



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:27 AM UTC

PDB ID : 8IRI / pdb_00008iri
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 5-millisecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.25 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

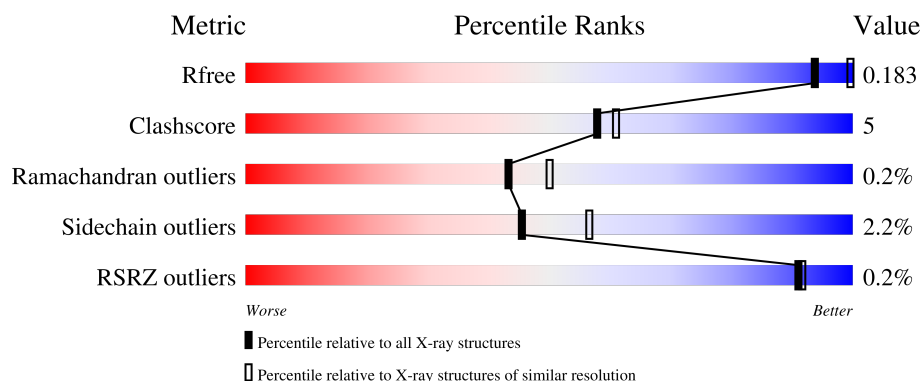
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



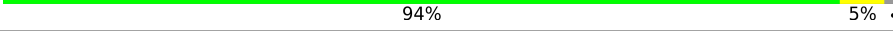
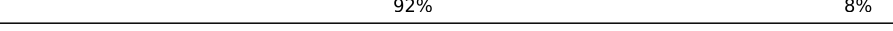
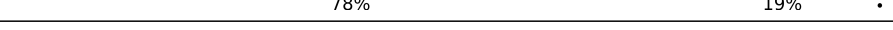
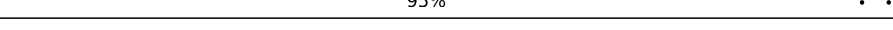
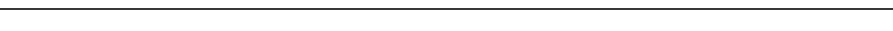
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	92%
1	a	344	88% 9%
2	B	505	93% 7%
2	b	505	92% 7%
3	C	455	91% 8%

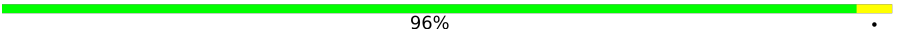
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	c	455	 92% 8%
4	D	342	 91% 9%
4	d	342	 92% 7%
5	E	84	 79% 18% .
5	e	84	 2% 89% 5% 6%
6	F	44	 66% 11% 23%
6	f	44	 2% 57% 14% 30%
7	H	65	 2% 94% 5% .
7	h	65	 2% 86% 12% .
8	I	38	 76% 16% 8%
8	i	38	 87% 13%
9	J	39	 82% 13% . .
9	j	39	 92% 8%
10	K	37	 78% 19% .
10	k	37	 81% 14% 5%
11	L	37	 95% . .
11	l	37	 89% 8% .
12	M	36	 81% 6% 6% 8%
12	m	36	 81% 11% . 6%
13	O	244	 84% 15%
13	o	244	 89% 10%
14	T	32	 81% 12% 6%
14	t	32	 78% 16% 6%
15	U	104	 83% 10% 8%
15	u	104	 88% . . 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	137	 96% .
16	v	137	 91% 9%
17	X	40	 88% 8% 5%
17	x	40	 88% 8% 5%
18	Y	30	 87% 10% .
18	y	30	 70% 27% .
19	Z	62	 85% 13% .
19	z	62	 81% 19%
20	R	34	 6% 76% 21% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[A]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	505	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	404[A]	X	-	-	-
23	CLA	D	404[B]	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[B]	X	-	-	-
23	CLA	a	406[A]	X	-	-	-
23	CLA	a	406[B]	X	-	-	-
23	CLA	a	409	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	403	X	-	-	-
27	GOL	D	403	-	-	X	-
27	GOL	a	419	-	-	X	-

2 Entry composition

There are 42 unique types of molecules in this entry. The entry contains 62604 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	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	221	0
			4330	2830	716	759	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	20	0
			4146	2721	692	720	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	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	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7

Continued on next page...

Continued from previous page...

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	15			

- 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	0	0
			662	432	107	123				
5	e	79	Total	C	N	O		0	2	0
			670	439	110	121				

- 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	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			506	339	81	84	2			
7	h	64	Total	C	N	O	S	0	1	0
			517	345	85	85	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
			277	185	43	48	1			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	36	Total	C	N	O	0	2	0
			311	207	49	55			
11	l	36	Total	C	N	O	0	2	0
			311	207	49	55			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	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	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	10	0
			1958	1221	335	398	4			
13	o	243	Total	C	N	O	S	0	8	0
			1933	1207	330	392	4			

- 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	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O		0	4	0
			800	508	133	159				
15	u	97	Total	C	N	O		0	4	0
			807	513	134	160				

- 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	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total	C	N	O	0	1	0
			289	194	46	49			
17	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			
18	y	29	Total	C	N	O	S	0	0	0
			215	142	37	33	3			

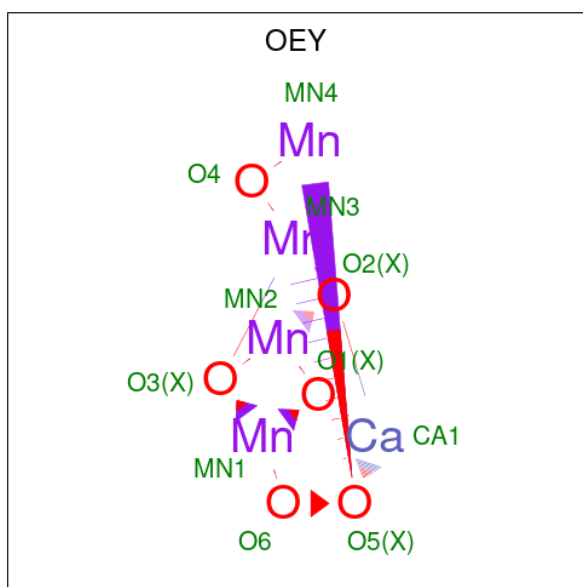
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	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	34	Total	C	N	O	0	0	0
			273	186	47	40			

- Molecule 21 is CA-MN4-O6 CLUSTER (CCD ID: OEY) (formula: CaMn_4O_6) (labeled as "Ligand of Interest" by depositor).

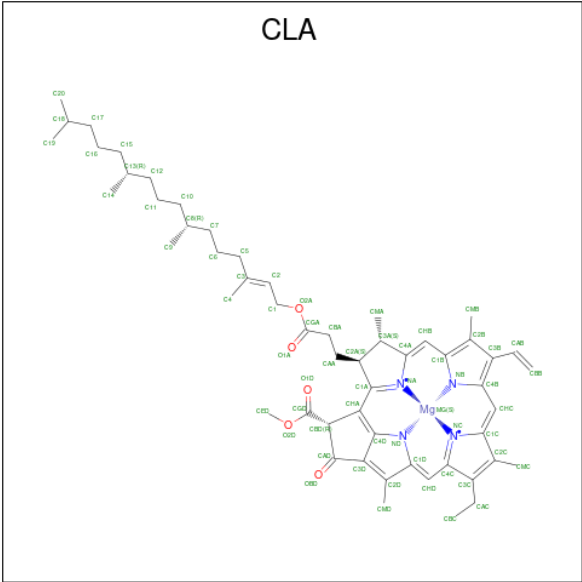


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	Ca	Mn	O	0	1
			11	1	4	6		
21	a	1	Total	Ca	Mn	O	0	1
			11	1	4	6		

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

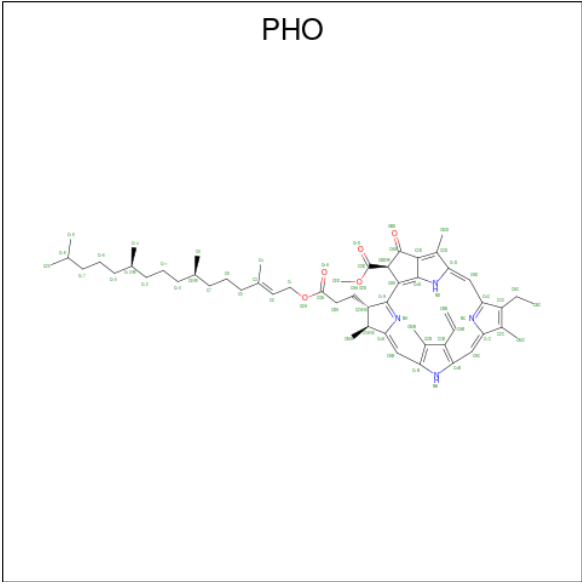
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

Continued on next page...

Continued from previous page...

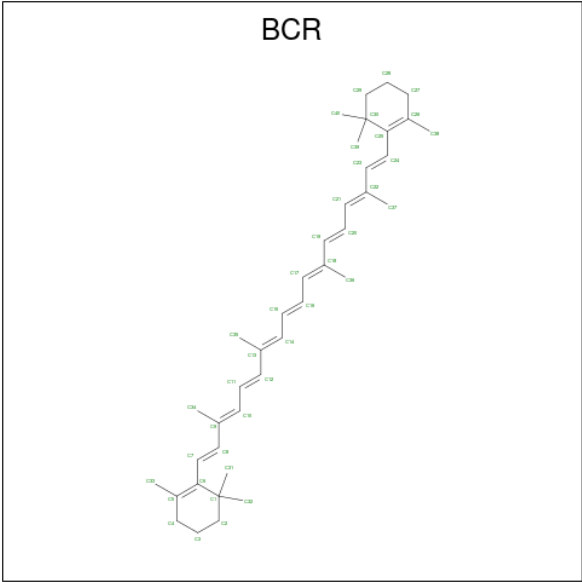
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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



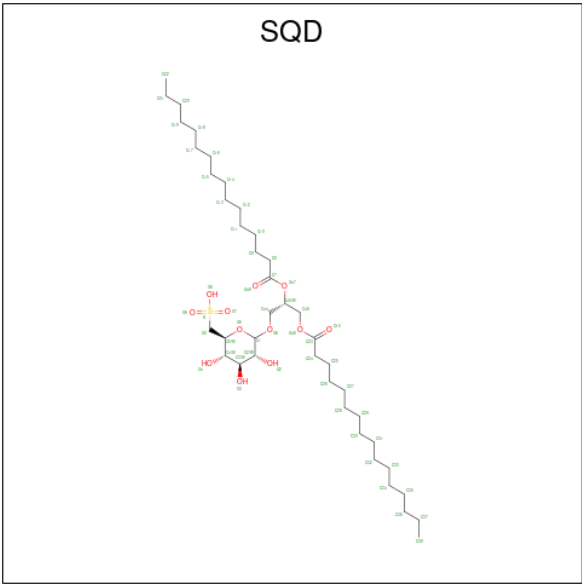
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



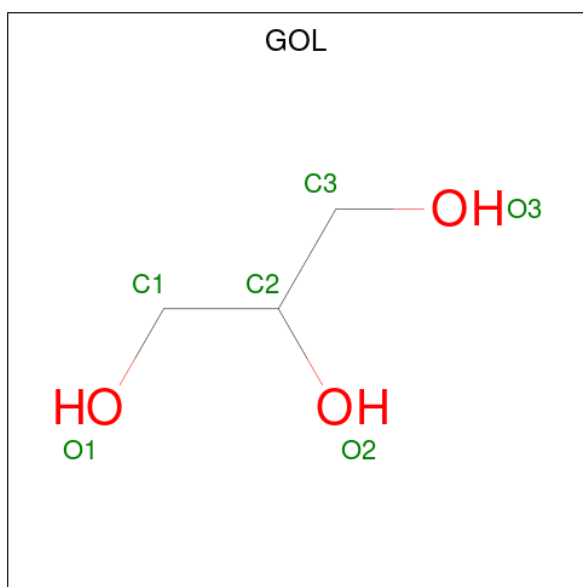
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	1
			108	82	24	2		
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	X	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0	0
			54	41	12	1		
26	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



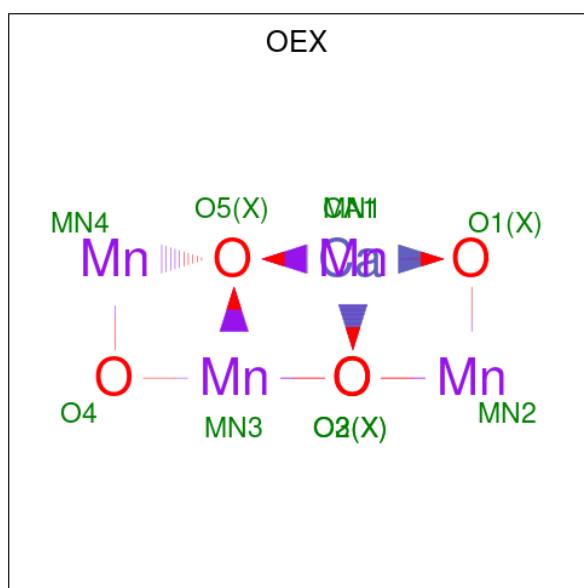
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	V	1	Total	C	O	0	1
			12	6	6		
27	a	1	Total	C	O	0	0
			6	3	3		
27	a	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		
27	b	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	c	1	Total	C	O	0	1
			12	6	6		
27	c	1	Total	C	O	0	0
			6	3	3		
27	d	1	Total	C	O	0	0
			6	3	3		
27	l	1	Total	C	O	0	1
			12	6	6		
27	o	1	Total	C	O	0	0
			6	3	3		
27	o	1	Total	C	O	0	0
			6	3	3		
27	v	1	Total	C	O	0	1
			12	6	6		

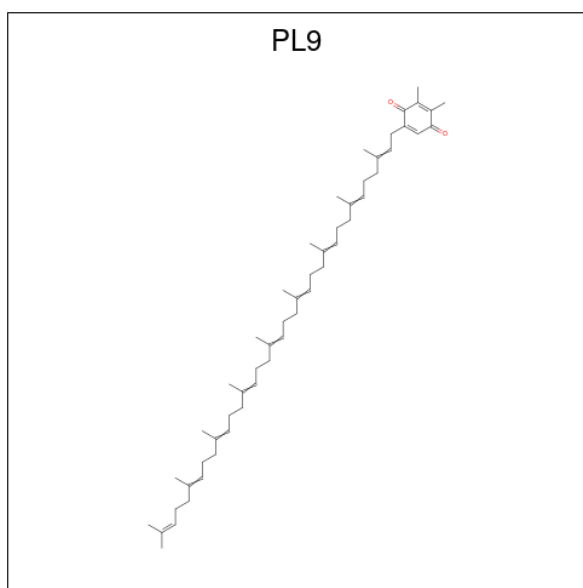
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $\text{C}_{53}\text{H}_{80}\text{O}_2$)

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



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

- Molecule 30 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

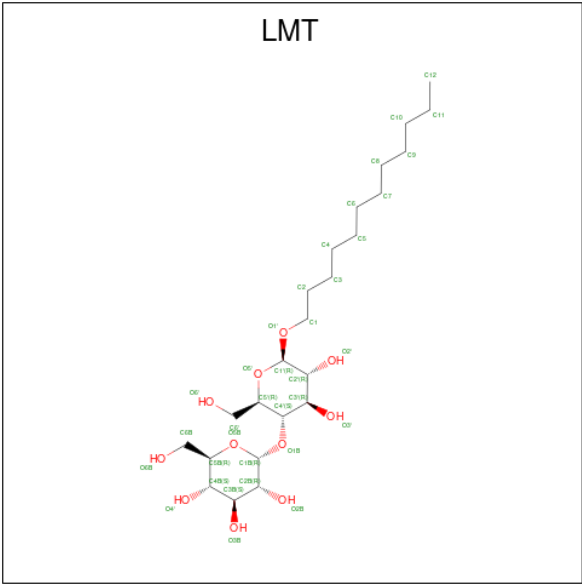
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			28	23	5		
30	B	1	Total	C	O	0	0
			33	28	5		
30	D	2	Total	C	O	0	0
			57	51	6		
30	I	1	Total	C	O	0	0
			40	35	5		
30	J	1	Total	C		0	0
			10	10			
30	K	1	Total	C	O	0	1
			68	58	10		
30	X	1	Total	C	O	0	0
			18	16	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	a	1	Total	C	O	0	0
			30	25	5		
30	b	1	Total	C	O	0	0
			33	28	5		
30	c	1	Total	C	O	0	1
			64	54	10		
30	d	2	Total	C	O	0	0
			53	47	6		
30	i	1	Total	C	O	0	0
			40	35	5		
30	j	1	Total	C		0	0
			10	10			
30	l	1	Total	C		0	0
			10	10			
30	m	1	Total	C		0	0
			10	10			
30	x	1	Total	C	O	0	0
			18	16	2		

- Molecule 31 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



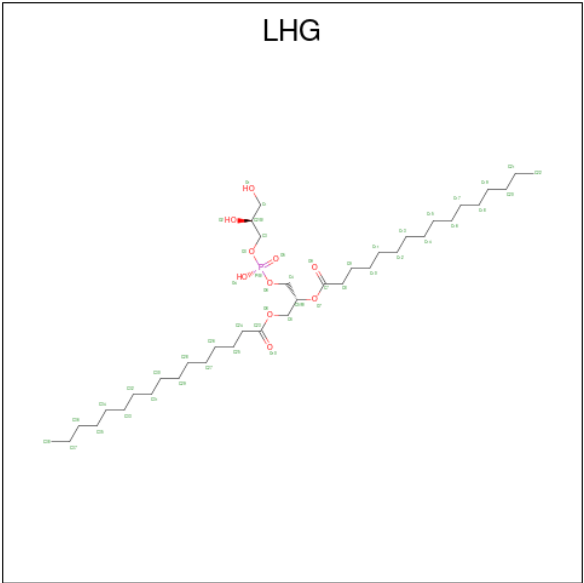
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	A	1	Total	C	O	0	0
			35	24	11		
31	A	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

Continued from previous page...

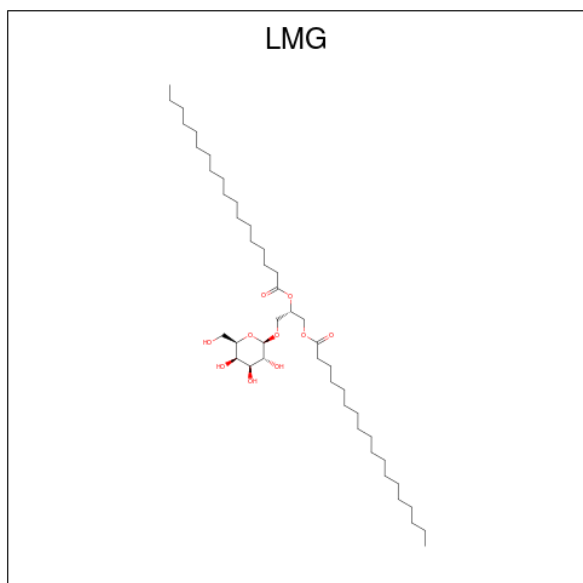
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			35	24	11		
31	B	1	Total	C	O	0	0
			25	19	6		
31	F	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	M	1	Total	C	O	0	0
			35	24	11		
31	b	1	Total	C	O	0	0
			25	19	6		
31	b	1	Total	C	O	0	0
			25	19	6		
31	c	1	Total	C	O	0	0
			35	24	11		
31	e	1	Total	C	O	0	0
			35	24	11		
31	m	1	Total	C	O	0	0
			35	24	11		
31	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	b	1	Total	C	O	P	0	1
			98	76	20	2		
32	d	1	Total	C	O	P	0	1
			98	76	20	2		
32	d	1	Total	C	O	P	0	1
			98	76	20	2		
32	d	1	Total	C	O	P	0	1
			98	76	20	2		

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



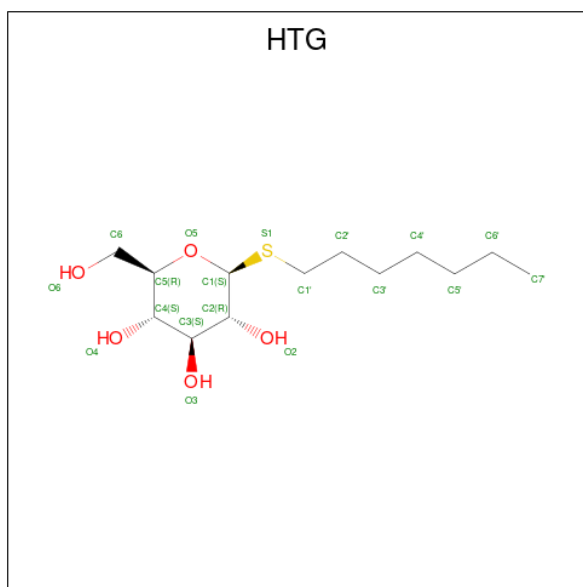
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		

Continued on next page...

Continued from previous page...

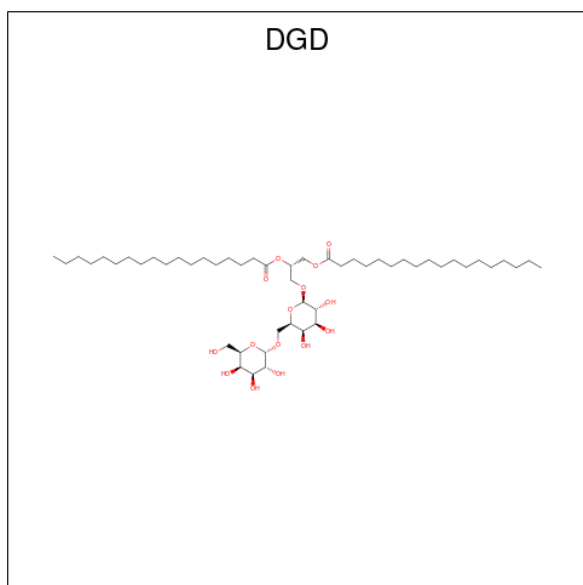
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	C	1	Total	C	O	0	0
			51	41	10		
33	D	1	Total	C	O	0	0
			51	41	10		
33	a	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	c	1	Total	C	O	0	0
			51	41	10		
33	d	1	Total	C	O	0	0
			51	41	10		
33	m	1	Total	C	O	0	0
			51	41	10		
33	Z	1	Total	C	O	0	0
			37	27	10		
33	z	1	Total	C	O	0	0
			39	29	10		

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34	d	1	Total C O S 16 10 5 1	0	0

- Molecule 35 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

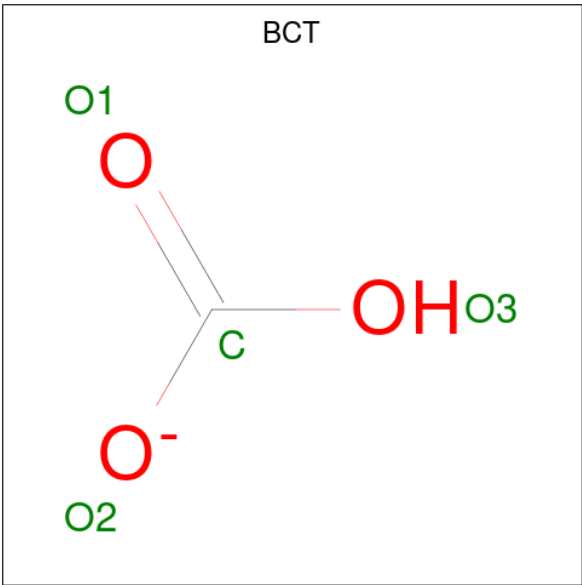
- Molecule 36 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 37 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

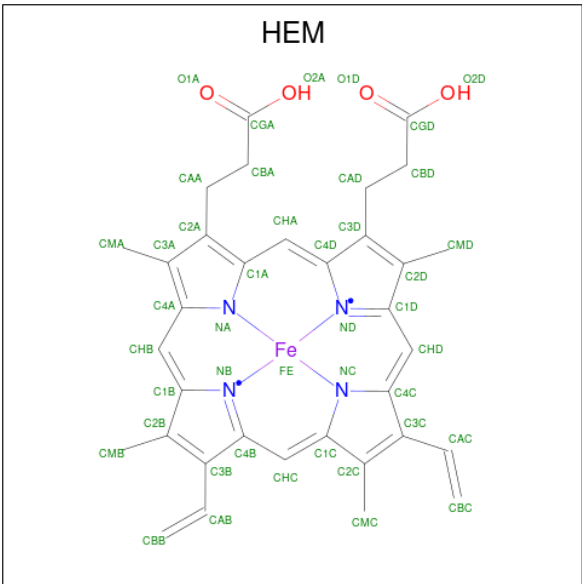
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total Fe 2 2	0	1
37	a	1	Total Fe 2 2	0	1

- Molecule 38 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	D	1	Total	C	O	0	1
			8	2	6		
38	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 39 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

Continued on next page...

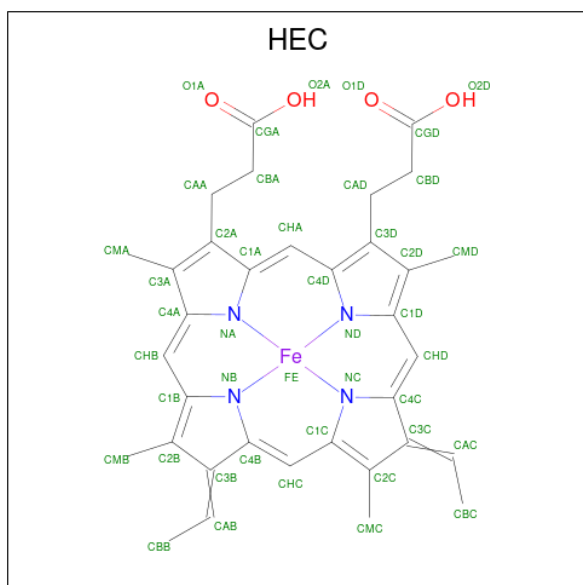
Continued from previous page...

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

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

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

- Molecule 41 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	137	Total	O	0	83
			218	218		
42	B	196	Total	O	0	3
			199	199		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	C	170	Total O 207 207	0	38
42	D	122	Total O 157 157	0	35
42	E	17	Total O 17 17	0	0
42	F	5	Total O 5 5	0	0
42	H	18	Total O 18 18	0	0
42	I	4	Total O 4 4	0	0
42	J	7	Total O 7 7	0	0
42	K	6	Total O 6 6	0	0
42	L	8	Total O 9 9	0	1
42	M	5	Total O 5 5	0	0
42	O	102	Total O 106 106	0	4
42	T	11	Total O 14 14	0	3
42	U	46	Total O 49 49	0	3
42	V	78	Total O 80 80	0	2
42	X	8	Total O 8 8	0	0
42	a	130	Total O 208 208	0	79
42	b	200	Total O 203 203	0	3
42	c	159	Total O 192 192	0	33
42	d	120	Total O 154 154	0	34
42	e	8	Total O 8 8	0	0
42	f	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	h	17	Total 17	O 17	0	0
42	i	2	Total 2	O 2	0	0
42	j	2	Total 2	O 2	0	0
42	k	3	Total 3	O 3	0	0
42	l	7	Total 8	O 8	0	1
42	m	13	Total 13	O 13	0	0
42	o	98	Total 102	O 102	0	4
42	t	8	Total 11	O 11	0	3
42	u	49	Total 50	O 50	0	1
42	v	58	Total 61	O 61	0	3
42	x	6	Total 6	O 6	0	0
42	y	2	Total 2	O 2	0	0

3 Residue-property plots [i](#)

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

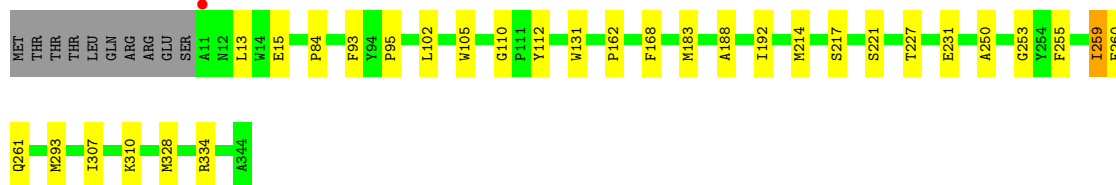
- Molecule 1: Photosystem II protein D1

Chain A:  92%



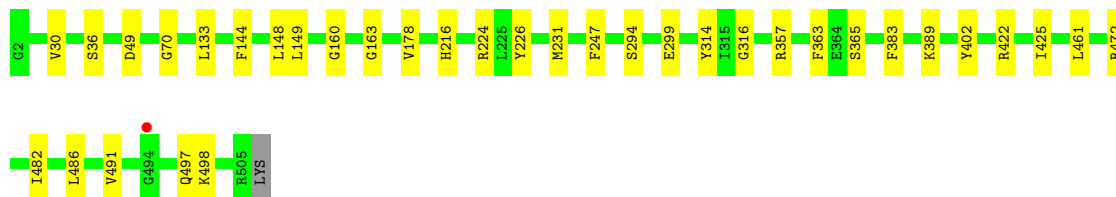
- Molecule 1: Photosystem II protein D1

Chain a:  88% 9%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain B:  93% 7%

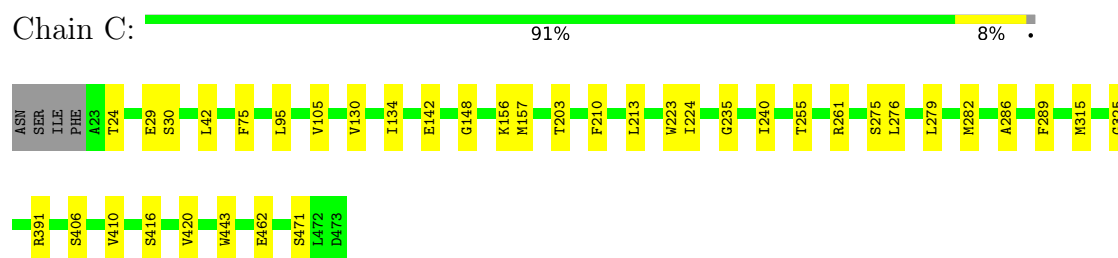


- Molecule 2: Photosystem II CP47 reaction center protein

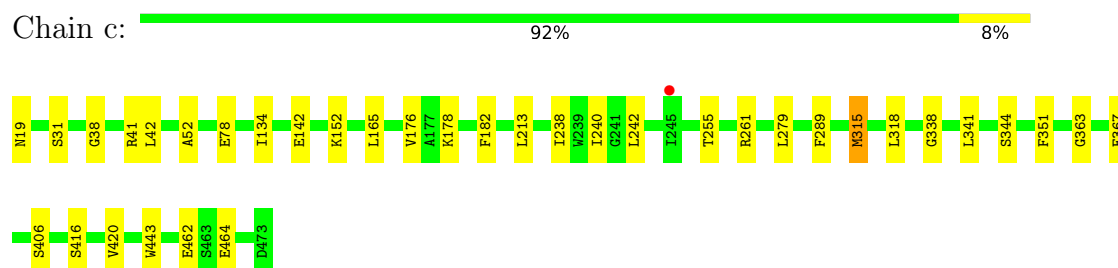
Chain b:  92% 7%



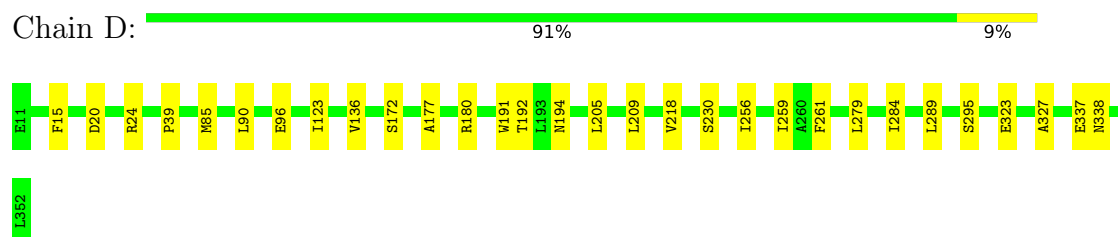
- Molecule 3: Photosystem II CP43 reaction center protein



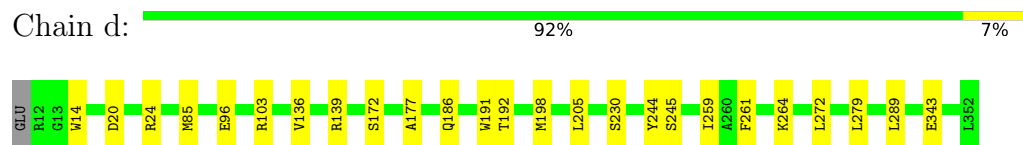
- Molecule 3: Photosystem II CP43 reaction center protein



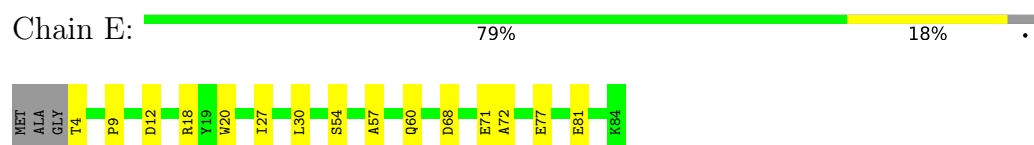
- Molecule 4: Photosystem II D2 protein



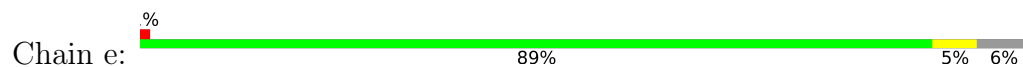
- Molecule 4: Photosystem II D2 protein



- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 5: Cytochrome b559 subunit alpha





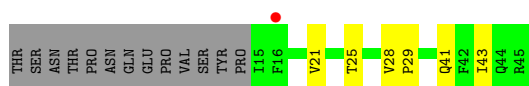
- Molecule 6: Cytochrome b559 subunit beta

Chain F: 66% 11% 23%



- Molecule 6: Cytochrome b559 subunit beta

Chain f: 2% 57% 14% 30%



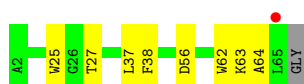
- Molecule 7: Photosystem II reaction center protein H

Chain H: 2% 94% 5%



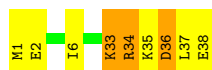
- Molecule 7: Photosystem II reaction center protein H

Chain h: 2% 86% 12%



- Molecule 8: Photosystem II reaction center protein I

Chain I: 76% 16% 8%



- Molecule 8: Photosystem II reaction center protein I

Chain i: 87% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain J: 82% 13%



- Molecule 9: Photosystem II reaction center protein J

Chain j: 92% 8%



- Molecule 10: Photosystem II reaction center protein K

Chain K: 78% 19% .



- Molecule 10: Photosystem II reaction center protein K

Chain k: 81% 14% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L: 95% . .



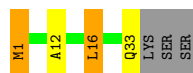
- Molecule 11: Photosystem II reaction center protein L

Chain l: 89% 8% .



- Molecule 12: Photosystem II reaction center protein M

Chain M: 81% 6% 6% 8%



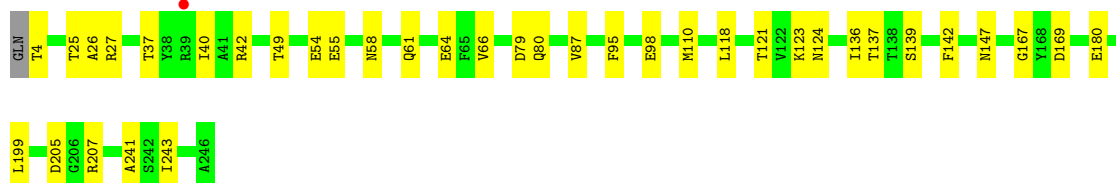
- Molecule 12: Photosystem II reaction center protein M

Chain m: 81% 11% . 6%



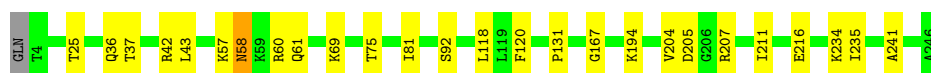
- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O: 84% 15%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o: 89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T: 81% 12% 6%



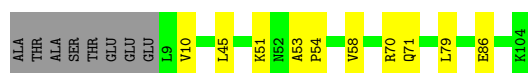
- Molecule 14: Photosystem II reaction center protein T

Chain t: 78% 16% 6%



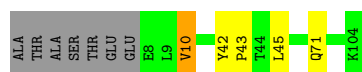
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U: 83% 10% 8%

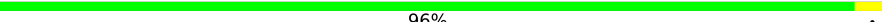


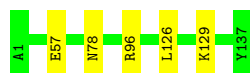
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u: 88% 7% 5%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



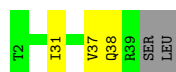
- Molecule 16: Cytochrome c-550

Chain v:  91% 9%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%



- Molecule 17: Photosystem II reaction center protein X

Chain x:  88% 8% 5%



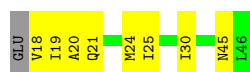
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  87% 10% .



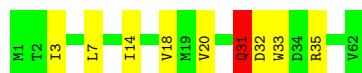
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  70% 27% .

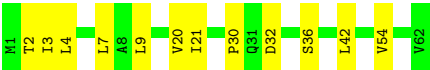
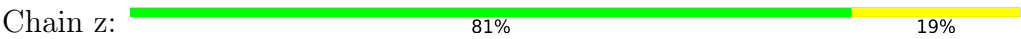


- Molecule 19: Photosystem II reaction center protein Z

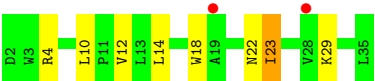
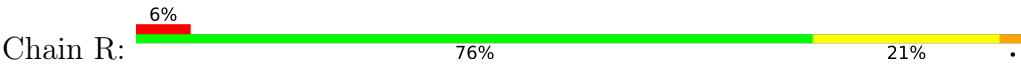
Chain Z:  85% 13% .



- 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	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.142 , 0.181 0.144 , 0.183	Depositor DCC
R_{free} test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	50.6	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62604	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% 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: GOL, CA, LMG, DGD, LHG, HTG, PHO, HEC, SQD, FME, BCR, OEY, PL9, CLA, LMT, MG, UNL, CL, HEM, BCT, OEX, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.27	0/4478	0.42	1/6098 (0.0%)
1	a	0.26	0/4470	0.40	0/6087
2	B	0.37	0/4293	0.51	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.29	0/4404	0.43	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.35	0/3741	0.47	0/5095
4	d	0.31	0/3749	0.44	0/5106
5	E	0.34	0/681	0.51	0/928
5	e	0.30	0/690	0.49	0/939
6	F	0.33	0/284	0.50	0/387
6	f	0.31	0/269	0.45	0/365
7	H	0.33	0/519	0.51	0/708
7	h	0.30	0/530	0.49	0/722
8	I	0.32	0/311	0.47	0/419
8	i	0.32	0/311	0.47	0/419
9	J	0.32	0/278	0.38	0/376
9	j	0.34	0/283	0.47	0/383
10	K	0.30	0/303	0.46	0/416
10	k	0.33	0/303	0.50	0/416
11	L	0.38	0/318	0.48	0/433
11	l	0.38	0/318	0.46	0/433
12	M	0.40	0/261	0.51	0/357
12	m	0.35	0/279	0.50	0/380
13	O	0.35	0/1991	0.51	0/2698
13	o	0.34	0/1966	0.52	0/2665
14	T	0.34	0/310	0.43	0/419
14	t	0.32	0/301	0.41	0/406
15	U	0.37	0/811	0.55	0/1095
15	u	0.37	0/818	0.52	0/1105
16	V	0.37	0/1142	0.51	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	v	0.31	0/1139	0.47	0/1542
17	X	0.23	0/292	0.35	0/395
17	x	0.25	0/284	0.40	0/384
18	Y	0.26	0/216	0.43	0/289
18	y	0.24	0/216	0.40	0/289
19	Z	0.22	0/490	0.38	0/669
19	z	0.22	0/490	0.41	0/669
20	R	0.25	0/279	0.34	0/383
All	All	0.31	0/50562	0.46	1/68780 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	TRP	CA-CB-CG	-5.18	103.75	113.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4338	0	4142	16	0
1	a	4330	0	4132	32	0
2	B	4146	0	3983	26	0
2	b	4134	0	3976	36	0
3	C	4260	0	4123	23	0
3	c	4308	0	4172	27	0
4	D	3620	0	3484	34	0
4	d	3628	0	3490	21	0
5	E	662	0	648	10	0
5	e	670	0	655	3	0
6	F	275	0	282	4	0
6	f	261	0	269	6	0
7	H	506	0	529	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	h	517	0	541	7	0
8	I	314	0	328	6	0
8	i	314	0	328	2	0
9	J	272	0	279	6	0
9	j	277	0	284	2	0
10	K	293	0	305	4	0
10	k	293	0	305	8	0
11	L	311	0	320	1	0
11	l	311	0	320	3	0
12	M	268	0	285	4	0
12	m	286	0	305	7	0
13	O	1958	0	1920	17	0
13	o	1933	0	1900	13	0
14	T	311	0	318	1	0
14	t	302	0	311	4	0
15	U	800	0	796	5	0
15	u	807	0	805	3	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	8	0
17	X	289	0	322	3	0
17	x	281	0	312	3	0
18	Y	215	0	246	2	0
18	y	215	0	246	6	0
19	Z	479	0	516	5	0
19	z	479	0	516	2	0
20	R	273	0	305	4	0
21	A	11	0	0	1	0
21	a	11	0	0	1	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	13	0
23	B	1040	0	1152	23	0
23	C	845	0	936	34	0
23	D	195	0	216	8	0
23	a	455	0	504	20	0
23	b	1040	0	1152	23	0
23	c	845	0	936	33	0
23	d	195	0	216	8	0
24	A	256	0	296	5	0
24	a	256	0	296	3	0
25	A	40	0	56	1	0
25	B	120	0	168	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	80	0	112	2	0
25	D	40	0	56	0	0
25	H	40	0	56	2	0
25	K	80	0	112	1	0
25	T	40	0	56	5	0
25	a	40	0	56	1	0
25	b	120	0	168	9	0
25	c	80	0	112	5	0
25	d	40	0	56	3	0
25	h	40	0	56	4	0
25	k	40	0	56	1	0
25	t	40	0	56	4	0
25	y	40	0	56	2	0
26	A	162	0	234	3	0
26	B	54	0	78	2	0
26	X	43	0	53	3	0
26	a	162	0	232	7	0
26	b	54	0	78	2	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	18	0	24	3	0
27	C	12	0	16	0	0
27	D	12	0	14	7	0
27	O	12	0	16	2	0
27	V	12	0	16	0	0
27	a	12	0	16	6	0
27	b	12	0	16	4	0
27	c	18	0	24	0	0
27	d	6	0	7	0	0
27	l	12	0	16	1	0
27	o	12	0	16	0	0
27	v	12	0	16	3	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	110	0	160	19	0
29	D	110	0	160	1	0
29	a	110	0	160	8	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	1	0
31	B	95	0	127	3	0
31	F	35	0	46	0	0
31	M	70	0	92	1	0
31	b	50	0	70	2	0
31	c	35	0	46	1	0
31	e	35	0	46	1	0
31	m	35	0	46	0	0
31	t	26	0	34	2	0
32	A	98	0	148	2	0
32	D	196	0	296	10	0
32	E	84	0	114	5	0
32	L	98	0	148	0	0
32	a	84	0	114	9	0
32	b	98	0	148	0	0
32	d	294	0	444	24	0
33	B	51	0	72	1	0
33	C	153	0	216	3	0
33	D	51	0	72	0	0
33	Z	37	0	44	1	0
33	a	51	0	72	1	0
33	c	102	0	144	1	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	3	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	310	0	410	4	0
35	H	62	0	82	1	0
35	c	310	0	410	8	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	2	0	0	0	0
37	a	2	0	0	0	0
38	D	8	0	0	0	0
38	d	8	0	0	0	0
39	F	43	0	30	2	0
39	f	43	0	30	0	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	218	0	0	1	0
42	B	199	0	0	1	0
42	C	207	0	0	0	0
42	D	157	0	0	3	0
42	E	17	0	0	0	0
42	F	5	0	0	0	0
42	H	18	0	0	0	0
42	I	4	0	0	0	0
42	J	7	0	0	1	0
42	K	6	0	0	0	0
42	L	9	0	0	0	0
42	M	5	0	0	0	0
42	O	106	0	0	0	0
42	T	14	0	0	0	0
42	U	49	0	0	0	0
42	V	80	0	0	0	0
42	X	8	0	0	0	0
42	a	208	0	0	2	0
42	b	203	0	0	1	0
42	c	192	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	d	154	0	0	1	0
42	e	8	0	0	0	0
42	f	3	0	0	0	0
42	h	17	0	0	0	0
42	i	2	0	0	0	0
42	j	2	0	0	0	0
42	k	3	0	0	1	0
42	l	8	0	0	0	0
42	m	13	0	0	0	0
42	o	102	0	0	0	0
42	t	11	0	0	1	0
42	u	50	0	0	1	0
42	v	61	0	0	0	0
42	x	6	0	0	0	0
42	y	2	0	0	0	0
All	All	62604	0	61443	553	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 (553) 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)
27:D:403:GOL:H11	12:M:1:FME:HG2	1.45	0.97
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.50	0.94
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
21:a:401[B]:OEY:O6	21:a:401[B]:OEY:O5	1.90	0.89
21:A:401[B]:OEY:O6	21:A:401[B]:OEY:O5	1.91	0.88
23:B:604:CLA:H42	23:B:605:CLA:H2	1.60	0.82
23:B:601:CLA:H12	23:B:601:CLA:H71	1.62	0.82
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.63	0.78
4:d:192[A]:THR:HG23	23:d:402[A]:CLA:HBC2	1.66	0.77
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
4:d:192[B]:THR:HG23	23:d:402[B]:CLA:HBC2	1.68	0.75
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.68	0.74
27:D:403:GOL:O2	42:D:501:HOH:O	2.07	0.72
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.70	0.72
23:A:404[B]:CLA:HBB1	23:D:404[B]:CLA:C4B	2.07	0.71
34:B:625:HTG:H61	1:a:102:LEU:HD12	1.73	0.71
23:a:409:CLA:H192	23:c:506:CLA:H142	1.73	0.71
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:408:CLA:H193	23:C:507:CLA:H101	1.74	0.70
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.75	0.69
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.27	0.68
32:D:409[A]:LHG:H112	32:D:409[A]:LHG:H382	1.76	0.68
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.76	0.67
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.76	0.67
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.77	0.67
32:D:409[B]:LHG:H382	32:D:409[B]:LHG:H112	1.77	0.67
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.76	0.67
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.77	0.66
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.78	0.66
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.27	0.66
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.77	0.65
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.79	0.65
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.79	0.64
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:HBB1	1.80	0.64
13:O:169:ASP:OD1	27:O:303:GOL:H12	1.98	0.64
31:B:631:LMT:H6E	31:t:101:LMT:H6D	1.80	0.64
23:a:409:CLA:H152	23:c:507:CLA:H142	1.79	0.64
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.80	0.64
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.30	0.64
29:A:414[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.63
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.78	0.63
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.31	0.63
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.28	0.63
23:C:507:CLA:H142	35:C:517[A]:DGD:HAF2	1.80	0.63
23:c:503:CLA:H61	23:c:513:CLA:H42	1.81	0.63
23:C:514:CLA:H202	33:C:521:LMG:H402	1.80	0.62
23:A:405[B]:CLA:HHC	23:A:405[B]:CLA:HBB1	1.81	0.62
26:a:411[A]:SQD:H152	32:d:407[A]:LHG:H172	1.82	0.62
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.80	0.62
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.81	0.62
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.00	0.62
27:a:419:GOL:O3	14:t:2:GLU:OE1	2.18	0.62
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.82	0.62
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.81	0.61
1:a:214[B]:MET:HB3	29:a:414[B]:PL9:H103	1.83	0.61
33:z:101:LMG:H302	33:z:101:LMG:H141	1.83	0.60
23:c:512:CLA:H191	33:z:101:LMG:H241	1.82	0.60
23:a:406[B]:CLA:HBB1	23:a:406[B]:CLA:HHC	1.84	0.60
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:17:ILE:H	10:K:17:ILE:HD13	1.68	0.59
35:c:519:DGD:HBH2	32:d:407[A]:LHG:H211	1.85	0.59
17:X:31:ILE:HD11	26:X:101:SQD:H102	1.84	0.59
26:a:411[A]:SQD:H141	32:d:407[A]:LHG:H152	1.84	0.59
23:C:507:CLA:H142	35:C:517[B]:DGD:HAF2	1.84	0.59
23:b:601:CLA:H72	23:b:601:CLA:H2	1.85	0.58
27:b:628:GOL:O1	27:b:628:GOL:O3	2.13	0.58
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.85	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.68	0.58
29:A:414[B]:PL9:H262	32:E:101[B]:LHG:H223	1.86	0.58
4:D:192[A]:THR:HG23	23:D:404[A]:CLA:HBC2	1.87	0.57
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.86	0.57
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.86	0.57
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.86	0.57
3:C:275:SER:HB3	23:C:510:CLA:HED3	1.87	0.57
23:a:407[A]:CLA:H191	32:a:420[A]:LHG:H111	1.85	0.57
4:D:85:MET:CE	4:D:96:GLU:HG2	2.34	0.57
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.34	0.57
18:y:20:ALA:O	18:y:24:MET:HG2	2.05	0.57
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.86	0.56
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.06	0.56
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.86	0.56
27:a:419:GOL:H11	12:m:1:FME:HE3	1.87	0.56
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.85	0.56
25:t:102:BCR:H382	25:t:102:BCR:H23C	1.87	0.56
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.69	0.56
20:R:18:TRP:O	20:R:22:ASN:ND2	2.37	0.56
2:b:285:ASN:O	2:b:289:GLN:HG2	2.05	0.56
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.87	0.56
35:c:517[A]:DGD:HG11	42:c:605[A]:HOH:O	2.06	0.56
33:c:521:LMG:H232	33:c:521:LMG:H391	1.87	0.56
23:a:405[B]:CLA:HBB1	23:d:402[B]:CLA:C4B	2.10	0.56
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.70	0.56
23:c:506:CLA:HMD1	23:c:508:CLA:HAB	1.87	0.55
32:d:406[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.88	0.55
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.88	0.55
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.39	0.55
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.11	0.55
23:a:407[B]:CLA:H203	33:d:411:LMG:H412	1.89	0.55
26:a:411[B]:SQD:H152	32:d:407[B]:LHG:H172	1.89	0.55
25:b:619:BCR:H331	25:b:619:BCR:C8	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:519:DGD:HBH2	32:d:407[B]:LHG:H211	1.88	0.55
23:c:509:CLA:HBC3	23:c:511:CLA:H71	1.88	0.54
27:D:403:GOL:H11	12:M:1:FME:CG	2.30	0.54
1:a:183[A]:MET:HA	23:a:405[A]:CLA:HMD1	1.89	0.54
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.88	0.54
32:D:409[A]:LHG:H382	32:D:409[A]:LHG:H132	1.89	0.54
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.88	0.54
23:a:407[B]:CLA:H191	32:a:420[B]:LHG:H111	1.88	0.54
35:c:518[B]:DGD:HAF1	35:c:518[B]:DGD:HA81	1.90	0.54
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.88	0.54
24:a:408[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.89	0.54
29:A:414[A]:PL9:H253	23:D:404[A]:CLA:H141	1.89	0.54
9:J:2:SER:N	42:J:201:HOH:O	2.40	0.53
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.90	0.53
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.42	0.53
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.39	0.53
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.22	0.53
29:A:414[B]:PL9:H253	23:D:404[B]:CLA:H141	1.90	0.52
23:a:407[A]:CLA:H203	33:d:411:LMG:H412	1.91	0.52
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	1.91	0.52
2:b:36:SER:OG	25:b:618:BCR:H362	2.09	0.52
27:l:102[A]:GOL:H32	14:t:25:GLU:HB2	1.90	0.52
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.45	0.52
4:D:327:ALA:HB2	27:D:414:GOL:H2	1.91	0.52
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.42	0.52
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.10	0.52
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.40	0.52
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.45	0.52
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.44	0.52
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.09	0.52
2:B:226:TYR:HA	2:B:231:MET:HG3	1.91	0.52
1:a:334[B]:ARG:NH2	42:a:503[B]:HOH:O	2.43	0.52
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.45	0.52
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.45	0.51
32:d:407[B]:LHG:H342	32:d:407[B]:LHG:H151	1.91	0.51
19:z:32:ASP:O	19:z:36:SER:OG	2.16	0.51
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.92	0.51
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.74	0.51
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.93	0.51
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.91	0.51
4:D:323[A]:GLU:O	27:D:414:GOL:O2	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:416[B]:PHO:H3A	23:D:404[B]:CLA:H142	1.93	0.51
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.93	0.51
8:I:35:LYS:O	8:I:37:LEU:N	2.43	0.51
27:a:419:GOL:O2	42:a:501:HOH:O	2.12	0.51
4:D:323[B]:GLU:O	27:D:414:GOL:O2	2.28	0.51
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.11	0.51
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.26	0.51
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.45	0.50
4:D:192[B]:THR:HG23	23:D:404[B]:CLA:HBC2	1.93	0.50
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.42	0.50
4:D:180:ARG:HD3	4:D:180:ARG:C	2.36	0.50
25:K:103:BCR:H321	25:K:103:BCR:HC8	1.93	0.50
1:a:15:GLU:HB2	31:c:501:LMT:H6'2	1.94	0.50
3:c:176:VAL:HG21	3:c:238:ILE:HG13	1.94	0.50
26:a:411[B]:SQD:H141	32:d:407[B]:LHG:H152	1.92	0.50
32:a:420[A]:LHG:HC31	5:e:9:PRO:HA	1.92	0.50
23:B:614:CLA:H192	14:t:8:PHE:CE1	2.47	0.50
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.94	0.50
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.46	0.50
35:c:517[B]:DGD:HG11	42:c:605[B]:HOH:O	2.12	0.49
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.94	0.49
4:D:261[B]:PHE:CZ	32:D:408[B]:LHG:HC81	2.47	0.49
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.94	0.49
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.12	0.49
15:u:10[A]:VAL:HG12	42:u:244:HOH:O	2.10	0.49
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.46	0.49
25:h:101:BCR:H331	25:h:101:BCR:C8	2.42	0.49
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.94	0.49
23:a:405[A]:CLA:H201	32:d:406[A]:LHG:H161	1.95	0.49
32:a:420[B]:LHG:HC31	5:e:9:PRO:HA	1.93	0.49
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.95	0.49
32:d:406[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.95	0.49
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	1.95	0.49
29:A:414[B]:PL9:H472	4:D:39:PRO:HD3	1.95	0.49
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.95	0.49
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.95	0.49
23:B:614:CLA:H71	23:B:614:CLA:H112	1.52	0.48
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.13	0.48
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.48	0.48
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.14	0.48
24:A:416[A]:PHO:H3A	23:D:404[A]:CLA:H142	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:418:GOL:H32	12:m:1:FME:HG3	1.94	0.48
2:b:233:ASN:O	2:b:236:THR:HG22	2.13	0.48
4:d:85:MET:CE	4:d:96:GLU:HG2	2.42	0.48
32:d:407[A]:LHG:H122	32:d:407[A]:LHG:C38	2.44	0.48
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.94	0.48
23:C:511:CLA:H112	23:C:511:CLA:H152	1.53	0.48
32:D:409[B]:LHG:H382	32:D:409[B]:LHG:H132	1.95	0.48
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.95	0.48
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.47	0.48
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.96	0.48
3:C:279:LEU:HD22	23:C:510:CLA:HED2	1.94	0.48
3:C:325:GLY:O	15:U:51:LYS:NZ	2.46	0.48
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.14	0.48
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.48	0.48
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.39	0.48
13:o:92:SER:HB3	13:o:131:PRO:HA	1.95	0.48
32:D:408[A]:LHG:HC62	11:L:15[A]:THR:HG23	1.96	0.48
13:O:42:ARG:O	13:O:241:ALA:HA	2.14	0.48
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.47	0.48
1:A:272[B]:HIS:CD2	4:D:218[B]:VAL:HG21	2.48	0.47
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.26	0.47
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.94	0.47
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.43	0.47
10:K:26:PRO:O	10:K:29:PRO:HD2	2.15	0.47
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.15	0.47
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.95	0.47
23:c:513:CLA:HMB2	23:c:513:CLA:H192	1.96	0.47
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.97	0.47
13:O:124:ASN:OD1	13:O:147:ASN:ND2	2.48	0.47
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.49	0.47
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.50	0.47
25:d:404:BCR:H15C	25:d:404:BCR:H351	1.78	0.47
32:d:407[A]:LHG:H342	32:d:407[A]:LHG:H151	1.97	0.47
2:B:133:LEU:HB2	27:B:627:GOL:H31	1.97	0.47
25:H:101:BCR:H331	25:H:101:BCR:C8	2.44	0.47
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.45	0.47
29:a:414[B]:PL9:H171	29:a:414[B]:PL9:H151	1.52	0.47
32:d:407[A]:LHG:H302	32:d:407[A]:LHG:H332	1.67	0.47
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.95	0.47
26:B:620:SQD:H1	26:B:620:SQD:H462	1.97	0.47
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	1.97	0.47
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	1.97	0.47
29:a:414[A]:PL9:H171	29:a:414[A]:PL9:H151	1.58	0.47
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.30	0.47
32:d:407[B]:LHG:H361	32:d:407[B]:LHG:H331	1.69	0.46
1:A:192[A]:ILE:HG13	1:A:293[A]:MET:HE1	1.97	0.46
26:A:410[B]:SQD:H122	26:A:410[B]:SQD:H152	1.68	0.46
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	1.98	0.46
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.15	0.46
25:B:619:BCR:H24C	25:B:619:BCR:H371	1.68	0.46
23:a:406[A]:CLA:HBA1	23:a:406[A]:CLA:C4A	2.45	0.46
2:b:299:GLU:HG2	2:b:402:TYR:HD2	1.80	0.46
2:b:497:GLN:HB2	2:b:504:THR:HB	1.97	0.46
3:c:363:GLY:O	3:c:367:GLU:HG2	2.16	0.46
2:B:482[B]:ILE:HD12	2:B:486[B]:LEU:HD22	1.98	0.46
4:D:261[B]:PHE:CE1	32:D:408[B]:LHG:HC81	2.51	0.46
8:I:33:LYS:HB3	8:I:34:ARG:H	1.57	0.46
26:a:411[A]:SQD:H271	32:d:407[A]:LHG:H141	1.97	0.46
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.51	0.46
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.74	0.46
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.96	0.46
6:F:27:ALA:HB1	39:F:102:HEM:HAC	1.98	0.46
29:a:414[B]:PL9:H28	32:a:420[B]:LHG:H222	1.98	0.46
32:d:407[B]:LHG:C38	32:d:407[B]:LHG:H122	2.46	0.46
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.98	0.46
24:a:416[A]:PHO:HBC3	4:d:279:LEU:HD22	1.96	0.46
23:b:605:CLA:HHC	23:b:605:CLA:CBB	2.46	0.46
32:d:407[A]:LHG:H331	32:d:407[A]:LHG:H361	1.46	0.46
24:a:416[B]:PHO:HBC2	24:a:416[B]:PHO:HHO	1.98	0.46
29:A:414[B]:PL9:H471	29:A:414[B]:PL9:H43	1.57	0.46
5:E:68:ASP:O	5:E:72:ALA:HB2	2.16	0.46
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.69	0.46
29:A:414[B]:PL9:H322	29:A:414[B]:PL9:H301	1.82	0.45
4:D:230[B]:SER:HB2	42:D:540:HOH:O	2.16	0.45
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	1.97	0.45
32:A:418[A]:LHG:H361	23:B:613:CLA:H51	1.98	0.45
2:B:422:ARG:O	2:B:425:ILE:HG12	2.16	0.45
23:C:507:CLA:H18	23:C:507:CLA:H152	1.48	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.98	0.45
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.50	0.45
2:b:307:GLU:OE2	42:b:701:HOH:O	2.21	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:402[B]:CLA:HAA2	23:d:402[B]:CLA:HBD	1.98	0.45
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.80	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.16	0.45
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.16	0.45
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.99	0.45
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.17	0.45
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.79	0.45
14:t:2:GLU:HG2	14:t:3:THR:N	2.32	0.45
19:Z:14:ILE:O	19:Z:18:VAL:HG23	2.17	0.45
4:D:261[A]:PHE:CZ	32:D:408[A]:LHG:HC81	2.52	0.45
29:a:414[A]:PL9:H351	6:f:25:THR:OG1	2.16	0.45
33:d:411:LMG:H221	33:d:411:LMG:H191	1.61	0.45
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	1.99	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.45
4:D:230[A]:SER:HB2	42:D:540:HOH:O	2.16	0.45
32:d:407[A]:LHG:H372	32:d:407[A]:LHG:H142	1.97	0.45
29:A:414[B]:PL9:H171	29:A:414[B]:PL9:H151	1.52	0.45
25:C:515:BCR:H352	33:C:521:LMG:H352	1.97	0.45
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.99	0.45
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.82	0.45
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	1.99	0.45
5:E:27:ILE:HD11	39:F:102:HEM:HBC2	1.98	0.45
13:O:79:ASP:OD1	13:O:80:GLN:N	2.45	0.45
23:b:615:CLA:H92	23:b:615:CLA:H61	1.68	0.45
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.24	0.45
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.83	0.45
3:c:182:PHE:HA	34:c:522:HTG:H61	2.00	0.45
15:u:45:LEU:HD21	15:u:71:GLN:HB3	1.98	0.45
3:C:223:TRP:CG	3:C:224:ILE:H	2.35	0.44
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.17	0.44
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.99	0.44
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.99	0.44
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.83	0.44
25:b:618:BCR:C8	25:b:618:BCR:H331	2.46	0.44
23:c:509:CLA:H18	35:c:518[A]:DGD:HAT2	1.99	0.44
13:o:58:ASN:C	13:o:60:ARG:H	2.24	0.44
3:C:279:LEU:HA	3:C:282:MET:HE3	1.99	0.44
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.51	0.44
2:b:422:ARG:O	2:b:425:ILE:HG12	2.17	0.44
27:b:628:GOL:H11	42:d:502:HOH:O	2.16	0.44
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414[A]:PL9:H151	29:A:414[A]:PL9:H171	1.55	0.44
29:A:414[A]:PL9:H301	29:A:414[A]:PL9:H322	1.76	0.44
25:C:516:BCR:H24C	25:C:516:BCR:H371	1.85	0.44
5:E:18:ARG:H	9:J:2:SER:N	2.15	0.44
23:b:611:CLA:H112	23:b:611:CLA:H72	1.78	0.44
23:c:509:CLA:H162	23:c:509:CLA:H122	1.69	0.44
23:A:408:CLA:H41	23:A:408:CLA:H61	1.64	0.44
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.46	0.44
23:b:609:CLA:NC	25:h:101:BCR:H332	2.32	0.44
3:C:210:PHE:HA	3:C:213:LEU:HD13	1.99	0.44
5:E:77:GLU:O	5:E:81:GLU:HG2	2.17	0.44
8:I:2:GLU:O	8:I:6:ILE:HG12	2.18	0.44
25:T:101:BCR:HC8	25:T:101:BCR:H311	1.99	0.44
25:d:404:BCR:C8	25:d:404:BCR:H331	2.48	0.44
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.99	0.44
1:a:214[A]:MET:HB3	29:a:414[A]:PL9:H103	1.98	0.44
23:C:509:CLA:H142	23:C:509:CLA:H111	1.81	0.44
13:O:25:THR:O	13:O:27:ARG:N	2.51	0.44
23:a:409:CLA:H203	23:c:507:CLA:H101	2.00	0.44
29:a:414[B]:PL9:H351	6:f:25:THR:OG1	2.18	0.44
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.53	0.44
3:c:31:SER:CB	3:c:41:ARG:HG2	2.47	0.44
4:d:261[B]:PHE:CZ	32:d:406[B]:LHG:HC81	2.52	0.44
7:h:38:PHE:HB2	25:h:101:BCR:H10C	2.00	0.44
2:B:461:LEU:HD21	4:D:284:ILE:HD11	1.99	0.44
23:B:614:CLA:H92	23:B:614:CLA:H61	1.80	0.44
26:a:411[B]:SQD:H271	32:d:407[B]:LHG:H141	2.00	0.44
24:A:416[B]:PHO:HBC3	4:D:279:LEU:HD22	2.00	0.44
23:B:606:CLA:H202	26:a:412:SQD:H302	1.99	0.44
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.73	0.44
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.63	0.44
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.76	0.44
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.82	0.44
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	2.00	0.43
3:C:130:VAL:O	3:C:134:ILE:HG12	2.19	0.43
3:C:279:LEU:HD12	3:C:282:MET:CE	2.48	0.43
29:a:414[A]:PL9:H28	32:a:420[A]:LHG:H222	1.99	0.43
2:b:29:LEU:HD23	26:b:620:SQD:H201	1.99	0.43
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	1.99	0.43
23:c:505:CLA:H151	23:c:509:CLA:H143	1.98	0.43
23:d:403:CLA:H162	7:h:37:LEU:HD21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:E:101[B]:LHG:H241	32:E:101[B]:LHG:HC61	1.83	0.43
8:I:36:ASP:OD1	8:I:36:ASP:N	2.52	0.43
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	2.00	0.43
1:a:259[A]:ILE:HG22	1:a:260[A]:PHE:CD1	2.53	0.43
23:a:409:CLA:H61	23:a:409:CLA:H41	1.88	0.43
2:b:358:ARG:HB2	27:b:628:GOL:H31	1.99	0.43
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.53	0.43
23:b:607:CLA:H91	23:b:607:CLA:H112	1.59	0.43
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.86	0.43
23:B:601:CLA:H72	23:B:601:CLA:C4D	2.48	0.43
23:B:602:CLA:H203	23:B:602:CLA:H162	1.76	0.43
23:b:604:CLA:H42	23:b:605:CLA:H2	2.01	0.43
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	2.00	0.43
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.48	0.43
29:A:414[A]:PL9:HC2	29:A:414[A]:PL9:HC8	1.71	0.43
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.88	0.43
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.84	0.43
25:B:618:BCR:H331	25:B:618:BCR:C8	2.48	0.43
34:B:623:HTG:H7'3	34:B:623:HTG:H4'2	1.80	0.43
29:D:407[A]:PL9:H401	29:D:407[A]:PL9:H422	1.75	0.43
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.54	0.43
3:c:443[B]:TRP:CZ2	23:c:509:CLA:HMD1	2.53	0.43
23:d:403:CLA:H41	23:d:403:CLA:H61	1.70	0.43
32:d:407[B]:LHG:H142	32:d:407[B]:LHG:H372	2.00	0.43
7:h:56:ASP:OD2	17:x:2:THR:OG1	2.36	0.43
2:B:49:ASP:OD2	13:o:57:LYS:NZ	2.49	0.43
3:C:276:LEU:HD23	23:C:510:CLA:HED1	2.01	0.43
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.54	0.43
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.19	0.43
2:b:234:ILE:HB	27:b:624:GOL:H31	2.01	0.43
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.43
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.49	0.43
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.00	0.43
23:b:616:CLA:H13	23:b:616:CLA:H102	1.81	0.43
3:c:315[B]:MET:HE3	3:c:351[B]:PHE:HZ	1.84	0.43
23:c:509:CLA:H18	35:c:518[B]:DGD:HAT2	2.01	0.43
13:o:204:VAL:HG22	13:o:211:ILE:HG22	2.00	0.43
24:A:407[B]:PHO:HAB	4:D:205[B]:LEU:HD13	1.99	0.43
26:A:410[A]:SQD:H122	26:A:410[A]:SQD:H152	1.52	0.43
32:A:418[B]:LHG:H361	23:B:613:CLA:H51	2.01	0.43
3:C:157:MET:HE2	3:C:157:MET:HA	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.01	0.43
23:b:614:CLA:H162	23:b:614:CLA:H122	1.68	0.43
19:Z:7:LEU:HD23	19:Z:7:LEU:HA	1.88	0.43
13:O:54:GLU:HG2	13:O:64:GLU:O	2.19	0.43
23:a:406[B]:CLA:C4A	23:a:406[B]:CLA:HBA1	2.48	0.43
23:a:406[B]:CLA:HED2	4:d:198:MET:SD	2.58	0.43
32:a:420[B]:LHG:H241	32:a:420[B]:LHG:HC61	1.88	0.43
23:c:507:CLA:H3A	23:c:507:CLA:HBA1	1.82	0.43
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.78	0.43
2:B:357[A]:ARG:HH12	27:B:624:GOL:H32	1.83	0.43
13:O:136:ILE:HD13	13:O:243:ILE:HD13	2.01	0.43
23:b:610:CLA:HHC	23:b:610:CLA:HBB1	2.00	0.43
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.44	0.42
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.54	0.42
23:a:407[B]:CLA:HMB2	23:d:402[B]:CLA:H122	2.01	0.42
11:l:20:GLY:O	11:l:24:ILE:HG12	2.19	0.42
17:x:28:LEU:HD23	17:x:28:LEU:HA	1.87	0.42
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	2.00	0.42
2:B:497:GLN:HE22	17:X:38:GLN:HB2	1.84	0.42
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	2.00	0.42
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.42
42:A:634[B]:HOH:O	3:C:410[B]:VAL:HB	2.20	0.42
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.01	0.42
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	2.00	0.42
23:b:614:CLA:H72	23:b:614:CLA:H112	1.66	0.42
3:c:464[B]:GLU:OE2	4:d:245[B]:SER:OG	2.37	0.42
10:k:24:VAL:HG21	18:y:25:ILE:HB	2.01	0.42
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.76	0.42
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.99	0.42
25:c:516:BCR:H24C	25:c:516:BCR:H371	1.87	0.42
23:C:511:CLA:H192	23:C:511:CLA:HBC3	2.01	0.42
5:E:57:ALA:H	5:E:60:GLN:HE21	1.66	0.42
1:A:82[A]:VAL:HB	1:A:174[A]:LEU:HB2	2.01	0.42
1:A:231:GLU:HB3	42:B:887:HOH:O	2.20	0.42
23:C:506:CLA:H93	23:C:506:CLA:H111	1.75	0.42
35:C:519:DGD:HBE2	35:C:519:DGD:HB81	1.69	0.42
5:E:9:PRO:HA	32:E:101[A]:LHG:HC31	2.01	0.42
2:b:154:GLY:HA2	2:b:158:LEU:HD12	2.01	0.42
4:d:14:TRP:CD1	34:d:410:HTG:H61	2.54	0.42
8:i:2:GLU:O	8:i:6:ILE:HG12	2.20	0.42
10:k:19:ASP:HB3	10:k:20:PRO:HD3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:42:ARG:O	13:o:241:ALA:HA	2.19	0.42
29:A:414[B]:PL9:H121	29:A:414[B]:PL9:HC8	1.69	0.42
23:C:503:CLA:HBD	23:C:503:CLA:HAA1	2.02	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.01	0.42
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.18	0.42
23:b:614:CLA:H62	23:b:614:CLA:H41	1.73	0.42
4:d:186[B]:GLN:HB2	23:d:402[B]:CLA:HBC1	2.02	0.42
6:f:21:VAL:O	6:f:25:THR:HG23	2.20	0.42
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.02	0.42
4:d:20:ASP:O	4:d:24:ARG:HG2	2.20	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
31:A:419:LMT:H6'2	31:A:419:LMT:O3'	2.20	0.42
2:B:357[A]:ARG:HH12	27:B:624:GOL:C3	2.32	0.42
32:D:409[A]:LHG:H302	32:D:409[A]:LHG:H332	1.81	0.42
25:T:101:BCR:H19C	25:b:618:BCR:H363	2.02	0.42
32:d:407[B]:LHG:H242	32:d:407[B]:LHG:H272	1.88	0.42
10:k:24:VAL:HG22	18:y:25:ILE:HD13	2.02	0.42
1:A:131:TRP:CD2	1:A:131:TRP:C	2.96	0.42
25:B:617:BCR:H24C	25:B:617:BCR:H371	1.76	0.42
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.01	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.01	0.42
2:b:149[B]:LEU:HD21	23:b:604:CLA:H171	2.02	0.42
3:c:165:LEU:HD23	3:c:165:LEU:HA	1.90	0.42
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.41
34:B:622:HTG:H4'1	31:B:630:LMT:H52	2.02	0.41
3:C:443[A]:TRP:CE2	23:C:509:CLA:HMD2	2.55	0.41
19:Z:31:GLN:CD	19:Z:31:GLN:H	2.28	0.41
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	2.01	0.41
23:a:405[B]:CLA:H203	23:a:405[B]:CLA:H162	1.77	0.41
23:c:506:CLA:H192	23:c:506:CLA:H162	1.92	0.41
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.02	0.41
20:R:10:LEU:O	20:R:14:LEU:HG	2.21	0.41
29:A:414[A]:PL9:H503	26:X:101:SQD:H341	2.01	0.41
23:B:615:CLA:H91	23:B:615:CLA:H112	1.91	0.41
3:C:148:GLY:O	3:C:156:LYS:NZ	2.46	0.41
32:a:420[A]:LHG:H241	32:a:420[A]:LHG:HC61	1.90	0.41
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	2.01	0.41
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.03	0.41
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.02	0.41
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.92	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:504:CLA:HBB2	23:C:513:CLA:H92	2.01	0.41
1:a:307:ILE:HD13	1:a:307:ILE:HG21	1.82	0.41
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.02	0.41
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	2.01	0.41
23:c:505:CLA:H92	23:c:505:CLA:H61	1.82	0.41
16:v:45[B]:ILE:HD13	27:v:202[B]:GOL:H11	2.02	0.41
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.86	0.41
23:C:510:CLA:H192	23:C:510:CLA:H162	1.83	0.41
4:D:24:ARG:NH2	26:X:101:SQD:O4	2.54	0.41
9:J:3:GLU:HB3	9:J:6:ARG:HH12	1.85	0.41
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:CBB	2.48	0.41
3:c:462[B]:GLU:HB2	42:c:700:HOH:O	2.20	0.41
23:c:513:CLA:H3A	23:c:513:CLA:HBA2	1.74	0.41
29:A:414[A]:PL9:H43	29:A:414[A]:PL9:H471	1.69	0.41
2:B:160:GLY:HA2	2:B:163:GLY:O	2.19	0.41
23:B:613:CLA:H162	23:B:613:CLA:H121	1.60	0.41
3:c:238:ILE:O	3:c:242:LEU:HG	2.20	0.41
32:d:407[A]:LHG:H131	32:d:407[A]:LHG:H102	1.91	0.41
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.18	0.41
13:o:120:PHE:CD1	13:o:235:ILE:HD13	2.56	0.41
23:A:404[B]:CLA:HBD	23:A:405[B]:CLA:HAC2	2.03	0.41
23:C:509:CLA:HBC2	32:D:409[B]:LHG:H351	2.03	0.41
23:C:511:CLA:HBA1	23:C:511:CLA:H3A	1.87	0.41
23:a:407[B]:CLA:H143	23:a:407[B]:CLA:H161	1.90	0.41
27:a:418:GOL:H12	42:t:201:HOH:O	2.20	0.41
25:c:516:BCR:H11C	25:c:516:BCR:H341	1.95	0.41
6:f:28:VAL:HB	6:f:29:PRO:HD3	2.03	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.90	0.41
1:A:60[B]:ILE:HD12	1:A:84[B]:PRO:HD2	2.03	0.41
23:C:514:CLA:H161	33:C:521:LMG:H421	2.03	0.41
13:O:121:THR:OG1	13:O:123:LYS:HG3	2.20	0.41
27:a:419:GOL:H31	12:m:1:FME:HG2	2.03	0.41
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.88	0.41
26:A:410[B]:SQD:H361	10:K:34:ALA:HA	2.03	0.41
2:B:491[A]:VAL:HG12	4:D:136[A]:VAL:HG13	2.03	0.41
31:B:628:LMT:H91	31:B:628:LMT:H62	1.57	0.41
35:C:518[A]:DGD:HAE2	35:C:518[A]:DGD:HA81	1.91	0.41
4:D:15:PHE:H	34:D:412:HTG:H61	1.85	0.41
23:D:404[B]:CLA:HAA2	23:D:404[B]:CLA:HBD	2.03	0.41
5:E:57:ALA:HB3	5:E:60:GLN:HG2	2.03	0.41
31:M:101:LMT:H6'2	12:m:32:GLN:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.03	0.41
25:t:102:BCR:H24C	25:t:102:BCR:H371	1.93	0.41
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.51	0.41
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:H121	1.79	0.41
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	2.03	0.41
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.85	0.41
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.56	0.41
33:a:417:LMG:H172	33:a:417:LMG:H201	1.83	0.41
2:b:247:PHE:CE2	23:b:602:CLA:H102	2.56	0.41
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.02	0.41
25:b:618:BCR:H361	25:b:618:BCR:H20C	1.85	0.41
26:b:620:SQD:H462	26:b:620:SQD:H1	2.03	0.41
23:C:505:CLA:H62	23:C:505:CLA:H41	1.73	0.40
27:D:403:GOL:H12	14:T:2:GLU:OE1	2.21	0.40
13:O:137:THR:C	13:O:139:SER:H	2.29	0.40
32:a:420[A]:LHG:H142	32:a:420[A]:LHG:H172	1.83	0.40
23:b:616:CLA:H91	25:b:619:BCR:H14C	2.03	0.40
23:c:512:CLA:H141	23:c:512:CLA:H162	1.89	0.40
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	2.04	0.40
23:c:514:CLA:NB	25:c:515:BCR:H383	2.36	0.40
4:d:343:GLU:HG2	16:v:135[A]:VAL:HG11	2.03	0.40
25:t:102:BCR:H331	25:t:102:BCR:HC7	1.50	0.40
15:u:42:TYR:HA	15:u:43:PRO:HA	1.88	0.40
26:B:620:SQD:H332	26:B:620:SQD:H301	1.92	0.40
23:C:507:CLA:HBA1	23:C:507:CLA:H3A	1.83	0.40
2:b:224:ARG:NH2	31:b:621:LMT:H1'	2.35	0.40
23:b:605:CLA:H62	23:b:605:CLA:H41	1.65	0.40
3:c:318:LEU:C	3:c:318:LEU:HD23	2.46	0.40
32:d:407[A]:LHG:H242	32:d:407[A]:LHG:H272	1.92	0.40
31:t:101:LMT:H81	31:t:101:LMT:H112	1.77	0.40
33:B:621:LMG:H141	33:B:621:LMG:H112	1.80	0.40
6:F:21:VAL:O	6:F:25:THR:HG23	2.21	0.40
25:A:409:BCR:H11C	25:A:409:BCR:H341	1.87	0.40
23:C:503:CLA:H141	23:C:503:CLA:H161	1.87	0.40
16:V:57:GLU:H	16:V:57:GLU:CD	2.29	0.40
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CZ3	2.55	0.40
25:a:410:BCR:H24C	25:a:410:BCR:H371	1.74	0.40
3:c:344[A]:SER:O	13:o:75:THR:HG22	2.21	0.40
35:c:518[A]:DGD:HBF2	35:c:518[A]:DGD:HBE1	1.91	0.40
25:d:404:BCR:H11C	25:d:404:BCR:H341	1.99	0.40
10:k:19:ASP:OD2	42:k:201:HOH:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PHE:CE2	23:B:602:CLA:H102	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	31
1	a	552/344 (160%)	545 (99%)	5 (1%)	2 (0%)	30	31
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	511 (98%)	10 (2%)	0	100	100
3	C	546/455 (120%)	539 (99%)	6 (1%)	1 (0%)	43	50
3	c	553/455 (122%)	542 (98%)	10 (2%)	1 (0%)	43	50
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	444 (98%)	10 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	7	4
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	31
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	98/104 (94%)	93 (95%)	5 (5%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100
17	X	37/40 (92%)	37 (100%)	0	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	3
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6040 (98%)	120 (2%)	11 (0%)	43	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	I	36	ASP
3	C	416	SER
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
13	O	26	ALA
7	h	63	LYS
1	a	259[A]	ILE
1	a	259[B]	ILE
1	A	259[A]	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	259[B]	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/279 (159%)	440 (99%)	4 (1%)	70	79
1	a	443/279 (159%)	442 (100%)	1 (0%)	87	92
2	B	421/403 (104%)	418 (99%)	3 (1%)	76	82
2	b	420/403 (104%)	410 (98%)	10 (2%)	43	54
3	C	430/356 (121%)	419 (97%)	11 (3%)	40	50
3	c	436/356 (122%)	429 (98%)	7 (2%)	55	66
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	80
4	d	369/277 (133%)	363 (98%)	6 (2%)	55	66
5	E	72/73 (99%)	69 (96%)	3 (4%)	26	31
5	e	72/73 (99%)	70 (97%)	2 (3%)	38	48
6	F	28/38 (74%)	28 (100%)	0	100	100
6	f	26/38 (68%)	26 (100%)	0	100	100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30	37
7	h	55/54 (102%)	55 (100%)	0	100	100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	47
9	J	26/27 (96%)	25 (96%)	1 (4%)	29	36
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	5
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	36 (100%)	0	100	100
12	M	30/32 (94%)	28 (93%)	2 (7%)	15	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	16
13	O	216/207 (104%)	208 (96%)	8 (4%)	30	37
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	42
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	3
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	55
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	55
16	V	123/117 (105%)	123 (100%)	0	100	100
16	v	123/117 (105%)	120 (98%)	3 (2%)	43	54
17	X	32/33 (97%)	32 (100%)	0	100	100
17	x	31/33 (94%)	31 (100%)	0	100	100
18	Y	22/23 (96%)	22 (100%)	0	100	100
18	y	22/23 (96%)	18 (82%)	4 (18%)	2	0
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18	19
19	z	52/52 (100%)	45 (86%)	7 (14%)	4	2
20	R	29/29 (100%)	26 (90%)	3 (10%)	7	5
All	All	5103/4403 (116%)	4992 (98%)	111 (2%)	45	56

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
1	A	244[A]	GLU
1	A	244[B]	GLU
2	B	294	SER
2	B	389	LYS
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	30	SER
3	C	142	GLU
3	C	240	ILE
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	315[B]	MET
3	C	462	GLU
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	4	THR
5	E	54	SER
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
13	O	4	THR
13	O	37	THR
13	O	49	THR
13	O	55	GLU
13	O	87	VAL
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
1	a	13	LEU
2	b	128	THR
2	b	161	LEU
2	b	298	LEU
2	b	315	ILE
2	b	362	PHE
2	b	472	ARG
2	b	486[A]	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	486[B]	LEU
2	b	491[A]	VAL
2	b	491[B]	VAL
3	c	19	ASN
3	c	142	GLU
3	c	152	LYS
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	230[A]	SER
4	d	230[B]	SER
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	11	SER
5	e	71	GLU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
18	y	18	VAL
18	y	19	ILE
18	y	30	ILE
18	y	45	ASN
19	Z	3	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Z	20	VAL
19	Z	31	GLN
20	R	4	ARG
20	R	23	ILE
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	21	ILE
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
5	E	60	GLN
11	L	8	GLN
13	O	231	HIS
1	a	12	ASN
2	b	14	ASN
2	b	331	ASN
3	c	19	ASN
3	c	415	ASN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN

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	$\# Z > 2$
12	FME	m	1	12	8,9,10	0.53	0	8,9,11	1.39	2 (25%)
8	FME	i	1	8	8,9,10	0.72	0	8,9,11	1.20	1 (12%)
12	FME	M	1	12	8,9,10	0.72	0	8,9,11	1.18	1 (12%)
8	FME	I	1	8	8,9,10	0.66	0	8,9,11	1.33	2 (25%)
14	FME	t	1	14	8,9,10	0.72	0	8,9,11	1.70	2 (25%)
14	FME	T	1	14	8,9,10	0.59	0	8,9,11	1.57	2 (25%)

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

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

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	O-C-CA	-2.79	117.60	124.77
14	t	1	FME	CA-N-CN	-2.68	118.70	122.82
14	T	1	FME	CB-CA-N	-2.50	105.96	110.52
12	M	1	FME	O-C-CA	-2.33	118.77	124.77
12	m	1	FME	O1-CN-N	-2.32	119.32	125.32
8	I	1	FME	O-C-CA	-2.27	118.94	124.77
8	I	1	FME	CA-N-CN	-2.26	119.34	122.82
12	m	1	FME	O-C-CA	-2.22	119.07	124.77
14	T	1	FME	CG-CB-CA	2.13	119.38	112.87
8	i	1	FME	O-C-CA	-2.08	119.42	124.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	3	0
12	M	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 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	$\# Z > 2$
31	LMT	b	627	-	25,25,36	0.86	0	30,30,47	1.15	2 (6%)
23	CLA	c	514	-	69,73,73	2.09	21 (30%)	82,113,113	2.73	31 (37%)
29	PL9	D	407[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)
34	HTG	D	412	-	16,16,19	0.94	1 (6%)	20,21,24	1.36	1 (5%)
35	DGD	c	519	-	63,63,67	0.86	4 (6%)	77,77,81	1.06	4 (5%)
31	LMT	t	101	-	26,26,36	0.90	1 (3%)	31,31,47	1.30	2 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	K	103	-	41,41,41	1.02	1 (2%)	56,56,56	1.78	13 (23%)
23	CLA	b	610	42	69,73,73	2.04	20 (28%)	82,113,113	2.83	34 (41%)
23	CLA	A	406[B]	42	69,73,73	2.07	19 (27%)	82,113,113	2.70	33 (40%)
32	LHG	d	413[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
24	PHO	a	416[B]	-	58,69,69	2.80	13 (22%)	55,99,99	2.90	15 (27%)
27	GOL	D	403	-	5,5,5	1.58	2 (40%)	5,5,5	1.04	1 (20%)
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.44	7 (15%)
23	CLA	C	512	3	69,73,73	2.01	20 (28%)	82,113,113	2.62	30 (36%)
26	SQD	A	410[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
31	LMT	m	103	-	36,36,36	1.01	3 (8%)	47,47,47	1.11	3 (6%)
38	BCT	D	402[B]	37	3,3,3	0.53	0	2,3,3	0.90	0
32	LHG	d	406[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
35	DGD	C	519	-	63,63,67	0.87	3 (4%)	77,77,81	1.04	5 (6%)
29	PL9	a	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
27	GOL	C	523[A]	-	5,5,5	1.16	0	5,5,5	0.94	0
26	SQD	a	411[B]	-	52,54,54	0.88	2 (3%)	62,65,65	1.62	10 (16%)
24	PHO	a	408[A]	-	58,69,69	2.77	13 (22%)	55,99,99	2.94	14 (25%)
34	HTG	B	622	-	19,19,19	1.05	2 (10%)	23,24,24	1.61	5 (21%)
23	CLA	D	404[B]	-	69,73,73	2.03	19 (27%)	82,113,113	2.71	29 (35%)
39	HEM	f	101	6,5	50,50,50	1.48	6 (12%)	67,82,82	1.65	16 (23%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.53	7 (11%)
31	LMT	B	631	-	25,25,36	0.88	2 (8%)	30,30,47	1.21	3 (10%)
25	BCR	c	515	-	41,41,41	1.00	1 (2%)	56,56,56	1.58	14 (25%)
27	GOL	l	102[B]	-	5,5,5	0.99	0	5,5,5	1.03	0
23	CLA	c	513	-	69,73,73	2.05	19 (27%)	82,113,113	2.68	34 (41%)
25	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.49	10 (17%)
23	CLA	c	512	3	69,73,73	2.04	21 (30%)	82,113,113	2.70	31 (37%)
23	CLA	c	510	-	69,73,73	2.01	20 (28%)	82,113,113	2.67	31 (37%)
32	LHG	D	408[A]	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.38	9 (16%)
31	LMT	F	101	-	36,36,36	1.04	1 (2%)	47,47,47	1.05	3 (6%)
41	HEC	v	201	16	46,50,50	1.88	5 (10%)	58,82,82	1.98	11 (18%)
32	LHG	d	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.97	3 (5%)
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.09	4 (5%)
39	HEM	F	102	6,5	50,50,50	1.54	8 (16%)	67,82,82	1.79	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	C	506	-	69,73,73	2.00	19 (27%)	82,113,113	2.71	30 (36%)
23	CLA	b	616	-	69,73,73	1.99	19 (27%)	82,113,113	2.80	33 (40%)
25	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.38	7 (12%)
31	LMT	A	419	-	36,36,36	1.00	2 (5%)	47,47,47	1.18	4 (8%)
31	LMT	B	628	-	36,36,36	1.15	3 (8%)	47,47,47	1.34	6 (12%)
23	CLA	B	609	-	69,73,73	2.03	18 (26%)	82,113,113	2.64	31 (37%)
25	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.54	9 (16%)
28	OEX	a	413[A]	42,3,1	0,15,15	-	-	-	-	-
32	LHG	D	409[B]	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	4 (7%)
35	DGD	h	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.10	8 (10%)
35	DGD	C	518[B]	-	63,63,67	0.90	3 (4%)	77,77,81	1.00	4 (5%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.47	6 (10%)
25	BCR	H	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	9 (16%)
25	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
23	CLA	a	406[B]	42	69,73,73	1.98	16 (23%)	82,113,113	2.69	31 (37%)
34	HTG	V	202	-	11,11,19	0.33	0	15,15,24	1.29	1 (6%)
27	GOL	A	411	-	5,5,5	1.09	0	5,5,5	0.96	0
38	BCT	d	401[B]	37	3,3,3	0.51	0	2,3,3	0.87	0
23	CLA	B	610	42	69,73,73	1.99	19 (27%)	82,113,113	2.77	34 (41%)
23	CLA	C	503	-	69,73,73	2.03	19 (27%)	82,113,113	2.55	31 (37%)
23	CLA	c	504	-	69,73,73	2.03	19 (27%)	82,113,113	2.72	29 (35%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	9 (16%)
23	CLA	C	502	-	69,73,73	1.96	19 (27%)	82,113,113	2.71	33 (40%)
21	OEY	A	401[B]	42,3,1	0,16,16	-	-	-	-	-
23	CLA	d	402[B]	-	69,73,73	2.00	19 (27%)	82,113,113	2.71	29 (35%)
23	CLA	B	602	-	69,73,73	2.01	20 (28%)	82,113,113	2.75	30 (36%)
26	SQD	A	410[B]	-	52,54,54	0.87	2 (3%)	62,65,65	1.65	10 (16%)
23	CLA	b	609	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	33 (40%)
33	LMG	d	411	40	51,51,55	0.92	2 (3%)	59,59,63	1.19	6 (10%)
41	HEC	V	201	16	46,50,50	1.90	5 (10%)	58,82,82	1.84	8 (13%)
31	LMT	c	501	-	36,36,36	0.96	0	47,47,47	1.06	2 (4%)
25	BCR	b	618	-	41,41,41	1.02	1 (2%)	56,56,56	1.24	7 (12%)
23	CLA	A	405[B]	42	69,73,73	2.03	18 (26%)	82,113,113	2.69	35 (42%)
27	GOL	B	624	-	5,5,5	0.81	0	5,5,5	1.21	1 (20%)
27	GOL	D	414	-	5,5,5	1.47	1 (20%)	5,5,5	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	LHG	A	418[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
27	GOL	b	624	-	5,5,5	1.32	1 (20%)	5,5,5	0.79	0
25	BCR	C	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.43	7 (12%)
31	LMT	M	102	-	36,36,36	1.04	3 (8%)	47,47,47	1.07	2 (4%)
23	CLA	C	507	-	69,73,73	2.03	21 (30%)	82,113,113	2.72	33 (40%)
23	CLA	b	611	-	69,73,73	1.91	18 (26%)	82,113,113	2.77	29 (35%)
23	CLA	B	607	42	69,73,73	2.00	18 (26%)	82,113,113	2.69	31 (37%)
27	GOL	c	527	-	5,5,5	1.19	0	5,5,5	0.99	0
27	GOL	v	202[A]	-	5,5,5	1.26	0	5,5,5	0.88	0
33	LMG	a	417	-	51,51,55	0.92	2 (3%)	59,59,63	1.25	6 (10%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.38	4 (17%)
23	CLA	c	507	-	69,73,73	2.01	19 (27%)	82,113,113	2.73	31 (37%)
27	GOL	O	303	-	5,5,5	0.93	0	5,5,5	1.17	1 (20%)
23	CLA	C	504	-	69,73,73	1.96	19 (27%)	82,113,113	2.73	29 (35%)
24	PHO	A	407[A]	-	58,69,69	2.66	12 (20%)	55,99,99	2.93	14 (25%)
28	OEX	A	413[A]	42,3,1	0,15,15	-	-	-	-	-
29	PL9	d	405[A]	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
32	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.13	4 (7%)
32	LHG	b	629[A]	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)
34	HTG	b	625	-	19,19,19	0.92	2 (10%)	23,24,24	1.42	2 (8%)
23	CLA	a	409	-	69,73,73	1.91	19 (27%)	82,113,113	2.85	34 (41%)
23	CLA	B	614	-	69,73,73	2.01	18 (26%)	82,113,113	2.87	35 (42%)
26	SQD	X	101	-	41,43,54	1.16	3 (7%)	51,54,65	2.13	13 (25%)
23	CLA	b	606	-	69,73,73	2.00	19 (27%)	82,113,113	2.76	31 (37%)
23	CLA	B	613	-	69,73,73	1.99	19 (27%)	82,113,113	2.68	32 (39%)
33	LMG	c	520	-	51,51,55	0.91	2 (3%)	59,59,63	1.12	5 (8%)
29	PL9	A	414[A]	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
23	CLA	b	602	-	69,73,73	2.04	18 (26%)	82,113,113	2.83	36 (43%)
23	CLA	a	405[A]	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	34 (41%)
23	CLA	b	607	42	69,73,73	1.91	20 (28%)	82,113,113	2.65	31 (37%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.37	7 (11%)
24	PHO	A	416[B]	-	58,69,69	2.81	15 (25%)	55,99,99	3.00	18 (32%)
23	CLA	C	508	42	69,73,73	1.95	19 (27%)	82,113,113	2.72	31 (37%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	V	203[B]	-	5,5,5	1.11	0	5,5,5	1.02	0
23	CLA	d	403	-	69,73,73	2.02	19 (27%)	82,113,113	2.70	32 (39%)
23	CLA	a	407[B]	42	69,73,73	2.02	19 (27%)	82,113,113	2.68	32 (39%)
32	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.13	4 (9%)
23	CLA	A	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
27	GOL	c	526[A]	-	5,5,5	1.04	0	5,5,5	1.05	0
35	DGD	C	517[A]	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
32	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	B	608	-	69,73,73	1.86	18 (26%)	82,113,113	2.69	36 (43%)
25	BCR	B	617	-	41,41,41	1.14	1 (2%)	56,56,56	1.24	7 (12%)
34	HTG	C	522	-	19,19,19	0.82	1 (5%)	23,24,24	1.24	1 (4%)
23	CLA	b	608	-	69,73,73	1.98	20 (28%)	82,113,113	2.74	33 (40%)
27	GOL	B	629	-	5,5,5	1.03	0	5,5,5	1.10	0
33	LMG	C	521	-	51,51,55	1.09	3 (5%)	59,59,63	1.38	6 (10%)
23	CLA	C	513	-	69,73,73	2.05	19 (27%)	82,113,113	2.72	33 (40%)
27	GOL	a	418	-	5,5,5	1.22	1 (20%)	5,5,5	1.07	1 (20%)
29	PL9	D	407[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.56	15 (22%)
25	BCR	d	404	-	41,41,41	1.15	2 (4%)	56,56,56	1.99	17 (30%)
34	HTG	b	622	-	19,19,19	1.14	2 (10%)	23,24,24	1.89	7 (30%)
23	CLA	A	406[A]	42	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
32	LHG	d	413[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.13	5 (9%)
24	PHO	a	416[A]	-	58,69,69	2.79	14 (24%)	55,99,99	3.05	17 (30%)
23	CLA	b	613	-	69,73,73	1.98	19 (27%)	82,113,113	2.64	30 (36%)
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.46	9 (16%)
27	GOL	o	302	-	5,5,5	1.09	0	5,5,5	1.06	0
31	LMT	B	630	-	36,36,36	0.99	1 (2%)	47,47,47	1.16	4 (8%)
25	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.43	10 (17%)
32	LHG	A	418[B]	-	48,48,48	0.90	3 (6%)	51,54,54	1.18	6 (11%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.06	4 (8%)
23	CLA	C	514	-	69,73,73	2.03	19 (27%)	82,113,113	2.67	30 (36%)
38	BCT	D	402[A]	37	3,3,3	0.55	0	2,3,3	1.29	0
31	LMT	A	417	-	36,36,36	0.93	2 (5%)	47,47,47	1.08	4 (8%)
23	CLA	D	405	-	69,73,73	2.08	18 (26%)	82,113,113	2.64	34 (41%)
32	LHG	d	406[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
25	BCR	a	410	-	41,41,41	1.10	1 (2%)	56,56,56	1.34	9 (16%)
34	HTG	c	522	-	19,19,19	0.87	1 (5%)	23,24,24	1.33	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	GOL	v	202[B]	-	5,5,5	1.07	0	5,5,5	1.01	0
27	GOL	C	523[B]	-	5,5,5	1.11	0	5,5,5	0.93	0
29	PL9	a	414[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.97	22 (32%)
26	SQD	a	411[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)
24	PHO	a	408[B]	-	58,69,69	2.72	13 (22%)	55,99,99	2.82	17 (30%)
25	BCR	T	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.70	14 (25%)
33	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.30	5 (8%)
23	CLA	c	506	-	69,73,73	1.99	18 (26%)	82,113,113	2.64	29 (35%)
33	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.10	3 (5%)
23	CLA	D	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	34 (41%)
23	CLA	b	601	42	69,73,73	2.06	20 (28%)	82,113,113	2.65	28 (34%)
23	CLA	c	509	-	69,73,73	2.09	20 (28%)	82,113,113	2.66	27 (32%)
27	GOL	d	412	-	5,5,5	1.34	1 (20%)	5,5,5	1.08	0
27	GOL	l	102[A]	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
35	DGD	c	518[B]	-	63,63,67	0.89	2 (3%)	77,77,81	0.95	4 (5%)
32	LHG	D	408[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.02	4 (7%)
31	LMT	M	101	-	36,36,36	1.11	3 (8%)	47,47,47	1.24	5 (10%)
23	CLA	b	605	-	69,73,73	1.94	19 (27%)	82,113,113	2.88	29 (35%)
23	CLA	B	604	-	69,73,73	2.02	21 (30%)	82,113,113	2.57	28 (34%)
23	CLA	B	612	-	69,73,73	2.03	18 (26%)	82,113,113	2.66	31 (37%)
35	DGD	c	517[A]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
23	CLA	b	604	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	28 (34%)
26	SQD	b	620	-	52,54,54	1.00	2 (3%)	62,65,65	1.70	11 (17%)
31	LMT	e	101	-	36,36,36	0.98	1 (2%)	47,47,47	1.02	1 (2%)
23	CLA	c	505	42	69,73,73	2.02	20 (28%)	82,113,113	2.63	30 (36%)
23	CLA	c	503	-	69,73,73	1.92	16 (23%)	82,113,113	2.58	28 (34%)
33	LMG	c	521	-	51,51,55	1.00	2 (3%)	59,59,63	1.37	6 (10%)
34	HTG	d	410	-	16,16,19	0.83	1 (6%)	20,21,24	1.36	1 (5%)
23	CLA	b	612	-	69,73,73	1.96	20 (28%)	82,113,113	2.64	32 (39%)
23	CLA	C	509	-	69,73,73	2.04	20 (28%)	82,113,113	2.64	28 (34%)
34	HTG	B	623	-	19,19,19	0.77	1 (5%)	23,24,24	1.29	1 (4%)
32	LHG	D	409[A]	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)
23	CLA	A	408	-	69,73,73	1.99	21 (30%)	82,113,113	2.77	37 (45%)
23	CLA	B	603	-	69,73,73	1.98	19 (27%)	82,113,113	2.80	32 (39%)
26	SQD	A	412	-	52,54,54	1.01	2 (3%)	62,65,65	1.24	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	D	406	-	41,41,41	1.12	1 (2%)	56,56,56	1.86	16 (28%)
23	CLA	c	511	-	69,73,73	2.01	20 (28%)	82,113,113	2.67	34 (41%)
23	CLA	C	510	-	69,73,73	1.99	20 (28%)	82,113,113	2.68	29 (35%)
35	DGD	C	518[A]	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)
25	BCR	K	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	12 (21%)
23	CLA	a	406[A]	42	69,73,73	2.01	17 (24%)	82,113,113	2.72	31 (37%)
23	CLA	c	502	-	69,73,73	1.99	21 (30%)	82,113,113	2.69	31 (37%)
38	BCT	d	401[A]	37	3,3,3	0.49	0	2,3,3	1.49	0
23	CLA	B	606	-	69,73,73	1.94	21 (30%)	82,113,113	2.78	34 (41%)
23	CLA	b	603	-	69,73,73	1.95	19 (27%)	82,113,113	2.77	33 (40%)
23	CLA	d	402[A]	-	69,73,73	1.94	19 (27%)	82,113,113	2.64	33 (40%)
23	CLA	B	601	42	69,73,73	2.05	20 (28%)	82,113,113	2.69	29 (35%)
31	LMT	b	621	-	25,25,36	0.96	1 (4%)	30,30,47	1.21	2 (6%)
23	CLA	b	615	-	69,73,73	1.96	18 (26%)	82,113,113	2.63	33 (40%)
26	SQD	a	412	-	52,54,54	1.03	3 (5%)	62,65,65	1.18	8 (12%)
26	SQD	f	102	-	41,43,54	1.17	2 (4%)	51,54,65	1.47	10 (19%)
21	OEY	a	401[B]	42,3,1	0,16,16	-	-	-	-	-
23	CLA	B	611	-	69,73,73	2.58	20 (28%)	82,113,113	3.70	34 (41%)
23	CLA	A	405[A]	42	69,73,73	2.00	18 (26%)	82,113,113	2.70	35 (42%)
23	CLA	C	505	42	69,73,73	1.96	18 (26%)	82,113,113	2.65	28 (34%)
27	GOL	a	419	-	5,5,5	1.29	1 (20%)	5,5,5	1.05	1 (20%)
27	GOL	b	628	-	5,5,5	0.54	0	5,5,5	1.54	1 (20%)
24	PHO	A	407[B]	-	58,69,69	2.74	13 (22%)	55,99,99	2.83	13 (23%)
32	LHG	L	101[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
29	PL9	d	405[B]	-	55,55,55	0.69	1 (1%)	68,69,69	1.63	17 (25%)
32	LHG	b	629[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.05	5 (9%)
23	CLA	C	511	-	69,73,73	2.00	20 (28%)	82,113,113	2.81	33 (40%)
27	GOL	B	627	-	5,5,5	0.98	0	5,5,5	1.07	1 (20%)
33	LMG	D	413	40	51,51,55	0.84	3 (5%)	59,59,63	1.08	3 (5%)
34	HTG	b	623	-	19,19,19	0.98	1 (5%)	23,24,24	1.64	2 (8%)
27	GOL	o	303	-	5,5,5	1.18	1 (20%)	5,5,5	1.13	0
29	PL9	A	414[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.97	23 (33%)
23	CLA	B	605	-	69,73,73	2.05	19 (27%)	82,113,113	2.85	31 (37%)
23	CLA	c	508	42	69,73,73	1.99	19 (27%)	82,113,113	2.71	31 (37%)
23	CLA	B	615	-	69,73,73	2.04	20 (28%)	82,113,113	2.75	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	616	-	69,73,73	1.99	20 (28%)	82,113,113	2.73	27 (32%)
23	CLA	a	405[B]	-	69,73,73	2.02	18 (26%)	82,113,113	2.78	35 (42%)
26	SQD	B	620	-	52,54,54	1.03	3 (5%)	62,65,65	1.79	13 (20%)
24	PHO	A	416[A]	-	58,69,69	2.81	14 (24%)	55,99,99	2.93	16 (29%)
32	LHG	d	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	b	614	-	69,73,73	1.99	20 (28%)	82,113,113	2.84	32 (39%)
27	GOL	O	302	-	5,5,5	1.04	0	5,5,5	0.93	0
27	GOL	V	203[A]	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
23	CLA	a	407[A]	42	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
32	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
23	CLA	A	404[B]	-	69,73,73	2.04	19 (27%)	82,113,113	2.75	34 (41%)
27	GOL	c	526[B]	-	5,5,5	1.00	0	5,5,5	1.03	0
35	DGD	C	517[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.06	6 (7%)
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.36	10 (17%)
32	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
35	DGD	H	102	-	63,63,67	0.90	4 (6%)	77,77,81	1.02	7 (9%)

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
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	c	514	-	1/1/15/20	12/39/115/115	-
29	PL9	D	407[A]	-	-	6/53/73/73	0/1/1/1
34	HTG	D	412	-	-	3/7/27/30	0/1/1/1
35	DGD	c	519	-	-	7/51/91/95	0/2/2/2
31	LMT	t	101	-	-	7/17/38/61	0/1/1/2
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
23	CLA	b	610	42	1/1/15/20	8/39/115/115	-
23	CLA	A	406[B]	42	-	4/39/115/115	-
32	LHG	d	413[A]	-	-	15/53/53/53	-
24	PHO	a	416[B]	-	-	1/37/103/103	0/5/6/6
27	GOL	D	403	-	-	1/4/4/4	-
33	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	C	512	3	1/1/15/20	4/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
31	LMT	m	103	-	-	6/21/61/61	0/2/2/2
32	LHG	d	406[B]	-	-	16/53/53/53	-
35	DGD	C	519	-	-	20/51/91/95	0/2/2/2
29	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
27	GOL	C	523[A]	-	-	0/4/4/4	-
26	SQD	a	411[B]	-	-	8/49/69/69	0/1/1/1
24	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	D	404[B]	-	1/1/15/20	2/39/115/115	-
39	HEM	f	101	6,5	-	6/14/54/54	-
33	LMG	C	501	-	-	11/46/66/70	0/1/1/1
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
27	GOL	l	102[B]	-	-	2/4/4/4	-
23	CLA	c	513	-	1/1/15/20	10/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
23	CLA	c	512	3	1/1/15/20	8/39/115/115	-
23	CLA	c	510	-	1/1/15/20	15/39/115/115	-
32	LHG	D	408[A]	-	-	17/53/53/53	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
41	HEC	v	201	16	-	6/14/54/54	-
32	LHG	d	407[B]	-	-	9/53/53/53	-
35	DGD	c	517[B]	-	-	17/51/91/95	0/2/2/2
39	HEM	F	102	6,5	-	4/14/54/54	-
23	CLA	C	506	-	1/1/15/20	6/39/115/115	-
23	CLA	b	616	-	1/1/15/20	8/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
31	LMT	A	419	-	-	16/21/61/61	0/2/2/2
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
23	CLA	B	609	-	1/1/15/20	0/39/115/115	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
32	LHG	D	409[B]	-	-	13/53/53/53	-
35	DGD	h	102	-	-	14/51/91/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	518[B]	-	-	11/51/91/95	0/2/2/2
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	H	101	-	-	3/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	a	406[B]	42	1/1/15/20	3/39/115/115	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
27	GOL	A	411	-	-	2/4/4/4	-
23	CLA	B	610	42	1/1/15/20	9/39/115/115	-
23	CLA	c	504	-	1/1/15/20	1/39/115/115	-
23	CLA	C	503	-	-	9/39/115/115	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	C	502	-	1/1/15/20	3/39/115/115	-
23	CLA	d	402[B]	-	1/1/15/20	4/39/115/115	-
23	CLA	B	602	-	1/1/15/20	10/39/115/115	-
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
23	CLA	b	609	-	1/1/15/20	4/39/115/115	-
33	LMG	d	411	40	-	10/46/66/70	0/1/1/1
41	HEC	V	201	16	-	6/14/54/54	-
31	LMT	c	501	-	-	10/21/61/61	0/2/2/2
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	A	405[B]	42	1/1/15/20	3/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
27	GOL	D	414	-	-	4/4/4/4	-
32	LHG	A	418[A]	-	-	14/53/53/53	-
27	GOL	b	624	-	-	2/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
31	LMT	M	102	-	-	8/21/61/61	0/2/2/2
23	CLA	C	507	-	1/1/15/20	12/39/115/115	-
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
23	CLA	B	607	42	1/1/15/20	1/39/115/115	-
27	GOL	c	527	-	-	3/4/4/4	-
27	GOL	v	202[A]	-	-	2/4/4/4	-
33	LMG	a	417	-	-	12/46/66/70	0/1/1/1
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
23	CLA	c	507	-	1/1/15/20	8/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	504	-	-	0/39/115/115	-
24	PHO	A	407[A]	-	-	0/37/103/103	0/5/6/6
29	PL9	d	405[A]	-	-	6/53/73/73	0/1/1/1
32	LHG	L	101[B]	-	-	17/53/53/53	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
32	LHG	b	629[A]	-	-	15/53/53/53	-
23	CLA	a	409	-	1/1/15/20	9/39/115/115	-
23	CLA	B	614	-	1/1/15/20	12/39/115/115	-
26	SQD	X	101	-	-	13/38/58/69	0/1/1/1
23	CLA	b	606	-	1/1/15/20	12/39/115/115	-
23	CLA	B	613	-	1/1/15/20	7/39/115/115	-
33	LMG	c	520	-	-	13/46/66/70	0/1/1/1
29	PL9	A	414[A]	-	-	14/53/73/73	0/1/1/1
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
23	CLA	a	405[A]	-	1/1/15/20	4/39/115/115	-
23	CLA	b	607	42	1/1/15/20	2/39/115/115	-
33	LMG	m	101	-	-	13/46/66/70	0/1/1/1
24	PHO	A	416[B]	-	-	1/37/103/103	0/5/6/6
23	CLA	C	508	42	1/1/15/20	10/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	d	403	-	1/1/15/20	8/39/115/115	-
23	CLA	a	407[B]	42	-	5/39/115/115	-
32	LHG	E	101[B]	-	-	19/46/46/53	-
23	CLA	A	404[A]	-	1/1/15/20	3/39/115/115	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
35	DGD	C	517[A]	-	-	15/51/91/95	0/2/2/2
32	LHG	a	420[B]	-	-	16/46/46/53	-
23	CLA	B	608	-	-	3/39/115/115	-
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
34	HTG	C	522	-	-	1/10/30/30	0/1/1/1
23	CLA	b	608	-	-	7/39/115/115	-
27	GOL	B	629	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	C	521	-	-	15/46/66/70	0/1/1/1
23	CLA	C	513	-	1/1/15/20	10/39/115/115	-
27	GOL	a	418	-	-	2/4/4/4	-
29	PL9	D	407[B]	-	-	9/53/73/73	0/1/1/1
25	BCR	d	404	-	-	5/29/63/63	0/2/2/2
34	HTG	b	622	-	-	4/10/30/30	0/1/1/1
23	CLA	A	406[A]	42	-	5/39/115/115	-
32	LHG	d	413[B]	-	-	13/53/53/53	-
24	PHO	a	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	b	613	-	1/1/15/20	5/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
27	GOL	o	302	-	-	2/4/4/4	-
31	LMT	B	630	-	-	10/21/61/61	0/2/2/2
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LHG	A	418[B]	-	-	14/53/53/53	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	C	514	-	1/1/15/20	7/39/115/115	-
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
23	CLA	D	405	-	1/1/15/20	13/39/115/115	-
32	LHG	d	406[A]	-	-	12/53/53/53	-
25	BCR	a	410	-	-	0/29/63/63	0/2/2/2
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1
27	GOL	v	202[B]	-	-	2/4/4/4	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
29	PL9	a	414[B]	-	-	14/53/73/73	0/1/1/1
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
24	PHO	a	408[B]	-	-	4/37/103/103	0/5/6/6
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LMG	B	621	-	-	14/46/66/70	0/1/1/1
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
23	CLA	D	404[A]	-	1/1/15/20	2/39/115/115	-
23	CLA	b	601	42	1/1/15/20	19/39/115/115	-
23	CLA	c	509	-	1/1/15/20	3/39/115/115	-
27	GOL	d	412	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	l	102[A]	-	-	2/4/4/4	-
35	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
32	LHG	D	408[B]	-	-	16/53/53/53	-
31	LMT	M	101	-	-	5/21/61/61	0/2/2/2
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
23	CLA	B	604	-	1/1/15/20	2/39/115/115	-
23	CLA	B	612	-	1/1/15/20	7/39/115/115	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
23	CLA	b	604	-	1/1/15/20	9/39/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
23	CLA	c	505	42	1/1/15/20	6/39/115/115	-
23	CLA	c	503	-	1/1/15/20	4/39/115/115	-
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
34	HTG	d	410	-	-	1/7/27/30	0/1/1/1
23	CLA	C	509	-	-	3/39/115/115	-
23	CLA	b	612	-	1/1/15/20	1/39/115/115	-
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
32	LHG	D	409[A]	-	-	13/53/53/53	-
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
25	BCR	D	406	-	-	4/29/63/63	0/2/2/2
23	CLA	c	511	-	1/1/15/20	11/39/115/115	-
23	CLA	C	510	-	1/1/15/20	6/39/115/115	-
35	DGD	C	518[A]	-	-	12/51/91/95	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	a	406[A]	42	1/1/15/20	4/39/115/115	-
23	CLA	c	502	-	1/1/15/20	5/39/115/115	-
23	CLA	B	606	-	1/1/15/20	5/39/115/115	-
23	CLA	b	603	-	1/1/15/20	3/39/115/115	-
23	CLA	d	402[A]	-	1/1/15/20	4/39/115/115	-
23	CLA	B	601	42	1/1/15/20	12/39/115/115	-
31	LMT	b	621	-	-	9/17/37/61	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-
26	SQD	a	412	-	-	14/49/69/69	0/1/1/1
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	A	405[A]	42	1/1/15/20	1/39/115/115	-
23	CLA	C	505	42	1/1/15/20	6/39/115/115	-
27	GOL	a	419	-	-	1/4/4/4	-
27	GOL	b	628	-	-	0/4/4/4	-
24	PHO	A	407[B]	-	-	0/37/103/103	0/5/6/6
32	LHG	L	101[A]	-	-	20/53/53/53	-
29	PL9	d	405[B]	-	-	7/53/73/73	0/1/1/1
32	LHG	b	629[B]	-	-	17/53/53/53	-
23	CLA	C	511	-	1/1/15/20	13/39/115/115	-
27	GOL	B	627	-	-	1/4/4/4	-
33	LMG	D	413	40	-	8/46/66/70	0/1/1/1
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
27	GOL	o	303	-	-	2/4/4/4	-
29	PL9	A	414[B]	-	-	12/53/73/73	0/1/1/1
23	CLA	B	605	-	1/1/15/20	4/39/115/115	-
23	CLA	c	508	42	1/1/15/20	10/39/115/115	-
23	CLA	B	615	-	1/1/15/20	8/39/115/115	-
23	CLA	B	616	-	1/1/15/20	6/39/115/115	-
23	CLA	a	405[B]	-	1/1/15/20	5/39/115/115	-
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
32	LHG	d	407[A]	-	-	12/53/53/53	-
23	CLA	b	614	-	1/1/15/20	11/39/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
23	CLA	a	407[A]	42	-	6/39/115/115	-
32	LHG	E	101[A]	-	-	21/46/46/53	-
23	CLA	A	404[B]	-	1/1/15/20	6/39/115/115	-
27	GOL	c	526[B]	-	-	0/4/4/4	-
35	DGD	C	517[B]	-	-	15/51/91/95	0/2/2/2
25	BCR	c	516	-	-	1/29/63/63	0/2/2/2
32	LHG	a	420[A]	-	-	16/46/46/53	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	H	102	-	-	11/51/91/95	0/2/2/2

