



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 08:43 PM JST

PDB ID : 8IRD / pdb_00008ird
Title : XFEL structure of cyanobacterial photosystem II following two flashes (2F)
with a 20-nanosecond delay
Authors : Li, H.; Suga, M.; Shen, J.R.
Deposited on : 2023-03-17
Resolution : 2.30 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:

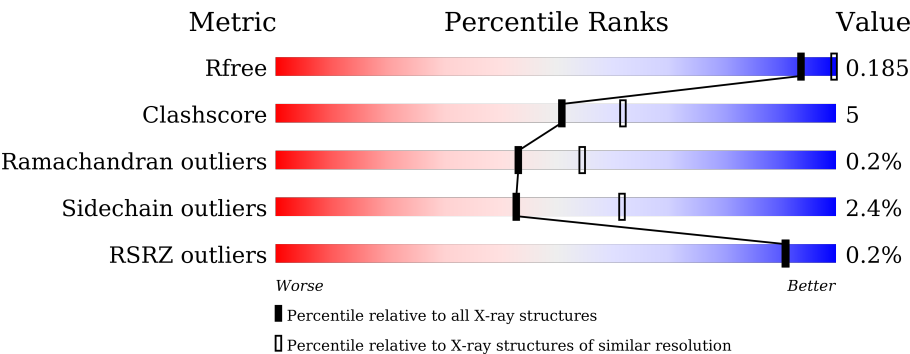
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



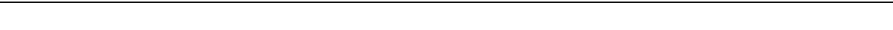
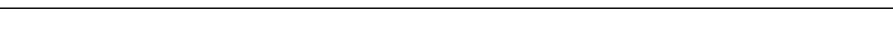
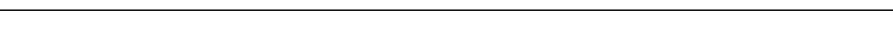
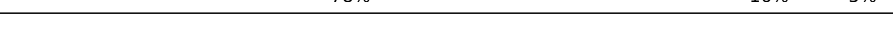
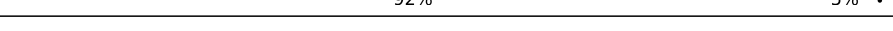
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 7% .
1	a	344	85% 11% .
2	B	505	91% 9% .
2	b	505	90% 8% .
3	C	455	91% 7% .
3	c	455	89% 10% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	 90% 10%
4	d	342	 92% 8%
5	E	84	 79% 18% .
5	e	84	 86% 8% 6%
6	F	44	 68% 9% 23%
6	f	44	 64% 7% 30%
7	H	65	 94% 5% .
7	h	65	 83% 14% . .
8	I	38	 76% 21% .
8	i	38	 87% 13%
9	J	39	 77% 21% .
9	j	39	 92% 8%
10	K	37	 81% 16% .
10	k	37	 78% 16% 5%
11	L	37	 92% 5% .
11	l	37	 81% 16% .
12	M	36	 78% 8% 6% 8%
12	m	36	 78% 14% . 6%
13	O	244	 84% 16%
13	o	244	 89% 10%
14	T	32	 75% 16% . 6%
14	t	32	 72% 22% 6%
15	U	104	 85% 8% 8%
15	u	104	 87% 6% . 7%
16	V	137	 96% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	137	 90% 10%
17	X	40	 88% 8% 5%
17	x	40	 90% 5% 5%
18	Y	30	 3% 80% 17% •
18	y	30	 60% 37% •
19	Z	62	 85% 13% •
19	z	62	 74% 24% •
20	R	34	 3% 71% 29%

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
26	GOL	D	402	-	-	X	-
26	GOL	D	413	-	X	-	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition [i](#)

There are 41 unique types of molecules in this entry. The entry contains 62600 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 FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

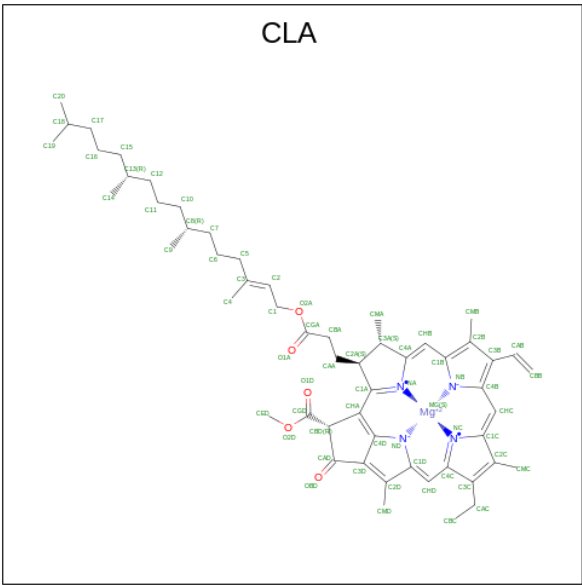
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

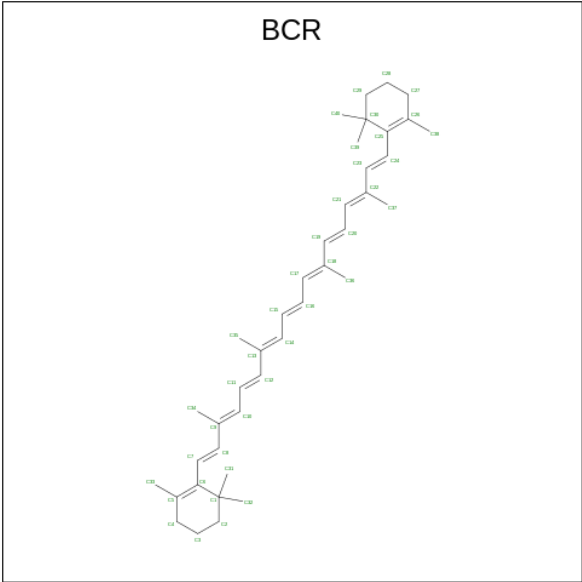
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 130	C 110	Mg 2	N 8	O 10	0	1
23	a	1	Total 65	C 55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

Continued on next page...

Continued from previous page...

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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



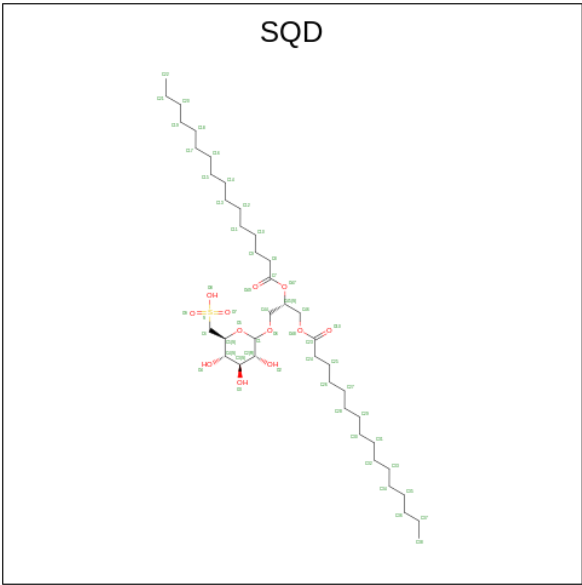
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	k	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	y	1	Total C 40 40	0	0

- Molecule 25 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



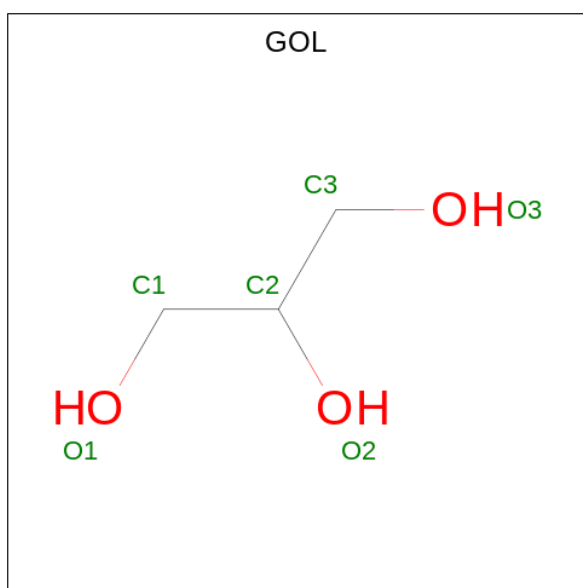
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O S 108 82 24 2	0	1
25	A	1	Total C O S 54 41 12 1	0	0
25	X	1	Total C O S 43 30 12 1	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 26 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



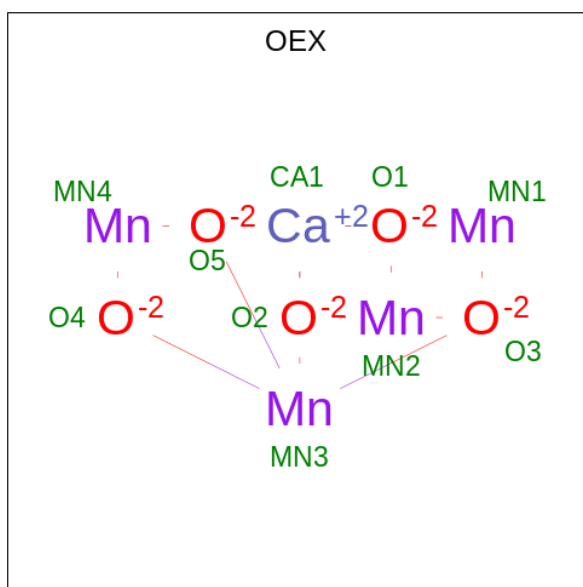
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	A	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	B	1	Total	C	O	0	0
			6	3	3		
26	C	1	Total	C	O	0	1
			12	6	6		
26	D	1	Total	C	O	0	0
			6	3	3		
26	D	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

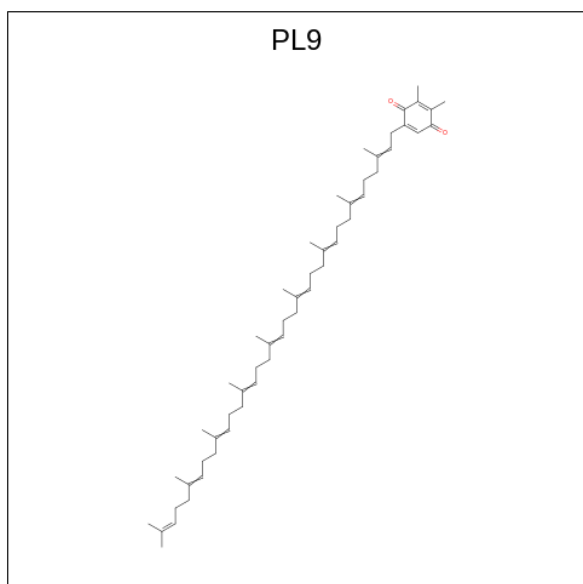
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
26	O	1	Total	C	O	0	0
			6	3	3		
26	O	1	Total	C	O	0	0
			6	3	3		
26	V	1	Total	C	O	0	1
			12	6	6		
26	a	1	Total	C	O	0	0
			6	3	3		
26	a	1	Total	C	O	0	0
			6	3	3		
26	a	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	b	1	Total	C	O	0	0
			6	3	3		
26	c	1	Total	C	O	0	1
			12	6	6		
26	c	1	Total	C	O	0	0
			6	3	3		
26	d	1	Total	C	O	0	0
			6	3	3		
26	l	1	Total	C	O	0	1
			12	6	6		
26	o	1	Total	C	O	0	0
			6	3	3		
26	o	1	Total	C	O	0	0
			6	3	3		
26	v	1	Total	C	O	0	1
			12	6	6		

- Molecule 27 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
27	A	1	Total	Ca	Mn	O	0	1
			20	2	8	10		
27	a	1	Total	Ca	Mn	O	0	1
			20	2	8	10		

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).

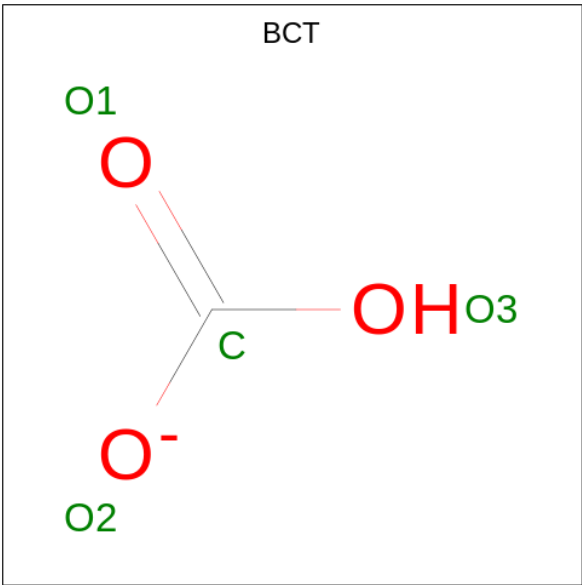


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	A	1	Total	C	O	0	1
			110	106	4		
28	D	1	Total	C	O	0	1
			110	106	4		
28	a	1	Total	C	O	0	1
			110	106	4		
28	d	1	Total	C	O	0	1
			110	106	4		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

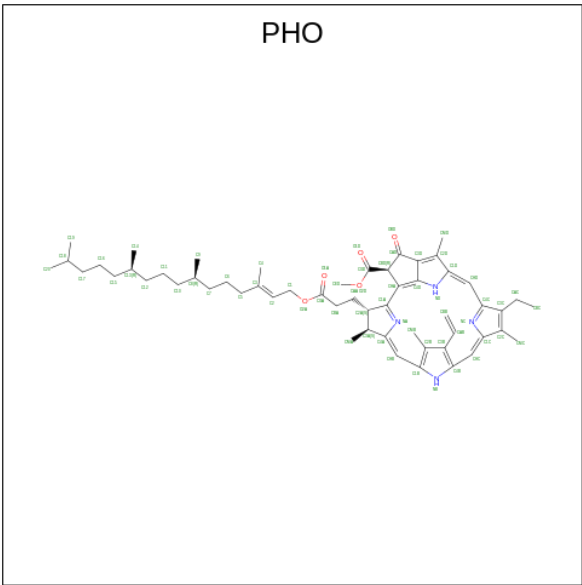
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	A	1	Total	C	O	0	0
			28	23	5		
29	B	2	Total	C	O	0	0
			73	63	10		
29	D	2	Total	C	O	0	0
			57	51	6		
29	I	1	Total	C	O	0	0
			40	35	5		
29	J	1	Total	C		0	0
			10	10			
29	K	1	Total	C	O	0	1
			68	58	10		
29	X	1	Total	C	O	0	0
			18	16	2		
29	a	1	Total	C	O	0	0
			30	25	5		
29	b	1	Total	C	O	0	0
			33	28	5		
29	c	1	Total	C	O	0	1
			64	54	10		
29	d	3	Total	C	O	0	0
			71	63	8		
29	j	1	Total	C		0	0
			10	10			
29	l	1	Total	C		0	0
			10	10			
29	m	1	Total	C		0	0
			10	10			

- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	1
			8	2	6		
30	d	1	Total	C	O	0	1
			8	2	6		

- Molecule 31 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅).



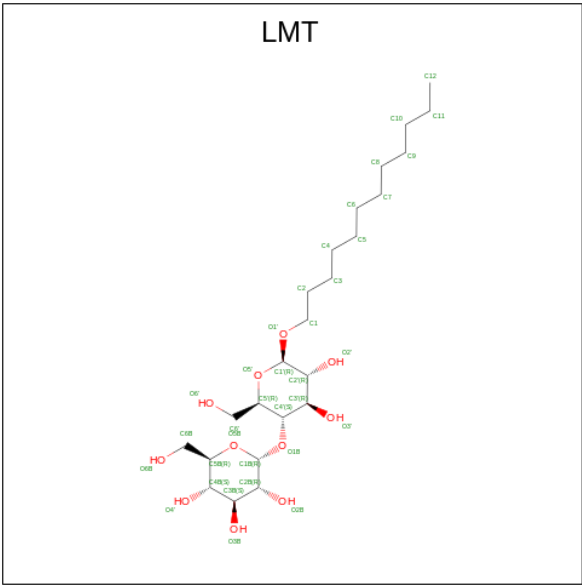
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	1
			128	110	8	10		
31	D	1	Total	C	N	O	0	1
			128	110	8	10		

Continued on next page...

Continued from previous page...

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

- Molecule 32 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



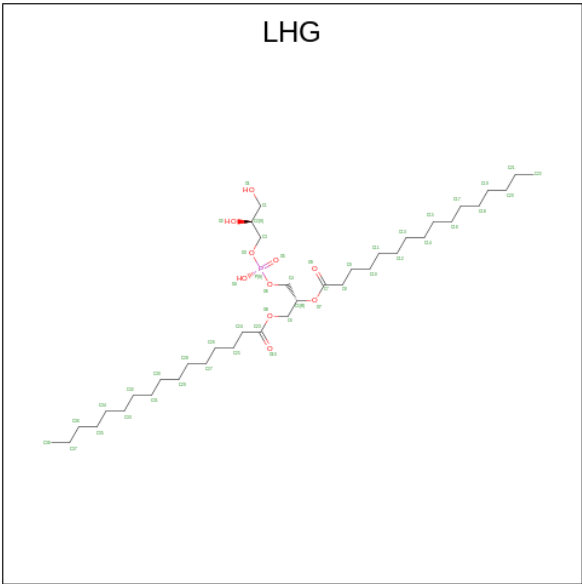
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			35	24	11		
32	A	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			35	24	11		
32	B	1	Total	C	O	0	0
			25	19	6		
32	F	1	Total	C	O	0	0
			35	24	11		
32	M	1	Total	C	O	0	0
			35	24	11		
32	T	1	Total	C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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	b	1	Total	C	O	0	0
			25	19	6		
32	b	1	Total	C	O	0	0
			25	19	6		
32	e	1	Total	C	O	0	0
			35	24	11		
32	m	1	Total	C	O	0	0
			35	24	11		
32	t	1	Total	C	O	0	0
			26	19	7		

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



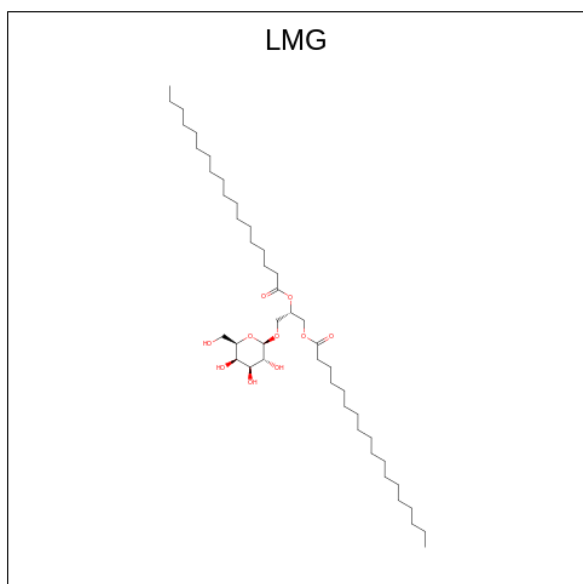
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	A	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	D	1	Total	C	O	P	0	1
			98	76	20	2		
33	E	1	Total	C	O	P	0	1
			84	62	20	2		
33	L	1	Total	C	O	P	0	1
			98	76	20	2		
33	a	1	Total	C	O	P	0	1
			84	62	20	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	b	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		
33	d	1	Total	C	O	P	0	1
			98	76	20	2		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



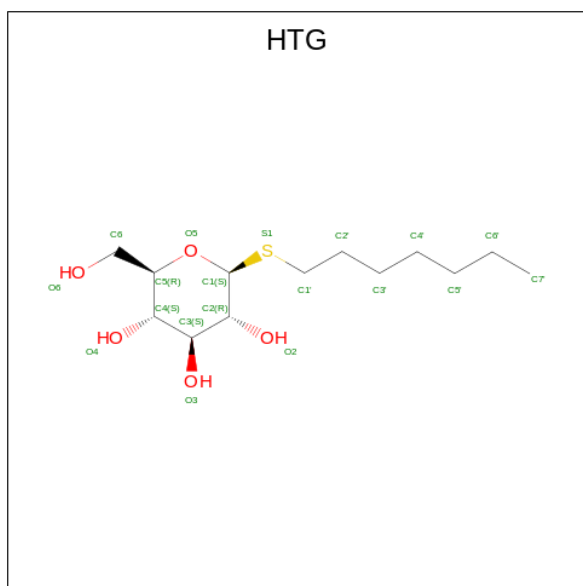
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		

Continued on next page...

