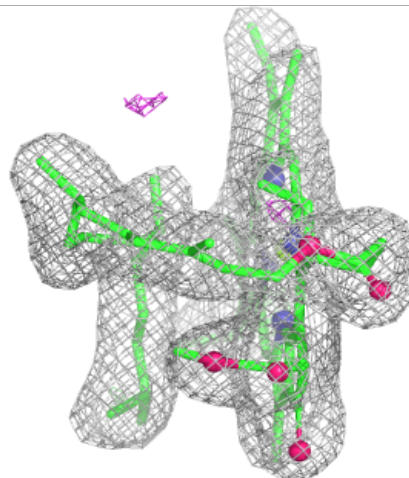
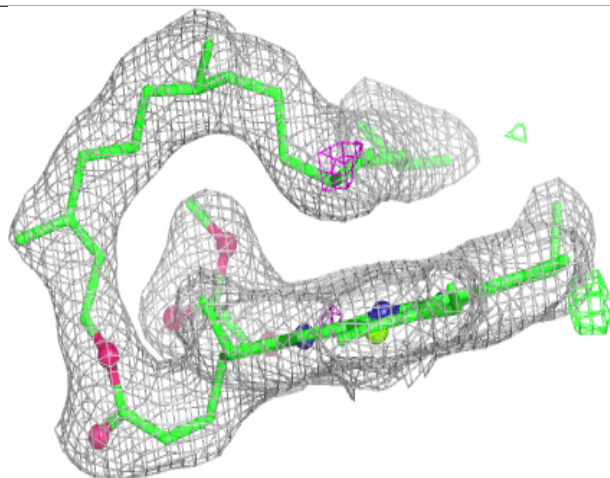
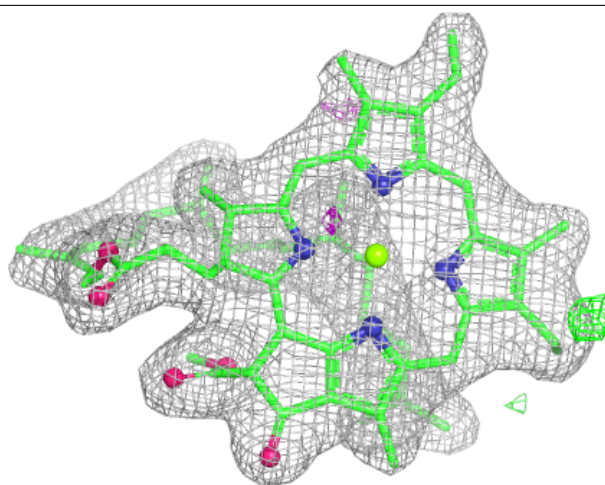
**Electron density around HTG b 602:**

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



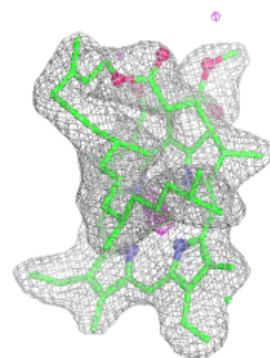
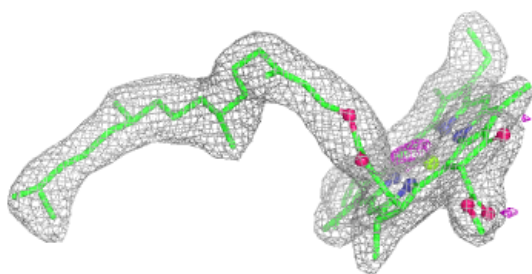
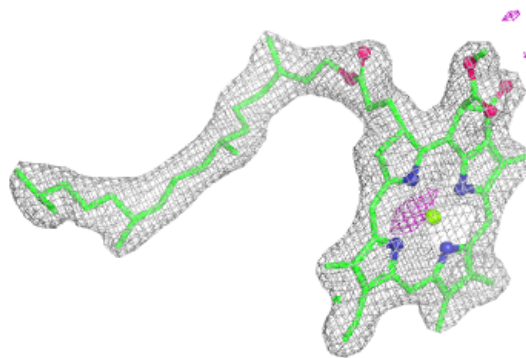
Electron density around CLA C 510:

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

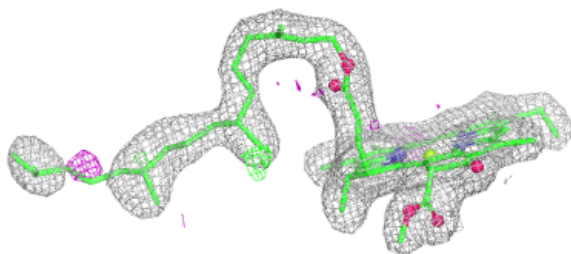
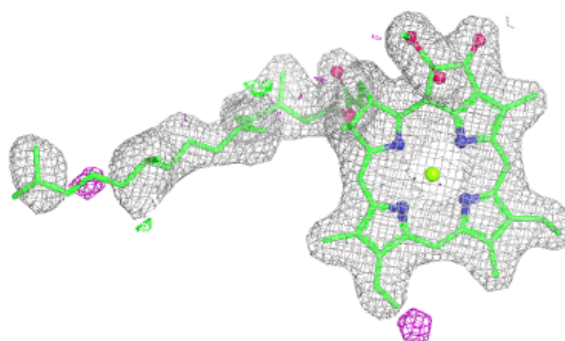


Electron density around CLA C 511:

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

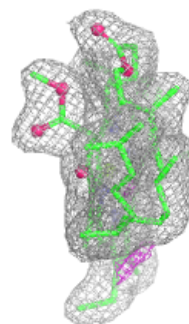
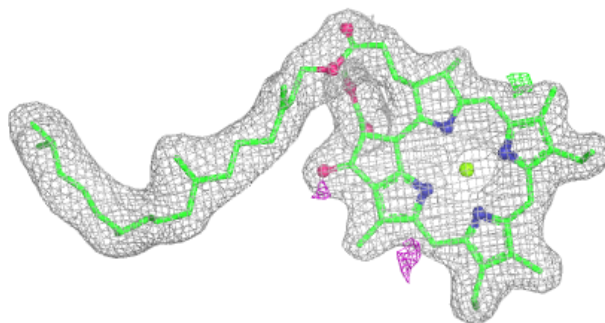
**Electron density around CLA A 407:**

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

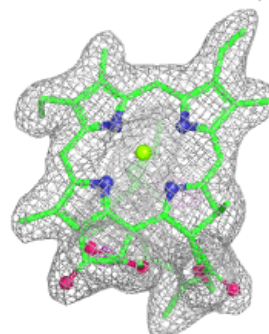
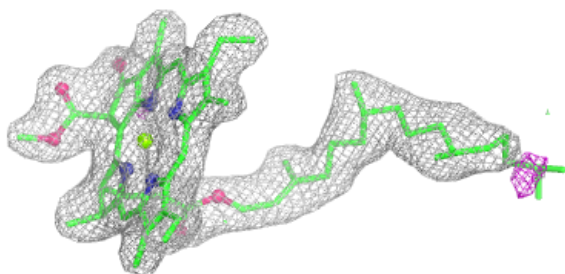
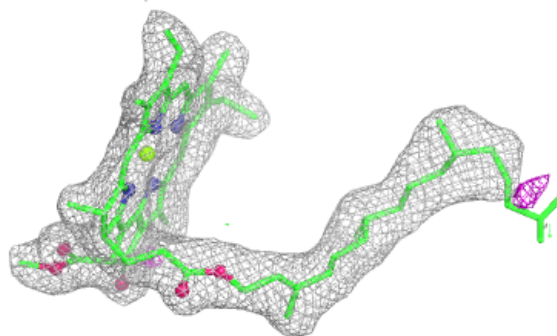


Electron density around CLA B 603:

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

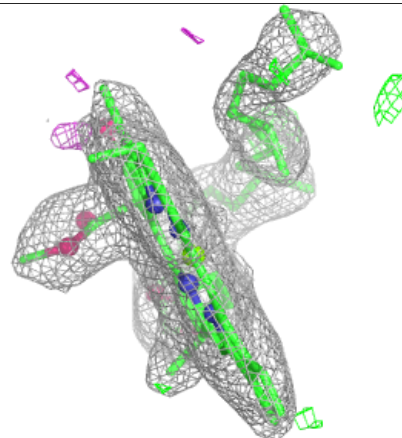
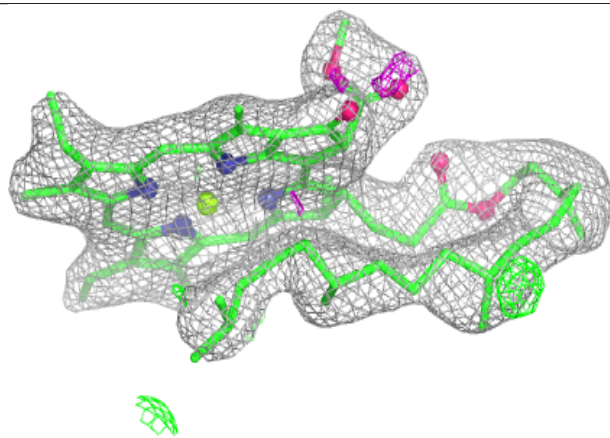
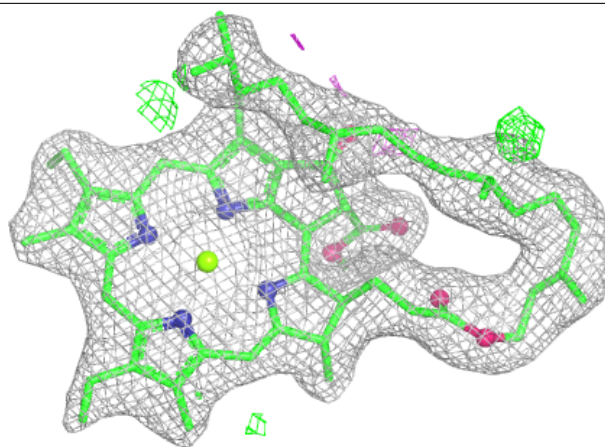
**Electron density around CLA c 512:**

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



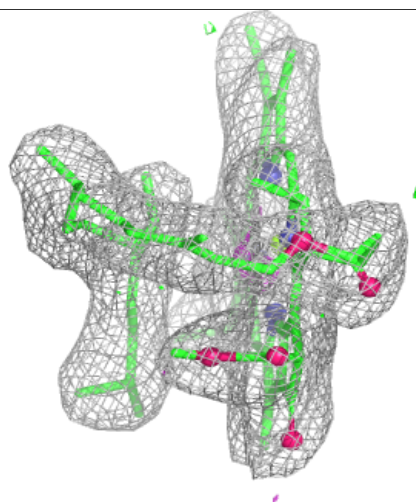
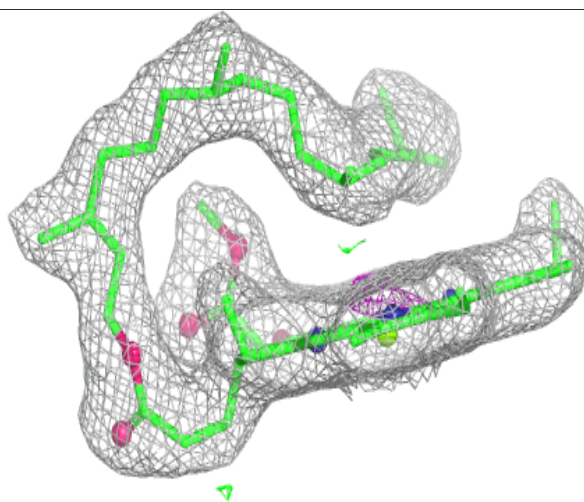
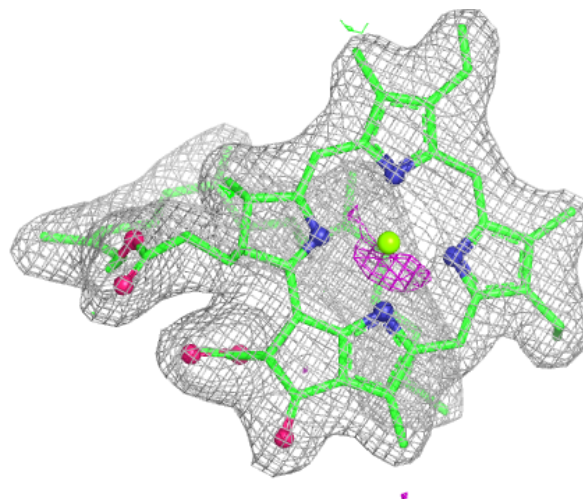
Electron density around CLA c 513:

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



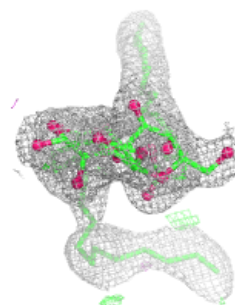
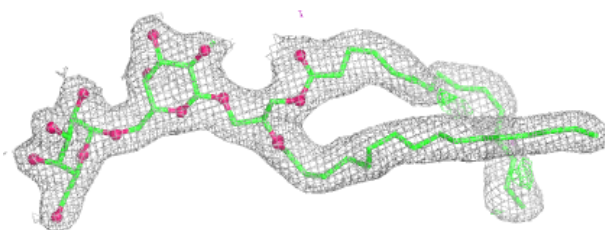
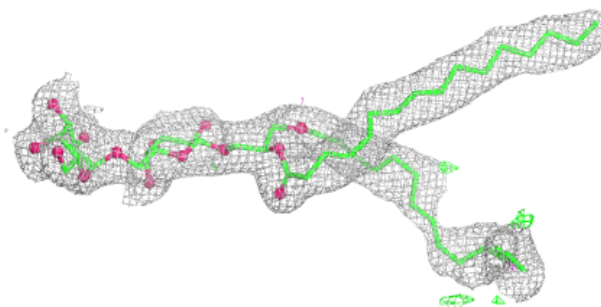
Electron density around CLA c 514:

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

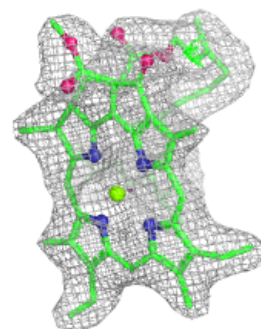
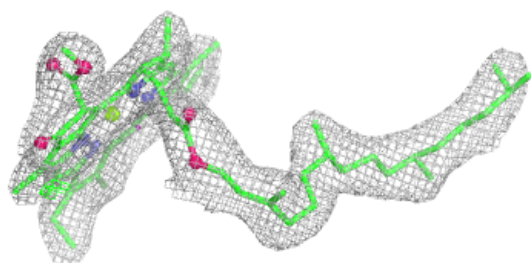
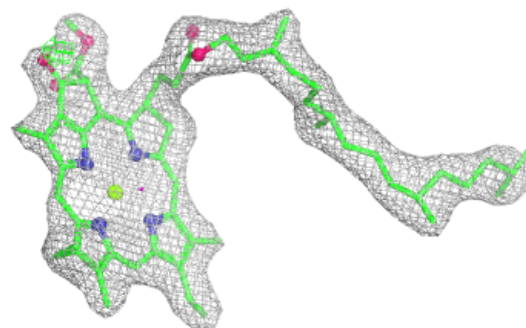


Electron density around DGD C 516:

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

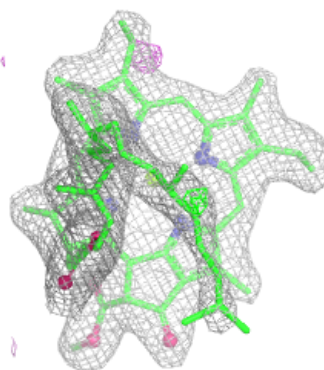
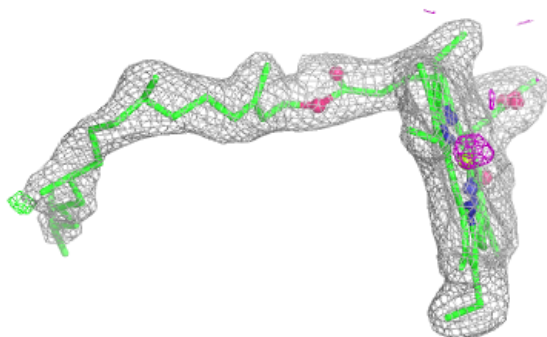
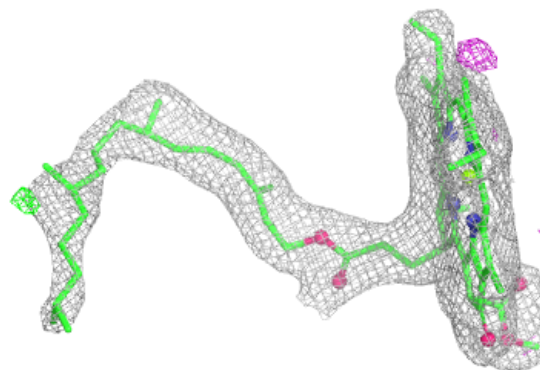
**Electron density around CLA c 515:**

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

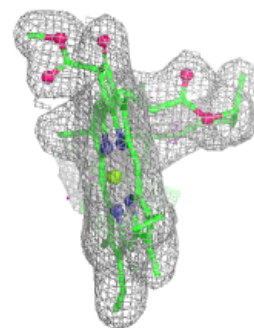
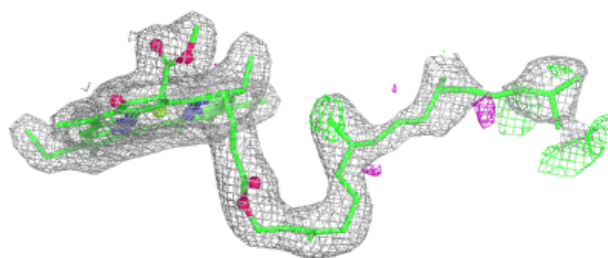
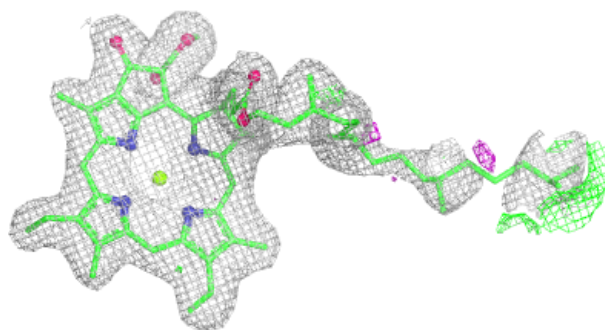


Electron density around CLA D 403:

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

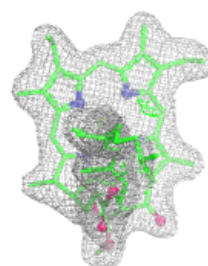
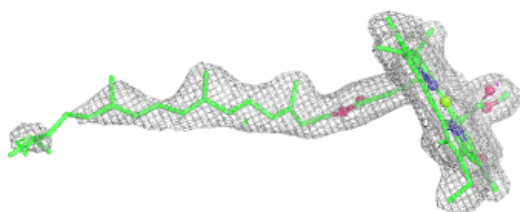
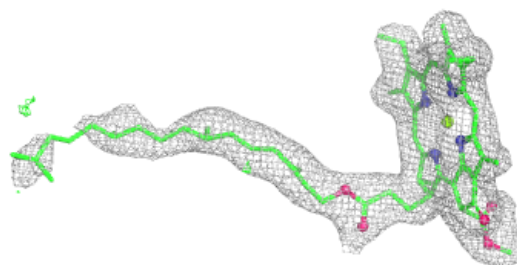
**Electron density around CLA a 410:**

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

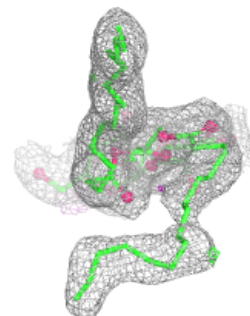
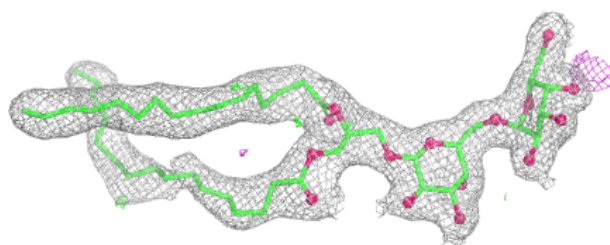
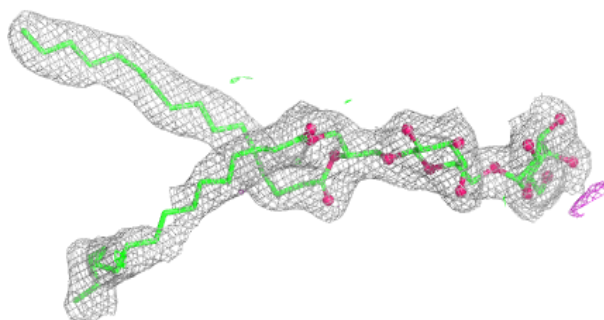


Electron density around CLA d 403:

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

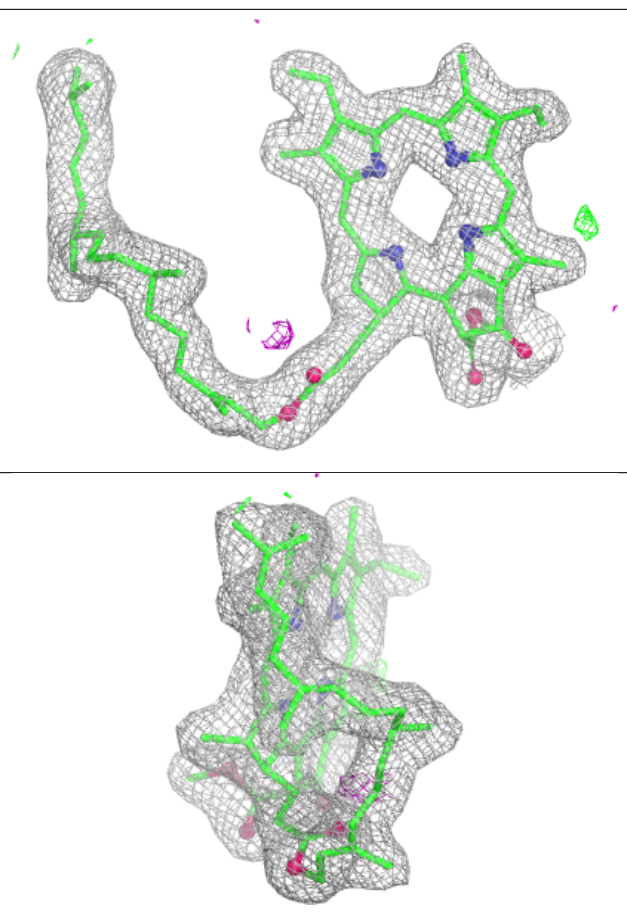
**Electron density around DGD c 519:**

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



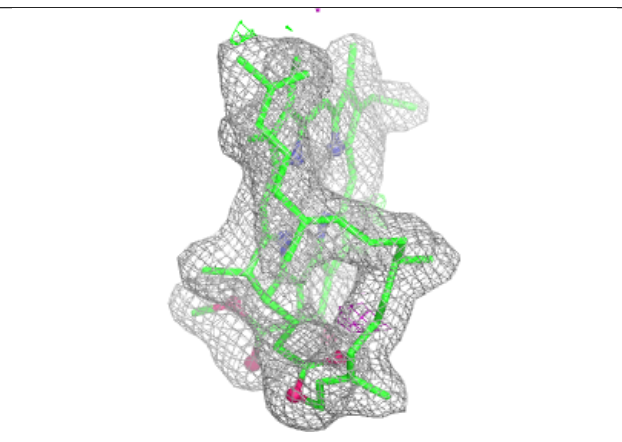
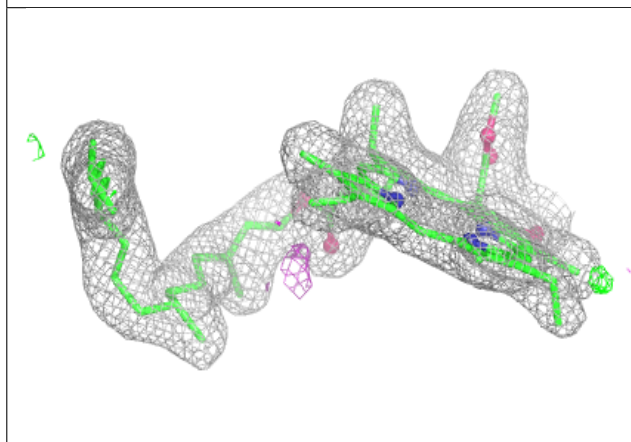
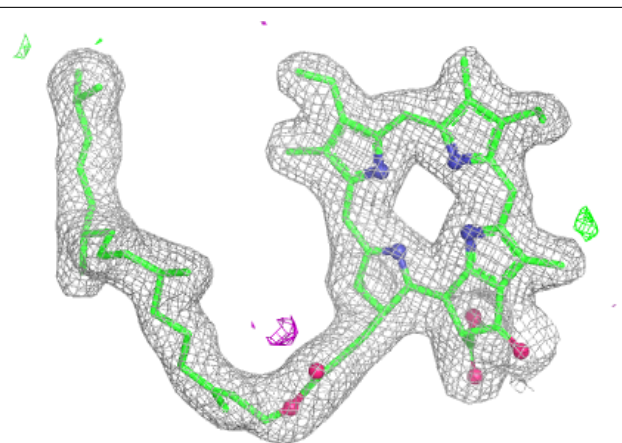
Electron density around PHO A 409 (A):

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



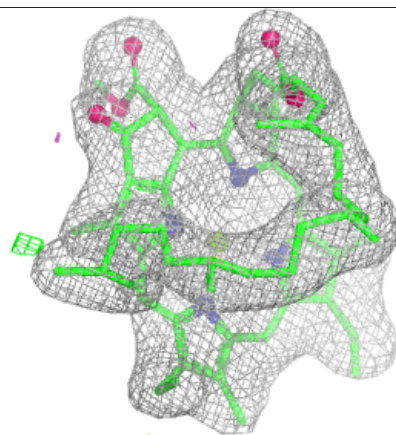
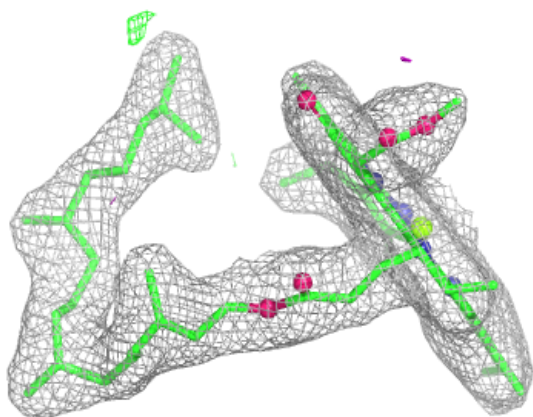
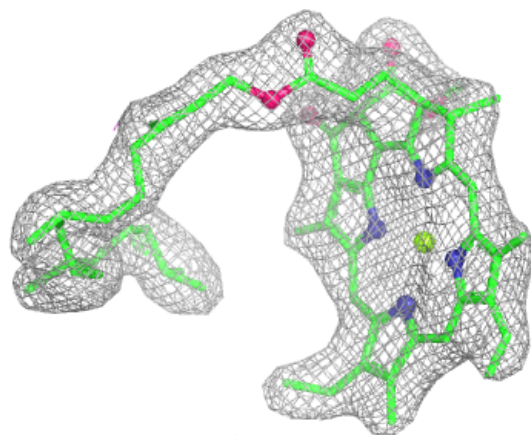
Electron density around PHO A 409 (B):

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



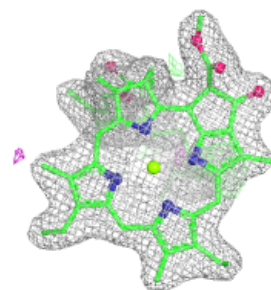
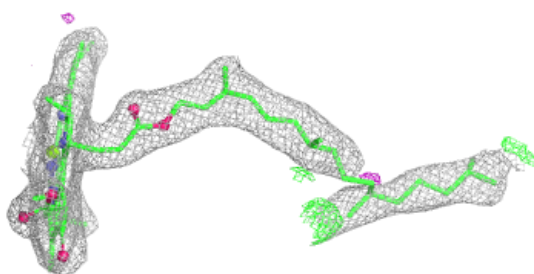
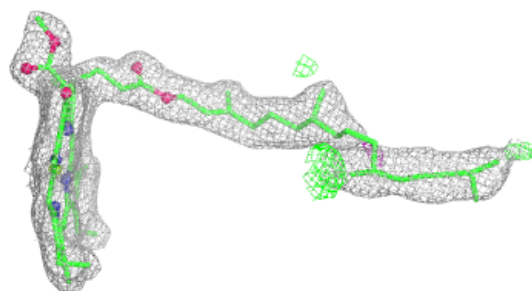
Electron density around CLA C 503:

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



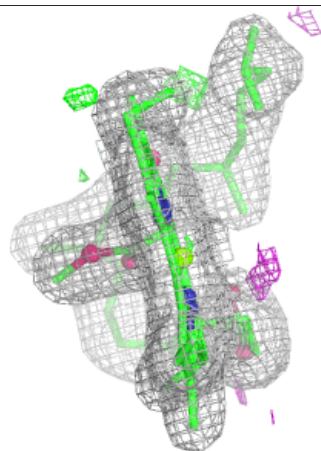
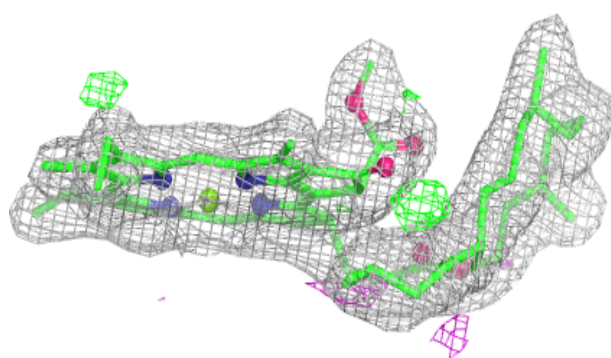
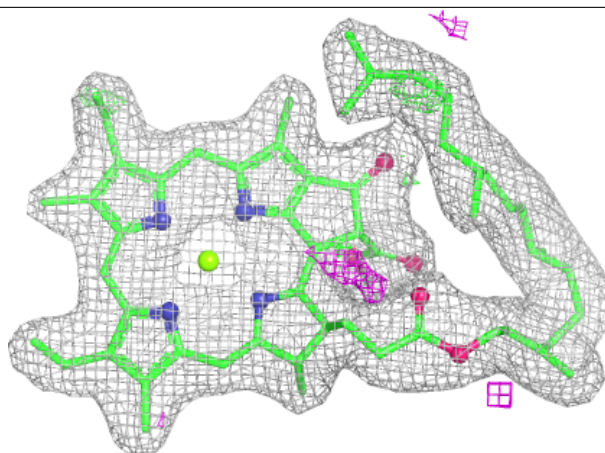
Electron density around CLA B 607:

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

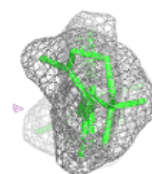
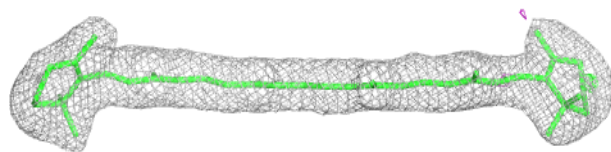
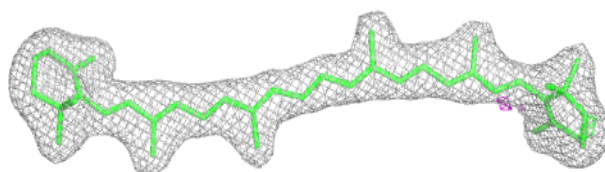


Electron density around CLA B 611:

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

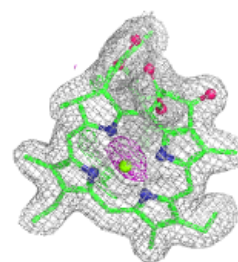
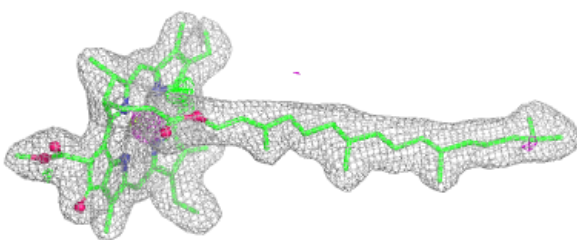
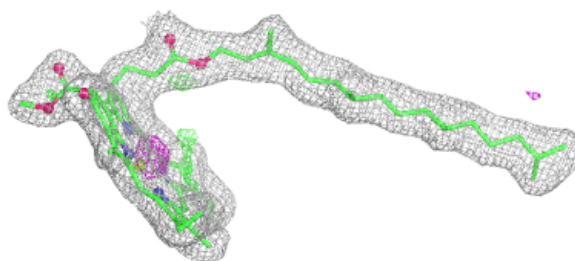
**Electron density around BCR B 619:**

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

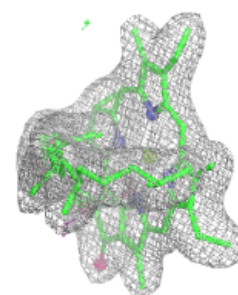
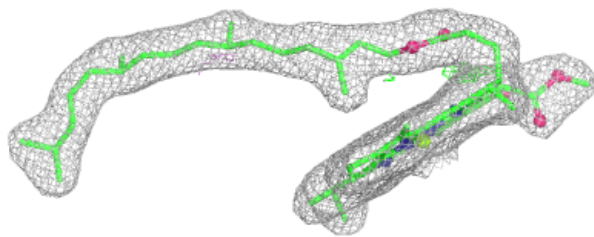
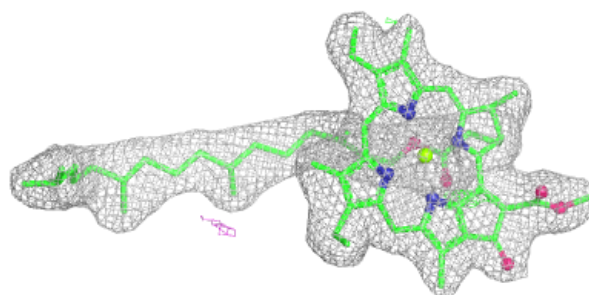


Electron density around CLA b 617:

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

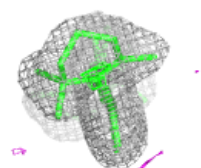
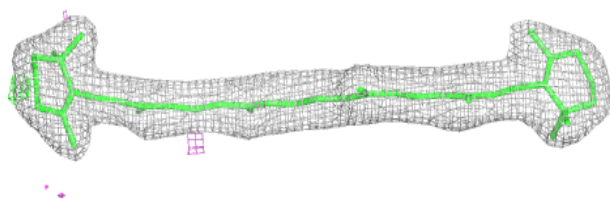
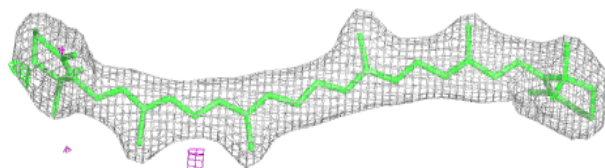
**Electron density around CLA b 618:**

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



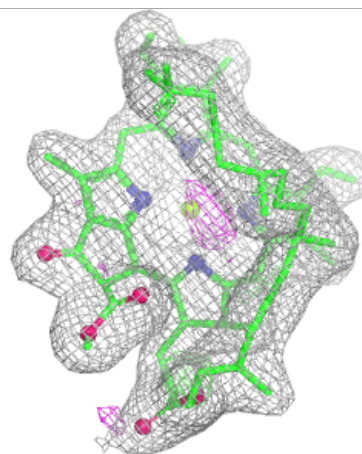
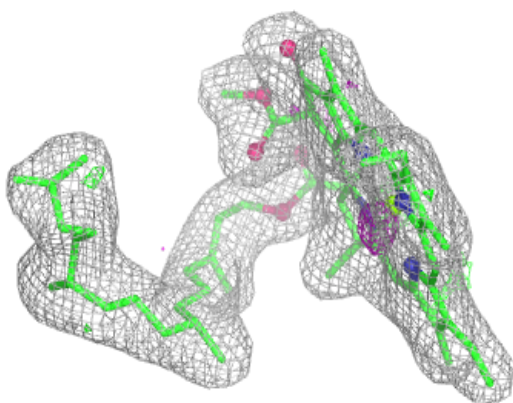
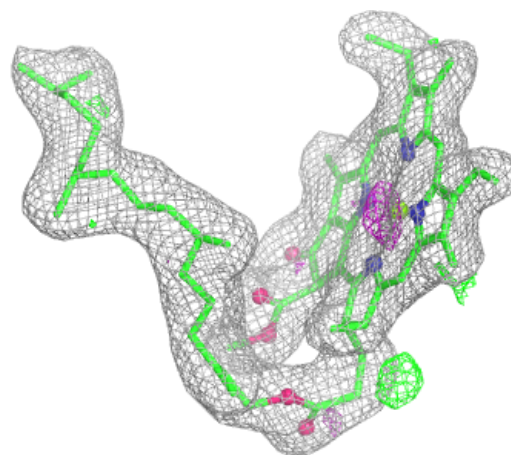
Electron density around BCR C 515:

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



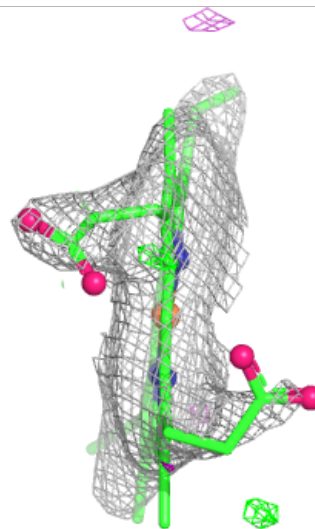
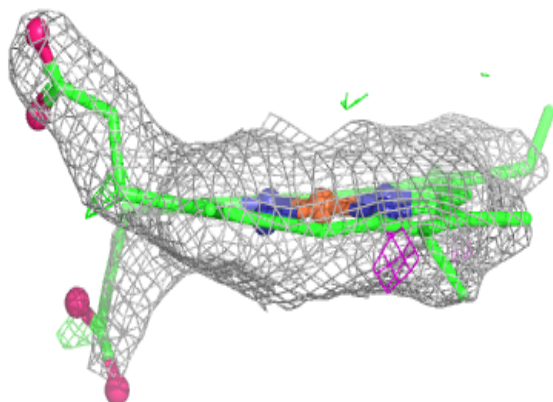
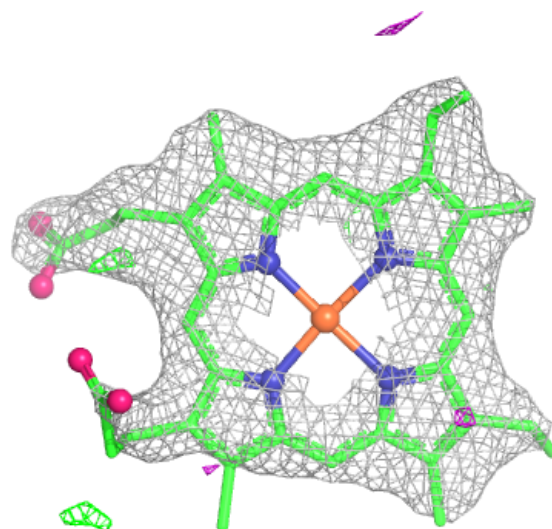
Electron density around CLA B 614:

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



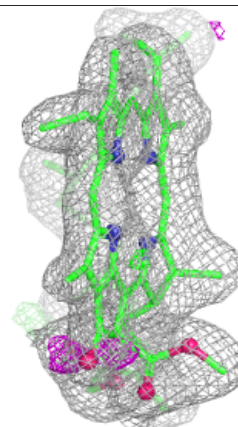
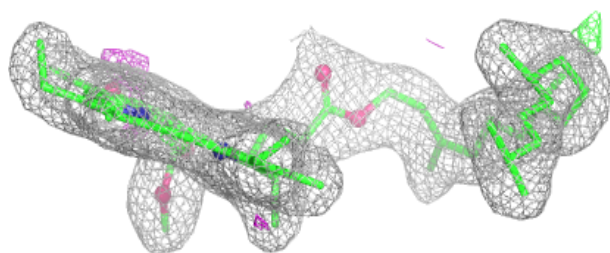
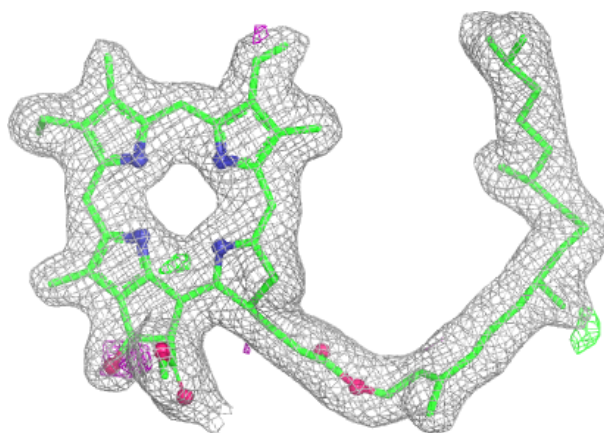
Electron density around HEM e 102:

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

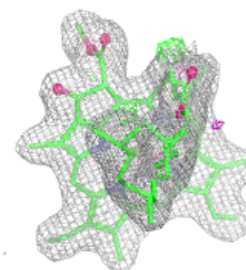
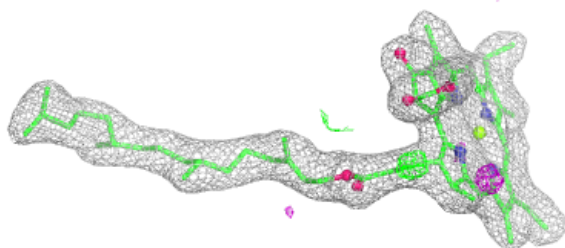
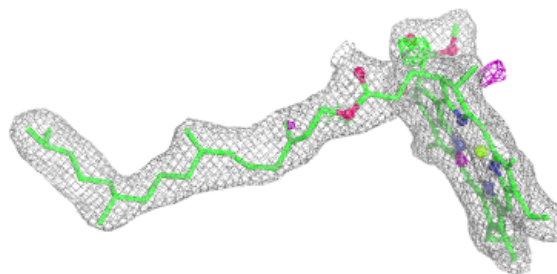


Electron density around PHO a 411:

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

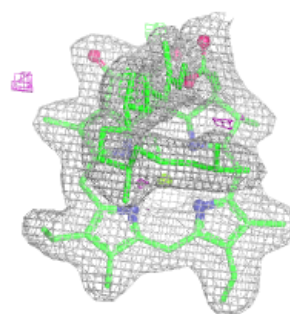
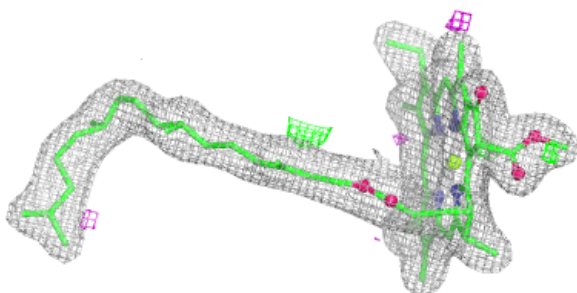
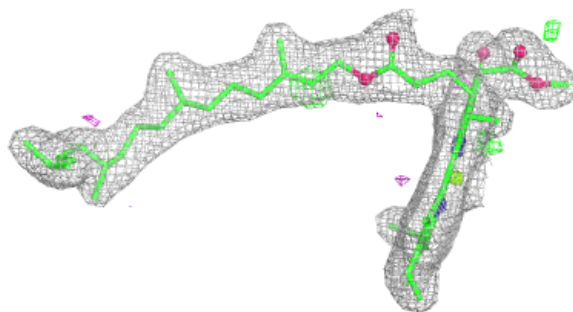
**Electron density around CLA B 605:**

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

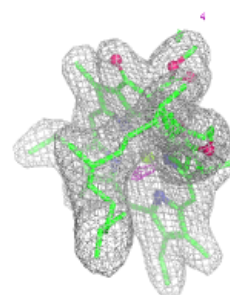
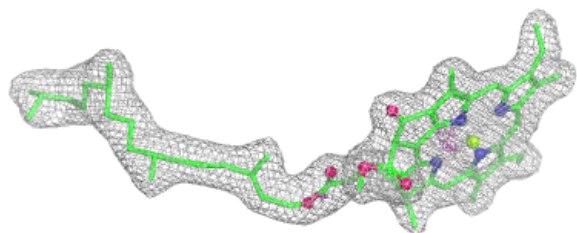
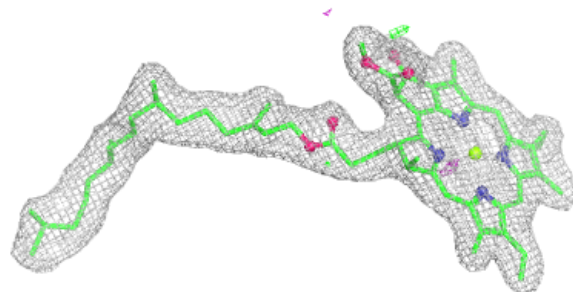


Electron density around CLA B 606:

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

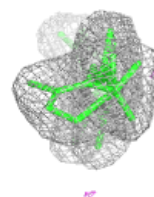
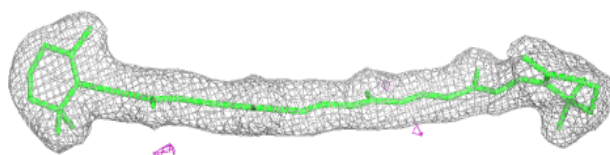
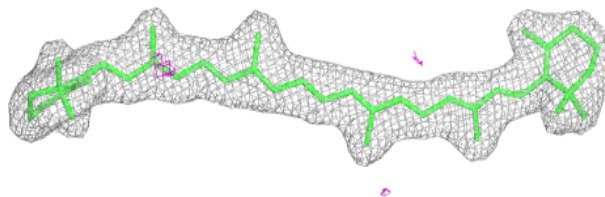
**Electron density around CLA a 409:**