All (1836) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[A]	PHO	C1B-C2B	9.37	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	9.34	1.49	1.39
24	a	416[B]	PHO	C1D-C2D	9.28	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	9.10	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.05	1.49	1.39
24	A	416[B]	PHO	C1D-C2D	9.01	1.49	1.39
24	a	416[B]	PHO	C1B-C2B	8.89	1.49	1.39
24	a	416[A]	PHO	C1B-C2B	8.84	1.49	1.39
24	A	416[A]	PHO	C1B-C2B	8.80	1.49	1.39
24	a	408[B]	PHO	C1B-C2B	8.80	1.49	1.39
24	a	416[A]	PHO	C1D-C2D	8.76	1.49	1.39
24	A	416[B]	PHO	C1B-C2B	8.76	1.49	1.39
24	A	416[A]	PHO	C1D-C2D	8.67	1.49	1.39
24	a	408[B]	PHO	C1D-C2D	8.61	1.49	1.39
24	A	407[A]	PHO	C1B-C2B	8.59	1.48	1.39
24	a	408[A]	PHO	C1D-C2D	8.55	1.48	1.39
24	a	416[A]	PHO	C3B-C4B	8.28	1.49	1.41
24	A	416[A]	PHO	C3B-C4B	8.05	1.49	1.41
23	B	611	CLA	CMB-C2B	8.03	1.67	1.50
24	a	416[B]	PHO	C3B-C4B	7.77	1.49	1.41
24	a	408[B]	PHO	C3B-C4B	7.63	1.49	1.41
24	a	408[A]	PHO	C3B-C4B	7.53	1.49	1.41
24	A	416[B]	PHO	C3B-C4B	7.44	1.49	1.41
24	A	407[B]	PHO	C3B-C4B	7.33	1.48	1.41
41	V	201	HEC	CAC-C3C	7.01	1.57	1.35
24	a	408[A]	PHO	C4D-CHA	7.01	1.50	1.39
23	B	611	CLA	C1B-C2B	6.98	1.59	1.43
24	A	407[A]	PHO	C3B-C4B	6.95	1.48	1.41
24	a	408[B]	PHO	C4D-CHA	6.93	1.49	1.39
41	v	201	HEC	CAC-C3C	6.88	1.57	1.35
24	A	416[B]	PHO	C3B-C2B	6.75	1.49	1.40
24	A	416[A]	PHO	C4D-CHA	6.72	1.49	1.39
24	A	416[B]	PHO	C4D-CHA	6.62	1.49	1.39
24	A	407[B]	PHO	C4D-CHA	6.60	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.57	1.49	1.39
24	a	408[A]	PHO	C3B-C2B	6.55	1.49	1.40
24	a	416[B]	PHO	C4D-CHA	6.54	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416[B]	PHO	C3B-C2B	6.52	1.49	1.40
24	a	416[A]	PHO	C4D-CHA	6.48	1.49	1.39
24	A	407[A]	PHO	C3B-C2B	6.28	1.48	1.40
41	V	201	HEC	CAB-C3B	6.20	1.55	1.35
41	v	201	HEC	CAB-C3B	6.12	1.54	1.35
24	A	416[A]	PHO	C3B-C2B	6.09	1.48	1.40
24	a	408[B]	PHO	C3B-C2B	6.07	1.48	1.40
23	B	611	CLA	C1D-ND	6.02	1.45	1.37
24	a	416[A]	PHO	C3B-C2B	6.02	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	5.91	1.48	1.40
23	B	610	CLA	C3C-C2C	5.70	1.49	1.36
24	A	416[B]	PHO	C3D-C2D	5.67	1.49	1.39
24	a	416[A]	PHO	OBD-CAD	5.65	1.29	1.22
24	A	416[A]	PHO	OBD-CAD	5.63	1.29	1.22
24	a	416[A]	PHO	C3D-C2D	5.62	1.49	1.39
24	a	408[A]	PHO	C3D-C2D	5.61	1.49	1.39
41	v	201	HEC	C3D-C2D	5.58	1.53	1.38
23	c	509	CLA	O2D-CGD	5.58	1.46	1.33
23	B	605	CLA	C3C-C2C	5.56	1.48	1.36
23	C	504	CLA	C3C-C2C	5.54	1.48	1.36
23	B	611	CLA	CHC-C1C	5.53	1.49	1.38
24	a	408[B]	PHO	C3D-C2D	5.52	1.49	1.39
23	a	406[A]	CLA	C3C-C2C	5.48	1.48	1.36
24	A	416[A]	PHO	C3D-C2D	5.48	1.49	1.39
24	a	416[B]	PHO	C3D-C2D	5.47	1.49	1.39
23	c	509	CLA	C3C-C2C	5.45	1.48	1.36
23	D	405	CLA	C1D-ND	5.44	1.45	1.37
24	a	416[B]	PHO	OBD-CAD	5.43	1.29	1.22
23	C	513	CLA	C3C-C2C	5.42	1.48	1.36
23	b	610	CLA	C3C-C2C	5.40	1.48	1.36
23	d	402[B]	CLA	C3C-C2C	5.40	1.48	1.36
23	B	611	CLA	C3C-C2C	5.40	1.48	1.36
23	b	605	CLA	C3C-C2C	5.38	1.48	1.36
23	B	612	CLA	CHC-C1C	5.38	1.49	1.38
23	b	609	CLA	O2D-CGD	5.37	1.46	1.33
23	c	504	CLA	C3C-C2C	5.36	1.48	1.36
23	b	612	CLA	C3C-C2C	5.35	1.48	1.36
23	c	513	CLA	C3C-C2C	5.35	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.34	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.34	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.33	1.48	1.36
23	C	506	CLA	CHC-C1C	5.33	1.49	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403	CLA	C3C-C2C	5.33	1.48	1.36
23	c	510	CLA	C3C-C2C	5.32	1.48	1.36
23	b	601	CLA	C3C-C2C	5.32	1.48	1.36
23	b	603	CLA	O2D-CGD	5.31	1.46	1.33
23	A	408	CLA	C3C-C2C	5.31	1.48	1.36
23	B	601	CLA	C3C-C2C	5.30	1.48	1.36
23	b	616	CLA	C3C-C2C	5.28	1.48	1.36
23	C	511	CLA	C3C-C2C	5.27	1.48	1.36
23	B	604	CLA	C3C-C2C	5.26	1.48	1.36
24	A	416[B]	PHO	OBD-CAD	5.26	1.29	1.22
23	C	513	CLA	CHC-C1C	5.24	1.49	1.38
23	b	602	CLA	C3C-C2C	5.23	1.48	1.36
23	D	405	CLA	C3C-C2C	5.23	1.48	1.36
23	a	407[B]	CLA	C3C-C2C	5.23	1.48	1.36
23	C	503	CLA	C3C-C2C	5.23	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.22	1.48	1.36
23	c	506	CLA	C3C-C2C	5.22	1.48	1.36
23	c	503	CLA	C3C-C2C	5.22	1.48	1.36
23	B	615	CLA	O2D-CGD	5.22	1.46	1.33
24	A	407[B]	PHO	C3D-C2D	5.22	1.48	1.39
23	a	407[A]	CLA	C3C-C2C	5.21	1.48	1.36
23	b	615	CLA	C3C-C2C	5.21	1.48	1.36
23	D	404[A]	CLA	C3C-C2C	5.21	1.48	1.36
23	A	404[B]	CLA	CHC-C1C	5.20	1.48	1.38
23	C	503	CLA	O2D-CGD	5.19	1.46	1.33
41	V	201	HEC	C3D-C2D	5.19	1.52	1.38
24	a	408[A]	PHO	O2D-CGD	5.19	1.46	1.33
23	b	606	CLA	C3C-C2C	5.18	1.47	1.36
23	c	507	CLA	O2D-CGD	5.18	1.46	1.33
23	a	405[B]	CLA	C1D-ND	5.18	1.44	1.37
23	B	613	CLA	CHC-C1C	5.18	1.48	1.38
23	B	605	CLA	O2D-CGD	5.18	1.46	1.33
23	D	404[B]	CLA	C3C-C2C	5.18	1.47	1.36
23	b	602	CLA	CHC-C1C	5.17	1.48	1.38
23	c	514	CLA	C3C-C2C	5.17	1.47	1.36
23	c	514	CLA	O2D-CGD	5.17	1.45	1.33
23	c	514	CLA	C1D-ND	5.16	1.44	1.37
23	b	614	CLA	C3C-C2C	5.16	1.47	1.36
23	C	503	CLA	C1D-ND	5.14	1.44	1.37
23	c	504	CLA	CHC-C1C	5.13	1.48	1.38
23	c	510	CLA	O2D-CGD	5.13	1.45	1.33
23	B	609	CLA	CHC-C1C	5.12	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	O2D-CGD	5.11	1.45	1.33
23	A	406[B]	CLA	CHC-C1C	5.11	1.48	1.38
23	A	405[B]	CLA	C3C-C2C	5.11	1.47	1.36
23	c	513	CLA	CHC-C1C	5.11	1.48	1.38
23	B	607	CLA	C3C-C2C	5.11	1.47	1.36
23	B	612	CLA	C3C-C2C	5.11	1.47	1.36
23	C	505	CLA	CHC-C1C	5.10	1.48	1.38
23	b	610	CLA	CHC-C1C	5.10	1.48	1.38
23	A	406[B]	CLA	O2D-CGD	5.10	1.45	1.33
23	B	616	CLA	C3C-C2C	5.09	1.47	1.36
23	b	603	CLA	C3C-C2C	5.09	1.47	1.36
23	A	405[A]	CLA	O2D-CGD	5.09	1.45	1.33
23	B	603	CLA	C3C-C2C	5.08	1.47	1.36
23	C	511	CLA	C1D-ND	5.08	1.44	1.37
23	c	505	CLA	C1D-ND	5.08	1.44	1.37
23	B	609	CLA	O2D-CGD	5.07	1.45	1.33
23	c	512	CLA	C3C-C2C	5.07	1.47	1.36
23	b	604	CLA	C3C-C2C	5.07	1.47	1.36
23	c	505	CLA	O2D-CGD	5.07	1.45	1.33
24	a	408[B]	PHO	O2D-CGD	5.07	1.45	1.33
23	a	405[B]	CLA	C3C-C2C	5.06	1.47	1.36
23	C	510	CLA	C3C-C2C	5.05	1.47	1.36
23	c	506	CLA	CHC-C1C	5.05	1.48	1.38
23	A	406[A]	CLA	C3C-C2C	5.04	1.47	1.36
23	b	606	CLA	C1D-ND	5.04	1.44	1.37
23	C	509	CLA	C3C-C2C	5.04	1.47	1.36
25	k	101	BCR	C23-C22	-5.03	1.35	1.46
23	A	406[A]	CLA	CHC-C1C	5.03	1.48	1.38
23	c	510	CLA	C1D-ND	5.03	1.44	1.37
23	D	405	CLA	CHC-C1C	5.02	1.48	1.38
23	c	502	CLA	C3C-C2C	5.01	1.47	1.36
23	A	405[B]	CLA	O2D-CGD	5.01	1.45	1.33
23	a	406[A]	CLA	C1D-ND	5.01	1.44	1.37
23	C	512	CLA	O2D-CGD	5.01	1.45	1.33
23	B	609	CLA	C3C-C2C	5.01	1.47	1.36
23	c	509	CLA	CHC-C1C	5.01	1.48	1.38
23	b	614	CLA	CHC-C1C	5.01	1.48	1.38
23	B	605	CLA	CHC-C1C	5.00	1.48	1.38
23	b	607	CLA	C3C-C2C	5.00	1.47	1.36
23	d	402[A]	CLA	C3C-C2C	5.00	1.47	1.36
23	c	513	CLA	C1D-ND	4.99	1.44	1.37
23	d	403	CLA	C1D-ND	4.99	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	f	101	HEM	FE-NB	4.99	2.10	1.94
23	c	509	CLA	C1D-ND	4.98	1.44	1.37
23	B	601	CLA	O2A-CGA	4.98	1.47	1.33
23	A	404[B]	CLA	O2D-CGD	4.98	1.45	1.33
23	C	502	CLA	CHC-C1C	4.98	1.48	1.38
23	d	403	CLA	CHC-C1C	4.98	1.48	1.38
23	C	506	CLA	C3C-C2C	4.98	1.47	1.36
23	b	613	CLA	C1D-ND	4.97	1.44	1.37
23	a	407[B]	CLA	O2D-CGD	4.97	1.45	1.33
23	c	508	CLA	C3C-C2C	4.97	1.47	1.36
24	a	416[B]	PHO	O2D-CGD	4.97	1.45	1.33
23	c	512	CLA	CHC-C1C	4.96	1.48	1.38
23	b	608	CLA	C3C-C2C	4.96	1.47	1.36
23	C	502	CLA	C3C-C2C	4.96	1.47	1.36
24	A	416[B]	PHO	O2D-CGD	4.96	1.45	1.33
23	c	504	CLA	C1D-ND	4.96	1.44	1.37
23	b	602	CLA	O2D-CGD	4.95	1.45	1.33
25	B	617	BCR	C23-C22	-4.95	1.35	1.46
23	C	508	CLA	C3C-C2C	4.95	1.47	1.36
23	C	512	CLA	C3C-C2C	4.93	1.47	1.36
23	a	405[A]	CLA	C3C-C2C	4.93	1.47	1.36
23	B	613	CLA	O2D-CGD	4.93	1.45	1.33
23	b	605	CLA	C1D-ND	4.93	1.44	1.37
23	B	606	CLA	C3C-C2C	4.93	1.47	1.36
23	B	615	CLA	C1D-ND	4.92	1.44	1.37
23	b	601	CLA	C1D-ND	4.92	1.44	1.37
23	B	611	CLA	O2D-CGD	4.92	1.45	1.33
23	C	505	CLA	C3C-C2C	4.92	1.47	1.36
23	b	613	CLA	C3C-C2C	4.92	1.47	1.36
39	F	102	HEM	FE-NB	4.92	2.10	1.94
23	A	404[B]	CLA	C1D-ND	4.91	1.44	1.37
23	B	611	CLA	CHC-C4B	4.91	1.50	1.39
23	C	513	CLA	C1D-ND	4.91	1.44	1.37
23	a	405[B]	CLA	CHC-C1C	4.91	1.48	1.38
24	A	407[A]	PHO	C3D-C2D	4.91	1.48	1.39
23	b	615	CLA	O2D-CGD	4.91	1.45	1.33
23	c	511	CLA	C3C-C2C	4.91	1.47	1.36
23	A	408	CLA	O2D-CGD	4.91	1.45	1.33
23	B	614	CLA	C4B-NB	-4.91	1.31	1.37
23	a	406[A]	CLA	O2D-CGD	4.90	1.45	1.33
23	c	507	CLA	C1D-ND	4.90	1.44	1.37
24	A	416[A]	PHO	O2D-CGD	4.90	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1D-ND	4.90	1.44	1.37
23	C	514	CLA	C3C-C2C	4.89	1.47	1.36
23	a	409	CLA	CHC-C1C	4.88	1.48	1.38
25	a	410	BCR	C23-C22	-4.87	1.35	1.46
23	D	404[B]	CLA	O2D-CGD	4.87	1.45	1.33
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	b	616	CLA	O2D-CGD	4.86	1.45	1.33
23	B	605	CLA	C1D-ND	4.86	1.44	1.37
23	C	507	CLA	C3C-C2C	4.86	1.47	1.36
23	B	613	CLA	C3C-C2C	4.86	1.47	1.36
23	b	610	CLA	O2D-CGD	4.86	1.45	1.33
24	A	407[A]	PHO	O2D-CGD	4.86	1.45	1.33
23	a	406[B]	CLA	C1D-ND	4.86	1.44	1.37
23	D	405	CLA	O2D-CGD	4.86	1.45	1.33
23	C	509	CLA	O2D-CGD	4.86	1.45	1.33
23	B	615	CLA	CHC-C1C	4.85	1.48	1.38
23	c	507	CLA	C3C-C2C	4.85	1.47	1.36
23	b	601	CLA	O2A-CGA	4.85	1.47	1.33
23	C	514	CLA	C1D-ND	4.84	1.44	1.37
23	b	611	CLA	O2D-CGD	4.84	1.45	1.33
23	c	512	CLA	C1D-ND	4.84	1.44	1.37
23	d	402[B]	CLA	O2D-CGD	4.84	1.45	1.33
25	C	515	BCR	C23-C22	-4.84	1.35	1.46
23	b	609	CLA	C3C-C2C	4.84	1.47	1.36
25	b	619	BCR	C23-C22	-4.84	1.35	1.46
23	c	508	CLA	O2D-CGD	4.83	1.45	1.33
23	c	511	CLA	O2D-CGD	4.83	1.45	1.33
23	D	404[A]	CLA	O2D-CGD	4.83	1.45	1.33
25	d	404	BCR	C23-C22	-4.83	1.35	1.46
23	B	601	CLA	O2D-CGD	4.83	1.45	1.33
23	C	511	CLA	CHC-C1C	4.82	1.48	1.38
24	A	407[B]	PHO	O2D-CGD	4.82	1.45	1.33
23	C	511	CLA	O2D-CGD	4.82	1.45	1.33
23	c	505	CLA	C3C-C2C	4.82	1.47	1.36
23	B	601	CLA	C1D-ND	4.81	1.44	1.37
23	c	512	CLA	O2D-CGD	4.81	1.45	1.33
23	A	405[B]	CLA	CHC-C1C	4.81	1.48	1.38
23	B	601	CLA	CHC-C1C	4.81	1.48	1.38
23	B	608	CLA	C3C-C2C	4.81	1.47	1.36
23	B	602	CLA	C3C-C2C	4.81	1.47	1.36
23	C	509	CLA	C1D-ND	4.80	1.44	1.37
23	a	405[B]	CLA	O2D-CGD	4.80	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416[A]	PHO	O2D-CGD	4.79	1.45	1.33
25	K	102	BCR	C23-C22	-4.79	1.35	1.46
25	B	619	BCR	C23-C22	-4.79	1.35	1.46
23	b	613	CLA	CHC-C1C	4.79	1.48	1.38
26	X	101	SQD	O47-C7	4.78	1.47	1.34
23	a	406[B]	CLA	O2D-CGD	4.78	1.45	1.33
23	B	604	CLA	O2D-CGD	4.77	1.45	1.33
23	b	611	CLA	C3C-C2C	4.77	1.47	1.36
24	A	407[B]	PHO	OBD-CAD	4.76	1.28	1.22
23	B	603	CLA	O2D-CGD	4.76	1.44	1.33
23	c	503	CLA	O2D-CGD	4.76	1.44	1.33
23	a	406[B]	CLA	CHC-C1C	4.75	1.48	1.38
23	b	616	CLA	CHC-C1C	4.75	1.48	1.38
23	a	407[B]	CLA	CHC-C1C	4.75	1.48	1.38
23	c	508	CLA	CHC-C1C	4.75	1.48	1.38
23	a	409	CLA	C3C-C2C	4.75	1.47	1.36
23	b	601	CLA	CHC-C1C	4.74	1.48	1.38
23	a	405[A]	CLA	C1D-ND	4.74	1.44	1.37
23	A	404[A]	CLA	C1D-ND	4.74	1.44	1.37
23	B	614	CLA	C3C-C2C	4.74	1.47	1.36
23	b	616	CLA	C1D-ND	4.73	1.44	1.37
23	a	405[A]	CLA	CHC-C1C	4.72	1.47	1.38
23	A	404[A]	CLA	O2D-CGD	4.72	1.44	1.33
23	b	602	CLA	CHD-C1D	4.72	1.47	1.38
26	f	102	SQD	O47-C7	4.72	1.47	1.34
33	c	521	LMG	O7-C10	4.72	1.47	1.34
23	C	512	CLA	CHC-C1C	4.72	1.47	1.38
23	B	602	CLA	O2D-CGD	4.71	1.44	1.33
25	t	102	BCR	C23-C22	-4.71	1.35	1.46
23	B	609	CLA	CHD-C1D	4.71	1.47	1.38
23	C	514	CLA	O2D-CGD	4.71	1.44	1.33
23	c	502	CLA	C1D-ND	4.70	1.44	1.37
23	b	605	CLA	O2D-CGD	4.70	1.44	1.33
23	b	604	CLA	CHC-C1C	4.70	1.47	1.38
23	b	615	CLA	CHC-C1C	4.70	1.47	1.38
23	B	614	CLA	C1D-ND	4.70	1.44	1.37
23	C	514	CLA	CHC-C1C	4.69	1.47	1.38
23	A	405[A]	CLA	CHC-C1C	4.69	1.47	1.38
23	a	407[A]	CLA	CHC-C1C	4.69	1.47	1.38
23	A	406[A]	CLA	O2D-CGD	4.68	1.44	1.33
23	B	615	CLA	C3C-C2C	4.67	1.46	1.36
23	B	606	CLA	CHC-C1C	4.67	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	O2D-CGD	4.67	1.44	1.33
23	C	510	CLA	O2D-CGD	4.66	1.44	1.33
23	C	504	CLA	CHC-C1C	4.66	1.47	1.38
23	B	610	CLA	CHC-C1C	4.66	1.47	1.38
23	C	509	CLA	CHC-C1C	4.66	1.47	1.38
23	C	508	CLA	CHC-C1C	4.65	1.47	1.38
23	b	611	CLA	CHC-C1C	4.65	1.47	1.38
26	A	412	SQD	O48-C23	4.65	1.46	1.33
25	D	406	BCR	C23-C22	-4.64	1.36	1.46
33	C	521	LMG	O7-C10	4.64	1.47	1.34
23	A	406[B]	CLA	C1D-ND	4.64	1.44	1.37
23	B	611	CLA	C4B-NB	-4.63	1.31	1.37
33	C	521	LMG	O8-C28	4.63	1.46	1.33
23	b	613	CLA	O2D-CGD	4.63	1.44	1.33
25	C	516	BCR	C23-C22	-4.63	1.36	1.46
23	C	506	CLA	O2D-CGD	4.63	1.44	1.33
23	b	606	CLA	CHC-C1C	4.62	1.47	1.38
23	D	404[A]	CLA	CHC-C1C	4.62	1.47	1.38
23	B	610	CLA	O2D-CGD	4.62	1.44	1.33
23	c	514	CLA	CHC-C1C	4.61	1.47	1.38
23	a	407[A]	CLA	O2D-CGD	4.60	1.44	1.33
23	B	603	CLA	C1D-ND	4.60	1.43	1.37
23	B	616	CLA	CHC-C1C	4.60	1.47	1.38
25	A	409	BCR	C23-C22	-4.59	1.36	1.46
23	c	513	CLA	O2D-CGD	4.59	1.44	1.33
23	b	604	CLA	O2D-CGD	4.59	1.44	1.33
23	b	608	CLA	O2D-CGD	4.59	1.44	1.33
32	E	101[A]	LHG	O8-C23	4.58	1.46	1.33
23	b	607	CLA	CHC-C1C	4.58	1.47	1.38
23	B	616	CLA	O2D-CGD	4.57	1.44	1.33
23	C	505	CLA	O2D-CGD	4.57	1.44	1.33
23	B	604	CLA	CHC-C1C	4.57	1.47	1.38
23	B	607	CLA	CHC-C1C	4.57	1.47	1.38
26	a	412	SQD	O48-C23	4.57	1.46	1.33
23	B	602	CLA	C1D-ND	4.57	1.43	1.37
23	A	404[A]	CLA	CHC-C1C	4.56	1.47	1.38
26	B	620	SQD	O47-C7	4.56	1.47	1.34
23	b	601	CLA	O2D-CGD	4.55	1.44	1.33
23	b	610	CLA	C1D-ND	4.54	1.43	1.37
23	d	402[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	c	503	CLA	C1D-ND	4.54	1.43	1.37
23	A	405[B]	CLA	C1D-ND	4.53	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[B]	PHO	OBD-CAD	4.53	1.28	1.22
23	a	406[A]	CLA	CHC-C1C	4.52	1.47	1.38
25	c	516	BCR	C23-C22	-4.52	1.36	1.46
32	E	101[B]	LHG	O8-C23	4.52	1.46	1.33
23	B	614	CLA	O2D-CGD	4.52	1.44	1.33
23	B	602	CLA	CHC-C1C	4.52	1.47	1.38
25	c	515	BCR	C23-C22	-4.51	1.36	1.46
23	c	502	CLA	CHC-C1C	4.51	1.47	1.38
32	a	420[A]	LHG	O8-C23	4.51	1.46	1.33
23	A	405[B]	CLA	CHD-C1D	4.51	1.47	1.38
23	C	507	CLA	CHD-C1D	4.51	1.47	1.38
23	C	506	CLA	CHD-C1D	4.51	1.47	1.38
23	B	615	CLA	CHD-C1D	4.50	1.47	1.38
23	B	607	CLA	O2D-CGD	4.50	1.44	1.33
23	d	402[B]	CLA	CHC-C1C	4.50	1.47	1.38
23	B	612	CLA	C1B-NB	-4.50	1.32	1.37
23	b	612	CLA	O2D-CGD	4.50	1.44	1.33
23	C	503	CLA	CHC-C1C	4.50	1.47	1.38
23	b	602	CLA	CHC-C4B	4.49	1.49	1.39
23	B	612	CLA	CHB-C1B	4.48	1.49	1.39
25	b	617	BCR	C23-C22	-4.48	1.36	1.46
23	B	606	CLA	O2D-CGD	4.48	1.44	1.33
23	C	504	CLA	C1D-ND	4.47	1.43	1.37
23	c	514	CLA	O2A-CGA	4.47	1.46	1.33
23	b	604	CLA	C1D-ND	4.47	1.43	1.37
23	C	502	CLA	CHD-C1D	4.47	1.47	1.38
23	b	609	CLA	CHC-C1C	4.46	1.47	1.38
23	D	404[B]	CLA	C1D-ND	4.45	1.43	1.37
23	B	605	CLA	CHC-C4B	4.45	1.49	1.39
23	b	603	CLA	CHC-C1C	4.45	1.47	1.38
23	A	406[B]	CLA	CHD-C1D	4.45	1.47	1.38
23	B	613	CLA	C1D-ND	4.45	1.43	1.37
23	d	403	CLA	O2D-CGD	4.45	1.44	1.33
23	B	614	CLA	CHC-C1C	4.45	1.47	1.38
23	C	507	CLA	CHC-C1C	4.44	1.47	1.38
33	z	101	LMG	O8-C28	4.44	1.46	1.33
23	B	603	CLA	CHC-C1C	4.44	1.47	1.38
25	y	101	BCR	C23-C22	-4.43	1.36	1.46
23	b	614	CLA	O2D-CGD	4.43	1.44	1.33
23	D	404[B]	CLA	CHC-C1C	4.43	1.47	1.38
23	C	513	CLA	CHD-C1D	4.42	1.47	1.38
23	C	510	CLA	C1D-ND	4.42	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	CHD-C1D	4.41	1.47	1.38
24	A	407[A]	PHO	OBD-CAD	4.41	1.28	1.22
23	D	404[B]	CLA	CHD-C1D	4.41	1.47	1.38
25	K	103	BCR	C23-C22	-4.40	1.36	1.46
23	C	513	CLA	O2D-CGD	4.40	1.44	1.33
23	c	505	CLA	CHC-C1C	4.39	1.47	1.38
23	b	608	CLA	CHC-C1C	4.39	1.47	1.38
23	c	508	CLA	C1D-ND	4.39	1.43	1.37
23	B	611	CLA	C3B-C2B	4.39	1.56	1.41
23	C	502	CLA	C1D-ND	4.38	1.43	1.37
32	a	420[B]	LHG	O8-C23	4.38	1.46	1.33
23	a	407[B]	CLA	C1D-ND	4.38	1.43	1.37
23	b	606	CLA	O2D-CGD	4.38	1.44	1.33
26	b	620	SQD	O48-C23	4.37	1.46	1.33
39	F	102	HEM	FE-NC	4.36	2.09	1.95
23	c	511	CLA	CHC-C1C	4.36	1.47	1.38
25	h	101	BCR	C23-C22	-4.36	1.36	1.46
23	a	406[A]	CLA	C3D-C2D	4.36	1.50	1.39
23	c	507	CLA	CHC-C1C	4.36	1.47	1.38
23	b	609	CLA	CHD-C1D	4.35	1.46	1.38
23	c	504	CLA	CHD-C1D	4.35	1.46	1.38
23	B	604	CLA	C1D-ND	4.35	1.43	1.37
26	b	620	SQD	O47-C7	4.35	1.46	1.34
26	f	102	SQD	O48-C23	4.35	1.46	1.33
23	C	508	CLA	O2D-CGD	4.35	1.43	1.33
23	c	508	CLA	O2A-CGA	4.34	1.46	1.33
23	B	614	CLA	CHB-C1B	4.34	1.49	1.39
23	a	405[A]	CLA	O2D-CGD	4.34	1.43	1.33
23	C	510	CLA	CHD-C1D	4.34	1.46	1.38
25	H	101	BCR	C23-C22	-4.34	1.36	1.46
23	c	512	CLA	CHB-C1B	4.34	1.49	1.39
23	b	612	CLA	CHC-C1C	4.33	1.47	1.38
23	c	513	CLA	O2A-CGA	4.33	1.46	1.33
23	B	615	CLA	O2A-CGA	4.33	1.46	1.33
23	d	403	CLA	C3D-C2D	4.32	1.50	1.39
23	c	502	CLA	CHD-C1D	4.32	1.46	1.38
23	a	409	CLA	O2D-CGD	4.32	1.43	1.33
25	b	618	BCR	C23-C22	-4.32	1.36	1.46
23	b	604	CLA	CHC-C4B	4.32	1.49	1.39
23	b	614	CLA	CHB-C1B	4.32	1.49	1.39
33	C	520	LMG	O8-C28	4.31	1.45	1.33
23	B	604	CLA	CHB-C1B	4.31	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	O2A-CGA	4.31	1.45	1.33
23	a	407[B]	CLA	O2A-CGA	4.31	1.45	1.33
23	C	514	CLA	O2A-CGA	4.31	1.45	1.33
23	C	503	CLA	CHD-C1D	4.30	1.46	1.38
23	b	604	CLA	CHD-C1D	4.30	1.46	1.38
33	B	621	LMG	O8-C28	4.30	1.45	1.33
23	C	505	CLA	CHB-C1B	4.30	1.49	1.39
23	B	610	CLA	C3D-C2D	4.29	1.50	1.39
23	D	404[B]	CLA	O2A-CGA	4.29	1.45	1.33
23	A	406[B]	CLA	C3D-C2D	4.29	1.50	1.39
23	c	513	CLA	CHD-C1D	4.29	1.46	1.38
23	B	607	CLA	CHB-C1B	4.29	1.49	1.39
32	a	420[A]	LHG	O7-C7	4.28	1.46	1.34
26	B	620	SQD	O48-C23	4.28	1.45	1.33
23	d	402[A]	CLA	CHC-C1C	4.28	1.47	1.38
23	B	612	CLA	CHD-C1D	4.28	1.46	1.38
23	D	405	CLA	CHC-C4B	4.28	1.49	1.39
23	b	602	CLA	CHD-C4C	4.28	1.48	1.39
23	d	403	CLA	CHD-C1D	4.28	1.46	1.38
23	C	507	CLA	C1D-ND	4.27	1.43	1.37
23	A	408	CLA	CHD-C4C	4.27	1.48	1.39
23	d	402[B]	CLA	O2A-CGA	4.27	1.45	1.33
23	B	607	CLA	C1B-NB	-4.27	1.32	1.37
23	B	606	CLA	C1D-ND	4.26	1.43	1.37
23	c	503	CLA	C3D-C2D	4.26	1.50	1.39
23	b	608	CLA	C3D-C2D	4.25	1.50	1.39
23	A	408	CLA	O2A-CGA	4.25	1.45	1.33
23	D	405	CLA	CHB-C1B	4.25	1.48	1.39
23	a	406[B]	CLA	O2A-CGA	4.25	1.45	1.33
23	B	604	CLA	CHD-C1D	4.24	1.46	1.38
23	c	504	CLA	O2A-CGA	4.24	1.45	1.33
23	A	408	CLA	C1D-ND	4.24	1.43	1.37
23	C	514	CLA	CHD-C1D	4.23	1.46	1.38
23	a	405[B]	CLA	CHD-C4C	4.23	1.48	1.39
23	c	512	CLA	O2A-CGA	4.23	1.45	1.33
23	b	607	CLA	CHD-C1D	4.23	1.46	1.38
23	B	610	CLA	C1D-ND	4.23	1.43	1.37
23	B	611	CLA	CHB-C1B	4.23	1.48	1.39
23	B	609	CLA	C1D-ND	4.23	1.43	1.37
25	T	101	BCR	C23-C22	-4.22	1.36	1.46
23	C	513	CLA	O2A-CGA	4.22	1.45	1.33
23	B	608	CLA	C3D-C2D	4.22	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	420[B]	LHG	O7-C7	4.22	1.46	1.34
23	b	601	CLA	CHD-C1D	4.22	1.46	1.38
23	a	409	CLA	O2A-CGA	4.22	1.45	1.33
32	E	101[A]	LHG	O7-C7	4.22	1.46	1.34
33	m	101	LMG	O8-C28	4.22	1.45	1.33
35	c	519	DGD	O1G-C1A	4.22	1.45	1.33
23	B	616	CLA	C1D-ND	4.21	1.43	1.37
23	B	602	CLA	CHD-C1D	4.21	1.46	1.38
39	f	101	HEM	FE-NC	4.21	2.09	1.95
23	C	513	CLA	CHC-C4B	4.21	1.48	1.39
23	C	509	CLA	C3D-C2D	4.21	1.50	1.39
32	d	407[A]	LHG	O8-C23	4.20	1.45	1.33
23	b	607	CLA	O2D-CGD	4.20	1.43	1.33
23	A	405[A]	CLA	C1D-ND	4.20	1.43	1.37
23	A	406[B]	CLA	CHD-C4C	4.20	1.48	1.39
23	B	612	CLA	O2D-CGD	4.19	1.43	1.33
23	b	615	CLA	O2A-CGA	4.19	1.45	1.33
23	D	404[A]	CLA	O2A-CGA	4.19	1.45	1.33
23	b	616	CLA	O2A-CGA	4.19	1.45	1.33
23	a	407[B]	CLA	CHD-C1D	4.19	1.46	1.38
23	b	611	CLA	O2A-CGA	4.19	1.45	1.33
23	c	511	CLA	C3D-C2D	4.18	1.50	1.39
23	C	503	CLA	C3D-C2D	4.18	1.50	1.39
35	c	518[B]	DGD	O1G-C1A	4.18	1.45	1.33
23	b	607	CLA	C1D-ND	4.18	1.43	1.37
23	c	508	CLA	CHD-C1D	4.18	1.46	1.38
23	c	507	CLA	O2A-CGA	4.17	1.45	1.33
33	c	521	LMG	O8-C28	4.17	1.45	1.33
23	d	403	CLA	O2A-CGA	4.17	1.45	1.33
23	D	404[B]	CLA	CHD-C4C	4.17	1.48	1.39
23	a	405[B]	CLA	CHD-C1D	4.16	1.46	1.38
23	C	508	CLA	O2A-CGA	4.16	1.45	1.33
23	C	512	CLA	O2A-CGA	4.16	1.45	1.33
23	b	610	CLA	CHD-C1D	4.16	1.46	1.38
23	c	509	CLA	C3D-C2D	4.16	1.50	1.39
32	E	101[B]	LHG	O7-C7	4.16	1.46	1.34
23	D	404[A]	CLA	CHD-C1D	4.16	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.15	1.50	1.39
23	b	610	CLA	CHD-C4C	4.15	1.48	1.39
23	c	510	CLA	CHC-C1C	4.15	1.46	1.38
23	b	610	CLA	CHB-C1B	4.15	1.48	1.39
23	c	502	CLA	CHD-C4C	4.14	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	CHD-C1D	4.14	1.46	1.38
33	d	411	LMG	O7-C10	4.14	1.46	1.34
23	c	514	CLA	CHD-C4C	4.14	1.48	1.39
23	A	405[B]	CLA	O2A-CGA	4.14	1.45	1.33
23	b	601	CLA	C3D-C2D	4.13	1.50	1.39
23	a	407[A]	CLA	C1D-ND	4.13	1.43	1.37
35	C	517[A]	DGD	O2G-C1B	4.13	1.46	1.34
23	c	513	CLA	C3D-C2D	4.13	1.50	1.39
24	a	408[A]	PHO	OBD-CAD	4.13	1.27	1.22
26	A	412	SQD	O47-C7	4.13	1.45	1.34
23	a	406[A]	CLA	O2A-CGA	4.13	1.45	1.33
23	b	616	CLA	CHD-C1D	4.12	1.46	1.38
23	a	405[A]	CLA	CHD-C4C	4.12	1.48	1.39
23	C	512	CLA	CHD-C1D	4.12	1.46	1.38
23	c	508	CLA	CHD-C4C	4.12	1.48	1.39
23	C	506	CLA	CHD-C4C	4.12	1.48	1.39
23	C	511	CLA	CHD-C4C	4.12	1.48	1.39
23	B	604	CLA	CHD-C4C	4.12	1.48	1.39
32	d	407[B]	LHG	O8-C23	4.12	1.45	1.33
23	c	510	CLA	CHB-C1B	4.12	1.48	1.39
23	A	406[A]	CLA	C1B-NB	-4.11	1.32	1.37
23	b	605	CLA	CHC-C1C	4.11	1.46	1.38
32	L	101[B]	LHG	O8-C23	4.11	1.45	1.33
23	c	505	CLA	CHD-C1D	4.11	1.46	1.38
33	Z	101	LMG	O7-C10	4.10	1.45	1.34
24	a	416[B]	PHO	O2A-CGA	4.10	1.45	1.33
23	c	512	CLA	CHD-C1D	4.10	1.46	1.38
23	C	503	CLA	CHC-C4B	4.10	1.48	1.39
23	C	504	CLA	O2D-CGD	4.10	1.43	1.33
23	B	611	CLA	C1C-C2C	4.10	1.52	1.44
26	a	412	SQD	O47-C7	4.09	1.45	1.34
33	c	520	LMG	O7-C10	4.09	1.45	1.34
23	A	408	CLA	CHC-C1C	4.09	1.46	1.38
23	C	507	CLA	O2A-CGA	4.08	1.45	1.33
23	c	505	CLA	C3D-C2D	4.08	1.50	1.39
23	c	511	CLA	CHB-C1B	4.08	1.48	1.39
32	D	409[B]	LHG	O7-C7	4.08	1.45	1.34
23	B	609	CLA	C3D-C2D	4.08	1.50	1.39
23	a	405[A]	CLA	CHD-C1D	4.08	1.46	1.38
23	A	405[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	d	402[B]	CLA	CHD-C1D	4.08	1.46	1.38
33	C	520	LMG	O7-C10	4.07	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	CHB-C1B	4.07	1.48	1.39
23	A	406[A]	CLA	CHD-C1D	4.07	1.46	1.38
35	C	519	DGD	O1G-C1A	4.07	1.45	1.33
32	D	409[B]	LHG	O8-C23	4.07	1.45	1.33
23	C	507	CLA	CHD-C4C	4.07	1.48	1.39
33	c	520	LMG	O8-C28	4.07	1.45	1.33
23	C	512	CLA	CHB-C1B	4.06	1.48	1.39
23	b	606	CLA	CHD-C1D	4.06	1.46	1.38
23	c	513	CLA	CHC-C4B	4.06	1.48	1.39
23	b	609	CLA	C1D-ND	4.06	1.43	1.37
23	A	408	CLA	CHD-C1D	4.06	1.46	1.38
23	B	605	CLA	CHB-C1B	4.05	1.48	1.39
23	c	509	CLA	O2A-CGA	4.05	1.45	1.33
26	a	411[A]	SQD	O47-C7	4.05	1.45	1.34
23	b	611	CLA	C1D-ND	4.05	1.43	1.37
23	c	504	CLA	CHD-C4C	4.05	1.48	1.39
23	c	507	CLA	CHD-C1D	4.05	1.46	1.38
23	a	407[B]	CLA	C3D-C2D	4.05	1.50	1.39
23	b	605	CLA	CHD-C4C	4.05	1.48	1.39
23	c	509	CLA	CHD-C1D	4.05	1.46	1.38
33	C	501	LMG	O8-C28	4.04	1.45	1.33
32	d	406[B]	LHG	O7-C7	4.04	1.45	1.34
23	B	609	CLA	O2A-CGA	4.04	1.45	1.33
23	b	608	CLA	CHD-C1D	4.04	1.46	1.38
23	B	608	CLA	CHC-C1C	4.04	1.46	1.38
23	D	405	CLA	C3D-C2D	4.03	1.50	1.39
23	b	601	CLA	CHD-C4C	4.03	1.48	1.39
23	b	611	CLA	CHB-C1B	4.03	1.48	1.39
33	a	417	LMG	O8-C28	4.03	1.45	1.33
23	b	603	CLA	C1D-ND	4.03	1.43	1.37
35	C	518[B]	DGD	O1G-C1A	4.03	1.45	1.33
23	b	615	CLA	CHD-C1D	4.03	1.46	1.38
23	c	504	CLA	O2D-CGD	4.03	1.43	1.33
24	A	416[A]	PHO	O2A-CGA	4.03	1.45	1.33
23	C	509	CLA	CHB-C1B	4.02	1.48	1.39
23	D	404[A]	CLA	CHB-C1B	4.02	1.48	1.39
23	a	406[B]	CLA	C3D-C2D	4.02	1.50	1.39
23	B	601	CLA	CHD-C1D	4.02	1.46	1.38
23	C	506	CLA	C1D-ND	4.02	1.43	1.37
35	c	517[B]	DGD	O2G-C1B	4.02	1.45	1.34
23	B	609	CLA	CHD-C4C	4.01	1.48	1.39
23	C	509	CLA	CHD-C1D	4.01	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	C1D-ND	4.01	1.43	1.37
23	c	504	CLA	CHC-C4B	4.01	1.48	1.39
23	a	407[A]	CLA	C3D-C2D	4.01	1.49	1.39
23	a	405[A]	CLA	CHB-C1B	4.01	1.48	1.39
35	c	518[A]	DGD	O1G-C1A	4.01	1.45	1.33
23	B	613	CLA	C3D-C2D	4.01	1.49	1.39
23	C	514	CLA	CHD-C4C	4.01	1.48	1.39
26	X	101	SQD	O48-C23	4.01	1.45	1.33
23	b	608	CLA	O2A-CGA	4.01	1.45	1.33
23	b	610	CLA	OBD-CAD	4.01	1.29	1.22
23	C	511	CLA	CHB-C1B	4.00	1.48	1.39
23	A	405[B]	CLA	CHD-C4C	4.00	1.48	1.39
23	A	406[A]	CLA	C3D-C2D	4.00	1.49	1.39
26	a	411[B]	SQD	O48-C23	4.00	1.45	1.33
23	A	408	CLA	C3D-C2D	4.00	1.49	1.39
23	c	504	CLA	CHB-C1B	4.00	1.48	1.39
23	c	506	CLA	CHD-C4C	4.00	1.48	1.39
23	b	604	CLA	CHD-C4C	3.99	1.48	1.39
33	z	101	LMG	O7-C10	3.99	1.45	1.34
23	B	607	CLA	CHC-C4B	3.99	1.48	1.39
23	A	404[B]	CLA	CHD-C4C	3.99	1.48	1.39
35	C	518[B]	DGD	O2G-C1B	3.99	1.45	1.34
23	b	614	CLA	C1D-ND	3.99	1.43	1.37
23	C	503	CLA	O2A-CGA	3.99	1.45	1.33
23	d	402[A]	CLA	CHB-C1B	3.99	1.48	1.39
33	C	501	LMG	O7-C10	3.99	1.45	1.34
33	a	417	LMG	O7-C10	3.99	1.45	1.34
35	c	518[B]	DGD	O2G-C1B	3.99	1.45	1.34
23	A	406[B]	CLA	O2A-CGA	3.98	1.45	1.33
23	B	602	CLA	CHD-C4C	3.98	1.48	1.39
23	C	511	CLA	O2A-CGA	3.98	1.45	1.33
23	c	511	CLA	CHC-C4B	3.98	1.48	1.39
23	b	612	CLA	C1D-ND	3.98	1.43	1.37
26	a	411[A]	SQD	O48-C23	3.98	1.44	1.33
23	C	510	CLA	C3D-C2D	3.98	1.49	1.39
23	d	402[B]	CLA	CHB-C1B	3.97	1.48	1.39
23	a	407[B]	CLA	CHD-C4C	3.97	1.48	1.39
23	B	606	CLA	CHB-C1B	3.97	1.48	1.39
23	B	601	CLA	CHC-C4B	3.97	1.48	1.39
23	C	514	CLA	C3D-C2D	3.97	1.49	1.39
23	c	502	CLA	C3D-C2D	3.97	1.49	1.39
32	A	418[B]	LHG	O8-C23	3.97	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407[A]	CLA	O2A-CGA	3.97	1.44	1.33
23	C	510	CLA	OBD-CAD	3.97	1.29	1.22
23	C	510	CLA	CHC-C1C	3.96	1.46	1.38
23	C	508	CLA	CHC-C4B	3.96	1.48	1.39
23	B	611	CLA	CHD-C1D	3.96	1.46	1.38
23	d	402[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	A	404[B]	CLA	CHD-C1D	3.96	1.46	1.38
23	C	504	CLA	CHD-C1D	3.96	1.46	1.38
23	B	602	CLA	O2A-CGA	3.96	1.44	1.33
23	b	602	CLA	C1D-ND	3.96	1.43	1.37
24	A	407[B]	PHO	O2A-CGA	3.96	1.44	1.33
23	C	506	CLA	CHC-C4B	3.96	1.48	1.39
23	c	511	CLA	CHD-C4C	3.96	1.48	1.39
23	b	612	CLA	CHB-C1B	3.96	1.48	1.39
23	C	508	CLA	C1D-ND	3.96	1.43	1.37
23	B	602	CLA	CHB-C1B	3.95	1.48	1.39
35	C	517[B]	DGD	O2G-C1B	3.95	1.45	1.34
23	C	510	CLA	CHB-C1B	3.95	1.48	1.39
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	B	616	CLA	C3D-C2D	3.95	1.49	1.39
23	C	512	CLA	C1D-ND	3.95	1.43	1.37
26	A	410[B]	SQD	O48-C23	3.95	1.44	1.33
23	B	609	CLA	CHC-C4B	3.95	1.48	1.39
23	A	405[A]	CLA	CHD-C1D	3.94	1.46	1.38
23	C	505	CLA	C1D-ND	3.94	1.43	1.37
23	B	605	CLA	CHD-C4C	3.94	1.48	1.39
23	b	614	CLA	CHD-C4C	3.94	1.48	1.39
32	L	101[B]	LHG	O7-C7	3.93	1.45	1.34
23	a	407[B]	CLA	OBD-CAD	3.93	1.29	1.22
23	c	505	CLA	O2A-CGA	3.93	1.44	1.33
23	b	610	CLA	CHC-C4B	3.93	1.48	1.39
23	B	613	CLA	OBD-CAD	3.93	1.29	1.22
23	c	503	CLA	CHC-C1C	3.93	1.46	1.38
33	d	411	LMG	O8-C28	3.93	1.44	1.33
32	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
23	B	615	CLA	CHD-C4C	3.92	1.48	1.39
23	C	502	CLA	O2A-CGA	3.92	1.44	1.33
23	D	404[A]	CLA	C1D-ND	3.92	1.43	1.37
23	c	506	CLA	CHB-C1B	3.92	1.48	1.39
35	c	517[B]	DGD	O1G-C1A	3.92	1.44	1.33
23	b	614	CLA	CHC-C4B	3.92	1.48	1.39
24	A	416[B]	PHO	O2A-CGA	3.91	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	409[A]	LHG	O8-C23	3.91	1.44	1.33
23	B	614	CLA	CHD-C4C	3.91	1.48	1.39
23	C	502	CLA	O2D-CGD	3.91	1.42	1.33
23	c	510	CLA	C3D-C2D	3.91	1.49	1.39
23	c	502	CLA	O2D-CGD	3.91	1.42	1.33
23	b	614	CLA	CHD-C1D	3.91	1.46	1.38
32	d	413[B]	LHG	O8-C23	3.90	1.44	1.33
23	c	506	CLA	C3D-C2D	3.90	1.49	1.39
23	a	406[A]	CLA	C1B-NB	-3.90	1.32	1.37
23	c	507	CLA	C3D-C2D	3.90	1.49	1.39
32	d	406[A]	LHG	O7-C7	3.90	1.45	1.34
23	c	507	CLA	CHD-C4C	3.90	1.48	1.39
23	c	502	CLA	O2A-CGA	3.90	1.44	1.33
23	b	606	CLA	CHB-C1B	3.90	1.48	1.39
23	C	505	CLA	CHD-C1D	3.90	1.46	1.38
23	c	511	CLA	O2A-CGA	3.90	1.44	1.33
23	c	509	CLA	CHD-C4C	3.90	1.48	1.39
32	b	629[B]	LHG	O8-C23	3.90	1.44	1.33
23	C	508	CLA	CHD-C1D	3.89	1.46	1.38
23	B	607	CLA	OBD-CAD	3.89	1.29	1.22
23	d	402[A]	CLA	CHD-C1D	3.89	1.46	1.38
23	B	613	CLA	CHB-C1B	3.89	1.48	1.39
26	a	411[B]	SQD	O47-C7	3.89	1.45	1.34
32	D	409[A]	LHG	O7-C7	3.89	1.45	1.34
23	C	502	CLA	CHC-C4B	3.89	1.48	1.39
23	c	511	CLA	CHD-C1D	3.89	1.46	1.38
23	c	513	CLA	CHD-C4C	3.89	1.48	1.39
23	B	616	CLA	O2A-CGA	3.89	1.44	1.33
23	B	606	CLA	CHD-C1D	3.89	1.46	1.38
25	B	618	BCR	C23-C22	-3.89	1.37	1.46
23	a	409	CLA	CHB-C1B	3.88	1.48	1.39
23	b	607	CLA	C1B-NB	-3.88	1.32	1.37
23	c	503	CLA	O2A-CGA	3.88	1.44	1.33
23	C	504	CLA	CHC-C4B	3.88	1.48	1.39
23	b	614	CLA	C3D-C2D	3.88	1.49	1.39
23	c	502	CLA	CHC-C4B	3.88	1.48	1.39
23	B	616	CLA	CHB-C1B	3.88	1.48	1.39
23	b	606	CLA	O2A-CGA	3.87	1.44	1.33
32	b	629[B]	LHG	O7-C7	3.87	1.45	1.34
23	A	405[B]	CLA	C3D-C2D	3.87	1.49	1.39
23	b	606	CLA	CHD-C4C	3.86	1.48	1.39
23	c	509	CLA	CHC-C4B	3.86	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C3D-C2D	3.86	1.49	1.39
23	c	514	CLA	C3D-C2D	3.86	1.49	1.39
23	C	513	CLA	CHD-C4C	3.86	1.48	1.39
24	a	416[A]	PHO	O2A-CGA	3.85	1.44	1.33
23	b	613	CLA	CHD-C1D	3.85	1.45	1.38
23	b	609	CLA	CHB-C1B	3.85	1.48	1.39
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	b	609	CLA	C3D-C2D	3.85	1.49	1.39
35	C	517[B]	DGD	O1G-C1A	3.85	1.44	1.33
23	b	615	CLA	CHB-C1B	3.85	1.48	1.39
23	a	406[A]	CLA	OBD-CAD	3.84	1.29	1.22
23	b	605	CLA	OBD-CAD	3.84	1.29	1.22
23	C	504	CLA	CHD-C4C	3.84	1.47	1.39
23	C	514	CLA	CHB-C1B	3.84	1.48	1.39
23	b	615	CLA	C3D-C2D	3.83	1.49	1.39
23	C	512	CLA	C3D-C2D	3.83	1.49	1.39
23	A	406[B]	CLA	CHC-C4B	3.83	1.48	1.39
23	B	601	CLA	CHD-C4C	3.83	1.47	1.39
23	a	406[B]	CLA	CHD-C1D	3.83	1.45	1.38
23	C	512	CLA	CHD-C4C	3.82	1.47	1.39
23	b	605	CLA	CHD-C1D	3.82	1.45	1.38
23	b	603	CLA	CHD-C1D	3.82	1.45	1.38
23	B	613	CLA	CHD-C1D	3.82	1.45	1.38
32	D	408[B]	LHG	O8-C23	3.82	1.44	1.33
23	b	616	CLA	C3D-C2D	3.82	1.49	1.39
23	A	405[A]	CLA	CHD-C4C	3.81	1.47	1.39
35	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34
23	B	614	CLA	O2A-CGA	3.81	1.44	1.33
23	a	407[A]	CLA	CHD-C4C	3.81	1.47	1.39
23	B	606	CLA	O2A-CGA	3.81	1.44	1.33
23	b	604	CLA	OBD-CAD	3.81	1.29	1.22
23	B	607	CLA	O2A-CGA	3.81	1.44	1.33
23	c	508	CLA	C3D-C2D	3.81	1.49	1.39
23	b	604	CLA	CHB-C1B	3.81	1.48	1.39
23	c	507	CLA	CHB-C1B	3.81	1.48	1.39
23	b	612	CLA	OBD-CAD	3.81	1.29	1.22
23	d	402[B]	CLA	CHD-C4C	3.80	1.47	1.39
35	C	518[A]	DGD	O1G-C1A	3.80	1.44	1.33
23	c	506	CLA	O2A-CGA	3.80	1.44	1.33
23	c	502	CLA	CHB-C1B	3.80	1.47	1.39
23	B	605	CLA	CHD-C1D	3.79	1.45	1.38
23	B	608	CLA	O2D-CGD	3.79	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	CHB-C1B	3.79	1.47	1.39
23	b	603	CLA	CHC-C4B	3.79	1.47	1.39
23	b	608	CLA	CHB-C1B	3.79	1.47	1.39
35	c	517[A]	DGD	O1G-C1A	3.79	1.44	1.33
23	c	510	CLA	O2A-CGA	3.78	1.44	1.33
32	D	408[B]	LHG	O7-C7	3.78	1.45	1.34
23	C	513	CLA	C3D-C2D	3.78	1.49	1.39
35	h	102	DGD	O2G-C1B	3.78	1.44	1.34
23	c	510	CLA	CHD-C1D	3.78	1.45	1.38
24	A	407[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	B	602	CLA	CHC-C4B	3.77	1.47	1.39
23	a	406[B]	CLA	CHD-C4C	3.77	1.47	1.39
23	C	502	CLA	CHB-C1B	3.77	1.47	1.39
23	A	406[A]	CLA	C1D-ND	3.77	1.42	1.37
23	b	612	CLA	C3D-C2D	3.77	1.49	1.39
26	A	410[A]	SQD	O48-C23	3.76	1.44	1.33
23	D	405	CLA	CHD-C4C	3.76	1.47	1.39
23	B	601	CLA	C3D-C2D	3.76	1.49	1.39
23	a	405[B]	CLA	O2A-CGA	3.76	1.44	1.33
23	B	608	CLA	C1D-ND	3.76	1.42	1.37
23	b	601	CLA	OBD-CAD	3.76	1.29	1.22
23	A	405[A]	CLA	CHC-C4B	3.76	1.47	1.39
24	A	416[A]	PHO	CHA-CBD	-3.76	1.47	1.51
23	C	507	CLA	C3D-C2D	3.76	1.49	1.39
32	d	406[B]	LHG	O8-C23	3.75	1.44	1.33
23	C	510	CLA	CHD-C4C	3.75	1.47	1.39
23	D	404[B]	CLA	CHB-C1B	3.75	1.47	1.39
23	c	514	CLA	CHB-C1B	3.75	1.47	1.39
23	c	506	CLA	C1D-ND	3.75	1.42	1.37
23	B	606	CLA	C3D-C2D	3.75	1.49	1.39
23	c	509	CLA	OBD-CAD	3.75	1.28	1.22
23	b	613	CLA	CHC-C4B	3.75	1.47	1.39
23	b	614	CLA	O2A-CGA	3.74	1.44	1.33
23	B	603	CLA	C1B-NB	-3.74	1.32	1.37
23	b	605	CLA	CHB-C1B	3.74	1.47	1.39
32	d	407[B]	LHG	O7-C7	3.74	1.44	1.34
33	B	621	LMG	O7-C10	3.74	1.44	1.34
23	a	405[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	A	406[A]	CLA	O2A-CGA	3.74	1.44	1.33
23	B	603	CLA	C3D-C2D	3.74	1.49	1.39
23	B	615	CLA	C3D-C2D	3.74	1.49	1.39
23	c	512	CLA	OBD-CAD	3.74	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	OBD-CAD	3.74	1.28	1.22
23	C	505	CLA	C3D-C2D	3.73	1.49	1.39
23	c	506	CLA	CHC-C4B	3.73	1.47	1.39
23	B	611	CLA	OBD-CAD	3.73	1.28	1.22
23	B	602	CLA	C3D-C2D	3.73	1.49	1.39
23	c	513	CLA	CHB-C1B	3.73	1.47	1.39
23	c	512	CLA	CHD-C4C	3.73	1.47	1.39
23	A	406[A]	CLA	CHD-C4C	3.73	1.47	1.39
26	A	410[B]	SQD	O47-C7	3.73	1.44	1.34
23	D	405	CLA	O2A-CGA	3.73	1.44	1.33
23	a	405[A]	CLA	C3D-C2D	3.72	1.49	1.39
23	B	611	CLA	O2A-CGA	3.72	1.44	1.33
23	b	613	CLA	CHB-C1B	3.72	1.47	1.39
23	C	502	CLA	CHD-C4C	3.72	1.47	1.39
23	b	609	CLA	CHD-C4C	3.72	1.47	1.39
23	b	609	CLA	O2A-CGA	3.71	1.44	1.33
23	b	615	CLA	CHD-C4C	3.71	1.47	1.39
35	h	102	DGD	O1G-C1A	3.71	1.44	1.33
23	c	503	CLA	CHD-C1D	3.71	1.45	1.38
23	B	612	CLA	O2A-CGA	3.71	1.44	1.33
23	C	514	CLA	OBD-CAD	3.71	1.28	1.22
23	a	406[B]	CLA	OBD-CAD	3.71	1.28	1.22
23	c	506	CLA	CHD-C1D	3.71	1.45	1.38
23	C	506	CLA	O2A-CGA	3.71	1.44	1.33
23	b	601	CLA	CHB-C1B	3.71	1.47	1.39
23	b	616	CLA	CHD-C4C	3.70	1.47	1.39
23	b	616	CLA	CHC-C4B	3.70	1.47	1.39
23	B	616	CLA	CHD-C1D	3.70	1.45	1.38
23	B	611	CLA	CHD-C4C	3.70	1.47	1.39
35	H	102	DGD	O1G-C1A	3.70	1.44	1.33
23	b	603	CLA	C3D-C2D	3.69	1.49	1.39
23	a	409	CLA	CHC-C4B	3.69	1.47	1.39
23	B	615	CLA	OBD-CAD	3.69	1.28	1.22
23	C	512	CLA	CHC-C4B	3.69	1.47	1.39
32	d	413[B]	LHG	O7-C7	3.69	1.44	1.34
23	A	404[A]	CLA	CHD-C4C	3.69	1.47	1.39
23	C	510	CLA	C4B-NB	-3.69	1.33	1.37
23	b	612	CLA	O2A-CGA	3.69	1.44	1.33
23	B	603	CLA	O2A-CGA	3.69	1.44	1.33
32	L	101[A]	LHG	O7-C7	3.69	1.44	1.34
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	B	603	CLA	CHD-C1D	3.68	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[B]	CLA	CHB-C1B	3.68	1.47	1.39
32	d	407[A]	LHG	O7-C7	3.68	1.44	1.34
23	c	510	CLA	CHD-C4C	3.68	1.47	1.39
23	b	607	CLA	C3D-C2D	3.68	1.49	1.39
23	C	509	CLA	OBD-CAD	3.67	1.28	1.22
23	B	610	CLA	C1B-NB	-3.67	1.33	1.37
23	a	409	CLA	CHD-C1D	3.67	1.45	1.38
23	D	404[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	A	404[A]	CLA	CHD-C1D	3.67	1.45	1.38
32	D	408[A]	LHG	O7-C7	3.67	1.44	1.34
23	C	503	CLA	CHD-C4C	3.67	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.67	1.49	1.39
23	c	513	CLA	OBD-CAD	3.66	1.28	1.22
23	C	510	CLA	O2A-CGA	3.66	1.44	1.33
23	B	608	CLA	CHB-C1B	3.66	1.47	1.39
23	b	604	CLA	C3D-C2D	3.66	1.49	1.39
23	A	404[B]	CLA	CHC-C4B	3.66	1.47	1.39
23	A	405[B]	CLA	CHB-C1B	3.66	1.47	1.39
35	C	517[A]	DGD	O1G-C1A	3.66	1.44	1.33
23	B	610	CLA	CHB-C1B	3.66	1.47	1.39
23	b	602	CLA	OBD-CAD	3.65	1.28	1.22
23	b	602	CLA	O2A-CGA	3.65	1.44	1.33
32	d	413[A]	LHG	O8-C23	3.65	1.44	1.33
23	b	608	CLA	C1B-NB	-3.65	1.33	1.37
23	b	604	CLA	O2A-CGA	3.65	1.44	1.33
23	c	508	CLA	CHC-C4B	3.65	1.47	1.39
23	D	404[B]	CLA	C3D-C2D	3.65	1.48	1.39
23	b	606	CLA	C3D-C2D	3.65	1.48	1.39
23	A	405[A]	CLA	CHB-C1B	3.65	1.47	1.39
23	B	604	CLA	OBD-CAD	3.64	1.28	1.22
23	a	407[B]	CLA	CHB-C1B	3.64	1.47	1.39
23	b	608	CLA	C1D-ND	3.64	1.42	1.37
23	A	406[A]	CLA	CHC-C4B	3.64	1.47	1.39
23	B	603	CLA	CHB-C1B	3.64	1.47	1.39
23	b	608	CLA	CHD-C4C	3.64	1.47	1.39
23	B	605	CLA	O2A-CGA	3.63	1.43	1.33
23	C	504	CLA	O2A-CGA	3.63	1.43	1.33
23	C	505	CLA	CHC-C4B	3.63	1.47	1.39
23	b	608	CLA	OBD-CAD	3.63	1.28	1.22
23	b	613	CLA	C1B-NB	-3.63	1.33	1.37
23	c	505	CLA	CHD-C4C	3.63	1.47	1.39
35	c	519	DGD	O2G-C1B	3.63	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CHB-C1B	3.63	1.47	1.39
23	c	509	CLA	CHB-C1B	3.62	1.47	1.39
24	a	408[B]	PHO	O2A-CGA	3.62	1.43	1.33
23	d	402[A]	CLA	CHD-C4C	3.62	1.47	1.39
23	A	406[B]	CLA	CHB-C1B	3.62	1.47	1.39
23	C	503	CLA	CHB-C1B	3.62	1.47	1.39
23	a	406[A]	CLA	CHD-C1D	3.62	1.45	1.38
23	B	607	CLA	CHD-C4C	3.62	1.47	1.39
23	b	613	CLA	CHD-C4C	3.62	1.47	1.39
33	D	413	LMG	O8-C28	3.61	1.43	1.33
23	C	508	CLA	C3D-C2D	3.61	1.48	1.39
23	b	615	CLA	C1D-ND	3.61	1.42	1.37
23	A	406[B]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	613	CLA	C3D-C2D	3.61	1.48	1.39
23	d	402[A]	CLA	OBD-CAD	3.61	1.28	1.22
32	b	629[A]	LHG	O7-C7	3.61	1.44	1.34
32	D	408[A]	LHG	O8-C23	3.61	1.43	1.33
23	C	506	CLA	CHB-C1B	3.61	1.47	1.39
23	D	404[B]	CLA	CHC-C4B	3.61	1.47	1.39
23	C	511	CLA	C3D-C2D	3.60	1.48	1.39
23	b	602	CLA	C3D-C2D	3.60	1.48	1.39
23	A	406[A]	CLA	CHB-C1B	3.60	1.47	1.39
23	C	508	CLA	CHB-C1B	3.60	1.47	1.39
32	A	418[A]	LHG	O7-C7	3.60	1.44	1.34
23	D	404[A]	CLA	C3D-C2D	3.60	1.48	1.39
23	b	611	CLA	C3D-C2D	3.60	1.48	1.39
23	A	405[B]	CLA	CHC-C4B	3.59	1.47	1.39
34	B	625	HTG	C1'-S1	-3.59	1.76	1.81
23	b	610	CLA	C3D-C2D	3.59	1.48	1.39
23	A	404[B]	CLA	O2A-CGA	3.59	1.43	1.33
23	B	603	CLA	CHD-C4C	3.59	1.47	1.39
23	A	404[B]	CLA	CHB-C1B	3.59	1.47	1.39
23	B	612	CLA	OBD-CAD	3.59	1.28	1.22
32	d	406[A]	LHG	O8-C23	3.58	1.43	1.33
23	a	407[A]	CLA	CHD-C1D	3.58	1.45	1.38
23	B	616	CLA	CHD-C4C	3.58	1.47	1.39
23	d	402[A]	CLA	C3D-C2D	3.58	1.48	1.39
23	c	510	CLA	C1B-NB	-3.58	1.33	1.37
23	C	507	CLA	CHB-C1B	3.58	1.47	1.39
23	B	608	CLA	CHD-C1D	3.58	1.45	1.38
23	d	403	CLA	CHC-C4B	3.58	1.47	1.39
23	B	608	CLA	O2A-CGA	3.58	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	OBD-CAD	3.58	1.28	1.22
23	A	404[B]	CLA	C1B-NB	-3.57	1.33	1.37
23	c	512	CLA	C3D-C2D	3.57	1.48	1.39
23	B	606	CLA	CHD-C4C	3.57	1.47	1.39
23	B	615	CLA	CHC-C4B	3.56	1.47	1.39
23	B	610	CLA	CHD-C1D	3.56	1.45	1.38
23	C	507	CLA	C4B-NB	-3.56	1.33	1.37
23	B	610	CLA	CHC-C4B	3.56	1.47	1.39
23	d	402[B]	CLA	C3D-C2D	3.55	1.48	1.39
32	A	418[B]	LHG	O7-C7	3.55	1.44	1.34
23	b	601	CLA	CHC-C4B	3.55	1.47	1.39
23	C	507	CLA	OBD-CAD	3.55	1.28	1.22
23	a	405[B]	CLA	C3D-C2D	3.55	1.48	1.39
23	a	405[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	b	607	CLA	CHB-C1B	3.55	1.47	1.39
23	a	407[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	a	406[A]	CLA	CHD-C4C	3.55	1.47	1.39
23	b	615	CLA	OBD-CAD	3.55	1.28	1.22
23	C	504	CLA	CHB-C1B	3.54	1.47	1.39
23	d	403	CLA	CHD-C4C	3.54	1.47	1.39
23	c	505	CLA	CHB-C1B	3.54	1.47	1.39
23	C	509	CLA	CHC-C4B	3.54	1.47	1.39
35	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	c	506	CLA	OBD-CAD	3.54	1.28	1.22
23	B	614	CLA	CHD-C1D	3.54	1.45	1.38
35	H	102	DGD	O2G-C1B	3.53	1.44	1.34
23	B	605	CLA	C3D-C2D	3.53	1.48	1.39
23	B	612	CLA	C3D-C2D	3.53	1.48	1.39
23	b	612	CLA	CHC-C4B	3.53	1.47	1.39
23	C	502	CLA	C3D-C2D	3.53	1.48	1.39
23	B	613	CLA	CHD-C4C	3.53	1.47	1.39
23	B	611	CLA	C3D-C2D	3.53	1.48	1.39
23	D	405	CLA	OBD-CAD	3.52	1.28	1.22
23	B	610	CLA	CHD-C4C	3.52	1.47	1.39
23	b	606	CLA	CHC-C4B	3.52	1.47	1.39
23	B	606	CLA	CHC-C4B	3.52	1.47	1.39
23	c	503	CLA	CHD-C4C	3.51	1.47	1.39
23	C	507	CLA	CHC-C4B	3.51	1.47	1.39
23	C	508	CLA	CHD-C4C	3.51	1.47	1.39
32	d	413[A]	LHG	O7-C7	3.51	1.44	1.34
23	b	613	CLA	O2A-CGA	3.51	1.43	1.33
23	C	505	CLA	O2A-CGA	3.51	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405[B]	CLA	OBD-CAD	3.50	1.28	1.22
35	C	519	DGD	O2G-C1B	3.50	1.44	1.34
32	A	418[A]	LHG	O8-C23	3.50	1.43	1.33
23	a	407[A]	CLA	OBD-CAD	3.50	1.28	1.22
23	D	404[A]	CLA	CHC-C4B	3.49	1.47	1.39
23	b	608	CLA	CHC-C4B	3.49	1.47	1.39
23	C	504	CLA	C3D-C2D	3.49	1.48	1.39
23	d	402[B]	CLA	OBD-CAD	3.49	1.28	1.22
23	b	611	CLA	CHC-C4B	3.49	1.47	1.39
23	B	602	CLA	C1B-NB	-3.49	1.33	1.37
23	B	609	CLA	CHB-C1B	3.48	1.47	1.39
23	d	403	CLA	CHB-C1B	3.48	1.47	1.39
23	B	604	CLA	O2A-CGA	3.48	1.43	1.33
23	b	603	CLA	CHB-C1B	3.48	1.47	1.39
23	B	613	CLA	CHC-C4B	3.48	1.47	1.39
23	d	402[B]	CLA	CHC-C4B	3.48	1.47	1.39
23	b	603	CLA	OBD-CAD	3.48	1.28	1.22
23	a	406[A]	CLA	CHB-C1B	3.47	1.47	1.39
23	C	505	CLA	CHD-C4C	3.47	1.47	1.39
23	a	407[B]	CLA	CHC-C4B	3.47	1.47	1.39
23	B	607	CLA	C3D-C2D	3.47	1.48	1.39
23	b	611	CLA	CHD-C4C	3.47	1.47	1.39
23	B	607	CLA	CHD-C1D	3.47	1.45	1.38
23	b	605	CLA	O2A-CGA	3.47	1.43	1.33
23	C	504	CLA	OBD-CAD	3.47	1.28	1.22
23	B	612	CLA	CHD-C4C	3.46	1.47	1.39
23	B	614	CLA	CHC-C4B	3.46	1.47	1.39
33	m	101	LMG	O7-C10	3.46	1.44	1.34
23	C	511	CLA	CHC-C4B	3.45	1.47	1.39
23	C	513	CLA	CHB-C1B	3.45	1.47	1.39
23	c	503	CLA	OBD-CAD	3.45	1.28	1.22
23	B	601	CLA	OBD-CAD	3.45	1.28	1.22
23	c	514	CLA	CHC-C4B	3.45	1.47	1.39
23	D	404[B]	CLA	OBD-CAD	3.44	1.28	1.22
23	B	601	CLA	CHB-C1B	3.44	1.47	1.39
23	c	504	CLA	C3D-C2D	3.44	1.48	1.39
23	C	509	CLA	CHD-C4C	3.44	1.47	1.39
23	C	503	CLA	OBD-CAD	3.43	1.28	1.22
23	b	605	CLA	C1B-NB	-3.43	1.33	1.37
23	A	408	CLA	CHC-C4B	3.43	1.47	1.39
23	c	508	CLA	CHB-C1B	3.43	1.47	1.39
23	b	612	CLA	C4B-NB	-3.43	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	CHD-C1D	3.42	1.45	1.38
34	b	623	HTG	C1'-S1	-3.42	1.76	1.81
23	b	602	CLA	CHB-C1B	3.42	1.47	1.39
23	B	604	CLA	CHC-C4B	3.42	1.47	1.39
23	B	603	CLA	CHC-C4B	3.42	1.47	1.39
23	b	616	CLA	C1B-NB	-3.41	1.33	1.37
34	B	622	HTG	C1'-S1	-3.41	1.76	1.81
23	c	507	CLA	CHC-C4B	3.40	1.47	1.39
23	b	615	CLA	CHC-C4B	3.40	1.47	1.39
23	c	514	CLA	OBD-CAD	3.40	1.28	1.22
23	b	607	CLA	CHD-C4C	3.40	1.46	1.39
32	b	629[A]	LHG	O8-C23	3.40	1.43	1.33
24	A	416[B]	PHO	CHA-CBD	-3.39	1.47	1.51
33	D	413	LMG	O7-C10	3.39	1.43	1.34
23	B	614	CLA	C3D-C2D	3.39	1.48	1.39
23	A	404[A]	CLA	C4B-NB	-3.39	1.33	1.37
23	B	612	CLA	C1C-C2C	3.39	1.51	1.44
23	A	405[B]	CLA	OBD-CAD	3.38	1.28	1.22
23	c	508	CLA	OBD-CAD	3.38	1.28	1.22
23	C	511	CLA	CHD-C1D	3.37	1.45	1.38
23	d	402[A]	CLA	CHC-C4B	3.37	1.47	1.39
23	b	604	CLA	C1B-NB	-3.37	1.33	1.37
23	b	603	CLA	CHD-C4C	3.37	1.46	1.39
23	a	409	CLA	CHD-C4C	3.37	1.46	1.39
23	b	614	CLA	OBD-CAD	3.36	1.28	1.22
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22
24	a	408[A]	PHO	O2A-CGA	3.36	1.43	1.33
23	a	406[B]	CLA	CHB-C1B	3.35	1.46	1.39
23	C	506	CLA	C3D-C2D	3.35	1.48	1.39
23	A	405[B]	CLA	C1B-NB	-3.35	1.33	1.37
23	A	404[B]	CLA	OBD-CAD	3.35	1.28	1.22
23	C	510	CLA	CHC-C4B	3.34	1.46	1.39
23	b	616	CLA	CHB-C1B	3.33	1.46	1.39
23	B	604	CLA	C3D-C2D	3.33	1.48	1.39
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
23	B	610	CLA	OBD-CAD	3.33	1.28	1.22
23	d	402[A]	CLA	C1D-ND	3.32	1.42	1.37
23	b	612	CLA	CHD-C4C	3.32	1.46	1.39
23	A	405[A]	CLA	C1B-NB	-3.32	1.33	1.37
23	a	409	CLA	C1B-NB	-3.32	1.33	1.37
23	b	611	CLA	CHD-C1D	3.31	1.44	1.38
23	B	613	CLA	O2A-CGA	3.31	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404[B]	CLA	C4B-NB	-3.31	1.33	1.37
23	c	512	CLA	CHC-C4B	3.31	1.46	1.39
23	C	514	CLA	CHC-C4B	3.30	1.46	1.39
23	B	616	CLA	CHC-C4B	3.30	1.46	1.39
23	B	607	CLA	C1D-ND	3.29	1.42	1.37
23	C	506	CLA	OBD-CAD	3.28	1.28	1.22
23	b	609	CLA	CHC-C4B	3.28	1.46	1.39
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	B	610	CLA	O2A-CGA	3.28	1.42	1.33
23	d	402[B]	CLA	C1B-NB	-3.28	1.33	1.37
23	B	603	CLA	OBD-CAD	3.28	1.28	1.22
23	c	505	CLA	C1B-NB	-3.28	1.33	1.37
23	b	608	CLA	C4B-NB	-3.27	1.33	1.37
23	c	505	CLA	CHC-C4B	3.27	1.46	1.39
39	f	101	HEM	C1B-NB	-3.27	1.34	1.40
23	C	512	CLA	C4B-NB	-3.26	1.33	1.37
23	B	616	CLA	C4B-NB	-3.26	1.33	1.37
23	C	508	CLA	C4B-NB	-3.26	1.33	1.37
23	a	407[A]	CLA	CHC-C4B	3.26	1.46	1.39
23	C	513	CLA	OBD-CAD	3.26	1.28	1.22
23	c	505	CLA	OBD-CAD	3.25	1.28	1.22
23	B	609	CLA	C1B-NB	-3.25	1.33	1.37
23	c	507	CLA	C1B-NB	-3.25	1.33	1.37
23	d	402[A]	CLA	C1B-NB	-3.25	1.33	1.37
34	b	622	HTG	C1'-S1	-3.25	1.76	1.81
39	f	101	HEM	C4D-ND	-3.25	1.34	1.40
23	b	614	CLA	C1B-NB	-3.24	1.33	1.37
23	C	502	CLA	OBD-CAD	3.24	1.28	1.22
23	D	404[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	b	607	CLA	CHC-C4B	3.24	1.46	1.39
23	B	608	CLA	OBD-CAD	3.24	1.28	1.22
23	c	505	CLA	C1B-C2B	3.23	1.50	1.43
23	a	406[A]	CLA	CHC-C4B	3.23	1.46	1.39
23	b	612	CLA	C1B-NB	-3.21	1.33	1.37
39	F	102	HEM	C1B-NB	-3.21	1.34	1.40
23	d	403	CLA	OBD-CAD	3.20	1.28	1.22
23	c	514	CLA	C4B-NB	-3.20	1.33	1.37
23	a	405[B]	CLA	CHC-C4B	3.20	1.46	1.39
23	c	503	CLA	CHC-C4B	3.20	1.46	1.39
23	a	405[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	D	404[B]	CLA	C1B-NB	-3.19	1.33	1.37
23	a	406[B]	CLA	C1B-NB	-3.18	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	C4B-NB	-3.18	1.33	1.37
23	B	608	CLA	CHC-C4B	3.17	1.46	1.39
23	B	614	CLA	OBD-CAD	3.17	1.27	1.22
23	B	612	CLA	CHC-C4B	3.17	1.46	1.39
23	b	603	CLA	O2A-CGA	3.17	1.42	1.33
23	a	409	CLA	C1D-ND	3.16	1.42	1.37
23	a	409	CLA	C4B-NB	-3.16	1.33	1.37
23	C	505	CLA	OBD-CAD	3.16	1.27	1.22
23	b	612	CLA	C1B-C2B	3.15	1.50	1.43
23	B	608	CLA	CHD-C4C	3.15	1.46	1.39
23	a	409	CLA	C3D-C2D	3.15	1.47	1.39
23	B	612	CLA	C4B-NB	-3.15	1.33	1.37
23	c	512	CLA	C1B-C2B	3.14	1.50	1.43
23	b	611	CLA	C1B-NB	-3.14	1.33	1.37
23	B	612	CLA	C1B-C2B	3.14	1.50	1.43
23	C	505	CLA	C1B-NB	-3.14	1.33	1.37
23	B	602	CLA	OBD-CAD	3.14	1.27	1.22
23	b	616	CLA	OBD-CAD	3.13	1.27	1.22
23	c	510	CLA	OBD-CAD	3.13	1.27	1.22
23	c	502	CLA	OBD-CAD	3.13	1.27	1.22
23	c	507	CLA	OBD-CAD	3.13	1.27	1.22
23	b	609	CLA	C1B-NB	-3.12	1.33	1.37
23	B	609	CLA	OBD-CAD	3.12	1.27	1.22
23	b	610	CLA	O2A-CGA	3.12	1.42	1.33
23	b	605	CLA	CHC-C4B	3.12	1.46	1.39
23	c	506	CLA	C1B-NB	-3.12	1.33	1.37
23	B	616	CLA	C1B-C2B	3.12	1.50	1.43
23	A	408	CLA	C4B-NB	-3.12	1.33	1.37
23	C	507	CLA	C1B-NB	-3.11	1.33	1.37
23	b	605	CLA	C3D-C2D	3.10	1.47	1.39
39	F	102	HEM	C4D-ND	-3.09	1.34	1.40
23	C	503	CLA	C1B-NB	-3.09	1.33	1.37
23	b	602	CLA	C1C-C2C	3.09	1.50	1.44
23	C	506	CLA	C1B-NB	-3.08	1.33	1.37
23	c	505	CLA	C4C-C3C	3.08	1.50	1.45
23	D	405	CLA	C1C-C2C	3.08	1.50	1.44
23	b	614	CLA	C1B-C2B	3.08	1.50	1.43
23	b	604	CLA	C1B-C2B	3.07	1.50	1.43
23	B	602	CLA	C1C-C2C	3.07	1.50	1.44
23	C	509	CLA	C1B-C2B	3.07	1.50	1.43
23	c	504	CLA	C1B-C2B	3.07	1.50	1.43
23	B	610	CLA	C4B-NB	-3.07	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C1B-C2B	3.06	1.50	1.43
23	C	514	CLA	C1B-NB	-3.05	1.33	1.37
23	c	510	CLA	CHC-C4B	3.05	1.46	1.39
23	b	603	CLA	C4B-NB	-3.05	1.33	1.37
23	D	404[A]	CLA	C1B-NB	-3.05	1.33	1.37
23	b	607	CLA	C1B-C2B	3.05	1.50	1.43
23	B	605	CLA	C1B-C2B	3.04	1.50	1.43
23	C	512	CLA	OBD-CAD	3.04	1.27	1.22
23	B	608	CLA	C4B-NB	-3.04	1.33	1.37
23	B	607	CLA	C4B-NB	-3.04	1.33	1.37
23	a	409	CLA	C1B-C2B	3.04	1.50	1.43
23	c	510	CLA	C1B-C2B	3.04	1.50	1.43
23	c	514	CLA	C1B-NB	-3.04	1.33	1.37
23	c	511	CLA	OBD-CAD	3.04	1.27	1.22
23	A	408	CLA	C1B-C2B	3.03	1.50	1.43
23	B	612	CLA	C1D-ND	3.03	1.41	1.37
23	A	406[A]	CLA	C1B-C2B	3.03	1.50	1.43
23	c	511	CLA	C4D-CHA	3.03	1.48	1.38
23	b	609	CLA	C4D-CHA	3.02	1.48	1.38
23	a	406[B]	CLA	CHC-C4B	3.02	1.46	1.39
23	A	408	CLA	CHB-C1B	3.02	1.46	1.39
23	B	611	CLA	C3B-C4B	3.02	1.51	1.42
23	B	604	CLA	C1B-C2B	3.02	1.50	1.43
23	b	615	CLA	C1B-NB	-3.02	1.33	1.37
23	c	513	CLA	C1B-NB	-3.01	1.33	1.37
23	b	603	CLA	C1B-C2B	3.01	1.50	1.43
23	C	511	CLA	OBD-CAD	3.01	1.27	1.22
23	A	404[A]	CLA	CHC-C4B	3.01	1.46	1.39
23	C	512	CLA	C4D-CHA	3.00	1.48	1.38
23	b	601	CLA	C1B-NB	-3.00	1.33	1.37
23	B	606	CLA	OBD-CAD	3.00	1.27	1.22
23	C	513	CLA	C1B-NB	-2.99	1.33	1.37
23	c	509	CLA	C1C-C2C	2.99	1.50	1.44
29	A	414[A]	PL9	C6-C5	2.99	1.49	1.35
24	A	407[A]	PHO	CBD-CGD	-2.99	1.48	1.52
23	a	405[B]	CLA	C1B-NB	-2.99	1.33	1.37
23	B	613	CLA	C4C-C3C	2.98	1.50	1.45
23	C	511	CLA	C1B-C2B	2.98	1.50	1.43
23	c	508	CLA	C4B-NB	-2.97	1.34	1.37
23	B	607	CLA	C4D-CHA	2.97	1.48	1.38
23	a	409	CLA	OBD-CAD	2.97	1.27	1.22
23	b	613	CLA	C1B-C2B	2.97	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4D-CHA	2.97	1.48	1.38
23	B	616	CLA	C1B-NB	-2.97	1.34	1.37
23	A	405[B]	CLA	C4D-CHA	2.97	1.48	1.38
23	A	408	CLA	OBD-CAD	2.97	1.27	1.22
23	b	607	CLA	O2A-CGA	2.97	1.42	1.33
23	c	511	CLA	C1B-NB	-2.97	1.34	1.37
23	C	502	CLA	C1B-NB	-2.96	1.34	1.37
23	A	404[A]	CLA	C1B-NB	-2.95	1.34	1.37
23	b	609	CLA	C4B-NB	-2.95	1.34	1.37
23	d	402[A]	CLA	C4B-NB	-2.95	1.34	1.37
23	C	508	CLA	C4D-CHA	2.95	1.48	1.38
23	c	510	CLA	C4B-NB	-2.95	1.34	1.37
23	C	512	CLA	C1B-C2B	2.94	1.50	1.43
23	C	509	CLA	C4C-C3C	2.93	1.50	1.45
23	c	508	CLA	C1B-NB	-2.93	1.34	1.37
23	c	503	CLA	C1B-C2B	2.93	1.50	1.43
23	C	511	CLA	C4B-NB	-2.92	1.34	1.37
23	B	604	CLA	C4D-CHA	2.92	1.48	1.38
23	C	502	CLA	C4D-CHA	2.92	1.48	1.38
23	C	514	CLA	C1B-C2B	2.92	1.50	1.43
29	a	414[A]	PL9	C6-C5	2.92	1.49	1.35
23	B	615	CLA	C1B-C2B	2.92	1.50	1.43
23	B	605	CLA	C1B-NB	-2.92	1.34	1.37
23	a	405[A]	CLA	C1B-NB	-2.92	1.34	1.37
23	a	407[B]	CLA	C1B-NB	-2.92	1.34	1.37
23	C	513	CLA	C1C-C2C	2.92	1.50	1.44
23	C	506	CLA	C1B-C2B	2.92	1.50	1.43
23	A	406[B]	CLA	C4B-NB	-2.92	1.34	1.37
23	a	405[A]	CLA	C4B-NB	-2.91	1.34	1.37
23	B	616	CLA	OBD-CAD	2.91	1.27	1.22
23	c	511	CLA	C1C-C2C	2.91	1.50	1.44
23	C	510	CLA	C1B-NB	-2.91	1.34	1.37
23	a	407[A]	CLA	C1B-NB	-2.91	1.34	1.37
23	B	605	CLA	OBD-CAD	2.90	1.27	1.22
29	a	414[B]	PL9	C6-C5	2.90	1.49	1.35
23	C	502	CLA	C1B-C2B	2.90	1.49	1.43
23	C	502	CLA	C1C-C2C	2.89	1.50	1.44
23	D	405	CLA	C3B-C4B	2.89	1.51	1.42
23	B	615	CLA	C1B-NB	-2.89	1.34	1.37
23	C	507	CLA	C4D-CHA	2.89	1.48	1.38
23	B	614	CLA	C4D-CHA	2.89	1.48	1.38
23	A	404[A]	CLA	C4C-C3C	2.88	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C1B-NB	-2.88	1.34	1.37
23	c	508	CLA	C4D-CHA	2.88	1.48	1.38
23	A	408	CLA	C4D-CHA	2.88	1.48	1.38
23	c	511	CLA	C1B-C2B	2.88	1.49	1.43
23	B	613	CLA	C1B-C2B	2.88	1.49	1.43
23	c	514	CLA	C1B-C2B	2.88	1.49	1.43
34	b	625	HTG	C1'-S1	-2.87	1.77	1.81
34	D	412	HTG	C1'-S1	-2.87	1.77	1.81
23	B	602	CLA	C1B-C2B	2.87	1.49	1.43
23	B	605	CLA	C4D-CHA	2.87	1.48	1.38
23	C	505	CLA	C4D-CHA	2.87	1.48	1.38
23	D	405	CLA	C1B-NB	-2.87	1.34	1.37
23	C	510	CLA	C1B-C2B	2.86	1.49	1.43
23	b	610	CLA	C1B-NB	-2.86	1.34	1.37
23	b	606	CLA	C1B-NB	-2.86	1.34	1.37
23	D	404[A]	CLA	C1B-C2B	2.86	1.49	1.43
23	B	610	CLA	C4D-CHA	2.85	1.48	1.38
23	C	508	CLA	C1C-C2C	2.85	1.50	1.44
23	C	504	CLA	C1B-NB	-2.85	1.34	1.37
23	a	405[B]	CLA	C4C-C3C	2.85	1.49	1.45
23	B	601	CLA	C1B-NB	-2.85	1.34	1.37
23	B	603	CLA	C4B-NB	-2.84	1.34	1.37
23	c	506	CLA	C1B-C2B	2.84	1.49	1.43
23	B	608	CLA	C1B-NB	-2.84	1.34	1.37
23	c	508	CLA	C1B-C2B	2.84	1.49	1.43
23	C	507	CLA	C4C-C3C	2.84	1.49	1.45
23	b	603	CLA	C4D-CHA	2.84	1.48	1.38
23	B	613	CLA	C4D-CHA	2.84	1.48	1.38
23	B	609	CLA	C3B-C4B	2.84	1.51	1.42
23	C	506	CLA	C4D-CHA	2.84	1.48	1.38
23	d	402[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	B	616	CLA	C1C-NC	-2.83	1.33	1.37
23	c	507	CLA	C4B-NB	-2.83	1.34	1.37
34	C	522	HTG	C1'-S1	-2.83	1.77	1.81
23	a	406[B]	CLA	C1B-C2B	2.83	1.49	1.43
23	A	404[A]	CLA	C1B-C2B	2.83	1.49	1.43
29	A	414[B]	PL9	C6-C5	2.82	1.49	1.35
23	c	503	CLA	C4B-NB	-2.82	1.34	1.37
23	D	404[B]	CLA	C1B-C2B	2.82	1.49	1.43
23	C	513	CLA	C4D-CHA	2.81	1.48	1.38
23	B	607	CLA	C1C-C2C	2.81	1.50	1.44
23	b	608	CLA	C1B-C2B	2.81	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C4D-CHA	2.80	1.48	1.38
23	c	509	CLA	C4D-CHA	2.80	1.48	1.38
23	b	606	CLA	C4B-NB	-2.79	1.34	1.37
23	C	512	CLA	C1C-C2C	2.79	1.50	1.44
23	b	613	CLA	C4D-CHA	2.79	1.48	1.38
23	a	407[A]	CLA	C1C-C2C	2.79	1.50	1.44
23	B	603	CLA	C4D-CHA	2.79	1.48	1.38
34	c	522	HTG	C1'-S1	-2.79	1.77	1.81
23	d	403	CLA	C4D-CHA	2.79	1.48	1.38
23	C	511	CLA	C1B-NB	-2.79	1.34	1.37
23	A	405[A]	CLA	C4D-CHA	2.79	1.48	1.38
24	a	408[A]	PHO	CBD-CGD	-2.79	1.49	1.52
23	C	508	CLA	OBD-CAD	2.79	1.27	1.22
23	c	513	CLA	C4D-CHA	2.79	1.47	1.38
23	b	610	CLA	C4C-C3C	2.78	1.49	1.45
23	a	407[A]	CLA	C4D-CHA	2.77	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.77	1.47	1.38
23	c	510	CLA	C4C-C3C	2.77	1.49	1.45
23	b	615	CLA	C4D-CHA	2.77	1.47	1.38
23	c	502	CLA	C4C-C3C	2.77	1.49	1.45
23	C	514	CLA	C1C-C2C	2.77	1.50	1.44
33	Z	101	LMG	O8-C28	2.76	1.46	1.33
23	B	608	CLA	C1B-C2B	2.76	1.49	1.43
23	a	405[B]	CLA	C1B-C2B	2.76	1.49	1.43
23	c	509	CLA	C1B-C2B	2.76	1.49	1.43
23	B	612	CLA	C4D-CHA	2.76	1.47	1.38
23	a	407[B]	CLA	C4D-CHA	2.76	1.47	1.38
23	b	605	CLA	C1B-C2B	2.76	1.49	1.43
23	b	602	CLA	C3B-C4B	2.76	1.50	1.42
23	A	405[A]	CLA	C1B-C2B	2.76	1.49	1.43
23	B	601	CLA	C1C-C2C	2.75	1.50	1.44
23	b	607	CLA	C4D-CHA	2.75	1.47	1.38
23	b	606	CLA	C4D-CHA	2.75	1.47	1.38
23	A	404[B]	CLA	C4D-CHA	2.75	1.47	1.38
23	B	614	CLA	C1B-C2B	2.75	1.49	1.43
23	B	606	CLA	C1B-C2B	2.74	1.49	1.43
23	C	510	CLA	C4D-CHA	2.74	1.47	1.38
23	D	404[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	b	606	CLA	C1B-C2B	2.74	1.49	1.43
23	B	609	CLA	C1B-C2B	2.74	1.49	1.43
23	b	604	CLA	C4D-CHA	2.73	1.47	1.38
23	a	407[A]	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)
23	B	604	CLA	C4C-C3C	2.73	1.49	1.45
23	d	402[B]	CLA	C1B-C2B	2.73	1.49	1.43
23	A	406[B]	CLA	C1B-NB	-2.73	1.34	1.37
23	b	605	CLA	C4D-CHA	2.73	1.47	1.38
23	a	406[A]	CLA	C1B-C2B	2.73	1.49	1.43
31	B	628	LMT	C3'-C2'	2.73	1.59	1.52
23	c	502	CLA	C1B-NB	-2.73	1.34	1.37
23	B	611	CLA	C4D-CHA	2.73	1.47	1.38
23	a	407[B]	CLA	C4B-NB	-2.72	1.34	1.37
23	c	506	CLA	C4D-CHA	2.72	1.47	1.38
23	B	602	CLA	C4C-C3C	2.72	1.49	1.45
23	B	604	CLA	C4B-NB	-2.72	1.34	1.37
23	b	611	CLA	OBD-CAD	2.72	1.27	1.22
23	B	615	CLA	C4D-CHA	2.72	1.47	1.38
23	b	613	CLA	OBD-CAD	2.71	1.27	1.22
23	A	406[A]	CLA	C3B-C4B	2.71	1.50	1.42
24	a	408[B]	PHO	C4B-NB	-2.71	1.33	1.38
23	D	404[A]	CLA	C4D-CHA	2.71	1.47	1.38
23	c	505	CLA	C4B-NB	-2.71	1.34	1.37
23	b	615	CLA	C1B-C2B	2.71	1.49	1.43
23	A	406[B]	CLA	C3B-C4B	2.71	1.50	1.42
23	C	511	CLA	C1C-C2C	2.70	1.50	1.44
23	A	405[B]	CLA	C1B-C2B	2.70	1.49	1.43
23	c	506	CLA	C4C-C3C	2.70	1.49	1.45
23	B	616	CLA	C3B-C2B	2.70	1.50	1.41
23	d	402[A]	CLA	C4D-CHA	2.70	1.47	1.38
23	c	506	CLA	C1C-C2C	2.69	1.50	1.44
23	B	613	CLA	C4B-NB	-2.69	1.34	1.37
23	a	405[B]	CLA	C3B-C4B	2.69	1.50	1.42
35	H	102	DGD	O5D-C1E	2.69	1.44	1.40
23	c	512	CLA	C1B-NB	-2.69	1.34	1.37
23	c	512	CLA	C4D-CHA	2.69	1.47	1.38
23	c	505	CLA	C4D-CHA	2.69	1.47	1.38
23	b	613	CLA	C1C-C2C	2.69	1.50	1.44
29	d	405[B]	PL9	C6-C5	2.69	1.48	1.35
29	D	407[B]	PL9	C6-C5	2.69	1.48	1.35
33	C	521	LMG	O1-C1	2.69	1.44	1.40
23	b	601	CLA	C4B-NB	-2.69	1.34	1.37
23	c	507	CLA	C1B-C2B	2.68	1.49	1.43
23	C	503	CLA	C1B-C2B	2.68	1.49	1.43
23	c	513	CLA	C3B-C4B	2.68	1.50	1.42
23	B	606	CLA	C1C-C2C	2.68	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C4D-CHA	2.67	1.47	1.38
23	A	406[A]	CLA	C4D-CHA	2.67	1.47	1.38
24	a	416[A]	PHO	C3A-C2A	-2.67	1.52	1.54
23	A	404[B]	CLA	C1B-C2B	2.67	1.49	1.43
23	C	511	CLA	C4D-CHA	2.67	1.47	1.38
23	c	504	CLA	C1C-C2C	2.67	1.49	1.44
23	d	403	CLA	C4B-NB	-2.67	1.34	1.37
23	c	504	CLA	OBD-CAD	2.66	1.27	1.22
23	b	611	CLA	C1B-C2B	2.66	1.49	1.43
23	A	405[B]	CLA	C3B-C4B	2.66	1.50	1.42
29	D	407[A]	PL9	C6-C5	2.66	1.48	1.35
23	C	509	CLA	C4D-CHA	2.66	1.47	1.38
23	B	605	CLA	C1C-C2C	2.66	1.49	1.44
23	B	614	CLA	C4C-C3C	2.65	1.49	1.45
23	B	609	CLA	C4D-CHA	2.65	1.47	1.38
34	d	410	HTG	C1'-S1	-2.65	1.77	1.81
23	a	405[A]	CLA	C4D-CHA	2.65	1.47	1.38
23	C	506	CLA	C3B-C4B	2.65	1.50	1.42
23	B	606	CLA	C1B-NB	-2.65	1.34	1.37
23	B	607	CLA	C1B-C2B	2.64	1.49	1.43
23	B	601	CLA	C4B-NB	-2.64	1.34	1.37
23	c	512	CLA	C1C-C2C	2.64	1.49	1.44
23	A	404[B]	CLA	C3B-C4B	2.64	1.50	1.42
23	D	405	CLA	C1B-C2B	2.64	1.49	1.43
34	b	622	HTG	O5-C1	2.64	1.46	1.42
23	c	503	CLA	C3B-C2B	2.64	1.50	1.41
23	A	404[A]	CLA	C4D-CHA	2.64	1.47	1.38
23	b	608	CLA	C4D-CHA	2.63	1.47	1.38
23	b	610	CLA	C4D-CHA	2.63	1.47	1.38
35	h	102	DGD	O5D-C1E	2.63	1.44	1.40
23	D	405	CLA	C4C-C3C	2.63	1.49	1.45
23	C	514	CLA	C4B-NB	-2.63	1.34	1.37
23	C	513	CLA	C3D-C4D	-2.63	1.38	1.44
23	a	407[A]	CLA	C4B-NB	-2.63	1.34	1.37
39	F	102	HEM	C1C-C2C	-2.63	1.40	1.45
23	b	601	CLA	C4D-CHA	2.62	1.47	1.38
23	C	509	CLA	C4B-NB	-2.62	1.34	1.37
23	A	405[A]	CLA	C1C-C2C	2.62	1.49	1.44
23	C	503	CLA	C4B-NB	-2.62	1.34	1.37
23	B	611	CLA	MG-NB	2.62	2.11	2.05
23	C	505	CLA	C3D-C4D	-2.62	1.38	1.44
23	D	404[B]	CLA	C4D-CHA	2.62	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C3B-C2B	2.62	1.50	1.41
23	C	514	CLA	C4D-CHA	2.62	1.47	1.38
23	b	610	CLA	C1B-C2B	2.62	1.49	1.43
23	a	406[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	a	406[A]	CLA	C4B-NB	-2.61	1.34	1.37
24	A	416[B]	PHO	C4B-NB	-2.61	1.33	1.38
23	c	504	CLA	C3B-C4B	2.61	1.50	1.42
23	A	408	CLA	C1B-NB	-2.60	1.34	1.37
23	c	509	CLA	C4C-C3C	2.60	1.49	1.45
24	A	416[A]	PHO	C3D-C4D	-2.60	1.37	1.41
23	A	405[A]	CLA	C4B-NB	-2.60	1.34	1.37
23	C	509	CLA	C3B-C2B	2.60	1.49	1.41
23	b	612	CLA	C4D-CHA	2.60	1.47	1.38
23	D	404[B]	CLA	C4C-C3C	2.60	1.49	1.45
23	c	514	CLA	C4C-C3C	2.60	1.49	1.45
23	a	409	CLA	C1C-C2C	2.60	1.49	1.44
23	C	508	CLA	C1B-NB	-2.60	1.34	1.37
23	B	613	CLA	C1B-NB	-2.60	1.34	1.37
23	d	402[B]	CLA	C4C-C3C	2.60	1.49	1.45
23	C	509	CLA	C1C-C2C	2.59	1.49	1.44
24	A	416[B]	PHO	C1D-ND	-2.58	1.34	1.38
23	B	603	CLA	C3B-C2B	2.58	1.49	1.41
23	C	508	CLA	C1B-C2B	2.58	1.49	1.43
23	B	612	CLA	C3B-C2B	2.57	1.49	1.41
23	b	614	CLA	C4D-CHA	2.57	1.47	1.38
23	d	402[A]	CLA	C1B-C2B	2.57	1.49	1.43
23	A	406[B]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	609	CLA	C1B-C2B	2.57	1.49	1.43
23	C	504	CLA	C3D-C4D	-2.57	1.38	1.44
23	c	514	CLA	C1C-C2C	2.57	1.49	1.44
23	c	504	CLA	C4D-CHA	2.56	1.47	1.38
26	X	101	SQD	O6-C1	2.56	1.44	1.40
23	A	405[A]	CLA	C3B-C4B	2.56	1.50	1.42
23	a	407[B]	CLA	C1B-C2B	2.55	1.49	1.43
23	b	602	CLA	C3D-C4D	-2.55	1.38	1.44
23	B	610	CLA	C1C-C2C	2.55	1.49	1.44
23	d	403	CLA	C1C-C2C	2.55	1.49	1.44
23	A	406[B]	CLA	C1B-C2B	2.55	1.49	1.43
23	C	512	CLA	C3B-C2B	2.55	1.49	1.41
23	d	402[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	b	611	CLA	C4B-NB	-2.54	1.34	1.37
23	b	610	CLA	C3D-C4D	-2.54	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C4D-CHA	2.54	1.47	1.38
23	c	510	CLA	C4D-CHA	2.54	1.47	1.38
23	b	601	CLA	C1C-C2C	2.54	1.49	1.44
23	b	604	CLA	C4B-NB	-2.54	1.34	1.37
23	b	616	CLA	C3B-C4B	2.54	1.50	1.42
23	b	602	CLA	C4D-CHA	2.54	1.47	1.38
23	c	506	CLA	C3B-C4B	2.54	1.50	1.42
23	B	610	CLA	C3D-C4D	-2.53	1.38	1.44
23	c	504	CLA	C1B-NB	-2.53	1.34	1.37
23	a	405[A]	CLA	C1B-C2B	2.53	1.49	1.43
23	b	605	CLA	C1D-C2D	2.53	1.50	1.45
23	c	507	CLA	C4C-C3C	2.53	1.49	1.45
23	C	513	CLA	C3B-C4B	2.53	1.50	1.42
23	B	606	CLA	C3D-C4D	-2.53	1.38	1.44
23	c	503	CLA	C4D-CHA	2.53	1.47	1.38
23	B	604	CLA	C3D-C4D	-2.53	1.38	1.44
23	C	504	CLA	C4B-NB	-2.52	1.34	1.37
23	b	609	CLA	C3D-C4D	-2.52	1.38	1.44
23	c	508	CLA	C1C-C2C	2.52	1.49	1.44
23	B	601	CLA	C3B-C4B	2.52	1.50	1.42
23	B	605	CLA	C3D-C4D	-2.52	1.38	1.44
23	C	502	CLA	C3D-C4D	-2.52	1.38	1.44
23	b	612	CLA	C1C-C2C	2.51	1.49	1.44
24	A	416[A]	PHO	C3A-C2A	-2.51	1.52	1.54
23	B	610	CLA	C1B-C2B	2.50	1.49	1.43
23	b	616	CLA	C4D-CHA	2.50	1.47	1.38
23	b	616	CLA	C3D-C4D	-2.50	1.38	1.44
23	c	514	CLA	C4D-CHA	2.50	1.47	1.38
23	C	504	CLA	C4D-CHA	2.50	1.47	1.38
24	a	416[A]	PHO	C4B-NB	-2.50	1.34	1.38
23	A	408	CLA	C3D-C4D	-2.50	1.38	1.44
23	C	506	CLA	C4C-C3C	2.50	1.49	1.45
23	c	509	CLA	C3B-C2B	2.50	1.49	1.41
27	D	403	GOL	C3-C2	2.50	1.61	1.51
23	c	504	CLA	C3D-C4D	-2.49	1.38	1.44
23	a	409	CLA	C4D-CHA	2.49	1.47	1.38
23	C	507	CLA	C3D-C4D	-2.49	1.38	1.44
23	B	601	CLA	C4D-CHA	2.49	1.46	1.38
23	C	511	CLA	C4C-C3C	2.49	1.49	1.45
23	c	509	CLA	C4B-NB	-2.49	1.34	1.37
23	B	602	CLA	C3D-C4D	-2.49	1.38	1.44
24	a	408[A]	PHO	C4B-NB	-2.48	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	625	HTG	C1-S1	-2.48	1.76	1.80
23	c	502	CLA	C1C-C2C	2.48	1.49	1.44
23	b	616	CLA	C1C-C2C	2.48	1.49	1.44
29	d	405[A]	PL9	C6-C5	2.48	1.47	1.35
23	c	504	CLA	C4C-C3C	2.48	1.49	1.45
23	B	608	CLA	C3D-C4D	-2.48	1.38	1.44
35	C	519	DGD	O2G-C2G	-2.48	1.40	1.46
31	t	101	LMT	O3'-C3'	-2.48	1.36	1.43
23	b	615	CLA	C3D-C4D	-2.48	1.38	1.44
23	B	608	CLA	C4D-CHA	2.47	1.46	1.38
23	b	612	CLA	C4C-C3C	2.47	1.49	1.45
23	A	405[B]	CLA	C4B-NB	-2.47	1.34	1.37
23	C	507	CLA	C1B-C2B	2.47	1.48	1.43
24	A	416[A]	PHO	C4B-NB	-2.47	1.34	1.38
23	A	404[B]	CLA	C4C-C3C	2.47	1.49	1.45
23	c	502	CLA	C4B-NB	-2.47	1.34	1.37
23	b	607	CLA	C4B-NB	-2.46	1.34	1.37
23	d	402[A]	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	510	CLA	C1C-C2C	2.46	1.49	1.44
23	b	601	CLA	C3B-C4B	2.46	1.49	1.42
23	B	605	CLA	C3B-C4B	2.46	1.49	1.42
23	a	409	CLA	C3B-C4B	2.46	1.49	1.42
23	b	615	CLA	C4C-C3C	2.46	1.49	1.45
23	b	611	CLA	C1C-C2C	2.46	1.49	1.44
27	a	419	GOL	C1-C2	2.46	1.61	1.51
39	f	101	HEM	C1D-ND	-2.46	1.34	1.38
23	d	402[A]	CLA	C1C-C2C	2.45	1.49	1.44
31	b	621	LMT	C3'-C2'	2.45	1.58	1.52
23	d	403	CLA	C1B-NB	-2.45	1.34	1.37
23	b	616	CLA	C1B-C2B	2.45	1.48	1.43
27	b	624	GOL	C3-C2	2.45	1.61	1.51
23	C	505	CLA	C3B-C2B	2.45	1.49	1.41
34	b	625	HTG	C1-S1	-2.45	1.76	1.80
23	A	406[A]	CLA	C4B-NB	-2.44	1.34	1.37
23	D	404[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	505	CLA	C1C-C2C	2.44	1.49	1.44
23	B	603	CLA	C1C-C2C	2.44	1.49	1.44
23	B	616	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	502	CLA	C4C-C3C	2.44	1.49	1.45
23	b	611	CLA	C3D-C4D	-2.44	1.38	1.44
27	D	414	GOL	O2-C2	-2.43	1.36	1.43
24	a	416[B]	PHO	C3A-C2A	-2.43	1.52	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C1C-C2C	2.43	1.49	1.44
23	c	510	CLA	C1C-C2C	2.43	1.49	1.44
23	b	604	CLA	C1C-C2C	2.43	1.49	1.44
23	b	606	CLA	C3B-C4B	2.43	1.49	1.42
23	c	512	CLA	C3B-C2B	2.43	1.49	1.41
24	A	416[B]	PHO	C3A-C2A	-2.42	1.52	1.54
23	B	616	CLA	C1C-C2C	2.42	1.49	1.44
23	C	503	CLA	C1C-C2C	2.42	1.49	1.44
23	B	603	CLA	C1B-C2B	2.42	1.48	1.43
23	B	608	CLA	C3B-C2B	2.42	1.49	1.41
23	c	513	CLA	C1B-C2B	2.42	1.48	1.43
23	b	607	CLA	OBD-CAD	2.42	1.26	1.22
23	b	607	CLA	C1C-C2C	2.41	1.49	1.44
23	c	507	CLA	C4D-CHA	2.41	1.46	1.38
23	B	615	CLA	C1C-C2C	2.41	1.49	1.44
27	d	412	GOL	O2-C2	-2.41	1.36	1.43
23	b	614	CLA	C4B-NB	-2.41	1.34	1.37
23	C	514	CLA	C3B-C2B	2.41	1.49	1.41
23	C	502	CLA	C3B-C4B	2.41	1.49	1.42
23	b	614	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	610	CLA	C1C-C2C	2.41	1.49	1.44
23	c	513	CLA	C1C-C2C	2.41	1.49	1.44
23	a	407[B]	CLA	C4C-C3C	2.41	1.49	1.45
23	a	407[A]	CLA	C3B-C4B	2.41	1.49	1.42
23	b	609	CLA	C1C-NC	-2.41	1.34	1.37
23	C	504	CLA	C1B-C2B	2.40	1.48	1.43
23	d	403	CLA	C1B-C2B	2.40	1.48	1.43
23	b	612	CLA	C3B-C2B	2.40	1.49	1.41
23	D	404[B]	CLA	C3B-C2B	2.40	1.49	1.41
23	C	504	CLA	C4C-C3C	2.40	1.49	1.45
23	B	614	CLA	C1B-NB	-2.40	1.34	1.37
23	D	404[A]	CLA	C3B-C2B	2.40	1.49	1.41
23	a	407[B]	CLA	C3B-C4B	2.40	1.49	1.42
23	b	602	CLA	C4C-C3C	2.40	1.49	1.45
23	A	405[B]	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	504	CLA	C3B-C4B	2.40	1.49	1.42
23	a	405[A]	CLA	C4C-C3C	2.39	1.49	1.45
23	b	601	CLA	C3B-C2B	2.39	1.49	1.41
23	a	406[B]	CLA	C4D-CHA	2.39	1.46	1.38
23	c	502	CLA	C1B-C2B	2.39	1.48	1.43
23	A	408	CLA	C3B-C2B	2.39	1.49	1.41
23	b	604	CLA	MG-NA	2.39	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	C4D-CHA	2.39	1.46	1.38
23	C	505	CLA	C4B-NB	-2.38	1.34	1.37
23	d	403	CLA	C3B-C4B	2.38	1.49	1.42
23	c	509	CLA	C1B-NB	-2.38	1.34	1.37
23	c	504	CLA	C4B-NB	-2.38	1.34	1.37
23	a	407[A]	CLA	C3D-C4D	-2.38	1.38	1.44
23	a	405[A]	CLA	C1C-C2C	2.38	1.49	1.44
23	b	613	CLA	C4C-C3C	2.38	1.49	1.45
23	b	611	CLA	C4D-CHA	2.37	1.46	1.38
23	D	404[A]	CLA	C1C-C2C	2.37	1.49	1.44
23	A	405[B]	CLA	C1C-C2C	2.36	1.49	1.44
23	B	614	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	614	CLA	C4C-C3C	2.36	1.49	1.45
35	H	102	DGD	O2G-C2G	-2.36	1.41	1.46
23	b	612	CLA	C3D-C4D	-2.36	1.38	1.44
23	C	512	CLA	C3D-C4D	-2.36	1.38	1.44
23	a	406[B]	CLA	C3B-C4B	2.35	1.49	1.42
23	a	405[B]	CLA	C3B-C2B	2.35	1.49	1.41
23	b	606	CLA	C1C-C2C	2.35	1.49	1.44
23	C	513	CLA	C1B-C2B	2.34	1.48	1.43
23	b	614	CLA	C1C-C2C	2.34	1.49	1.44
23	B	609	CLA	C1C-C2C	2.34	1.49	1.44
23	b	610	CLA	C3B-C4B	2.34	1.49	1.42
23	b	611	CLA	C3B-C2B	2.34	1.49	1.41
23	C	511	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	606	CLA	C4C-C3C	2.34	1.49	1.45
23	b	603	CLA	C1C-C2C	2.34	1.49	1.44
24	a	408[A]	PHO	C1D-ND	-2.34	1.34	1.38
31	B	630	LMT	O2B-C2B	-2.34	1.37	1.43
23	a	406[B]	CLA	C4B-NB	-2.34	1.34	1.37
23	B	604	CLA	C1B-NB	-2.34	1.34	1.37
23	d	402[B]	CLA	C1C-C2C	2.34	1.49	1.44
23	a	409	CLA	C4C-C3C	2.34	1.49	1.45
23	c	502	CLA	C3D-C4D	-2.34	1.38	1.44
23	c	514	CLA	C3D-C4D	-2.33	1.38	1.44
23	c	505	CLA	C1C-C2C	2.33	1.49	1.44
23	c	507	CLA	C3B-C2B	2.33	1.49	1.41
24	A	407[B]	PHO	C1D-ND	-2.33	1.34	1.38
23	A	404[A]	CLA	C1C-C2C	2.33	1.49	1.44
23	C	512	CLA	C3B-C4B	2.32	1.49	1.42
39	f	101	HEM	C1C-C2C	-2.32	1.40	1.45
23	B	601	CLA	C1B-C2B	2.32	1.48	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	MG-NA	2.32	2.11	2.06
23	B	604	CLA	C1C-C2C	2.32	1.49	1.44
23	c	514	CLA	C3B-C4B	2.32	1.49	1.42
23	c	510	CLA	C3B-C2B	2.32	1.49	1.41
23	B	613	CLA	C1C-C2C	2.32	1.49	1.44
23	c	512	CLA	C4B-NB	-2.31	1.34	1.37
23	c	512	CLA	C4C-C3C	2.31	1.49	1.45
23	B	601	CLA	C3B-C2B	2.31	1.48	1.41
23	d	402[B]	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	613	CLA	C4B-NB	-2.30	1.34	1.37
31	B	628	LMT	O3'-C3'	-2.30	1.37	1.43
23	c	505	CLA	C3B-C2B	2.30	1.48	1.41
24	a	416[B]	PHO	C4B-NB	-2.30	1.34	1.38
23	C	508	CLA	C3D-C4D	-2.30	1.39	1.44
23	A	406[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	C	512	CLA	C4C-C3C	2.30	1.48	1.45
27	D	403	GOL	O2-C2	-2.30	1.36	1.43
23	A	404[B]	CLA	C3D-C4D	-2.29	1.39	1.44
23	c	502	CLA	C3B-C4B	2.29	1.49	1.42
23	b	603	CLA	C3B-C2B	2.29	1.48	1.41
23	d	402[B]	CLA	C3B-C2B	2.29	1.48	1.41
23	a	406[A]	CLA	C3B-C4B	2.29	1.49	1.42
23	A	406[B]	CLA	C4C-C3C	2.29	1.48	1.45
23	b	615	CLA	C4B-NB	-2.29	1.34	1.37
23	c	507	CLA	C1C-C2C	2.29	1.49	1.44
23	B	613	CLA	C3B-C2B	2.28	1.48	1.41
23	B	602	CLA	C3B-C2B	2.28	1.48	1.41
23	B	604	CLA	C1A-CHA	2.28	1.52	1.43
23	B	612	CLA	C4C-C3C	2.28	1.48	1.45
34	B	622	HTG	O5-C1	2.28	1.46	1.42
23	b	613	CLA	C3B-C2B	2.28	1.48	1.41
23	B	615	CLA	C3B-C4B	2.27	1.49	1.42
24	a	416[B]	PHO	C1B-NB	-2.27	1.34	1.38
23	b	608	CLA	C3D-C4D	-2.27	1.39	1.44
23	C	507	CLA	C1C-C2C	2.27	1.49	1.44
23	c	511	CLA	C3B-C2B	2.27	1.48	1.41
31	A	419	LMT	O3'-C3'	-2.27	1.37	1.43
35	C	518[A]	DGD	O5D-C1E	2.27	1.44	1.40
23	B	606	CLA	C3B-C4B	2.27	1.49	1.42
23	c	511	CLA	C4B-NB	-2.27	1.34	1.37
23	D	404[B]	CLA	C3D-C4D	-2.27	1.39	1.44
23	A	405[A]	CLA	C3D-C4D	-2.26	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	416[A]	PHO	C1D-ND	-2.26	1.34	1.38
23	B	609	CLA	C3D-C4D	-2.26	1.39	1.44
31	M	101	LMT	O3'-C3'	-2.26	1.37	1.43
23	c	503	CLA	C1B-NB	-2.26	1.34	1.37
23	b	606	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	609	CLA	C3B-C4B	2.26	1.49	1.42
23	D	404[B]	CLA	C1C-C2C	2.26	1.49	1.44
23	D	405	CLA	C3D-C4D	-2.26	1.39	1.44
29	D	407[B]	PL9	C2-C3	2.26	1.40	1.34
31	M	101	LMT	O1'-C1'	-2.26	1.36	1.40
23	b	603	CLA	C3B-C4B	2.25	1.49	1.42
23	A	404[B]	CLA	C1C-C2C	2.25	1.49	1.44
41	V	201	HEC	CMB-C2B	2.25	1.55	1.50
23	b	609	CLA	C1C-C2C	2.25	1.49	1.44
23	b	614	CLA	C3B-C4B	2.25	1.49	1.42
23	C	513	CLA	C4B-NB	-2.24	1.34	1.37
31	A	419	LMT	O2'-C2'	-2.24	1.37	1.43
31	B	631	LMT	O3'-C3'	-2.24	1.37	1.43
23	a	407[B]	CLA	C3D-C4D	-2.24	1.39	1.44
39	F	102	HEM	C1D-ND	-2.24	1.34	1.38
23	B	601	CLA	C4C-C3C	2.24	1.48	1.45
23	C	506	CLA	C1C-C2C	2.24	1.49	1.44
23	b	608	CLA	C1C-C2C	2.24	1.49	1.44
23	b	608	CLA	C3B-C2B	2.24	1.48	1.41
31	e	101	LMT	O3'-C3'	-2.24	1.37	1.43
41	v	201	HEC	CMD-C2D	2.23	1.55	1.50
24	A	407[B]	PHO	C1B-NB	-2.23	1.34	1.38
23	A	404[B]	CLA	C3B-C2B	2.23	1.48	1.41
23	C	511	CLA	C3B-C2B	2.23	1.48	1.41
23	A	406[B]	CLA	C1C-C2C	2.23	1.49	1.44
23	c	513	CLA	C4B-NB	-2.23	1.34	1.37
23	C	506	CLA	C4B-NB	-2.23	1.34	1.37
23	a	405[B]	CLA	C3D-C4D	-2.23	1.39	1.44
27	o	303	GOL	C1-C2	2.23	1.60	1.51
31	M	102	LMT	O3'-C3'	-2.22	1.37	1.43
29	a	414[A]	PL9	C2-C3	2.22	1.40	1.34
23	c	507	CLA	C3D-C4D	-2.22	1.39	1.44
23	b	608	CLA	C3B-C4B	2.22	1.49	1.42
35	c	519	DGD	O2G-C2G	-2.22	1.41	1.46
23	b	601	CLA	C4C-C3C	2.22	1.48	1.45
23	c	513	CLA	C3D-C4D	-2.22	1.39	1.44
23	A	408	CLA	C1C-C2C	2.22	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C3B-C2B	2.22	1.48	1.41
23	A	404[A]	CLA	C3B-C2B	2.22	1.48	1.41
23	B	603	CLA	C3D-C4D	-2.22	1.39	1.44
23	C	509	CLA	C3D-C4D	-2.22	1.39	1.44
23	C	507	CLA	C3B-C2B	2.22	1.48	1.41
23	c	505	CLA	C1C-NC	-2.21	1.34	1.37
23	D	404[A]	CLA	C4C-C3C	2.21	1.48	1.45
23	b	616	CLA	C4B-NB	-2.21	1.35	1.37
23	C	514	CLA	C3D-C4D	-2.21	1.39	1.44
23	b	603	CLA	C1B-NB	-2.21	1.35	1.37
23	b	604	CLA	C3B-C4B	2.21	1.49	1.42
23	b	601	CLA	C1B-C2B	2.21	1.48	1.43
35	c	518[A]	DGD	O2G-C2G	-2.21	1.41	1.46
25	d	404	BCR	C30-C25	-2.20	1.51	1.53
23	C	503	CLA	C3B-C4B	2.20	1.49	1.42
23	C	503	CLA	C4D-CHA	2.20	1.46	1.38
23	b	605	CLA	C3B-C2B	2.20	1.48	1.41
24	A	407[B]	PHO	CBD-CGD	-2.20	1.49	1.52
23	c	508	CLA	C3D-C4D	-2.20	1.39	1.44
23	c	512	CLA	C3B-C4B	2.20	1.49	1.42
23	c	511	CLA	C3B-C4B	2.20	1.49	1.42
23	C	514	CLA	C3B-C4B	2.19	1.49	1.42
23	C	508	CLA	C3B-C2B	2.19	1.48	1.41
23	c	511	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	602	CLA	C1B-C2B	2.19	1.48	1.43
31	M	102	LMT	O2'-C2'	-2.18	1.37	1.43
39	F	102	HEM	C3B-C4B	2.18	1.49	1.44
23	B	615	CLA	C3D-C4D	-2.18	1.39	1.44
24	a	408[B]	PHO	C3A-C2A	-2.18	1.52	1.54
23	b	612	CLA	C3B-C4B	2.18	1.49	1.42
23	b	607	CLA	C3D-C4D	-2.18	1.39	1.44
23	c	506	CLA	C3D-C4D	-2.18	1.39	1.44
23	a	405[A]	CLA	C3B-C2B	2.18	1.48	1.41
23	b	616	CLA	C3B-C2B	2.18	1.48	1.41
23	c	514	CLA	C3B-C2B	2.18	1.48	1.41
23	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
33	D	413	LMG	O7-C8	-2.17	1.41	1.46
23	C	506	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	510	CLA	C3D-C4D	-2.17	1.39	1.44
31	A	417	LMT	O2'-C2'	-2.17	1.37	1.43
23	C	507	CLA	C1D-C2D	2.17	1.49	1.45
34	B	623	HTG	C1'-S1	-2.16	1.78	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	416[A]	PHO	C1B-NB	-2.16	1.34	1.38
23	c	505	CLA	C3D-C4D	-2.16	1.39	1.44
41	v	201	HEC	CMC-C2C	2.16	1.55	1.50
24	A	416[B]	PHO	C3D-C4D	-2.16	1.38	1.41
23	B	607	CLA	C1A-CHA	2.16	1.52	1.43
23	C	507	CLA	C3B-C4B	2.16	1.49	1.42
23	B	611	CLA	C3D-C4D	-2.15	1.39	1.44
23	b	605	CLA	C1C-C2C	2.15	1.48	1.44
23	C	512	CLA	C1C-NC	-2.15	1.34	1.37
23	C	509	CLA	C3B-C4B	2.15	1.49	1.42
23	B	615	CLA	C4B-NB	-2.15	1.35	1.37
23	c	509	CLA	C3D-C4D	-2.15	1.39	1.44
31	A	417	LMT	O3'-C3'	-2.15	1.37	1.43
23	C	503	CLA	C3B-C2B	2.14	1.48	1.41
23	C	511	CLA	C3B-C4B	2.14	1.49	1.42
23	C	513	CLA	C3B-C2B	2.14	1.48	1.41
23	c	509	CLA	C3B-C4B	2.14	1.49	1.42
31	m	103	LMT	O2B-C2B	-2.13	1.37	1.43
31	M	101	LMT	O2B-C2B	-2.13	1.37	1.43
31	F	101	LMT	O3'-C3'	-2.13	1.37	1.43
23	B	610	CLA	C3B-C4B	2.13	1.48	1.42
23	B	615	CLA	C4C-C3C	2.13	1.48	1.45
23	a	407[A]	CLA	C4C-C3C	2.13	1.48	1.45
23	A	406[A]	CLA	C3D-C4D	-2.12	1.39	1.44
23	C	510	CLA	C4C-C3C	2.12	1.48	1.45
29	a	414[B]	PL9	C2-C3	2.12	1.40	1.34
24	A	407[A]	PHO	C1B-NB	-2.12	1.34	1.38
23	A	406[B]	CLA	C3D-C4D	-2.12	1.39	1.44
23	C	509	CLA	C1B-NB	-2.12	1.35	1.37
41	V	201	HEC	CMD-C2D	2.12	1.55	1.50
32	d	413[A]	LHG	O7-C5	-2.12	1.41	1.46
23	B	607	CLA	C3B-C2B	2.12	1.48	1.41
23	d	403	CLA	C3D-C4D	-2.12	1.39	1.44
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
23	B	602	CLA	C4B-NB	-2.11	1.35	1.37
23	a	409	CLA	C1D-C2D	2.11	1.49	1.45
23	C	503	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	604	CLA	C1A-CHA	2.11	1.51	1.43
31	m	103	LMT	O3'-C3'	-2.11	1.37	1.43
23	C	508	CLA	C4C-C3C	2.11	1.48	1.45
23	a	405[A]	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	615	CLA	MG-NA	2.11	2.11	2.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C4C-C3C	2.11	1.48	1.45
23	B	613	CLA	C1A-CHA	2.10	1.51	1.43
23	B	606	CLA	C4B-NB	-2.10	1.35	1.37
23	B	614	CLA	C3B-C2B	2.10	1.48	1.41
23	b	610	CLA	C4B-NB	-2.10	1.35	1.37
23	d	402[A]	CLA	C3B-C2B	2.10	1.48	1.41
23	B	610	CLA	C4C-C3C	2.10	1.48	1.45
23	b	606	CLA	C3B-C2B	2.10	1.48	1.41
23	b	615	CLA	C3B-C4B	2.09	1.48	1.42
23	b	604	CLA	C3B-C2B	2.09	1.48	1.41
23	A	408	CLA	C3B-C4B	2.09	1.48	1.42
32	D	408[A]	LHG	O7-C5	-2.08	1.41	1.46
24	a	408[B]	PHO	CHA-CBD	-2.08	1.49	1.51
26	a	412	SQD	O6-C1	2.08	1.43	1.40
24	A	407[A]	PHO	C4B-NB	-2.08	1.34	1.38
23	A	408	CLA	C4C-C3C	2.07	1.48	1.45
23	b	608	CLA	C1C-NC	-2.07	1.34	1.37
23	A	406[A]	CLA	C1C-NC	-2.07	1.34	1.37
23	b	605	CLA	C4C-C3C	2.06	1.48	1.45
32	A	418[B]	LHG	O7-C5	-2.06	1.41	1.46
35	c	519	DGD	O5D-C1E	2.06	1.43	1.40
35	C	518[B]	DGD	O5D-C1E	2.06	1.43	1.40
23	B	602	CLA	C3B-C4B	2.06	1.48	1.42
23	c	513	CLA	C4C-C3C	2.05	1.48	1.45
25	B	619	BCR	C30-C25	-2.05	1.51	1.53
23	b	607	CLA	C4C-C3C	2.05	1.48	1.45
23	b	614	CLA	C3B-C2B	2.05	1.48	1.41
23	A	408	CLA	C1C-NC	-2.05	1.34	1.37
39	F	102	HEM	C3C-C4C	-2.05	1.42	1.46
23	B	603	CLA	C4C-C3C	2.05	1.48	1.45
29	A	414[A]	PL9	C2-C3	2.05	1.39	1.34
23	c	502	CLA	C1C-NC	-2.05	1.34	1.37
23	C	510	CLA	C1C-NC	-2.05	1.34	1.37
23	A	404[A]	CLA	C3D-C4D	-2.04	1.39	1.44
32	b	629[A]	LHG	O7-C5	-2.04	1.41	1.46
23	B	606	CLA	MG-NA	2.04	2.11	2.06
23	c	508	CLA	C1D-C2D	2.04	1.49	1.45
23	c	510	CLA	C3B-C4B	2.04	1.48	1.42
27	V	203[A]	GOL	C1-C2	2.04	1.59	1.51
23	B	616	CLA	C4C-C3C	2.04	1.48	1.45
23	a	406[A]	CLA	C1C-C2C	2.04	1.48	1.44
23	c	502	CLA	C1D-C2D	2.04	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C4B-NB	-2.04	1.34	1.38
23	B	605	CLA	C4B-NB	-2.04	1.35	1.37
23	B	606	CLA	C3B-C2B	2.03	1.48	1.41
24	a	408[A]	PHO	CHA-CBD	-2.03	1.49	1.51
24	a	416[B]	PHO	C1D-ND	-2.03	1.34	1.38
23	d	403	CLA	C4C-C3C	2.03	1.48	1.45
31	B	628	LMT	O5'-C5'	-2.03	1.39	1.44
31	B	631	LMT	O2'-C2'	-2.03	1.37	1.43
23	b	613	CLA	C3B-C4B	2.03	1.48	1.42
23	b	607	CLA	C3B-C2B	2.03	1.48	1.41
23	B	608	CLA	C4C-C3C	2.03	1.48	1.45
23	b	603	CLA	C4C-C3C	2.03	1.48	1.45
23	b	610	CLA	C3B-C2B	2.03	1.48	1.41
23	c	512	CLA	O2A-C1	-2.03	1.40	1.46
23	c	512	CLA	MG-NA	2.03	2.11	2.06
24	a	416[A]	PHO	C1D-ND	-2.03	1.35	1.38
29	A	414[B]	PL9	C2-C1	-2.02	1.39	1.44
32	L	101[A]	LHG	O7-C5	-2.02	1.41	1.46
23	b	605	CLA	C3B-C4B	2.02	1.48	1.42
23	b	607	CLA	CBD-CAD	-2.02	1.47	1.56
23	c	514	CLA	C1D-C2D	2.02	1.49	1.45
23	B	605	CLA	MG-NA	2.02	2.11	2.06
23	C	510	CLA	C3B-C4B	2.02	1.48	1.42
26	B	620	SQD	O6-C1	2.02	1.43	1.40
31	M	102	LMT	O3B-C3B	-2.02	1.38	1.43
23	a	407[B]	CLA	C1C-C2C	2.02	1.48	1.44
23	c	508	CLA	C4C-C3C	2.01	1.48	1.45
23	C	502	CLA	C3B-C2B	2.01	1.48	1.41
23	b	601	CLA	C3D-C4D	-2.01	1.39	1.44
24	a	408[B]	PHO	C1D-ND	-2.01	1.35	1.38
31	m	103	LMT	C3'-C2'	2.01	1.57	1.52
27	a	418	GOL	C3-C2	2.01	1.59	1.51
23	B	609	CLA	C4C-C3C	2.01	1.48	1.45
24	A	416[B]	PHO	C1B-NB	-2.00	1.35	1.38
24	a	416[A]	PHO	CHA-CBD	-2.00	1.49	1.51