Continued from previous page...

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



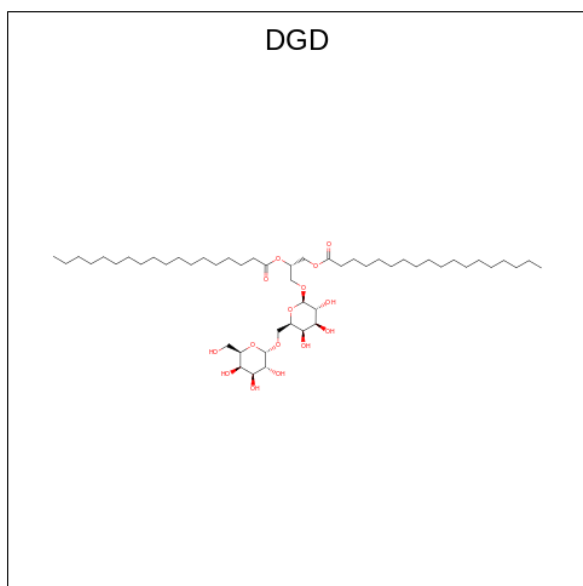
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			16	10	5	1		
35	V	1	Total	C	O		0	0
			11	6	5			
35	b	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	d	1	Total	C	O	S	0	0
			16	10	5	1		
35	o	1	Total	C	O	S	0	0
			19	13	5	1		

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



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

Continued on next page...

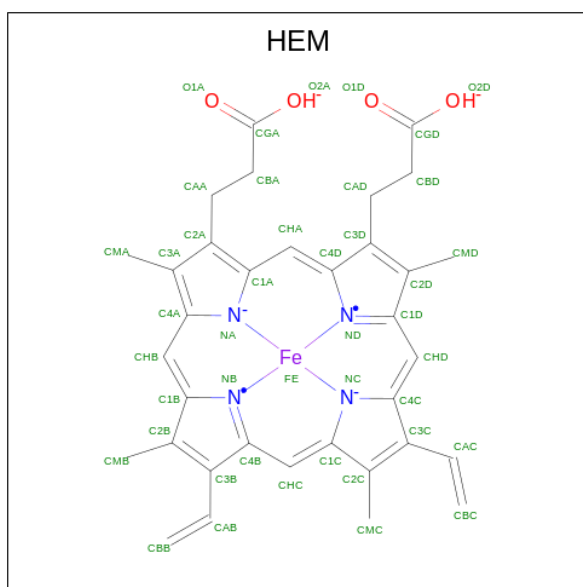
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	c	1	Total 62	C 47	O 15	0	0
36	h	1	Total 62	C 47	O 15	0	0

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 38 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

Continued on next page...

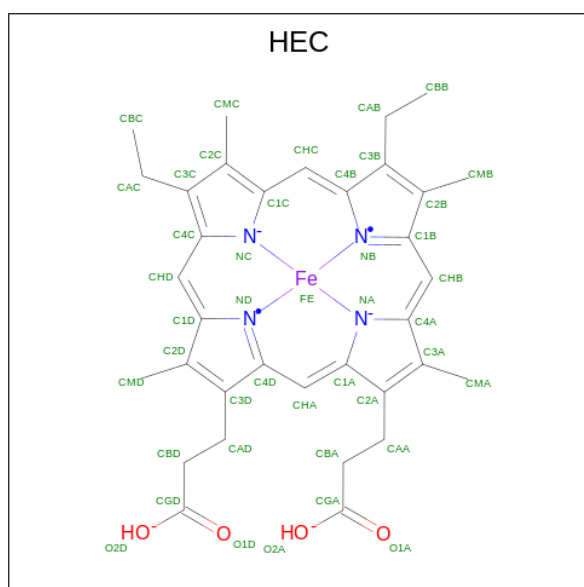
Continued from previous page...

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

- Molecule 39 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	A	133	Total O 215 215	0	83
41	B	190	Total O 193 193	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	C	165	Total 202	O 202	0	37
41	D	127	Total 162	O 162	0	35
41	E	15	Total 15	O 15	0	0
41	F	6	Total 6	O 6	0	0
41	H	23	Total 23	O 23	0	0
41	I	6	Total 6	O 6	0	0
41	J	7	Total 7	O 7	0	0
41	K	6	Total 6	O 6	0	0
41	L	7	Total 8	O 8	0	1
41	M	5	Total 5	O 5	0	0
41	O	102	Total 106	O 106	0	4
41	T	10	Total 13	O 13	0	3
41	U	47	Total 49	O 49	0	2
41	V	80	Total 82	O 82	0	2
41	X	8	Total 8	O 8	0	0
41	a	129	Total 207	O 207	0	79
41	b	206	Total 209	O 209	0	3
41	c	159	Total 192	O 192	0	33
41	d	118	Total 152	O 152	0	34
41	e	9	Total 9	O 9	0	0
41	f	3	Total 3	O 3	0	0

Continued on next page...

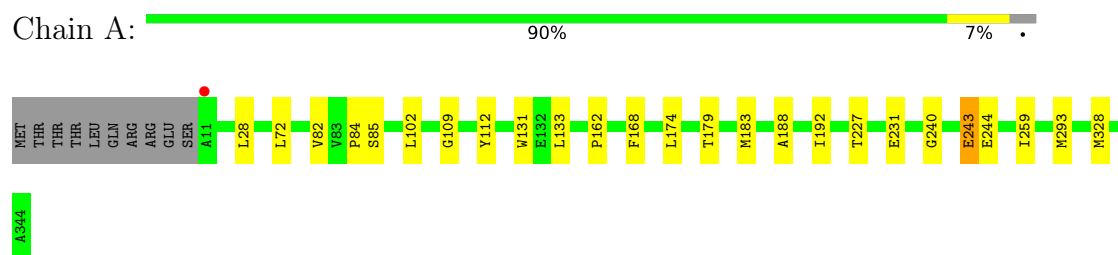
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	h	18	Total 18	O 18	0	0
41	i	2	Total 2	O 2	0	0
41	j	1	Total 1	O 1	0	0
41	k	3	Total 3	O 3	0	0
41	l	7	Total 8	O 8	0	1
41	m	12	Total 12	O 12	0	0
41	o	95	Total 99	O 99	0	4
41	t	8	Total 11	O 11	0	3
41	u	50	Total 51	O 51	0	1
41	v	58	Total 61	O 61	0	3
41	x	6	Total 6	O 6	0	0
41	y	2	Total 2	O 2	0	0

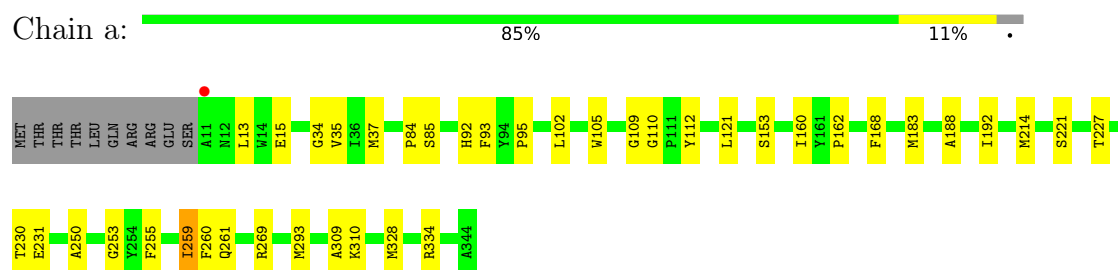
3 Residue-property plots

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

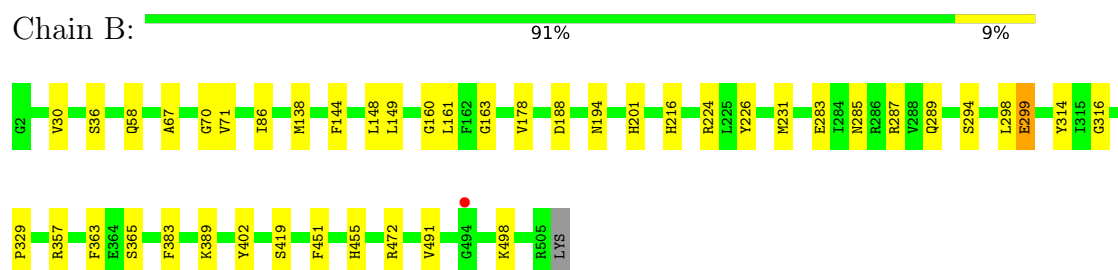
• Molecule 1: Photosystem II protein D1



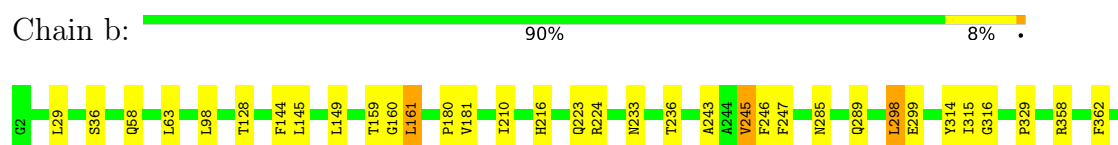
• Molecule 1: Photosystem II protein D1



• Molecule 2: Photosystem II CP47 reaction center protein



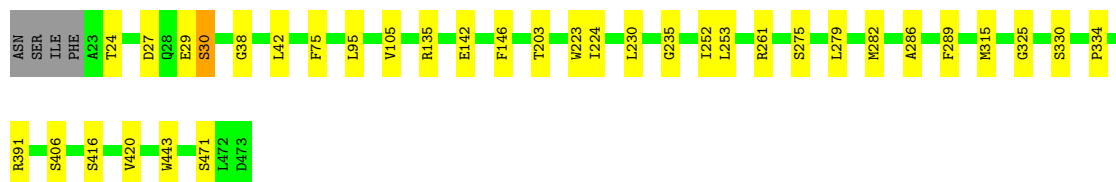
• Molecule 2: Photosystem II CP47 reaction center protein





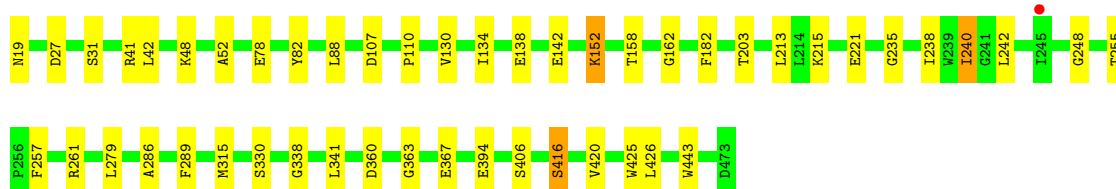
- Molecule 3: Photosystem II CP43 reaction center protein

Chain C: 91% 7% .



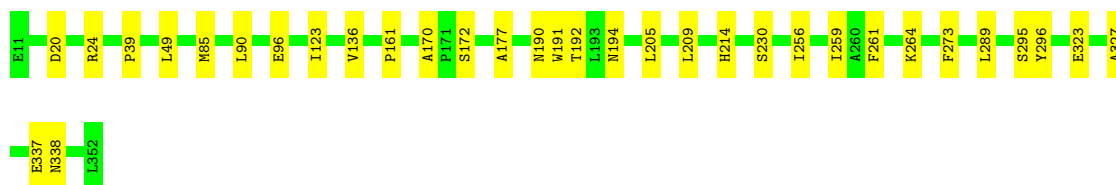
- Molecule 3: Photosystem II CP43 reaction center protein

Chain c: 89% 10% .



- Molecule 4: Photosystem II D2 protein

Chain D: 90% 10%



- Molecule 4: Photosystem II D2 protein

Chain d: 92% 8%

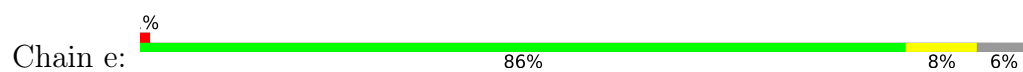


- Molecule 5: Cytochrome b559 subunit alpha

Chain E: 79% 18% .



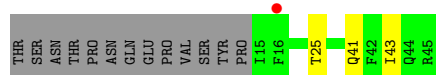
- Molecule 5: Cytochrome b559 subunit alpha



- Molecule 6: Cytochrome b559 subunit beta



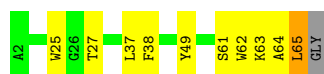
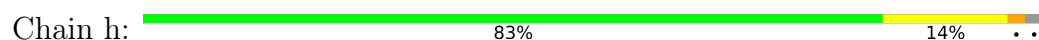
- Molecule 6: Cytochrome b559 subunit beta



- Molecule 7: Photosystem II reaction center protein H



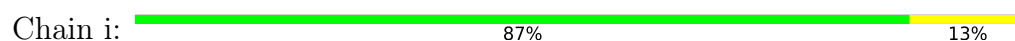
- Molecule 7: Photosystem II reaction center protein H



- Molecule 8: Photosystem II reaction center protein I

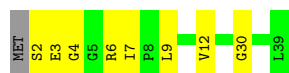


- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J

Chain J:  77% 21% .



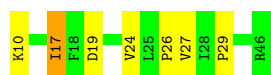
- Molecule 9: Photosystem II reaction center protein J

Chain j:  92% 8%



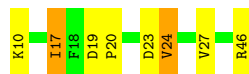
- Molecule 10: Photosystem II reaction center protein K

Chain K:  81% 16% .



- Molecule 10: Photosystem II reaction center protein K

Chain k:  78% 16% 5%



- Molecule 11: Photosystem II reaction center protein L

Chain L:  92% 5% .



- Molecule 11: Photosystem II reaction center protein L

Chain l:  81% 16% .



- Molecule 12: Photosystem II reaction center protein M

Chain M:  78% 8% 6% 8%



- Molecule 12: Photosystem II reaction center protein M

Chain m:  78% 14% 6%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:  84% 16%



- Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:  89% 10%



- Molecule 14: Photosystem II reaction center protein T

Chain T:  75% 16% 6%



- Molecule 14: Photosystem II reaction center protein T

Chain t:  3% 72% 22% 6%



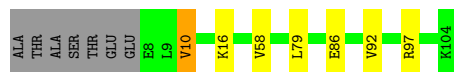
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:  85% 8% 8%

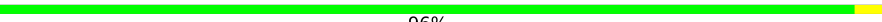


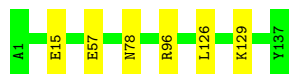
- Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:  87% 6% 7%



- Molecule 16: Cytochrome c-550

Chain V:  96% .



- Molecule 16: Cytochrome c-550

Chain v:  90% 10%



- Molecule 17: Photosystem II reaction center protein X

Chain X:  88% 8% 5%



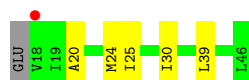
- Molecule 17: Photosystem II reaction center protein X

Chain x:  90% 5% 5%



- Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:  80% 17% 3%



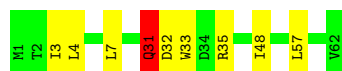
- Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:  60% 37% .



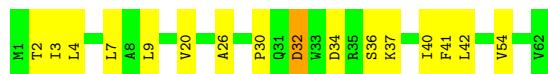
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  85% 13% .



- Molecule 19: Photosystem II reaction center protein Z

Chain z:  74% 24% .



- Molecule 20: Photosystem II protein Y

Chain R:  3% 71% 29%



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 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.30) 99.7 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.142 , 0.183 0.143 , 0.185	Depositor DCC
R_{free} test set	18693 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å ²)	50.8	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	62600	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 1.66% 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: CA, CLA, SQD, FE2, HTG, PHO, HEC, GOL, LMG, LMT, FME, PL9, OEX, HEM, LHG, BCT, MG, DGD, BCR, CL, UNL