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

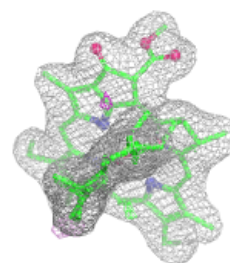
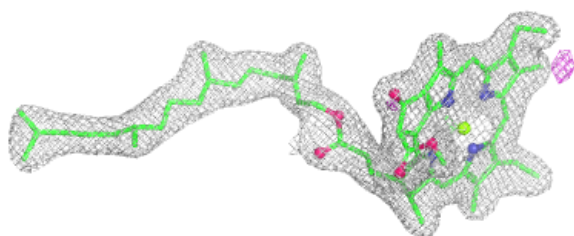
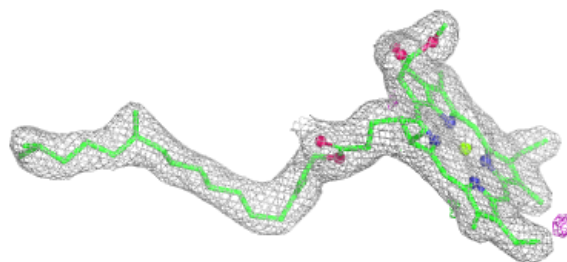


Electron density around BCR B 618:

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

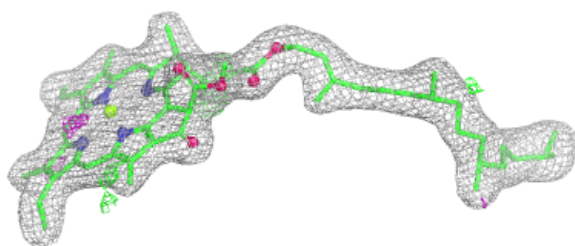
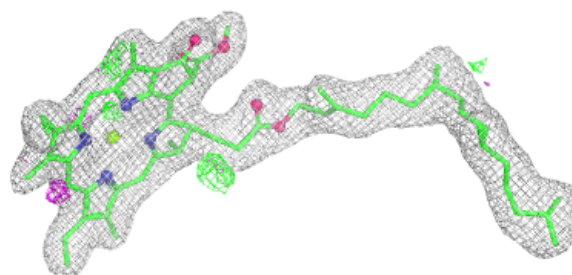
**Electron density around CLA C 502:**

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

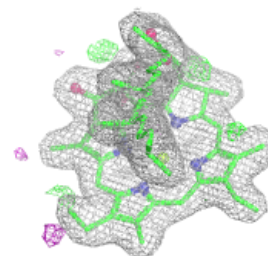
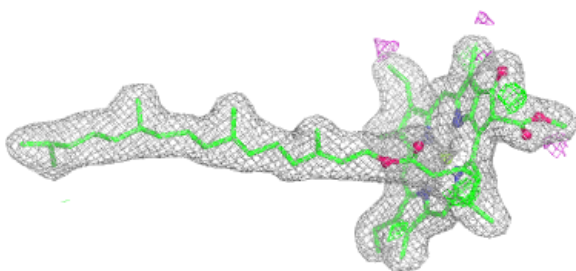
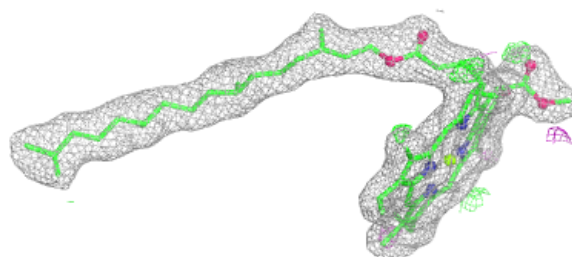


Electron density around CLA A 405:

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

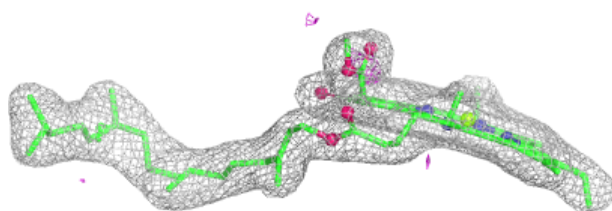
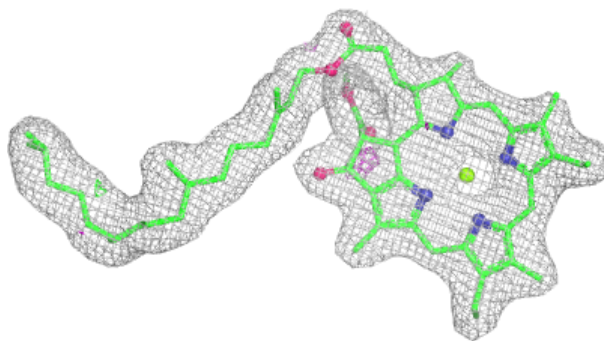
**Electron density around CLA B 608:**

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

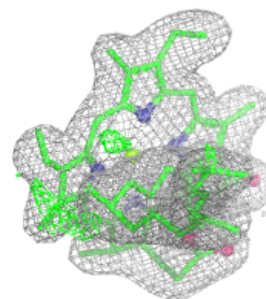
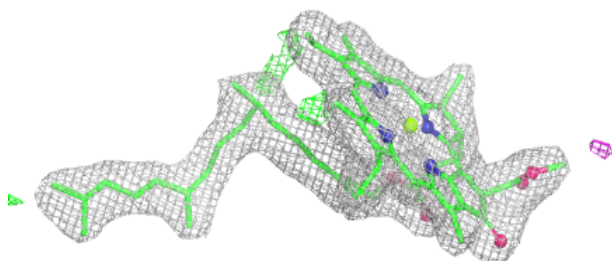
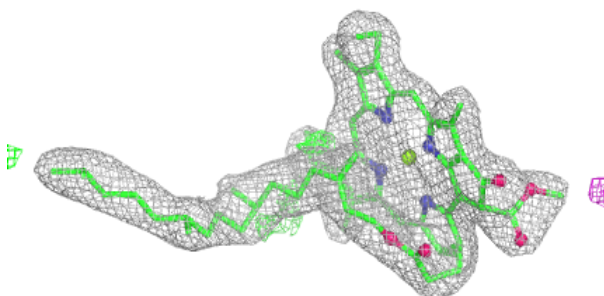


Electron density around CLA b 612:

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

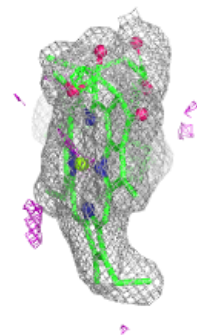
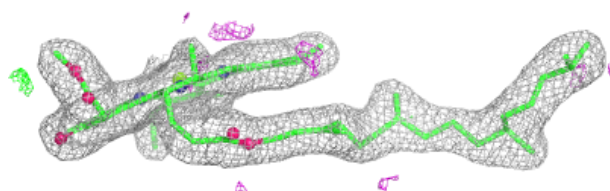
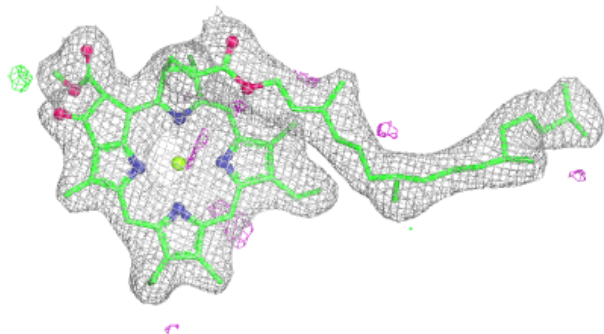
**Electron density around CLA c 509:**

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

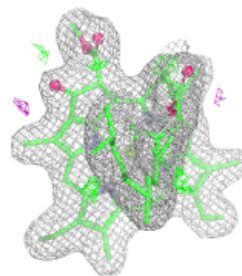
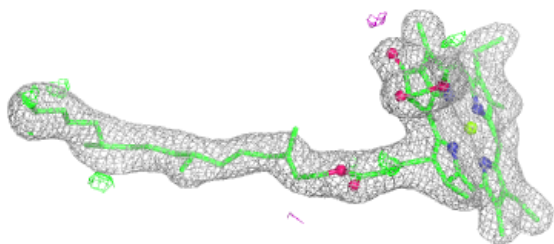
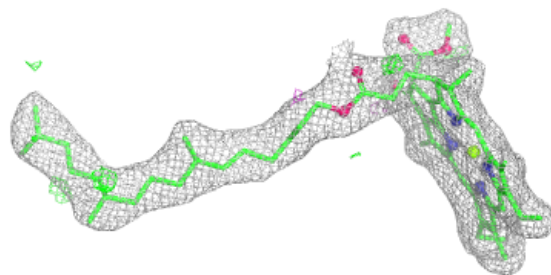


Electron density around CLA b 613:

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

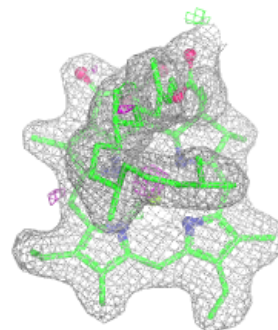
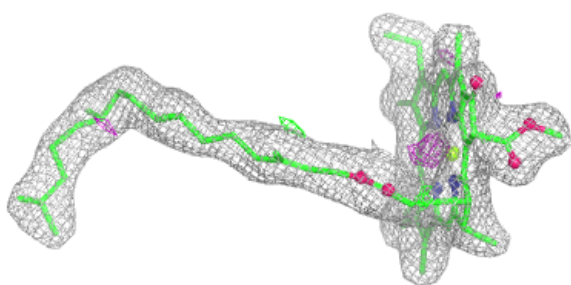
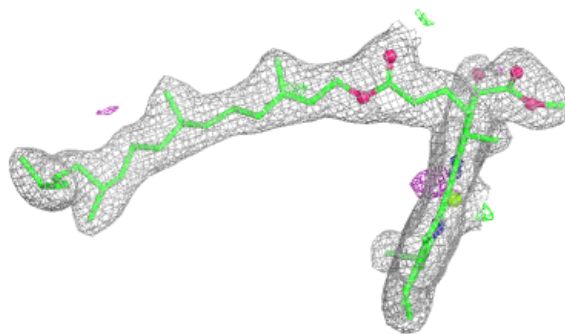
**Electron density around CLA b 614:**

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

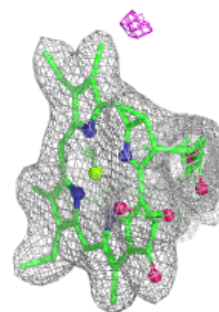
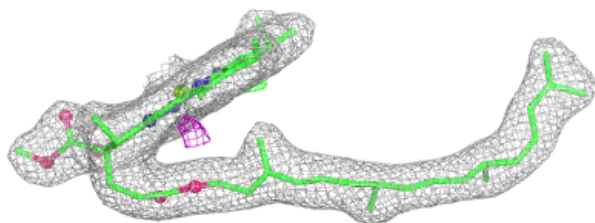
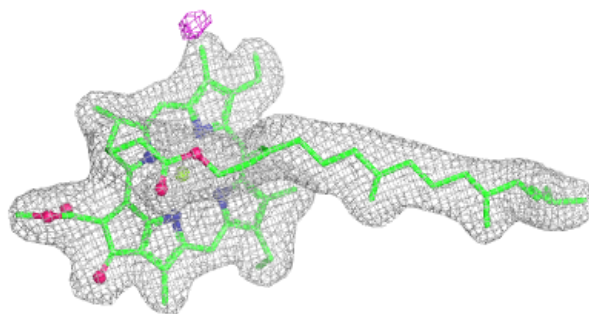


Electron density around CLA b 615:

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

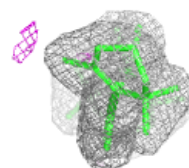
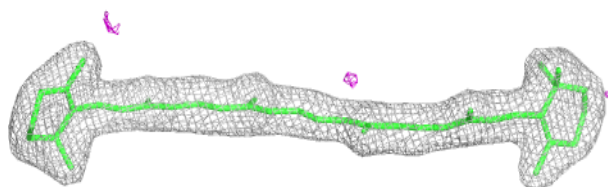
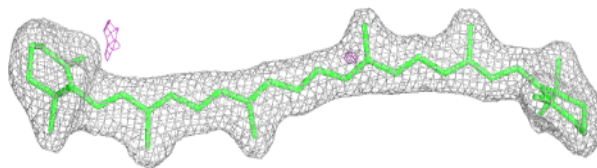
**Electron density around CLA B 609:**

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

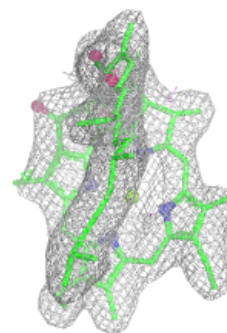
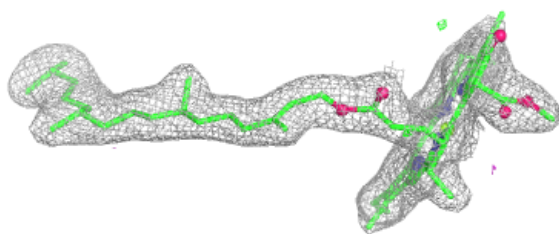
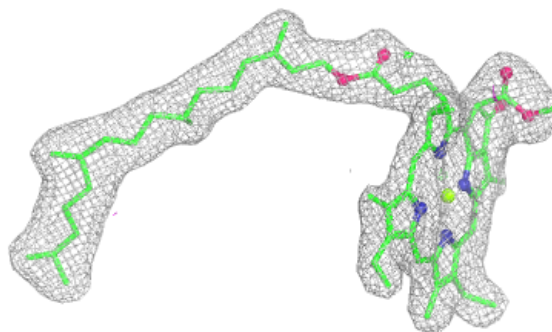


Electron density around BCR a 413:

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

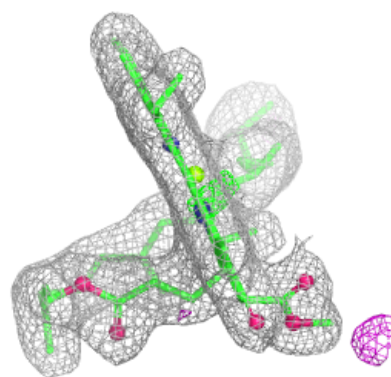
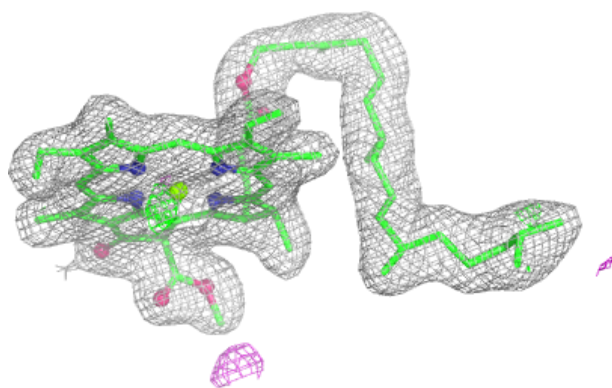
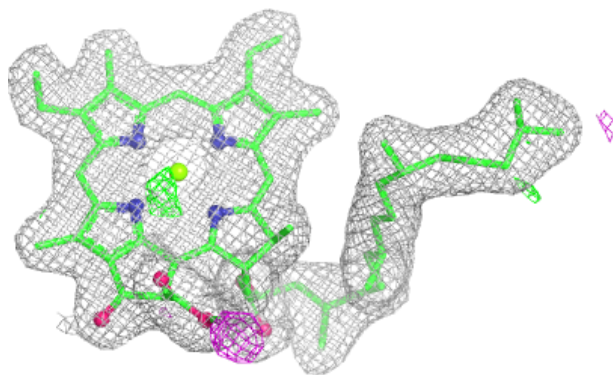
**Electron density around CLA B 610:**

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

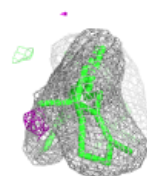
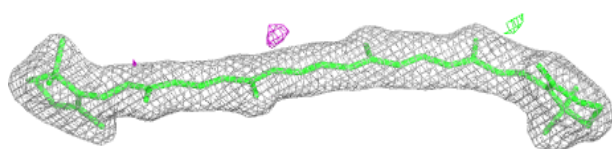
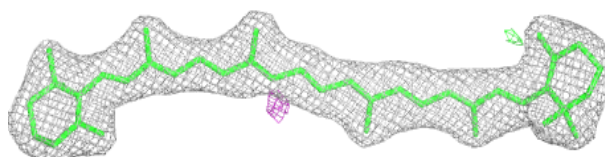


Electron density around CLA A 406:

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

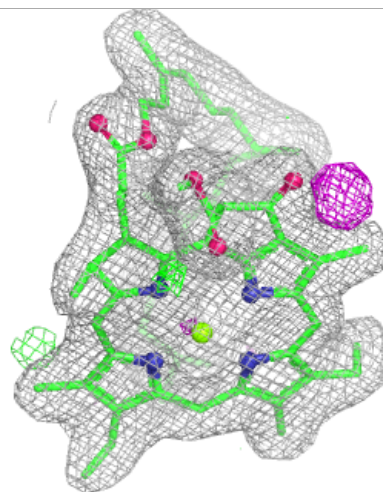
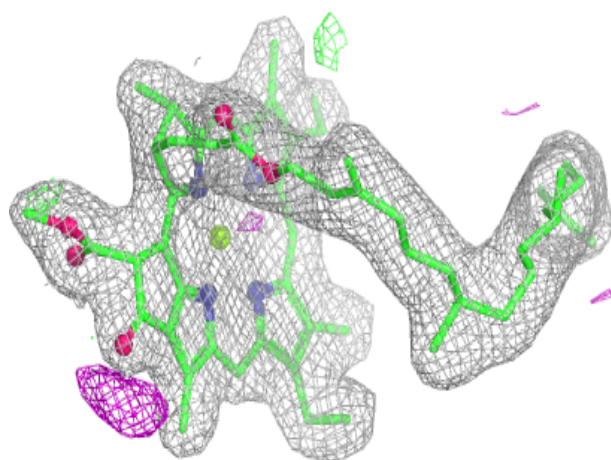
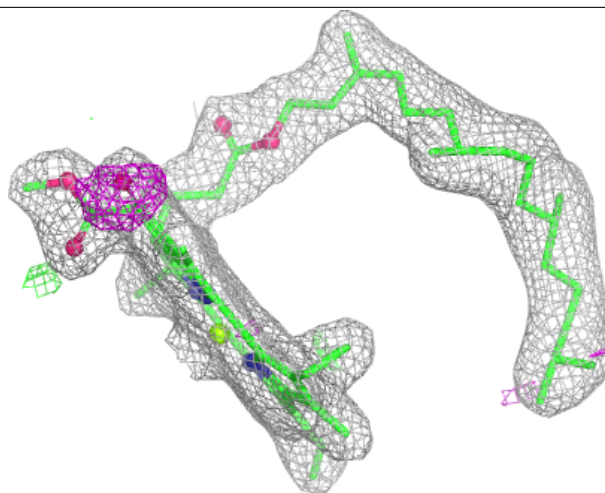
**Electron density around BCR b 629:**

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



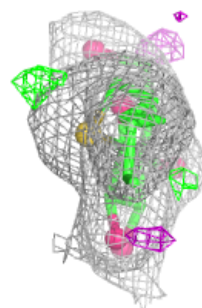
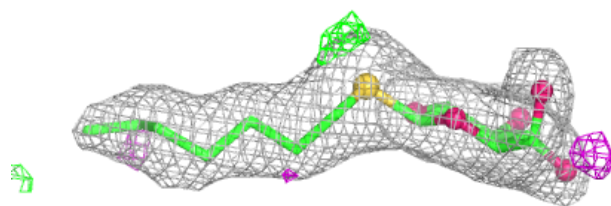
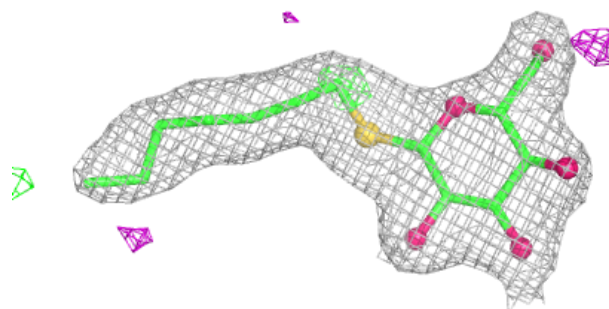
Electron density around CLA B 612:

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



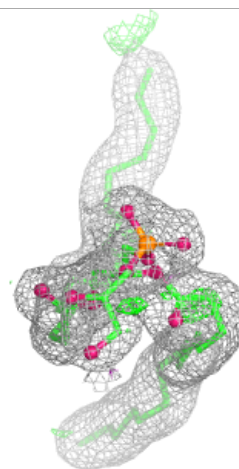
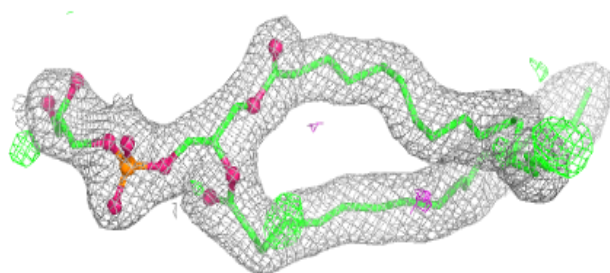
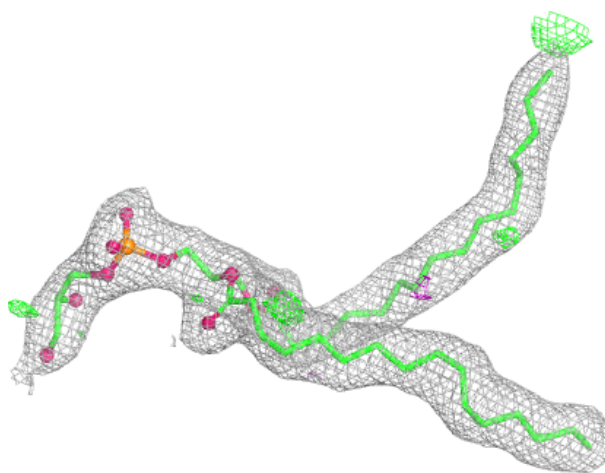
Electron density around HTG B 623:

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



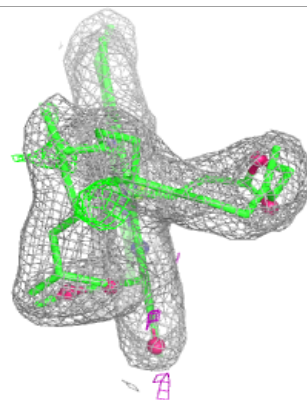
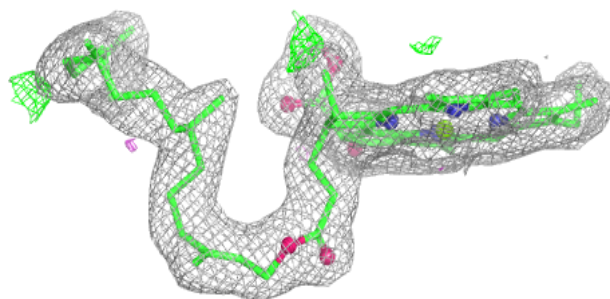
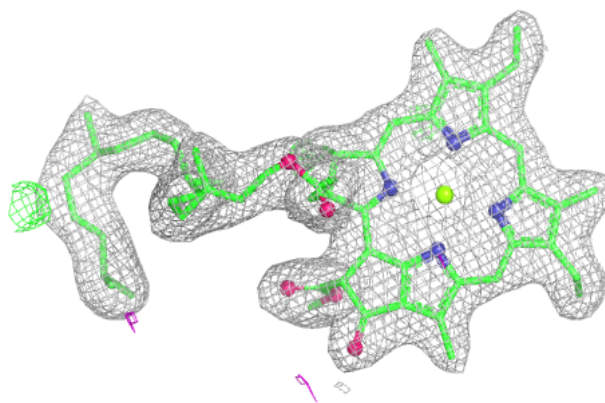
Electron density around LHG D 408:

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

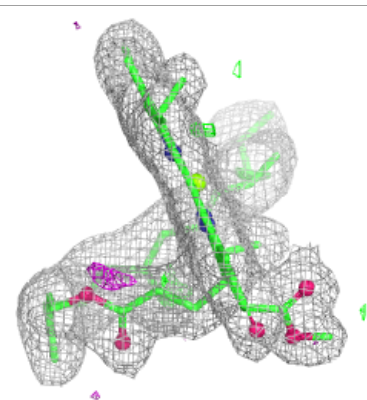
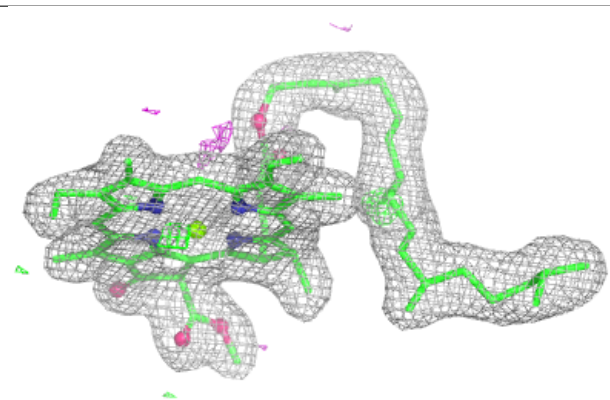
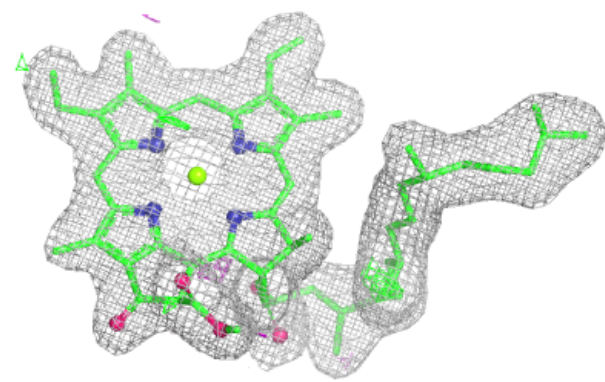


Electron density around CLA B 613:

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

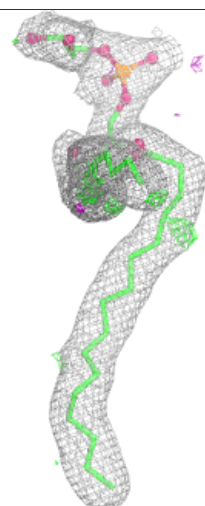
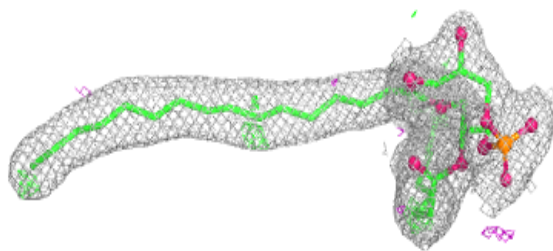
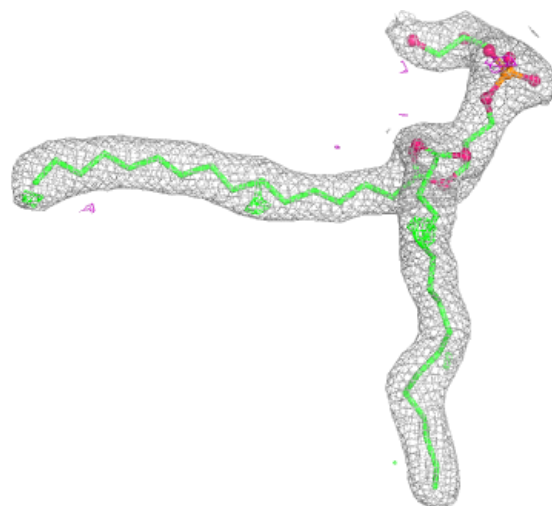
**Electron density around CLA d 401:**

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



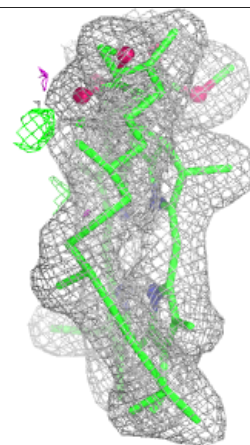
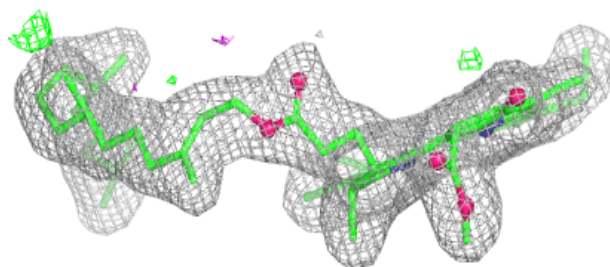
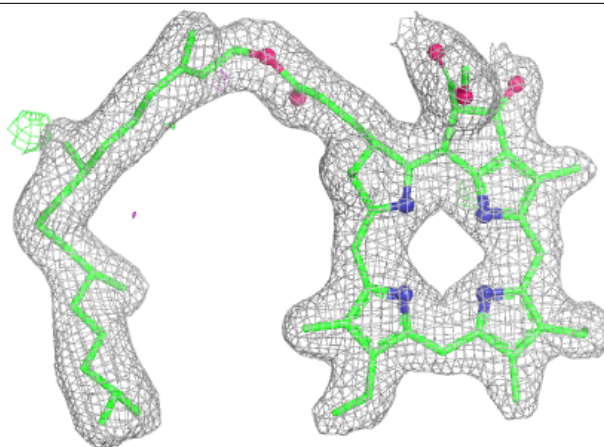
Electron density around LHG L 101:

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



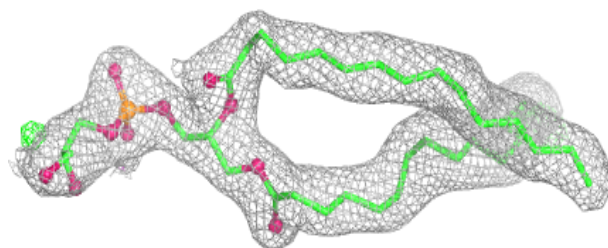
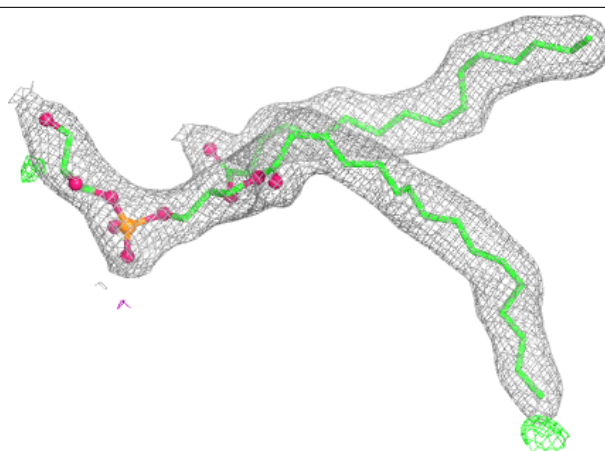
Electron density around PHO A 408:

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



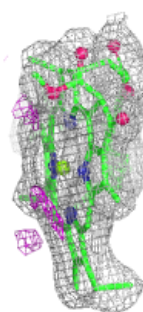
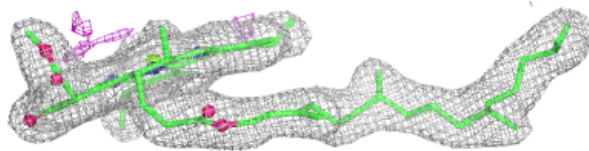
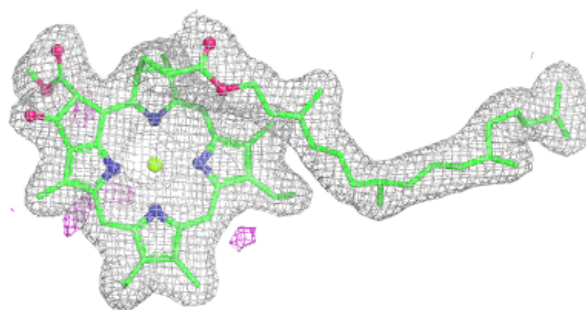
Electron density around LHG d 407:

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



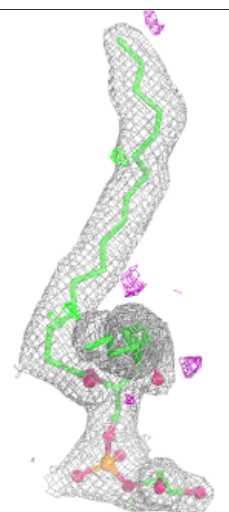
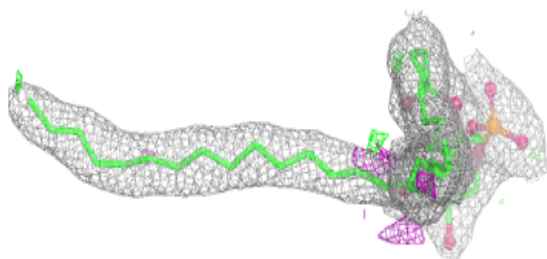
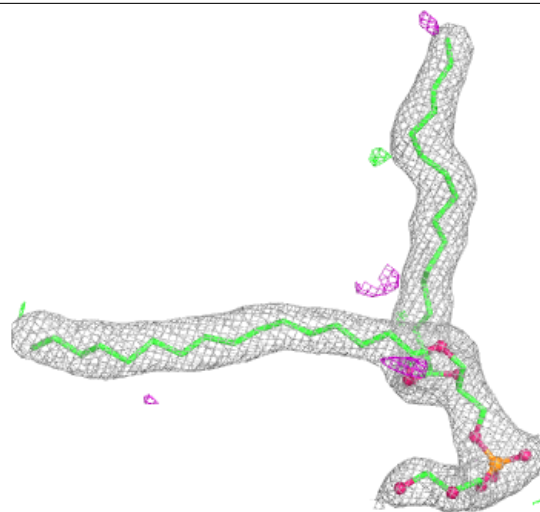
Electron density around CLA B 604:

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



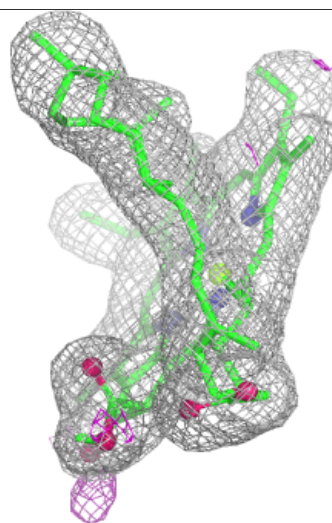
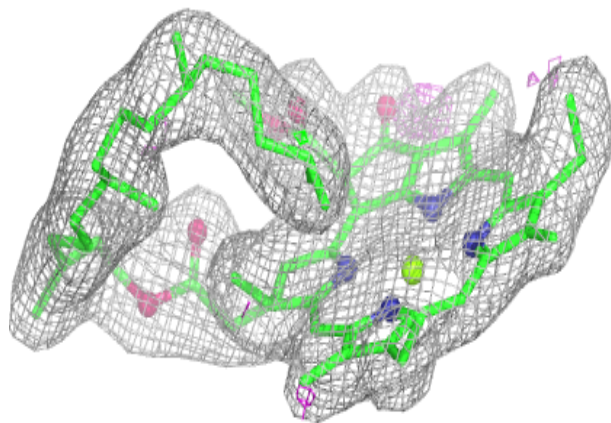
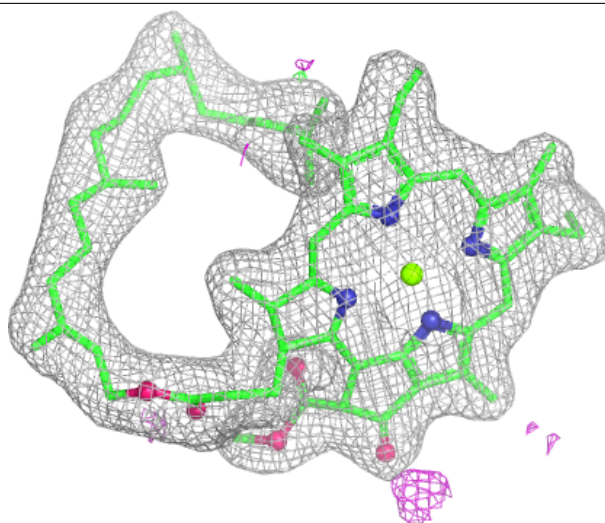
Electron density around LHG 1 101:

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



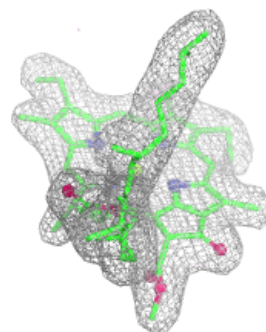
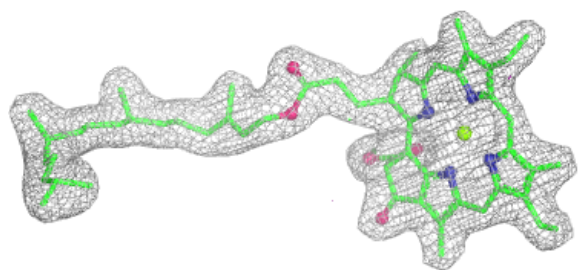
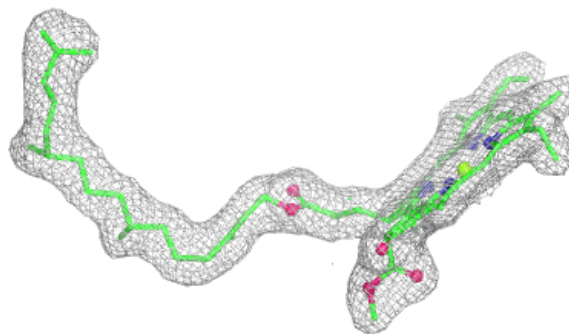
Electron density around CLA B 616:

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

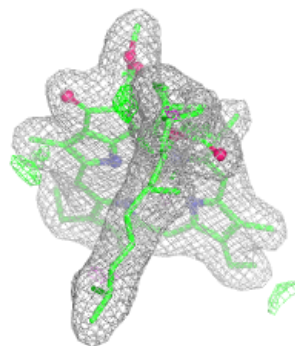
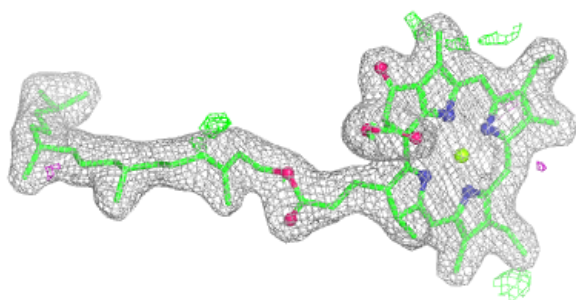
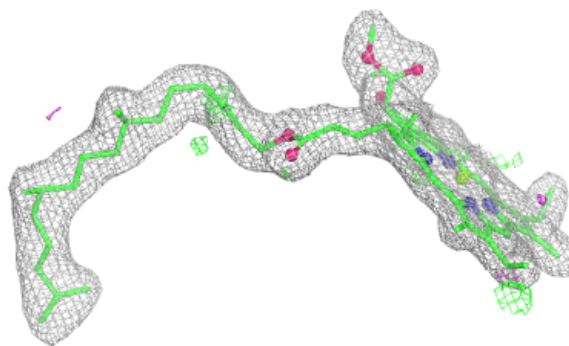


Electron density around CLA d 402:

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

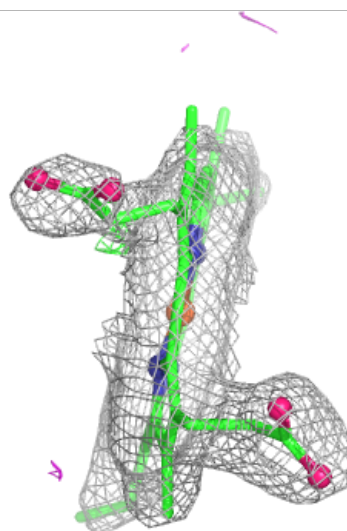
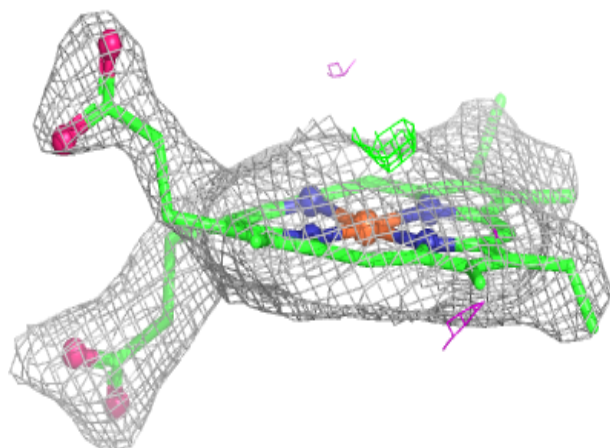
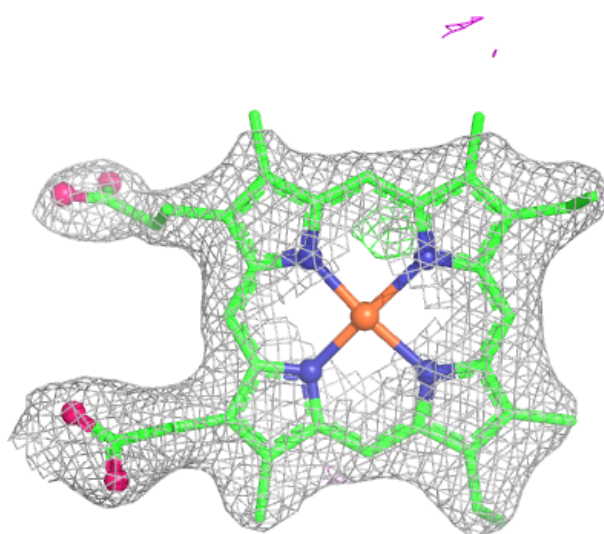
**Electron density around CLA D 402:**

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



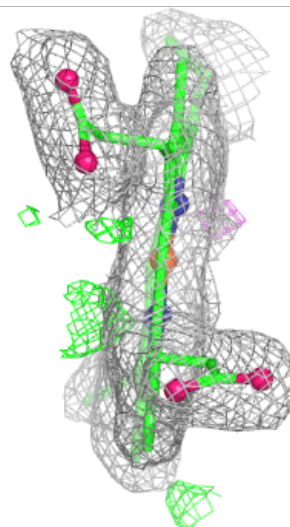
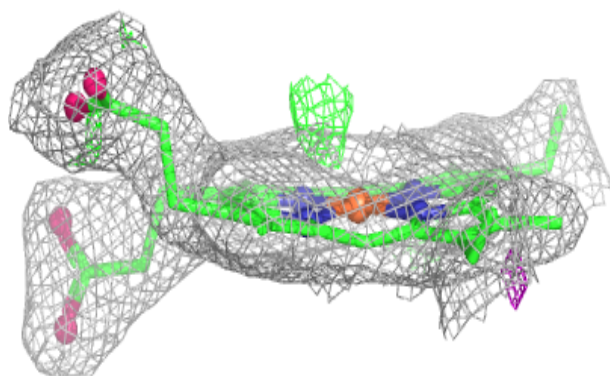
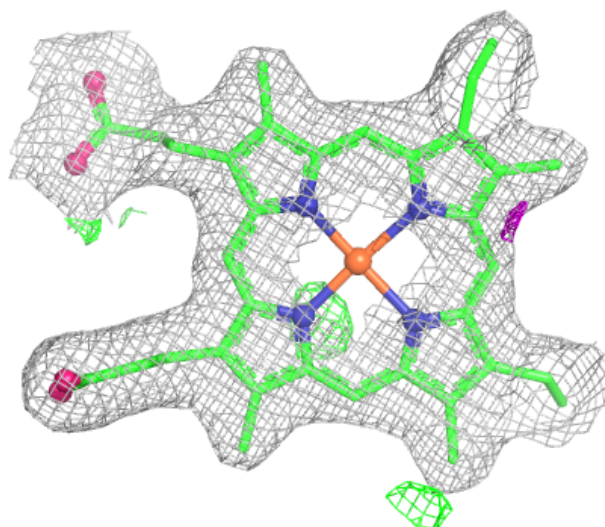
Electron density around HEM F 102:

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



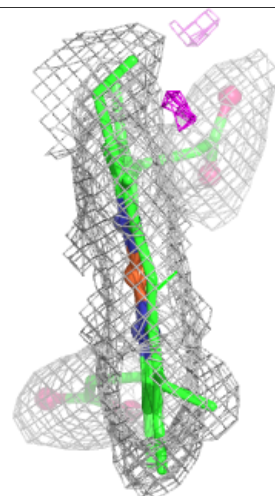
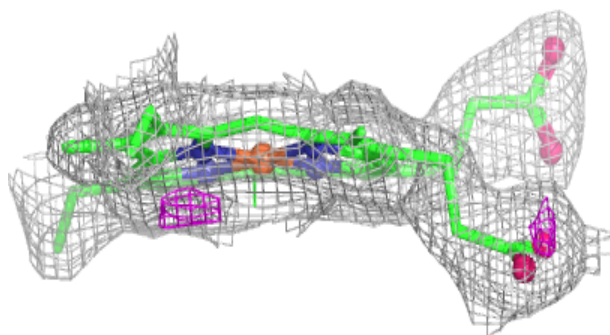
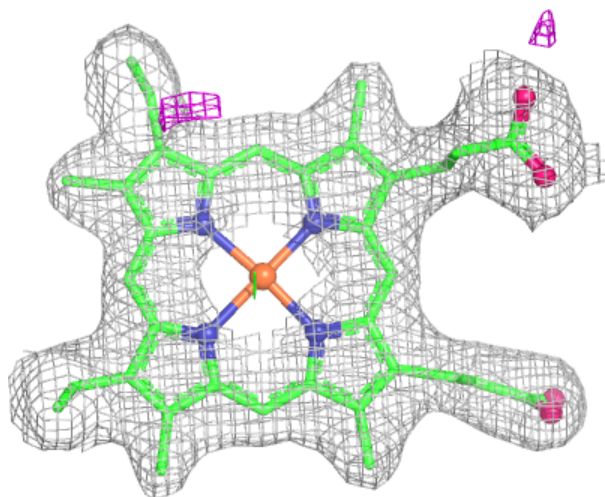
Electron density around HEC V 206:

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



Electron density around HEC v 205:

$2mF_o-DF_c$ (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.