All (3400) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C3B-C2B-C1B	-14.56	90.00	107.17
23	B	611	CLA	C1D-ND-C4D	-11.73	98.08	106.31
24	A	407[A]	PHO	C2D-C1D-ND	11.49	117.73	109.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	11.26	122.00	110.33
23	b	605	CLA	C1D-ND-C4D	-11.23	98.43	106.31
24	A	407[B]	PHO	C2D-C1D-ND	11.11	117.46	109.43
24	a	416[B]	PHO	C2D-C1D-ND	11.07	117.43	109.43
24	A	416[B]	PHO	C2D-C1D-ND	11.05	117.42	109.43
24	a	416[A]	PHO	C2D-C1D-ND	10.99	117.38	109.43
24	a	408[A]	PHO	C2D-C1D-ND	10.81	117.24	109.43
24	a	408[B]	PHO	C2D-C1D-ND	10.65	117.12	109.43
23	a	409	CLA	C1D-ND-C4D	-10.60	98.87	106.31
24	A	416[A]	PHO	C2D-C1D-ND	10.58	117.08	109.43
23	c	512	CLA	C1D-ND-C4D	-10.41	99.01	106.31
23	B	612	CLA	C1D-ND-C4D	-10.33	99.07	106.31
23	B	615	CLA	C1D-ND-C4D	-10.19	99.17	106.31
41	v	201	HEC	CBB-CAB-C3B	-10.16	107.13	127.43
23	b	614	CLA	C1D-ND-C4D	-10.12	99.21	106.31
23	C	504	CLA	C1D-ND-C4D	-10.02	99.28	106.31
23	a	405[B]	CLA	C1D-ND-C4D	-9.99	99.30	106.31
23	C	511	CLA	C1D-ND-C4D	-9.98	99.31	106.31
23	c	504	CLA	C1D-ND-C4D	-9.95	99.33	106.31
23	b	611	CLA	C1D-ND-C4D	-9.94	99.34	106.31
23	C	506	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	B	605	CLA	C1D-ND-C4D	-9.76	99.47	106.31
23	b	603	CLA	C1D-ND-C4D	-9.74	99.48	106.31
23	B	601	CLA	C1D-ND-C4D	-9.74	99.48	106.31
23	A	406[B]	CLA	C1D-ND-C4D	-9.73	99.48	106.31
23	b	602	CLA	C1D-ND-C4D	-9.73	99.49	106.31
23	a	407[B]	CLA	C1D-ND-C4D	-9.60	99.58	106.31
23	a	406[B]	CLA	C1D-ND-C4D	-9.59	99.58	106.31
23	A	404[B]	CLA	C1D-ND-C4D	-9.59	99.58	106.31
41	V	201	HEC	CBB-CAB-C3B	-9.59	108.27	127.43
23	b	610	CLA	C1D-ND-C4D	-9.57	99.60	106.31
23	d	402[B]	CLA	C1D-ND-C4D	-9.56	99.60	106.31
23	b	607	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	B	614	CLA	C1D-ND-C4D	-9.52	99.63	106.31
23	C	505	CLA	C1D-ND-C4D	-9.51	99.64	106.31
23	B	607	CLA	C1D-ND-C4D	-9.49	99.66	106.31
23	c	514	CLA	C1D-ND-C4D	-9.46	99.68	106.31
23	c	507	CLA	C1D-ND-C4D	-9.45	99.68	106.31
23	B	603	CLA	C1D-ND-C4D	-9.44	99.69	106.31
23	d	403	CLA	C1D-ND-C4D	-9.44	99.69	106.31
23	C	514	CLA	C1D-ND-C4D	-9.43	99.69	106.31
24	a	408[A]	PHO	O2D-CGD-CBD	9.43	121.31	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C1D-ND-C4D	-9.40	99.72	106.31
23	C	510	CLA	C1D-ND-C4D	-9.38	99.73	106.31
23	C	502	CLA	C1D-ND-C4D	-9.31	99.78	106.31
23	a	407[A]	CLA	C1D-ND-C4D	-9.26	99.82	106.31
23	D	404[B]	CLA	C1D-ND-C4D	-9.26	99.82	106.31
23	D	404[A]	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	c	506	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	B	602	CLA	C1D-ND-C4D	-9.23	99.84	106.31
23	B	606	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	d	402[A]	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	A	406[A]	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	a	406[A]	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	B	613	CLA	C1D-ND-C4D	-9.11	99.92	106.31
23	A	405[B]	CLA	C1D-ND-C4D	-9.11	99.92	106.31
23	b	615	CLA	C1D-ND-C4D	-9.07	99.95	106.31
24	a	416[A]	PHO	O2D-CGD-CBD	9.07	120.91	110.95
23	C	512	CLA	C1D-ND-C4D	-8.99	100.00	106.31
23	A	405[A]	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	A	408	CLA	C1D-ND-C4D	-8.98	100.01	106.31
23	B	608	CLA	C1D-ND-C4D	-8.98	100.01	106.31
23	a	405[A]	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	c	502	CLA	C1D-ND-C4D	-8.90	100.07	106.31
24	A	416[B]	PHO	O2D-CGD-CBD	8.89	120.72	110.95
23	b	608	CLA	C1D-ND-C4D	-8.88	100.08	106.31
23	b	612	CLA	C1D-ND-C4D	-8.86	100.09	106.31
23	c	513	CLA	C1D-ND-C4D	-8.82	100.12	106.31
24	a	408[B]	PHO	O2D-CGD-CBD	8.81	120.63	110.95
23	c	510	CLA	C1D-ND-C4D	-8.81	100.13	106.31
23	c	503	CLA	C1D-ND-C4D	-8.76	100.16	106.31
24	A	407[A]	PHO	C3B-C4B-NB	8.75	113.17	107.46
23	b	606	CLA	C1D-ND-C4D	-8.73	100.19	106.31
23	D	405	CLA	C1D-ND-C4D	-8.71	100.20	106.31
23	C	508	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	b	616	CLA	C1D-ND-C4D	-8.66	100.23	106.31
24	A	416[A]	PHO	O2D-CGD-CBD	8.64	120.44	110.95
23	B	609	CLA	C1D-ND-C4D	-8.64	100.25	106.31
23	c	509	CLA	C1D-ND-C4D	-8.63	100.26	106.31
23	c	508	CLA	C1D-ND-C4D	-8.61	100.27	106.31
23	A	404[A]	CLA	C1D-ND-C4D	-8.57	100.30	106.31
23	b	613	CLA	C1D-ND-C4D	-8.56	100.30	106.31
23	c	505	CLA	C1D-ND-C4D	-8.54	100.32	106.31
23	C	513	CLA	C1D-ND-C4D	-8.53	100.32	106.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C1D-ND-C4D	-8.53	100.33	106.31
24	a	416[B]	PHO	O2D-CGD-CBD	8.51	120.30	110.95
23	C	509	CLA	C1D-ND-C4D	-8.49	100.35	106.31
23	B	616	CLA	C1D-ND-C4D	-8.46	100.38	106.31
23	C	503	CLA	C1D-ND-C4D	-8.43	100.40	106.31
23	b	609	CLA	C1D-ND-C4D	-8.38	100.44	106.31
24	A	407[B]	PHO	O2D-CGD-CBD	8.28	120.05	110.95
23	B	610	CLA	C1D-ND-C4D	-8.16	100.58	106.31
23	c	511	CLA	C1D-ND-C4D	-8.13	100.61	106.31
24	a	408[A]	PHO	C3B-C4B-NB	8.10	112.75	107.46
23	b	604	CLA	C1D-ND-C4D	-7.96	100.73	106.31
24	a	416[A]	PHO	C3B-C4B-NB	7.89	112.61	107.46
24	A	407[B]	PHO	C3B-C4B-NB	7.84	112.58	107.46
23	B	611	CLA	CHD-C4C-C3C	-7.76	113.45	124.77
23	C	513	CLA	C4A-NA-C1A	-7.75	103.14	106.68
26	X	101	SQD	O6-C1-C2	7.72	119.99	108.27
23	B	611	CLA	CHB-C1B-NB	-7.71	112.49	124.05
23	B	611	CLA	CMB-C2B-C1B	7.68	137.11	125.42
24	A	416[A]	PHO	C3B-C4B-NB	7.61	112.43	107.46
23	C	504	CLA	C4A-NA-C1A	-7.58	103.22	106.68
23	B	604	CLA	C1D-ND-C4D	-7.44	101.09	106.31
24	A	416[B]	PHO	C3B-C4B-NB	7.37	112.27	107.46
24	a	408[B]	PHO	C3B-C4B-NB	7.33	112.24	107.46
23	c	502	CLA	CMD-C2D-C1D	7.32	137.62	124.73
23	b	605	CLA	CMD-C2D-C1D	7.31	137.61	124.73
23	B	611	CLA	C2D-C1D-ND	7.31	117.36	110.13
23	B	605	CLA	CHD-C4C-C3C	-7.31	114.11	124.77
24	A	416[A]	PHO	C2B-C1B-NB	7.26	114.68	109.43
23	c	508	CLA	O2D-CGD-CBD	7.26	123.92	111.23
24	A	407[A]	PHO	O2D-CGD-CBD	7.23	118.89	110.95
23	B	610	CLA	O2D-CGD-CBD	7.22	123.86	111.23
23	B	614	CLA	CMD-C2D-C1D	7.17	137.35	124.73
23	C	508	CLA	CMD-C2D-C1D	7.12	137.26	124.73
23	a	405[B]	CLA	CMD-C2D-C1D	7.09	137.22	124.73
23	B	607	CLA	C2D-C1D-ND	7.08	117.14	110.13
23	C	502	CLA	O2D-CGD-CBD	7.08	123.60	111.23
23	b	616	CLA	O2D-CGD-CBD	7.06	123.58	111.23
23	D	404[A]	CLA	C4A-NA-C1A	-7.05	103.46	106.68
23	B	609	CLA	C4A-NA-C1A	-6.98	103.50	106.68
23	B	611	CLA	CMD-C2D-C1D	6.96	136.98	124.73
23	b	614	CLA	O2D-CGD-CBD	6.94	123.36	111.23
23	b	606	CLA	C4A-NA-C1A	-6.93	103.52	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	CMD-C2D-C1D	6.90	136.88	124.73
23	b	602	CLA	C4A-NA-C1A	-6.88	103.54	106.68
23	B	616	CLA	O2D-CGD-CBD	6.88	123.25	111.23
23	C	511	CLA	CMD-C2D-C1D	6.86	136.82	124.73
23	b	611	CLA	CMD-C2D-C1D	6.86	136.81	124.73
23	B	606	CLA	O2D-CGD-CBD	6.86	123.22	111.23
23	b	616	CLA	CHD-C4C-C3C	-6.85	114.78	124.77
24	a	416[B]	PHO	C3B-C4B-NB	6.85	111.93	107.46
23	b	616	CLA	CMD-C2D-C1D	6.84	136.77	124.73
23	a	409	CLA	C2D-C1D-ND	6.83	116.88	110.13
23	b	611	CLA	CHD-C4C-C3C	-6.82	114.82	124.77
23	c	512	CLA	CHD-C4C-C3C	-6.80	114.86	124.77
23	A	404[B]	CLA	CMD-C2D-C1D	6.80	136.70	124.73
23	c	504	CLA	C4A-NA-C1A	-6.78	103.59	106.68
23	B	615	CLA	C4A-NA-C1A	-6.78	103.59	106.68
23	b	605	CLA	C2D-C1D-ND	6.77	116.83	110.13
23	b	610	CLA	O2D-CGD-CBD	6.76	123.05	111.23
23	B	606	CLA	CMD-C2D-C1D	6.76	136.63	124.73
24	a	416[A]	PHO	C2B-C1B-NB	6.74	114.30	109.43
23	c	507	CLA	CMD-C2D-C1D	6.73	136.59	124.73
23	b	606	CLA	CMD-C2D-C1D	6.73	136.57	124.73
23	b	614	CLA	C2D-C1D-ND	6.71	116.77	110.13
23	c	514	CLA	CMD-C2D-C1D	6.71	136.54	124.73
23	b	615	CLA	C4A-NA-C1A	-6.71	103.62	106.68
23	B	605	CLA	CMD-C2D-C1D	6.70	136.53	124.73
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.73
23	b	607	CLA	C2D-C1D-ND	6.70	116.76	110.13
23	b	610	CLA	CHD-C4C-C3C	-6.69	115.02	124.77
23	B	605	CLA	C4A-NA-C1A	-6.67	103.64	106.68
23	C	507	CLA	CMD-C2D-C1D	6.67	136.47	124.73
23	B	616	CLA	CHD-C4C-C3C	-6.66	115.06	124.77
24	a	416[B]	PHO	C2B-C1B-NB	6.65	114.24	109.43
26	A	410[A]	SQD	O6-C1-C2	6.64	118.36	108.27
23	b	611	CLA	C2D-C1D-ND	6.63	116.69	110.13
23	C	508	CLA	O2D-CGD-CBD	6.63	122.83	111.23
23	c	508	CLA	CMD-C2D-C1D	6.63	136.41	124.73
23	b	604	CLA	O2D-CGD-CBD	6.62	122.81	111.23
23	B	603	CLA	CHD-C4C-C3C	-6.62	115.12	124.77
23	a	406[A]	CLA	CHD-C4C-C3C	-6.62	115.12	124.77
23	B	612	CLA	C2D-C1D-ND	6.61	116.67	110.13
23	B	615	CLA	C2D-C1D-ND	6.61	116.67	110.13
23	b	603	CLA	CHD-C4C-C3C	-6.59	115.17	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	b	605	CLA	CHD-C4C-C3C	-6.57	115.19	124.77
23	C	513	CLA	CHD-C4C-C3C	-6.55	115.22	124.77
23	B	602	CLA	O2D-CGD-CBD	6.54	122.66	111.23
23	B	610	CLA	C2D-C1D-ND	6.52	116.58	110.13
23	D	404[B]	CLA	C4A-NA-C1A	-6.51	103.71	106.68
23	c	504	CLA	CMD-C2D-C1D	6.50	136.18	124.73
23	C	505	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	a	406[A]	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	d	403	CLA	C2D-C1D-ND	6.47	116.53	110.13
23	C	504	CLA	CHD-C4C-C3C	-6.46	115.36	124.77
23	b	603	CLA	C2D-C1D-ND	6.45	116.51	110.13
23	A	408	CLA	C2D-C1D-ND	6.44	116.50	110.13
23	B	601	CLA	CMD-C2D-C1D	6.44	136.07	124.73
23	B	614	CLA	C2D-C1D-ND	6.44	116.50	110.13
23	c	503	CLA	C2D-C1D-ND	6.43	116.49	110.13
23	b	610	CLA	CMD-C2D-C1D	6.42	136.04	124.73
23	B	613	CLA	C2D-C1D-ND	6.42	116.48	110.13
23	a	407[A]	CLA	C2D-C1D-ND	6.42	116.48	110.13
23	a	407[A]	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
23	a	406[B]	CLA	CMD-C2D-C1D	6.40	136.00	124.73
23	B	605	CLA	C2D-C1D-ND	6.40	116.46	110.13
23	b	616	CLA	C4A-NA-C1A	-6.38	103.77	106.68
23	a	409	CLA	CHD-C4C-C3C	-6.37	115.48	124.77
23	C	512	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
24	A	416[B]	PHO	C2B-C1B-NB	6.36	114.03	109.43
23	B	606	CLA	C4A-NA-C1A	-6.36	103.78	106.68
23	b	602	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
23	B	603	CLA	C2D-C1D-ND	6.35	116.41	110.13
23	B	610	CLA	CHD-C4C-C3C	-6.34	115.52	124.77
23	b	606	CLA	CHD-C4C-C3C	-6.34	115.53	124.77
23	B	604	CLA	CMD-C2D-C1D	6.34	135.88	124.73
24	a	408[A]	PHO	C2B-C1B-NB	6.33	114.01	109.43
23	b	608	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	a	406[B]	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	C	513	CLA	CMD-C2D-C1D	6.32	135.87	124.73
23	c	511	CLA	C4A-NA-C1A	-6.31	103.80	106.68
23	D	404[A]	CLA	C2D-C1D-ND	6.30	116.37	110.13
23	B	615	CLA	CHD-C4C-C3C	-6.30	115.58	124.77
23	b	613	CLA	CMD-C2D-C1D	6.30	135.82	124.73
23	C	504	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	A	404[A]	CLA	C4A-NA-C1A	-6.29	103.81	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	CMD-C2D-C1D	6.29	135.80	124.73
23	c	504	CLA	C2D-C1D-ND	6.28	116.34	110.13
24	A	407[A]	PHO	C4D-ND-C1D	-6.28	101.35	108.87
23	c	509	CLA	CHD-C4C-C3C	-6.27	115.63	124.77
23	d	402[B]	CLA	C4A-NA-C1A	-6.27	103.82	106.68
23	b	602	CLA	O2D-CGD-CBD	6.26	122.18	111.23
23	B	606	CLA	C2D-C1D-ND	6.26	116.32	110.13
23	C	506	CLA	CMD-C2D-C1D	6.26	135.75	124.73
26	X	101	SQD	O47-C7-C8	6.26	125.02	111.48
23	c	513	CLA	C4A-NA-C1A	-6.25	103.83	106.68
23	b	613	CLA	C4A-NA-C1A	-6.25	103.83	106.68
23	C	510	CLA	C2D-C1D-ND	6.24	116.30	110.13
23	B	608	CLA	C2D-C1D-ND	6.24	116.30	110.13
23	c	509	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	d	402[B]	CLA	CMD-C2D-C1D	6.22	135.68	124.73
23	c	504	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
23	c	505	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	c	503	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
23	C	505	CLA	CMD-C2D-C1D	6.20	135.65	124.73
23	D	405	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
23	b	610	CLA	C2D-C1D-ND	6.20	116.26	110.13
23	B	606	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
23	b	607	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
23	D	404[B]	CLA	CMD-C2D-C1D	6.19	135.63	124.73
23	b	601	CLA	O2D-CGD-CBD	6.17	122.02	111.23
23	a	406[B]	CLA	CHD-C4C-C3C	-6.17	115.78	124.77
23	a	407[B]	CLA	CMD-C2D-C1D	6.17	135.59	124.73
24	a	408[B]	PHO	C2B-C1B-NB	6.17	113.89	109.43
23	b	601	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
26	B	620	SQD	O6-C1-C2	6.16	117.63	108.27
23	B	601	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
23	c	510	CLA	CMD-C2D-C1D	6.14	135.55	124.73
23	A	404[B]	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	c	513	CLA	CHD-C4C-C3C	-6.13	115.83	124.77
23	B	603	CLA	O2D-CGD-CBD	6.13	121.94	111.23
23	C	511	CLA	CHD-C4C-C3C	-6.12	115.84	124.77
23	C	508	CLA	CHD-C4C-C3C	-6.12	115.84	124.77
23	A	405[A]	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	b	607	CLA	CMD-C2D-C1D	6.11	135.50	124.73
23	c	511	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	C	514	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	D	404[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C2D-C1D-ND	6.09	116.15	110.13
23	C	502	CLA	CMD-C2D-C1D	6.09	135.45	124.73
23	B	601	CLA	C2D-C1D-ND	6.09	116.15	110.13
23	b	613	CLA	CHD-C4C-C3C	-6.08	115.90	124.77
23	B	604	CLA	C1-C2-C3	-6.08	116.23	126.20
23	B	612	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	a	405[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	C	509	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	c	507	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	C	508	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	A	406[A]	CLA	C2D-C1D-ND	6.05	116.11	110.13
25	K	103	BCR	C33-C5-C6	-6.05	117.89	124.48
23	b	616	CLA	C2D-C1D-ND	6.04	116.11	110.13
23	b	615	CLA	CMD-C2D-C1D	6.04	135.36	124.73
23	b	602	CLA	CMD-C2D-C1D	6.03	135.35	124.73
23	a	405[A]	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	C	509	CLA	CHD-C4C-C3C	-6.03	115.99	124.77
23	A	404[B]	CLA	CHD-C4C-C3C	-6.02	115.99	124.77
23	a	407[A]	CLA	C4A-NA-C1A	-6.02	103.93	106.68
23	C	512	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	D	405	CLA	O2D-CGD-CBD	6.01	121.74	111.23
23	A	406[B]	CLA	C4A-NA-C1A	-6.01	103.94	106.68
23	b	612	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
23	B	609	CLA	CMD-C2D-C1D	6.01	135.30	124.73
23	b	601	CLA	C2D-C1D-ND	6.00	116.07	110.13
26	A	410[B]	SQD	O6-C1-C2	6.00	117.39	108.27
24	A	407[A]	PHO	C2B-C1B-NB	6.00	113.77	109.43
23	D	404[B]	CLA	C2D-C1D-ND	6.00	116.06	110.13
23	D	405	CLA	CMD-C2D-C1D	6.00	135.29	124.73
23	d	403	CLA	O2D-CGD-CBD	6.00	121.71	111.23
34	b	623	HTG	C1'-S1-C1	5.98	113.37	100.45
23	c	506	CLA	C4A-NA-C1A	-5.98	103.95	106.68
23	B	603	CLA	CMD-C2D-C1D	5.98	135.26	124.73
23	a	405[B]	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	C	514	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	b	613	CLA	C2D-C1D-ND	5.95	116.02	110.13
23	C	511	CLA	C2D-C1D-ND	5.95	116.01	110.13
23	b	614	CLA	CHD-C4C-C3C	-5.94	116.11	124.77
23	c	505	CLA	C2D-C1D-ND	5.93	116.00	110.13
23	b	602	CLA	C2D-C1D-ND	5.93	116.00	110.13
23	C	505	CLA	CHD-C4C-C3C	-5.93	116.13	124.77
23	c	511	CLA	CMD-C2D-C1D	5.93	135.17	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.73
23	C	511	CLA	O2D-CGD-CBD	5.92	121.57	111.23
23	A	406[B]	CLA	C2D-C1D-ND	5.92	115.98	110.13
23	B	609	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
23	c	510	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
23	A	405[B]	CLA	CMD-C2D-C1D	5.90	135.12	124.73
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.73
23	B	604	CLA	C2C-C1C-NC	5.89	116.17	109.98
23	B	602	CLA	C2D-C1D-ND	5.89	115.95	110.13
23	d	402[B]	CLA	C2D-C1D-ND	5.89	115.95	110.13
23	b	608	CLA	CHD-C4C-C3C	-5.88	116.20	124.77
23	A	405[B]	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	A	408	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
26	a	411[A]	SQD	O6-C1-C2	5.87	117.19	108.27
23	C	502	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
23	D	405	CLA	C2D-C1D-ND	5.87	115.94	110.13
23	B	607	CLA	CHD-C4C-C3C	-5.87	116.22	124.77
23	B	608	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
25	D	406	BCR	C7-C8-C9	-5.86	117.57	126.23
23	c	510	CLA	C2D-C1D-ND	5.85	115.92	110.13
23	a	407[B]	CLA	C2D-C1D-ND	5.85	115.92	110.13
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
23	C	507	CLA	C2C-C1C-NC	5.85	116.12	109.98
23	B	616	CLA	C2D-C1D-ND	5.85	115.91	110.13
23	B	602	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
23	C	509	CLA	C2C-C1C-NC	5.84	116.11	109.98
23	b	605	CLA	O2D-CGD-CBD	5.83	121.42	111.23
23	C	506	CLA	C2D-C1D-ND	5.82	115.89	110.13
23	d	403	CLA	CMD-C2D-C1D	5.82	134.98	124.73
23	c	507	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
26	b	620	SQD	O6-C1-C2	5.82	117.11	108.27
23	c	513	CLA	C2D-C1D-ND	5.82	115.88	110.13
23	b	604	CLA	CMD-C2D-C1D	5.82	134.97	124.73
23	A	405[B]	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
23	b	611	CLA	O2D-CGD-CBD	5.81	121.38	111.23
23	c	506	CLA	CHD-C4C-C3C	-5.81	116.31	124.77
23	d	402[A]	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	a	407[B]	CLA	C4A-NA-C1A	-5.80	104.03	106.68
24	a	416[B]	PHO	C4D-ND-C1D	-5.79	101.94	108.87
23	c	502	CLA	C4A-NA-C1A	-5.79	104.04	106.68
23	A	408	CLA	CMD-C2D-C1D	5.79	134.92	124.73
24	a	416[A]	PHO	C1-C2-C3	-5.78	116.72	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	C2D-C1D-ND	5.78	115.85	110.13
23	d	402[A]	CLA	C2C-C1C-NC	5.78	116.05	109.98
23	c	508	CLA	C2D-C1D-ND	5.78	115.84	110.13
23	C	503	CLA	CHD-C4C-C3C	-5.77	116.35	124.77
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	A	406[A]	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	a	409	CLA	O2D-CGD-CBD	5.76	121.30	111.23
23	b	609	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
23	C	510	CLA	CHD-C4C-C3C	-5.76	116.38	124.77
23	C	506	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
23	c	502	CLA	C2D-C1D-ND	5.75	115.82	110.13
23	B	602	CLA	C4A-NA-C1A	-5.75	104.06	106.68
24	A	407[B]	PHO	C4D-ND-C1D	-5.74	101.99	108.87
23	C	510	CLA	CMD-C2D-C1D	5.74	134.84	124.73
24	a	416[A]	PHO	C4D-ND-C1D	-5.74	101.99	108.87
24	A	416[B]	PHO	C4D-ND-C1D	-5.74	101.99	108.87
23	d	403	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
23	B	603	CLA	C4A-NA-C1A	-5.74	104.06	106.68
23	c	509	CLA	O2D-CGD-CBD	5.73	121.25	111.23
23	C	502	CLA	C2D-C1D-ND	5.73	115.80	110.13
23	C	514	CLA	CMD-C2D-C1D	5.72	134.81	124.73
23	C	508	CLA	C3B-C2B-C1B	-5.71	100.44	107.17
23	C	503	CLA	C2D-C1D-ND	5.71	115.78	110.13
23	D	405	CLA	C4A-NA-C1A	-5.71	104.08	106.68
23	c	506	CLA	O2D-CGD-CBD	5.70	121.20	111.23
23	B	614	CLA	C3B-C2B-C1B	-5.70	100.45	107.17
23	B	601	CLA	O2D-CGD-CBD	5.69	121.18	111.23
26	A	410[A]	SQD	C1-O5-C5	-5.69	102.61	113.72
24	A	407[A]	PHO	C3D-C4D-ND	5.69	115.00	107.71
23	b	609	CLA	C4A-NA-C1A	-5.68	104.09	106.68
23	c	514	CLA	C2D-C1D-ND	5.68	115.75	110.13
23	B	604	CLA	CHD-C4C-C3C	-5.68	116.50	124.77
23	A	404[A]	CLA	C2D-C1D-ND	5.67	115.73	110.13
24	A	416[B]	PHO	C3D-C4D-ND	5.66	114.97	107.71
23	B	607	CLA	O2D-CGD-CBD	5.66	121.13	111.23
23	C	512	CLA	CMD-C2D-C1D	5.66	134.69	124.73
23	c	503	CLA	C2C-C1C-NC	5.65	115.92	109.98
23	B	605	CLA	O2D-CGD-CBD	5.65	121.10	111.23
23	d	402[B]	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
23	B	602	CLA	CMD-C2D-C1D	5.63	134.65	124.73
23	B	611	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
23	A	408	CLA	C3B-C2B-C1B	-5.61	100.55	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	C2C-C1C-NC	5.61	115.88	109.98
23	b	615	CLA	CHD-C4C-C3C	-5.59	116.62	124.77
23	C	506	CLA	C4A-NA-C1A	-5.59	104.13	106.68
23	b	608	CLA	O2D-CGD-CBD	5.59	121.00	111.23
23	C	513	CLA	O2D-CGD-CBD	5.59	121.00	111.23
23	c	508	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
23	c	512	CLA	CMD-C2D-C1D	5.58	134.55	124.73
23	c	513	CLA	O2D-CGD-CBD	5.57	120.96	111.23
23	B	609	CLA	C2D-C1D-ND	5.57	115.64	110.13
23	B	614	CLA	C2C-C1C-NC	5.56	115.82	109.98
23	c	514	CLA	C4A-NA-C1A	-5.56	104.14	106.68
23	b	606	CLA	C2D-C1D-ND	5.55	115.62	110.13
23	D	404[B]	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
23	D	404[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
23	b	604	CLA	CHD-C4C-C3C	-5.53	116.70	124.77
23	C	503	CLA	O2D-CGD-CBD	5.53	120.90	111.23
23	A	406[B]	CLA	CHD-C4C-C3C	-5.53	116.72	124.77
23	a	405[A]	CLA	C2C-C1C-NC	5.53	115.79	109.98
23	A	406[B]	CLA	CMD-C2D-C1D	5.53	134.46	124.73
24	a	416[A]	PHO	C3D-C4D-ND	5.52	114.79	107.71
23	b	601	CLA	C4A-NA-C1A	-5.52	104.16	106.68
23	b	604	CLA	C2C-C1C-NC	5.52	115.78	109.98
23	a	405[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
23	d	402[A]	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
24	A	416[A]	PHO	C4D-ND-C1D	-5.49	102.29	108.87
23	a	409	CLA	CMD-C2D-C1D	5.48	134.39	124.73
23	a	407[A]	CLA	CMD-C2D-C1D	5.48	134.38	124.73
23	B	608	CLA	O2D-CGD-CBD	5.48	120.81	111.23
24	a	416[B]	PHO	C3D-C4D-ND	5.47	114.72	107.71
23	B	612	CLA	O2D-CGD-CBD	5.46	120.78	111.23
23	B	615	CLA	CMD-C2D-C1D	5.46	134.34	124.73
23	c	511	CLA	C2D-C1D-ND	5.45	115.52	110.13
25	t	102	BCR	C33-C5-C6	-5.45	118.53	124.48
23	B	614	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
23	b	612	CLA	C1-C2-C3	-5.44	117.28	126.20
23	b	614	CLA	O2D-CGD-O1D	-5.44	113.26	123.85
23	B	610	CLA	CMD-C2D-C1D	5.44	134.31	124.73
23	C	502	CLA	O2D-CGD-O1D	-5.44	113.26	123.85
23	c	513	CLA	C2B-C1B-NB	5.44	115.96	110.33
23	B	614	CLA	CHD-C4C-C3C	-5.43	116.85	124.77
23	d	402[A]	CLA	CMD-C2D-C1D	5.43	134.30	124.73
23	C	506	CLA	O2D-CGD-CBD	5.43	120.73	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	v	201	HEC	CBC-CAC-C3C	-5.43	116.58	127.43
23	A	408	CLA	C3D-C2D-C1D	-5.43	98.43	105.83
23	a	405[A]	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	B	613	CLA	CMD-C2D-C1D	5.42	134.26	124.73
23	C	503	CLA	CMD-C2D-C1D	5.41	134.26	124.73
23	b	607	CLA	C3D-C2D-C1D	-5.41	98.45	105.83
23	C	505	CLA	C2C-C1C-NC	5.39	115.64	109.98
23	B	608	CLA	CMD-C2D-C1D	5.39	134.22	124.73
23	A	408	CLA	C2C-C1C-NC	5.38	115.63	109.98
23	B	614	CLA	O2D-CGD-CBD	5.38	120.63	111.23
23	c	514	CLA	CHD-C4C-C3C	-5.37	116.94	124.77
23	b	616	CLA	C3D-C2D-C1D	-5.37	98.50	105.83
26	B	620	SQD	O47-C7-C8	5.37	123.09	111.48
23	c	503	CLA	O2D-CGD-CBD	5.36	120.61	111.23
23	B	610	CLA	C3D-C2D-C1D	-5.36	98.52	105.83
23	c	507	CLA	C2C-C1C-NC	5.36	115.61	109.98
23	b	608	CLA	C4A-NA-C1A	-5.36	104.23	106.68
23	b	609	CLA	C2D-C1D-ND	5.35	115.42	110.13
23	b	612	CLA	C2D-C1D-ND	5.35	115.42	110.13
24	A	407[B]	PHO	C3D-C4D-ND	5.34	114.55	107.71
23	b	604	CLA	C2D-C1D-ND	5.34	115.41	110.13
23	c	505	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
23	d	402[B]	CLA	C2C-C1C-NC	5.33	115.58	109.98
24	a	408[B]	PHO	C4D-ND-C1D	-5.33	102.48	108.87
33	C	501	LMG	C7-O1-C1	-5.32	102.39	113.80
23	B	613	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
23	B	610	CLA	C4A-NA-C1A	-5.31	104.25	106.68
23	B	601	CLA	C4A-NA-C1A	-5.30	104.26	106.68
23	A	408	CLA	C2B-C1B-NB	5.30	115.83	110.33
23	B	613	CLA	C1-C2-C3	-5.30	117.51	126.20
26	A	410[A]	SQD	C1-C2-C3	-5.30	98.86	110.01
23	b	603	CLA	C4A-NA-C1A	-5.30	104.26	106.68
23	B	602	CLA	C2C-C1C-NC	5.29	115.54	109.98
23	b	603	CLA	CMD-C2D-C1D	5.29	134.04	124.73
23	b	605	CLA	C3D-C2D-C1D	-5.28	98.62	105.83
24	A	416[A]	PHO	C3D-C4D-ND	5.28	114.48	107.71
23	C	514	CLA	C4A-NA-C1A	-5.28	104.27	106.68
23	c	510	CLA	C1-C2-C3	-5.28	117.55	126.20
23	b	613	CLA	C2C-C1C-NC	5.28	115.52	109.98
23	a	407[B]	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
23	B	613	CLA	C2C-C1C-NC	5.27	115.52	109.98
23	a	405[B]	CLA	CHD-C4C-C3C	-5.27	117.09	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C2B-C1B-NB	5.26	115.78	110.33
23	B	605	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	b	611	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	c	505	CLA	C2C-C1C-NC	5.26	115.50	109.98
23	C	507	CLA	CHD-C4C-C3C	-5.26	117.11	124.77
23	c	506	CLA	CMD-C2D-C1D	5.25	133.97	124.73
34	D	412	HTG	C1'-S1-C1	5.25	111.78	100.45
23	D	404[B]	CLA	C2C-C1C-NC	5.25	115.49	109.98
23	C	507	CLA	C2D-C1D-ND	5.24	115.32	110.13
23	C	512	CLA	O2D-CGD-CBD	5.24	120.40	111.23
23	A	405[A]	CLA	C4A-NA-C1A	-5.24	104.29	106.68
26	b	620	SQD	O47-C7-C8	5.24	122.82	111.48
23	d	403	CLA	C2B-C1B-NB	5.24	115.76	110.33
23	D	404[A]	CLA	C2C-C1C-NC	5.23	115.48	109.98
23	C	507	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
23	c	505	CLA	O2D-CGD-CBD	5.23	120.37	111.23
23	B	616	CLA	C3B-C4B-NB	5.22	115.19	110.53
23	c	513	CLA	CMD-C2D-C1D	5.21	133.90	124.73
23	b	609	CLA	CMD-C2D-C1D	5.20	133.89	124.73
23	A	404[A]	CLA	C2C-C1C-NC	5.20	115.44	109.98
34	c	522	HTG	C1'-S1-C1	5.20	111.67	100.45
23	c	509	CLA	C2C-C1C-NC	5.20	115.44	109.98
23	a	406[B]	CLA	C2C-C1C-NC	5.19	115.43	109.98
23	C	502	CLA	C4A-NA-C1A	-5.18	104.32	106.68
23	C	509	CLA	CMD-C2D-C1D	5.18	133.84	124.73
24	a	408[A]	PHO	C4D-ND-C1D	-5.17	102.68	108.87
23	b	605	CLA	CHD-C1D-ND	-5.17	117.53	124.80
23	d	403	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
23	c	504	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	C	513	CLA	C2D-C1D-ND	5.16	115.23	110.13
23	B	607	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	b	604	CLA	C1-C2-C3	-5.15	117.76	126.20
23	c	502	CLA	CHD-C1D-ND	-5.14	117.56	124.80
23	a	409	CLA	C2C-C1C-NC	5.13	115.37	109.98
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.77
26	f	102	SQD	O47-C7-C8	5.12	122.55	111.48
23	A	405[A]	CLA	O2D-CGD-CBD	5.11	120.17	111.23
23	B	607	CLA	CMD-C2D-C1D	5.11	133.72	124.73
23	c	508	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
23	b	609	CLA	C2C-C1C-NC	5.09	115.33	109.98
34	b	622	HTG	C1-O5-C5	5.09	121.69	112.56
23	C	505	CLA	C3D-C2D-C1D	-5.09	98.88	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[B]	PL9	C7-C8-C9	-5.08	118.07	126.83
23	c	509	CLA	C3D-C2D-C1D	-5.08	98.89	105.83
23	b	603	CLA	C2C-C1C-NC	5.08	115.32	109.98
23	c	508	CLA	C2C-C1C-NC	5.08	115.32	109.98
23	c	508	CLA	C4A-NA-C1A	-5.08	104.36	106.68
23	a	406[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	b	612	CLA	CMD-C2D-C1D	5.08	133.67	124.73
23	A	404[B]	CLA	C4A-NA-C1A	-5.07	104.36	106.68
26	a	411[A]	SQD	O47-C7-C8	5.07	122.45	111.48
23	B	614	CLA	C4A-NA-C1A	-5.07	104.37	106.68
23	C	512	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
23	B	606	CLA	C2C-C1C-NC	5.06	115.30	109.98
23	D	404[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
26	b	620	SQD	C1-O5-C5	-5.06	103.83	113.72
23	c	511	CLA	C1-C2-C3	-5.06	117.91	126.20
23	d	403	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	C	510	CLA	C2C-C1C-NC	5.06	115.29	109.98
23	b	614	CLA	C4A-NA-C1A	-5.05	104.37	106.68
23	C	513	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
23	c	507	CLA	C4A-NA-C1A	-5.05	104.37	106.68
23	c	503	CLA	C3B-C2B-C1B	-5.04	101.22	107.17
23	b	606	CLA	C2B-C1B-NB	5.04	115.56	110.33
23	A	406[B]	CLA	C3D-C4D-ND	5.04	118.18	109.99
23	b	614	CLA	CMD-C2D-C1D	5.04	133.60	124.73
23	B	603	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	D	405	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
26	a	411[B]	SQD	O6-C1-C2	5.03	115.92	108.27
24	A	407[B]	PHO	C2B-C1B-NB	5.03	113.06	109.43
23	B	606	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
23	C	509	CLA	C3C-C4C-NC	5.02	116.86	110.43
25	b	617	BCR	C7-C8-C9	-5.01	118.82	126.23
23	c	505	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
23	C	507	CLA	C4A-NA-C1A	-5.01	104.39	106.68
23	C	513	CLA	C2B-C1B-NB	5.00	115.51	110.33
23	C	508	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	c	514	CLA	C2C-C1C-NC	5.00	115.23	109.98
23	B	611	CLA	O2D-CGD-CBD	5.00	119.97	111.23
23	b	605	CLA	C3D-C4D-ND	4.99	118.10	109.99
23	B	604	CLA	O2D-CGD-CBD	4.99	119.96	111.23
23	C	511	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	D	404[B]	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
23	b	606	CLA	O2D-CGD-CBD	4.98	119.93	111.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
23	C	507	CLA	C1C-C2C-C3C	-4.97	101.75	106.98
23	B	607	CLA	C4A-NA-C1A	-4.97	104.41	106.68
23	b	613	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	B	616	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	a	407[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	c	509	CLA	CMD-C2D-C1D	4.96	133.46	124.73
23	B	615	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	b	607	CLA	C2C-C1C-NC	4.95	115.19	109.98
24	a	408[B]	PHO	C3D-C4D-ND	4.95	114.06	107.71
26	a	411[A]	SQD	C1-O5-C5	-4.95	104.05	113.72
23	b	602	CLA	C2B-C1B-NB	4.95	115.46	110.33
23	c	511	CLA	O2D-CGD-CBD	4.95	119.88	111.23
23	B	613	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
24	a	408[A]	PHO	C3D-C4D-ND	4.94	114.04	107.71
23	A	406[B]	CLA	O2D-CGD-CBD	4.94	119.86	111.23
23	A	405[A]	CLA	C2C-C1C-NC	4.93	115.17	109.98
23	b	615	CLA	C2C-C1C-NC	4.93	115.17	109.98
23	c	502	CLA	CHD-C4C-C3C	-4.93	117.58	124.77
23	a	407[B]	CLA	C3D-C4D-ND	4.93	118.00	109.99
23	b	610	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	C	507	CLA	C2B-C1B-NB	4.92	115.43	110.33
24	a	416[B]	PHO	C1-C2-C3	-4.92	118.14	126.20
23	c	513	CLA	C3B-C2B-C1B	-4.91	101.38	107.17
23	B	603	CLA	C2C-C1C-NC	4.91	115.14	109.98
39	f	101	HEM	CHC-C4B-NB	4.91	129.71	124.42
23	C	503	CLA	C2C-C1C-NC	4.91	115.14	109.98
25	T	101	BCR	C11-C10-C9	-4.91	120.40	127.28
23	a	407[B]	CLA	C2B-C1B-NB	4.90	115.41	110.33
23	b	606	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	a	406[A]	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	b	611	CLA	C2C-C1C-NC	4.89	115.12	109.98
23	B	612	CLA	CMD-C2D-C1D	4.89	133.35	124.73
34	d	410	HTG	C1'-S1-C1	4.89	111.01	100.45
23	c	510	CLA	O2D-CGD-CBD	4.89	119.78	111.23
23	C	504	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	A	406[B]	CLA	C2B-C1B-NB	4.89	115.39	110.33
23	B	616	CLA	C3C-C4C-NC	4.89	116.69	110.43
29	a	414[B]	PL9	C7-C3-C4	4.88	120.93	116.91
23	B	613	CLA	O2D-CGD-CBD	4.88	119.76	111.23
25	d	404	BCR	C7-C8-C9	-4.88	119.02	126.23
23	c	509	CLA	C3B-C2B-C1B	-4.87	101.43	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	O2D-CGD-CBD	4.87	119.74	111.23
26	X	101	SQD	C1-O5-C5	-4.87	104.21	113.72
23	a	409	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
23	B	611	CLA	CMC-C2C-C1C	4.86	132.63	125.03
23	a	405[B]	CLA	C3B-C4B-NB	4.86	114.87	110.53
23	c	502	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	a	409	CLA	C3D-C4D-ND	4.86	117.88	109.99
23	c	506	CLA	C2C-C1C-NC	4.86	115.08	109.98
23	B	607	CLA	C2C-C1C-NC	4.85	115.08	109.98
23	B	603	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
23	C	510	CLA	C3B-C2B-C1B	-4.85	101.46	107.17
23	c	507	CLA	O2D-CGD-CBD	4.85	119.70	111.23
23	C	507	CLA	O2D-CGD-CBD	4.84	119.70	111.23
29	a	414[A]	PL9	C7-C8-C9	-4.84	118.50	126.83
23	a	405[A]	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
23	A	404[B]	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
23	b	604	CLA	C1C-C2C-C3C	-4.83	101.90	106.98
23	B	608	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
23	C	506	CLA	C2C-C1C-NC	4.83	115.05	109.98
23	C	509	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
23	C	514	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
23	B	609	CLA	C2C-C1C-NC	4.82	115.04	109.98
23	c	514	CLA	C2B-C1B-NB	4.82	115.32	110.33
23	a	406[B]	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
26	a	411[B]	SQD	O47-C7-C8	4.81	121.89	111.48
23	b	616	CLA	C1D-CHD-C4C	-4.81	115.80	126.02
23	c	503	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
29	A	414[A]	PL9	C7-C8-C9	-4.80	118.56	126.83
23	c	509	CLA	C4A-NA-C1A	-4.80	104.49	106.68
23	B	608	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	602	CLA	C3D-C4D-ND	4.79	117.78	109.99
23	c	508	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	608	CLA	CMD-C2D-C1D	4.78	133.15	124.73
23	c	510	CLA	C3D-C2D-C1D	-4.78	99.30	105.83
23	a	407[B]	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
23	a	409	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	b	603	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
23	A	405[B]	CLA	C2C-C1C-NC	4.78	115.00	109.98
23	b	608	CLA	C2B-C1B-NB	4.77	115.28	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	616	CLA	CMD-C2D-C1D	4.77	133.13	124.73
23	c	510	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
23	C	512	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	B	604	CLA	C3C-C4C-NC	4.77	116.54	110.43
23	A	406[A]	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	b	608	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.73
23	b	612	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	c	510	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	B	612	CLA	C3D-C4D-ND	4.77	117.73	109.99
23	B	616	CLA	C4A-NA-C1A	-4.76	104.51	106.68
23	D	404[B]	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	d	402[A]	CLA	C4A-NA-C1A	-4.76	104.51	106.68
23	B	608	CLA	C2C-C1C-NC	4.76	114.98	109.98
23	b	610	CLA	O2A-CGA-CBA	4.75	126.33	111.83
23	d	403	CLA	C4A-NA-C1A	-4.75	104.51	106.68
23	b	614	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	a	406[B]	CLA	C1C-C2C-C3C	-4.75	101.99	106.98
23	c	514	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
23	b	606	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	b	610	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	b	605	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	C	514	CLA	C2C-C1C-NC	4.73	114.95	109.98
23	A	405[B]	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	C	504	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
23	C	510	CLA	C4A-NA-C1A	-4.73	104.52	106.68
23	a	406[A]	CLA	O2D-CGD-CBD	4.73	119.49	111.23
23	C	511	CLA	C1C-C2C-C3C	-4.73	102.01	106.98
23	B	611	CLA	C3D-C4D-ND	4.73	117.67	109.99
23	C	511	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
24	A	416[B]	PHO	C1-C2-C3	-4.72	118.46	126.20
23	a	405[B]	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	c	505	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
23	B	610	CLA	O2A-CGA-CBA	4.72	126.23	111.83
23	b	606	CLA	C2C-C1C-NC	4.72	114.94	109.98
23	C	510	CLA	O2D-CGD-CBD	4.72	119.48	111.23
23	b	602	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	b	608	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
34	C	522	HTG	C1'-S1-C1	4.71	110.62	100.45
23	B	613	CLA	C3B-C2B-C1B	-4.70	101.62	107.17
23	b	608	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	a	407[B]	CLA	CHD-C1D-ND	-4.70	118.19	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	C	503	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	A	405[B]	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
23	C	511	CLA	C1-C2-C3	-4.69	118.51	126.20
23	A	404[A]	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	B	612	CLA	C3C-C4C-NC	4.69	116.44	110.43
23	C	511	CLA	C3D-C4D-ND	4.69	117.61	109.99
23	C	514	CLA	C2B-C1B-NB	4.68	115.18	110.33
23	C	508	CLA	C4A-NA-C1A	-4.68	104.54	106.68
23	A	406[B]	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	B	615	CLA	O2D-CGD-CBD	4.68	119.42	111.23
25	b	617	BCR	C33-C5-C6	-4.68	119.38	124.48
23	a	407[B]	CLA	O2D-CGD-CBD	4.68	119.40	111.23
23	C	511	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
23	B	601	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
23	c	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	C	506	CLA	C2B-C1B-NB	4.67	115.17	110.33
23	d	402[B]	CLA	O2D-CGD-CBD	4.67	119.39	111.23
23	A	406[A]	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	C	505	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
23	b	614	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	d	402[B]	CLA	C3D-C4D-ND	4.65	117.55	109.99
34	B	623	HTG	C1'-S1-C1	4.65	110.50	100.45
23	b	616	CLA	C2B-C1B-NB	4.65	115.14	110.33
23	C	506	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
23	A	408	CLA	C4A-NA-C1A	-4.64	104.56	106.68
23	b	603	CLA	C1D-CHD-C4C	-4.64	116.15	126.02
23	A	406[B]	CLA	CHD-C1D-ND	-4.64	118.27	124.80
23	c	508	CLA	CHD-C1D-ND	-4.64	118.28	124.80
23	b	604	CLA	C4A-NA-C1A	-4.64	104.56	106.68
23	b	614	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	a	405[B]	CLA	C4A-NA-C1A	-4.63	104.57	106.68
23	c	511	CLA	C2C-C1C-NC	4.63	114.84	109.98
23	B	604	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
23	d	402[A]	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	C	506	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	b	615	CLA	C3D-C4D-ND	4.62	117.49	109.99
23	b	612	CLA	C3B-C2B-C1B	-4.62	101.73	107.17
23	c	514	CLA	O2D-CGD-CBD	4.62	119.30	111.23
23	b	606	CLA	C1D-CHD-C4C	-4.62	116.21	126.02
23	a	405[B]	CLA	C3D-C4D-ND	4.62	117.49	109.99
23	C	514	CLA	C3D-C2D-C1D	-4.61	99.54	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	O2D-CGD-CBD	4.61	119.28	111.23
23	c	502	CLA	O2D-CGD-CBD	4.61	119.28	111.23
23	B	610	CLA	C3C-C4C-NC	4.61	116.33	110.43
23	b	602	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	C	508	CLA	C2C-C1C-NC	4.60	114.81	109.98
23	c	508	CLA	C1C-C2C-C3C	-4.60	102.15	106.98
23	C	505	CLA	O2D-CGD-CBD	4.60	119.26	111.23
23	c	502	CLA	O2D-CGD-O1D	-4.59	114.91	123.85
23	c	514	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	b	601	CLA	C2B-C1B-NB	4.59	115.09	110.33
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	A	405[A]	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
29	A	414[B]	PL9	C32-C33-C34	-4.59	117.12	127.62
23	b	603	CLA	O2D-CGD-CBD	4.58	119.25	111.23
23	c	512	CLA	O2D-CGD-CBD	4.58	119.24	111.23
23	b	601	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	C	503	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	c	502	CLA	C2B-C1B-NB	4.57	115.06	110.33
23	A	404[B]	CLA	C2C-C1C-NC	4.57	114.78	109.98
23	B	615	CLA	CMB-C2B-C1B	4.57	132.37	125.42
23	C	507	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	b	603	CLA	C3D-C4D-ND	4.56	117.41	109.99
23	B	602	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	b	601	CLA	C3D-C4D-ND	4.56	117.39	109.99
23	B	616	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
23	c	514	CLA	CHD-C1D-ND	-4.55	118.40	124.80
23	c	502	CLA	C1-C2-C3	-4.55	118.74	126.20
39	F	102	HEM	CHC-C4B-NB	4.55	129.32	124.42
23	A	405[B]	CLA	C4A-NA-C1A	-4.55	104.61	106.68
39	F	102	HEM	CAD-CBD-CGD	4.55	125.72	113.67
23	a	406[B]	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	a	407[A]	CLA	O2D-CGD-CBD	4.54	119.17	111.23
23	A	405[A]	CLA	C2B-C1B-NB	4.53	115.03	110.33
23	c	512	CLA	C3D-C4D-ND	4.53	117.36	109.99
23	B	611	CLA	C1D-CHD-C4C	-4.53	116.39	126.02
23	c	502	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	d	402[B]	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	b	612	CLA	O2D-CGD-CBD	4.53	119.15	111.23
23	c	505	CLA	C3B-C4B-NB	4.53	114.57	110.53
23	C	514	CLA	C3D-C4D-ND	4.53	117.35	109.99
23	c	504	CLA	C2C-C1C-NC	4.53	114.74	109.98
23	c	507	CLA	C3D-C4D-ND	4.53	117.35	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	C	512	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	b	609	CLA	O2D-CGD-CBD	4.52	119.14	111.23
23	B	601	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	b	610	CLA	C1-C2-C3	-4.52	118.79	126.20
23	c	514	CLA	C3D-C4D-ND	4.52	117.33	109.99
29	A	414[A]	PL9	C32-C33-C34	-4.51	117.31	127.62
23	A	405[B]	CLA	O2D-CGD-CBD	4.51	119.11	111.23
23	b	609	CLA	C2B-C1B-NB	4.51	115.00	110.33
23	b	611	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
23	A	408	CLA	CHD-C1D-ND	-4.50	118.47	124.80
23	A	406[B]	CLA	C2C-C1C-NC	4.50	114.71	109.98
23	A	406[A]	CLA	CMB-C2B-C1B	4.50	132.27	125.42
23	C	511	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	b	607	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	a	405[B]	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	A	405[A]	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	B	615	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	C	507	CLA	CHD-C1D-ND	-4.50	118.48	124.80
23	a	405[B]	CLA	C2C-C1C-NC	4.49	114.70	109.98
23	c	512	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
23	C	502	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	b	608	CLA	C1C-C2C-C3C	-4.49	102.26	106.98
23	D	404[A]	CLA	C3C-C4C-NC	4.49	116.18	110.43
23	b	611	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	c	504	CLA	O2D-CGD-CBD	4.49	119.08	111.23
23	B	609	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	a	409	CLA	C2B-C1B-NB	4.49	114.98	110.33
23	c	502	CLA	C2C-C1C-NC	4.49	114.69	109.98
23	b	601	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
33	d	411	LMG	O7-C10-C11	4.48	121.18	111.48
33	B	621	LMG	O7-C10-C11	4.48	121.18	111.48
23	B	607	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
23	C	514	CLA	O2D-CGD-CBD	4.48	119.05	111.23
25	K	103	BCR	C16-C17-C18	-4.48	121.00	127.28
23	C	504	CLA	C3D-C4D-ND	4.47	117.26	109.99
33	C	501	LMG	O1-C1-C2	4.47	115.07	108.27
23	c	504	CLA	CMB-C2B-C1B	4.47	132.22	125.42
23	a	407[A]	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
23	C	513	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
23	b	611	CLA	C4A-NA-C1A	-4.46	104.64	106.68
23	b	614	CLA	C2C-C1C-NC	4.46	114.67	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	C4A-NA-C1A	-4.46	104.64	106.68
23	b	611	CLA	C3C-C4C-NC	4.46	116.14	110.43
23	C	504	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	c	505	CLA	CHD-C1D-ND	-4.46	118.53	124.80
23	B	606	CLA	O2D-CGD-O1D	-4.45	115.18	123.85
23	c	506	CLA	C3D-C4D-ND	4.45	117.21	109.99
23	b	612	CLA	C3C-C4C-NC	4.44	116.12	110.43
23	B	604	CLA	C2D-C1D-ND	4.43	114.51	110.13
23	B	609	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	B	607	CLA	C3C-C4C-NC	4.43	116.10	110.43
23	c	506	CLA	C3C-C4C-NC	4.42	116.10	110.43
23	B	609	CLA	C2B-C1B-NB	4.42	114.91	110.33
23	a	407[A]	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	C	511	CLA	CHD-C1D-ND	-4.42	118.58	124.80
25	k	101	BCR	C29-C30-C25	4.42	116.86	110.44
23	B	615	CLA	C2C-C1C-NC	4.42	114.62	109.98
23	a	405[A]	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	b	606	CLA	C4-C3-C5	4.41	122.89	115.23
31	t	101	LMT	C3'-C4'-C5'	-4.41	101.14	110.93
23	a	405[A]	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	C	507	CLA	C3D-C4D-ND	4.41	117.16	109.99
23	c	502	CLA	C3D-C4D-ND	4.41	117.16	109.99
23	a	406[A]	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	a	409	CLA	C4A-NA-C1A	-4.41	104.67	106.68
23	B	609	CLA	O2D-CGD-CBD	4.41	118.93	111.23
23	c	507	CLA	CHD-C1D-ND	-4.40	118.60	124.80
23	b	614	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	B	612	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
23	C	503	CLA	C4A-NA-C1A	-4.40	104.67	106.68
23	a	407[A]	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	d	403	CLA	C3D-C4D-ND	4.40	117.13	109.99
23	B	606	CLA	CHD-C1D-ND	-4.39	118.62	124.80
23	c	514	CLA	C3B-C4B-NB	4.39	114.45	110.53
23	a	406[A]	CLA	C2B-C1B-NB	4.39	114.88	110.33
23	b	615	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
23	c	505	CLA	C1-O2A-CGA	4.39	127.28	116.65
24	A	416[A]	PHO	C1-C2-C3	-4.39	119.00	126.20
23	A	405[A]	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	A	408	CLA	O2D-CGD-CBD	4.39	118.90	111.23
23	a	406[B]	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	a	405[B]	CLA	C4B-C3B-C2B	-4.38	101.85	107.30
23	A	405[B]	CLA	C1C-C2C-C3C	-4.38	102.37	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	409	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
23	c	507	CLA	C1-C2-C3	-4.38	119.02	126.20
23	A	404[B]	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	B	614	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	b	609	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	B	602	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
23	c	511	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
23	B	608	CLA	C3D-C4D-ND	4.37	117.08	109.99
23	b	608	CLA	C3B-C4B-NB	4.37	114.43	110.53
29	a	414[B]	PL9	C7-C3-C2	-4.37	118.24	123.39
23	B	616	CLA	C1D-CHD-C4C	-4.36	116.74	126.02
23	d	402[A]	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
23	c	504	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	c	511	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	a	407[B]	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	B	602	CLA	C3D-C4D-ND	4.36	117.07	109.99
23	A	404[B]	CLA	C3B-C4B-NB	4.36	114.42	110.53
23	a	409	CLA	CMC-C2C-C1C	4.36	131.84	125.03
33	m	101	LMG	O7-C10-C11	4.36	120.91	111.48
23	C	502	CLA	C3D-C4D-ND	4.36	117.07	109.99
23	c	503	CLA	O2D-CGD-O1D	-4.35	115.37	123.85
23	C	504	CLA	C2C-C1C-NC	4.35	114.56	109.98
23	a	407[B]	CLA	C2C-C1C-NC	4.35	114.56	109.98
32	E	101[A]	LHG	O7-C7-C8	4.35	120.90	111.48
23	C	510	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	b	605	CLA	O2D-CGD-O1D	-4.35	115.38	123.85
23	B	612	CLA	C1-C2-C3	-4.34	119.08	126.20
23	B	603	CLA	C1D-CHD-C4C	-4.34	116.79	126.02
23	D	404[B]	CLA	C3D-C4D-ND	4.34	117.04	109.99
29	a	414[B]	PL9	C32-C33-C34	-4.34	117.70	127.62
23	b	614	CLA	C1-C2-C3	-4.34	119.09	126.20
23	c	504	CLA	C1D-CHD-C4C	-4.34	116.81	126.02
23	b	604	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
25	H	101	BCR	C38-C26-C25	-4.33	119.76	124.48
23	B	610	CLA	C3B-C2B-C1B	-4.33	102.07	107.17
23	B	614	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	B	601	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	D	405	CLA	C3C-C4C-NC	4.32	115.97	110.43
23	C	503	CLA	C1C-C2C-C3C	-4.32	102.44	106.98
23	B	603	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	C	509	CLA	C3B-C4B-NB	4.32	114.38	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	CMB-C2B-C1B	4.31	131.99	125.42
23	C	511	CLA	C3B-C4B-NB	4.31	114.38	110.53
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.38	110.53
23	B	608	CLA	C2B-C1B-NB	4.31	114.80	110.33
23	A	405[B]	CLA	C3D-C4D-ND	4.31	116.99	109.99
23	b	608	CLA	C3D-C4D-ND	4.31	116.99	109.99
23	B	614	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
23	c	506	CLA	C2B-C1B-NB	4.31	114.79	110.33
23	c	509	CLA	C2B-C1B-NB	4.31	114.79	110.33
23	C	505	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	b	610	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	C	502	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	A	404[B]	CLA	C4B-C3B-C2B	-4.30	101.95	107.30
23	A	408	CLA	C3C-C4C-NC	4.30	115.94	110.43
23	A	406[A]	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	B	605	CLA	C3C-C4C-NC	4.29	115.93	110.43
23	a	406[B]	CLA	C4A-NA-C1A	-4.29	104.72	106.68
23	A	405[B]	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
23	B	610	CLA	C2C-C1C-NC	4.29	114.49	109.98
23	c	503	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	a	407[A]	CLA	C2C-C1C-NC	4.29	114.49	109.98
23	A	404[B]	CLA	C1D-CHD-C4C	-4.29	116.91	126.02
23	B	602	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
24	A	416[B]	PHO	C1A-C2A-C3A	-4.29	98.76	102.84
33	a	417	LMG	O7-C10-C11	4.28	120.75	111.48
23	c	506	CLA	C3D-C2D-C1D	-4.28	99.98	105.83
23	B	614	CLA	C1-C2-C3	-4.28	119.19	126.20
23	b	603	CLA	C3C-C4C-NC	4.28	115.91	110.43
23	b	612	CLA	C3D-C4D-ND	4.28	116.94	109.99
23	C	510	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
23	b	607	CLA	C3C-C4C-NC	4.27	115.91	110.43
23	b	609	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
26	a	411[A]	SQD	C1-C2-C3	-4.27	101.02	110.01
23	C	505	CLA	C3C-C4C-NC	4.27	115.90	110.43
23	a	405[A]	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	B	603	CLA	C3C-C4C-NC	4.27	115.89	110.43
23	C	512	CLA	C2B-C1B-NB	4.26	114.75	110.33
23	A	408	CLA	C3B-C4B-NB	4.26	114.33	110.53
23	a	405[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	C	505	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	a	406[B]	CLA	C2B-C1B-NB	4.26	114.75	110.33
23	A	406[A]	CLA	CHD-C1D-ND	-4.26	118.81	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	404[B]	CLA	C1-C2-C3	-4.26	119.22	126.20
23	b	615	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	b	604	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	b	616	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
26	A	410[B]	SQD	C1-C2-C3	-4.26	101.05	110.01
23	a	406[A]	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	A	406[A]	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	C	506	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	a	406[A]	CLA	C4A-NA-C1A	-4.25	104.74	106.68
23	a	407[A]	CLA	CHD-C1D-ND	-4.25	118.81	124.80
23	c	504	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
32	E	101[B]	LHG	O7-C7-C8	4.25	120.68	111.48
23	D	404[A]	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	A	404[B]	CLA	CHD-C1D-ND	-4.25	118.82	124.80
23	B	609	CLA	CHD-C1D-ND	-4.25	118.83	124.80
23	A	406[B]	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	b	610	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
23	A	404[B]	CLA	C3D-C4D-ND	4.24	116.88	109.99
25	B	619	BCR	C24-C23-C22	-4.24	119.96	126.23
23	A	404[A]	CLA	CHD-C1D-ND	-4.24	118.83	124.80
23	B	611	CLA	CHD-C4C-NC	4.24	130.80	124.23
23	C	505	CLA	CHD-C1D-ND	-4.24	118.84	124.80
23	d	403	CLA	CHD-C1D-ND	-4.24	118.84	124.80
23	B	616	CLA	C3D-C4D-ND	4.24	116.88	109.99
23	d	402[B]	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
23	C	510	CLA	C1-C2-C3	-4.24	119.26	126.20
32	A	418[A]	LHG	O8-C23-O10	-4.23	113.04	123.63
23	b	605	CLA	C3B-C2B-C1B	-4.23	102.18	107.17
23	c	513	CLA	C3D-C4D-ND	4.23	116.86	109.99
23	b	609	CLA	C3C-C4C-NC	4.23	115.85	110.43
23	c	503	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
23	c	512	CLA	C1D-CHD-C4C	-4.23	117.04	126.02
23	a	406[B]	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
23	a	406[A]	CLA	CAA-C2A-C3A	-4.22	101.59	113.00
23	d	402[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	C	506	CLA	CMB-C2B-C1B	4.22	131.85	125.42
23	A	405[B]	CLA	CAA-C2A-C3A	-4.22	101.59	113.00
29	a	414[A]	PL9	C32-C33-C34	-4.22	117.96	127.62
23	C	503	CLA	C2B-C1B-NB	4.22	114.70	110.33
23	B	605	CLA	C3D-C4D-ND	4.22	116.84	109.99
33	c	521	LMG	O6-C5-C4	4.21	117.29	109.70
23	B	613	CLA	C3D-C4D-ND	4.21	116.84	109.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C4A-NA-C1A	-4.21	104.76	106.68
29	a	414[A]	PL9	C7-C3-C2	-4.21	118.42	123.39
23	c	510	CLA	C2B-C1B-NB	4.21	114.69	110.33
33	c	521	LMG	O7-C10-C11	4.21	120.59	111.48
23	B	603	CLA	C3D-C4D-ND	4.21	116.83	109.99
23	A	404[A]	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	d	403	CLA	C2C-C1C-NC	4.21	114.40	109.98
23	c	507	CLA	C3B-C4B-NB	4.21	114.29	110.53
23	B	605	CLA	C2C-C1C-NC	4.21	114.40	109.98
23	D	404[A]	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	b	602	CLA	O2D-CGD-O1D	-4.21	115.66	123.85
23	a	405[A]	CLA	CAA-C2A-C3A	-4.20	101.65	113.00
23	C	506	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
23	A	408	CLA	C1C-C2C-C3C	-4.20	102.57	106.98
23	b	612	CLA	C4A-NA-C1A	-4.20	104.77	106.68
25	d	404	BCR	C40-C30-C25	-4.20	103.66	110.24
23	d	402[A]	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
23	C	512	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	a	405[B]	CLA	CHD-C1D-ND	-4.19	118.90	124.80
23	D	405	CLA	C2C-C1C-NC	4.19	114.38	109.98
23	a	405[A]	CLA	C1D-CHD-C4C	-4.19	117.12	126.02
23	A	408	CLA	C3D-C4D-ND	4.19	116.80	109.99
25	B	618	BCR	C29-C30-C25	4.19	116.52	110.44
23	C	508	CLA	CHD-C1D-ND	-4.19	118.91	124.80
23	c	513	CLA	C1D-CHD-C4C	-4.18	117.13	126.02
23	c	507	CLA	C1C-C2C-C3C	-4.18	102.58	106.98
25	d	404	BCR	C29-C30-C25	4.18	116.51	110.44
23	d	402[A]	CLA	O2D-CGD-CBD	4.18	118.53	111.23
23	C	503	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	B	608	CLA	C4A-NA-C1A	-4.18	104.77	106.68
23	B	609	CLA	C3C-C4C-NC	4.18	115.78	110.43
23	B	605	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
23	C	513	CLA	C3D-C4D-ND	4.17	116.77	109.99
23	c	506	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
23	b	607	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
23	C	505	CLA	C4A-NA-C1A	-4.17	104.78	106.68
23	a	406[A]	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
23	c	509	CLA	C3C-C4C-NC	4.17	115.77	110.43
23	A	404[A]	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	c	507	CLA	C3B-C2B-C1B	-4.16	102.26	107.17
25	C	515	BCR	C7-C8-C9	-4.16	120.08	126.23
23	C	508	CLA	C3C-C4C-NC	4.16	115.76	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	b	602	CLA	CHD-C1D-ND	-4.16	118.95	124.80
23	b	604	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	b	611	CLA	C2B-C1B-NB	4.16	114.64	110.33
23	D	404[A]	CLA	O2D-CGD-CBD	4.15	118.49	111.23
23	B	606	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
23	c	509	CLA	C1C-C2C-C3C	-4.15	102.61	106.98
23	C	513	CLA	C1-C2-C3	-4.14	119.41	126.20
23	B	611	CLA	C3C-C4C-NC	4.14	115.74	110.43
23	C	513	CLA	C1D-CHD-C4C	-4.14	117.21	126.02
25	K	102	BCR	C7-C8-C9	-4.14	120.11	126.23
23	C	504	CLA	C1D-CHD-C4C	-4.14	117.22	126.02
23	b	609	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	C	510	CLA	C3C-C4C-NC	4.14	115.73	110.43
23	b	613	CLA	C3C-C4C-NC	4.13	115.73	110.43
23	B	614	CLA	C3D-C4D-ND	4.13	116.71	109.99
23	D	404[B]	CLA	O2D-CGD-CBD	4.13	118.45	111.23
23	b	601	CLA	C2C-C1C-NC	4.12	114.31	109.98
23	b	603	CLA	C2B-C1B-NB	4.12	114.60	110.33
24	A	407[B]	PHO	C1A-C2A-C3A	-4.12	98.91	102.84
23	B	613	CLA	C1C-C2C-C3C	-4.12	102.64	106.98
23	d	402[B]	CLA	C3C-C4C-NC	4.12	115.71	110.43
23	B	605	CLA	C1D-CHD-C4C	-4.12	117.27	126.02
23	B	607	CLA	C3D-C4D-ND	4.12	116.68	109.99
33	C	521	LMG	O6-C5-C4	4.11	117.11	109.70
23	b	613	CLA	C3B-C2B-C1B	-4.11	102.33	107.17
23	B	602	CLA	O2D-CGD-O1D	-4.11	115.85	123.85
23	D	404[A]	CLA	CHD-C1D-ND	-4.11	119.02	124.80
33	C	501	LMG	O7-C10-C11	4.11	120.36	111.48
23	B	613	CLA	C3B-C4B-NB	4.11	114.19	110.53
23	b	612	CLA	C3B-C4B-NB	4.11	114.19	110.53
23	a	406[A]	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
23	D	405	CLA	O2D-CGD-O1D	-4.10	115.87	123.85
26	A	412	SQD	O47-C7-C8	4.10	120.34	111.48
23	B	616	CLA	O2D-CGD-O1D	-4.10	115.88	123.85
23	c	504	CLA	C3C-C4C-NC	4.09	115.67	110.43
23	b	607	CLA	C4A-NA-C1A	-4.09	104.81	106.68
23	B	615	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
23	a	406[B]	CLA	O2D-CGD-CBD	4.09	118.38	111.23
23	C	502	CLA	C2B-C1B-NB	4.09	114.57	110.33
23	c	508	CLA	C2B-C1B-NB	4.09	114.57	110.33
23	a	405[B]	CLA	C1-C2-C3	-4.09	119.50	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	CHD-C1D-ND	-4.09	119.05	124.80
23	B	612	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
23	d	402[A]	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	b	601	CLA	CHD-C1D-ND	-4.08	119.06	124.80
23	c	512	CLA	C2C-C1C-NC	4.08	114.27	109.98
23	C	509	CLA	C3D-C4D-ND	4.08	116.62	109.99
23	c	505	CLA	C2B-C1B-NB	4.08	114.56	110.33
24	A	407[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	c	510	CLA	C3D-C4D-ND	4.08	116.61	109.99
23	B	615	CLA	C3C-C4C-NC	4.07	115.65	110.43
23	b	610	CLA	C1D-CHD-C4C	-4.07	117.37	126.02
23	B	606	CLA	C3C-C4C-NC	4.07	115.64	110.43
39	F	102	HEM	CHD-C4C-NC	4.07	128.88	124.45
23	C	502	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
23	c	504	CLA	C2B-C1B-NB	4.07	114.55	110.33
23	B	604	CLA	C1D-CHD-C4C	-4.07	117.37	126.02
23	B	605	CLA	CHD-C1D-ND	-4.07	119.08	124.80
23	D	404[A]	CLA	C1-C2-C3	-4.06	119.54	126.20
26	a	412	SQD	O47-C7-C8	4.06	120.27	111.48
23	B	607	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
23	a	406[A]	CLA	CMB-C2B-C1B	4.06	131.60	125.42
23	b	610	CLA	C3C-C4C-NC	4.06	115.63	110.43
41	V	201	HEC	CBC-CAC-C3C	-4.06	119.32	127.43
23	C	512	CLA	C3C-C4C-NC	4.06	115.62	110.43
23	B	605	CLA	C4-C3-C5	4.05	122.27	115.23
23	c	503	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
23	B	606	CLA	C3D-C4D-ND	4.05	116.57	109.99
23	c	509	CLA	C3D-C4D-ND	4.05	116.57	109.99
23	c	514	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
23	C	510	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	B	615	CLA	C3B-C2B-C1B	-4.05	102.40	107.17
23	c	511	CLA	C2B-C1B-NB	4.05	114.52	110.33
23	c	508	CLA	C3D-C4D-ND	4.05	116.56	109.99
23	C	504	CLA	CHD-C1D-ND	-4.05	119.11	124.80
23	A	404[B]	CLA	CAA-C2A-C3A	-4.04	102.07	113.00
23	a	409	CLA	C3C-C4C-NC	4.04	115.61	110.43
23	B	602	CLA	C2B-C1B-NB	4.04	114.52	110.33
34	V	202	HTG	C1-O5-C5	4.04	117.60	112.19
29	a	414[A]	PL9	C7-C3-C4	4.04	120.24	116.91
23	B	611	CLA	C1-C2-C3	-4.04	119.58	126.20
23	C	502	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
29	A	414[A]	PL9	C7-C3-C2	-4.03	118.63	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	506	CLA	C3C-C4C-NC	4.03	115.60	110.43
23	B	608	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	C	509	CLA	C2B-C1B-NB	4.03	114.51	110.33
23	C	508	CLA	CMB-C2B-C1B	4.03	131.56	125.42
23	D	404[B]	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	A	404[A]	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
23	c	511	CLA	C1C-C2C-C3C	-4.03	102.75	106.98
23	B	601	CLA	C2C-C1C-NC	4.02	114.20	109.98
23	b	607	CLA	CHD-C1D-ND	-4.02	119.15	124.80
23	b	611	CLA	CHD-C1D-ND	-4.02	119.15	124.80
23	C	511	CLA	C1D-CHD-C4C	-4.02	117.48	126.02
23	c	503	CLA	C2B-C1B-NB	4.02	114.49	110.33
26	A	410[B]	SQD	C1-O5-C5	-4.02	105.88	113.72
23	B	606	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
23	C	514	CLA	CHD-C1D-ND	-4.01	119.16	124.80
33	C	521	LMG	O7-C10-C11	4.01	120.16	111.48
23	B	602	CLA	CMC-C2C-C1C	4.01	131.30	125.03
23	B	612	CLA	C2C-C1C-NC	4.01	114.19	109.98
23	b	605	CLA	C2B-C1B-NB	4.01	114.48	110.33
23	b	601	CLA	C1D-CHD-C4C	-4.01	117.50	126.02
23	b	606	CLA	C3D-C4D-ND	4.01	116.50	109.99
23	b	605	CLA	C4A-NA-C1A	-4.01	104.85	106.68
25	d	404	BCR	C15-C14-C13	-4.00	121.66	127.28
23	A	405[B]	CLA	CHD-C1D-ND	-4.00	119.17	124.80
23	b	613	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
23	D	405	CLA	C3D-C4D-ND	4.00	116.49	109.99
23	c	505	CLA	C3D-C4D-ND	4.00	116.49	109.99
23	B	604	CLA	C4A-NA-C1A	-4.00	104.85	106.68
23	a	405[B]	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
23	d	402[B]	CLA	C2B-C1B-NB	4.00	114.47	110.33
23	d	402[B]	CLA	C1-C2-C3	-4.00	119.65	126.20
23	B	614	CLA	CAC-C3C-C4C	3.99	129.99	124.79
35	C	518[A]	DGD	O2G-C1B-C2B	3.99	120.12	111.48
23	b	606	CLA	O2D-CGD-O1D	-3.99	116.07	123.85
26	B	620	SQD	C3-C4-C5	3.99	117.47	110.23
23	c	503	CLA	C3C-C4C-NC	3.99	115.55	110.43
23	C	504	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	D	404[B]	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	C	507	CLA	C1-C2-C3	-3.99	119.66	126.20
23	b	612	CLA	C4-C3-C5	3.99	122.15	115.23
23	C	508	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
25	C	515	BCR	C33-C5-C6	-3.98	120.14	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	601	CLA	C3C-C4C-NC	3.98	115.53	110.43
23	B	610	CLA	C2B-C1B-NB	3.98	114.45	110.33
23	B	602	CLA	C3C-C4C-NC	3.98	115.53	110.43
23	B	613	CLA	CHD-C1D-ND	-3.98	119.20	124.80
32	b	629[B]	LHG	O7-C7-C8	3.98	120.08	111.48
23	C	514	CLA	C3B-C4B-NB	3.98	114.08	110.53
23	a	406[B]	CLA	C1D-CHD-C4C	-3.98	117.57	126.02
23	c	509	CLA	C1D-CHD-C4C	-3.97	117.57	126.02
23	C	514	CLA	C3C-C4C-NC	3.97	115.52	110.43
23	b	616	CLA	C3D-C4D-ND	3.97	116.44	109.99
23	C	513	CLA	C3C-C4C-NC	3.97	115.51	110.43
23	d	403	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
23	C	509	CLA	C4A-NA-C1A	-3.97	104.87	106.68
23	d	402[B]	CLA	CHD-C1D-ND	-3.97	119.22	124.80
23	b	616	CLA	O2A-CGA-CBA	3.97	123.93	111.83
23	D	405	CLA	C2B-C1B-NB	3.97	114.44	110.33
23	a	405[A]	CLA	O2D-CGD-CBD	3.96	118.16	111.23
23	b	610	CLA	C2B-C1B-NB	3.96	114.43	110.33
35	C	517[A]	DGD	O2G-C1B-C2B	3.96	120.05	111.48
23	b	615	CLA	C2B-C1B-NB	3.96	114.43	110.33
23	A	404[A]	CLA	CAA-C2A-C3A	-3.96	102.30	113.00
23	b	615	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
23	c	513	CLA	C1-C2-C3	-3.95	119.72	126.20
23	b	604	CLA	C2B-C1B-NB	3.95	114.42	110.33
23	c	511	CLA	C3D-C4D-ND	3.95	116.40	109.99
23	c	512	CLA	CHD-C1D-ND	-3.95	119.25	124.80
23	c	503	CLA	CMD-C2D-C1D	3.94	131.68	124.73
23	C	503	CLA	CHD-C1D-ND	-3.94	119.25	124.80
23	b	602	CLA	C3C-C4C-NC	3.94	115.48	110.43
23	b	613	CLA	O2A-CGA-O1A	-3.94	113.77	123.63
23	A	406[B]	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
23	b	604	CLA	C3D-C4D-ND	3.93	116.38	109.99
23	B	608	CLA	C3B-C4B-NB	3.93	114.04	110.53
23	C	510	CLA	C3B-C4B-NB	3.93	114.04	110.53
23	c	506	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
23	A	404[A]	CLA	O2A-CGA-CBA	3.93	123.81	111.83
23	B	610	CLA	O2A-CGA-O1A	-3.93	113.81	123.63
23	D	404[B]	CLA	C2B-C1B-NB	3.92	114.40	110.33
23	C	514	CLA	C1C-C2C-C3C	-3.92	102.85	106.98
23	C	510	CLA	C2B-C1B-NB	3.92	114.39	110.33
23	C	514	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.92	102.86	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407[A]	CLA	C3C-C4C-NC	3.92	115.45	110.43
25	D	406	BCR	C29-C30-C25	3.92	116.13	110.44
23	C	503	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	C	512	CLA	C4A-NA-C1A	-3.92	104.89	106.68
23	A	406[A]	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	b	607	CLA	C3B-C4B-NB	3.91	114.02	110.53
23	C	511	CLA	C4A-NA-C1A	-3.91	104.90	106.68
23	C	512	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
23	B	616	CLA	C4C-C3C-C2C	-3.91	101.21	106.89
23	B	612	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	b	604	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	C	509	CLA	CAC-C3C-C4C	3.90	129.87	124.79
33	Z	101	LMG	O7-C10-C11	3.90	119.92	111.48
23	b	602	CLA	CAA-C2A-C3A	-3.90	102.46	113.00
23	c	510	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
23	D	404[A]	CLA	C3B-C4B-NB	3.90	114.01	110.53
23	B	606	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
23	b	615	CLA	C3C-C4C-NC	3.90	115.42	110.43
23	B	613	CLA	C2B-C1B-NB	3.90	114.37	110.33
23	b	608	CLA	CHD-C1D-ND	-3.89	119.32	124.80
23	b	612	CLA	C2B-C1B-NB	3.89	114.36	110.33
23	c	509	CLA	C1-C2-C3	-3.89	119.82	126.20
25	A	409	BCR	C24-C23-C22	-3.89	120.48	126.23
32	L	101[B]	LHG	O7-C7-C8	3.89	119.89	111.48
23	c	512	CLA	C2B-C1B-NB	3.89	114.36	110.33
23	a	409	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
23	b	605	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
23	b	610	CLA	O2D-CGD-O1D	-3.88	116.29	123.85
23	b	610	CLA	O2A-CGA-O1A	-3.88	113.92	123.63
23	c	507	CLA	C2B-C1B-NB	3.88	114.35	110.33
23	C	512	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
23	b	613	CLA	C3B-C4B-NB	3.88	113.99	110.53
35	C	518[B]	DGD	O2G-C1B-C2B	3.88	119.86	111.48
23	B	615	CLA	CED-O2D-CGD	3.87	124.69	115.92
23	C	508	CLA	C3D-C4D-ND	3.87	116.27	109.99
23	b	607	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	C	506	CLA	C1-C2-C3	-3.86	119.88	126.20
23	c	508	CLA	CMC-C2C-C1C	3.86	131.06	125.03
23	b	613	CLA	C3D-C4D-ND	3.85	116.25	109.99
23	b	614	CLA	C3C-C4C-NC	3.85	115.37	110.43
23	b	608	CLA	O2D-CGD-O1D	-3.85	116.36	123.85
23	b	604	CLA	O2D-CGD-O1D	-3.85	116.36	123.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	CMC-C2C-C1C	3.85	131.04	125.03
23	A	405[A]	CLA	CMC-C2C-C1C	3.84	131.04	125.03
29	D	407[A]	PL9	C42-C43-C44	-3.84	118.83	127.62
23	c	511	CLA	C3C-C4C-NC	3.84	115.35	110.43
23	b	603	CLA	CAA-C2A-C3A	-3.84	102.62	113.00
33	c	521	LMG	C3-C4-C5	3.84	117.20	110.23
23	b	616	CLA	C2C-C1C-NC	3.84	114.02	109.98
23	b	606	CLA	CHD-C1D-ND	-3.84	119.40	124.80
23	A	405[B]	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	B	614	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
23	b	609	CLA	CAC-C3C-C4C	3.84	129.78	124.79
23	C	502	CLA	C3C-C4C-NC	3.83	115.34	110.43
23	C	508	CLA	C2B-C1B-NB	3.83	114.30	110.33
23	a	406[A]	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	b	612	CLA	O2D-CGD-O1D	-3.83	116.39	123.85
23	c	502	CLA	CMB-C2B-C1B	3.83	131.25	125.42
23	B	611	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	b	614	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	B	613	CLA	C4A-NA-C1A	-3.83	104.93	106.68
33	Z	101	LMG	C1-C2-C3	3.83	118.06	110.01
26	B	620	SQD	O7-S-C6	3.83	112.47	106.76
23	C	503	CLA	C1-C2-C3	-3.82	119.93	126.20
23	c	506	CLA	CHD-C1D-ND	-3.82	119.42	124.80
23	B	604	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
23	c	514	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
23	b	613	CLA	C2B-C1B-NB	3.82	114.29	110.33
23	A	404[A]	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	a	405[B]	CLA	CAC-C3C-C4C	3.81	129.75	124.79
23	A	405[A]	CLA	CBC-CAC-C3C	-3.81	102.10	112.42
23	b	609	CLA	C3B-C4B-NB	3.81	113.93	110.53
23	C	504	CLA	O2D-CGD-CBD	3.81	117.88	111.23
23	c	511	CLA	CHD-C1D-ND	-3.80	119.45	124.80
23	b	602	CLA	C2C-C1C-NC	3.80	113.98	109.98
23	c	513	CLA	C2C-C1C-NC	3.80	113.98	109.98
23	A	404[A]	CLA	O2D-CGD-CBD	3.80	117.88	111.23
23	b	611	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
23	B	610	CLA	C3D-C4D-ND	3.80	116.16	109.99
26	f	102	SQD	C1-O5-C5	3.80	121.14	113.72
23	d	402[A]	CLA	C2B-C1B-NB	3.80	114.26	110.33
23	a	406[A]	CLA	C3C-C4C-NC	3.80	115.29	110.43
23	c	510	CLA	C3B-C4B-NB	3.80	113.92	110.53
23	B	615	CLA	C2B-C1B-NB	3.79	114.26	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	O2D-CGD-O1D	-3.79	116.47	123.85
23	B	616	CLA	C2B-C1B-NB	3.79	114.25	110.33
23	B	603	CLA	CHD-C1D-ND	-3.79	119.47	124.80
23	B	609	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
23	d	402[B]	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
23	B	613	CLA	C3C-C4C-NC	3.78	115.28	110.43
23	C	510	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
23	B	615	CLA	CHD-C1D-ND	-3.78	119.48	124.80
32	d	413[A]	LHG	O8-C23-O10	-3.78	114.17	123.63
23	A	405[A]	CLA	CHD-C1D-ND	-3.78	119.48	124.80
23	b	613	CLA	CHD-C1D-ND	-3.78	119.48	124.80
23	d	402[B]	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
23	b	616	CLA	C3C-C4C-NC	3.78	115.27	110.43
23	c	510	CLA	C3C-C4C-NC	3.78	115.27	110.43
23	b	603	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
23	B	602	CLA	CHD-C1D-ND	-3.77	119.49	124.80
23	b	616	CLA	O2D-CGD-O1D	-3.77	116.50	123.85
23	b	606	CLA	C3C-C4C-NC	3.77	115.26	110.43
23	d	403	CLA	C3C-C4C-NC	3.77	115.26	110.43
23	b	609	CLA	C1-C2-C3	-3.77	120.02	126.20
23	C	507	CLA	CMC-C2C-C1C	3.77	130.93	125.03
34	b	625	HTG	C1-O5-C5	3.76	119.31	112.56
23	B	611	CLA	C4A-NA-C1A	-3.76	104.96	106.68
25	y	101	BCR	C33-C5-C6	-3.76	120.38	124.48
23	b	601	CLA	O2D-CGD-O1D	-3.76	116.53	123.85
23	b	606	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
29	d	405[A]	PL9	C42-C43-C44	-3.76	119.02	127.62
23	B	605	CLA	O2A-CGA-O1A	-3.75	114.24	123.63
23	B	607	CLA	CHD-C1D-ND	-3.75	119.52	124.80
39	F	102	HEM	C1B-NB-C4B	3.75	109.65	105.21
23	a	409	CLA	O2D-CGD-O1D	-3.75	116.56	123.85
23	b	608	CLA	C1D-CHD-C4C	-3.74	118.06	126.02
29	A	414[A]	PL9	C22-C23-C24	-3.74	119.05	127.62
23	d	402[B]	CLA	C3B-C4B-NB	3.74	113.87	110.53
23	b	613	CLA	O2A-CGA-CBA	3.74	123.24	111.83
25	D	406	BCR	C38-C26-C25	-3.74	120.41	124.48
23	c	512	CLA	C3C-C4C-NC	3.74	115.22	110.43
23	C	509	CLA	C4C-C3C-C2C	-3.74	101.45	106.89
23	a	409	CLA	CHD-C1D-ND	-3.74	119.54	124.80
29	A	414[A]	PL9	C7-C3-C4	3.74	119.99	116.91
23	A	404[B]	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	a	405[A]	CLA	CHD-C1D-ND	-3.73	119.55	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	d	413[A]	LHG	O8-C23-C24	3.73	123.21	111.83
23	B	601	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
24	a	408[A]	PHO	O1D-CGD-CBD	-3.73	119.07	124.72
23	b	605	CLA	CHD-C4C-NC	3.73	130.01	124.23
23	B	606	CLA	C2B-C1B-NB	3.73	114.19	110.33
23	A	404[B]	CLA	O2D-CGD-CBD	3.72	117.74	111.23
23	D	405	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
26	X	101	SQD	C44-O6-C1	-3.72	105.82	113.80
33	C	520	LMG	O8-C28-C29	3.72	123.18	111.83
23	b	610	CLA	C4A-NA-C1A	-3.71	104.99	106.68
23	B	614	CLA	CMC-C2C-C1C	3.71	130.83	125.03
23	B	605	CLA	C1-C2-C3	-3.71	120.12	126.20
26	a	411[A]	SQD	C44-O6-C1	-3.71	105.84	113.80
32	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.48
23	b	611	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	b	612	CLA	C3D-C2D-C1D	-3.70	100.78	105.83
23	C	509	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	c	508	CLA	C3C-C4C-NC	3.70	115.17	110.43
23	B	604	CLA	C3D-C4D-ND	3.69	115.99	109.99
23	b	601	CLA	C3C-C4C-NC	3.69	115.16	110.43
23	B	608	CLA	CMA-C3A-C4A	-3.69	101.86	111.77
23	b	607	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
32	d	413[B]	LHG	O7-C7-C8	3.69	119.46	111.48
23	B	605	CLA	CHD-C4C-NC	3.69	129.95	124.23
23	b	616	CLA	CHD-C4C-NC	3.69	129.95	124.23
23	b	615	CLA	CHD-C1D-ND	-3.69	119.62	124.80
23	b	605	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
23	c	511	CLA	CMC-C2C-C1C	3.68	130.79	125.03
23	D	404[A]	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
35	c	517[B]	DGD	O2G-C1B-C2B	3.68	119.44	111.48
23	c	507	CLA	C1D-CHD-C4C	-3.68	118.21	126.02
23	B	616	CLA	C4B-C3B-C2B	-3.68	102.73	107.30
35	c	518[B]	DGD	O2G-C1B-C2B	3.67	119.43	111.48
23	b	603	CLA	C3B-C4B-NB	3.67	113.81	110.53
23	c	512	CLA	CHD-C4C-NC	3.67	129.93	124.23
29	a	414[A]	PL9	C15-C14-C16	3.67	121.60	115.23
23	B	610	CLA	C4C-C3C-C2C	-3.67	101.55	106.89
23	a	407[A]	CLA	C1D-CHD-C4C	-3.67	118.23	126.02
23	a	405[A]	CLA	O2A-CGA-O1A	-3.66	114.47	123.63
23	c	514	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	a	407[A]	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	b	616	CLA	CHD-C1D-ND	-3.66	119.66	124.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[A]	CLA	CAA-C2A-C3A	-3.65	103.13	113.00
23	B	604	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
23	B	614	CLA	C3B-C4B-NB	3.65	113.78	110.53
23	C	505	CLA	C3B-C4B-NB	3.64	113.78	110.53
34	B	622	HTG	O5-C1-C2	3.64	115.34	110.32
23	b	615	CLA	CMB-C2B-C1B	3.64	130.96	125.42
23	B	604	CLA	C2B-C1B-NB	3.64	114.10	110.33
23	B	603	CLA	CAA-C2A-C3A	-3.64	103.17	113.00
23	C	510	CLA	CAC-C3C-C4C	3.64	129.52	124.79
23	a	405[A]	CLA	C3C-C4C-NC	3.64	115.09	110.43
29	a	414[B]	PL9	C27-C28-C29	-3.64	119.30	127.62
23	C	502	CLA	CHD-C1D-ND	-3.64	119.69	124.80
23	C	508	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
35	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.48
41	v	201	HEC	C4D-ND-C1D	3.63	111.75	105.82
25	C	516	BCR	C7-C8-C9	-3.63	120.86	126.23
23	c	505	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
23	d	402[A]	CLA	CHD-C1D-ND	-3.63	119.69	124.80
23	b	607	CLA	C2B-C1B-NB	3.63	114.09	110.33
23	a	407[B]	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
23	c	502	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
29	a	414[B]	PL9	C7-C8-C9	-3.63	120.58	126.83
23	B	609	CLA	C3B-C2B-C1B	-3.63	102.90	107.17
29	d	405[A]	PL9	C37-C38-C39	-3.63	119.33	127.62
25	b	619	BCR	C24-C23-C22	-3.62	120.87	126.23
23	b	604	CLA	C3B-C4B-NB	3.62	113.77	110.53
23	A	404[B]	CLA	C3C-C4C-NC	3.62	115.06	110.43
23	A	406[B]	CLA	C1D-CHD-C4C	-3.62	118.33	126.02
23	C	509	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
23	a	405[A]	CLA	C1-C2-C3	-3.61	120.28	126.20
23	C	502	CLA	CAC-C3C-C4C	3.61	129.49	124.79
23	c	509	CLA	O2D-CGD-O1D	-3.61	116.82	123.85
23	b	612	CLA	C4C-C3C-C2C	-3.61	101.64	106.89
23	C	512	CLA	CHD-C1D-ND	-3.61	119.73	124.80
23	d	402[A]	CLA	O2A-CGA-CBA	3.61	122.83	111.83
26	A	410[B]	SQD	O47-C7-C8	3.60	119.28	111.48
23	b	614	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
23	B	613	CLA	O2A-CGA-O1A	-3.60	114.62	123.63
23	B	602	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
23	b	611	CLA	C3B-C4B-NB	3.60	113.74	110.53
33	m	101	LMG	C8-O7-C10	-3.60	109.18	117.80
23	b	608	CLA	CBC-CAC-C3C	-3.60	102.67	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	411[B]	SQD	C1-O5-C5	-3.60	106.70	113.72
23	A	405[A]	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
23	C	508	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
23	d	402[A]	CLA	C3B-C4B-NB	3.59	113.73	110.53
23	B	608	CLA	CAC-C3C-C4C	3.59	129.46	124.79
29	a	414[A]	PL9	C30-C29-C31	3.58	121.44	115.23
23	A	406[A]	CLA	C3C-C4C-NC	3.58	115.02	110.43
29	A	414[B]	PL9	C22-C23-C24	-3.58	119.43	127.62
23	b	614	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
23	b	609	CLA	CHD-C1D-ND	-3.58	119.77	124.80
23	b	606	CLA	C3B-C4B-NB	3.58	113.72	110.53
23	B	612	CLA	O2D-CGD-O1D	-3.58	116.89	123.85
23	A	406[A]	CLA	C1D-CHD-C4C	-3.57	118.42	126.02
23	b	614	CLA	C3B-C4B-NB	3.57	113.72	110.53
41	V	201	HEC	CBD-CAD-C3D	-3.57	102.67	112.53
23	b	612	CLA	CAC-C3C-C4C	3.57	129.43	124.79
29	A	414[B]	PL9	C27-C28-C29	-3.56	119.46	127.62
35	c	518[A]	DGD	O2G-C1B-C2B	3.56	119.19	111.48
29	A	414[A]	PL9	C15-C14-C16	3.56	121.41	115.23
23	b	610	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
25	c	515	BCR	C11-C10-C9	-3.56	122.28	127.28
23	C	503	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
23	B	608	CLA	O2D-CGD-O1D	-3.56	116.93	123.85
23	b	615	CLA	C1C-C2C-C3C	-3.55	103.24	106.98
23	C	506	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
23	A	404[A]	CLA	C3C-C4C-NC	3.55	114.98	110.43
26	A	410[A]	SQD	O47-C7-C8	3.55	119.16	111.48
23	b	609	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
33	c	520	LMG	O7-C10-C11	3.55	119.15	111.48
29	D	407[B]	PL9	C42-C43-C44	-3.54	119.51	127.62
23	D	404[B]	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
23	c	513	CLA	CHD-C1D-ND	-3.54	119.82	124.80
23	b	610	CLA	CAA-C2A-C3A	-3.54	103.43	113.00
23	a	405[B]	CLA	C3B-C2B-C1B	-3.54	103.00	107.17
23	c	503	CLA	C4A-NA-C1A	-3.54	105.06	106.68
23	B	614	CLA	O2A-CGA-O1A	-3.54	114.78	123.63
23	D	404[B]	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
23	c	510	CLA	C1C-C2C-C3C	-3.54	103.26	106.98
23	B	610	CLA	CAA-C2A-C3A	-3.54	103.44	113.00
29	a	414[A]	PL9	C27-C28-C29	-3.54	119.53	127.62
23	C	511	CLA	CHD-C4C-NC	3.54	129.71	124.23
23	b	612	CLA	C1D-CHD-C4C	-3.53	118.51	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[A]	PL9	C37-C38-C39	-3.53	119.54	127.62
23	b	613	CLA	C1D-CHD-C4C	-3.53	118.51	126.02
23	B	612	CLA	CAC-C3C-C4C	3.53	129.39	124.79
25	k	101	BCR	C7-C8-C9	-3.53	121.01	126.23
33	C	521	LMG	C3-C4-C5	3.53	116.63	110.23
23	c	505	CLA	C3C-C4C-NC	3.53	114.95	110.43
25	d	404	BCR	C38-C26-C25	-3.53	120.63	124.48
23	b	613	CLA	O2D-CGD-CBD	3.53	117.40	111.23
23	c	502	CLA	CAC-C3C-C4C	3.53	129.38	124.79
25	b	619	BCR	C38-C26-C25	-3.53	120.63	124.48
23	c	512	CLA	C3B-C4B-NB	3.53	113.68	110.53
23	B	604	CLA	C4C-C3C-C2C	-3.53	101.76	106.89
23	C	513	CLA	CHD-C1D-ND	-3.52	119.84	124.80
29	A	414[A]	PL9	C27-C28-C29	-3.52	119.56	127.62
23	c	507	CLA	C4B-C3B-C2B	-3.52	102.92	107.30
29	A	414[B]	PL9	C7-C3-C2	-3.52	119.24	123.39
23	B	610	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
26	a	411[A]	SQD	O9-S-C6	3.52	112.01	106.76
23	d	402[A]	CLA	C1-C2-C3	-3.52	120.43	126.20
23	c	510	CLA	CHD-C1D-ND	-3.52	119.85	124.80
35	C	517[B]	DGD	O2G-C1B-C2B	3.52	119.09	111.48
23	D	404[B]	CLA	CAC-C3C-C4C	3.51	129.36	124.79
23	B	612	CLA	C4C-C3C-C2C	-3.51	101.78	106.89
25	h	101	BCR	C38-C26-C25	-3.51	120.65	124.48
23	b	609	CLA	C1D-CHD-C4C	-3.51	118.56	126.02
23	b	610	CLA	CHD-C1D-ND	-3.51	119.86	124.80
34	b	622	HTG	O2-C2-C1	3.51	116.53	110.30
23	B	609	CLA	CMB-C2B-C1B	3.51	130.76	125.42
32	D	408[B]	LHG	O7-C7-C8	3.50	119.06	111.48
23	C	505	CLA	C2B-C1B-NB	3.50	113.96	110.33
23	B	607	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
33	a	417	LMG	C8-O7-C10	-3.50	109.42	117.80
32	D	409[B]	LHG	O7-C7-C8	3.50	119.05	111.48
23	b	604	CLA	CMC-C2C-C1C	3.50	130.50	125.03
23	B	604	CLA	CAC-C3C-C4C	3.50	129.34	124.79
23	d	403	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
29	A	414[B]	PL9	C37-C38-C39	-3.50	119.62	127.62
23	A	404[A]	CLA	O2A-CGA-O1A	-3.50	114.89	123.63
23	a	406[A]	CLA	C3B-C4B-NB	3.49	113.65	110.53
32	A	418[A]	LHG	O7-C7-C8	3.49	119.04	111.48
23	B	610	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
23	c	511	CLA	C1D-CHD-C4C	-3.49	118.61	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	611	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
23	C	509	CLA	C1-C2-C3	-3.49	120.49	126.20
29	d	405[A]	PL9	C40-C39-C41	3.49	121.28	115.23
23	a	405[A]	CLA	O2A-CGA-CBA	3.48	122.45	111.83
23	b	603	CLA	CHD-C1D-ND	-3.48	119.91	124.80
23	A	404[B]	CLA	C3B-C2B-C1B	-3.48	103.07	107.17
23	B	613	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
26	a	411[B]	SQD	C1-C2-C3	-3.48	102.70	110.01
23	b	602	CLA	C1D-CHD-C4C	-3.47	118.64	126.02
23	b	608	CLA	C4B-C3B-C2B	-3.47	102.99	107.30
23	C	509	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
23	C	510	CLA	CMC-C2C-C1C	3.47	130.45	125.03
24	A	416[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
25	T	101	BCR	C15-C16-C17	-3.46	116.43	123.52
23	B	610	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
23	C	507	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
23	A	405[A]	CLA	C3C-C4C-NC	3.46	114.86	110.43
31	b	627	LMT	C3'-C4'-C5'	-3.46	103.26	110.93
29	a	414[A]	PL9	C37-C38-C39	-3.46	119.71	127.62
23	c	507	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	c	512	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
23	B	607	CLA	C4-C3-C5	3.45	121.22	115.23
23	c	514	CLA	CAC-C3C-C4C	3.45	129.28	124.79
23	a	406[A]	CLA	CHD-C4C-NC	3.45	129.58	124.23
23	D	405	CLA	C3B-C2B-C1B	-3.45	103.10	107.17
39	f	101	HEM	CHA-C4D-ND	3.45	128.63	124.37
23	b	607	CLA	O2D-CGD-CBD	3.45	117.26	111.23
23	B	611	CLA	C4B-C3B-C2B	3.45	111.59	107.30
23	D	405	CLA	CHD-C1D-ND	-3.45	119.95	124.80
23	c	510	CLA	C1-O2A-CGA	3.44	124.99	116.65
23	a	407[B]	CLA	C1D-CHD-C4C	-3.44	118.70	126.02
23	a	406[B]	CLA	CHD-C4C-NC	3.44	129.57	124.23
23	D	404[A]	CLA	C2B-C1B-NB	3.44	113.90	110.33
29	A	414[B]	PL9	C17-C18-C19	-3.44	119.75	127.62
23	c	505	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
32	A	418[B]	LHG	C5-O7-C7	-3.44	109.57	117.80
23	B	609	CLA	C4B-C3B-C2B	-3.44	103.03	107.30
23	C	512	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
23	b	613	CLA	C4B-C3B-C2B	-3.44	103.03	107.30
23	C	502	CLA	CMB-C2B-C1B	3.43	130.65	125.42
23	b	615	CLA	O2D-CGD-CBD	3.43	117.23	111.23
26	A	412	SQD	O48-C23-C24	3.43	122.30	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CMC-C2C-C1C	3.43	130.40	125.03
32	A	418[B]	LHG	O7-C7-C8	3.43	118.91	111.48
23	D	404[B]	CLA	C3B-C4B-NB	3.43	113.59	110.53
23	C	506	CLA	C1D-CHD-C4C	-3.43	118.73	126.02
29	a	414[B]	PL9	C15-C14-C16	3.43	121.18	115.23
24	a	408[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
23	B	605	CLA	C2B-C1B-NB	3.43	113.88	110.33
31	B	628	LMT	C1'-O5'-C5'	-3.42	107.03	113.72
32	A	418[A]	LHG	O8-C23-C24	3.42	122.28	111.83
31	B	630	LMT	O1'-C1'-C2'	3.42	113.47	108.27
23	c	513	CLA	C3C-C4C-NC	3.42	114.81	110.43
23	b	608	CLA	CMC-C2C-C1C	3.42	130.38	125.03
33	B	621	LMG	O8-C28-C29	3.42	122.26	111.83
23	b	610	CLA	C4C-C3C-C2C	-3.42	101.92	106.89
32	d	407[A]	LHG	O7-C7-C8	3.41	118.86	111.48
23	a	405[A]	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	b	605	CLA	C3C-C4C-NC	3.41	114.80	110.43
23	B	601	CLA	C4C-C3C-C2C	-3.41	101.92	106.89
29	A	414[B]	PL9	C15-C14-C16	3.41	121.15	115.23
23	B	611	CLA	C2A-C1A-CHA	-3.41	117.95	123.87
23	a	406[B]	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	A	406[A]	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
23	B	605	CLA	CMB-C2B-C1B	3.41	130.61	125.42
23	B	607	CLA	C2B-C1B-NB	3.41	113.86	110.33
23	B	602	CLA	CAA-C2A-C3A	-3.40	103.80	113.00
25	h	101	BCR	C7-C8-C9	-3.40	121.20	126.23
23	B	607	CLA	C4B-C3B-C2B	-3.40	103.08	107.30
23	A	406[A]	CLA	C3B-C4B-NB	3.40	113.56	110.53
23	A	404[A]	CLA	C1-C2-C3	-3.40	120.63	126.20
26	X	101	SQD	O8-S-C6	3.39	112.51	105.97
39	F	102	HEM	CHB-C1B-NB	3.39	128.56	124.37
23	C	512	CLA	C3B-C4B-NB	3.38	113.55	110.53
23	A	405[B]	CLA	C3B-C4B-NB	3.38	113.55	110.53
23	a	407[B]	CLA	CBC-CAC-C3C	-3.38	103.25	112.42
25	T	101	BCR	C12-C13-C14	-3.38	113.69	119.01
23	C	513	CLA	C2C-C1C-NC	3.38	113.53	109.98
23	c	511	CLA	C3B-C4B-NB	3.38	113.55	110.53
23	C	504	CLA	C1-C2-C3	-3.38	120.67	126.20
23	B	610	CLA	CHD-C1D-ND	-3.37	120.05	124.80
23	b	609	CLA	CBC-CAC-C3C	-3.37	103.27	112.42
23	d	402[B]	CLA	O2A-CGA-CBA	3.37	122.12	111.83
23	B	613	CLA	C4-C3-C5	3.37	121.08	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	D	406	BCR	C10-C11-C12	-3.37	113.43	123.20
26	A	410[A]	SQD	C44-O6-C1	-3.37	106.57	113.80
26	A	410[B]	SQD	C44-O6-C1	-3.37	106.57	113.80
23	C	510	CLA	C1D-CHD-C4C	-3.37	118.86	126.02
23	B	616	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
25	K	103	BCR	C15-C14-C13	-3.36	122.56	127.28
23	B	612	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
23	c	506	CLA	CAC-C3C-C4C	3.36	129.16	124.79
29	a	414[A]	PL9	C17-C18-C19	-3.36	119.94	127.62
23	D	404[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
26	B	620	SQD	O48-C23-C24	3.35	122.06	111.83
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.79
23	c	513	CLA	O2A-CGA-CBA	3.35	122.06	111.83
26	A	412	SQD	O8-S-C6	3.35	112.44	105.97
23	b	613	CLA	C1-C2-C3	-3.35	120.71	126.20
23	a	406[B]	CLA	CMB-C2B-C1B	3.35	130.52	125.42
23	d	403	CLA	C1D-CHD-C4C	-3.35	118.90	126.02
29	D	407[A]	PL9	C17-C18-C19	-3.35	119.96	127.62
23	c	506	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
23	B	614	CLA	O2A-CGA-CBA	3.34	122.03	111.83
32	b	629[A]	LHG	O7-C7-C8	3.34	118.72	111.48
23	C	506	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
23	A	408	CLA	C1-C2-C3	-3.33	120.73	126.20
25	B	617	BCR	C33-C5-C6	-3.33	120.85	124.48
39	f	101	HEM	CHD-C1D-ND	3.33	128.01	124.42
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
23	c	502	CLA	C3C-C4C-NC	3.33	114.70	110.43
23	B	608	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
23	a	406[B]	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
23	C	504	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
23	b	608	CLA	C3C-C4C-NC	3.33	114.69	110.43
23	a	405[B]	CLA	CHC-C1C-C2C	-3.33	117.49	126.95
23	d	402[A]	CLA	C1D-CHD-C4C	-3.33	118.95	126.02
33	C	520	LMG	O7-C10-C11	3.33	118.67	111.48
29	D	407[B]	PL9	C25-C24-C26	3.32	121.00	115.23
25	b	617	BCR	C29-C30-C25	3.32	115.26	110.44
23	B	608	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
23	a	405[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	b	602	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
23	B	604	CLA	C3B-C4B-NB	3.32	113.49	110.53
26	X	101	SQD	C1-C2-C3	-3.32	103.03	110.01
23	c	513	CLA	C1C-C2C-C3C	-3.32	103.49	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[B]	CLA	O2D-CGD-CBD	3.32	117.03	111.23
23	b	612	CLA	C4B-C3B-C2B	-3.31	103.18	107.30
29	a	414[B]	PL9	C17-C18-C19	-3.31	120.04	127.62
23	B	607	CLA	C3B-C4B-NB	3.31	113.49	110.53
26	a	412	SQD	O48-C23-C24	3.31	121.93	111.83
26	a	411[A]	SQD	C45-O47-C7	-3.31	109.88	117.80
41	V	201	HEC	C4D-ND-C1D	3.31	111.21	105.82
23	c	508	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	c	513	CLA	CHD-C4C-NC	3.31	129.36	124.23
23	C	507	CLA	C3B-C4B-NB	3.31	113.48	110.53
23	c	506	CLA	CMB-C2B-C1B	3.30	130.45	125.42
23	b	603	CLA	CMA-C3A-C2A	-3.30	101.21	113.98
23	D	404[B]	CLA	O2A-CGA-CBA	3.30	121.91	111.83
23	b	610	CLA	CHD-C4C-NC	3.30	129.35	124.23
33	a	417	LMG	C7-O1-C1	-3.30	106.72	113.80
23	B	602	CLA	C3B-C4B-NB	3.30	113.47	110.53
23	a	405[A]	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
23	a	406[B]	CLA	C3C-C4C-NC	3.30	114.65	110.43
23	b	601	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
23	c	512	CLA	C4-C3-C5	3.30	120.95	115.23
23	B	611	CLA	CHB-C4A-NA	3.29	129.15	124.40
23	B	605	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
23	c	503	CLA	C3B-C4B-NB	3.29	113.47	110.53
23	B	615	CLA	CMC-C2C-C1C	3.28	130.17	125.03
23	B	615	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
23	c	514	CLA	C4B-C3B-C2B	-3.28	103.22	107.30
23	c	512	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
23	B	610	CLA	CMB-C2B-C1B	3.28	130.41	125.42
23	a	409	CLA	CAA-C2A-C3A	-3.28	104.14	113.00
29	d	405[B]	PL9	C42-C43-C44	-3.28	120.12	127.62
23	C	513	CLA	C4-C3-C5	3.28	120.92	115.23
23	c	505	CLA	CAC-C3C-C4C	3.28	129.06	124.79
23	c	504	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
23	b	609	CLA	C4C-C3C-C2C	-3.28	102.12	106.89
23	B	612	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
23	B	608	CLA	C1D-CHD-C4C	-3.27	119.06	126.02
23	a	409	CLA	C4-C3-C5	3.27	120.91	115.23
26	A	410[A]	SQD	O9-S-C6	3.27	111.64	106.76
23	A	406[A]	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
24	a	416[A]	PHO	C4-C3-C5	3.27	120.90	115.23
23	b	604	CLA	CMB-C2B-C1B	3.27	130.39	125.42
25	D	406	BCR	C28-C27-C26	-3.27	108.23	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[B]	CLA	CMB-C2B-C1B	3.27	130.39	125.42
23	B	613	CLA	CAC-C3C-C4C	3.27	129.04	124.79
23	C	505	CLA	C1D-CHD-C4C	-3.27	119.08	126.02
23	d	402[B]	CLA	C4C-C3C-C2C	-3.26	102.14	106.89
23	B	605	CLA	O2D-CGD-O1D	-3.26	117.49	123.85
33	c	521	LMG	C9-C8-C7	-3.26	104.17	111.78
23	A	405[B]	CLA	CBC-CAC-C3C	-3.26	103.58	112.42
23	d	402[A]	CLA	C4-C3-C5	3.26	120.89	115.23
23	c	504	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
23	B	613	CLA	O2A-CGA-CBA	3.26	121.78	111.83
23	c	513	CLA	CMB-C2B-C1B	3.26	130.38	125.42
23	b	607	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
23	b	605	CLA	O2A-CGA-O1A	-3.26	115.48	123.63
33	m	101	LMG	O8-C28-C29	3.26	121.76	111.83
25	d	404	BCR	C37-C22-C23	3.26	123.06	118.09
23	A	406[B]	CLA	CAA-C2A-C3A	-3.25	104.20	113.00
39	f	101	HEM	C1B-NB-C4B	3.25	109.06	105.21
23	c	510	CLA	C4-C3-C5	3.25	120.87	115.23
23	B	610	CLA	CAA-CBA-CGA	-3.25	103.98	113.21
23	B	614	CLA	CHC-C1C-C2C	-3.25	117.71	126.95
23	A	408	CLA	C1D-CHD-C4C	-3.25	119.11	126.02
23	b	612	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
23	A	405[B]	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
23	C	513	CLA	CHD-C4C-NC	3.25	129.27	124.23
24	a	408[A]	PHO	O2A-CGA-O1A	-3.25	115.51	123.63
23	c	510	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
32	d	413[B]	LHG	O8-C23-C24	3.24	121.71	111.83
23	B	611	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
23	D	405	CLA	C1C-C2C-C3C	-3.24	103.58	106.98
23	C	512	CLA	C1-C2-C3	-3.23	120.90	126.20
23	c	505	CLA	CHC-C1C-C2C	-3.23	117.76	126.95
39	f	101	HEM	CAD-CBD-CGD	3.23	122.23	113.67
23	C	502	CLA	C1C-C2C-C3C	-3.23	103.58	106.98
23	A	406[A]	CLA	C4B-C3B-C2B	-3.22	103.29	107.30
23	d	402[A]	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
23	C	512	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
23	a	409	CLA	O2A-CGA-CBA	3.22	121.65	111.83
32	d	407[B]	LHG	O7-C7-C8	3.22	118.44	111.48
23	a	409	CLA	C3B-C4B-NB	3.22	113.40	110.53
23	A	406[B]	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
23	B	605	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
23	c	504	CLA	C1-C2-C3	-3.22	120.93	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	D	407[A]	PL9	C25-C24-C26	3.22	120.81	115.23
23	a	407[A]	CLA	CAA-C2A-C3A	-3.22	104.31	113.00
33	C	521	LMG	O8-C28-C29	3.21	121.64	111.83
24	a	408[A]	PHO	O2A-CGA-CBA	3.21	121.63	111.83
23	c	512	CLA	C1-C2-C3	-3.21	120.93	126.20
33	Z	101	LMG	O6-C1-C2	3.21	116.97	110.37
23	b	606	CLA	CHD-C4C-NC	3.21	129.21	124.23
23	C	509	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
23	B	614	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
32	d	406[B]	LHG	O7-C7-C8	3.21	118.42	111.48
23	A	408	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
23	b	616	CLA	CMB-C2B-C1B	3.21	130.30	125.42
23	A	405[B]	CLA	CHD-C4C-NC	3.20	129.20	124.23
31	M	101	LMT	C1'-O5'-C5'	-3.20	107.46	113.72
23	A	406[B]	CLA	C3C-C4C-NC	3.20	114.53	110.43
23	c	511	CLA	C4-C3-C5	3.20	120.79	115.23
23	B	615	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
23	B	616	CLA	O2A-CGA-CBA	3.20	121.59	111.83
23	b	602	CLA	C1-C2-C3	-3.20	120.96	126.20
23	D	404[A]	CLA	C4B-C3B-C2B	-3.20	103.33	107.30
23	B	601	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
23	C	511	CLA	CBC-CAC-C3C	-3.20	103.75	112.42
23	C	507	CLA	C3C-C4C-NC	3.20	114.52	110.43
23	b	609	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
23	B	609	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
29	A	414[A]	PL9	O1-C4-C3	-3.19	117.37	120.73
25	K	102	BCR	C20-C21-C22	-3.19	122.81	127.28
23	a	405[B]	CLA	CAA-C2A-C3A	-3.19	104.39	113.00
23	C	510	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
23	b	607	CLA	CBC-CAC-C3C	-3.18	103.79	112.42
23	b	601	CLA	C1-O2A-CGA	3.18	124.35	116.65
23	b	616	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
23	c	506	CLA	CMC-C2C-C1C	3.18	130.00	125.03
23	D	404[B]	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
23	A	405[B]	CLA	C3C-C4C-NC	3.18	114.50	110.43
23	B	609	CLA	C1D-CHD-C4C	-3.18	119.26	126.02
23	c	509	CLA	O2A-CGA-CBA	3.18	121.53	111.83
23	a	407[A]	CLA	C3B-C4B-NB	3.18	113.37	110.53
23	A	408	CLA	CAA-C2A-C3A	-3.18	104.41	113.00
23	b	615	CLA	C4C-C3C-C2C	-3.18	102.27	106.89
23	D	405	CLA	C4C-C3C-C2C	-3.18	102.27	106.89
23	B	612	CLA	C1D-CHD-C4C	-3.18	119.27	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	405	CLA	CMB-C2B-C1B	3.18	130.25	125.42
23	C	505	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	b	614	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
23	C	507	CLA	C1D-CHD-C4C	-3.17	119.28	126.02
23	a	407[B]	CLA	CAA-C2A-C3A	-3.17	104.44	113.00
23	C	513	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	A	405[B]	CLA	CMB-C2B-C1B	3.17	130.24	125.42
23	a	406[A]	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	c	509	CLA	CHD-C1D-ND	-3.17	120.34	124.80
33	Z	101	LMG	C4-C3-C2	3.17	116.39	110.83
23	b	615	CLA	C11-C10-C8	-3.17	105.44	115.97
23	a	409	CLA	CBC-CAC-C3C	-3.17	103.84	112.42
23	b	614	CLA	C2A-C1A-CHA	-3.17	118.37	123.87
23	b	603	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
23	b	608	CLA	C1-C2-C3	-3.16	121.01	126.20
25	T	101	BCR	C2-C1-C6	3.16	115.03	110.44
29	a	414[B]	PL9	C37-C38-C39	-3.16	120.38	127.62
23	C	510	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
29	D	407[B]	PL9	C17-C18-C19	-3.16	120.39	127.62
25	b	619	BCR	C11-C10-C9	-3.16	122.85	127.28
23	d	402[A]	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
23	C	510	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
32	D	409[A]	LHG	O8-C23-C24	3.16	121.46	111.83
23	A	404[A]	CLA	C4B-C3B-C2B	-3.16	103.38	107.30
23	B	616	CLA	CHC-C1C-C2C	-3.16	117.98	126.95
23	c	506	CLA	C4C-C3C-C2C	-3.16	102.30	106.89
23	C	504	CLA	CMB-C2B-C1B	3.16	130.22	125.42
26	b	620	SQD	C3-C4-C5	3.15	115.95	110.23
26	B	620	SQD	C1-O5-C5	-3.15	107.56	113.72
23	B	612	CLA	C3B-C4B-NB	3.15	113.34	110.53
23	B	612	CLA	C2B-C1B-NB	3.15	113.60	110.33
29	a	414[B]	PL9	C30-C29-C31	3.15	120.70	115.23
24	a	408[B]	PHO	O1D-CGD-CBD	-3.15	119.94	124.72
25	D	406	BCR	C37-C22-C23	3.15	122.90	118.09
24	A	416[B]	PHO	C4-C3-C5	3.15	120.70	115.23
23	B	603	CLA	O2A-CGA-CBA	3.15	121.44	111.83
23	d	402[B]	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
23	c	508	CLA	C1D-CHD-C4C	-3.15	119.32	126.02
23	a	407[A]	CLA	CHD-C4C-NC	3.15	129.12	124.23
34	b	622	HTG	O5-C5-C4	3.15	115.37	109.70
23	b	603	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
23	b	608	CLA	CHD-C4C-NC	3.15	129.11	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
23	C	504	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
23	a	405[B]	CLA	C3C-C4C-NC	3.15	114.46	110.43
23	c	513	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
39	F	102	HEM	CBD-CAD-C3D	-3.14	103.84	112.53
23	B	603	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
23	b	609	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
23	a	407[B]	CLA	C3B-C4B-NB	3.14	113.33	110.53
25	d	404	BCR	C10-C11-C12	-3.14	114.10	123.20
23	C	504	CLA	CHD-C4C-NC	3.14	129.10	124.23
29	d	405[A]	PL9	C22-C23-C24	-3.14	120.44	127.62
23	C	508	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
23	a	407[B]	CLA	CAC-C3C-C4C	3.14	128.87	124.79
24	A	407[B]	PHO	O1D-CGD-CBD	-3.14	119.97	124.72
23	c	507	CLA	CHC-C1C-C2C	-3.14	118.04	126.95
23	D	404[A]	CLA	C1D-CHD-C4C	-3.13	119.36	126.02
23	B	614	CLA	C2A-C1A-CHA	-3.13	118.43	123.87
23	C	511	CLA	C4-C3-C5	3.13	120.67	115.23
29	A	414[A]	PL9	C17-C18-C19	-3.13	120.45	127.62
23	c	505	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	C	514	CLA	CMC-C2C-C1C	3.13	129.93	125.03
23	c	505	CLA	C4C-C3C-C2C	-3.13	102.33	106.89
23	A	405[A]	CLA	CMB-C2B-C1B	3.13	130.18	125.42
23	A	405[A]	CLA	CAC-C3C-C4C	3.13	128.86	124.79
23	d	403	CLA	CAA-C2A-C3A	-3.13	104.55	113.00
29	a	414[A]	PL9	C25-C24-C26	3.12	120.65	115.23
23	A	405[A]	CLA	C3B-C4B-NB	3.12	113.32	110.53
32	D	408[A]	LHG	O8-C23-O10	-3.12	115.82	123.63
23	c	509	CLA	C3B-C4B-NB	3.12	113.32	110.53
23	C	506	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
23	b	616	CLA	C1C-C2C-C3C	-3.12	103.70	106.98
23	B	607	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
29	a	414[B]	PL9	C25-C24-C26	3.12	120.64	115.23
23	C	511	CLA	C3C-C4C-NC	3.12	114.43	110.43
23	B	615	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	A	416[A]	PHO	C4-C3-C5	3.12	120.64	115.23
23	b	604	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
26	a	411[B]	SQD	C45-O47-C7	-3.11	110.34	117.80
23	D	404[B]	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
25	y	101	BCR	C38-C26-C25	-3.11	121.09	124.48
23	C	511	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
23	b	601	CLA	CHD-C4C-NC	3.11	129.05	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C15-C14-C13	-3.11	122.92	127.28
29	a	414[A]	PL9	C42-C43-C44	-3.11	120.50	127.62
34	B	625	HTG	O5-C5-C4	3.11	115.30	109.70
23	B	612	CLA	CMC-C2C-C1C	3.11	129.89	125.03
23	b	603	CLA	C4-C3-C5	3.11	120.62	115.23
39	F	102	HEM	CHD-C1D-ND	3.11	127.77	124.42
23	c	504	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
23	B	616	CLA	CAC-C3C-C4C	3.10	128.82	124.79
32	D	409[A]	LHG	O7-C7-C8	3.10	118.19	111.48
23	b	611	CLA	CHD-C4C-NC	3.10	129.04	124.23
23	c	509	CLA	C4C-C3C-C2C	-3.10	102.39	106.89
23	B	609	CLA	C3B-C4B-NB	3.10	113.29	110.53
23	b	612	CLA	CHD-C1D-ND	-3.09	120.45	124.80
23	C	514	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
23	a	407[A]	CLA	CMB-C2B-C1B	3.09	130.12	125.42
23	a	406[A]	CLA	CMA-C3A-C2A	-3.09	102.03	113.98
23	b	606	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
25	c	516	BCR	C7-C8-C9	-3.09	121.66	126.23
23	C	504	CLA	C4-C3-C5	3.09	120.59	115.23
23	b	601	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
29	d	405[B]	PL9	C37-C38-C39	-3.09	120.56	127.62
23	B	601	CLA	C1C-C2C-C3C	-3.09	103.73	106.98
23	C	508	CLA	CBC-CAC-C3C	-3.09	104.05	112.42
23	b	602	CLA	CHD-C4C-NC	3.09	129.01	124.23
23	c	510	CLA	CAC-C3C-C4C	3.09	128.80	124.79
23	C	507	CLA	CBC-CAC-C3C	-3.08	104.06	112.42
32	D	409[B]	LHG	O8-C23-C24	3.08	121.23	111.83
23	c	513	CLA	C4-C3-C5	3.08	120.58	115.23
23	b	602	CLA	CMB-C2B-C1B	3.08	130.11	125.42
23	b	614	CLA	CAC-C3C-C4C	3.08	128.80	124.79
29	d	405[B]	PL9	C40-C39-C41	3.08	120.58	115.23
23	B	610	CLA	C1-C2-C3	-3.08	121.15	126.20
29	d	405[B]	PL9	C10-C9-C11	3.08	120.58	115.23
25	d	404	BCR	C3-C4-C5	-3.08	108.56	114.06
23	c	503	CLA	CMB-C2B-C1B	3.08	130.11	125.42
23	c	510	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	c	507	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
23	d	403	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
23	c	503	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
23	a	405[A]	CLA	C4-C3-C5	3.08	120.57	115.23
23	c	506	CLA	C1D-CHD-C4C	-3.08	119.48	126.02
25	B	618	BCR	C38-C26-C25	-3.08	121.13	124.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	z	101	LMG	O7-C10-C11	3.08	118.14	111.48
32	E	101[B]	LHG	O8-C23-C24	3.08	121.21	111.83
23	C	503	CLA	C1D-CHD-C4C	-3.07	119.48	126.02
26	a	411[B]	SQD	C44-O6-C1	-3.07	107.20	113.80
23	b	604	CLA	C6-C5-C3	-3.07	105.98	113.47
39	F	102	HEM	CBA-CAA-C2A	-3.07	104.04	112.53
23	C	507	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
23	B	612	CLA	C11-C12-C13	-3.07	105.77	115.97
23	B	614	CLA	C3C-C4C-NC	3.07	114.36	110.43
24	A	416[B]	PHO	O2D-CGD-O1D	-3.07	117.88	123.85
23	B	609	CLA	CBC-CAC-C3C	-3.07	104.11	112.42
23	b	605	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
23	A	406[B]	CLA	C2A-C1A-CHA	-3.07	118.55	123.87
25	c	516	BCR	C32-C1-C6	-3.07	105.44	110.24
35	C	519	DGD	O1G-C1A-C2A	3.06	121.18	111.83
23	B	615	CLA	C3B-C4B-NB	3.06	113.27	110.53
23	A	406[B]	CLA	O2A-CGA-O1A	-3.06	115.97	123.63
23	A	404[B]	CLA	O2A-CGA-CBA	3.06	121.17	111.83
23	a	405[B]	CLA	O2A-CGA-CBA	3.06	121.17	111.83
23	B	603	CLA	CHD-C4C-NC	3.06	128.98	124.23
23	b	612	CLA	C2A-C1A-CHA	-3.06	118.56	123.87
23	a	407[B]	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
23	b	611	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
35	C	517[A]	DGD	C2G-O2G-C1B	-3.06	110.47	117.80
23	B	603	CLA	O2A-CGA-O1A	-3.06	115.98	123.63
23	C	510	CLA	O2A-CGA-CBA	3.06	121.16	111.83
23	a	407[B]	CLA	C3C-C4C-NC	3.06	114.35	110.43
31	B	628	LMT	C4B-C3B-C2B	3.06	116.20	110.83
23	B	614	CLA	CBC-CAC-C3C	-3.06	104.14	112.42
23	b	605	CLA	C3B-C4B-NB	3.05	113.26	110.53
25	c	515	BCR	C15-C14-C13	-3.05	123.00	127.28
32	D	409[A]	LHG	O8-C23-O10	-3.05	115.99	123.63
23	C	502	CLA	CMC-C2C-C1C	3.05	129.80	125.03
32	a	420[A]	LHG	O7-C7-C8	3.05	118.08	111.48
25	C	516	BCR	C32-C1-C6	-3.05	105.46	110.24
23	c	505	CLA	C4A-NA-C1A	-3.05	105.29	106.68
31	m	103	LMT	C3'-C4'-C5'	-3.05	104.17	110.93
29	d	405[B]	PL9	C17-C18-C19	-3.05	120.64	127.62
23	D	405	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	b	615	CLA	C3B-C4B-NB	3.05	113.25	110.53
35	h	102	DGD	O1G-C1A-O1A	-3.05	116.00	123.63
23	b	610	CLA	CMB-C2B-C1B	3.05	130.06	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	505	CLA	CMB-C2B-C1B	3.05	130.06	125.42
23	C	508	CLA	CMC-C2C-C1C	3.05	129.79	125.03
23	a	406[B]	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	b	602	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	a	405[B]	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
23	C	509	CLA	CHD-C1D-ND	-3.04	120.53	124.80
23	a	406[B]	CLA	CHC-C1C-C2C	-3.04	118.32	126.95
23	d	402[B]	CLA	C4-C3-C5	3.04	120.50	115.23
23	a	405[B]	CLA	CAA-C2A-C1A	-3.04	102.03	111.97
23	C	507	CLA	CAA-C2A-C3A	-3.04	104.80	113.00
23	b	615	CLA	C4-C3-C5	3.03	120.50	115.23
39	f	101	HEM	CBD-CAD-C3D	-3.03	104.14	112.53
23	a	405[B]	CLA	C4C-C3C-C2C	-3.03	102.47	106.89
29	a	414[A]	PL9	C35-C34-C36	3.03	120.49	115.23
23	b	611	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
25	K	103	BCR	C10-C11-C12	-3.03	114.41	123.20
23	c	509	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
23	B	602	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
32	d	413[A]	LHG	O7-C7-C8	3.03	118.04	111.48
23	b	607	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	A	406[A]	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
23	C	514	CLA	C1-C2-C3	-3.03	121.23	126.20
23	A	404[B]	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	A	408	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
23	b	604	CLA	C1D-CHD-C4C	-3.03	119.59	126.02
32	E	101[A]	LHG	O8-C23-C24	3.03	121.06	111.83
25	T	101	BCR	C16-C17-C18	-3.02	123.04	127.28
26	B	620	SQD	O9-S-C6	3.02	111.27	106.76
23	B	607	CLA	CMC-C2C-C1C	3.02	129.76	125.03
23	b	603	CLA	CHD-C4C-NC	3.02	128.92	124.23
23	B	609	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
41	v	201	HEC	CBD-CAD-C3D	-3.02	104.18	112.53
23	b	605	CLA	C1-C2-C3	-3.02	121.25	126.20
23	c	512	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
23	B	607	CLA	CBC-CAC-C3C	-3.02	104.24	112.42
23	a	409	CLA	CHD-C4C-NC	3.02	128.91	124.23
33	C	501	LMG	C8-O7-C10	-3.02	110.58	117.80
25	a	410	BCR	C29-C30-C25	3.02	114.82	110.44
23	A	408	CLA	CHC-C1C-C2C	-3.01	118.38	126.95
29	a	414[B]	PL9	C22-C23-C24	-3.01	120.73	127.62
31	B	628	LMT	C2'-C3'-C4'	3.01	116.52	109.68
25	H	101	BCR	C11-C10-C9	-3.01	123.06	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	CLA	C4-C3-C5	3.01	120.45	115.23
23	A	404[B]	CLA	CHC-C1C-C2C	-3.01	118.40	126.95
23	B	608	CLA	C1-C2-C3	-3.01	121.27	126.20
23	D	404[A]	CLA	O2A-CGA-CBA	3.01	121.00	111.83
32	d	413[B]	LHG	C5-O7-C7	-3.01	110.60	117.80
23	b	616	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
23	D	404[A]	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
23	d	402[A]	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
32	d	413[B]	LHG	O8-C23-O10	-3.00	116.13	123.63
23	C	506	CLA	C4-C3-C5	3.00	120.43	115.23
23	c	514	CLA	O2A-CGA-CBA	3.00	120.98	111.83
23	a	405[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
23	c	510	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
23	a	407[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
23	B	607	CLA	C1D-CHD-C4C	-3.00	119.65	126.02
23	b	602	CLA	C2A-C1A-CHA	-3.00	118.67	123.87
23	b	614	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
32	a	420[B]	LHG	O7-C7-C8	2.99	117.96	111.48
23	c	511	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
29	A	414[B]	PL9	C20-C19-C21	2.99	120.42	115.23
25	A	409	BCR	C11-C10-C9	-2.99	123.08	127.28
23	B	606	CLA	C3B-C4B-NB	2.99	113.20	110.53
23	b	614	CLA	CMC-C2C-C1C	2.99	129.70	125.03
23	B	609	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	C	512	CLA	CHD-C4C-NC	2.99	128.86	124.23
23	B	604	CLA	CMB-C2B-C1B	2.98	129.96	125.42
24	a	416[A]	PHO	O2D-CGD-O1D	-2.98	118.05	123.85
24	a	416[A]	PHO	CBA-CAA-C2A	-2.98	105.00	113.78
23	C	505	CLA	C1-O2A-CGA	2.98	123.86	116.65
23	c	507	CLA	CHD-C4C-NC	2.98	128.85	124.23
23	c	502	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
23	B	615	CLA	CAC-C3C-C4C	2.98	128.66	124.79
23	a	405[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
23	C	513	CLA	O2A-CGA-CBA	2.98	120.91	111.83
25	c	515	BCR	C28-C27-C26	-2.98	108.75	114.06
34	B	622	HTG	C1-O5-C5	2.97	117.90	112.56
23	b	609	CLA	CHC-C1C-C2C	-2.97	118.50	126.95
29	a	414[A]	PL9	C10-C9-C11	2.97	120.39	115.23
35	c	519	DGD	O2G-C1B-C2B	2.97	117.91	111.48
35	h	102	DGD	O1G-C1A-C2A	2.97	120.90	111.83
26	a	411[A]	SQD	O47-C7-O49	-2.97	116.75	123.70
23	d	402[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	508	CLA	O1D-CGD-CBD	-2.97	118.66	124.52
23	c	502	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
25	c	515	BCR	C16-C17-C18	-2.97	123.11	127.28
23	A	404[A]	CLA	CMC-C2C-C1C	2.97	129.68	125.03
23	B	608	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
23	c	507	CLA	CAC-C3C-C4C	2.97	128.65	124.79
23	D	404[A]	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	A	414[A]	PL9	C20-C19-C21	2.97	120.38	115.23
33	z	101	LMG	O8-C28-C29	2.97	120.89	111.83
23	a	405[B]	CLA	C2A-C1A-CHA	-2.97	118.72	123.87
23	b	603	CLA	CBC-CAC-C3C	-2.97	104.38	112.42
23	A	408	CLA	CMB-C2B-C1B	2.97	129.93	125.42
23	B	606	CLA	CMC-C2C-C1C	2.96	129.66	125.03
35	h	102	DGD	O2G-C1B-C2B	2.96	117.89	111.48
23	b	613	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	B	604	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
23	a	407[B]	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
29	D	407[A]	PL9	C37-C38-C39	-2.96	120.85	127.62
23	c	504	CLA	C3B-C4B-NB	2.96	113.17	110.53
31	A	419	LMT	O5B-C5B-C4B	2.96	115.02	109.70
26	X	101	SQD	O48-C23-C24	2.95	120.84	111.83
23	D	405	CLA	CMA-C3A-C2A	-2.95	102.56	113.98
32	A	418[A]	LHG	C5-O7-C7	-2.95	110.73	117.80
23	a	409	CLA	O2A-CGA-O1A	-2.95	116.25	123.63
23	a	409	CLA	CMA-C3A-C2A	-2.95	102.58	113.98
23	b	603	CLA	CMB-C2B-C1B	2.95	129.91	125.42
32	A	418[B]	LHG	O8-C23-C24	2.95	120.82	111.83
26	A	410[A]	SQD	O48-C23-C24	2.95	120.82	111.83
23	c	512	CLA	O2A-CGA-CBA	2.95	120.82	111.83
23	A	405[A]	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	A	406[B]	CLA	O2A-CGA-CBA	2.94	120.81	111.83
24	A	407[B]	PHO	CMA-C3A-C4A	-2.94	108.27	114.61
23	C	502	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	b	616	CLA	CBC-CAC-C3C	-2.94	104.44	112.42
23	C	502	CLA	C3B-C4B-NB	2.94	113.16	110.53
23	b	616	CLA	C3B-C4B-NB	2.94	113.16	110.53
23	A	406[A]	CLA	O2A-CGA-CBA	2.94	120.80	111.83
23	B	613	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	c	514	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	c	512	CLA	C4B-C3B-C2B	-2.94	103.65	107.30
23	b	614	CLA	CMB-C2B-C1B	2.94	129.89	125.42
23	A	404[A]	CLA	C2A-C1A-CHA	-2.94	118.77	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	CMB-C2B-C1B	2.93	129.89	125.42
23	A	405[B]	CLA	CHC-C1C-C2C	-2.93	118.61	126.95
23	b	605	CLA	C4-C3-C5	2.93	120.32	115.23
23	A	405[A]	CLA	CHD-C4C-NC	2.93	128.78	124.23
39	f	101	HEM	CHD-C4C-NC	2.93	127.64	124.45
29	a	414[A]	PL9	C22-C23-C24	-2.93	120.92	127.62
23	A	405[B]	CLA	CMC-C2C-C1C	2.93	129.61	125.03
23	a	406[B]	CLA	CBC-CAC-C3C	-2.93	104.48	112.42
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	C	506	CLA	CAC-C3C-C4C	2.93	128.60	124.79
23	c	511	CLA	CHD-C4C-NC	2.93	128.77	124.23
23	b	605	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
26	A	410[B]	SQD	O48-C23-C24	2.93	120.75	111.83
34	B	625	HTG	C3-C4-C5	2.92	115.53	110.23
23	B	613	CLA	CMC-C2C-C1C	2.92	129.60	125.03
23	b	614	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
29	a	414[B]	PL9	C42-C43-C44	-2.92	120.93	127.62
23	B	615	CLA	CHD-C4C-NC	2.92	128.76	124.23
24	a	416[B]	PHO	C4-C3-C5	2.92	120.30	115.23
23	A	406[B]	CLA	C3B-C4B-NB	2.92	113.14	110.53
23	B	603	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
32	L	101[A]	LHG	O8-C23-C24	2.92	120.75	111.83
23	C	509	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
23	b	615	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
23	c	503	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	C	511	CLA	CHC-C1C-C2C	-2.92	118.65	126.95
23	A	405[B]	CLA	CED-O2D-CGD	2.92	122.53	115.92
33	c	521	LMG	O8-C28-C29	2.92	120.72	111.83
23	A	406[B]	CLA	CHD-C4C-NC	2.91	128.75	124.23
23	C	509	CLA	C4-C3-C5	2.91	120.29	115.23
23	C	512	CLA	C4-C3-C5	2.91	120.29	115.23
23	A	404[B]	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
23	c	514	CLA	CAA-C2A-C3A	-2.91	105.13	113.00
23	b	606	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
23	b	608	CLA	O2A-CGA-CBA	2.91	120.71	111.83
23	D	405	CLA	CMC-C2C-C1C	2.91	129.58	125.03
23	b	610	CLA	CAA-CBA-CGA	-2.91	104.94	113.21
23	c	511	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
23	C	507	CLA	C4-C3-C5	2.91	120.28	115.23
32	A	418[B]	LHG	O8-C23-O10	-2.91	116.36	123.63
23	c	503	CLA	CHD-C4C-NC	2.90	128.74	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	CHD-C4C-NC	2.90	128.73	124.23
23	A	406[A]	CLA	CMC-C2C-C1C	2.90	129.57	125.03
29	d	405[A]	PL9	C10-C9-C11	2.90	120.27	115.23
26	f	102	SQD	O48-C23-C24	2.90	120.68	111.83
23	C	511	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	C	510	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
23	B	604	CLA	C6-C5-C3	-2.90	106.40	113.47
23	d	402[A]	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
23	a	405[A]	CLA	CMC-C2C-C1C	2.90	129.56	125.03
23	a	406[B]	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
24	A	407[A]	PHO	C1-C2-C3	-2.90	121.45	126.20
33	c	520	LMG	O8-C28-C29	2.90	120.67	111.83
23	B	611	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
23	B	616	CLA	C1-O2A-CGA	2.90	123.66	116.65
23	B	614	CLA	CHD-C4C-NC	2.90	128.72	124.23
23	A	405[B]	CLA	C4-C3-C5	2.90	120.25	115.23
29	D	407[B]	PL9	C27-C28-C29	-2.90	121.00	127.62
23	C	505	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
25	C	515	BCR	C15-C14-C13	-2.89	123.22	127.28
23	D	404[B]	CLA	O2A-CGA-O1A	-2.89	116.39	123.63
23	B	603	CLA	C4-C3-C5	2.89	120.25	115.23
23	b	612	CLA	O2A-CGA-CBA	2.89	120.66	111.83
33	d	411	LMG	O8-C28-O10	-2.89	116.39	123.63
23	b	607	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
23	C	504	CLA	O2A-CGA-O1A	-2.89	116.40	123.63
23	b	611	CLA	C2A-C1A-CHA	-2.89	118.85	123.87
23	b	602	CLA	C1-O2A-CGA	2.89	123.65	116.65
35	c	519	DGD	O1G-C1A-C2A	2.89	120.65	111.83
24	A	416[A]	PHO	O2D-CGD-O1D	-2.89	118.22	123.85
29	A	414[B]	PL9	C30-C29-C31	2.89	120.24	115.23
26	B	620	SQD	C4-C3-C2	2.89	115.89	110.83
23	B	603	CLA	C3B-C4B-NB	2.88	113.10	110.53
24	a	408[B]	PHO	CBC-CAC-C3C	-2.88	108.75	112.87
35	C	517[A]	DGD	O6D-C1D-O3G	-2.88	103.24	110.04
32	d	406[A]	LHG	O7-C7-C8	2.88	117.71	111.48
34	b	625	HTG	O5-C5-C4	2.88	114.89	109.70
31	B	631	LMT	C3'-C4'-C5'	-2.88	104.55	110.93
24	a	416[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	b	611	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
23	B	602	CLA	CAC-C3C-C4C	2.88	128.53	124.79
23	b	601	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
23	C	502	CLA	C4B-C3B-C2B	-2.88	103.73	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	BCR	C7-C8-C9	-2.88	121.98	126.23
23	a	405[A]	CLA	CAC-C3C-C4C	2.88	128.53	124.79
25	D	406	BCR	C40-C30-C25	-2.87	105.73	110.24
29	a	414[B]	PL9	C35-C34-C36	2.87	120.22	115.23
23	b	614	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
23	B	606	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
23	C	506	CLA	CMC-C2C-C1C	2.87	129.52	125.03
23	b	616	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
25	k	101	BCR	C39-C30-C25	-2.87	105.74	110.24
23	B	606	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
23	D	405	CLA	C4-C3-C5	2.87	120.21	115.23
23	B	601	CLA	C3B-C4B-NB	2.87	113.09	110.53
26	a	411[B]	SQD	O47-C7-O49	-2.87	117.00	123.70
23	a	406[A]	CLA	O2A-CGA-CBA	2.87	120.58	111.83
29	D	407[A]	PL9	C10-C9-C11	2.87	120.20	115.23
23	a	406[A]	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
23	C	506	CLA	O2A-CGA-CBA	2.86	120.56	111.83
26	A	412	SQD	C4-C3-C2	-2.86	105.81	110.83
31	M	102	LMT	C1'-O5'-C5'	-2.86	108.14	113.72
23	B	608	CLA	CHB-C4A-NA	2.86	128.52	124.40
23	c	512	CLA	CMC-C2C-C1C	2.86	129.50	125.03
29	D	407[A]	PL9	C53-C6-C1	2.86	121.13	115.28
23	B	615	CLA	C2A-C1A-CHA	-2.86	118.91	123.87
23	C	503	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
23	a	407[A]	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	b	621	LMT	C1'-O5'-C5'	-2.85	108.15	113.72
23	c	508	CLA	O2A-CGA-CBA	2.85	120.53	111.83
23	B	601	CLA	CHD-C4C-NC	2.85	128.65	124.23
25	B	619	BCR	C38-C26-C25	-2.85	121.38	124.48
23	D	404[A]	CLA	C4-C3-C5	2.85	120.17	115.23
33	D	413	LMG	O8-C28-O10	-2.85	116.50	123.63
23	c	514	CLA	CHC-C1C-C2C	-2.85	118.86	126.95
23	c	506	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
29	d	405[A]	PL9	C27-C28-C29	-2.85	121.11	127.62
27	b	628	GOL	C3-C2-C1	-2.85	101.36	111.80
23	B	607	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
23	c	506	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
24	a	408[B]	PHO	CMA-C3A-C4A	-2.84	108.49	114.61
35	C	517[B]	DGD	C2G-O2G-C1B	-2.84	110.99	117.80
23	B	613	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
23	A	406[B]	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
23	c	514	CLA	C2A-C1A-CHA	-2.84	118.94	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	O2A-CGA-CBA	2.84	120.48	111.83
23	C	512	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	b	613	CLA	CHC-C1C-C2C	-2.84	118.89	126.95
39	f	101	HEM	CHB-C1B-NB	2.84	127.88	124.37
35	C	519	DGD	O2G-C1B-C2B	2.84	117.62	111.48
23	C	513	CLA	CMC-C2C-C1C	2.84	129.47	125.03
23	d	403	CLA	CMB-C2B-C1B	2.84	129.74	125.42
25	H	101	BCR	C16-C17-C18	-2.84	123.30	127.28
32	b	629[B]	LHG	O8-C23-C24	2.83	120.48	111.83
25	A	409	BCR	C33-C5-C6	-2.83	121.39	124.48
23	D	404[B]	CLA	CHC-C1C-C2C	-2.83	118.89	126.95
29	D	407[B]	PL9	C10-C9-C11	2.83	120.14	115.23
23	d	402[B]	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
23	a	407[A]	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
23	C	514	CLA	CHD-C4C-NC	2.83	128.62	124.23
23	C	513	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
23	A	404[B]	CLA	C2A-C1A-CHA	-2.83	118.96	123.87
23	A	404[A]	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
23	C	510	CLA	C16-C15-C13	-2.83	106.57	115.97
23	A	404[A]	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
23	b	606	CLA	C4B-C3B-C2B	-2.83	103.79	107.30
23	D	405	CLA	CAC-C3C-C4C	2.82	128.46	124.79
23	b	611	CLA	C1-C2-C3	-2.82	121.57	126.20
23	B	606	CLA	CHD-C4C-NC	2.82	128.61	124.23
25	k	101	BCR	C24-C23-C22	-2.82	122.06	126.23
23	C	511	CLA	CMC-C2C-C1C	2.82	129.44	125.03
34	B	625	HTG	C1'-S1-C1	2.82	106.54	100.45
23	d	402[B]	CLA	C2A-C1A-CHA	-2.82	118.97	123.87
23	c	509	CLA	CHD-C4C-NC	2.82	128.60	124.23
39	F	102	HEM	CHA-C4D-ND	2.82	127.85	124.37
23	c	502	CLA	C3B-C4B-NB	2.82	113.05	110.53
25	H	101	BCR	C16-C15-C14	-2.81	117.76	123.52
23	A	405[B]	CLA	C1-C2-C3	-2.81	121.59	126.20
23	B	608	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
24	a	416[A]	PHO	CMB-C2B-C3B	2.81	130.30	124.68
24	A	407[A]	PHO	O1D-CGD-CBD	-2.81	120.46	124.72
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
25	C	515	BCR	C38-C26-C25	-2.81	121.42	124.48
25	B	618	BCR	C40-C30-C25	-2.81	105.84	110.24
23	C	508	CLA	C4-C3-C5	2.81	120.10	115.23
23	a	407[B]	CLA	C1-C2-C3	-2.81	121.60	126.20
25	A	409	BCR	C8-C7-C6	-2.81	119.50	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d	405[B]	PL9	C22-C23-C24	-2.81	121.20	127.62
29	A	414[B]	PL9	C10-C9-C11	2.81	120.10	115.23
23	A	405[A]	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	c	504	CLA	CHD-C4C-NC	2.81	128.58	124.23
25	K	103	BCR	C28-C27-C26	-2.81	109.05	114.06
23	C	508	CLA	CAC-C3C-C4C	2.81	128.44	124.79
25	B	618	BCR	C2-C1-C6	2.81	114.51	110.44
24	a	416[B]	PHO	CMB-C2B-C3B	2.80	130.29	124.68
23	A	408	CLA	CMA-C3A-C2A	-2.80	103.14	113.98
23	a	407[A]	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
35	c	518[B]	DGD	O1G-C1A-C2A	2.80	120.38	111.83
23	b	608	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
23	B	605	CLA	C2A-C1A-CHA	-2.80	119.01	123.87
23	a	407[A]	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
23	a	406[B]	CLA	C1-C2-C3	-2.80	121.61	126.20
23	b	605	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
23	c	510	CLA	CHD-C4C-NC	2.80	128.57	124.23
29	D	407[B]	PL9	C37-C38-C39	-2.80	121.22	127.62
23	B	610	CLA	C4B-C3B-C2B	-2.80	103.83	107.30
23	c	503	CLA	CHD-C1D-ND	-2.80	120.87	124.80
23	a	407[B]	CLA	CHD-C4C-NC	2.79	128.56	124.23
23	c	506	CLA	C3B-C4B-NB	2.79	113.02	110.53
23	B	610	CLA	C3B-C4B-NB	2.79	113.02	110.53
23	c	503	CLA	O2A-CGA-CBA	2.79	120.34	111.83
23	A	405[A]	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	B	609	CLA	CMC-C2C-C1C	2.79	129.39	125.03
23	B	612	CLA	O2A-CGA-CBA	2.79	120.33	111.83
23	b	612	CLA	CHC-C1C-C2C	-2.79	119.03	126.95
32	b	629[A]	LHG	O8-C23-C24	2.78	120.32	111.83
23	B	615	CLA	C4-C3-C5	2.78	120.06	115.23
23	C	506	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
23	b	603	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
23	B	605	CLA	CMC-C2C-C1C	2.78	129.38	125.03
23	B	601	CLA	O2A-CGA-CBA	2.78	120.31	111.83
23	B	602	CLA	C2A-C1A-CHA	-2.78	119.04	123.87
23	C	514	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
23	B	601	CLA	CAC-C3C-C4C	2.78	128.41	124.79
23	c	503	CLA	C1-C2-C3	-2.77	121.65	126.20
23	d	403	CLA	C4-C3-C5	2.77	120.04	115.23
23	c	513	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
25	D	406	BCR	C16-C17-C18	-2.77	123.39	127.28
33	d	411	LMG	O8-C28-C29	2.77	120.28	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	609	CLA	CMB-C2B-C1B	2.77	129.64	125.42
23	B	613	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
23	b	614	CLA	CBC-CAC-C3C	-2.77	104.92	112.42
24	A	407[B]	PHO	C1-C2-C3	-2.77	121.67	126.20
23	b	614	CLA	CHD-C4C-NC	2.76	128.52	124.23
23	c	509	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
34	B	622	HTG	O2-C2-C3	-2.76	103.87	110.38
32	a	420[A]	LHG	O8-C23-C24	2.76	120.25	111.83
39	F	102	HEM	O2A-CGA-CBA	2.76	122.72	114.00
23	D	404[B]	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
23	B	615	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
29	A	414[A]	PL9	C35-C34-C36	2.76	120.01	115.23
23	d	402[B]	CLA	CAA-C2A-C3A	-2.75	105.56	113.00
23	A	405[A]	CLA	CMA-C3A-C2A	-2.75	103.33	113.98
23	C	511	CLA	O2A-CGA-CBA	2.75	120.23	111.83
32	D	408[A]	LHG	O7-C7-C8	2.75	117.44	111.48
23	b	601	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
23	A	406[B]	CLA	CBC-CAC-C3C	-2.75	104.96	112.42
24	A	416[B]	PHO	C4D-CHA-CBD	2.75	109.78	108.45
23	B	610	CLA	O1D-CGD-CBD	-2.75	119.09	124.52
23	d	402[B]	CLA	CAC-C3C-C4C	2.75	128.37	124.79
29	D	407[A]	PL9	C51-C49-C50	2.75	120.92	114.59
29	D	407[B]	PL9	C20-C19-C21	2.75	120.00	115.23
31	M	101	LMT	C3'-C4'-C5'	-2.75	104.84	110.93
23	B	602	CLA	CMB-C2B-C1B	2.75	129.60	125.42
26	b	620	SQD	O8-S-C6	2.75	111.28	105.97
23	b	603	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
23	A	406[A]	CLA	C4-C3-C5	2.75	119.99	115.23
29	A	414[A]	PL9	C30-C29-C31	2.75	119.99	115.23
23	B	609	CLA	O2A-CGA-CBA	2.74	120.20	111.83
32	D	408[A]	LHG	O8-C23-C24	2.74	120.20	111.83
31	B	628	LMT	O1'-C1'-C2'	2.74	112.44	108.27
33	C	521	LMG	O1-C1-C2	2.74	112.44	108.27
23	b	616	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
23	A	406[B]	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
23	B	603	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
23	a	407[B]	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
23	C	504	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
23	b	612	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
25	K	103	BCR	C15-C16-C17	-2.74	117.92	123.52
35	c	517[B]	DGD	C2G-O2G-C1B	-2.74	111.25	117.80
33	D	413	LMG	O8-C28-C29	2.74	120.18	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
23	a	409	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
32	L	101[A]	LHG	O8-C23-O10	-2.73	116.80	123.63
23	D	404[B]	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
23	A	408	CLA	O2A-CGA-CBA	2.73	120.16	111.83
23	c	514	CLA	CMC-C2C-C1C	2.73	129.30	125.03
23	b	607	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
29	d	405[A]	PL9	C36-C34-C33	-2.72	115.05	121.17
23	b	604	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
23	c	507	CLA	CBC-CAC-C3C	-2.72	105.04	112.42
23	C	512	CLA	CAC-C3C-C4C	2.72	128.33	124.79
23	c	506	CLA	C1-C2-C3	-2.72	121.74	126.20
35	h	102	DGD	O3G-C1D-C2D	2.72	112.40	108.27
23	b	615	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
23	C	502	CLA	CHD-C4C-NC	2.72	128.45	124.23
23	a	405[A]	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
25	t	102	BCR	C21-C20-C19	-2.72	115.33	123.20
23	b	603	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
23	D	405	CLA	CAA-C2A-C3A	-2.72	105.66	113.00
23	D	404[B]	CLA	CMC-C2C-C1C	2.72	129.28	125.03
23	B	603	CLA	CMA-C3A-C2A	-2.71	103.49	113.98
23	a	405[B]	CLA	CHD-C4C-NC	2.71	128.44	124.23
23	b	610	CLA	CHC-C1C-C2C	-2.71	119.24	126.95
23	b	607	CLA	C4-C3-C5	2.71	119.94	115.23
23	C	514	CLA	CBC-CAC-C3C	-2.71	105.07	112.42
23	c	512	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
23	a	407[A]	CLA	O2A-CGA-CBA	2.71	120.10	111.83
23	B	608	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
23	C	507	CLA	CAC-C3C-C4C	2.71	128.31	124.79
23	B	601	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
33	D	413	LMG	O7-C10-C11	2.71	117.34	111.48
32	d	407[A]	LHG	O8-C23-C24	2.71	120.09	111.83
29	D	407[A]	PL9	C2-C1-C6	2.71	122.22	119.00
23	c	513	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
23	b	615	CLA	C6-C5-C3	-2.71	106.87	113.47
31	A	417	LMT	O5B-C5B-C4B	2.71	114.58	109.70
23	C	502	CLA	CHC-C1C-C2C	-2.71	119.26	126.95
23	c	514	CLA	CMB-C2B-C1B	2.71	129.54	125.42
29	d	405[B]	PL9	C27-C28-C29	-2.71	121.43	127.62
23	B	606	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
29	a	414[A]	PL9	C53-C6-C1	2.71	120.82	115.28
23	A	406[B]	CLA	C4C-C3C-C2C	-2.71	102.95	106.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	507	CLA	CMC-C2C-C1C	2.70	129.26	125.03
23	A	404[B]	CLA	C1-C2-C3	-2.70	121.77	126.20
29	A	414[B]	PL9	C12-C13-C14	-2.70	121.43	127.62
23	b	603	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
23	B	603	CLA	CMC-C2C-C1C	2.70	129.26	125.03
23	B	606	CLA	C4-C3-C5	2.70	119.92	115.23
23	C	514	CLA	O2A-CGA-CBA	2.70	120.07	111.83
25	d	404	BCR	C40-C30-C39	2.70	116.36	108.63
23	c	504	CLA	O2A-CGA-O1A	-2.70	116.88	123.63
23	d	403	CLA	CBC-CAC-C3C	-2.70	105.10	112.42
25	t	102	BCR	C1-C6-C7	2.70	122.97	115.65
32	a	420[B]	LHG	O8-C23-C24	2.70	120.06	111.83
23	D	404[A]	CLA	CAC-C3C-C4C	2.70	128.30	124.79
26	X	101	SQD	O5-C1-O6	2.70	116.42	110.04
24	a	408[B]	PHO	C1A-C2A-C3A	-2.70	100.27	102.84
23	a	406[B]	CLA	C1-O2A-CGA	2.70	123.18	116.65
23	C	512	CLA	O2A-CGA-CBA	2.69	120.05	111.83
24	A	407[A]	PHO	O2A-CGA-CBA	2.69	120.05	111.83
29	A	414[B]	PL9	C42-C43-C44	-2.69	121.46	127.62
23	c	507	CLA	C4C-C3C-C2C	-2.69	102.97	106.89
23	B	613	CLA	C1D-CHD-C4C	-2.69	120.30	126.02
26	a	411[B]	SQD	O9-S-C6	2.69	110.78	106.76
29	A	414[A]	PL9	C2-C1-C6	2.69	122.20	119.00
23	B	611	CLA	CMB-C2B-C3B	2.69	132.88	126.55
23	c	511	CLA	O2A-CGA-O1A	-2.69	116.90	123.63
35	C	518[A]	DGD	O1G-C1A-O1A	-2.69	116.90	123.63
23	c	508	CLA	C4-C3-C5	2.69	119.89	115.23
23	C	508	CLA	CHD-C4C-NC	2.68	128.39	124.23
23	d	403	CLA	O2A-CGA-CBA	2.68	120.01	111.83
23	D	404[B]	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
32	L	101[B]	LHG	O8-C23-C24	2.68	120.01	111.83
25	B	618	BCR	C37-C22-C23	2.68	122.18	118.09
23	a	407[B]	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
23	B	609	CLA	CAC-C3C-C4C	2.68	128.28	124.79
23	b	611	CLA	CMC-C2C-C1C	2.68	129.22	125.03
29	a	414[B]	PL9	C53-C6-C1	2.68	120.76	115.28
23	C	512	CLA	CMB-C2B-C1B	2.68	129.50	125.42
24	a	416[B]	PHO	O2D-CGD-O1D	-2.68	118.64	123.85
23	d	403	CLA	C3B-C4B-NB	2.68	112.92	110.53
23	d	402[A]	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
25	a	410	BCR	C38-C26-C25	-2.67	121.57	124.48
23	b	604	CLA	C1-O2A-CGA	2.67	123.12	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	c	520	LMG	O1-C7-C8	-2.67	104.32	110.82
23	B	614	CLA	CMB-C2B-C1B	2.67	129.49	125.42
25	K	102	BCR	C38-C26-C25	-2.67	121.57	124.48
23	a	407[B]	CLA	C4-C3-C5	2.67	119.86	115.23
23	D	404[A]	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	b	613	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	D	404[A]	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
25	C	516	BCR	C2-C1-C6	2.67	114.31	110.44
23	a	406[A]	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
23	C	502	CLA	C1-C2-C3	-2.67	121.83	126.20
25	T	101	BCR	C15-C14-C13	2.67	131.02	127.28
23	a	406[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
29	A	414[B]	PL9	C7-C3-C4	2.67	119.11	116.91
25	h	101	BCR	C33-C5-C6	-2.66	121.58	124.48
23	C	507	CLA	CHD-C4C-NC	2.66	128.36	124.23
23	C	511	CLA	O2A-CGA-O1A	-2.66	116.97	123.63
26	X	101	SQD	O47-C7-O49	-2.66	117.48	123.70
23	d	402[A]	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
23	C	503	CLA	C3B-C4B-NB	2.66	112.90	110.53
23	b	608	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
31	A	419	LMT	O5'-C5'-C4'	2.66	115.22	109.72
23	d	402[A]	CLA	CAC-C3C-C4C	2.66	128.25	124.79
23	A	408	CLA	CHB-C4A-NA	2.66	128.24	124.40
23	C	514	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
23	a	409	CLA	CAC-C3C-C4C	2.66	128.25	124.79
25	B	617	BCR	C7-C8-C9	-2.65	122.31	126.23
23	a	406[B]	CLA	C2A-C1A-CHA	-2.65	119.26	123.87
23	c	504	CLA	C4-C3-C5	2.65	119.83	115.23
23	C	503	CLA	CMC-C2C-C1C	2.65	129.18	125.03
23	C	509	CLA	O2A-CGA-CBA	2.65	119.92	111.83
29	d	405[B]	PL9	C7-C8-C9	-2.65	122.26	126.83
29	A	414[B]	PL9	C53-C6-C1	2.65	120.71	115.28
23	D	405	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
23	b	606	CLA	C1-C2-C3	-2.65	121.86	126.20
25	B	619	BCR	C21-C20-C19	-2.65	115.52	123.20
25	T	101	BCR	C35-C13-C12	2.65	122.13	118.09
23	B	606	CLA	O2A-CGA-CBA	2.65	119.91	111.83
23	d	403	CLA	CHD-C4C-NC	2.65	128.34	124.23
23	C	514	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
23	A	406[A]	CLA	C1-C2-C3	-2.65	121.86	126.20
23	B	608	CLA	CMA-C3A-C2A	-2.64	103.76	113.98
29	a	414[A]	PL9	C47-C48-C49	-2.64	118.83	127.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
25	h	101	BCR	C10-C11-C12	-2.64	115.54	123.20
23	a	407[B]	CLA	O2A-CGA-CBA	2.64	119.89	111.83
35	C	518[B]	DGD	O1G-C1A-C2A	2.64	119.89	111.83
23	b	607	CLA	CHD-C4C-NC	2.64	128.33	124.23
35	H	102	DGD	O6E-C5E-C6E	2.64	112.98	106.44
23	b	604	CLA	CAC-C3C-C4C	2.64	128.22	124.79
23	B	606	CLA	CMB-C2B-C1B	2.64	129.44	125.42
23	C	510	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
25	c	515	BCR	C20-C21-C22	-2.64	123.58	127.28
23	C	514	CLA	CAC-C3C-C4C	2.63	128.22	124.79
25	K	102	BCR	C29-C30-C25	2.63	114.27	110.44
23	c	511	CLA	O2A-CGA-CBA	2.63	119.86	111.83
23	c	513	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	C	503	CLA	CMB-C2B-C1B	2.63	129.43	125.42
23	c	504	CLA	CHC-C1C-C2C	-2.63	119.47	126.95
23	b	605	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	B	602	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
23	b	602	CLA	C11-C12-C13	-2.63	107.22	115.97
25	b	618	BCR	C15-C14-C13	-2.63	123.59	127.28
34	b	623	HTG	O5-C1-C2	2.63	113.94	110.32
23	a	406[A]	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
23	C	503	CLA	CBC-CAC-C3C	-2.63	105.30	112.42
23	D	405	CLA	CHD-C4C-NC	2.63	128.30	124.23
23	C	504	CLA	CAC-C3C-C4C	2.62	128.21	124.79
23	B	601	CLA	C1-O2A-CGA	2.62	123.00	116.65
23	c	509	CLA	CMB-C2B-C1B	2.62	129.41	125.42
25	b	618	BCR	C37-C22-C21	-2.62	118.57	122.82
23	b	605	CLA	CMB-C2B-C1B	2.62	129.41	125.42
23	c	508	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
23	b	614	CLA	O2A-CGA-CBA	2.62	119.82	111.83
25	c	516	BCR	C21-C20-C19	-2.62	115.61	123.20
23	C	514	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
25	K	102	BCR	C24-C23-C22	-2.62	122.36	126.23
23	b	615	CLA	C1-C2-C3	-2.62	121.91	126.20
23	C	513	CLA	CMB-C2B-C1B	2.62	129.40	125.42
25	t	102	BCR	C29-C30-C25	2.62	114.24	110.44
23	c	510	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
25	b	619	BCR	C7-C8-C9	-2.61	122.37	126.23
25	c	515	BCR	C36-C18-C19	2.61	122.08	118.09
23	D	404[A]	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
23	C	503	CLA	C2A-C1A-CHA	-2.61	119.34	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C1-O2A-CGA	2.61	122.97	116.65
23	B	616	CLA	CHD-C1D-ND	-2.61	121.13	124.80
23	a	405[A]	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
25	k	101	BCR	C2-C1-C6	2.61	114.23	110.44
23	c	506	CLA	O2A-CGA-CBA	2.61	119.78	111.83
23	C	503	CLA	CAC-C3C-C4C	2.61	128.18	124.79
32	d	406[B]	LHG	O8-C23-C24	2.61	119.78	111.83
26	A	410[A]	SQD	O48-C23-O10	-2.61	117.11	123.63
23	d	403	CLA	C1-O2A-CGA	2.60	122.95	116.65
24	A	407[A]	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
34	b	622	HTG	C1'-S1-C1	2.60	106.07	100.45
23	a	406[A]	CLA	CAA-CBA-CGA	2.60	120.59	113.21
23	c	511	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
23	A	405[A]	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
23	a	409	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
23	A	404[B]	CLA	CAC-C3C-C4C	2.60	128.17	124.79
23	c	512	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
23	C	512	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
25	B	619	BCR	C7-C8-C9	-2.60	122.39	126.23
23	A	404[B]	CLA	CAA-C2A-C1A	-2.60	103.46	111.97
25	C	516	BCR	C33-C5-C6	-2.60	121.65	124.48
23	A	406[A]	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
24	A	416[B]	PHO	O2A-CGA-CBA	2.60	119.75	111.83
24	a	408[B]	PHO	O2A-CGA-CBA	2.59	119.75	111.83
23	B	611	CLA	C3B-C4B-NB	2.59	112.85	110.53
23	A	408	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
23	c	504	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
23	A	404[B]	CLA	CMC-C2C-C1C	2.59	129.09	125.03
35	c	518[A]	DGD	O1G-C1A-C2A	2.59	119.74	111.83
23	A	405[A]	CLA	C4-C3-C5	2.59	119.73	115.23
23	B	606	CLA	O2A-CGA-O1A	-2.59	117.14	123.63
24	a	408[A]	PHO	CMB-C2B-C3B	2.59	129.86	124.68
23	b	610	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
23	c	508	CLA	CAC-C3C-C4C	2.59	128.16	124.79
29	a	414[A]	PL9	C40-C39-C41	2.59	119.72	115.23
23	a	407[B]	CLA	CMB-C2B-C1B	2.59	129.36	125.42
23	C	506	CLA	C3B-C4B-NB	2.59	112.84	110.53
23	B	616	CLA	CHD-C4C-NC	2.59	128.24	124.23
23	c	502	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
23	b	614	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
25	K	102	BCR	C2-C1-C6	2.58	114.19	110.44
23	A	405[A]	CLA	O2A-CGA-O1A	-2.58	117.17	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	608	CLA	C11-C12-C13	-2.58	107.39	115.97
26	b	620	SQD	O48-C23-C24	2.58	119.70	111.83
23	b	607	CLA	C1-C2-C3	-2.58	121.97	126.20
29	a	414[B]	PL9	C40-C39-C41	2.58	119.70	115.23
32	d	407[B]	LHG	O8-C23-C24	2.58	119.70	111.83
31	A	419	LMT	O5'-C5'-C6'	2.58	112.83	106.44
23	d	403	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
29	a	414[A]	PL9	C10-C9-C8	-2.58	117.01	123.63
29	d	405[B]	PL9	C12-C13-C14	-2.58	121.73	127.62
29	A	414[A]	PL9	C40-C39-C41	2.58	119.70	115.23
23	b	609	CLA	CMC-C2C-C1C	2.58	129.06	125.03
23	a	407[A]	CLA	C1-C2-C3	-2.58	121.98	126.20
29	A	414[A]	PL9	C47-C48-C49	-2.58	119.05	127.64
23	c	509	CLA	C4B-C3B-C2B	-2.57	104.10	107.30
23	C	503	CLA	O2A-CGA-CBA	2.57	119.68	111.83
23	c	504	CLA	C2A-C1A-CHA	-2.57	119.40	123.87
23	B	602	CLA	CHD-C4C-NC	2.57	128.22	124.23
29	a	414[B]	PL9	C20-C19-C21	2.57	119.69	115.23
23	c	505	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
29	d	405[B]	PL9	C35-C34-C36	2.57	119.69	115.23
41	v	201	HEC	CHA-C1A-NA	2.57	127.25	124.45
29	D	407[B]	PL9	C45-C44-C46	2.57	119.69	115.23
23	C	507	CLA	O2A-CGA-CBA	2.57	119.67	111.83
35	H	102	DGD	O1G-C1A-C2A	2.57	119.67	111.83
23	a	409	CLA	CMB-C2B-C1B	2.57	129.33	125.42
23	b	610	CLA	C4-C3-C5	2.57	119.69	115.23
25	H	101	BCR	C24-C23-C22	-2.57	122.44	126.23
23	C	512	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
23	c	512	CLA	CMB-C2B-C1B	2.56	129.32	125.42
23	b	611	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
25	B	617	BCR	C31-C1-C6	-2.56	106.23	110.24
23	b	609	CLA	C1-O2A-CGA	2.56	122.84	116.65
25	y	101	BCR	C10-C11-C12	-2.56	115.79	123.20
32	d	406[B]	LHG	O8-C23-O10	-2.56	117.23	123.63
23	C	506	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
29	a	414[B]	PL9	C10-C9-C11	2.56	119.67	115.23
24	A	407[A]	PHO	CMA-C3A-C4A	-2.56	109.11	114.61
23	C	513	CLA	CMA-C3A-C4A	-2.55	104.91	111.77
23	c	508	CLA	CHD-C4C-NC	2.55	128.19	124.23
23	B	615	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
23	c	502	CLA	C1D-CHD-C4C	-2.55	120.59	126.02
25	b	618	BCR	C37-C22-C23	2.55	121.99	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	519	DGD	O5E-C6E-C5E	-2.55	102.64	111.33
23	b	605	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
23	b	603	CLA	O2A-CGA-CBA	2.55	119.61	111.83
23	c	509	CLA	O2A-CGA-O1A	-2.55	117.25	123.63
23	C	503	CLA	CHD-C4C-NC	2.55	128.19	124.23
23	b	603	CLA	C7-C6-C5	-2.55	106.47	113.26
23	c	507	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
29	D	407[A]	PL9	C42-C41-C39	-2.55	104.75	113.19
29	A	414[B]	PL9	C45-C44-C46	2.55	119.65	115.23
23	B	602	CLA	CHC-C1C-C2C	-2.55	119.72	126.95
26	a	411[B]	SQD	O48-C23-C24	2.55	119.59	111.83
35	c	517[A]	DGD	C2G-O2G-C1B	-2.55	111.70	117.80
29	D	407[B]	PL9	C40-C39-C41	2.54	119.64	115.23
23	A	404[B]	CLA	C4-C3-C5	2.54	119.64	115.23
33	a	417	LMG	O6-C5-C4	2.54	114.28	109.70
23	C	505	CLA	CBC-CAC-C3C	-2.54	105.53	112.42
26	b	620	SQD	O47-C7-O49	-2.54	117.77	123.70
23	B	608	CLA	CMC-C2C-C1C	2.54	129.00	125.03
29	A	414[A]	PL9	C10-C9-C8	-2.54	117.11	123.63
23	C	511	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
23	b	608	CLA	CMA-C3A-C4A	-2.54	104.95	111.77
26	B	620	SQD	O48-C23-O10	-2.54	117.28	123.63
24	a	408[B]	PHO	C1-C2-C3	-2.54	122.04	126.20
23	C	503	CLA	C4B-C3B-C2B	-2.54	104.15	107.30
23	B	615	CLA	C11-C10-C8	-2.53	107.54	115.97
23	a	407[A]	CLA	CMC-C2C-C1C	2.53	128.99	125.03
23	C	513	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
23	c	511	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
26	f	102	SQD	O5-C1-C2	2.53	115.57	110.37
23	b	609	CLA	C16-C15-C13	-2.53	107.55	115.97
32	D	409[B]	LHG	O8-C23-O10	-2.53	117.30	123.63
23	A	406[A]	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
23	C	514	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
23	a	405[A]	CLA	CHD-C4C-NC	2.53	128.15	124.23
23	b	602	CLA	CMA-C3A-C4A	-2.53	104.97	111.77
23	B	601	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
29	A	414[B]	PL9	C35-C34-C36	2.53	119.62	115.23
32	A	418[B]	LHG	O7-C7-O9	-2.53	117.80	123.70
25	d	404	BCR	C16-C17-C18	-2.53	123.73	127.28
23	C	505	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
23	A	405[B]	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
23	A	404[B]	CLA	CBC-CAC-C3C	-2.53	105.57	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[A]	CLA	CMA-C3A-C2A	-2.53	104.22	113.98
23	C	505	CLA	CHC-C1C-C2C	-2.53	119.77	126.95
23	B	610	CLA	CHD-C4C-NC	2.52	128.15	124.23
23	a	405[B]	CLA	C4-C3-C5	2.52	119.61	115.23
26	A	410[B]	SQD	O9-S-C6	2.52	110.53	106.76
25	y	101	BCR	C37-C22-C23	2.52	121.94	118.09
31	A	419	LMT	O1'-C1'-C2'	2.52	112.10	108.27
39	F	102	HEM	C3B-C4B-NB	-2.52	107.66	109.47
35	C	517[B]	DGD	O1G-C1A-O1A	-2.52	117.32	123.63
23	a	406[A]	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
25	D	406	BCR	C30-C25-C24	2.52	122.49	115.65
23	D	405	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
23	c	508	CLA	C3B-C4B-NB	2.52	112.78	110.53
23	B	610	CLA	CHC-C1C-C2C	-2.52	119.79	126.95
25	c	516	BCR	C33-C5-C6	-2.52	121.74	124.48
23	B	602	CLA	C11-C12-C13	-2.52	107.60	115.97
23	b	615	CLA	C6-C7-C8	-2.52	107.60	115.97
23	B	604	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
25	k	101	BCR	C36-C18-C19	2.52	121.93	118.09
23	b	608	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
31	e	101	LMT	O1'-C1'-C2'	2.51	112.09	108.27
25	K	103	BCR	C37-C22-C23	2.51	121.93	118.09
23	a	405[B]	CLA	CMA-C3A-C2A	-2.51	104.26	113.98
23	b	601	CLA	C2A-C1A-CHA	-2.51	119.50	123.87
23	b	601	CLA	C3B-C4B-NB	2.51	112.77	110.53
23	b	607	CLA	C2A-C1A-CHA	-2.51	119.50	123.87
33	C	520	LMG	O8-C28-O10	-2.51	117.34	123.63
23	c	507	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
25	t	102	BCR	C7-C6-C5	-2.51	115.77	121.56
23	B	607	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
23	B	603	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
23	A	405[A]	CLA	CAA-CBA-CGA	2.51	120.34	113.21
25	K	103	BCR	C3-C4-C5	-2.51	109.58	114.06
23	a	409	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
26	b	620	SQD	C44-O6-C1	-2.51	108.42	113.80
25	b	618	BCR	C8-C7-C6	-2.51	120.30	127.00
29	d	405[A]	PL9	C17-C18-C19	-2.51	121.89	127.62
33	C	501	LMG	C6-C5-C4	2.51	119.17	113.02
23	C	510	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
23	A	404[A]	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
23	B	605	CLA	OBD-CAD-C3D	-2.50	122.56	128.42
25	y	101	BCR	C21-C20-C19	-2.50	115.95	123.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	503	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
23	B	608	CLA	C11-C12-C13	-2.50	107.65	115.97
23	c	509	CLA	C4-C3-C5	2.50	119.56	115.23
23	a	405[B]	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
35	H	102	DGD	O1G-C1A-O1A	-2.50	117.38	123.63
31	c	501	LMT	C3'-C4'-C5'	-2.50	105.40	110.93
32	A	418[A]	LHG	O7-C7-O9	-2.50	117.87	123.70
23	B	612	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
23	A	408	CLA	CAC-C3C-C4C	2.49	128.03	124.79
23	a	409	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	D	404[B]	CLA	C4-C3-C5	2.49	119.56	115.23
23	C	509	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	a	405[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	C	506	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
26	A	412	SQD	O48-C23-O10	-2.49	117.39	123.63
25	y	101	BCR	C15-C14-C13	-2.49	123.78	127.28
33	c	521	LMG	O8-C28-O10	-2.49	117.39	123.63
25	K	102	BCR	C33-C5-C6	-2.49	121.77	124.48
23	c	507	CLA	O2A-CGA-O1A	-2.49	117.40	123.63
23	b	612	CLA	OBD-CAD-C3D	-2.49	122.60	128.42
23	C	503	CLA	C4C-C3C-C2C	-2.49	103.27	106.89
23	A	408	CLA	C1-O2A-CGA	2.49	122.67	116.65
32	L	101[B]	LHG	C5-O7-C7	-2.49	111.85	117.80
26	f	102	SQD	C4-C3-C2	-2.48	106.47	110.83
26	a	412	SQD	C1-O5-C5	2.48	118.57	113.72
23	A	406[A]	CLA	CMA-C3A-C2A	-2.48	104.38	113.98
23	D	405	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
23	b	608	CLA	CAC-C3C-C4C	2.48	128.02	124.79
23	A	404[B]	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
32	d	406[B]	LHG	C5-O7-C7	-2.48	111.87	117.80
23	a	405[B]	CLA	O2A-CGA-O1A	-2.48	117.43	123.63
23	B	609	CLA	CHD-C4C-NC	2.48	128.07	124.23
35	C	517[B]	DGD	O1G-C1A-C2A	2.48	119.38	111.83
23	B	611	CLA	C1C-C2C-C3C	-2.47	104.38	106.98
23	c	511	CLA	CAC-C3C-C4C	2.47	128.01	124.79
23	a	407[B]	CLA	CMC-C2C-C1C	2.47	128.90	125.03
31	B	631	LMT	O1'-C1'-C2'	2.47	112.03	108.27
23	B	610	CLA	CMA-C3A-C2A	-2.47	104.44	113.98
25	T	101	BCR	C21-C20-C19	-2.47	116.05	123.20
33	m	101	LMG	O7-C10-O9	-2.47	117.94	123.70
23	c	505	CLA	CHD-C4C-NC	2.47	128.05	124.23
23	d	402[B]	CLA	O2A-CGA-O1A	-2.46	117.46	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C2A-C1A-CHA	-2.46	119.59	123.87
31	m	103	LMT	C3B-C4B-C5B	-2.46	105.77	110.23
35	c	517[B]	DGD	O6D-C1D-O3G	-2.46	104.22	110.04
23	B	606	CLA	C1-C2-C3	-2.46	122.16	126.20
23	B	614	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
29	d	405[A]	PL9	C12-C13-C14	-2.46	121.99	127.62
25	c	515	BCR	C37-C22-C21	-2.46	118.83	122.82
23	b	611	CLA	CMB-C2B-C1B	2.46	129.16	125.42
23	c	504	CLA	CAC-C3C-C4C	2.46	127.98	124.79
23	B	607	CLA	O2A-CGA-O1A	-2.45	117.49	123.63
23	B	608	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
23	a	406[B]	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
24	a	408[B]	PHO	O2A-CGA-O1A	-2.45	117.49	123.63
23	B	611	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
25	c	515	BCR	C31-C1-C6	-2.45	106.40	110.24
23	d	402[A]	CLA	CMC-C2C-C1C	2.45	128.86	125.03
23	C	502	CLA	C1-O2A-CGA	2.45	122.58	116.65
23	b	607	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
23	B	614	CLA	CED-O2D-CGD	2.45	121.46	115.92
33	C	501	LMG	O6-C1-O1	-2.45	104.27	110.04
23	a	406[B]	CLA	O2A-CGA-CBA	2.44	119.29	111.83
29	A	414[A]	PL9	C42-C43-C44	-2.44	122.03	127.62
25	T	101	BCR	C33-C5-C6	-2.44	121.82	124.48
23	c	514	CLA	C1-C2-C3	-2.44	122.20	126.20
23	b	608	CLA	CHB-C4A-NA	2.44	127.92	124.40
33	c	520	LMG	C8-O7-C10	-2.44	111.96	117.80
25	d	404	BCR	C33-C5-C6	-2.44	121.82	124.48
23	A	408	CLA	C2A-C1A-CHA	-2.44	119.63	123.87
23	C	506	CLA	CHD-C4C-NC	2.44	128.01	124.23
32	D	408[B]	LHG	O8-C23-C24	2.44	119.27	111.83
32	b	629[A]	LHG	O8-C23-O10	-2.44	117.53	123.63
23	B	614	CLA	C4C-C3C-C2C	-2.43	103.35	106.89
32	d	407[A]	LHG	O8-C23-O10	-2.43	117.54	123.63
31	M	102	LMT	C3'-C4'-C5'	-2.43	105.54	110.93
35	h	102	DGD	O4D-C4D-C3D	-2.43	104.65	110.38
24	a	416[A]	PHO	O1D-CGD-CBD	-2.43	121.04	124.72
25	a	410	BCR	C40-C30-C25	-2.43	106.43	110.24
23	C	508	CLA	O2A-CGA-CBA	2.43	119.23	111.83
26	f	102	SQD	O47-C7-O49	-2.43	118.03	123.70
23	c	512	CLA	C2A-C1A-CHA	-2.43	119.66	123.87
23	B	605	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
23	b	612	CLA	C4D-CHA-C1A	-2.43	118.35	121.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	603	CLA	C1-C2-C3	-2.42	122.23	126.20
23	B	611	CLA	CMA-C3A-C2A	-2.42	104.61	113.98
23	B	604	CLA	CMC-C2C-C1C	2.42	128.82	125.03
29	D	407[A]	PL9	C20-C19-C21	2.42	119.43	115.23
35	C	518[B]	DGD	C2G-O2G-C1B	-2.42	112.00	117.80
23	b	616	CLA	OBD-CAD-C3D	-2.42	122.76	128.42
24	A	407[B]	PHO	O2A-CGA-CBA	2.42	119.21	111.83
23	B	608	CLA	CHD-C4C-NC	2.42	127.98	124.23
23	b	604	CLA	C4C-C3C-C2C	-2.42	103.37	106.89
29	a	414[B]	PL9	C47-C48-C49	-2.42	119.58	127.64
23	b	609	CLA	O2A-CGA-CBA	2.42	119.20	111.83
23	C	509	CLA	O2A-CGA-O1A	-2.42	117.59	123.63
23	b	607	CLA	C1-O2A-CGA	2.41	122.50	116.65
23	B	605	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
23	b	615	CLA	C2A-C1A-CHA	-2.41	119.68	123.87
24	a	416[B]	PHO	O1D-CGD-CBD	-2.41	121.06	124.72
23	c	505	CLA	CED-O2D-CGD	2.41	121.39	115.92
23	C	505	CLA	CHD-C4C-NC	2.41	127.97	124.23
23	C	514	CLA	C4-C3-C5	2.41	119.41	115.23
23	C	512	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
23	C	502	CLA	C4-C3-C5	2.41	119.41	115.23
23	c	508	CLA	C4C-C3C-C2C	-2.41	103.39	106.89
23	b	607	CLA	CAC-C3C-C4C	2.41	127.92	124.79
23	A	408	CLA	C4-C3-C5	2.41	119.41	115.23
35	C	519	DGD	O3G-C3G-C2G	-2.41	104.97	110.82
23	c	514	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
33	m	101	LMG	C7-O1-C1	-2.41	108.64	113.80
25	D	406	BCR	C21-C20-C19	-2.41	116.23	123.20
23	b	615	CLA	CHD-C4C-NC	2.40	127.96	124.23
31	F	101	LMT	C1'-O5'-C5'	-2.40	109.03	113.72
23	C	507	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
31	A	417	LMT	O1'-C1'-C2'	2.40	111.92	108.27
23	c	508	CLA	O2A-CGA-O1A	-2.40	117.62	123.63
23	B	613	CLA	CMB-C2B-C1B	2.40	129.08	125.42
23	B	608	CLA	O2A-CGA-CBA	2.40	119.16	111.83
23	b	614	CLA	CMA-C3A-C2A	-2.40	104.70	113.98
23	b	608	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
23	B	605	CLA	O2A-CGA-CBA	2.40	119.15	111.83
25	d	404	BCR	C29-C28-C27	-2.40	106.00	111.28
25	C	516	BCR	C11-C10-C9	-2.40	123.91	127.28
25	y	101	BCR	C24-C23-C22	-2.40	122.69	126.23
24	a	408[A]	PHO	CMA-C3A-C4A	-2.40	109.45	114.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C1-O2A-CGA	2.40	122.45	116.65
29	D	407[A]	PL9	C40-C39-C41	2.40	119.39	115.23
23	c	513	CLA	C3B-C4B-NB	2.40	112.67	110.53
23	B	604	CLA	C6-C7-C8	-2.40	108.00	115.97
23	b	613	CLA	C4-C3-C5	2.39	119.39	115.23
23	B	615	CLA	C6-C7-C8	-2.39	108.00	115.97
23	a	407[B]	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
23	D	405	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
35	c	517[A]	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
34	B	622	HTG	C6-C5-C4	-2.39	107.15	113.02
23	B	604	CLA	C11-C12-C13	-2.39	108.02	115.97
23	c	514	CLA	CHD-C4C-NC	2.39	127.94	124.23
23	B	613	CLA	CHB-C4A-NA	2.39	127.85	124.40
26	a	411[A]	SQD	O48-C23-C24	2.39	119.11	111.83
25	h	101	BCR	C37-C22-C21	-2.39	118.95	122.82
23	b	615	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
23	A	408	CLA	CMA-C3A-C4A	-2.39	105.36	111.77
29	d	405[B]	PL9	C20-C19-C21	2.39	119.37	115.23
23	A	404[B]	CLA	CAA-CBA-CGA	-2.39	106.43	113.21
23	c	502	CLA	O2A-CGA-O1A	-2.39	117.66	123.63
23	C	502	CLA	O2A-CGA-CBA	2.38	119.11	111.83
23	D	405	CLA	O2A-CGA-CBA	2.38	119.10	111.83
25	b	619	BCR	C15-C14-C13	-2.38	123.94	127.28
23	A	406[B]	CLA	C1-C2-C3	-2.38	122.29	126.20
26	X	101	SQD	O6-C44-C45	2.38	116.61	110.82
25	k	101	BCR	C20-C21-C22	-2.38	123.94	127.28
23	b	610	CLA	C3B-C4B-NB	2.38	112.66	110.53
23	B	603	CLA	C5-C3-C2	-2.38	115.82	121.17
34	B	622	HTG	C1'-S1-C1	2.38	105.59	100.45
23	A	406[A]	CLA	CAC-C3C-C4C	2.38	127.89	124.79
23	b	615	CLA	C11-C12-C13	-2.38	108.05	115.97
23	D	405	CLA	OBD-CAD-C3D	-2.38	122.85	128.42
23	B	601	CLA	CAA-C2A-C3A	-2.38	106.57	113.00
29	d	405[B]	PL9	C51-C49-C50	2.38	120.06	114.59
32	D	408[B]	LHG	O8-C23-O10	-2.38	117.68	123.63
23	A	405[B]	CLA	CMA-C3A-C4A	-2.38	105.39	111.77
23	b	611	CLA	CAC-C3C-C4C	2.38	127.88	124.79
35	C	518[A]	DGD	C2G-O2G-C1B	-2.38	112.11	117.80
23	B	614	CLA	C4-C3-C5	2.37	119.35	115.23
25	K	102	BCR	C36-C18-C19	2.37	121.72	118.09
31	B	630	LMT	O5'-C5'-C6'	2.37	112.32	106.44
23	C	513	CLA	C2A-C1A-CHA	-2.37	119.75	123.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	O2A-CGA-O1A	-2.37	117.69	123.63
23	B	614	CLA	CMA-C3A-C2A	-2.37	104.81	113.98
23	B	605	CLA	C7-C6-C5	-2.37	106.95	113.26
23	b	602	CLA	C11-C10-C8	-2.37	108.09	115.97
23	A	406[B]	CLA	CAC-C3C-C4C	2.37	127.87	124.79
23	B	602	CLA	C1-C2-C3	-2.37	122.32	126.20
23	B	604	CLA	CHD-C1D-ND	-2.37	121.47	124.80
25	c	516	BCR	C38-C26-C25	-2.37	121.90	124.48
32	d	406[A]	LHG	C6-C5-C4	-2.37	106.27	111.78
23	b	615	CLA	O2A-CGA-O1A	-2.36	117.71	123.63
23	B	609	CLA	C16-C15-C13	-2.36	108.11	115.97
23	b	611	CLA	O2A-CGA-CBA	2.36	119.04	111.83
23	a	405[B]	CLA	CMA-C3A-C4A	-2.36	105.42	111.77
24	a	416[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
25	c	516	BCR	C11-C10-C9	-2.36	123.97	127.28
25	k	101	BCR	C10-C11-C12	-2.36	116.36	123.20
23	b	606	CLA	CMC-C2C-C1C	2.36	128.72	125.03
24	A	416[B]	PHO	CMB-C2B-C3B	2.36	129.40	124.68
23	C	510	CLA	CHD-C4C-NC	2.36	127.89	124.23
23	B	610	CLA	CAC-C3C-C4C	2.36	127.86	124.79
24	A	416[A]	PHO	C4D-CHA-CBD	2.36	109.59	108.45
23	c	507	CLA	O2A-CGA-CBA	2.36	119.03	111.83
24	a	416[A]	PHO	O2A-CGA-CBA	2.36	119.03	111.83
23	b	612	CLA	CMC-C2C-C1C	2.36	128.72	125.03
23	B	609	CLA	C1-O2A-CGA	2.36	122.36	116.65
23	B	607	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
23	C	502	CLA	CBC-CAC-C3C	-2.36	106.03	112.42
23	A	405[B]	CLA	CMA-C3A-C2A	-2.36	104.87	113.98
25	t	102	BCR	C35-C13-C12	2.36	121.69	118.09
29	D	407[A]	PL9	C7-C8-C9	-2.36	122.77	126.83
34	b	622	HTG	O2-C2-C3	-2.35	104.83	110.38
23	c	513	CLA	C4B-C3B-C2B	-2.35	104.37	107.30
25	k	101	BCR	C3-C4-C5	-2.35	109.86	114.06
23	d	402[A]	CLA	CMB-C2B-C1B	2.35	129.00	125.42
23	B	612	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
23	C	505	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
23	a	409	CLA	C1-C2-C3	-2.35	122.35	126.20
32	b	629[B]	LHG	O7-C7-O9	-2.35	118.21	123.70
29	d	405[B]	PL9	C47-C48-C49	-2.35	119.81	127.64
23	b	616	CLA	CMC-C2C-C1C	2.35	128.70	125.03
25	K	103	BCR	C36-C18-C17	-2.35	119.01	122.82
32	d	413[B]	LHG	O7-C7-O9	-2.35	118.22	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C11-C10-C8	-2.35	108.17	115.97
23	c	513	CLA	O2A-CGA-O1A	-2.35	117.76	123.63
25	d	404	BCR	C30-C25-C24	2.35	122.01	115.65
23	B	603	CLA	C7-C6-C5	-2.35	107.01	113.26
23	C	509	CLA	CMC-C2C-C1C	2.34	128.70	125.03
23	b	615	CLA	O2A-CGA-CBA	2.34	118.98	111.83
23	b	612	CLA	CHD-C4C-NC	2.34	127.86	124.23
23	B	604	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
23	a	407[B]	CLA	C2A-C1A-CHA	-2.34	119.80	123.87
23	b	601	CLA	O2A-CGA-CBA	2.34	118.97	111.83
23	c	511	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
23	b	610	CLA	CMA-C3A-C2A	-2.34	104.94	113.98
25	c	515	BCR	C15-C16-C17	-2.34	118.73	123.52
25	T	101	BCR	C1-C6-C7	2.34	121.99	115.65
35	C	518[A]	DGD	O2G-C1B-O1B	-2.34	118.24	123.70
23	A	405[B]	CLA	OBD-CAD-C3D	-2.34	122.95	128.42
26	B	620	SQD	O5-C1-C2	-2.34	105.57	110.37
23	B	612	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	A	408	CLA	CHD-C4C-NC	2.34	127.86	124.23
31	F	101	LMT	C3B-C4B-C5B	-2.34	106.00	110.23
23	B	608	CLA	C2A-C1A-CHA	-2.34	119.81	123.87
29	d	405[A]	PL9	C7-C8-C9	-2.34	122.81	126.83
23	c	507	CLA	C4-C3-C5	2.33	119.28	115.23
23	d	403	CLA	C2A-C1A-CHA	-2.33	119.81	123.87
23	B	607	CLA	CMB-C2B-C1B	2.33	128.97	125.42
23	b	616	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
23	c	510	CLA	C2A-C1A-CHA	-2.33	119.82	123.87
29	a	414[A]	PL9	C20-C19-C21	2.33	119.28	115.23
23	b	610	CLA	CMC-C2C-C1C	2.33	128.68	125.03
24	a	408[B]	PHO	CMB-C2B-C3B	2.33	129.34	124.68
41	V	201	HEC	CMD-C2D-C1D	2.33	128.96	125.42
26	A	410[A]	SQD	O9-S-O7	-2.33	106.25	113.82
23	b	613	CLA	CAC-C3C-C4C	2.33	127.82	124.79
26	X	101	SQD	O48-C23-O10	-2.33	117.81	123.63
25	y	101	BCR	C1-C6-C7	2.33	121.96	115.65
26	A	410[A]	SQD	O8-S-C6	2.33	110.46	105.97
23	D	404[A]	CLA	CMC-C2C-C1C	2.33	128.67	125.03
29	A	414[A]	PL9	C12-C13-C14	-2.33	122.30	127.62
23	C	508	CLA	CHC-C1C-C2C	-2.32	120.34	126.95
23	b	609	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
23	C	505	CLA	CMB-C2B-C1B	2.32	128.95	125.42
23	C	511	CLA	CMB-C2B-C1B	2.32	128.95	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	618	BCR	C3-C4-C5	-2.32	109.92	114.06
25	t	102	BCR	C11-C10-C9	-2.32	124.03	127.28
23	a	405[B]	CLA	CHC-C1C-NC	2.32	127.80	124.31
23	b	605	CLA	CBC-CAC-C3C	-2.32	106.13	112.42
35	C	517[A]	DGD	O6E-C5E-C4E	2.32	113.88	109.70
41	v	201	HEC	CMD-C2D-C1D	2.32	128.95	125.42
35	C	517[A]	DGD	C3G-C2G-C1G	-2.32	106.38	111.78
31	B	631	LMT	O5'-C5'-C4'	2.32	114.52	109.72
26	a	412	SQD	C3-C4-C5	2.32	114.43	110.23
24	A	416[B]	PHO	CMA-C3A-C4A	-2.31	109.62	114.61
25	h	101	BCR	C20-C21-C22	-2.31	124.03	127.28
23	d	403	CLA	CMC-C2C-C1C	2.31	128.65	125.03
23	B	606	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
39	F	102	HEM	C4C-NC-C1C	2.31	109.59	105.82
23	B	609	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
26	f	102	SQD	O48-C23-O10	-2.31	117.84	123.63
25	d	404	BCR	C30-C25-C26	-2.31	119.48	122.64
41	V	201	HEC	CAD-CBD-CGD	-2.31	107.53	113.67
23	c	513	CLA	CAC-C3C-C4C	2.31	127.80	124.79
23	A	405[B]	CLA	CHB-C4A-NA	2.31	127.73	124.40
25	k	101	BCR	C15-C14-C13	-2.31	124.04	127.28
23	c	503	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
23	A	404[B]	CLA	CMA-C3A-C2A	-2.31	105.05	113.98
29	A	414[B]	PL9	C40-C39-C41	2.31	119.24	115.23
23	a	409	CLA	C1-O2A-CGA	2.31	122.24	116.65
27	B	624	GOL	C3-C2-C1	-2.31	103.33	111.80
23	b	606	CLA	OBD-CAD-C3D	-2.31	123.02	128.42
26	b	620	SQD	C1-C2-C3	-2.31	105.16	110.01
24	a	416[B]	PHO	C4A-C3A-C2A	-2.31	100.64	102.84
23	B	605	CLA	C4B-C3B-C2B	-2.31	104.44	107.30
33	d	411	LMG	C8-O7-C10	-2.31	112.28	117.80
23	C	502	CLA	O2A-CGA-O1A	-2.31	117.86	123.63
24	A	407[A]	PHO	CMB-C2B-C3B	2.30	129.29	124.68
25	c	515	BCR	C38-C26-C25	-2.30	121.97	124.48
23	B	604	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
23	b	606	CLA	O2A-CGA-O1A	-2.30	117.87	123.63
26	A	410[B]	SQD	C45-O47-C7	-2.30	112.29	117.80
29	A	414[A]	PL9	C45-C44-C46	2.30	119.22	115.23
26	a	411[A]	SQD	O9-S-O7	-2.30	106.34	113.82
24	a	416[B]	PHO	O2A-CGA-CBA	2.30	118.85	111.83
25	T	101	BCR	C38-C26-C25	-2.30	121.98	124.48
23	D	404[A]	CLA	CMB-C2B-C1B	2.30	128.92	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	414[B]	PL9	C25-C24-C26	2.30	119.21	115.23
23	b	608	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
23	c	512	CLA	CBC-CAC-C3C	-2.30	106.20	112.42
23	b	602	CLA	CHB-C1B-C2B	-2.29	120.77	127.43
29	d	405[B]	PL9	C7-C3-C4	2.29	118.80	116.91
23	c	510	CLA	O2A-CGA-CBA	2.29	118.82	111.83
23	D	404[B]	CLA	CHD-C4C-NC	2.29	127.78	124.23
23	C	504	CLA	CMC-C2C-C1C	2.29	128.61	125.03
26	B	620	SQD	C44-O6-C1	-2.29	108.89	113.80
39	f	101	HEM	C4D-ND-C1D	2.29	107.92	105.21
25	A	409	BCR	C16-C17-C18	-2.29	124.07	127.28
23	C	505	CLA	O2A-CGA-O1A	-2.29	117.91	123.63
29	d	405[A]	PL9	C20-C19-C21	2.29	119.20	115.23
23	B	601	CLA	C2A-C1A-CHA	-2.29	119.90	123.87
25	b	619	BCR	C21-C20-C19	-2.29	116.58	123.20
23	C	513	CLA	CHB-C4A-NA	2.29	127.70	124.40
25	T	101	BCR	C7-C6-C5	-2.28	116.29	121.56
32	E	101[A]	LHG	O7-C7-O9	-2.28	118.37	123.70
23	c	502	CLA	C4-C3-C5	2.28	119.19	115.23
35	C	518[B]	DGD	O1G-C1A-O1A	-2.28	117.92	123.63
23	b	609	CLA	CHD-C4C-NC	2.28	127.77	124.23
25	K	103	BCR	C38-C26-C25	-2.28	122.00	124.48
23	B	601	CLA	CMC-C2C-C1C	2.28	128.59	125.03
24	a	408[B]	PHO	O2D-CGD-O1D	-2.28	119.42	123.85
23	B	601	CLA	CHB-C4A-NA	2.27	127.68	124.40
23	a	405[A]	CLA	C7-C6-C5	-2.27	107.20	113.26
29	D	407[B]	PL9	C22-C23-C24	-2.27	122.42	127.62
35	c	517[B]	DGD	O3G-C3G-C2G	-2.27	105.29	110.82
23	C	511	CLA	CHB-C4A-NA	2.27	127.68	124.40
23	a	406[A]	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
25	d	404	BCR	C21-C20-C19	-2.27	116.62	123.20
29	d	405[A]	PL9	C47-C48-C49	-2.27	120.08	127.64
23	B	614	CLA	OBD-CAD-C3D	-2.26	123.13	128.42
23	d	402[B]	CLA	CHD-C4C-NC	2.26	127.74	124.23
26	f	102	SQD	O7-S-C6	2.26	110.13	106.76
23	B	610	CLA	C2A-C1A-CHA	-2.26	119.94	123.87
23	C	508	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
32	A	418[A]	LHG	O4-P-O5	2.26	122.96	112.44
25	T	101	BCR	C36-C18-C19	2.26	121.54	118.09
23	b	607	CLA	CMA-C3A-C2A	-2.26	105.25	113.98
23	A	408	CLA	CMC-C2C-C1C	2.26	128.56	125.03
23	B	616	CLA	O2A-CGA-O1A	-2.26	117.98	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	K	102	BCR	C3-C4-C5	-2.26	110.03	114.06
23	B	610	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	C	513	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
23	a	406[A]	CLA	CMC-C2C-C1C	2.26	128.56	125.03
25	C	515	BCR	C16-C17-C18	-2.25	124.12	127.28
23	D	404[A]	CLA	CED-O2D-CGD	2.25	121.03	115.92
33	d	411	LMG	C7-O1-C1	-2.25	108.96	113.80
23	c	510	CLA	CMC-C2C-C1C	2.25	128.56	125.03
32	d	406[A]	LHG	O8-C23-O10	-2.25	117.99	123.63
25	D	406	BCR	C11-C10-C9	-2.25	124.12	127.28
23	b	605	CLA	O2A-CGA-CBA	2.25	118.70	111.83
23	b	602	CLA	CHB-C4A-NA	2.25	127.65	124.40
23	c	513	CLA	CHB-C4A-NA	2.25	127.65	124.40
23	c	502	CLA	CHD-C4C-NC	2.25	127.72	124.23
23	B	606	CLA	CAC-C3C-C4C	2.25	127.72	124.79
23	C	511	CLA	C4C-C3C-C2C	-2.25	103.61	106.89
31	F	101	LMT	C2'-C3'-C4'	2.25	114.79	109.68
39	F	102	HEM	O2D-CGD-CBD	2.25	121.11	114.00
24	a	408[A]	PHO	C1-C2-C3	-2.25	122.51	126.20
29	D	407[B]	PL9	C53-C6-C1	2.25	119.88	115.28
25	K	103	BCR	C1-C6-C7	2.25	121.75	115.65
29	D	407[A]	PL9	C12-C13-C14	-2.25	122.48	127.62
23	A	405[A]	CLA	O2A-CGA-CBA	2.25	118.68	111.83
29	A	414[A]	PL9	C35-C34-C33	-2.25	117.86	123.63
23	B	610	CLA	CMC-C2C-C1C	2.24	128.54	125.03
23	d	403	CLA	CGD-CBD-CAD	-2.24	103.58	110.85
23	b	607	CLA	CMC-C2C-C1C	2.24	128.54	125.03
23	A	404[A]	CLA	CHD-C4C-NC	2.24	127.71	124.23
23	d	402[A]	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
29	a	414[B]	PL9	C45-C44-C46	2.24	119.12	115.23
24	A	416[A]	PHO	O1D-CGD-CBD	-2.24	121.33	124.72
31	b	627	LMT	C1'-O5'-C5'	-2.24	109.35	113.72
23	A	405[B]	CLA	O2A-CGA-CBA	2.24	118.65	111.83
23	a	405[B]	CLA	C7-C6-C5	-2.24	107.30	113.26
23	C	505	CLA	CAA-C2A-C3A	-2.24	106.96	113.00
24	A	407[B]	PHO	C4-C3-C5	2.24	119.11	115.23
23	B	613	CLA	CHD-C4C-NC	2.24	127.70	124.23
25	K	102	BCR	C32-C1-C6	-2.23	106.74	110.24
23	c	505	CLA	CBC-CAC-C3C	-2.23	106.36	112.42
23	A	405[B]	CLA	C4C-C3C-C2C	-2.23	103.64	106.89
25	K	103	BCR	C7-C6-C5	-2.23	116.41	121.56
23	A	404[B]	CLA	CHB-C1B-C2B	-2.23	120.94	127.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	OBD-CAD-C3D	-2.23	123.20	128.42
26	a	412	SQD	O48-C23-O10	-2.23	118.05	123.63
23	c	503	CLA	C2A-C1A-CHA	-2.23	120.00	123.87
39	f	101	HEM	CHA-C1A-NA	2.23	127.91	123.86
26	a	411[B]	SQD	C3-C4-C5	2.23	114.28	110.23
23	C	503	CLA	C4-C3-C5	2.23	119.10	115.23
23	A	406[B]	CLA	CMA-C3A-C2A	-2.23	105.37	113.98
29	d	405[B]	PL9	C7-C3-C2	-2.23	120.76	123.39
24	a	416[B]	PHO	C1A-C2A-C3A	-2.23	100.72	102.84
24	A	416[A]	PHO	CED-O2D-CGD	2.23	120.97	115.92
35	c	518[A]	DGD	O1G-C1A-O1A	-2.23	118.06	123.63
32	E	101[B]	LHG	C5-O7-C7	-2.23	112.47	117.80
25	t	102	BCR	C2-C1-C6	2.23	113.67	110.44
29	D	407[B]	PL9	C51-C49-C50	2.22	119.71	114.59
23	c	506	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
26	X	101	SQD	O7-S-C6	2.22	110.08	106.76
33	d	411	LMG	O7-C10-O9	-2.22	118.50	123.70
23	B	612	CLA	C6-C5-C3	-2.22	108.05	113.47
32	d	413[A]	LHG	O7-C7-O9	-2.22	118.51	123.70
31	B	630	LMT	C3B-C4B-C5B	-2.22	106.20	110.23
23	C	502	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
31	B	628	LMT	C1B-C2B-C3B	2.22	114.68	110.01
23	c	513	CLA	CMA-C3A-C4A	-2.22	105.80	111.77
23	B	607	CLA	CHD-C4C-NC	2.22	127.67	124.23
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
35	C	519	DGD	O2G-C1B-O1B	-2.22	118.51	123.70
34	b	622	HTG	O5-C1-C2	2.22	113.38	110.32
25	B	617	BCR	C24-C23-C22	-2.22	122.95	126.23
23	B	607	CLA	CMA-C3A-C2A	-2.22	105.40	113.98
31	c	501	LMT	O5B-C1B-C2B	2.22	114.93	110.37
35	H	102	DGD	O2G-C1B-C2B	2.22	116.28	111.48
23	C	512	CLA	C1-O2A-CGA	2.22	122.02	116.65
23	A	405[B]	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
23	C	504	CLA	CBC-CAC-C3C	-2.22	106.42	112.42
23	c	502	CLA	O2A-CGA-CBA	2.21	118.59	111.83
23	C	504	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
32	d	406[A]	LHG	O8-C23-C24	2.21	118.59	111.83
25	d	404	BCR	C28-C27-C26	-2.21	110.11	114.06
23	D	404[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
25	H	101	BCR	C37-C22-C21	-2.21	119.23	122.82
33	B	621	LMG	O8-C28-O10	-2.21	118.09	123.63
41	v	201	HEC	CMC-C2C-C1C	-2.21	122.05	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	515	BCR	C36-C18-C17	-2.21	119.23	122.82
23	C	504	CLA	O2A-CGA-CBA	2.21	118.58	111.83
23	c	508	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
26	X	101	SQD	O5-C1-C2	-2.21	105.83	110.37
23	C	509	CLA	CMB-C2B-C1B	2.21	128.78	125.42
29	A	414[B]	PL9	C10-C9-C8	-2.21	117.95	123.63
29	a	414[A]	PL9	C35-C34-C33	-2.21	117.95	123.63
23	c	503	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
24	A	407[A]	PHO	C4-C3-C5	2.21	119.06	115.23
23	b	615	CLA	CAC-C3C-C4C	2.21	127.66	124.79
23	b	609	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
23	c	508	CLA	C1-C2-C3	-2.21	122.58	126.20
26	f	102	SQD	O5-C5-C4	2.21	113.67	109.70
29	D	407[B]	PL9	C2-C1-C6	2.20	121.62	119.00
23	A	406[B]	CLA	CHB-C4A-NA	2.20	127.58	124.40
35	h	102	DGD	O2G-C1B-O1B	-2.20	118.55	123.70
23	C	513	CLA	CHB-C1B-C2B	-2.20	121.03	127.43
23	B	612	CLA	CHD-C4C-NC	2.20	127.64	124.23
23	c	514	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
33	c	520	LMG	O8-C28-O10	-2.20	118.12	123.63
31	b	621	LMT	C2'-C3'-C4'	2.20	114.67	109.68
25	K	102	BCR	C39-C30-C25	-2.20	106.79	110.24
23	C	510	CLA	C11-C12-C13	-2.20	108.66	115.97
23	d	403	CLA	CAC-C3C-C4C	2.20	127.65	124.79
23	b	601	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
25	c	516	BCR	C29-C30-C25	2.20	113.63	110.44
27	O	303	GOL	C3-C2-C1	-2.20	103.74	111.80
35	C	518[A]	DGD	O1G-C1A-C2A	2.19	118.53	111.83
23	c	507	CLA	C1-O2A-CGA	2.19	121.96	116.65
24	A	416[B]	PHO	O1D-CGD-CBD	-2.19	121.39	124.72
39	f	101	HEM	C4C-NC-C1C	2.19	109.40	105.82
35	c	517[A]	DGD	O3G-C3G-C2G	-2.19	105.48	110.82
29	A	414[B]	PL9	C47-C48-C49	-2.19	120.33	127.64
29	d	405[A]	PL9	C51-C49-C50	2.19	119.63	114.59
23	b	613	CLA	CED-O2D-CGD	2.19	120.89	115.92
32	b	629[B]	LHG	C5-O7-C7	-2.19	112.56	117.80
23	c	511	CLA	C4-C3-C2	-2.19	118.00	123.63
29	A	414[B]	PL9	C35-C34-C33	-2.19	118.00	123.63
23	c	502	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
35	C	517[B]	DGD	O3G-C3G-C2G	-2.19	105.50	110.82
23	A	408	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
32	D	408[B]	LHG	O7-C7-O9	-2.19	118.59	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	605	CLA	CED-O2D-CGD	2.18	120.87	115.92
29	A	414[A]	PL9	C25-C24-C26	2.18	119.02	115.23
23	B	613	CLA	C4-C3-C2	-2.18	118.02	123.63
23	B	613	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
23	C	514	CLA	C1-O2A-CGA	2.18	121.94	116.65
32	E	101[B]	LHG	O7-C7-O9	-2.18	118.60	123.70
35	c	519	DGD	O3G-C3G-C2G	-2.18	105.51	110.82
23	B	601	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
23	A	405[B]	CLA	C2A-C1A-CHA	-2.18	120.08	123.87
33	C	521	LMG	C9-C8-C7	-2.18	106.70	111.78
23	a	406[B]	CLA	C4-C3-C5	2.18	119.01	115.23
25	a	410	BCR	C33-C5-C6	-2.18	122.11	124.48
23	d	403	CLA	CHB-C4A-NA	2.18	127.54	124.40
33	a	417	LMG	O8-C28-C29	2.18	118.48	111.83
29	a	414[B]	PL9	C51-C49-C50	2.18	119.60	114.59
23	B	612	CLA	C4-C3-C5	2.18	119.01	115.23
23	C	511	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
33	m	101	LMG	O8-C28-O10	-2.18	118.19	123.63
23	c	502	CLA	C1-O2A-CGA	2.17	121.92	116.65
23	C	504	CLA	C2A-C1A-CHA	-2.17	120.09	123.87
24	a	408[A]	PHO	O2D-CGD-O1D	-2.17	119.62	123.85
23	B	608	CLA	C11-C10-C8	-2.17	108.74	115.97
25	B	617	BCR	C28-C27-C26	-2.17	110.18	114.06
23	C	503	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
25	C	515	BCR	C37-C22-C23	2.17	121.41	118.09
26	b	620	SQD	O5-C1-C2	-2.17	105.91	110.37
23	B	612	CLA	C4A-NA-C1A	-2.17	105.69	106.68
25	A	409	BCR	C15-C14-C13	-2.17	124.23	127.28
23	c	511	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
23	B	608	CLA	CMB-C2B-C1B	2.17	128.72	125.42
23	B	615	CLA	O2A-CGA-CBA	2.17	118.44	111.83
23	b	610	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	B	614	CLA	C4B-C3B-C2B	-2.16	104.61	107.30
35	c	517[A]	DGD	O6D-C1D-O3G	-2.16	104.93	110.04
24	a	416[A]	PHO	C4-C3-C2	-2.16	118.07	123.63
25	d	404	BCR	C39-C30-C25	-2.16	106.85	110.24
29	d	405[A]	PL9	O2-C1-C6	-2.16	117.04	120.48
23	b	614	CLA	C4D-CHA-C1A	-2.16	118.66	121.24
24	A	416[A]	PHO	OBD-CAD-C3D	-2.16	124.52	127.89
23	c	506	CLA	CHD-C4C-NC	2.16	127.58	124.23
25	b	619	BCR	C16-C17-C18	-2.16	124.25	127.28
23	D	404[A]	CLA	OBD-CAD-C3D	-2.16	123.37	128.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	410	BCR	C10-C11-C12	-2.16	116.94	123.20
27	D	403	GOL	C3-C2-C1	-2.16	103.88	111.80
23	c	514	CLA	C1-O2A-CGA	2.16	121.88	116.65
25	B	619	BCR	C10-C11-C12	-2.16	116.95	123.20
23	a	407[A]	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
35	H	102	DGD	C2G-O2G-C1B	-2.16	112.64	117.80
25	H	101	BCR	C10-C11-C12	-2.16	116.95	123.20
29	d	405[B]	PL9	C15-C14-C16	2.15	118.97	115.23
23	A	406[B]	CLA	CMC-C2C-C1C	2.15	128.40	125.03
23	a	409	CLA	CHB-C4A-NA	2.15	127.50	124.40
23	B	616	CLA	CBC-CAC-C3C	-2.15	106.59	112.42
35	C	517[A]	DGD	O3G-C3G-C2G	-2.15	105.59	110.82
23	B	606	CLA	OBD-CAD-C3D	-2.15	123.39	128.42
25	B	618	BCR	C37-C22-C21	-2.15	119.33	122.82
23	C	507	CLA	CMB-C2B-C1B	2.15	128.69	125.42
29	D	407[A]	PL9	C27-C28-C29	-2.15	122.71	127.62
23	b	613	CLA	C2A-C1A-CHA	-2.15	120.14	123.87
24	a	416[B]	PHO	CMA-C3A-C4A	-2.15	109.98	114.61
35	c	518[B]	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
23	c	502	CLA	CBC-CAC-C3C	-2.15	106.60	112.42
25	H	101	BCR	C31-C1-C6	-2.15	106.88	110.24
35	c	517[A]	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
23	c	505	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
25	h	101	BCR	C16-C17-C18	-2.14	124.27	127.28
23	B	602	CLA	CMA-C3A-C2A	-2.14	105.70	113.98
25	h	101	BCR	C34-C9-C8	2.14	121.36	118.09
23	B	611	CLA	C4D-CHA-C1A	-2.14	118.69	121.24
24	A	416[B]	PHO	O2A-CGA-O1A	-2.14	118.27	123.63
23	c	505	CLA	C4-C3-C5	2.14	118.94	115.23
23	d	402[A]	CLA	CHD-C4C-NC	2.14	127.55	124.23
23	C	507	CLA	CGD-CBD-CAD	-2.14	103.92	110.85
23	c	513	CLA	CBA-CAA-C2A	-2.14	107.43	113.79
23	C	507	CLA	C2A-C1A-CHA	-2.14	120.16	123.87
25	A	409	BCR	C38-C26-C25	-2.14	122.15	124.48
25	b	617	BCR	C21-C20-C19	-2.14	117.01	123.20
23	b	601	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
29	D	407[B]	PL9	C7-C8-C9	-2.13	123.16	126.83
23	d	403	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
23	b	604	CLA	CHD-C4C-NC	2.13	127.54	124.23
23	c	513	CLA	CBC-CAC-C3C	-2.13	106.64	112.42
32	L	101[A]	LHG	O4-P-O5	2.13	122.36	112.44
24	A	416[A]	PHO	C6-C5-C3	-2.13	108.28	113.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	516	BCR	C37-C22-C23	2.13	121.34	118.09
23	B	607	CLA	C6-C7-C8	-2.13	108.88	115.97
25	c	515	BCR	C37-C22-C23	2.13	121.34	118.09
23	a	407[A]	CLA	C4-C3-C5	2.13	118.92	115.23
23	b	602	CLA	C4-C3-C5	2.13	118.92	115.23
33	a	417	LMG	O7-C10-O9	-2.13	118.73	123.70
24	a	408[B]	PHO	CBA-CAA-C2A	-2.13	107.51	113.78
23	c	511	CLA	C2A-C1A-CHA	-2.13	120.18	123.87
41	v	201	HEC	CHA-C4D-ND	2.12	127.71	123.86
23	a	405[B]	CLA	CMC-C2C-C1C	2.12	128.35	125.03
26	B	620	SQD	C9-C8-C7	-2.12	105.91	113.69
26	A	410[B]	SQD	O48-C23-O10	-2.12	118.31	123.63
23	D	405	CLA	C3B-C4B-NB	2.12	112.43	110.53
25	D	406	BCR	C30-C25-C26	-2.12	119.73	122.64
23	B	609	CLA	C2A-C1A-CHA	-2.12	120.18	123.87
25	B	618	BCR	C24-C23-C22	-2.12	123.09	126.23
23	c	510	CLA	C4-C3-C2	-2.12	118.18	123.63
29	a	414[A]	PL9	C45-C44-C46	2.12	118.91	115.23
23	a	405[A]	CLA	CMB-C2B-C3B	2.12	131.54	126.55
23	b	609	CLA	CGD-CBD-CAD	-2.12	103.98	110.85
25	c	515	BCR	C29-C30-C25	2.12	113.52	110.44
23	b	610	CLA	C4-C3-C2	-2.12	118.18	123.63
25	D	406	BCR	C40-C30-C39	2.12	114.70	108.63
23	b	613	CLA	CMC-C2C-C1C	2.12	128.34	125.03
23	A	406[A]	CLA	CHB-C4A-NA	2.12	127.46	124.40
29	A	414[B]	PL9	C2-C3-C4	2.12	121.62	118.78
39	F	102	HEM	C4B-C3B-C2B	-2.12	105.33	107.28
23	A	406[B]	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
23	b	615	CLA	CHA-C1A-NA	-2.12	121.60	126.39
23	b	602	CLA	C7-C6-C5	-2.11	107.63	113.26
25	a	410	BCR	C3-C4-C5	-2.11	110.29	114.06
33	B	621	LMG	O6-C5-C4	2.11	113.51	109.70
23	c	503	CLA	CMC-C2C-C1C	2.11	128.34	125.03
23	b	608	CLA	C4-C3-C5	2.11	118.89	115.23
23	b	602	CLA	CHC-C1C-C2C	-2.11	120.95	126.95
23	B	606	CLA	C11-C10-C8	-2.11	108.95	115.97
31	M	101	LMT	O1'-C1'-C2'	2.11	111.48	108.27
25	D	406	BCR	C39-C30-C25	-2.11	106.93	110.24
35	H	102	DGD	C3E-C4E-C5E	-2.11	106.41	110.23
23	C	507	CLA	C4C-C3C-C2C	-2.11	103.82	106.89
23	A	405[A]	CLA	CHB-C4A-NA	2.11	127.44	124.40
29	D	407[B]	PL9	C15-C14-C16	2.11	118.89	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	406[B]	CLA	CAA-CBA-CGA	2.11	119.20	113.21
32	b	629[A]	LHG	O7-C7-O9	-2.11	118.77	123.70
31	M	101	LMT	O5B-C5B-C6B	2.11	111.67	106.44
23	C	513	CLA	OBD-CAD-C3D	-2.11	123.49	128.42
23	b	610	CLA	CHB-C4A-NA	2.11	127.44	124.40
23	B	616	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	c	502	CLA	CMC-C2C-C1C	2.11	128.32	125.03
39	f	101	HEM	CHA-C4D-C3D	-2.11	121.34	125.23
23	D	404[A]	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
25	b	618	BCR	C29-C30-C25	2.11	113.50	110.44
23	A	404[A]	CLA	C7-C6-C5	-2.11	107.65	113.26
39	f	101	HEM	CMD-C2D-C1D	2.11	128.32	125.03
26	B	620	SQD	O9-S-O7	-2.10	106.98	113.82
35	c	518[B]	DGD	O2G-C1B-O1B	-2.10	118.78	123.70
23	C	513	CLA	C4B-C3B-C2B	-2.10	104.69	107.30
23	b	616	CLA	C4-C3-C5	2.10	118.88	115.23
25	b	618	BCR	C29-C28-C27	-2.10	106.65	111.28
23	c	510	CLA	O2A-C1-C2	2.10	116.20	108.11
25	b	617	BCR	C20-C21-C22	-2.10	124.33	127.28
31	B	628	LMT	O1B-C4'-C3'	2.10	112.58	107.23
23	B	606	CLA	CHB-C1B-C2B	-2.10	121.32	127.43
35	c	519	DGD	O2G-C1B-O1B	-2.10	118.79	123.70
23	A	408	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
33	Z	101	LMG	C1-O6-C5	2.10	117.83	113.72
33	Z	101	LMG	C9-C8-C7	-2.10	106.88	111.78
23	C	513	CLA	CHC-C1C-C2C	-2.10	120.97	126.95
23	a	406[A]	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	d	407[B]	LHG	O8-C23-O10	-2.10	118.37	123.63
23	B	603	CLA	CAC-C3C-C4C	2.10	127.52	124.79
25	D	406	BCR	C3-C4-C5	-2.10	110.31	114.06
25	B	617	BCR	C16-C17-C18	-2.10	124.33	127.28
33	Z	101	LMG	C3-C4-C5	2.10	114.04	110.23
41	V	201	HEC	C1D-C2D-C3D	-2.10	104.41	106.82
29	d	405[A]	PL9	C45-C44-C46	2.10	118.87	115.23
23	D	405	CLA	C1-C2-C3	-2.10	122.76	126.20
23	B	612	CLA	CMA-C3A-C2A	-2.10	105.86	113.98
26	a	412	SQD	O47-C7-O49	-2.10	118.80	123.70
32	L	101[B]	LHG	O8-C23-O10	-2.10	118.38	123.63
31	m	103	LMT	O1'-C1'-C2'	2.10	111.46	108.27
41	v	201	HEC	C2A-C1A-NA	-2.10	108.30	110.32
25	B	619	BCR	C2-C1-C6	2.10	113.48	110.44
25	c	516	BCR	C37-C22-C23	2.10	121.29	118.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	c	517[A]	DGD	O1G-C1A-C2A	2.10	118.23	111.83
23	a	407[A]	CLA	CAC-C3C-C4C	2.09	127.52	124.79
23	B	611	CLA	C2C-C1C-NC	2.09	112.18	109.98
27	a	419	GOL	C3-C2-C1	-2.09	104.12	111.80
25	C	515	BCR	C21-C20-C19	-2.09	117.14	123.20
25	b	619	BCR	C39-C30-C25	-2.09	106.96	110.24
23	d	402[A]	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
23	c	505	CLA	CAA-C2A-C3A	-2.09	107.35	113.00
25	D	406	BCR	C37-C22-C21	-2.09	119.43	122.82
23	c	513	CLA	CHA-C1A-NA	-2.09	121.66	126.39
23	A	408	CLA	C11-C12-C13	-2.09	109.03	115.97
23	C	508	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
23	b	616	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
23	c	513	CLA	CHB-C1B-C2B	-2.09	121.37	127.43
25	b	619	BCR	C16-C15-C14	-2.09	119.25	123.52
29	d	405[A]	PL9	C2-C1-C6	2.08	121.48	119.00
39	F	102	HEM	CHA-C1A-NA	2.08	127.64	123.86
34	b	622	HTG	C6-C5-C4	-2.08	107.90	113.02
23	b	602	CLA	CAA-CBA-CGA	-2.08	107.29	113.21
23	C	508	CLA	CBB-CAB-C3B	-2.08	117.12	127.53
25	B	617	BCR	C15-C14-C13	-2.08	124.36	127.28
23	C	506	CLA	C11-C10-C8	-2.08	109.05	115.97
23	C	512	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
23	a	406[B]	CLA	CHB-C4A-NA	2.08	127.40	124.40
29	A	414[A]	PL9	C53-C6-C1	2.08	119.54	115.28
23	b	616	CLA	CHB-C1B-C2B	-2.08	121.39	127.43
26	a	411[A]	SQD	C3-C4-C5	2.08	114.00	110.23
25	a	410	BCR	C24-C23-C22	-2.08	123.16	126.23
23	C	511	CLA	C4-C3-C2	-2.08	118.30	123.63
23	D	404[A]	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
23	A	406[A]	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
33	B	621	LMG	C4-C3-C2	-2.08	107.19	110.83
23	b	606	CLA	C2A-C1A-CHA	-2.07	120.27	123.87
23	b	613	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
23	C	503	CLA	CED-O2D-CGD	2.07	120.62	115.92
23	c	505	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
24	A	407[B]	PHO	CBC-CAC-C3C	-2.07	109.90	112.87
24	a	416[A]	PHO	O2A-CGA-O1A	-2.07	118.44	123.63
25	B	618	BCR	C10-C11-C12	-2.07	117.19	123.20
23	c	512	CLA	CAC-C3C-C4C	2.07	127.49	124.79
23	b	602	CLA	CAC-C3C-C4C	2.07	127.48	124.79
26	A	410[B]	SQD	O7-S-C6	2.07	109.85	106.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	630	LMT	O5'-C5'-C4'	2.07	114.00	109.72
35	h	102	DGD	C6D-C5D-C4D	2.07	116.41	112.07
35	C	517[B]	DGD	O6D-C1D-O3G	-2.07	105.16	110.04
23	C	504	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
23	A	408	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
23	a	407[B]	CLA	CHB-C4A-NA	2.07	127.38	124.40
23	b	612	CLA	CMB-C2B-C1B	2.07	128.57	125.42
23	C	506	CLA	CHA-C1A-NA	-2.07	121.71	126.39
25	c	516	BCR	C2-C1-C6	2.07	113.44	110.44
23	b	604	CLA	O2A-CGA-CBA	2.07	118.13	111.83
31	A	417	LMT	C4B-C3B-C2B	-2.06	107.21	110.83
25	B	618	BCR	C7-C8-C9	-2.06	123.18	126.23
23	a	407[A]	CLA	CAA-CBA-CGA	2.06	119.06	113.21
23	B	606	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
23	B	603	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
23	b	606	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
23	B	611	CLA	CAC-C3C-C4C	2.06	127.47	124.79
23	A	404[B]	CLA	CED-O2D-CGD	2.06	120.59	115.92
23	A	405[A]	CLA	C1-C2-C3	-2.06	122.82	126.20
23	B	606	CLA	C2A-C1A-CHA	-2.06	120.30	123.87
25	K	102	BCR	C37-C22-C21	-2.06	119.48	122.82
23	B	615	CLA	C1-O2A-CGA	2.06	121.63	116.65
23	B	607	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
23	D	405	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
29	a	414[B]	PL9	C12-C13-C14	-2.06	122.92	127.62
23	b	610	CLA	CAC-C3C-C2C	2.06	131.34	127.56
23	c	511	CLA	C7-C6-C5	-2.06	107.78	113.26
25	c	515	BCR	C33-C5-C6	-2.06	122.24	124.48
23	c	514	CLA	C4-C3-C5	2.06	118.80	115.23
29	d	405[B]	PL9	C36-C34-C33	-2.05	116.55	121.17
24	A	416[A]	PHO	O2A-CGA-CBA	2.05	118.10	111.83
23	c	511	CLA	CHA-C1A-NA	-2.05	121.74	126.39
23	C	508	CLA	C7-C6-C5	-2.05	107.79	113.26
23	b	616	CLA	C1-C2-C3	-2.05	122.83	126.20
23	b	613	CLA	CHA-C1A-NA	-2.05	121.74	126.39
39	f	101	HEM	O2D-CGD-CBD	2.05	120.48	114.00
26	a	412	SQD	O8-S-C6	2.05	109.94	105.97
23	b	616	CLA	CHA-C1A-NA	-2.05	121.74	126.39
25	c	516	BCR	C15-C14-C13	-2.05	124.40	127.28
32	A	418[B]	LHG	O4-P-O5	2.05	121.98	112.44
29	D	407[A]	PL9	C47-C48-C49	-2.05	120.81	127.64
23	c	508	CLA	C1-O2A-CGA	2.05	121.61	116.65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
29	d	405[A]	PL9	C40-C39-C38	-2.05	118.37	123.63
39	f	101	HEM	C3B-C4B-NB	-2.05	108.00	109.47
29	a	414[B]	PL9	C35-C34-C33	-2.05	118.37	123.63
23	B	615	CLA	OBD-CAD-C3D	-2.05	123.63	128.42
23	B	608	CLA	C6-C7-C8	-2.05	109.17	115.97
23	b	611	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
24	a	408[B]	PHO	C4A-C3A-C2A	-2.04	100.89	102.84
23	c	506	CLA	C4-C3-C5	2.04	118.77	115.23
23	d	402[A]	CLA	CBB-CAB-C3B	-2.04	117.32	127.53
27	a	418	GOL	C3-C2-C1	-2.04	104.31	111.80
23	C	513	CLA	CHA-C1A-NA	-2.04	121.77	126.39
23	a	407[A]	CLA	CHA-C1A-NA	-2.04	121.77	126.39
23	b	603	CLA	CMC-C2C-C1C	2.04	128.22	125.03
25	h	101	BCR	C16-C15-C14	-2.04	119.35	123.52
41	v	201	HEC	CAD-CBD-CGD	-2.04	108.26	113.67
29	A	414[A]	PL9	C10-C9-C11	2.04	118.77	115.23
23	C	502	CLA	C11-C12-C13	-2.04	109.19	115.97
31	A	417	LMT	O5'-C1'-C2'	-2.04	106.18	110.37
29	a	414[A]	PL9	C47-C46-C44	-2.04	106.43	113.19
33	m	101	LMG	O6-C1-C2	2.04	114.56	110.37
23	B	609	CLA	CHA-C1A-NA	-2.04	121.78	126.39
41	v	201	HEC	C1D-C2D-C3D	-2.04	104.48	106.82
35	H	102	DGD	C1E-O6E-C5E	-2.04	109.74	113.72
25	H	101	BCR	C34-C9-C8	2.04	121.20	118.09
23	b	601	CLA	CAC-C3C-C4C	2.04	127.44	124.79
23	B	613	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
23	b	603	CLA	CGD-CBD-CAD	-2.03	104.26	110.85
23	c	510	CLA	CED-O2D-CGD	2.03	120.53	115.92
24	A	416[B]	PHO	C6-C5-C3	-2.03	108.52	113.47
35	h	102	DGD	C3B-C2B-C1B	-2.03	106.25	113.69
41	V	201	HEC	C2A-C1A-NA	-2.03	108.36	110.32
26	a	412	SQD	O5-C5-C4	2.03	113.36	109.70
27	l	102[A]	GOL	C3-C2-C1	-2.03	104.36	111.80
33	z	101	LMG	C8-O7-C10	-2.03	112.94	117.80
27	B	627	GOL	C3-C2-C1	-2.03	104.37	111.80
35	c	518[A]	DGD	O6E-C1E-O5D	-2.03	105.26	110.04
32	b	629[B]	LHG	O8-C23-O10	-2.02	118.56	123.63
29	a	414[A]	PL9	C51-C49-C50	2.02	119.25	114.59
26	b	620	SQD	C4-C3-C2	2.02	114.38	110.83
23	b	602	CLA	O2A-CGA-CBA	2.02	118.00	111.83
34	B	625	HTG	C6-C5-C4	-2.02	108.06	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	101	BCR	C28-C27-C26	-2.02	110.45	114.06
23	c	508	CLA	CHA-C1A-NA	-2.02	121.82	126.39
23	b	602	CLA	CMA-C3A-C2A	-2.02	106.17	113.98
23	B	614	CLA	C4-C3-C2	-2.02	118.44	123.63
25	K	103	BCR	C34-C9-C8	2.02	121.17	118.09
23	C	508	CLA	C1-C2-C3	-2.02	122.89	126.20
26	f	102	SQD	O6-C1-C2	2.02	111.34	108.27
31	M	101	LMT	C3B-C4B-C5B	-2.02	106.57	110.23
23	b	607	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
25	T	101	BCR	C34-C9-C10	-2.02	119.55	122.82
23	c	512	CLA	CMA-C3A-C4A	2.02	117.19	111.77
39	f	101	HEM	O2A-CGA-CBA	2.02	120.37	114.00
32	D	409[A]	LHG	O4-P-O5	2.01	121.82	112.44
29	A	414[A]	PL9	C51-C49-C50	2.01	119.22	114.59
33	C	501	LMG	O7-C10-O9	-2.01	119.00	123.70
23	C	507	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
23	B	602	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
23	B	608	CLA	CBC-CAC-C3C	-2.01	106.97	112.42
29	D	407[A]	PL9	C45-C44-C46	2.01	118.72	115.23
32	D	409[B]	LHG	O4-P-O5	2.01	121.80	112.44
23	c	504	CLA	CMC-C2C-C1C	2.01	128.17	125.03
23	B	611	CLA	CBC-CAC-C3C	-2.01	106.97	112.42
24	A	416[B]	PHO	CED-O2D-CGD	2.01	120.47	115.92
23	C	508	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	B	610	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
31	t	101	LMT	O5'-C5'-C6'	2.01	111.42	106.44
25	a	410	BCR	C11-C10-C9	-2.01	124.46	127.28
23	b	609	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	C	511	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
35	c	517[A]	DGD	O2G-C1B-O1B	-2.01	119.01	123.70
23	a	405[B]	CLA	CHB-C1B-C2B	-2.01	121.61	127.43
25	t	102	BCR	C7-C8-C9	-2.00	123.27	126.23
25	b	617	BCR	C11-C12-C13	-2.00	120.87	126.36
23	b	612	CLA	C4-C3-C2	-2.00	118.48	123.63
29	D	407[A]	PL9	C22-C23-C24	-2.00	123.04	127.62
23	d	402[B]	CLA	CMC-C2C-C1C	2.00	128.16	125.03
33	z	101	LMG	O8-C28-O10	-2.00	118.62	123.63

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	A	404[B]	CLA	ND
23	A	405[A]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	404[A]	CLA	ND
23	D	404[B]	CLA	ND
23	D	405	CLA	ND
23	a	405[A]	CLA	ND
23	a	405[B]	CLA	ND
23	a	406[A]	CLA	ND
23	a	406[B]	CLA	ND
23	a	409	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	c	514	CLA	ND
23	d	402[A]	CLA	ND
23	d	402[B]	CLA	ND
23	d	403	CLA	ND

All (1584) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C6-C7-C8-C9
23	B	603	CLA	C4-C3-C5-C6
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	a	405[B]	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	409	CLA	C4-C3-C5-C6
23	b	601	CLA	C11-C10-C8-C9
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	C11-C12-C13-C14
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
25	K	103	BCR	C1-C6-C7-C8
25	K	103	BCR	C5-C6-C7-C8
25	d	404	BCR	C21-C22-C23-C24
26	A	410[B]	SQD	C8-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-C7-O47-C45
26	X	101	SQD	O49-C7-O47-C45
26	X	101	SQD	C8-C7-O47-C45
26	a	412	SQD	O6-C44-C45-O47
26	a	412	SQD	C5-C6-S-O7
26	a	412	SQD	C5-C6-S-O8
26	a	412	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	B	624	GOL	C1-C2-C3-O3
27	B	624	GOL	O2-C2-C3-O3
27	B	629	GOL	O1-C1-C2-C3
27	D	414	GOL	C1-C2-C3-O3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	o	302	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3
29	A	414[A]	PL9	C9-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	414[A]	PL9	C23-C24-C26-C27
29	a	414[A]	PL9	C25-C24-C26-C27
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	419	LMT	C2'-C1'-O1'-C1
31	A	419	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
32	A	418[B]	LHG	C4-O6-P-O5
32	D	408[A]	LHG	O2-C2-C3-O3
32	D	408[A]	LHG	C3-O3-P-O4
32	D	408[A]	LHG	C3-O3-P-O5
32	D	408[A]	LHG	C3-O3-P-O6
32	D	408[A]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	O2-C2-C3-O3
32	D	408[B]	LHG	C3-O3-P-O4
32	D	408[B]	LHG	C3-O3-P-O6
32	D	408[B]	LHG	C4-O6-P-O3
32	D	408[B]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	420[A]	LHG	C3-O3-P-O4
32	a	420[A]	LHG	C3-O3-P-O6
32	a	420[A]	LHG	C4-O6-P-O3
32	a	420[A]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	O10-C23-O8-C6
32	a	420[A]	LHG	C24-C23-O8-C6
32	a	420[B]	LHG	C3-O3-P-O4
32	a	420[B]	LHG	C3-O3-P-O6
32	a	420[B]	LHG	C4-O6-P-O3
32	a	420[B]	LHG	C4-O6-P-O5
32	a	420[B]	LHG	O10-C23-O8-C6
32	a	420[B]	LHG	C24-C23-O8-C6
32	b	629[A]	LHG	C4-O6-P-O3
32	b	629[A]	LHG	C4-O6-P-O4
32	b	629[A]	LHG	C4-O6-P-O5
32	b	629[B]	LHG	C4-O6-P-O3
32	b	629[B]	LHG	C4-O6-P-O4
32	b	629[B]	LHG	C4-O6-P-O5
32	d	406[A]	LHG	C3-O3-P-O4
32	d	406[A]	LHG	C3-O3-P-O5
32	d	406[A]	LHG	C3-O3-P-O6
32	d	406[A]	LHG	C4-O6-P-O4
32	d	406[B]	LHG	O2-C2-C3-O3
32	d	406[B]	LHG	C3-O3-P-O4
32	d	406[B]	LHG	C3-O3-P-O5
32	d	406[B]	LHG	C3-O3-P-O6
32	d	406[B]	LHG	C4-O6-P-O3
32	d	406[B]	LHG	C4-O6-P-O4
32	d	413[A]	LHG	C3-O3-P-O5
32	d	413[B]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
39	F	102	HEM	C2C-C3C-CAC-CBC
39	F	102	HEM	C4C-C3C-CAC-CBC
41	V	201	HEC	C2B-C3B-CAB-CBB
41	V	201	HEC	C4B-C3B-CAB-CBB
41	V	201	HEC	C2C-C3C-CAC-CBC
41	V	201	HEC	C4C-C3C-CAC-CBC
41	v	201	HEC	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
41	v	201	HEC	C4B-C3B-CAB-CBB
41	v	201	HEC	C2C-C3C-CAC-CBC
41	v	201	HEC	C4C-C3C-CAC-CBC
31	A	419	LMT	O5B-C1B-O1B-C4'
31	B	630	LMT	C4'-C5'-C6'-O6'
31	M	102	LMT	C4B-C5B-C6B-O6B
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
33	C	521	LMG	O9-C10-O7-C8
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
31	M	102	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O5B-C5B-C6B-O6B
23	D	405	CLA	CBD-CGD-O2D-CED
26	B	620	SQD	C8-C7-O47-C45
33	c	521	LMG	C11-C10-O7-C8
23	A	408	CLA	C4-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C30-C29-C31-C32
23	A	408	CLA	C2-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6
23	a	409	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C28-C29-C31-C32
31	B	630	LMT	O5B-C5B-C6B-O6B
23	B	614	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
34	D	412	HTG	O5-C5-C6-O6
25	T	101	BCR	C13-C14-C15-C16
31	m	103	LMT	C4B-C5B-C6B-O6B
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	D	405	CLA	C3-C5-C6-C7
32	d	406[A]	LHG	O2-C2-C3-O3
32	d	413[B]	LHG	O2-C2-C3-O3
31	b	621	LMT	O5'-C5'-C6'-O6'
33	C	521	LMG	O6-C5-C6-O5
31	B	628	LMT	C4'-C5'-C6'-O6'
31	m	103	LMT	O5B-C5B-C6B-O6B
31	c	501	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	514	CLA	CBD-CGD-O2D-CED
26	A	410[A]	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
31	B	628	LMT	O5B-C5B-C6B-O6B
33	c	521	LMG	C4-C5-C6-O5
31	F	101	LMT	O5'-C5'-C6'-O6'
34	B	625	HTG	O5-C5-C6-O6
31	M	102	LMT	C4'-C5'-C6'-O6'
34	b	625	HTG	S1-C1'-C2'-C3'
23	C	508	CLA	C4-C3-C5-C6
23	D	405	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	a	414[A]	PL9	C15-C14-C16-C17
29	a	414[A]	PL9	C30-C29-C31-C32
29	a	414[B]	PL9	C15-C14-C16-C17
29	a	414[B]	PL9	C25-C24-C26-C27
29	a	414[B]	PL9	C30-C29-C31-C32
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C18-C19-C21-C22
29	a	414[A]	PL9	C13-C14-C16-C17
29	a	414[A]	PL9	C28-C29-C31-C32
29	a	414[B]	PL9	C13-C14-C16-C17
29	a	414[B]	PL9	C28-C29-C31-C32
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	407[A]	PL9	C39-C41-C42-C43
29	a	414[A]	PL9	C9-C11-C12-C13
29	a	414[A]	PL9	C14-C16-C17-C18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	a	414[B]	PL9	C9-C11-C12-C13
29	a	414[B]	PL9	C14-C16-C17-C18
31	B	630	LMT	C4B-C5B-C6B-O6B
31	A	419	LMT	O5B-C5B-C6B-O6B
31	M	102	LMT	O5B-C5B-C6B-O6B
34	D	412	HTG	C4-C5-C6-O6
26	B	620	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C5'-C6'-O6'
23	c	502	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
31	A	419	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	C4'-C5'-C6'-O6'
23	c	514	CLA	CBD-CGD-O2D-CED
34	D	412	HTG	S1-C1'-C2'-C3'
31	b	627	LMT	C4'-C5'-C6'-O6'
31	e	101	LMT	C4'-C5'-C6'-O6'
33	z	101	LMG	O9-C10-O7-C8
32	d	406[A]	LHG	C1-C2-C3-O3
32	d	413[B]	LHG	C1-C2-C3-O3
23	a	409	CLA	CBA-CGA-O2A-C1
31	B	628	LMT	O5'-C5'-C6'-O6'
31	F	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C20-C19-C21-C22
23	B	605	CLA	C2-C3-C5-C6
23	D	405	CLA	C2-C3-C5-C6
23	C	503	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
31	b	627	LMT	O5'-C5'-C6'-O6'
26	X	101	SQD	C2-C1-O6-C44
31	A	417	LMT	C2'-C1'-O1'-C1
35	h	102	DGD	C6B-C7B-C8B-C9B
26	X	101	SQD	C23-C24-C25-C26
31	A	419	LMT	C4B-C5B-C6B-O6B
25	b	619	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C10
33	c	521	LMG	O6-C5-C6-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	b	625	HTG	O5-C5-C6-O6
23	b	606	CLA	C10-C11-C12-C13
33	B	621	LMG	C39-C40-C41-C42
23	D	405	CLA	O1D-CGD-O2D-CED
35	C	519	DGD	C6B-C7B-C8B-C9B
23	b	614	CLA	C8-C10-C11-C12
27	b	624	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
23	A	408	CLA	C12-C13-C15-C16
23	b	606	CLA	C12-C13-C15-C16
31	B	628	LMT	C5'-C4'-O1B-C1B
29	A	414[A]	PL9	C30-C29-C31-C32
31	e	101	LMT	O5B-C5B-C6B-O6B
29	D	407[B]	PL9	C39-C41-C42-C43
29	a	414[B]	PL9	C24-C26-C27-C28
29	d	405[A]	PL9	C39-C41-C42-C43
29	d	405[B]	PL9	C39-C41-C42-C43
31	A	419	LMT	O1'-C1-C2-C3
23	B	601	CLA	C10-C11-C12-C13
31	B	631	LMT	C4'-C5'-C6'-O6'
26	A	410[B]	SQD	C7-C8-C9-C10
33	Z	101	LMG	C10-C11-C12-C13
35	c	518[A]	DGD	C1B-C2B-C3B-C4B
35	c	518[B]	DGD	C1B-C2B-C3B-C4B
23	B	602	CLA	C13-C15-C16-C17
23	b	601	CLA	C10-C11-C12-C13
23	c	513	CLA	C15-C16-C17-C18
23	B	606	CLA	C2A-CAA-CBA-CGA
26	B	620	SQD	C30-C31-C32-C33
23	b	604	CLA	C8-C10-C11-C12
31	B	628	LMT	C4B-C5B-C6B-O6B
32	E	101[A]	LHG	C23-C24-C25-C26
23	a	409	CLA	O1A-CGA-O2A-C1
34	b	622	HTG	S1-C1'-C2'-C3'
26	X	101	SQD	O5-C1-O6-C44
31	b	621	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
23	A	408	CLA	C5-C6-C7-C8
23	B	601	CLA	C5-C6-C7-C8
23	b	611	CLA	C8-C10-C11-C12
31	A	419	LMT	C4'-C5'-C6'-O6'
23	B	606	CLA	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C13-C15-C16-C17
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	C13-C15-C16-C17
23	D	405	CLA	C10-C11-C12-C13
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
31	e	101	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O1'-C1-C2-C3
23	a	405[A]	CLA	C15-C16-C17-C18
23	a	405[B]	CLA	C15-C16-C17-C18
32	D	408[A]	LHG	C1-C2-C3-O3
32	d	406[B]	LHG	C1-C2-C3-O3
23	b	606	CLA	C2A-CAA-CBA-CGA
32	D	409[A]	LHG	C33-C34-C35-C36
23	B	608	CLA	C13-C15-C16-C17
23	B	615	CLA	C5-C6-C7-C8
23	C	508	CLA	C5-C6-C7-C8
23	b	611	CLA	C15-C16-C17-C18
23	b	614	CLA	C10-C11-C12-C13
31	A	417	LMT	O1'-C1-C2-C3
32	E	101[B]	LHG	C23-C24-C25-C26
23	C	503	CLA	C13-C15-C16-C17
23	b	604	CLA	C5-C6-C7-C8
23	c	507	CLA	C15-C16-C17-C18
31	B	631	LMT	O1'-C1-C2-C3
23	B	614	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
31	B	630	LMT	C2'-C1'-O1'-C1
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
26	A	410[A]	SQD	C7-C8-C9-C10
34	b	623	HTG	C1'-C2'-C3'-C4'
25	K	102	BCR	C7-C8-C9-C34
25	d	404	BCR	C37-C22-C23-C24
31	B	628	LMT	C6-C7-C8-C9
25	D	406	BCR	C21-C22-C23-C24
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
23	B	610	CLA	C2A-CAA-CBA-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	c	517[B]	DGD	C4D-C5D-C6D-O5D
23	B	614	CLA	C5-C6-C7-C8
33	B	621	LMG	C37-C38-C39-C40
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	O1-C1-C2-C3
27	B	629	GOL	C1-C2-C3-O3
27	D	414	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	418	GOL	O1-C1-C2-C3
27	d	412	GOL	O1-C1-C2-C3
27	d	412	GOL	C1-C2-C3-O3
27	v	202[A]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
26	B	620	SQD	C7-C8-C9-C10
34	B	625	HTG	C4-C5-C6-O6
23	B	603	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
31	B	630	LMT	O5'-C1'-O1'-C1
34	B	622	HTG	C1'-C2'-C3'-C4'
26	A	410[B]	SQD	C11-C10-C9-C8
31	A	419	LMT	C5'-C4'-O1B-C1B
26	A	410[A]	SQD	C12-C13-C14-C15
32	D	409[B]	LHG	C33-C34-C35-C36
23	B	615	CLA	C10-C11-C12-C13
33	c	520	LMG	C10-C11-C12-C13
23	B	616	CLA	C2-C1-O2A-CGA
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
23	a	409	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
23	c	514	CLA	C10-C11-C12-C13
32	L	101[A]	LHG	C15-C16-C17-C18
32	L	101[A]	LHG	C17-C18-C19-C20
32	d	413[B]	LHG	C16-C17-C18-C19
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
26	X	101	SQD	C30-C31-C32-C33
26	f	102	SQD	C32-C33-C34-C35
32	L	101[B]	LHG	C12-C13-C14-C15
35	C	518[B]	DGD	CCB-CDB-CEB-CFB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C8-C10-C11-C12
31	t	101	LMT	C4-C5-C6-C7
33	C	501	LMG	C36-C37-C38-C39
33	D	413	LMG	C19-C20-C21-C22
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
35	h	102	DGD	C7B-C8B-C9B-CAB
35	c	517[A]	DGD	O6D-C5D-C6D-O5D
26	A	410[B]	SQD	C15-C16-C17-C18
32	b	629[B]	LHG	C14-C15-C16-C17
35	H	102	DGD	CCB-CDB-CEB-CFB
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
27	B	629	GOL	O1-C1-C2-O2
27	O	302	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
31	B	628	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2-C1-O1'-C1'
31	t	101	LMT	C2-C1-O1'-C1'
32	D	409[B]	LHG	C32-C33-C34-C35
33	B	621	LMG	C17-C18-C19-C20
34	B	623	HTG	C3'-C4'-C5'-C6'
23	C	514	CLA	O1D-CGD-O2D-CED
23	C	508	CLA	C4B-C3B-CAB-CBB
23	D	404[B]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
32	d	413[A]	LHG	C16-C17-C18-C19
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	c	502	CLA	O1D-CGD-O2D-CED
23	A	405[A]	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12
31	A	419	LMT	C1-C2-C3-C4
33	B	621	LMG	C11-C10-O7-C8
33	m	101	LMG	C11-C10-O7-C8
31	M	101	LMT	O5'-C5'-C6'-O6'
23	C	511	CLA	C11-C12-C13-C15
26	b	620	SQD	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	b	627	LMT	C7-C8-C9-C10
32	d	407[B]	LHG	C27-C28-C29-C30
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
32	E	101[B]	LHG	O2-C2-C3-O3
31	B	630	LMT	C5-C6-C7-C8
32	d	413[A]	LHG	C32-C33-C34-C35
31	A	419	LMT	C3-C4-C5-C6
32	a	420[A]	LHG	C26-C27-C28-C29
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
32	D	408[A]	LHG	C16-C17-C18-C19
33	D	413	LMG	C36-C37-C38-C39
23	b	606	CLA	C15-C16-C17-C18
23	B	615	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
23	d	402[A]	CLA	C16-C17-C18-C20
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
31	c	501	LMT	O5'-C5'-C6'-O6'
26	b	620	SQD	C27-C28-C29-C30
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
32	D	409[A]	LHG	C32-C33-C34-C35
32	D	408[B]	LHG	C1-C2-C3-O3
33	Z	101	LMG	O6-C5-C6-O5
23	c	513	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
31	c	501	LMT	C1-C2-C3-C4
29	A	414[B]	PL9	C39-C41-C42-C43
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
33	C	501	LMG	C10-C11-C12-C13
31	b	627	LMT	C3-C4-C5-C6
32	L	101[A]	LHG	C12-C13-C14-C15
32	L	101[A]	LHG	C13-C14-C15-C16
32	b	629[A]	LHG	C16-C17-C18-C19
33	C	521	LMG	C18-C19-C20-C21
35	C	517[A]	DGD	C4B-C5B-C6B-C7B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
26	A	410[A]	SQD	C15-C16-C17-C18
32	E	101[A]	LHG	C24-C25-C26-C27
32	L	101[B]	LHG	C13-C14-C15-C16
32	a	420[B]	LHG	C26-C27-C28-C29
32	d	413[A]	LHG	C29-C30-C31-C32
33	D	413	LMG	C35-C36-C37-C38
33	d	411	LMG	C29-C30-C31-C32
35	H	102	DGD	C5B-C6B-C7B-C8B
23	c	512	CLA	O1D-CGD-O2D-CED
31	M	102	LMT	C7-C8-C9-C10
32	L	101[B]	LHG	C15-C16-C17-C18
33	C	501	LMG	C12-C13-C14-C15
23	c	510	CLA	C16-C17-C18-C19
33	a	417	LMG	C10-C11-C12-C13
23	c	508	CLA	C2B-C3B-CAB-CBB
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
23	b	605	CLA	C5-C6-C7-C8
32	L	101[B]	LHG	C17-C18-C19-C20
33	C	501	LMG	C17-C18-C19-C20
31	B	628	LMT	C3'-C4'-O1B-C1B
33	a	417	LMG	C30-C31-C32-C33
31	B	628	LMT	C5-C6-C7-C8
32	L	101[A]	LHG	C25-C26-C27-C28
32	L	101[B]	LHG	C25-C26-C27-C28
33	C	501	LMG	C20-C21-C22-C23
26	A	412	SQD	C17-C18-C19-C20
31	e	101	LMT	C5-C6-C7-C8
33	B	621	LMG	O9-C10-O7-C8
33	m	101	LMG	O9-C10-O7-C8
23	C	511	CLA	C4-C3-C5-C6
29	d	405[B]	PL9	C15-C14-C16-C17
31	e	101	LMT	C4-C5-C6-C7
35	h	102	DGD	C9A-CAA-CBA-CCA
29	a	414[B]	PL9	C23-C24-C26-C27
26	X	101	SQD	C24-C25-C26-C27
26	a	412	SQD	C31-C32-C33-C34
33	C	520	LMG	C16-C17-C18-C19
32	D	409[B]	LHG	C24-C23-O8-C6
31	b	627	LMT	C1-C2-C3-C4
26	X	101	SQD	C29-C30-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	631	LMT	C4-C5-C6-C7
33	m	101	LMG	C35-C36-C37-C38
23	B	615	CLA	C13-C15-C16-C17
24	a	416[B]	PHO	C2C-C3C-CAC-CBC
32	D	408[B]	LHG	C16-C17-C18-C19
35	h	102	DGD	CAA-CBA-CCA-CDA
26	A	412	SQD	O5-C1-O6-C44
31	M	101	LMT	O5'-C1'-O1'-C1
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
31	M	101	LMT	C3-C4-C5-C6
26	A	412	SQD	C2-C1-O6-C44
31	B	631	LMT	C2'-C1'-O1'-C1
33	Z	101	LMG	C2-C1-O1-C7
31	B	628	LMT	C7-C8-C9-C10
32	b	629[A]	LHG	C14-C15-C16-C17
33	D	413	LMG	C30-C31-C32-C33
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
35	c	518[B]	DGD	CBB-CCB-CDB-CEB
35	c	519	DGD	CBB-CCB-CDB-CEB
32	E	101[A]	LHG	O2-C2-C3-O3
31	B	631	LMT	C11-C10-C9-C8
32	E	101[B]	LHG	C24-C25-C26-C27
23	B	610	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
26	a	412	SQD	C25-C26-C27-C28
31	t	101	LMT	O5'-C5'-C6'-O6'
33	a	417	LMG	C34-C35-C36-C37
26	A	410[B]	SQD	C12-C13-C14-C15
32	b	629[B]	LHG	C16-C17-C18-C19
23	c	513	CLA	CBD-CGD-O2D-CED
26	A	412	SQD	C26-C27-C28-C29
31	B	631	LMT	C3-C4-C5-C6
32	d	413[B]	LHG	C32-C33-C34-C35
35	c	517[A]	DGD	C7A-C8A-C9A-CAA
26	b	620	SQD	C31-C32-C33-C34
33	C	521	LMG	C19-C20-C21-C22
23	B	610	CLA	C16-C17-C18-C20
23	c	503	CLA	C16-C17-C18-C19
32	A	418[B]	LHG	C12-C13-C14-C15
32	d	407[B]	LHG	C25-C26-C27-C28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	d	406[B]	LHG	C34-C35-C36-C37
32	d	407[A]	LHG	C29-C30-C31-C32
23	A	406[B]	CLA	C13-C15-C16-C17
33	C	501	LMG	C39-C40-C41-C42
32	D	409[B]	LHG	C29-C30-C31-C32
33	C	501	LMG	C29-C30-C31-C32
33	D	413	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
32	A	418[A]	LHG	C12-C13-C14-C15
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
32	d	406[B]	LHG	C11-C10-C9-C8
32	d	407[A]	LHG	C27-C28-C29-C30
23	A	404[B]	CLA	C13-C15-C16-C17
32	d	407[A]	LHG	C25-C26-C27-C28
23	c	510	CLA	C3-C5-C6-C7
26	A	410[A]	SQD	O6-C44-C45-O47
33	a	417	LMG	C4-C5-C6-O5
33	c	521	LMG	C29-C28-O8-C9
32	D	409[B]	LHG	O10-C23-O8-C6
32	A	418[B]	LHG	C34-C35-C36-C37
32	d	413[A]	LHG	C24-C25-C26-C27
33	d	411	LMG	O6-C5-C6-O5
31	b	627	LMT	C5-C6-C7-C8
32	b	629[A]	LHG	C27-C28-C29-C30
35	c	517[A]	DGD	C4D-C5D-C6D-O5D
32	D	408[A]	LHG	C12-C13-C14-C15
33	c	520	LMG	C34-C35-C36-C37
23	d	402[A]	CLA	C16-C17-C18-C19
33	C	501	LMG	C19-C20-C21-C22
33	C	521	LMG	C17-C18-C19-C20
33	c	520	LMG	C31-C32-C33-C34
23	C	507	CLA	C4-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
31	b	621	LMT	C3'-C4'-O1B-C1B
32	D	409[A]	LHG	C15-C16-C17-C18
33	C	521	LMG	C13-C14-C15-C16
33	m	101	LMG	C39-C40-C41-C42
23	b	610	CLA	C2A-CAA-CBA-CGA
23	c	511	CLA	CBD-CGD-O2D-CED
35	C	519	DGD	C2B-C3B-C4B-C5B
23	c	514	CLA	O1D-CGD-O2D-CED
23	B	605	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	e	101	LMT	C1-C2-C3-C4
32	A	418[A]	LHG	C34-C35-C36-C37
32	D	409[B]	LHG	C15-C16-C17-C18
34	b	623	HTG	O5-C5-C6-O6
27	B	629	GOL	O2-C2-C3-O3
27	D	414	GOL	O2-C2-C3-O3
27	o	302	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
23	c	513	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	O10-C23-O48-C46
32	d	407[A]	LHG	C34-C35-C36-C37
33	B	621	LMG	C34-C35-C36-C37
26	B	620	SQD	C11-C10-C9-C8
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	a	407[B]	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
23	b	601	CLA	C8-C10-C11-C12
33	C	520	LMG	C34-C35-C36-C37
35	c	518[A]	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	CAB-CBB-CCB-CDB
32	d	406[A]	LHG	C34-C35-C36-C37
33	m	101	LMG	C38-C39-C40-C41
23	C	512	CLA	C3-C5-C6-C7
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	511	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	D	405	CLA	C12-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
31	B	630	LMT	C6-C7-C8-C9
23	b	606	CLA	C16-C17-C18-C20
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	604	CLA	C5-C6-C7-C8
35	c	518[A]	DGD	C4A-C5A-C6A-C7A
23	c	508	CLA	C5-C6-C7-C8
29	D	407[B]	PL9	C15-C14-C16-C17
29	a	414[A]	PL9	C12-C11-C9-C10
33	c	520	LMG	C4-C5-C6-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	411	LMG	C11-C12-C13-C14
31	B	628	LMT	C1-C2-C3-C4
23	c	507	CLA	C10-C11-C12-C13
23	B	610	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	510	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
33	c	520	LMG	C33-C34-C35-C36
35	c	517[B]	DGD	C2A-C1A-O1G-C1G
23	a	406[B]	CLA	C2C-C3C-CAC-CBC
35	c	517[B]	DGD	O6E-C5E-C6E-O5E
31	A	419	LMT	C3'-C4'-O1B-C1B
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
35	c	517[B]	DGD	C7A-C8A-C9A-CAA
33	m	101	LMG	C2-C1-O1-C7
23	C	503	CLA	C15-C16-C17-C18
26	A	412	SQD	O6-C44-C45-C46
26	a	411[A]	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	E	101[A]	LHG	C4-C5-C6-O8
32	E	101[B]	LHG	C4-C5-C6-O8
32	a	420[B]	LHG	C4-C5-C6-O8
32	D	409[A]	LHG	C13-C14-C15-C16
33	a	417	LMG	C29-C30-C31-C32
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
33	a	417	LMG	C21-C22-C23-C24
33	d	411	LMG	C35-C36-C37-C38
32	A	418[A]	LHG	O2-C2-C3-O3
32	d	413[B]	LHG	C29-C30-C31-C32
23	B	601	CLA	CBA-CGA-O2A-C1
35	c	517[A]	DGD	C2A-C1A-O1G-C1G
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
35	c	517[A]	DGD	O6E-C5E-C6E-O5E
35	H	102	DGD	C7A-C8A-C9A-CAA
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
35	h	102	DGD	CBA-CCA-CDA-CEA
23	c	506	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C2-C3-C5-C6
23	B	613	CLA	C13-C15-C16-C17
25	D	406	BCR	C37-C22-C23-C24
23	c	503	CLA	C16-C17-C18-C20
32	d	413[A]	LHG	C25-C26-C27-C28
33	c	521	LMG	O10-C28-O8-C9
23	B	602	CLA	C15-C16-C17-C18
23	b	605	CLA	C13-C15-C16-C17
33	m	101	LMG	C14-C15-C16-C17
32	D	409[A]	LHG	C29-C30-C31-C32
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	CAB-CBB-CCB-CDB
23	C	507	CLA	C5-C6-C7-C8
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
27	l	102[A]	GOL	O1-C1-C2-C3
31	B	630	LMT	C2-C3-C4-C5
31	b	621	LMT	C11-C10-C9-C8
33	C	520	LMG	C17-C18-C19-C20
23	c	512	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C24-C23-O48-C46
35	c	519	DGD	C2A-C1A-O1G-C1G
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	a	406[A]	CLA	C2C-C3C-CAC-CBC
26	f	102	SQD	C25-C26-C27-C28
32	b	629[B]	LHG	C27-C28-C29-C30
23	b	610	CLA	C15-C16-C17-C18
26	a	411[A]	SQD	C9-C10-C11-C12
32	A	418[A]	LHG	C26-C27-C28-C29
35	c	519	DGD	CBA-CCA-CDA-CEA
31	c	501	LMT	C4'-C5'-C6'-O6'
32	D	408[B]	LHG	C12-C13-C14-C15
32	d	413[B]	LHG	C24-C25-C26-C27
35	H	102	DGD	C9B-CAB-CBB-CCB
32	d	406[B]	LHG	C13-C14-C15-C16
23	A	405[B]	CLA	C15-C16-C17-C18
32	d	407[A]	LHG	C28-C29-C30-C31
33	D	413	LMG	C12-C13-C14-C15
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
24	a	408[B]	PHO	C2-C3-C5-C6
31	m	103	LMT	O5'-C5'-C6'-O6'
31	A	419	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	c	518[B]	DGD	C6A-C7A-C8A-C9A
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
35	c	517[B]	DGD	O1A-C1A-O1G-C1G
26	a	411[A]	SQD	C12-C13-C14-C15
32	d	413[B]	LHG	C33-C34-C35-C36
33	C	520	LMG	C31-C32-C33-C34
33	z	101	LMG	C14-C15-C16-C17
26	A	410[B]	SQD	O6-C44-C45-O47
26	X	101	SQD	O47-C45-C46-O48
32	D	408[A]	LHG	C10-C11-C12-C13
33	C	520	LMG	C11-C12-C13-C14
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
31	c	501	LMT	C2-C3-C4-C5
26	X	101	SQD	C34-C35-C36-C37
32	D	408[B]	LHG	C10-C11-C12-C13
32	L	101[B]	LHG	C27-C28-C29-C30
32	b	629[A]	LHG	C9-C10-C11-C12
23	C	513	CLA	C3-C5-C6-C7
35	h	102	DGD	CDB-CEB-CFB-CGB
23	C	511	CLA	C10-C11-C12-C13
32	E	101[B]	LHG	C25-C26-C27-C28
32	E	101[A]	LHG	C25-C26-C27-C28
26	b	620	SQD	C26-C27-C28-C29
32	D	409[B]	LHG	C17-C18-C19-C20
35	c	518[B]	DGD	C4A-C5A-C6A-C7A
23	C	513	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
32	d	406[B]	LHG	C24-C23-O8-C6
32	d	413[A]	LHG	C33-C34-C35-C36
32	A	418[B]	LHG	C29-C30-C31-C32
32	D	409[B]	LHG	C13-C14-C15-C16
34	B	622	HTG	C2'-C3'-C4'-C5'
26	B	620	SQD	C34-C35-C36-C37
29	D	407[A]	PL9	C45-C44-C46-C47
29	a	414[B]	PL9	C12-C11-C9-C10
29	d	405[A]	PL9	C13-C14-C16-C17
32	d	407[B]	LHG	C28-C29-C30-C31
26	A	410[A]	SQD	C11-C10-C9-C8
27	B	624	GOL	O1-C1-C2-O2
27	B	627	GOL	O1-C1-C2-O2
27	a	418	GOL	O1-C1-C2-O2
27	v	202[A]	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	A	419	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
23	B	610	CLA	C11-C12-C13-C14
23	B	613	CLA	C11-C12-C13-C14
23	C	505	CLA	C14-C13-C15-C16
23	C	511	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	c	514	CLA	C6-C7-C8-C9
23	c	512	CLA	C8-C10-C11-C12
23	a	407[A]	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
32	d	407[A]	LHG	C33-C34-C35-C36
32	d	413[B]	LHG	C25-C26-C27-C28
23	A	404[A]	CLA	C13-C15-C16-C17
23	C	509	CLA	C5-C6-C7-C8
31	B	628	LMT	C9-C10-C11-C12
26	b	620	SQD	C11-C10-C9-C8
32	D	409[A]	LHG	C17-C18-C19-C20
31	M	101	LMT	C2'-C1'-O1'-C1
33	C	520	LMG	C37-C38-C39-C40
34	B	625	HTG	C2'-C3'-C4'-C5'
31	c	501	LMT	C9-C10-C11-C12
31	e	101	LMT	C9-C10-C11-C12
32	L	101[B]	LHG	O6-C4-C5-C6
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C12-C13-C15
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
35	c	517[A]	DGD	O1A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	E	101[A]	LHG	C13-C14-C15-C16
33	a	417	LMG	C35-C36-C37-C38
23	B	601	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
23	b	615	CLA	C10-C11-C12-C13
33	C	501	LMG	C13-C14-C15-C16
29	A	414[A]	PL9	C12-C11-C9-C8
29	D	407[A]	PL9	C13-C14-C16-C17
35	c	519	DGD	O1A-C1A-O1G-C1G
23	c	513	CLA	C10-C11-C12-C13
26	a	411[B]	SQD	C12-C13-C14-C15
23	B	612	CLA	C10-C11-C12-C13
32	d	407[B]	LHG	C9-C10-C11-C12
23	C	511	CLA	CBA-CGA-O2A-C1
23	C	512	CLA	CBA-CGA-O2A-C1
26	B	620	SQD	C29-C30-C31-C32
31	b	621	LMT	C3-C4-C5-C6
23	C	508	CLA	C13-C15-C16-C17
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	410[B]	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	b	620	SQD	C44-C45-C46-O48
32	a	420[A]	LHG	C4-C5-C6-O8
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
35	h	102	DGD	C9B-CAB-CBB-CCB
23	b	615	CLA	C5-C6-C7-C8
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
35	c	518[A]	DGD	CBB-CCB-CDB-CEB
34	b	622	HTG	C3'-C4'-C5'-C6'
23	c	514	CLA	C4-C3-C5-C6
24	a	408[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C45-C44-C46-C47
32	a	420[A]	LHG	C23-C24-C25-C26
29	D	407[A]	PL9	C43-C44-C46-C47
29	D	407[B]	PL9	C13-C14-C16-C17
29	d	405[B]	PL9	C28-C29-C31-C32
26	A	412	SQD	O10-C23-O48-C46
35	c	519	DGD	C2B-C3B-C4B-C5B
23	b	601	CLA	C13-C15-C16-C17
32	d	407[B]	LHG	C29-C30-C31-C32
23	B	608	CLA	C16-C17-C18-C20
23	d	402[B]	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	a	411[B]	SQD	C35-C36-C37-C38
23	a	407[A]	CLA	C2B-C3B-CAB-CBB
25	D	406	BCR	C23-C24-C25-C30
25	b	617	BCR	C1-C6-C7-C8
32	d	407[B]	LHG	C2-C3-O3-P
33	z	101	LMG	C19-C20-C21-C22
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
35	C	519	DGD	CDB-CEB-CFB-CGB
32	a	420[A]	LHG	C10-C11-C12-C13
33	B	621	LMG	C15-C16-C17-C18
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
23	b	602	CLA	C10-C11-C12-C13
32	L	101[B]	LHG	C24-C25-C26-C27
23	b	606	CLA	C16-C17-C18-C19
26	X	101	SQD	C7-C8-C9-C10
26	a	411[A]	SQD	O6-C44-C45-O47
26	a	411[B]	SQD	O6-C44-C45-O47
33	c	521	LMG	O1-C7-C8-O7
29	a	414[B]	PL9	C4-C3-C7-C8
23	C	502	CLA	O1D-CGD-O2D-CED
33	C	521	LMG	C35-C36-C37-C38
33	d	411	LMG	C28-C29-C30-C31
31	t	101	LMT	C7-C8-C9-C10
32	L	101[A]	LHG	C27-C28-C29-C30
29	A	414[B]	PL9	C12-C11-C9-C8
29	d	405[B]	PL9	C13-C14-C16-C17
26	b	620	SQD	C13-C14-C15-C16
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
32	a	420[B]	LHG	C23-C24-C25-C26
23	C	513	CLA	C6-C7-C8-C9
31	b	627	LMT	C6-C7-C8-C9
32	b	629[B]	LHG	C9-C10-C11-C12
35	C	519	DGD	CAB-CBB-CCB-CDB
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
26	A	412	SQD	C30-C31-C32-C33
31	t	101	LMT	O1'-C1-C2-C3
33	C	521	LMG	C4-C5-C6-O5
29	A	414[A]	PL9	C39-C41-C42-C43
29	a	414[A]	PL9	C24-C26-C27-C28
26	a	412	SQD	C16-C17-C18-C19
35	C	519	DGD	O6D-C5D-C6D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	b	622	HTG	C1'-C2'-C3'-C4'
26	A	412	SQD	C27-C28-C29-C30
35	h	102	DGD	C2B-C3B-C4B-C5B
35	C	517[A]	DGD	C1B-C2B-C3B-C4B
33	C	521	LMG	C12-C13-C14-C15
27	D	403	GOL	O1-C1-C2-O2
23	b	601	CLA	CAA-CBA-CGA-O2A
33	B	621	LMG	O6-C5-C6-O5
23	A	406[A]	CLA	C16-C17-C18-C20
32	A	418[A]	LHG	C1-C2-C3-O3
31	M	102	LMT	C9-C10-C11-C12
23	c	506	CLA	C12-C13-C15-C16
26	f	102	SQD	C23-C24-C25-C26
33	d	411	LMG	C10-C11-C12-C13
32	D	409[A]	LHG	C27-C28-C29-C30
32	b	629[A]	LHG	C34-C35-C36-C37
25	K	102	BCR	C7-C8-C9-C10
23	C	511	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	c	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	518[B]	DGD	C5D-C6D-O5D-C1E
32	D	408[B]	LHG	C26-C27-C28-C29
32	L	101[A]	LHG	C11-C10-C9-C8
33	C	501	LMG	C18-C19-C20-C21
33	B	621	LMG	C32-C33-C34-C35
29	d	405[A]	PL9	C45-C44-C46-C47
29	d	405[B]	PL9	C45-C44-C46-C47
23	C	512	CLA	O1A-CGA-O2A-C1
32	d	406[B]	LHG	O10-C23-O8-C6
29	a	414[A]	PL9	C12-C11-C9-C8
39	f	101	HEM	C2B-C3B-CAB-CBB
32	a	420[B]	LHG	C10-C11-C12-C13
33	C	501	LMG	C11-C12-C13-C14
26	A	410[A]	SQD	C18-C19-C20-C21
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
32	b	629[A]	LHG	C13-C14-C15-C16
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	C	510	CLA	O1D-CGD-O2D-CED
33	z	101	LMG	C13-C14-C15-C16
32	D	408[A]	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C30-C31-C32-C33
35	c	517[A]	DGD	CCB-CDB-CEB-CFB
32	E	101[A]	LHG	O6-C4-C5-O7
32	L	101[A]	LHG	O6-C4-C5-O7
32	L	101[B]	LHG	O6-C4-C5-O7
26	a	411[A]	SQD	C27-C28-C29-C30
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
35	c	519	DGD	O6D-C5D-C6D-O5D
26	a	411[B]	SQD	O6-C44-C45-C46
26	a	412	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
23	B	601	CLA	C13-C15-C16-C17
32	L	101[A]	LHG	C24-C25-C26-C27
31	F	101	LMT	C4-C5-C6-C7
32	b	629[B]	LHG	C25-C26-C27-C28
32	d	406[A]	LHG	C13-C14-C15-C16
32	D	409[A]	LHG	C10-C11-C12-C13
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
26	a	411[A]	SQD	C34-C35-C36-C37
23	C	511	CLA	C8-C10-C11-C12
33	Z	101	LMG	C11-C12-C13-C14
26	B	620	SQD	O47-C45-C46-O48
26	b	620	SQD	O47-C45-C46-O48
32	a	420[A]	LHG	O7-C5-C6-O8
23	c	507	CLA	C11-C10-C8-C9
31	b	621	LMT	C7-C8-C9-C10
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
26	a	411[B]	SQD	C9-C10-C11-C12
35	c	517[B]	DGD	C4B-C5B-C6B-C7B
31	A	417	LMT	O5B-C5B-C6B-O6B
31	F	101	LMT	C6-C7-C8-C9
32	D	408[B]	LHG	C13-C14-C15-C16
33	z	101	LMG	C20-C21-C22-C23
32	a	420[A]	LHG	C7-C8-C9-C10
23	B	601	CLA	C15-C16-C17-C18
35	C	519	DGD	C8A-C9A-CAA-CBA
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
23	C	513	CLA	C10-C11-C12-C13
26	b	620	SQD	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	E	101[B]	LHG	C13-C14-C15-C16
33	d	411	LMG	C18-C19-C20-C21
35	H	102	DGD	CDB-CEB-CFB-CGB
29	a	414[B]	PL9	C12-C11-C9-C8
32	A	418[A]	LHG	C32-C33-C34-C35
33	d	411	LMG	C16-C17-C18-C19
23	a	406[B]	CLA	C15-C16-C17-C18
35	c	518[B]	DGD	C1A-C2A-C3A-C4A
31	F	101	LMT	C2-C3-C4-C5
32	d	407[A]	LHG	C9-C10-C11-C12
33	m	101	LMG	C37-C38-C39-C40
26	A	410[A]	SQD	C34-C35-C36-C37
32	d	406[B]	LHG	C16-C17-C18-C19
23	c	513	CLA	O1D-CGD-O2D-CED
32	d	406[A]	LHG	C11-C10-C9-C8
23	A	406[B]	CLA	C16-C17-C18-C20
23	d	402[B]	CLA	C16-C17-C18-C19
23	C	513	CLA	C4B-C3B-CAB-CBB
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
23	a	407[B]	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	b	609	CLA	C4B-C3B-CAB-CBB
33	m	101	LMG	C30-C31-C32-C33
23	C	511	CLA	C13-C15-C16-C17
32	D	408[B]	LHG	C28-C29-C30-C31
26	a	411[A]	SQD	C35-C36-C37-C38
25	y	101	BCR	C21-C22-C23-C24
23	b	604	CLA	C13-C15-C16-C17
23	d	403	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	C15-C16-C17-C18
32	L	101[B]	LHG	C26-C27-C28-C29
31	e	101	LMT	C3-C4-C5-C6
32	L	101[A]	LHG	O6-C4-C5-C6
32	d	413[A]	LHG	C18-C19-C20-C21
23	b	613	CLA	CBD-CGD-O2D-CED
33	c	520	LMG	C32-C33-C34-C35
33	c	521	LMG	C31-C32-C33-C34
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	D	405	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	d	402[A]	CLA	C11-C12-C13-C15
23	d	402[B]	CLA	C11-C12-C13-C15
32	L	101[B]	LHG	C11-C12-C13-C14
23	c	510	CLA	O1A-CGA-O2A-C1
32	d	407[B]	LHG	O10-C23-O8-C6
32	d	406[A]	LHG	C16-C17-C18-C19
32	d	407[B]	LHG	C24-C23-O8-C6
32	A	418[B]	LHG	C17-C18-C19-C20
32	D	409[B]	LHG	C10-C11-C12-C13
31	b	627	LMT	O1'-C1-C2-C3
32	b	629[B]	LHG	C12-C13-C14-C15
32	b	629[B]	LHG	C13-C14-C15-C16
33	a	417	LMG	C33-C34-C35-C36
32	D	409[B]	LHG	C2-C3-O3-P
29	D	407[B]	PL9	C20-C19-C21-C22
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
31	c	501	LMT	C3-C4-C5-C6
23	B	614	CLA	C14-C13-C15-C16
23	D	405	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C9
26	a	411[B]	SQD	C27-C28-C29-C30
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
33	c	520	LMG	C30-C31-C32-C33
26	X	101	SQD	C32-C33-C34-C35
32	L	101[A]	LHG	C26-C27-C28-C29
35	c	518[A]	DGD	C7B-C8B-C9B-CAB
34	B	623	HTG	C4'-C5'-C6'-C7'
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	420[B]	LHG	O7-C5-C6-O8
23	B	606	CLA	C8-C10-C11-C12
33	C	521	LMG	C38-C39-C40-C41
26	X	101	SQD	C44-C45-C46-O48
23	C	506	CLA	C4-C3-C5-C6
29	D	407[B]	PL9	C45-C44-C46-C47
29	a	414[A]	PL9	C43-C44-C46-C47
29	a	414[B]	PL9	C43-C44-C46-C47
23	b	607	CLA	C3-C5-C6-C7
32	A	418[B]	LHG	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
26	A	410[A]	SQD	C13-C14-C15-C16
23	d	403	CLA	CBA-CGA-O2A-C1
35	C	519	DGD	C7A-C8A-C9A-CAA
23	B	608	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C20
32	D	408[A]	LHG	C34-C35-C36-C37
23	B	601	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
35	C	519	DGD	O1A-C1A-O1G-C1G
31	A	419	LMT	C4-C5-C6-C7
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O1D
32	D	408[A]	LHG	C4-O6-P-O3
32	D	408[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C4-O6-P-O4
32	a	420[B]	LHG	C4-O6-P-O4
32	d	406[B]	LHG	C4-O6-P-O5
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
33	d	411	LMG	C36-C37-C38-C39
33	B	621	LMG	C20-C21-C22-C23
23	C	507	CLA	C15-C16-C17-C18
23	C	508	CLA	C2B-C3B-CAB-CBB
23	D	404[B]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	609	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C28-C29-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	417	LMG	C36-C37-C38-C39
32	D	409[A]	LHG	C2-C3-O3-P
32	d	407[A]	LHG	C2-C3-O3-P
32	d	407[A]	LHG	C32-C33-C34-C35
23	b	604	CLA	C15-C16-C17-C18
32	D	408[A]	LHG	C26-C27-C28-C29
27	A	411	GOL	O1-C1-C2-O2
31	A	417	LMT	C9-C10-C11-C12
29	a	414[A]	PL9	C4-C3-C7-C8
27	l	102[B]	GOL	O1-C1-C2-C3
32	A	418[A]	LHG	O1-C1-C2-C3
32	d	413[A]	LHG	C34-C35-C36-C37
26	b	620	SQD	C16-C17-C18-C19
33	B	621	LMG	C29-C30-C31-C32
23	C	506	CLA	C2-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6
29	D	407[B]	PL9	C18-C19-C21-C22
23	C	507	CLA	C16-C17-C18-C20
32	d	413[A]	LHG	C11-C12-C13-C14
32	E	101[A]	LHG	O6-C4-C5-C6
26	b	620	SQD	C28-C29-C30-C31
35	C	518[A]	DGD	C7B-C8B-C9B-CAB
23	B	606	CLA	C11-C10-C8-C9
23	a	409	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	d	402[A]	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C10-C8-C7
23	c	509	CLA	C12-C13-C15-C16
31	c	501	LMT	C7-C8-C9-C10
32	d	407[B]	LHG	C34-C35-C36-C37
35	C	519	DGD	CBA-CCA-CDA-CEA
35	H	102	DGD	O2G-C1B-C2B-C3B
33	B	621	LMG	C14-C15-C16-C17
26	a	411[B]	SQD	C34-C35-C36-C37
23	D	405	CLA	C8-C10-C11-C12
26	A	412	SQD	C31-C32-C33-C34
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
29	D	407[A]	PL9	C15-C14-C16-C17
34	b	623	HTG	C4'-C5'-C6'-C7'
32	D	408[B]	LHG	C11-C10-C9-C8
32	D	408[A]	LHG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	D	408[B]	LHG	C34-C35-C36-C37
26	f	102	SQD	O47-C45-C46-O48
32	E	101[B]	LHG	O7-C5-C6-O8
34	b	625	HTG	C4-C5-C6-O6
23	b	616	CLA	C5-C6-C7-C8
23	c	510	CLA	CBA-CGA-O2A-C1
32	b	629[B]	LHG	C34-C35-C36-C37
32	A	418[B]	LHG	C18-C19-C20-C21
32	b	629[A]	LHG	C28-C29-C30-C31
32	d	407[A]	LHG	C10-C11-C12-C13
33	c	521	LMG	C39-C40-C41-C42
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
23	c	512	CLA	C3-C5-C6-C7
23	c	511	CLA	C4-C3-C5-C6
35	C	519	DGD	CAA-CBA-CCA-CDA
35	H	102	DGD	CCA-CDA-CEA-CFA
23	a	406[A]	CLA	C15-C16-C17-C18
23	c	508	CLA	C8-C10-C11-C12
31	e	101	LMT	C4B-C5B-C6B-O6B
32	D	409[B]	LHG	C27-C28-C29-C30
32	a	420[B]	LHG	C24-C25-C26-C27
34	B	625	HTG	C4'-C5'-C6'-C7'
35	c	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	519	DGD	C8B-C9B-CAB-CBB
32	d	413[B]	LHG	C27-C28-C29-C30
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
31	e	101	LMT	O1'-C1-C2-C3
29	a	414[A]	PL9	C45-C44-C46-C47
29	a	414[B]	PL9	C45-C44-C46-C47
23	B	610	CLA	C13-C15-C16-C17
33	B	621	LMG	O8-C28-C29-C30
29	d	405[B]	PL9	C43-C44-C46-C47
26	A	410[A]	SQD	C16-C17-C18-C19
23	B	612	CLA	CBA-CGA-O2A-C1
31	B	631	LMT	C2-C3-C4-C5
27	c	527	GOL	O1-C1-C2-O2
31	e	101	LMT	C2-C1-O1'-C1'
23	A	406[A]	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
32	D	408[A]	LHG	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	408[A]	PHO	C2C-C3C-CAC-CBC
23	B	610	CLA	C4B-C3B-CAB-CBB
23	D	404[A]	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C3-C5-C6-C7
32	b	629[B]	LHG	C17-C18-C19-C20
23	b	616	CLA	CBA-CGA-O2A-C1
35	C	519	DGD	C2A-C1A-O1G-C1G
32	L	101[A]	LHG	C23-C24-C25-C26
23	b	601	CLA	C4-C3-C5-C6
23	b	616	CLA	C4-C3-C5-C6
23	c	511	CLA	C2-C3-C5-C6
29	d	405[A]	PL9	C43-C44-C46-C47
33	C	520	LMG	C36-C37-C38-C39
23	D	405	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
32	D	409[A]	LHG	O10-C23-O8-C6
23	c	504	CLA	C8-C10-C11-C12
23	b	613	CLA	O1D-CGD-O2D-CED
39	f	101	HEM	C4B-C3B-CAB-CBB
35	c	517[B]	DGD	CCB-CDB-CEB-CFB
23	a	406[A]	CLA	C4C-C3C-CAC-CBC
32	b	629[B]	LHG	C10-C11-C12-C13
23	B	613	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
23	c	511	CLA	C12-C13-C15-C16
23	b	610	CLA	C13-C15-C16-C17
23	B	612	CLA	O1A-CGA-O2A-C1
32	D	409[A]	LHG	C24-C23-O8-C6
26	a	412	SQD	C26-C27-C28-C29
35	C	519	DGD	C7B-C8B-C9B-CAB
35	H	102	DGD	C8A-C9A-CAA-CBA
23	a	409	CLA	C15-C16-C17-C18
32	L	101[B]	LHG	C11-C10-C9-C8
32	d	413[B]	LHG	C17-C18-C19-C20
35	C	519	DGD	C6A-C7A-C8A-C9A
23	B	614	CLA	C4-C3-C5-C6
23	B	601	CLA	CAA-CBA-CGA-O2A
29	D	407[B]	PL9	C43-C44-C46-C47
35	C	519	DGD	C9A-CAA-CBA-CCA
31	M	101	LMT	C2-C3-C4-C5
26	a	411[A]	SQD	C11-C12-C13-C14
23	b	613	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	t	102	BCR	C13-C14-C15-C16
32	A	418[B]	LHG	C31-C32-C33-C34
23	b	609	CLA	C4-C3-C5-C6
23	a	406[B]	CLA	C4C-C3C-CAC-CBC
23	b	608	CLA	C16-C17-C18-C19
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
32	d	413[A]	LHG	C1-C2-C3-O3
33	c	521	LMG	O1-C7-C8-C9
23	A	406[B]	CLA	C14-C13-C15-C16
23	A	408	CLA	C11-C12-C13-C14
23	B	602	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C14-C13-C15-C16
23	a	407[B]	CLA	C11-C12-C13-C14
23	d	402[B]	CLA	C11-C12-C13-C14
24	a	408[B]	PHO	C14-C13-C15-C16
32	D	409[B]	LHG	C28-C29-C30-C31
35	h	102	DGD	O2G-C1B-C2B-C3B
33	C	521	LMG	C20-C21-C22-C23
33	m	101	LMG	C32-C33-C34-C35
35	c	517[A]	DGD	C4B-C5B-C6B-C7B
33	B	621	LMG	C18-C19-C20-C21
26	A	410[B]	SQD	C34-C35-C36-C37
27	a	419	GOL	O2-C2-C3-O3
27	d	412	GOL	O1-C1-C2-O2
27	d	412	GOL	O2-C2-C3-O3
32	E	101[A]	LHG	C12-C13-C14-C15
26	a	411[A]	SQD	C10-C11-C12-C13
32	d	406[A]	LHG	C9-C10-C11-C12
23	B	604	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	C1A-C2A-CAA-CBA
23	a	407[A]	CLA	C1A-C2A-CAA-CBA
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
23	b	610	CLA	C16-C17-C18-C19
32	a	420[B]	LHG	C7-C8-C9-C10
23	B	611	CLA	C8-C10-C11-C12
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
23	B	602	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	404[A]	CLA	C2B-C3B-CAB-CBB
23	a	407[B]	CLA	C2B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	609	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
25	D	406	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
23	D	405	CLA	CBA-CGA-O2A-C1
32	D	408[A]	LHG	C17-C18-C19-C20
23	c	511	CLA	O1A-CGA-O2A-C1
26	f	102	SQD	C11-C10-C9-C8
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
23	A	406[A]	CLA	C16-C17-C18-C19
39	F	102	HEM	CAD-CBD-CGD-O1D
23	b	601	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
32	A	418[A]	LHG	C29-C30-C31-C32
23	B	602	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C12-C13-C15
32	b	629[A]	LHG	C10-C11-C12-C13
35	H	102	DGD	O1G-C1G-C2G-O2G
32	A	418[B]	LHG	C33-C34-C35-C36
29	A	414[A]	PL9	C4-C3-C7-C8
29	A	414[B]	PL9	C4-C3-C7-C8
23	c	507	CLA	C13-C15-C16-C17
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
35	C	519	DGD	CDA-CEA-CFA-CGA
35	H	102	DGD	C4E-C5E-C6E-O5E
33	d	411	LMG	C19-C20-C21-C22
26	b	620	SQD	C33-C34-C35-C36
41	v	201	HEC	CAD-CBD-CGD-O2D
29	D	407[A]	PL9	C35-C34-C36-C37
33	z	101	LMG	O7-C10-C11-C12
26	A	410[B]	SQD	C16-C17-C18-C19
32	L	101[A]	LHG	C10-C11-C12-C13
23	c	510	CLA	C15-C16-C17-C18
23	c	505	CLA	C14-C13-C15-C16
23	c	513	CLA	C13-C15-C16-C17
33	c	520	LMG	C28-C29-C30-C31
32	a	420[A]	LHG	C24-C25-C26-C27
32	b	629[B]	LHG	C28-C29-C30-C31
29	A	414[A]	PL9	C25-C24-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
23	c	514	CLA	C2-C3-C5-C6
31	m	103	LMT	C7-C8-C9-C10
23	b	608	CLA	C13-C15-C16-C17
41	v	201	HEC	CAD-CBD-CGD-O1D
35	C	519	DGD	C2A-C3A-C4A-C5A
33	a	417	LMG	C7-C8-C9-O8
23	C	508	CLA	C2A-CAA-CBA-CGA
23	C	503	CLA	C16-C17-C18-C19
32	A	418[A]	LHG	O1-C1-C2-O2
32	d	413[A]	LHG	C27-C28-C29-C30
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
32	E	101[B]	LHG	O6-C4-C5-O7
23	c	505	CLA	C4-C3-C5-C6
32	d	413[A]	LHG	C17-C18-C19-C20
23	B	602	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	b	602	CLA	C8-C10-C11-C12
32	d	406[A]	LHG	C25-C26-C27-C28
39	f	101	HEM	CAD-CBD-CGD-O1D
41	V	201	HEC	CAD-CBD-CGD-O2D
23	A	404[B]	CLA	C16-C17-C18-C19
23	b	610	CLA	C16-C17-C18-C20
33	C	520	LMG	C29-C30-C31-C32
24	a	408[A]	PHO	CHA-CBD-CGD-O1D
33	a	417	LMG	O8-C28-C29-C30
32	D	408[B]	LHG	O6-C4-C5-C6
32	d	406[B]	LHG	O6-C4-C5-C6
33	m	101	LMG	O6-C1-O1-C7
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
23	B	615	CLA	C12-C13-C15-C16
39	F	102	HEM	CAD-CBD-CGD-O2D
32	d	413[A]	LHG	C9-C10-C11-C12
32	A	418[A]	LHG	C17-C18-C19-C20
41	V	201	HEC	CAD-CBD-CGD-O1D
23	B	616	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
32	d	413[B]	LHG	C18-C19-C20-C21
23	B	613	CLA	C15-C16-C17-C18
35	C	519	DGD	C4A-C5A-C6A-C7A
35	C	518[B]	DGD	C5D-C6D-O5D-C1E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
32	E	101[B]	LHG	C11-C10-C9-C8
35	c	517[A]	DGD	CDB-CEB-CFB-CGB
23	C	502	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C2-C1-O2A-CGA
23	c	508	CLA	C2-C1-O2A-CGA
23	B	601	CLA	C3-C5-C6-C7
23	A	408	CLA	C16-C17-C18-C19
34	b	623	HTG	S1-C1'-C2'-C3'
32	d	413[B]	LHG	C23-C24-C25-C26
35	c	517[B]	DGD	C2A-C3A-C4A-C5A
23	c	507	CLA	C3A-C2A-CAA-CBA
29	D	407[B]	PL9	C35-C34-C36-C37
23	B	602	CLA	C8-C10-C11-C12
32	A	418[B]	LHG	O1-C1-C2-C3
31	A	417	LMT	C2B-C1B-O1B-C4'
23	b	601	CLA	C3-C5-C6-C7
31	B	630	LMT	C7-C8-C9-C10
24	a	408[A]	PHO	O2A-C1-C2-C3
24	a	408[B]	PHO	O2A-C1-C2-C3
23	C	512	CLA	C8-C10-C11-C12
32	b	629[A]	LHG	C25-C26-C27-C28
31	e	101	LMT	C2-C3-C4-C5
35	c	518[B]	DGD	C7B-C8B-C9B-CAB
34	d	410	HTG	S1-C1'-C2'-C3'
39	f	101	HEM	CAA-CBA-CGA-O2A
26	a	412	SQD	O10-C23-O48-C46
23	b	605	CLA	C3-C5-C6-C7
33	c	520	LMG	C29-C30-C31-C32
32	b	629[B]	LHG	C32-C33-C34-C35
26	B	620	SQD	C12-C13-C14-C15
32	L	101[A]	LHG	C11-C12-C13-C14
32	b	629[B]	LHG	O7-C7-C8-C9
31	e	101	LMT	C2B-C1B-O1B-C4'
34	C	522	HTG	S1-C1'-C2'-C3'
23	B	605	CLA	C6-C7-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	b	608	CLA	C14-C13-C15-C16
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
31	B	631	LMT	C1-C2-C3-C4
32	A	418[A]	LHG	O8-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	O7-C10-C11-C12
31	m	103	LMT	C9-C10-C11-C12
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
23	C	511	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
23	B	602	CLA	C11-C12-C13-C15
23	B	616	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	a	407[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	b	608	CLA	C6-C7-C8-C10
23	c	505	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
39	f	101	HEM	CAD-CBD-CGD-O2D
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C30
32	A	418[B]	LHG	C32-C33-C34-C35
32	a	420[A]	LHG	O8-C23-C24-C25
31	M	102	LMT	C3-C4-C5-C6
23	C	507	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	B	613	CLA	CAA-CBA-CGA-O2A
32	a	420[B]	LHG	O8-C23-C24-C25
23	b	601	CLA	CAA-CBA-CGA-O1A
26	a	412	SQD	C24-C23-O48-C46
24	a	408[A]	PHO	C2-C3-C5-C6
29	D	407[B]	PL9	C28-C29-C31-C32
34	B	622	HTG	C2'-C1'-S1-C1
23	a	405[B]	CLA	C2A-CAA-CBA-CGA
39	f	101	HEM	CAA-CBA-CGA-O1A
32	L	101[A]	LHG	O7-C7-C8-C9
32	b	629[A]	LHG	O7-C7-C8-C9
23	C	507	CLA	C16-C17-C18-C19
26	a	412	SQD	C18-C19-C20-C21
34	c	522	HTG	C4'-C5'-C6'-C7'
35	C	517[B]	DGD	C6A-C7A-C8A-C9A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	a	408[A]	PHO	C4-C3-C5-C6
26	A	412	SQD	O48-C23-C24-C25
32	L	101[B]	LHG	O7-C7-C8-C9
23	b	607	CLA	C8-C10-C11-C12
23	B	614	CLA	C2-C3-C5-C6
35	c	518[B]	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	C6A-C7A-C8A-C9A
32	A	418[B]	LHG	O8-C23-C24-C25
23	c	511	CLA	CBA-CGA-O2A-C1
31	b	627	LMT	C2-C1-O1'-C1'
23	b	610	CLA	C3-C5-C6-C7
23	c	505	CLA	C5-C6-C7-C8
32	d	413[A]	LHG	C30-C31-C32-C33
23	C	506	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	c	512	CLA	C11-C10-C8-C9
25	c	516	BCR	C7-C8-C9-C34
33	D	413	LMG	O7-C10-C11-C12
24	a	416[A]	PHO	C2C-C3C-CAC-CBC
23	d	403	CLA	C4B-C3B-CAB-CBB
35	h	102	DGD	C3B-C4B-C5B-C6B
23	C	513	CLA	C4-C3-C5-C6
31	A	419	LMT	C7-C8-C9-C10
25	b	619	BCR	C21-C22-C23-C24
25	d	404	BCR	C7-C8-C9-C10
26	B	620	SQD	C24-C25-C26-C27
23	b	610	CLA	C5-C6-C7-C8
23	B	612	CLA	CAA-CBA-CGA-O2A
23	b	613	CLA	CAA-CBA-CGA-O2A
26	f	102	SQD	C26-C27-C28-C29
33	c	520	LMG	C39-C40-C41-C42
23	C	503	CLA	C16-C17-C18-C20
23	C	513	CLA	CAA-CBA-CGA-O2A
33	c	520	LMG	O7-C10-C11-C12
35	C	519	DGD	O1G-C1A-C2A-C3A
23	c	511	CLA	O1D-CGD-O2D-CED
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C2-C1-O2A-CGA
23	a	405[A]	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
32	E	101[B]	LHG	O7-C7-C8-C9
23	B	612	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C15
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
33	m	101	LMG	C11-C12-C13-C14
35	h	102	DGD	CCB-CDB-CEB-CFB
35	C	517[A]	DGD	C3A-C4A-C5A-C6A
23	b	613	CLA	C5-C6-C7-C8
33	C	521	LMG	C11-C12-C13-C14
23	c	510	CLA	C13-C15-C16-C17
32	A	418[A]	LHG	C18-C19-C20-C21
32	d	407[A]	LHG	C30-C31-C32-C33
32	d	406[B]	LHG	C11-C12-C13-C14
33	a	417	LMG	C14-C15-C16-C17
29	d	405[A]	PL9	C34-C36-C37-C38
33	C	521	LMG	C33-C34-C35-C36
33	Z	101	LMG	O9-C10-C11-C12
31	b	621	LMT	C5'-C4'-O1B-C1B
32	E	101[A]	LHG	O7-C7-C8-C9
29	d	405[B]	PL9	C18-C19-C21-C22
32	A	418[B]	LHG	C30-C31-C32-C33
32	b	629[A]	LHG	O9-C7-C8-C9
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
33	z	101	LMG	C10-C11-C12-C13
32	d	407[A]	LHG	O10-C23-O8-C6
23	B	601	CLA	C8-C10-C11-C12
23	b	612	CLA	C10-C11-C12-C13
23	B	612	CLA	C11-C10-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	b	601	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16
35	c	519	DGD	C2A-C3A-C4A-C5A
32	A	418[B]	LHG	O10-C23-C24-C25
23	B	615	CLA	C8-C10-C11-C12
23	c	510	CLA	C8-C10-C11-C12
32	L	101[A]	LHG	O9-C7-C8-C9
23	A	404[B]	CLA	C15-C16-C17-C18
23	b	615	CLA	C13-C15-C16-C17
26	f	102	SQD	O5-C5-C6-S
31	A	417	LMT	C7-C8-C9-C10
23	C	509	CLA	C13-C15-C16-C17
27	D	414	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	l	102[A]	GOL	O1-C1-C2-O2
27	l	102[B]	GOL	O1-C1-C2-O2
32	A	418[A]	LHG	C30-C31-C32-C33
23	C	511	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
32	A	418[A]	LHG	O10-C23-C24-C25
32	a	420[A]	LHG	O10-C23-C24-C25
32	a	420[B]	LHG	O10-C23-C24-C25
33	c	520	LMG	C36-C37-C38-C39
32	D	409[A]	LHG	C28-C29-C30-C31
33	C	521	LMG	C8-C7-O1-C1
35	C	517[A]	DGD	C5D-C6D-O5D-C1E
35	C	517[B]	DGD	C5D-C6D-O5D-C1E
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	517[A]	DGD	C5D-C6D-O5D-C1E
32	E	101[A]	LHG	C11-C10-C9-C8
32	L	101[B]	LHG	O9-C7-C8-C9
32	b	629[B]	LHG	O9-C7-C8-C9
33	c	520	LMG	O9-C10-C11-C12
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
23	B	602	CLA	C2A-CAA-CBA-CGA
33	c	521	LMG	C32-C33-C34-C35
35	C	517[A]	DGD	CBA-CCA-CDA-CEA
33	m	101	LMG	O1-C7-C8-C9
35	h	102	DGD	O1G-C1G-C2G-C3G
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A
26	A	412	SQD	O10-C23-C24-C25
35	C	519	DGD	O1A-C1A-C2A-C3A
29	d	405[A]	PL9	C11-C12-C13-C14
26	A	410[B]	SQD	C18-C19-C20-C21
26	a	411[B]	SQD	O47-C7-C8-C9
32	D	409[B]	LHG	O8-C23-C24-C25
35	c	518[A]	DGD	CDA-CEA-CFA-CGA
33	Z	101	LMG	C19-C20-C21-C22
25	H	101	BCR	C9-C10-C11-C12
32	E	101[B]	LHG	O9-C7-C8-C9
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
24	a	408[A]	PHO	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	L	101[A]	LHG	C32-C33-C34-C35
32	E	101[B]	LHG	O8-C23-C24-C25
23	a	405[B]	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
33	D	413	LMG	O9-C10-C11-C12
32	E	101[A]	LHG	O8-C23-C24-C25
34	B	622	HTG	C3'-C4'-C5'-C6'
23	b	602	CLA	C2A-CAA-CBA-CGA
32	b	629[A]	LHG	C17-C18-C19-C20
26	a	412	SQD	O48-C23-C24-C25
32	D	409[A]	LHG	O8-C23-C24-C25
33	C	520	LMG	O7-C10-C11-C12
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
32	E	101[A]	LHG	O9-C7-C8-C9
35	c	518[B]	DGD	C4B-C5B-C6B-C7B
23	c	502	CLA	CAA-CBA-CGA-O2A
23	B	612	CLA	CAA-CBA-CGA-O1A
26	a	412	SQD	C15-C16-C17-C18

There are no ring outliers.