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	0.26	0/4478	0.42	0/6098
1	a	0.24	0/4470	0.40	0/6087
2	B	0.37	0/4293	0.50	0/5851
2	b	0.33	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	0.33	0/3741	0.46	0/5095
4	d	0.30	0/3749	0.46	0/5106
5	E	0.35	0/681	0.53	0/928
5	e	0.31	0/690	0.49	0/939
6	F	0.32	0/284	0.45	0/387
6	f	0.29	0/269	0.43	0/365
7	H	0.33	0/519	0.50	0/708
7	h	0.30	0/530	0.49	0/722
8	I	0.31	0/311	0.44	0/419
8	i	0.35	0/311	0.51	0/419
9	J	0.34	0/278	0.41	0/376
9	j	0.28	0/283	0.42	0/383
10	K	0.32	0/303	0.48	0/416
10	k	0.32	0/303	0.46	0/416
11	L	0.38	0/318	0.47	0/433
11	l	0.38	0/318	0.45	0/433
12	M	0.40	0/261	0.51	0/357
12	m	0.36	0/279	0.48	0/380
13	O	0.35	0/1991	0.51	0/2698
13	o	0.34	0/1966	0.52	0/2665
14	T	0.36	0/310	0.43	0/419
14	t	0.33	0/301	0.43	0/406
15	U	0.37	0/811	0.54	0/1095
15	u	0.36	0/818	0.57	0/1105
16	V	0.35	0/1142	0.48	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	0.25	0/292	0.38	0/395
17	x	0.28	0/284	0.39	0/384
18	Y	0.25	0/216	0.43	0/289
18	y	0.25	0/216	0.41	0/289
19	Z	0.24	0/490	0.39	0/669
19	z	0.23	0/490	0.42	0/669
20	R	0.25	0/279	0.35	0/383
All	All	0.31	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	23	0
1	a	4330	0	4132	39	0
2	B	4146	0	3983	32	0
2	b	4134	0	3976	41	0
3	C	4260	0	4123	24	0
3	c	4308	0	4172	36	0
4	D	3620	0	3484	33	0
4	d	3628	0	3490	22	0
5	E	662	0	648	12	0
5	e	670	0	655	5	0
6	F	275	0	282	3	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	7	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	3	0
10	k	293	0	305	6	0
11	L	311	0	320	3	0
11	l	311	0	320	5	0
12	M	268	0	285	7	0
12	m	286	0	305	8	0
13	O	1958	0	1920	23	0
13	o	1933	0	1900	13	0
14	T	311	0	318	3	0
14	t	302	0	311	6	0
15	U	800	0	796	4	0
15	u	807	0	805	4	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	11	0
17	X	289	0	322	3	0
17	x	281	0	312	2	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	7	0
19	z	479	0	516	5	0
20	R	273	0	305	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	18	0
23	B	1040	0	1152	26	0
23	C	845	0	936	30	0
23	D	195	0	216	9	0
23	a	325	0	360	22	0
23	b	1040	0	1152	29	0
23	c	845	0	936	45	0
23	d	325	0	360	15	0
24	A	40	0	56	1	0
24	B	120	0	168	5	0
24	C	80	0	112	1	0
24	D	40	0	56	1	0
24	H	40	0	56	1	0
24	K	40	0	56	1	0
24	T	40	0	56	5	0
24	Y	40	0	56	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	1	0
24	b	120	0	168	8	0
24	c	80	0	112	3	0
24	d	40	0	56	2	0
24	h	40	0	56	5	0
24	k	40	0	56	1	0
24	t	40	0	56	7	0
24	y	40	0	56	1	0
25	A	162	0	234	3	0
25	X	43	0	53	1	0
25	a	162	0	233	10	0
25	b	54	0	78	2	0
25	f	43	0	53	1	0
25	l	54	0	78	2	0
26	A	6	0	8	0	0
26	B	12	0	16	2	0
26	C	12	0	16	0	0
26	D	12	0	16	7	0
26	O	12	0	16	3	0
26	V	12	0	16	0	0
26	a	18	0	24	5	0
26	b	12	0	16	2	0
26	c	18	0	24	0	0
26	d	6	0	8	0	0
26	l	12	0	16	2	0
26	o	12	0	16	0	0
26	v	12	0	16	3	0
27	A	20	0	0	0	0
27	a	20	0	0	0	0
28	A	110	0	160	21	0
28	D	110	0	160	2	0
28	a	110	0	160	8	0
28	d	110	0	160	0	0
29	A	28	0	0	0	0
29	B	73	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	K	68	0	0	0	0
29	X	18	0	0	0	0
29	a	30	0	0	1	0
29	b	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	c	64	0	0	0	0
29	d	71	0	0	0	0
29	j	10	0	0	0	0
29	l	10	0	0	0	0
29	m	10	0	0	0	0
30	A	8	0	0	0	0
30	d	8	0	0	0	0
31	A	128	0	148	2	0
31	D	128	0	148	3	0
31	a	256	0	296	4	0
32	A	70	0	91	2	0
32	B	95	0	127	3	0
32	F	35	0	46	0	0
32	M	35	0	45	2	0
32	T	35	0	46	0	0
32	a	35	0	46	1	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	2	0
32	t	26	0	34	3	0
33	A	98	0	148	2	0
33	D	196	0	296	11	0
33	E	84	0	114	6	0
33	L	98	0	148	1	0
33	a	84	0	114	8	0
33	b	98	0	148	0	0
33	d	294	0	444	22	0
34	B	51	0	72	2	0
34	C	153	0	216	3	0
34	D	51	0	72	0	0
34	Z	37	0	44	3	0
34	c	153	0	216	3	0
34	d	51	0	72	3	0
34	m	51	0	72	0	0
34	z	39	0	48	2	0
35	B	38	0	52	2	0
35	C	19	0	26	0	0
35	D	16	0	17	0	0
35	V	11	0	10	0	0
35	b	57	0	78	3	0
35	c	19	0	26	1	0
35	d	16	0	17	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	o	19	0	26	1	0
36	C	310	0	410	6	0
36	H	62	0	82	1	0
36	c	310	0	410	10	0
36	h	62	0	82	2	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
37	O	1	0	0	0	0
37	c	2	0	0	0	0
37	f	1	0	0	0	0
37	o	1	0	0	0	0
38	F	43	0	30	1	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	215	0	0	1	0
41	B	193	0	0	2	0
41	C	202	0	0	1	0
41	D	162	0	0	4	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	23	0	0	0	0
41	I	6	0	0	0	0
41	J	7	0	0	1	0
41	K	6	0	0	0	0
41	L	8	0	0	0	0
41	M	5	0	0	0	0
41	O	106	0	0	0	0
41	T	13	0	0	0	0
41	U	49	0	0	0	0
41	V	82	0	0	0	0
41	X	8	0	0	0	0
41	a	207	0	0	3	0
41	b	209	0	0	0	0
41	c	192	0	0	3	0
41	d	152	0	0	0	0
41	e	9	0	0	0	0
41	f	3	0	0	0	0
41	h	18	0	0	0	0
41	i	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	1	0	0	0	0
41	k	3	0	0	0	0
41	l	8	0	0	0	0
41	m	12	0	0	0	0
41	o	99	0	0	0	0
41	t	11	0	0	1	0
41	u	51	0	0	1	0
41	v	61	0	0	0	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	62600	0	61445	629	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 (629) 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)
23:B:604:CLA:H42	23:B:605:CLA:H2	1.44	0.95
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.53	0.91
26:D:402:GOL:H11	12:M:1:FME:HG2	1.57	0.86
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:HBB1	1.64	0.80
4:d:192[A]:THR:HG23	23:d:403[A]:CLA:HBC2	1.66	0.77
23:B:601:CLA:H12	23:B:601:CLA:H71	1.65	0.77
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.67	0.77
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.66	0.77
23:A:406[A]:CLA:H152	28:A:413[A]:PL9:H252	1.67	0.76
23:A:406[B]:CLA:H152	28:A:413[B]:PL9:H252	1.68	0.76
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.68	0.75
4:d:192[B]:THR:HG23	23:d:403[B]:CLA:HBC2	1.69	0.75
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.69	0.74
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.69	0.74
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.71	0.71
23:a:407:CLA:H192	23:c:506:CLA:H142	1.74	0.70
23:A:407:CLA:H193	23:C:507:CLA:H101	1.74	0.69
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.75	0.69
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.75	0.69
23:C:514:CLA:H202	34:C:521:LMG:H402	1.74	0.69
32:B:627:LMT:H52	35:o:301:HTG:H4'1	1.76	0.68
2:b:98:LEU:HB2	35:b:622:HTG:H7'1	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:TYR:HA	2:B:231:MET:HG3	1.74	0.68
23:c:512:CLA:H191	34:z:101:LMG:H241	1.75	0.68
33:D:408[A]:LHG:H382	33:D:408[A]:LHG:H112	1.76	0.68
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.77	0.66
23:a:407:CLA:H152	23:c:507:CLA:H142	1.76	0.66
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.78	0.66
23:c:503:CLA:H61	23:c:513:CLA:H42	1.77	0.66
32:B:629:LMT:H6E	32:t:101:LMT:H6D	1.76	0.65
19:z:32:ASP:O	19:z:36:SER:OG	2.12	0.65
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.78	0.65
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.79	0.65
23:d:402[A]:CLA:HHC	23:d:402[A]:CLA:HBB1	1.80	0.64
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.80	0.64
28:A:413[A]:PL9:H262	33:E:101[A]:LHG:H223	1.80	0.63
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.80	0.63
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.80	0.63
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.80	0.63
25:a:409[A]:SQD:H152	33:d:408[A]:LHG:H172	1.82	0.62
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.81	0.62
23:b:601:CLA:H72	23:b:601:CLA:H2	1.81	0.62
23:C:507:CLA:H142	36:C:517[B]:DGD:HAF2	1.80	0.62
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.82	0.62
23:b:610:CLA:HHC	23:b:610:CLA:HBB1	1.81	0.62
23:C:507:CLA:H142	36:C:517[A]:DGD:HAF2	1.81	0.62
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.30	0.61
16:v:134[B]:LYS:HE2	26:v:202[B]:GOL:H32	1.81	0.61
10:k:17:ILE:HD13	10:k:17:ILE:H	1.64	0.61
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.82	0.61
26:D:402:GOL:H31	12:M:1:FME:HE3	1.82	0.60
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.35	0.60
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.82	0.60
3:c:88:LEU:HD13	23:c:504:CLA:HED3	1.84	0.60
28:A:413[B]:PL9:H262	33:E:101[B]:LHG:H223	1.83	0.60
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.84	0.60
10:K:17:ILE:H	10:K:17:ILE:HD13	1.66	0.59
25:a:409[A]:SQD:H141	33:d:408[A]:LHG:H152	1.84	0.59
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.36	0.59
24:b:619:BCR:H331	24:b:619:BCR:HC8	1.84	0.59
36:c:519:DGD:HBH2	33:d:408[A]:LHG:H211	1.86	0.58
34:z:101:LMG:H302	34:z:101:LMG:H141	1.85	0.58
24:y:101:BCR:H321	24:y:101:BCR:HC8	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:408[B]:LHG:H112	33:D:408[B]:LHG:H382	1.86	0.58
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.33	0.57
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.39	0.57
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.05	0.57
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.85	0.57
12:M:32:GLN:HG2	32:m:103:LMT:H6'2	1.86	0.57
4:D:192[A]:THR:HG23	23:D:403[A]:CLA:HBC2	1.87	0.57
1:a:15:GLU:HB2	32:a:416:LMT:H6'2	1.86	0.57
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.87	0.57
26:a:417:GOL:H32	12:m:1:FME:HG3	1.85	0.57
23:b:606:CLA:H72	24:b:619:BCR:HC7	1.86	0.57
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.86	0.57
23:a:405[A]:CLA:H191	33:a:419[A]:LHG:H111	1.85	0.57
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.04	0.57
26:a:418:GOL:O2	41:a:501:HOH:O	2.10	0.57
31:A:416[B]:PHO:H3A	23:D:403[B]:CLA:H142	1.88	0.56
35:B:623:HTG:H61	1:a:102:LEU:HD12	1.87	0.56
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.86	0.56
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.35	0.56
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.40	0.56
36:c:517[A]:DGD:HG11	41:c:606[A]:HOH:O	2.06	0.56
26:a:418:GOL:O3	14:t:2:GLU:OE1	2.24	0.55
23:a:405[B]:CLA:H203	34:d:412:LMG:H412	1.88	0.55
3:c:82:TYR:OH	3:c:394[A]:GLU:OE2	2.24	0.55
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.19	0.55
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.87	0.55
23:c:514:CLA:HBB1	24:c:515:BCR:H24C	1.88	0.55
24:B:618:BCR:H363	24:t:102:BCR:H19C	1.88	0.55
26:a:418:GOL:H11	12:m:1:FME:HE3	1.88	0.55
13:o:92:SER:HB3	13:o:131:PRO:HA	1.88	0.55
17:X:31:ILE:HD11	25:X:101:SQD:H102	1.88	0.55
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.07	0.55
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.41	0.55
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.89	0.54
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.35	0.54
24:b:619:BCR:H331	24:b:619:BCR:C8	2.37	0.54
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.15	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.89	0.54
25:a:409[B]:SQD:H141	33:d:408[B]:LHG:H152	1.88	0.54
16:v:134[A]:LYS:HE2	26:v:202[A]:GOL:H32	1.88	0.54
2:b:285:ASN:O	2:b:289:GLN:HG2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:408[A]:LHG:H382	33:D:408[A]:LHG:H132	1.89	0.54
13:O:42:ARG:HH12	26:O:302:GOL:H12	1.71	0.54
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.89	0.54
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.90	0.54
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.88	0.54
3:C:252:ILE:HG22	3:C:253:LEU:HD23	1.90	0.54
23:a:405[A]:CLA:H203	34:d:412:LMG:H412	1.90	0.54
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.90	0.54
28:A:413[A]:PL9:H253	23:D:403[A]:CLA:H141	1.89	0.54
5:E:27:ILE:HD11	38:F:102:HEM:HBC2	1.89	0.54
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.20	0.53
1:a:214[B]:MET:HB3	28:a:413[B]:PL9:H103	1.90	0.53
33:d:407[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.91	0.53
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.90	0.53
23:A:404[B]:CLA:HBB1	23:D:403[B]:CLA:C4B	2.14	0.53
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.39	0.53
13:O:169:ASP:OD1	26:O:303:GOL:H12	2.09	0.53
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.91	0.53
4:D:205[B]:LEU:HD13	31:D:401[B]:PHO:HAB	1.89	0.53
23:B:606:CLA:H202	25:a:411:SQD:H302	1.91	0.53
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.90	0.53
23:c:511:CLA:HBB1	23:c:511:CLA:HMB1	1.91	0.52
26:D:402:GOL:O2	41:D:501:HOH:O	2.19	0.52
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.35	0.52
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.91	0.52
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.91	0.52
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.90	0.52
2:b:29:LEU:HD23	25:b:620:SQD:H201	1.90	0.52
24:C:515:BCR:H352	34:C:521:LMG:H352	1.91	0.52
28:A:413[A]:PL9:H472	4:D:39:PRO:HD3	1.92	0.52
28:A:413[B]:PL9:H472	4:D:39:PRO:HD3	1.92	0.52
28:A:413[B]:PL9:H253	23:D:403[B]:CLA:H141	1.90	0.52
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.92	0.52
3:C:325:GLY:O	15:U:51:LYS:NZ	2.38	0.52
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.10	0.52
23:a:404[B]:CLA:HBB1	23:d:403[B]:CLA:C4B	2.15	0.52
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.44	0.52
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.44	0.52
2:b:233:ASN:O	2:b:236:THR:HG22	2.10	0.52
25:l:101:SQD:H462	25:l:101:SQD:H1	1.91	0.52
5:E:77:GLU:O	5:E:81:GLU:HG2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:41:ARG:NH1	23:c:512:CLA:HMD1	2.24	0.51
18:y:20:ALA:O	18:y:24:MET:HG2	2.11	0.51
33:A:418[A]:LHG:H361	23:B:613:CLA:H51	1.92	0.51
2:B:357[A]:ARG:HH12	26:B:622:GOL:H32	1.75	0.51
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.45	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.51
29:a:414:UNL:O6	41:a:502:HOH:O	2.19	0.51
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.92	0.51
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	1.93	0.51
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.93	0.51
33:d:408[B]:LHG:H342	33:d:408[B]:LHG:H151	1.93	0.51
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.92	0.51
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.93	0.51
23:a:405[B]:CLA:H191	33:a:419[B]:LHG:H111	1.91	0.51
4:d:85:MET:CE	4:d:96:GLU:HG2	2.40	0.51
20:R:18:TRP:O	20:R:22:ASN:ND2	2.38	0.51
5:E:73:LYS:NZ	5:E:77:GLU:OE2	2.42	0.50
26:b:628:GOL:O3	26:b:628:GOL:O1	2.26	0.50
4:D:323[A]:GLU:O	26:D:413:GOL:O2	2.29	0.50
33:D:408[B]:LHG:H382	33:D:408[B]:LHG:H132	1.94	0.50
2:b:145:LEU:HD22	23:b:604:CLA:H162	1.93	0.50
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.45	0.50
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.41	0.50
36:c:519:DGD:HBH2	33:d:408[B]:LHG:H211	1.93	0.50
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.44	0.50
15:u:10[A]:VAL:HG12	41:u:243:HOH:O	2.11	0.50
32:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.92	0.50
1:A:183[B]:MET:HA	23:A:404[B]:CLA:HMD1	1.92	0.50
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.93	0.50
1:A:102:LEU:HD12	35:b:625:HTG:H61	1.94	0.50
33:a:419[B]:LHG:HC31	5:e:9:PRO:HA	1.92	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.47	0.50
9:J:2:SER:N	41:J:201:HOH:O	2.44	0.50
25:a:409[A]:SQD:H321	23:c:509:CLA:H102	1.93	0.50
2:B:357[A]:ARG:HH12	26:B:622:GOL:C3	2.25	0.49
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.93	0.49
31:a:415[A]:PHO:HBC3	4:d:279:LEU:HD22	1.93	0.49
18:y:31:ALA:O	18:y:35:ILE:HG13	2.11	0.49
23:A:406[B]:CLA:HHC	23:A:406[B]:CLA:HBB1	1.94	0.49
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.12	0.49
33:a:419[A]:LHG:HC31	5:e:9:PRO:HA	1.92	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192[B]:THR:HG23	23:D:403[B]:CLA:HBC2	1.93	0.49
1:a:334[B]:ARG:NH2	41:a:504[B]:HOH:O	2.44	0.49
23:a:404[A]:CLA:H201	33:d:407[A]:LHG:H161	1.95	0.49
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.95	0.49
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.42	0.49
31:a:415[B]:PHO:HHD	31:a:415[B]:PHO:HBC2	1.95	0.49
34:c:520:LMG:H181	10:k:27:VAL:HG11	1.95	0.49
33:d:407[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.95	0.49
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	1.95	0.49
31:a:406[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.94	0.49
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.13	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.12	0.49
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.95	0.49
23:C:503:CLA:HBD	23:C:503:CLA:HAA1	1.94	0.49
23:C:511:CLA:H112	23:C:511:CLA:H152	1.49	0.49
2:B:36[B]:SER:OG	24:B:618:BCR:H362	2.13	0.48
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.48
5:E:9:PRO:HA	33:E:101[B]:LHG:HC31	1.95	0.48
31:A:416[A]:PHO:H3A	23:D:403[A]:CLA:H142	1.94	0.48
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.43	0.48
33:d:408[A]:LHG:C38	33:d:408[A]:LHG:H122	2.44	0.48
23:b:604:CLA:H42	23:b:605:CLA:H2	1.96	0.48
3:c:363:GLY:O	3:c:367:GLU:HG2	2.14	0.48
7:h:38:PHE:HB2	24:h:101:BCR:C10	2.43	0.48
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.47	0.48
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.11	0.48
24:h:101:BCR:H331	24:h:101:BCR:C8	2.44	0.48
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.72	0.48
26:l:103[A]:GOL:H32	14:t:25:GLU:HB2	1.95	0.48
4:D:123:ILE:HD11	36:H:102:DGD:HAH2	1.95	0.48
23:A:405[B]:CLA:HHC	23:A:405[B]:CLA:HBB1	1.96	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.14	0.48
3:c:31:SER:CB	3:c:41:ARG:HG2	2.44	0.48
36:c:518[B]:DGD:HAF1	36:c:518[B]:DGD:HA81	1.95	0.48
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.79	0.48
3:C:275:SER:HB3	23:C:510:CLA:HED3	1.95	0.48
33:D:407[A]:LHG:HC62	11:L:15[A]:THR:HG23	1.96	0.48
23:a:404[B]:CLA:H152	31:a:406[B]:PHO:H52	1.96	0.48
28:a:413[B]:PL9:H171	28:a:413[B]:PL9:H151	1.52	0.48
23:c:509:CLA:H18	36:c:518[A]:DGD:HAT2	1.95	0.48
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:607:CLA:H91	23:b:607:CLA:H112	1.60	0.47
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.96	0.47
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.45	0.47
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.96	0.47
24:T:102:BCR:H321	24:T:102:BCR:HC8	1.97	0.47
28:A:413[B]:PL9:H322	28:A:413[B]:PL9:H301	1.72	0.47
28:a:413[B]:PL9:H351	6:f:25:THR:OG1	2.15	0.47
24:b:617:BCR:H24C	24:b:617:BCR:H371	1.69	0.47
36:c:517[B]:DGD:HG11	41:c:606[B]:HOH:O	2.13	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
33:d:408[A]:LHG:H342	33:d:408[A]:LHG:H151	1.97	0.47
36:h:102:DGD:HB62	36:h:102:DGD:HB32	1.71	0.47
23:a:404[B]:CLA:HMC3	4:d:182:LEU:HD13	1.96	0.47
33:d:408[A]:LHG:H302	33:d:408[A]:LHG:H332	1.67	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.96	0.47
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	1.97	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.47
23:B:610:CLA:H122	23:B:615:CLA:HAA1	1.96	0.47
8:I:35:LYS:O	8:I:37:LEU:N	2.48	0.47
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.15	0.47
28:a:413[A]:PL9:H171	28:a:413[A]:PL9:H151	1.58	0.47
24:t:102:BCR:HC7	24:t:102:BCR:H331	1.45	0.47
25:a:409[B]:SQD:H152	33:d:408[B]:LHG:H172	1.97	0.46
24:t:102:BCR:H382	24:t:102:BCR:H23C	1.97	0.46
24:t:102:BCR:HC8	24:t:102:BCR:H321	1.97	0.46
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	1.97	0.46
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	1.98	0.46
1:A:192[A]:ILE:HG13	1:A:293[A]:MET:HE1	1.97	0.46
1:A:231:GLU:HB3	41:B:877:HOH:O	2.16	0.46
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.80	0.46
5:E:9:PRO:HA	33:E:101[A]:LHG:HC31	1.97	0.46
13:O:25:THR:O	13:O:27:ARG:N	2.47	0.46
25:a:409[B]:SQD:H321	23:c:509:CLA:H102	1.97	0.46
23:b:614:CLA:H112	23:b:614:CLA:H72	1.60	0.46
10:k:24:VAL:HG21	18:y:25:ILE:HB	1.97	0.46
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.97	0.46
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.97	0.46
1:a:309:ALA:HB3	16:v:1:ALA:O	2.16	0.46
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.80	0.46
1:A:28:LEU:HD12	25:A:411:SQD:H121	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ASN:O	2:B:289:GLN:HG2	2.14	0.46
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.46
23:d:402[A]:CLA:HBA1	23:d:402[A]:CLA:C4A	2.45	0.46
25:a:409[A]:SQD:H271	33:d:408[A]:LHG:H141	1.97	0.46
28:a:413[A]:PL9:H351	6:f:25:THR:OG1	2.15	0.46
25:b:620:SQD:H341	25:b:620:SQD:H311	1.58	0.46
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.16	0.46
33:d:408[B]:LHG:H331	33:d:408[B]:LHG:H361	1.60	0.46
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.16	0.46
25:A:409[B]:SQD:H152	25:A:409[B]:SQD:H122	1.71	0.46
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.98	0.46
33:d:408[A]:LHG:H331	33:d:408[A]:LHG:H361	1.46	0.46
5:E:14:ILE:HD12	9:J:12:VAL:HG11	1.98	0.46
3:c:48:LYS:HG3	3:c:138:GLU:HG3	1.98	0.46
24:T:102:BCR:HC7	24:T:102:BCR:H331	1.64	0.46
23:b:616:CLA:H13	23:b:616:CLA:H102	1.77	0.46
28:A:413[B]:PL9:H471	28:A:413[B]:PL9:H43	1.59	0.45
33:A:418[A]:LHG:H171	23:B:613:CLA:H141	1.98	0.45
4:D:264[A]:LYS:NZ	41:D:504[A]:HOH:O	2.49	0.45
23:A:404[B]:CLA:H143	31:D:401[B]:PHO:H61	1.99	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.98	0.45
33:d:408[B]:LHG:H122	33:d:408[B]:LHG:C38	2.46	0.45
7:h:49:TYR:CG	36:h:102:DGD:HB22	2.52	0.45
24:t:102:BCR:H11C	24:t:102:BCR:H341	1.85	0.45
34:B:620:LMG:HC71	34:B:620:LMG:O9	2.16	0.45
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	1.98	0.45
4:D:261[B]:PHE:CZ	33:D:407[B]:LHG:HC81	2.51	0.45
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.16	0.45
8:I:36:ASP:OD1	8:I:36:ASP:N	2.50	0.45
12:m:5[B]:GLN:H	12:m:5[B]:GLN:CD	2.23	0.45
24:B:619:BCR:H371	24:B:619:BCR:H24C	1.72	0.45
2:b:159:THR:HA	2:b:181:VAL:O	2.17	0.45
23:b:612:CLA:HBB1	23:b:612:CLA:HMB1	1.98	0.45
3:c:443[A]:TRP:CE2	23:c:509:CLA:HMD2	2.52	0.45
23:B:612:CLA:H61	23:B:612:CLA:H102	1.85	0.45
23:C:507:CLA:H18	23:C:507:CLA:H152	1.52	0.45
4:D:261[A]:PHE:CZ	33:D:407[A]:LHG:HC81	2.52	0.45
2:b:36:SER:OG	24:b:618:BCR:H362	2.16	0.45
3:C:146:PHE:HZ	23:C:513:CLA:HBB2	1.81	0.45
4:D:85:MET:CE	4:D:96:GLU:HG2	2.42	0.45
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.98	0.45