169 monomers are involved in 333 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	514	CLA	2	0
29	D	407[A]	PL9	1	0
34	D	412	HTG	1	0
35	c	519	DGD	2	0
31	t	101	LMT	2	0
25	K	103	BCR	1	0
23	b	610	CLA	1	0
23	A	406[B]	CLA	1	0
24	a	416[B]	PHO	1	0
27	D	403	GOL	4	0
33	Z	101	LMG	1	0
23	C	512	CLA	1	0
26	A	410[A]	SQD	1	0
32	d	406[B]	LHG	2	0
35	C	519	DGD	1	0
29	a	414[A]	PL9	4	0
26	a	411[B]	SQD	3	0
34	B	622	HTG	1	0
23	D	404[B]	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	B	631	LMT	1	0
25	c	515	BCR	3	0
23	c	513	CLA	4	0
25	k	101	BCR	1	0
23	c	512	CLA	7	0
23	c	510	CLA	1	0
32	D	408[A]	LHG	2	0
25	h	101	BCR	4	0
32	d	407[B]	LHG	9	0
35	c	517[B]	DGD	1	0
39	F	102	HEM	2	0
23	C	506	CLA	4	0
23	b	616	CLA	3	0
25	A	409	BCR	1	0
31	A	419	LMT	1	0
31	B	628	LMT	1	0
23	B	609	CLA	2	0
25	t	102	BCR	4	0
32	D	409[B]	LHG	3	0
25	H	101	BCR	2	0
25	B	619	BCR	1	0
23	a	406[B]	CLA	3	0
23	C	503	CLA	3	0
23	c	504	CLA	3	0
25	y	101	BCR	2	0
23	C	502	CLA	4	0
21	A	401[B]	OEY	1	0
23	d	402[B]	CLA	5	0
23	B	602	CLA	2	0
26	A	410[B]	SQD	2	0
23	b	609	CLA	4	0
33	d	411	LMG	3	0
31	c	501	LMT	1	0
25	b	618	BCR	4	0
23	A	405[B]	CLA	5	0
27	B	624	GOL	2	0
27	D	414	GOL	3	0
32	A	418[A]	LHG	1	0
27	b	624	GOL	1	0
25	C	515	BCR	1	0
23	C	507	CLA	5	0
23	b	611	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	v	202[A]	GOL	1	0
33	a	417	LMG	1	0
34	B	625	HTG	1	0
23	c	507	CLA	4	0
27	O	303	GOL	1	0
23	C	504	CLA	4	0
24	A	407[A]	PHO	1	0
23	a	409	CLA	4	0
23	B	614	CLA	3	0
26	X	101	SQD	3	0
23	b	606	CLA	1	0
23	B	613	CLA	4	0
29	A	414[A]	PL9	11	0
35	c	518[A]	DGD	2	0
23	b	602	CLA	1	0
23	a	405[A]	CLA	2	0
23	b	607	CLA	1	0
24	A	416[B]	PHO	2	0
23	C	508	CLA	2	0
25	C	516	BCR	1	0
23	d	403	CLA	2	0
23	a	407[B]	CLA	4	0
32	E	101[B]	LHG	2	0
23	A	404[A]	CLA	2	0
35	C	517[A]	DGD	1	0
32	a	420[B]	LHG	4	0
25	B	617	BCR	1	0
33	C	521	LMG	3	0
23	C	513	CLA	2	0
27	a	418	GOL	2	0
25	d	404	BCR	3	0
34	b	622	HTG	2	0
23	A	406[A]	CLA	1	0
24	a	416[A]	PHO	1	0
25	b	619	BCR	5	0
31	B	630	LMT	1	0
25	B	618	BCR	3	0
32	A	418[B]	LHG	1	0
33	z	101	LMG	2	0
23	C	514	CLA	2	0
32	d	406[A]	LHG	2	0
25	a	410	BCR	1	0

Continued on next page...

Continued from previous page...

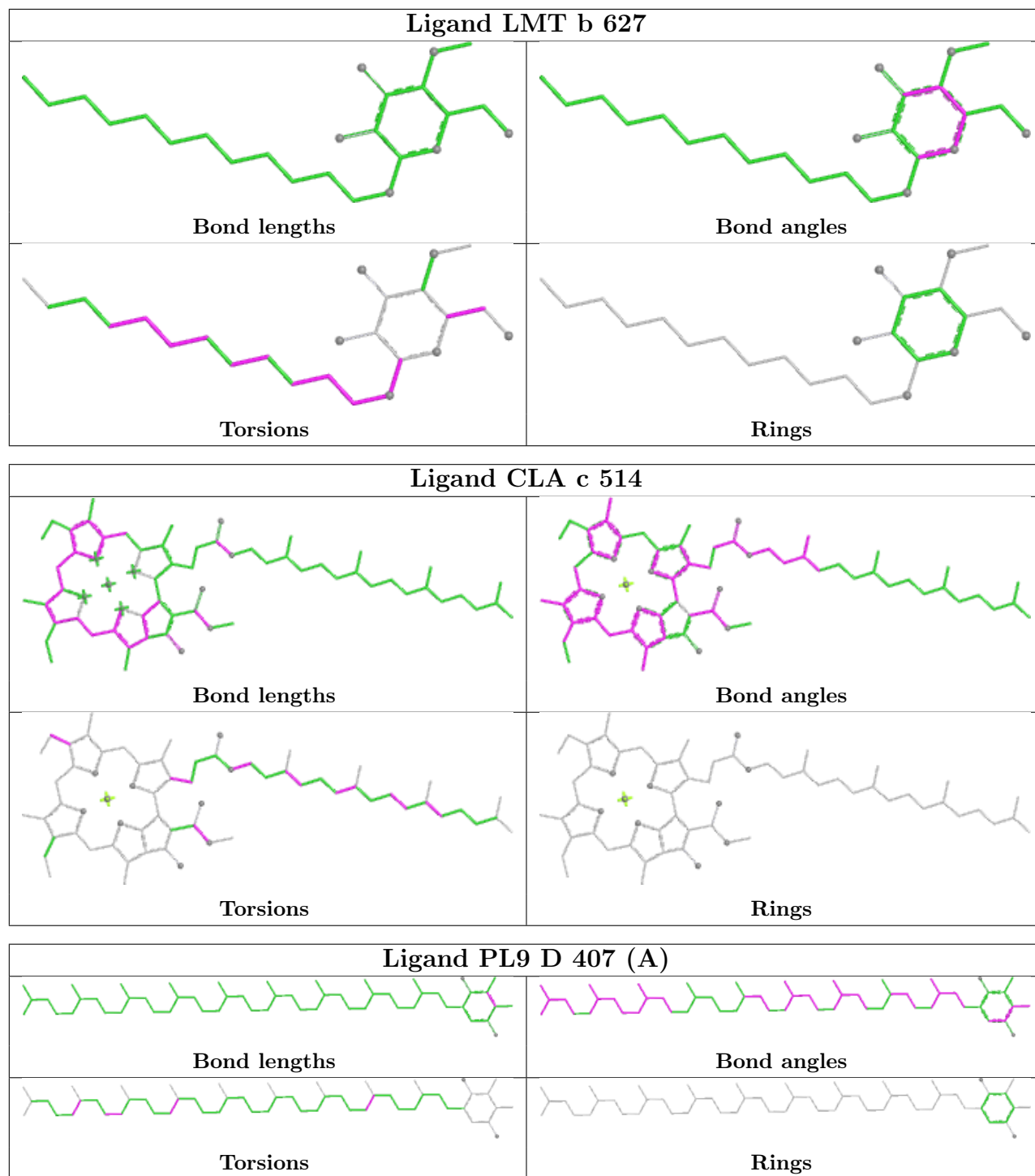
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	c	522	HTG	1	0
27	v	202[B]	GOL	2	0
29	a	414[B]	PL9	4	0
26	a	411[A]	SQD	3	0
24	a	408[B]	PHO	1	0
25	T	101	BCR	5	0
33	B	621	LMG	1	0
23	c	506	CLA	6	0
23	D	404[A]	CLA	3	0
23	b	601	CLA	1	0
23	c	509	CLA	6	0
27	l	102[A]	GOL	1	0
35	c	518[B]	DGD	2	0
32	D	408[B]	LHG	2	0
31	M	101	LMT	1	0
23	b	605	CLA	5	0
23	B	604	CLA	1	0
35	c	517[A]	DGD	1	0
23	b	604	CLA	2	0
26	b	620	SQD	2	0
31	e	101	LMT	1	0
23	c	505	CLA	2	0
23	c	503	CLA	1	0
33	c	521	LMG	1	0
34	d	410	HTG	1	0
23	C	509	CLA	4	0
34	B	623	HTG	1	0
32	D	409[A]	LHG	3	0
23	A	408	CLA	2	0
23	c	511	CLA	1	0
23	C	510	CLA	5	0
35	C	518[A]	DGD	1	0
23	a	406[A]	CLA	3	0
23	c	502	CLA	2	0
23	B	606	CLA	2	0
23	d	402[A]	CLA	1	0
23	B	601	CLA	2	0
31	b	621	LMT	2	0
23	b	615	CLA	1	0
26	a	412	SQD	1	0
21	a	401[B]	OEY	1	0
23	A	405[A]	CLA	1	0

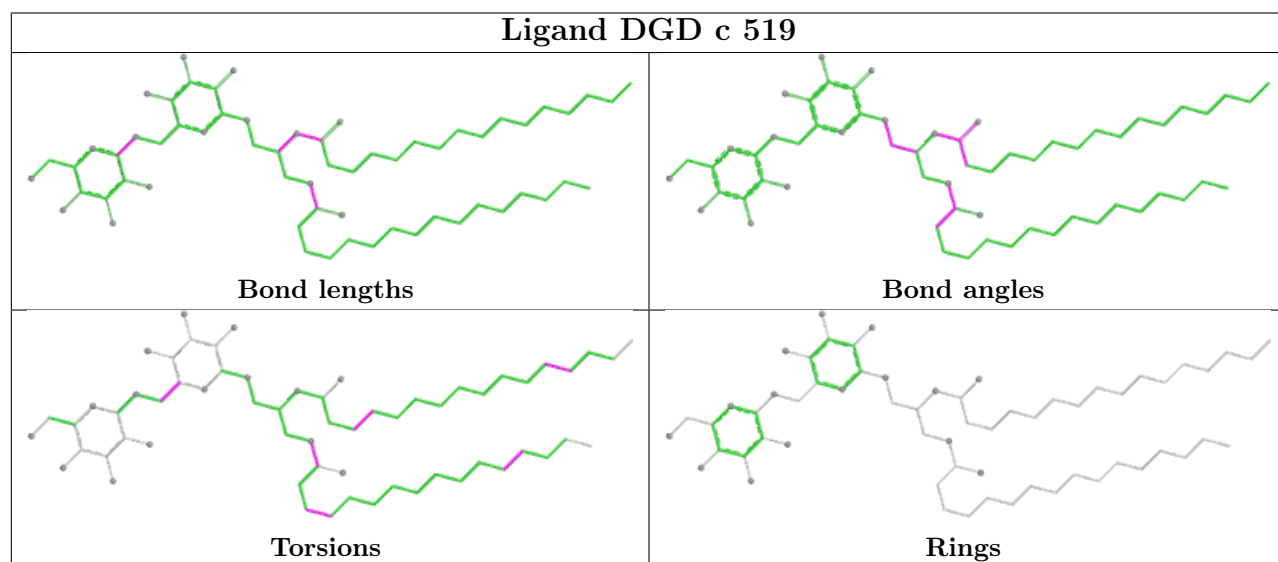
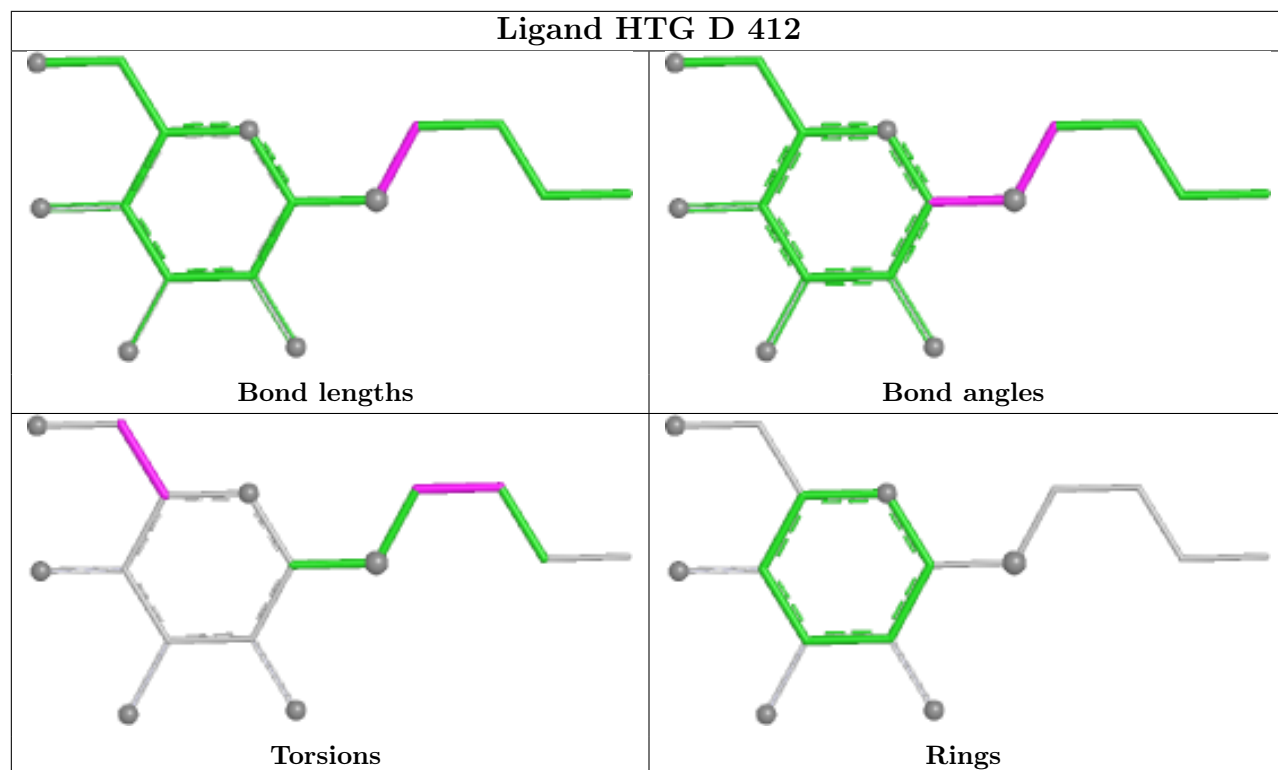
Continued on next page...

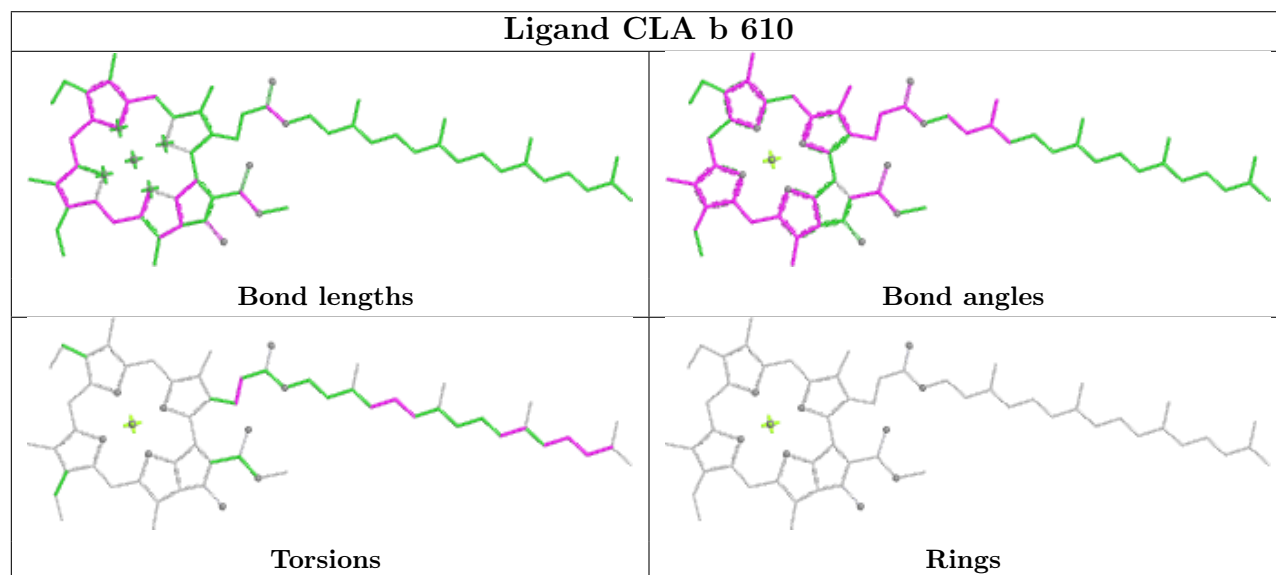
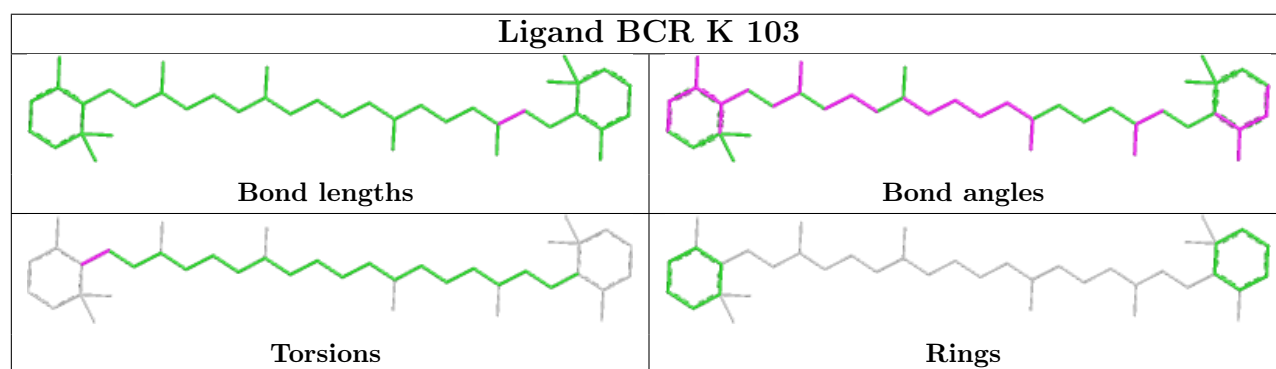
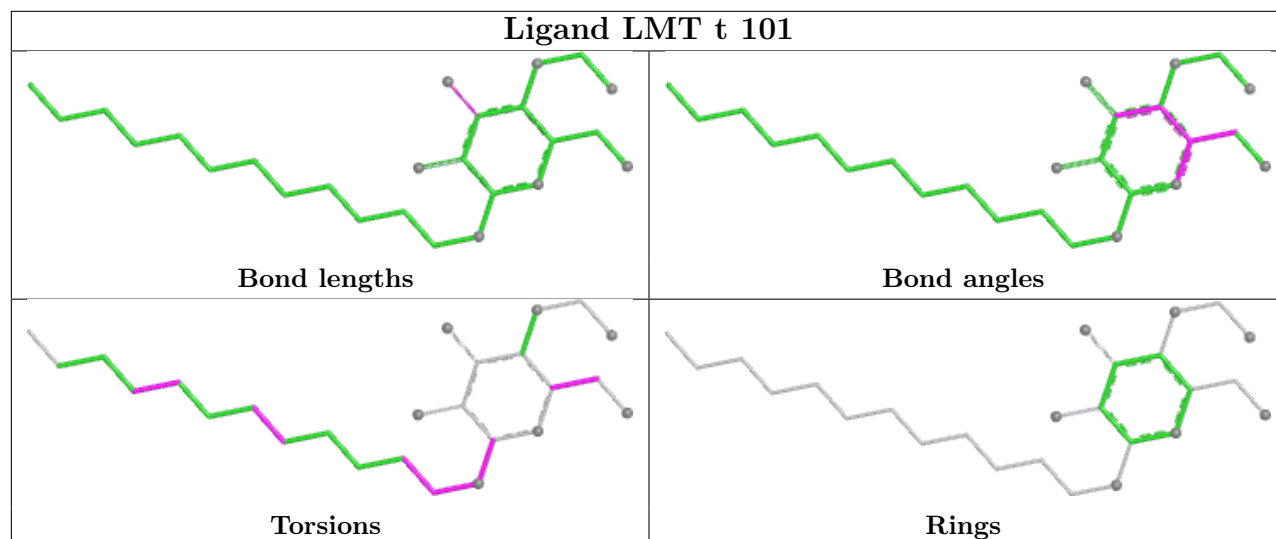
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	C	505	CLA	1	0
27	a	419	GOL	4	0
27	b	628	GOL	3	0
24	A	407[B]	PHO	1	0
23	C	511	CLA	4	0
27	B	627	GOL	1	0
29	A	414[B]	PL9	8	0
23	B	605	CLA	3	0
23	c	508	CLA	2	0
23	B	615	CLA	4	0
23	B	616	CLA	3	0
23	a	405[B]	CLA	2	0
26	B	620	SQD	2	0
24	A	416[A]	PHO	1	0
32	d	407[A]	LHG	11	0
23	b	614	CLA	3	0
27	O	302	GOL	1	0
23	a	407[A]	CLA	2	0
32	E	101[A]	LHG	3	0
23	A	404[B]	CLA	3	0
35	C	517[B]	DGD	1	0
25	c	516	BCR	2	0
32	a	420[A]	LHG	5	0
35	H	102	DGD	1	0

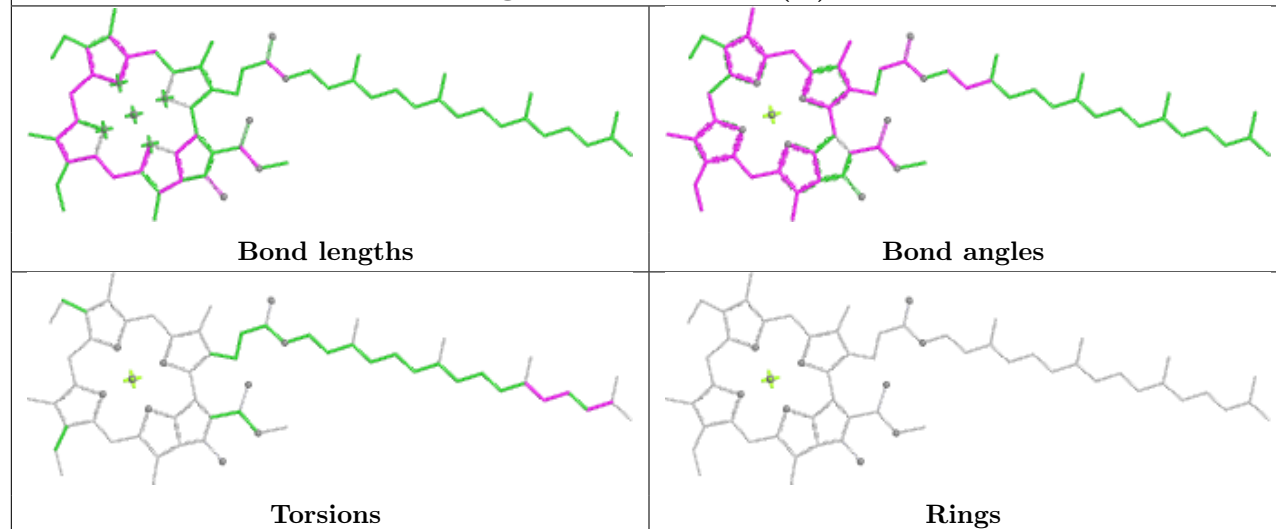
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



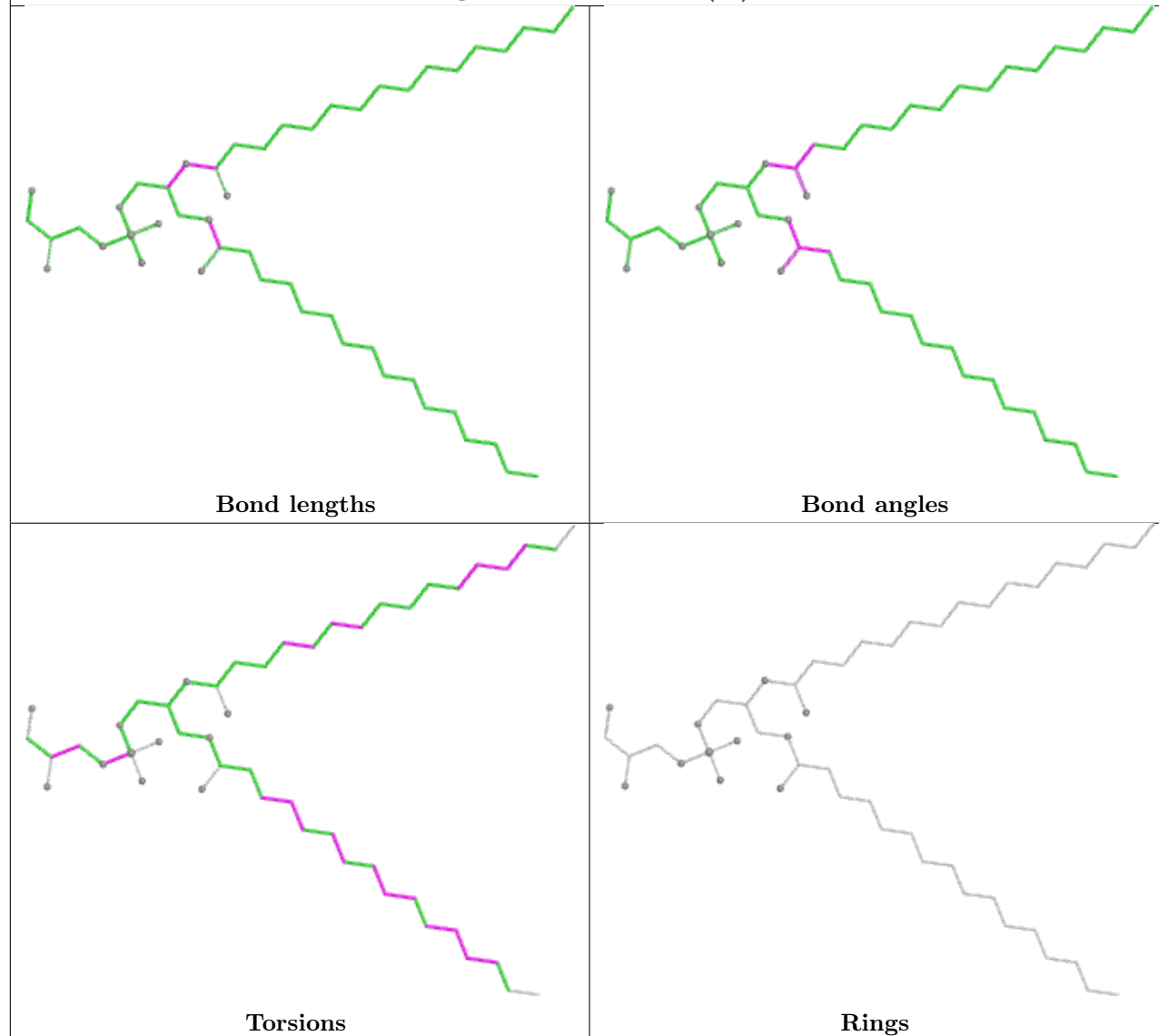




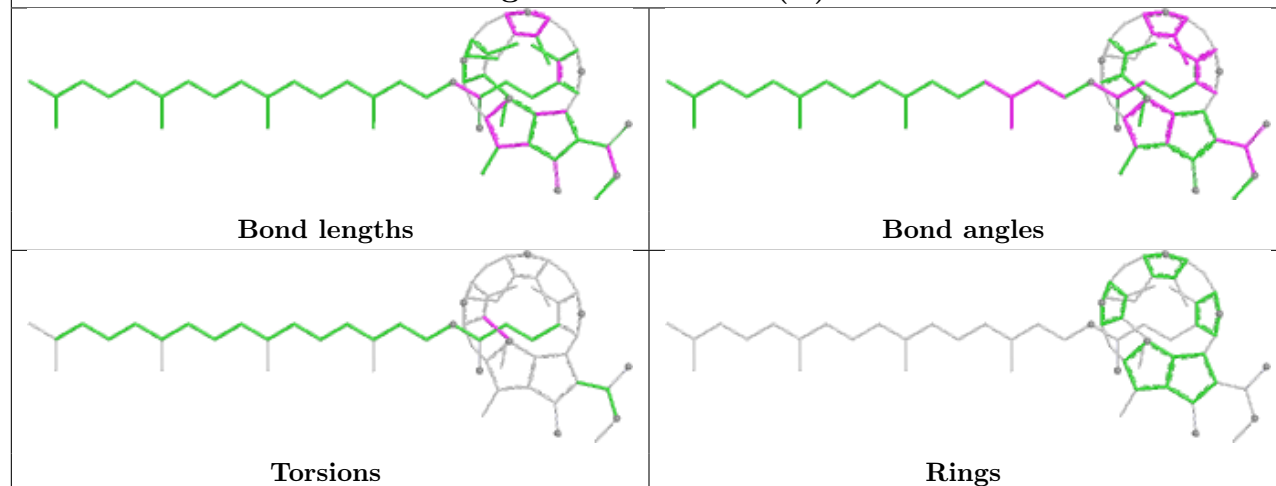
Ligand CLA A 406 (B)



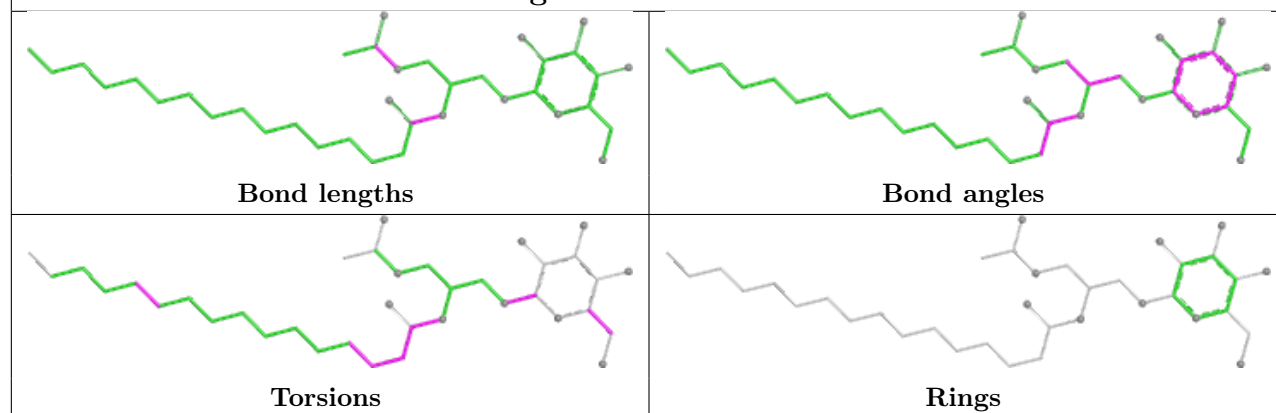
Ligand LHG d 413 (A)



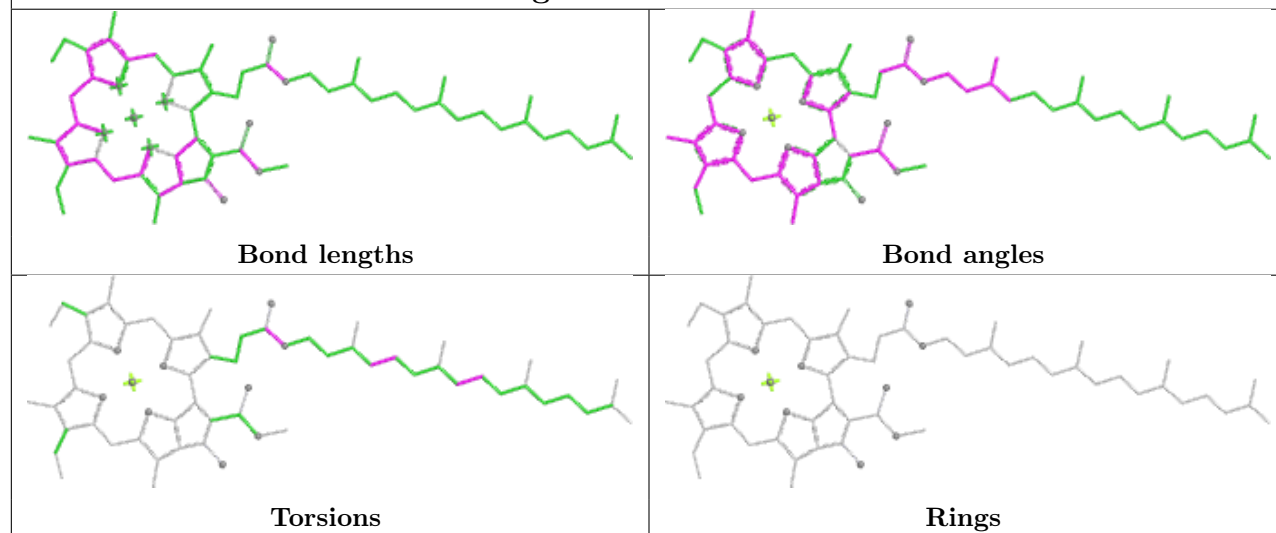
Ligand PHO a 416 (B)

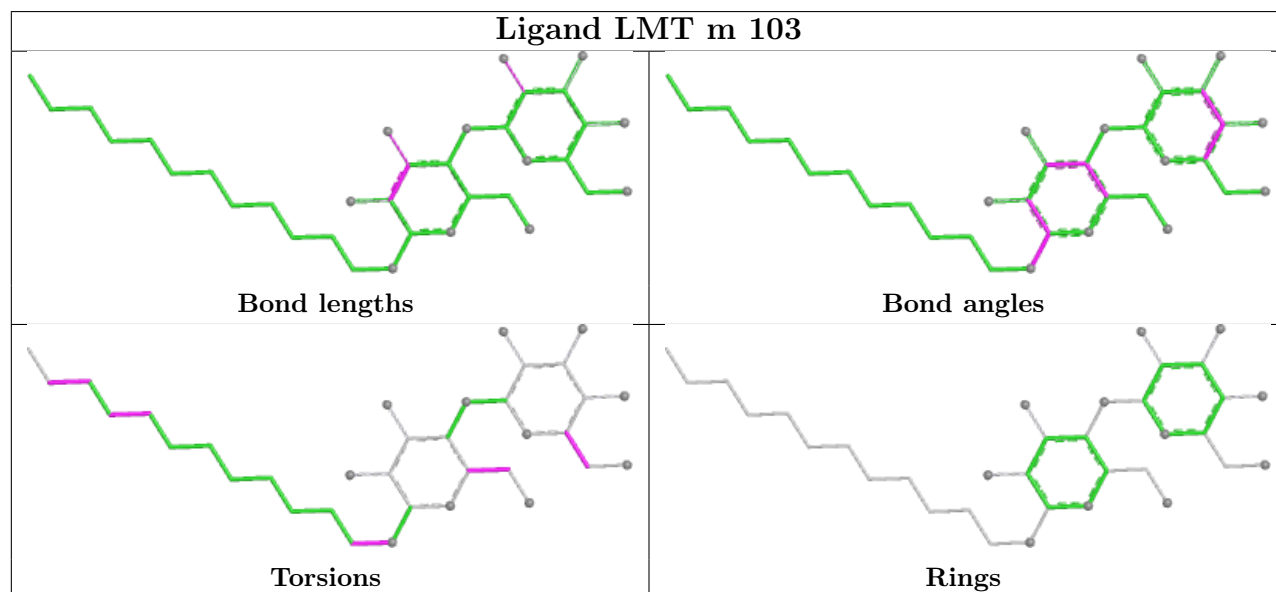
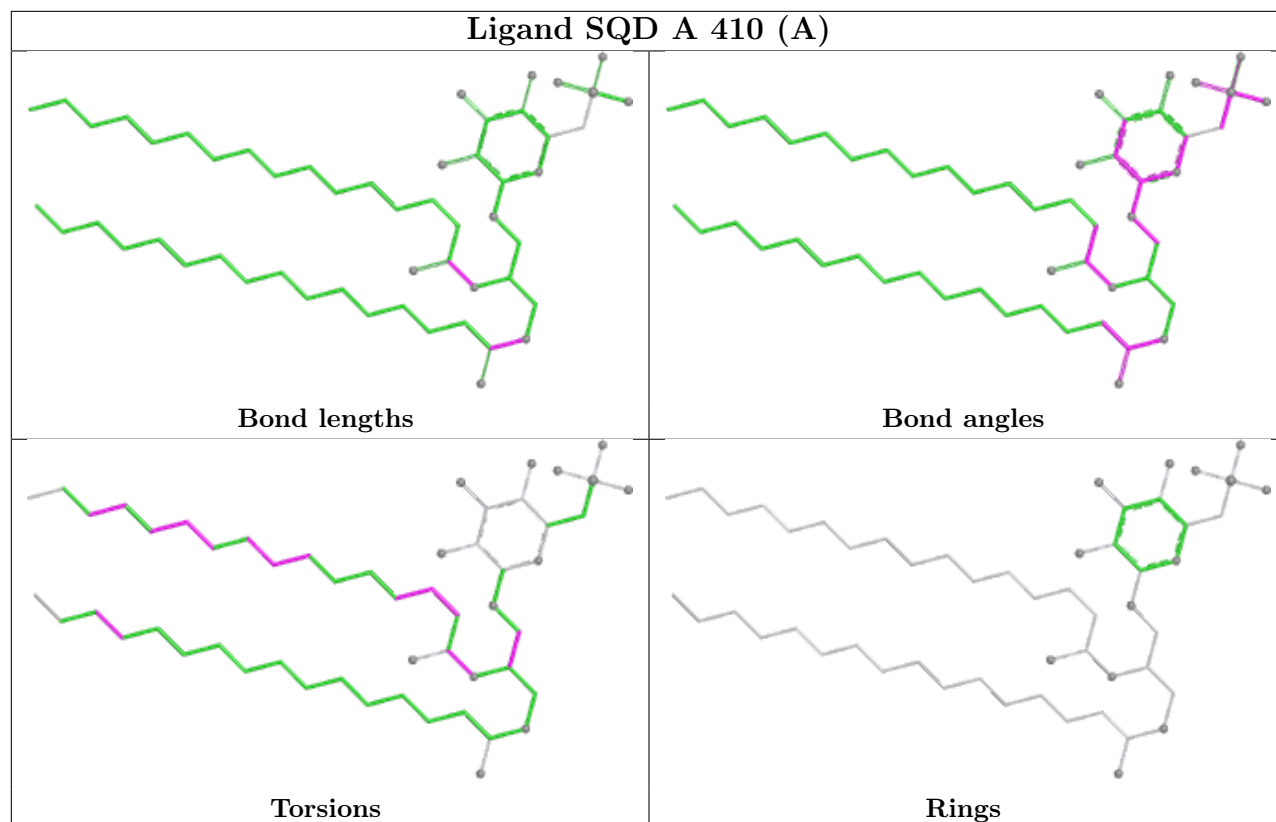


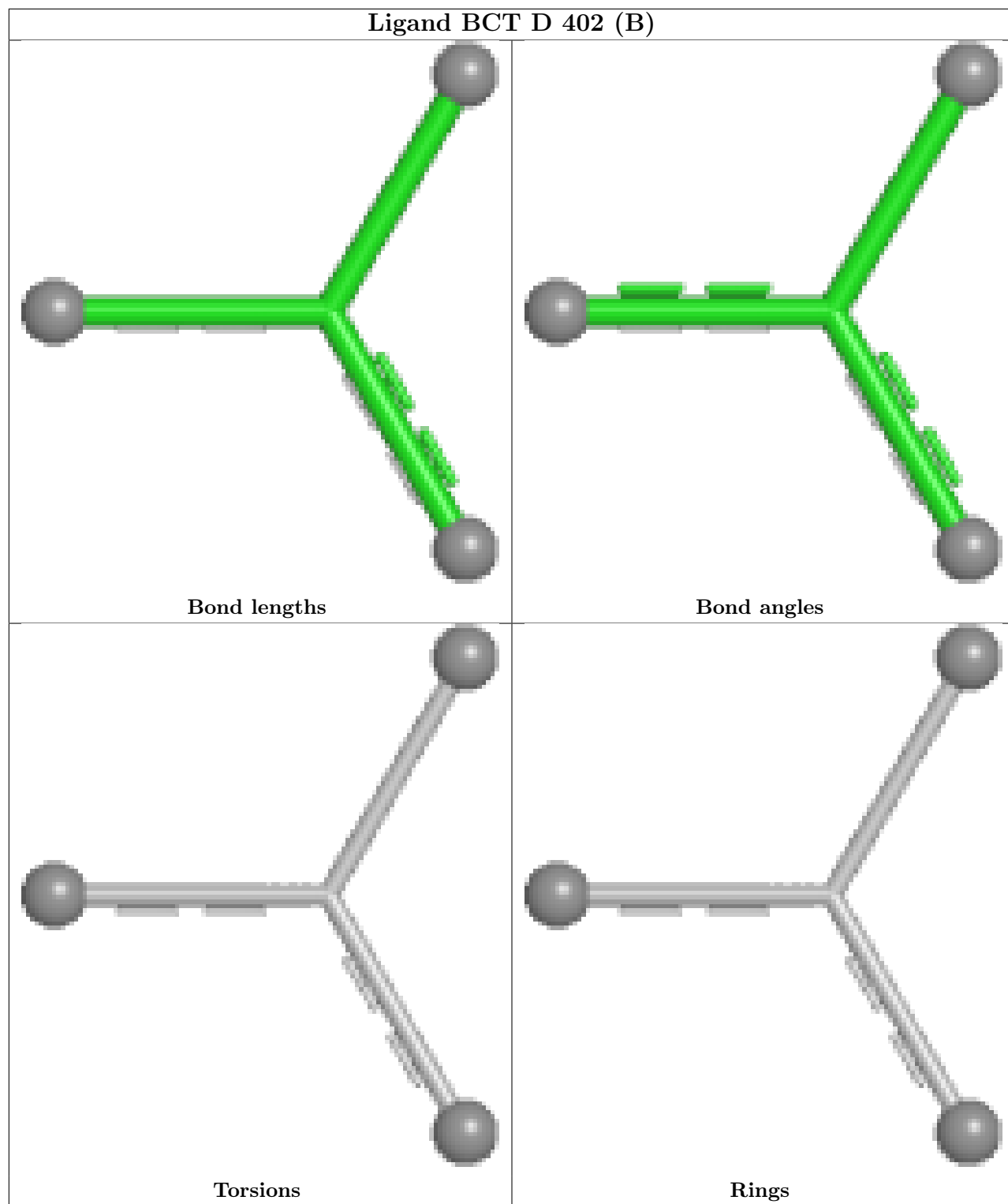
Ligand LMG Z 101



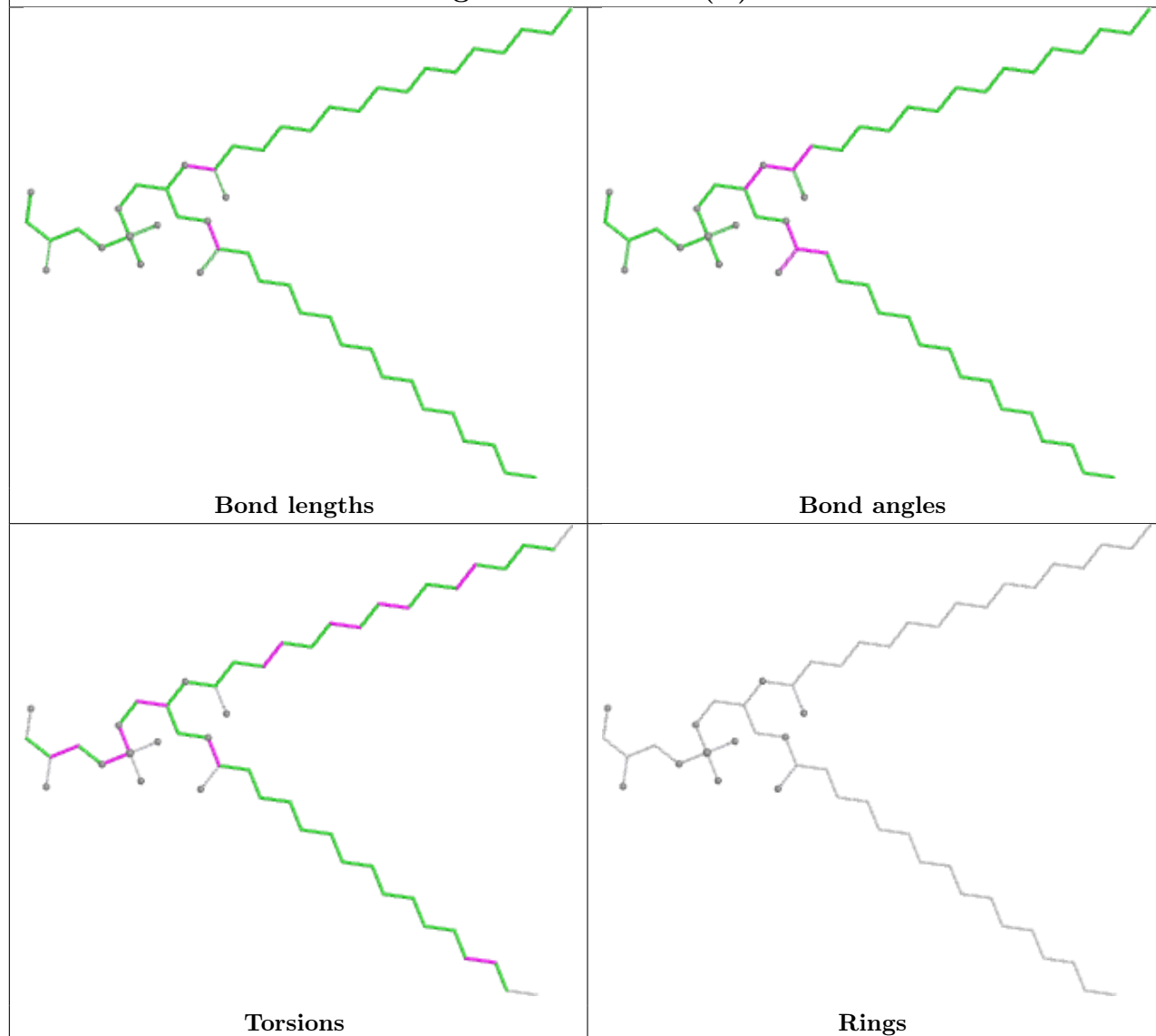
Ligand CLA C 512



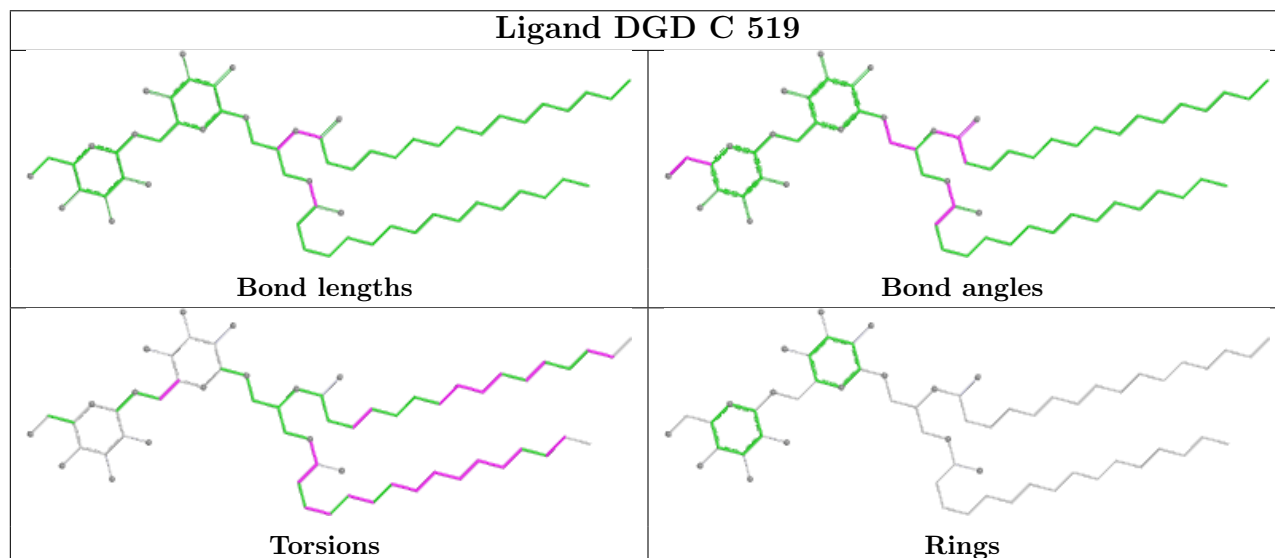


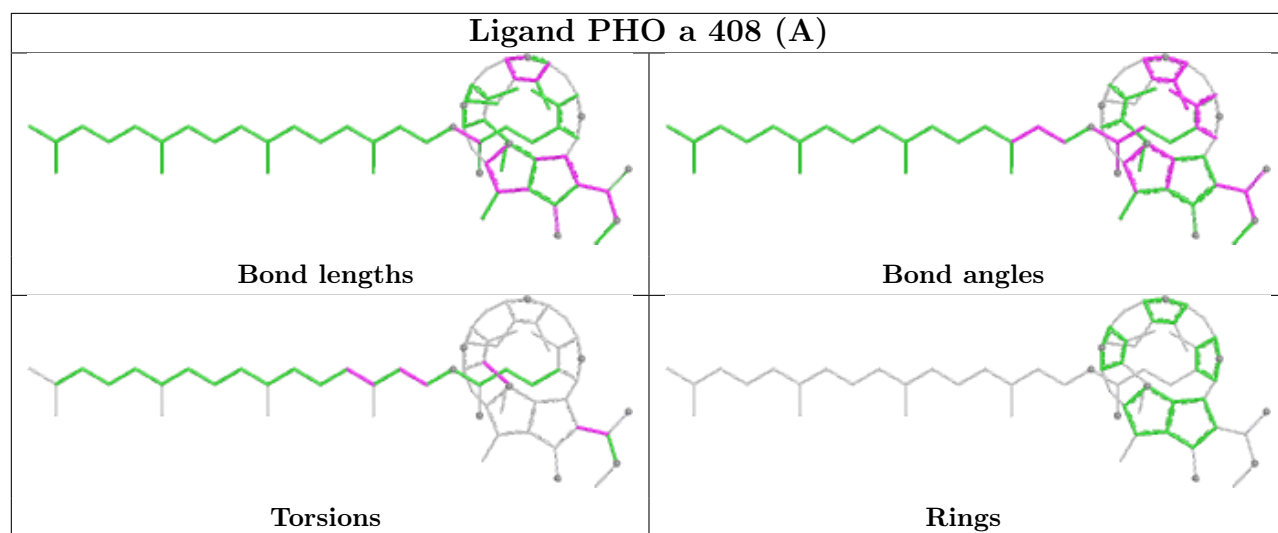
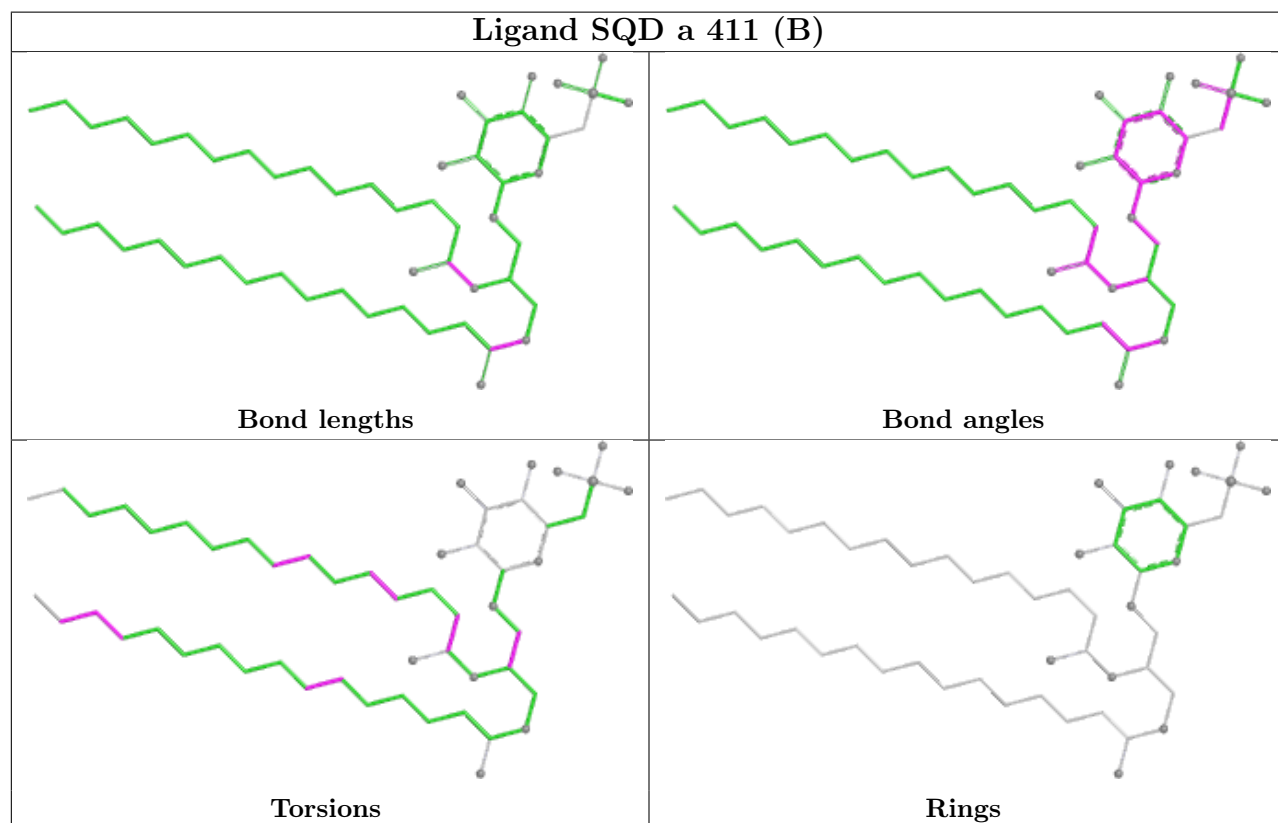
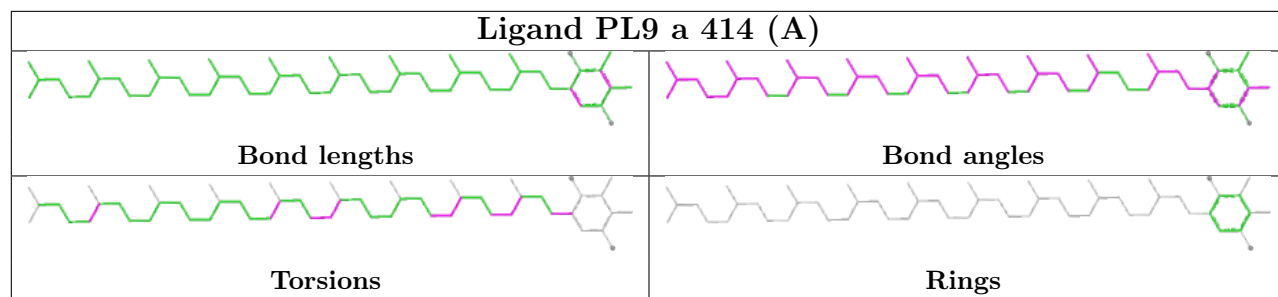


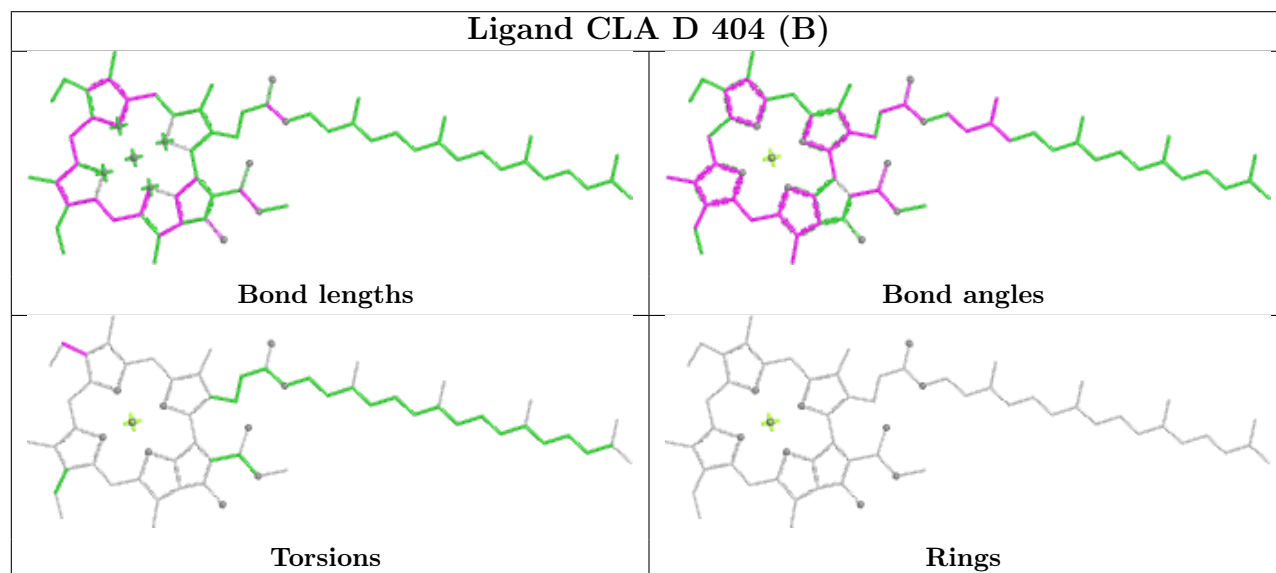
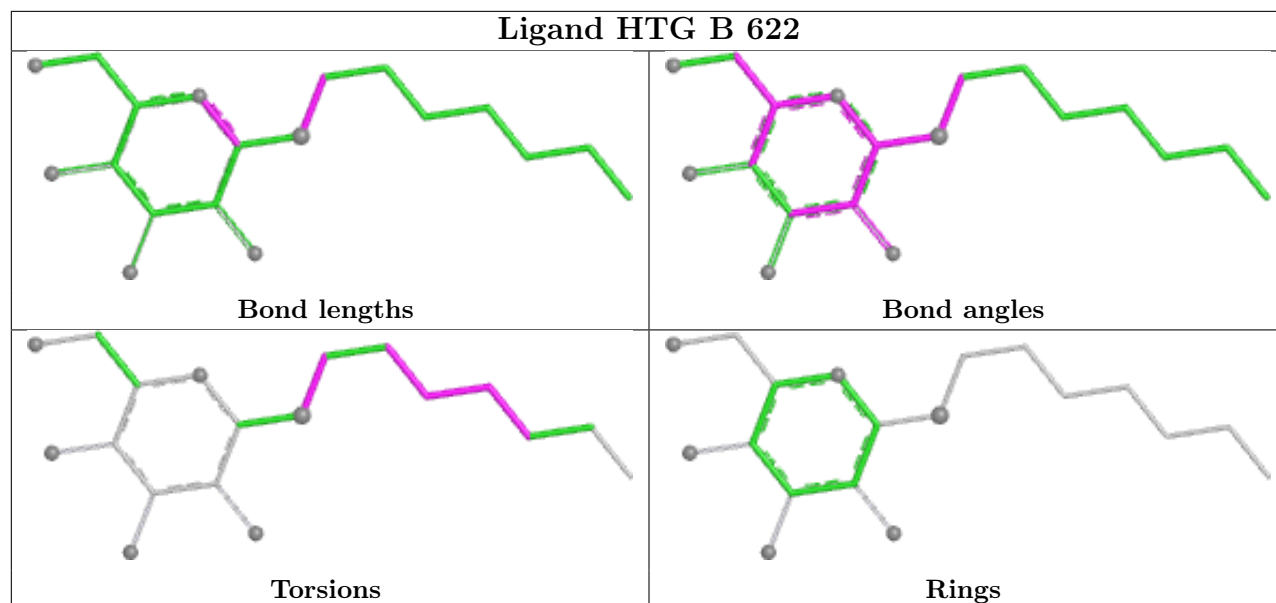
Ligand LHG d 406 (B)



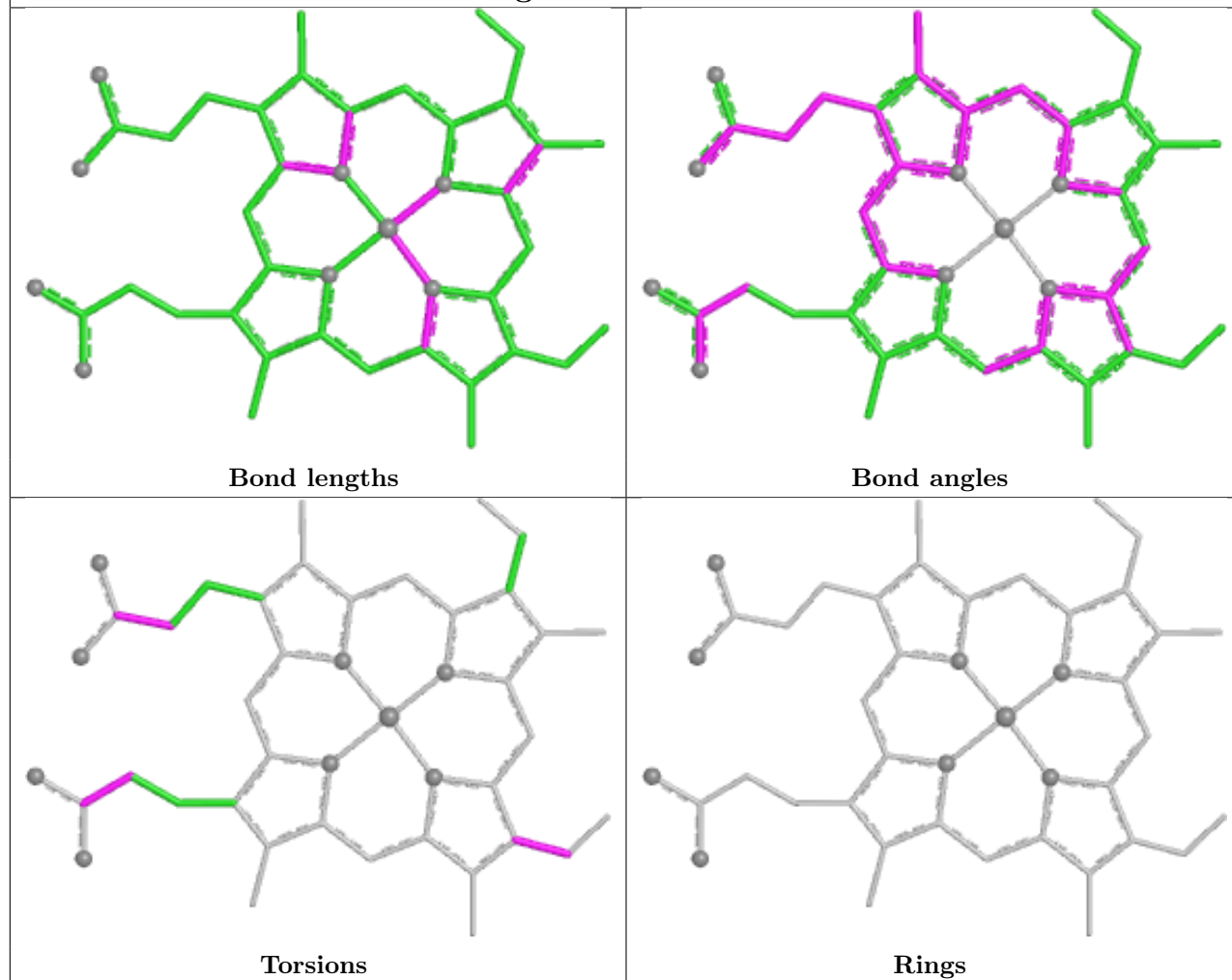
Ligand DGD C 519



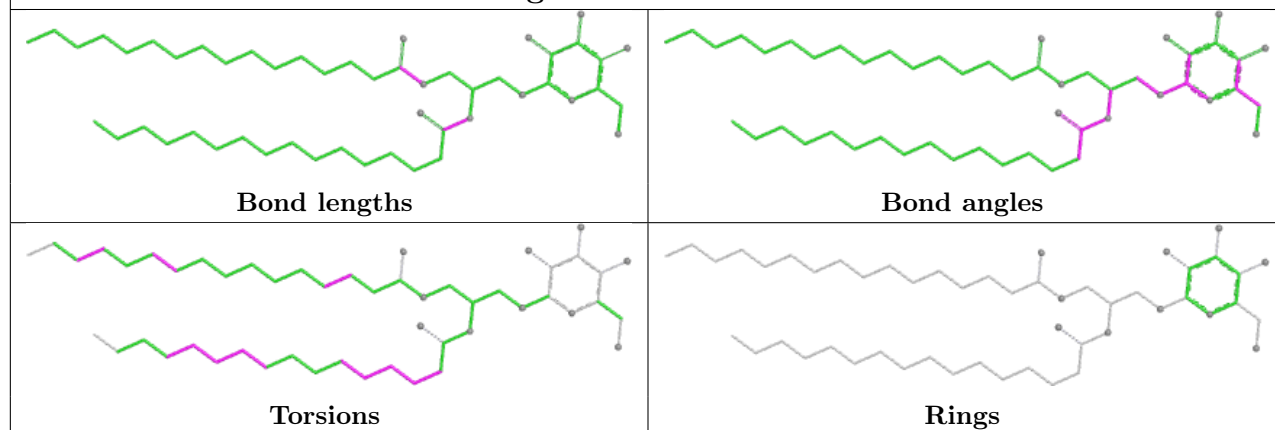


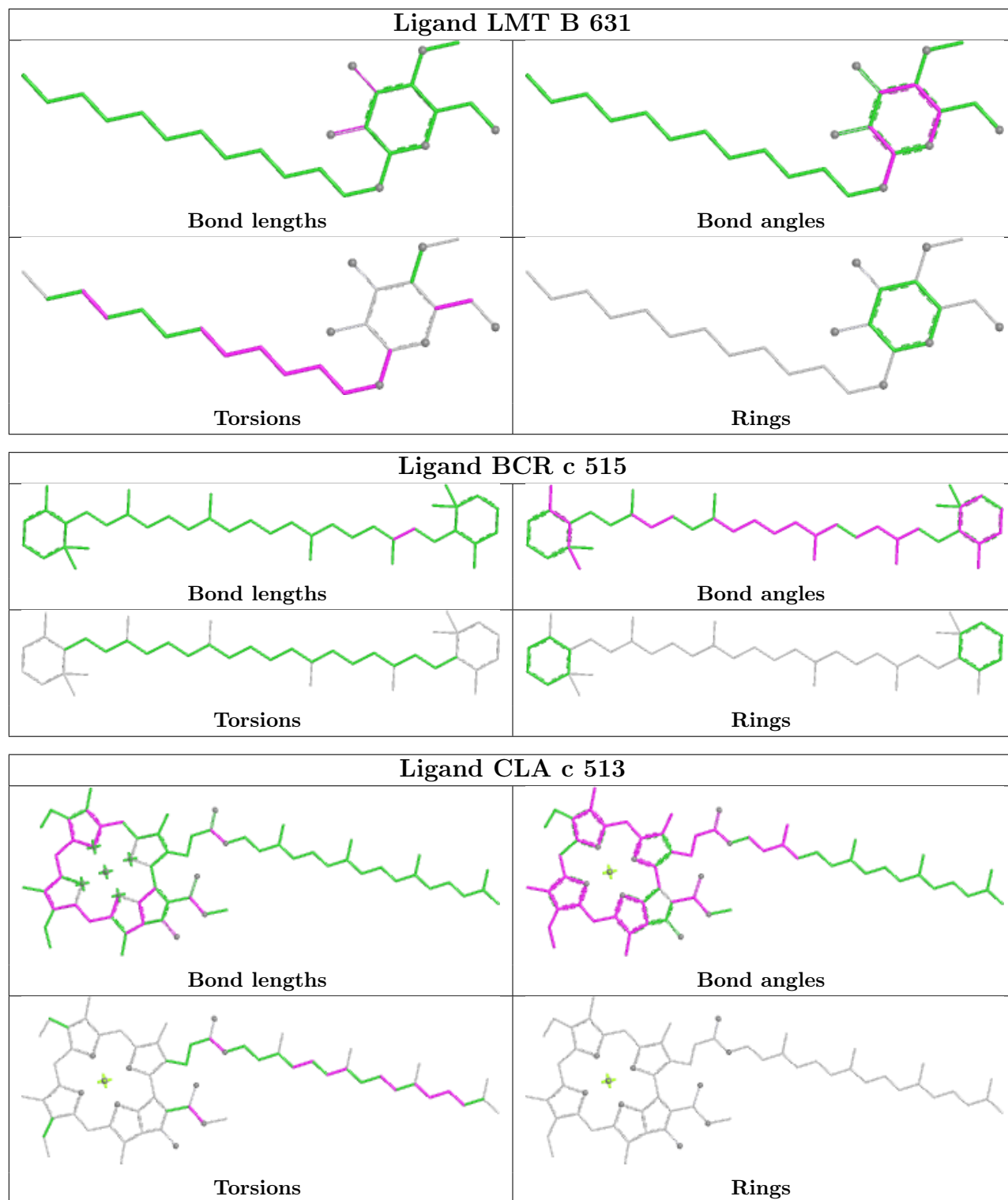


Ligand HEM f 101

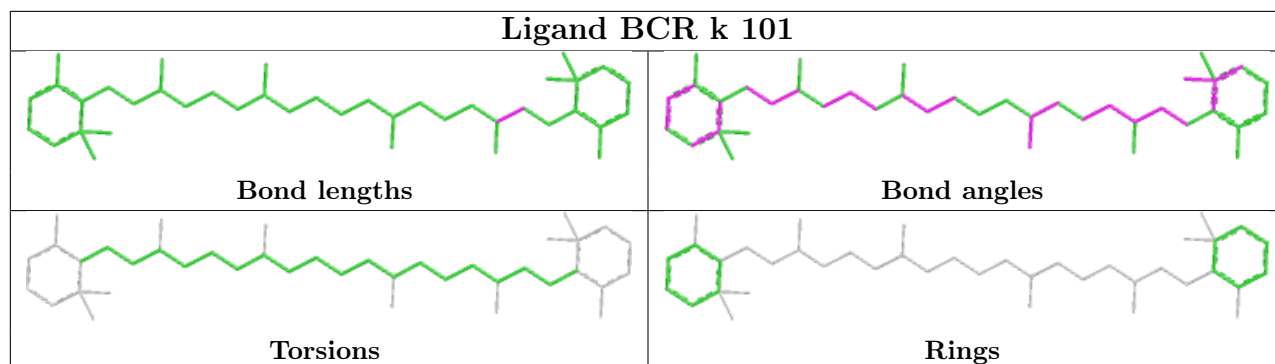


Ligand LMG C 501

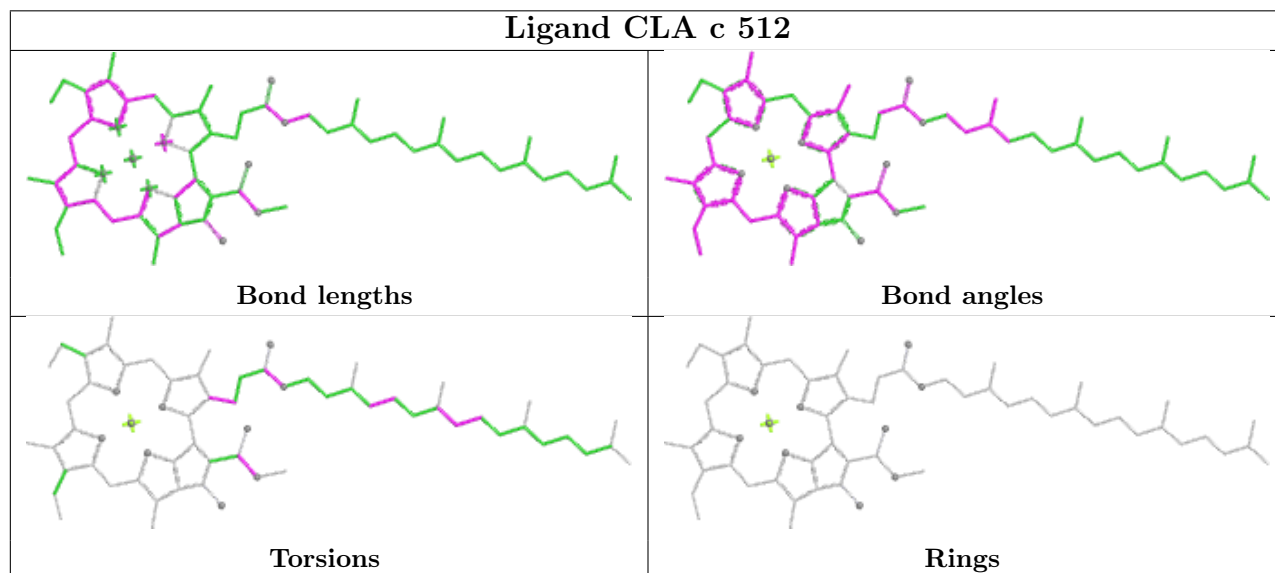




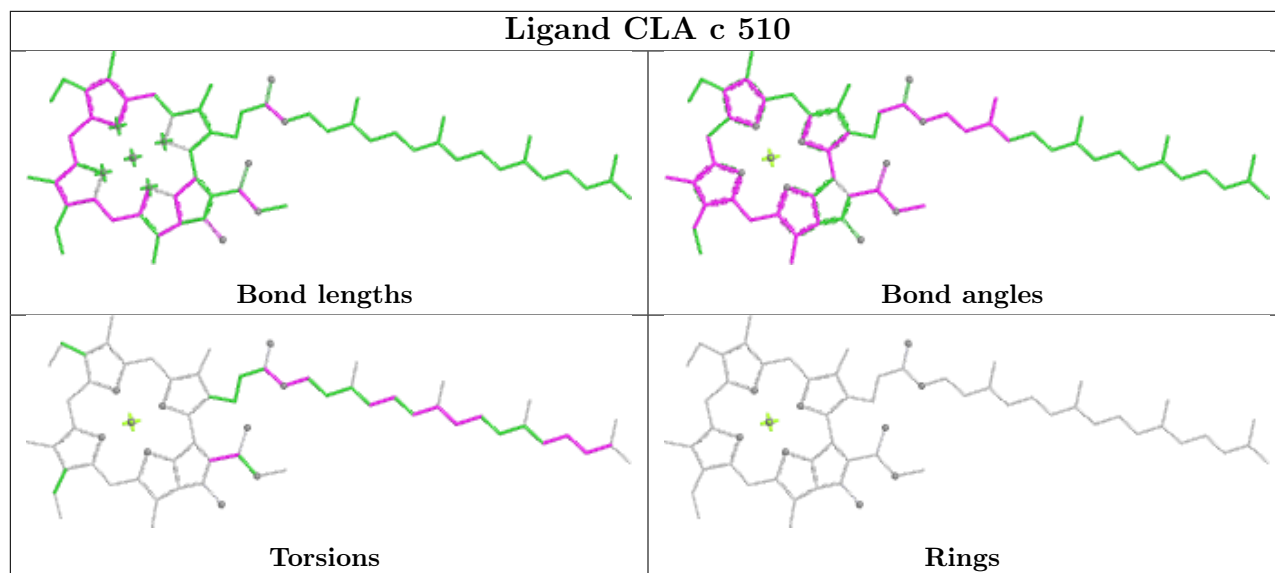
Ligand BCR k 101

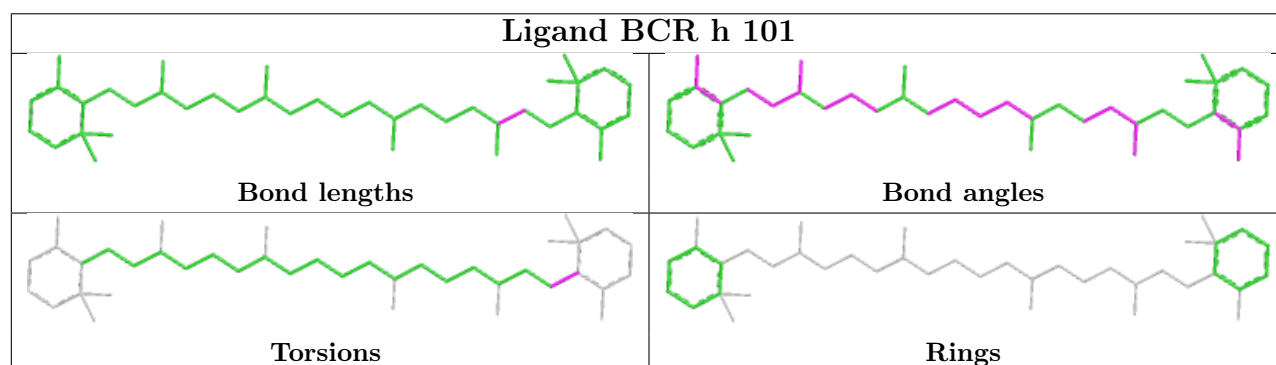
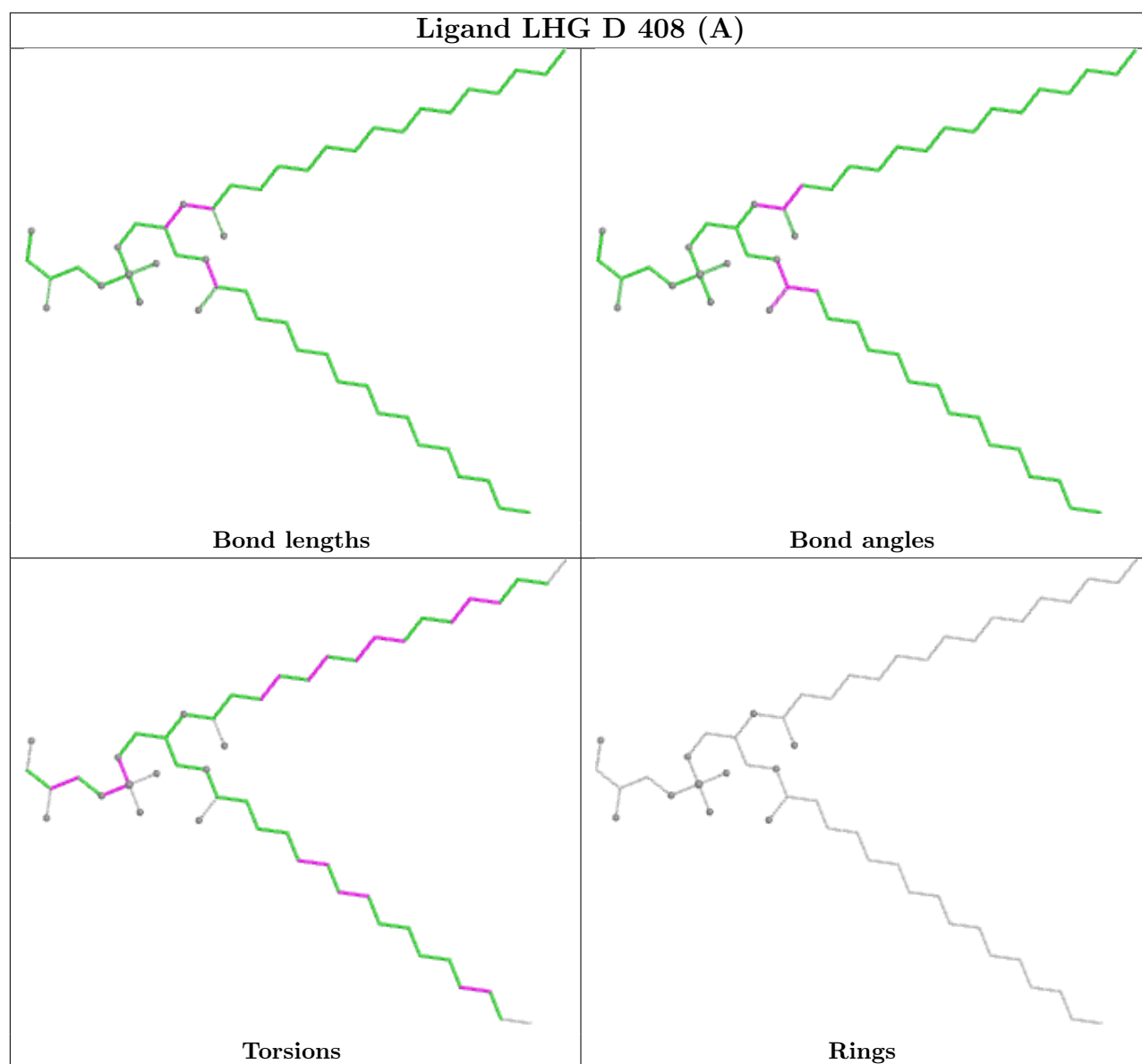


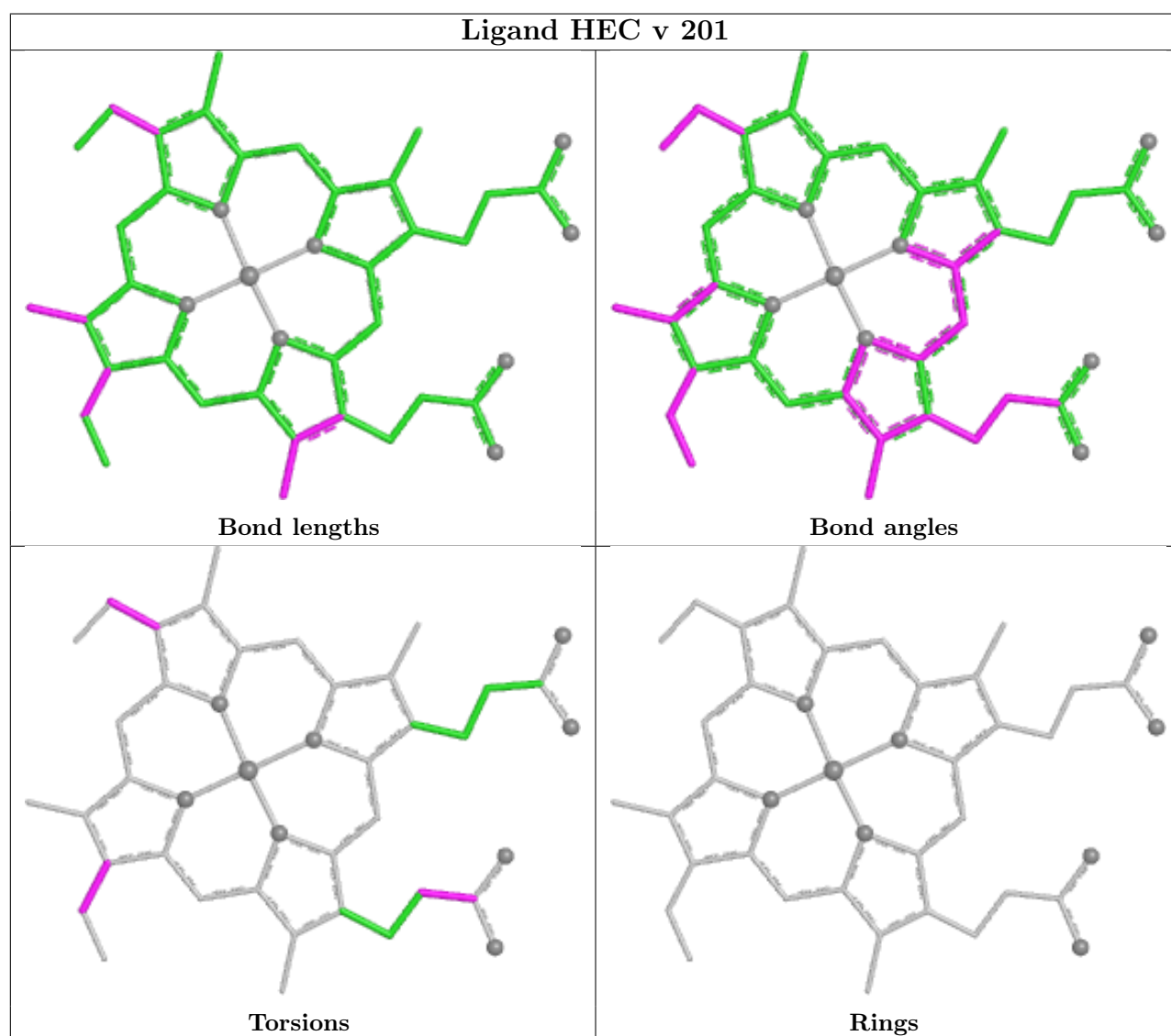
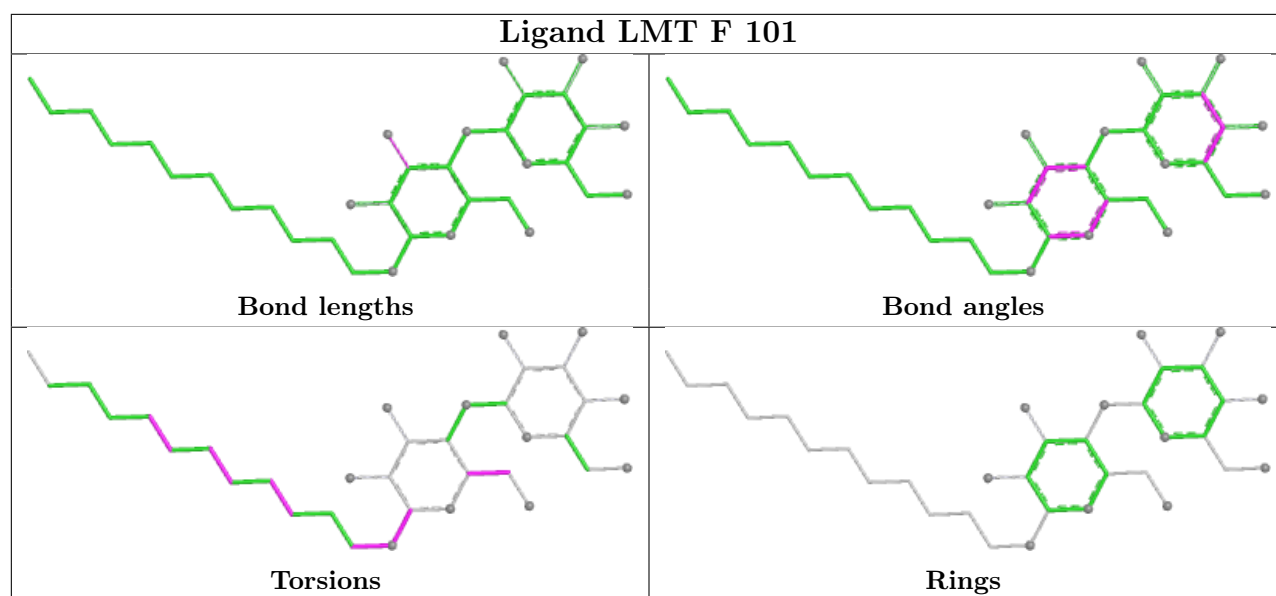
Ligand CLA c 512



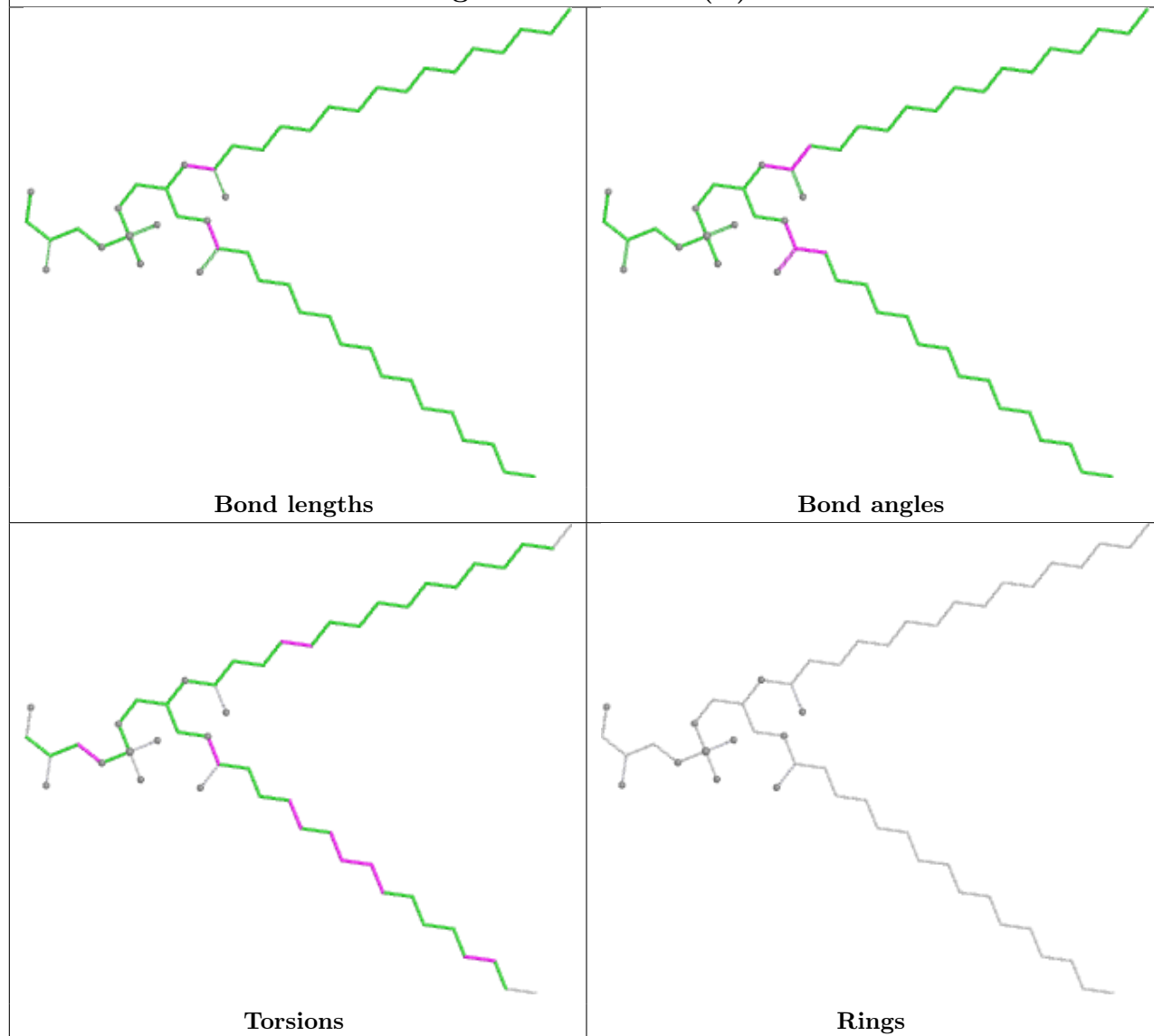
Ligand CLA c 510



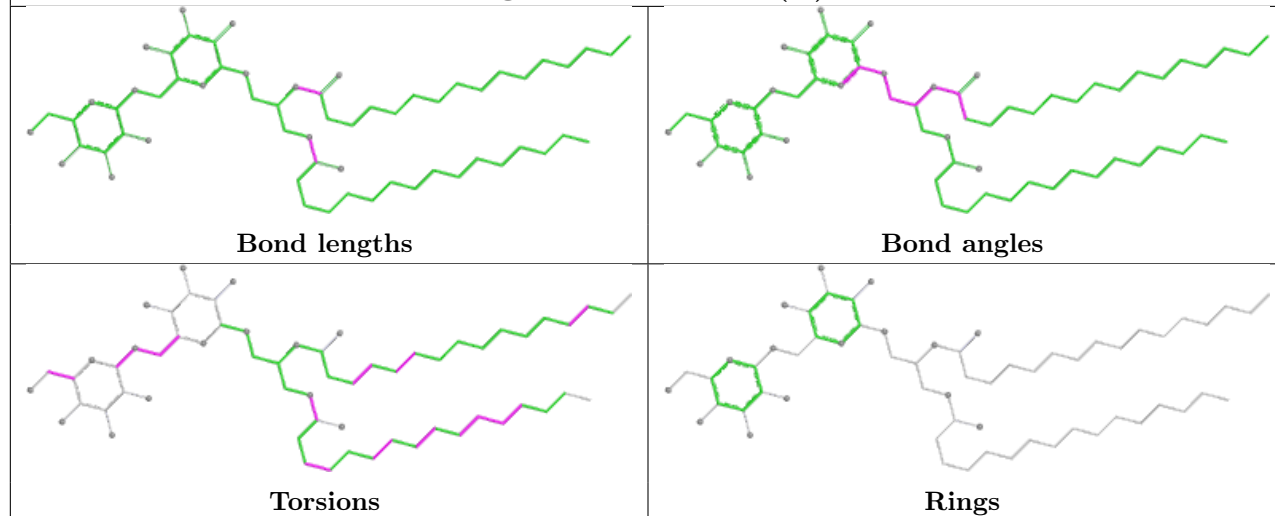


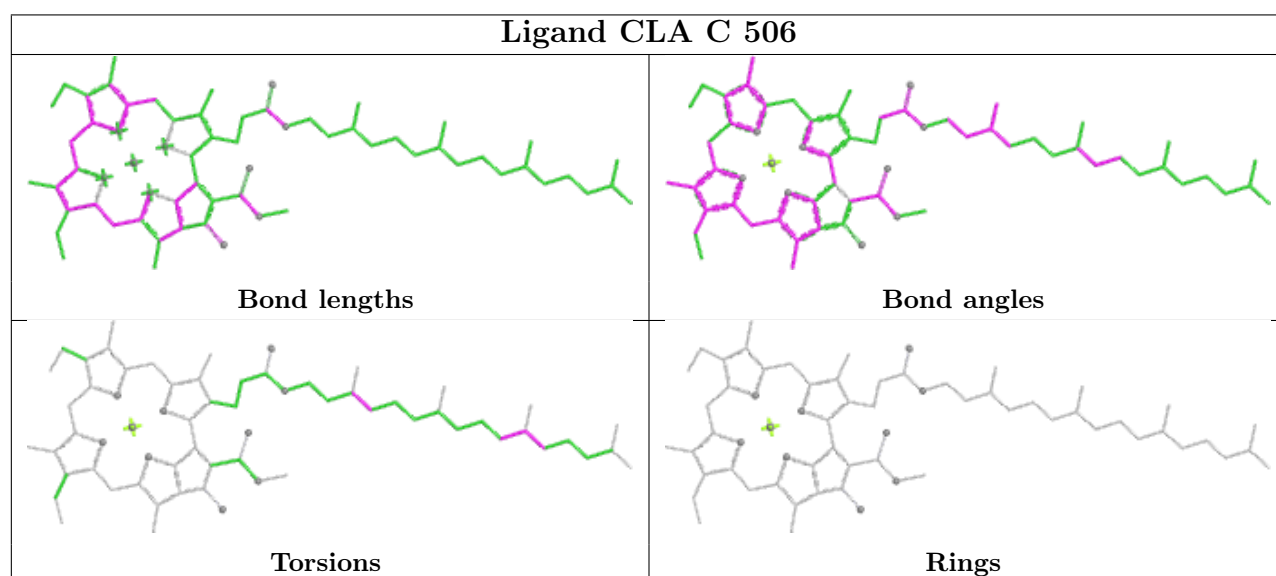
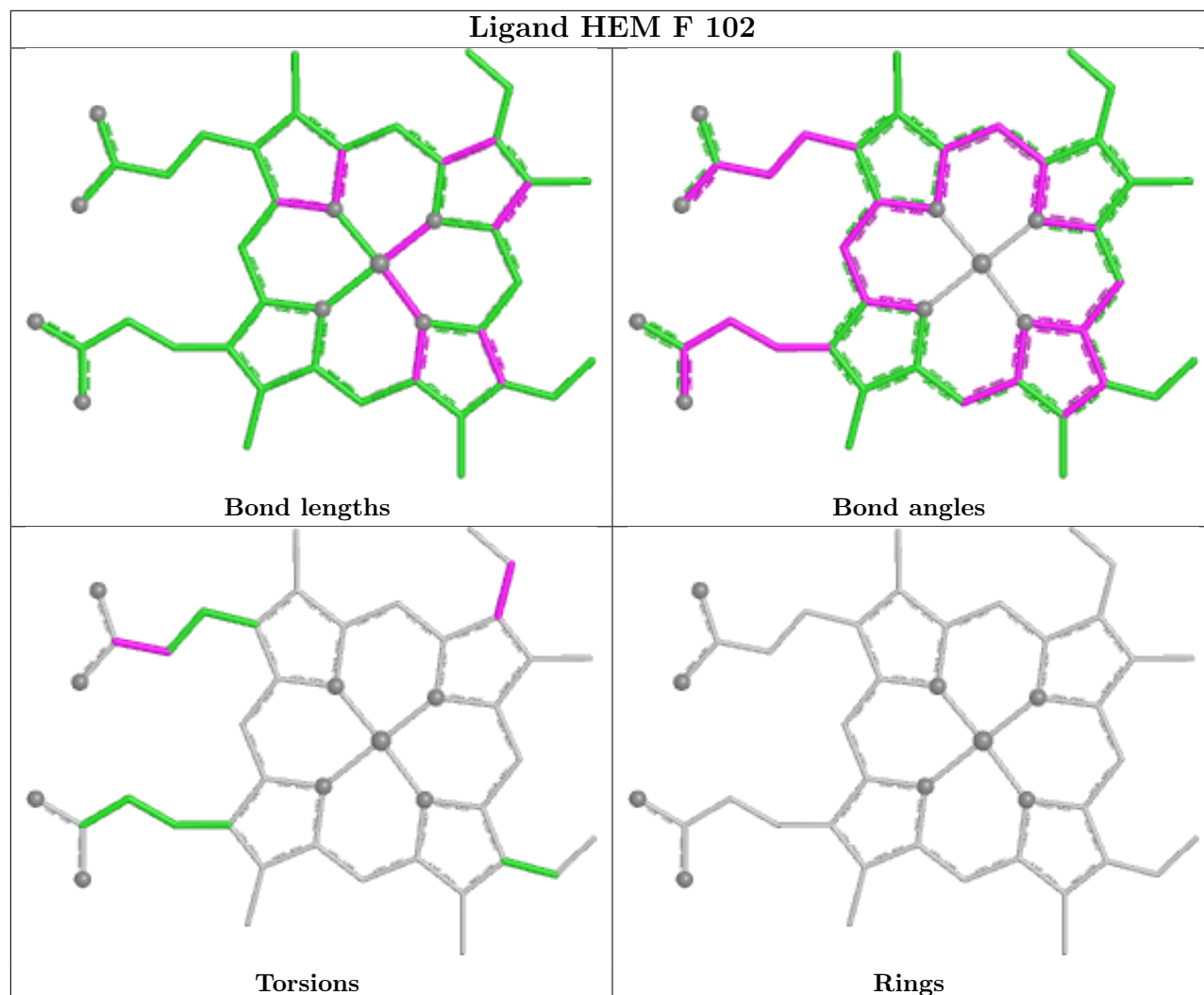


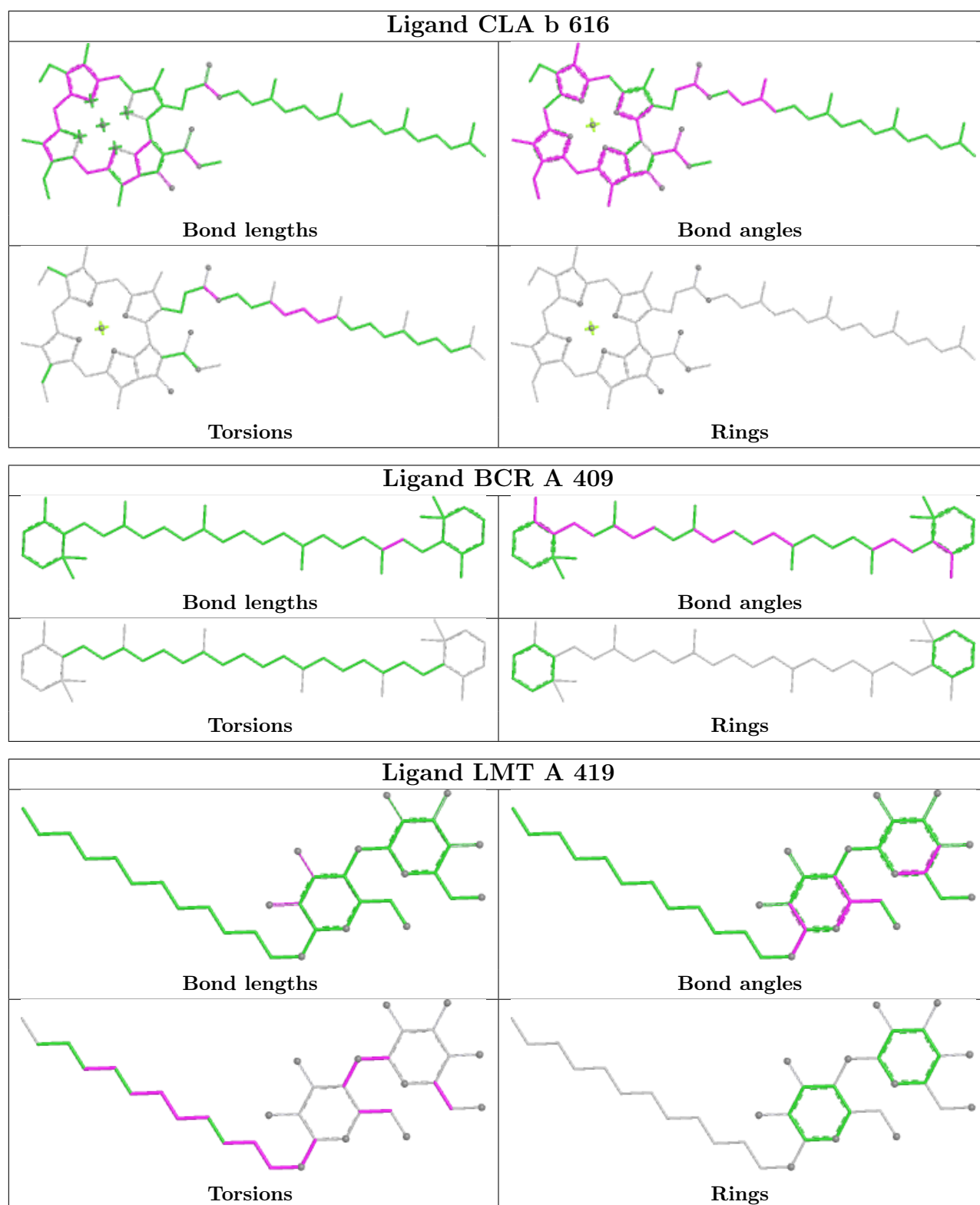
Ligand LHG d 407 (B)

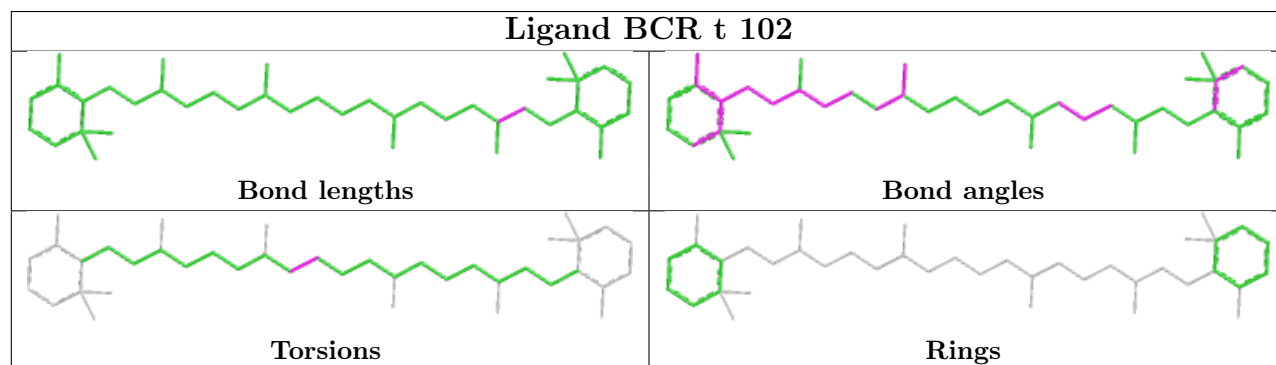
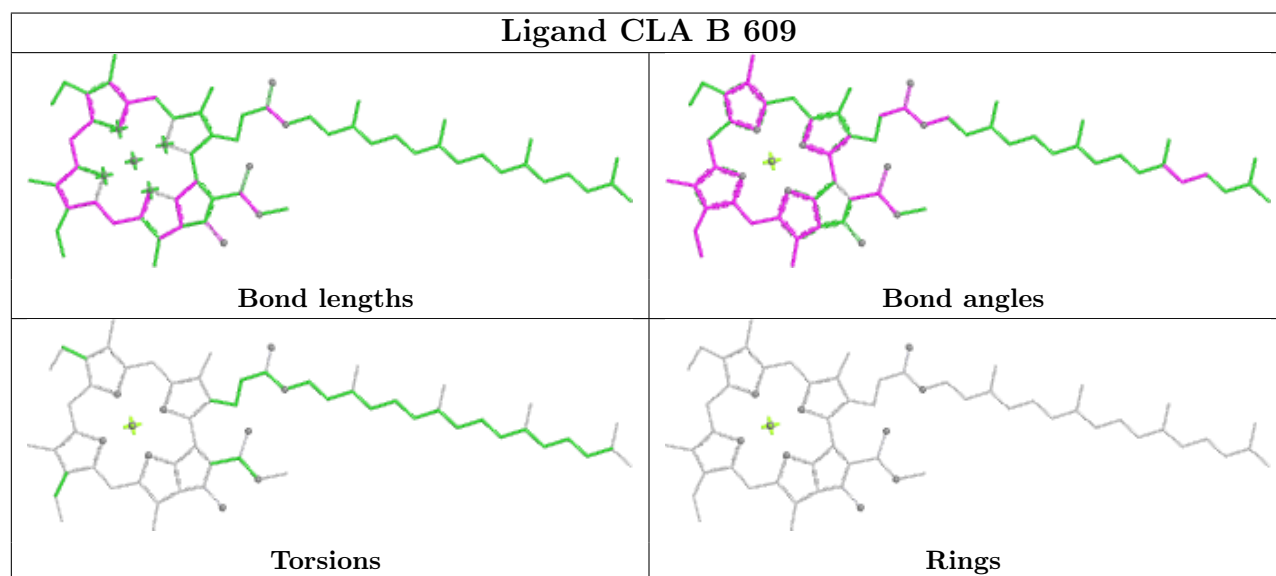
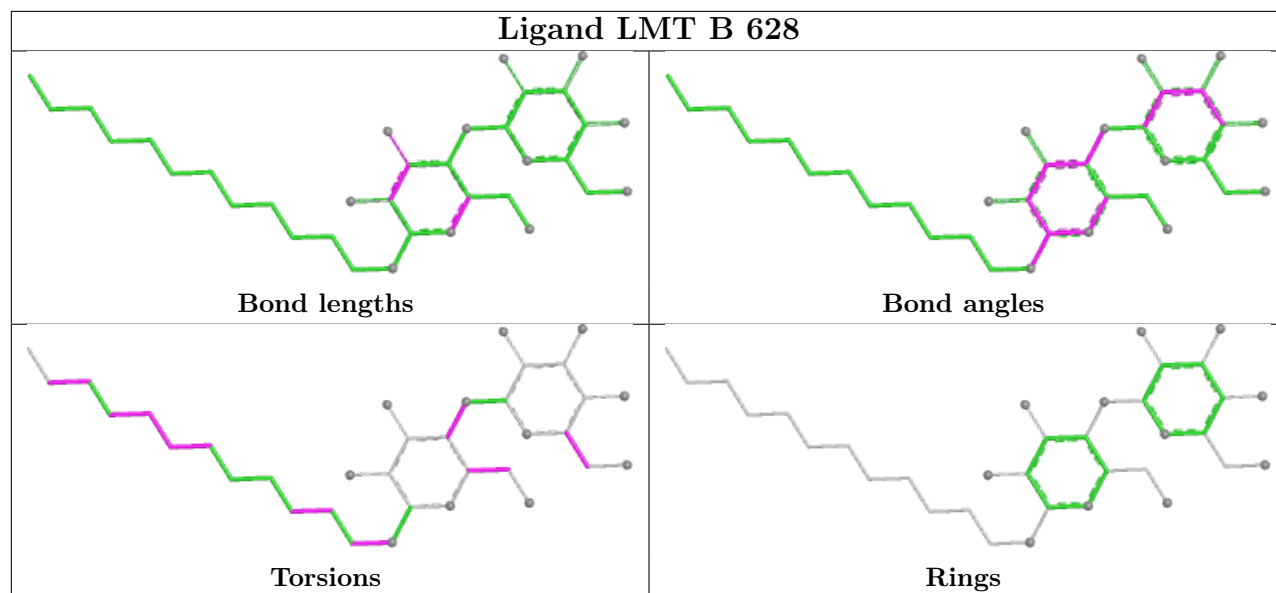


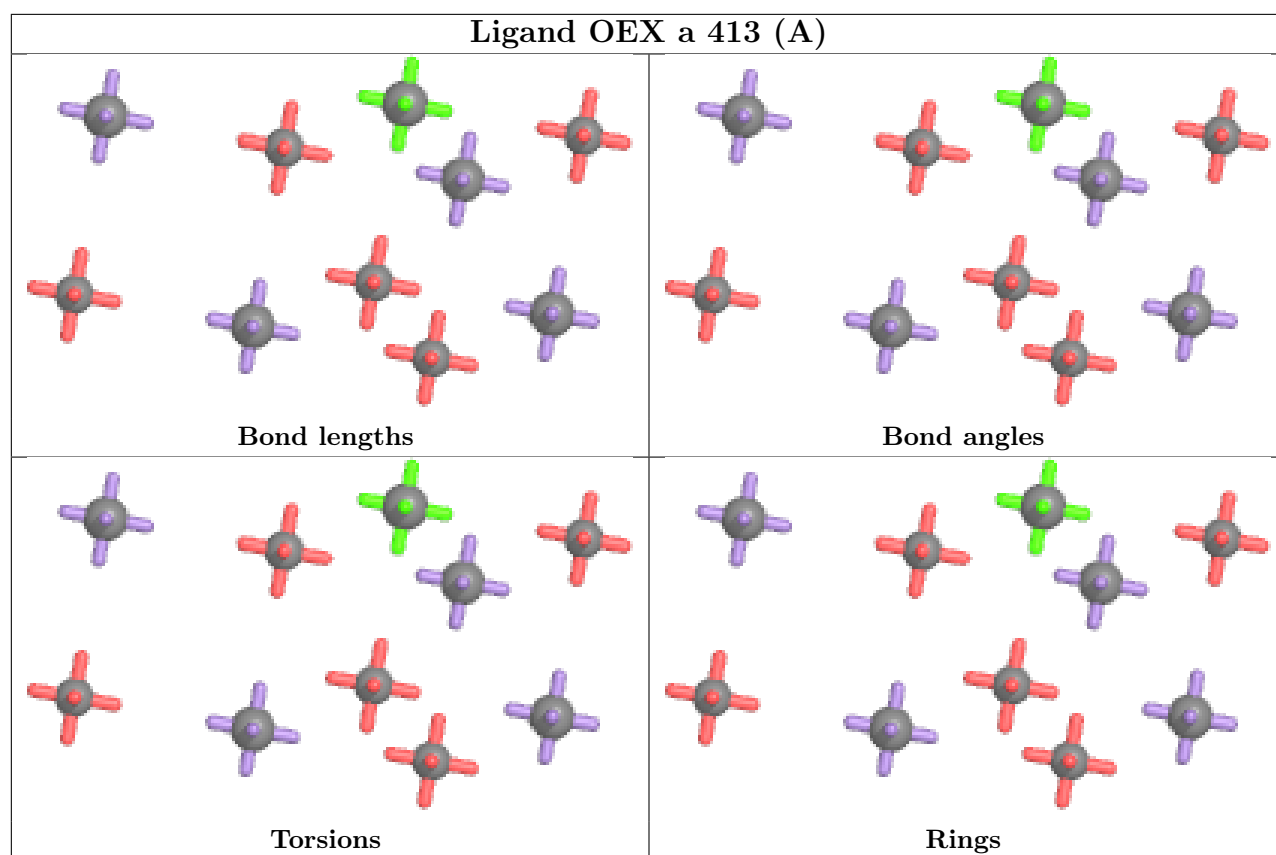
Ligand DGD c 517 (B)



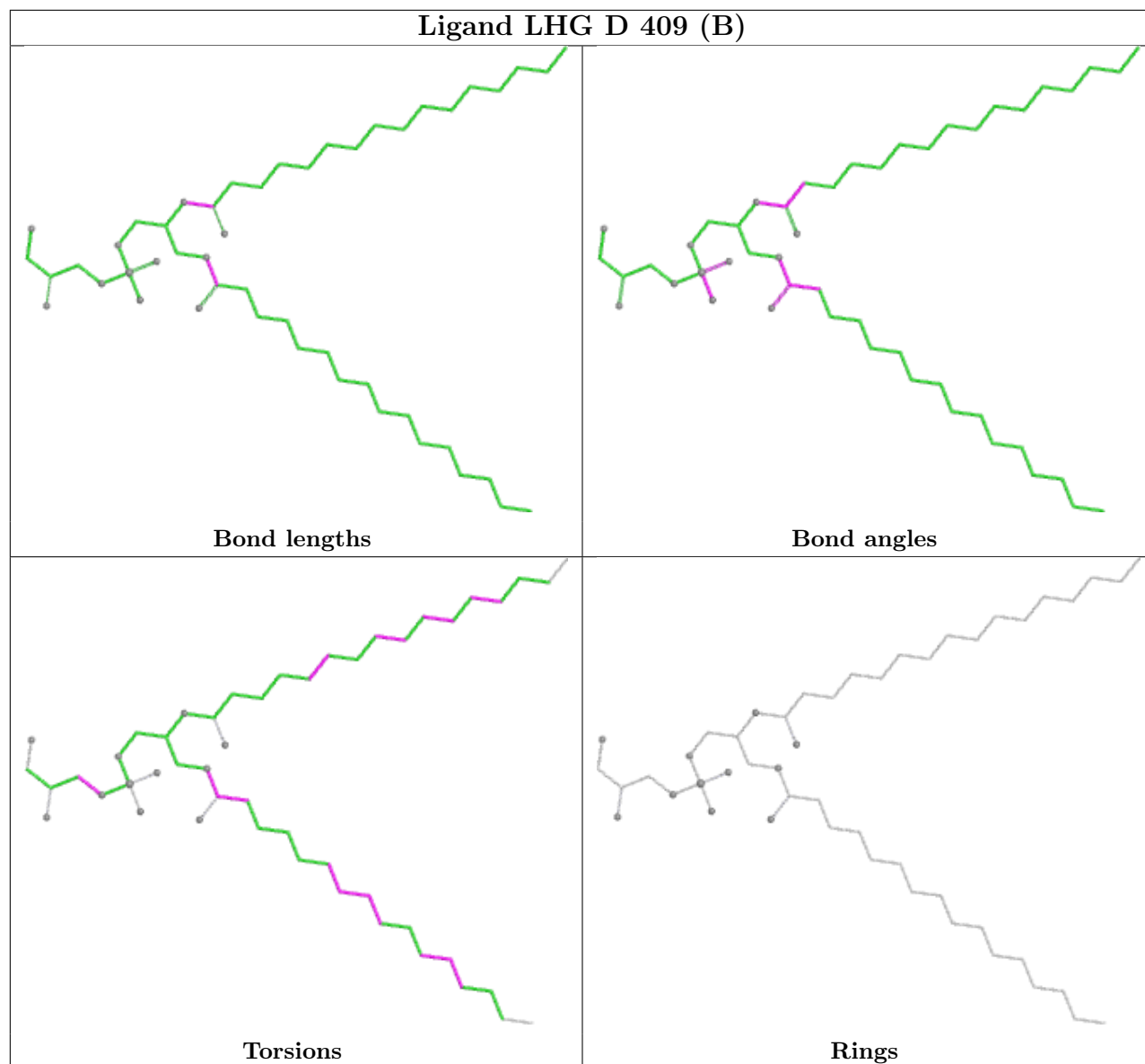




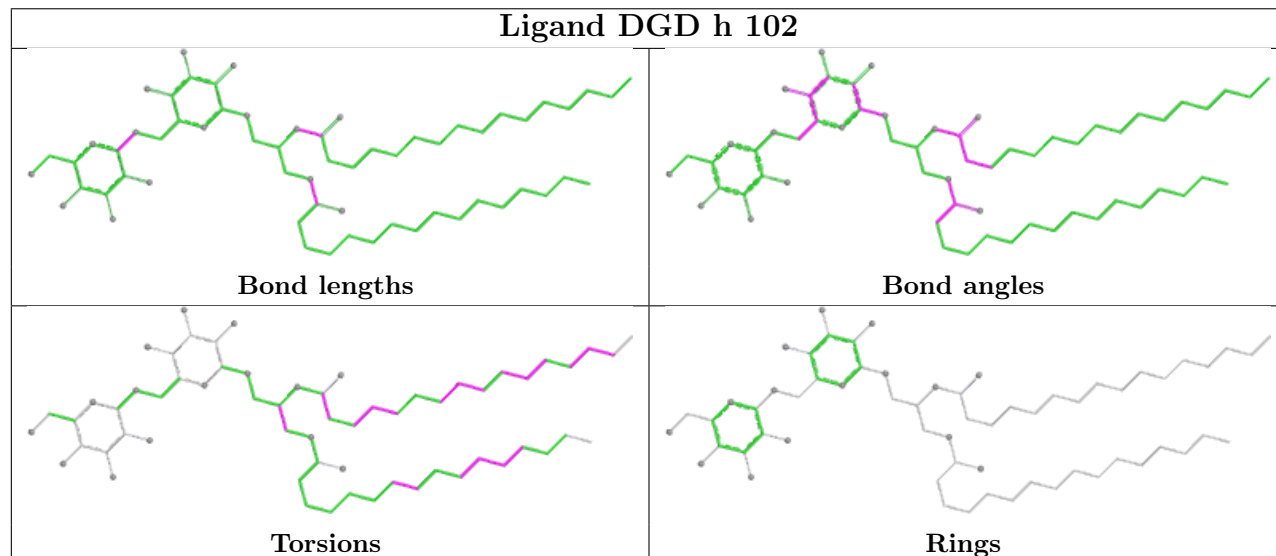


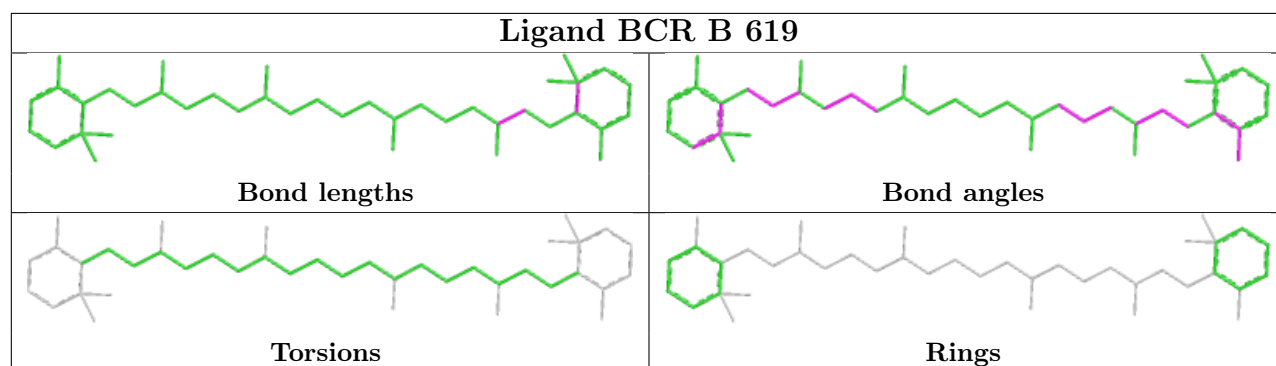
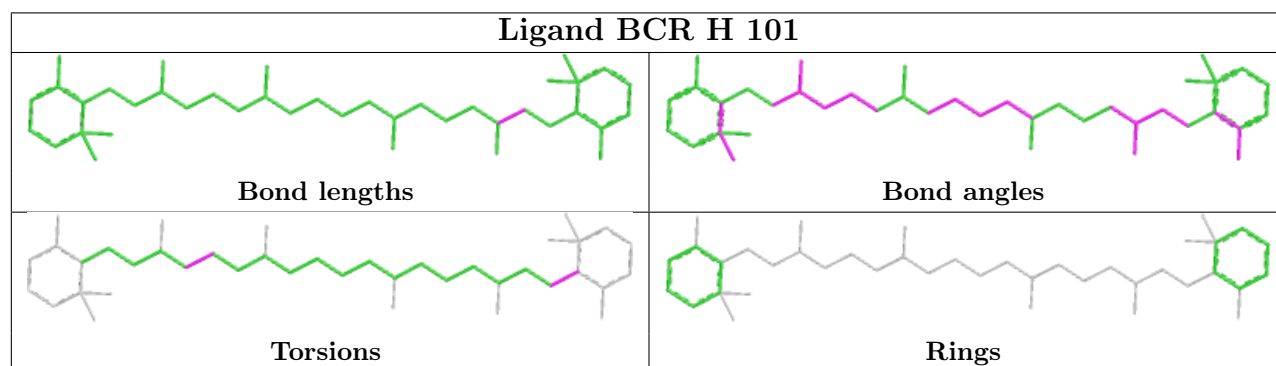
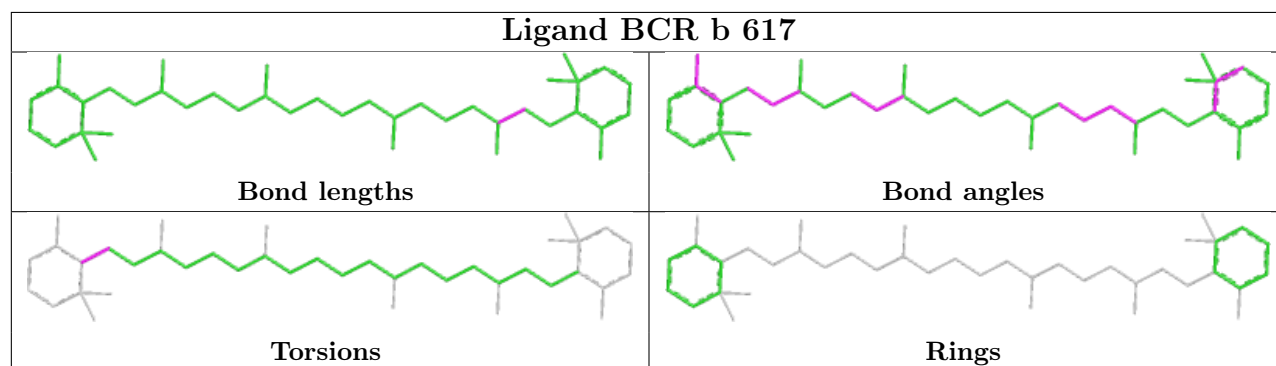
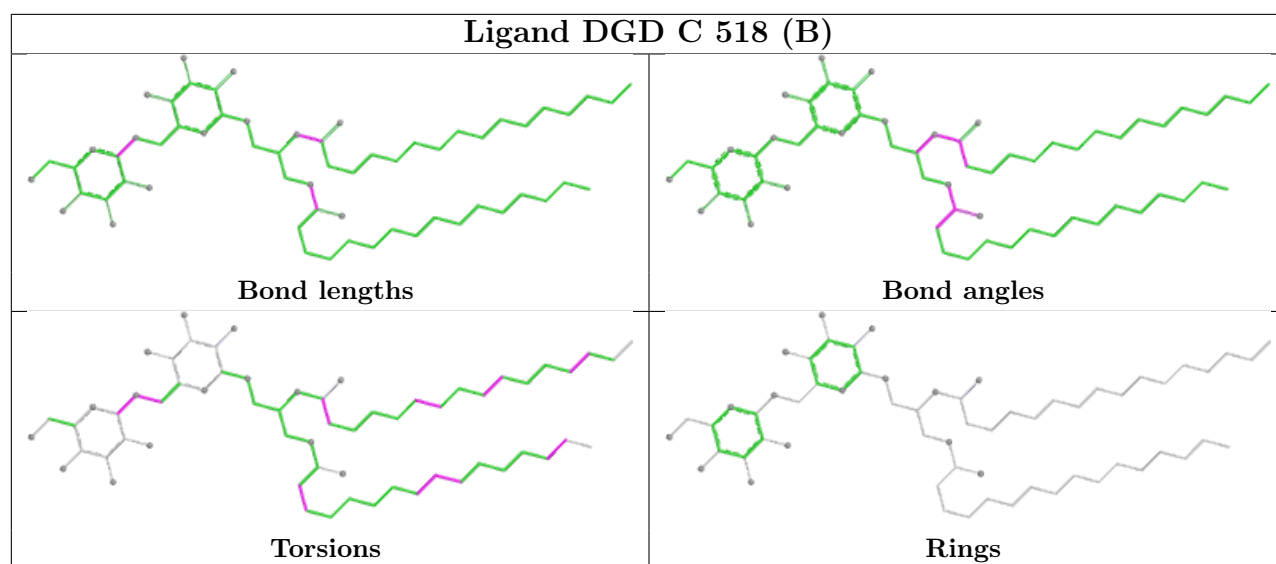


Ligand LHG D 409 (B)

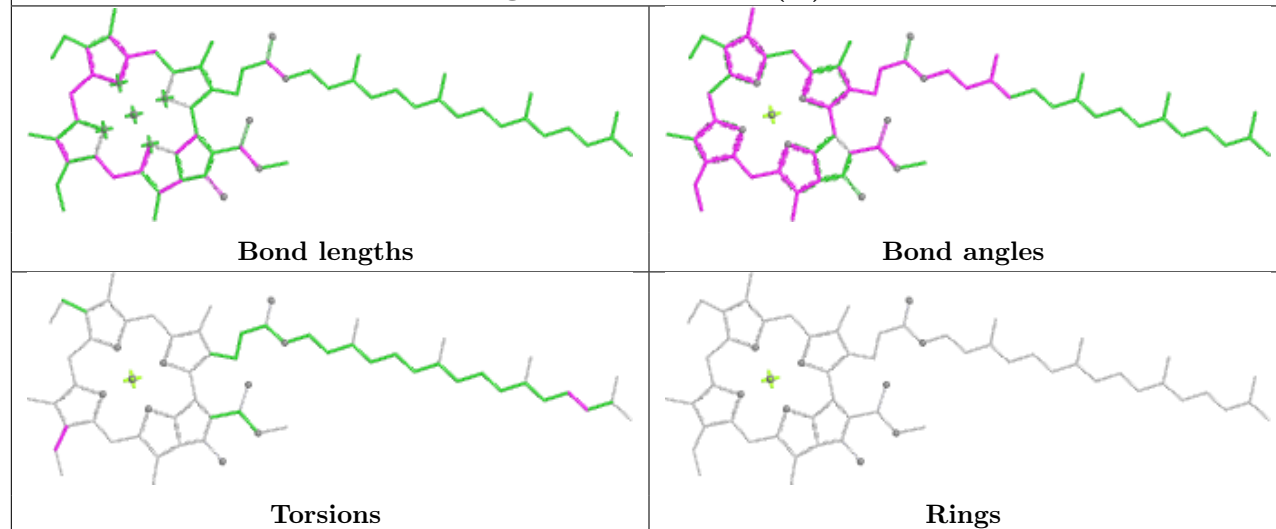


Ligand DGD h 102

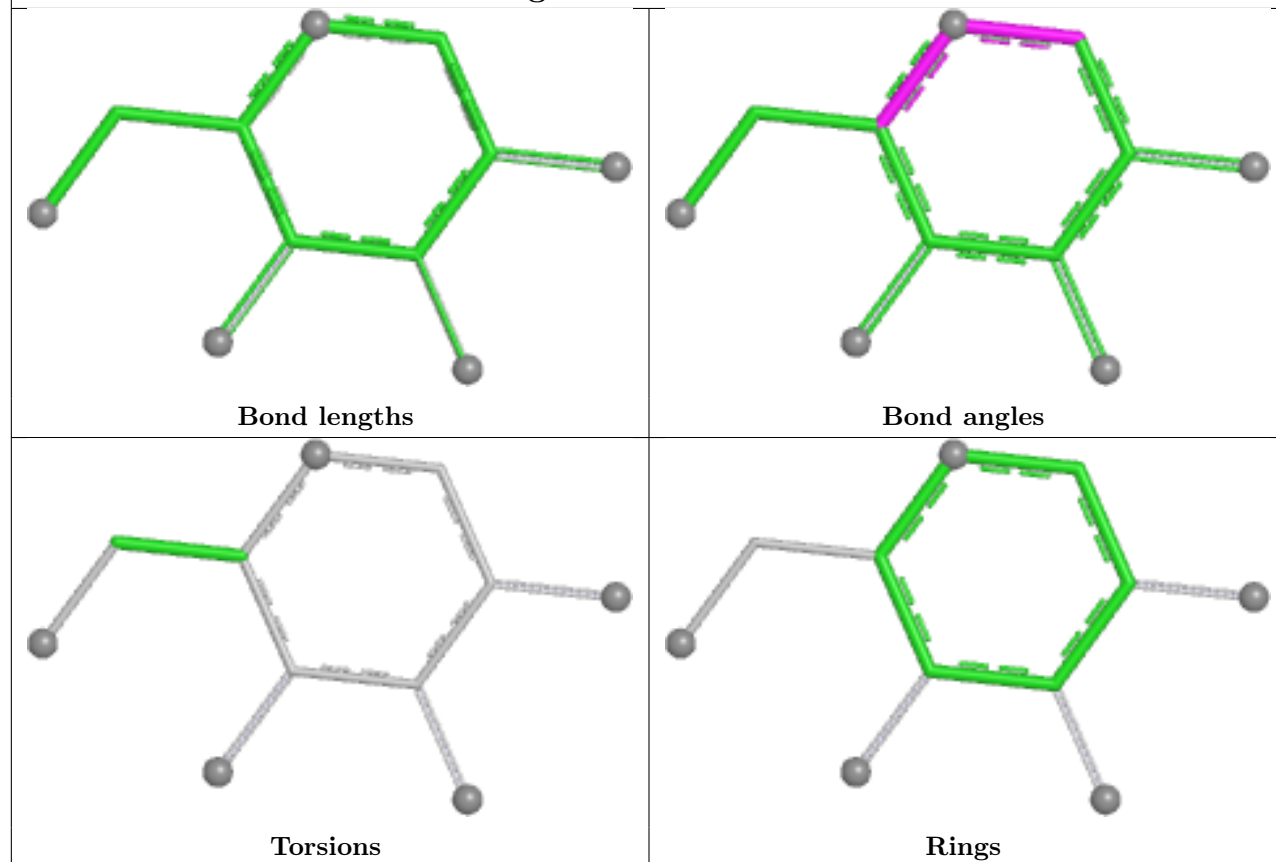


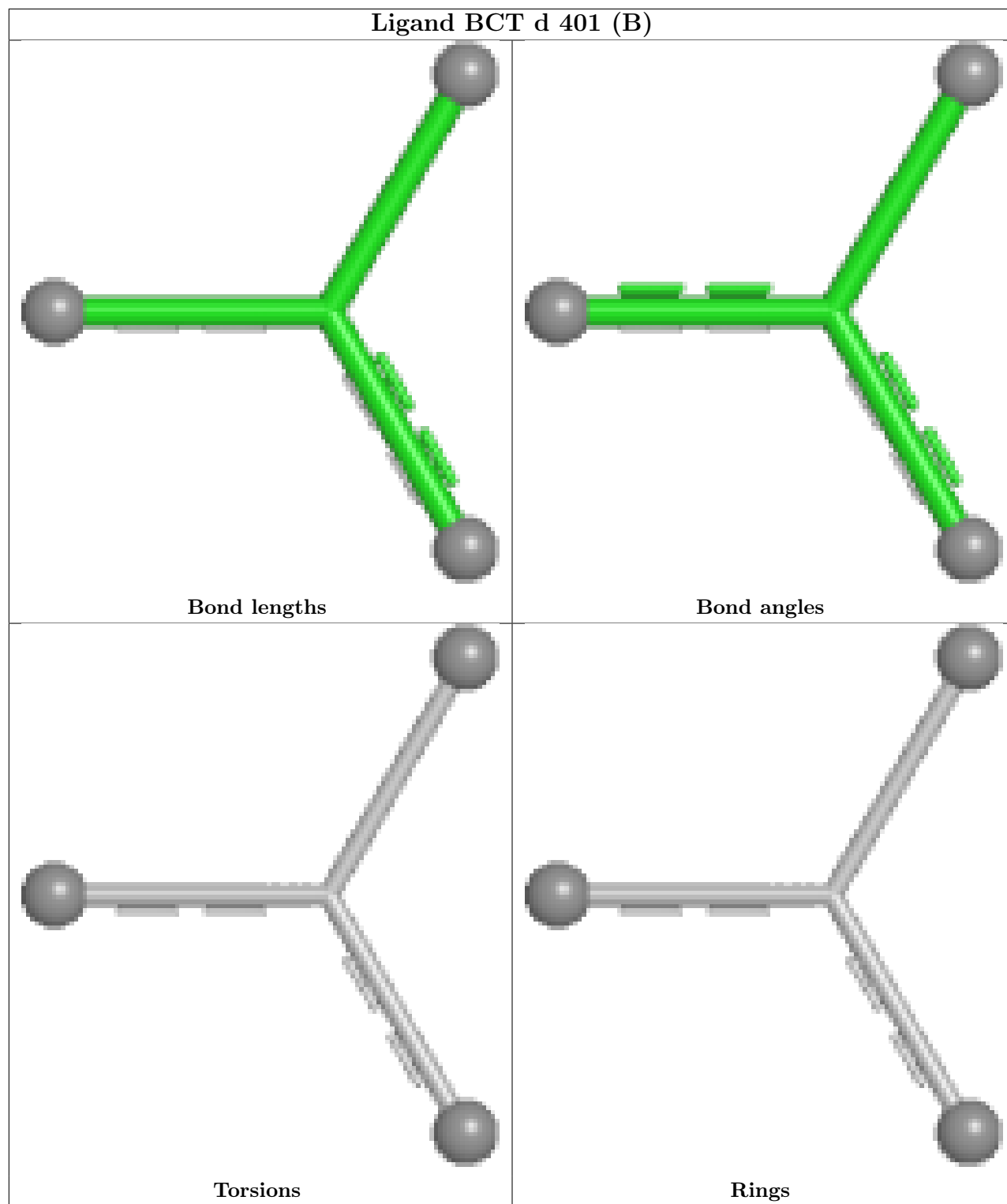


Ligand CLA a 406 (B)

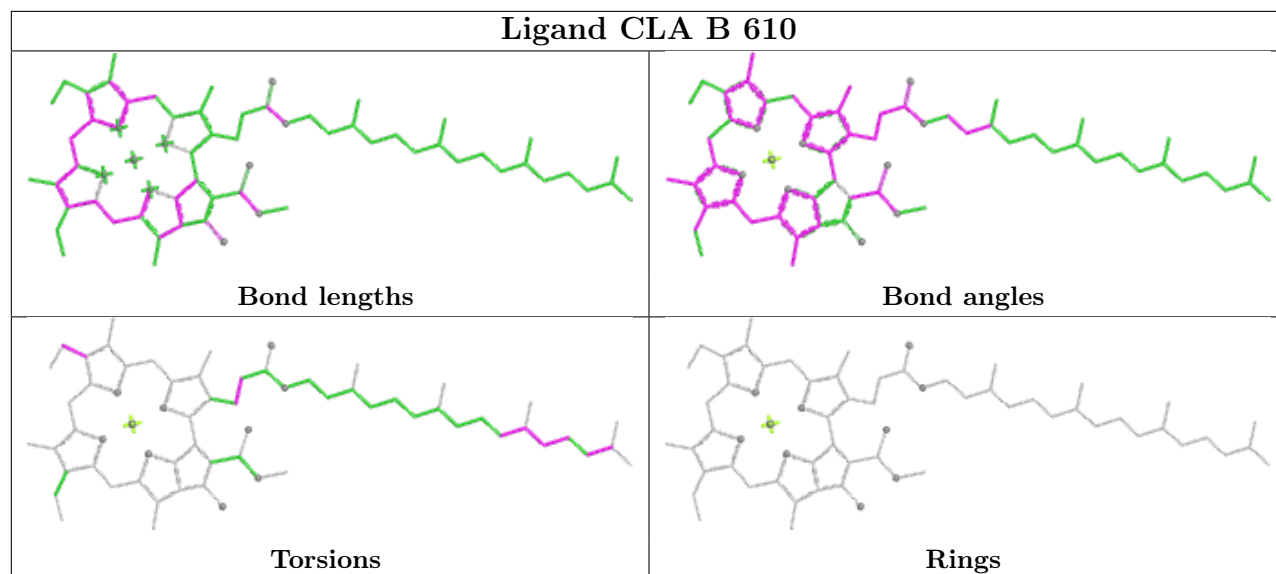


Ligand HTG V 202

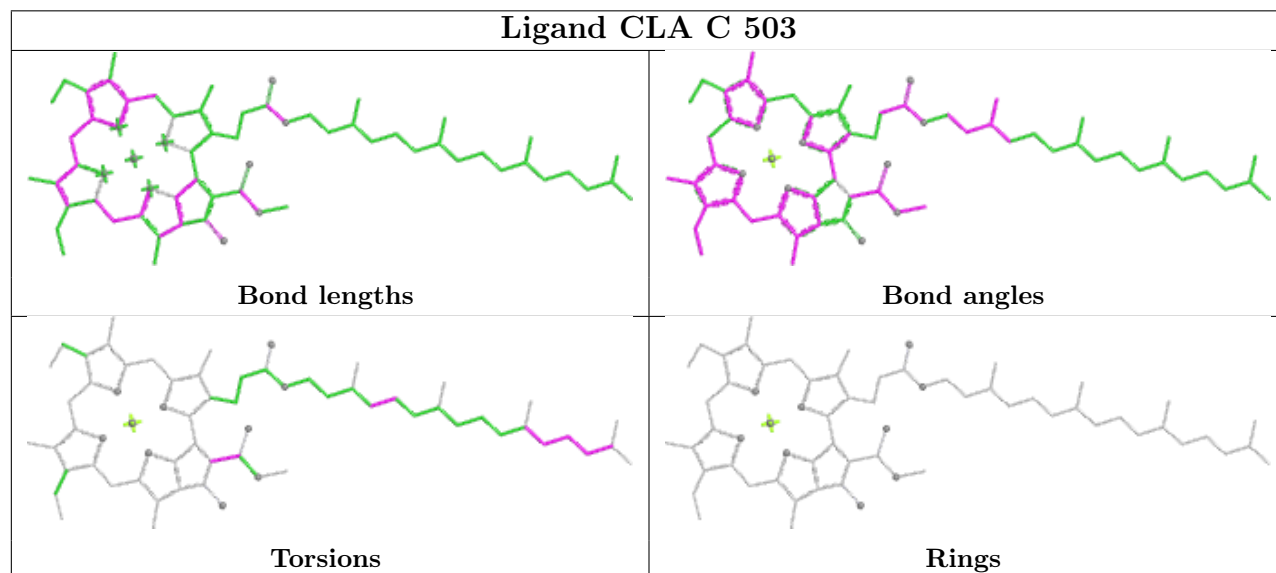




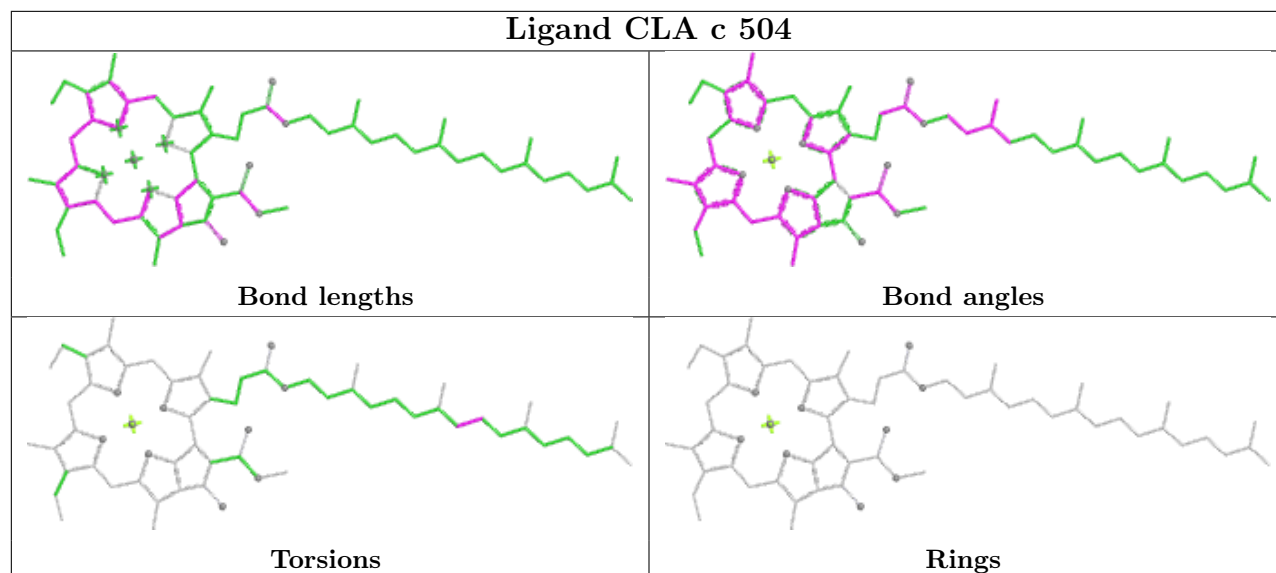
Ligand CLA B 610

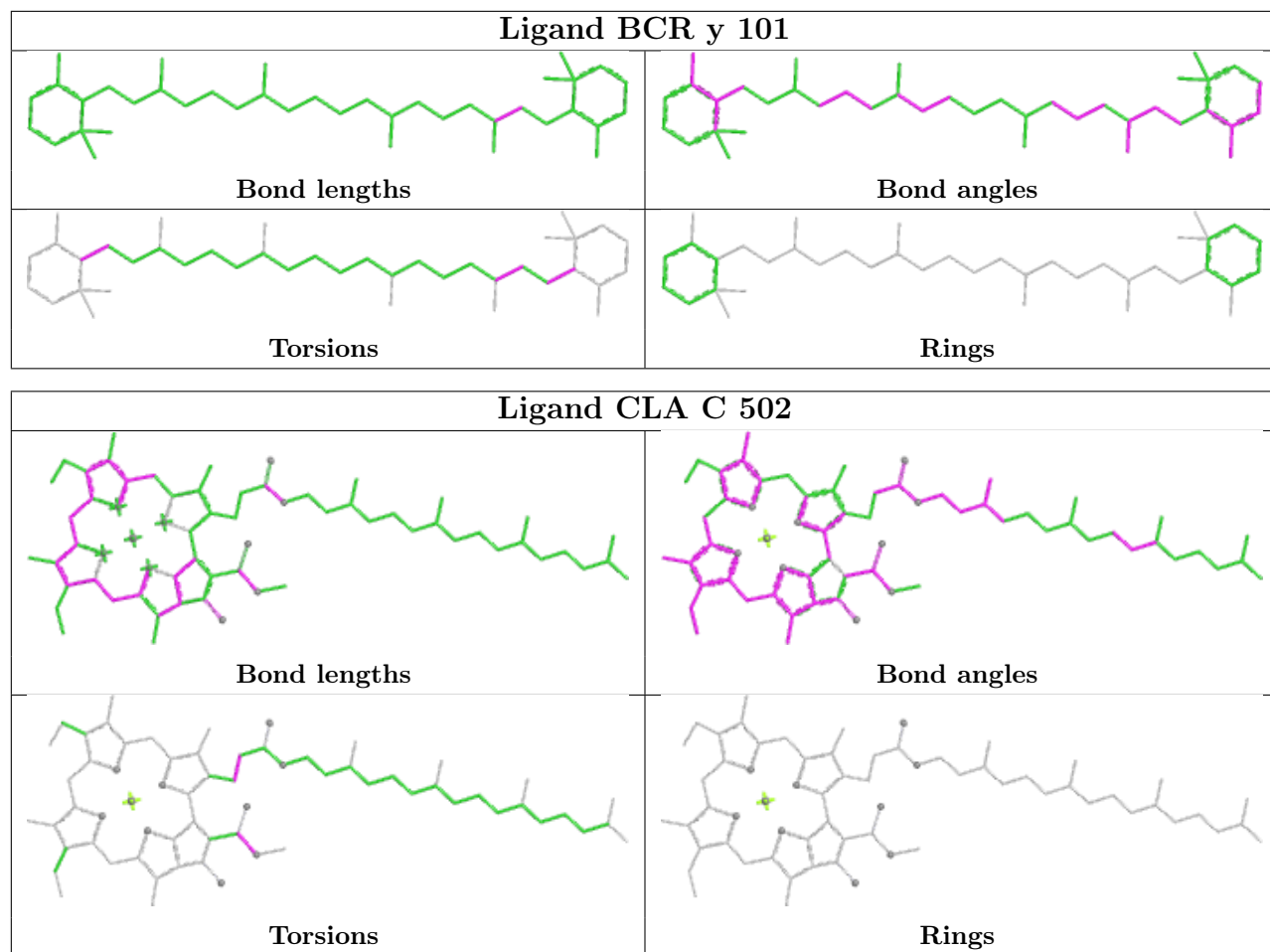


Ligand CLA C 503

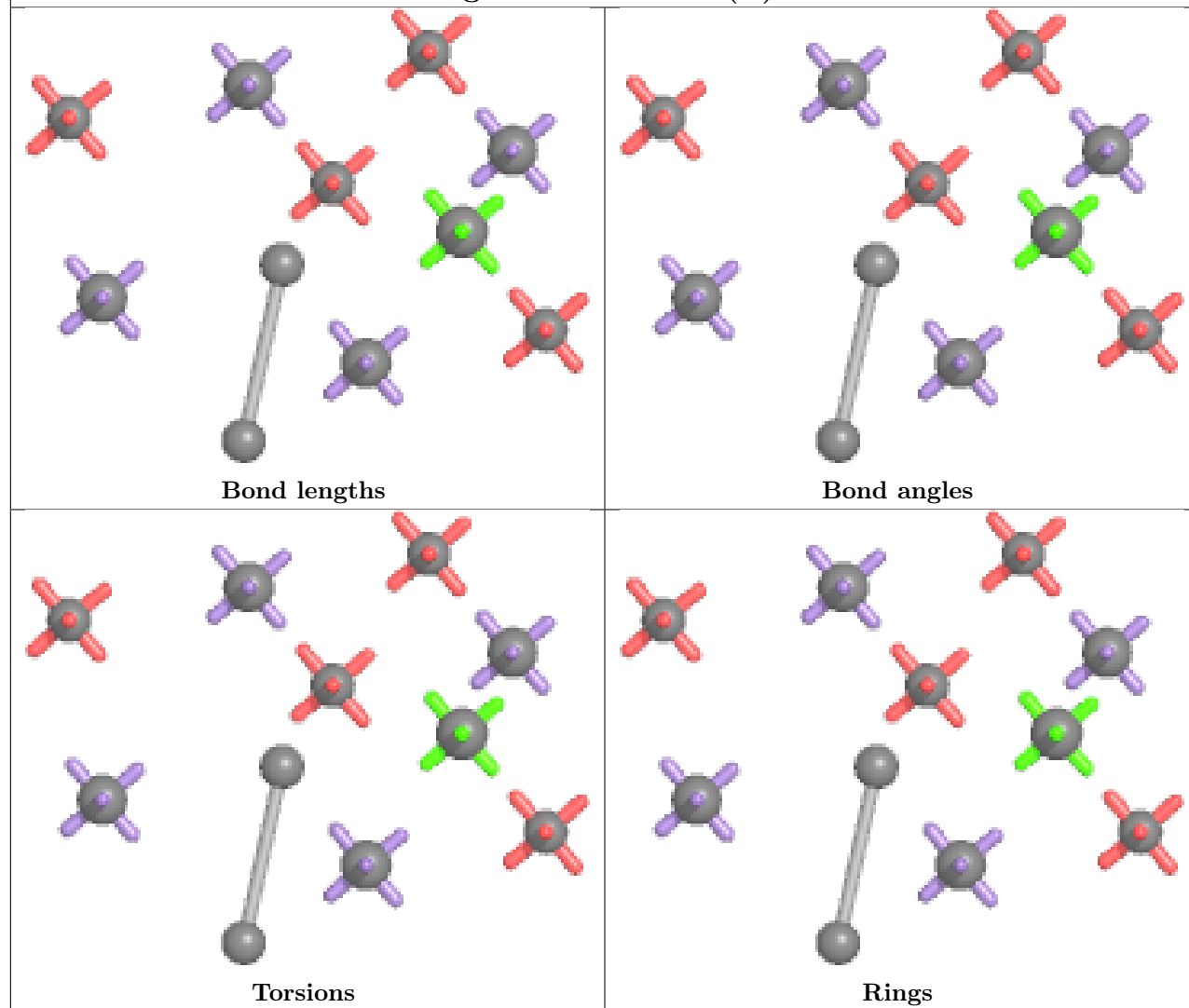


Ligand CLA c 504

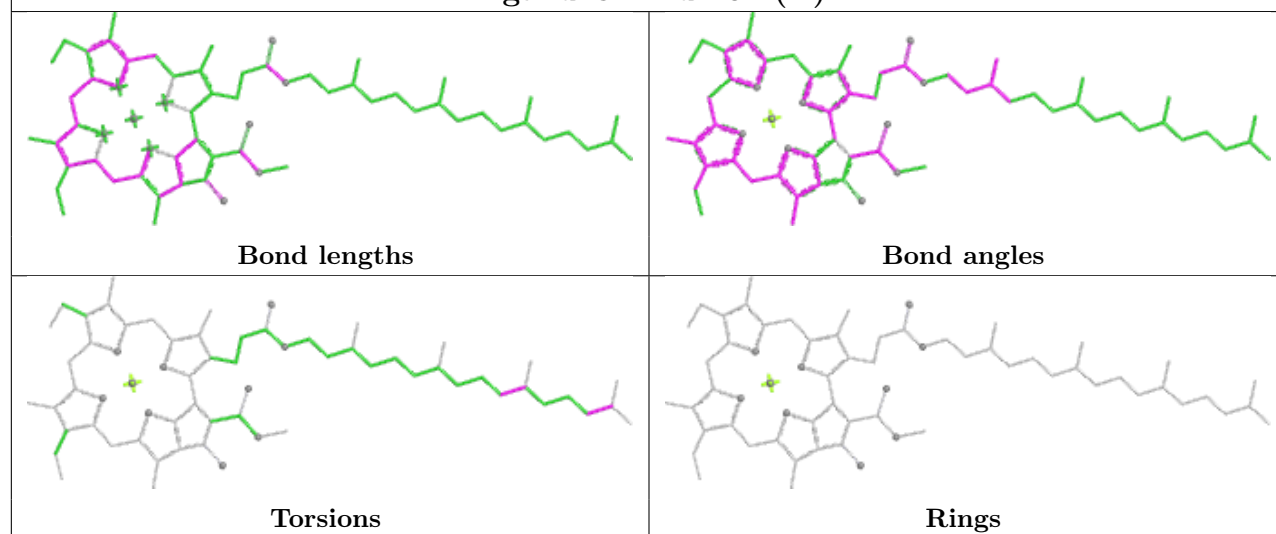


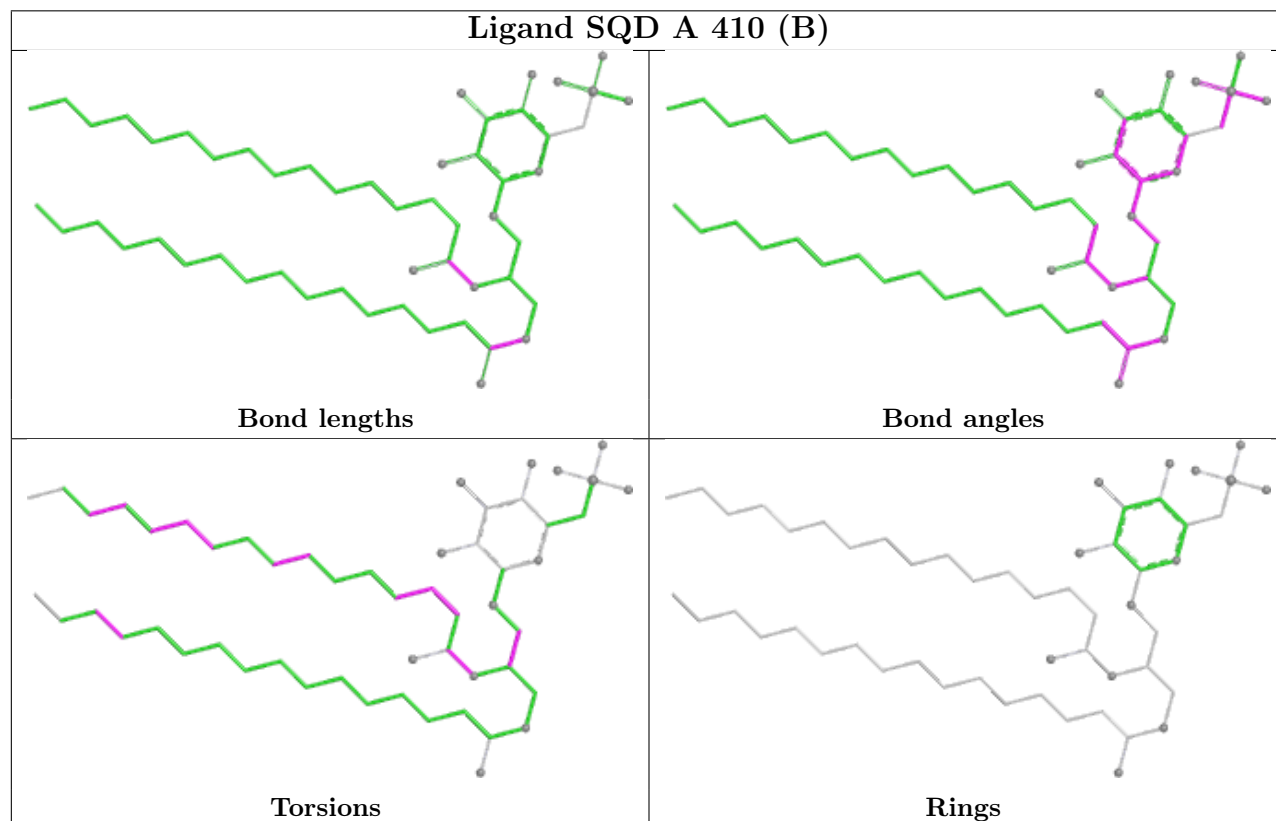
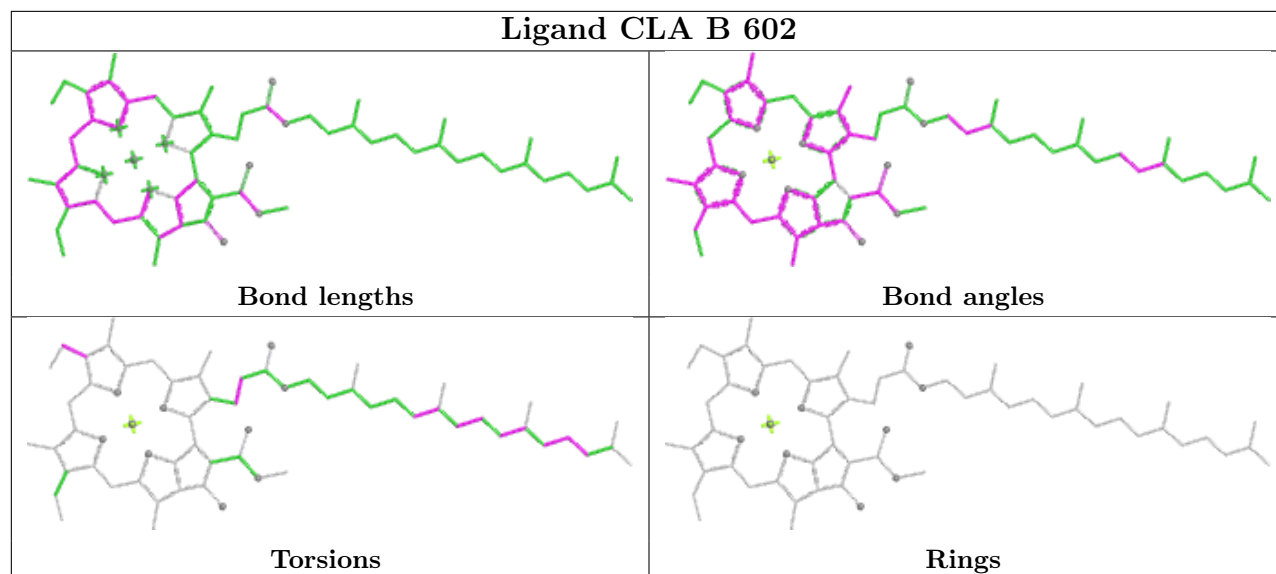


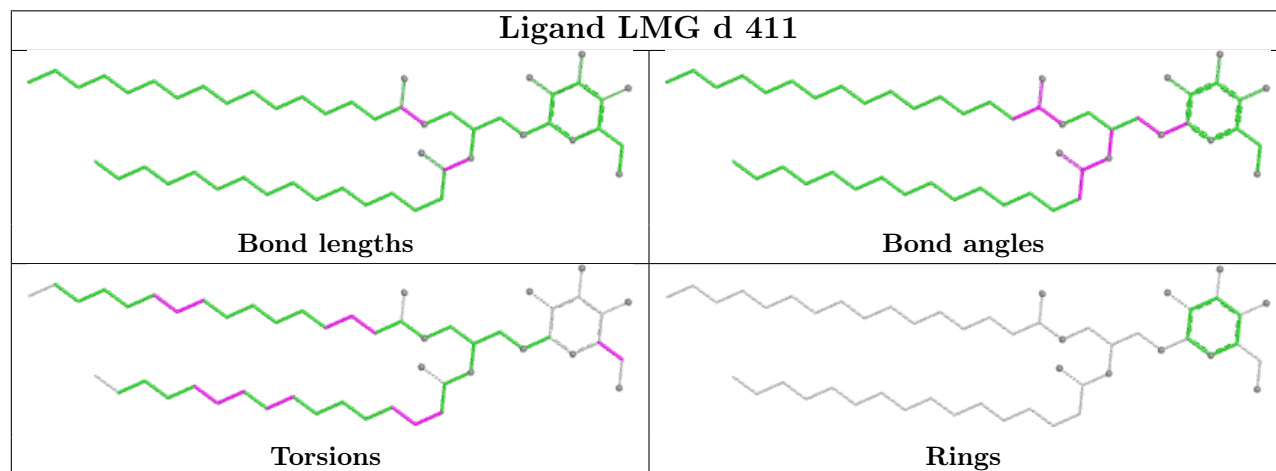
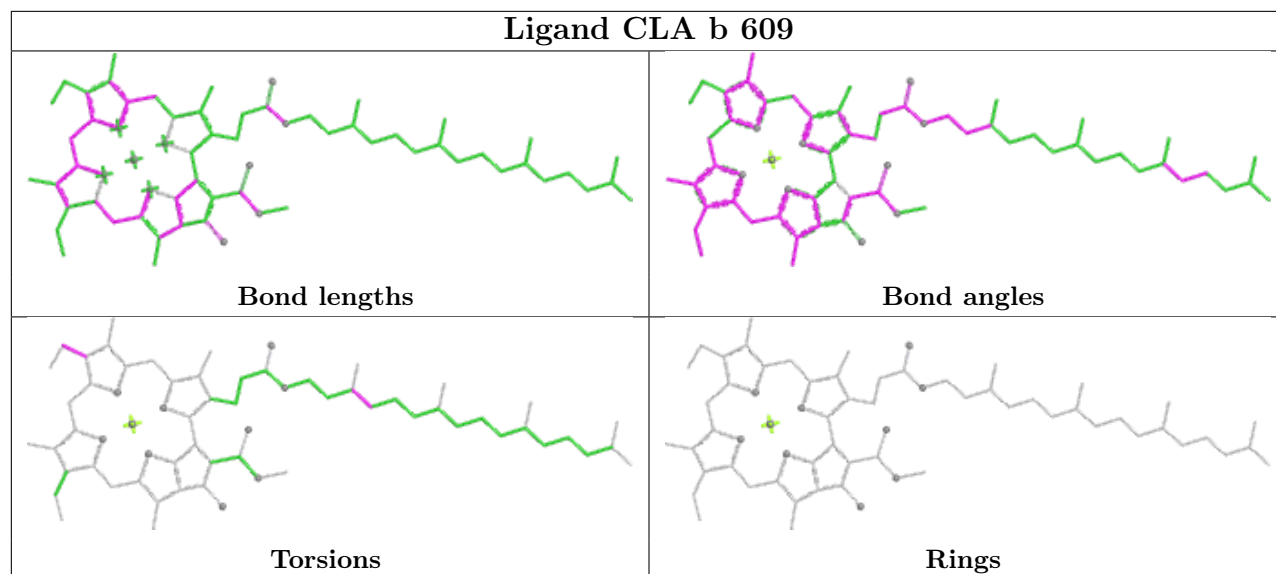
Ligand OEY A 401 (B)



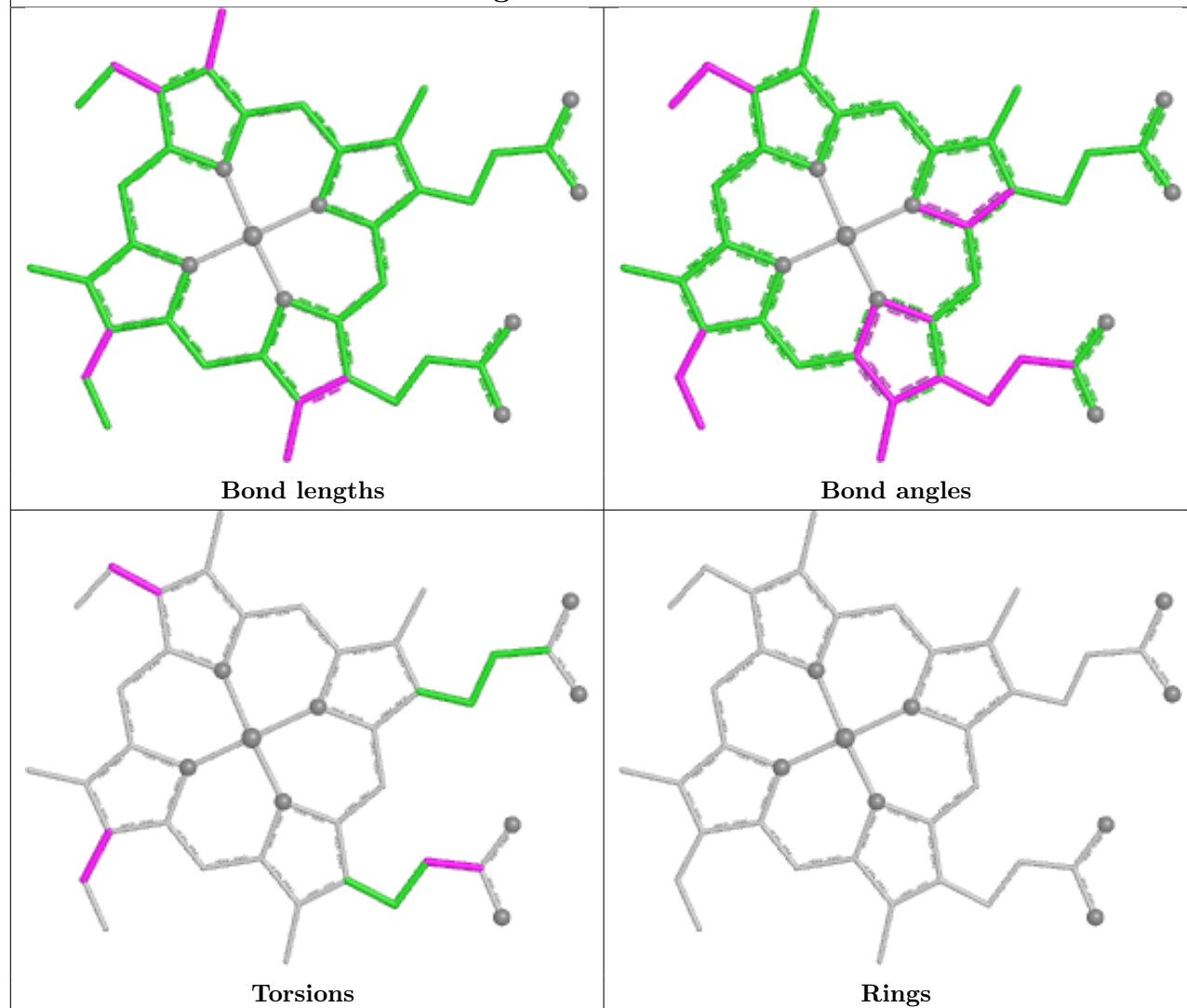
Ligand CLA d 402 (B)



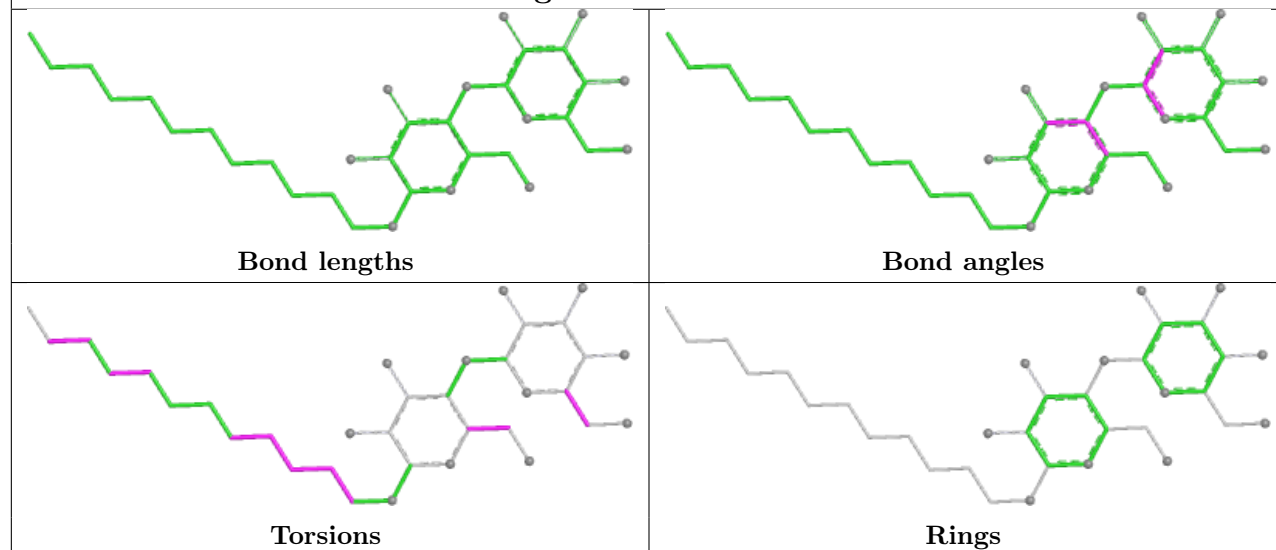


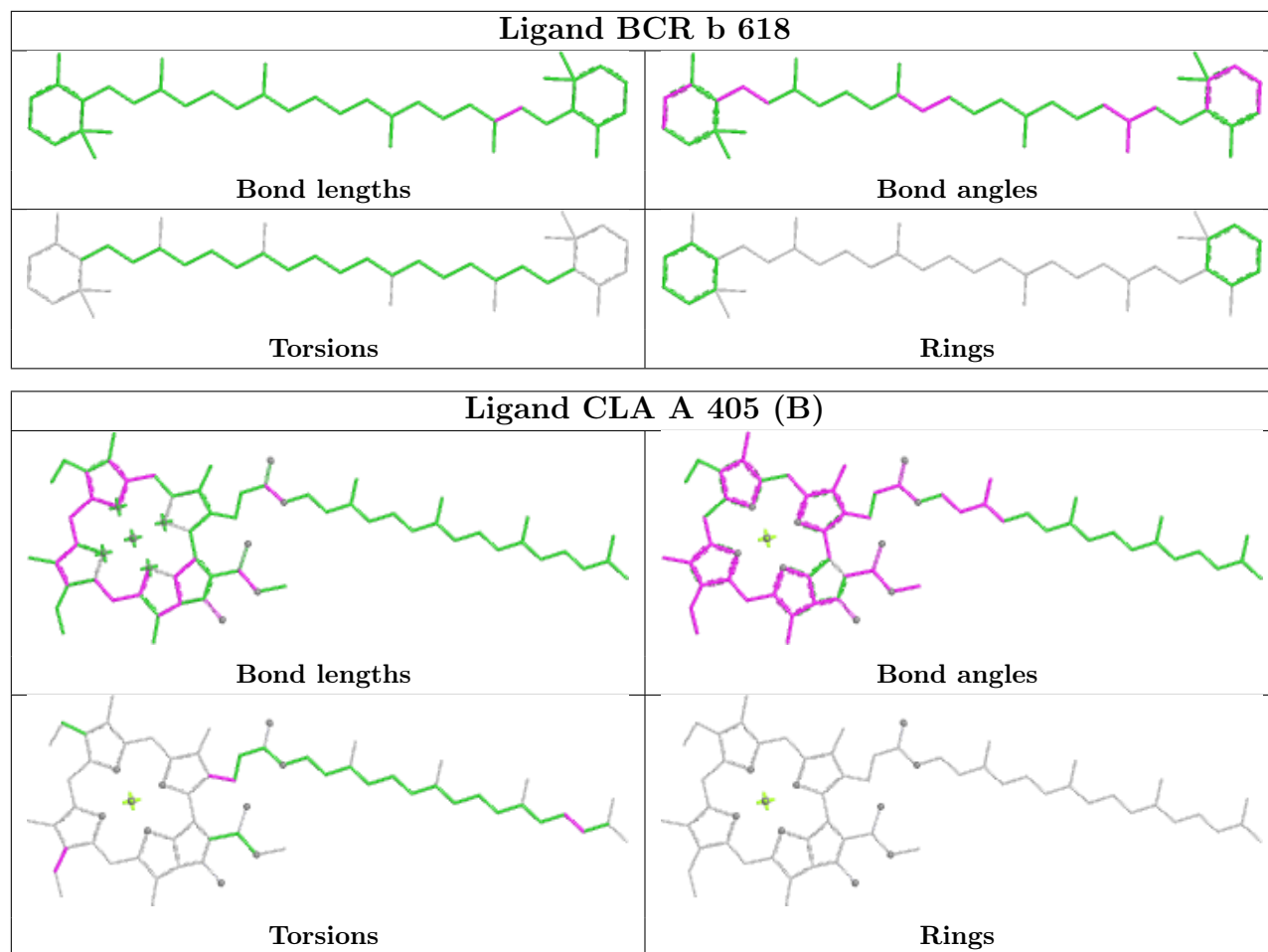


Ligand HEC V 201

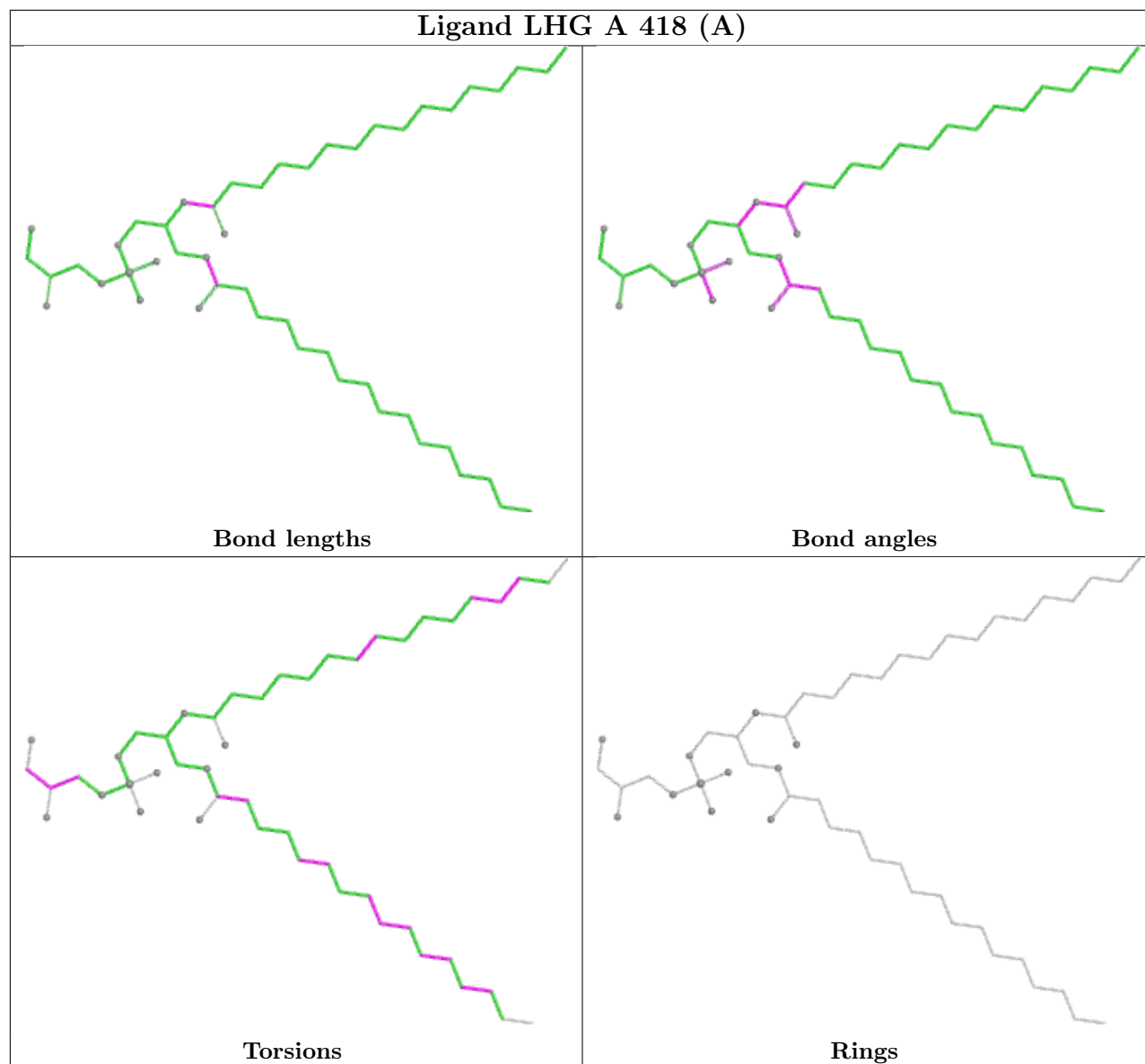


Ligand LMT c 501

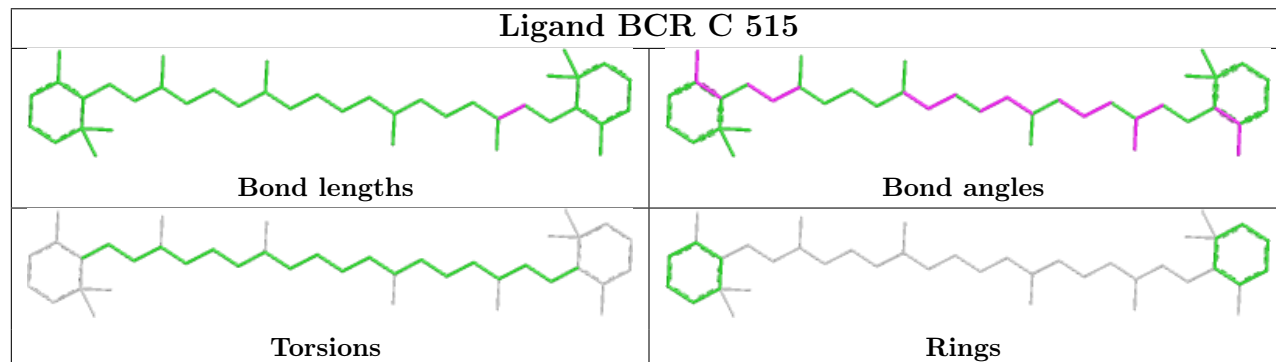


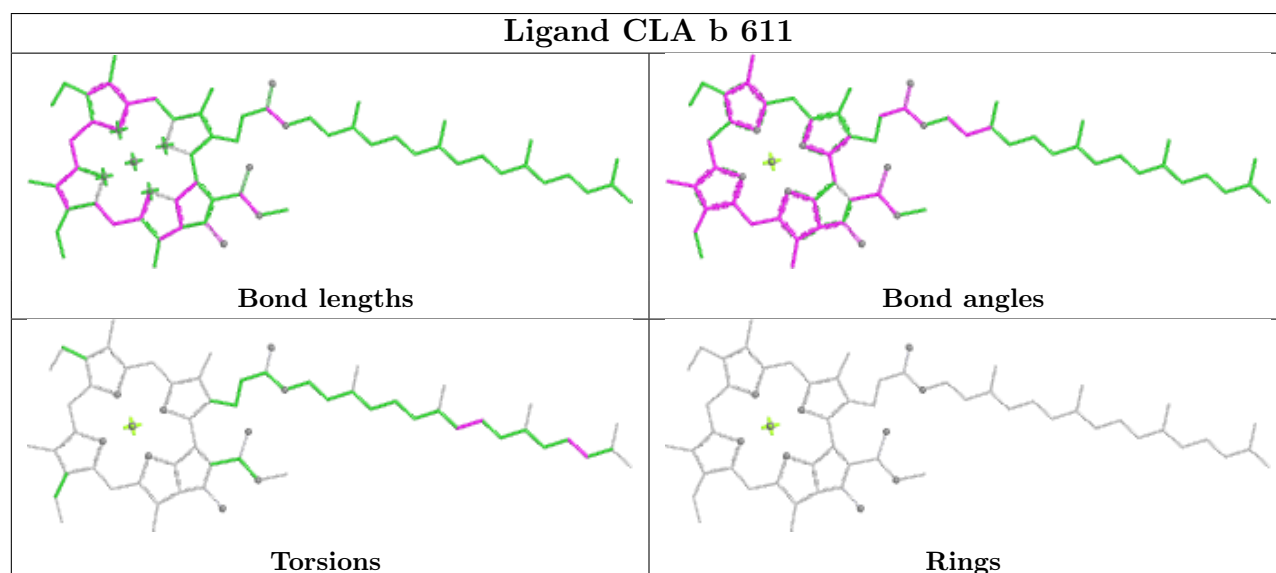
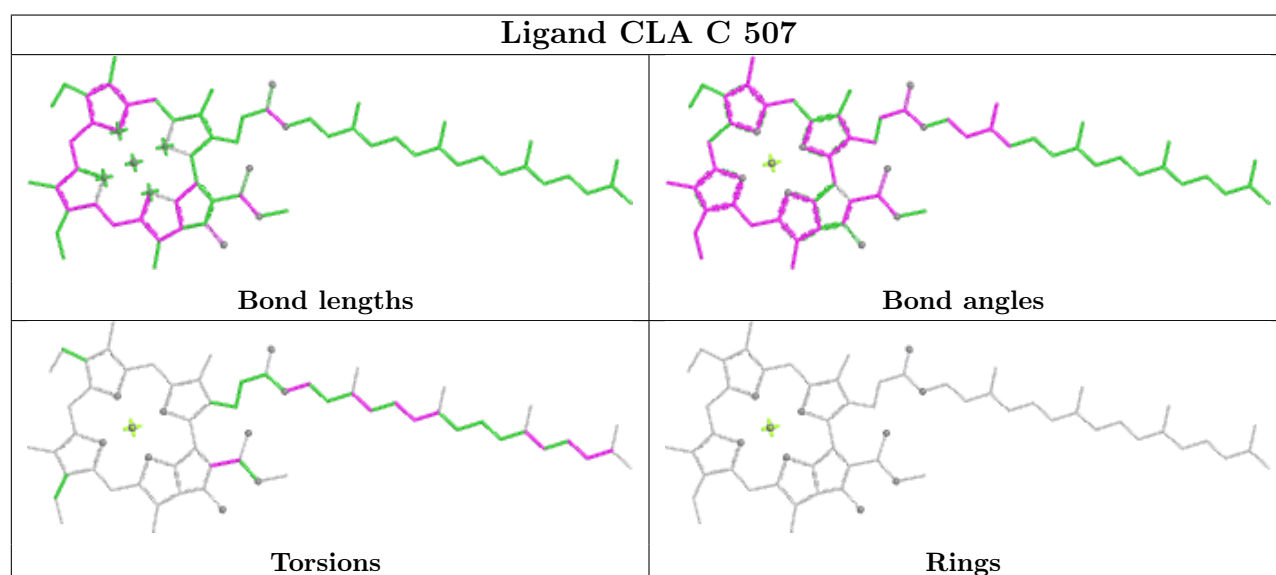
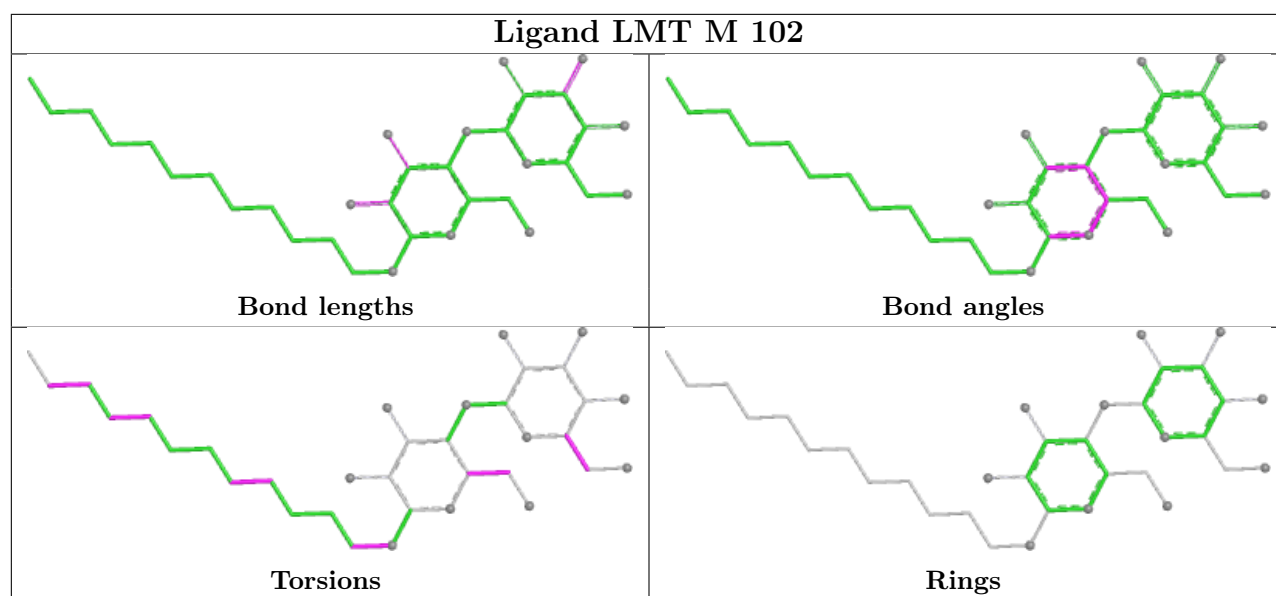


Ligand LHG A 418 (A)

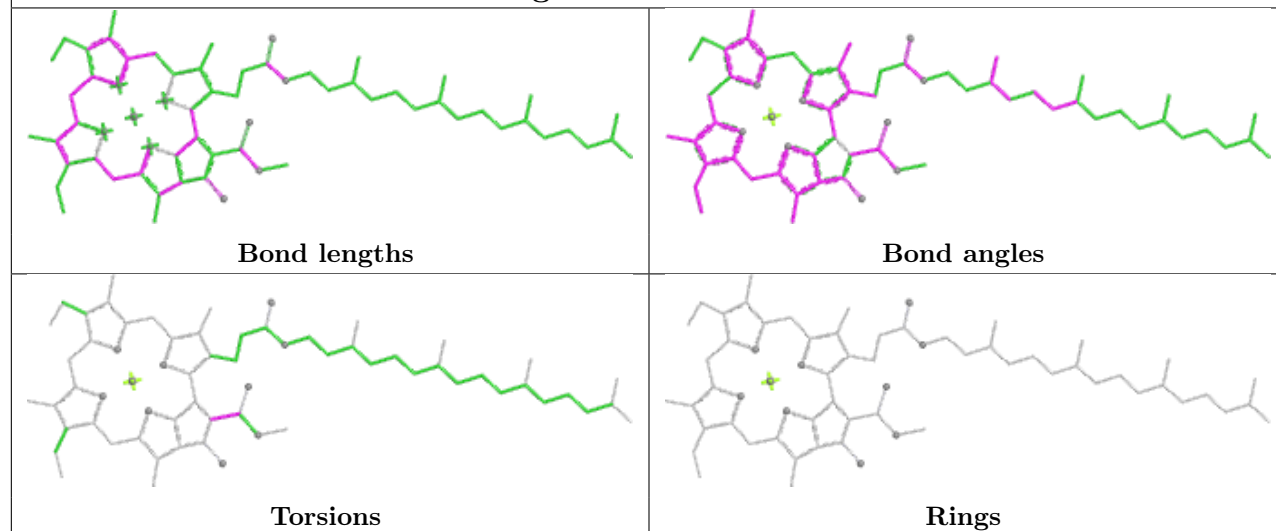


Ligand BCR C 515

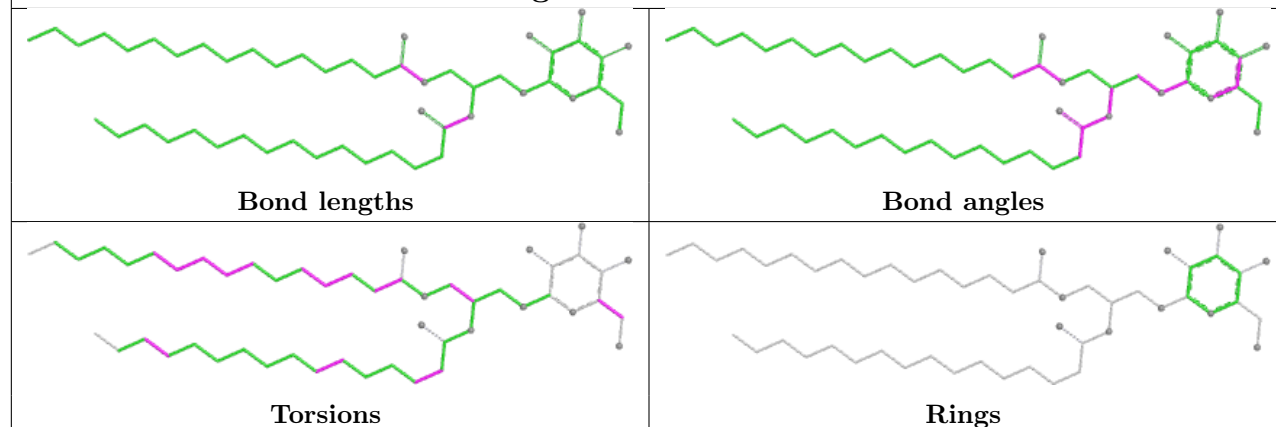




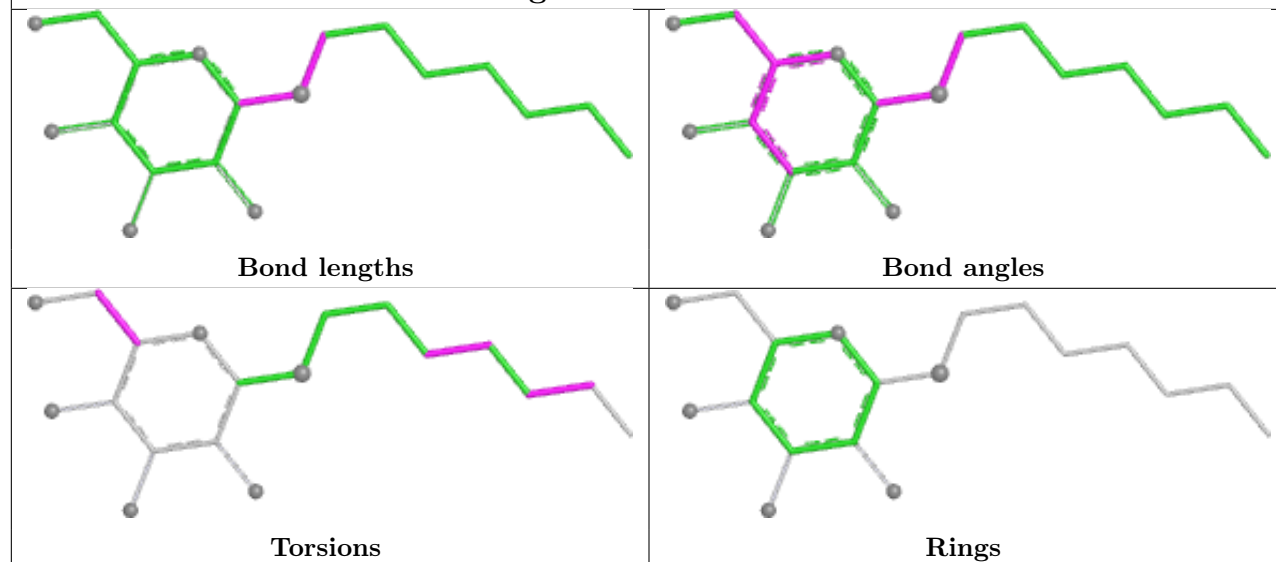
Ligand CLA B 607



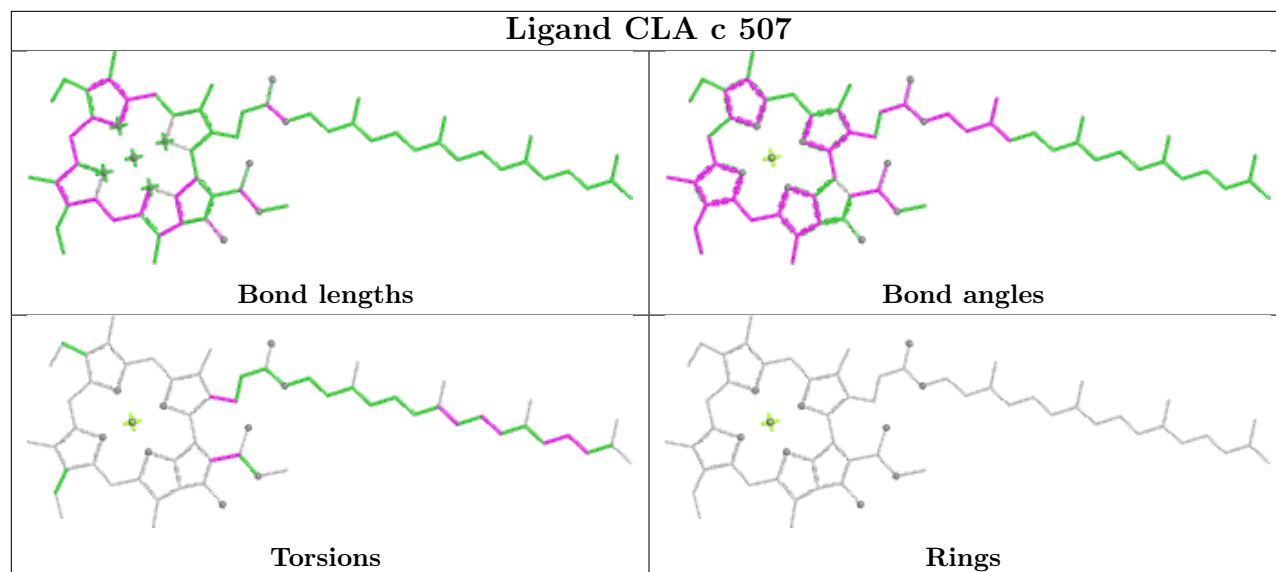
Ligand LMG a 417



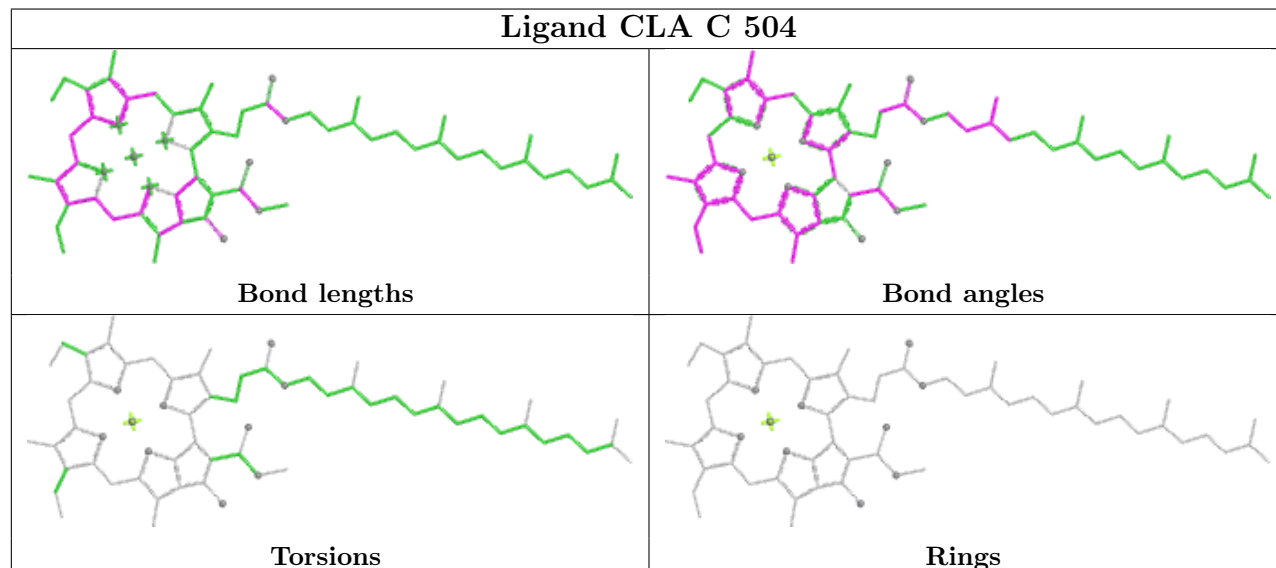
Ligand HTG B 625



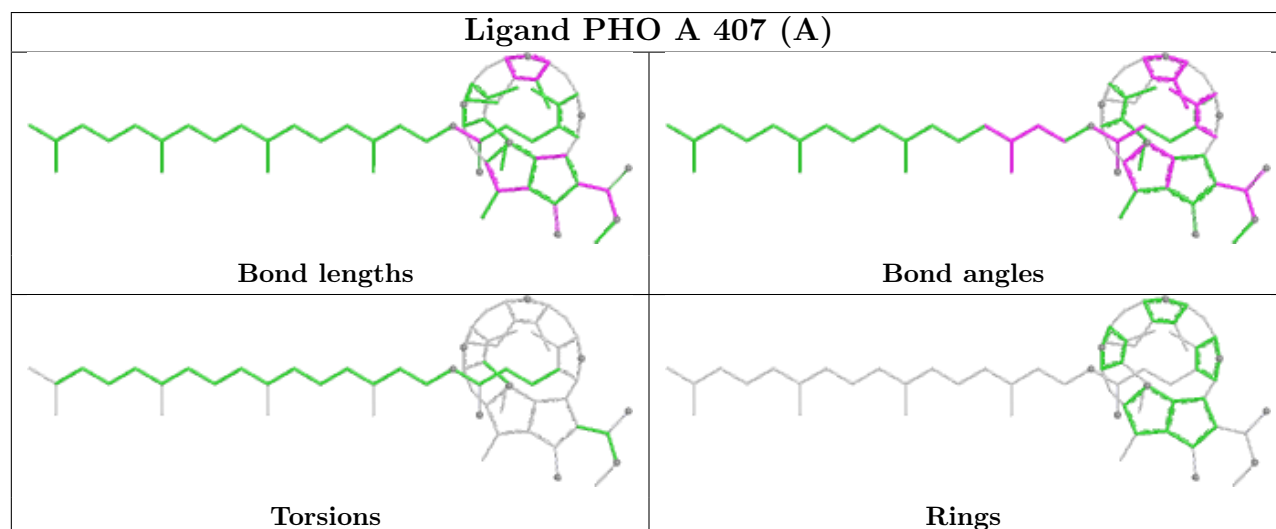
Ligand CLA c 507



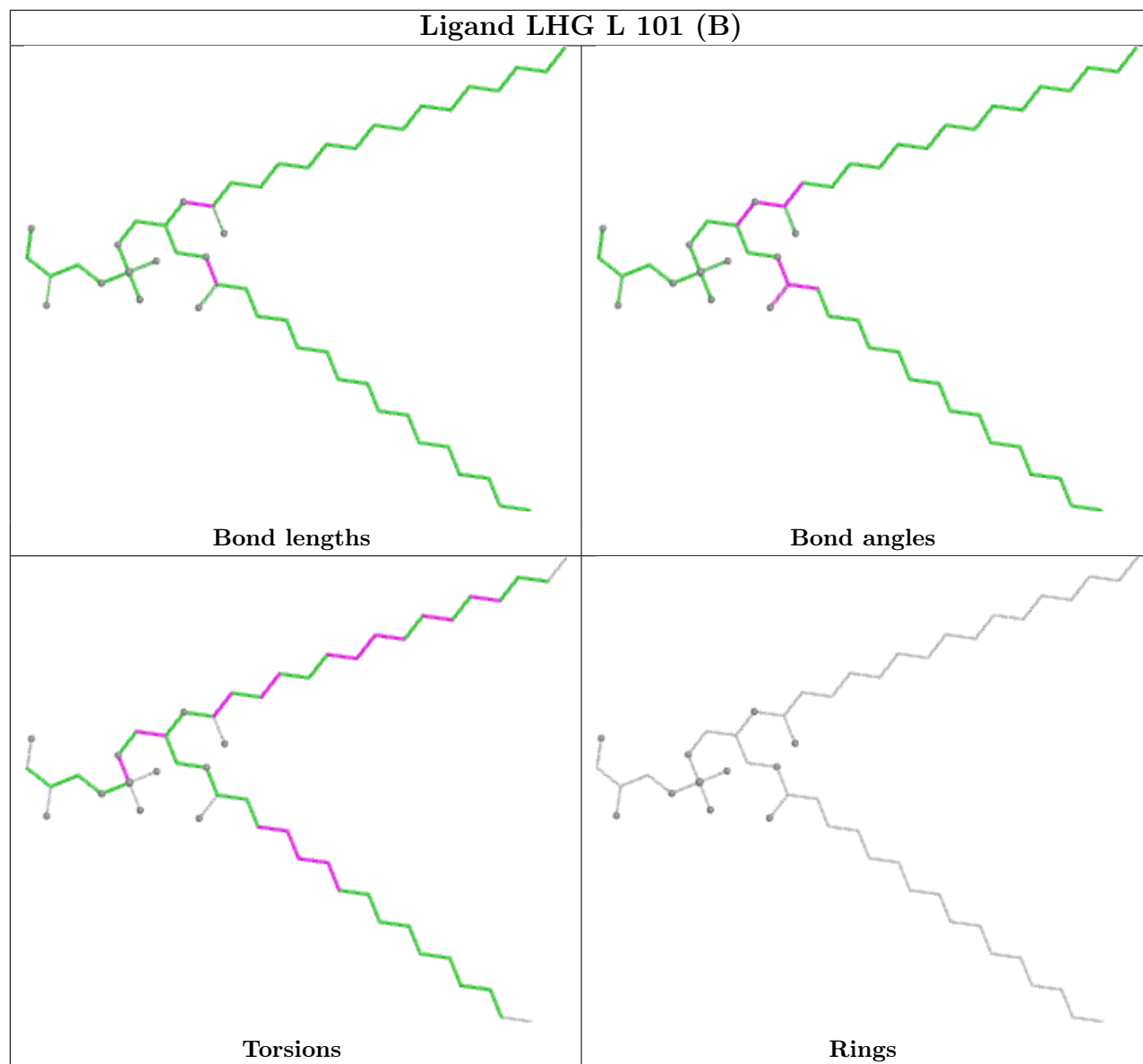
Ligand CLA C 504



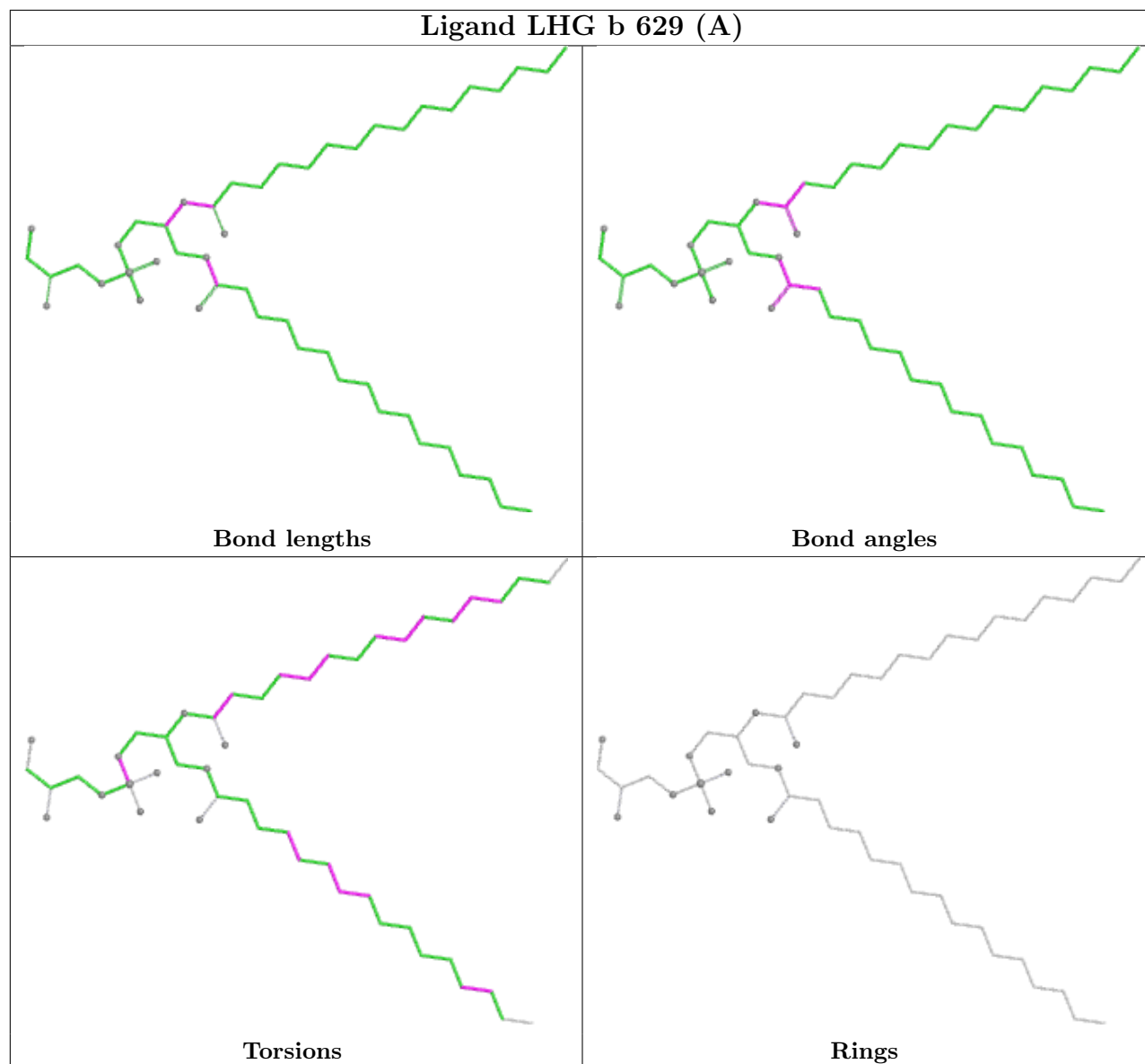
Ligand PHO A 407 (A)



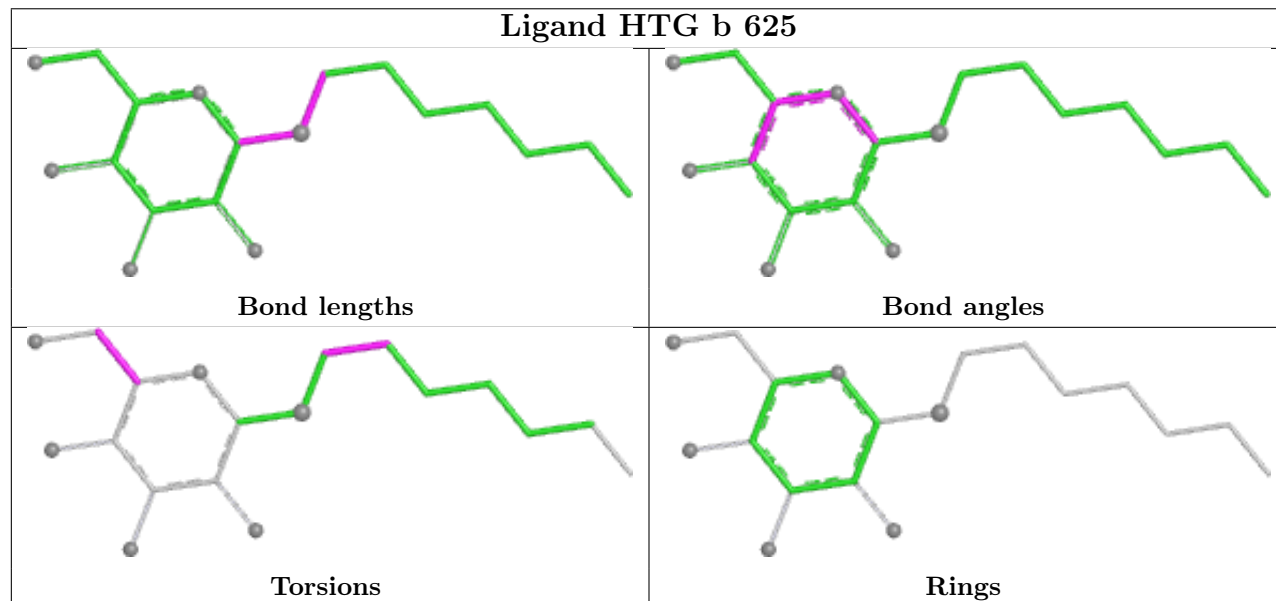
Ligand OEX A 413 (A)	
Bond lengths	Bond angles
Torsions	Rings
Ligand PL9 d 405 (A)	
Bond lengths	Bond angles
Torsions	Rings

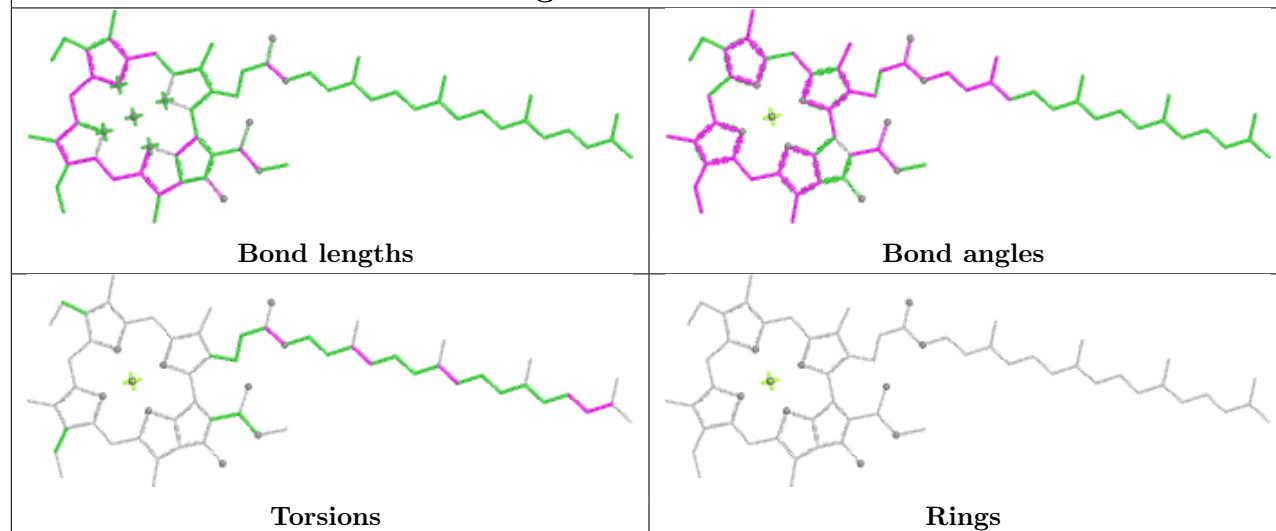
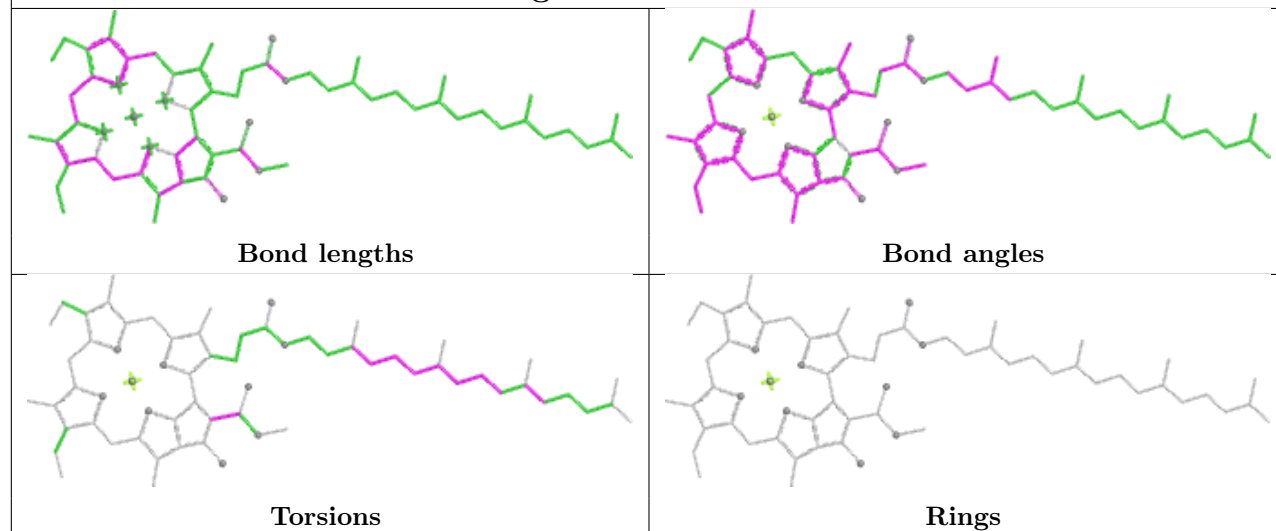


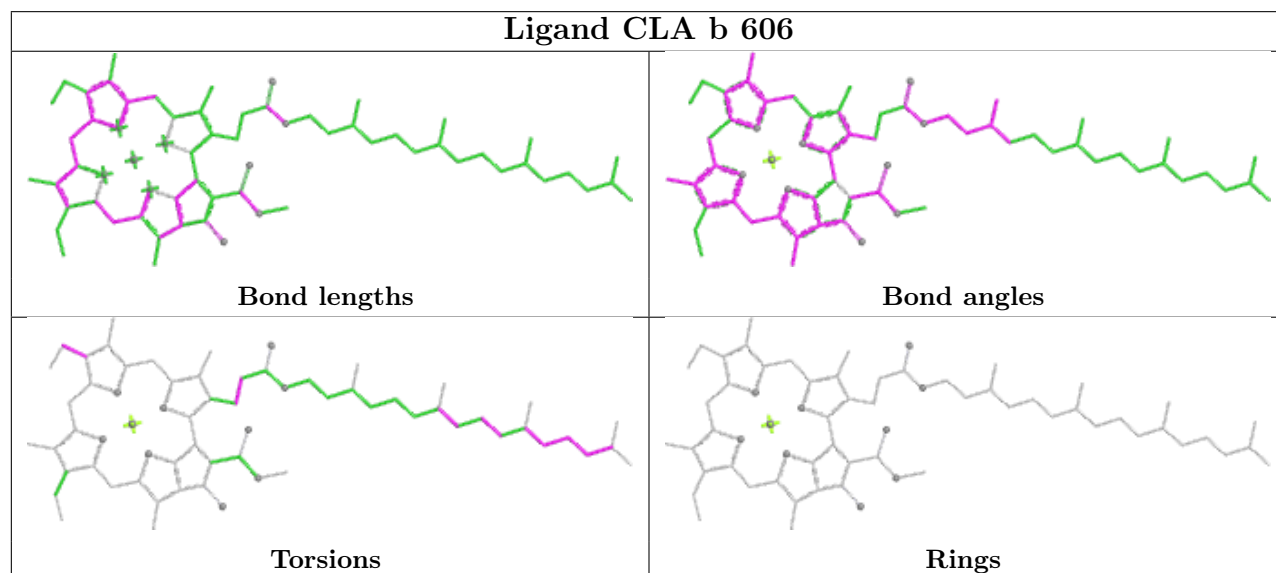
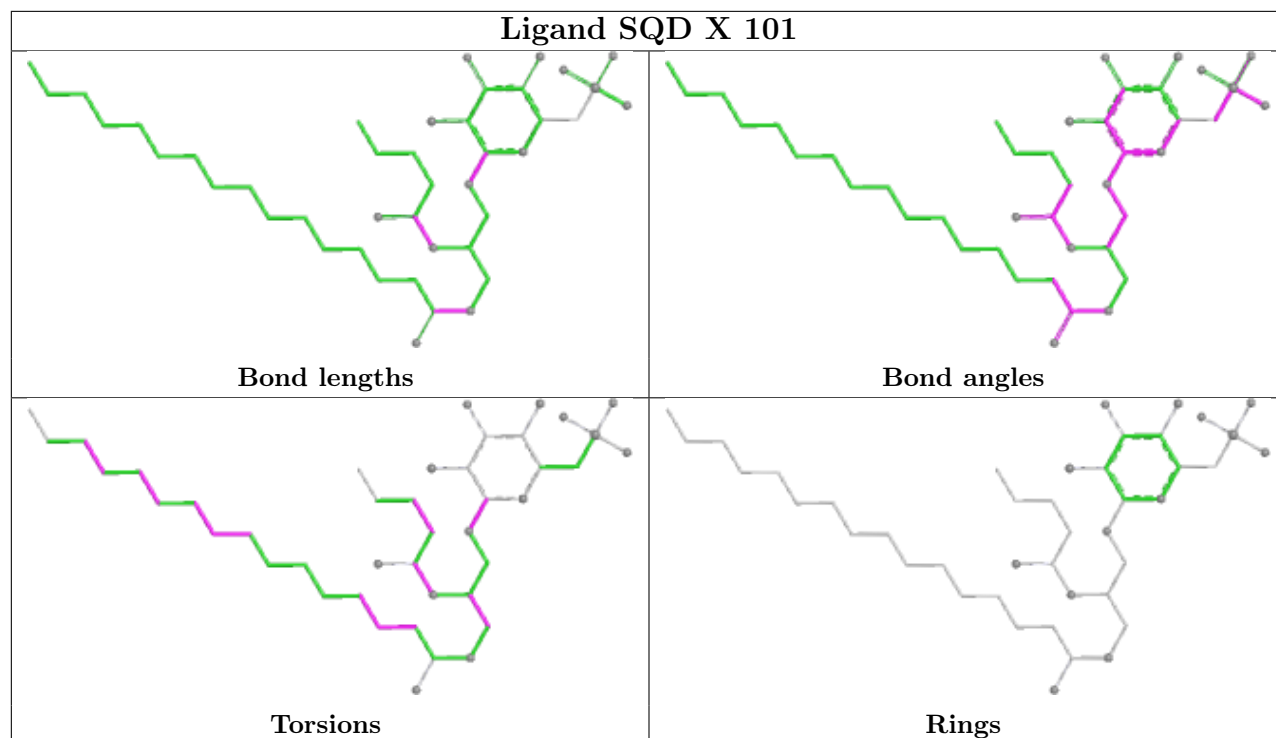
Ligand LHG b 629 (A)

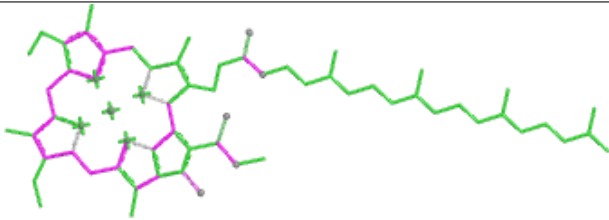
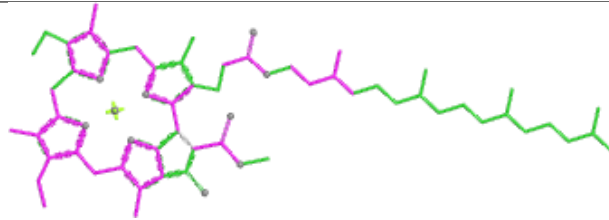
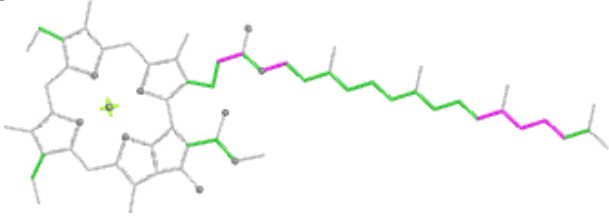
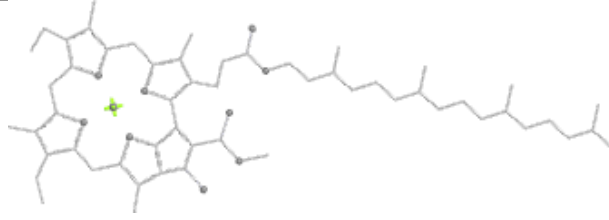


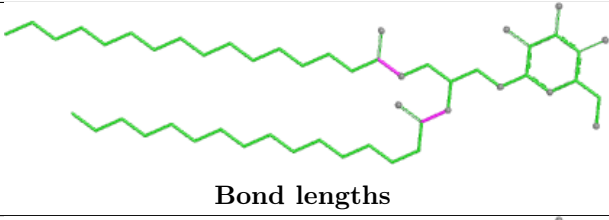
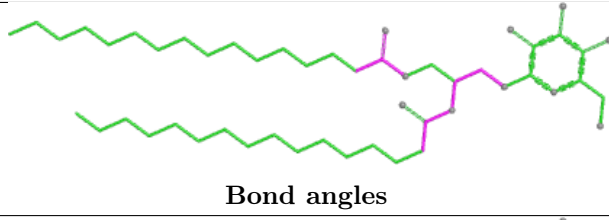
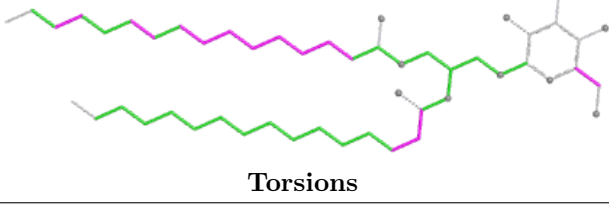
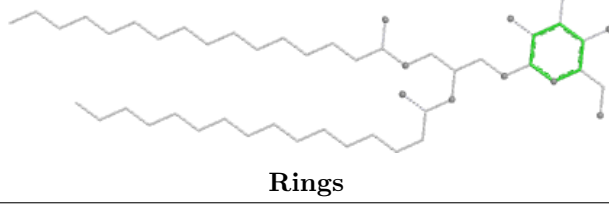
Ligand HTG b 625

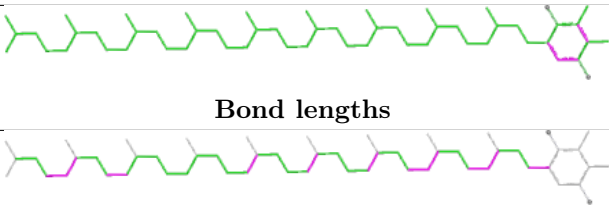
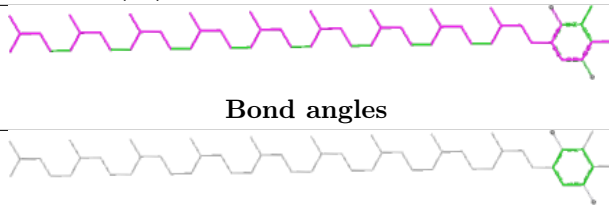
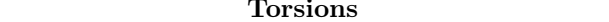
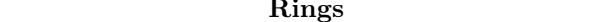


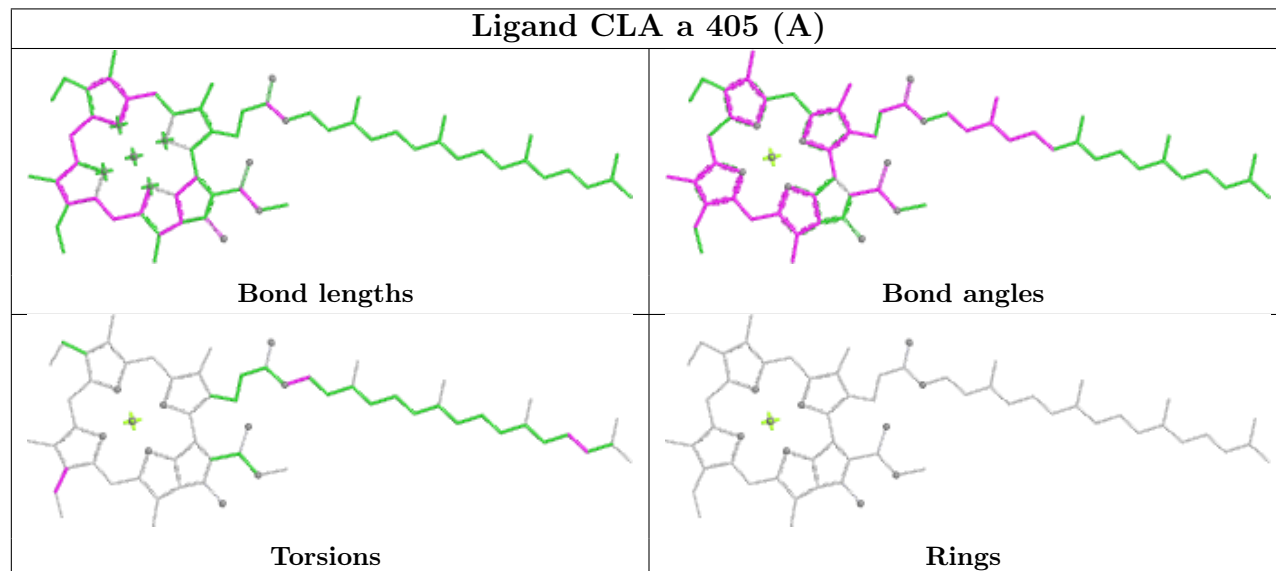
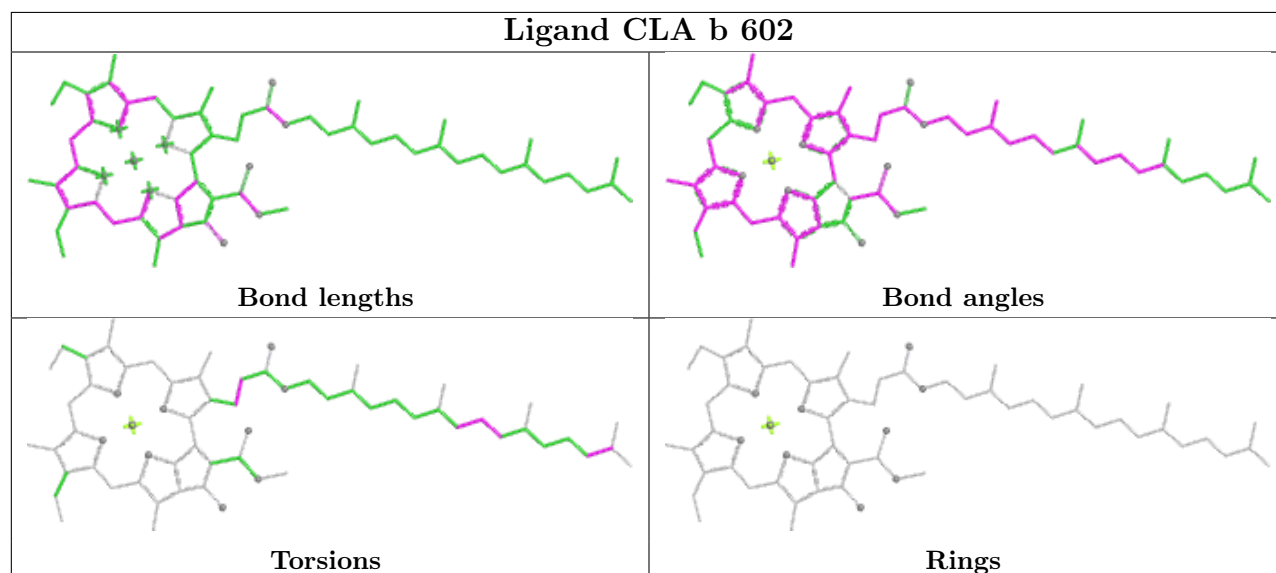
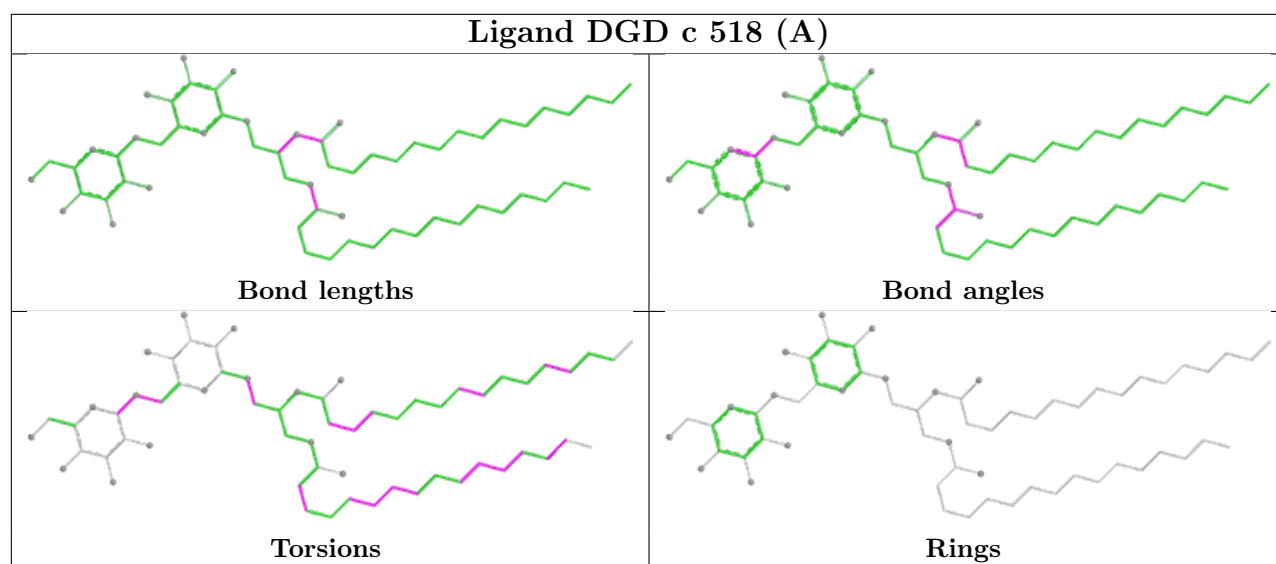
Ligand CLA a 409**Ligand CLA B 614**

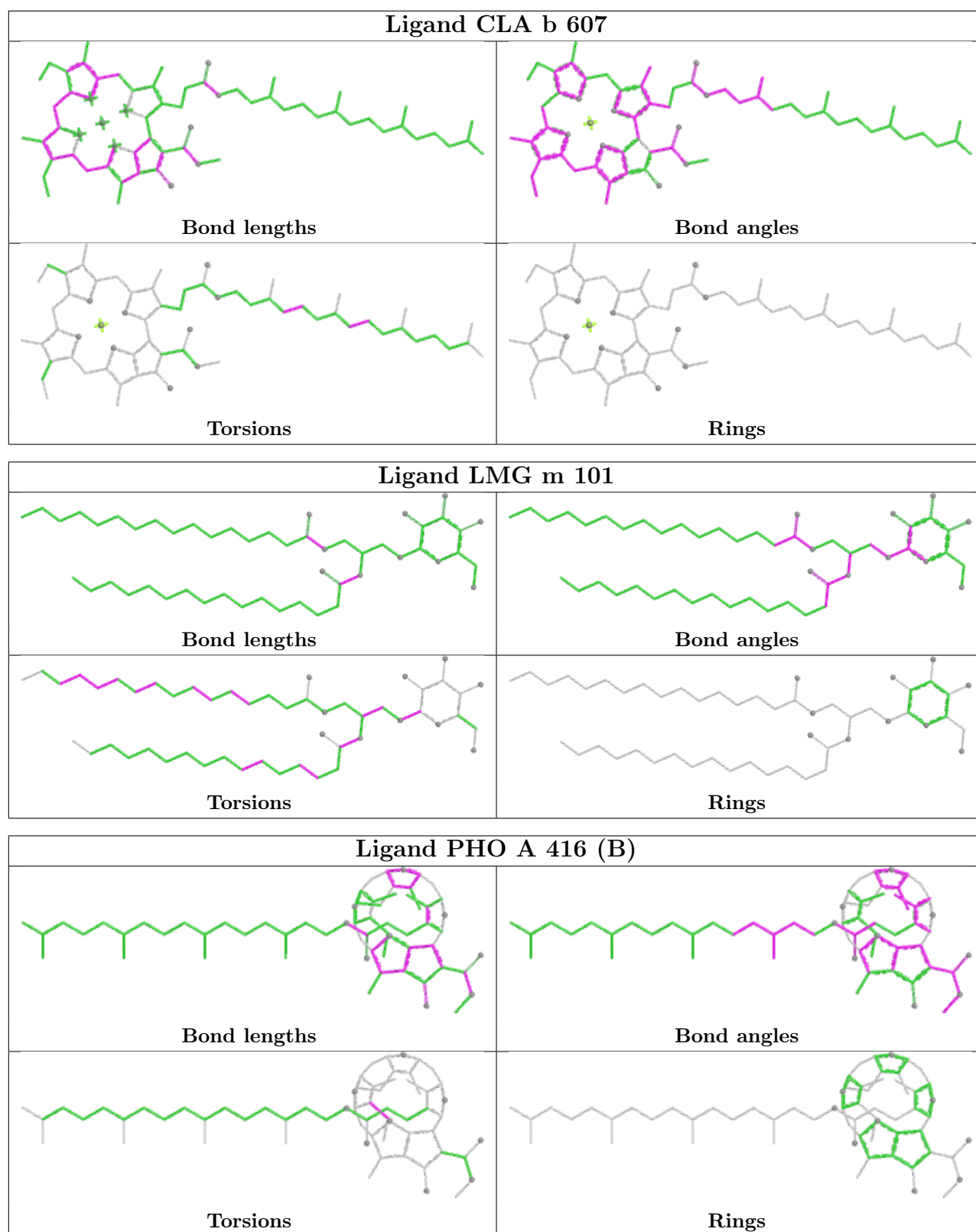


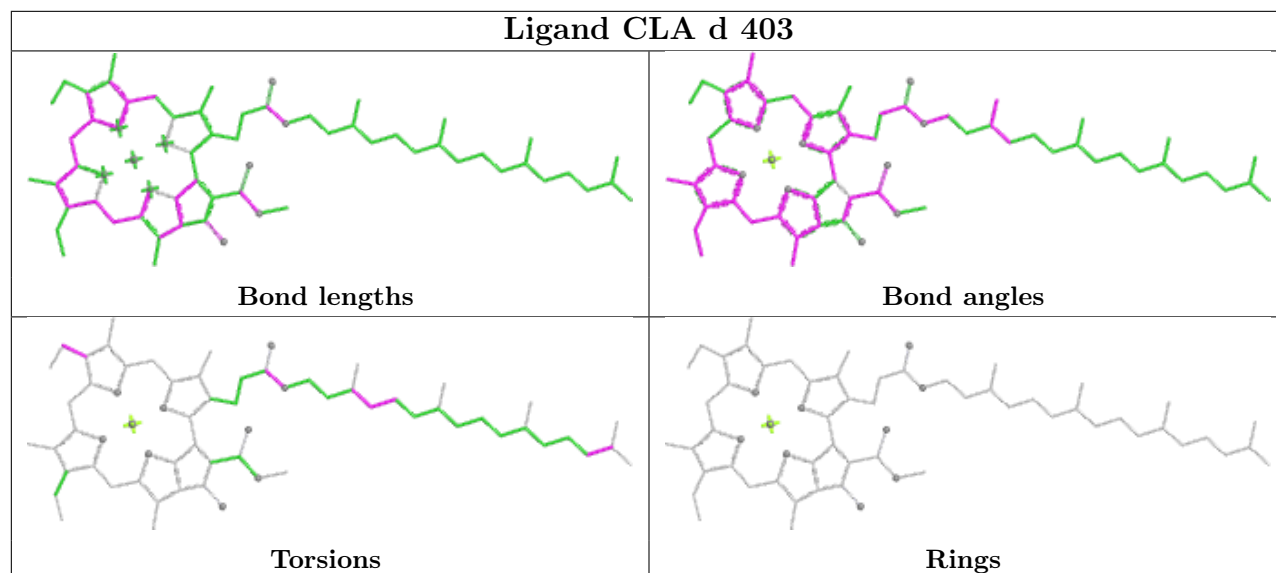
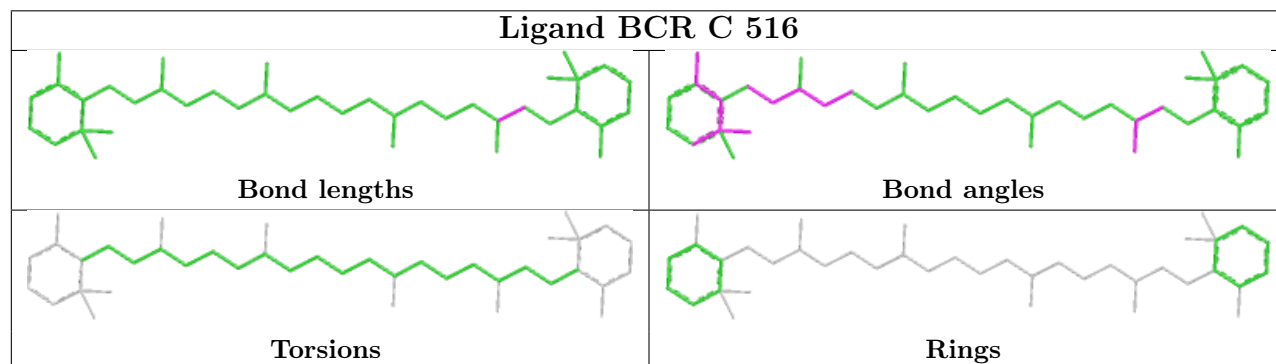
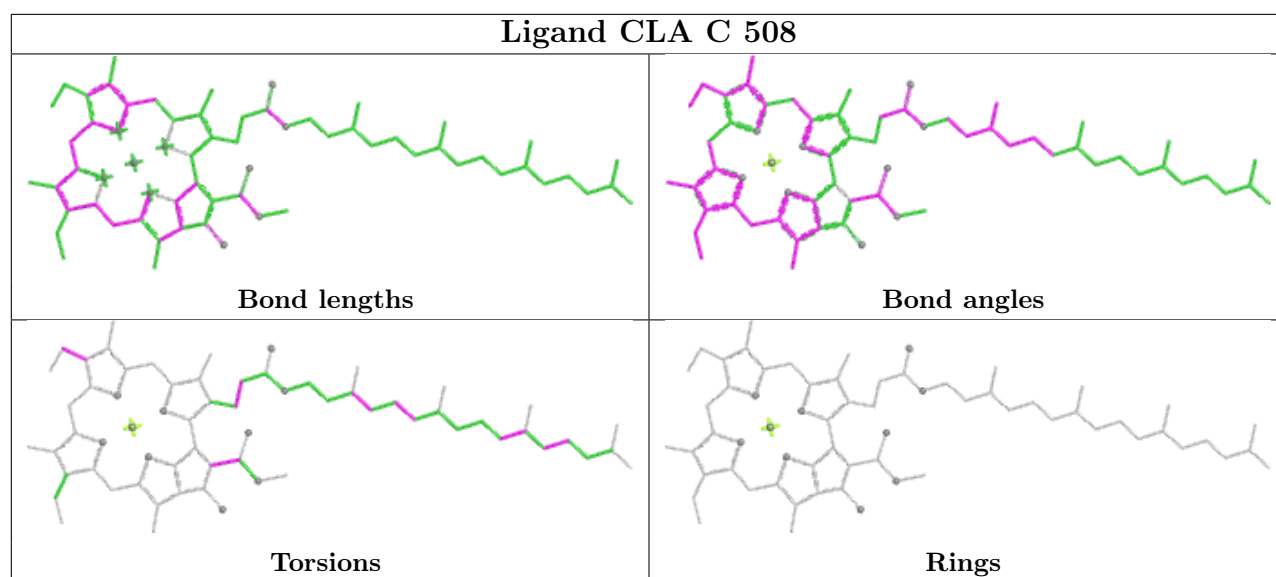
Ligand CLA B 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LMG c 520	
	
Bond lengths	Bond angles
	
Torsions	Rings

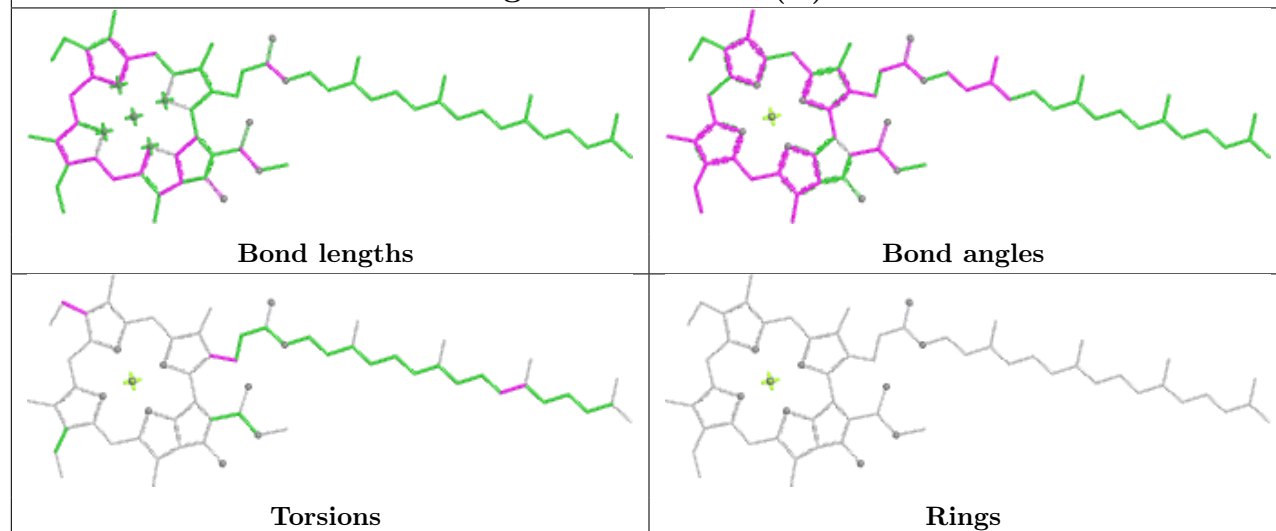
Ligand PL9 A 414 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings



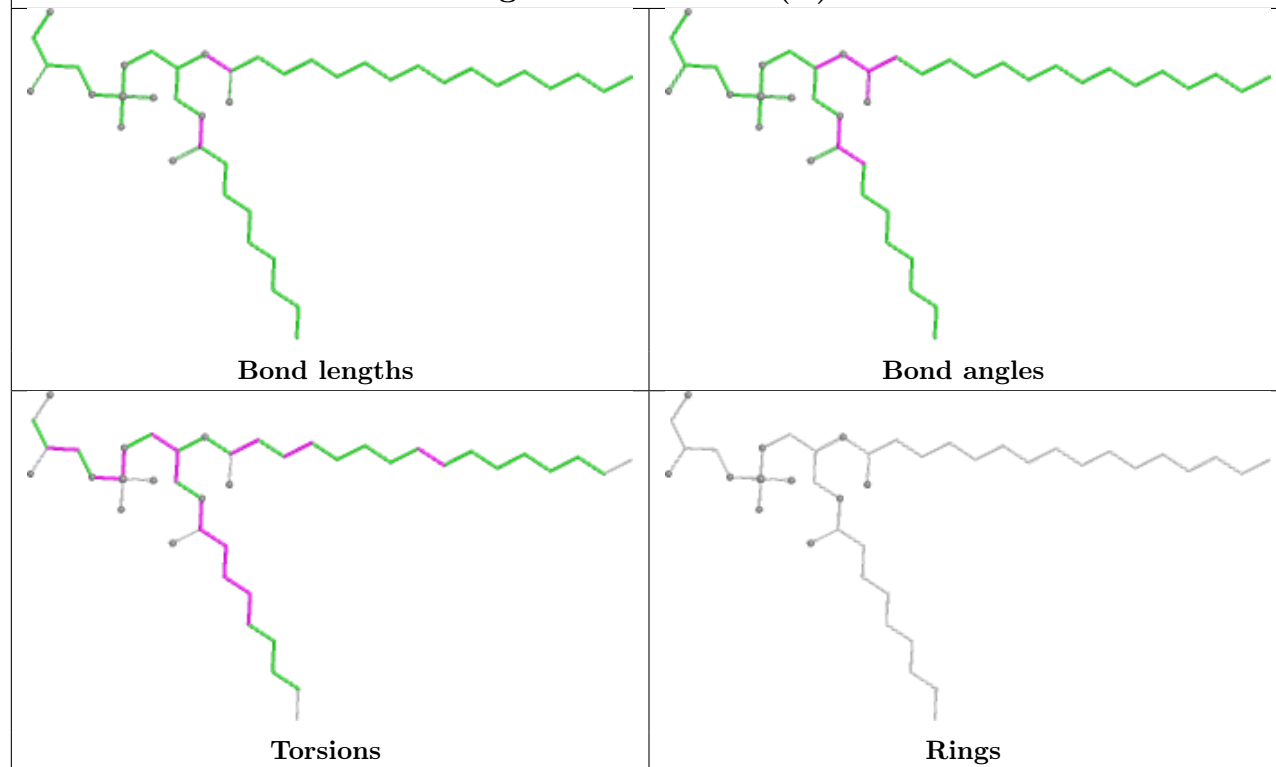


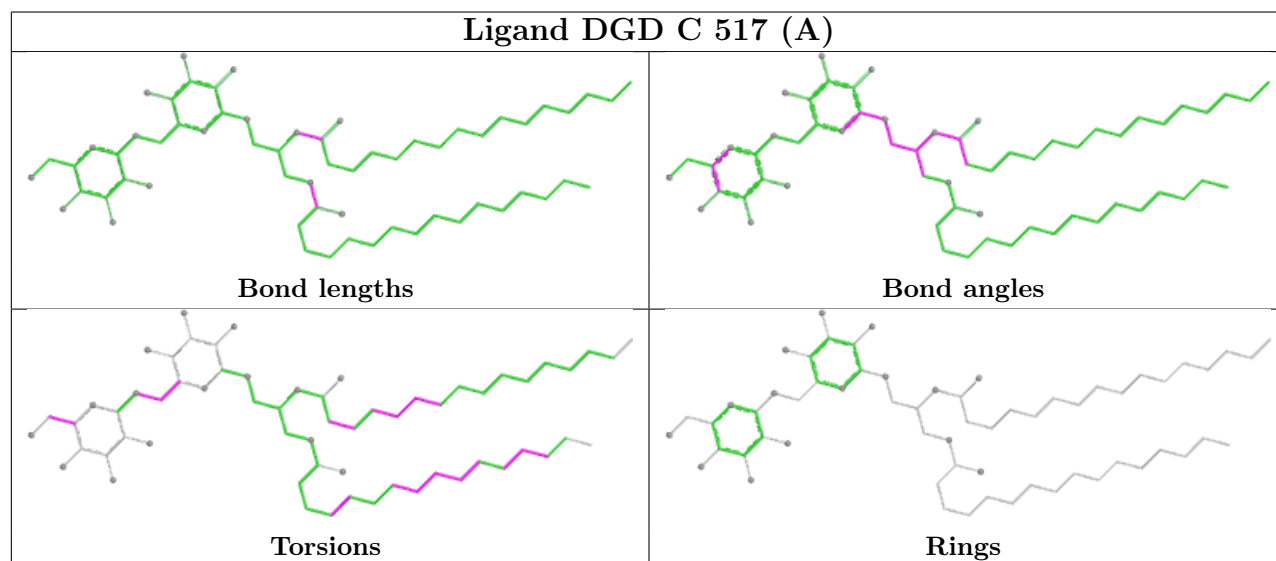
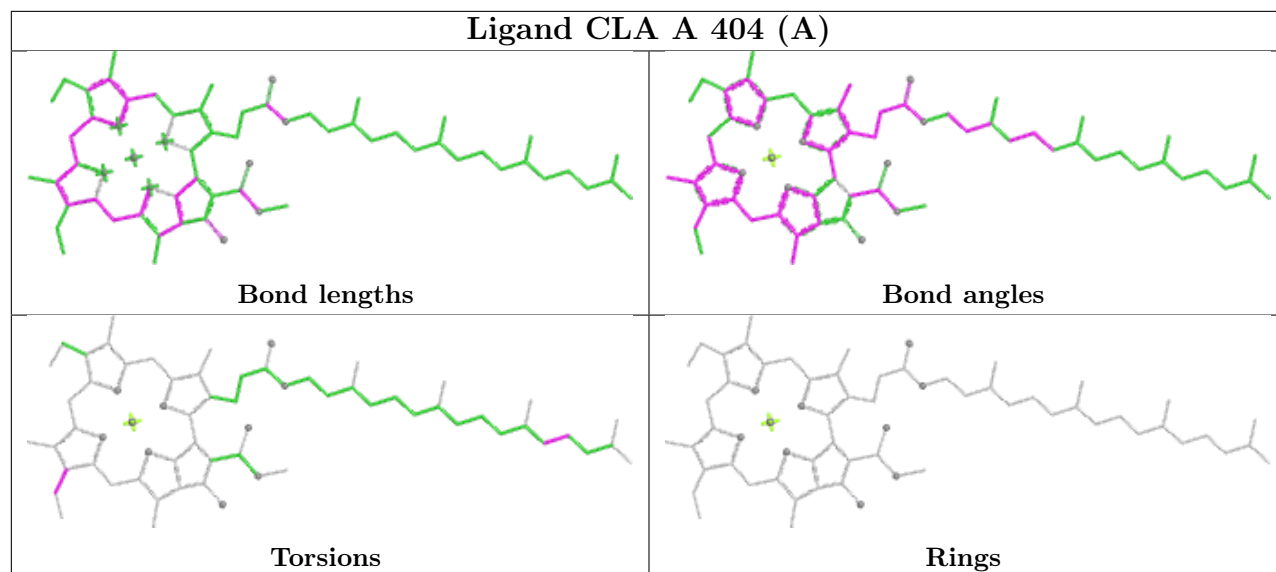


Ligand CLA a 407 (B)

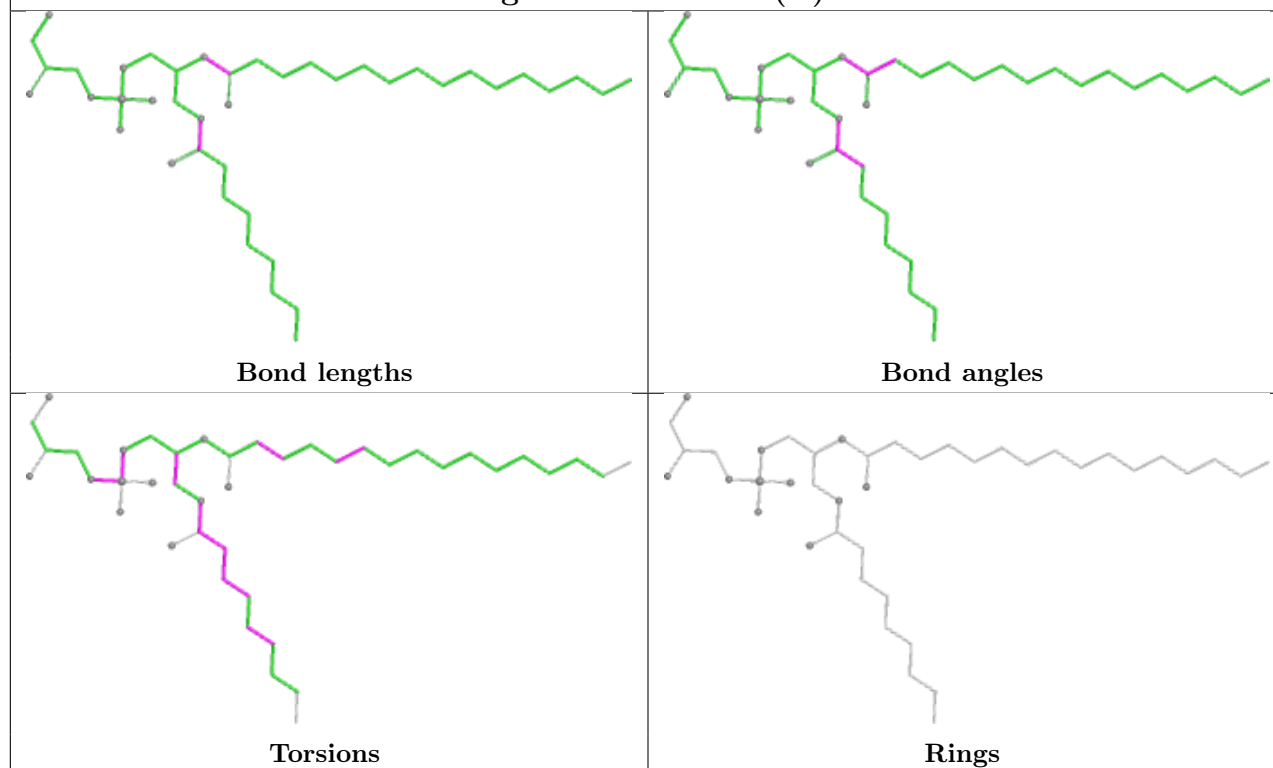


Ligand LHG E 101 (B)

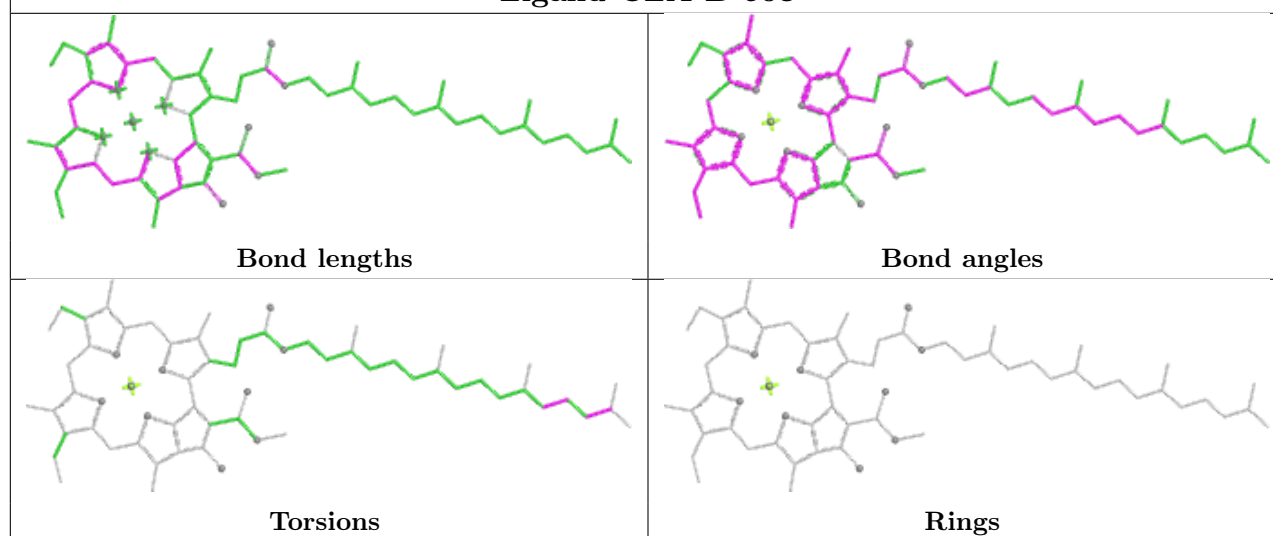




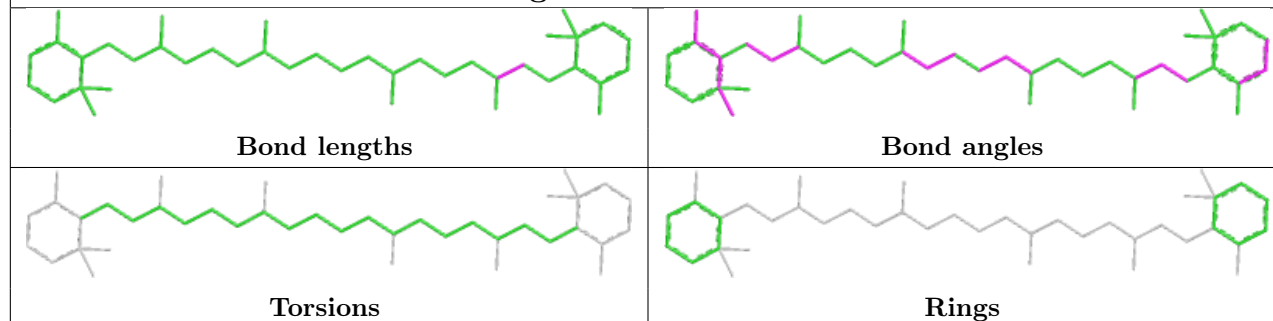
Ligand LHG a 420 (B)

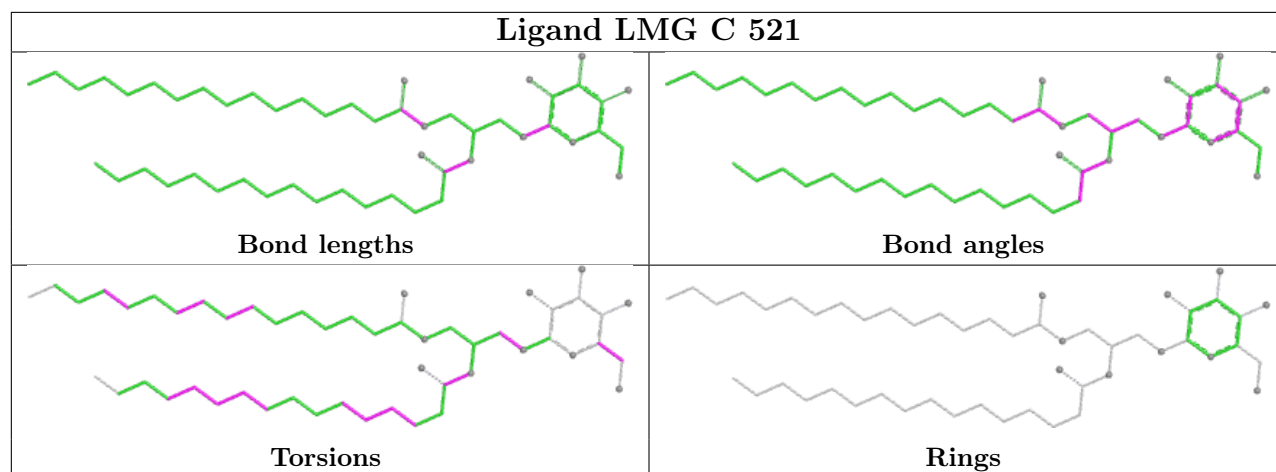
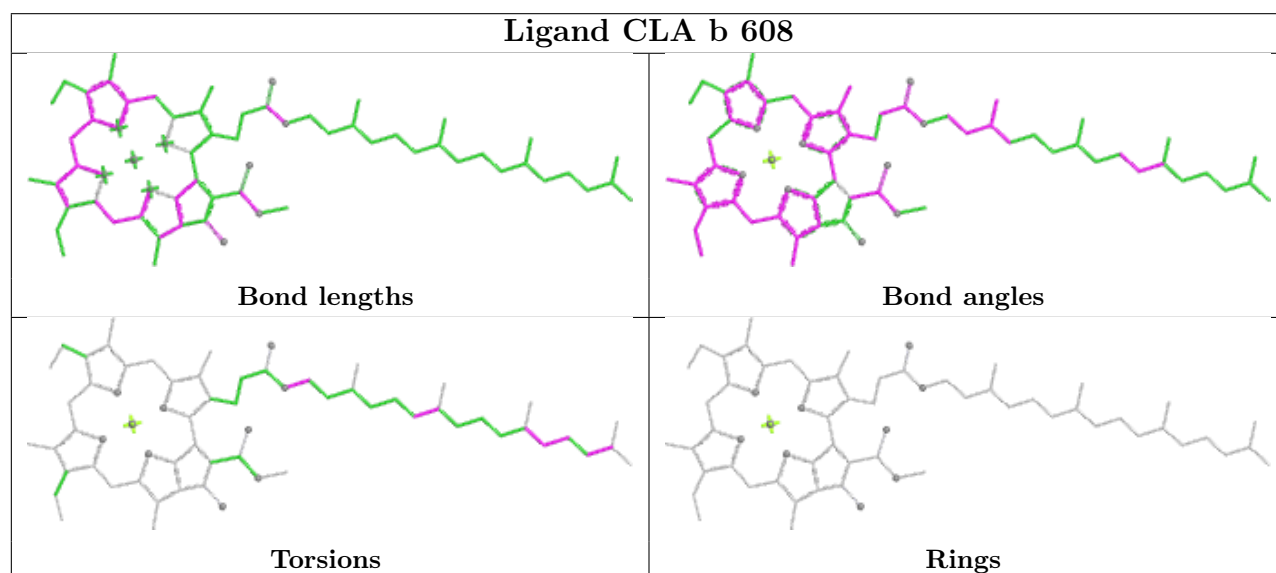
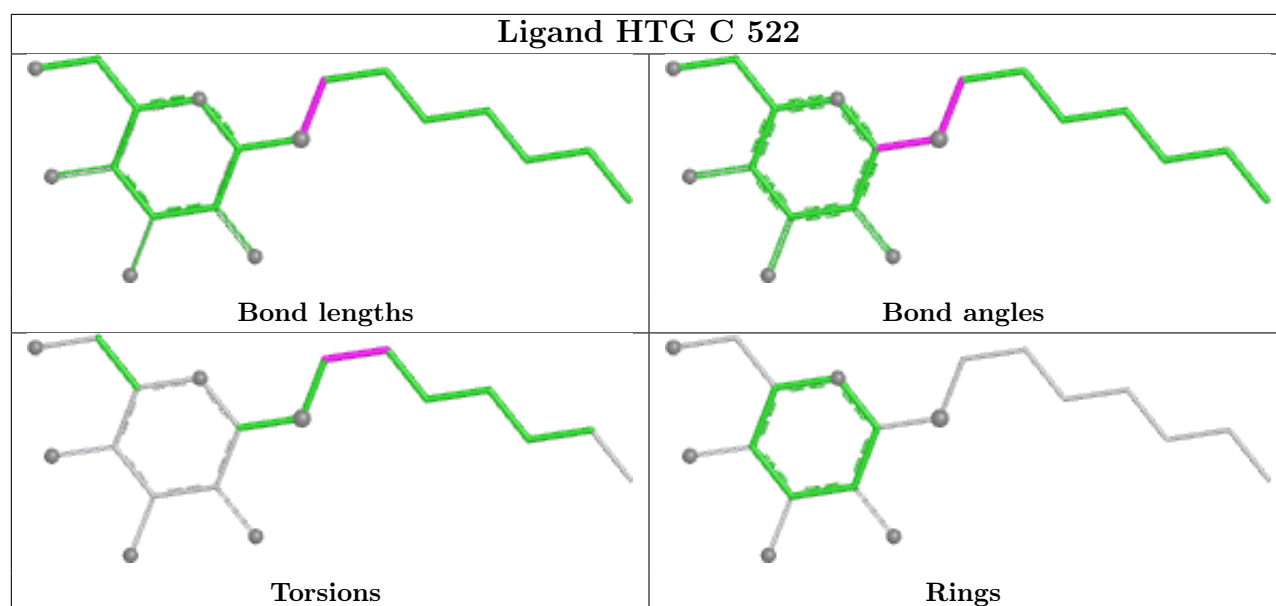


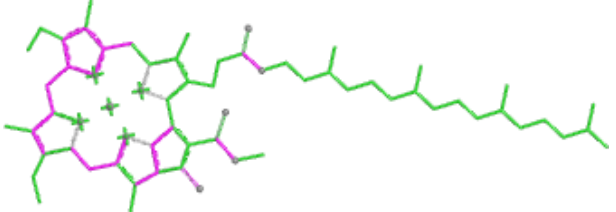
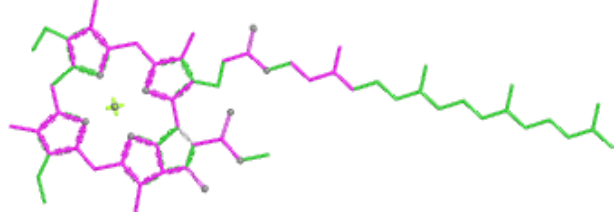
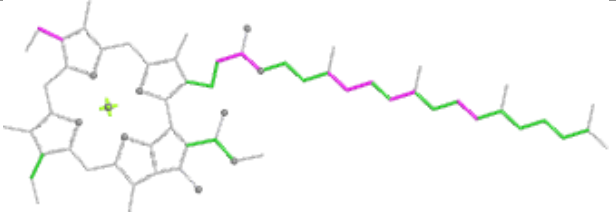
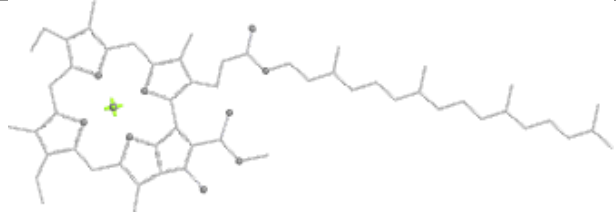
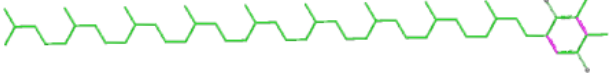
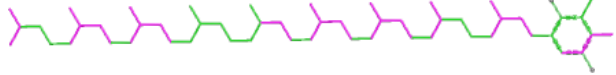
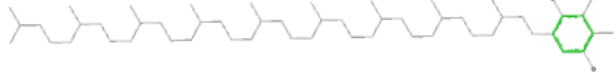
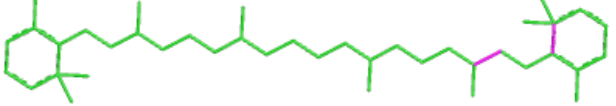
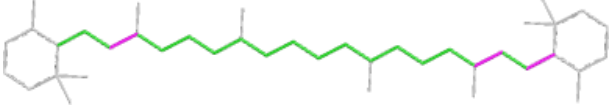
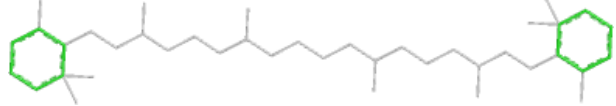
Ligand CLA B 608

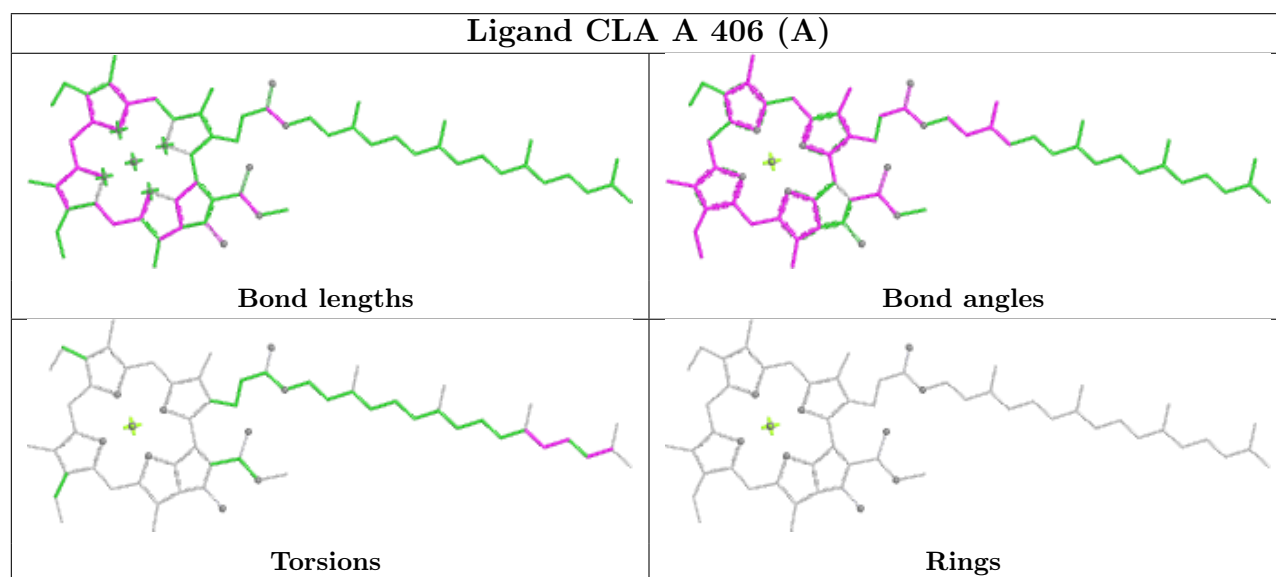
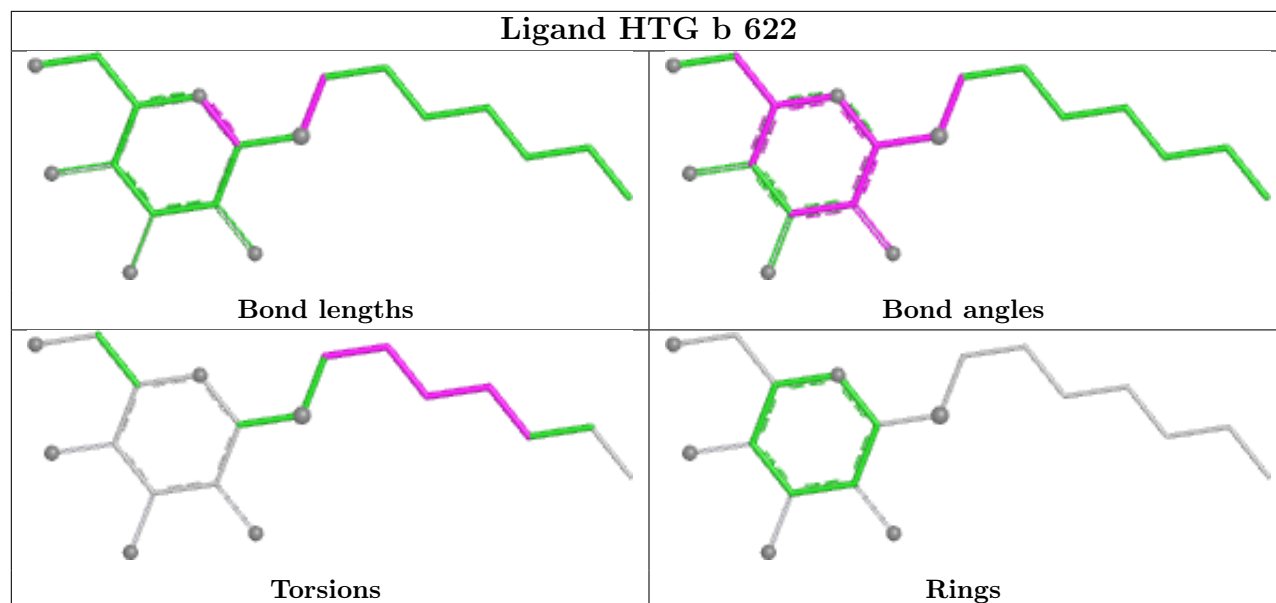


Ligand BCR B 617

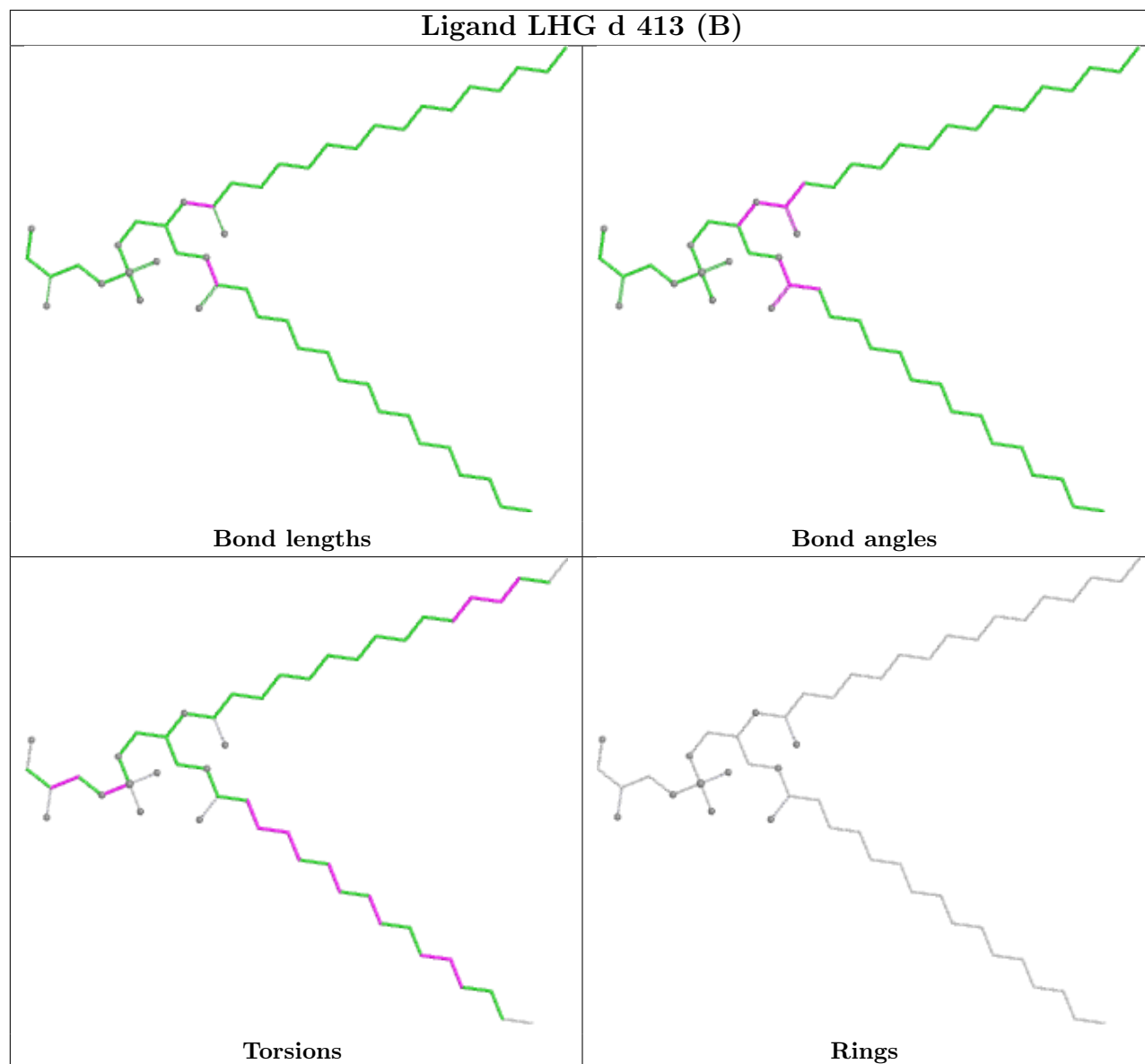




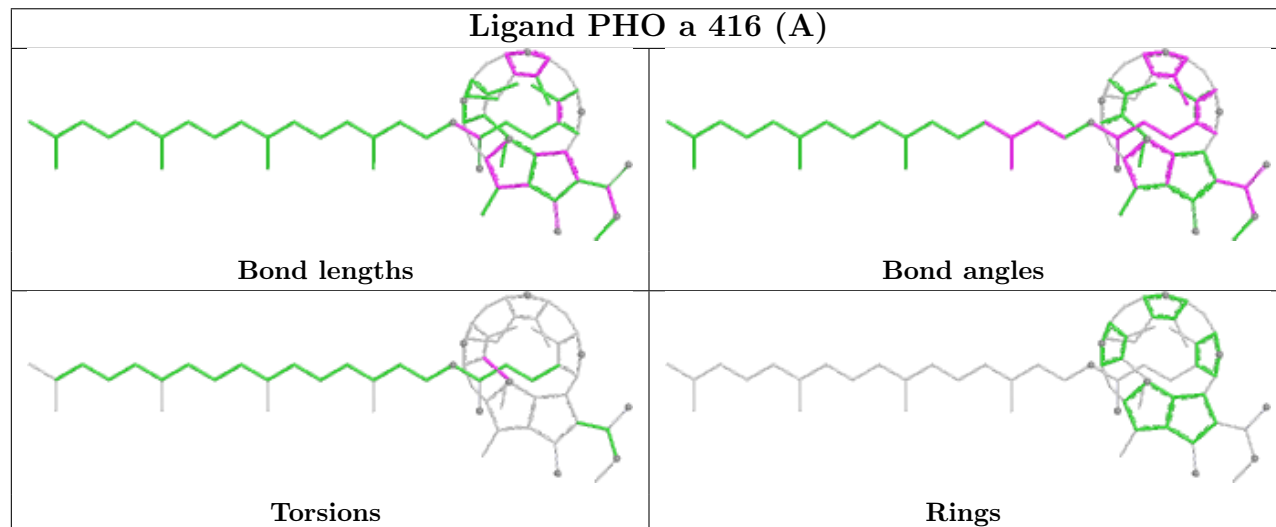
Ligand CLA C 513	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PL9 D 407 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR d 404	
 Bond lengths	 Bond angles
 Torsions	 Rings

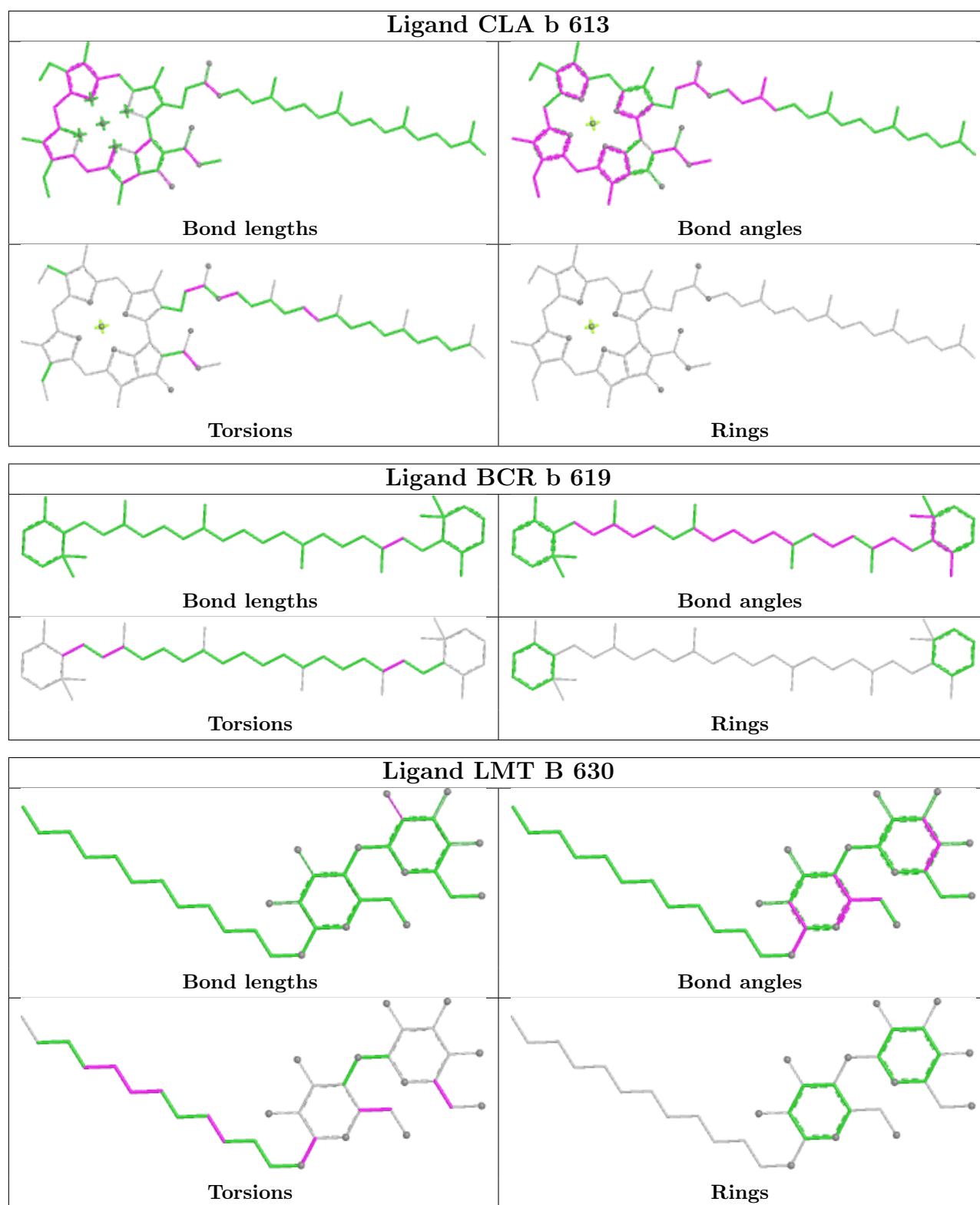


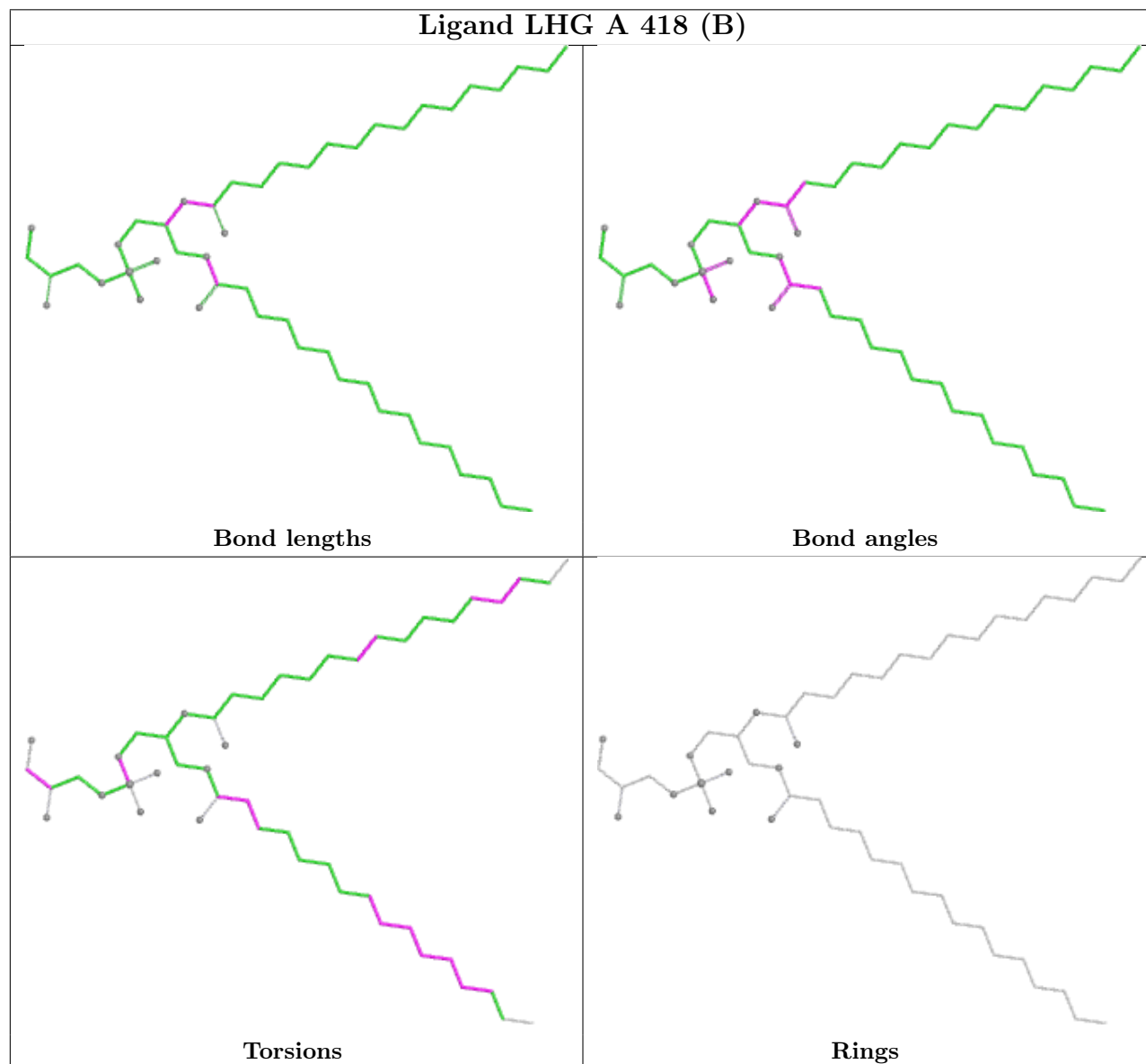
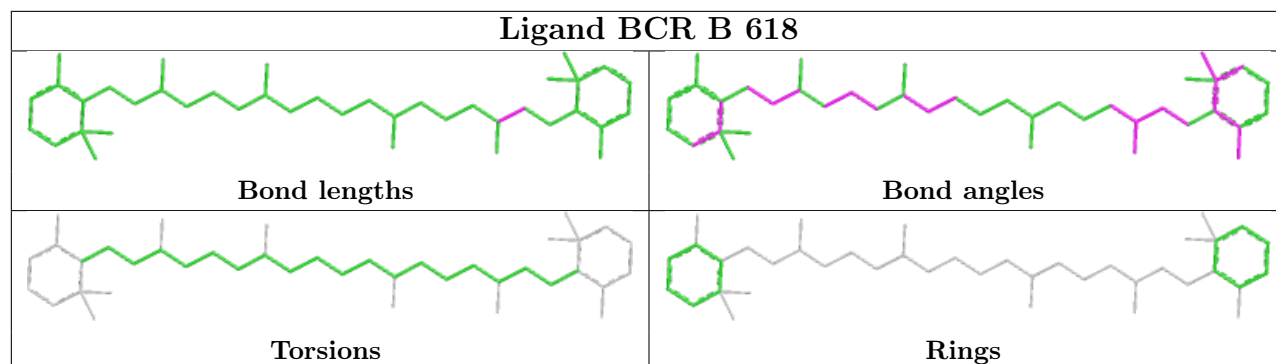
Ligand LHG d 413 (B)

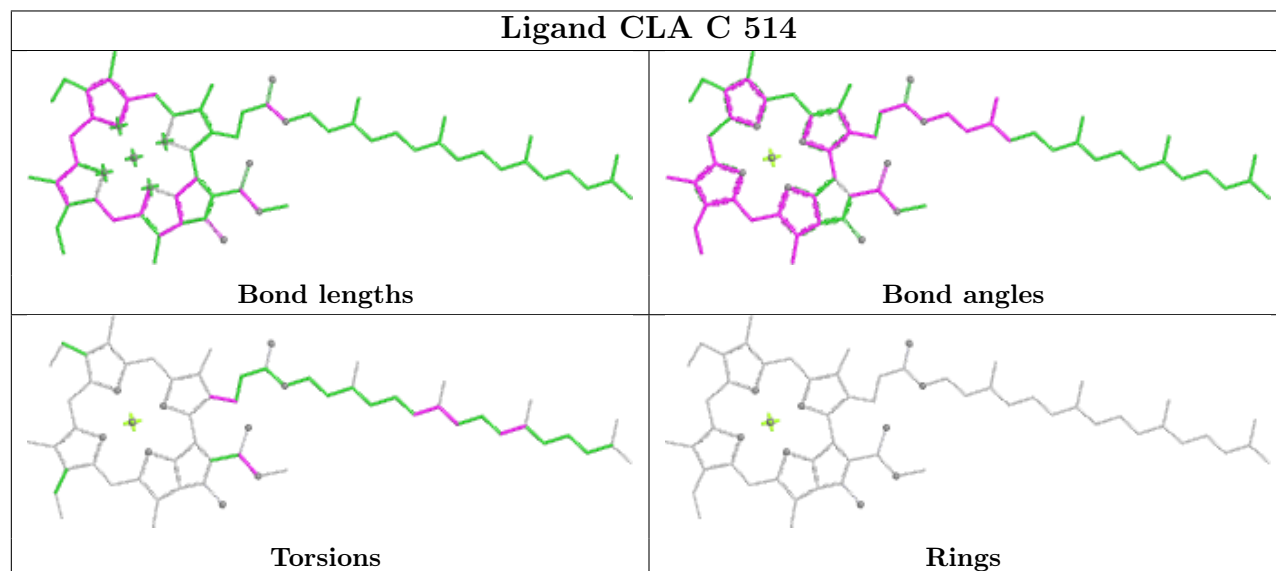
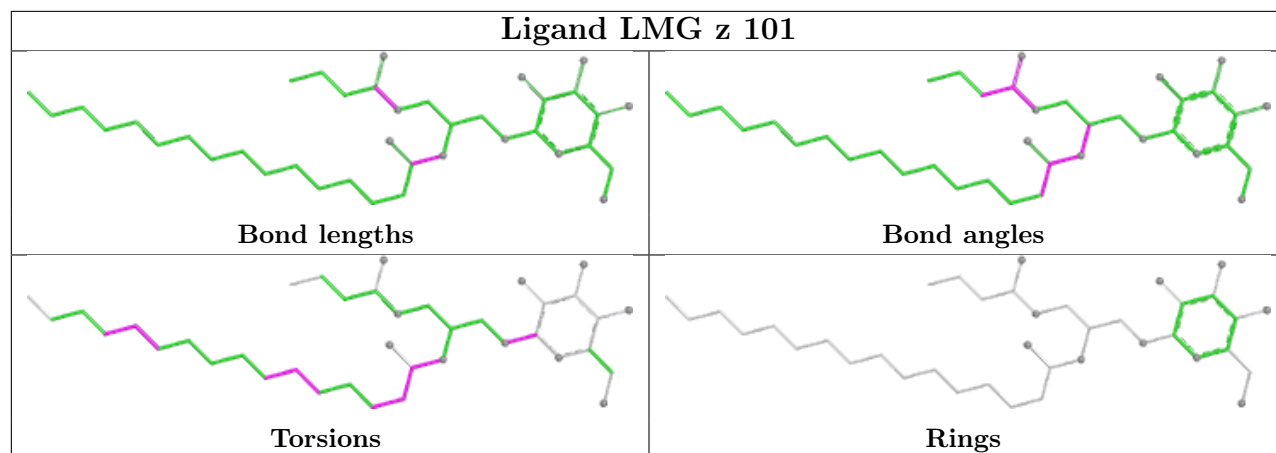


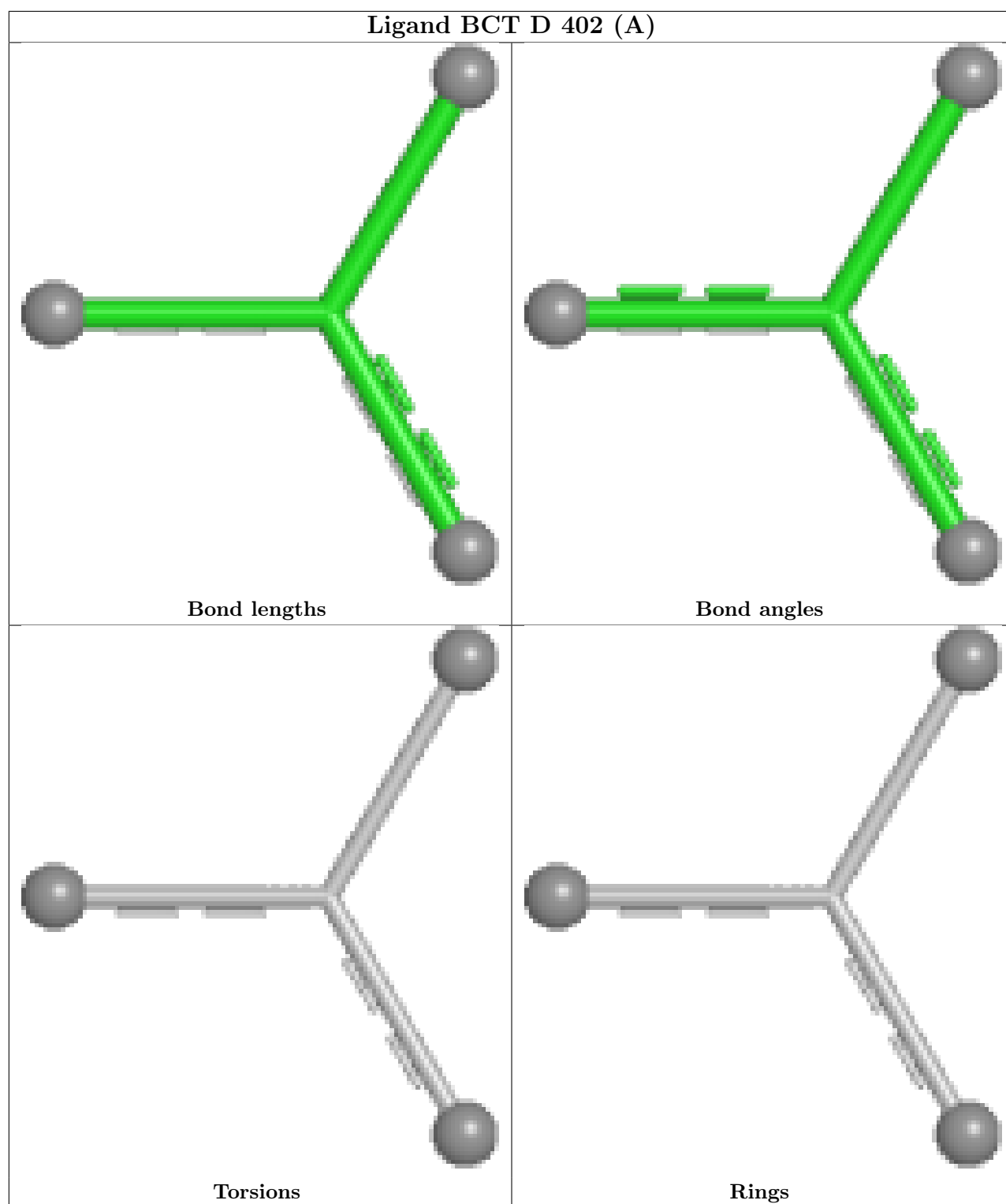
Ligand PHO a 416 (A)

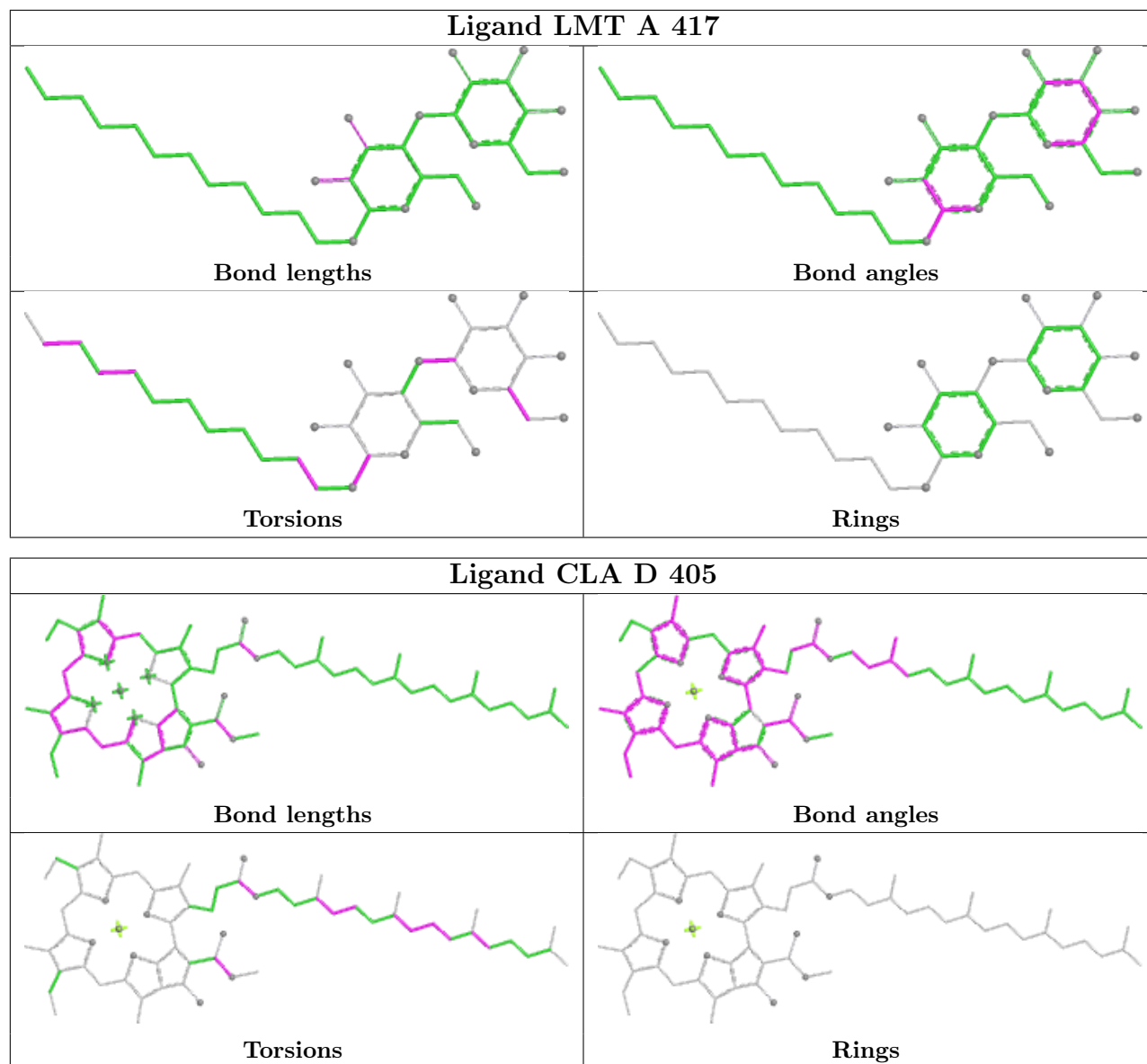




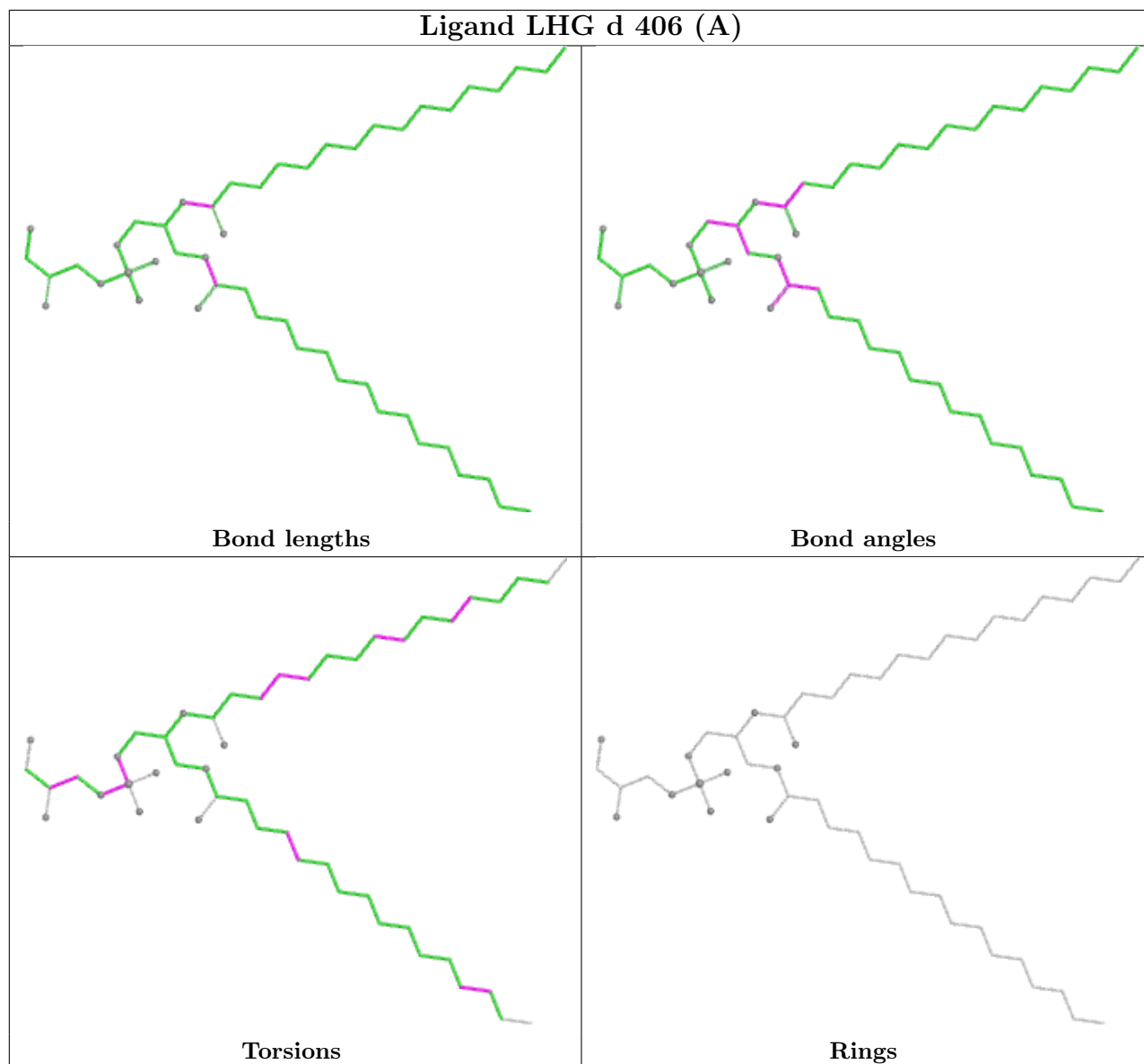




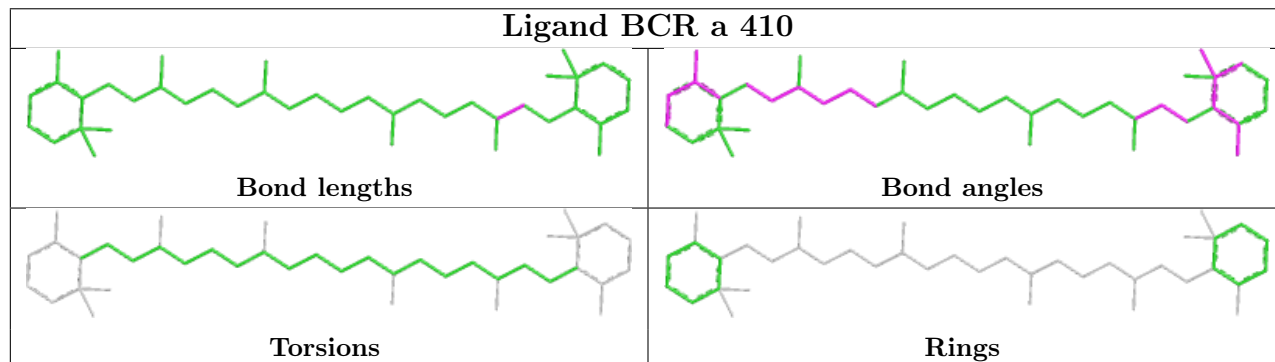


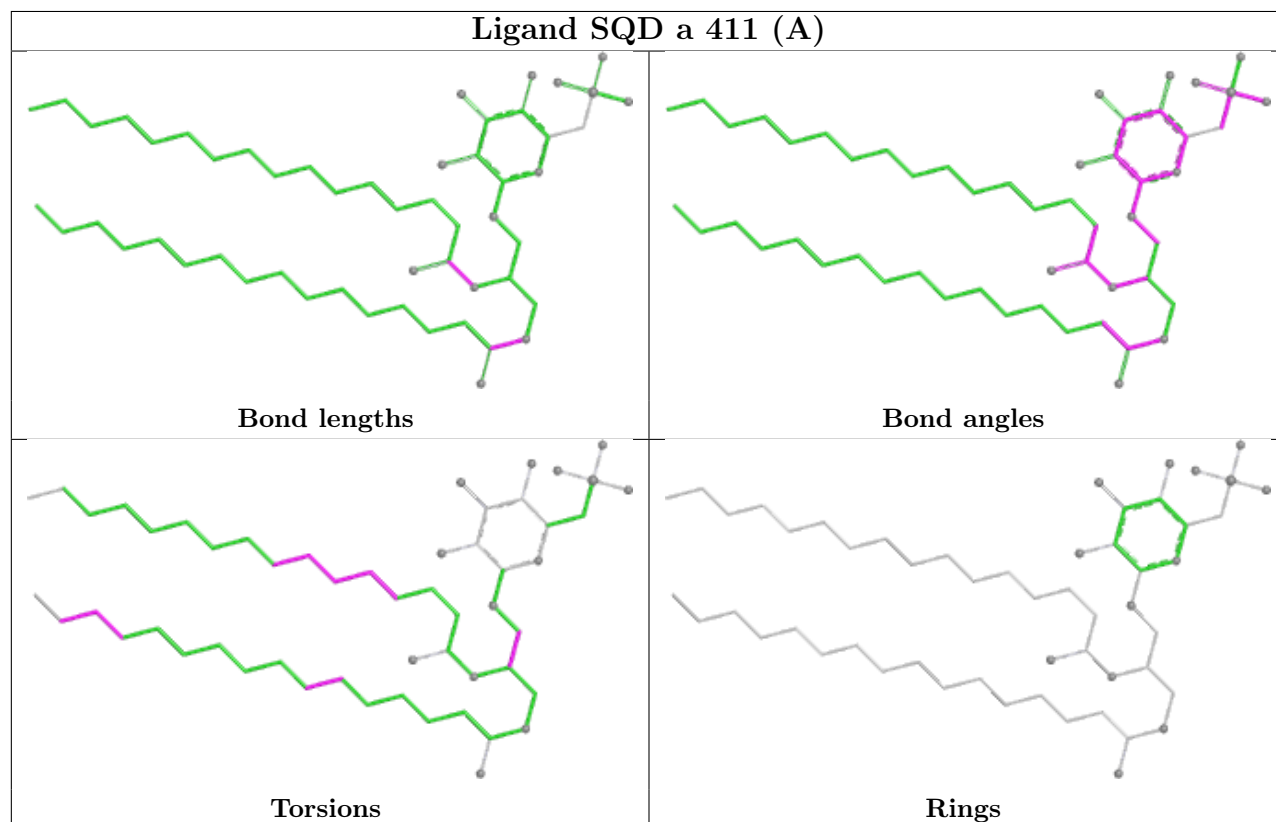
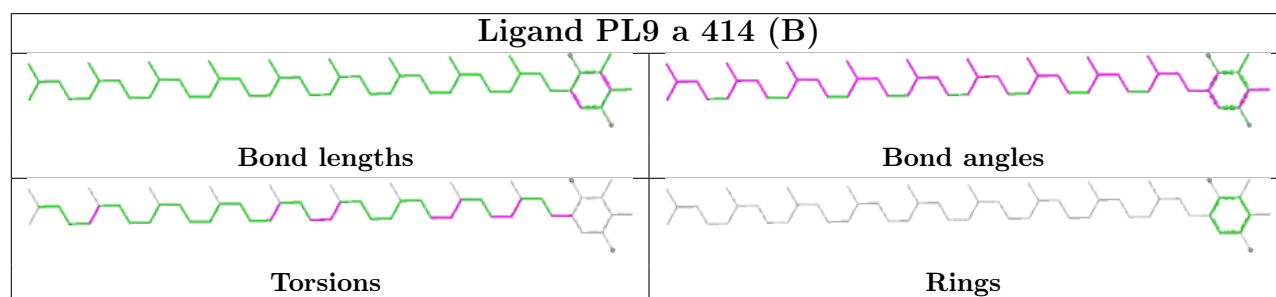
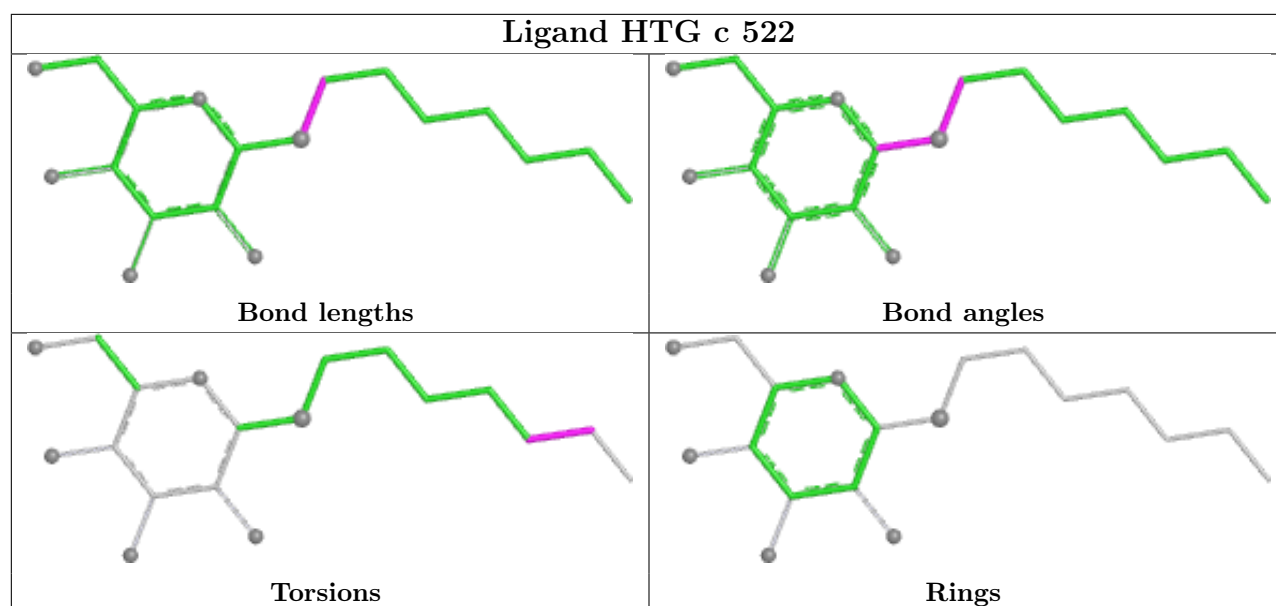


Ligand LHG d 406 (A)

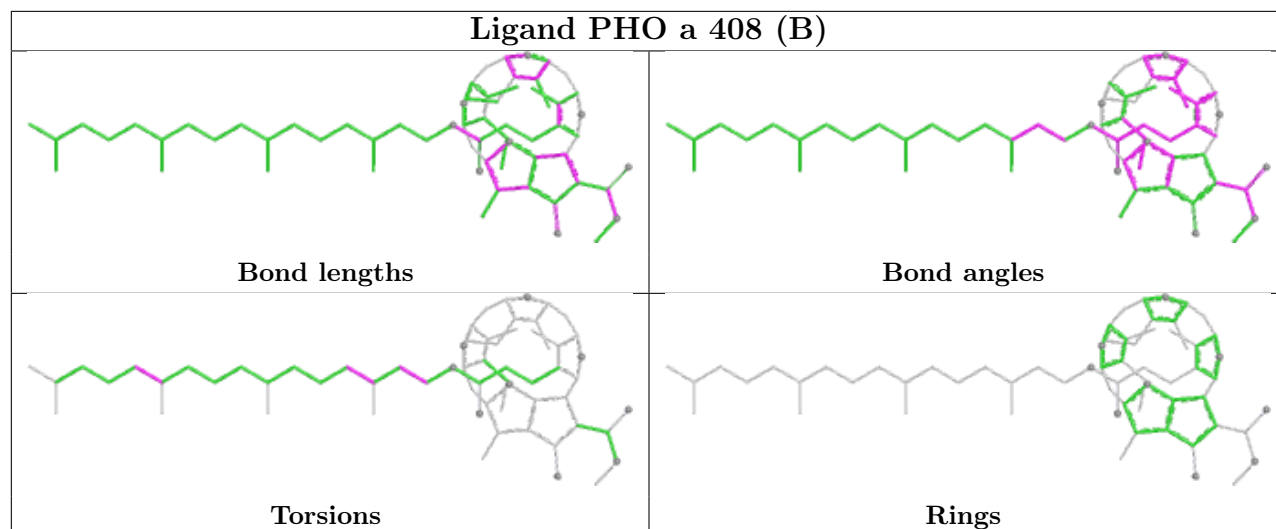


Ligand BCR a 410

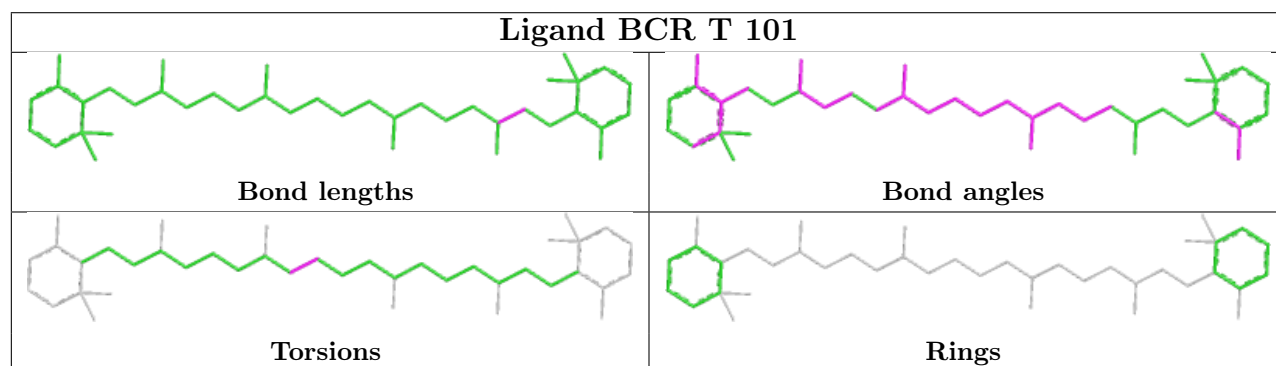




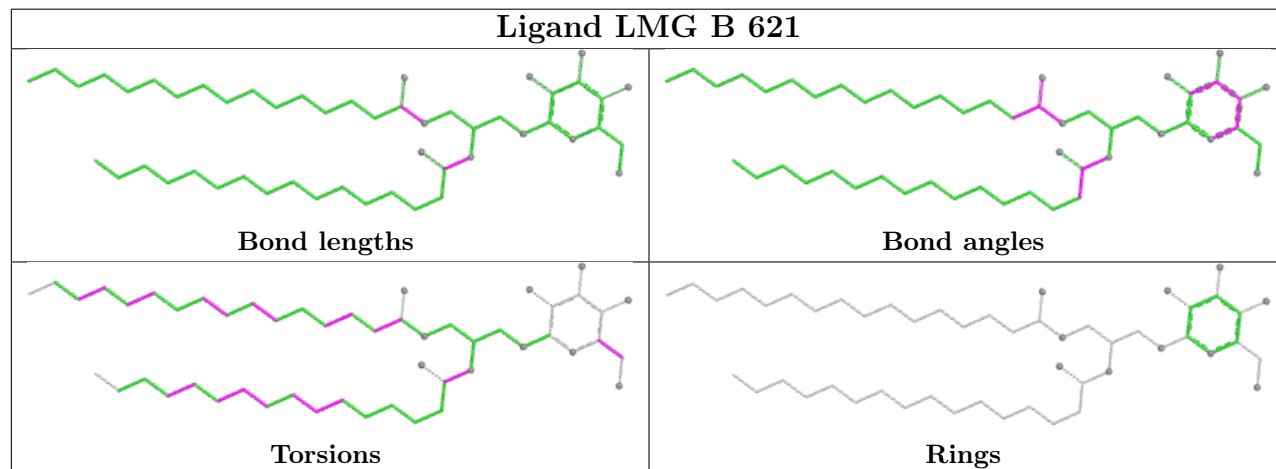
Ligand PHO a 408 (B)



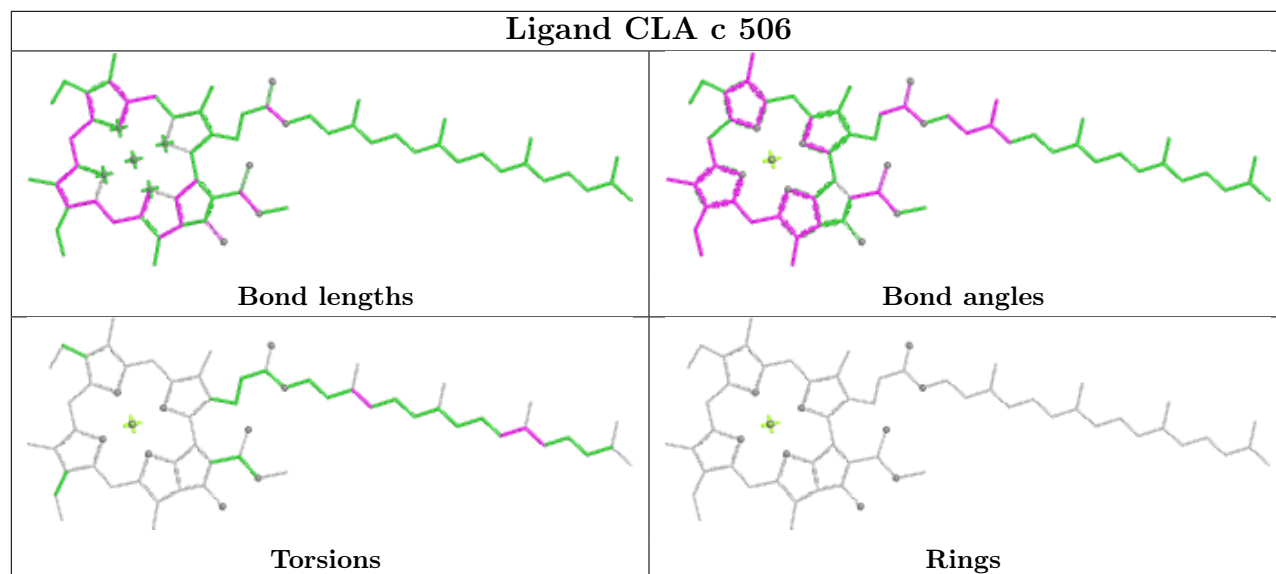
Ligand BCR T 101



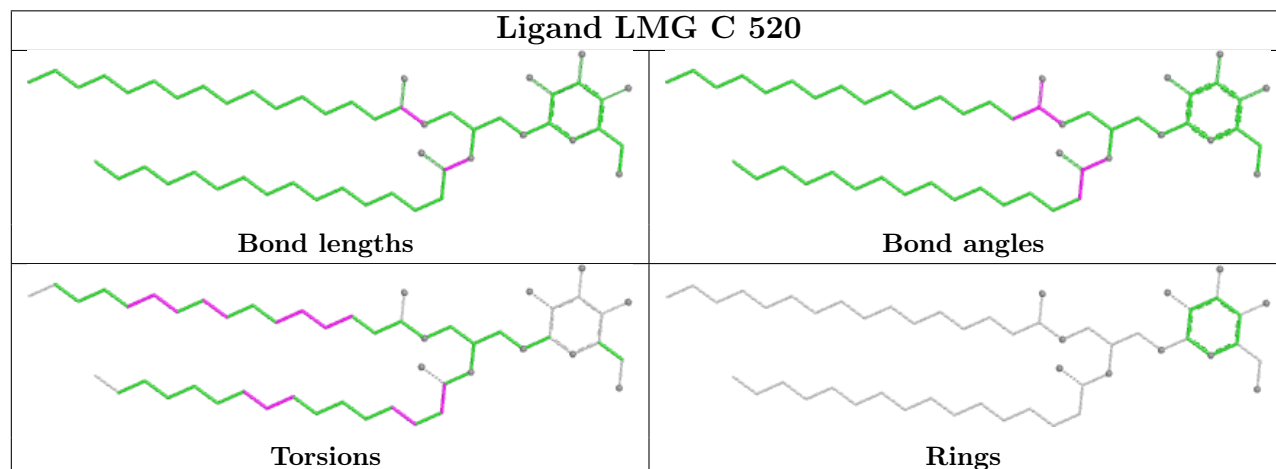
Ligand LMG B 621



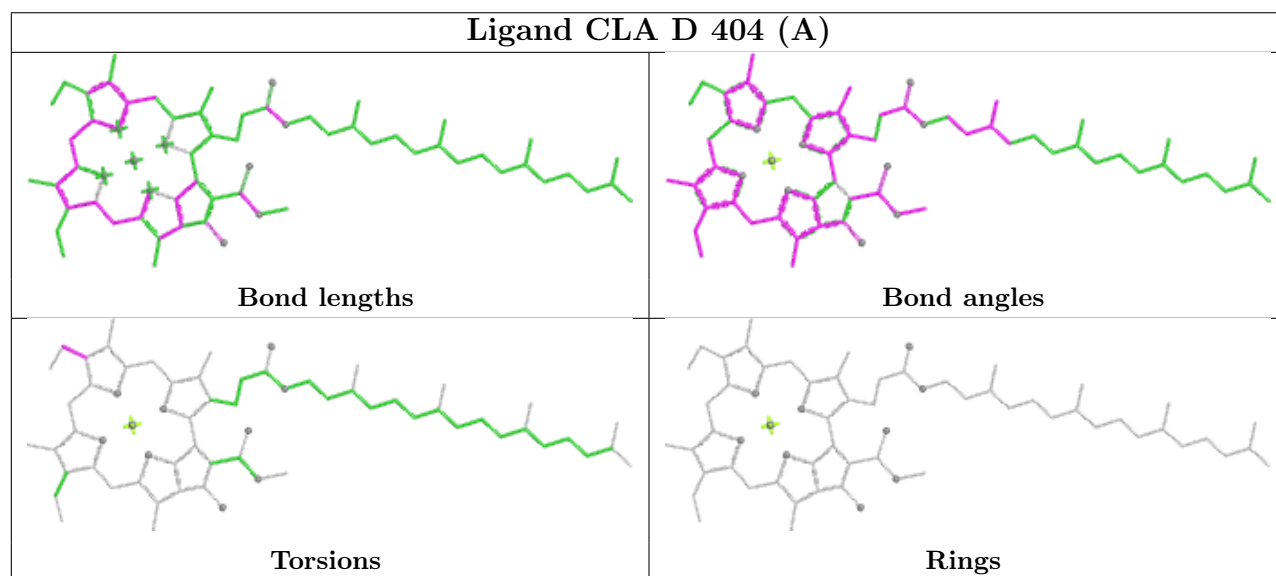
Ligand CLA c 506

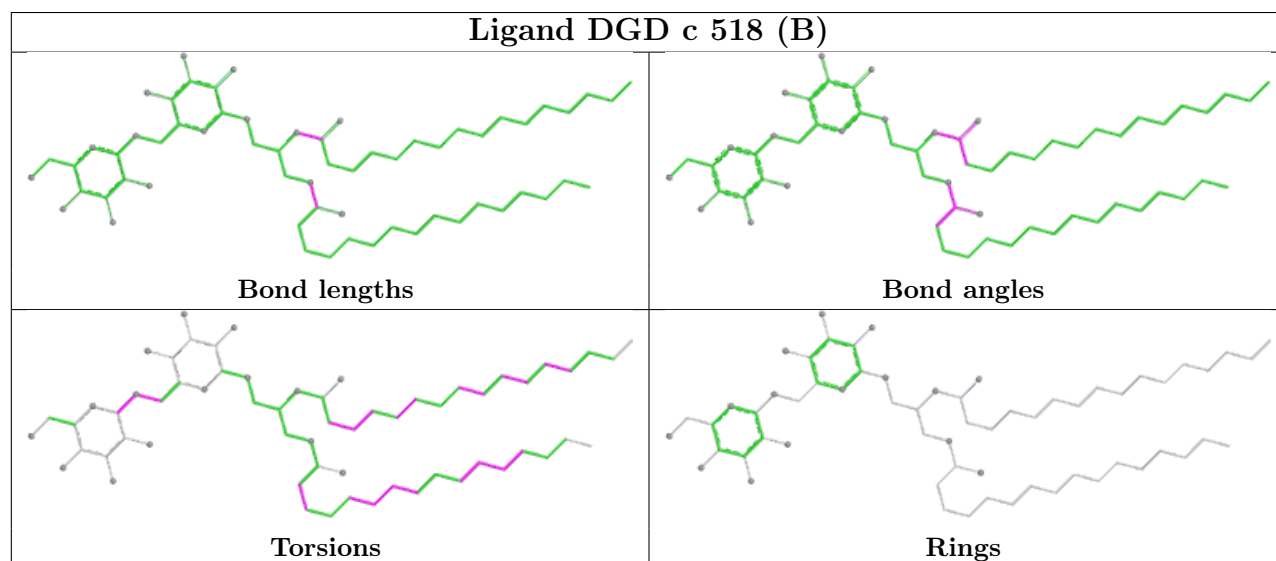
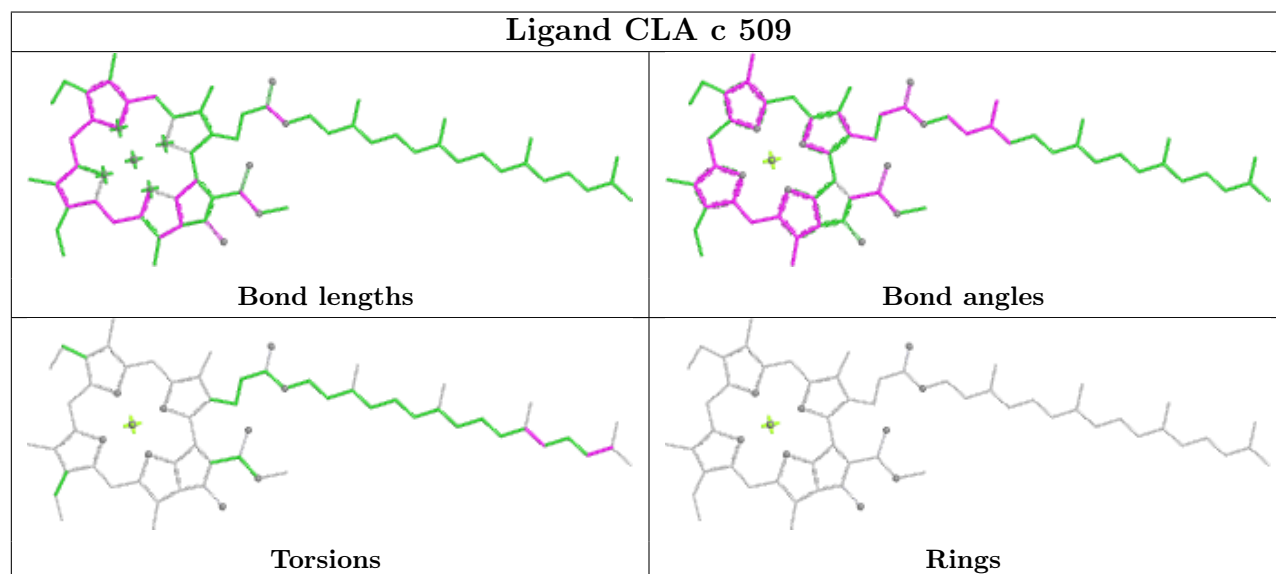
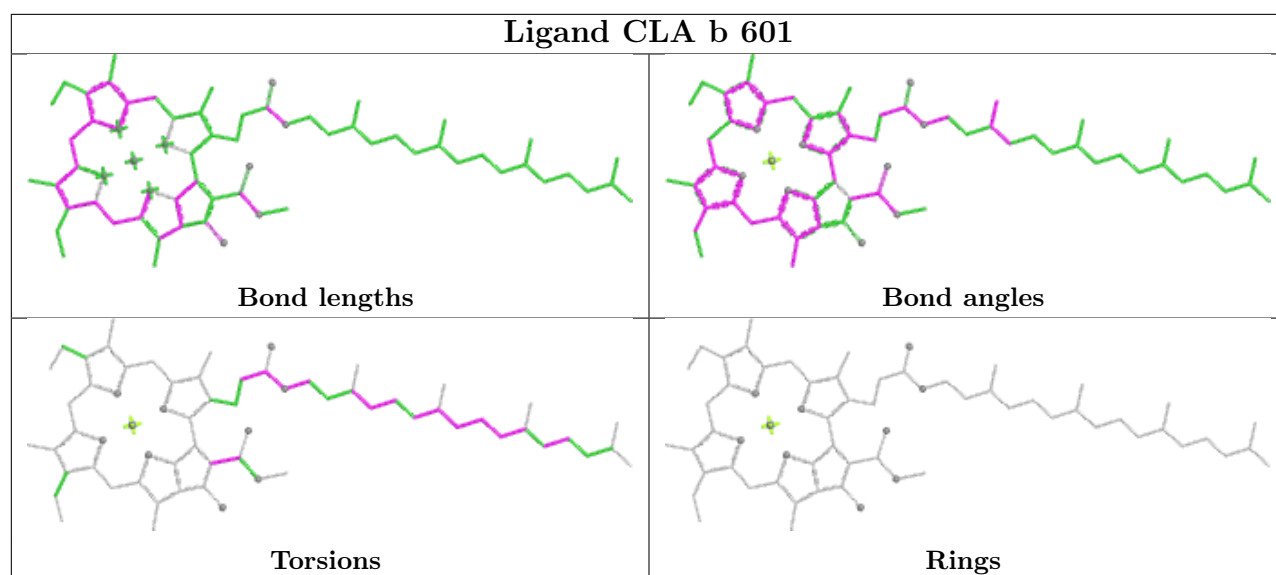


Ligand LMG C 520

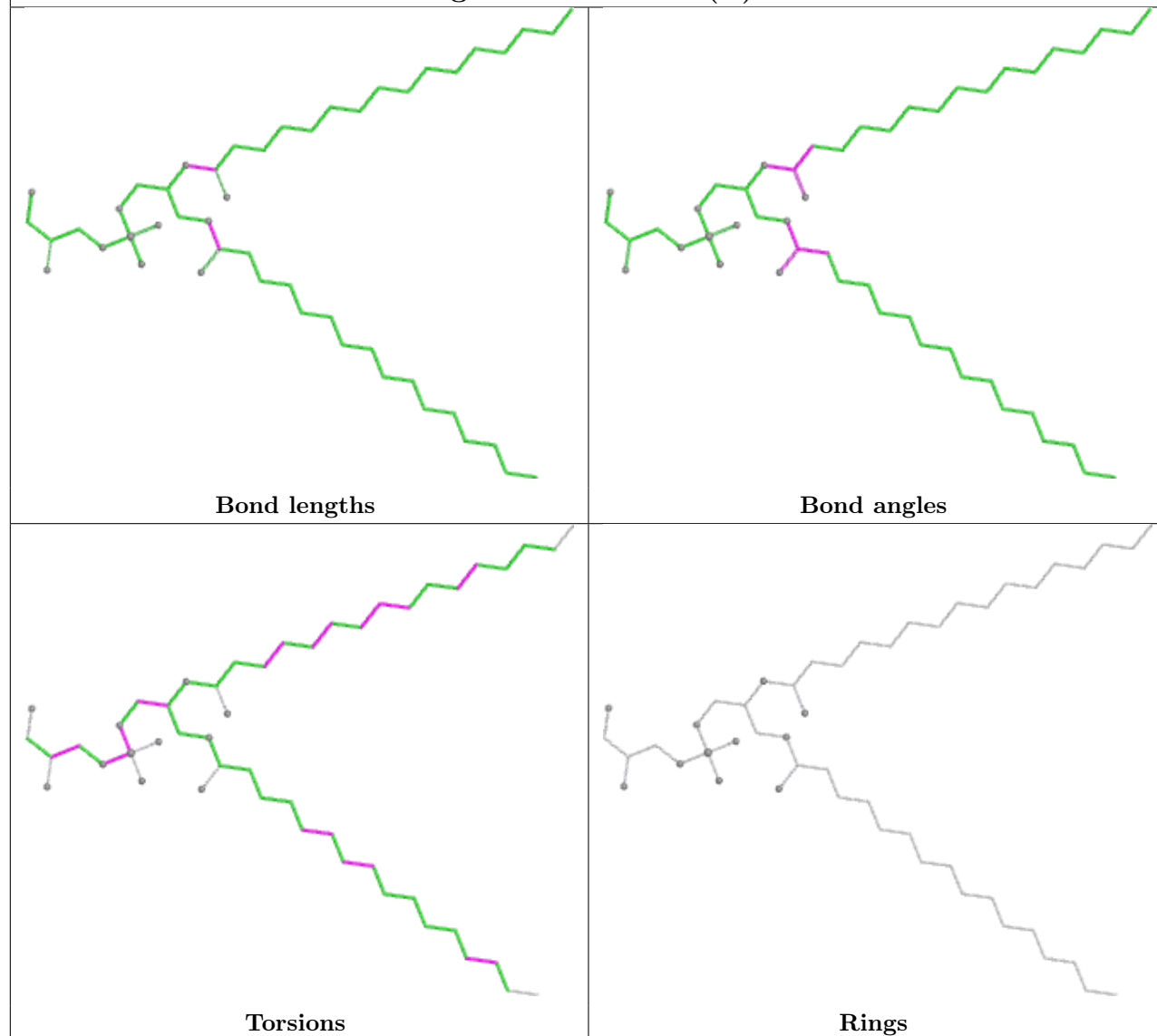


Ligand CLA D 404 (A)

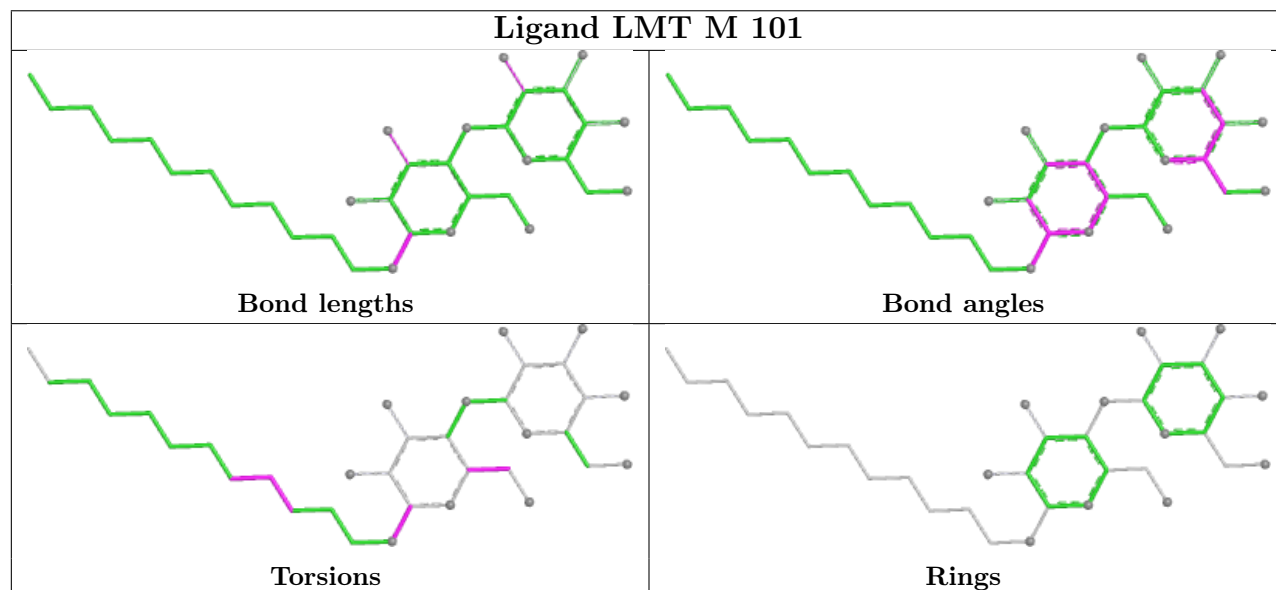


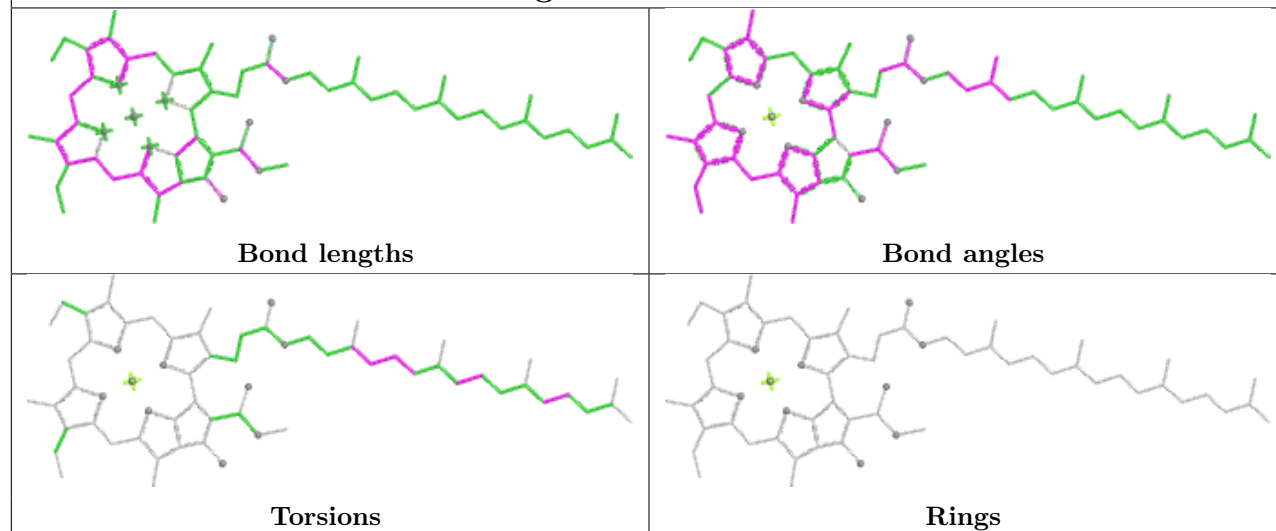
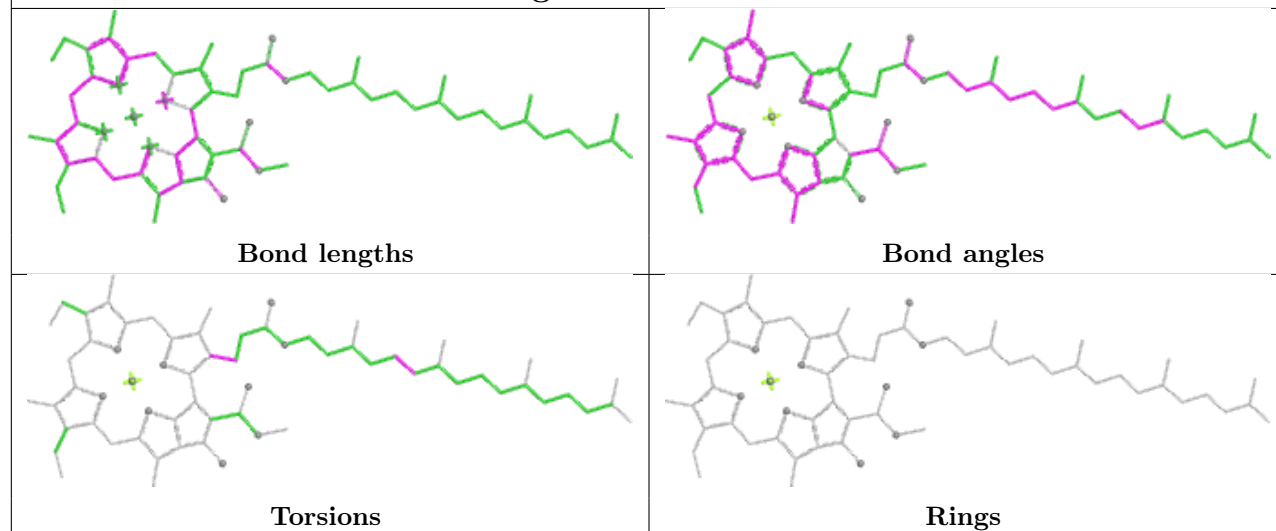
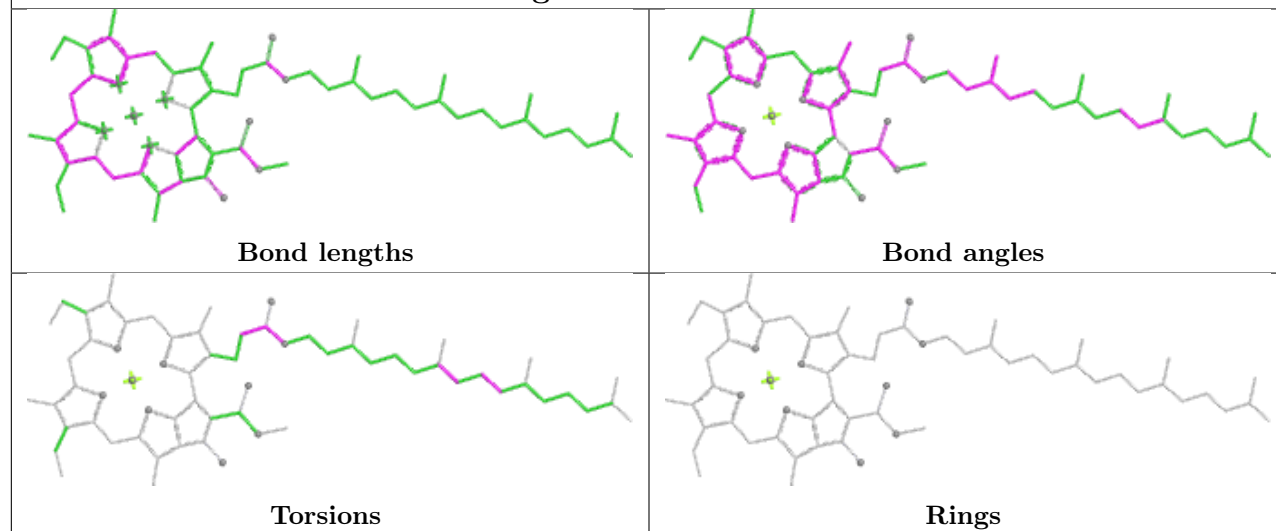