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	1.99	0.45
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	1.98	0.45
3:c:182:PHE:HA	35:c:522:HTG:H61	1.98	0.45
33:d:408[A]:LHG:H142	33:d:408[A]:LHG:H372	1.97	0.45
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.41	0.45
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.83	0.45
23:A:407:CLA:H61	23:A:407:CLA:H41	1.55	0.45
28:A:413[B]:PL9:HC8	28:A:413[B]:PL9:H121	1.66	0.45
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	1.98	0.45
36:C:518[B]:DGD:HAT1	36:C:519:DGD:HBE1	1.99	0.45
4:D:273[B]:PHE:CE2	33:L:101[B]:LHG:H121	2.52	0.45
1:a:153[B]:SER:CB	23:a:404[B]:CLA:H43	2.47	0.45
23:c:506:CLA:H112	23:c:506:CLA:H72	1.70	0.45
13:o:58:ASN:C	13:o:60:ARG:H	2.25	0.45
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.52	0.45
33:E:101[A]:LHG:H241	33:E:101[A]:LHG:HC61	1.83	0.45
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.99	0.45
3:c:215:LYS:HD3	3:c:221:GLU:O	2.16	0.45
16:v:41:HIS:HA	16:v:45[A]:ILE:O	2.17	0.45
19:Z:31:GLN:CD	19:Z:31:GLN:H	2.25	0.45
23:B:613:CLA:H121	23:B:613:CLA:H162	1.78	0.44
3:C:443[B]:TRP:CE2	23:C:509:CLA:HMD2	2.53	0.44
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	1.99	0.44
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.51	0.44
23:c:510:CLA:H43	23:c:510:CLA:H12	1.86	0.44
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.99	0.44
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.81	0.44
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.85	0.44
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.44
4:d:126:MET:HE3	4:d:143[B]:ALA:O	2.17	0.44
28:A:413[A]:PL9:H151	28:A:413[A]:PL9:H171	1.55	0.44
28:A:413[A]:PL9:H322	28:A:413[A]:PL9:H301	1.76	0.44
28:A:413[B]:PL9:HC8	28:A:413[B]:PL9:HC2	1.84	0.44
4:D:230[A]:SER:HB2	41:D:566:HOH:O	2.16	0.44
13:O:137:THR:C	13:O:139:SER:H	2.25	0.44
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.98	0.44
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.98	0.44
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.98	0.44
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.00	0.44
23:B:610:CLA:H162	23:B:612:CLA:O1A	2.18	0.44
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.18	0.44
34:c:501:LMG:H201	34:c:501:LMG:H172	1.80	0.44
23:c:510:CLA:H91	23:c:510:CLA:H111	1.80	0.44
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.32	0.44
1:A:131:TRP:CD2	1:A:131:TRP:C	2.94	0.44
6:F:21:VAL:O	6:F:25:THR:HG23	2.17	0.44
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.44
1:a:214[A]:MET:HB3	28:a:413[A]:PL9:H103	1.98	0.44
2:b:497:GLN:HB2	2:b:504:THR:HB	1.99	0.44
23:b:609:CLA:NC	24:h:101:BCR:H332	2.33	0.44
24:c:515:BCR:H15C	24:c:515:BCR:H351	1.83	0.44
24:d:405:BCR:C8	24:d:405:BCR:H331	2.48	0.44
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.42	0.44
23:b:615:CLA:H92	23:b:615:CLA:H61	1.64	0.44
1:A:179[B]:THR:O	1:A:183[B]:MET:HG3	2.18	0.44
7:h:62:TRP:O	7:h:65:LEU:HB2	2.17	0.44
14:t:2:GLU:HG2	14:t:3:THR:N	2.33	0.44
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.48	0.44
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.17	0.44
4:D:327:ALA:HB2	26:D:413:GOL:H2	2.00	0.44
24:T:102:BCR:H11C	24:T:102:BCR:H341	1.85	0.44
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	1.99	0.44
23:d:404:CLA:H162	7:h:37:LEU:HD21	1.99	0.44
23:A:404[B]:CLA:HBD	23:A:405[B]:CLA:HAC2	2.00	0.43
28:A:413[B]:PL9:H171	28:A:413[B]:PL9:H151	1.52	0.43
3:C:279:LEU:HD12	3:C:282:MET:HE3	1.99	0.43
23:C:509:CLA:HBC2	33:D:408[B]:LHG:H351	2.00	0.43
23:D:404:CLA:H3A	23:D:404:CLA:HBA1	1.84	0.43
32:M:101:LMT:H6D	11:l:9:PRO:HA	2.00	0.43
13:O:27:ARG:NH1	13:O:203:LYS:HG2	2.33	0.43
25:a:409[B]:SQD:H302	23:c:509:CLA:H71	2.00	0.43
28:a:413[A]:PL9:H28	33:a:419[A]:LHG:H222	1.99	0.43
2:b:247:PHE:HB2	23:b:608:CLA:HBC1	1.99	0.43
23:b:604:CLA:HBB1	23:b:607:CLA:HAB	2.00	0.43
3:c:443[B]:TRP:CE2	23:c:509:CLA:HMD2	2.53	0.43
34:d:412:LMG:H221	34:d:412:LMG:H191	1.68	0.43
7:h:62:TRP:C	7:h:64:ALA:H	2.26	0.43
24:t:102:BCR:HC8	24:t:102:BCR:H311	2.00	0.43
2:B:363:PHE:HB3	2:B:365:SER:O	2.17	0.43
23:B:614:CLA:H92	23:B:614:CLA:H61	1.75	0.43
23:C:505:CLA:H41	23:C:505:CLA:H62	1.72	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:54:GLU:HG2	13:O:64:GLU:O	2.18	0.43
1:a:259[A]:ILE:HG22	1:a:260[A]:PHE:CD1	2.53	0.43
10:k:19:ASP:HB3	10:k:20:PRO:HD3	2.00	0.43
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.00	0.43
13:O:93:LEU:O	13:O:128:SER:HA	2.18	0.43
23:a:405[B]:CLA:HMB2	23:d:403[B]:CLA:H122	2.00	0.43
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.53	0.43
3:c:152:LYS:HD2	41:c:746:HOH:O	2.18	0.43
14:t:20:ALA:O	14:t:24[B]:ARG:HB3	2.19	0.43
32:A:419:LMT:H6'2	32:A:419:LMT:O3'	2.18	0.43
4:D:230[B]:SER:HB2	41:D:566:HOH:O	2.19	0.43
1:a:269[B]:ARG:NE	4:d:222[B]:LEU:HD22	2.33	0.43
23:a:404[B]:CLA:H203	23:a:404[B]:CLA:H162	1.85	0.43
2:b:224:ARG:HH21	32:b:621:LMT:H1'	1.83	0.43
28:A:413[A]:PL9:H221	28:A:413[A]:PL9:H201	1.88	0.43
28:A:413[A]:PL9:HC2	28:A:413[A]:PL9:HC8	1.71	0.43
2:B:160:GLY:HA2	2:B:163:GLY:O	2.17	0.43
2:B:357[A]:ARG:HD2	41:B:779:HOH:O	2.18	0.43
28:D:406[A]:PL9:H401	28:D:406[A]:PL9:H422	1.75	0.43
5:E:18:ARG:H	9:J:2:SER:N	2.16	0.43
1:a:34:GLY:HA2	1:a:37:MET:HB3	1.99	0.43
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.54	0.43
23:b:613:CLA:H172	24:b:618:BCR:H312	2.00	0.43
34:c:521:LMG:H232	34:c:521:LMG:H391	2.00	0.43
18:y:22:LEU:HA	18:y:25:ILE:HG22	1.99	0.43
19:Z:33:TRP:HZ2	34:Z:101:LMG:HC61	1.84	0.43
2:B:283:GLU:O	2:B:287:ARG:HG3	2.18	0.43
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.84	0.43
1:a:121:LEU:HD11	23:c:506:CLA:H172	2.01	0.43
1:a:160[B]:ILE:HD11	36:c:517[B]:DGD:HBT1	2.01	0.43
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.54	0.43
23:c:505:CLA:ND	36:c:518[A]:DGD:HB32	2.34	0.43
36:C:518[B]:DGD:HAE2	36:C:518[B]:DGD:HA81	1.91	0.43
23:a:404[B]:CLA:H193	33:d:407[B]:LHG:H321	2.00	0.43
26:a:417:GOL:H12	41:t:201:HOH:O	2.18	0.43
25:A:409[A]:SQD:H122	25:A:409[A]:SQD:H152	1.52	0.43
2:b:422:ARG:NH2	13:o:169:ASP:OD2	2.48	0.43
24:B:619:BCR:H331	24:B:619:BCR:C8	2.48	0.43
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.01	0.43
32:M:101:LMT:H6'2	12:m:32:GLN:HG2	2.01	0.43
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:385:ARG:HG2	13:o:165:ALA:O	2.19	0.43
23:c:513:CLA:H3A	23:c:513:CLA:HBA2	1.74	0.43
23:c:513:CLA:H121	23:c:514:CLA:H142	2.01	0.43
4:d:55:VAL:O	4:d:66:SER:HB3	2.19	0.43
33:d:408[B]:LHG:H372	33:d:408[B]:LHG:H142	2.00	0.43
13:o:120:PHE:CD1	13:o:235:ILE:HD13	2.54	0.43
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	2.00	0.42
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.92	0.42
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.44	0.42
23:D:403[B]:CLA:HAA2	23:D:403[B]:CLA:HBD	2.01	0.42
14:T:20:ALA:O	14:T:24[B]:ARG:HB3	2.19	0.42
1:a:85[B]:SER:HA	1:a:109[B]:GLY:HA3	2.01	0.42
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.54	0.42
24:a:408:BCR:H371	24:a:408:BCR:H24C	1.79	0.42
23:b:605:CLA:H41	23:b:605:CLA:H62	1.54	0.42
23:c:509:CLA:H18	36:c:518[B]:DGD:HAT2	2.00	0.42
23:C:504:CLA:H62	23:C:504:CLA:H101	1.68	0.42
4:D:205[A]:LEU:HD13	31:D:401[A]:PHO:HAB	2.00	0.42
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.01	0.42
24:Y:101:BCR:HC7	24:Y:101:BCR:H331	1.82	0.42
23:d:403[B]:CLA:HAA2	23:d:403[B]:CLA:HBD	2.01	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.42
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.55	0.42
23:d:402[B]:CLA:HBB1	23:d:402[B]:CLA:CHC	2.42	0.42
20:R:8:VAL:O	20:R:11:PRO:HD2	2.20	0.42
23:A:404[B]:CLA:HBD	23:A:404[B]:CLA:HAA2	2.01	0.42
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.76	0.42
3:C:330:SER:HB3	13:O:100:GLY:O	2.18	0.42
16:V:57:GLU:CD	16:V:57:GLU:H	2.27	0.42
23:c:509:CLA:HBC3	23:c:511:CLA:H71	2.01	0.42
23:c:513:CLA:H142	23:c:513:CLA:H111	1.91	0.42
26:l:103[B]:GOL:H32	14:t:25:GLU:HB2	2.00	0.42
15:u:92:VAL:HG12	15:u:97:ARG:HD2	2.02	0.42
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.91	0.42
19:Z:7:LEU:HD23	19:Z:7:LEU:HA	1.87	0.42
4:D:49:LEU:HD13	24:D:405:BCR:C15	2.48	0.42
25:a:409[A]:SQD:H302	23:c:509:CLA:H71	2.00	0.42
2:b:160:GLY:HA3	2:b:180:PRO:HB3	2.00	0.42
19:Z:48:ILE:HD11	34:Z:101:LMG:H202	2.02	0.42
1:A:82[A]:VAL:HB	1:A:174[A]:LEU:HB2	2.01	0.42
28:A:413[B]:PL9:H221	28:A:413[B]:PL9:H201	1.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:509:CLA:HBC2	33:D:408[A]:LHG:H351	2.01	0.42
1:a:153[B]:SER:HB3	23:a:404[B]:CLA:H43	2.01	0.42
4:d:14:TRP:CD1	35:d:411:HTG:H61	2.54	0.42
17:x:23:LEU:HD23	17:x:23:LEU:HA	1.86	0.42
32:A:417:LMT:H6'1	41:A:504:HOH:O	2.18	0.42
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.01	0.42
23:b:613:CLA:H111	23:b:613:CLA:H72	1.84	0.42
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	2.02	0.42
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.02	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.89	0.42
23:B:602:CLA:H203	23:B:602:CLA:H162	1.75	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.42
13:O:169:ASP:H	26:O:303:GOL:H12	1.84	0.42
24:T:102:BCR:H24C	24:T:102:BCR:H371	1.84	0.42
23:c:506:CLA:H192	23:c:506:CLA:H162	1.92	0.42
23:d:402[B]:CLA:HBA1	23:d:402[B]:CLA:C4A	2.49	0.42
15:u:16:LYS:NZ	15:u:86:GLU:O	2.46	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.49	0.42
26:D:402:GOL:H11	12:M:1:FME:CG	2.40	0.42
33:D:408[A]:LHG:H302	33:D:408[A]:LHG:H332	1.81	0.42
16:v:134[B]:LYS:HB3	26:v:202[B]:GOL:H32	2.02	0.42
35:B:621:HTG:H4'2	35:B:621:HTG:H7'3	1.83	0.42
23:C:506:CLA:H111	23:C:506:CLA:H93	1.68	0.42
4:D:214[B]:HIS:HA	28:D:406[B]:PL9:O2	2.20	0.42
12:M:20:VAL:CG2	12:m:20:VAL:HG11	2.50	0.42
24:T:102:BCR:H19C	24:b:618:BCR:H363	2.02	0.42
14:t:8:PHE:CD2	32:t:101:LMT:H121	2.55	0.42
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.45	0.41
3:C:391[A]:ARG:NH1	41:C:609:HOH:O	2.53	0.41
1:a:92[B]:HIS:HE2	3:c:360[B]:ASP:CG	2.27	0.41
23:b:605:CLA:HBB1	23:b:605:CLA:CHC	2.46	0.41
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.02	0.41
24:k:101:BCR:H371	24:k:101:BCR:H24C	1.65	0.41
20:R:2:ASP:HB3	20:R:5:VAL:HG23	2.02	0.41
2:B:201:HIS:CE1	23:B:603:CLA:HMB2	2.54	0.41
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.88	0.41
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.86	0.41
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.54	0.41
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:513:CLA:HMB2	23:c:513:CLA:H192	2.02	0.41
24:K:102:BCR:H24C	24:K:102:BCR:H371	1.63	0.41
33:a:419[A]:LHG:H241	33:a:419[A]:LHG:HC61	1.90	0.41
2:b:299:GLU:HG2	2:b:402:TYR:HD2	1.86	0.41
23:b:613:CLA:H203	23:b:613:CLA:H161	1.88	0.41
32:t:101:LMT:H112	32:t:101:LMT:H81	1.61	0.41
34:C:521:LMG:H331	34:C:521:LMG:H362	1.84	0.41
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.50	0.41
24:b:619:BCR:H11C	24:b:619:BCR:H341	1.91	0.41
3:c:425[A]:TRP:CD1	23:c:505:CLA:HMA3	2.54	0.41
24:c:516:BCR:H24C	24:c:516:BCR:H371	1.89	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.02	0.41
24:A:408:BCR:H24C	24:A:408:BCR:H371	1.71	0.41
2:B:30:VAL:HG12	23:B:605:CLA:HHD	2.03	0.41
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.51	0.41
23:B:614:CLA:H71	23:B:614:CLA:H112	1.52	0.41
1:a:310:LYS:HD2	16:v:1:ALA:HB1	2.02	0.41
23:a:404[B]:CLA:H122	23:a:404[B]:CLA:H161	1.88	0.41
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.84	0.41
3:c:107:ASP:O	3:c:110:PRO:HD2	2.20	0.41
23:d:402[A]:CLA:HHC	23:d:402[A]:CLA:CBB	2.48	0.41
24:h:101:BCR:H11C	24:h:101:BCR:H341	1.97	0.41
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.93	0.41
28:A:413[A]:PL9:H43	28:A:413[A]:PL9:H471	1.69	0.41
23:a:407:CLA:H61	23:a:407:CLA:H41	1.80	0.41
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.02	0.41
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.20	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.86	0.41
33:d:408[A]:LHG:H131	33:d:408[A]:LHG:H102	1.91	0.41
24:h:101:BCR:H24C	24:h:101:BCR:H371	1.71	0.41
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.41
33:E:101[A]:LHG:O2	6:F:19:ARG:NH1	2.54	0.41
8:I:2:GLU:O	8:I:6:ILE:HG12	2.20	0.41
3:c:238:ILE:O	3:c:242:LEU:HG	2.20	0.41
4:d:12:ARG:NE	4:d:12:ARG:HA	2.36	0.41
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.85	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.72	0.41
2:B:216:HIS:CE1	23:B:609:CLA:C1A	3.03	0.41
24:B:617:BCR:H15C	24:B:617:BCR:H351	1.90	0.41
32:B:626:LMT:H41	32:B:626:LMT:H71	1.95	0.41
3:C:279:LEU:HD22	23:C:510:CLA:HED2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:419[B]:LHG:H241	33:a:419[B]:LHG:HC61	1.90	0.41
2:b:245:VAL:HG22	23:b:612:CLA:H202	2.03	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.83	0.41
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.21	0.41
20:R:24:LEU:N	20:R:25:PRO:HD2	2.35	0.41
19:z:26:ALA:HB3	19:z:40:ILE:HD11	2.03	0.41
28:A:413[A]:PL9:H451	17:X:28:LEU:HD11	2.02	0.41
2:B:451:PHE:CE2	2:B:455:HIS:CE1	3.09	0.41
2:B:491[A]:VAL:HG12	4:D:136[A]:VAL:HG13	2.03	0.41
3:C:27:ASP:OD1	3:C:30:SER:OG	2.38	0.41
36:C:518[A]:DGD:HAE2	36:C:518[A]:DGD:HA81	1.91	0.41
36:C:519:DGD:HB81	36:C:519:DGD:HBE2	1.79	0.41
33:D:407[B]:LHG:HC62	11:L:15[B]:THR:HG23	2.03	0.41
24:H:101:BCR:H331	24:H:101:BCR:C8	2.51	0.41
13:O:24:ASP:HA	13:O:203:LYS:HE2	2.03	0.41
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.56	0.41
13:O:130:GLN:H	13:O:130:GLN:CD	2.27	0.41
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.20	0.41
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.56	0.41
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.03	0.41
28:a:413[B]:PL9:H503	17:x:24:THR:OG1	2.21	0.41
3:c:257:PHE:O	3:c:261:ARG:HG3	2.21	0.41
3:c:426:LEU:HD23	3:c:426:LEU:HA	1.95	0.41
23:d:404:CLA:H61	23:d:404:CLA:H41	1.69	0.41
34:Z:101:LMG:H141	34:Z:101:LMG:H111	1.84	0.41
28:A:413[A]:PL9:HC8	28:A:413[A]:PL9:H121	1.79	0.41
9:J:2:SER:HB2	9:J:3:GLU:H	1.74	0.41
13:O:147:ASN:OD1	13:O:194:LYS:HE3	2.21	0.41
1:a:230:THR:HG21	11:l:8:GLN:NE2	2.36	0.41
23:a:405[B]:CLA:C4A	23:a:405[B]:CLA:HBA1	2.51	0.41
23:a:407:CLA:H203	23:c:507:CLA:H101	2.03	0.41
2:b:98:LEU:HB2	35:b:622:HTG:C7'	2.46	0.41
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.87	0.41
23:b:606:CLA:H151	23:b:616:CLA:H112	2.02	0.41
23:c:513:CLA:HBB1	23:c:513:CLA:HHC	2.03	0.41
4:d:186[B]:GLN:HB2	23:d:403[B]:CLA:HBC1	2.03	0.41
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.02	0.41
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.93	0.40
23:a:404[B]:CLA:CBD	23:d:402[B]:CLA:HAC2	2.51	0.40
33:a:419[A]:LHG:H142	33:a:419[A]:LHG:H172	1.83	0.40
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:330:SER:HB3	13:o:100:GLY:O	2.21	0.40
5:e:68:ASP:O	5:e:72:ALA:HB2	2.21	0.40
25:f:102:SQD:H462	25:f:102:SQD:O7	2.21	0.40
8:i:2:GLU:O	8:i:6:ILE:HG12	2.22	0.40
2:B:67:ALA:HA	2:B:71:VAL:O	2.21	0.40
23:C:507:CLA:HBA1	23:C:507:CLA:H3A	1.72	0.40
4:D:323[B]:GLU:O	26:D:413:GOL:O2	2.39	0.40
18:Y:39:LEU:HD23	18:Y:39:LEU:HA	1.90	0.40
2:b:358:ARG:HB2	26:b:628:GOL:H31	2.02	0.40
33:d:408[A]:LHG:H242	33:d:408[A]:LHG:H272	1.92	0.40
34:B:620:LMG:H112	34:B:620:LMG:H141	1.84	0.40
5:E:68:ASP:O	5:E:72:ALA:HB2	2.22	0.40
2:b:58:GLN:C	2:b:329:PRO:HB3	2.46	0.40
2:b:149[B]:LEU:HD21	23:b:604:CLA:H171	2.03	0.40
23:c:507:CLA:HBA1	23:c:507:CLA:H3A	1.84	0.40
11:l:20:GLY:O	11:l:24:ILE:HG12	2.21	0.40
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CZ3	2.55	0.40
36:c:518[A]:DGD:HBF2	36:c:518[A]:DGD:HBE1	1.91	0.40
25:l:101:SQD:H381	32:m:103:LMT:H121	2.03	0.40
19:Z:57:LEU:HA	19:Z:57:LEU:HD23	1.87	0.40
23:A:407:CLA:H171	23:C:507:CLA:H121	2.01	0.40
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.21	0.40
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.04	0.40
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.57	0.40
23:b:612:CLA:H122	23:b:612:CLA:H162	1.91	0.40
23:c:506:CLA:HBD	23:c:506:CLA:HAA1	2.03	0.40
23:c:506:CLA:HMD3	23:c:508:CLA:HAB	2.04	0.40
4:d:126:MET:HE3	4:d:143[A]:ALA:O	2.21	0.40
24:d:405:BCR:H351	24:d:405:BCR:H15C	1.74	0.40
24:t:102:BCR:H24C	24:t:102:BCR:H371	1.89	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%)	542 (98%)	9 (2%)	2 (0%)	30	38
1	a	552/344 (160%)	541 (98%)	9 (2%)	2 (0%)	30	38
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	546/455 (120%)	536 (98%)	9 (2%)	1 (0%)	43	55
3	c	553/455 (122%)	539 (98%)	13 (2%)	1 (0%)	43	55
4	D	453/342 (132%)	435 (96%)	18 (4%)	0	100	100
4	d	454/342 (133%)	439 (97%)	15 (3%)	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	7
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	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%)	7 (3%)	2 (1%)	16	20
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%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	93 (95%)	5 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36 (97%)	1 (3%)	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	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	7
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6019 (98%)	140 (2%)	12 (0%)	43	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
13	O	138	THR
7	h	63	LYS
1	a	259[A]	ILE
1	a	259[B]	ILE
1	A	259[A]	ILE
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	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	443/279 (159%)	441 (100%)	2 (0%)	81	90
2	B	421/403 (104%)	415 (99%)	6 (1%)	59	76
2	b	420/403 (104%)	408 (97%)	12 (3%)	37	55
3	C	430/356 (121%)	422 (98%)	8 (2%)	50	69
3	c	436/356 (122%)	426 (98%)	10 (2%)	44	63
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	86
4	d	369/277 (133%)	362 (98%)	7 (2%)	50	69
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	76
5	e	72/73 (99%)	71 (99%)	1 (1%)	59	76
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	45
7	h	55/54 (102%)	53 (96%)	2 (4%)	31	47
8	I	34/34 (100%)	32 (94%)	2 (6%)	18	26
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	55
9	J	26/27 (96%)	24 (92%)	2 (8%)	12	16
9	j	26/27 (96%)	25 (96%)	1 (4%)	29	44
10	K	30/30 (100%)	26 (87%)	4 (13%)	4	4
10	k	30/30 (100%)	27 (90%)	3 (10%)	7	9
11	L	36/35 (103%)	36 (100%)	0	100	100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38	56
12	M	30/32 (94%)	27 (90%)	3 (10%)	7	9
12	m	32/32 (100%)	30 (94%)	2 (6%)	16	23
13	O	216/207 (104%)	211 (98%)	5 (2%)	44	63
13	o	213/207 (103%)	206 (97%)	7 (3%)	33	50
14	T	32/28 (114%)	28 (88%)	4 (12%)	4	5
14	t	31/28 (111%)	31 (100%)	0	100	100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44	63
15	u	87/89 (98%)	85 (98%)	2 (2%)	44	63
16	V	123/117 (105%)	122 (99%)	1 (1%)	73	86
16	v	123/117 (105%)	119 (97%)	4 (3%)	33	50

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	21 (96%)	1 (4%)	24	37
18	y	22/23 (96%)	19 (86%)	3 (14%)	3	4
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	44
19	z	52/52 (100%)	44 (85%)	8 (15%)	2	3
20	R	29/29 (100%)	27 (93%)	2 (7%)	14	20
All	All	5103/4403 (116%)	4985 (98%)	118 (2%)	43	63

All (118) 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	161	LEU
2	B	294	SER
2	B	299	GLU
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	30	SER
3	C	142	GLU
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
9	J	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
12	M	20	VAL
13	O	49	THR
13	O	55	GLU
13	O	87	VAL
13	O	98[A]	GLU
13	O	98[B]	GLU
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
16	V	15	GLU
18	Y	30	ILE
1	a	13	LEU
1	a	35	VAL
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	245	VAL
2	b	298	LEU
2	b	315	ILE
2	b	362	PHE
2	b	486[A]	LEU
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	158	THR
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	416	SER
4	d	26	ARG
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	71	GLU
7	h	61	SER
7	h	65	LEU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
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
16	v	109	GLU
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	32	ASP
19	z	34	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
3	C	322	GLN
3	C	415	ASN
1	a	75	ASN
2	b	331	ASN
3	c	19	ASN
3	c	155	ASN
3	c	201	ASN
10	k	40	GLN
11	l	8	GLN
13	o	58	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
14	FME	T	1	14	8,9,10	0.59	0	7,9,11	1.62	2 (28%)
8	FME	I	1	8	8,9,10	0.62	0	7,9,11	1.24	1 (14%)
8	FME	i	1	8	8,9,10	0.64	0	7,9,11	1.22	1 (14%)
12	FME	M	1	12	8,9,10	0.54	0	7,9,11	1.38	1 (14%)
12	FME	m	1	12	8,9,10	0.53	0	7,9,11	1.43	1 (14%)
14	FME	t	1	14	8,9,10	0.76	0	7,9,11	1.33	1 (14%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	t	1	FME	O-C-CA	-2.36	118.58	124.78
14	T	1	FME	CA-N-CN	2.35	126.44	122.82
12	m	1	FME	O1-CN-N	-2.33	119.12	125.27
8	I	1	FME	O-C-CA	-2.19	119.03	124.78
12	M	1	FME	O-C-CA	-2.13	119.21	124.78
14	T	1	FME	C-CA-N	2.09	113.50	109.73
8	i	1	FME	O-C-CA	-2.05	119.40	124.78

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	FME	O-C-CA-CB
12	M	1	FME	O-C-CA-CB
12	m	1	FME	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	i	1	FME	CA-CB-CG-SD
12	m	1	FME	O1-CN-N-CA
8	i	1	FME	C-CA-CB-CG