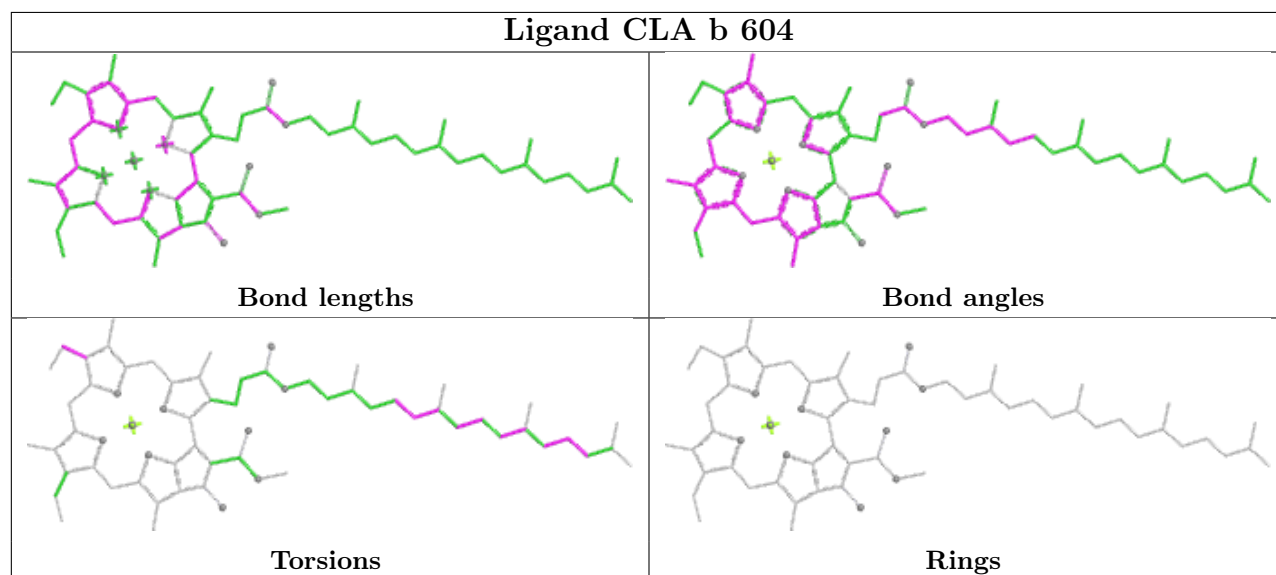
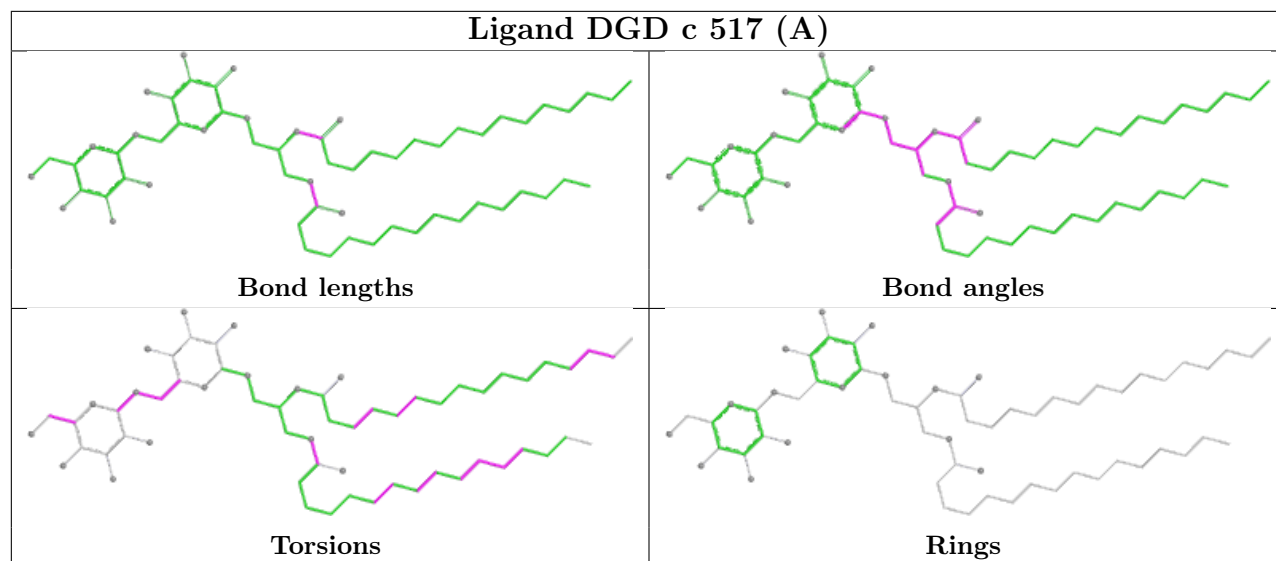
Ligand LHG D 408 (B)

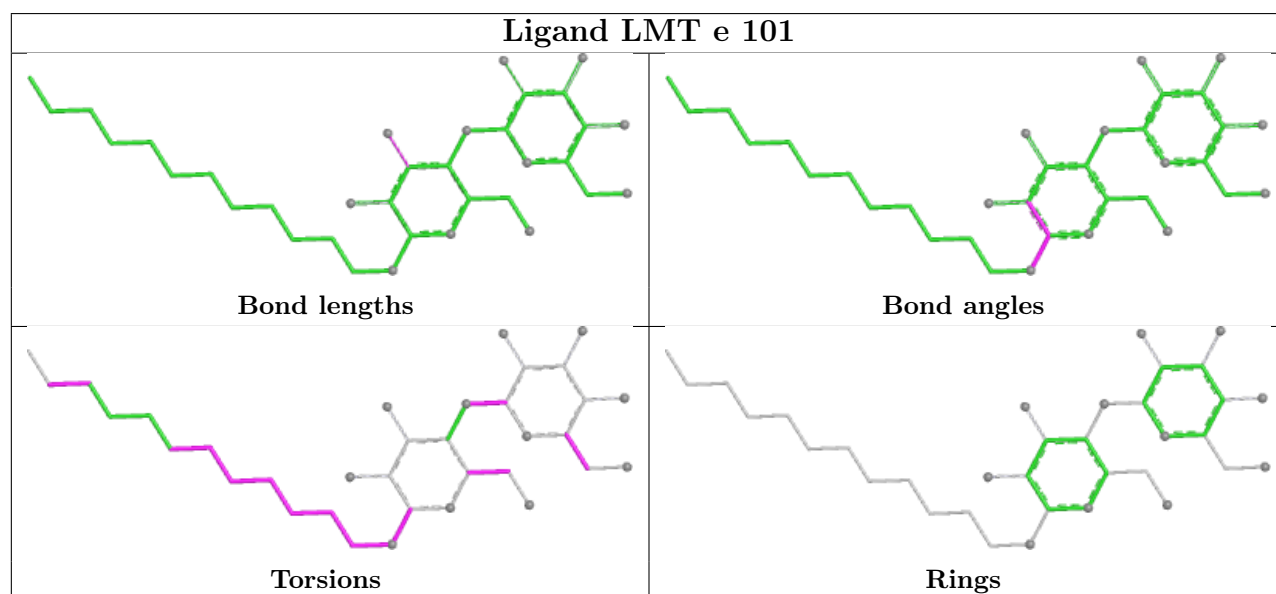
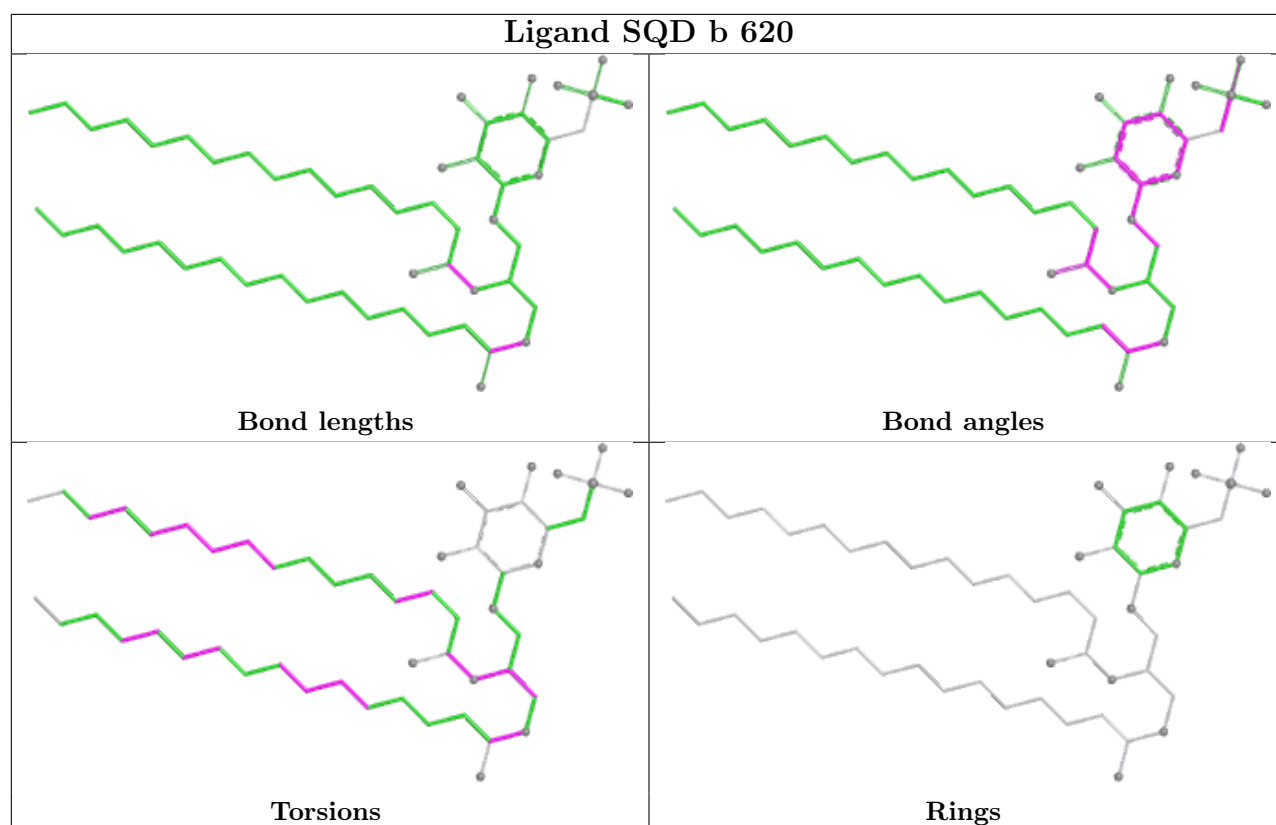


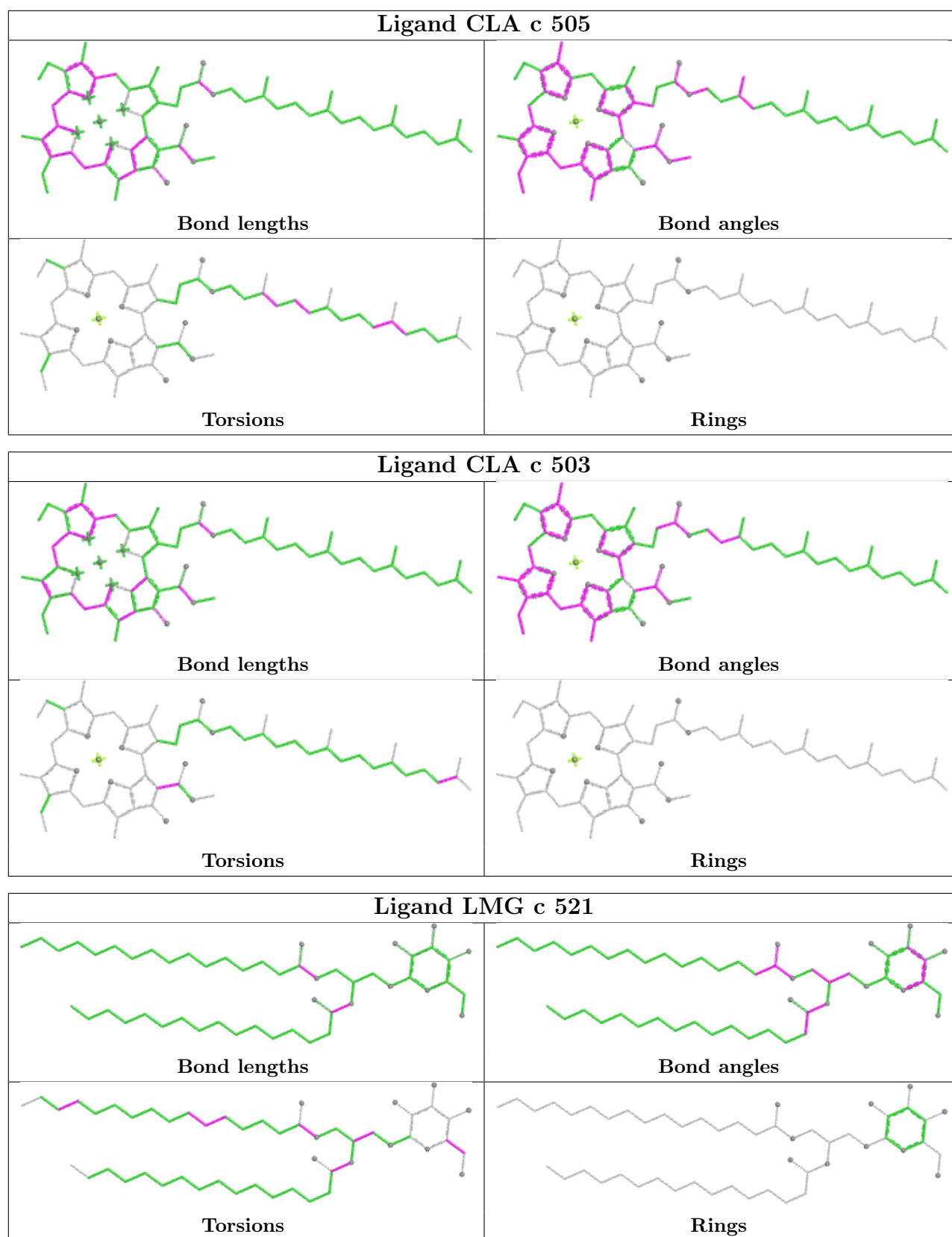
Ligand LMT M 101

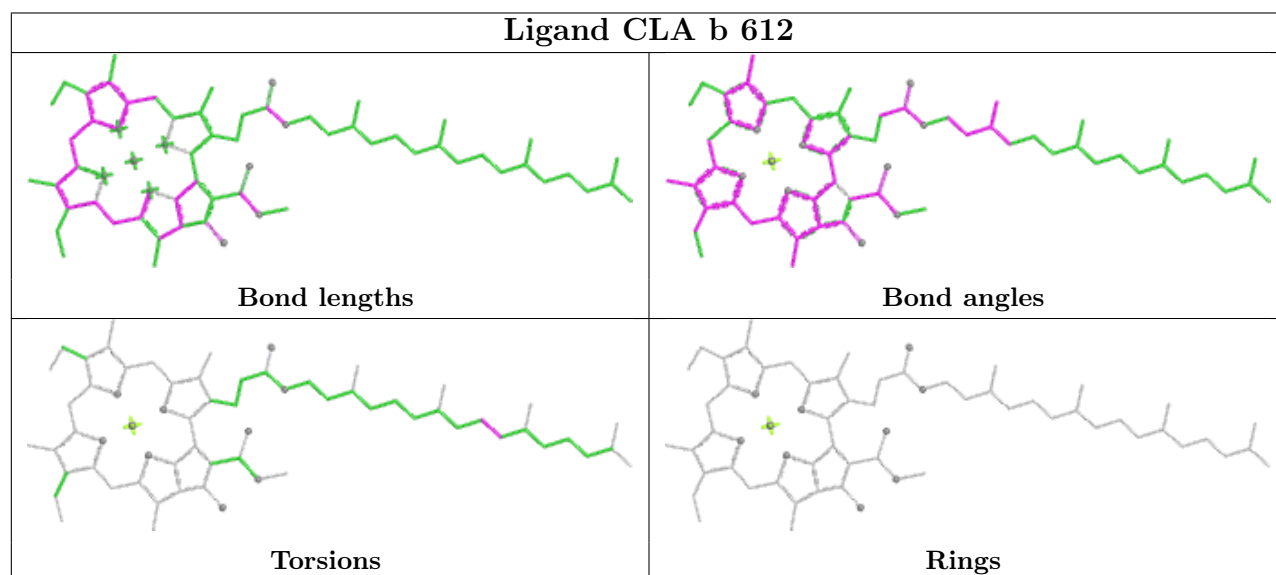
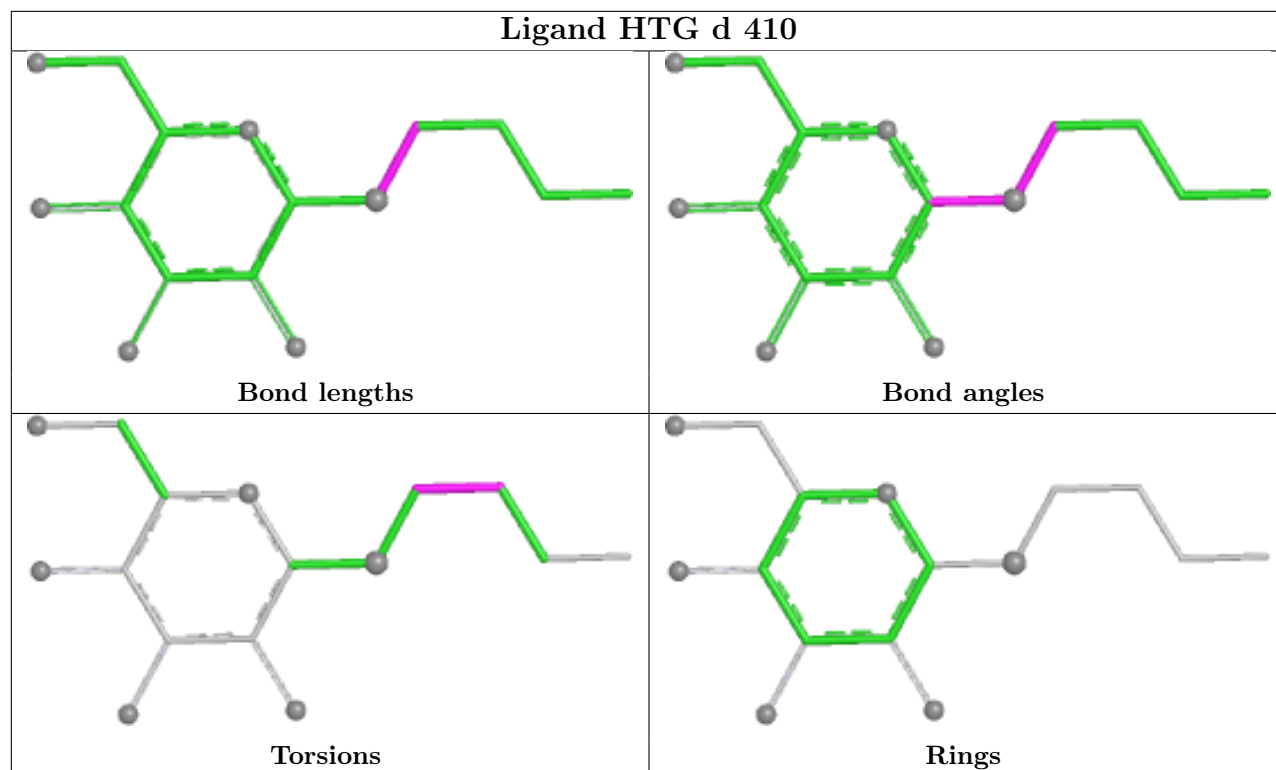


Ligand CLA b 605**Ligand CLA B 604****Ligand CLA B 612**

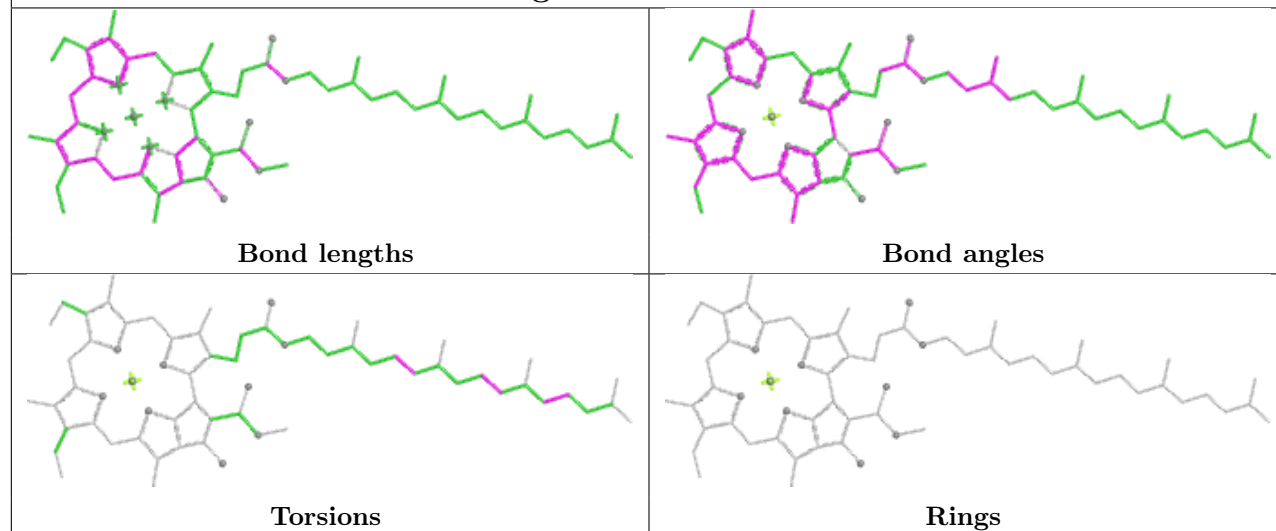




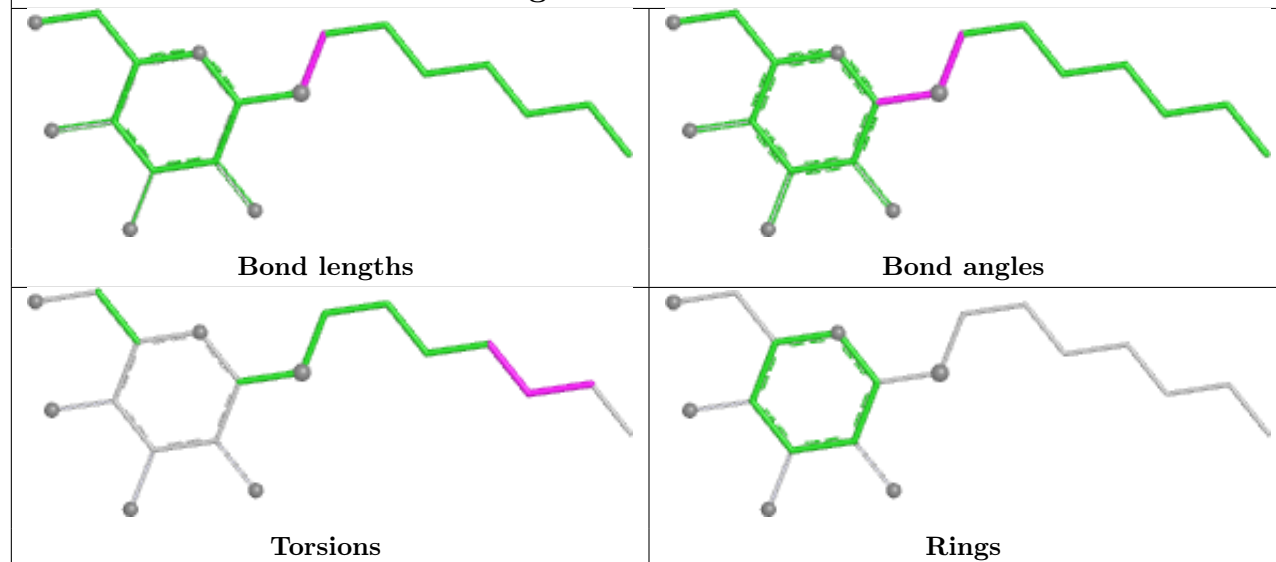


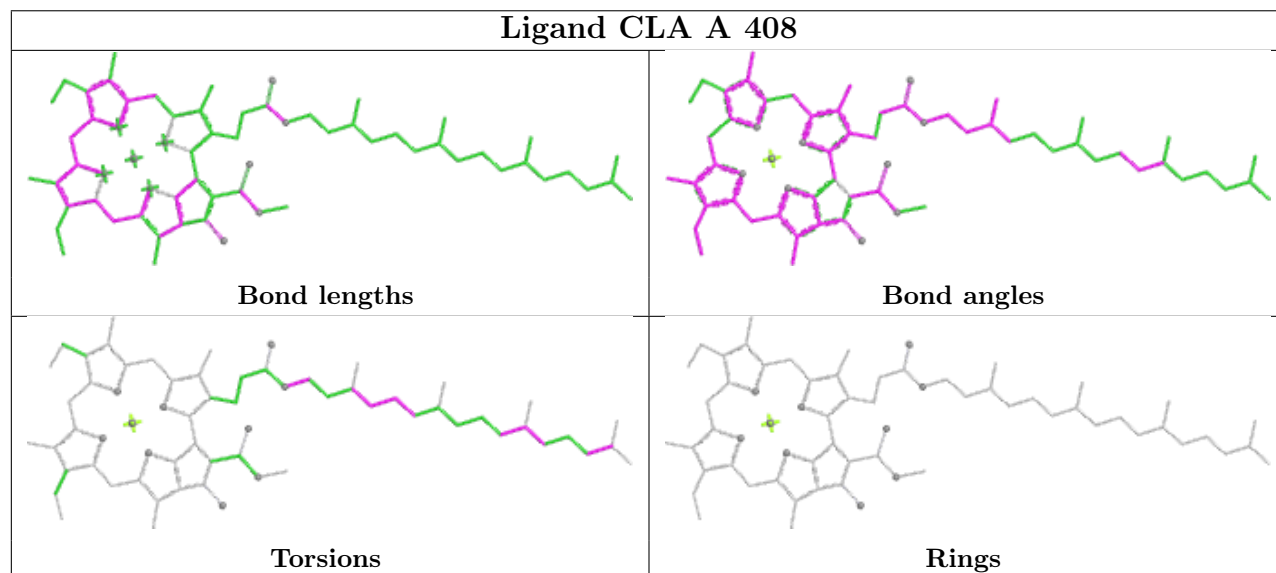
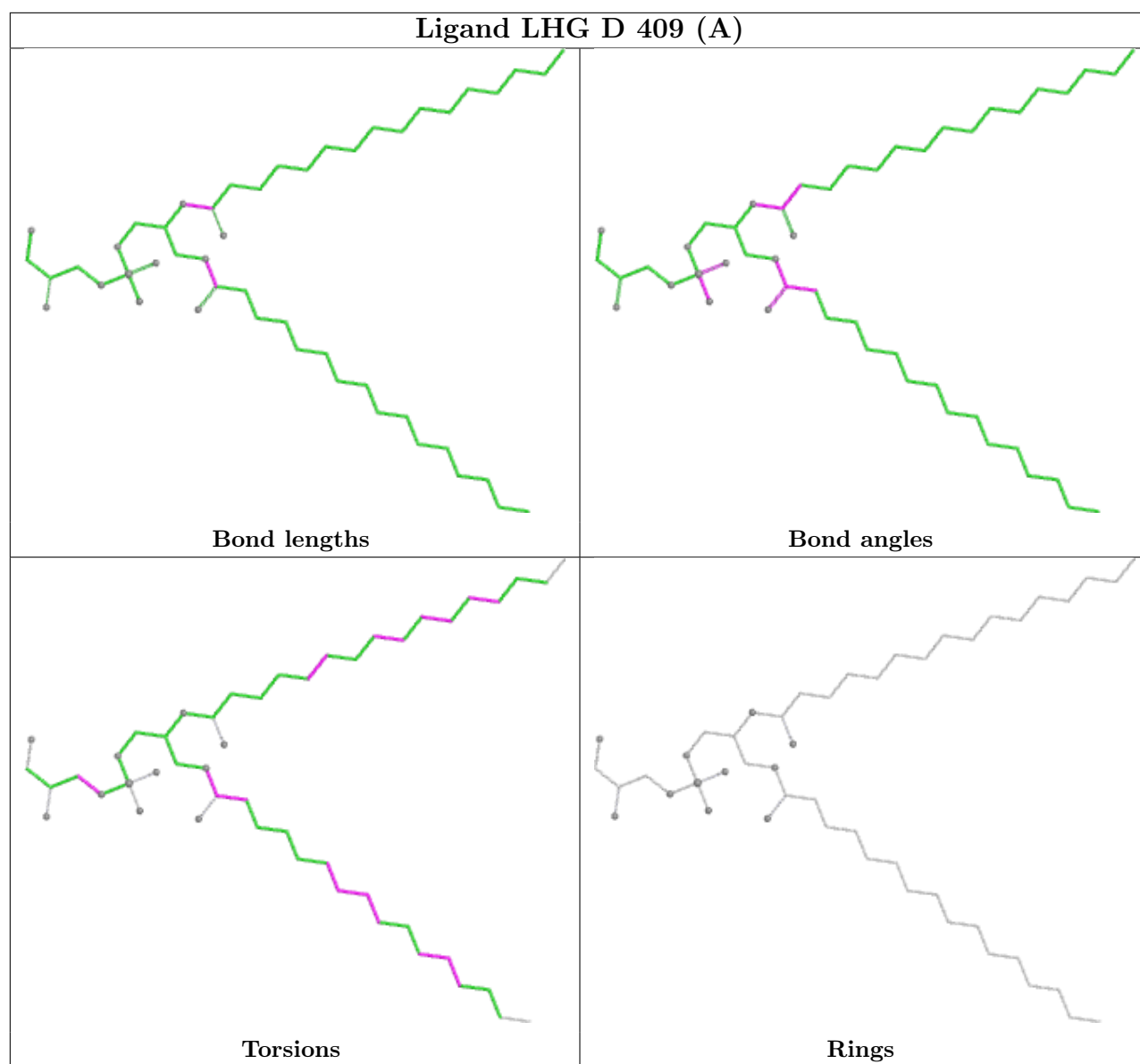


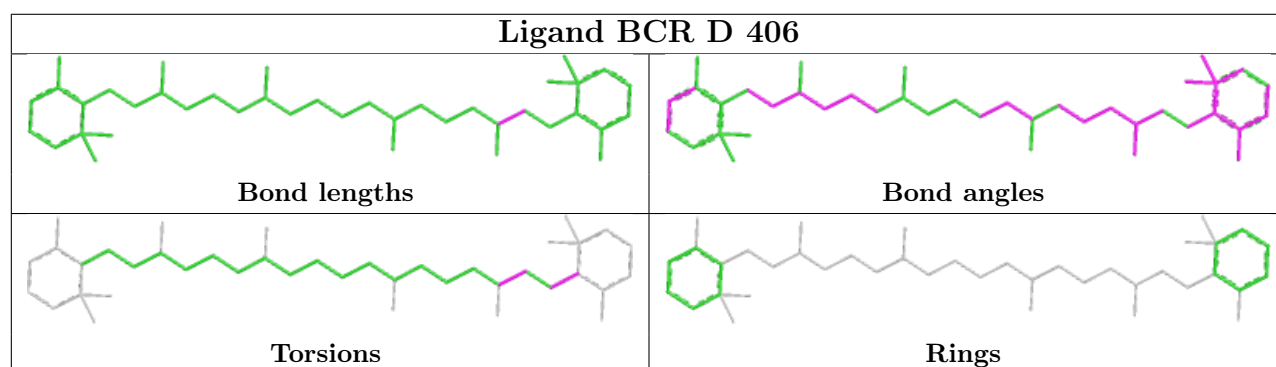
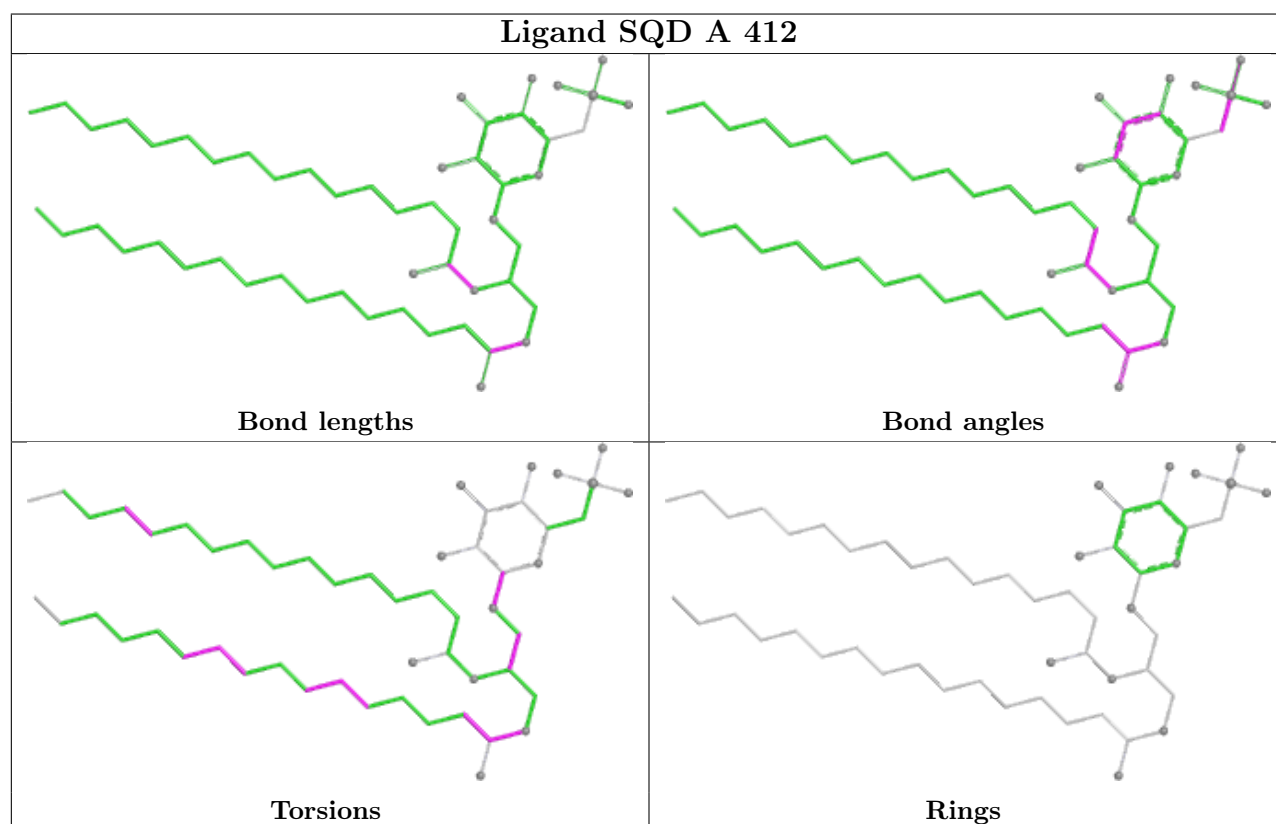
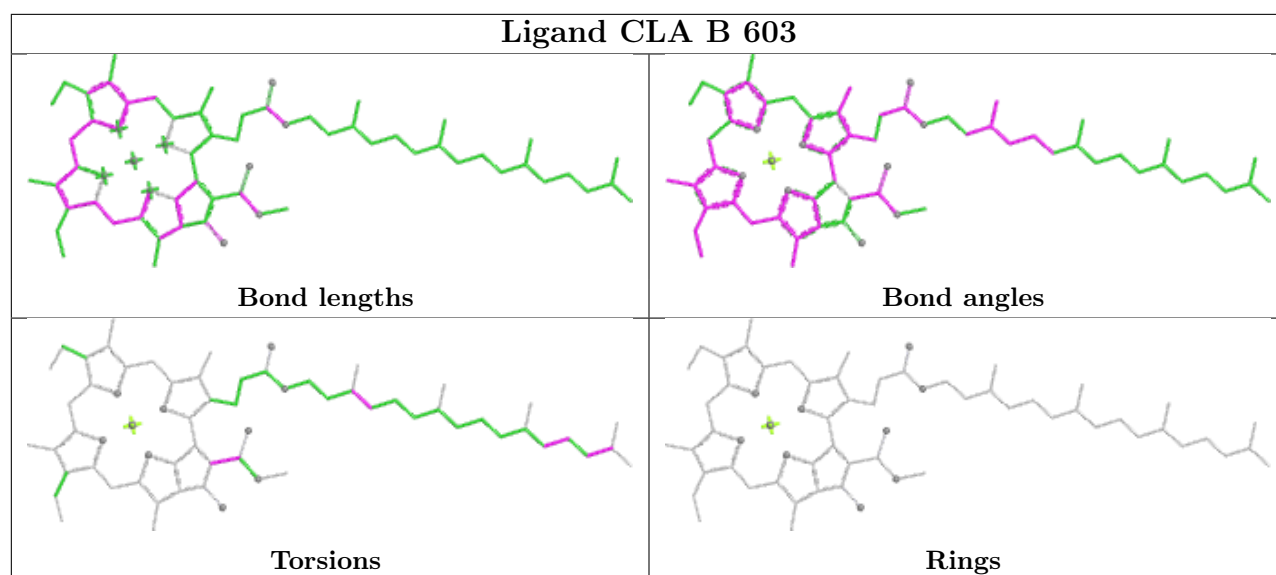
Ligand CLA C 509



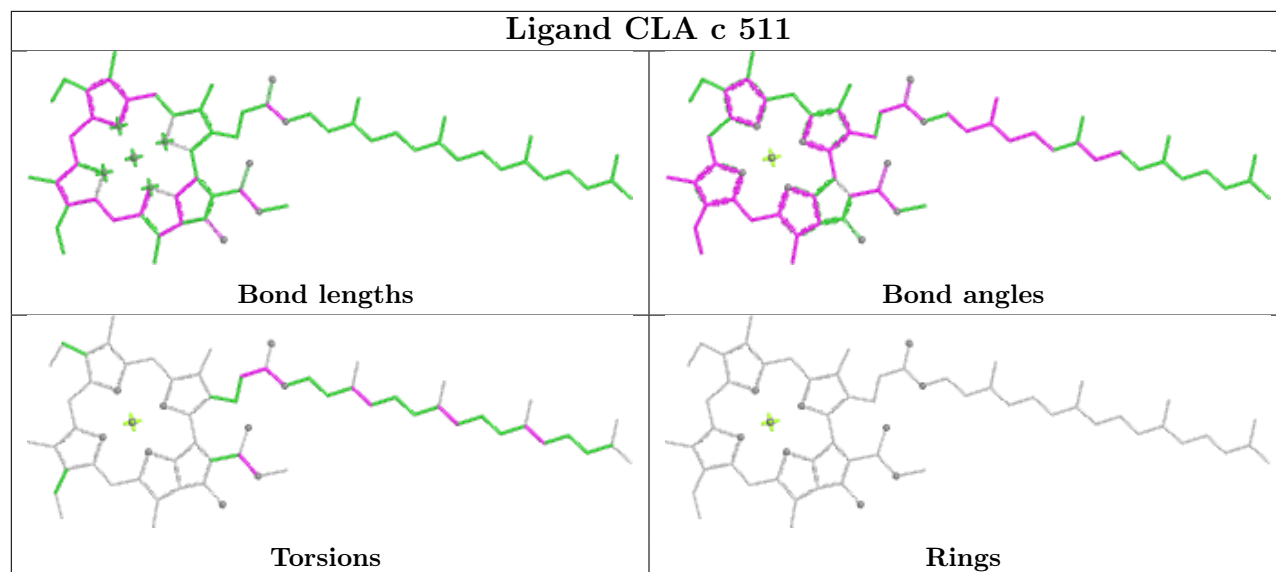
Ligand HTG B 623



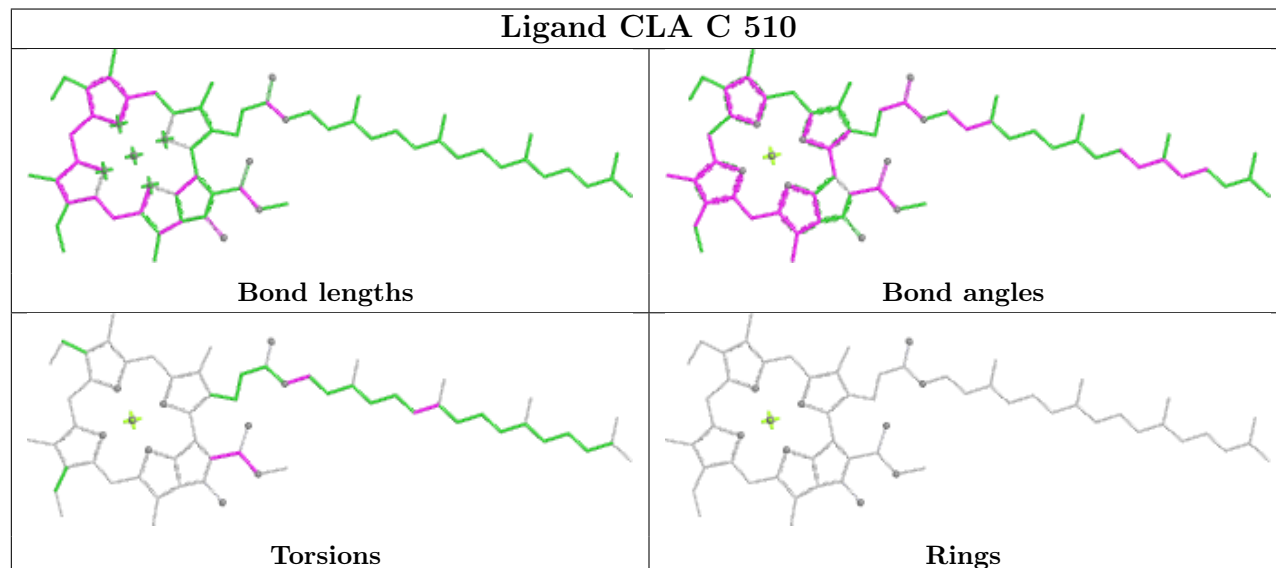




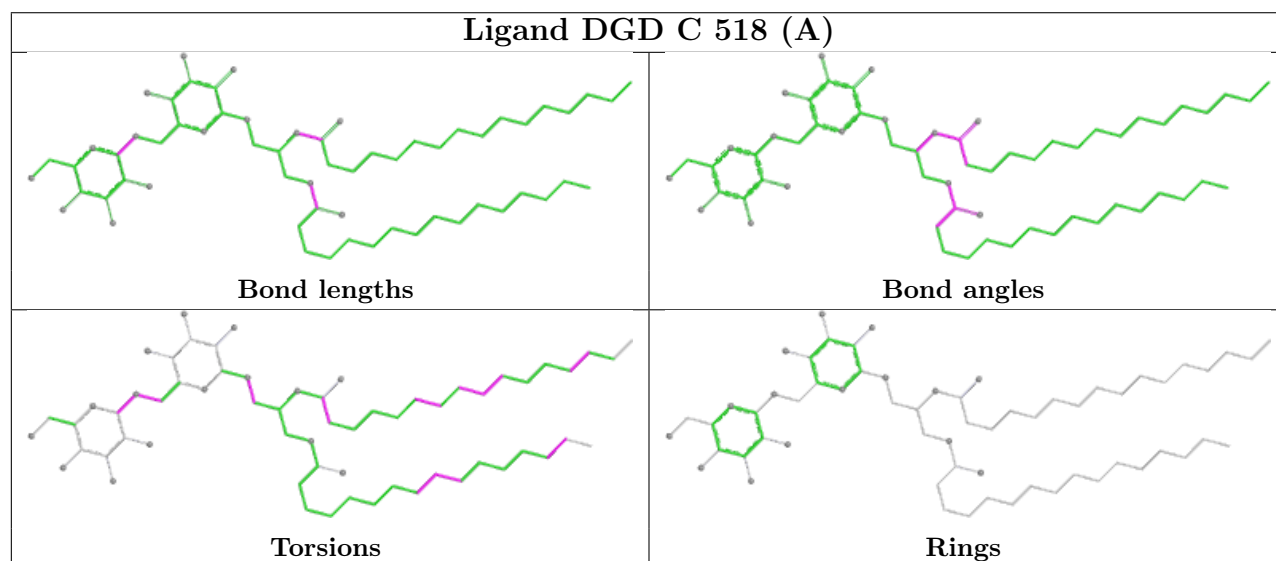
Ligand CLA c 511

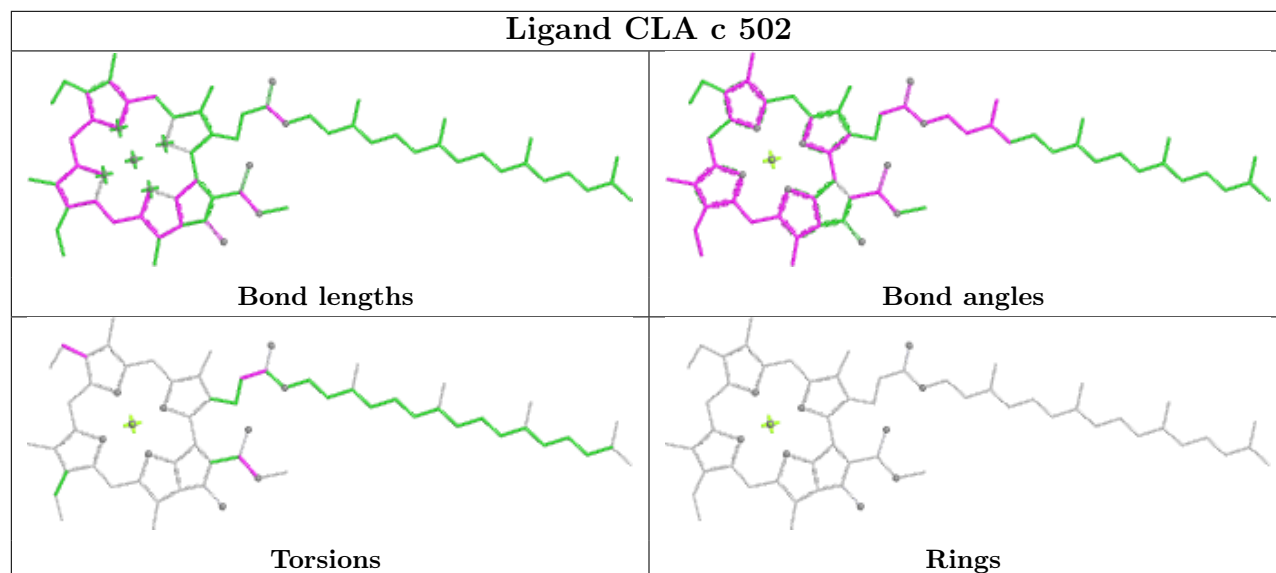
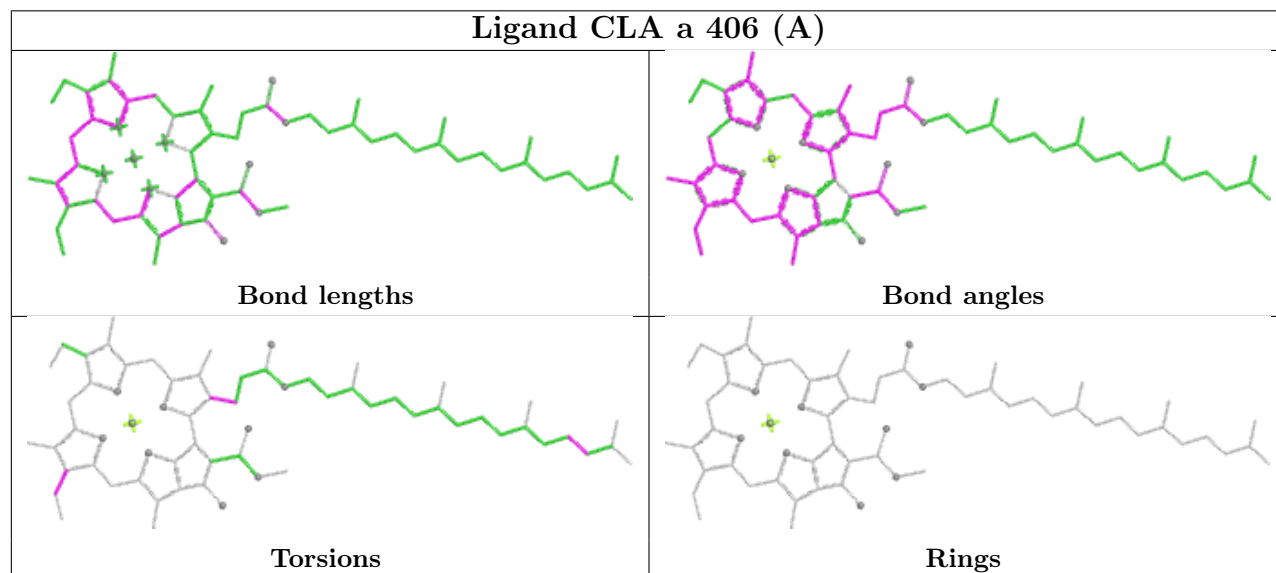
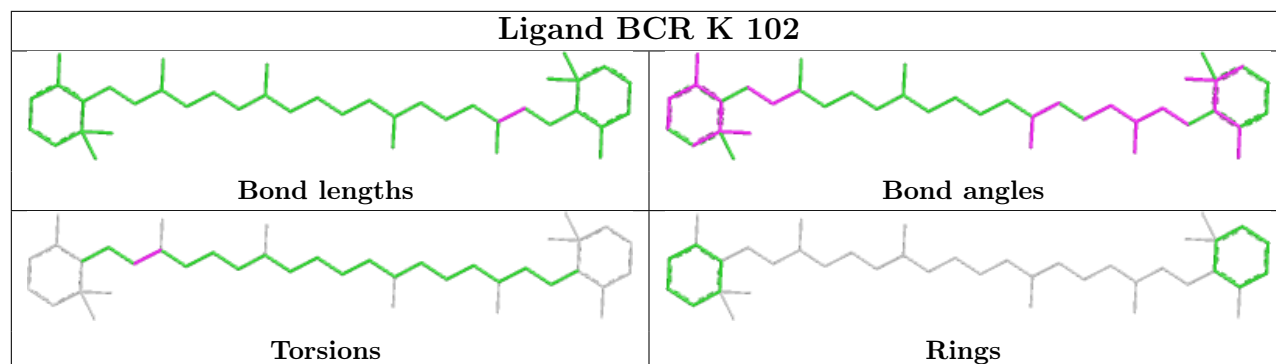


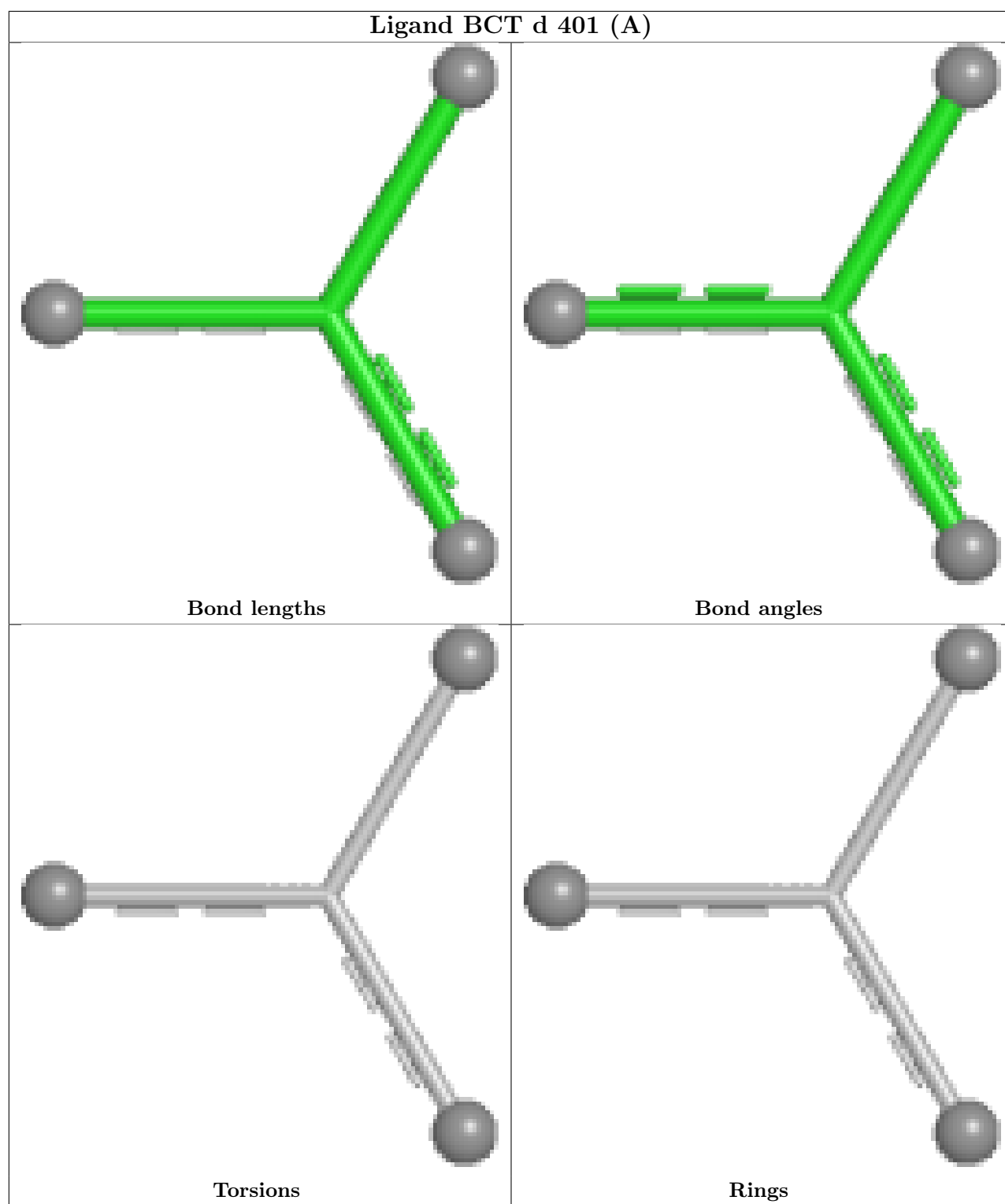
Ligand CLA C 510



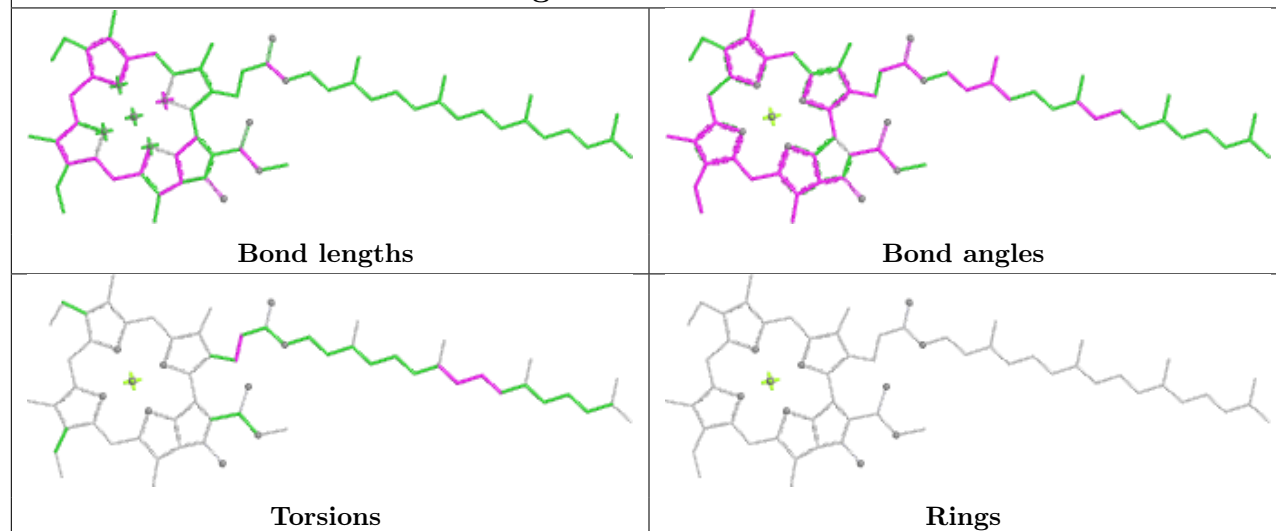
Ligand DGD C 518 (A)



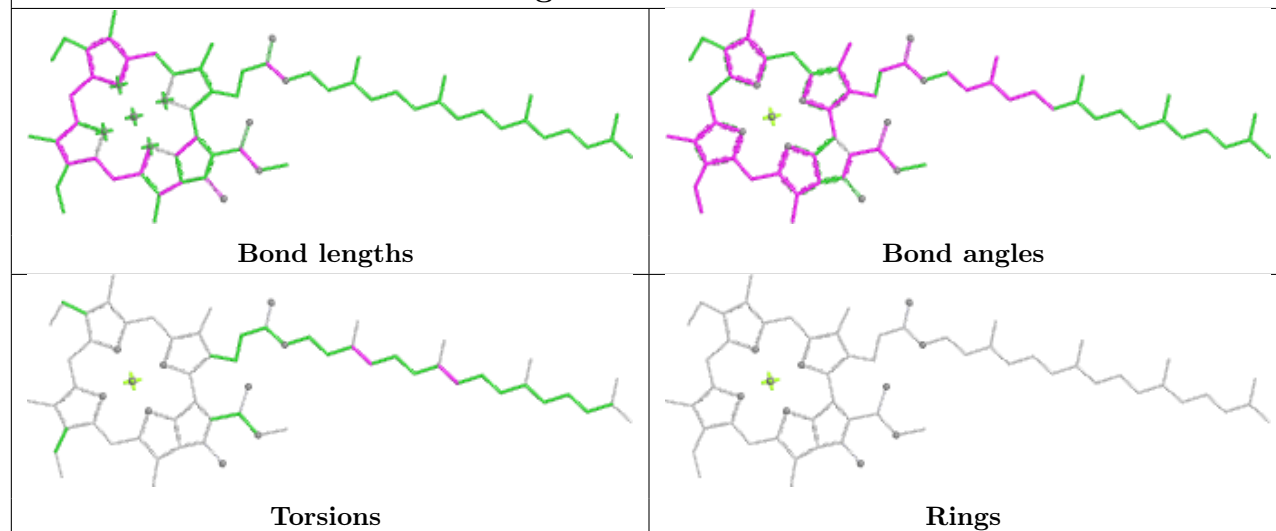




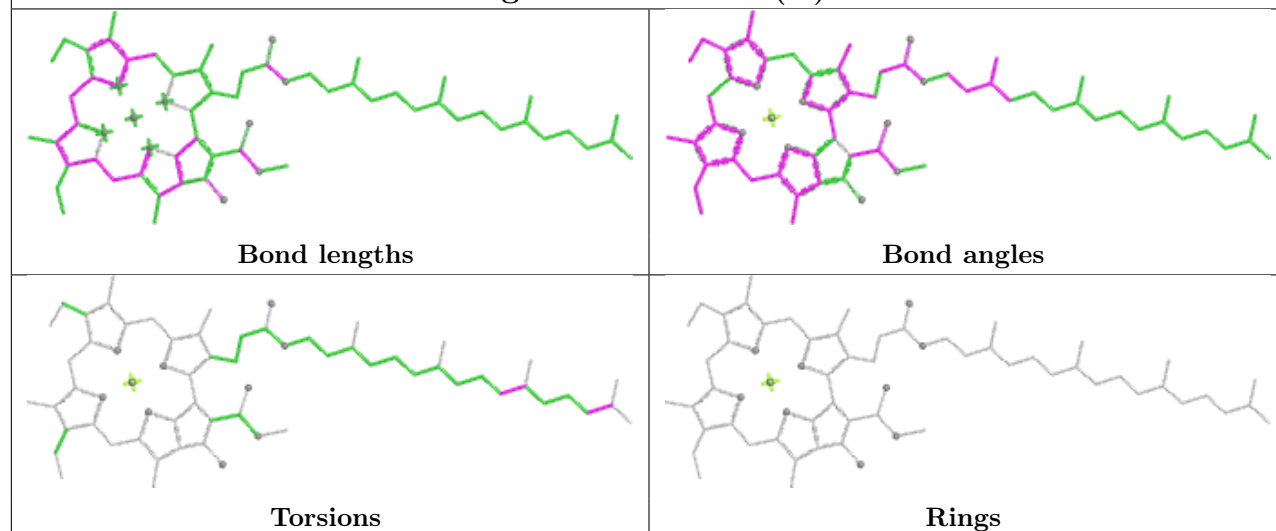
Ligand CLA B 606



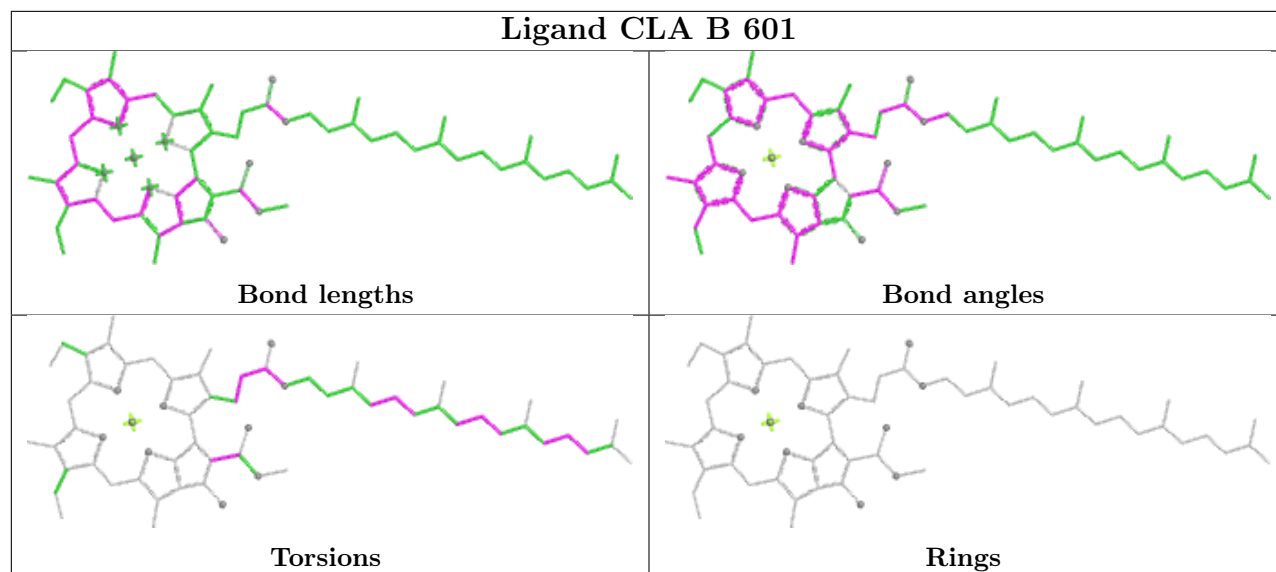
Ligand CLA b 603



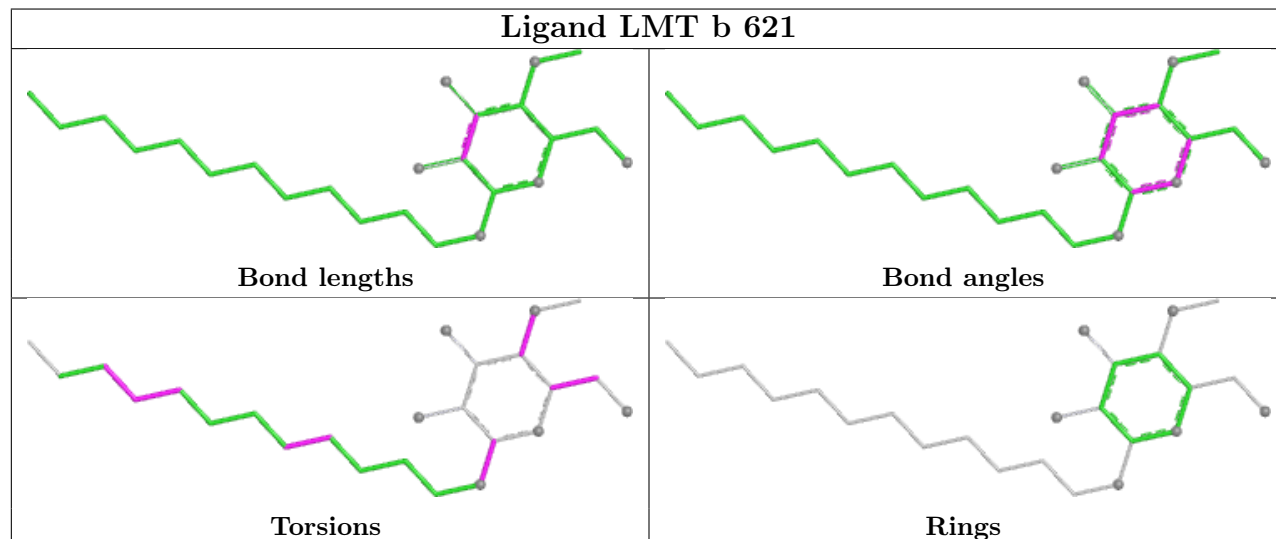
Ligand CLA d 402 (A)



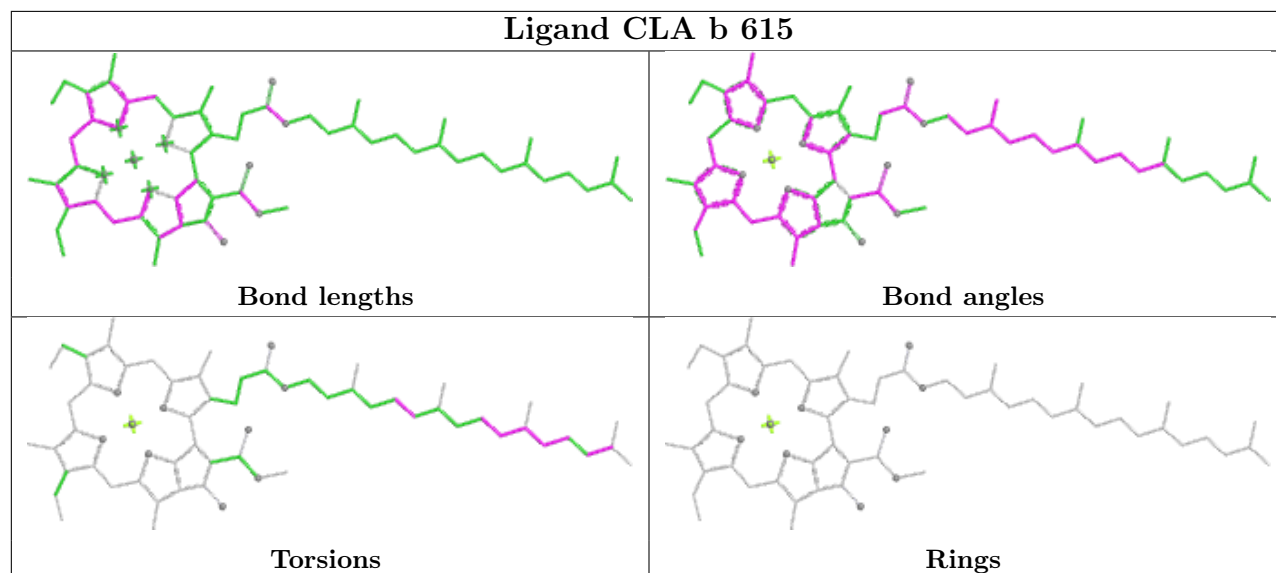
Ligand CLA B 601

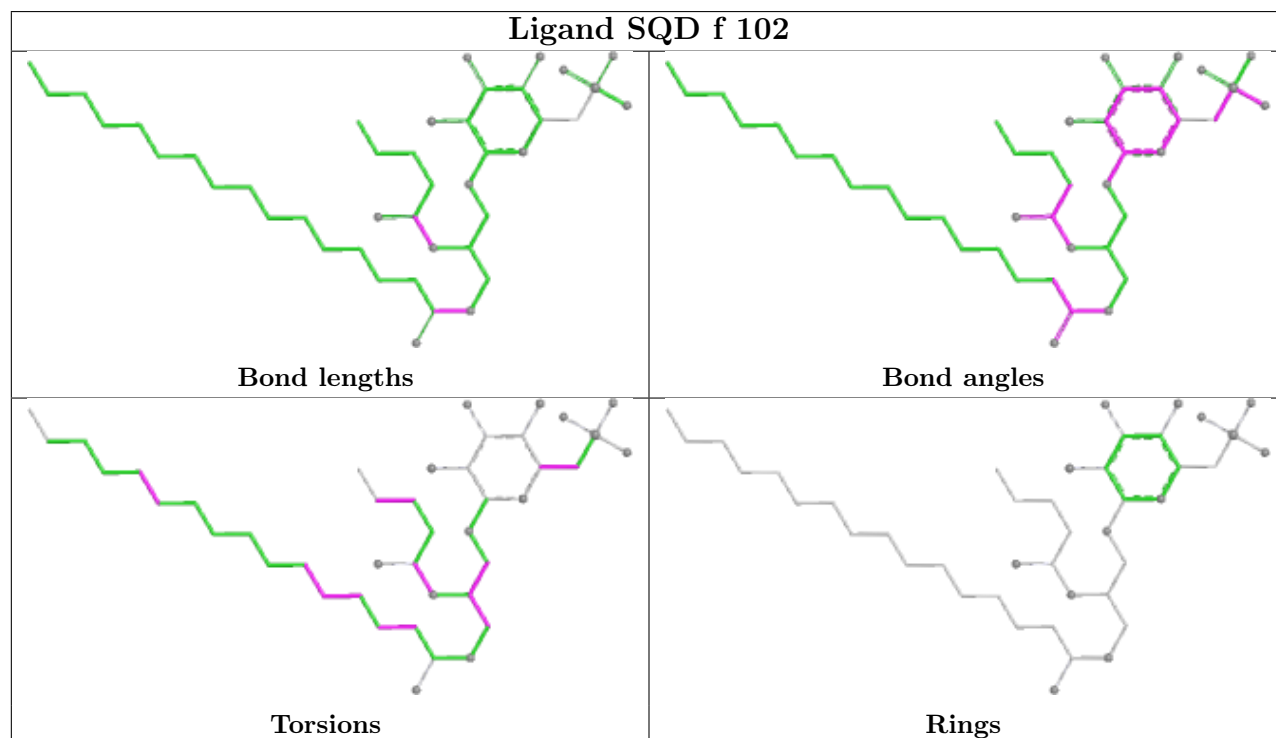
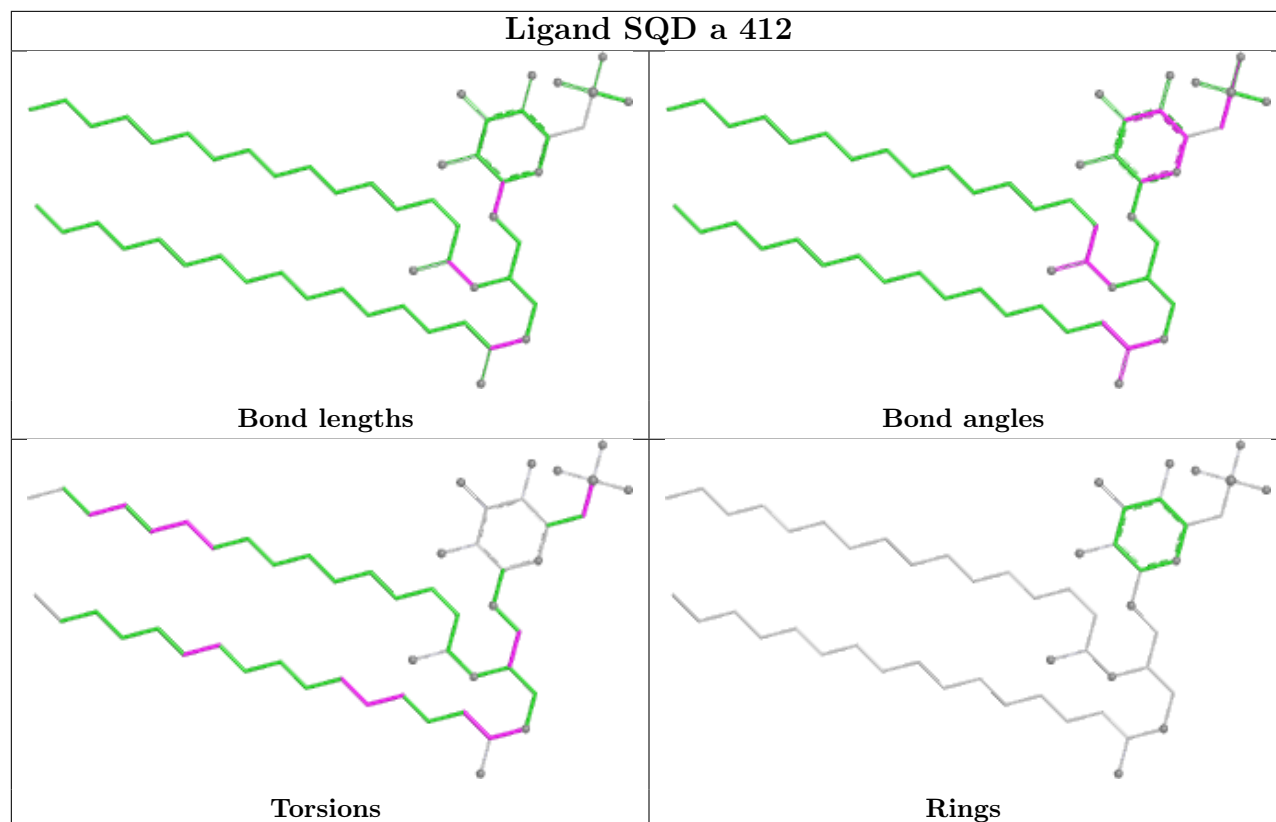


Ligand LMT b 621

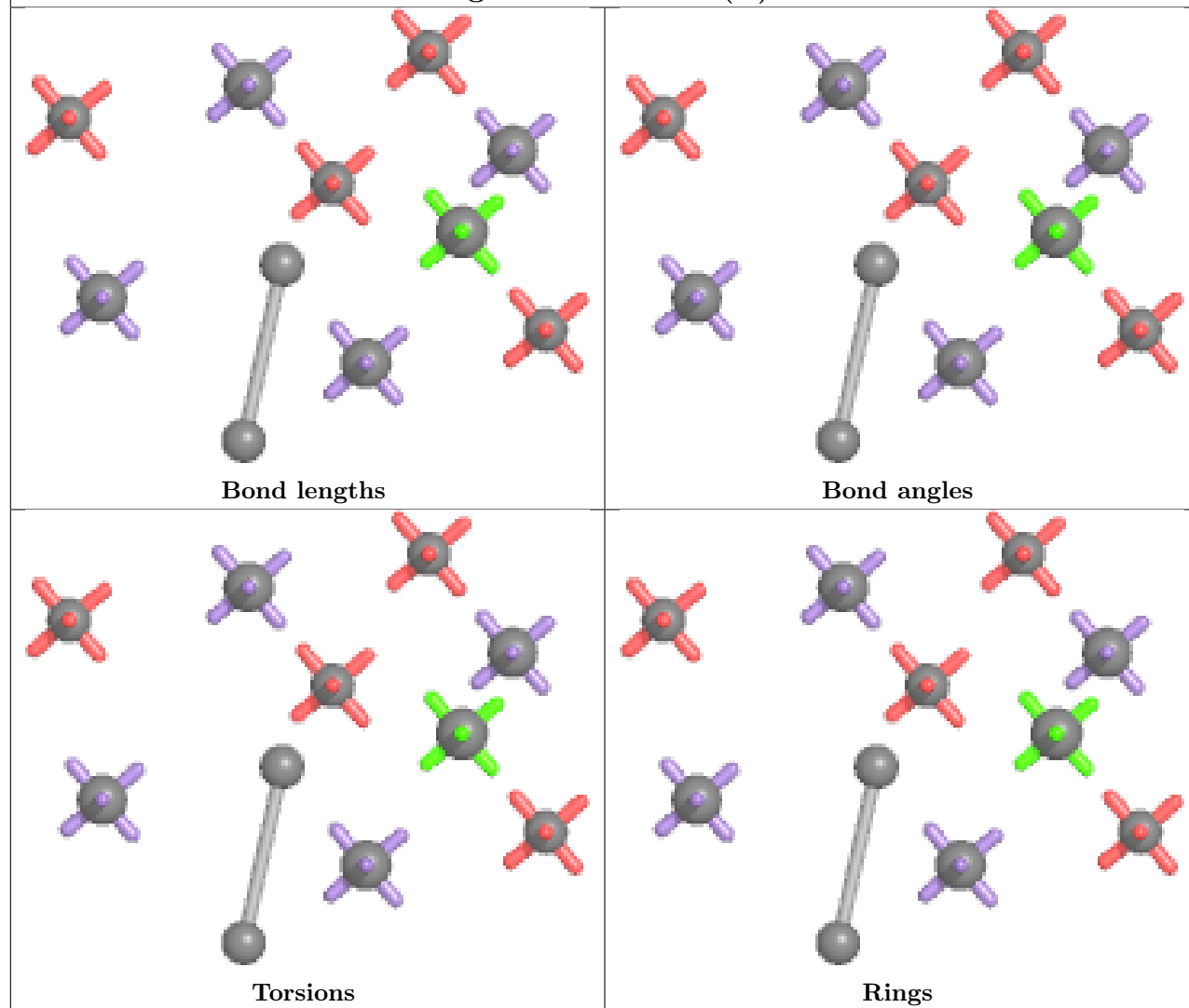


Ligand CLA b 615

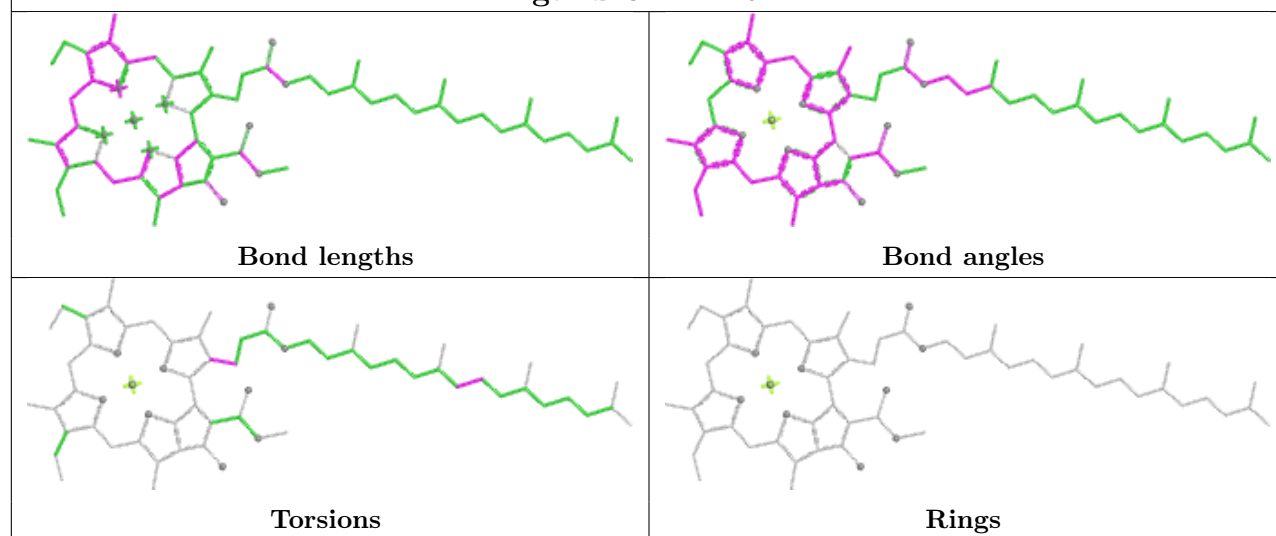




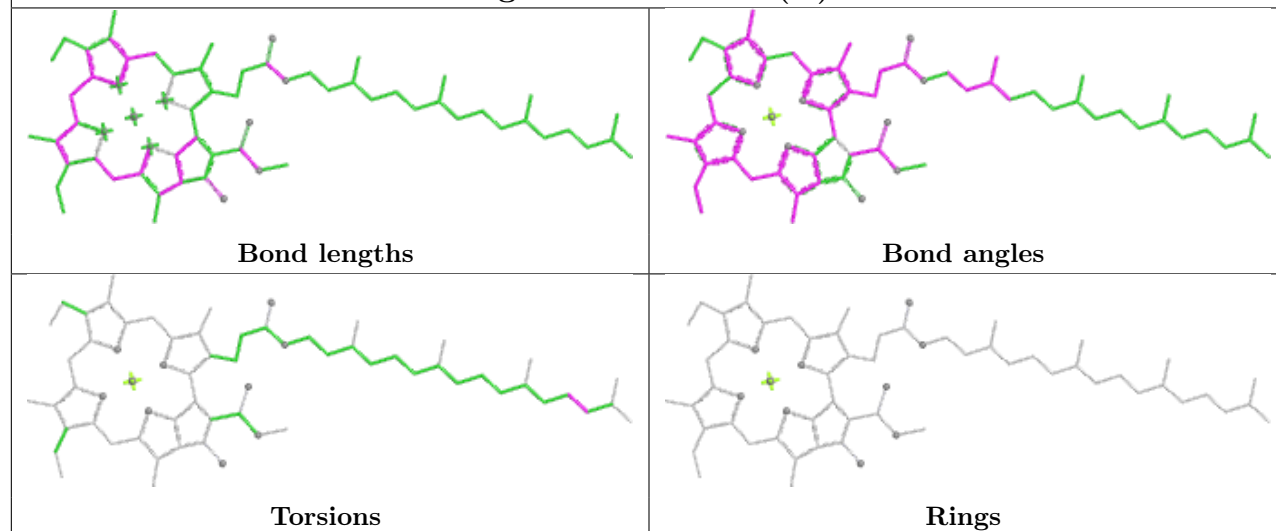
Ligand OEY a 401 (B)



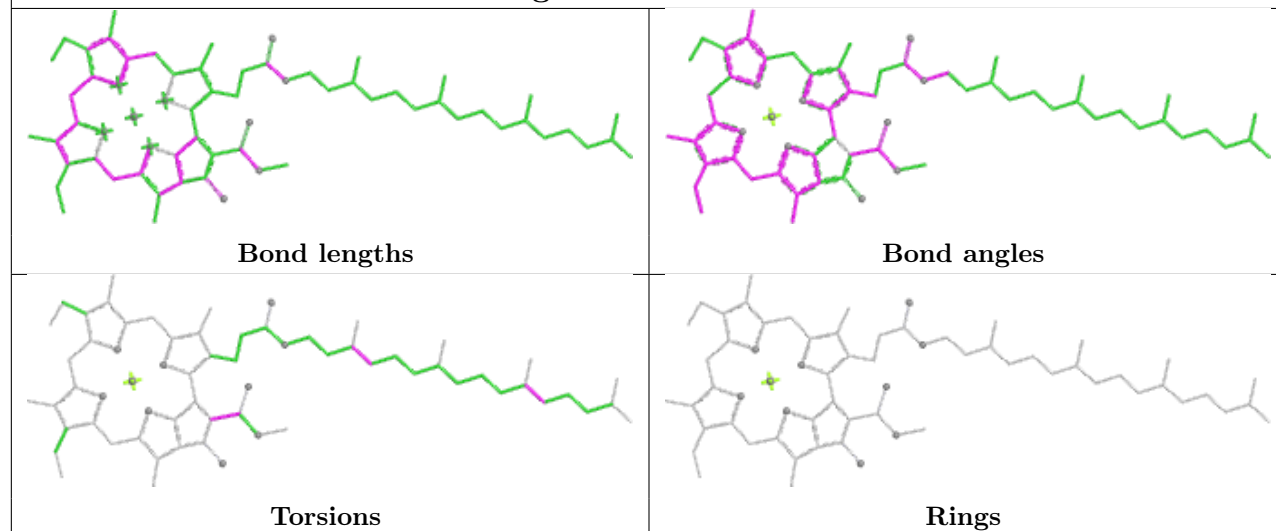
Ligand CLA B 611



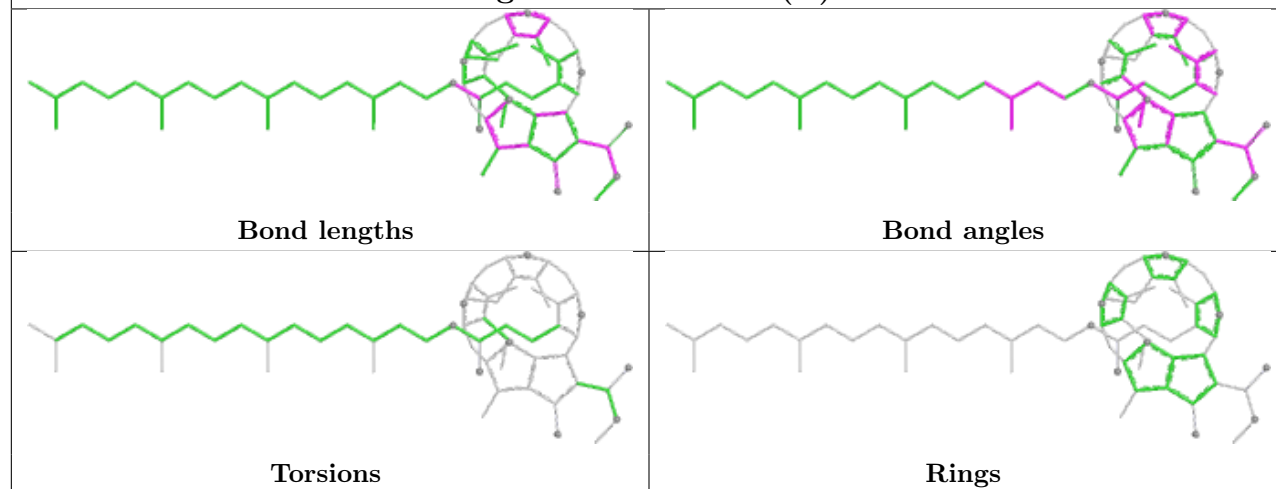
Ligand CLA A 405 (A)

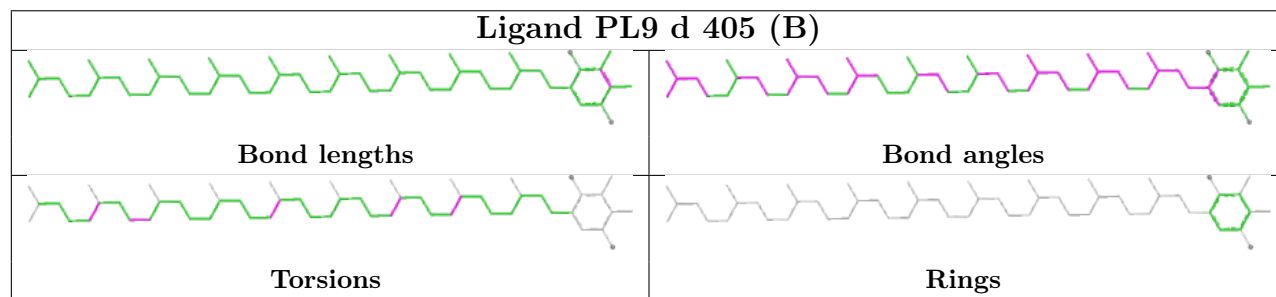
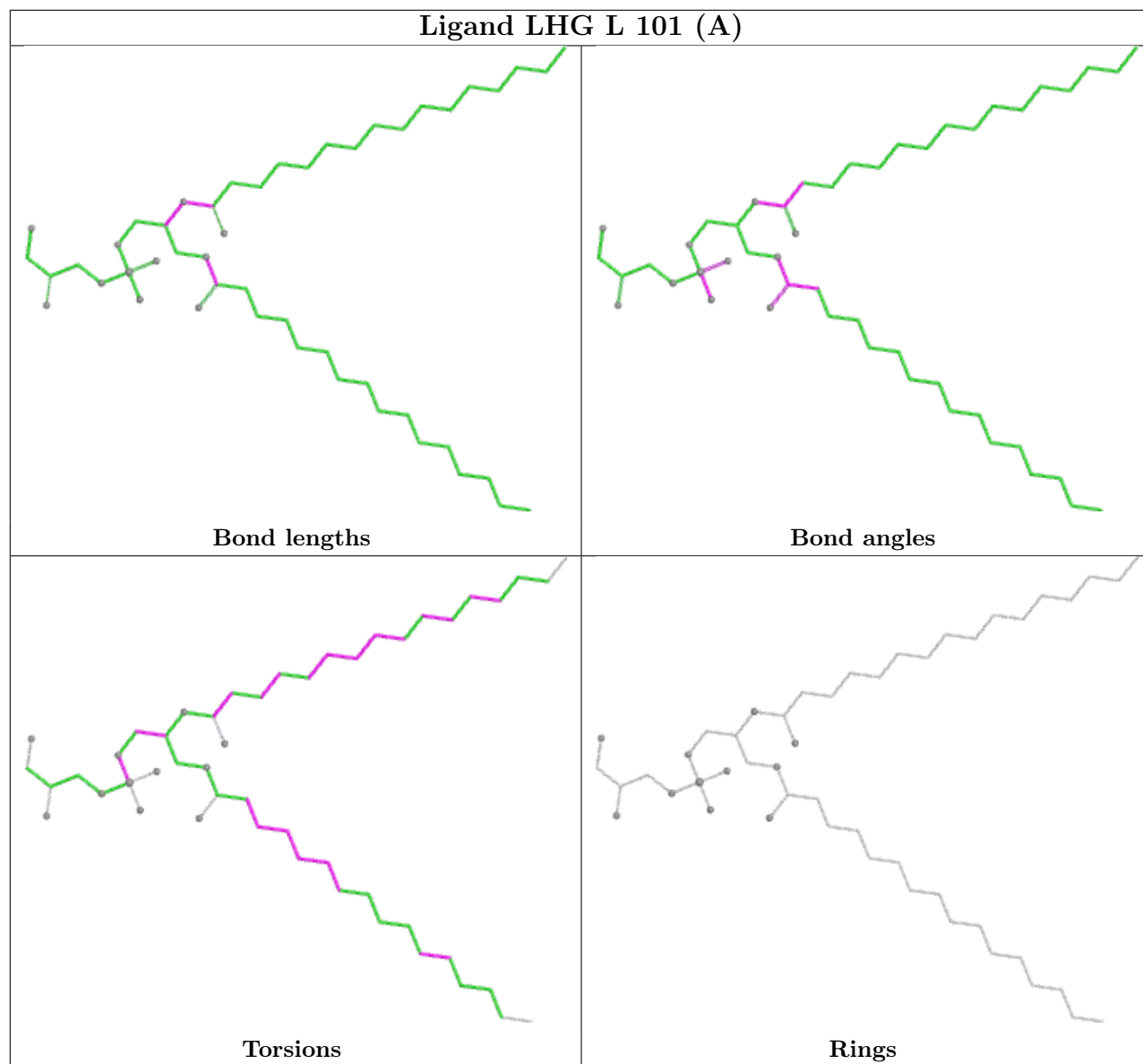


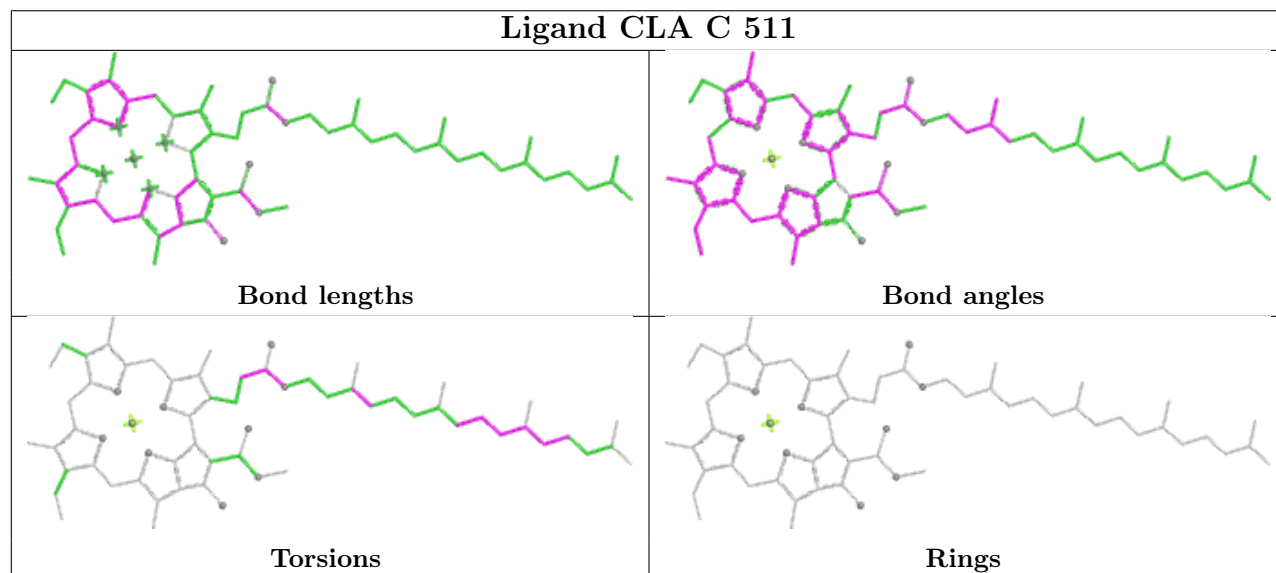
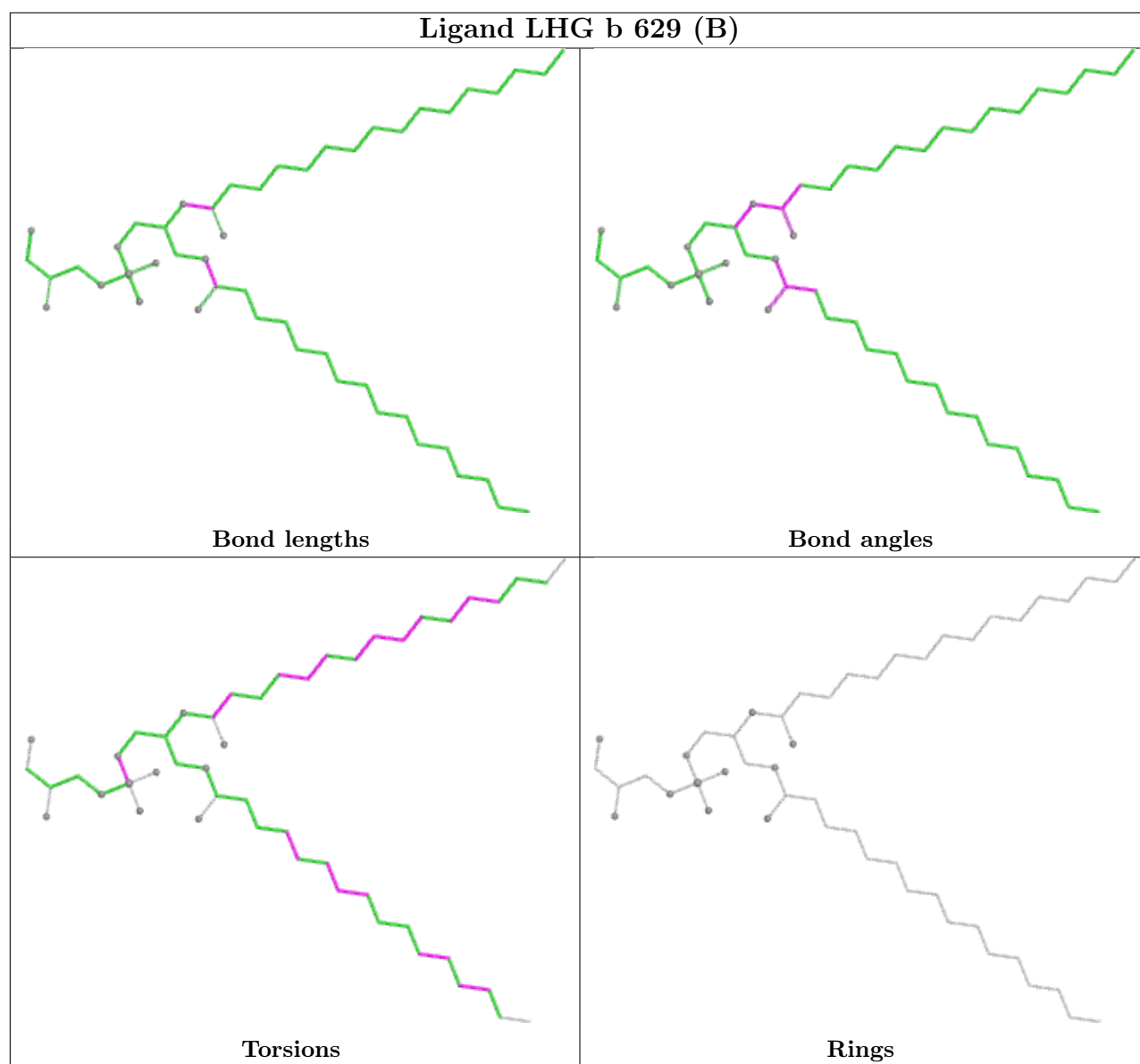
Ligand CLA C 505

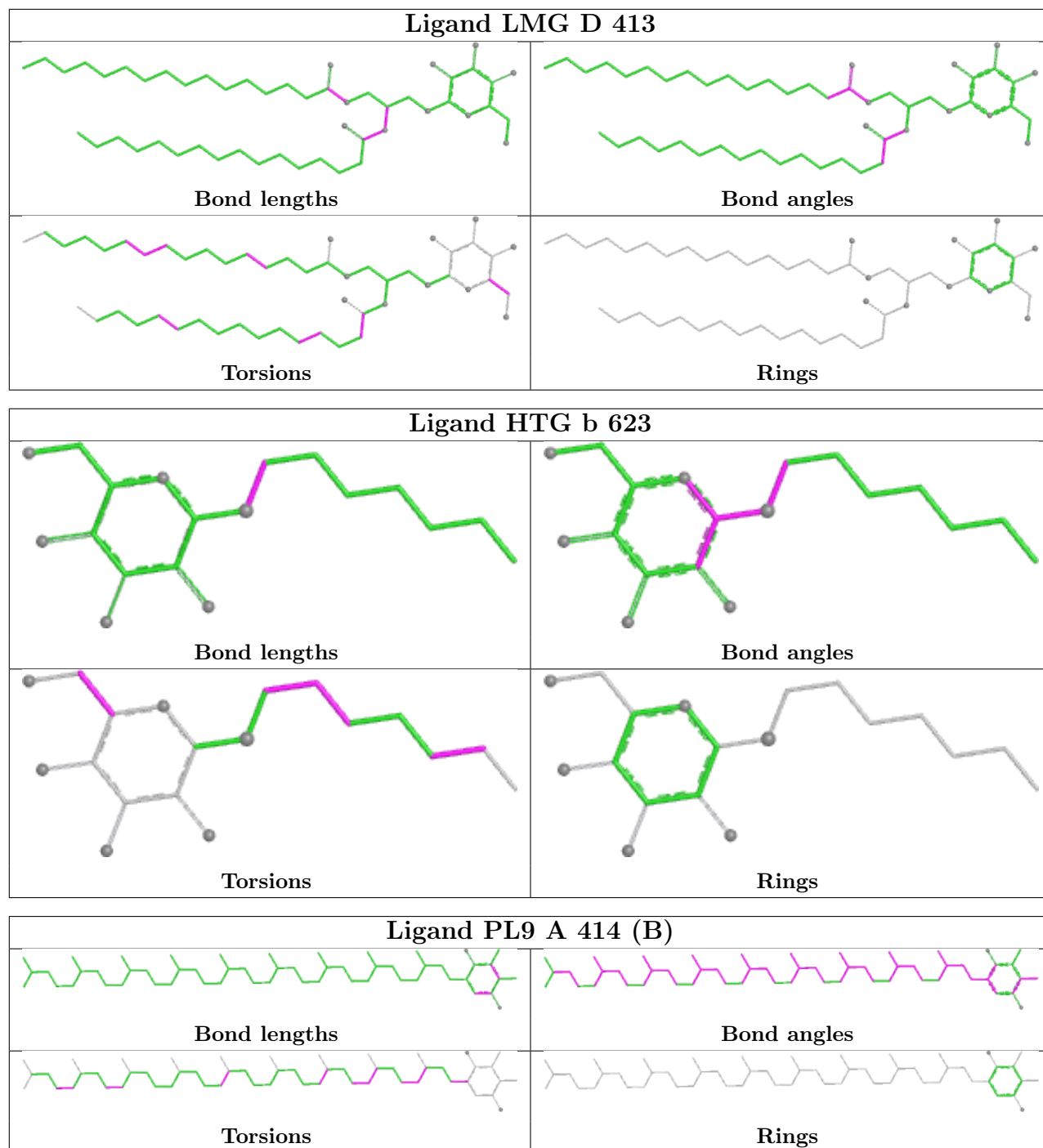


Ligand PHO A 407 (B)

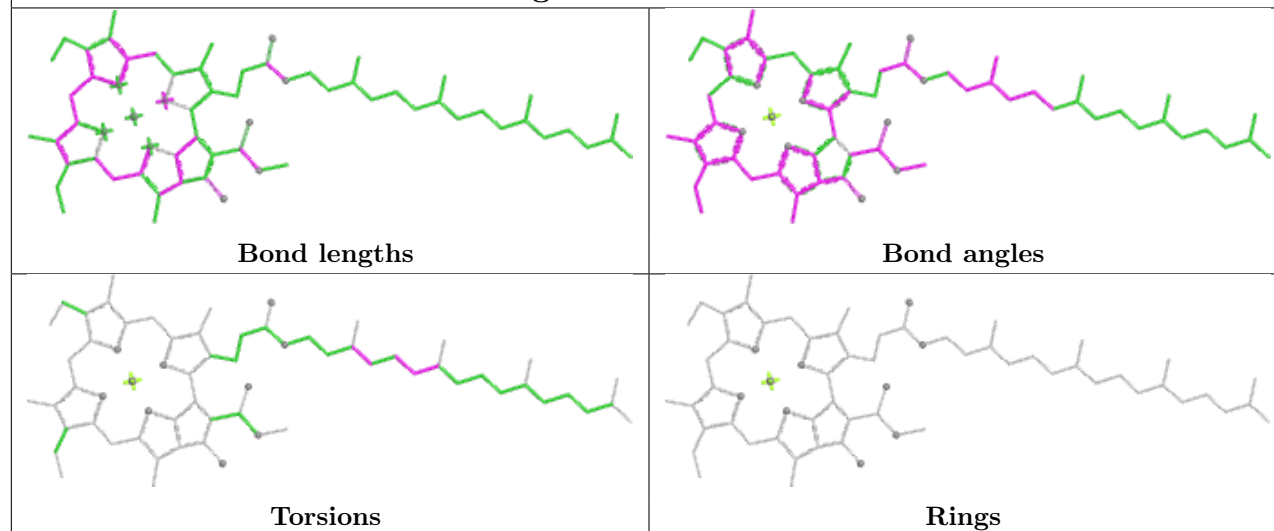




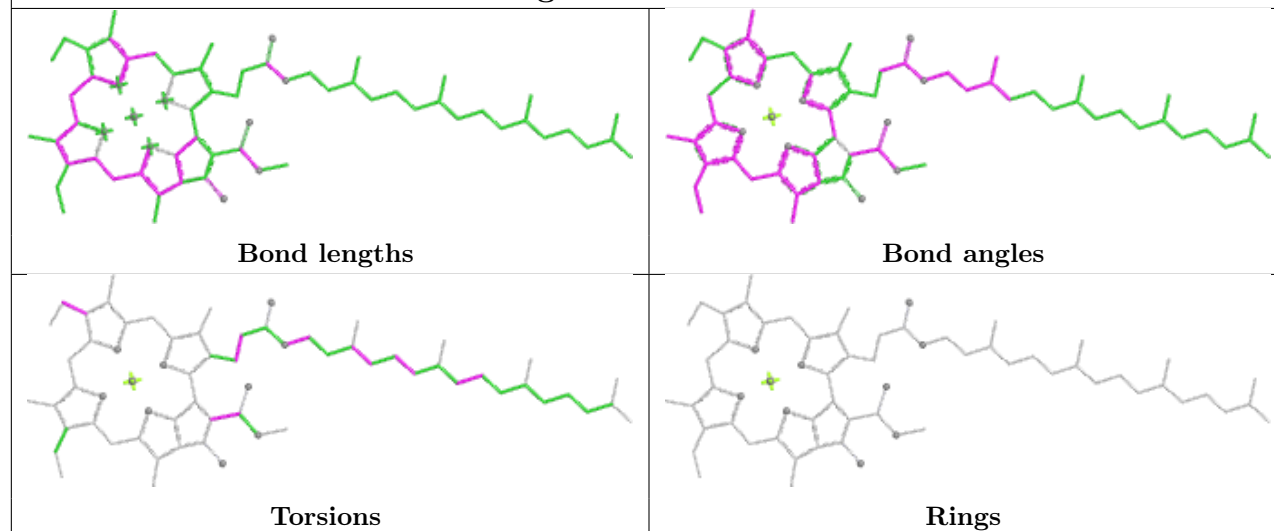




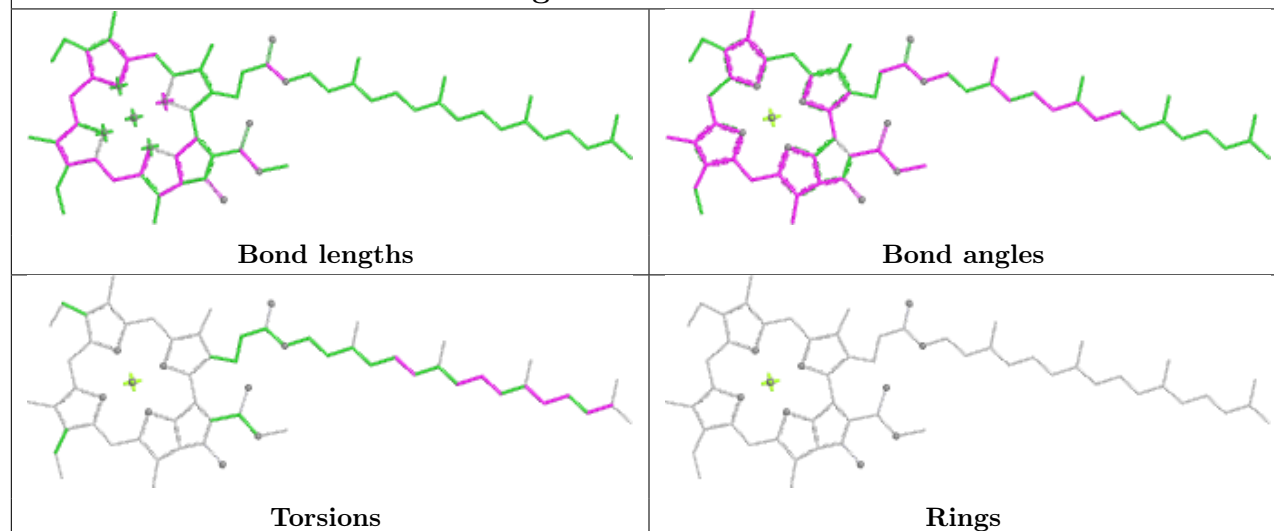
Ligand CLA B 605



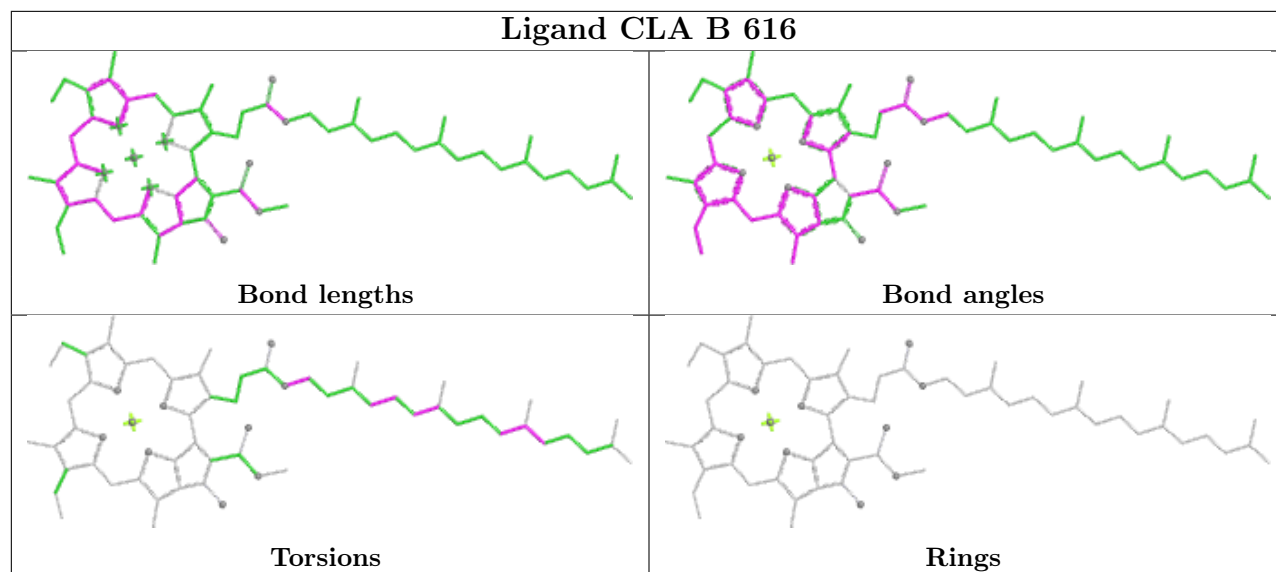
Ligand CLA c 508



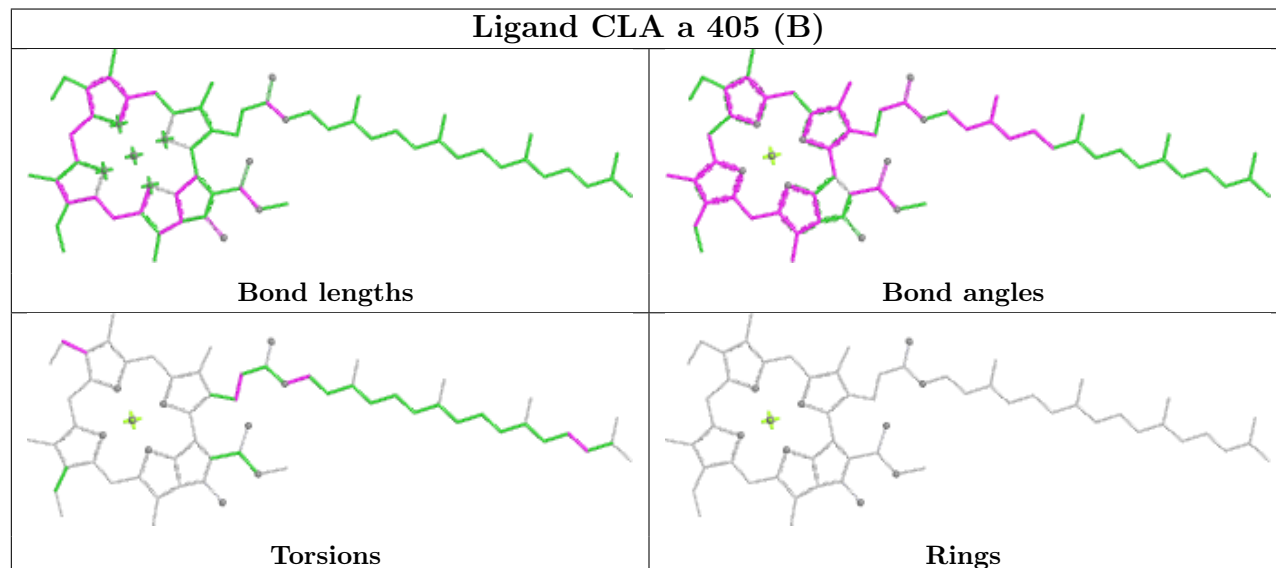
Ligand CLA B 615

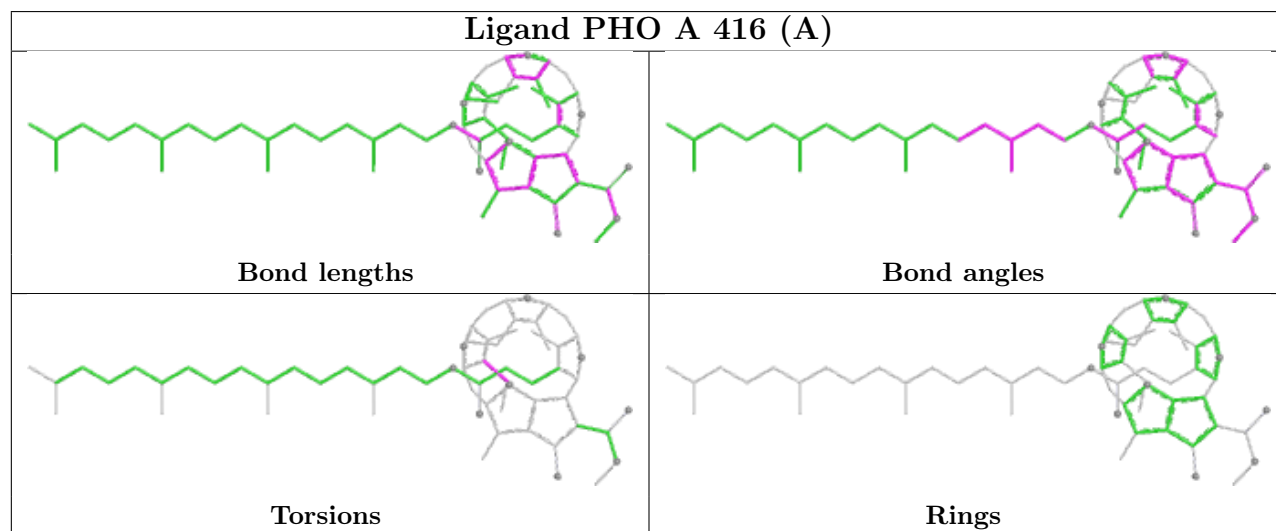
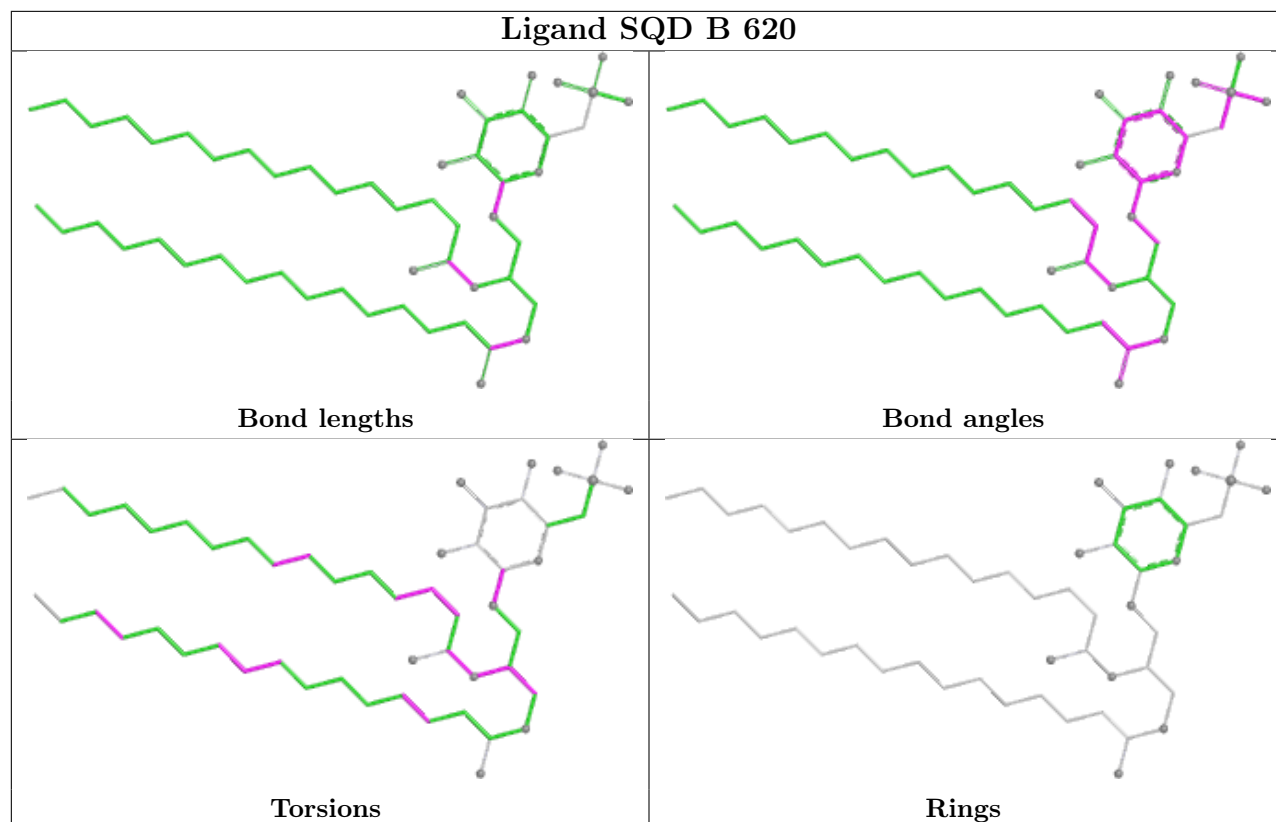


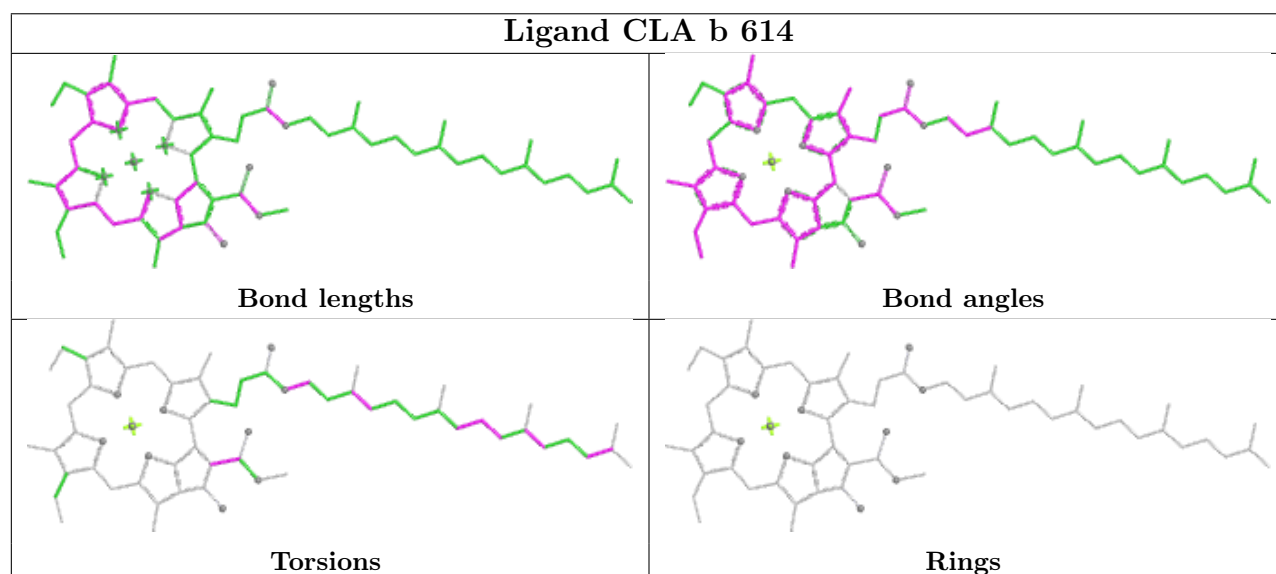
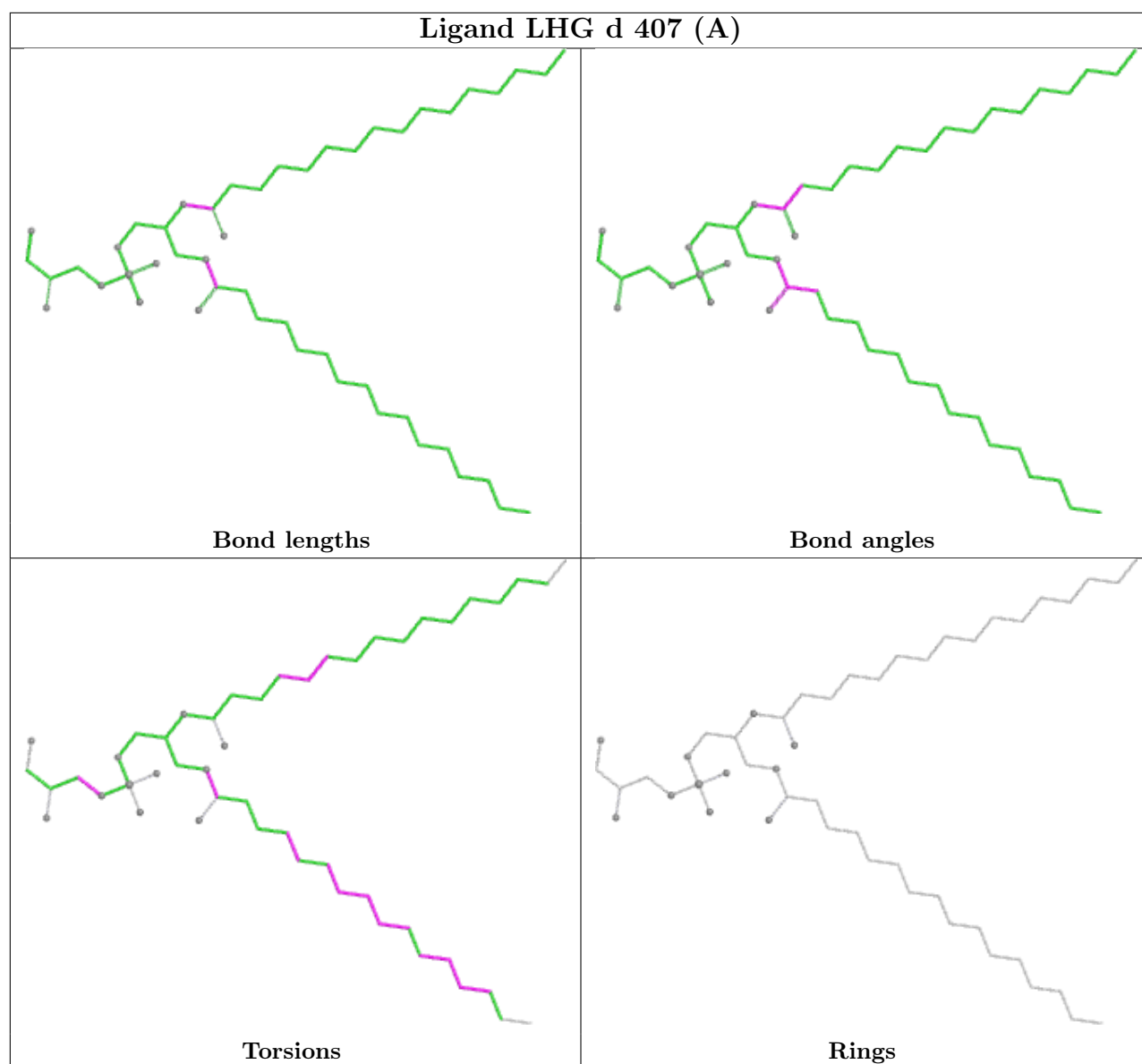
Ligand CLA B 616



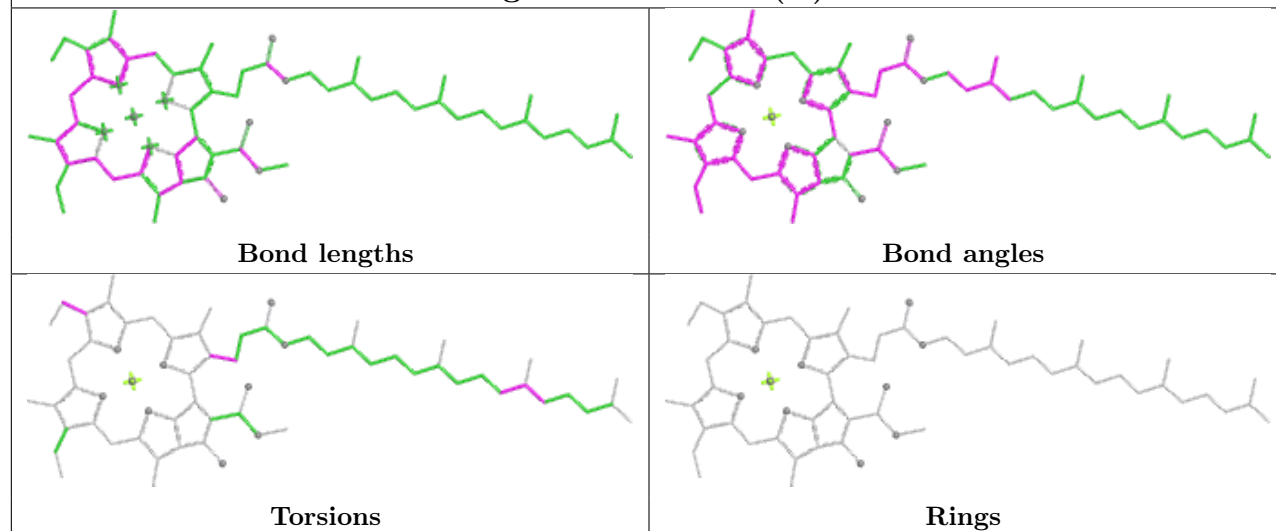
Ligand CLA a 405 (B)



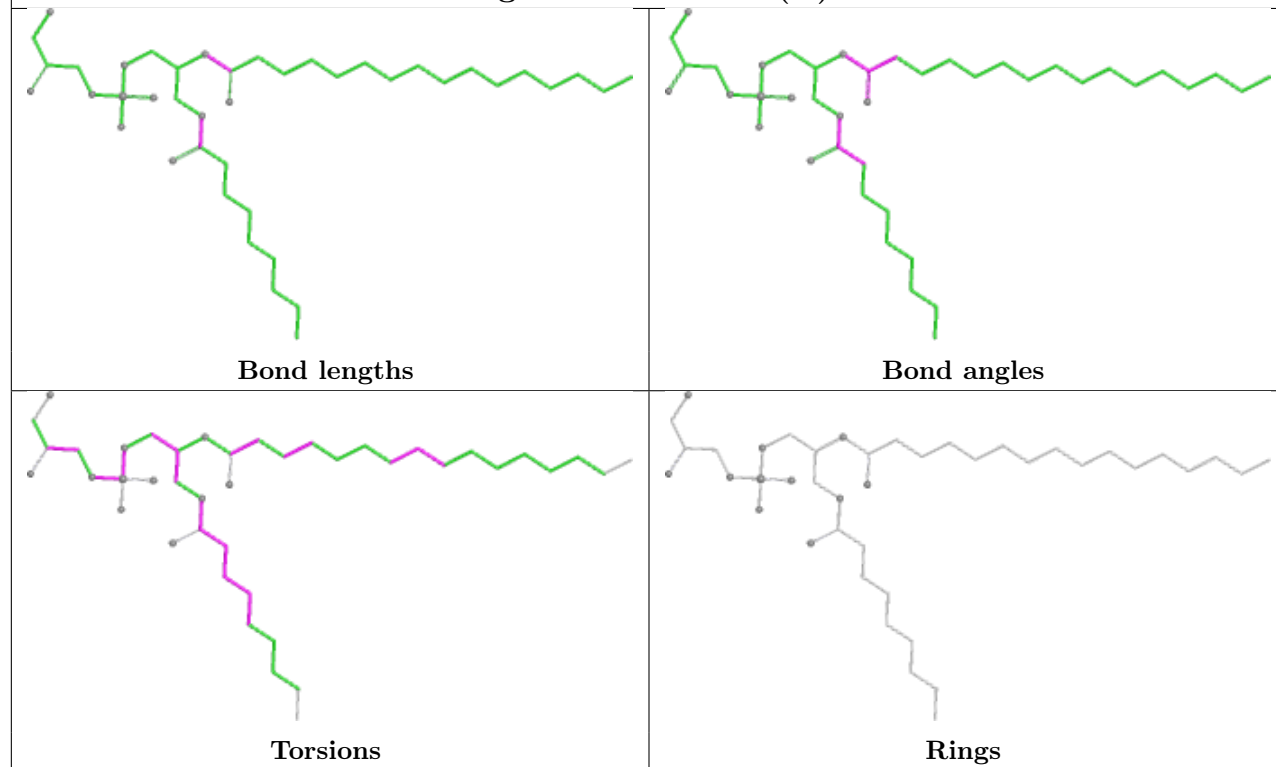


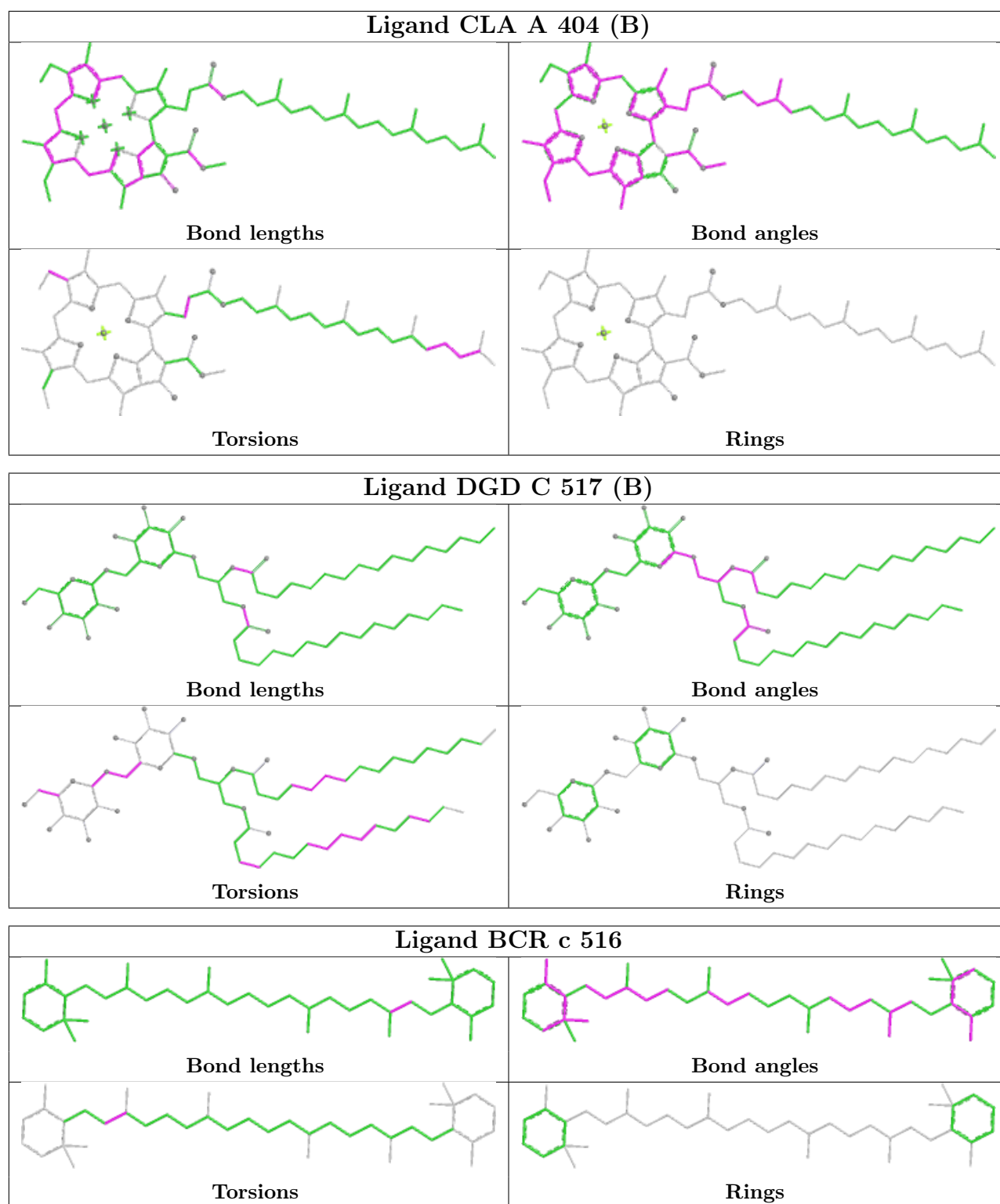


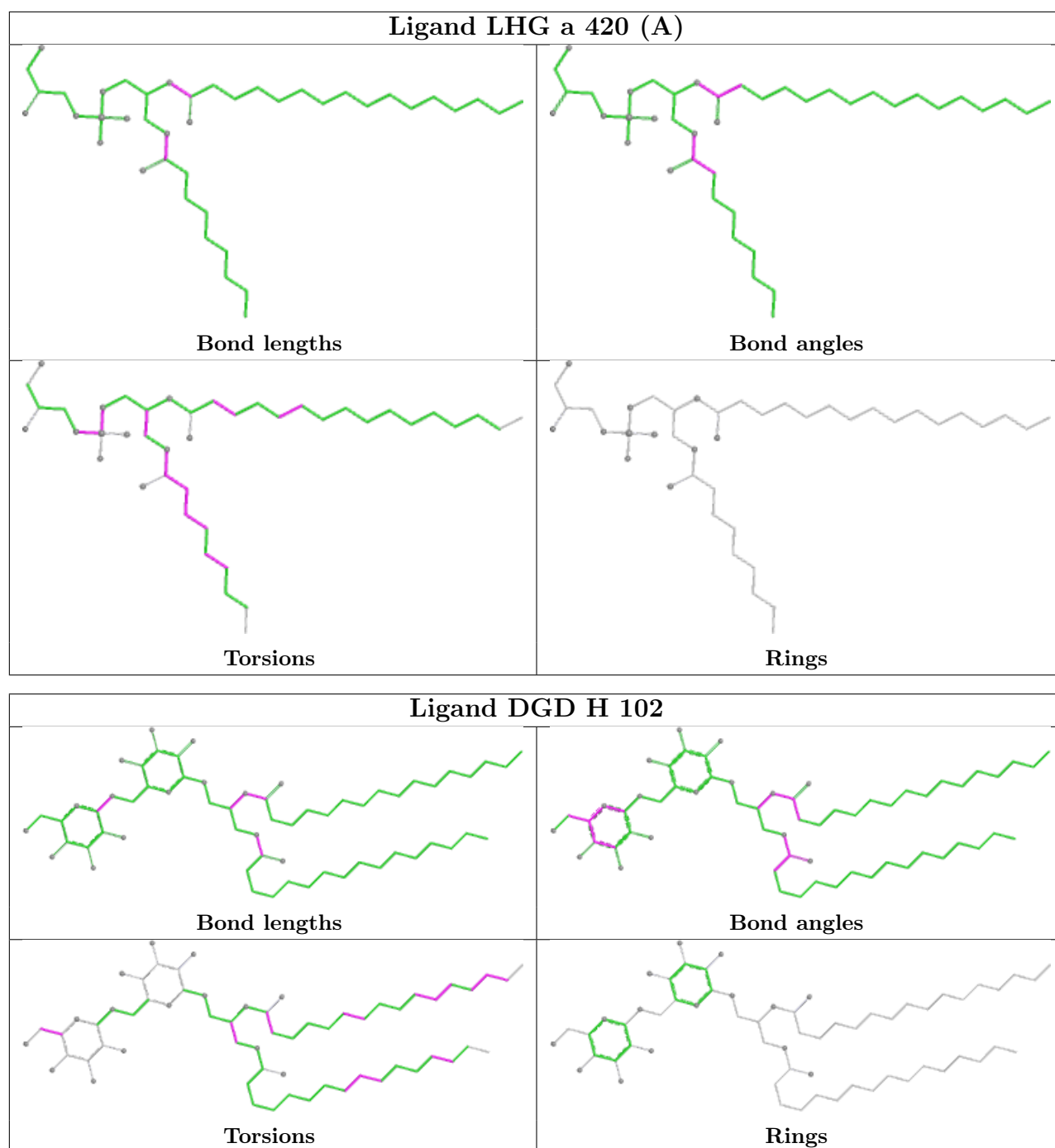
Ligand CLA a 407 (A)



Ligand LHG E 101 (A)







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	1 (0%) 90 90	19, 25, 60, 122	222 (66%)
1	a	334/344 (97%)	-0.61	1 (0%) 90 90	19, 28, 63, 131	221 (66%)
2	B	504/505 (99%)	-0.56	1 (0%) 91 92	22, 52, 81, 113	20 (3%)
2	b	504/505 (99%)	-0.46	1 (0%) 91 92	23, 56, 96, 158	19 (3%)
3	C	451/455 (99%)	-0.56	0 100 100	21, 58, 81, 134	97 (21%)
3	c	455/455 (100%)	-0.49	1 (0%) 91 92	24, 65, 86, 121	100 (21%)
4	D	342/342 (100%)	-0.70	0 100 100	19, 43, 63, 128	114 (33%)
4	d	341/342 (99%)	-0.66	0 100 100	20, 49, 74, 126	116 (34%)
5	E	81/84 (96%)	-0.33	0 100 100	51, 68, 98, 147	0
5	e	79/84 (94%)	-0.31	1 (1%) 75 76	32, 76, 122, 142	2 (2%)
6	F	34/44 (77%)	-0.58	0 100 100	53, 61, 89, 111	0
6	f	31/44 (70%)	-0.29	1 (3%) 50 50	54, 67, 95, 134	1 (3%)
7	H	64/65 (98%)	-0.34	1 (1%) 70 71	52, 61, 85, 107	0
7	h	64/65 (98%)	-0.30	1 (1%) 70 71	38, 71, 93, 105	1 (1%)
8	I	37/38 (97%)	-0.17	0 100 100	55, 63, 119, 145	0
8	i	37/38 (97%)	-0.32	0 100 100	53, 63, 113, 130	0
9	J	38/39 (97%)	-0.38	0 100 100	50, 66, 116, 159	0
9	j	39/39 (100%)	-0.23	0 100 100	56, 76, 128, 155	0
10	K	37/37 (100%)	-0.69	0 100 100	56, 66, 84, 102	0
10	k	37/37 (100%)	-0.45	0 100 100	64, 74, 95, 111	0
11	L	36/37 (97%)	-0.65	0 100 100	21, 43, 113, 128	2 (5%)
11	l	36/37 (97%)	-0.56	0 100 100	23, 45, 100, 117	2 (5%)
12	M	32/36 (88%)	-0.64	0 100 100	25, 47, 75, 125	1 (3%)
12	m	33/36 (91%)	-0.57	0 100 100	23, 46, 69, 139	2 (6%)

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%)	-0.51	1 (0%) 88 89	20, 64, 116, 165	10 (4%)
13	o	243/244 (99%)	-0.45	0 100 100	22, 67, 121, 155	8 (3%)
14	T	29/32 (90%)	-0.68	0 100 100	25, 46, 53, 63	6 (20%)
14	t	29/32 (90%)	-0.66	0 100 100	26, 46, 59, 71	5 (17%)
15	U	96/104 (92%)	-0.64	0 100 100	24, 56, 88, 101	4 (4%)
15	u	97/104 (93%)	-0.66	0 100 100	28, 60, 82, 119	4 (4%)
16	V	137/137 (100%)	-0.71	0 100 100	22, 55, 78, 102	6 (4%)
16	v	137/137 (100%)	-0.55	0 100 100	26, 69, 101, 131	6 (4%)
17	X	38/40 (95%)	-0.22	0 100 100	33, 72, 92, 112	1 (2%)
17	x	38/40 (95%)	-0.03	0 100 100	66, 78, 124, 154	0
18	Y	29/30 (96%)	-0.15	0 100 100	66, 82, 115, 121	0
18	y	29/30 (96%)	-0.18	0 100 100	75, 88, 107, 113	0
19	Z	62/62 (100%)	-0.28	0 100 100	65, 79, 131, 149	0
19	z	62/62 (100%)	0.10	0 100 100	80, 92, 137, 164	0
20	R	34/34 (100%)	0.60	2 (5%) 28 26	89, 113, 135, 148	0
All	All	5283/5384 (98%)	-0.52	12 (0%) 91 92	19, 56, 100, 165	970 (18%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.9
5	e	79[A]	PHE	3.4
6	f	16[A]	PHE	2.9
2	b	499	VAL	2.8
1	a	11	ALA	2.6
2	B	494	GLY	2.3
20	R	19	ALA	2.3
20	R	28	VAL	2.3
7	h	65	LEU	2.2
3	c	245[A]	ILE	2.2
13	O	39[A]	ARG	2.1
1	A	11	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
14	FME	T	1	10/11	0.95	0.08	44,52,66,69	0
8	FME	I	1	10/11	0.96	0.07	58,70,80,82	0
14	FME	t	1	10/11	0.96	0.07	41,47,64,74	0
12	FME	m	1	10/11	0.97	0.07	48,62,89,111	0
8	FME	i	1	10/11	0.97	0.07	51,70,75,80	0
12	FME	M	1	10/11	0.98	0.06	47,58,93,94	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
30	UNL	m	102	10/-	0.69	0.20	68,74,92,95	0
31	LMT	F	101	35/35	0.69	0.15	99,125,174,181	0
27	GOL	a	418	6/6	0.70	0.14	74,91,102,106	0
30	UNL	a	415	30/-	0.70	0.12	82,107,135,143	0
30	UNL	A	415	28/-	0.71	0.13	75,106,122,143	0
30	UNL	j	101	10/-	0.71	0.18	74,84,94,103	0
30	UNL	K	101[A]	34/-	0.71	0.14	76,100,114,120	34
30	UNL	K	101[B]	34/-	0.71	0.14	75,100,114,120	34
30	UNL	J	101	10/-	0.72	0.23	62,77,82,84	0
31	LMT	e	101	35/35	0.72	0.14	101,141,173,185	0
34	HTG	C	522	19/19	0.72	0.13	100,120,131,134	0
31	LMT	A	417	35/35	0.74	0.13	63,110,133,143	0
31	LMT	c	501	35/35	0.74	0.13	96,127,142,156	0
31	LMT	A	419	35/35	0.74	0.12	84,125,147,154	0
32	LHG	a	420[A]	42/49	0.74	0.13	86,128,146,160	42
32	LHG	a	420[B]	42/49	0.74	0.13	86,128,146,161	42

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
31	LMT	B	630	35/35	0.74	0.13	64,112,141,149	0
27	GOL	o	302	6/6	0.75	0.18	79,96,106,107	0
26	SQD	f	102	43/54	0.75	0.13	98,125,174,183	0
30	UNL	I	101	40/-	0.75	0.15	70,98,154,158	0
30	UNL	c	525[B]	32/-	0.77	0.14	85,105,118,125	32
30	UNL	c	525[A]	32/-	0.77	0.14	85,105,118,124	32
36	CA	F	103	1/1	0.77	0.23	123,123,123,123	0
30	UNL	l	101	10/-	0.78	0.15	65,71,90,94	0
27	GOL	B	627	6/6	0.79	0.14	68,83,98,114	0
27	GOL	A	411	6/6	0.79	0.15	62,73,77,86	0
30	UNL	D	411	40/-	0.80	0.13	62,92,143,144	0
31	LMT	b	621	25/35	0.80	0.12	80,108,155,168	0
30	UNL	b	626	33/-	0.80	0.12	66,92,150,160	0
30	UNL	i	101	40/-	0.80	0.13	69,101,149,158	0
36	CA	f	103	1/1	0.80	0.14	118,118,118,118	0
34	HTG	B	623	19/19	0.81	0.14	61,90,112,112	0
30	UNL	d	409	36/-	0.81	0.11	68,91,127,139	0
34	HTG	D	412	16/19	0.81	0.12	86,106,131,142	0
27	GOL	d	412	6/6	0.81	0.21	50,69,79,87	0
33	LMG	C	521	51/55	0.81	0.11	59,109,155,182	0
27	GOL	b	624	6/6	0.82	0.17	85,90,98,109	0
27	GOL	o	303	6/6	0.82	0.13	76,84,95,96	0
29	PL9	a	414[B]	55/55	0.83	0.14	73,95,109,111	55
29	PL9	a	414[A]	55/55	0.83	0.14	74,95,109,111	55
34	HTG	b	623	19/19	0.83	0.11	77,129,156,158	0
34	HTG	c	522	19/19	0.83	0.09	99,118,138,139	0
31	LMT	M	102	35/35	0.83	0.10	70,116,169,173	0
31	LMT	t	101	26/35	0.83	0.12	68,101,143,157	0
29	PL9	A	414[B]	55/55	0.84	0.13	59,83,98,106	55
27	GOL	O	302	6/6	0.84	0.10	81,88,98,99	0
27	GOL	v	202[A]	6/6	0.84	0.12	65,79,82,84	6
34	HTG	V	202	11/19	0.84	0.09	75,108,122,129	0
27	GOL	v	202[B]	6/6	0.84	0.12	65,79,82,84	6
31	LMT	B	631	25/35	0.84	0.12	56,79,145,158	0
34	HTG	d	410	16/19	0.84	0.11	84,118,135,151	0
30	UNL	B	626	33/-	0.84	0.13	49,100,140,150	0
29	PL9	A	414[A]	55/55	0.84	0.13	59,83,98,106	55
27	GOL	l	102[A]	6/6	0.85	0.15	61,90,91,96	6
27	GOL	l	102[B]	6/6	0.85	0.15	61,90,91,96	6
27	GOL	O	303	6/6	0.85	0.12	73,86,96,96	0
26	SQD	a	412	54/54	0.85	0.10	66,94,138,154	0
31	LMT	B	628	35/35	0.85	0.10	64,104,142,147	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
31	LMT	m	103	35/35	0.86	0.11	59,91,105,123	0
34	HTG	b	622	19/19	0.86	0.11	55,79,115,117	0
33	LMG	c	521	51/55	0.86	0.10	74,127,151,183	0
33	LMG	Z	101	37/55	0.86	0.13	73,119,150,165	0
31	LMT	b	627	25/35	0.86	0.12	49,93,146,152	0
27	GOL	c	527	6/6	0.86	0.17	96,104,109,110	0
26	SQD	A	412	54/54	0.86	0.10	61,84,127,151	0
26	SQD	b	620	54/54	0.87	0.10	60,93,127,136	0
31	LMT	M	101	35/35	0.88	0.10	59,95,122,132	0
33	LMG	z	101	39/55	0.88	0.10	70,121,149,162	0
26	SQD	B	620	54/54	0.88	0.10	61,88,137,149	0
23	CLA	b	601	65/65	0.89	0.09	60,85,120,153	0
32	LHG	E	101[A]	42/49	0.89	0.10	71,96,110,120	42
32	LHG	E	101[B]	42/49	0.89	0.10	71,96,110,120	42
34	HTG	B	622	19/19	0.89	0.11	60,85,119,121	0
27	GOL	B	629	6/6	0.89	0.11	71,76,90,96	0
27	GOL	D	414	6/6	0.89	0.15	46,63,67,82	0
26	SQD	X	101	43/54	0.89	0.11	71,104,131,133	0
27	GOL	c	526[B]	6/6	0.90	0.09	65,69,74,75	6
27	GOL	D	403	6/6	0.90	0.23	47,76,78,81	0
33	LMG	C	501	51/55	0.90	0.09	70,86,112,128	0
27	GOL	C	523[A]	6/6	0.90	0.10	56,60,64,69	6
27	GOL	C	523[B]	6/6	0.90	0.10	56,60,65,69	6
27	GOL	c	526[A]	6/6	0.90	0.09	65,69,74,75	6
27	GOL	V	203[B]	6/6	0.91	0.12	57,65,72,73	6
23	CLA	c	514	65/65	0.91	0.10	69,94,124,151	0
27	GOL	a	419	6/6	0.91	0.23	51,78,82,88	0
23	CLA	B	601	65/65	0.91	0.09	56,76,108,146	0
27	GOL	V	203[A]	6/6	0.91	0.12	57,64,72,73	6
30	UNL	D	410	17/-	0.91	0.09	56,71,101,118	0
33	LMG	a	417	51/55	0.92	0.08	67,93,108,115	0
33	LMG	c	520	51/55	0.92	0.09	61,88,133,163	0
25	BCR	T	101	40/40	0.92	0.07	40,57,73,80	0
33	LMG	m	101	51/55	0.92	0.08	50,72,94,107	0
27	GOL	B	624	6/6	0.92	0.11	63,69,80,88	0
33	LMG	B	621	51/55	0.92	0.08	48,68,90,106	0
30	UNL	d	408	17/-	0.92	0.10	64,78,111,121	0
25	BCR	d	404	40/40	0.92	0.08	50,64,99,110	0
34	HTG	B	625	19/19	0.92	0.08	65,76,101,101	0
33	LMG	d	411	51/55	0.93	0.09	52,74,116,144	0
26	SQD	A	410[A]	54/54	0.93	0.09	54,78,112,115	54
33	LMG	C	520	51/55	0.93	0.08	53,83,109,128	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	SQD	A	410[B]	54/54	0.93	0.09	54,78,112,115	54
33	LMG	D	413	51/55	0.93	0.09	47,67,117,134	0
23	CLA	C	514	65/65	0.93	0.08	59,85,113,121	0
35	DGD	C	518[A]	62/66	0.93	0.08	47,64,107,111	62
35	DGD	C	518[B]	62/66	0.93	0.08	47,63,107,111	62
32	LHG	A	418[A]	49/49	0.93	0.09	48,60,79,83	49
32	LHG	A	418[B]	49/49	0.93	0.09	48,60,80,83	49
36	CA	o	301	1/1	0.93	0.07	108,108,108,108	0
25	BCR	K	103	40/40	0.94	0.08	54,63,84,87	0
29	PL9	D	407[A]	55/55	0.94	0.07	37,47,57,68	55
29	PL9	D	407[B]	55/55	0.94	0.07	37,47,57,68	55
23	CLA	C	505	65/65	0.94	0.08	41,56,107,134	0
25	BCR	c	515	40/40	0.94	0.08	65,78,91,96	0
23	CLA	C	507	65/65	0.94	0.08	52,70,118,141	0
25	BCR	k	101	40/40	0.94	0.09	58,73,86,88	0
32	LHG	D	409[A]	49/49	0.94	0.09	47,60,109,113	49
32	LHG	D	409[B]	49/49	0.94	0.09	47,60,109,113	49
25	BCR	t	102	40/40	0.94	0.06	42,62,75,83	0
23	CLA	b	616	65/65	0.94	0.08	48,63,121,133	0
23	CLA	c	513	65/65	0.94	0.09	60,79,121,133	0
23	CLA	C	513	65/65	0.94	0.09	58,74,116,126	0
32	LHG	d	407[A]	49/49	0.94	0.09	52,62,108,122	49
32	LHG	d	407[B]	49/49	0.94	0.09	52,62,108,122	49
34	HTG	b	625	19/19	0.94	0.07	61,78,94,103	0
32	LHG	d	413[A]	49/49	0.94	0.08	49,64,78,85	49
32	LHG	d	413[B]	49/49	0.94	0.08	48,64,79,85	49
25	BCR	D	406	40/40	0.94	0.08	43,57,102,106	0
25	BCR	H	101	40/40	0.94	0.08	48,65,85,89	0
35	DGD	c	518[A]	62/66	0.94	0.07	53,68,114,129	62
35	DGD	c	518[B]	62/66	0.94	0.07	54,68,114,129	62
35	DGD	c	519	62/66	0.94	0.07	49,61,101,125	0
26	SQD	a	411[A]	54/54	0.94	0.09	59,78,111,118	54
26	SQD	a	411[B]	54/54	0.94	0.09	59,78,111,118	54
25	BCR	K	102	40/40	0.94	0.09	56,64,76,79	0
23	CLA	B	614	65/65	0.95	0.07	36,47,102,121	0
23	CLA	d	403	65/65	0.95	0.09	50,66,117,142	0
25	BCR	A	409	40/40	0.95	0.06	37,51,65,67	0
25	BCR	B	618	40/40	0.95	0.06	39,55,70,78	0
25	BCR	B	619	40/40	0.95	0.07	46,58,93,96	0
25	BCR	C	515	40/40	0.95	0.08	54,73,89,94	0
23	CLA	B	616	65/65	0.95	0.09	41,57,131,139	0
23	CLA	D	405	65/65	0.95	0.08	46,59,121,138	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	a	407[A]	65/65	0.95	0.07	39,52,118,132	65
23	CLA	a	407[B]	65/65	0.95	0.07	39,52,118,132	65
23	CLA	a	409	65/65	0.95	0.10	43,56,138,157	0
29	PL9	d	405[A]	55/55	0.95	0.07	36,49,60,73	55
29	PL9	d	405[B]	55/55	0.95	0.07	36,49,60,73	55
25	BCR	a	410	40/40	0.95	0.06	42,53,63,67	0
25	BCR	b	619	40/40	0.95	0.07	46,63,86,89	0
23	CLA	A	408	65/65	0.95	0.08	37,49,126,140	0
25	BCR	c	516	40/40	0.95	0.07	56,64,78,81	0
23	CLA	b	606	65/65	0.95	0.07	44,59,112,127	0
25	BCR	h	101	40/40	0.95	0.09	59,72,94,97	0
23	CLA	b	614	65/65	0.95	0.07	40,50,98,117	0
23	CLA	B	606	65/65	0.95	0.08	44,57,111,135	0
30	UNL	X	102	18/-	0.95	0.10	55,71,104,104	0
25	BCR	y	101	40/40	0.95	0.07	56,70,83,96	0
27	GOL	b	628	6/6	0.95	0.08	72,79,85,88	0
23	CLA	c	505	65/65	0.95	0.07	47,63,102,132	0
35	DGD	C	519	62/66	0.95	0.07	42,59,95,109	0
35	DGD	H	102	62/66	0.95	0.08	43,61,76,93	0
35	DGD	c	517[A]	62/66	0.95	0.07	46,63,97,105	62
35	DGD	c	517[B]	62/66	0.95	0.07	46,63,97,105	62
32	LHG	b	629[A]	49/49	0.95	0.08	47,56,75,91	49
32	LHG	b	629[B]	49/49	0.95	0.08	47,56,75,92	49
23	CLA	c	507	65/65	0.95	0.08	46,70,118,131	0
35	DGD	h	102	62/66	0.95	0.07	52,64,77,86	0
23	CLA	c	508	65/65	0.95	0.08	49,67,83,90	0
23	CLA	c	509	65/65	0.95	0.07	42,62,124,152	0
23	CLA	C	509	65/65	0.95	0.07	45,54,113,140	0
38	BCT	d	401[A]	4/4	0.95	0.06	53,54,63,71	4
38	BCT	d	401[B]	4/4	0.95	0.06	53,53,63,70	4
23	CLA	b	609	65/65	0.96	0.07	49,64,77,92	0
23	CLA	b	612	65/65	0.96	0.07	41,53,69,76	0
23	CLA	A	404[B]	65/65	0.96	0.06	34,41,59,67	65
23	CLA	C	506	65/65	0.96	0.07	49,59,87,103	0
23	CLA	c	502	65/65	0.96	0.07	51,67,81,95	0
30	UNL	x	101	18/-	0.96	0.10	64,80,124,134	0
23	CLA	c	504	65/65	0.96	0.07	52,70,82,98	0
23	CLA	B	602	65/65	0.96	0.07	43,55,72,95	0
23	CLA	c	506	65/65	0.96	0.07	49,64,90,97	0
23	CLA	C	508	65/65	0.96	0.08	50,61,84,92	0
23	CLA	B	603	65/65	0.96	0.07	42,52,71,81	0
23	CLA	C	512	65/65	0.96	0.07	49,62,80,89	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	c	512	65/65	0.96	0.07	53,68,86,97	0
23	CLA	A	406[A]	65/65	0.96	0.06	37,45,105,116	65
23	CLA	B	607	65/65	0.96	0.06	36,44,74,81	0
23	CLA	B	609	65/65	0.96	0.06	46,58,72,81	0
24	PHO	A	416[A]	64/64	0.96	0.06	37,48,53,60	64
24	PHO	A	416[B]	64/64	0.96	0.06	37,47,53,60	64
24	PHO	a	416[A]	64/64	0.96	0.06	44,55,61,65	64
24	PHO	a	416[B]	64/64	0.96	0.06	44,55,61,65	64
23	CLA	a	405[A]	65/65	0.96	0.06	34,44,60,74	65
25	BCR	B	617	40/40	0.96	0.05	38,50,61,65	0
32	LHG	D	408[A]	49/49	0.96	0.07	43,53,64,73	49
35	DGD	C	517[A]	62/66	0.96	0.06	46,57,97,102	62
35	DGD	C	517[B]	62/66	0.96	0.06	46,57,97,102	62
32	LHG	D	408[B]	49/49	0.96	0.07	43,53,64,73	49
23	CLA	a	405[B]	65/65	0.96	0.06	36,44,63,74	65
23	CLA	B	611	65/65	0.96	0.06	33,42,64,68	0
23	CLA	A	406[B]	65/65	0.96	0.06	37,45,105,116	65
25	BCR	C	516	40/40	0.96	0.06	52,64,80,85	0
23	CLA	A	404[A]	65/65	0.96	0.06	34,41,59,67	65
23	CLA	C	502	65/65	0.96	0.07	48,60,71,76	0
23	CLA	b	602	65/65	0.96	0.07	48,61,80,91	0
23	CLA	b	604	65/65	0.96	0.07	40,52,102,119	0
32	LHG	d	406[A]	49/49	0.96	0.07	44,55,68,76	49
32	LHG	d	406[B]	49/49	0.96	0.07	44,55,68,76	49
23	CLA	C	504	65/65	0.96	0.06	47,61,72,85	0
23	CLA	b	607	65/65	0.96	0.06	37,47,79,93	0
25	BCR	b	617	40/40	0.96	0.06	43,54,60,67	0
25	BCR	b	618	40/40	0.96	0.05	43,55,77,84	0
23	CLA	b	615	65/65	0.97	0.06	47,61,82,92	0
23	CLA	C	503	65/65	0.97	0.06	41,54,72,86	0
23	CLA	B	604	65/65	0.97	0.06	37,45,117,138	0
23	CLA	c	503	65/65	0.97	0.06	41,57,81,96	0
23	CLA	B	610	65/65	0.97	0.07	39,52,67,79	0
23	CLA	a	406[A]	65/65	0.97	0.05	35,42,61,70	65
23	CLA	a	406[B]	65/65	0.97	0.05	35,43,61,70	65
23	CLA	B	605	65/65	0.97	0.06	39,48,62,78	0
23	CLA	B	612	65/65	0.97	0.06	31,47,58,74	0
23	CLA	B	613	65/65	0.97	0.06	35,44,93,108	0
23	CLA	c	510	65/65	0.97	0.07	42,60,84,98	0
23	CLA	c	511	65/65	0.97	0.06	47,61,80,91	0
32	LHG	L	101[A]	49/49	0.97	0.06	45,54,69,88	49
32	LHG	L	101[B]	49/49	0.97	0.06	45,54,69,89	49

Continued on next page...

Continued from previous page...

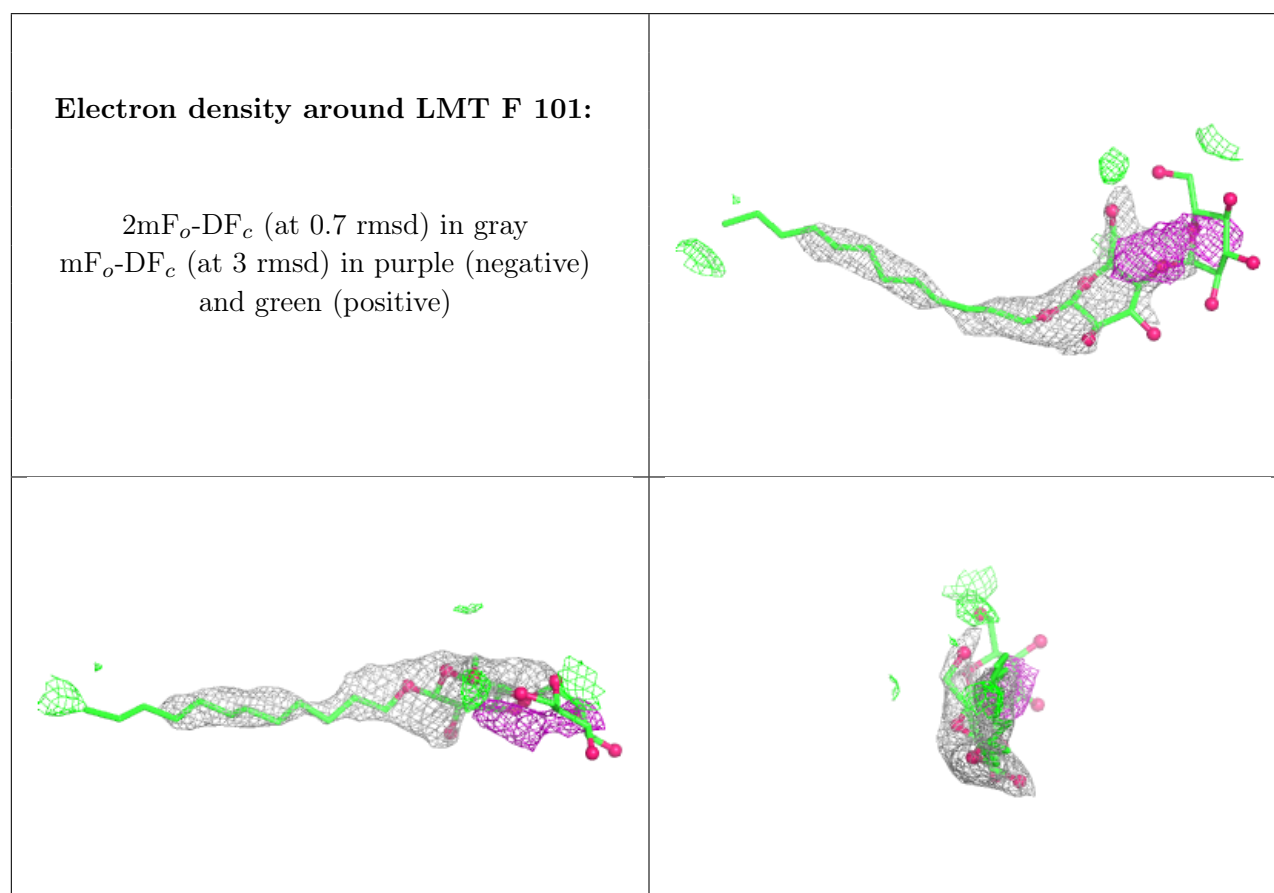
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	CLA	A	405[A]	65/65	0.97	0.06	33,41,58,69	65
23	CLA	C	510	65/65	0.97	0.07	48,58,80,86	0
23	CLA	b	603	65/65	0.97	0.06	46,55,82,93	0
23	CLA	C	511	65/65	0.97	0.06	46,57,76,81	0
24	PHO	A	407[A]	64/64	0.97	0.05	33,44,51,54	64
24	PHO	A	407[B]	64/64	0.97	0.05	33,44,51,54	64
23	CLA	b	605	65/65	0.97	0.07	36,49,74,76	0
23	CLA	B	615	65/65	0.97	0.06	44,54,76,83	0
24	PHO	a	408[A]	64/64	0.97	0.04	38,47,53,58	64
24	PHO	a	408[B]	64/64	0.97	0.04	38,47,52,58	64
23	CLA	A	405[B]	65/65	0.97	0.06	33,41,58,69	65
23	CLA	b	608	65/65	0.97	0.06	40,54,84,96	0
23	CLA	B	608	65/65	0.97	0.05	37,48,67,73	0
36	CA	C	524	1/1	0.97	0.05	77,77,77,77	0
23	CLA	b	610	65/65	0.97	0.07	48,57,67,72	0
36	CA	O	301	1/1	0.97	0.04	104,104,104,104	0
36	CA	c	523	1/1	0.97	0.07	76,76,76,76	0
23	CLA	b	611	65/65	0.97	0.06	38,48,70,75	0
23	CLA	D	404[A]	65/65	0.97	0.06	34,42,64,74	65
38	BCT	D	402[A]	4/4	0.97	0.06	50,52,56,67	4
38	BCT	D	402[B]	4/4	0.97	0.06	50,52,56,68	4
23	CLA	b	613	65/65	0.97	0.05	40,48,85,98	0
23	CLA	D	404[B]	65/65	0.97	0.06	34,42,64,75	65
22	CL	a	404[B]	1/1	0.98	0.06	52,52,52,52	1
22	CL	a	403[A]	1/1	0.98	0.06	47,47,47,47	1
22	CL	a	403[B]	1/1	0.98	0.06	47,47,47,47	1
22	CL	a	404[A]	1/1	0.98	0.06	52,52,52,52	1
23	CLA	d	402[A]	65/65	0.98	0.05	38,45,69,85	65
23	CLA	d	402[B]	65/65	0.98	0.05	38,45,69,85	65
39	HEM	F	102	43/43	0.98	0.06	54,70,82,90	0
39	HEM	f	101	43/43	0.98	0.08	65,85,116,138	0
41	HEC	V	201	43/43	0.98	0.07	38,50,58,66	0
41	HEC	v	201	43/43	0.98	0.07	48,62,68,75	0
21	OEY	A	401[B]	11/11	0.99	0.03	37,44,47,47	11
22	CL	A	402[A]	1/1	0.99	0.06	41,41,41,41	1
22	CL	A	402[B]	1/1	0.99	0.06	41,41,41,41	1
36	CA	c	524	1/1	0.99	0.04	76,76,76,76	0
28	OEX	A	413[A]	10/10	0.99	0.03	37,43,47,48	10
40	MG	J	102	1/1	0.99	0.03	56,56,56,56	0
40	MG	j	102	1/1	0.99	0.03	63,63,63,63	0
22	CL	A	403[A]	1/1	0.99	0.04	45,45,45,45	1
22	CL	A	403[B]	1/1	0.99	0.04	45,45,45,45	1

Continued on next page...

Continued from previous page...

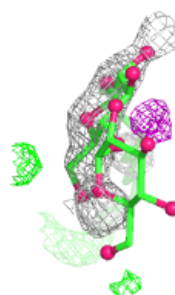
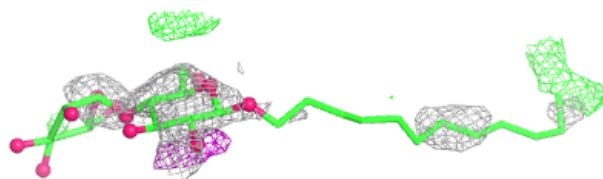
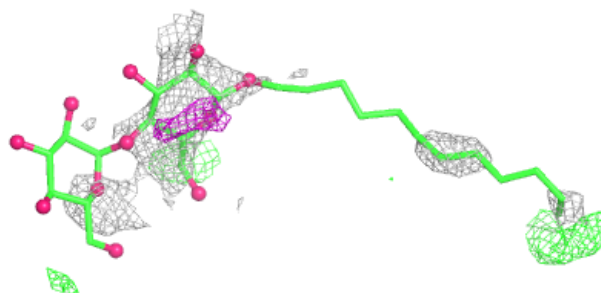
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	FE2	a	402[A]	1/1	1.00	0.01	52,52,52,52	1
37	FE2	a	402[B]	1/1	1.00	0.01	52,52,52,52	1
21	OEY	a	401[B]	11/11	1.00	0.02	45,48,52,55	11
28	OEX	a	413[A]	10/10	1.00	0.02	47,48,51,52	10
37	FE2	D	401[A]	1/1	1.00	0.02	48,48,48,48	1
37	FE2	D	401[B]	1/1	1.00	0.02	48,48,48,48	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.

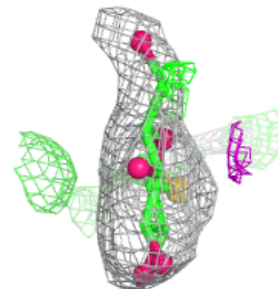
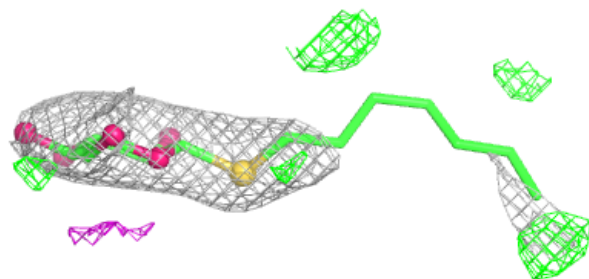
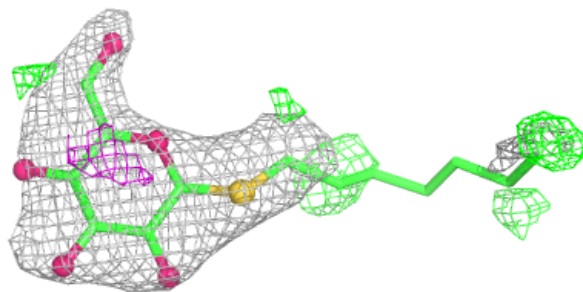


Electron density around LMT e 101:

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

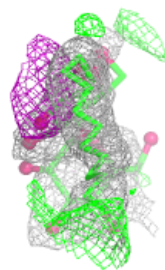
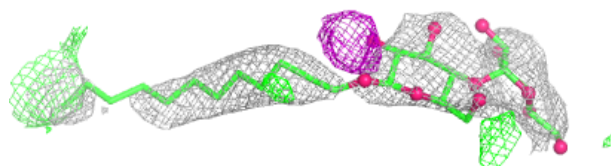
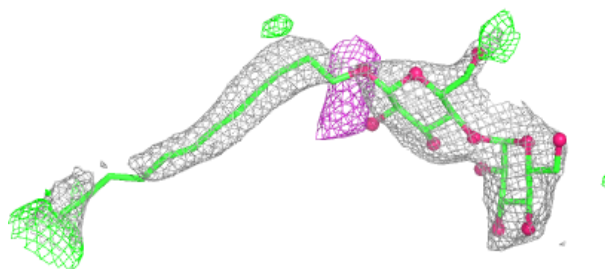
**Electron density around HTG C 522:**

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

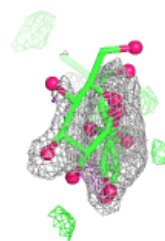
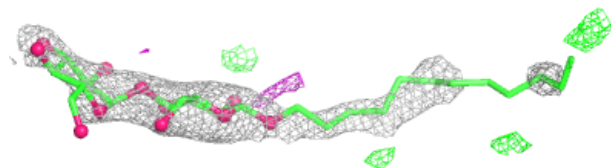
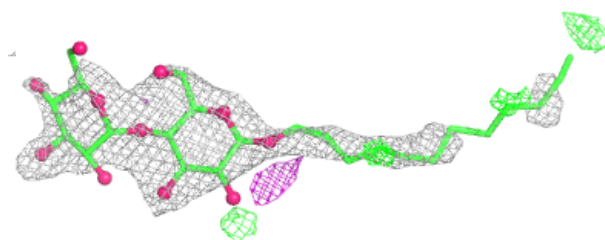


Electron density around LMT A 417:

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

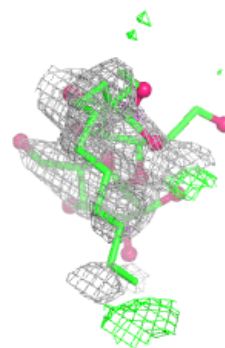
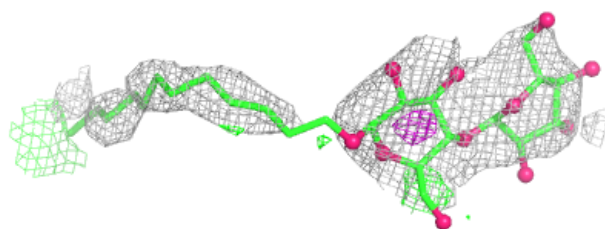
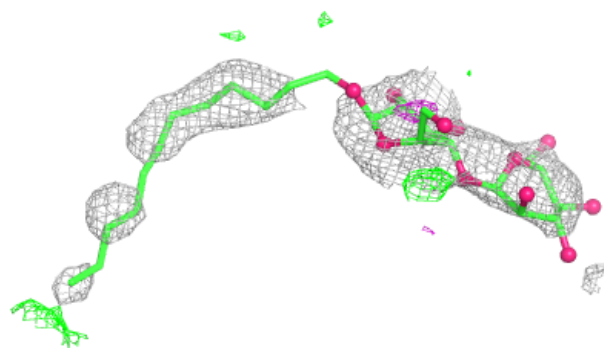
**Electron density around LMT c 501:**

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

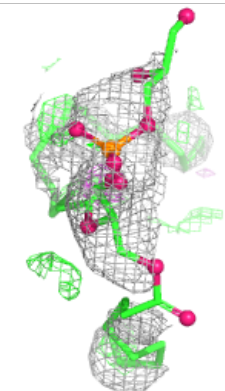
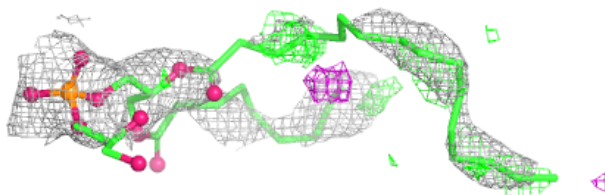
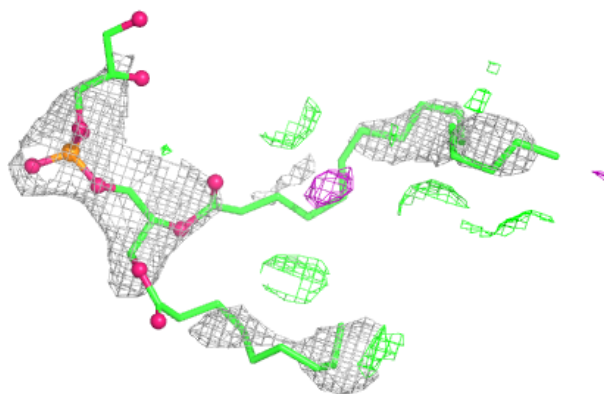


Electron density around LMT A 419:

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

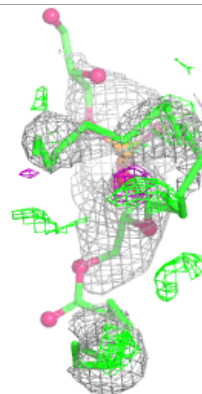
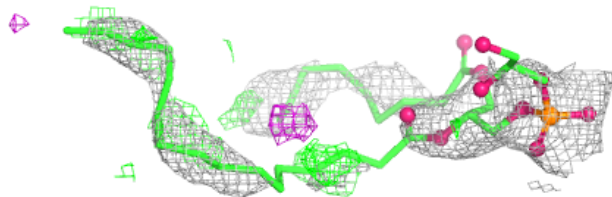
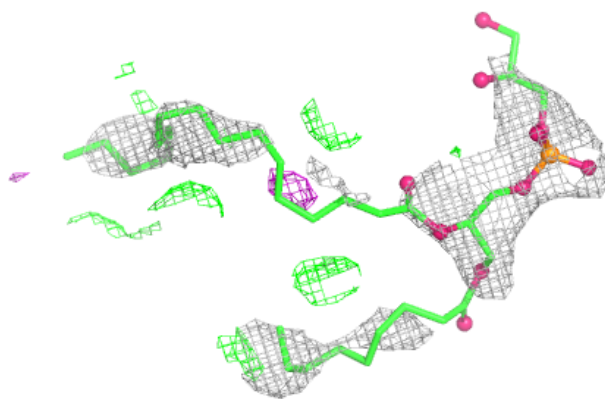
**Electron density around LHG a 420 (A):**

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

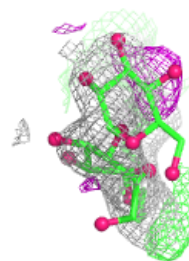
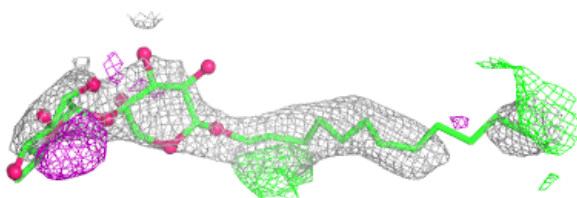
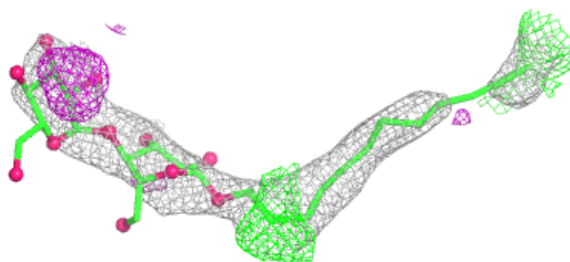


Electron density around LHG a 420 (B):

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

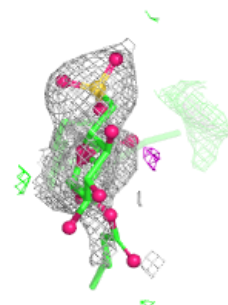
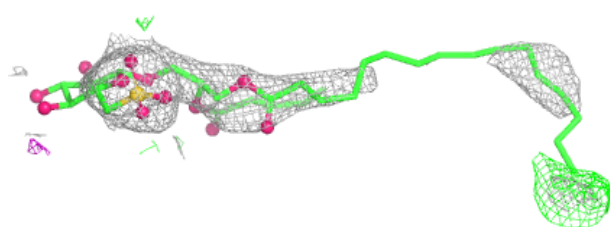
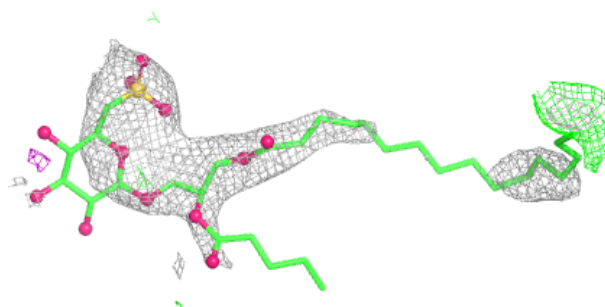
**Electron density around LMT B 630:**

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

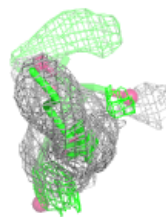
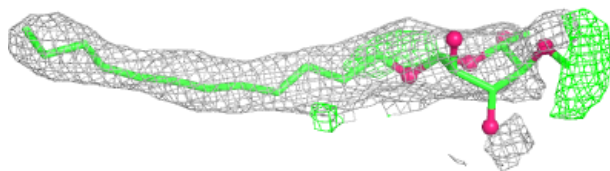
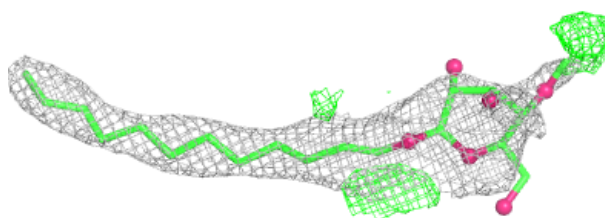


Electron density around SQD f 102:

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

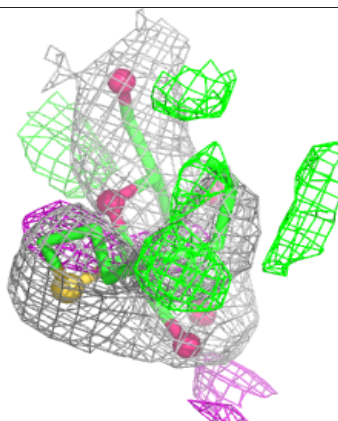
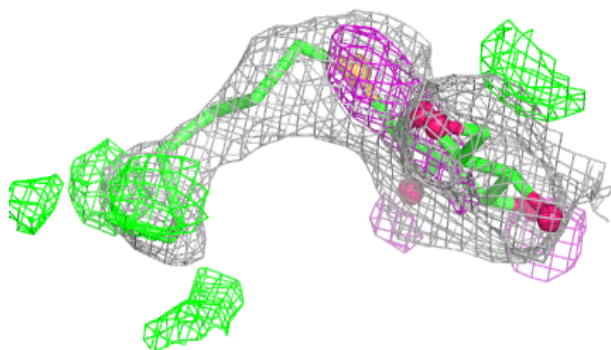
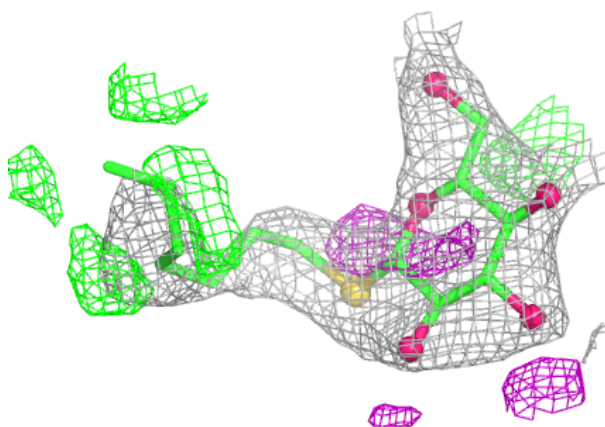
**Electron density around LMT b 621:**

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

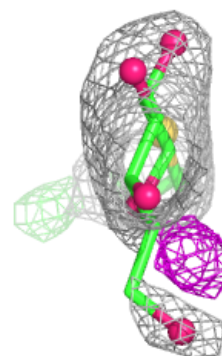
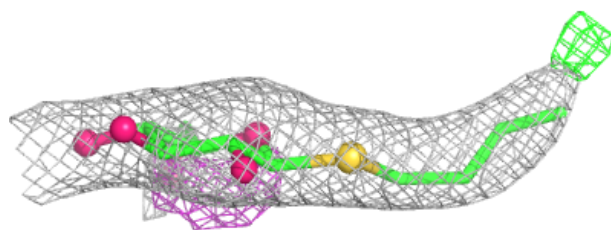
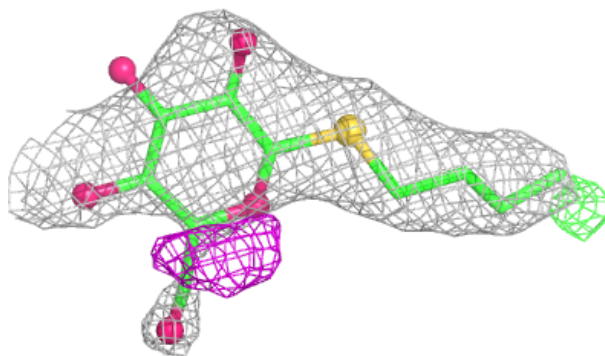


Electron density around HTG B 623:

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

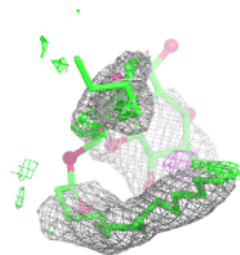
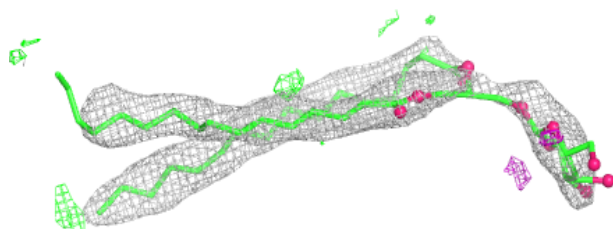
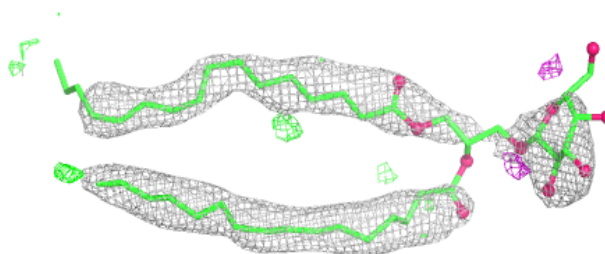
**Electron density around HTG D 412:**

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

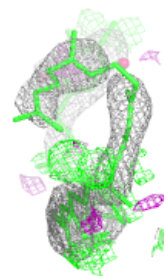
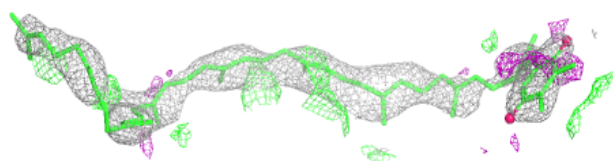
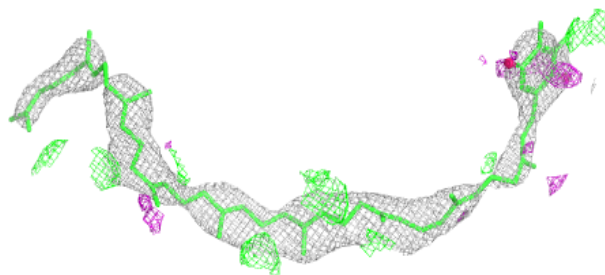


Electron density around LMG C 521:

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

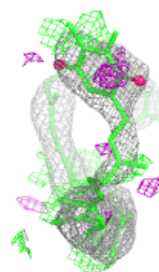
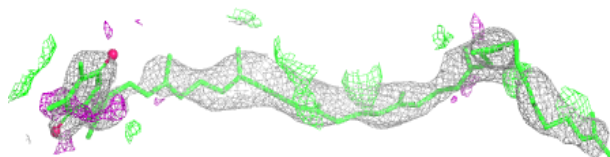
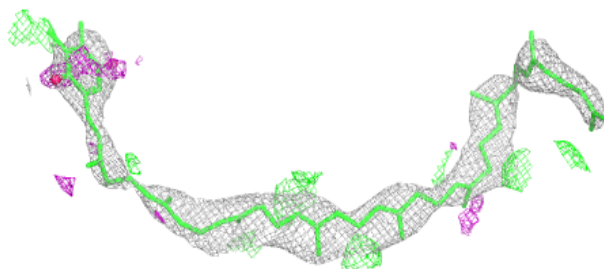
**Electron density around PL9 a 414 (B):**

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

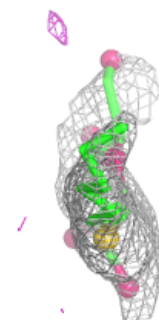
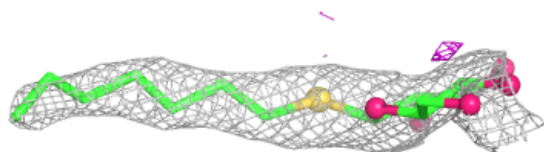
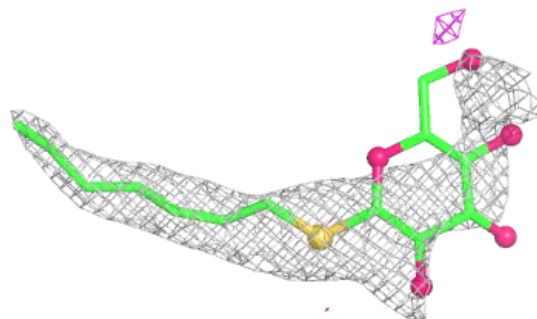


Electron density around PL9 a 414 (A):

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

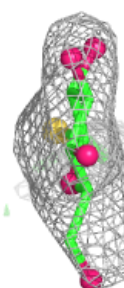
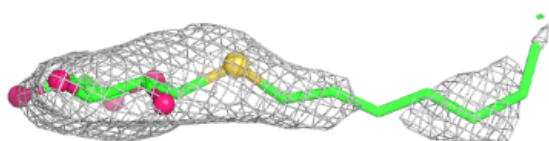
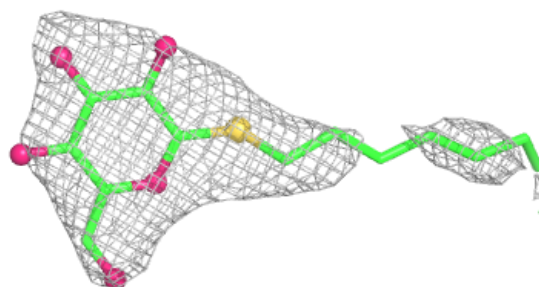
**Electron density around HTG b 623:**

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

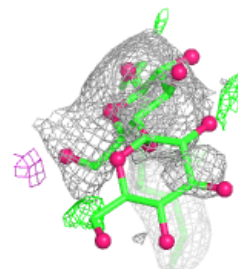
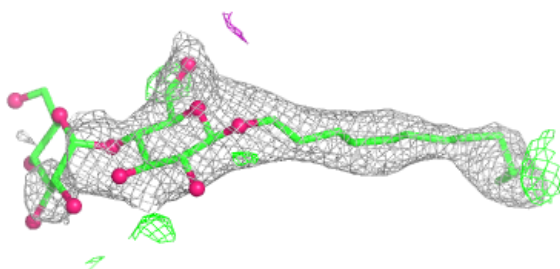
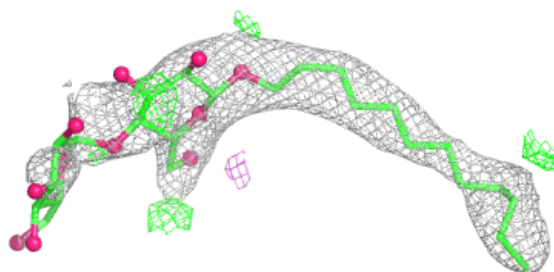


Electron density around HTG c 522:

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

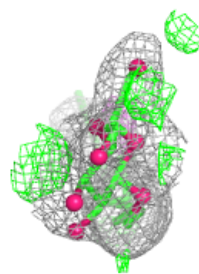
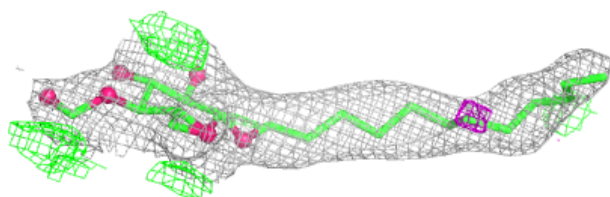
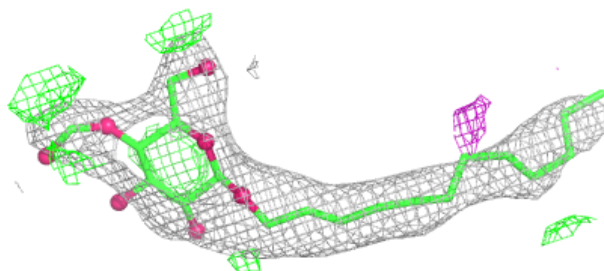
**Electron density around LMT M 102:**

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

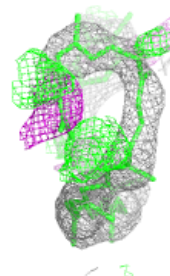
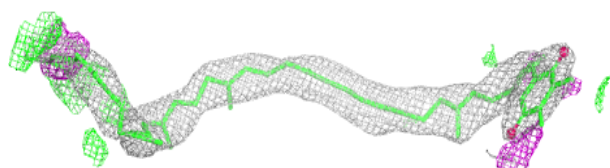
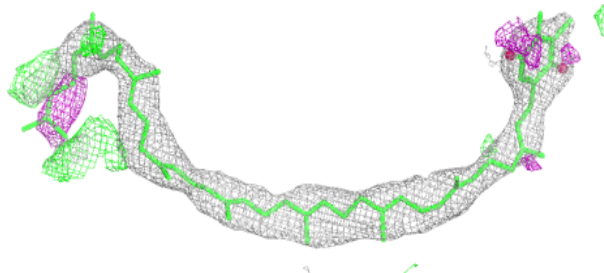


Electron density around LMT t 101:

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

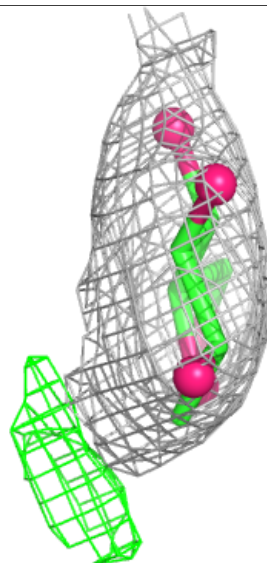
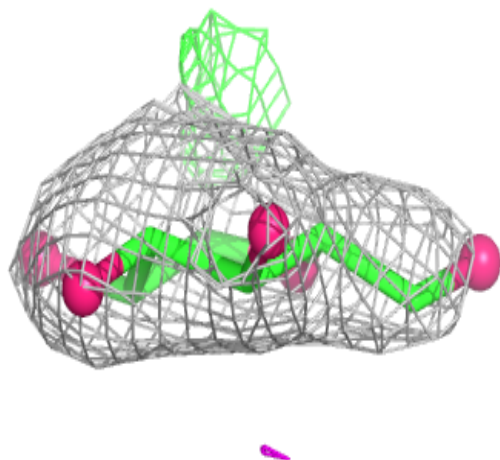
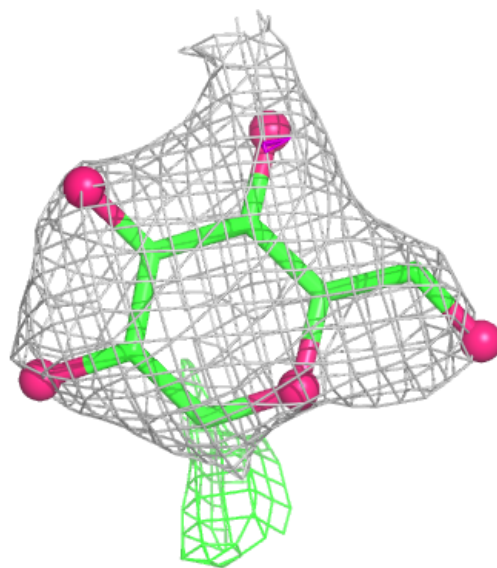
**Electron density around PL9 A 414 (B):**

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



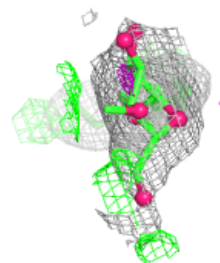
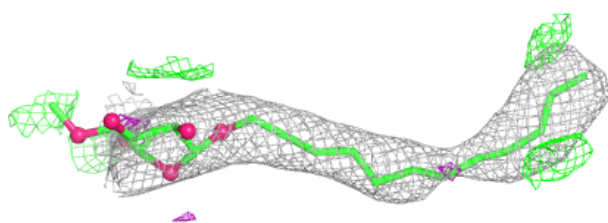
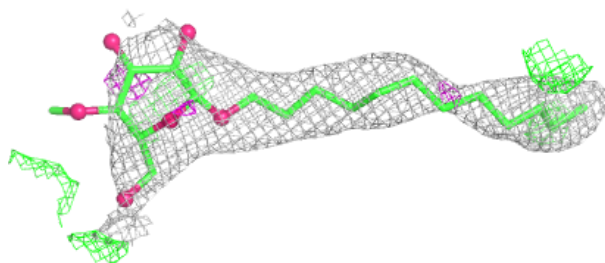
Electron density around HTG V 202:

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

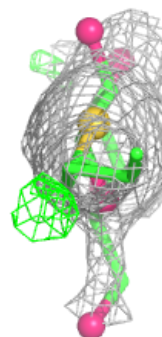
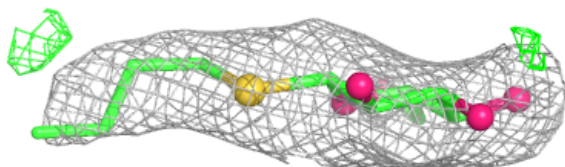
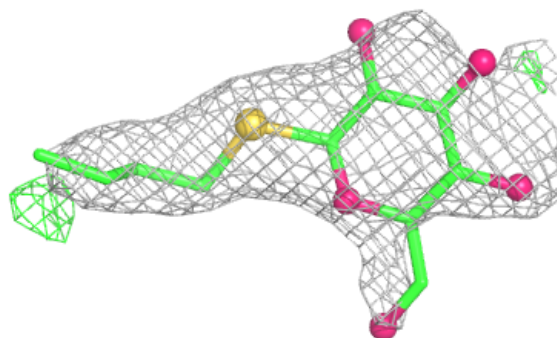


Electron density around LMT B 631:

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

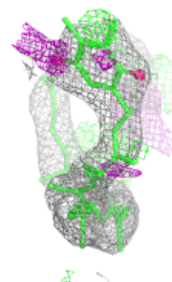
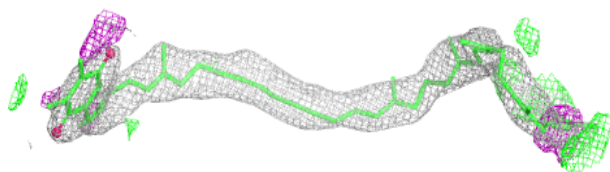
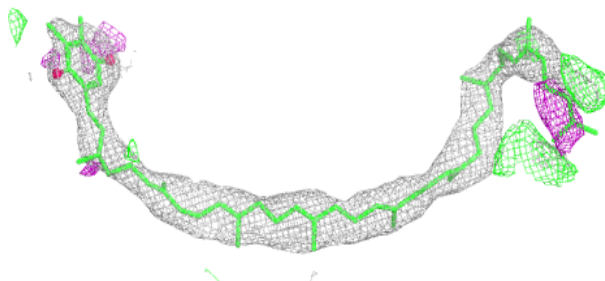
**Electron density around HTG d 410:**

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

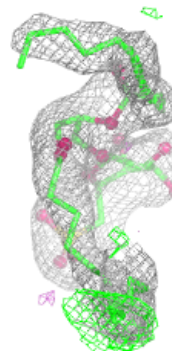
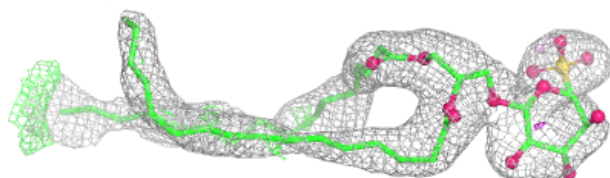
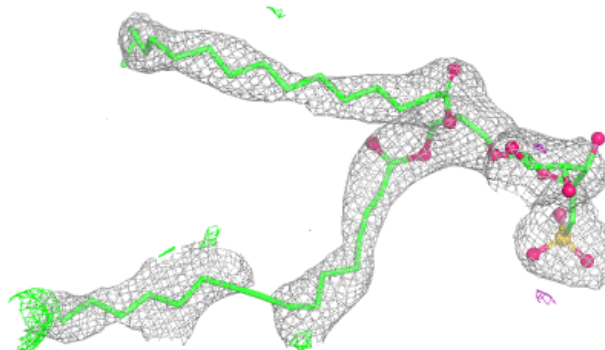


Electron density around PL9 A 414 (A):

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

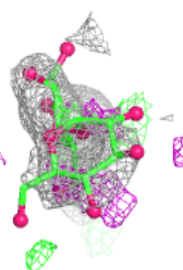
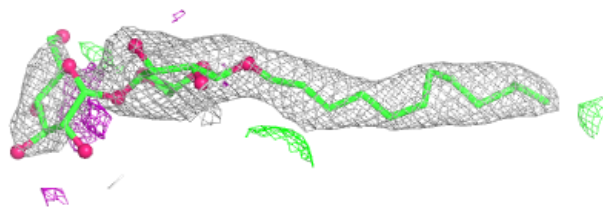
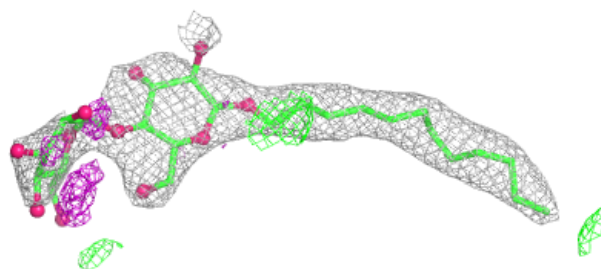
**Electron density around SQD a 412:**

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

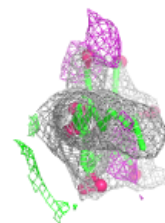
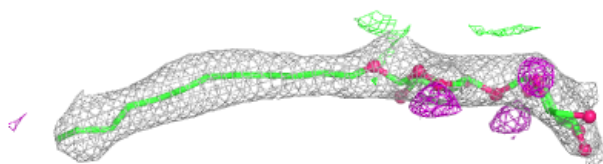
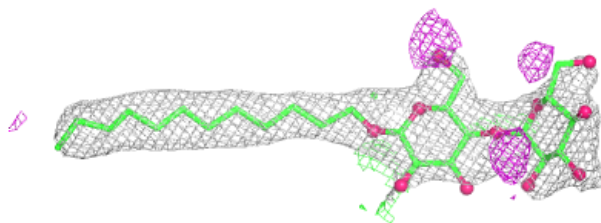


Electron density around LMT B 628:

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

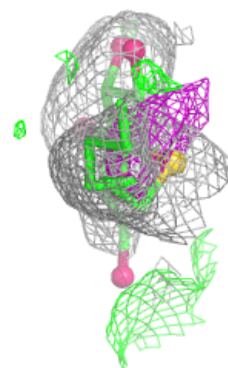
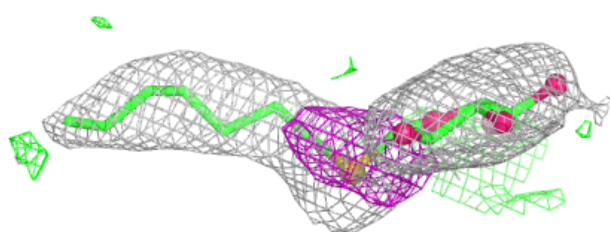
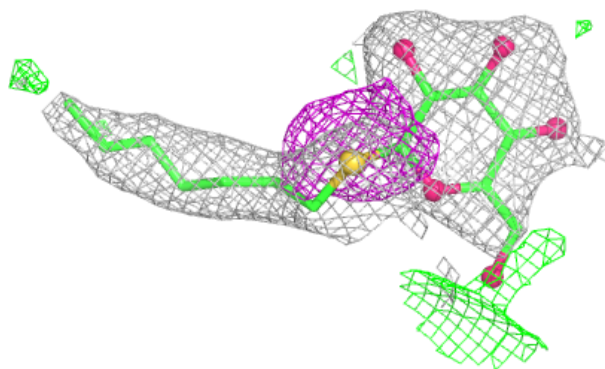
**Electron density around LMT m 103:**

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

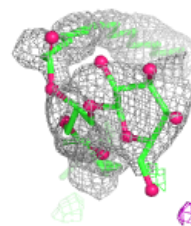
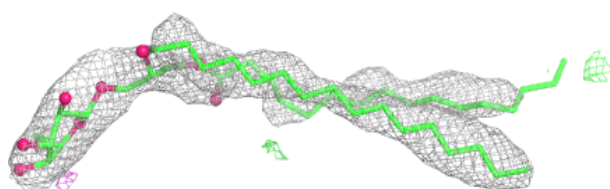
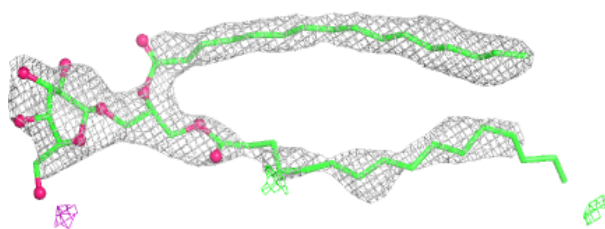


Electron density around HTG b 622:

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

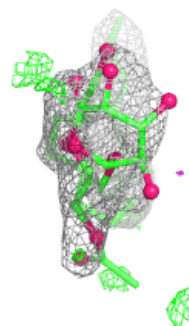
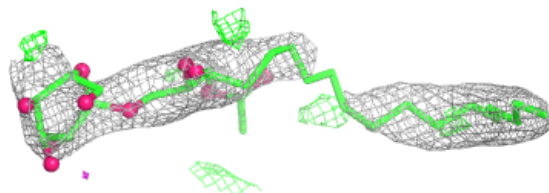
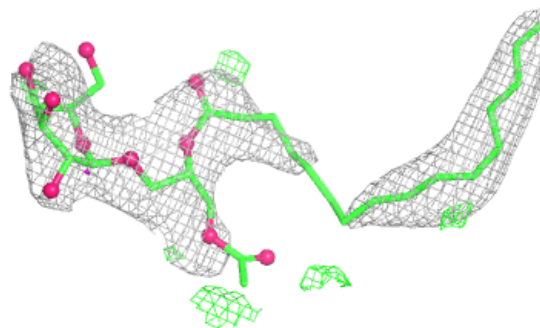
**Electron density around LMG c 521:**

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

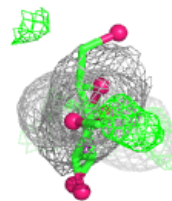
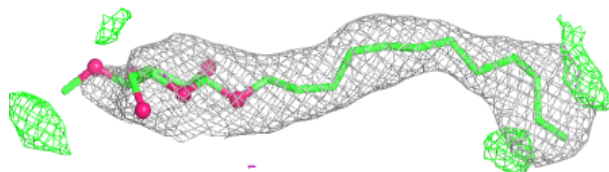
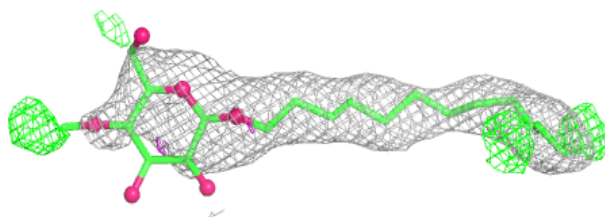


Electron density around LMG Z 101:

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

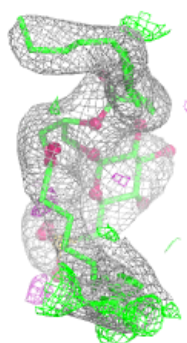
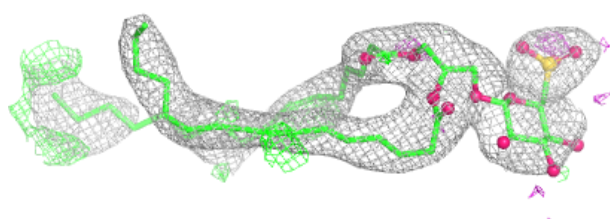
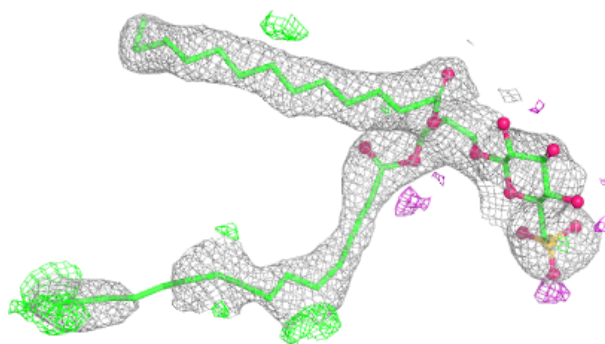
**Electron density around LMT b 627:**

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

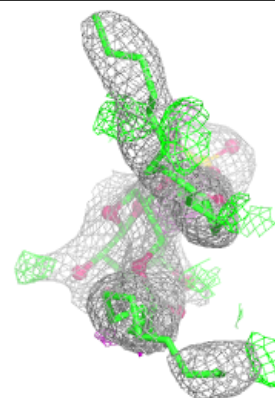
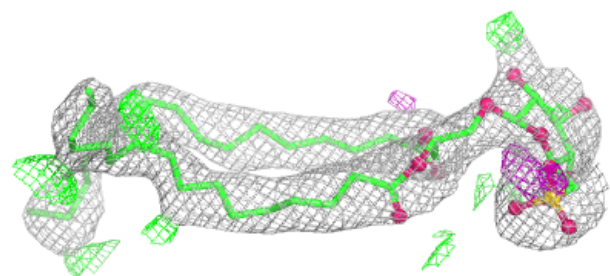
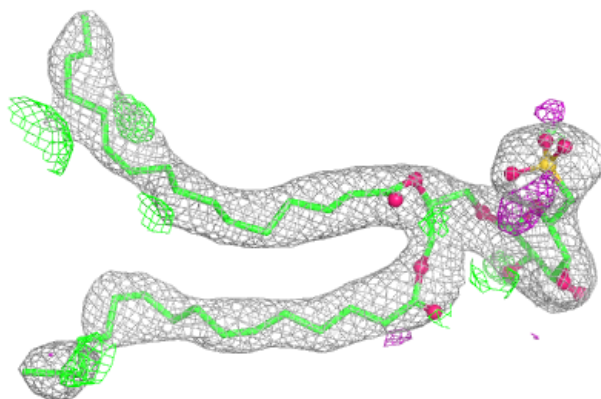


Electron density around SQD A 412:

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

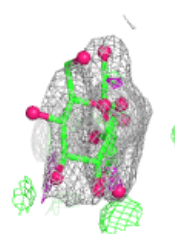
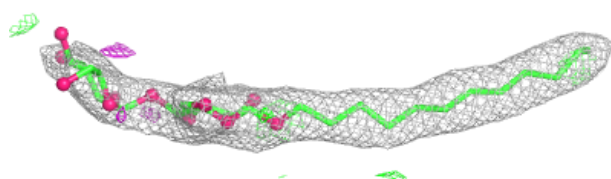
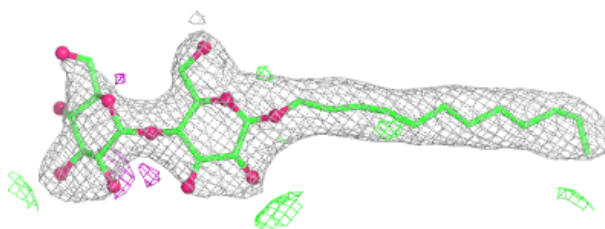
**Electron density around SQD b 620:**

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

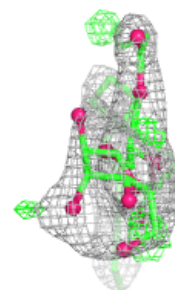
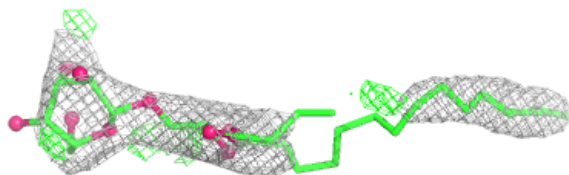
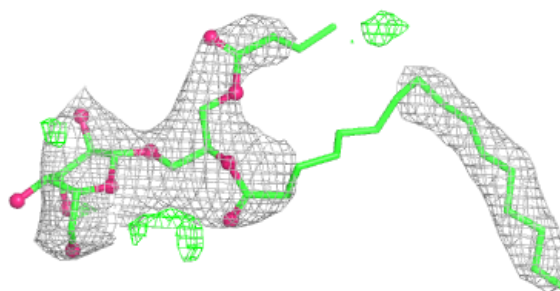


Electron density around LMT M 101:

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

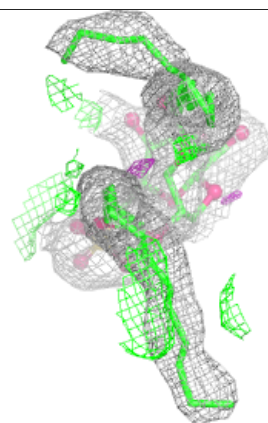
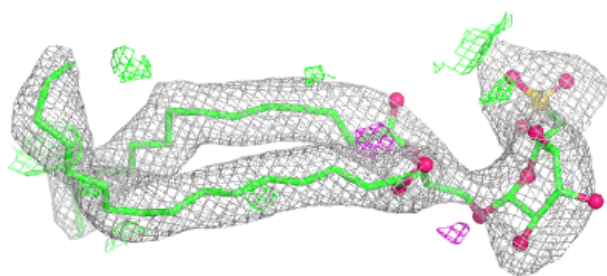
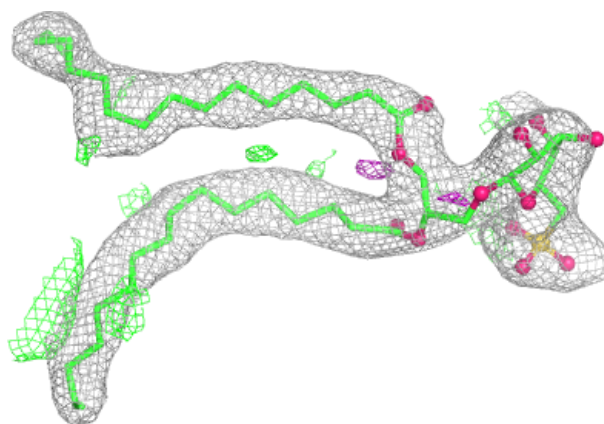
**Electron density around LMG z 101:**

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



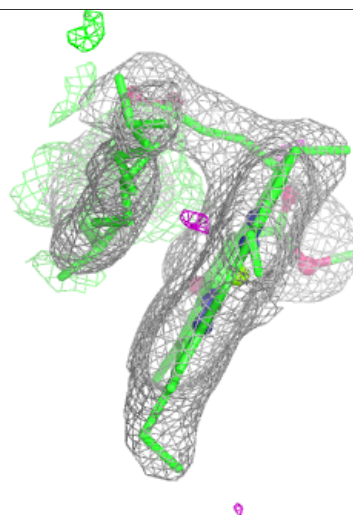
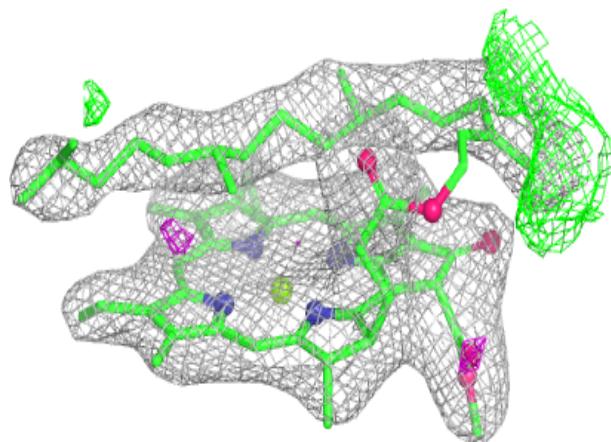
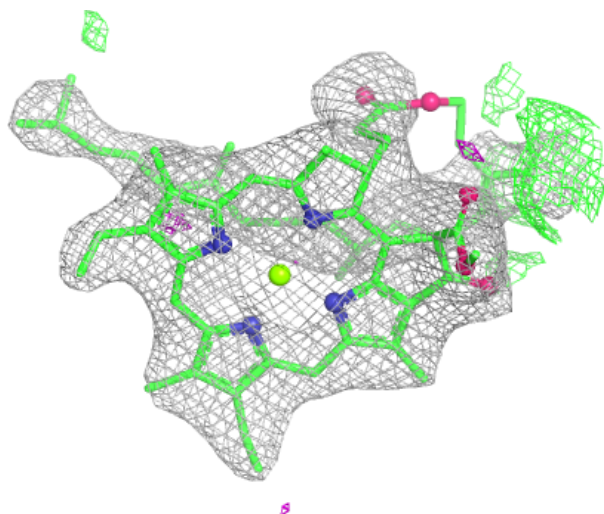
Electron density around SQD B 620:

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



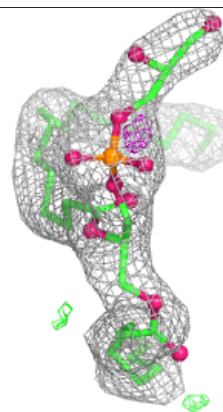
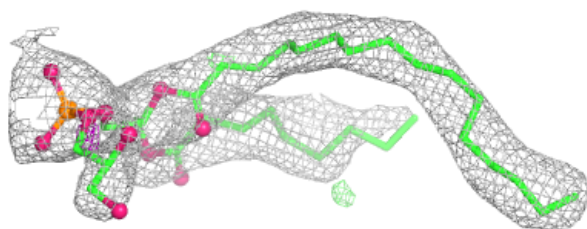
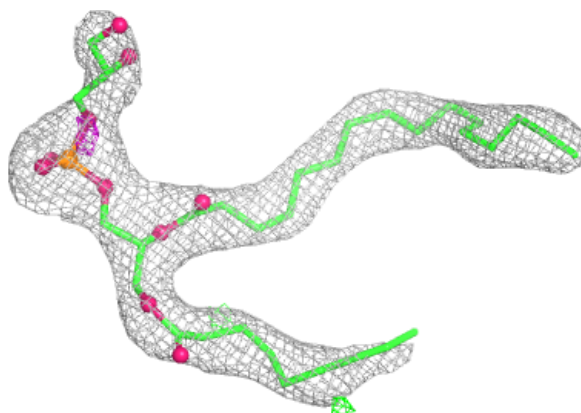
Electron density around CLA b 601:

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

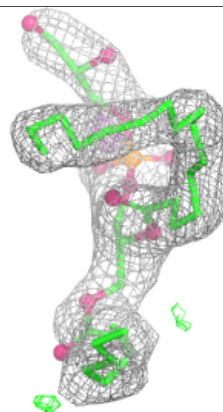
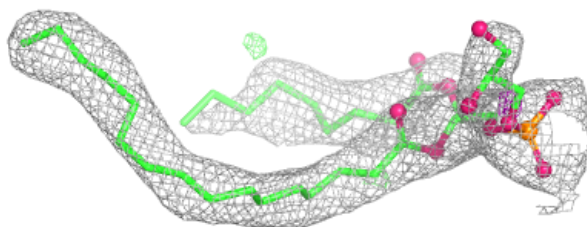
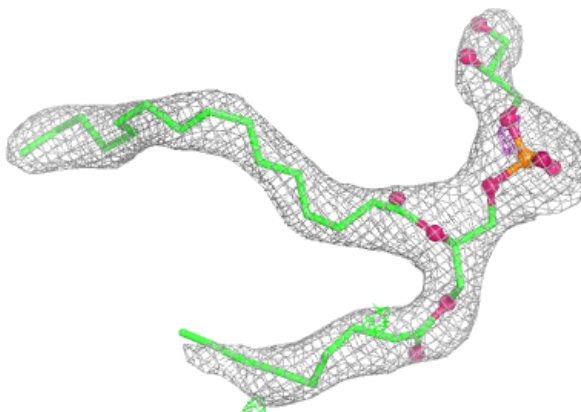


Electron density around LHG E 101 (A):

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

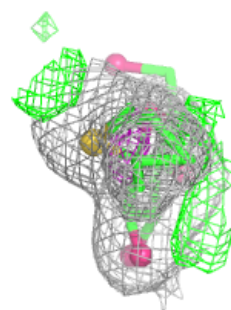
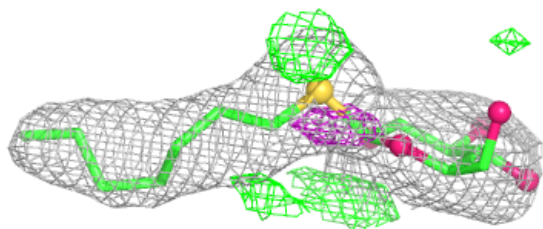
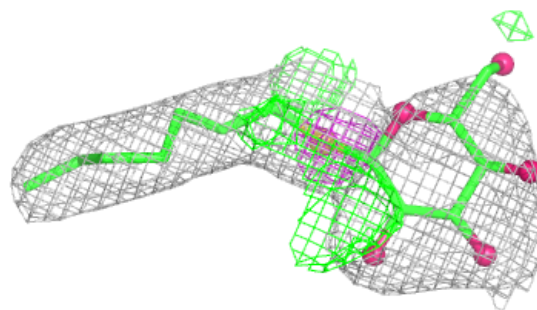
**Electron density around LHG E 101 (B):**

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

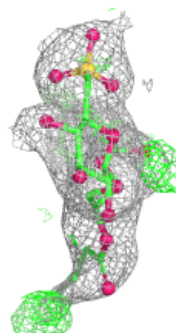
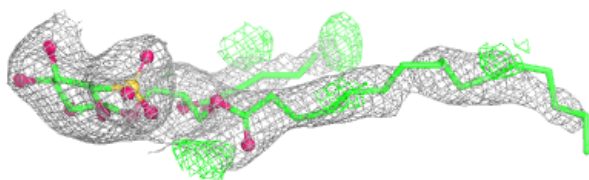
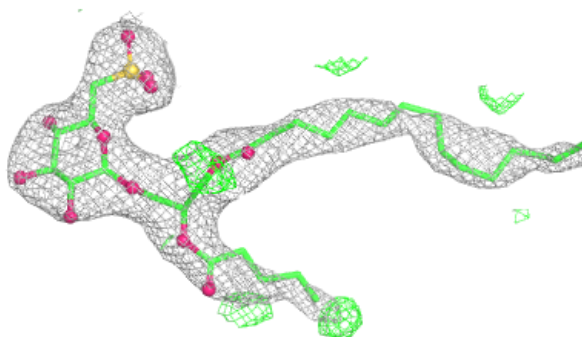


Electron density around HTG B 622:

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

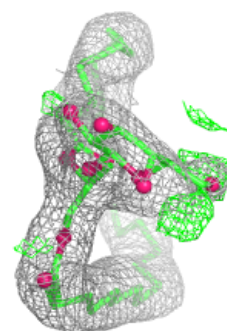
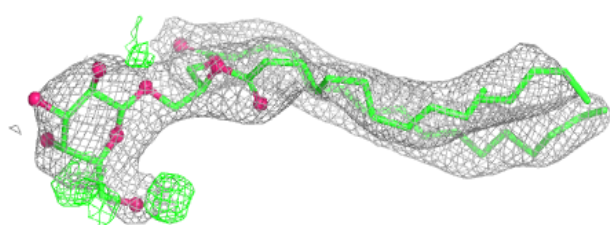
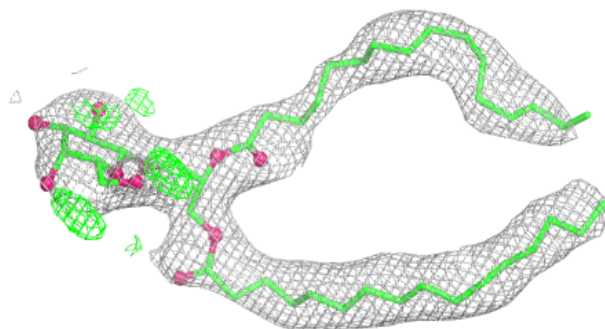
**Electron density around SQD X 101:**

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

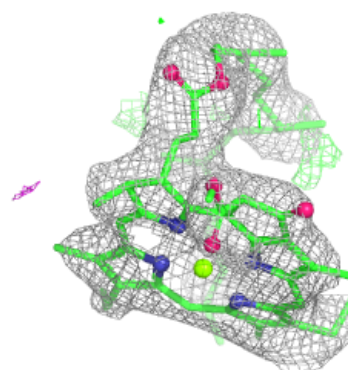
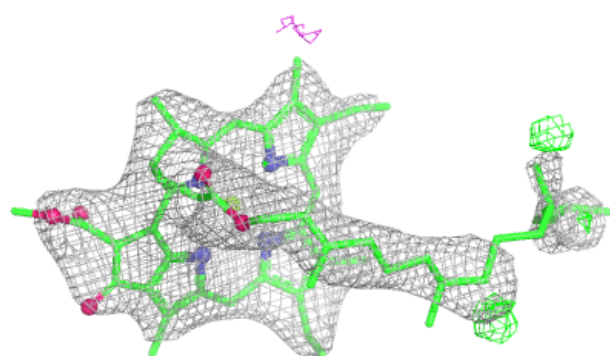
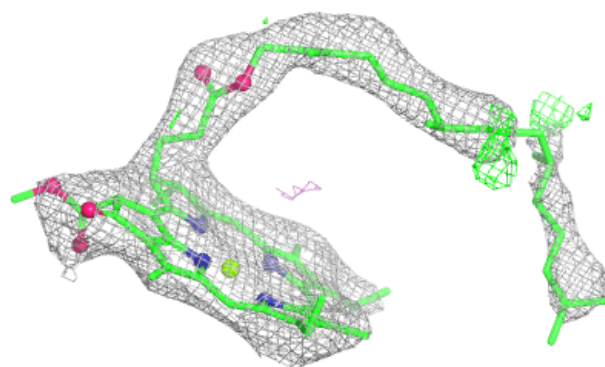


Electron density around LMG C 501:

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

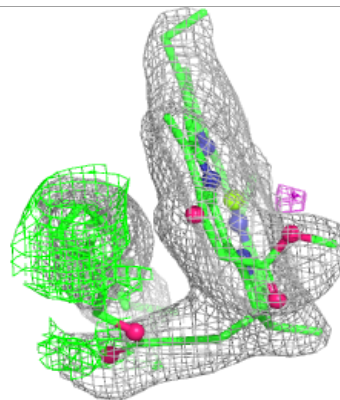
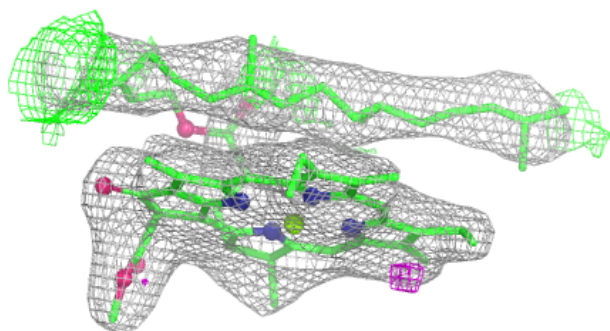
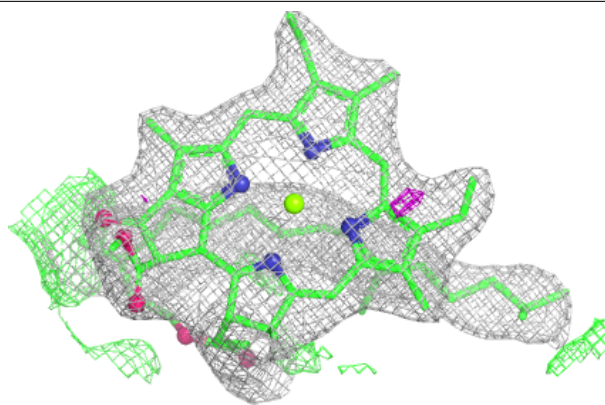
**Electron density around CLA c 514:**

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

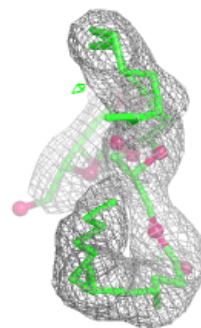
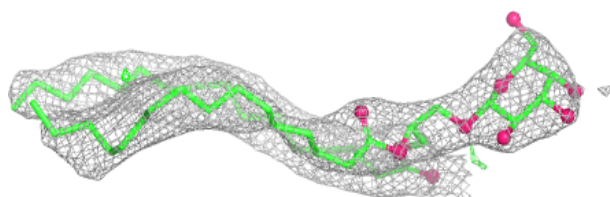
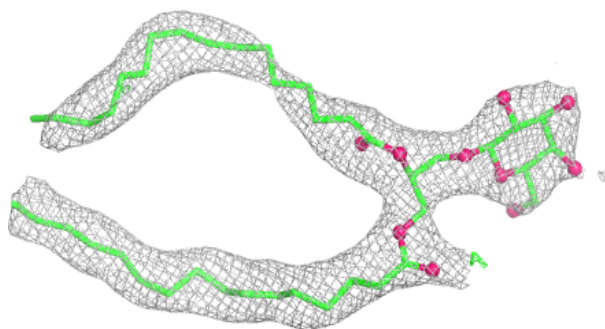


Electron density around CLA B 601:

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

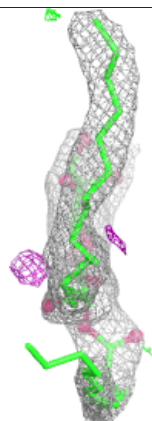
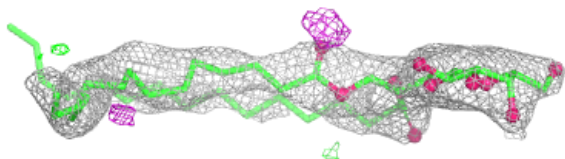
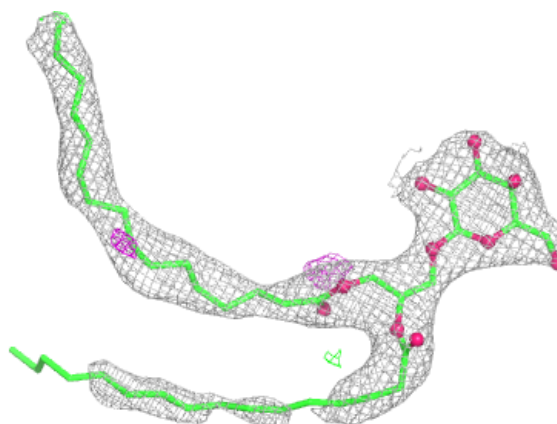
**Electron density around LMG a 417:**

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

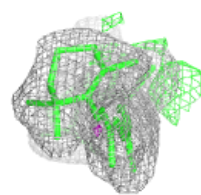
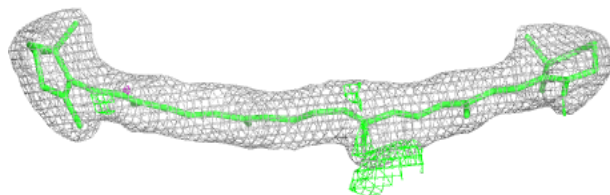
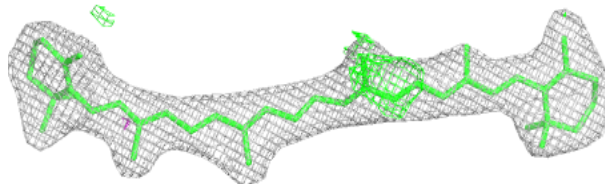


Electron density around LMG c 520:

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

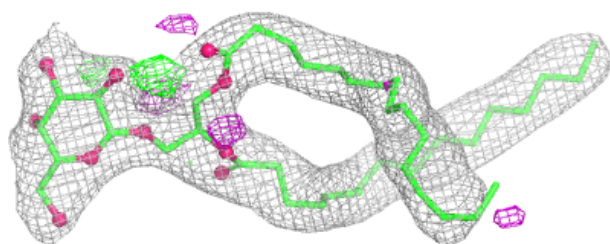
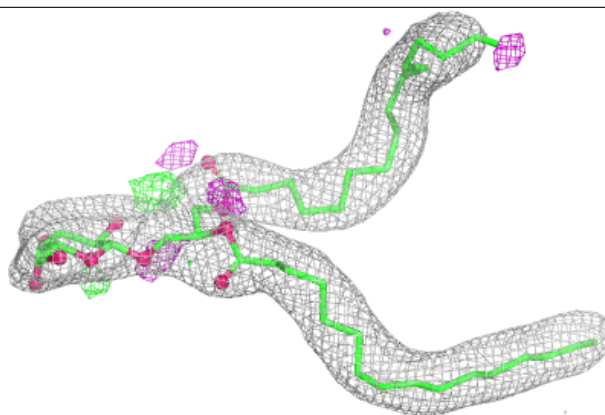
**Electron density around BCR T 101:**

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

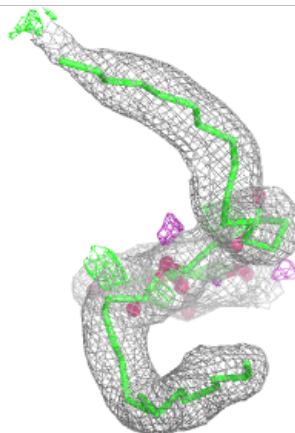
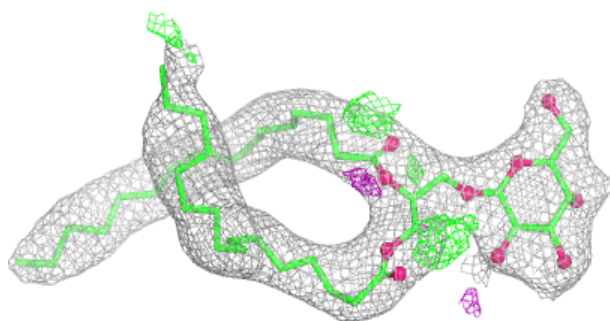
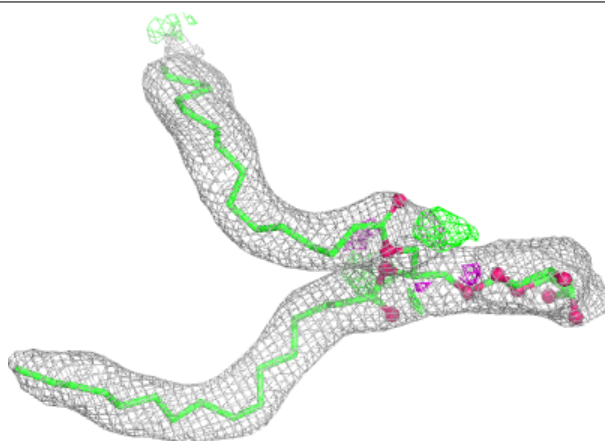


Electron density around LMG m 101:

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

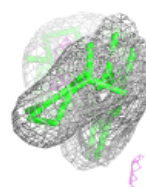
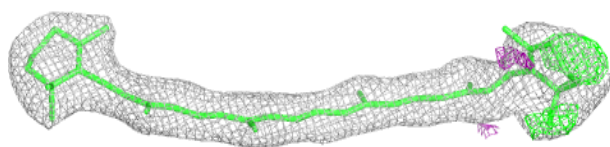
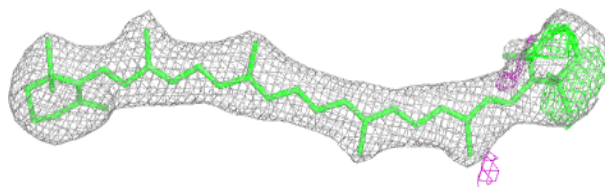
**Electron density around LMG B 621:**

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

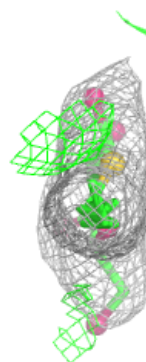
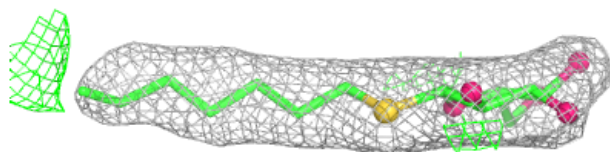
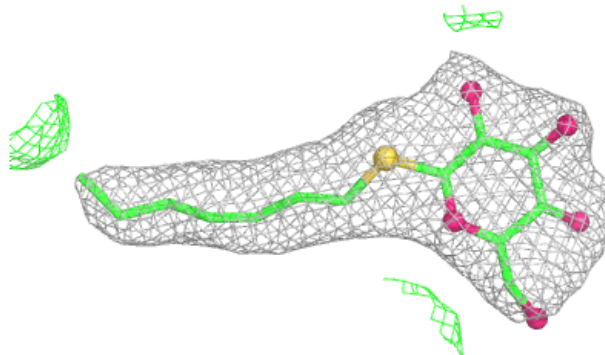


Electron density around BCR d 404:

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

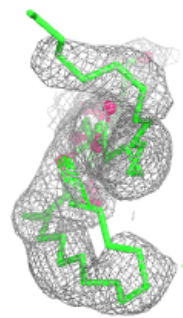
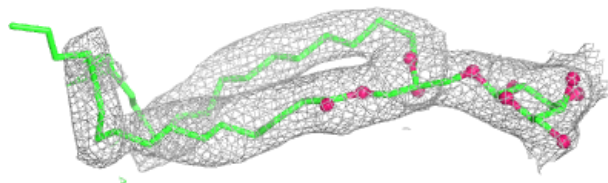
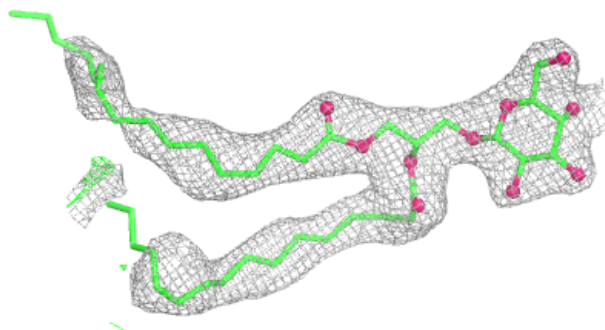
**Electron density around HTG B 625:**

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



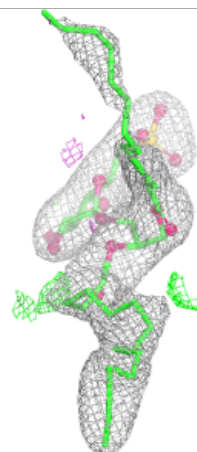
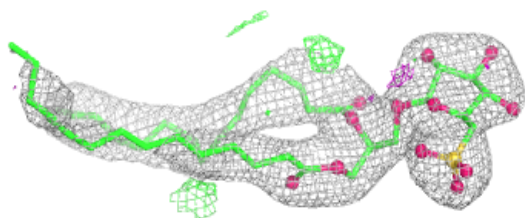
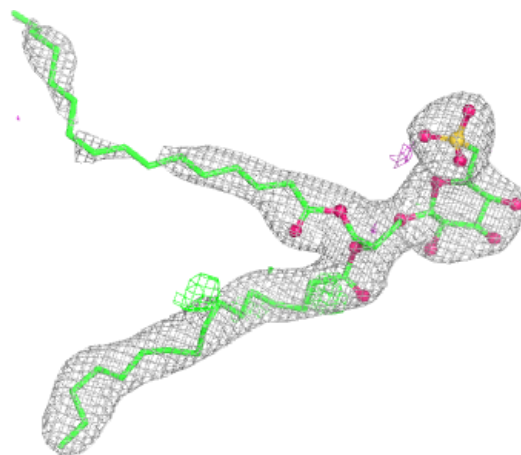
Electron density around LMG d 411:

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



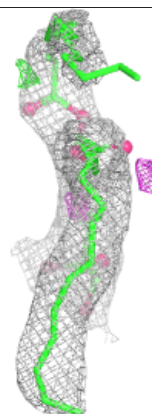
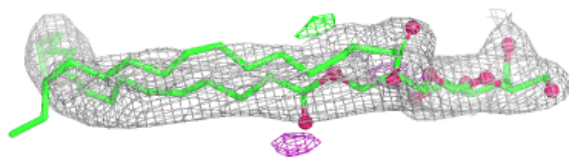
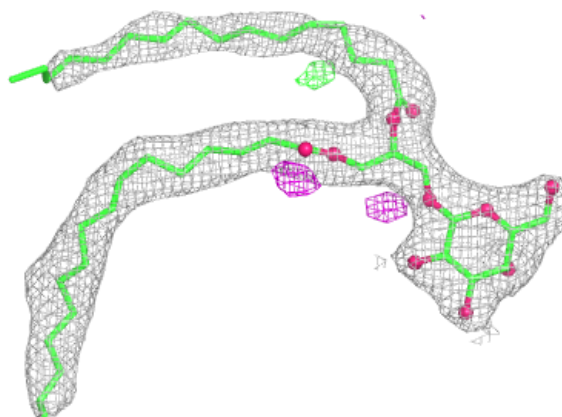
Electron density around SQD A 410 (A):

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



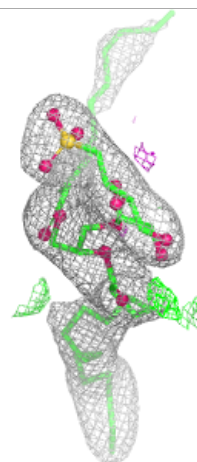
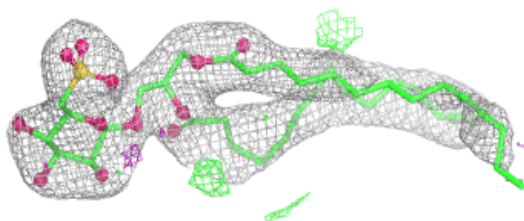
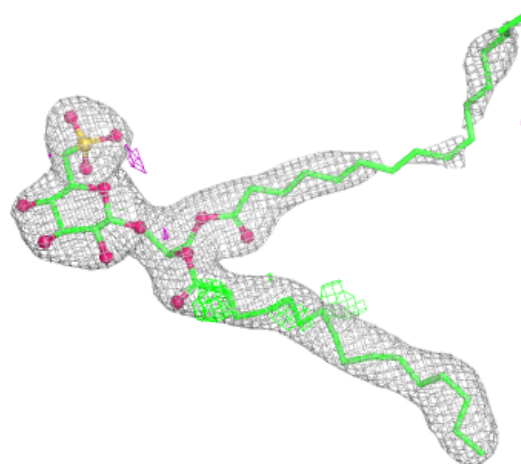
Electron density around LMG C 520:

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



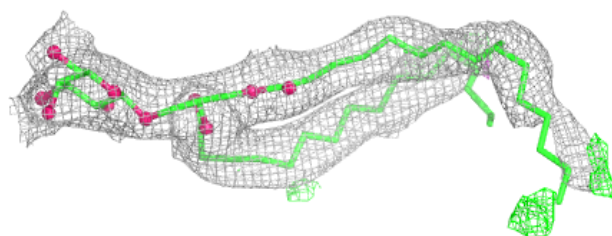
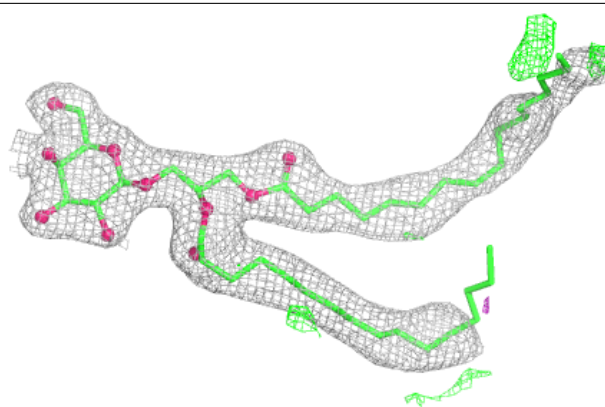
Electron density around SQD A 410 (B):

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

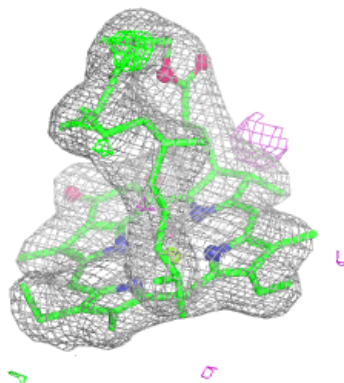
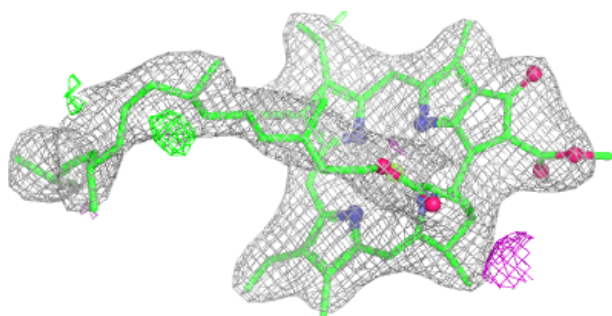
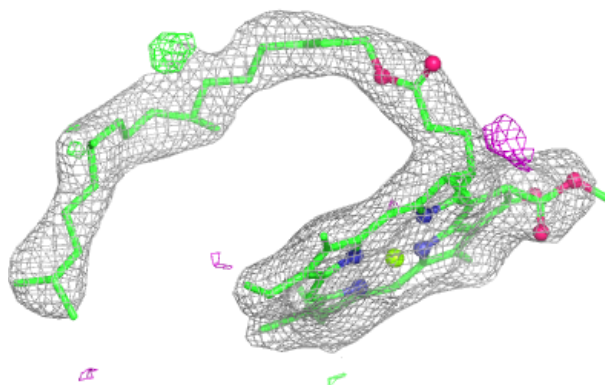


Electron density around LMG D 413:

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

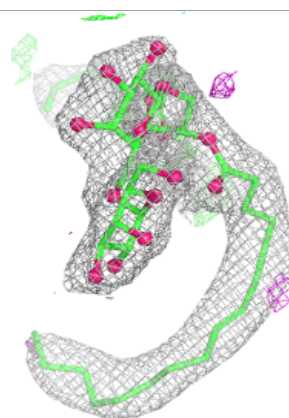
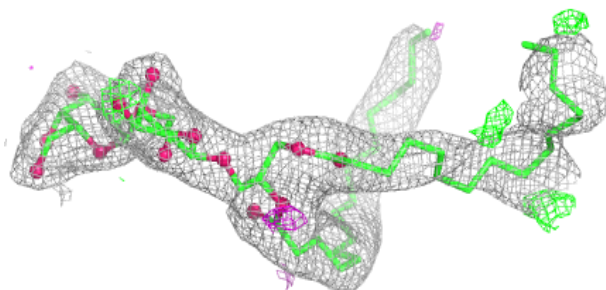
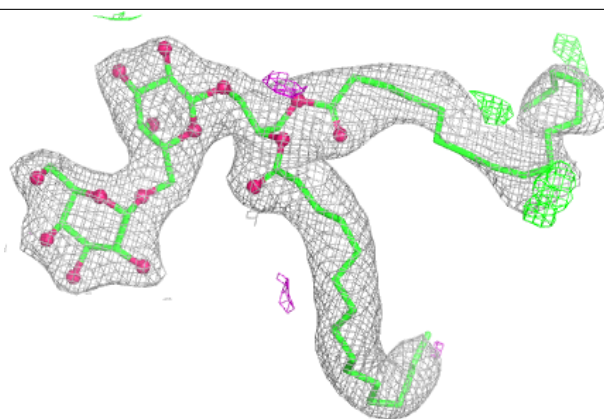
**Electron density around CLA C 514:**

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

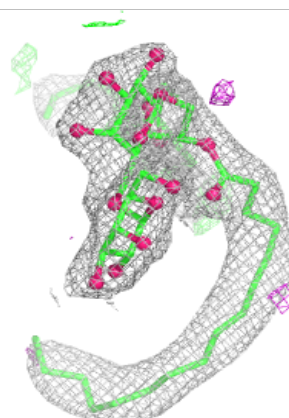
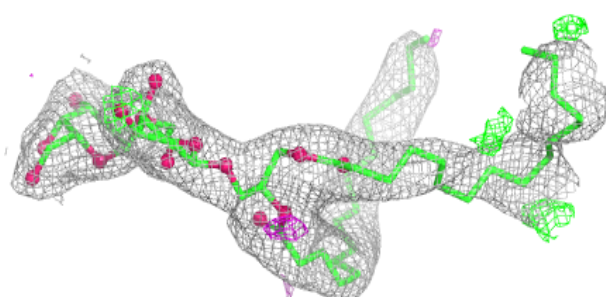
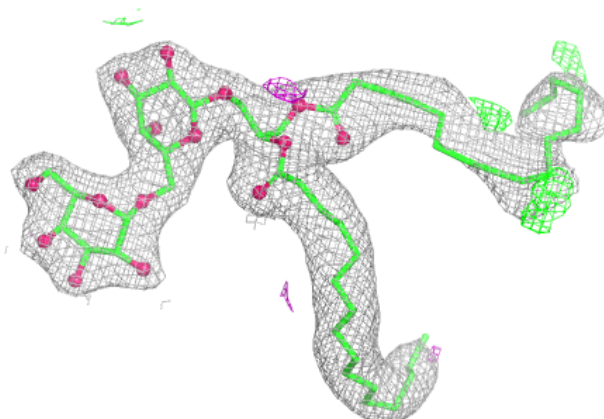


Electron density around DGD C 518 (A):

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

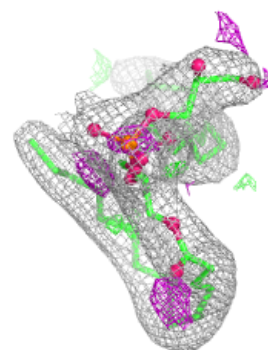
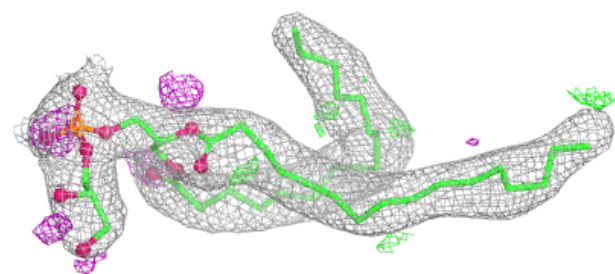
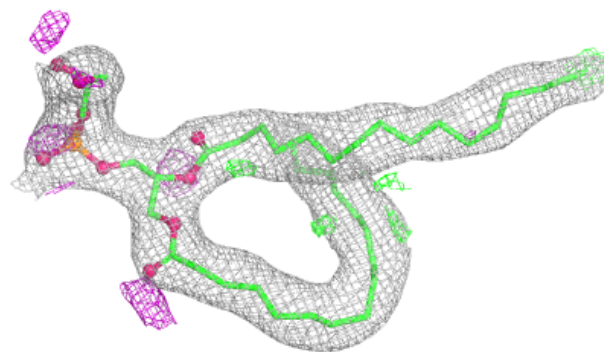
**Electron density around DGD C 518 (B):**

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

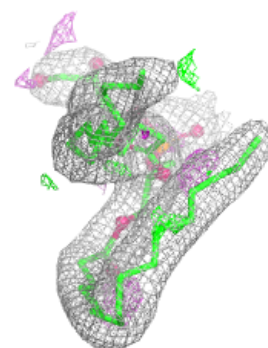
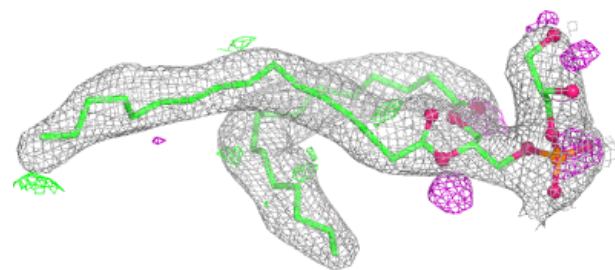
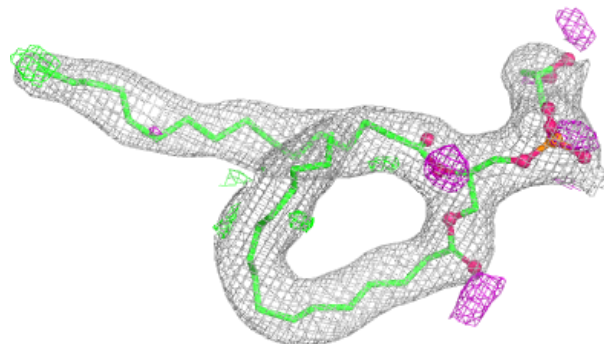


Electron density around LHG A 418 (A):

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

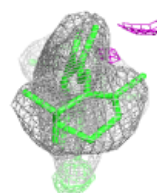
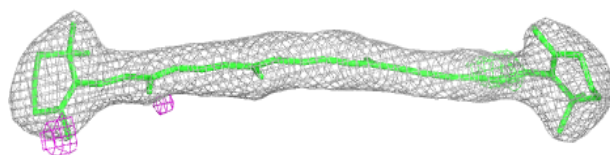
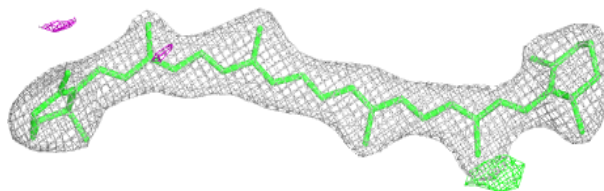
**Electron density around LHG A 418 (B):**

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

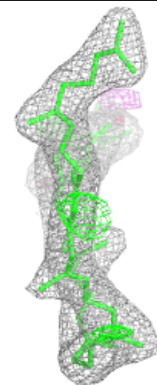
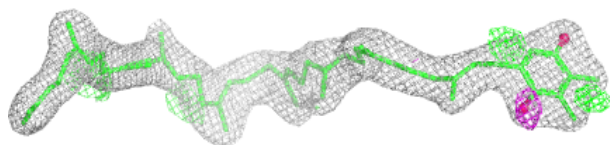
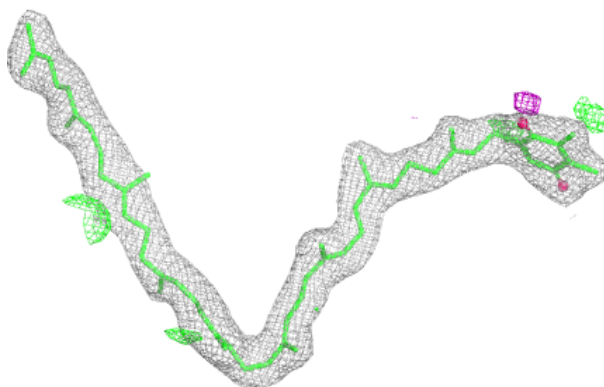


Electron density around BCR K 103:

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

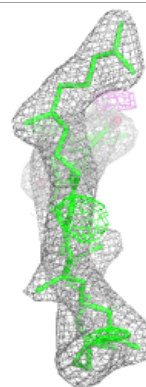
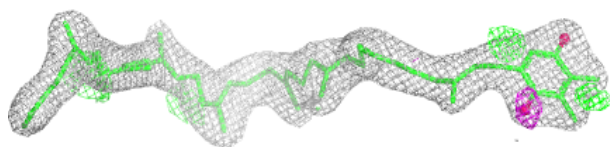
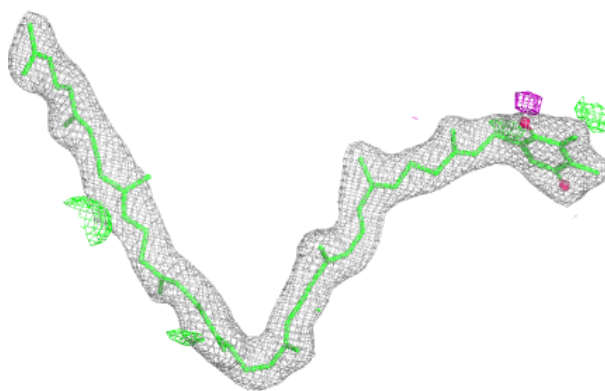
**Electron density around PL9 D 407 (A):**

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

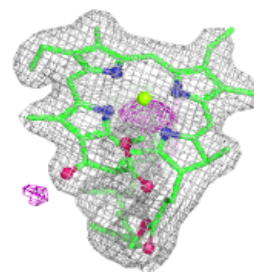
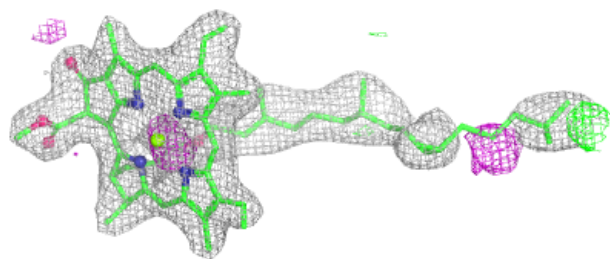
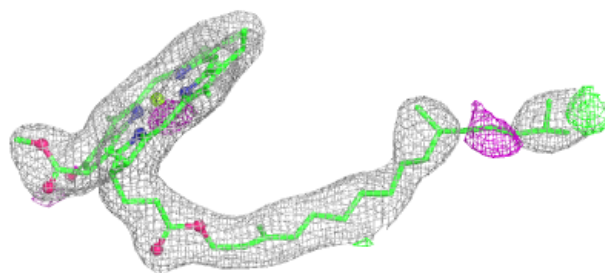


Electron density around PL9 D 407 (B):

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

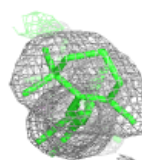
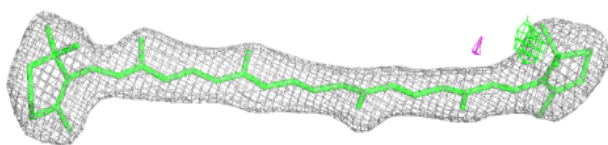
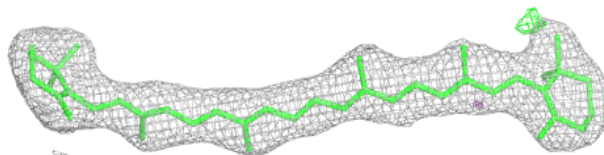
**Electron density around CLA C 505:**

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

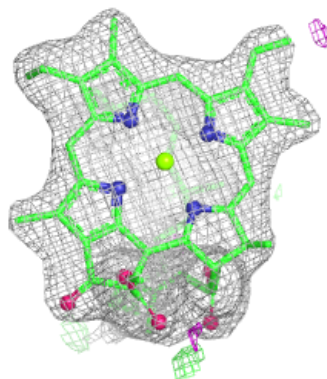
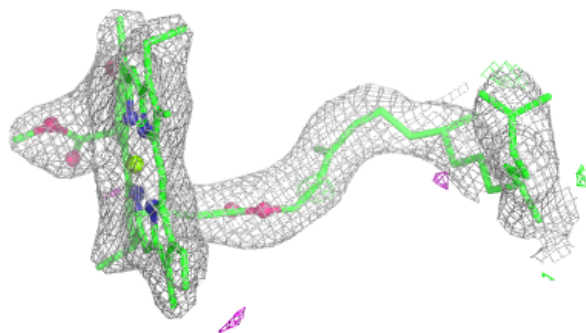
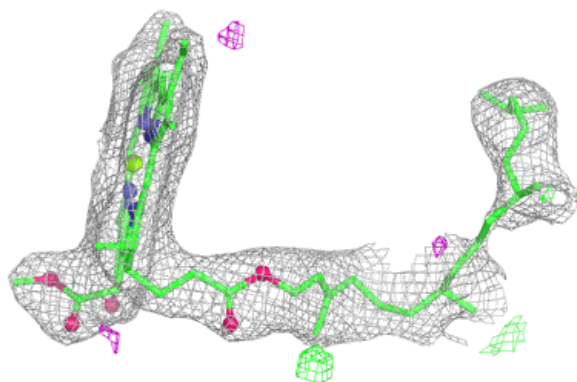


Electron density around BCR c 515:

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

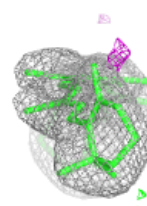
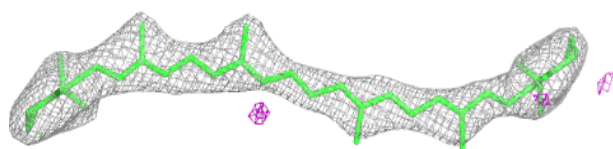
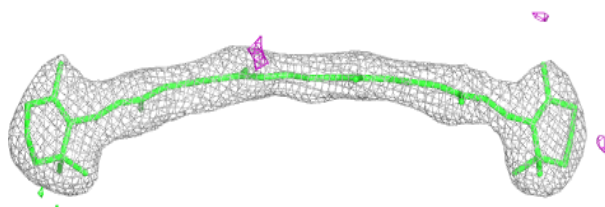
**Electron density around CLA C 507:**

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

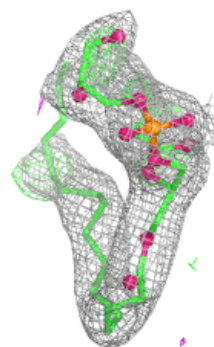
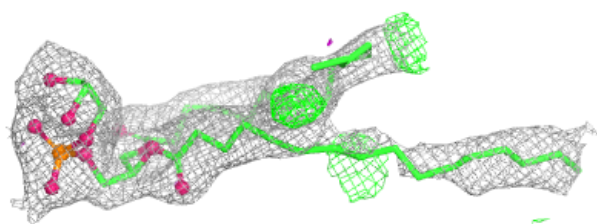
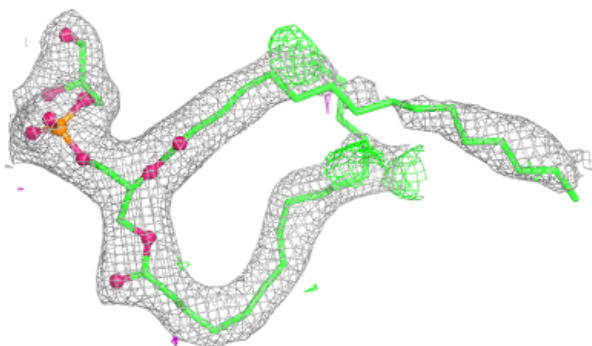


Electron density around BCR k 101:

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

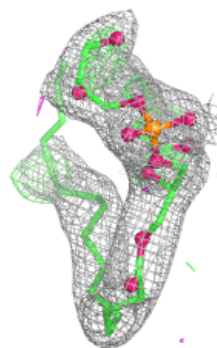
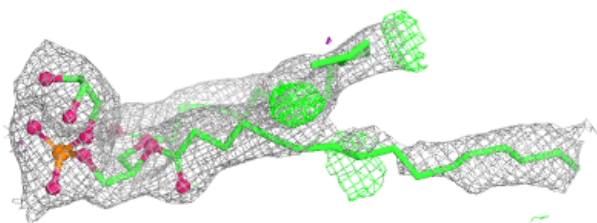
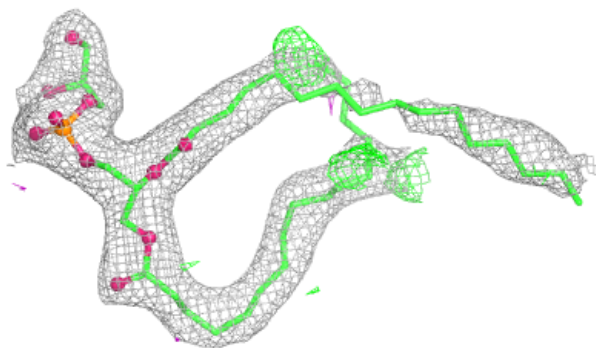
**Electron density around LHG D 409 (A):**

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

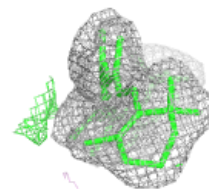
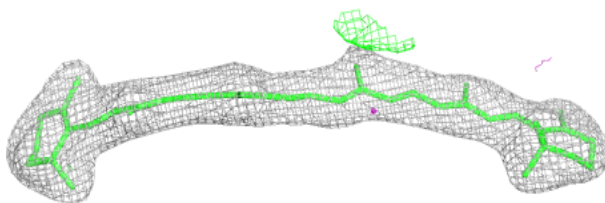
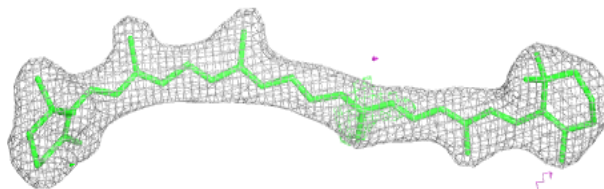


Electron density around LHG D 409 (B):

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

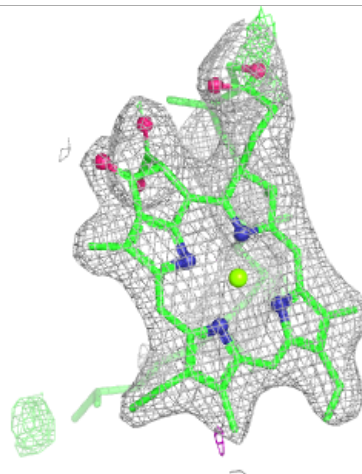
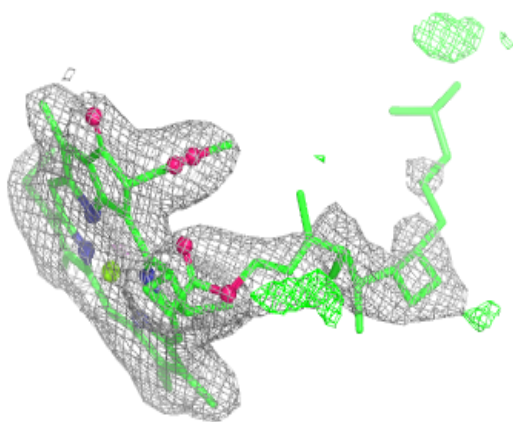
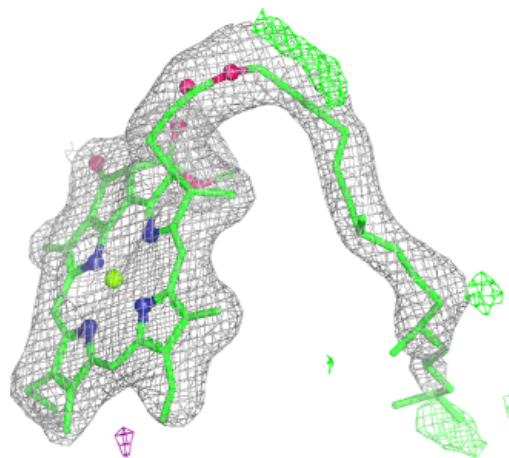
**Electron density around BCR t 102:**

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



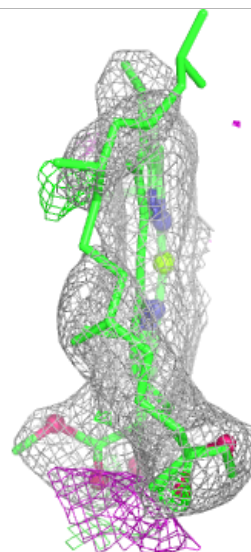
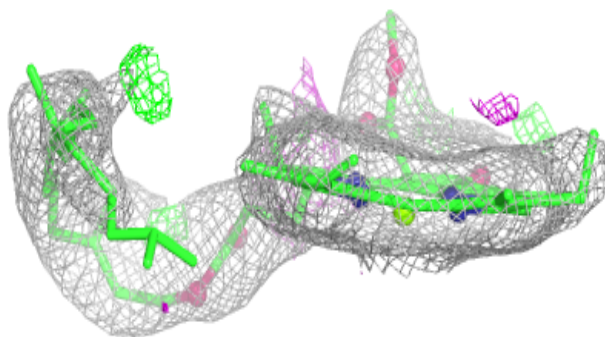
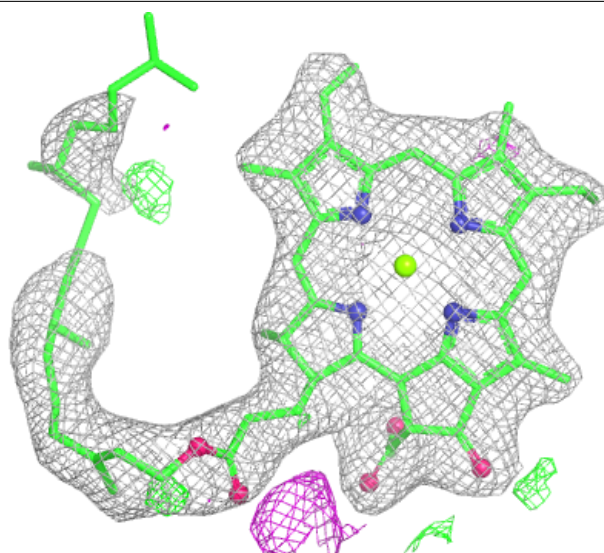
Electron density around CLA b 616:

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



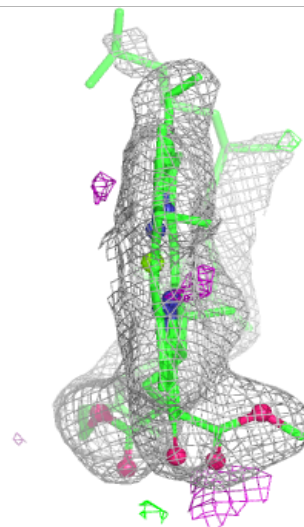
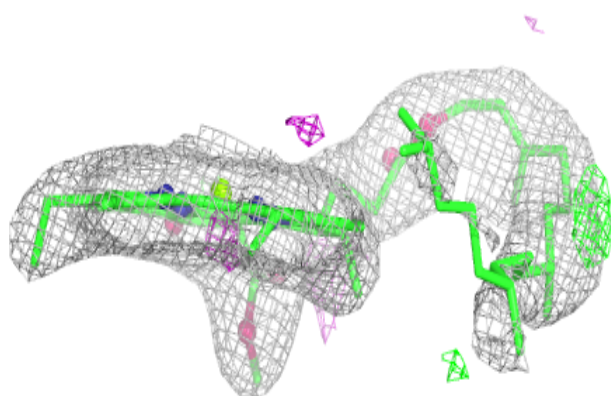
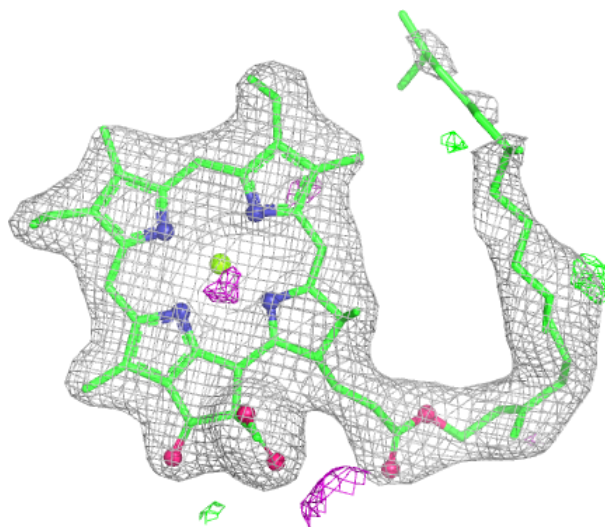
Electron density around CLA c 513:

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



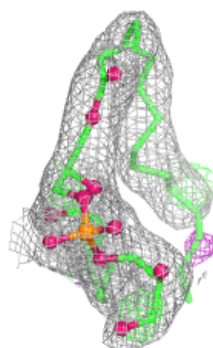
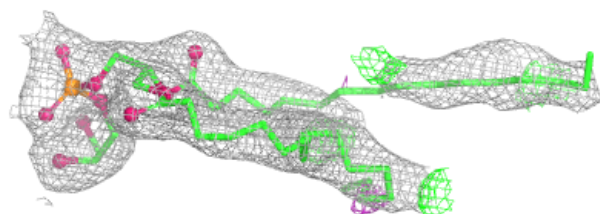
Electron density around CLA C 513:

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

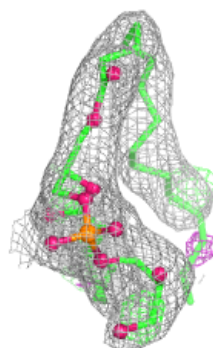
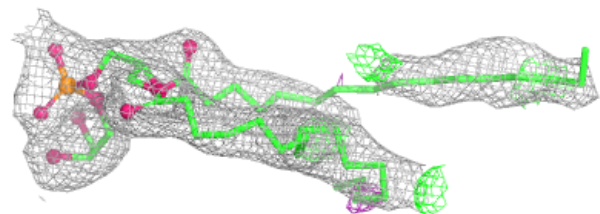
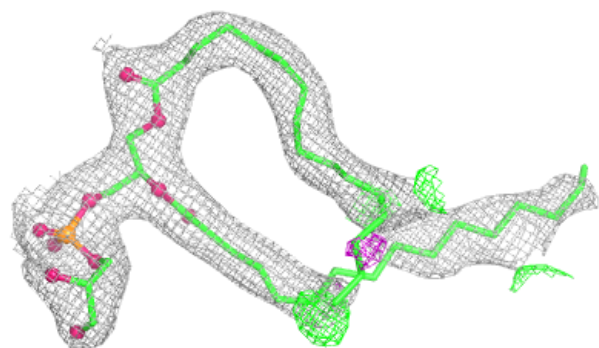


Electron density around LHG d 407 (A):

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

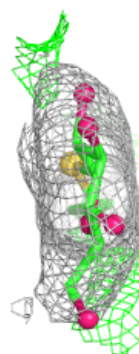
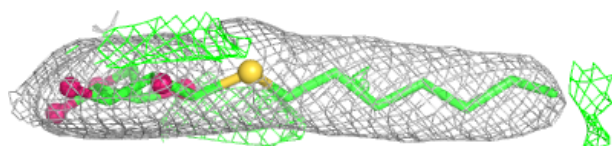
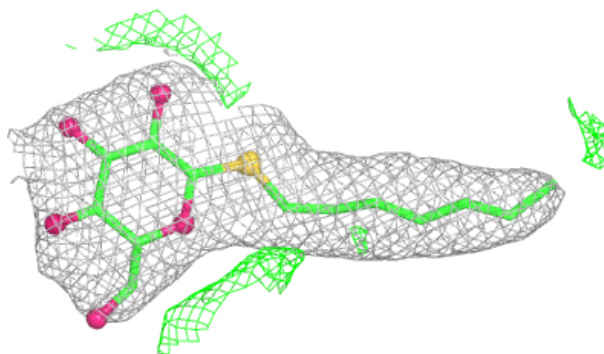
**Electron density around LHG d 407 (B):**

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

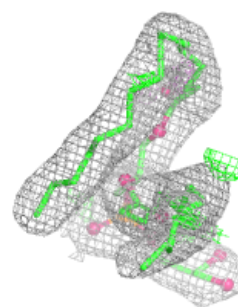
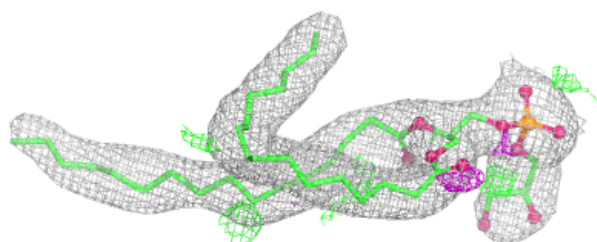
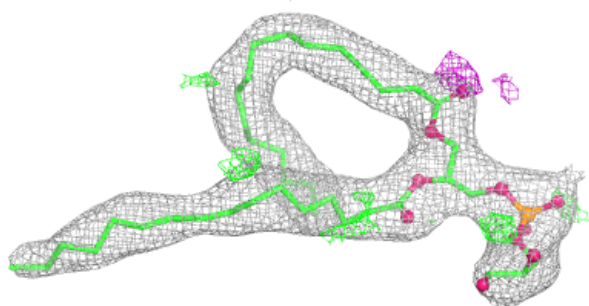


Electron density around HTG b 625:

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

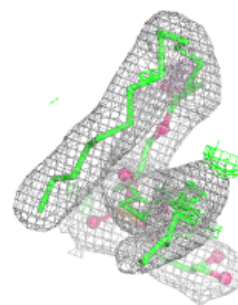
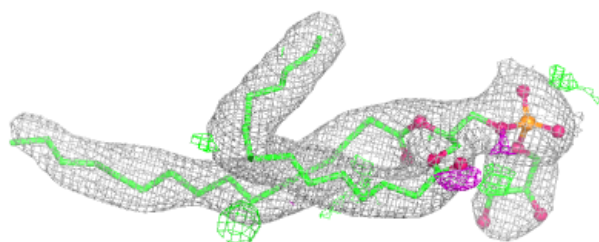
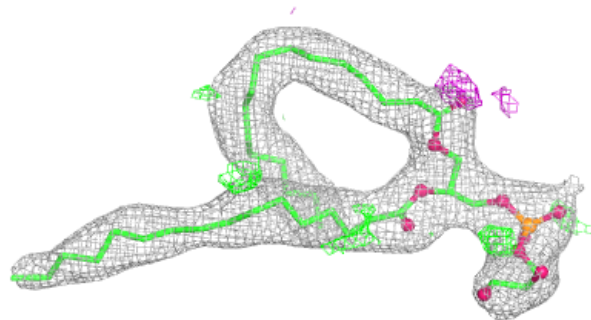
**Electron density around LHG d 413 (A):**

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

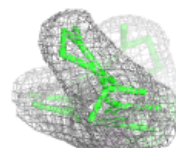
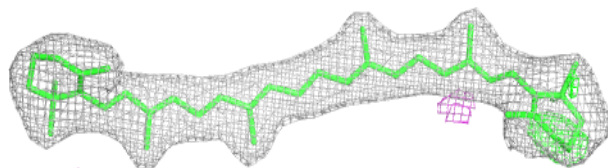
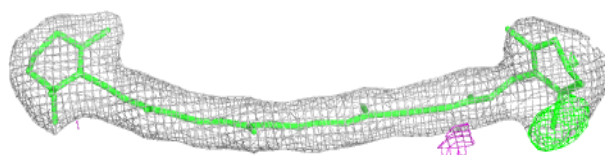


Electron density around LHG d 413 (B):

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

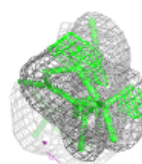
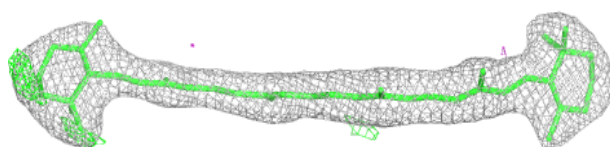
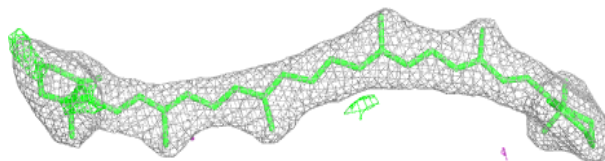
**Electron density around BCR D 406:**

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

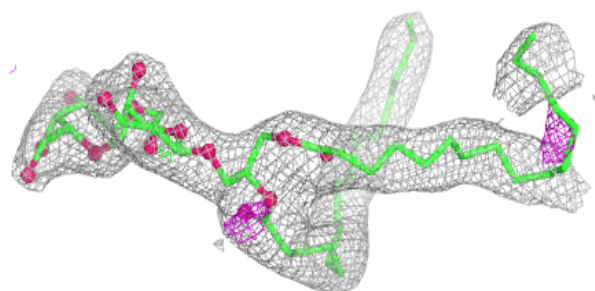
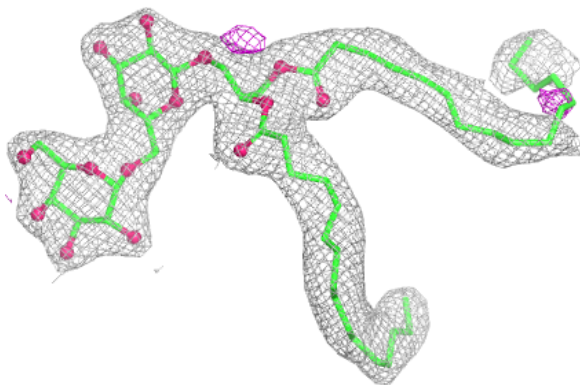


Electron density around BCR H 101:

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

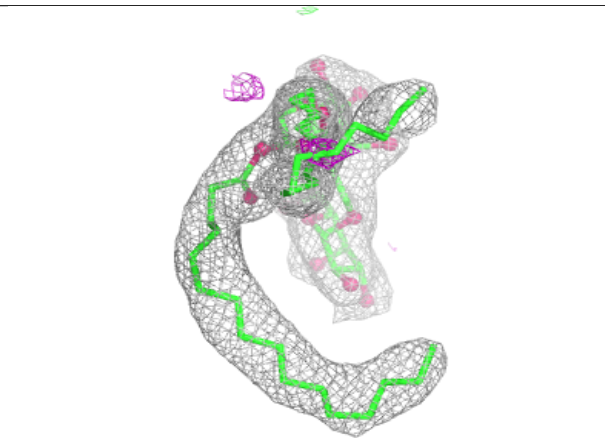
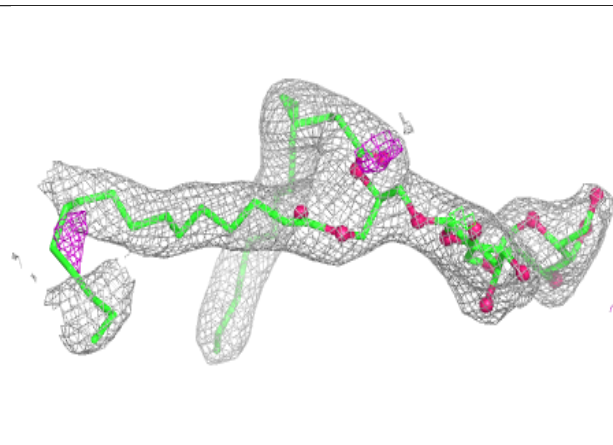
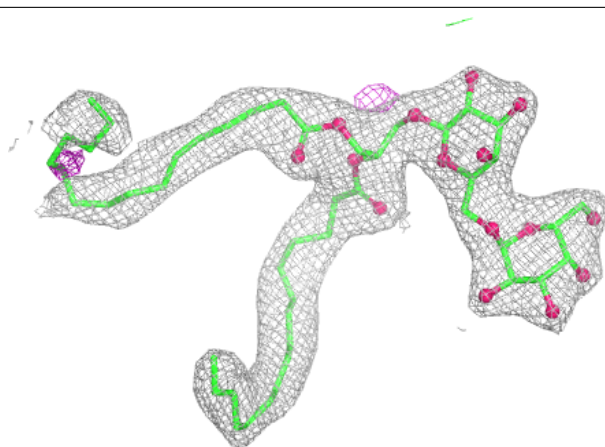
**Electron density around DGD c 518 (A):**

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

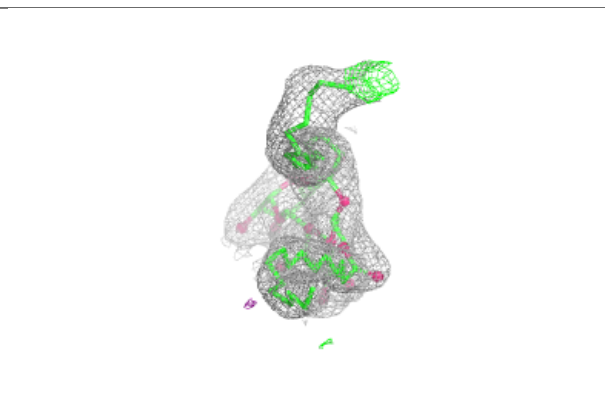
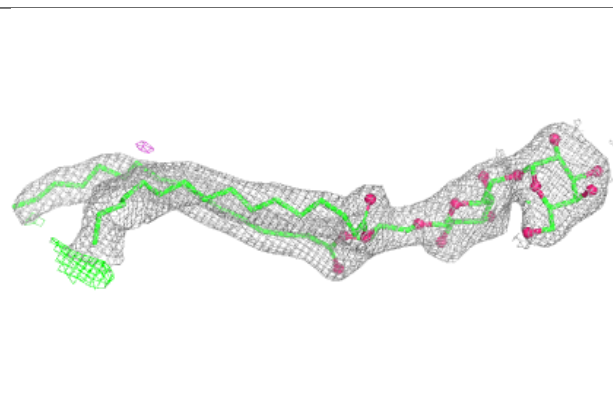
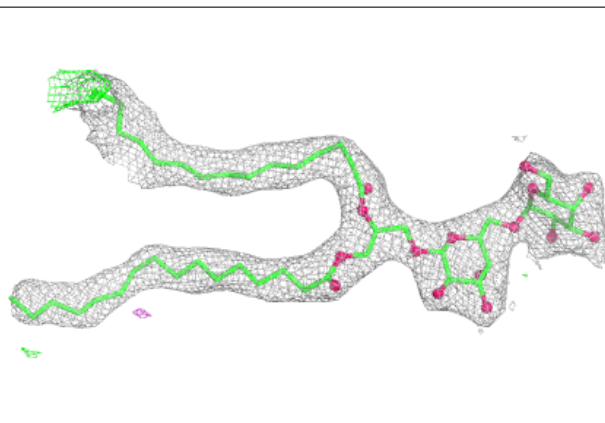


Electron density around DGD c 518 (B):

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

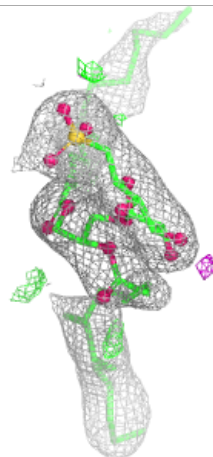
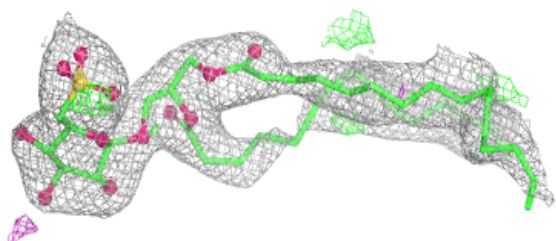
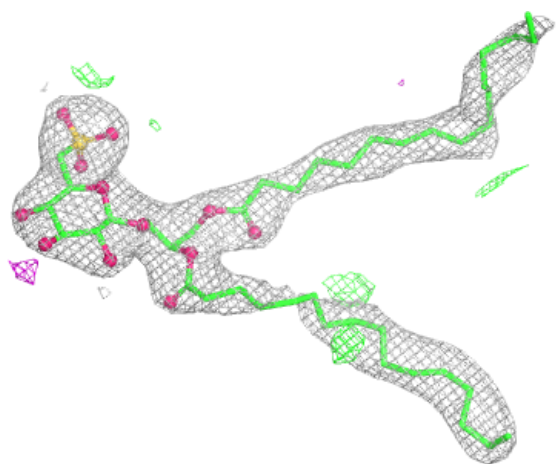
**Electron density around DGD c 519:**

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



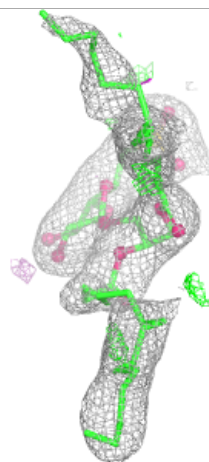
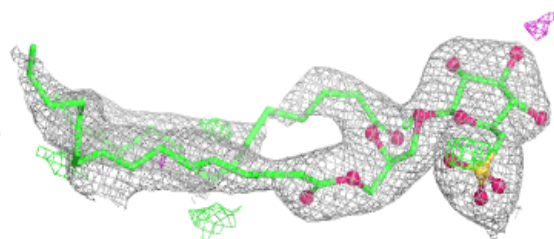
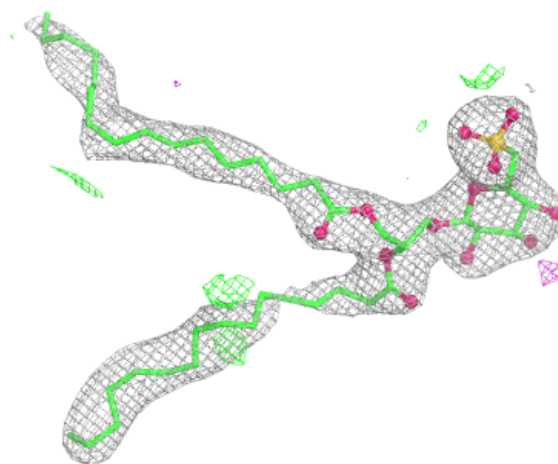
Electron density around SQD a 411 (A):

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



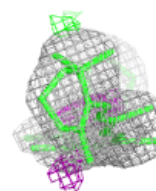
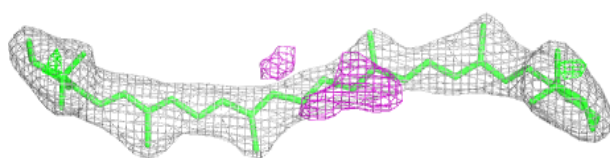
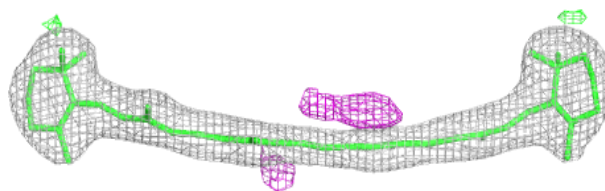
Electron density around SQD a 411 (B):

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

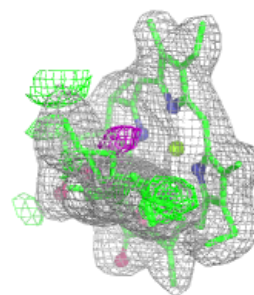
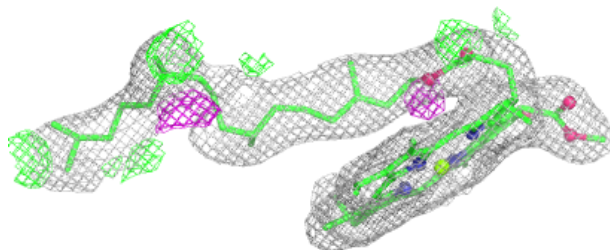
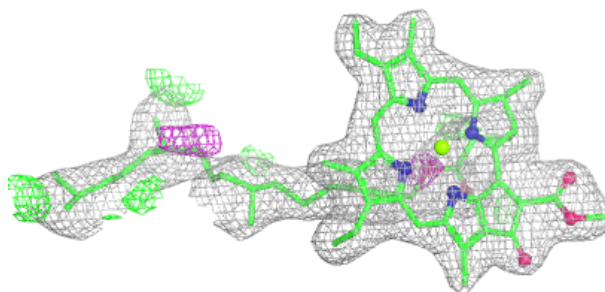


Electron density around BCR K 102:

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

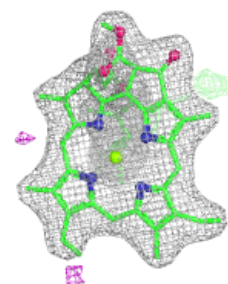
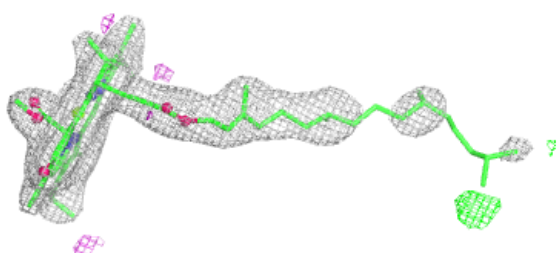
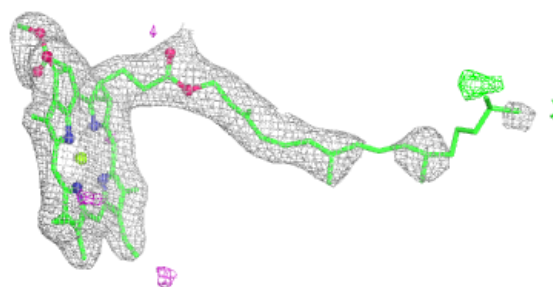
**Electron density around CLA B 614:**

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

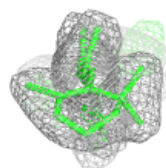
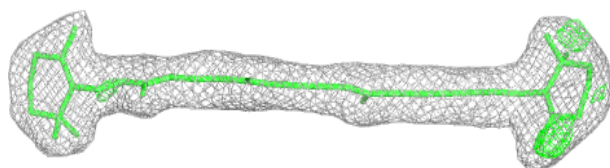
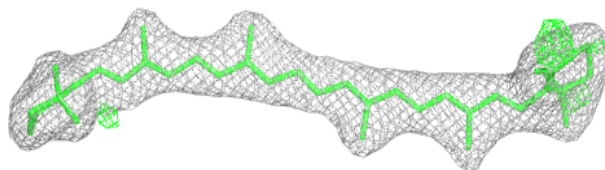


Electron density around CLA d 403:

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

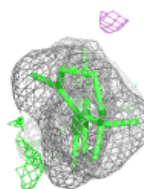
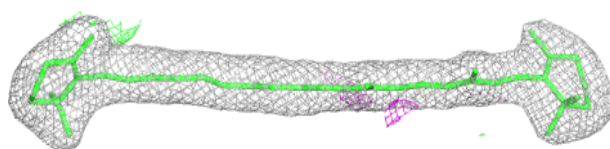
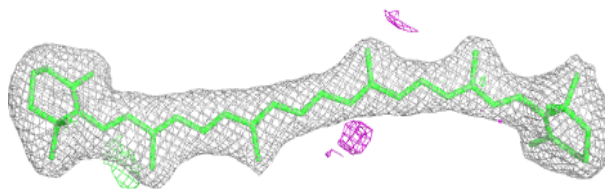
**Electron density around BCR A 409:**

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

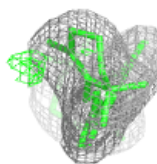
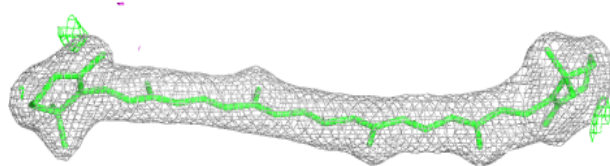
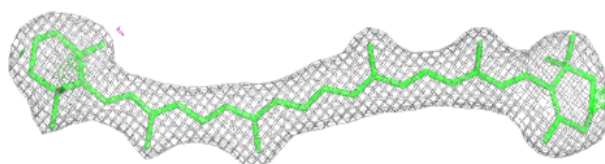


Electron density around BCR B 618:

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

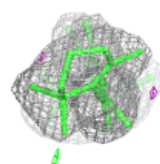
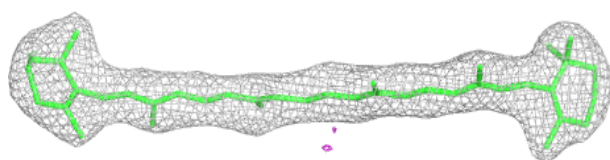
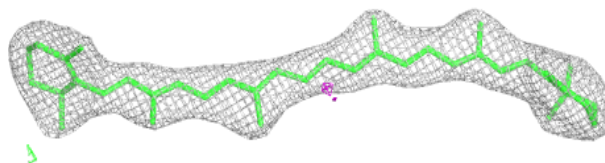
**Electron density around BCR B 619:**

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



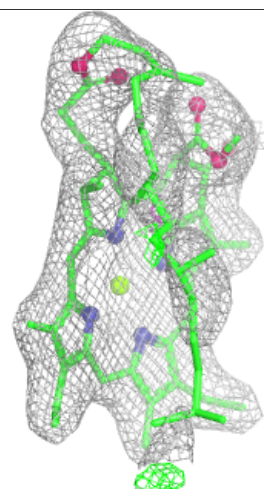
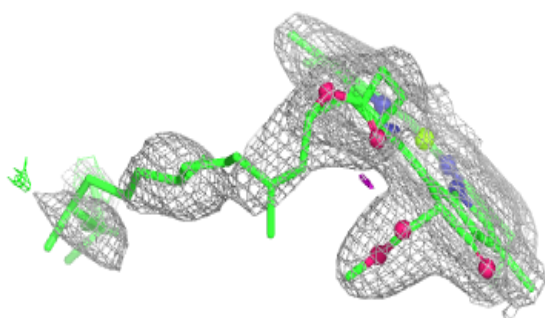
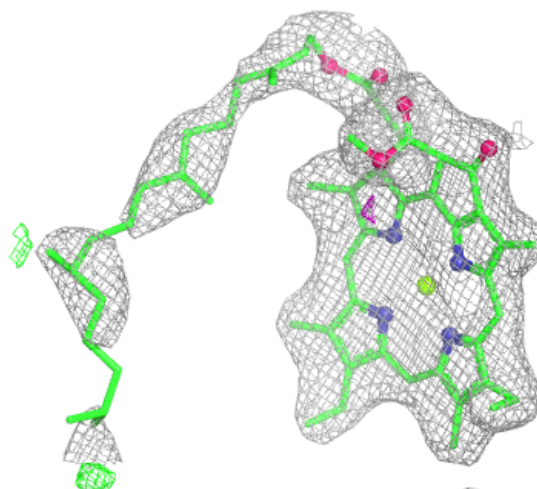
Electron density around BCR C 515:

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



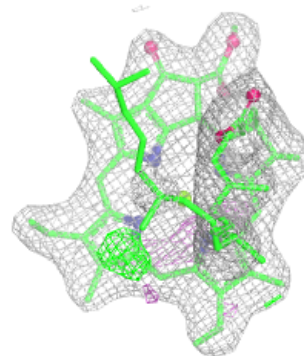
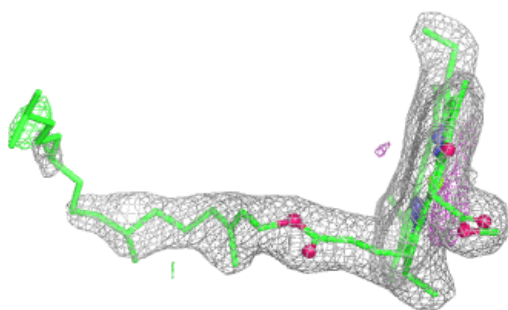
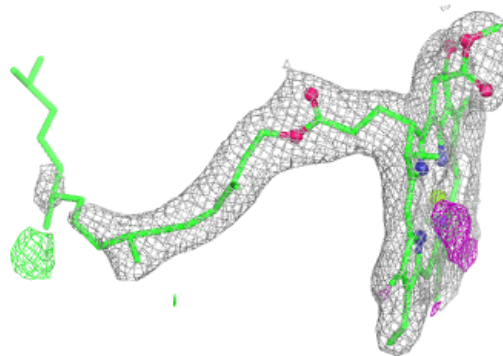
Electron density around CLA B 616:

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

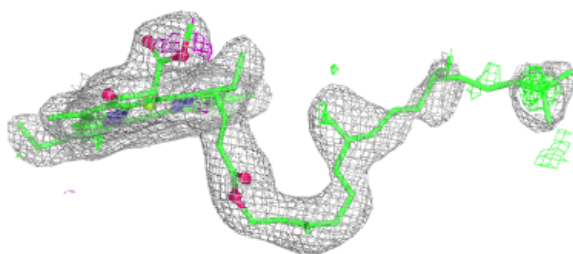
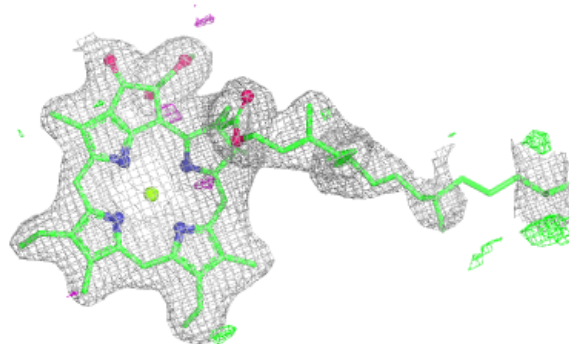


Electron density around CLA D 405:

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

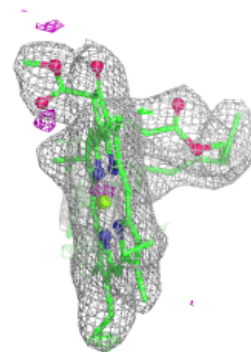
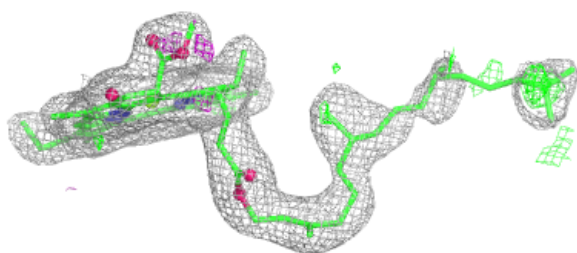
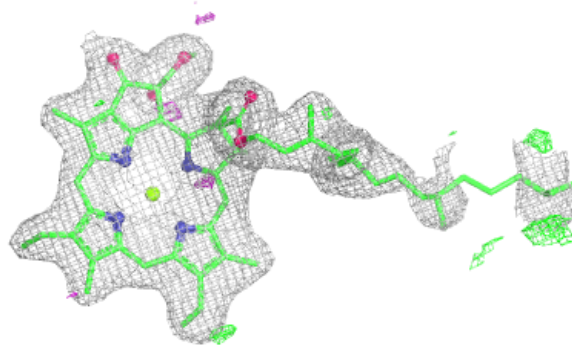
**Electron density around CLA a 407 (A):**

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

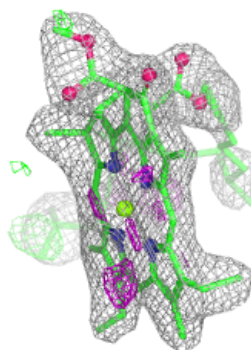
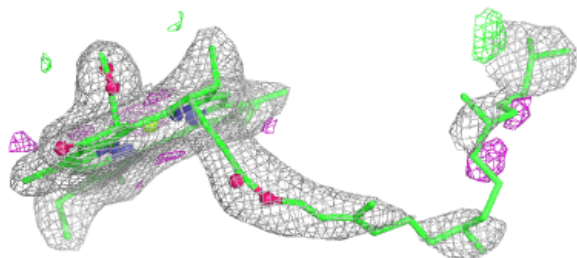
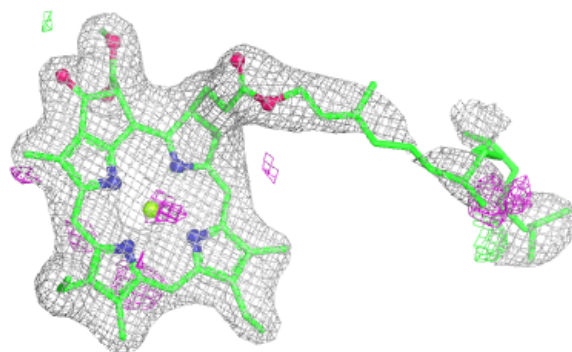


Electron density around CLA a 407 (B):

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

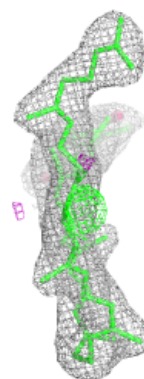
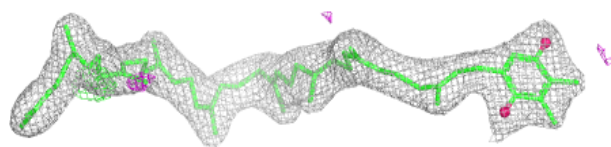
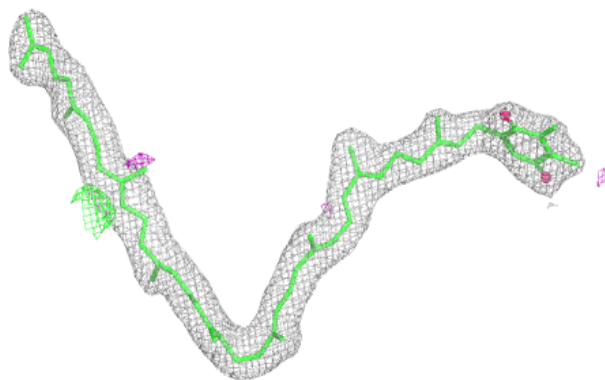
**Electron density around CLA a 409:**

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

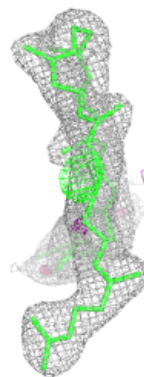
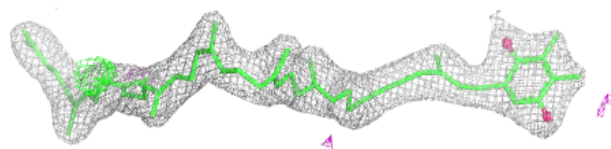
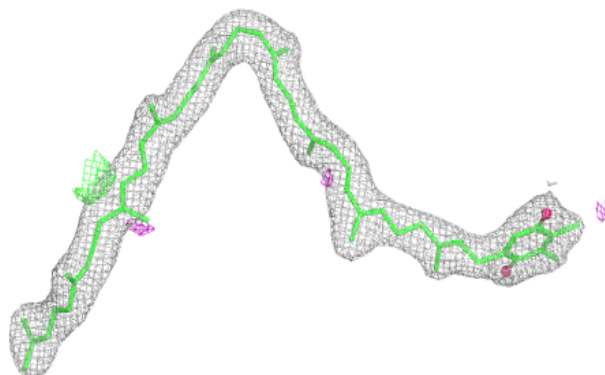


Electron density around PL9 d 405 (A):

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

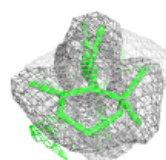
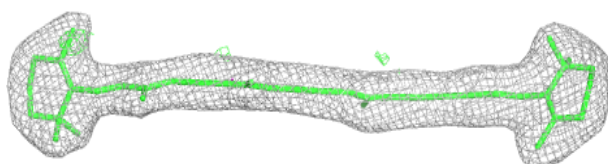
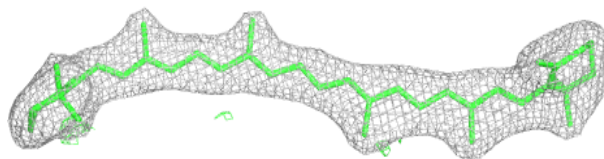
**Electron density around PL9 d 405 (B):**

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

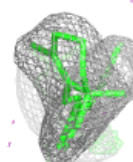
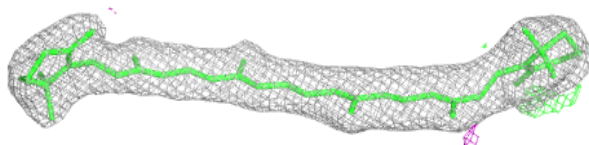
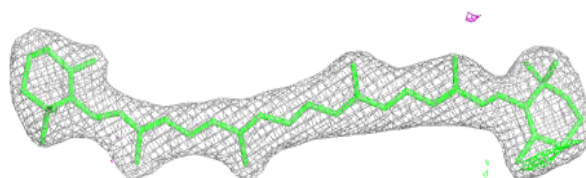


Electron density around BCR a 410:

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

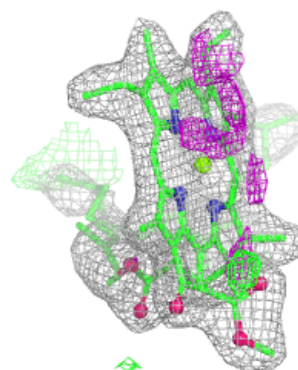
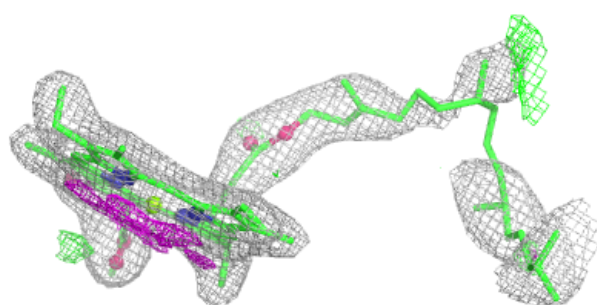
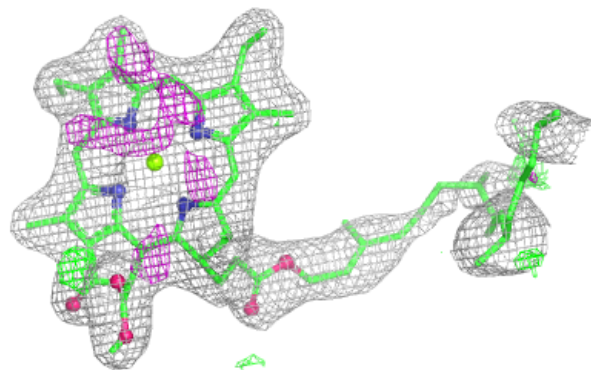
**Electron density around BCR b 619:**

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

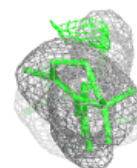
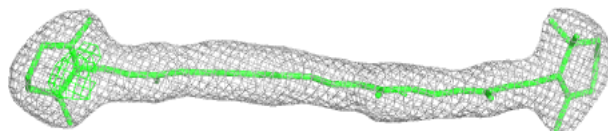
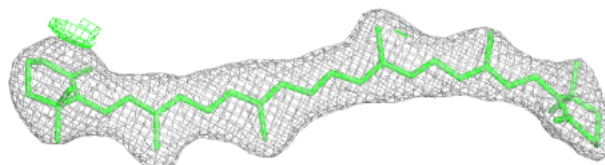


Electron density around CLA A 408:

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

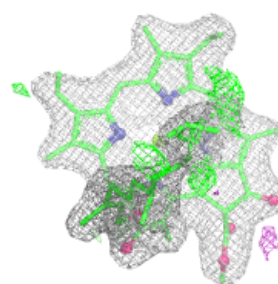
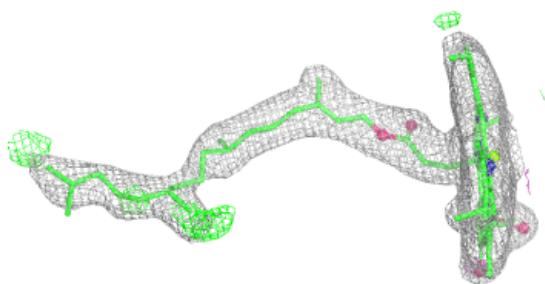
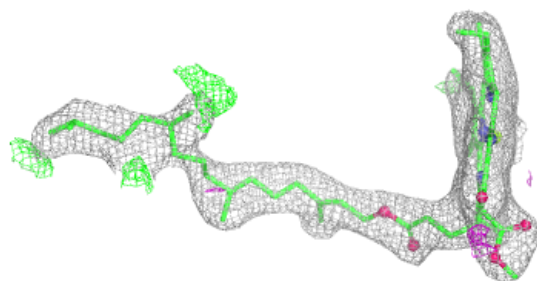
**Electron density around BCR c 516:**

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

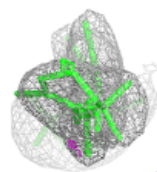
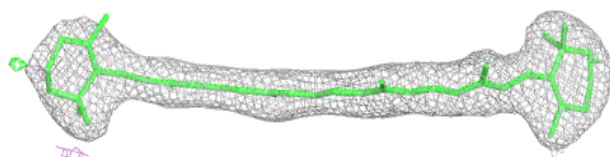
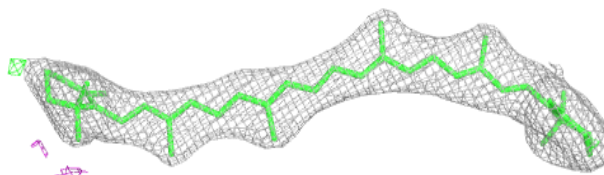


Electron density around CLA b 606:

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

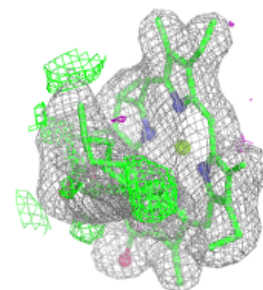
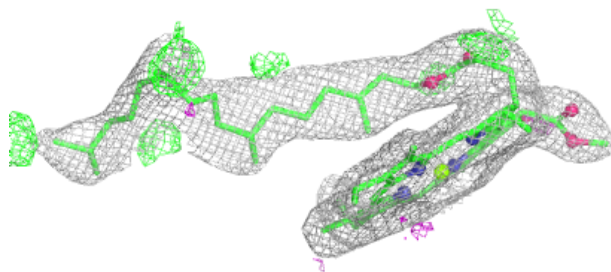
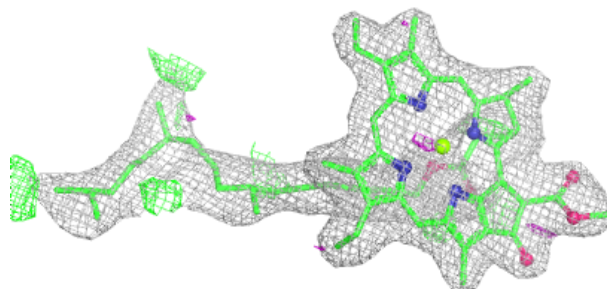
**Electron density around BCR h 101:**

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

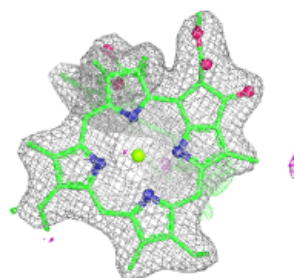
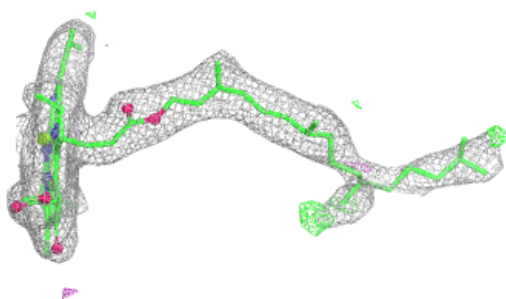
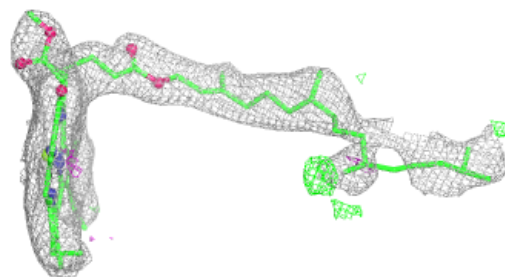


Electron density around CLA b 614:

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

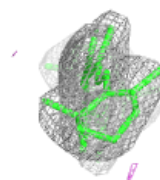
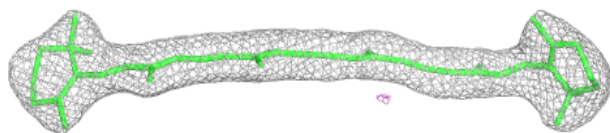
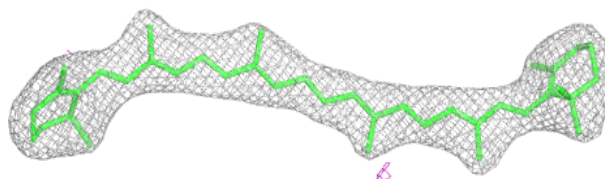
**Electron density around CLA B 606:**

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

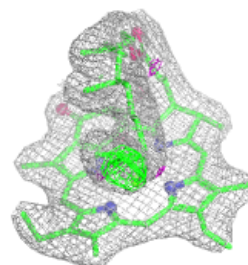
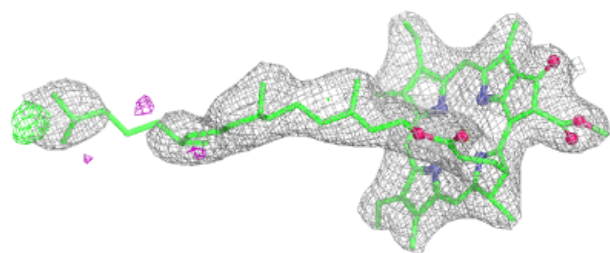
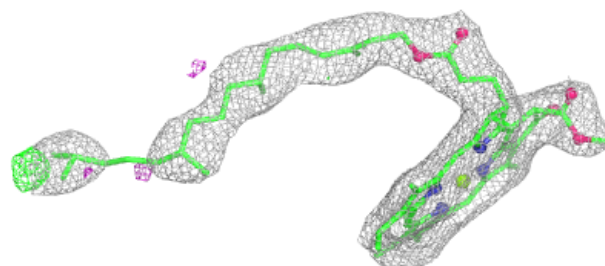


Electron density around BCR y 101:

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

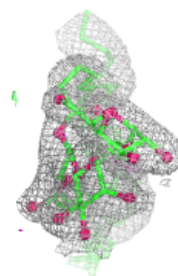
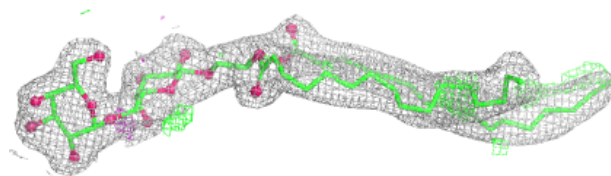
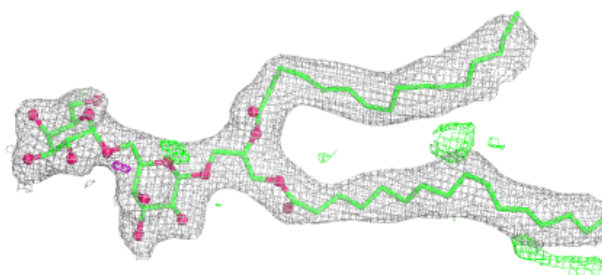
**Electron density around CLA c 505:**

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

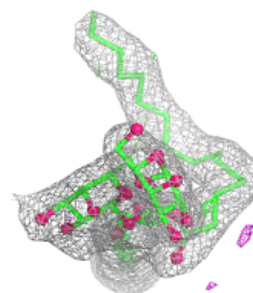
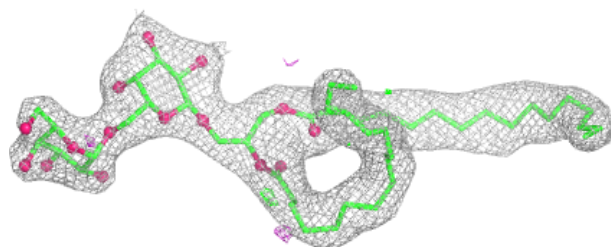
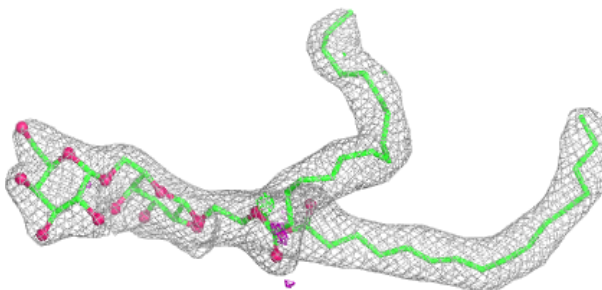


Electron density around DGD C 519:

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

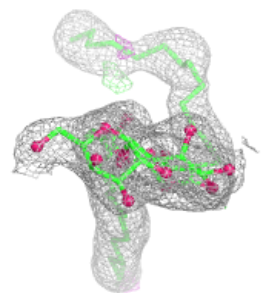
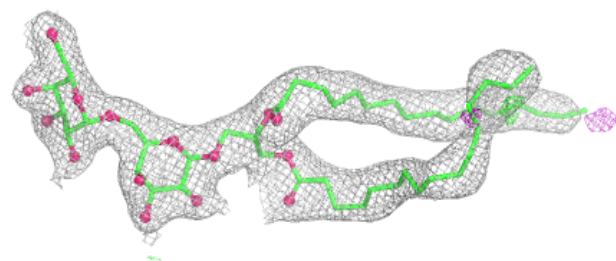
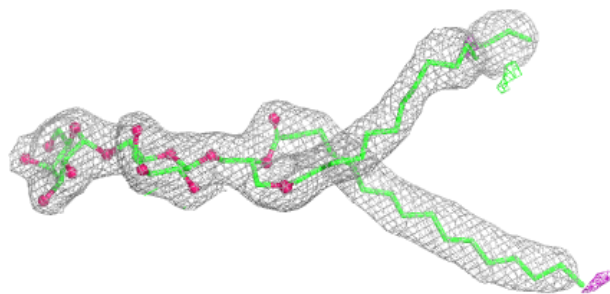
**Electron density around DGD H 102:**

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

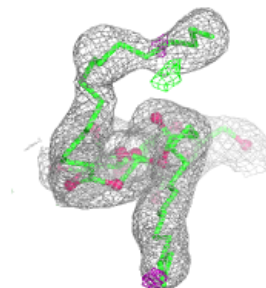
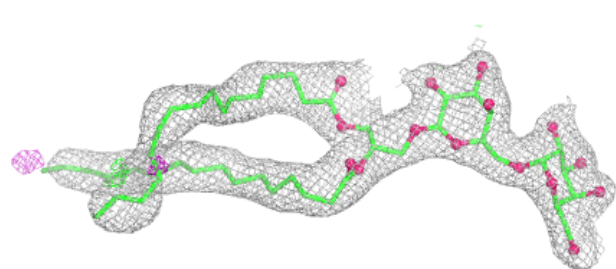
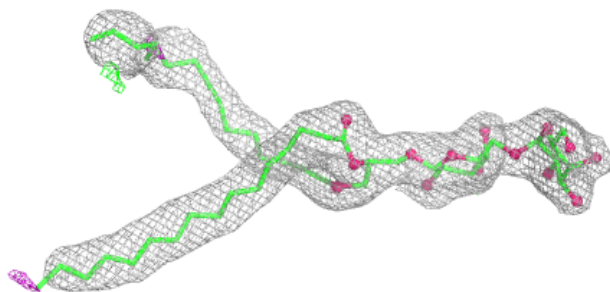


Electron density around DGD c 517 (A):

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

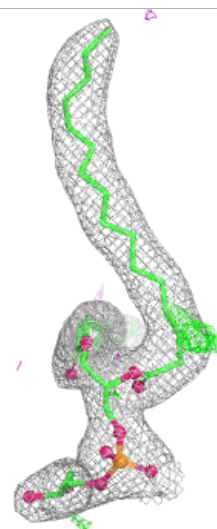
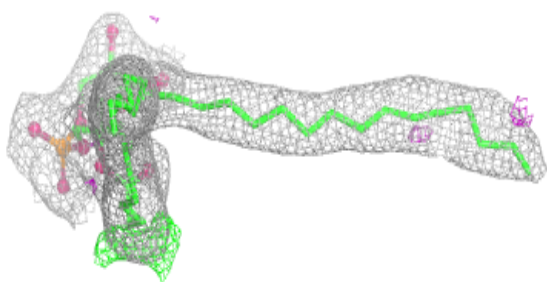
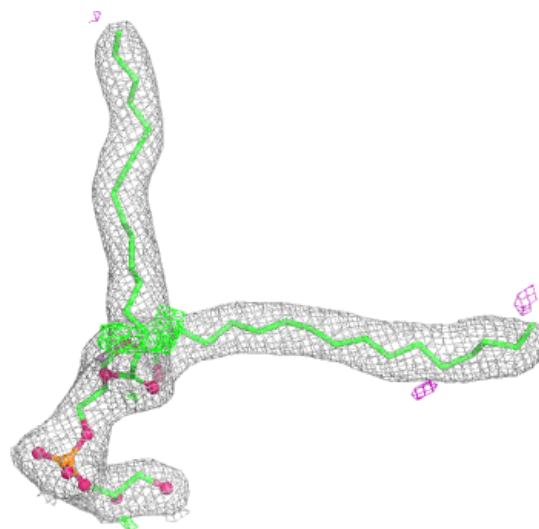
**Electron density around DGD c 517 (B):**

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



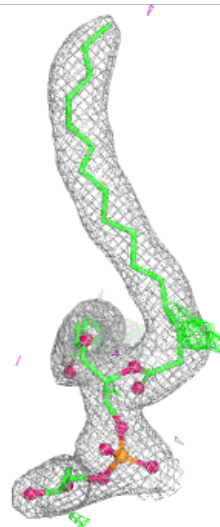
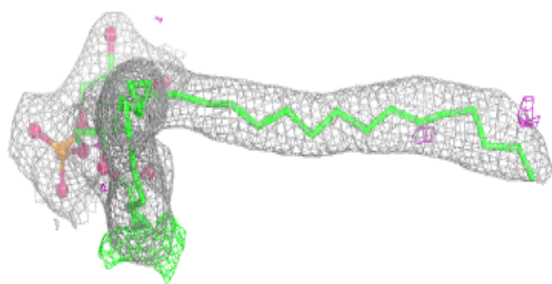
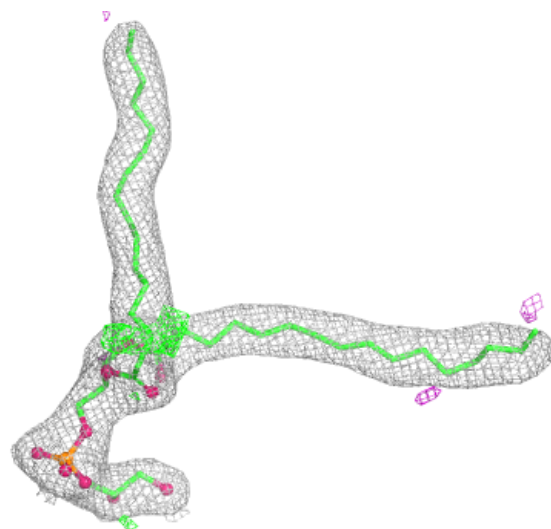
Electron density around LHG b 629 (A):

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



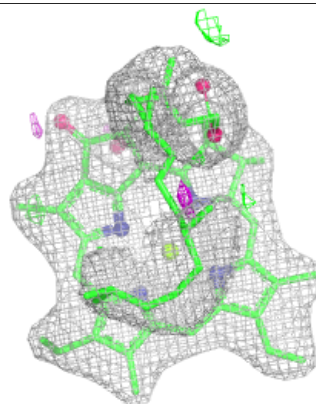
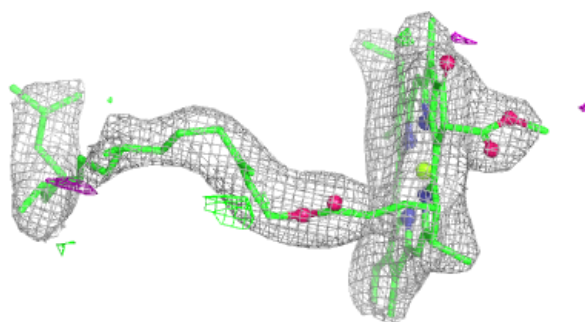
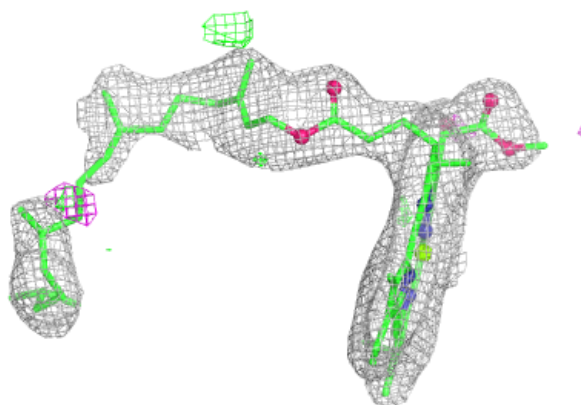
Electron density around LHG b 629 (B):

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

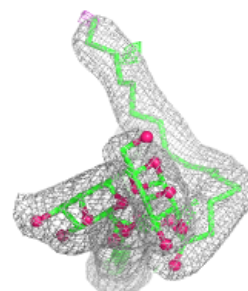
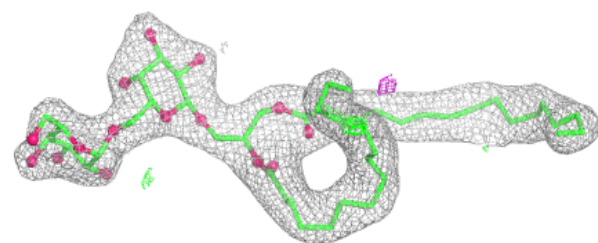
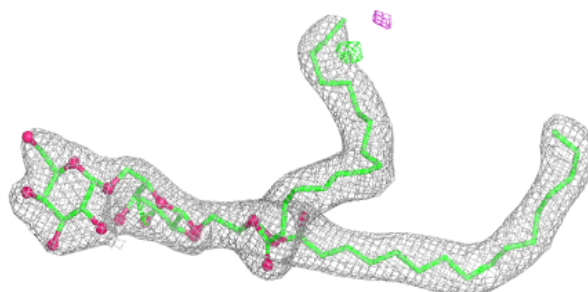


Electron density around CLA c 507:

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

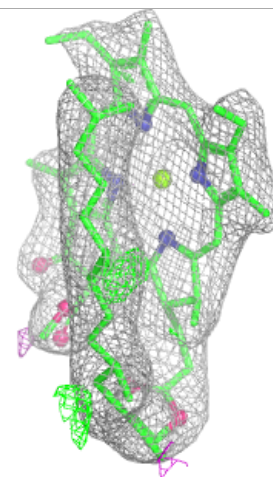
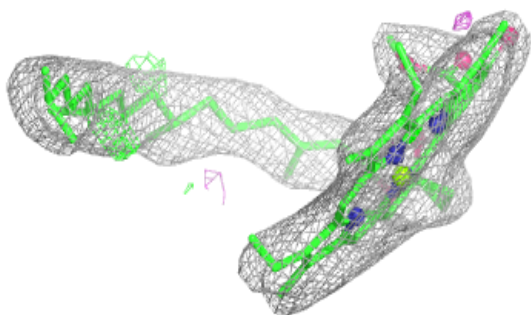
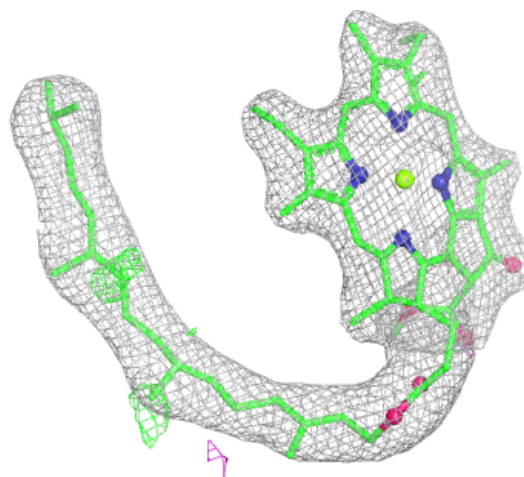
**Electron density around DGD h 102:**

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



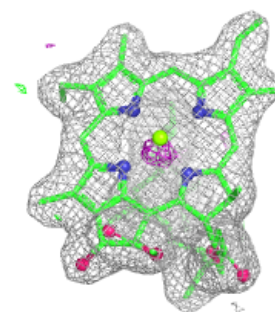
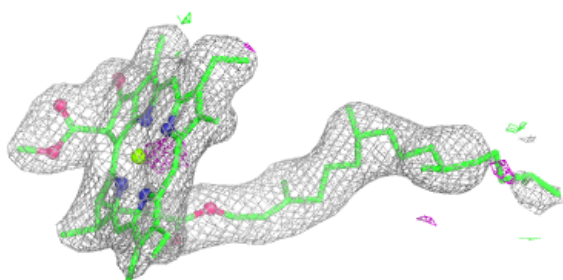
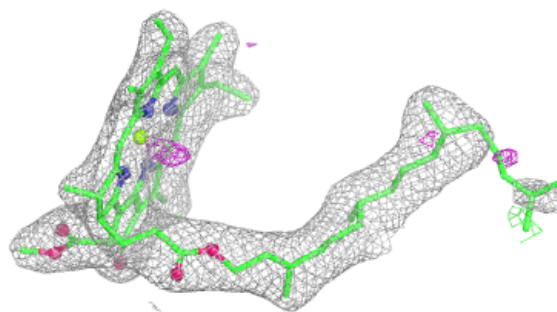
Electron density around CLA c 508:

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

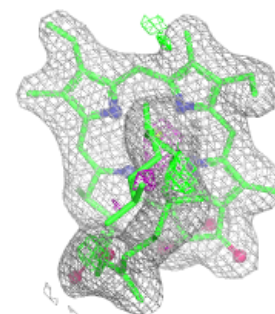
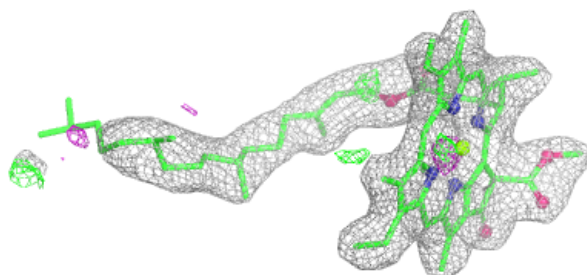
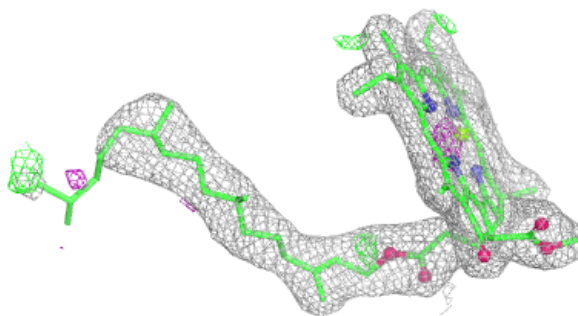


Electron density around CLA c 509:

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

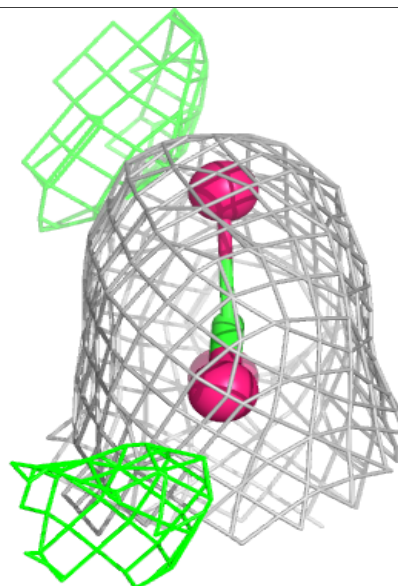
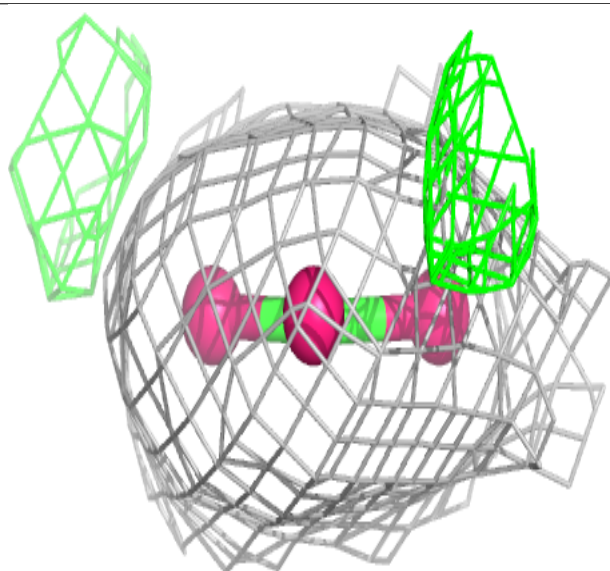
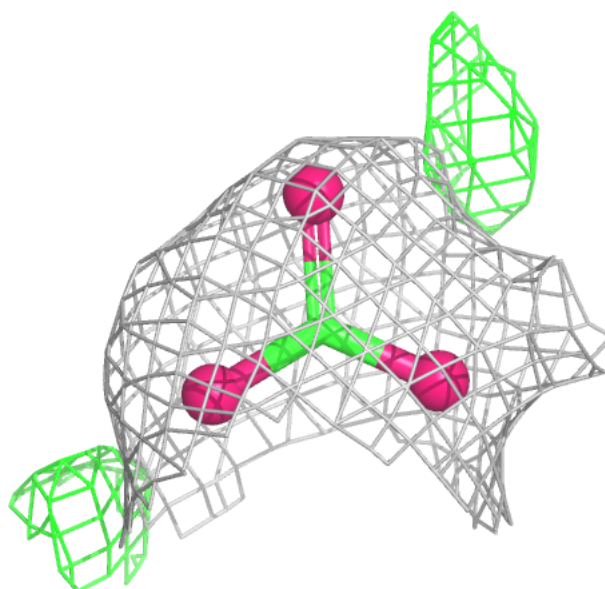
**Electron density around CLA C 509:**

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



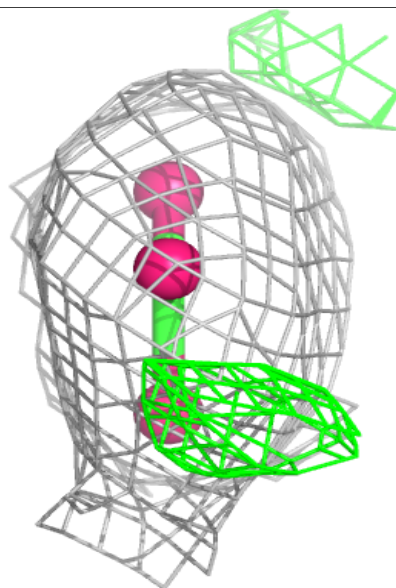
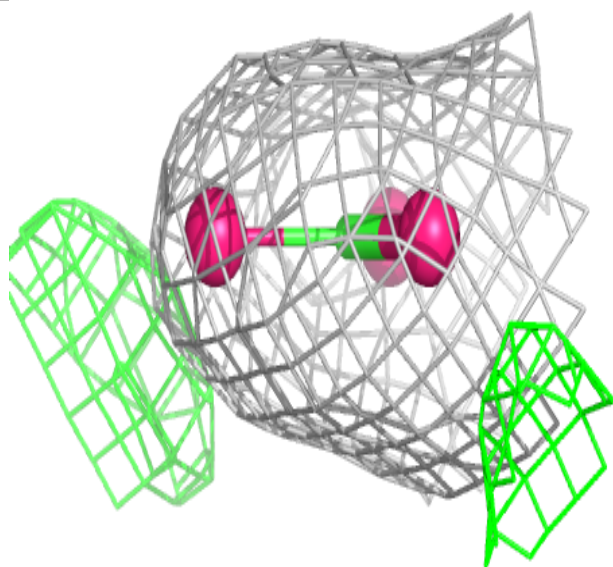
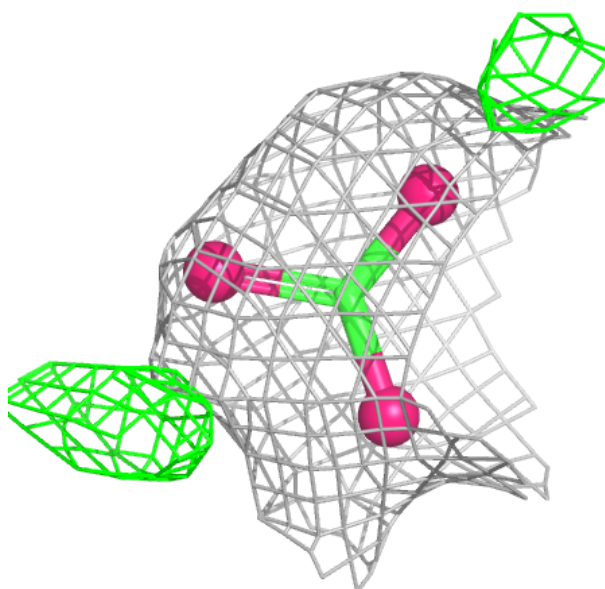
Electron density around BCT d 401 (A):

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



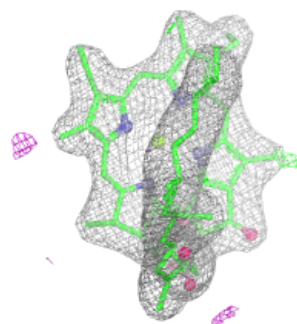
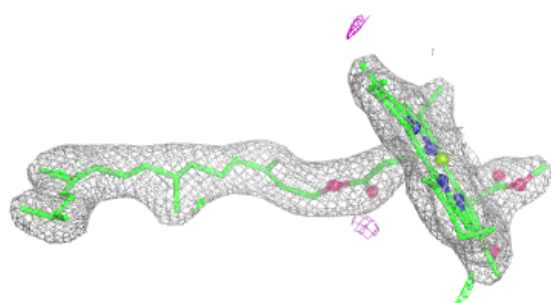
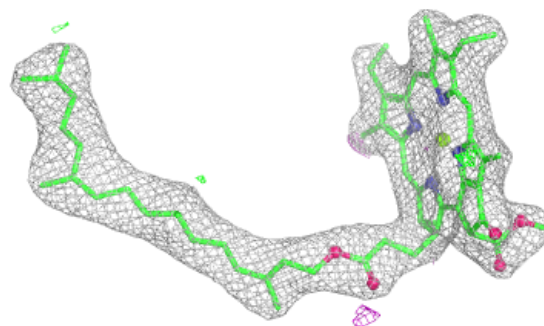
Electron density around BCT d 401 (B):

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

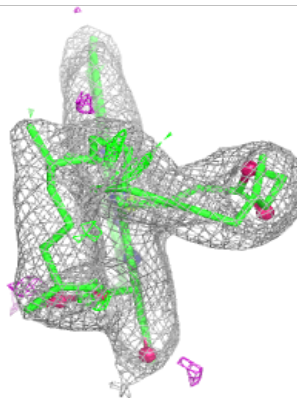
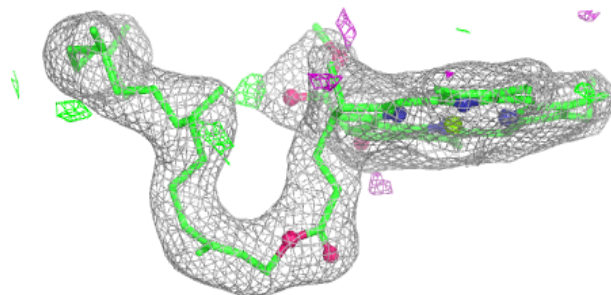
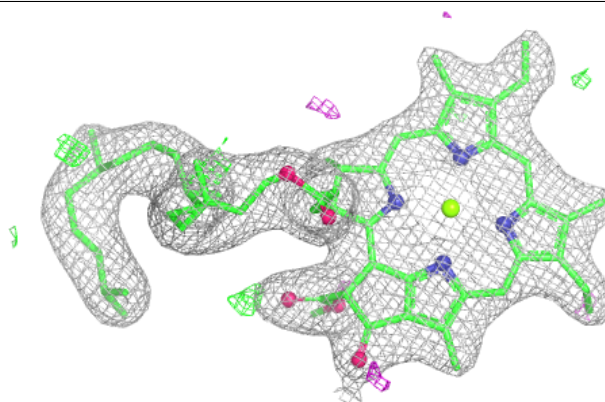


Electron density around CLA b 609:

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

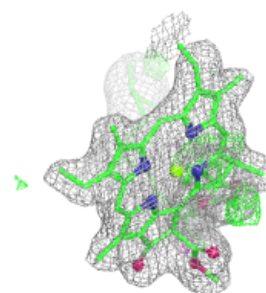
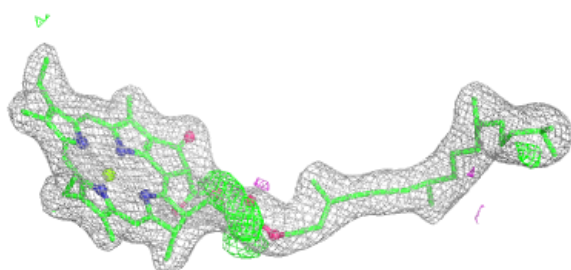
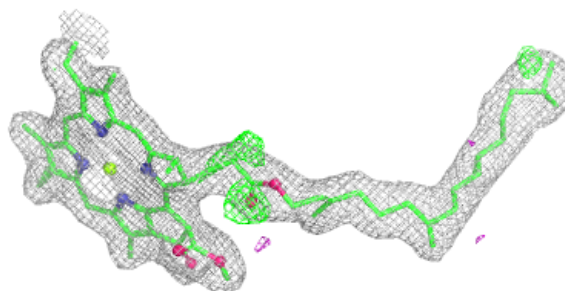
**Electron density around CLA b 612:**

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

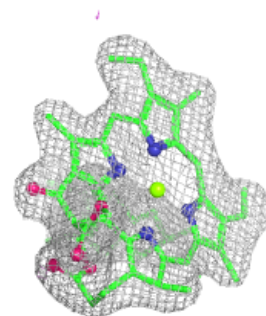
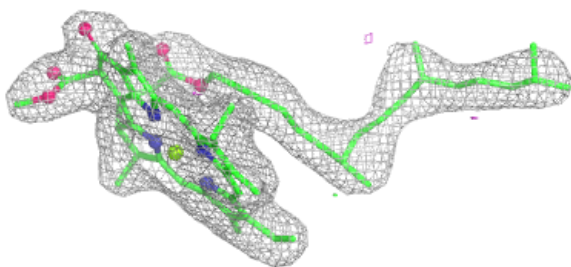
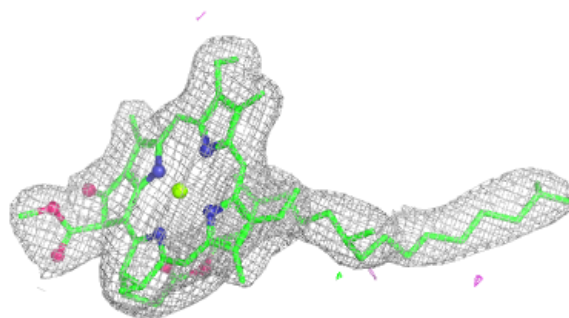


Electron density around CLA A 404 (B):

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

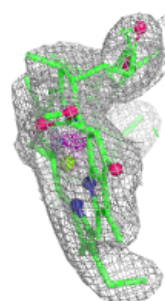
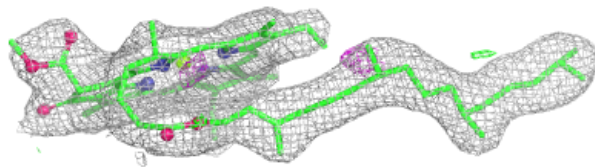
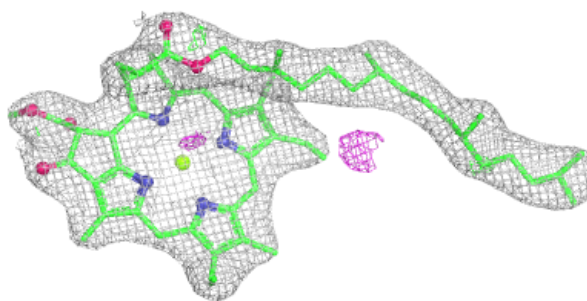
**Electron density around CLA C 506:**

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



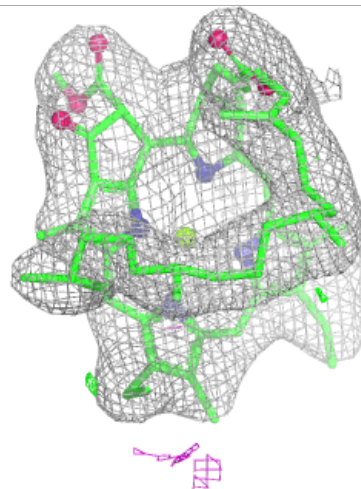
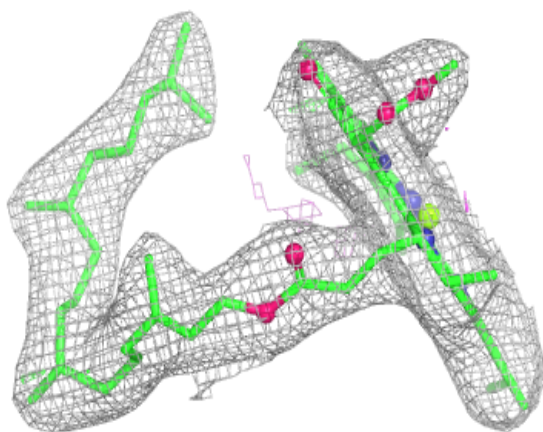
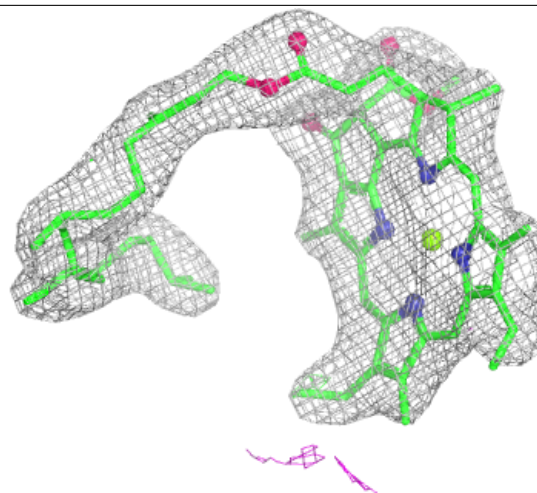
Electron density around CLA c 502:

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



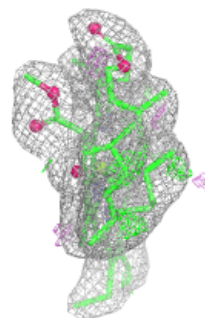
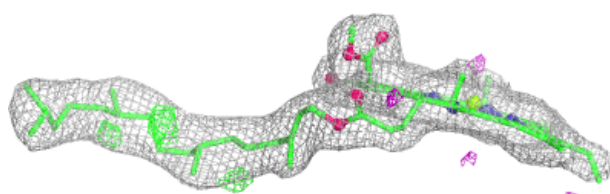
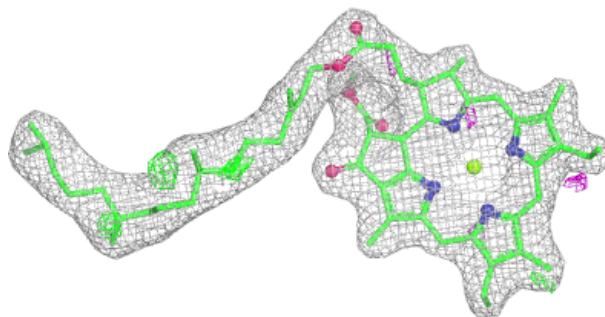
Electron density around CLA c 504:

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

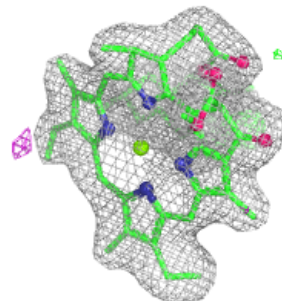
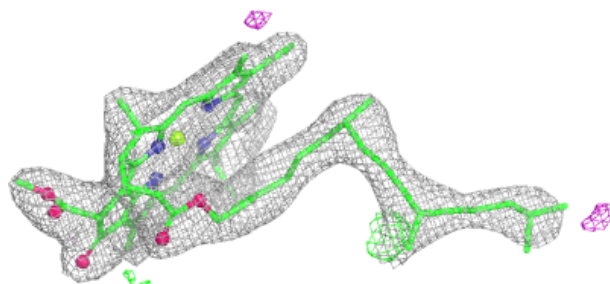
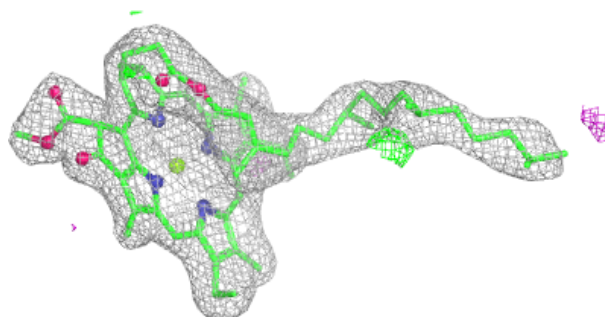


Electron density around CLA B 602:

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

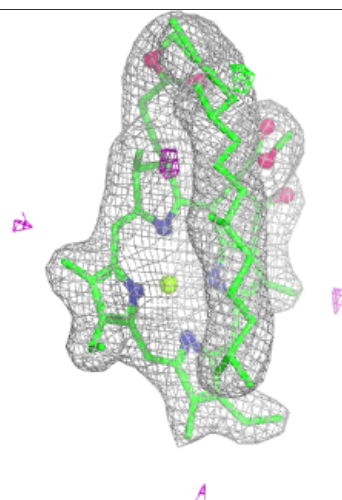
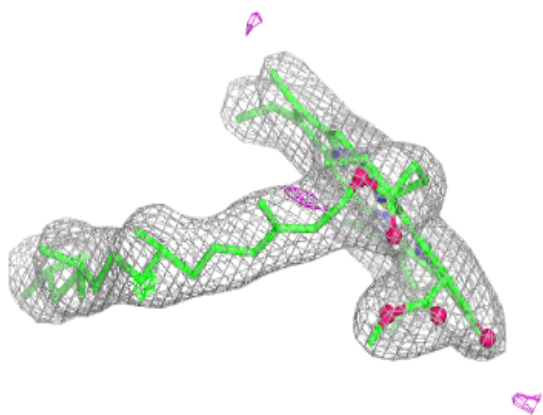
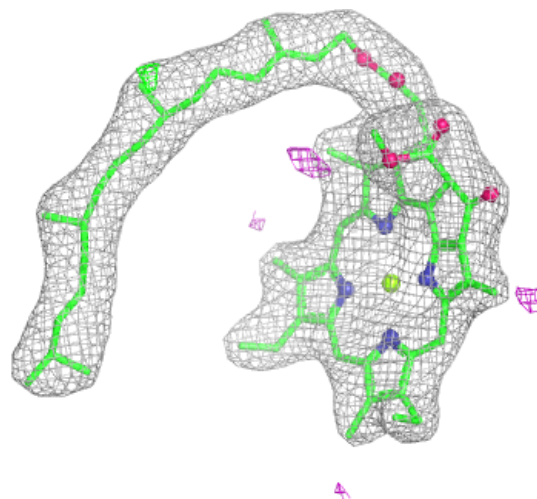
**Electron density around CLA c 506:**

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



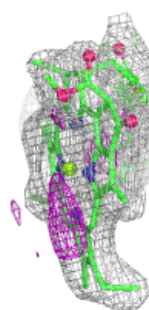
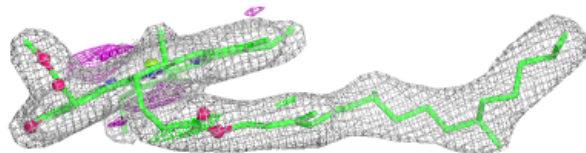
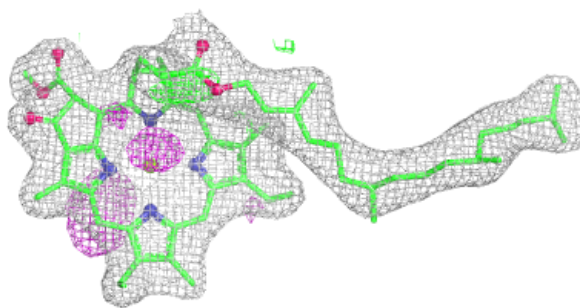
Electron density around CLA C 508:

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

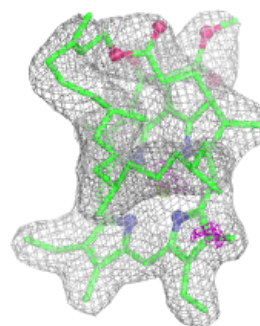
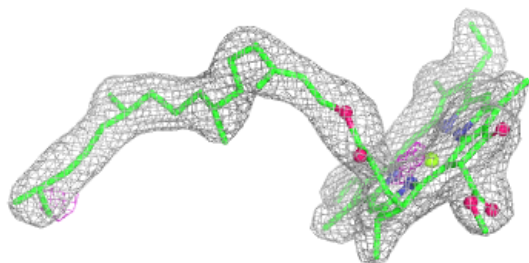
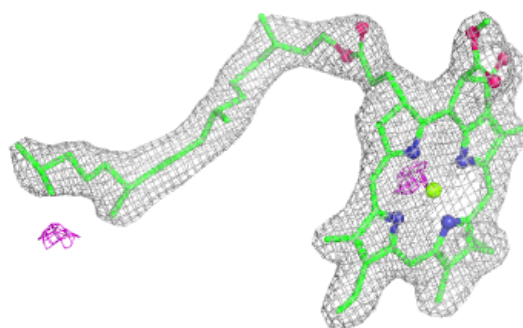


Electron density around CLA B 603:

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

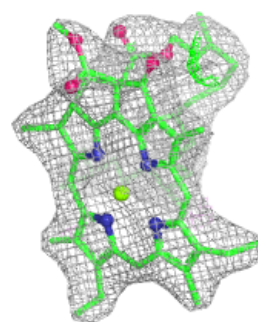
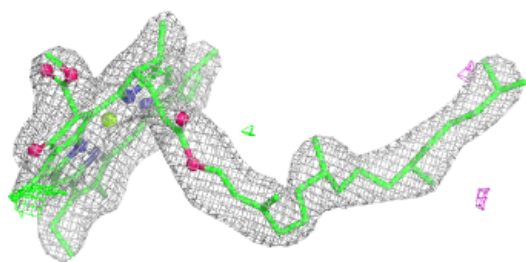
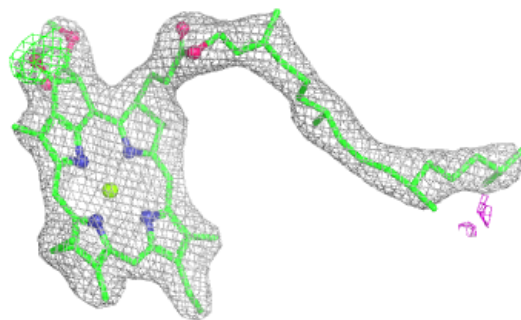
**Electron density around CLA C 512:**

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

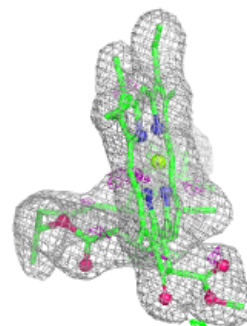
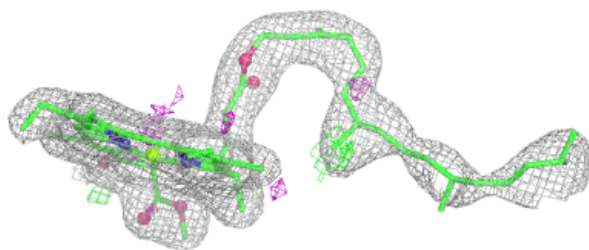
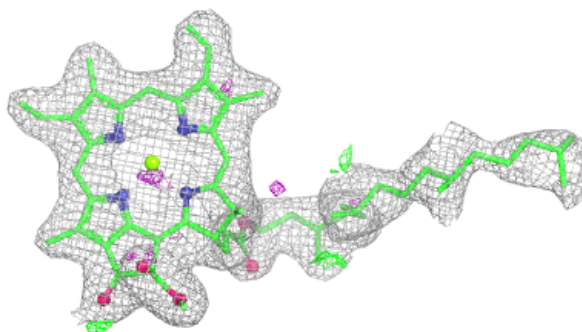


Electron density around CLA c 512:

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

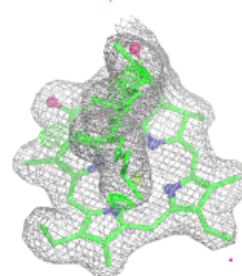
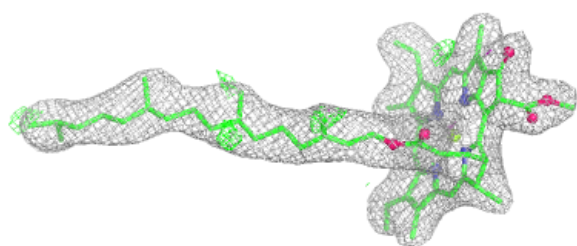
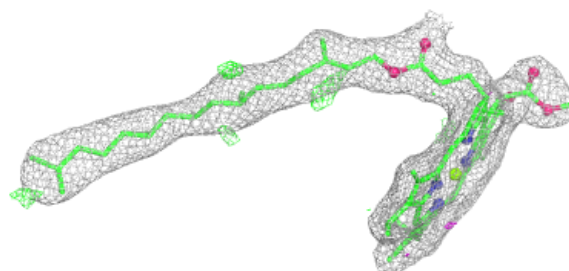
**Electron density around CLA A 406 (A):**

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

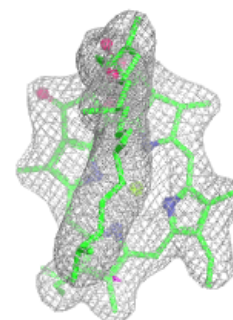
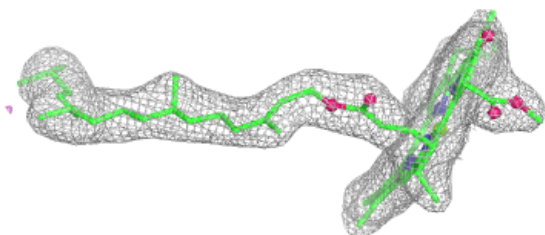
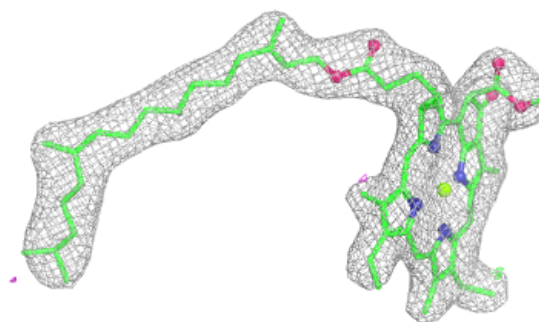


Electron density around CLA B 607:

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

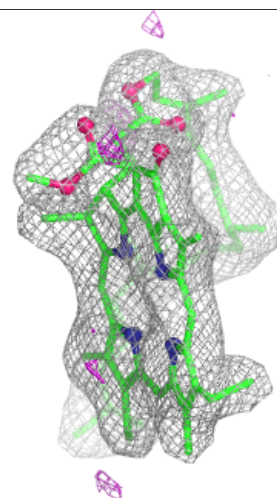
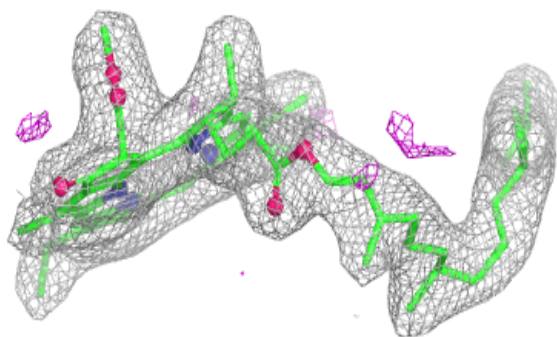
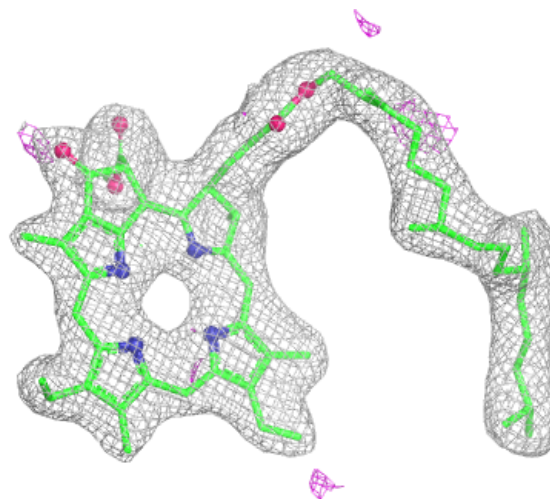
**Electron density around CLA B 609:**

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



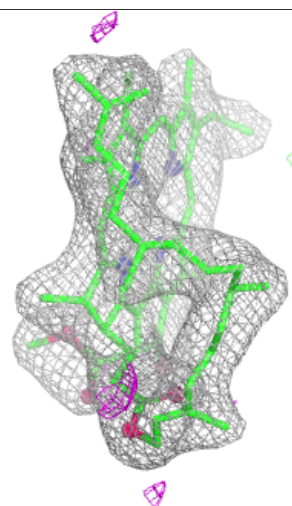
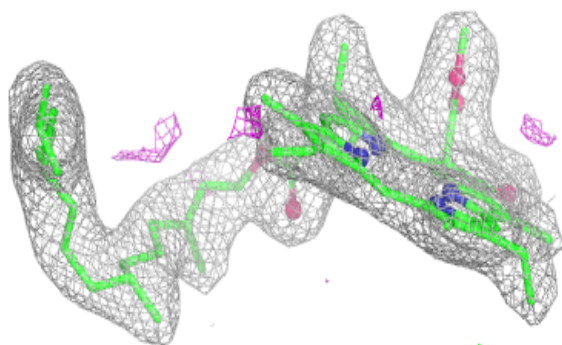
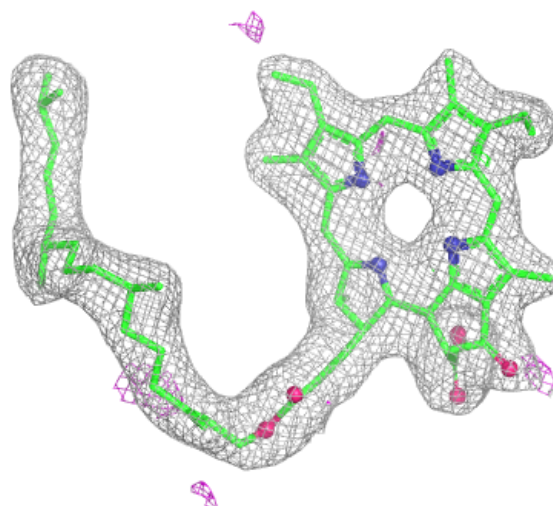
Electron density around PHO A 416 (A):

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



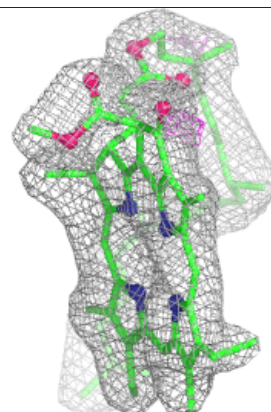
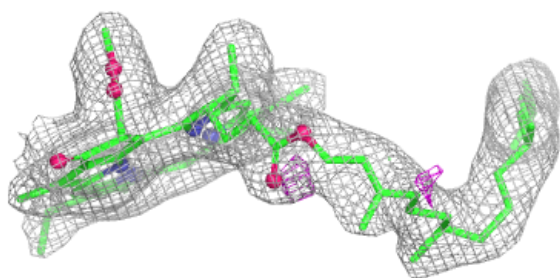
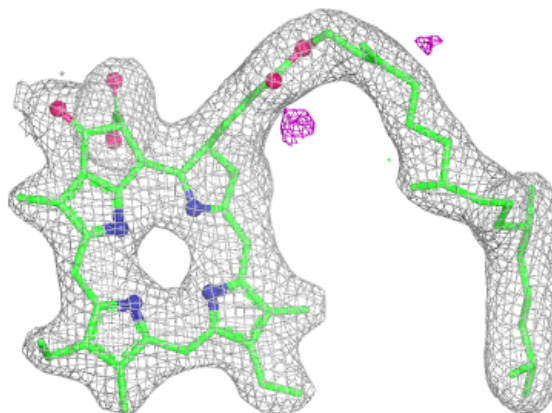
Electron density around PHO A 416 (B):

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

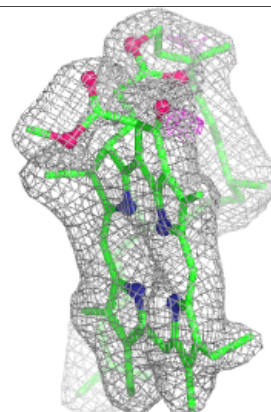
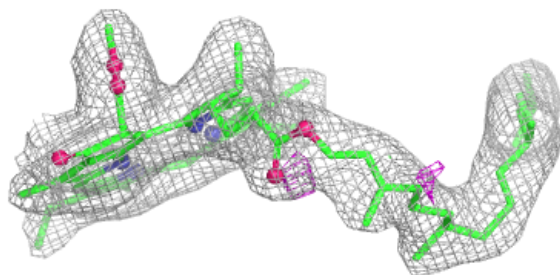
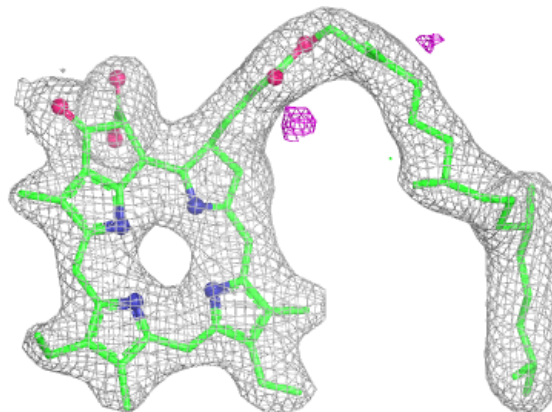


Electron density around PHO a 416 (A):

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

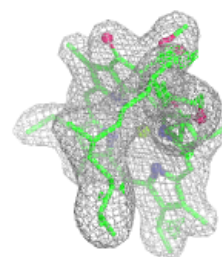
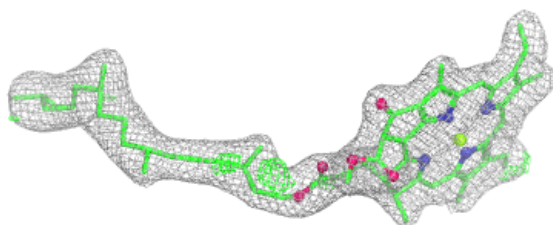
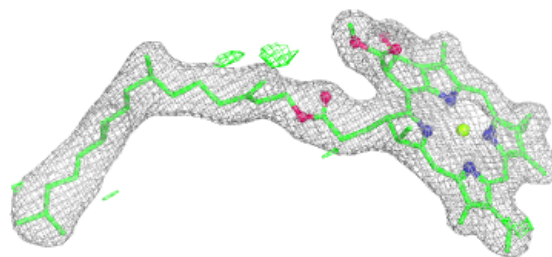
**Electron density around PHO a 416 (B):**

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

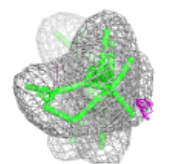
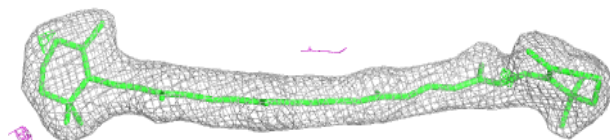
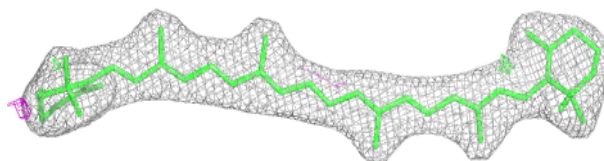


Electron density around CLA a 405 (A):

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

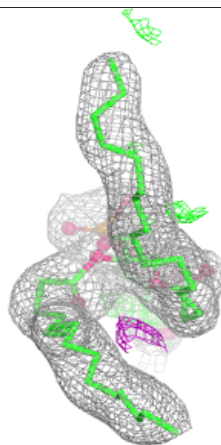
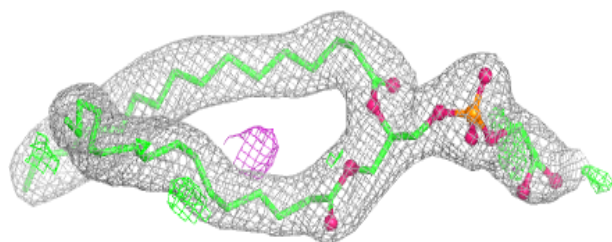
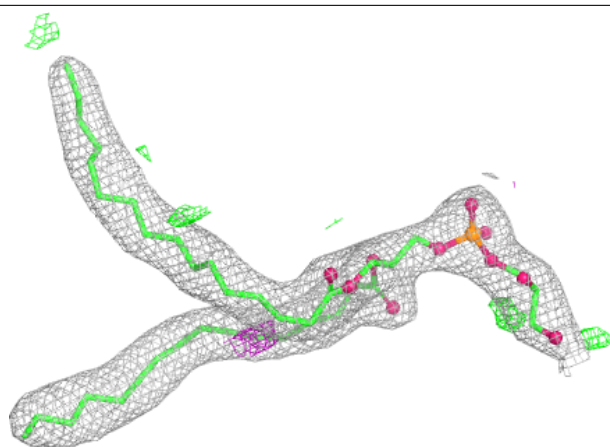
**Electron density around BCR B 617:**

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

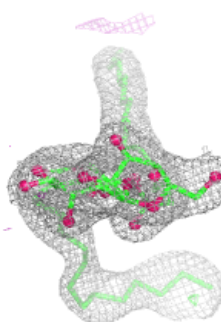
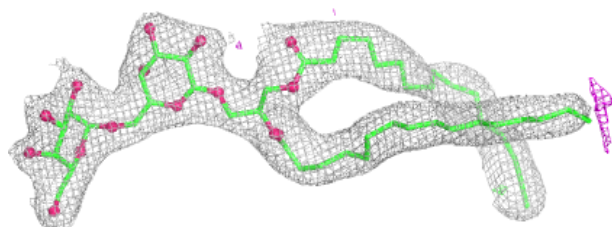
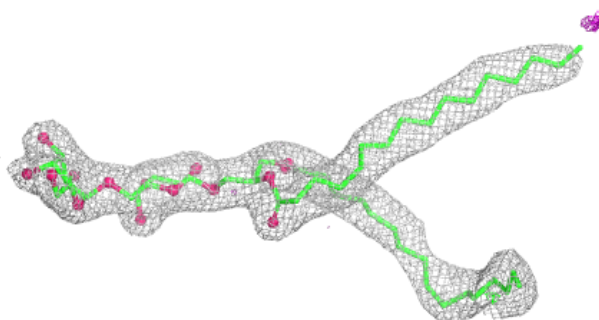


Electron density around LHG D 408 (A):

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

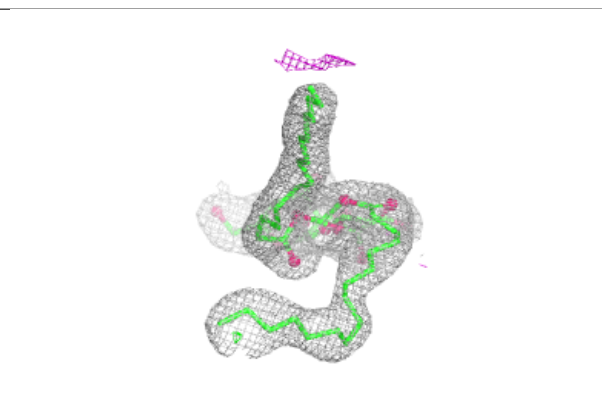
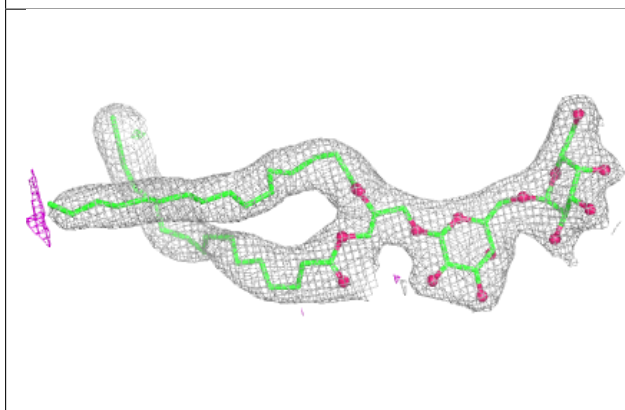
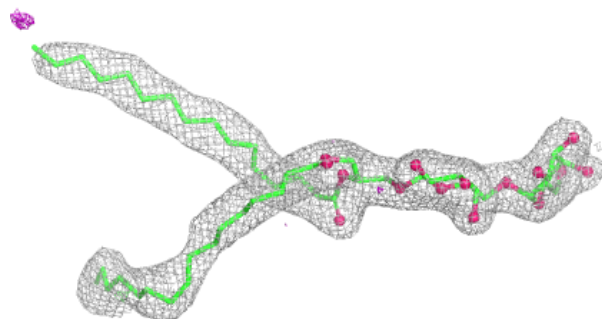
**Electron density around DGD C 517 (A):**

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

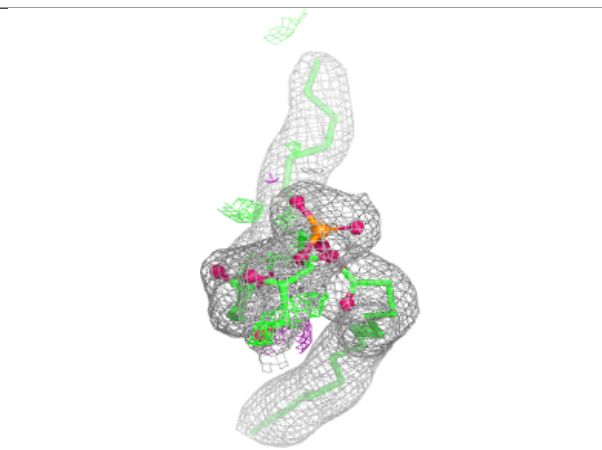
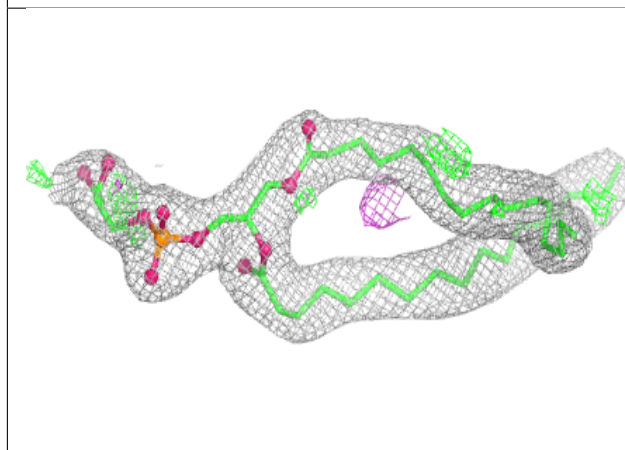
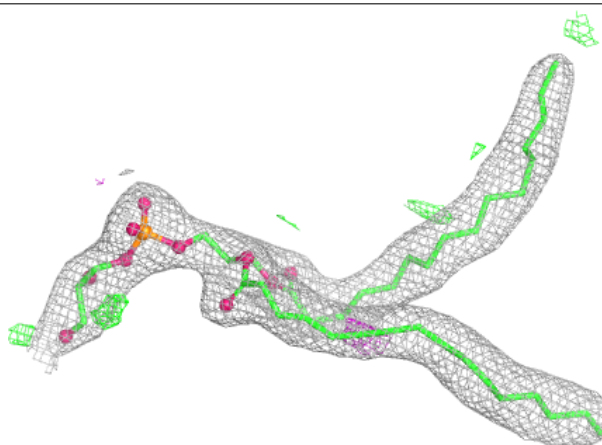


Electron density around DGD C 517 (B):

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

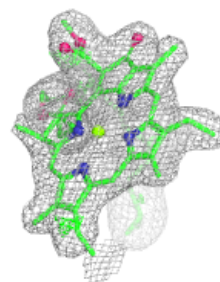
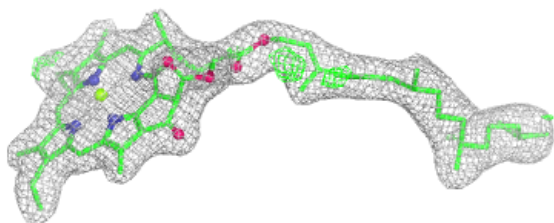
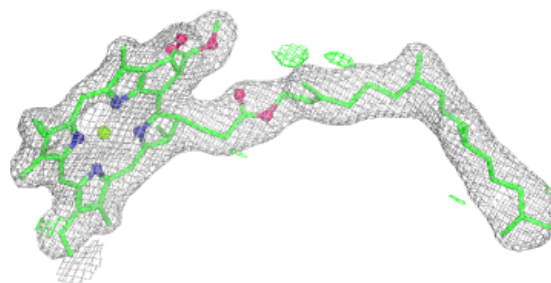
**Electron density around LHG D 408 (B):**

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



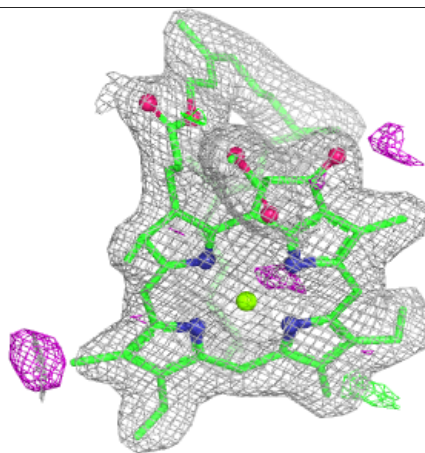
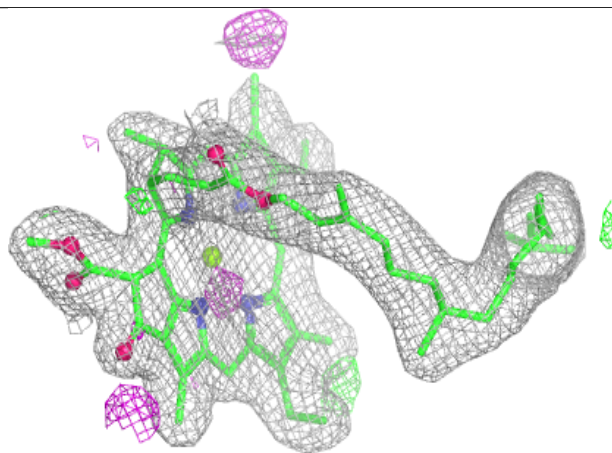
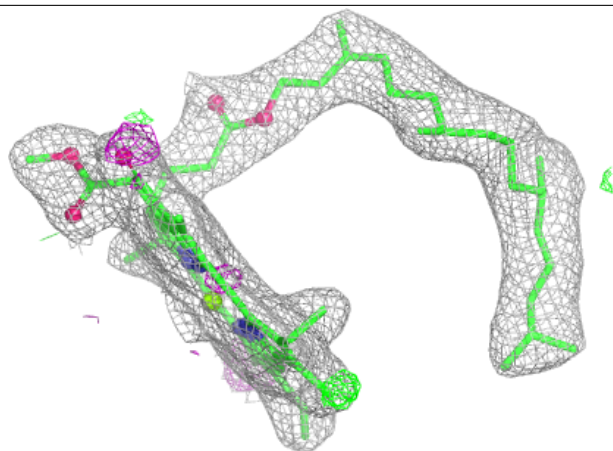
Electron density around CLA a 405 (B):

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



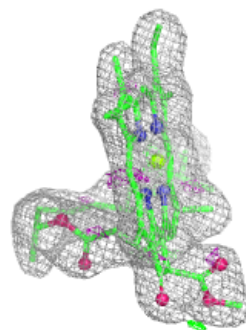
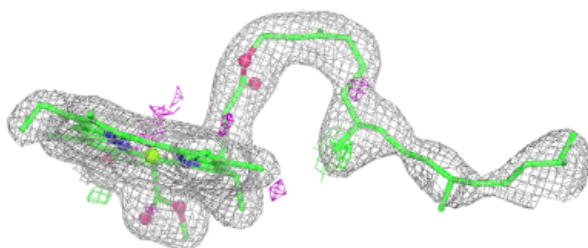
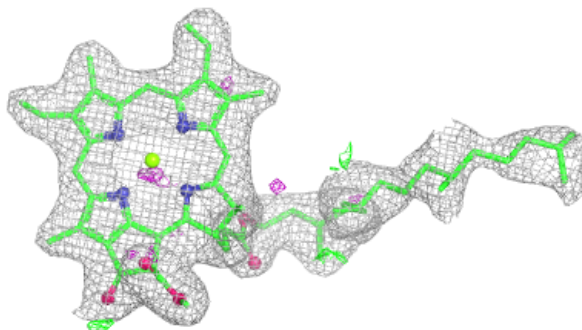
Electron density around CLA B 611:

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

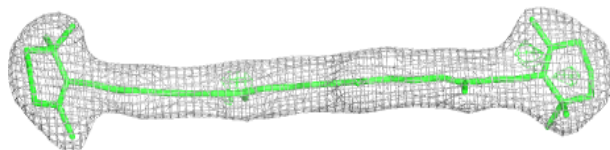
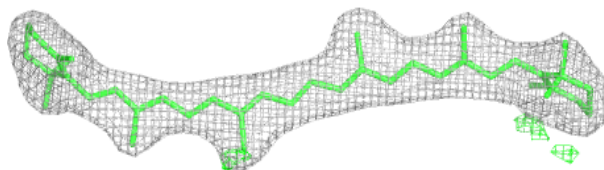


Electron density around CLA A 406 (B):

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

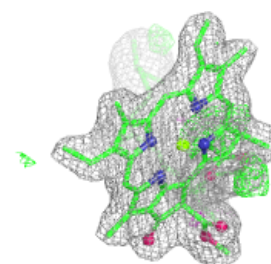
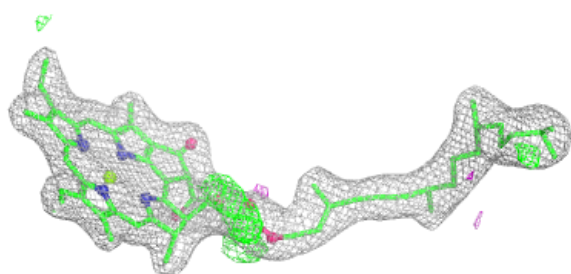
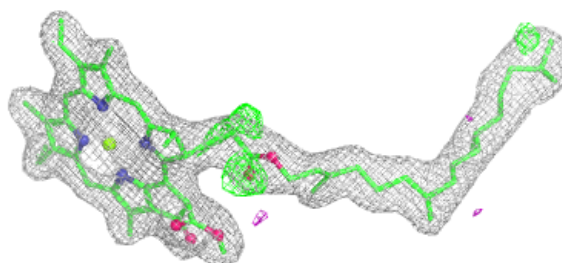
**Electron density around BCR C 516:**

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

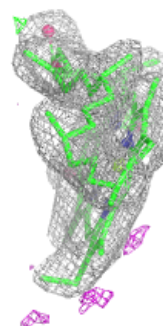
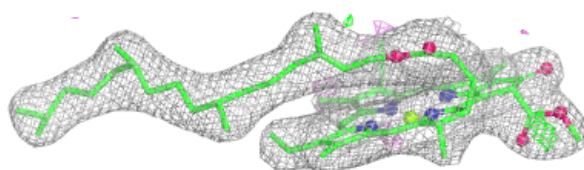
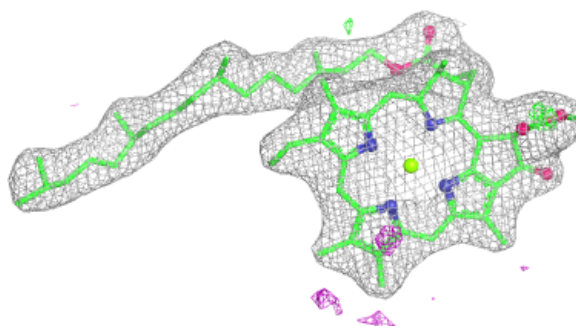


Electron density around CLA A 404 (A):

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

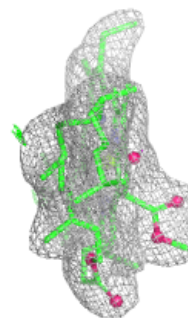
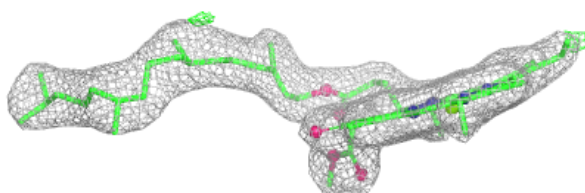
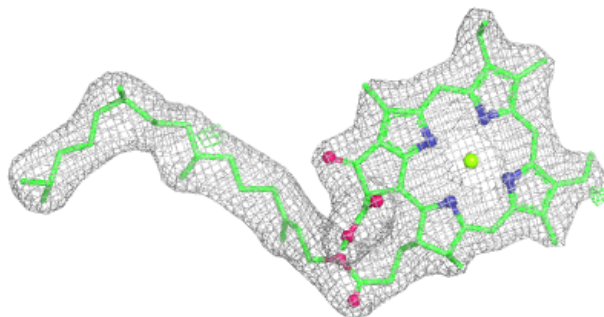
**Electron density around CLA C 502:**

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

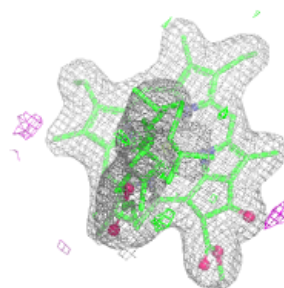
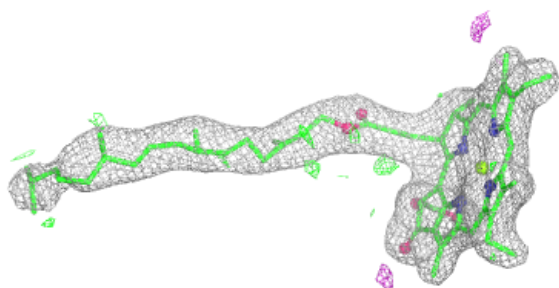
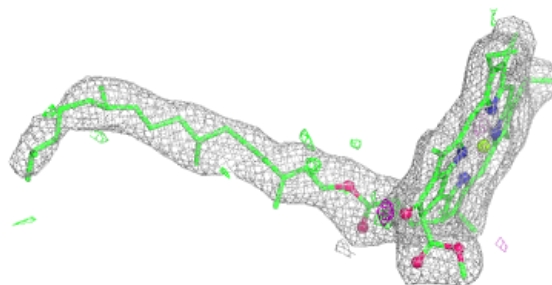


Electron density around CLA b 602:

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

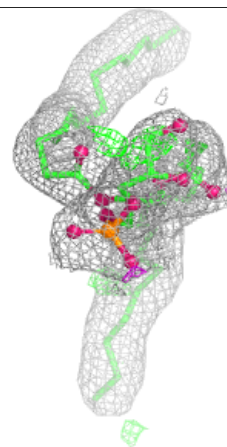
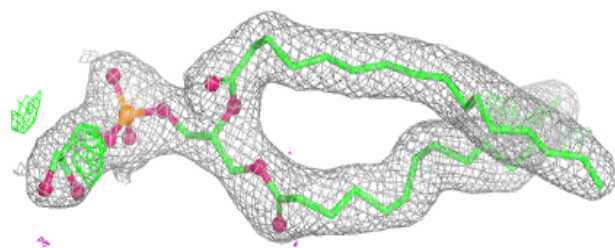
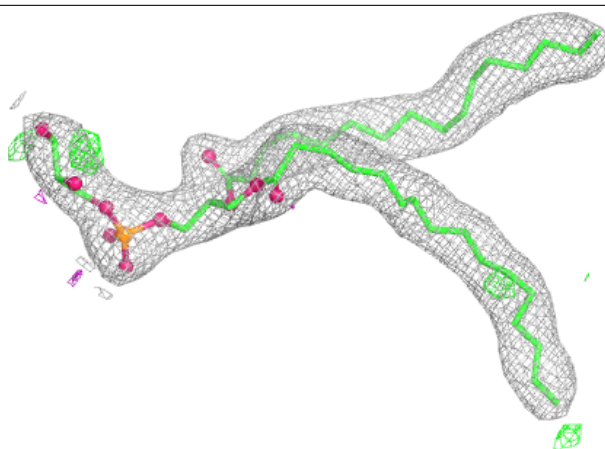
**Electron density around CLA b 604:**

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



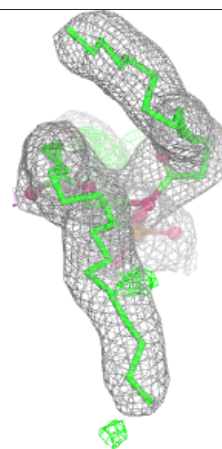
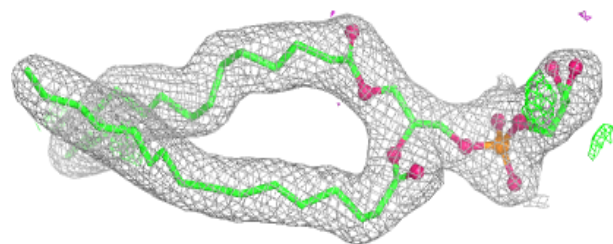
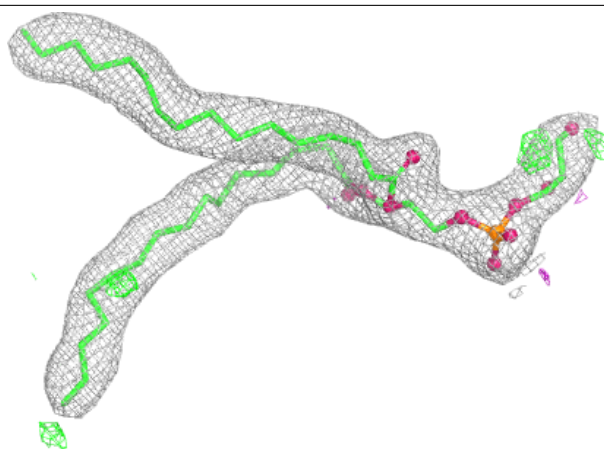
Electron density around LHG d 406 (A):

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



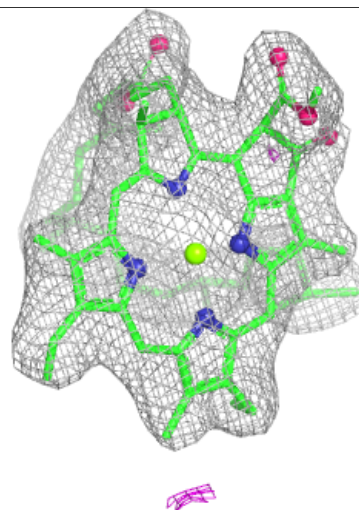
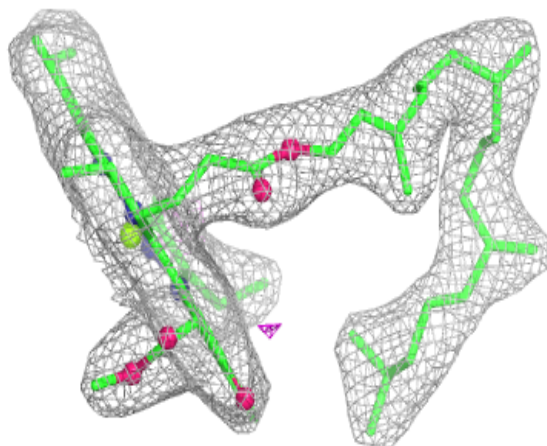
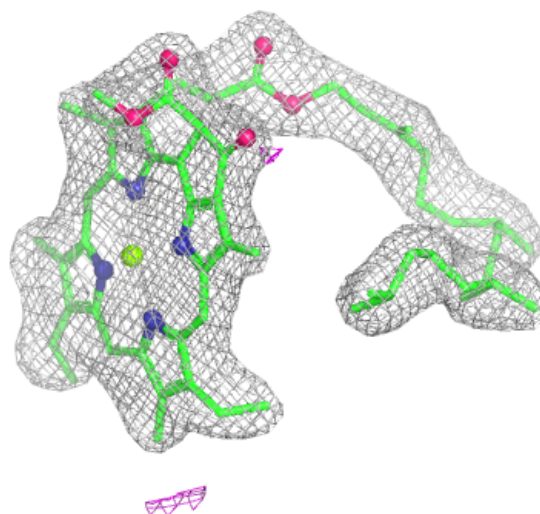
Electron density around LHG d 406 (B):

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



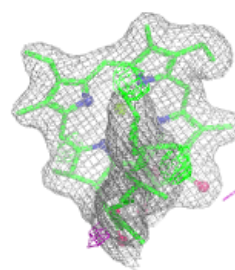
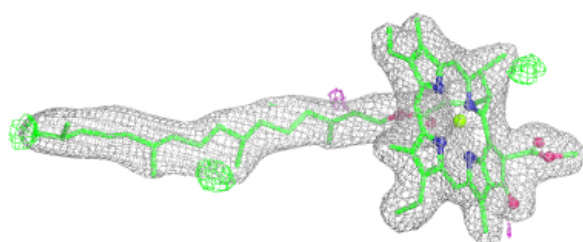
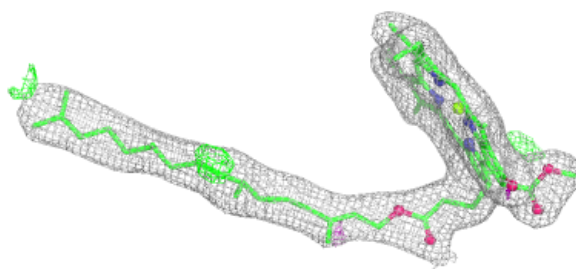
Electron density around CLA C 504:

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

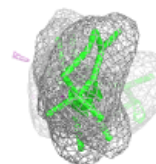
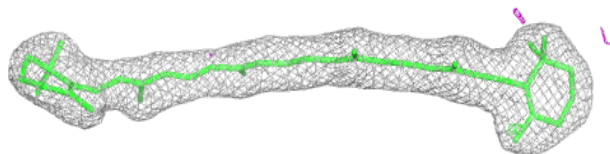
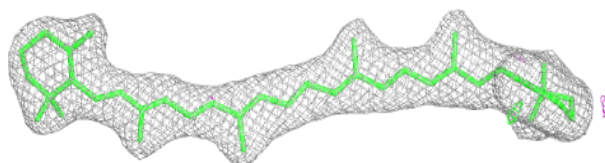


Electron density around CLA b 607:

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

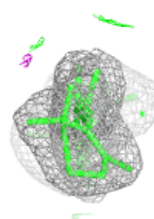
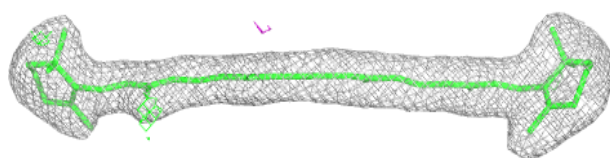
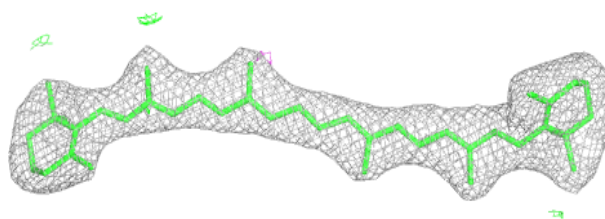
**Electron density around BCR b 617:**

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



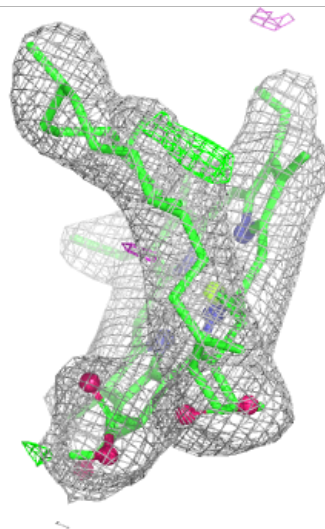
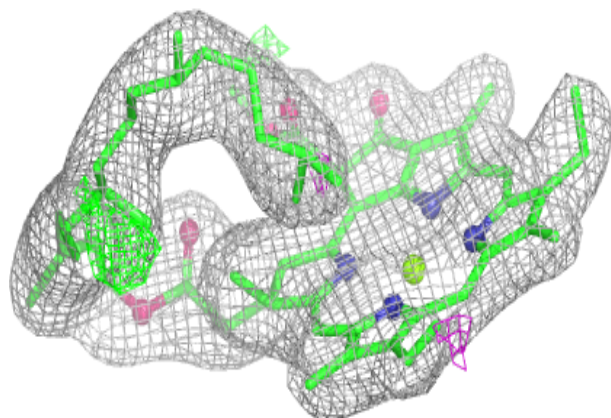
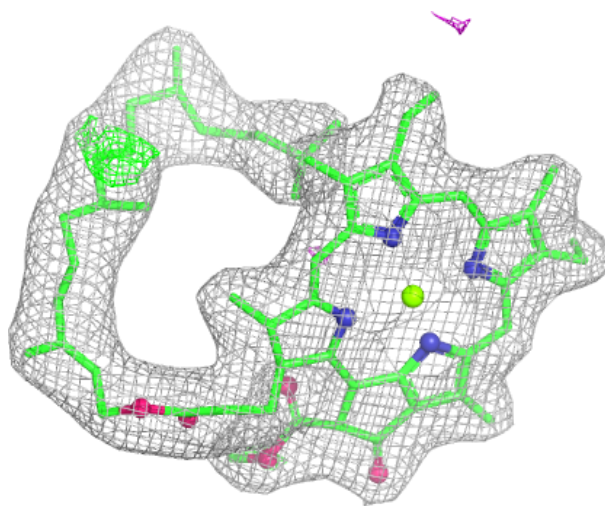
Electron density around BCR b 618:

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



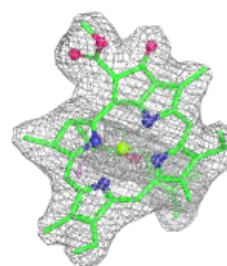
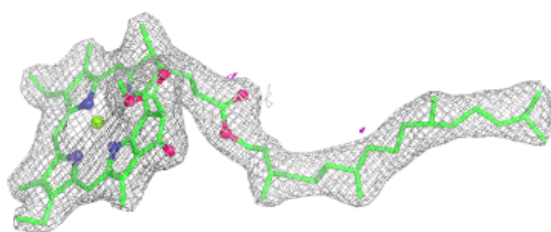
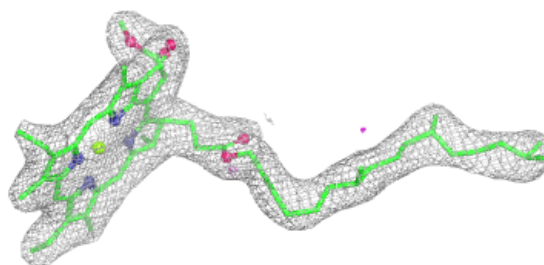
Electron density around CLA b 615:

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

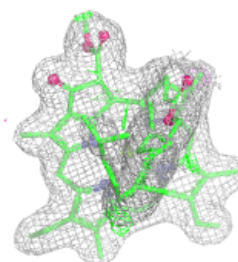
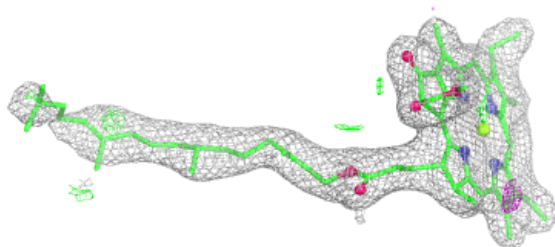
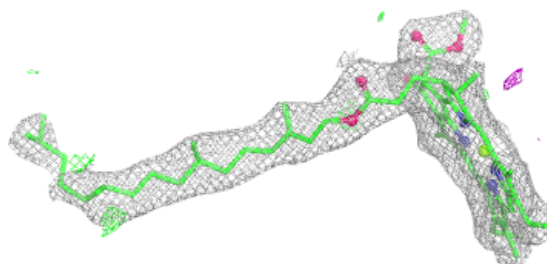


Electron density around CLA C 503:

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

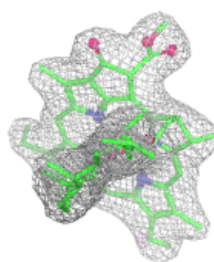
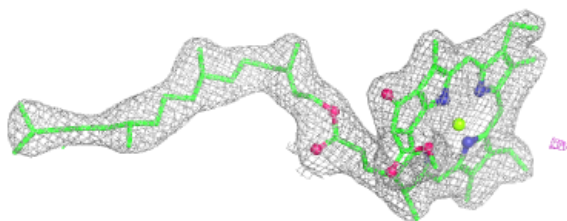
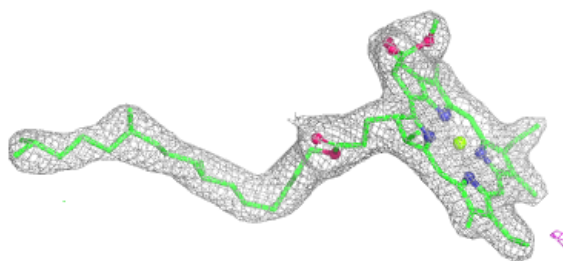
**Electron density around CLA B 604:**

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



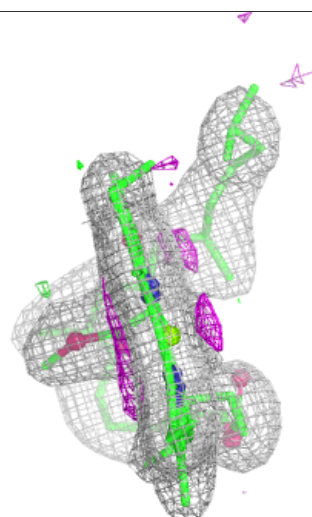
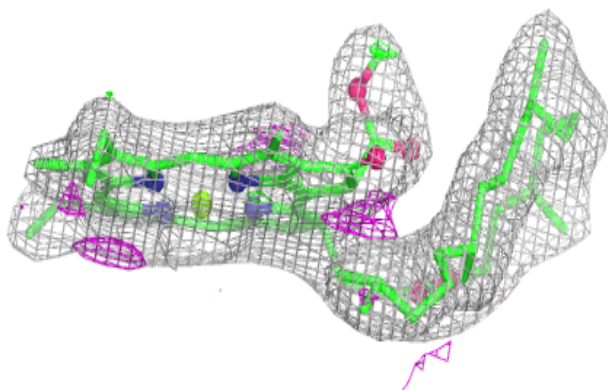
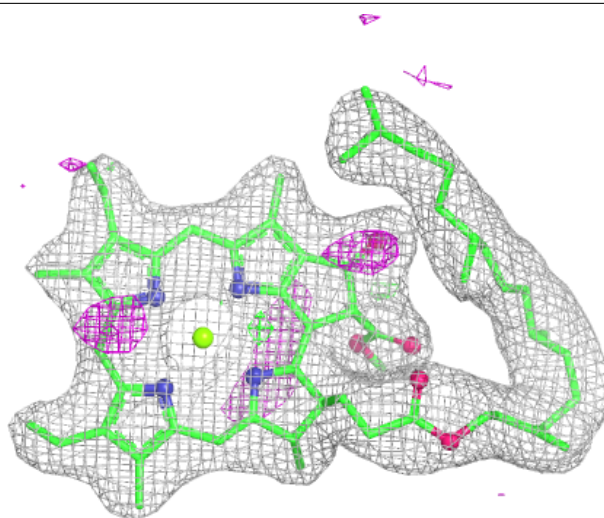
Electron density around CLA c 503:

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



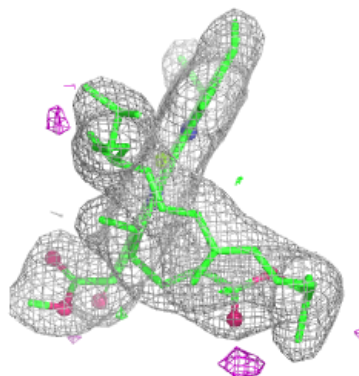
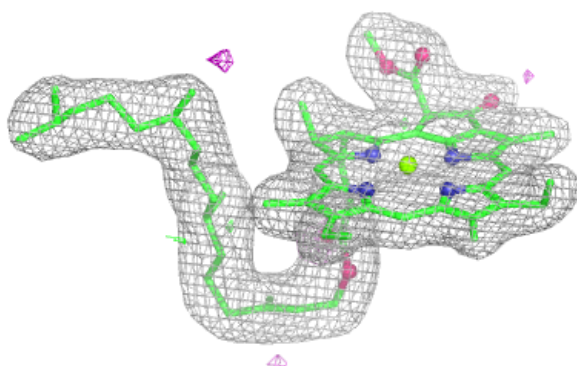
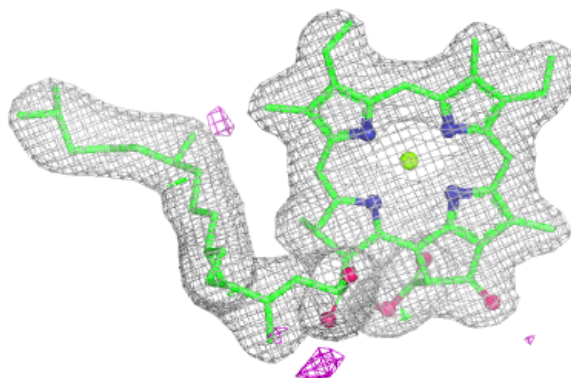
Electron density around CLA B 610:

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

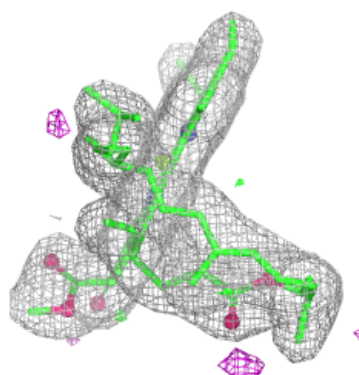
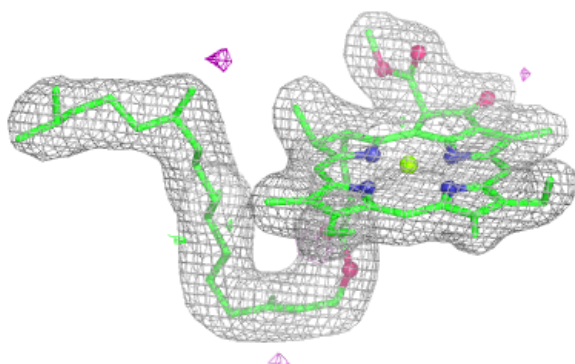
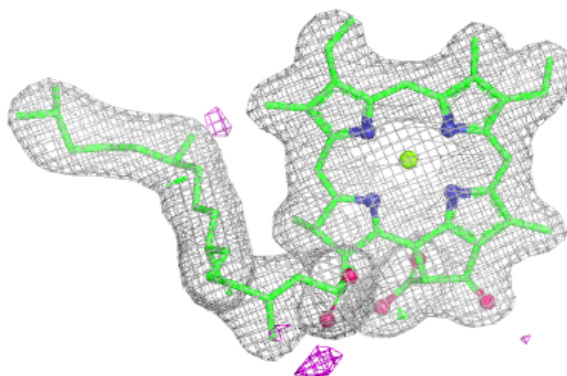


Electron density around CLA a 406 (A):

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

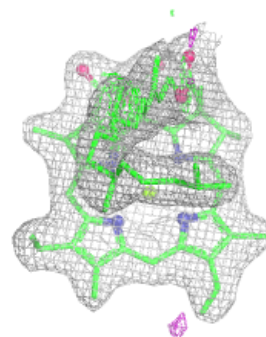
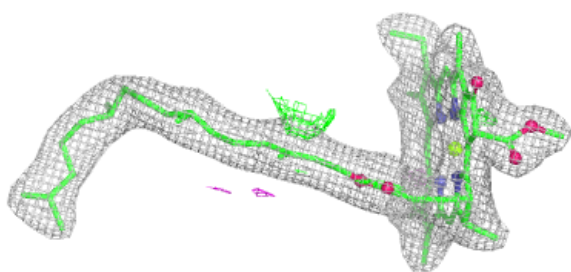
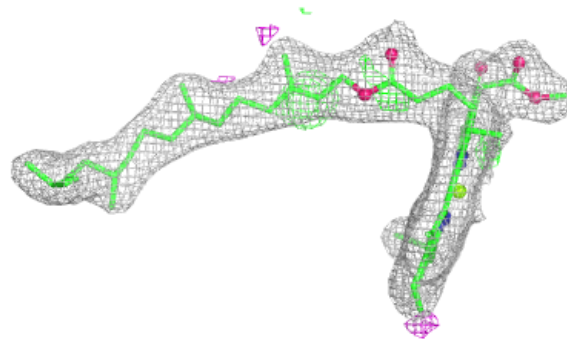
**Electron density around CLA a 406 (B):**

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

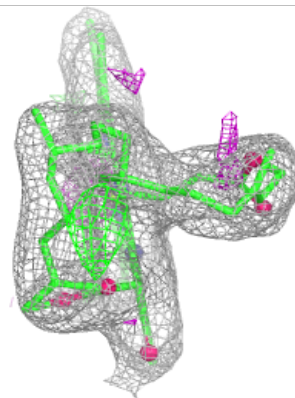
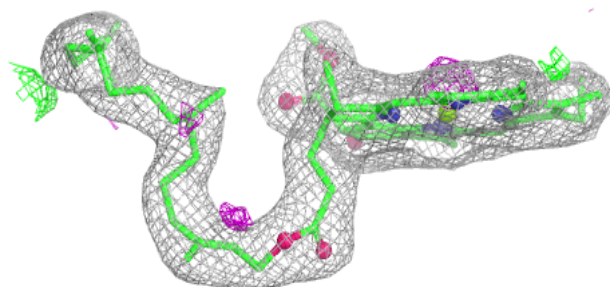
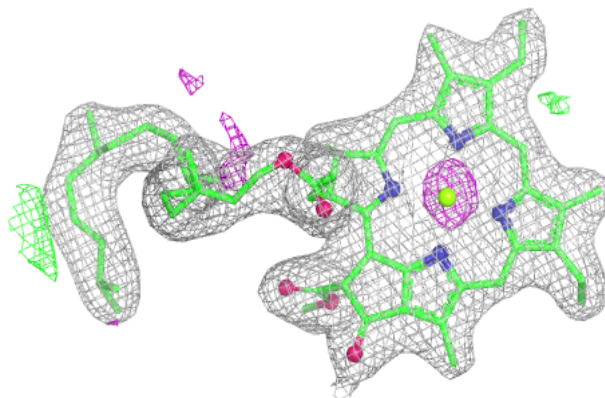


Electron density around CLA B 605:

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

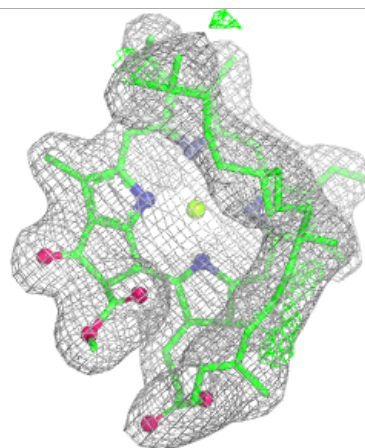
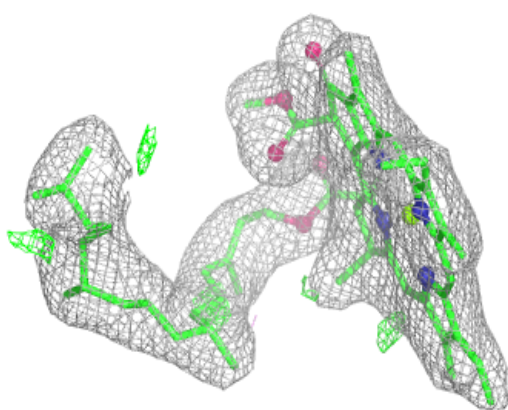
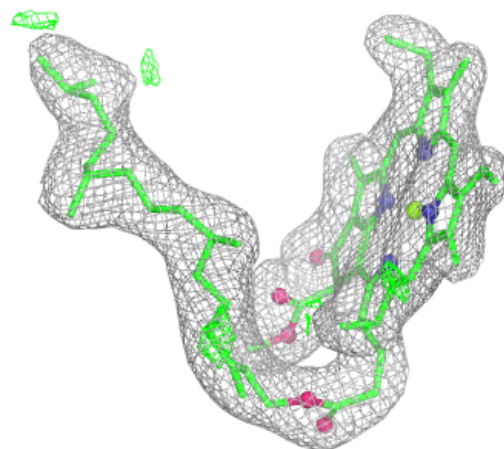
**Electron density around CLA B 612:**

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



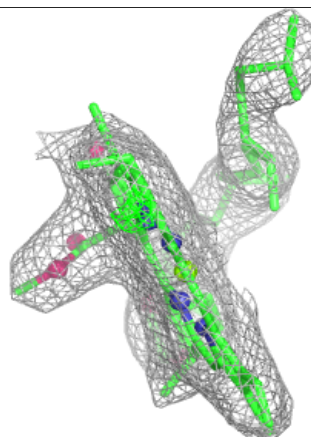
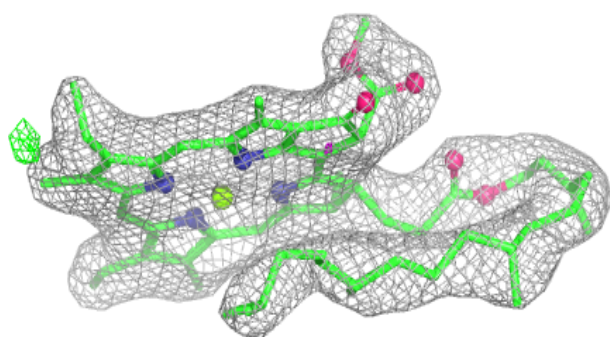
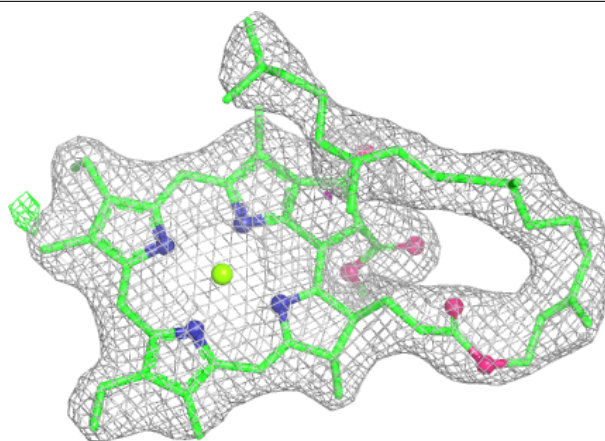
Electron density around CLA B 613:

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



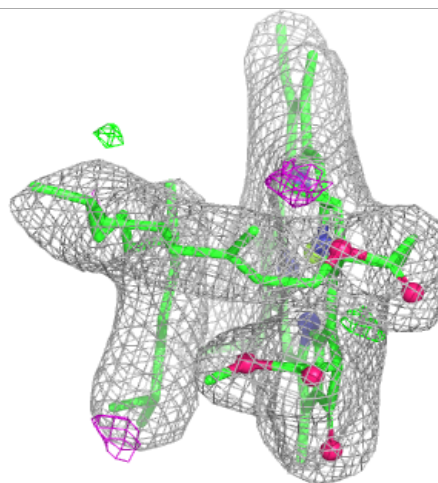
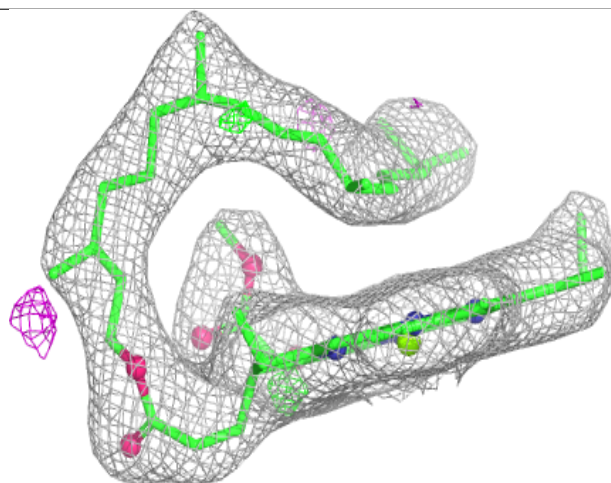
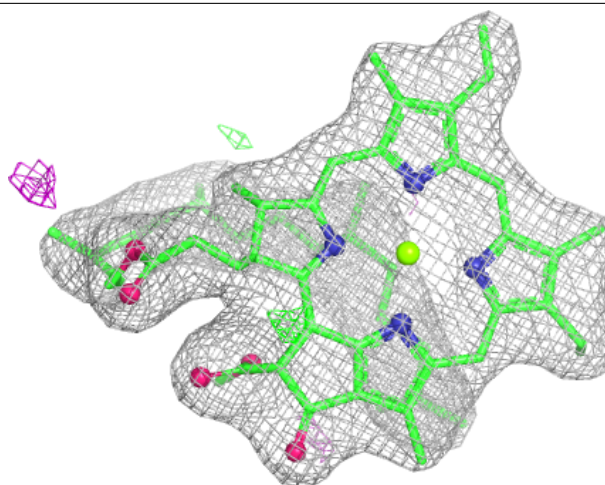
Electron density around CLA c 510:

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



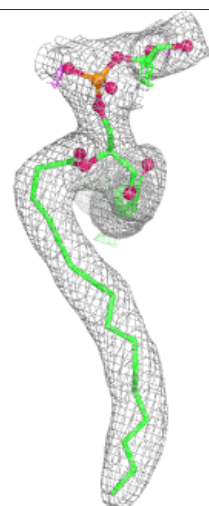
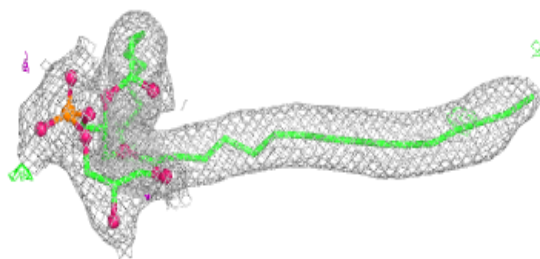
Electron density around CLA c 511:

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



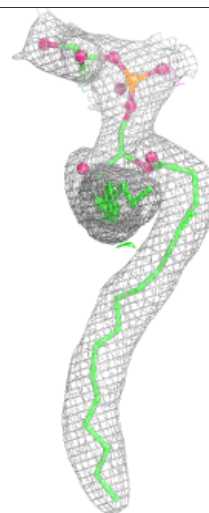
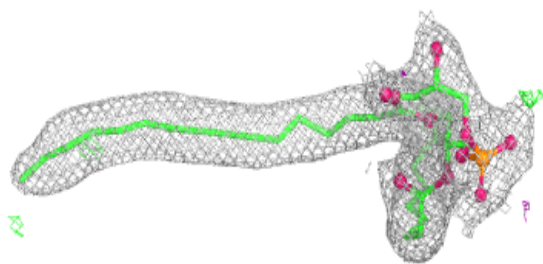
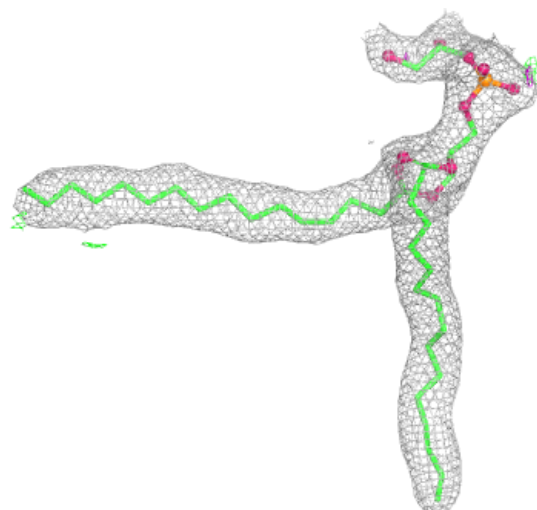
Electron density around LHG L 101 (A):

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



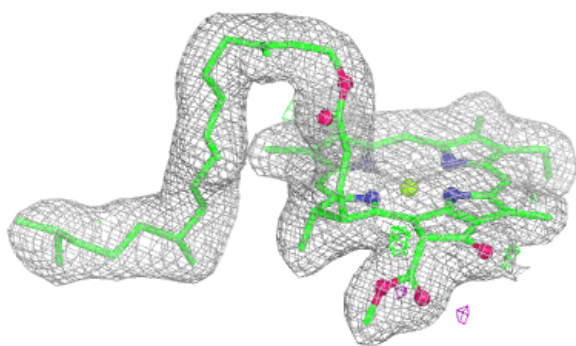
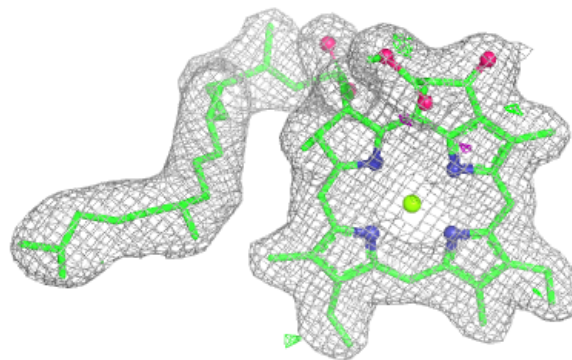
Electron density around LHG L 101 (B):

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



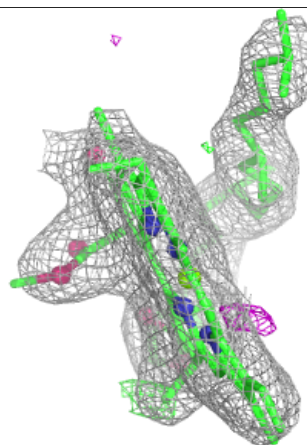
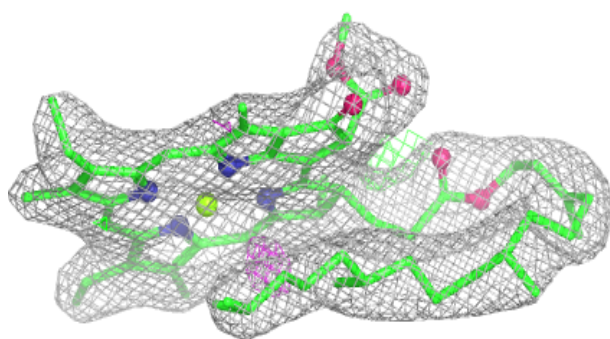
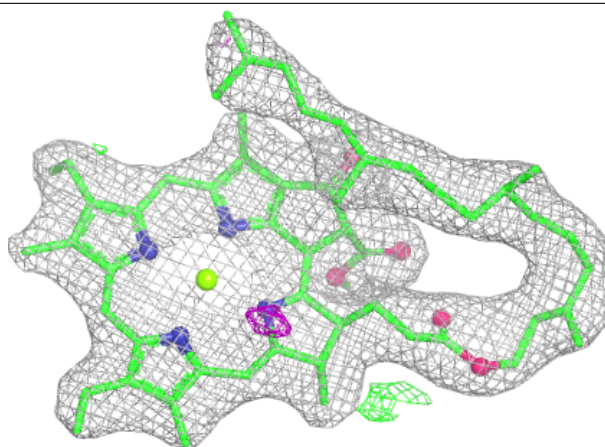
Electron density around CLA A 405 (A):

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



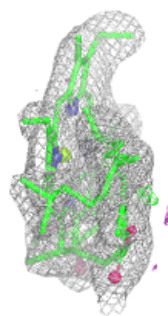
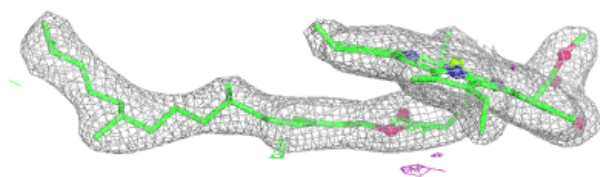
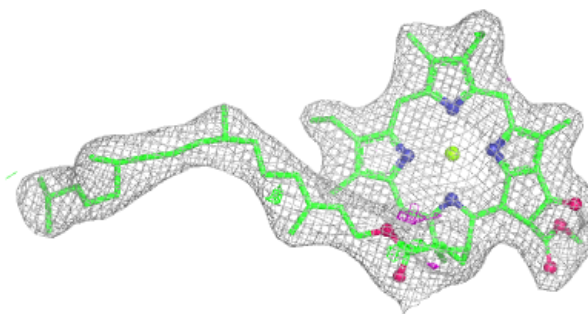
Electron density around CLA C 510:

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



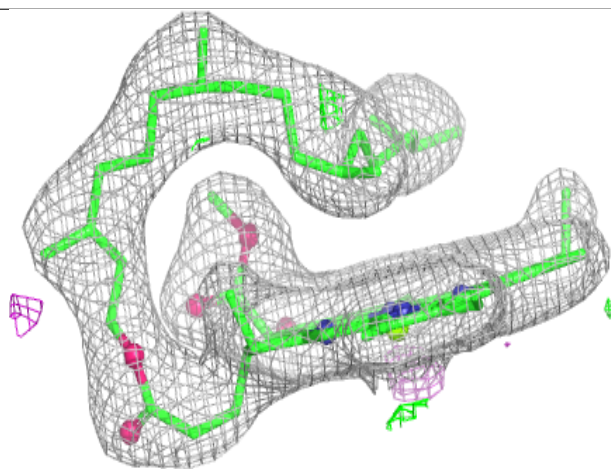
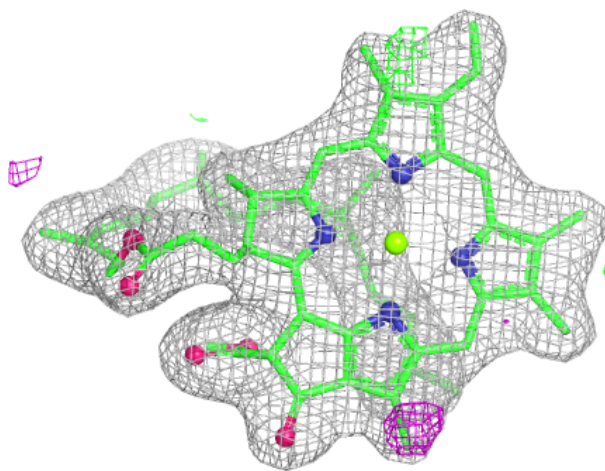
Electron density around CLA b 603:

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



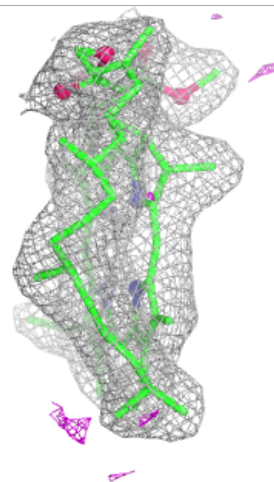
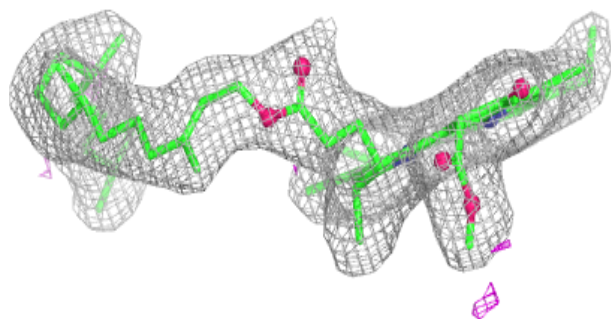
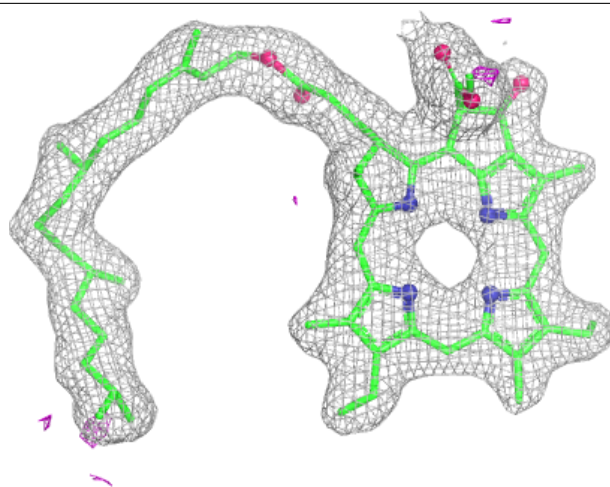
Electron density around CLA C 511:

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



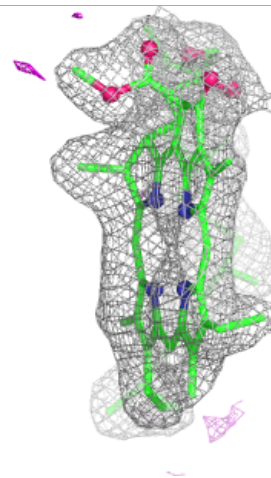
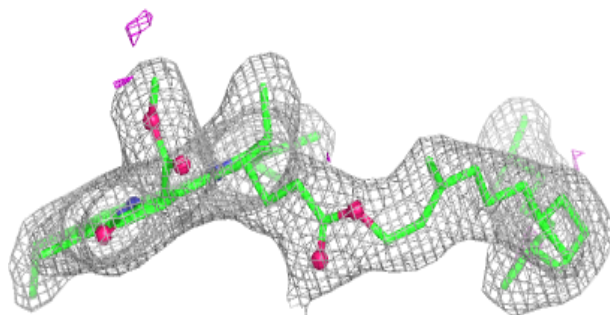
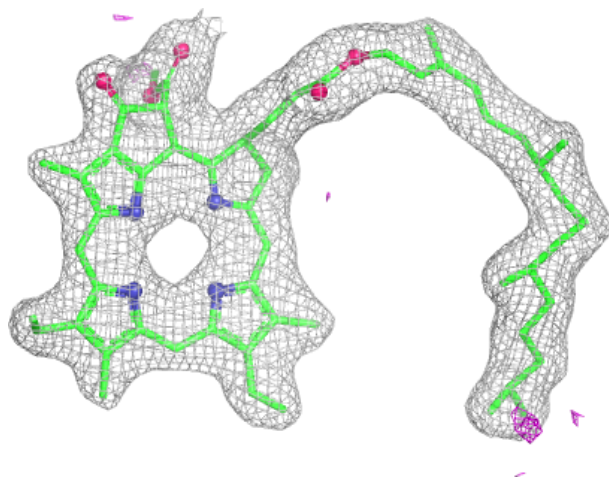
Electron density around PHO A 407 (A):

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



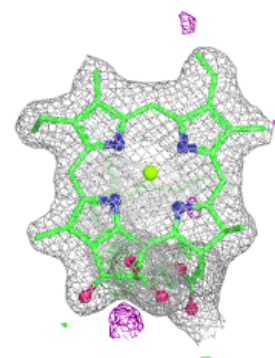
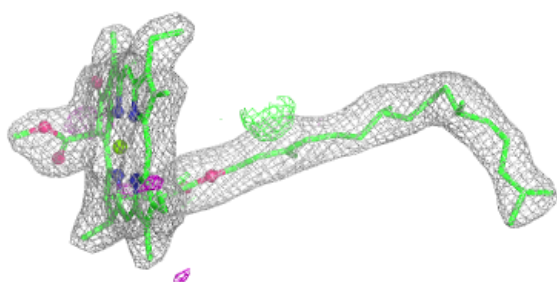
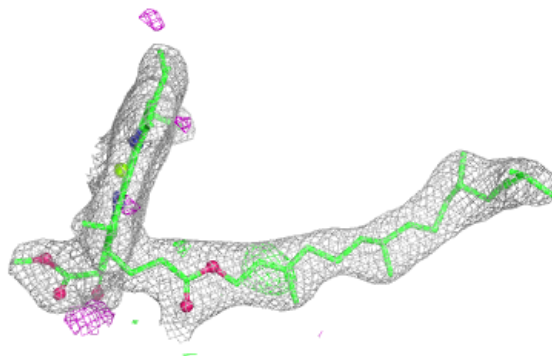
Electron density around PHO A 407 (B):

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



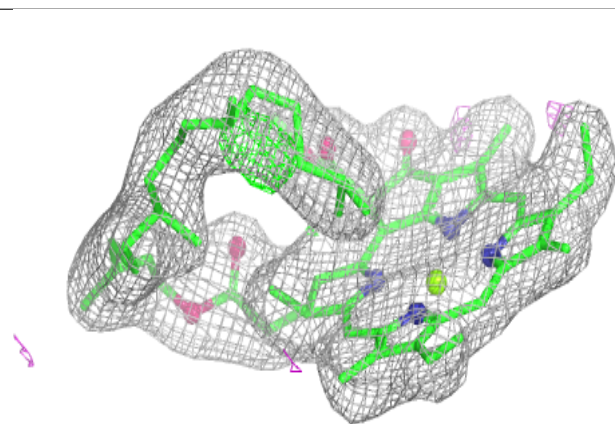
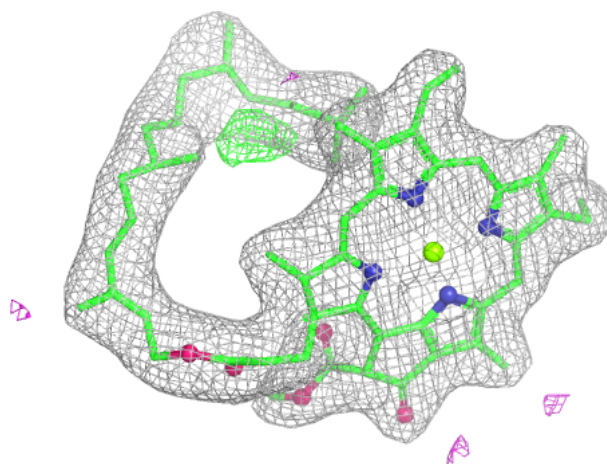
Electron density around CLA b 605:

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



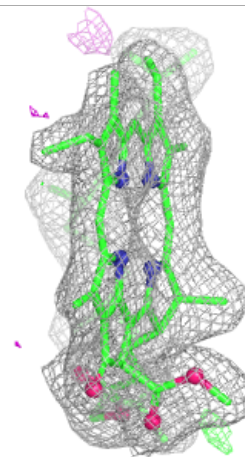
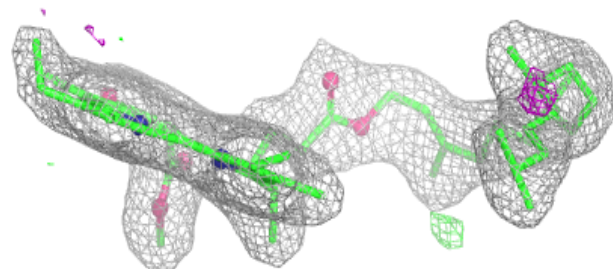
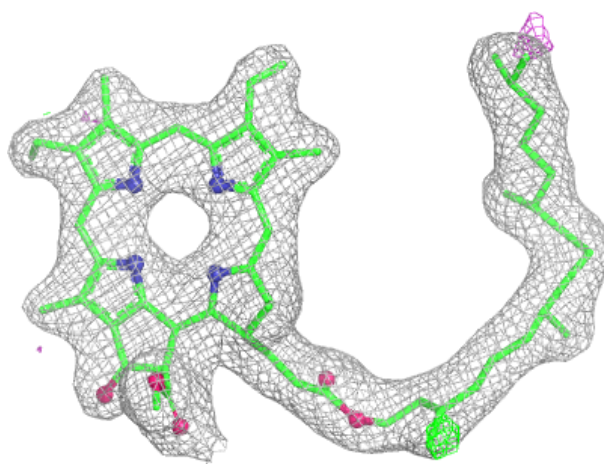
Electron density around CLA B 615:

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



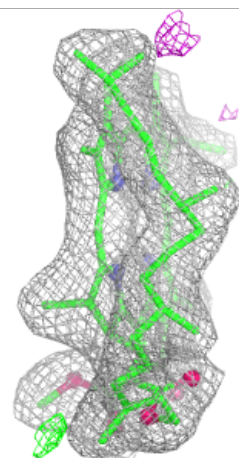
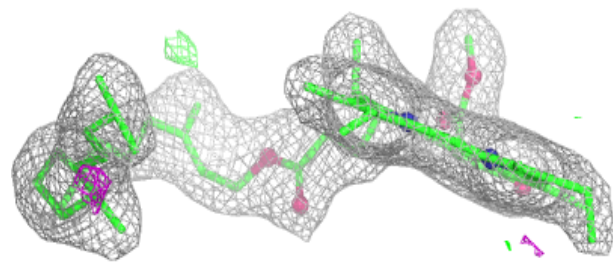
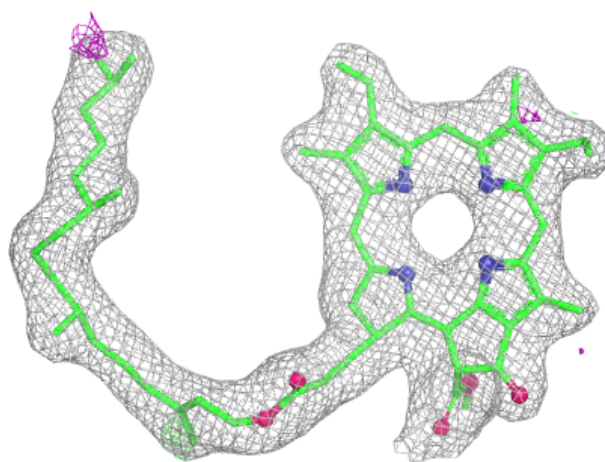
Electron density around PHO a 408 (A):

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



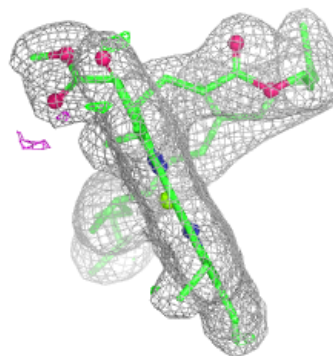
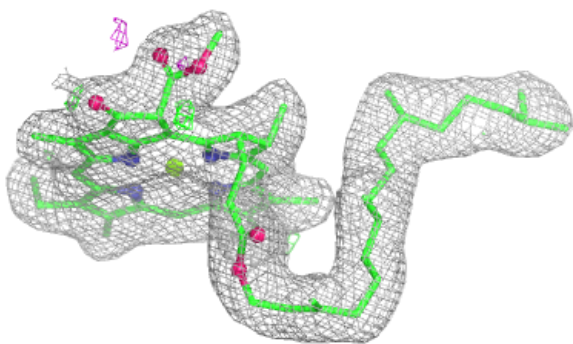
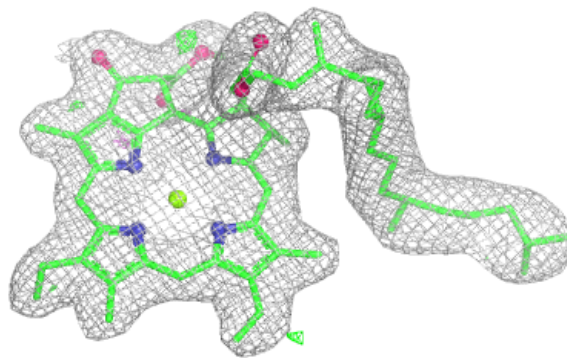
Electron density around PHO a 408 (B):

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

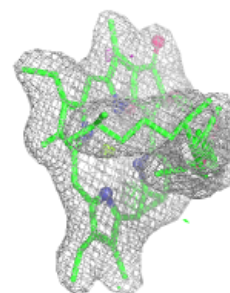
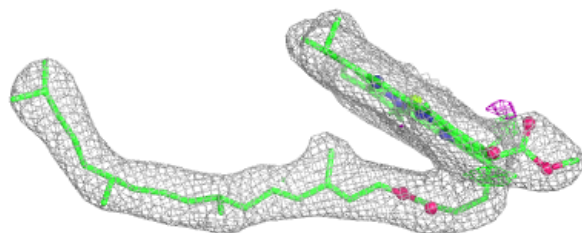
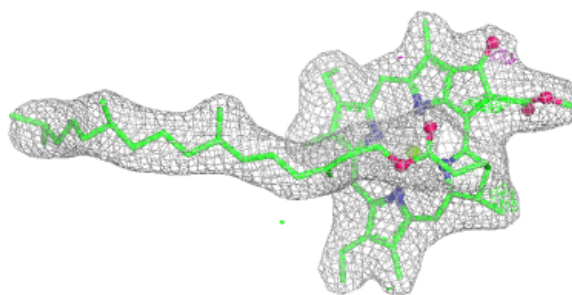


Electron density around CLA A 405 (B):

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

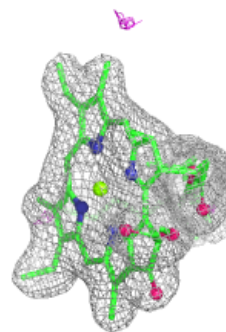
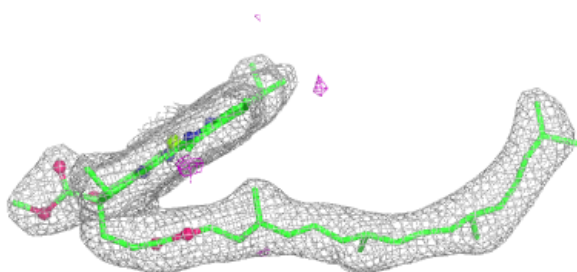
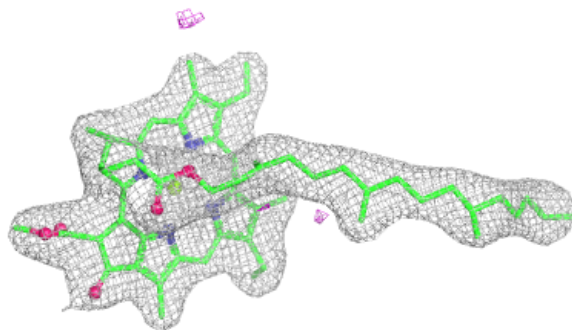
**Electron density around CLA b 608:**

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



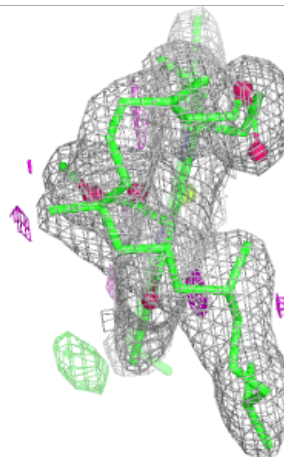
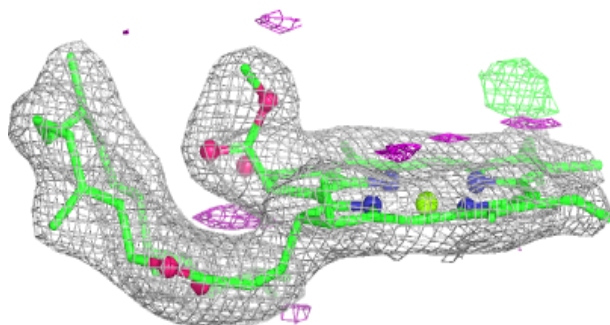
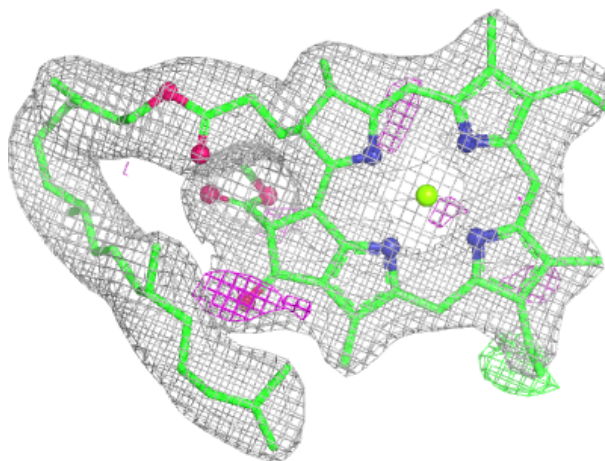
Electron density around CLA B 608:

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



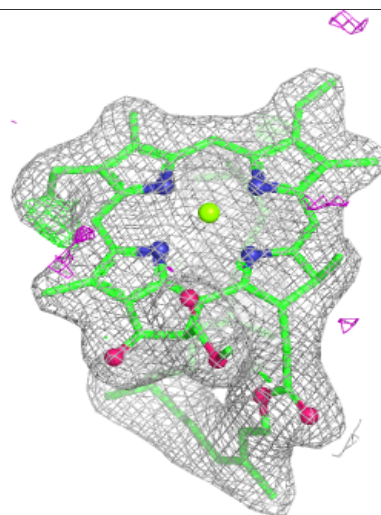
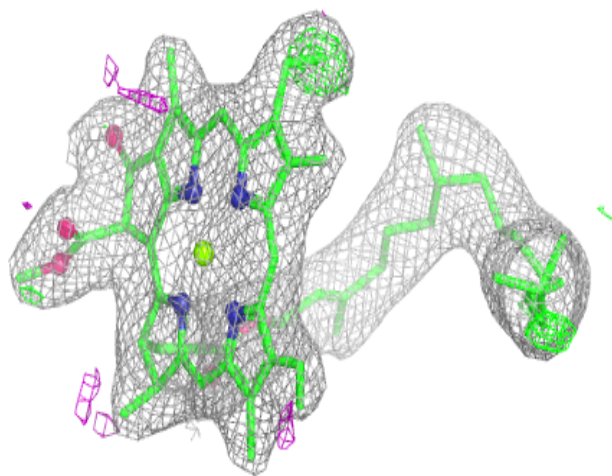
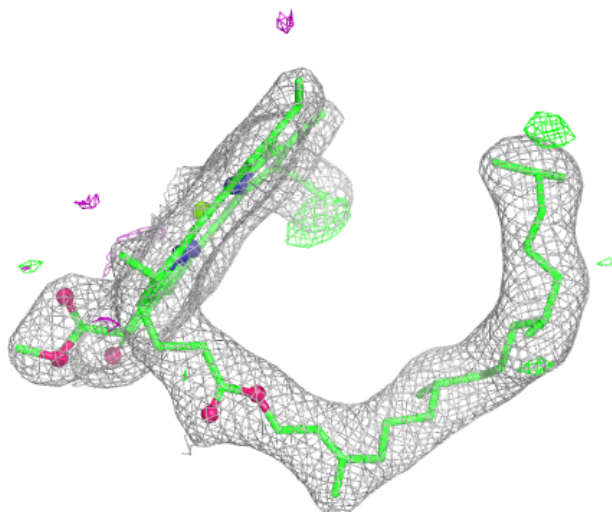
Electron density around CLA b 610:

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



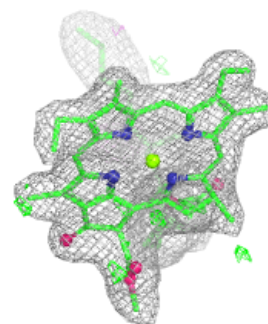
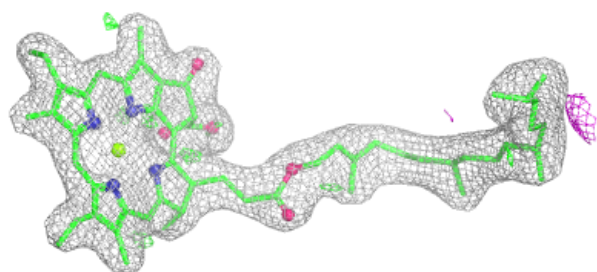
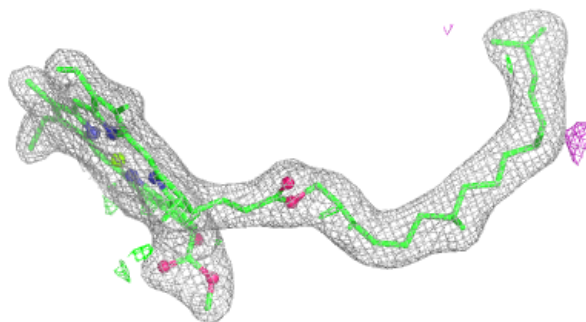
Electron density around CLA b 611:

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



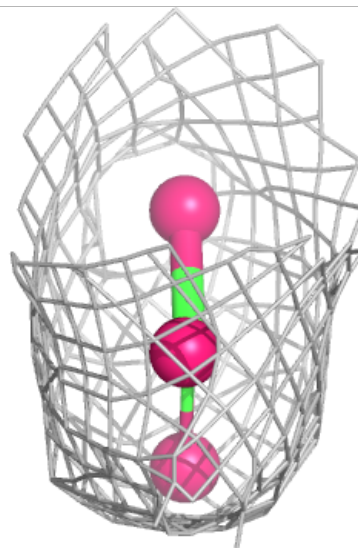
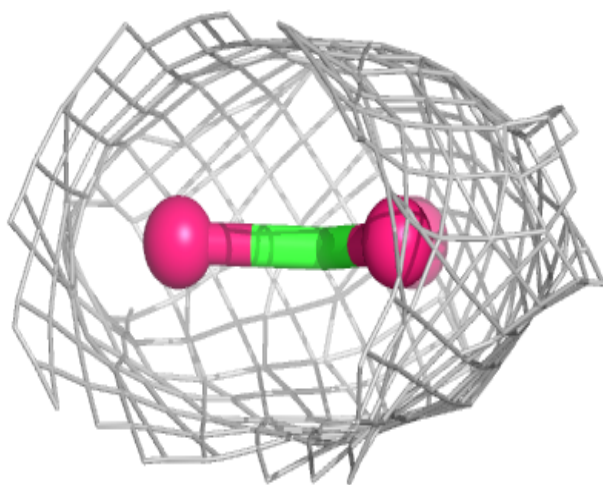
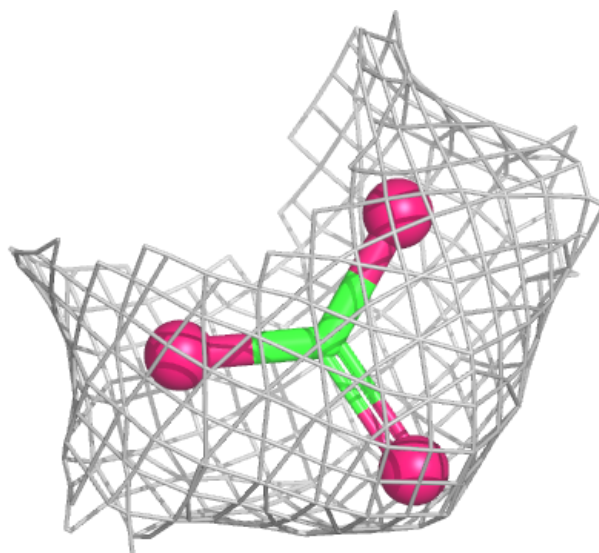
Electron density around CLA D 404 (A):

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



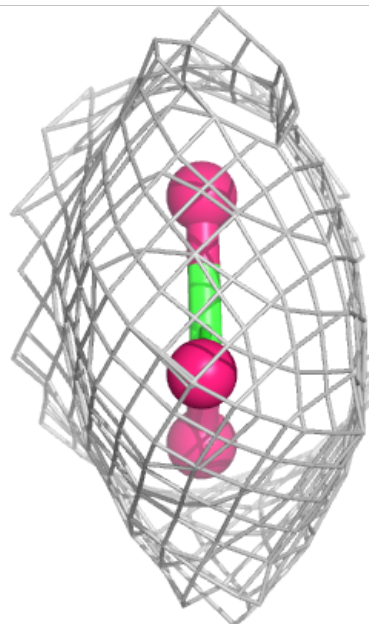
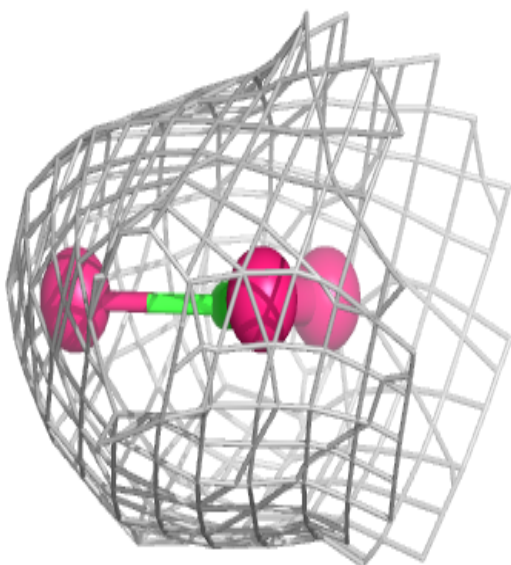
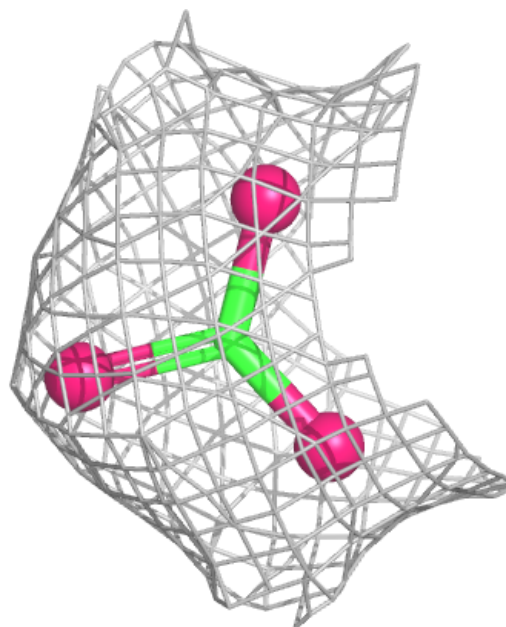
Electron density around BCT D 402 (A):

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



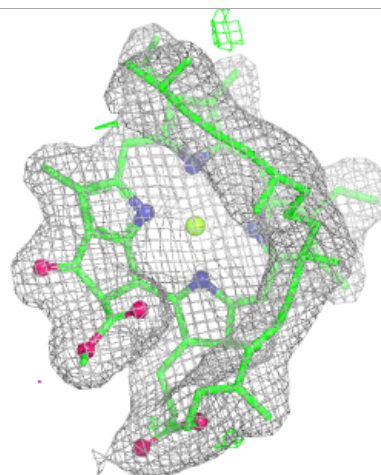
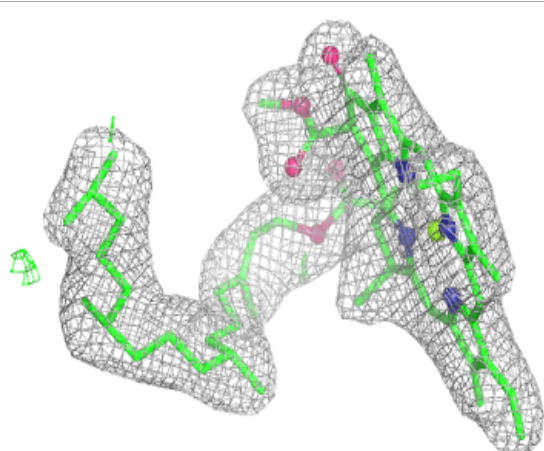
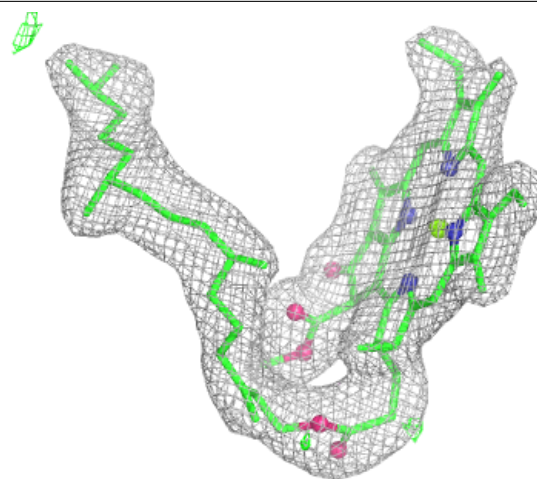
Electron density around BCT D 402 (B):

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



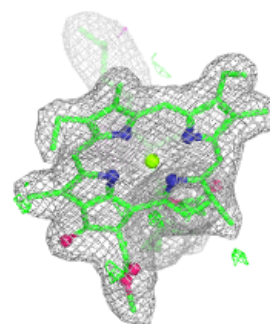
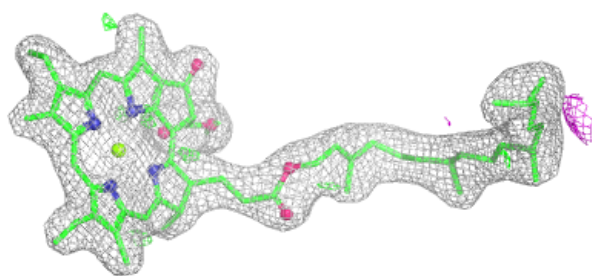
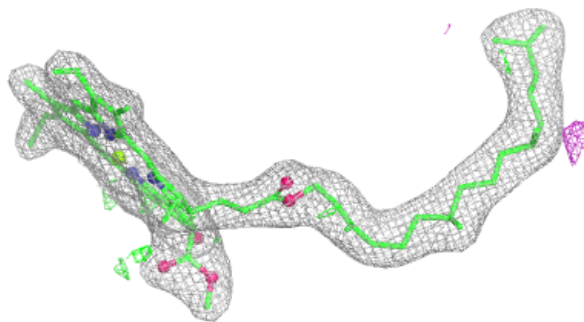
Electron density around CLA b 613:

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



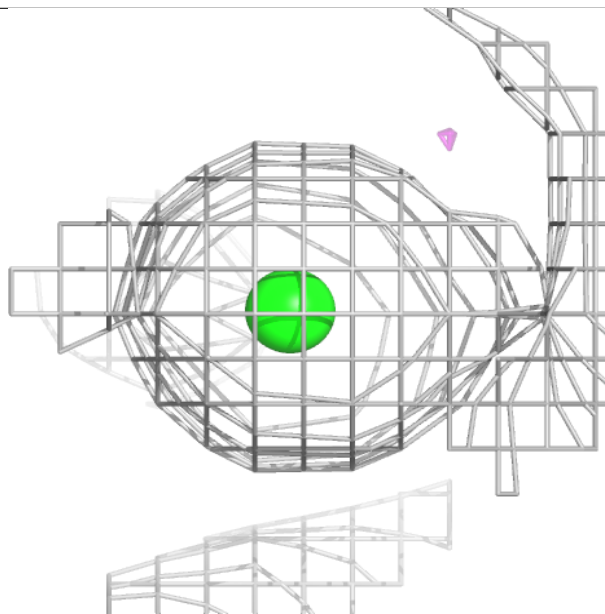
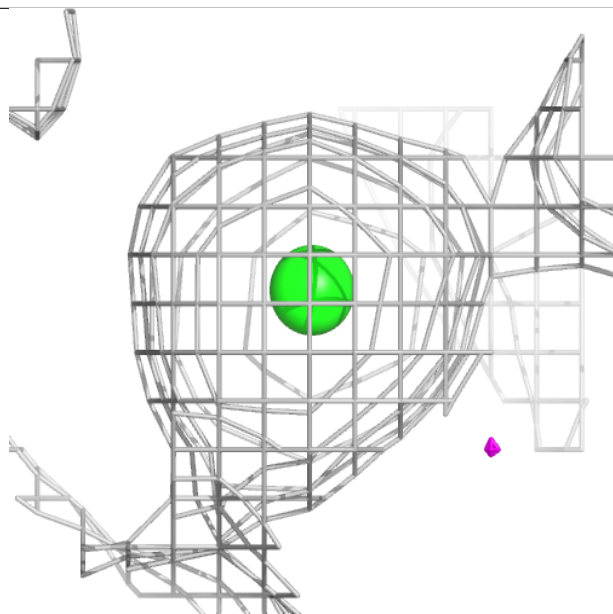
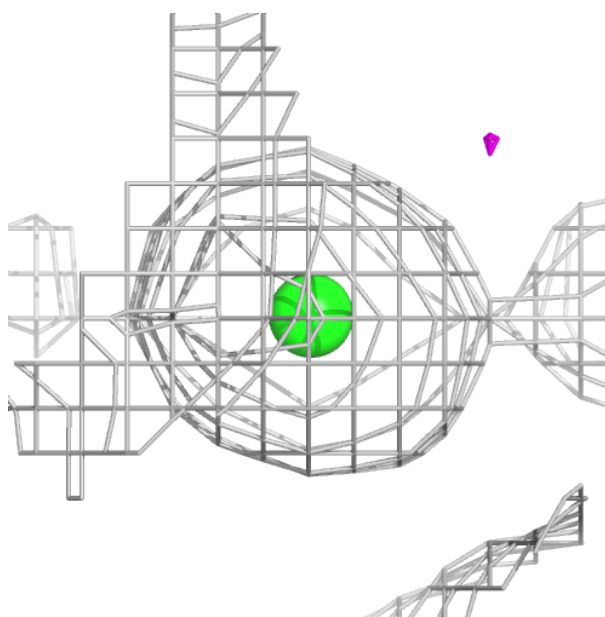
Electron density around CLA D 404 (B):

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



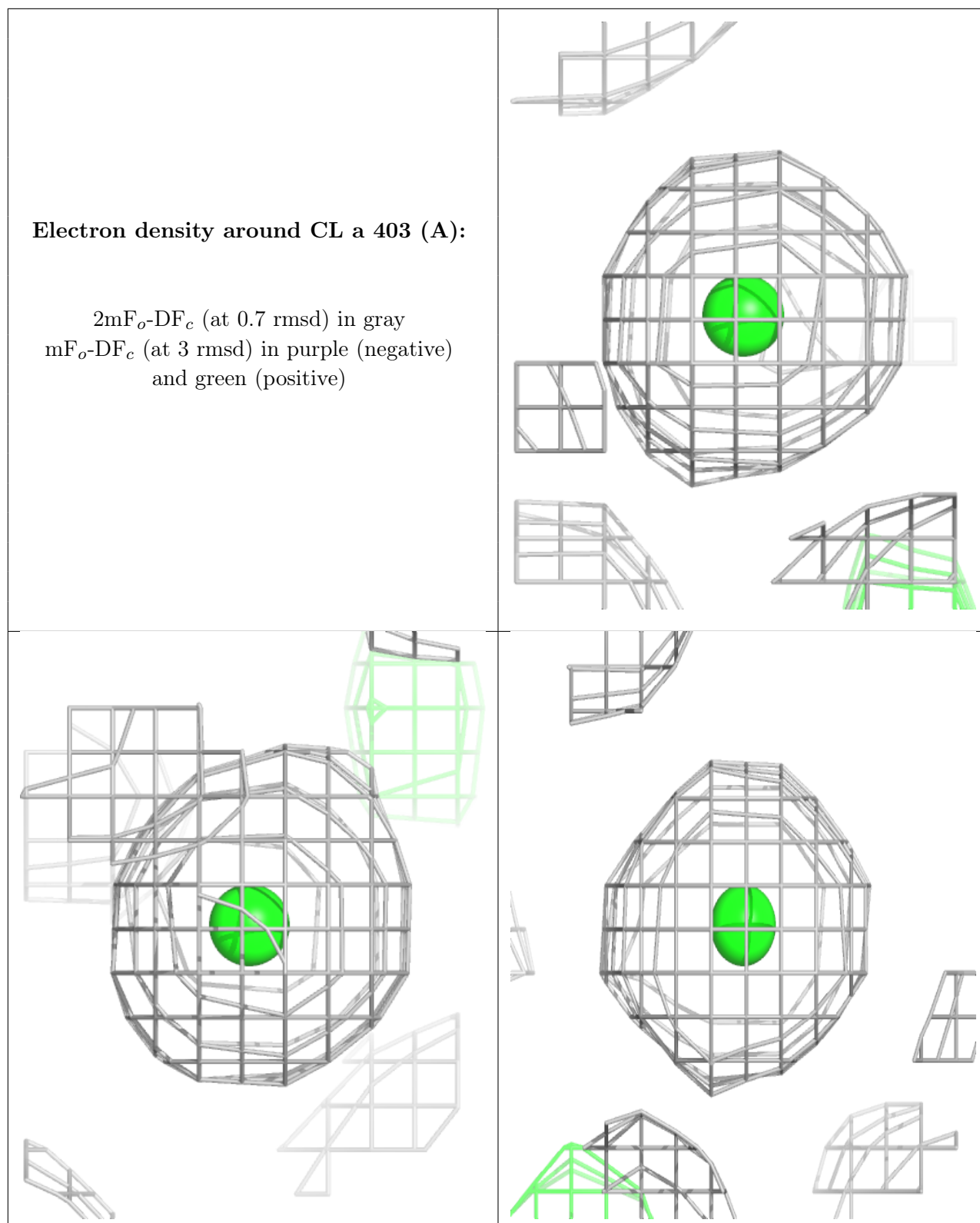
Electron density around CL a 404 (B):

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



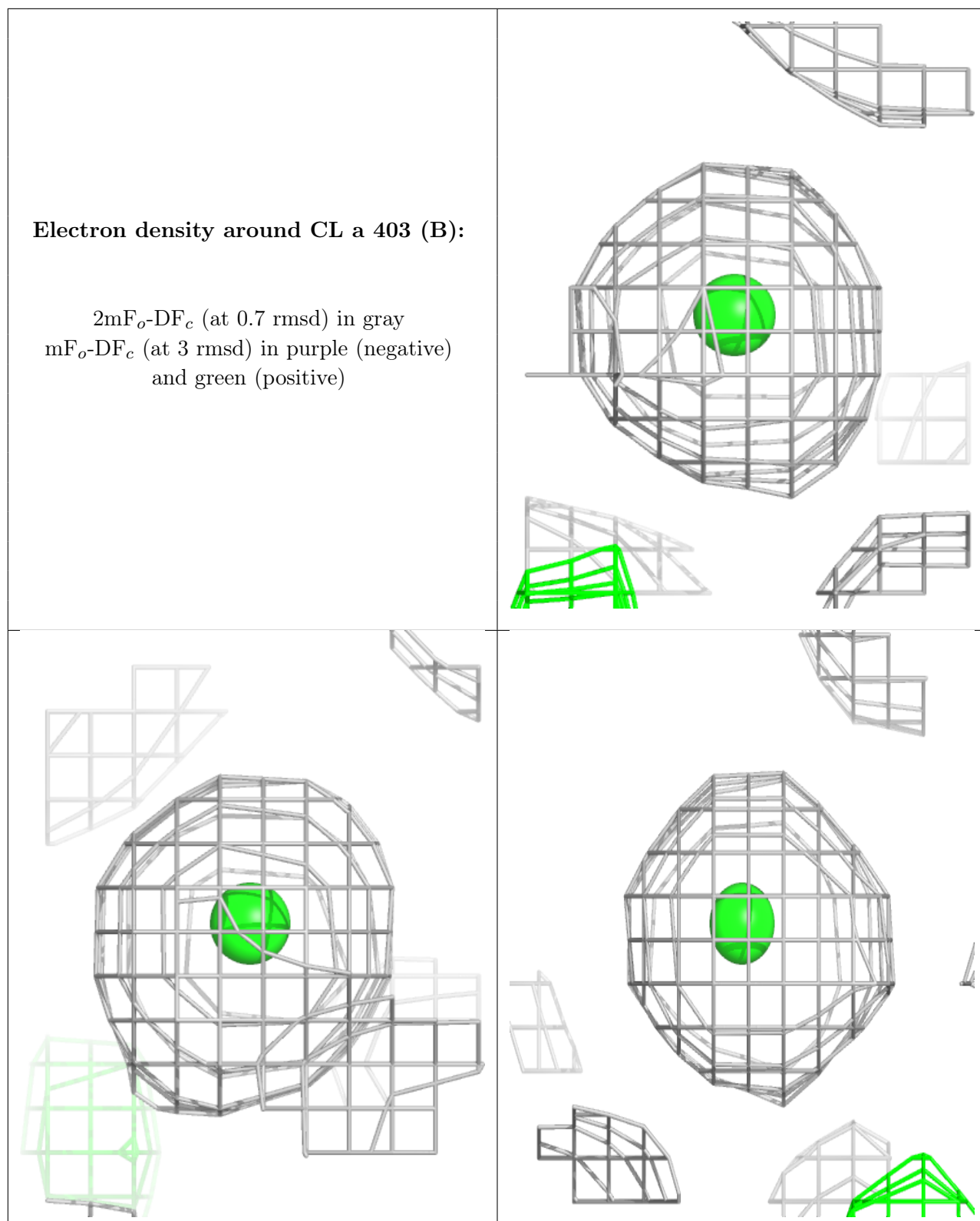
Electron density around CL a 403 (A):

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



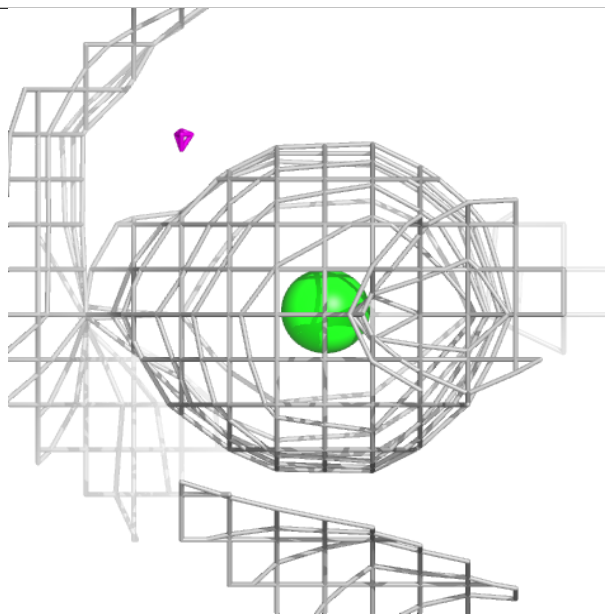
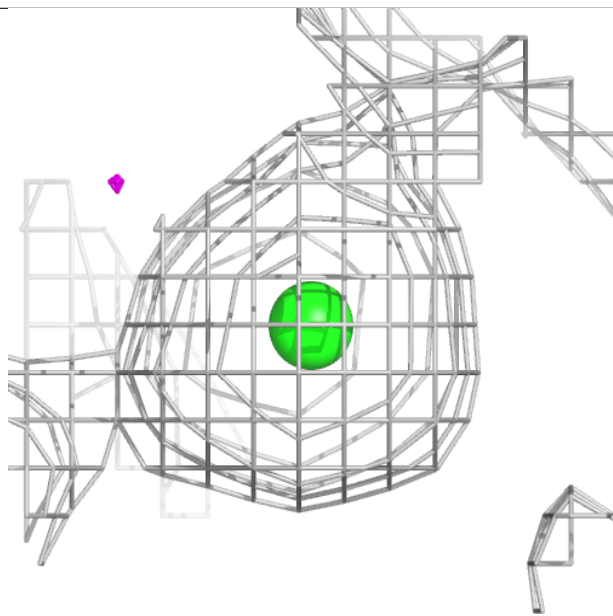
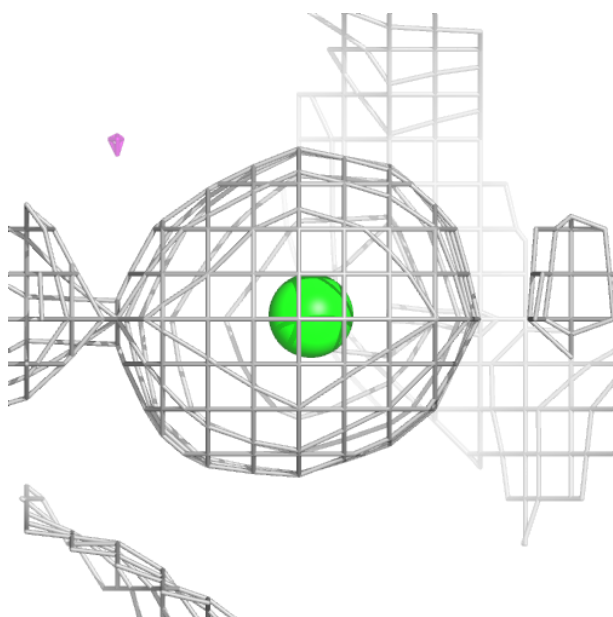
Electron density around CL a 403 (B):

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



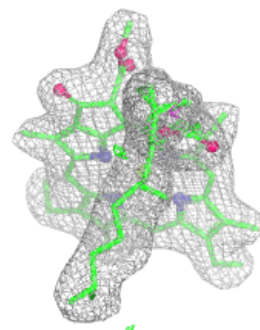
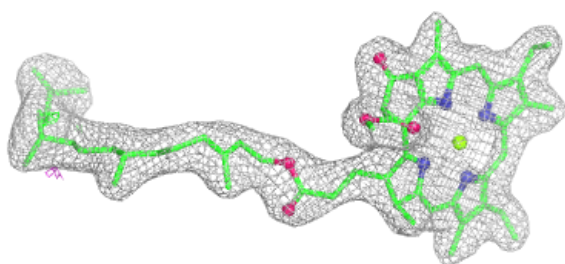
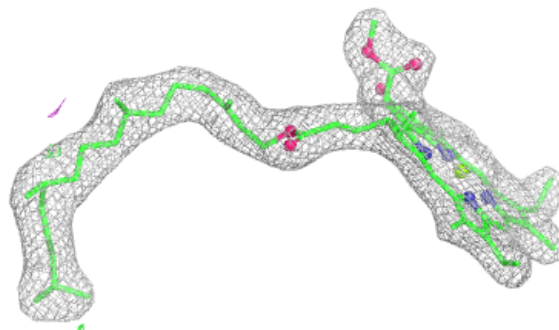
Electron density around CL a 404 (A):

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

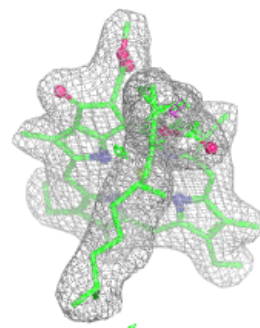
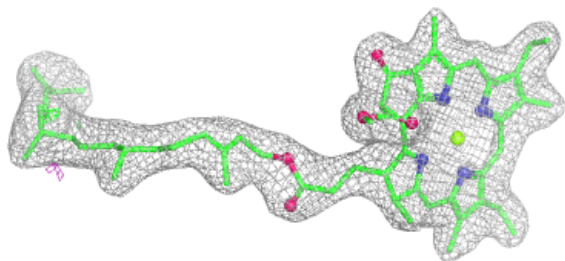
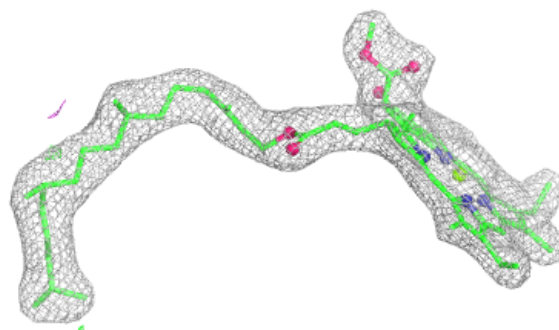


Electron density around CLA d 402 (A):

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

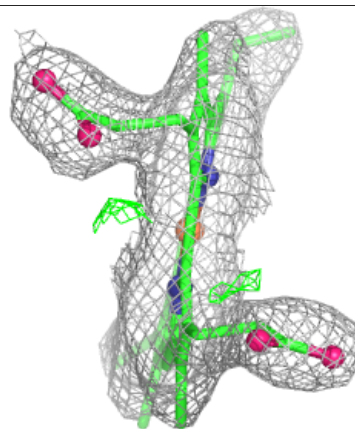
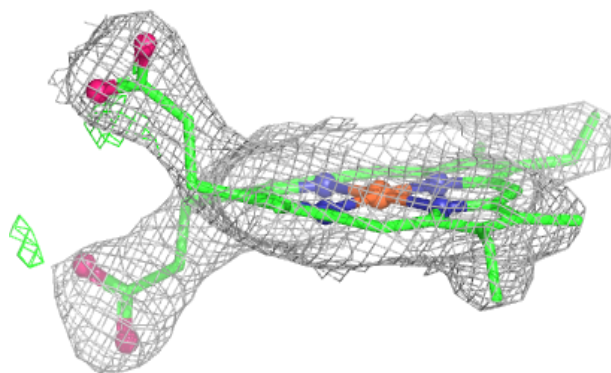
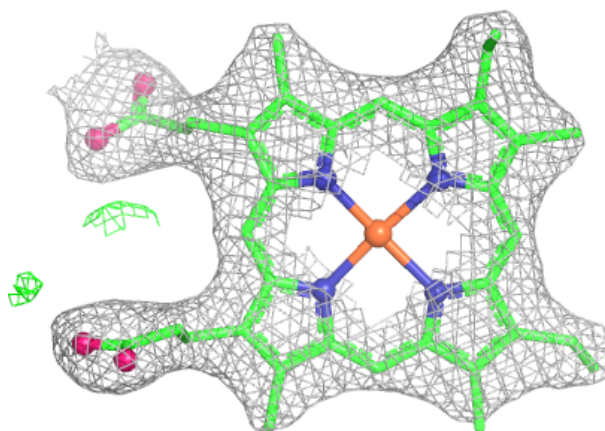
**Electron density around CLA d 402 (B):**

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



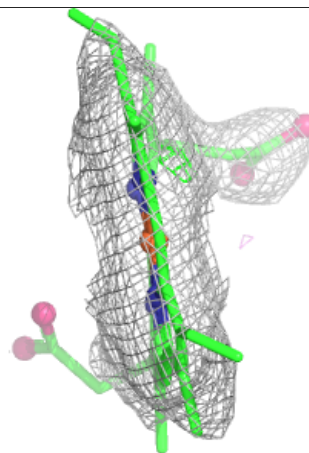
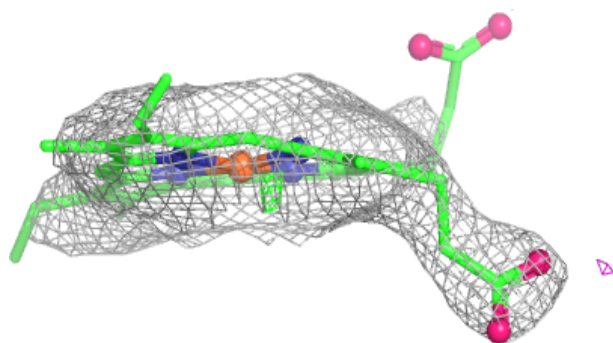
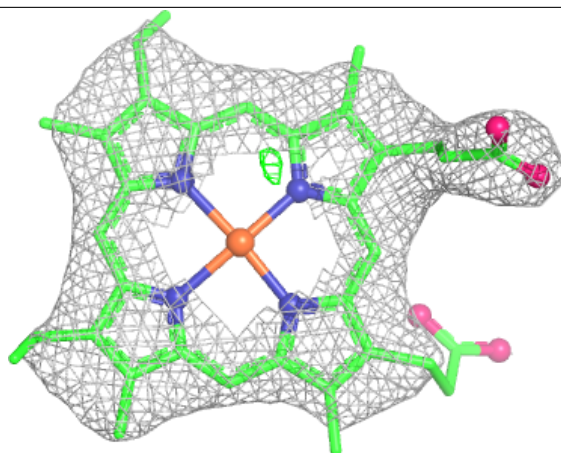
Electron density around HEM F 102:

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



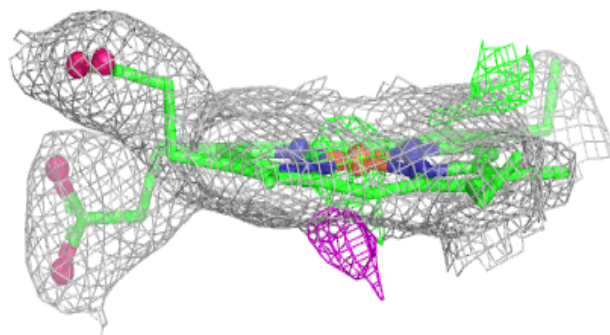
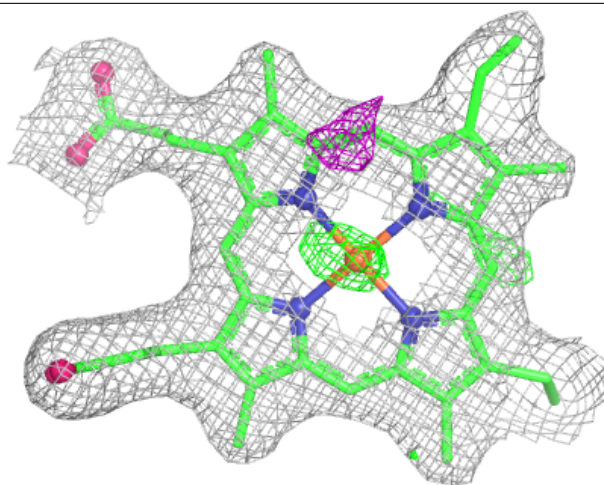
Electron density around HEM f 101:

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



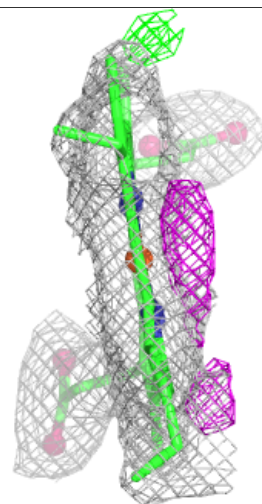
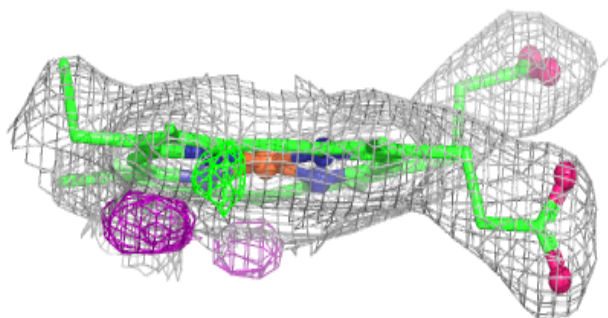
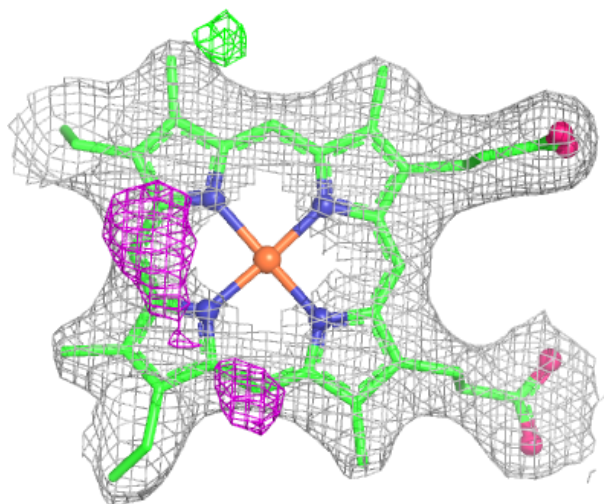
Electron density around HEC V 201:

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



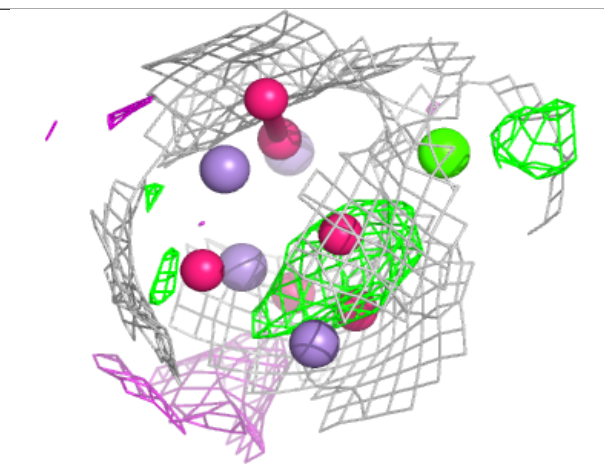
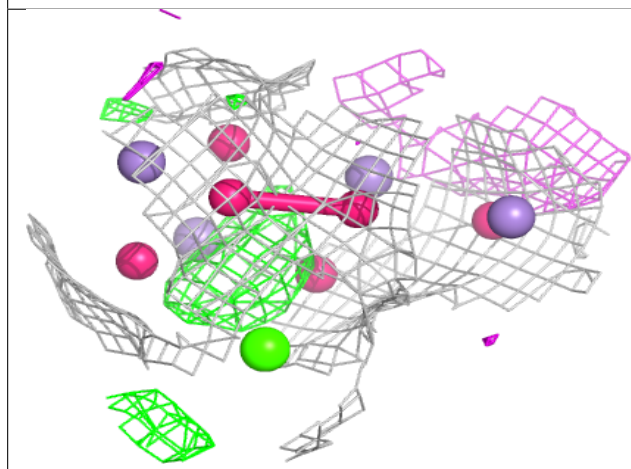
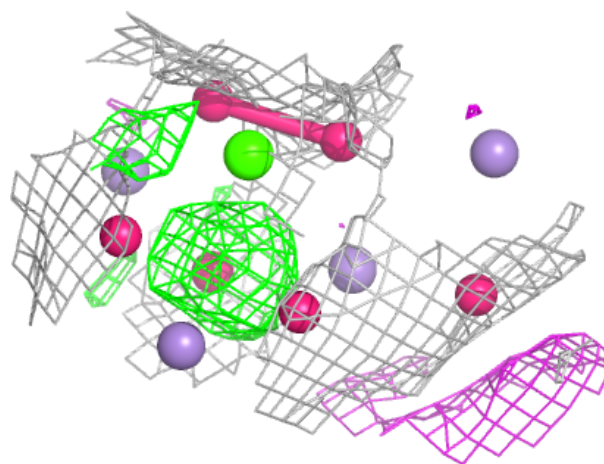
Electron density around HEC v 201:

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



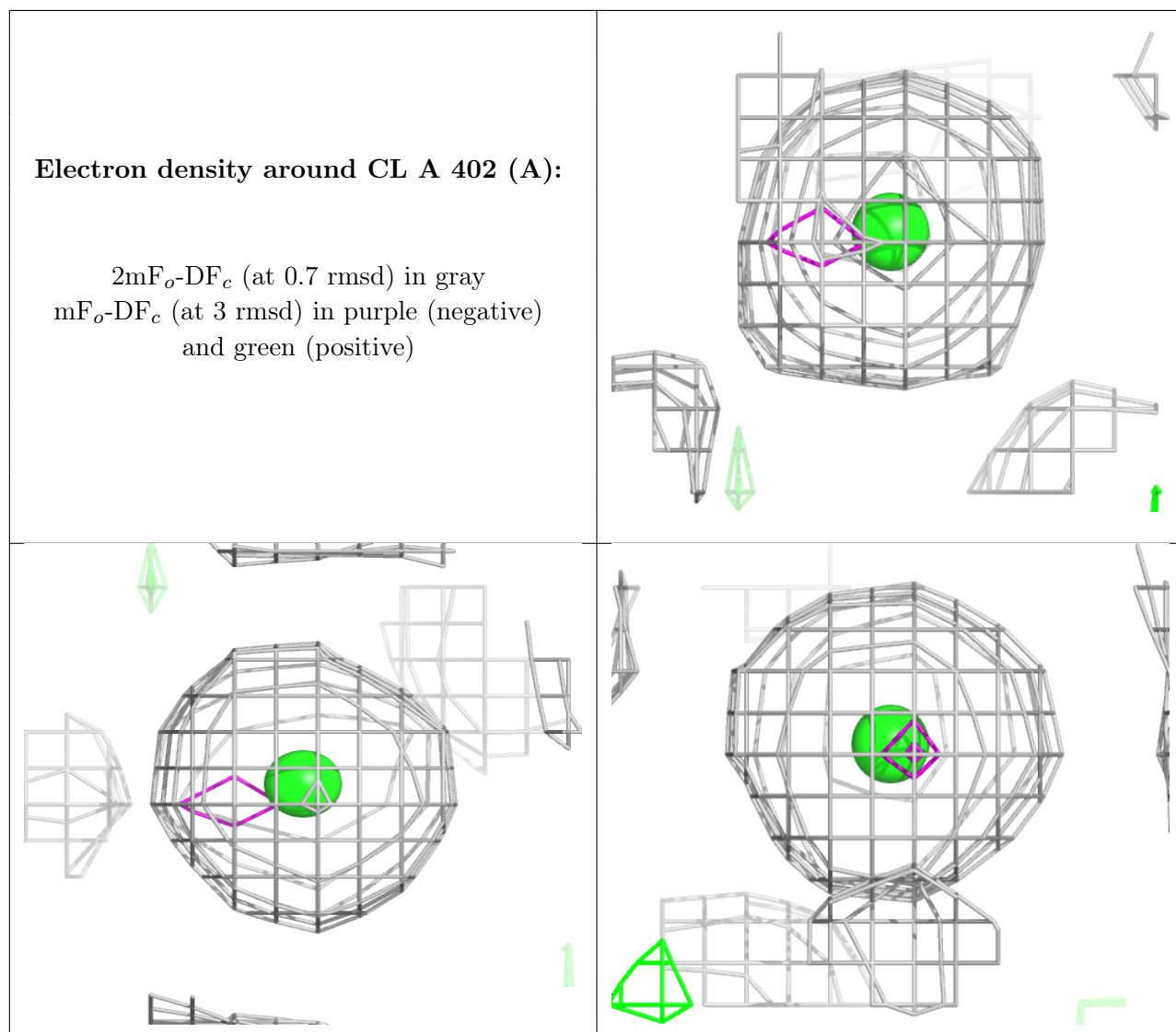
Electron density around OEY A 401 (B):

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



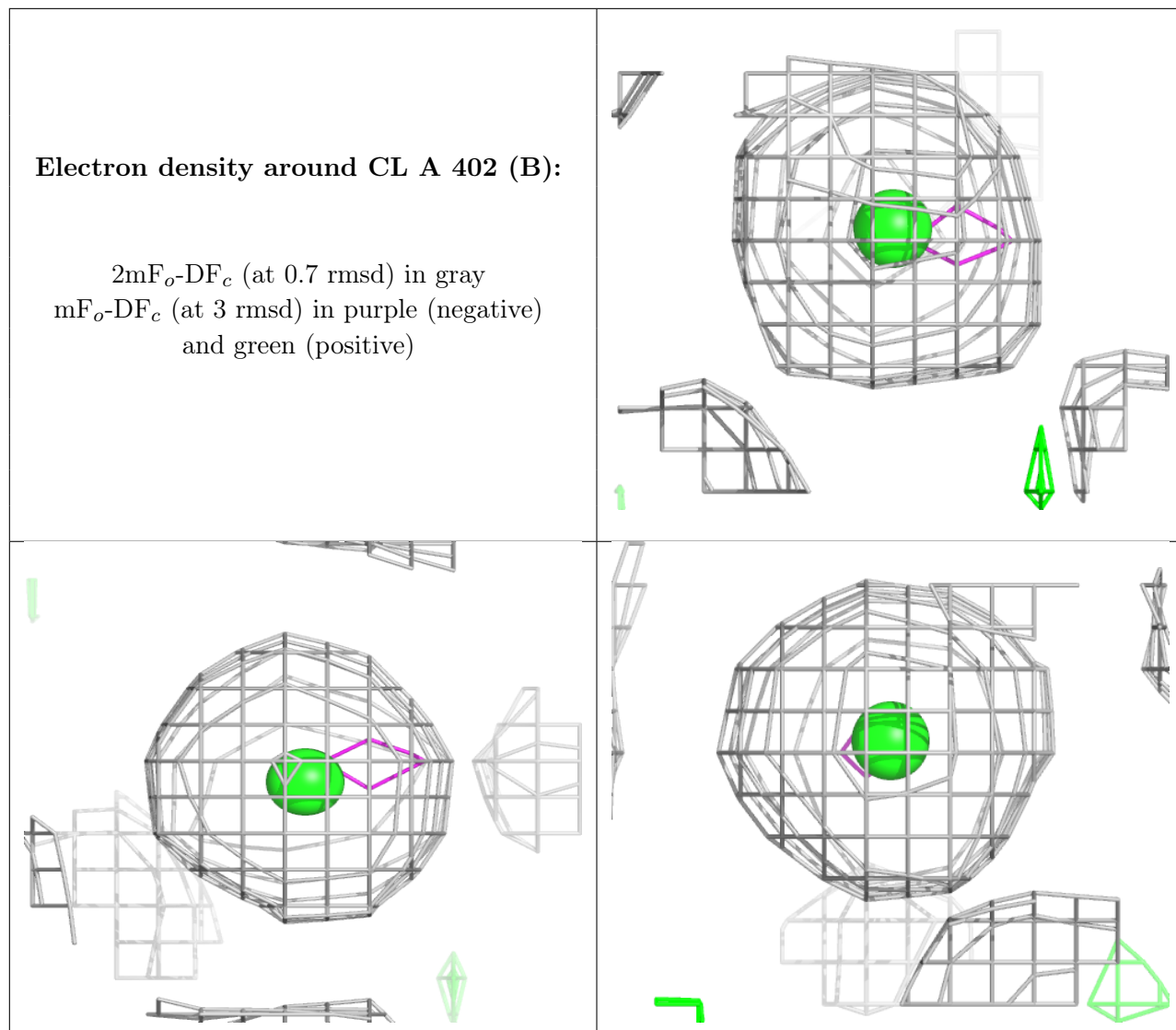
Electron density around CL A 402 (A):

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



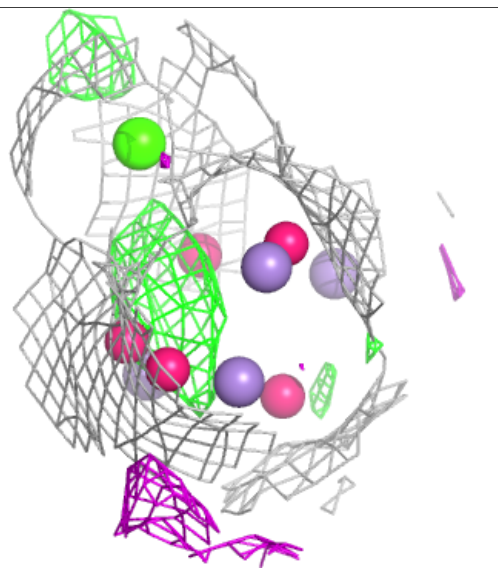
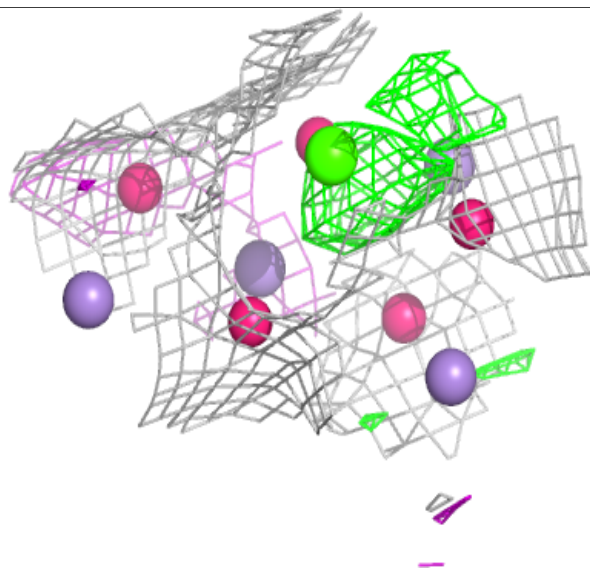
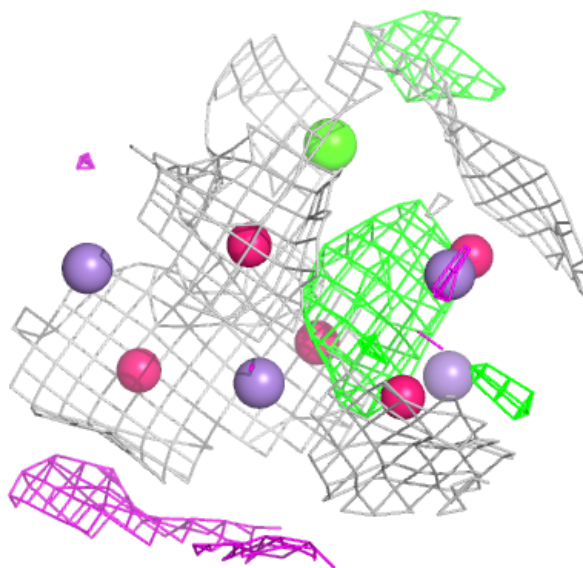
Electron density around CL A 402 (B):

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



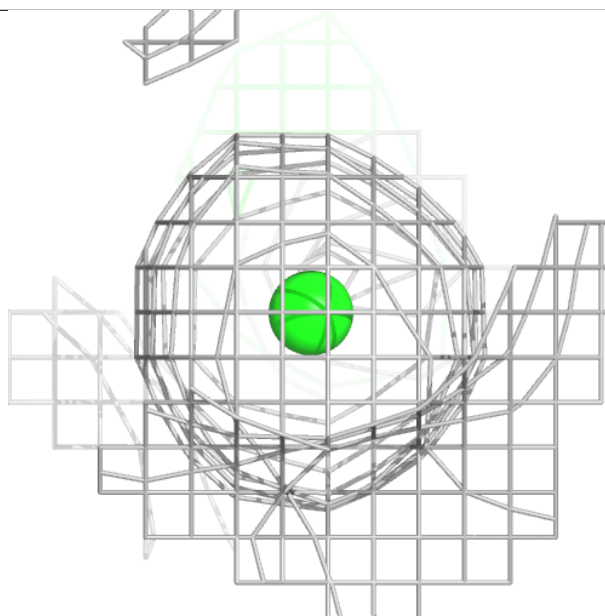
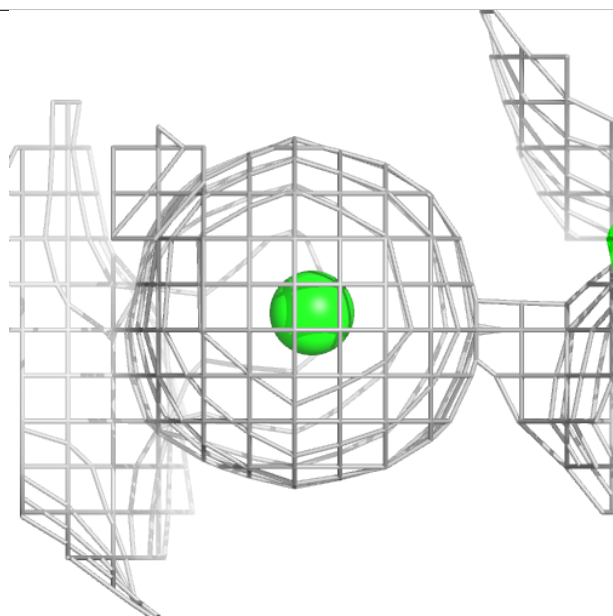
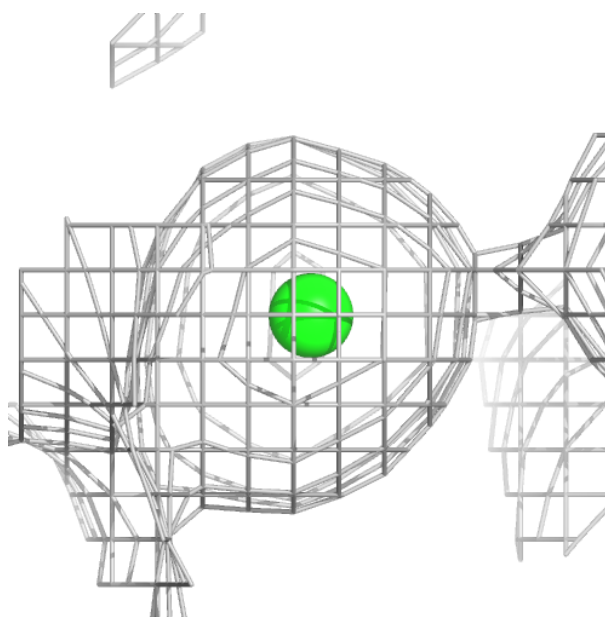
Electron density around OEX A 413 (A):

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



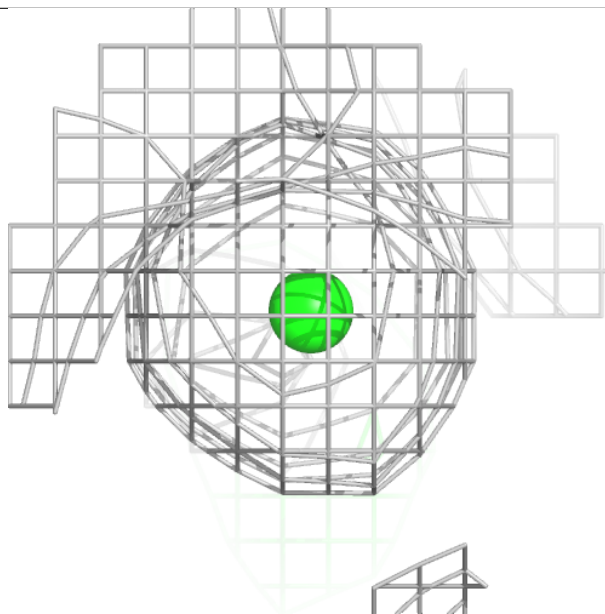
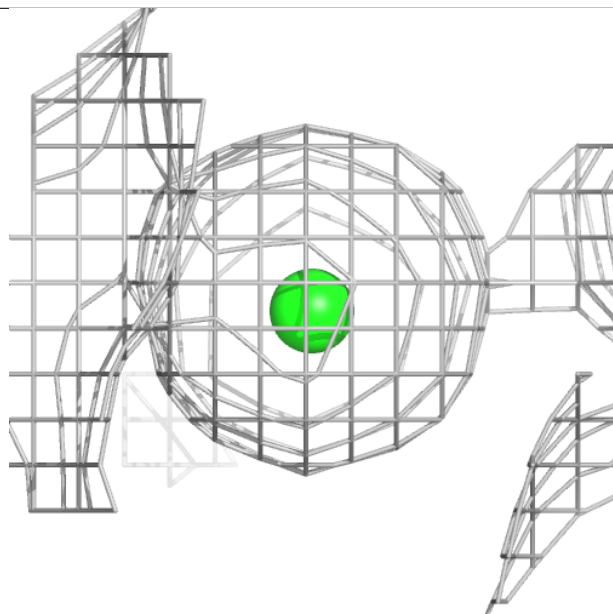
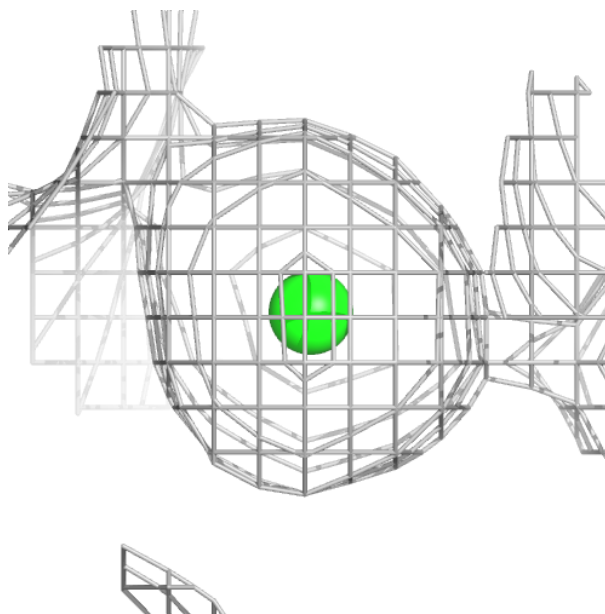
Electron density around CL A 403 (A):

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



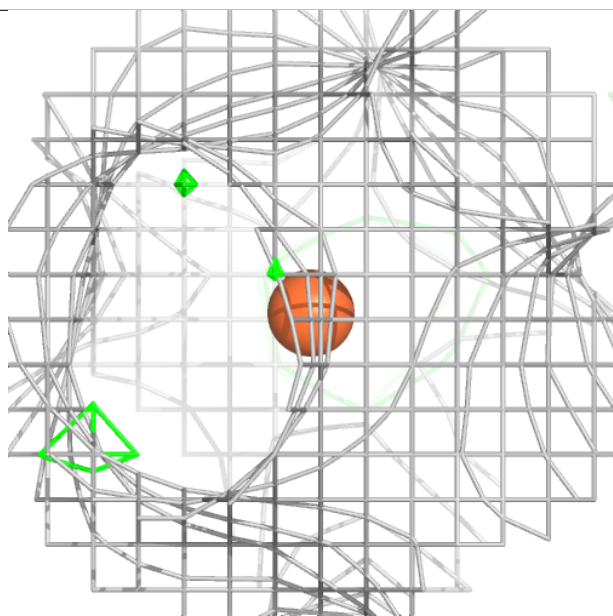
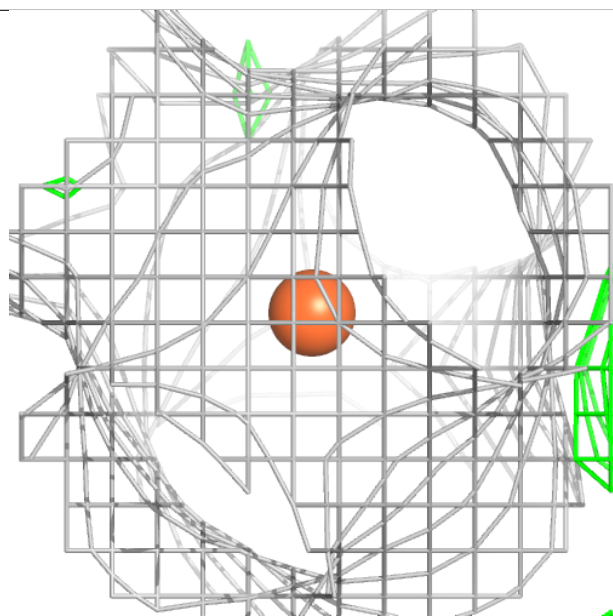
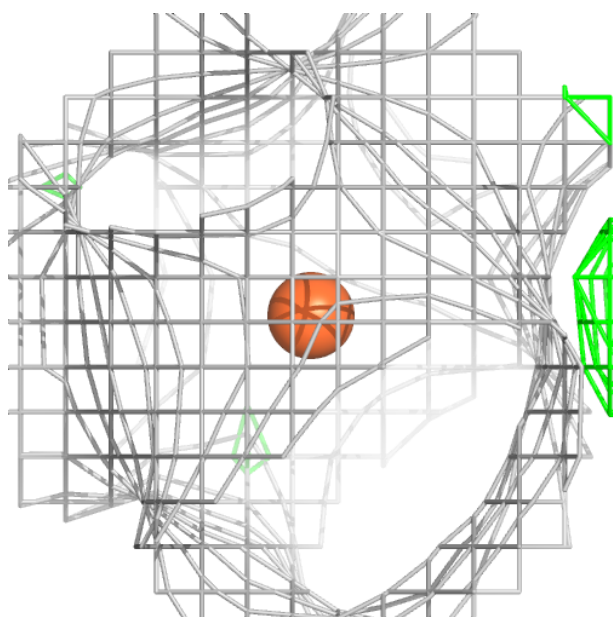
Electron density around CL A 403 (B):

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



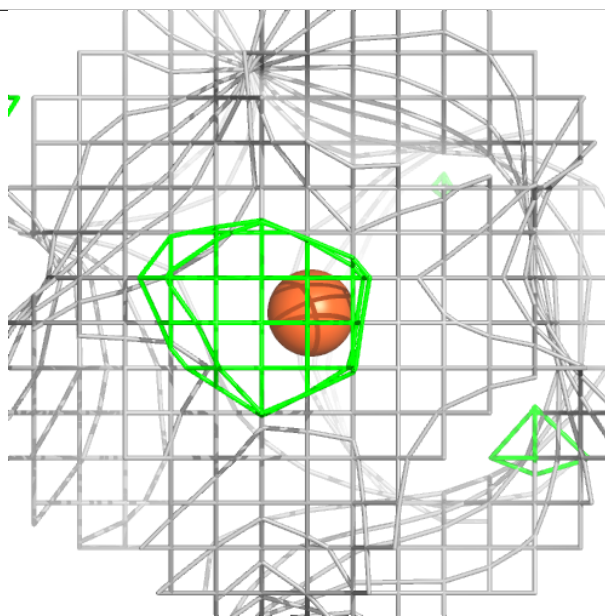
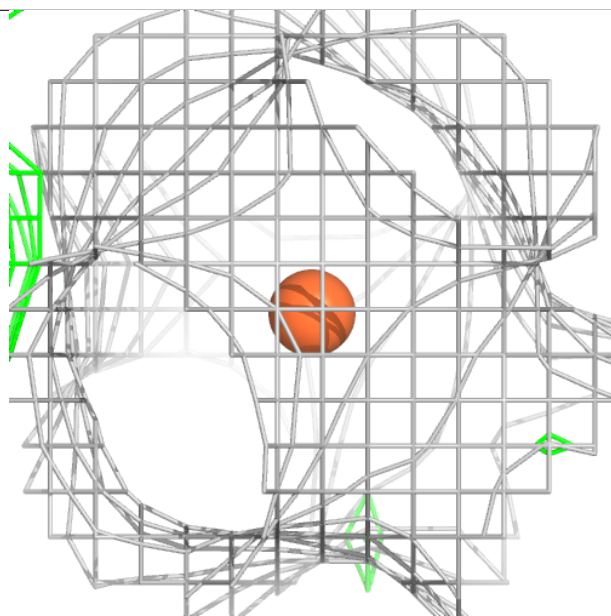
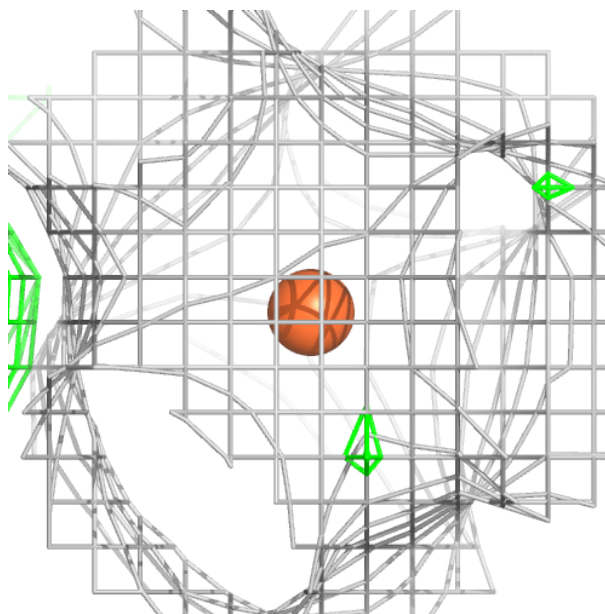
Electron density around FE2 a 402 (A):

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



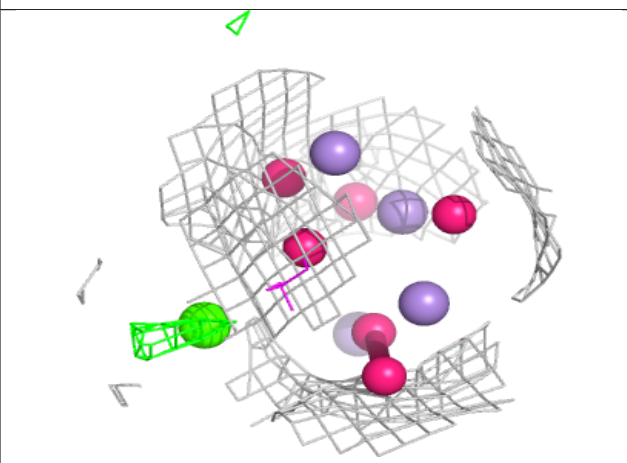
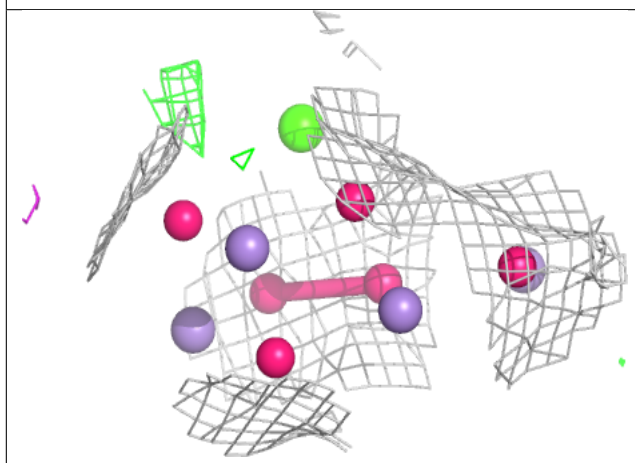
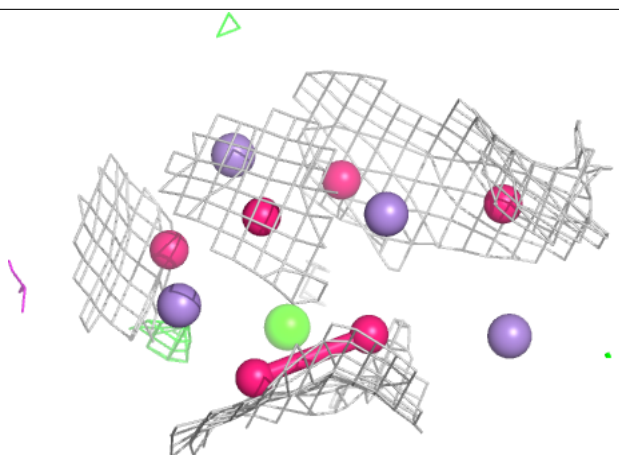
Electron density around FE2 a 402 (B):

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



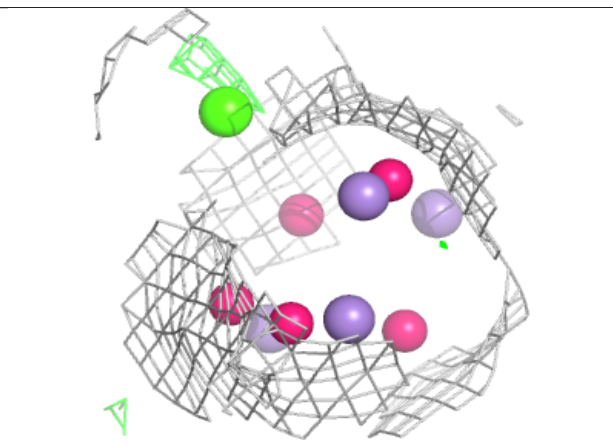
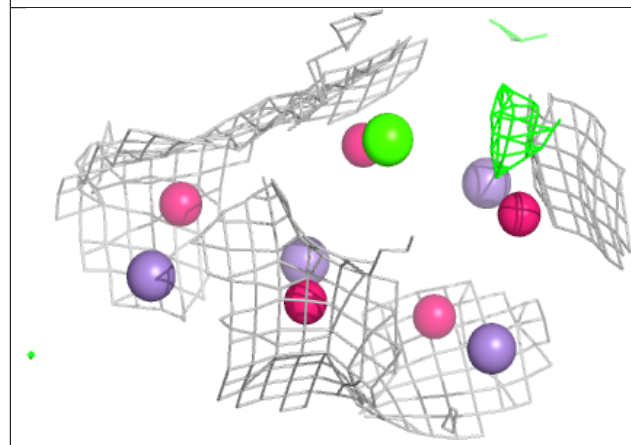
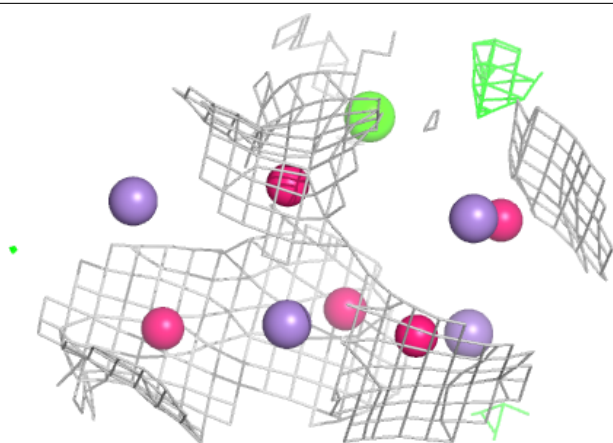
Electron density around OEY a 401 (B):

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



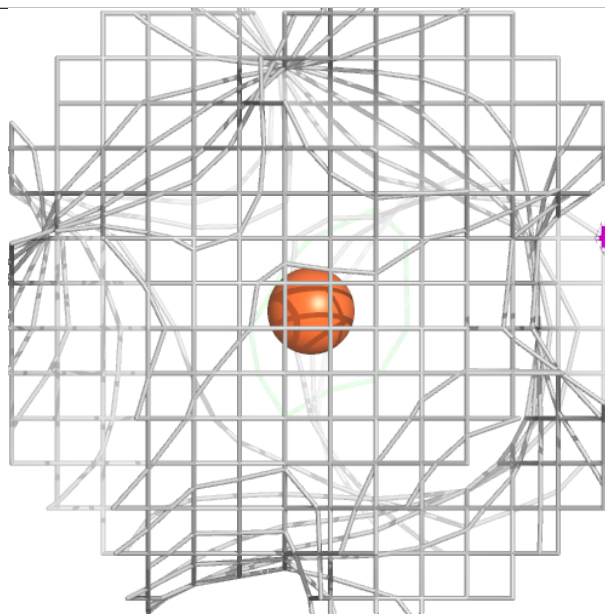
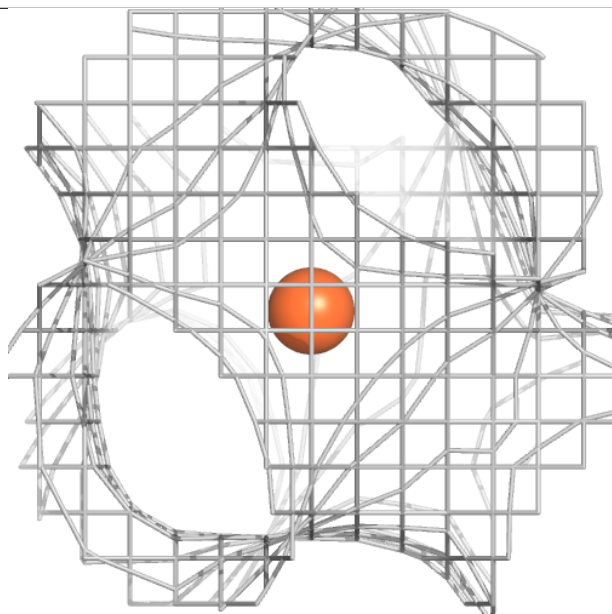
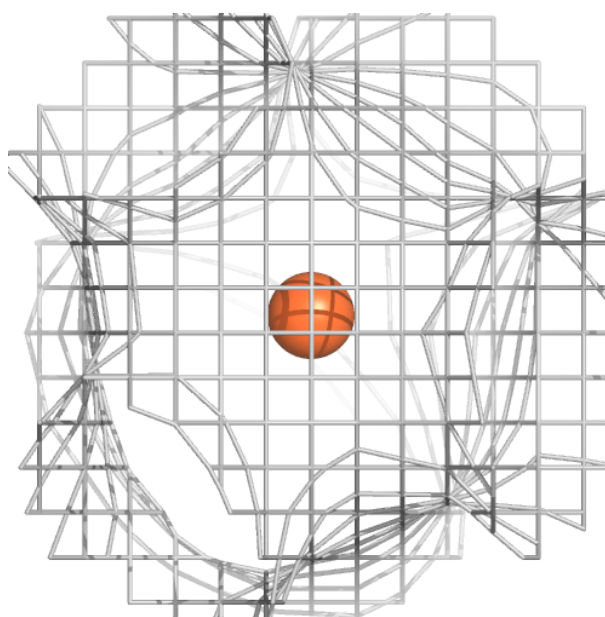
Electron density around OEX a 413 (A):

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



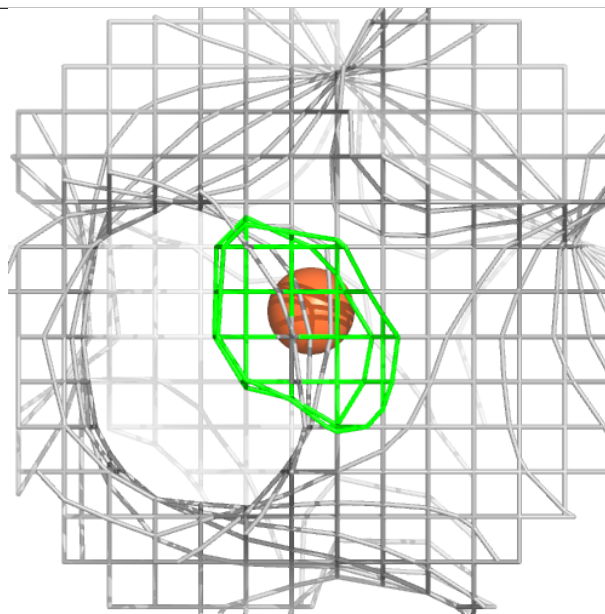
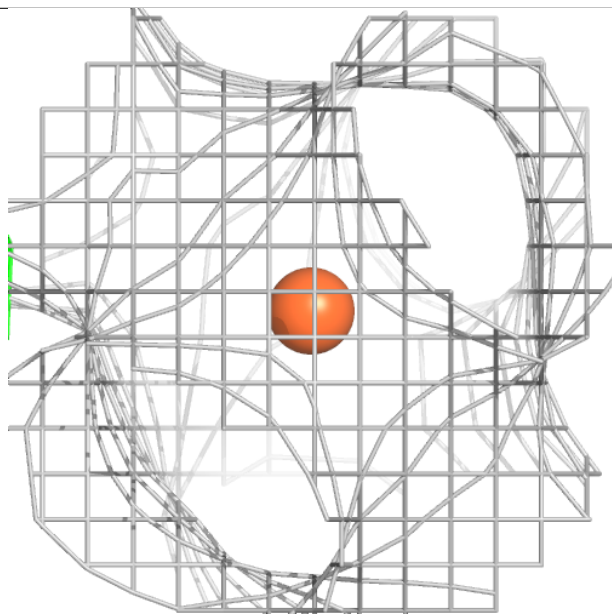
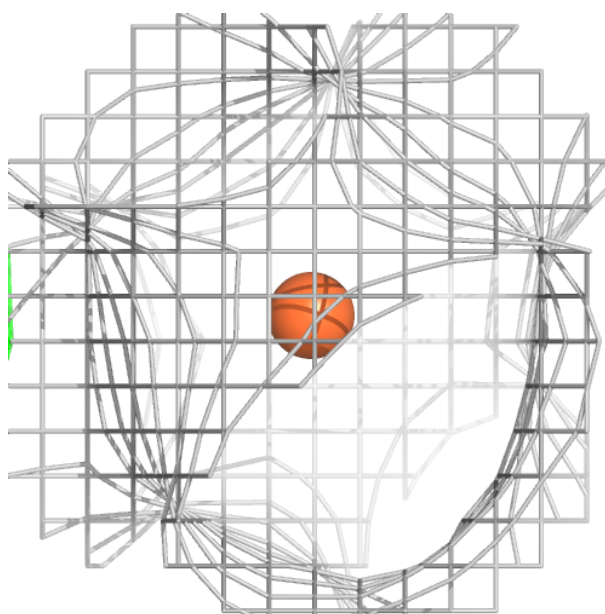
Electron density around FE2 D 401 (A):

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



Electron density around FE2 D 401 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.