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
24	BCR	T	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	13 (23%)
34	LMG	C	520	-	51,51,55	0.94	2 (3%)	59,59,63	1.12	4 (6%)
32	LMT	a	416	-	36,36,36	1.00	2 (5%)	47,47,47	1.05	2 (4%)
23	CLA	B	606	2	69,73,73	1.93	20 (28%)	83,113,113	3.01	31 (37%)
26	GOL	d	413	-	5,5,5	0.98	0	5,5,5	1.07	0
27	OEX	A	412[B]	3,1,41	0,14,14	-	-	-	-	-
38	HEM	f	101	5,6	50,50,50	1.47	6 (12%)	66,82,82	1.77	11 (16%)
23	CLA	c	503	3	69,73,73	2.05	20 (28%)	83,113,113	2.71	27 (32%)
23	CLA	B	605	2	69,73,73	2.03	18 (26%)	83,113,113	3.05	34 (40%)
23	CLA	A	407	1	69,73,73	1.94	21 (30%)	83,113,113	2.90	35 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	404[A]	1	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
27	OEX	a	412[A]	3,1,41	0,14,14	-	-	-		
23	CLA	B	608	2	69,73,73	1.97	20 (28%)	83,113,113	2.86	35 (42%)
23	CLA	c	514	3	69,73,73	2.11	21 (30%)	83,113,113	2.88	30 (36%)
36	DGD	c	519	-	63,63,67	0.85	4 (6%)	77,77,81	1.08	5 (6%)
23	CLA	c	511	3	69,73,73	2.03	20 (28%)	83,113,113	2.89	32 (38%)
34	LMG	D	412	39	51,51,55	0.80	2 (3%)	59,59,63	1.05	3 (5%)
36	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
31	PHO	A	416[B]	-	58,69,69	2.80	15 (25%)	56,99,99	2.91	16 (28%)
33	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	5 (9%)
23	CLA	c	504	3	69,73,73	2.05	20 (28%)	83,113,113	2.84	29 (34%)
23	CLA	b	610	41	69,73,73	2.07	20 (28%)	83,113,113	2.95	31 (37%)
24	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	10 (17%)
27	OEX	A	412[A]	3,1,41	0,14,14	-	-	-		
23	CLA	C	504	3	69,73,73	1.99	19 (27%)	83,113,113	2.87	29 (34%)
24	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.52	10 (17%)
26	GOL	a	410	-	5,5,5	0.92	0	5,5,5	0.97	0
26	GOL	D	413	-	5,5,5	1.51	2 (40%)	5,5,5	0.89	0
24	BCR	d	405	-	41,41,41	1.15	2 (4%)	56,56,56	1.97	18 (32%)
23	CLA	b	616	2	69,73,73	2.00	19 (27%)	83,113,113	2.92	32 (38%)
38	HEM	F	102	5,6	50,50,50	1.52	7 (14%)	66,82,82	1.96	18 (27%)
23	CLA	B	614	2	69,73,73	1.97	19 (27%)	83,113,113	2.98	32 (38%)
23	CLA	b	605	2	69,73,73	1.96	20 (28%)	83,113,113	2.94	30 (36%)
31	PHO	A	416[A]	-	58,69,69	2.79	15 (25%)	56,99,99	2.85	15 (26%)
33	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
24	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.44	11 (19%)
30	BCT	A	415[B]	21	2,3,3	0.68	0	2,3,3	0.84	0
23	CLA	a	404[A]	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	33 (39%)
30	BCT	d	401[B]	21	2,3,3	0.64	0	2,3,3	1.18	0
32	LMT	A	417	-	36,36,36	0.94	3 (8%)	47,47,47	1.06	2 (4%)
24	BCR	B	617	-	41,41,41	1.05	1 (2%)	56,56,56	1.46	8 (14%)
33	LHG	D	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	3 (5%)
32	LMT	b	627	-	25,25,36	0.89	0	30,30,47	1.05	2 (6%)
26	GOL	c	526[B]	-	5,5,5	0.96	0	5,5,5	0.99	0
34	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.41	8 (13%)
23	CLA	C	510	3	69,73,73	2.06	20 (28%)	83,113,113	2.86	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	b	606	2	69,73,73	2.02	19 (27%)	83,113,113	2.91	29 (34%)
34	LMG	d	412	39	51,51,55	0.90	2 (3%)	59,59,63	1.13	5 (8%)
33	LHG	D	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	4 (7%)
25	SQD	f	102	-	42,43,54	1.21	3 (7%)	51,54,65	1.61	11 (21%)
23	CLA	c	506	3	69,73,73	2.05	19 (27%)	83,113,113	2.80	29 (34%)
23	CLA	C	502	3	69,73,73	1.96	19 (27%)	83,113,113	2.89	33 (39%)
23	CLA	C	503	3	69,73,73	2.07	20 (28%)	83,113,113	2.70	30 (36%)
24	BCR	c	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.64	12 (21%)
25	SQD	a	409[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
23	CLA	b	601	41	69,73,73	2.11	19 (27%)	83,113,113	2.83	30 (36%)
30	BCT	A	415[A]	21	2,3,3	0.64	0	2,3,3	1.30	0
36	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.11	5 (6%)
31	PHO	a	406[B]	-	58,69,69	2.75	12 (20%)	56,99,99	2.76	15 (26%)
26	GOL	v	202[B]	-	5,5,5	1.10	0	5,5,5	0.80	0
30	BCT	d	401[A]	21	2,3,3	0.59	0	2,3,3	1.49	0
40	HEC	V	201	16	50,50,50	1.73	8 (16%)	68,82,82	1.46	9 (13%)
32	LMT	t	101	-	26,26,36	0.93	2 (7%)	31,31,47	1.29	2 (6%)
33	LHG	D	408[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
26	GOL	B	625	-	5,5,5	0.96	0	5,5,5	1.10	1 (20%)
26	GOL	c	526[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
28	PL9	D	406[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.66	17 (25%)
23	CLA	d	402[B]	41	69,73,73	2.10	19 (27%)	83,113,113	2.86	32 (38%)
24	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	12 (21%)
24	BCR	c	516	-	41,41,41	1.01	1 (2%)	56,56,56	1.39	9 (16%)
23	CLA	A	406[B]	41	69,73,73	2.10	20 (28%)	83,113,113	2.87	33 (39%)
33	LHG	d	414[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	4 (7%)
33	LHG	D	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
34	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.20	6 (10%)
28	PL9	A	413[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.96	24 (35%)
25	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	2.17	14 (27%)
34	LMG	z	101	-	39,39,55	1.10	2 (5%)	47,47,63	1.06	2 (4%)
23	CLA	b	604	2	69,73,73	2.08	20 (28%)	83,113,113	2.78	29 (34%)
35	HTG	C	522	-	19,19,19	0.85	1 (5%)	23,24,24	1.36	2 (8%)
28	PL9	a	413[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.93	20 (29%)
23	CLA	B	607	41	69,73,73	1.94	20 (28%)	83,113,113	2.90	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
31	PHO	a	406[A]	-	58,69,69	2.74	13 (22%)	56,99,99	2.81	14 (25%)
23	CLA	b	609	2	69,73,73	2.03	19 (27%)	83,113,113	2.77	30 (36%)
25	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.71	12 (19%)
26	GOL	v	202[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
35	HTG	V	202	-	11,11,19	0.32	0	15,15,24	1.25	1 (6%)
24	BCR	a	408	-	41,41,41	1.03	1 (2%)	56,56,56	1.42	8 (14%)
23	CLA	c	507	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	31 (37%)
31	PHO	a	415[B]	-	58,69,69	2.80	14 (24%)	56,99,99	2.96	15 (26%)
35	HTG	D	411	-	16,16,19	1.04	1 (6%)	20,21,24	1.52	1 (5%)
23	CLA	b	612	2	69,73,73	1.99	19 (27%)	83,113,113	2.77	30 (36%)
25	SQD	l	101	-	53,54,54	1.07	4 (7%)	62,65,65	1.79	12 (19%)
40	HEC	v	201	16	50,50,50	1.78	7 (14%)	68,82,82	1.39	8 (11%)
23	CLA	B	601	41	69,73,73	2.07	21 (30%)	83,113,113	2.89	27 (32%)
28	PL9	D	406[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
26	GOL	b	628	-	5,5,5	0.54	0	5,5,5	1.38	1 (20%)
23	CLA	d	402[A]	41	69,73,73	2.04	17 (24%)	83,113,113	2.86	32 (38%)
23	CLA	C	506	3	69,73,73	2.02	19 (27%)	83,113,113	2.90	30 (36%)
23	CLA	C	507	3	69,73,73	1.98	21 (30%)	83,113,113	2.87	31 (37%)
24	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	10 (17%)
23	CLA	D	403[B]	4	69,73,73	2.00	20 (28%)	83,113,113	2.93	30 (36%)
33	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	4 (9%)
23	CLA	A	406[A]	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	32 (38%)
33	LHG	b	629[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	3 (5%)
32	LMT	B	629	-	25,25,36	0.90	2 (8%)	30,30,47	1.19	3 (10%)
23	CLA	a	407	1	69,73,73	1.98	18 (26%)	83,113,113	2.96	30 (36%)
33	LHG	A	418[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.14	5 (9%)
33	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
24	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.60	11 (19%)
23	CLA	b	602	2	69,73,73	2.09	19 (27%)	83,113,113	3.08	35 (42%)
28	PL9	A	413[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	B	613	2	69,73,73	1.95	19 (27%)	83,113,113	2.87	29 (34%)
24	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.34	8 (14%)
26	GOL	a	417	-	5,5,5	1.30	1 (20%)	5,5,5	1.06	0
24	BCR	A	408	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	c	502	3	69,73,73	2.04	20 (28%)	83,113,113	2.91	31 (37%)
26	GOL	O	302	-	5,5,5	0.94	0	5,5,5	0.90	0
26	GOL	l	103[B]	-	5,5,5	0.85	0	5,5,5	1.06	0
28	PL9	a	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
32	LMT	B	626	-	36,36,36	1.19	4 (11%)	47,47,47	1.39	5 (10%)
32	LMT	T	101	-	36,36,36	1.07	3 (8%)	47,47,47	1.07	2 (4%)
35	HTG	B	623	-	19,19,19	1.06	2 (10%)	23,24,24	1.34	3 (13%)
36	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.13	5 (6%)
25	SQD	A	411	-	53,54,54	1.05	3 (5%)	62,65,65	1.24	7 (11%)
31	PHO	a	415[A]	-	58,69,69	2.77	13 (22%)	56,99,99	2.94	17 (30%)
23	CLA	C	505	41	69,73,73	1.96	20 (28%)	83,113,113	2.87	33 (39%)
23	CLA	B	612	2	69,73,73	1.99	19 (27%)	83,113,113	2.78	31 (37%)
23	CLA	B	604	2	69,73,73	1.96	20 (28%)	83,113,113	2.69	35 (42%)
26	GOL	C	523[B]	-	5,5,5	1.22	0	5,5,5	0.77	0
23	CLA	C	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.90	31 (37%)
33	LHG	b	629[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
23	CLA	B	609	2	69,73,73	2.04	17 (24%)	83,113,113	2.76	30 (36%)
23	CLA	D	403[A]	4	69,73,73	2.00	20 (28%)	83,113,113	2.86	32 (38%)
23	CLA	d	403[B]	4	69,73,73	2.01	19 (27%)	83,113,113	2.75	27 (32%)
26	GOL	A	410	-	5,5,5	1.09	0	5,5,5	0.79	0
32	LMT	b	621	-	25,25,36	0.96	1 (4%)	30,30,47	1.19	3 (10%)
33	LHG	A	418[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
33	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	B	616	2	69,73,73	2.03	19 (27%)	83,113,113	2.91	27 (32%)
36	DGD	H	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.07	8 (10%)
24	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.70	14 (25%)
26	GOL	l	103[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
23	CLA	C	512	3	69,73,73	2.01	21 (30%)	83,113,113	2.74	27 (32%)
28	PL9	d	406[B]	-	55,55,55	0.63	1 (1%)	68,69,69	1.72	19 (27%)
24	BCR	b	617	-	41,41,41	1.03	1 (2%)	56,56,56	1.43	9 (16%)
23	CLA	B	603	2	69,73,73	2.01	19 (27%)	83,113,113	2.93	32 (38%)
23	CLA	b	611	2	69,73,73	1.96	20 (28%)	83,113,113	2.89	31 (37%)
23	CLA	c	513	3	69,73,73	2.06	18 (26%)	83,113,113	2.90	31 (37%)
32	LMT	B	627	-	36,36,36	1.03	3 (8%)	47,47,47	1.15	4 (8%)
32	LMT	e	101	-	36,36,36	1.03	4 (11%)	47,47,47	0.98	1 (2%)
23	CLA	A	405[B]	41	69,73,73	2.02	20 (28%)	83,113,113	2.78	34 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	d	403[A]	4	69,73,73	1.95	20 (28%)	83,113,113	2.76	32 (38%)
26	GOL	B	622	-	5,5,5	0.86	0	5,5,5	1.15	1 (20%)
34	LMG	c	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.21	4 (6%)
32	LMT	F	101	-	36,36,36	1.06	1 (2%)	47,47,47	1.00	1 (2%)
23	CLA	C	514	3	69,73,73	2.06	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	a	405[B]	41	69,73,73	2.04	19 (27%)	83,113,113	2.89	31 (37%)
26	GOL	V	203[B]	-	5,5,5	1.07	0	5,5,5	0.92	0
35	HTG	B	621	-	19,19,19	0.84	1 (5%)	23,24,24	1.37	1 (4%)
34	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.35	7 (11%)
25	SQD	A	409[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.73	12 (19%)
32	LMT	A	419	-	36,36,36	1.05	2 (5%)	47,47,47	1.18	4 (8%)
23	CLA	c	510	3	69,73,73	2.01	21 (30%)	83,113,113	2.92	32 (38%)
28	PL9	d	406[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
35	HTG	b	625	-	19,19,19	1.07	2 (10%)	23,24,24	1.52	4 (17%)
32	LMT	m	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.09	3 (6%)
23	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.79	28 (33%)
23	CLA	b	615	2	69,73,73	2.01	18 (26%)	83,113,113	2.84	30 (36%)
23	CLA	c	509	3	69,73,73	2.13	20 (28%)	83,113,113	2.71	28 (33%)
26	GOL	o	303	-	5,5,5	1.15	0	5,5,5	0.97	0
35	HTG	b	623	-	19,19,19	1.04	1 (5%)	23,24,24	1.94	3 (13%)
23	CLA	b	607	41	69,73,73	1.96	21 (30%)	83,113,113	2.77	30 (36%)
23	CLA	C	511	3	69,73,73	2.02	20 (28%)	83,113,113	2.87	32 (38%)
36	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.00	3 (3%)
33	LHG	a	419[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	B	602	2	69,73,73	2.03	20 (28%)	83,113,113	2.84	29 (34%)
23	CLA	A	405[A]	41	69,73,73	2.02	18 (26%)	83,113,113	2.85	33 (39%)
24	BCR	D	405	-	41,41,41	1.11	1 (2%)	56,56,56	1.77	15 (26%)
26	GOL	a	418	-	5,5,5	1.26	1 (20%)	5,5,5	0.96	0
35	HTG	c	522	-	19,19,19	0.93	1 (5%)	23,24,24	1.60	2 (8%)
31	PHO	D	401[B]	-	58,69,69	2.76	15 (25%)	56,99,99	2.76	14 (25%)
36	DGD	C	518[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.03	5 (6%)
26	GOL	b	624	-	5,5,5	1.18	1 (20%)	5,5,5	0.81	0
26	GOL	D	402	-	5,5,5	1.36	2 (40%)	5,5,5	0.82	0
23	CLA	a	405[A]	41	69,73,73	1.98	19 (27%)	83,113,113	2.83	30 (36%)
26	GOL	V	203[A]	-	5,5,5	1.34	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	615	2	69,73,73	2.05	19 (27%)	83,113,113	2.95	32 (38%)
25	SQD	A	409[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
34	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.28	4 (6%)
34	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.28	7 (11%)
36	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.00	6 (7%)
26	GOL	o	304	-	5,5,5	1.00	1 (20%)	5,5,5	1.08	0
26	GOL	c	527	-	5,5,5	1.14	0	5,5,5	0.98	0
23	CLA	b	603	2	69,73,73	2.00	20 (28%)	83,113,113	2.86	31 (37%)
24	BCR	b	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.33	9 (16%)
33	LHG	a	419[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
24	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.42	7 (12%)
23	CLA	B	610	41	69,73,73	2.04	19 (27%)	83,113,113	2.90	32 (38%)
31	PHO	D	401[A]	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	14 (25%)
34	LMG	C	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.55	8 (13%)
34	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.46	5 (11%)
23	CLA	a	404[B]	1	69,73,73	2.07	20 (28%)	83,113,113	2.87	32 (38%)
23	CLA	c	508	41	69,73,73	2.04	18 (26%)	83,113,113	2.91	30 (36%)
23	CLA	B	611	2	69,73,73	2.52	20 (28%)	83,113,113	3.86	29 (34%)
26	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
35	HTG	b	622	-	19,19,19	1.18	2 (10%)	23,24,24	1.94	7 (30%)
36	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.08	5 (6%)
36	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
33	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	3 (5%)
23	CLA	d	404	4	69,73,73	2.04	20 (28%)	83,113,113	2.94	34 (40%)
25	SQD	a	411	-	53,54,54	1.07	3 (5%)	62,65,65	1.23	8 (12%)
33	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.12	5 (9%)
32	LMT	M	101	-	36,36,36	1.12	2 (5%)	47,47,47	1.26	6 (12%)
23	CLA	D	404	4	69,73,73	2.13	19 (27%)	83,113,113	2.88	34 (40%)
23	CLA	c	512	3	69,73,73	2.09	20 (28%)	83,113,113	2.82	33 (39%)
25	SQD	a	409[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.60	12 (19%)
24	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.75	14 (25%)
35	HTG	o	301	-	19,19,19	1.11	2 (10%)	23,24,24	1.59	5 (21%)
23	CLA	b	613	2	69,73,73	2.01	19 (27%)	83,113,113	2.83	32 (38%)
23	CLA	A	404[B]	1	69,73,73	2.09	20 (28%)	83,113,113	2.83	32 (38%)
26	GOL	O	303	-	5,5,5	1.14	1 (20%)	5,5,5	1.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.27	6 (10%)
23	CLA	b	614	2	69,73,73	2.02	20 (28%)	83,113,113	3.01	31 (37%)
27	OEX	a	412[B]	3,1,41	0,14,14	-	-	-	-	-
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
24	BCR	B	618	-	41,41,41	0.98	2 (4%)	56,56,56	1.33	6 (10%)
23	CLA	b	608	2	69,73,73	2.03	20 (28%)	83,113,113	2.76	31 (37%)
33	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
35	HTG	d	411	-	16,16,19	0.95	1 (6%)	20,21,24	1.59	1 (5%)
23	CLA	c	505	41	69,73,73	2.09	20 (28%)	83,113,113	2.86	32 (38%)
23	CLA	C	508	41	69,73,73	1.95	19 (27%)	83,113,113	2.74	29 (34%)
33	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)

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
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
34	LMG	C	520	-	-	12/46/66/70	0/1/1/1
32	LMT	a	416	-	-	11/21/61/61	0/2/2/2
23	CLA	B	606	2	-	7/39/115/115	-
26	GOL	d	413	-	-	1/4/4/4	-
38	HEM	f	101	5,6	-	6/14/54/54	-
23	CLA	c	503	3	-	6/39/115/115	-
23	CLA	B	605	2	-	9/39/115/115	-
23	CLA	A	407	1	-	7/39/115/115	-
23	CLA	A	404[A]	1	-	3/39/115/115	-
23	CLA	B	608	2	-	4/39/115/115	-
23	CLA	c	514	3	-	11/39/115/115	-
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
23	CLA	c	511	3	-	11/39/115/115	-
34	LMG	D	412	39	-	9/46/66/70	0/1/1/1
36	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
31	PHO	A	416[B]	-	-	1/37/103/103	0/5/6/6
33	LHG	d	408[B]	-	-	16/53/53/53	-
23	CLA	c	504	3	-	1/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	610	41	-	10/39/115/115	-
24	BCR	H	101	-	-	3/29/63/63	0/2/2/2
23	CLA	C	504	3	-	4/39/115/115	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
26	GOL	a	410	-	-	4/4/4/4	-
26	GOL	D	413	-	-	4/4/4/4	-
24	BCR	d	405	-	-	5/29/63/63	0/2/2/2
23	CLA	b	616	2	-	9/39/115/115	-
38	HEM	F	102	5,6	-	5/14/54/54	-
23	CLA	B	614	2	-	15/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
31	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
33	LHG	d	408[A]	-	-	13/53/53/53	-
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404[A]	1	-	4/39/115/115	-
32	LMT	A	417	-	-	6/21/61/61	0/2/2/2
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2
33	LHG	D	408[B]	-	-	13/53/53/53	-
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
26	GOL	c	526[B]	-	-	0/4/4/4	-
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
23	CLA	C	510	3	-	7/39/115/115	-
23	CLA	b	606	2	-	15/39/115/115	-
34	LMG	d	412	39	-	10/46/66/70	0/1/1/1
33	LHG	D	407[B]	-	-	19/53/53/53	-
25	SQD	f	102	-	-	10/38/58/69	0/1/1/1
23	CLA	c	506	3	-	7/39/115/115	-
23	CLA	C	502	3	-	4/39/115/115	-
23	CLA	C	503	3	-	10/39/115/115	-
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
25	SQD	a	409[A]	-	-	9/49/69/69	0/1/1/1
23	CLA	b	601	41	-	19/39/115/115	-
36	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
31	PHO	a	406[B]	-	-	4/37/103/103	0/5/6/6
26	GOL	v	202[B]	-	-	2/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
32	LMT	t	101	-	-	10/17/38/61	0/1/1/2
33	LHG	D	408[A]	-	-	14/53/53/53	-
26	GOL	B	625	-	-	4/4/4/4	-
26	GOL	c	526[A]	-	-	0/4/4/4	-
28	PL9	D	406[B]	-	-	7/53/73/73	0/1/1/1
23	CLA	d	402[B]	41	-	3/39/115/115	-
24	BCR	h	101	-	-	2/29/63/63	0/2/2/2
24	BCR	c	516	-	-	2/29/63/63	0/2/2/2
23	CLA	A	406[B]	41	-	4/39/115/115	-
33	LHG	d	414[B]	-	-	9/53/53/53	-
33	LHG	D	407[A]	-	-	17/53/53/53	-
34	LMG	c	520	-	-	13/46/66/70	0/1/1/1
28	PL9	A	413[B]	-	-	14/53/73/73	0/1/1/1
25	SQD	X	101	-	-	12/38/58/69	0/1/1/1
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	b	604	2	-	12/39/115/115	-
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
28	PL9	a	413[B]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	607	41	-	4/39/115/115	-
36	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
31	PHO	a	406[A]	-	-	6/37/103/103	0/5/6/6
23	CLA	b	609	2	-	1/39/115/115	-
25	SQD	b	620	-	-	18/49/69/69	0/1/1/1
26	GOL	v	202[A]	-	-	2/4/4/4	-
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1
24	BCR	a	408	-	-	1/29/63/63	0/2/2/2
23	CLA	c	507	3	-	9/39/115/115	-
31	PHO	a	415[B]	-	-	3/37/103/103	0/5/6/6
35	HTG	D	411	-	-	3/7/27/30	0/1/1/1
23	CLA	b	612	2	-	5/39/115/115	-
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
25	SQD	l	101	-	-	14/49/69/69	0/1/1/1
23	CLA	B	601	41	-	12/39/115/115	-
28	PL9	D	406[A]	-	-	6/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	GOL	b	628	-	-	0/4/4/4	-
23	CLA	d	402[A]	41	-	8/39/115/115	-
23	CLA	C	506	3	-	7/39/115/115	-
23	CLA	C	507	3	-	13/39/115/115	-
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
23	CLA	D	403[B]	4	-	2/39/115/115	-
33	LHG	E	101[B]	-	-	20/46/46/53	-
23	CLA	A	406[A]	41	-	5/39/115/115	-
33	LHG	b	629[B]	-	-	17/53/53/53	-
32	LMT	B	629	-	-	11/17/37/61	0/1/1/2
23	CLA	a	407	1	-	11/39/115/115	-
33	LHG	A	418[B]	-	-	16/53/53/53	-
33	LHG	d	414[A]	-	-	17/53/53/53	-
24	BCR	t	102	-	-	0/29/63/63	0/2/2/2
23	CLA	b	602	2	-	3/39/115/115	-
28	PL9	A	413[A]	-	-	15/53/73/73	0/1/1/1
23	CLA	B	613	2	-	7/39/115/115	-
24	BCR	C	516	-	-	0/29/63/63	0/2/2/2
26	GOL	a	417	-	-	2/4/4/4	-
24	BCR	A	408	-	-	0/29/63/63	0/2/2/2
23	CLA	c	502	3	-	6/39/115/115	-
26	GOL	O	302	-	-	2/4/4/4	-
26	GOL	l	103[B]	-	-	2/4/4/4	-
28	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
32	LMT	B	626	-	-	12/21/61/61	0/2/2/2
32	LMT	T	101	-	-	7/21/61/61	0/2/2/2
35	HTG	B	623	-	-	4/10/30/30	0/1/1/1
36	DGD	h	102	-	-	15/51/91/95	0/2/2/2
25	SQD	A	411	-	-	15/49/69/69	0/1/1/1
31	PHO	a	415[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	C	505	41	-	9/39/115/115	-
23	CLA	B	612	2	-	7/39/115/115	-
23	CLA	B	604	2	-	2/39/115/115	-
26	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	C	513	3	-	9/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LHG	b	629[A]	-	-	14/53/53/53	-
23	CLA	B	609	2	-	1/39/115/115	-
23	CLA	D	403[A]	4	-	2/39/115/115	-
23	CLA	d	403[B]	4	-	4/39/115/115	-
26	GOL	A	410	-	-	2/4/4/4	-
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
33	LHG	A	418[A]	-	-	14/53/53/53	-
33	LHG	E	101[A]	-	-	22/46/46/53	-
23	CLA	B	616	2	-	7/39/115/115	-
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
24	BCR	y	101	-	-	4/29/63/63	0/2/2/2
26	GOL	l	103[A]	-	-	1/4/4/4	-
23	CLA	C	512	3	-	5/39/115/115	-
28	PL9	d	406[B]	-	-	8/53/73/73	0/1/1/1
24	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	603	2	-	7/39/115/115	-
23	CLA	b	611	2	-	4/39/115/115	-
23	CLA	c	513	3	-	13/39/115/115	-
32	LMT	B	627	-	-	10/21/61/61	0/2/2/2
32	LMT	e	101	-	-	15/21/61/61	0/2/2/2
23	CLA	A	405[B]	41	-	5/39/115/115	-
23	CLA	d	403[A]	4	-	4/39/115/115	-
26	GOL	B	622	-	-	4/4/4/4	-
34	LMG	c	501	-	-	12/46/66/70	0/1/1/1
32	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	C	514	3	-	6/39/115/115	-
23	CLA	a	405[B]	41	-	7/39/115/115	-
26	GOL	V	203[B]	-	-	2/4/4/4	-
35	HTG	B	621	-	-	2/10/30/30	0/1/1/1
34	LMG	c	521	-	-	11/46/66/70	0/1/1/1
25	SQD	A	409[B]	-	-	10/49/69/69	0/1/1/1
32	LMT	A	419	-	-	15/21/61/61	0/2/2/2
23	CLA	c	510	3	-	15/39/115/115	-
28	PL9	d	406[A]	-	-	7/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	HTG	b	625	-	-	3/10/30/30	0/1/1/1
32	LMT	m	103	-	-	8/21/61/61	0/2/2/2
23	CLA	C	509	3	-	5/39/115/115	-
23	CLA	b	615	2	-	8/39/115/115	-
23	CLA	c	509	3	-	4/39/115/115	-
26	GOL	o	303	-	-	2/4/4/4	-
35	HTG	b	623	-	-	4/10/30/30	0/1/1/1
23	CLA	b	607	41	-	7/39/115/115	-
23	CLA	C	511	3	-	13/39/115/115	-
36	DGD	C	519	-	-	20/51/91/95	0/2/2/2
33	LHG	a	419[B]	-	-	16/46/46/53	-
23	CLA	B	602	2	-	11/39/115/115	-
23	CLA	A	405[A]	41	-	3/39/115/115	-
24	BCR	D	405	-	-	4/29/63/63	0/2/2/2
26	GOL	a	418	-	-	2/4/4/4	-
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
31	PHO	D	401[B]	-	-	3/37/103/103	0/5/6/6
36	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
26	GOL	b	624	-	-	2/4/4/4	-
26	GOL	D	402	-	-	2/4/4/4	-
23	CLA	a	405[A]	41	-	8/39/115/115	-
26	GOL	V	203[A]	-	-	2/4/4/4	-
23	CLA	B	615	2	-	8/39/115/115	-
25	SQD	A	409[A]	-	-	12/49/69/69	0/1/1/1
34	LMG	B	620	-	-	17/46/66/70	0/1/1/1
34	LMG	m	101	-	-	11/46/66/70	0/1/1/1
36	DGD	c	518[B]	-	-	13/51/91/95	0/2/2/2
26	GOL	o	304	-	-	4/4/4/4	-
26	GOL	c	527	-	-	2/4/4/4	-
23	CLA	b	603	2	-	4/39/115/115	-
24	BCR	b	619	-	-	2/29/63/63	0/2/2/2
33	LHG	a	419[A]	-	-	16/46/46/53	-
24	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	B	610	41	-	9/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PHO	D	401[A]	-	-	3/37/103/103	0/5/6/6
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
34	LMG	Z	101	-	-	12/31/51/70	0/1/1/1
23	CLA	a	404[B]	1	-	6/39/115/115	-
23	CLA	c	508	41	-	9/39/115/115	-
23	CLA	B	611	2	-	6/39/115/115	-
26	GOL	C	523[A]	-	-	0/4/4/4	-
35	HTG	b	622	-	-	5/10/30/30	0/1/1/1
36	DGD	c	517[B]	-	-	20/51/91/95	0/2/2/2
36	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
33	LHG	L	101[B]	-	-	18/53/53/53	-
23	CLA	d	404	4	-	8/39/115/115	-
25	SQD	a	411	-	-	15/49/69/69	0/1/1/1
33	LHG	d	407[B]	-	-	16/53/53/53	-
32	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	D	404	4	-	14/39/115/115	-
23	CLA	c	512	3	-	6/39/115/115	-
25	SQD	a	409[B]	-	-	9/49/69/69	0/1/1/1
24	BCR	Y	101	-	-	5/29/63/63	0/2/2/2
35	HTG	o	301	-	-	4/10/30/30	0/1/1/1
23	CLA	b	613	2	-	2/39/115/115	-
23	CLA	A	404[B]	1	-	6/39/115/115	-
26	GOL	O	303	-	-	2/4/4/4	-
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	614	2	-	16/39/115/115	-
36	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	608	2	-	4/39/115/115	-
33	LHG	L	101[A]	-	-	20/53/53/53	-
35	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	c	505	41	-	6/39/115/115	-
23	CLA	C	508	41	-	9/39/115/115	-
33	LHG	d	407[A]	-	-	13/53/53/53	-

All (1880) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	401[B]	PHO	C1D-C2D	9.40	1.50	1.39
31	a	406[A]	PHO	C1B-C2B	9.21	1.49	1.39
31	a	415[B]	PHO	C1B-C2B	9.13	1.49	1.39
31	D	401[B]	PHO	C1B-C2B	8.90	1.49	1.39
31	D	401[A]	PHO	C1D-C2D	8.89	1.49	1.39
31	A	416[B]	PHO	C1D-C2D	8.80	1.49	1.39
31	a	406[B]	PHO	C1D-C2D	8.79	1.49	1.39
31	a	415[A]	PHO	C1B-C2B	8.69	1.49	1.39
31	a	406[B]	PHO	C1B-C2B	8.69	1.49	1.39
31	A	416[A]	PHO	C1B-C2B	8.65	1.49	1.39
31	A	416[B]	PHO	C1B-C2B	8.64	1.49	1.39
31	a	415[B]	PHO	C1D-C2D	8.63	1.49	1.39
31	a	415[A]	PHO	C1D-C2D	8.62	1.49	1.39
31	A	416[A]	PHO	C1D-C2D	8.53	1.49	1.39
31	D	401[A]	PHO	C1B-C2B	8.45	1.48	1.39
31	a	406[A]	PHO	C1D-C2D	8.40	1.48	1.39
40	v	201	HEC	C3D-C2D	8.10	1.54	1.36
40	V	201	HEC	C3D-C2D	7.47	1.52	1.36
31	a	415[A]	PHO	C3B-C4B	7.31	1.49	1.41
23	B	611	CLA	C1D-ND	7.25	1.46	1.37
31	A	416[B]	PHO	C3B-C4B	7.11	1.49	1.41
31	A	416[A]	PHO	C3B-C4B	7.11	1.49	1.41
31	a	406[B]	PHO	C3B-C4B	6.86	1.49	1.41
31	a	406[A]	PHO	C3B-C4B	6.66	1.49	1.41
31	a	406[A]	PHO	C4D-CHA	6.54	1.50	1.39
31	a	415[B]	PHO	C3B-C2B	6.52	1.49	1.40
23	B	611	CLA	C1B-C2B	6.48	1.58	1.43
31	a	415[B]	PHO	C3B-C4B	6.48	1.48	1.41
31	a	406[B]	PHO	C3B-C2B	6.42	1.49	1.40
31	a	406[B]	PHO	C4D-CHA	6.41	1.49	1.39
31	D	401[B]	PHO	C4D-CHA	6.40	1.49	1.39
31	a	406[A]	PHO	C3B-C2B	6.39	1.49	1.40
31	A	416[B]	PHO	C4D-CHA	6.29	1.49	1.39
31	A	416[A]	PHO	C4D-CHA	6.27	1.49	1.39
23	B	611	CLA	CMB-C2B	6.24	1.64	1.50
31	D	401[B]	PHO	C3B-C4B	6.17	1.48	1.41
31	D	401[A]	PHO	C3B-C4B	6.16	1.48	1.41
31	A	416[B]	PHO	C3B-C2B	6.16	1.48	1.40
31	a	415[B]	PHO	C4D-CHA	6.15	1.49	1.39
31	D	401[B]	PHO	C3B-C2B	6.13	1.48	1.40
31	D	401[A]	PHO	C4D-CHA	6.13	1.49	1.39
31	D	401[A]	PHO	C3B-C2B	6.13	1.48	1.40
31	a	415[B]	PHO	C3C-C2C	6.05	1.49	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	415[A]	PHO	C4D-CHA	6.05	1.49	1.39
23	C	511	CLA	C1D-ND	5.97	1.45	1.37
23	B	611	CLA	C3C-C2C	5.96	1.49	1.36
31	A	416[A]	PHO	C3B-C2B	5.94	1.48	1.40
31	A	416[B]	PHO	C3C-C2C	5.89	1.49	1.36
31	a	415[A]	PHO	C3B-C2B	5.88	1.48	1.40
31	a	415[A]	PHO	C3C-C2C	5.86	1.49	1.36
31	D	401[B]	PHO	C3C-C2C	5.81	1.49	1.36
23	c	512	CLA	C1D-ND	5.80	1.44	1.37
23	c	505	CLA	C1D-ND	5.72	1.44	1.37
31	A	416[A]	PHO	C3C-C2C	5.72	1.48	1.36
23	c	509	CLA	C3C-C2C	5.71	1.48	1.36
31	D	401[A]	PHO	C3C-C2C	5.71	1.48	1.36
23	C	504	CLA	C3C-C2C	5.71	1.48	1.36
23	c	509	CLA	O2D-CGD	5.70	1.47	1.33
23	c	509	CLA	C1D-ND	5.69	1.44	1.37
23	D	404	CLA	C3C-C2C	5.66	1.48	1.36
23	d	402[B]	CLA	C1D-ND	5.66	1.44	1.37
23	B	610	CLA	C3C-C2C	5.66	1.48	1.36
23	c	513	CLA	C3C-C2C	5.64	1.48	1.36
23	d	402[B]	CLA	C3C-C2C	5.62	1.48	1.36
23	d	404	CLA	C3C-C2C	5.61	1.48	1.36
23	D	404	CLA	C1D-ND	5.60	1.44	1.37
23	b	601	CLA	C1D-ND	5.59	1.44	1.37
23	d	402[A]	CLA	C3C-C2C	5.58	1.48	1.36
23	c	503	CLA	C1D-ND	5.57	1.44	1.37
23	c	503	CLA	C3C-C2C	5.54	1.48	1.36
31	a	406[B]	PHO	C3C-C2C	5.52	1.48	1.36
23	c	514	CLA	C1D-ND	5.52	1.44	1.37
23	A	404[B]	CLA	C1D-ND	5.51	1.44	1.37
23	A	406[B]	CLA	C3C-C2C	5.51	1.48	1.36
23	a	404[B]	CLA	C3C-C2C	5.50	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.48	1.48	1.36
31	a	415[B]	PHO	C3D-C2D	5.47	1.49	1.39
23	C	513	CLA	C3C-C2C	5.47	1.48	1.36
23	C	503	CLA	C1D-ND	5.47	1.44	1.37
31	a	415[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	b	610	CLA	C3C-C2C	5.46	1.48	1.36
31	a	406[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	c	504	CLA	C3C-C2C	5.45	1.48	1.36
23	c	506	CLA	C3C-C2C	5.45	1.48	1.36
23	c	511	CLA	C1D-ND	5.44	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C3C-C2C	5.44	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.43	1.48	1.36
23	d	402[A]	CLA	C1D-ND	5.42	1.44	1.37
23	C	514	CLA	C1D-ND	5.42	1.44	1.37
23	b	609	CLA	O2D-CGD	5.41	1.46	1.33
23	d	403[B]	CLA	C3C-C2C	5.41	1.48	1.36
31	a	406[B]	PHO	C3D-C2D	5.40	1.49	1.39
23	D	403[B]	CLA	C3C-C2C	5.40	1.48	1.36
23	b	614	CLA	C3C-C2C	5.40	1.48	1.36
23	c	514	CLA	C3C-C2C	5.39	1.48	1.36
23	c	512	CLA	C3C-C2C	5.38	1.48	1.36
23	b	601	CLA	C3C-C2C	5.38	1.48	1.36
23	a	407	CLA	C3C-C2C	5.37	1.48	1.36
23	B	601	CLA	C3C-C2C	5.36	1.48	1.36
23	b	605	CLA	C3C-C2C	5.36	1.48	1.36
31	a	406[A]	PHO	C3C-C2C	5.36	1.48	1.36
23	c	502	CLA	C1D-ND	5.36	1.44	1.37
23	b	612	CLA	C3C-C2C	5.35	1.48	1.36
23	B	605	CLA	C3C-C2C	5.34	1.48	1.36
23	C	509	CLA	C3C-C2C	5.34	1.48	1.36
23	C	511	CLA	C3C-C2C	5.34	1.48	1.36
23	b	606	CLA	C3C-C2C	5.34	1.48	1.36
23	B	611	CLA	CHC-C1C	5.33	1.49	1.38
31	A	416[A]	PHO	C3D-C2D	5.33	1.49	1.39
23	a	405[A]	CLA	C3C-C2C	5.31	1.48	1.36
23	D	403[A]	CLA	C3C-C2C	5.30	1.48	1.36
31	a	415[A]	PHO	OBD-CAD	5.30	1.29	1.22
23	b	604	CLA	C1D-ND	5.30	1.44	1.37
31	A	416[B]	PHO	C3D-C2D	5.29	1.48	1.39
23	a	405[B]	CLA	C3C-C2C	5.29	1.48	1.36
31	A	416[A]	PHO	OBD-CAD	5.28	1.29	1.22
23	C	509	CLA	C1D-ND	5.28	1.44	1.37
23	b	607	CLA	C3C-C2C	5.28	1.47	1.36
24	k	101	BCR	C23-C22	-5.27	1.34	1.45
24	C	515	BCR	C23-C22	-5.27	1.34	1.45
23	c	505	CLA	C3C-C2C	5.27	1.47	1.36
23	c	510	CLA	O2D-CGD	5.26	1.46	1.33
23	C	510	CLA	C3C-C2C	5.26	1.47	1.36
23	C	513	CLA	CHC-C1C	5.25	1.49	1.38
24	K	102	BCR	C23-C22	-5.24	1.34	1.45
31	a	406[A]	PHO	O2D-CGD	5.24	1.46	1.33
23	b	613	CLA	O2D-CGD	5.24	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	O2D-CGD	5.22	1.45	1.33
23	a	405[B]	CLA	C1D-ND	5.21	1.44	1.37
23	b	615	CLA	C3C-C2C	5.20	1.47	1.36
23	d	404	CLA	C1D-ND	5.19	1.44	1.37
23	B	606	CLA	C3C-C2C	5.19	1.47	1.36
23	B	603	CLA	C3C-C2C	5.19	1.47	1.36
23	B	609	CLA	C3C-C2C	5.18	1.47	1.36
23	C	502	CLA	C3C-C2C	5.17	1.47	1.36
23	c	513	CLA	CHC-C1C	5.17	1.49	1.38
23	a	404[B]	CLA	C1D-ND	5.17	1.44	1.37
23	c	511	CLA	O2D-CGD	5.16	1.45	1.33
23	b	610	CLA	CHC-C1C	5.16	1.49	1.38
23	b	606	CLA	C1D-ND	5.15	1.44	1.37
23	b	602	CLA	C3C-C2C	5.15	1.47	1.36
23	B	612	CLA	C3C-C2C	5.15	1.47	1.36
23	A	405[A]	CLA	O2D-CGD	5.14	1.45	1.33
23	c	510	CLA	C3C-C2C	5.14	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.13	1.47	1.36
23	C	506	CLA	C3C-C2C	5.13	1.47	1.36
23	a	404[A]	CLA	C1D-ND	5.13	1.44	1.37
23	b	610	CLA	C1D-ND	5.13	1.44	1.37
23	A	404[A]	CLA	C1D-ND	5.13	1.44	1.37
23	c	502	CLA	C3C-C2C	5.12	1.47	1.36
23	B	601	CLA	O2A-CGA	5.12	1.48	1.33
31	a	415[B]	PHO	OBD-CAD	5.12	1.29	1.22
23	a	407	CLA	CHC-C1C	5.11	1.48	1.38
23	c	505	CLA	O2D-CGD	5.11	1.45	1.33
23	B	605	CLA	O2D-CGD	5.11	1.45	1.33
23	C	508	CLA	C3C-C2C	5.10	1.47	1.36
23	c	507	CLA	C3C-C2C	5.10	1.47	1.36
23	A	406[B]	CLA	C1D-ND	5.10	1.44	1.37
23	d	403[A]	CLA	C3C-C2C	5.09	1.47	1.36
23	C	505	CLA	C3C-C2C	5.09	1.47	1.36
23	c	504	CLA	C1D-ND	5.08	1.44	1.37
23	C	509	CLA	O2D-CGD	5.08	1.45	1.33
23	b	602	CLA	CHC-C1C	5.07	1.48	1.38
23	b	615	CLA	O2D-CGD	5.07	1.45	1.33
23	C	514	CLA	C3C-C2C	5.07	1.47	1.36
23	c	508	CLA	C3C-C2C	5.07	1.47	1.36
23	B	602	CLA	C3C-C2C	5.07	1.47	1.36
23	B	615	CLA	C1D-ND	5.06	1.44	1.37
23	A	406[B]	CLA	O2D-CGD	5.06	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	CHC-C1C	5.06	1.48	1.38
23	B	614	CLA	C3C-C2C	5.05	1.47	1.36
23	b	603	CLA	C3C-C2C	5.05	1.47	1.36
23	B	614	CLA	C1D-ND	5.05	1.44	1.37
23	c	511	CLA	C3C-C2C	5.05	1.47	1.36
23	b	602	CLA	O2D-CGD	5.04	1.45	1.33
31	A	416[B]	PHO	O2D-CGD	5.04	1.45	1.33
31	a	415[B]	PHO	O2D-CGD	5.03	1.45	1.33
23	B	601	CLA	CHC-C1C	5.02	1.48	1.38
23	a	404[A]	CLA	C3C-C2C	5.02	1.47	1.36
24	d	405	BCR	C23-C22	-5.02	1.35	1.45
23	B	602	CLA	CHC-C1C	5.01	1.48	1.38
23	A	405[B]	CLA	C3C-C2C	5.01	1.47	1.36
23	B	615	CLA	C3C-C2C	5.01	1.47	1.36
31	A	416[B]	PHO	OBD-CAD	5.01	1.29	1.22
23	B	615	CLA	O2D-CGD	5.01	1.45	1.33
23	B	604	CLA	O2D-CGD	5.01	1.45	1.33
40	V	201	HEC	FE-ND	5.00	2.10	1.94
23	A	406[B]	CLA	CHC-C1C	5.00	1.48	1.38
23	b	603	CLA	O2D-CGD	5.00	1.45	1.33
23	A	404[B]	CLA	CHC-C1C	5.00	1.48	1.38
23	b	613	CLA	CHC-C1C	5.00	1.48	1.38
23	b	609	CLA	C3C-C2C	5.00	1.47	1.36
23	c	502	CLA	CHC-C1C	4.99	1.48	1.38
23	b	611	CLA	C3C-C2C	4.99	1.47	1.36
23	B	605	CLA	C1D-ND	4.99	1.43	1.37
23	b	613	CLA	C1D-ND	4.99	1.43	1.37
23	c	513	CLA	C1D-ND	4.99	1.43	1.37
23	d	402[B]	CLA	O2D-CGD	4.99	1.45	1.33
23	c	507	CLA	C1D-ND	4.98	1.43	1.37
23	B	616	CLA	C3C-C2C	4.98	1.47	1.36
23	b	601	CLA	O2D-CGD	4.98	1.45	1.33
23	b	616	CLA	C1D-ND	4.98	1.43	1.37
24	T	102	BCR	C23-C22	-4.98	1.35	1.45
23	b	609	CLA	CHC-C1C	4.97	1.48	1.38
23	C	503	CLA	O2D-CGD	4.97	1.45	1.33
23	D	404	CLA	O2D-CGD	4.97	1.45	1.33
23	B	601	CLA	O2D-CGD	4.97	1.45	1.33
38	F	102	HEM	FE-NB	4.96	2.10	1.94
23	A	405[A]	CLA	C3C-C2C	4.96	1.47	1.36
23	a	404[B]	CLA	CHC-C1C	4.95	1.48	1.38
23	d	402[A]	CLA	O2D-CGD	4.95	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	416[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	B	607	CLA	C3C-C2C	4.95	1.47	1.36
23	C	513	CLA	C1D-ND	4.95	1.43	1.37
23	a	405[B]	CLA	O2D-CGD	4.95	1.45	1.33
23	b	615	CLA	C1D-ND	4.95	1.43	1.37
23	a	404[B]	CLA	O2D-CGD	4.95	1.45	1.33
23	A	406[A]	CLA	CHC-C1C	4.95	1.48	1.38
23	B	607	CLA	CHC-C1C	4.94	1.48	1.38
23	A	407	CLA	O2D-CGD	4.94	1.45	1.33
23	c	514	CLA	O2D-CGD	4.94	1.45	1.33
23	C	507	CLA	C3C-C2C	4.94	1.47	1.36
23	C	510	CLA	O2D-CGD	4.94	1.45	1.33
23	b	616	CLA	O2D-CGD	4.93	1.45	1.33
31	a	406[B]	PHO	O2D-CGD	4.92	1.45	1.33
23	a	405[B]	CLA	CHC-C1C	4.92	1.48	1.38
31	D	401[A]	PHO	O2D-CGD	4.91	1.45	1.33
24	t	102	BCR	C23-C22	-4.90	1.35	1.45
31	D	401[B]	PHO	O2D-CGD	4.90	1.45	1.33
23	c	504	CLA	CHC-C1C	4.89	1.48	1.38
23	B	616	CLA	C1D-ND	4.89	1.43	1.37
23	b	613	CLA	C3C-C2C	4.89	1.47	1.36
23	b	616	CLA	C3C-C2C	4.89	1.47	1.36
23	c	507	CLA	O2D-CGD	4.88	1.45	1.33
23	b	601	CLA	O2A-CGA	4.88	1.47	1.33
23	D	403[A]	CLA	O2D-CGD	4.88	1.45	1.33
23	b	608	CLA	O2D-CGD	4.88	1.45	1.33
25	X	101	SQD	O47-C7	4.87	1.48	1.34
23	C	505	CLA	O2D-CGD	4.87	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	4.86	1.45	1.33
23	D	404	CLA	CHC-C1C	4.86	1.48	1.38
23	B	603	CLA	C1D-ND	4.86	1.43	1.37
23	B	608	CLA	C3C-C2C	4.85	1.47	1.36
23	b	604	CLA	C3C-C2C	4.85	1.47	1.36
23	C	504	CLA	CHC-C1C	4.85	1.48	1.38
23	c	503	CLA	O2D-CGD	4.84	1.45	1.33
31	a	415[A]	PHO	O2D-CGD	4.84	1.45	1.33
23	D	403[B]	CLA	O2D-CGD	4.84	1.45	1.33
23	A	405[B]	CLA	C1D-ND	4.83	1.43	1.37
23	B	608	CLA	C1D-ND	4.83	1.43	1.37
23	B	605	CLA	CHC-C1C	4.82	1.48	1.38
31	D	401[B]	PHO	C3D-C2D	4.82	1.48	1.39
23	b	611	CLA	O2D-CGD	4.82	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	C1D-ND	4.82	1.43	1.37
23	c	508	CLA	O2D-CGD	4.82	1.45	1.33
23	A	405[B]	CLA	O2D-CGD	4.82	1.45	1.33
23	b	610	CLA	O2D-CGD	4.82	1.45	1.33
23	d	404	CLA	CHC-C1C	4.81	1.48	1.38
23	b	603	CLA	CHC-C1C	4.81	1.48	1.38
23	A	407	CLA	C3C-C2C	4.81	1.47	1.36
23	C	502	CLA	CHC-C1C	4.81	1.48	1.38
23	b	615	CLA	CHC-C1C	4.80	1.48	1.38
23	B	610	CLA	O2D-CGD	4.80	1.44	1.33
23	c	508	CLA	CHC-C1C	4.80	1.48	1.38
23	B	603	CLA	O2D-CGD	4.79	1.44	1.33
31	D	401[A]	PHO	C3D-C2D	4.79	1.48	1.39
23	c	508	CLA	C1D-ND	4.78	1.43	1.37
23	c	506	CLA	CHC-C1C	4.78	1.48	1.38
34	c	521	LMG	O7-C10	4.78	1.47	1.34
24	D	405	BCR	C23-C22	-4.78	1.35	1.45
23	d	403[B]	CLA	O2D-CGD	4.77	1.44	1.33
23	A	404[A]	CLA	O2D-CGD	4.77	1.44	1.33
23	b	608	CLA	C3C-C2C	4.77	1.46	1.36
23	C	512	CLA	C3C-C2C	4.77	1.46	1.36
23	C	506	CLA	O2D-CGD	4.75	1.44	1.33
23	c	504	CLA	CHD-C1D	4.75	1.47	1.38
23	B	609	CLA	CHC-C1C	4.74	1.48	1.38
23	C	514	CLA	O2D-CGD	4.74	1.44	1.33
23	C	505	CLA	CHC-C1C	4.74	1.48	1.38
23	B	611	CLA	O2D-CGD	4.74	1.44	1.33
23	C	502	CLA	C1D-ND	4.74	1.43	1.37
23	C	513	CLA	O2D-CGD	4.74	1.44	1.33
23	B	613	CLA	C1B-NB	-4.73	1.32	1.37
23	b	602	CLA	C1D-ND	4.73	1.43	1.37
23	A	406[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	C	507	CLA	O2D-CGD	4.72	1.44	1.33
25	a	411	SQD	O48-C23	4.72	1.47	1.33
23	d	404	CLA	O2D-CGD	4.72	1.44	1.33
23	B	610	CLA	CHC-C1C	4.72	1.48	1.38
24	C	516	BCR	C23-C22	-4.72	1.35	1.45
24	c	515	BCR	C23-C22	-4.71	1.35	1.45
23	B	616	CLA	CHC-C1C	4.71	1.48	1.38
23	b	614	CLA	CHC-C1C	4.71	1.48	1.38
23	C	506	CLA	CHC-C1C	4.71	1.48	1.38
23	b	607	CLA	CHC-C1C	4.71	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CHC-C1C	4.70	1.48	1.38
23	B	613	CLA	CHC-C1C	4.70	1.48	1.38
23	B	606	CLA	O2D-CGD	4.69	1.44	1.33
23	C	503	CLA	C3C-C2C	4.68	1.46	1.36
23	b	605	CLA	C1D-ND	4.68	1.43	1.37
23	b	602	CLA	CHD-C1D	4.67	1.47	1.38
23	B	616	CLA	O2D-CGD	4.67	1.44	1.33
23	b	605	CLA	O2D-CGD	4.67	1.44	1.33
23	B	606	CLA	CHC-C1C	4.67	1.48	1.38
34	C	521	LMG	O7-C10	4.66	1.47	1.34
23	b	612	CLA	C1D-ND	4.66	1.43	1.37
23	C	508	CLA	CHC-C1C	4.65	1.48	1.38
23	B	602	CLA	O2D-CGD	4.65	1.44	1.33
23	C	503	CLA	CHC-C1C	4.65	1.48	1.38
25	f	102	SQD	O47-C7	4.65	1.47	1.34
23	a	405[A]	CLA	O2D-CGD	4.65	1.44	1.33
23	B	609	CLA	O2D-CGD	4.65	1.44	1.33
23	b	614	CLA	C1D-ND	4.65	1.43	1.37
23	c	511	CLA	CHC-C1C	4.64	1.48	1.38
23	d	402[B]	CLA	CHC-C1C	4.64	1.48	1.38
24	b	619	BCR	C23-C22	-4.64	1.36	1.45
31	D	401[B]	PHO	OBD-CAD	4.64	1.28	1.22
23	a	404[A]	CLA	CHC-C1C	4.64	1.47	1.38
23	B	601	CLA	C1D-ND	4.64	1.43	1.37
23	a	407	CLA	O2D-CGD	4.64	1.44	1.33
24	B	619	BCR	C23-C22	-4.64	1.36	1.45
23	C	511	CLA	O2D-CGD	4.63	1.44	1.33
23	B	615	CLA	CHC-C1C	4.63	1.47	1.38
23	b	604	CLA	CHC-C1C	4.63	1.47	1.38
23	c	506	CLA	O2D-CGD	4.62	1.44	1.33
25	l	101	SQD	O47-C7	4.62	1.47	1.34
24	y	101	BCR	C23-C22	-4.62	1.36	1.45
23	b	606	CLA	O2D-CGD	4.62	1.44	1.33
38	f	101	HEM	FE-NB	4.62	2.09	1.94
23	c	512	CLA	CHB-C1B	4.61	1.49	1.39
23	c	514	CLA	CHC-C1C	4.61	1.47	1.38
23	c	512	CLA	CHC-C1C	4.61	1.47	1.38
23	A	405[A]	CLA	CHC-C1C	4.61	1.47	1.38
23	a	405[A]	CLA	CHC-C1C	4.61	1.47	1.38
23	C	504	CLA	O2D-CGD	4.60	1.44	1.33
23	B	613	CLA	C3C-C2C	4.59	1.46	1.36
23	b	616	CLA	CHC-C1C	4.59	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	C1D-ND	4.59	1.43	1.37
23	B	606	CLA	C1D-ND	4.59	1.43	1.37
23	d	403[A]	CLA	O2D-CGD	4.59	1.44	1.33
23	a	407	CLA	O2A-CGA	4.58	1.46	1.33
23	c	514	CLA	CHD-C1D	4.58	1.47	1.38
24	A	408	BCR	C23-C22	-4.57	1.36	1.45
33	E	101[A]	LHG	O8-C23	4.57	1.46	1.33
23	b	603	CLA	C1D-ND	4.57	1.43	1.37
23	B	609	CLA	CHD-C1D	4.57	1.47	1.38
23	c	508	CLA	O2A-CGA	4.57	1.46	1.33
23	b	607	CLA	O2D-CGD	4.56	1.44	1.33
34	C	521	LMG	O8-C28	4.55	1.46	1.33
23	A	405[A]	CLA	C1D-ND	4.55	1.43	1.37
23	A	406[B]	CLA	CHD-C1D	4.54	1.47	1.38
23	D	403[A]	CLA	CHC-C1C	4.54	1.47	1.38
23	b	601	CLA	CHC-C1C	4.54	1.47	1.38
23	B	613	CLA	O2D-CGD	4.54	1.44	1.33
34	z	101	LMG	O8-C28	4.54	1.46	1.33
24	c	516	BCR	C23-C22	-4.54	1.36	1.45
23	c	510	CLA	C1D-ND	4.53	1.43	1.37
31	a	406[B]	PHO	OBD-CAD	4.52	1.28	1.22
23	b	612	CLA	O2D-CGD	4.52	1.44	1.33
23	C	512	CLA	CHC-C1C	4.51	1.47	1.38
23	c	513	CLA	O2D-CGD	4.50	1.44	1.33
23	B	611	CLA	C4B-NB	-4.50	1.32	1.37
23	b	604	CLA	O2D-CGD	4.50	1.44	1.33
33	a	419[A]	LHG	O8-C23	4.50	1.46	1.33
23	b	611	CLA	C1D-ND	4.50	1.43	1.37
23	b	606	CLA	CHC-C1C	4.49	1.47	1.38
24	b	618	BCR	C23-C22	-4.49	1.36	1.45
23	C	510	CLA	CHD-C1D	4.49	1.47	1.38
23	B	615	CLA	CHD-C1D	4.48	1.47	1.38
23	C	514	CLA	CHC-C1C	4.48	1.47	1.38
23	a	405[A]	CLA	C1D-ND	4.48	1.43	1.37
23	c	512	CLA	CHD-C1D	4.48	1.47	1.38
23	A	404[A]	CLA	CHC-C1C	4.48	1.47	1.38
24	b	617	BCR	C23-C22	-4.48	1.36	1.45
23	c	512	CLA	O2D-CGD	4.48	1.44	1.33
23	d	402[B]	CLA	O2A-CGA	4.48	1.46	1.33
23	C	506	CLA	C1D-ND	4.47	1.43	1.37
23	A	405[B]	CLA	CHC-C1C	4.47	1.47	1.38
23	C	506	CLA	CHD-C1D	4.47	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	E	101[B]	LHG	O8-C23	4.47	1.46	1.33
23	B	608	CLA	O2D-CGD	4.47	1.44	1.33
23	c	503	CLA	CHC-C1C	4.47	1.47	1.38
23	b	601	CLA	CHD-C1D	4.47	1.47	1.38
23	B	604	CLA	CHD-C1D	4.45	1.47	1.38
23	b	604	CLA	CHD-C1D	4.45	1.47	1.38
23	C	513	CLA	CHC-C4B	4.44	1.49	1.39
23	C	503	CLA	C3D-C2D	4.44	1.51	1.39
25	A	411	SQD	O48-C23	4.44	1.46	1.33
23	d	402[A]	CLA	CHC-C1C	4.44	1.47	1.38
24	H	101	BCR	C23-C22	-4.44	1.36	1.45
24	Y	101	BCR	C23-C22	-4.43	1.36	1.45
23	b	608	CLA	CHC-C1C	4.43	1.47	1.38
23	b	614	CLA	O2D-CGD	4.42	1.44	1.33
23	B	609	CLA	O2A-CGA	4.42	1.46	1.33
23	c	514	CLA	O2A-CGA	4.42	1.46	1.33
25	b	620	SQD	O48-C23	4.41	1.46	1.33
23	d	403[B]	CLA	C1D-ND	4.40	1.43	1.37
23	C	503	CLA	CHD-C1D	4.40	1.46	1.38
23	D	403[B]	CLA	O2A-CGA	4.40	1.46	1.33
23	B	602	CLA	C1D-ND	4.39	1.43	1.37
23	a	404[A]	CLA	O2D-CGD	4.38	1.43	1.33
23	b	610	CLA	CHC-C4B	4.38	1.49	1.39
23	c	506	CLA	C1D-ND	4.38	1.43	1.37
24	a	408	BCR	C23-C22	-4.37	1.36	1.45
24	h	101	BCR	C23-C22	-4.37	1.36	1.45
23	B	609	CLA	C1D-ND	4.37	1.43	1.37
23	c	502	CLA	O2D-CGD	4.37	1.43	1.33
25	b	620	SQD	O47-C7	4.37	1.46	1.34
23	C	502	CLA	O2D-CGD	4.37	1.43	1.33
23	C	509	CLA	CHC-C1C	4.36	1.47	1.38
23	B	616	CLA	C3D-C2D	4.35	1.51	1.39
23	C	507	CLA	CHD-C1D	4.35	1.46	1.38
23	c	513	CLA	O2A-CGA	4.35	1.46	1.33
23	B	612	CLA	O2D-CGD	4.35	1.43	1.33
33	a	419[B]	LHG	O8-C23	4.35	1.46	1.33
23	C	507	CLA	C1D-ND	4.35	1.43	1.37
23	B	611	CLA	CHC-C4B	4.34	1.49	1.39
23	b	612	CLA	CHB-C1B	4.34	1.49	1.39
23	A	406[A]	CLA	C1B-NB	-4.33	1.32	1.37
23	C	511	CLA	CHC-C1C	4.33	1.47	1.38
24	B	617	BCR	C23-C22	-4.33	1.36	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	CHD-C4C	4.32	1.49	1.39
23	C	514	CLA	O2A-CGA	4.32	1.46	1.33
23	c	507	CLA	CHD-C1D	4.32	1.46	1.38
23	d	403[B]	CLA	O2A-CGA	4.32	1.46	1.33
23	d	404	CLA	O2A-CGA	4.31	1.45	1.33
34	m	101	LMG	O8-C28	4.31	1.45	1.33
23	d	402[A]	CLA	C3D-C2D	4.30	1.50	1.39
23	A	407	CLA	O2A-CGA	4.30	1.45	1.33
23	d	403[B]	CLA	CHD-C1D	4.30	1.46	1.38
23	C	508	CLA	O2D-CGD	4.29	1.43	1.33
23	c	513	CLA	CHD-C1D	4.29	1.46	1.38
23	B	611	CLA	OBD-CAD	4.29	1.29	1.22
23	C	510	CLA	C3D-C2D	4.29	1.50	1.39
33	a	419[A]	LHG	O7-C7	4.28	1.46	1.34
34	B	620	LMG	O8-C28	4.28	1.45	1.33
23	b	608	CLA	C1D-ND	4.28	1.43	1.37
23	A	404[B]	CLA	CHD-C1D	4.28	1.46	1.38
23	c	507	CLA	O2A-CGA	4.28	1.45	1.33
34	C	520	LMG	O8-C28	4.27	1.45	1.33
23	c	505	CLA	CHD-C1D	4.27	1.46	1.38
23	D	404	CLA	CHD-C1D	4.27	1.46	1.38
23	B	606	CLA	CHB-C1B	4.26	1.49	1.39
23	a	405[B]	CLA	O2A-CGA	4.26	1.45	1.33
23	C	504	CLA	C1D-ND	4.26	1.43	1.37
25	f	102	SQD	O48-C23	4.26	1.45	1.33
23	B	614	CLA	O2D-CGD	4.26	1.43	1.33
23	D	403[A]	CLA	C1D-ND	4.25	1.43	1.37
34	c	521	LMG	O8-C28	4.25	1.45	1.33
23	b	602	CLA	CHC-C4B	4.24	1.48	1.39
23	C	512	CLA	C1D-ND	4.24	1.43	1.37
23	c	505	CLA	C3D-C2D	4.24	1.50	1.39
23	A	405[B]	CLA	O2A-CGA	4.23	1.45	1.33
23	B	605	CLA	CHC-C4B	4.23	1.48	1.39
23	B	616	CLA	CHB-C1B	4.23	1.48	1.39
23	C	508	CLA	O2A-CGA	4.23	1.45	1.33
23	d	402[B]	CLA	C3D-C2D	4.22	1.50	1.39
40	v	201	HEC	FE-ND	4.22	2.07	1.94
23	C	508	CLA	CHD-C1D	4.22	1.46	1.38
23	c	512	CLA	O2A-CGA	4.22	1.45	1.33
23	c	510	CLA	C1B-NB	-4.22	1.32	1.37
23	b	601	CLA	C3D-C2D	4.22	1.50	1.39
33	E	101[A]	LHG	O7-C7	4.22	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	CHD-C1D	4.21	1.46	1.38
23	d	403[A]	CLA	CHC-C1C	4.21	1.47	1.38
23	A	407	CLA	CHD-C1D	4.20	1.46	1.38
25	A	411	SQD	O47-C7	4.20	1.46	1.34
23	c	506	CLA	CHD-C1D	4.20	1.46	1.38
23	c	502	CLA	CHD-C1D	4.20	1.46	1.38
23	C	512	CLA	O2A-CGA	4.20	1.45	1.33
23	B	608	CLA	C4B-NB	-4.20	1.32	1.37
23	A	404[B]	CLA	CHD-C4C	4.20	1.48	1.39
23	b	611	CLA	O2A-CGA	4.20	1.45	1.33
23	B	603	CLA	C3D-C2D	4.20	1.50	1.39
23	c	508	CLA	CHD-C1D	4.19	1.46	1.38
33	d	408[A]	LHG	O8-C23	4.19	1.45	1.33
23	A	405[B]	CLA	CHD-C1D	4.19	1.46	1.38
33	a	419[B]	LHG	O7-C7	4.19	1.46	1.34
23	D	403[A]	CLA	CHD-C1D	4.19	1.46	1.38
23	b	609	CLA	OBD-CAD	4.19	1.29	1.22
38	f	101	HEM	FE-NC	4.19	2.09	1.95
36	c	517[B]	DGD	O2G-C1B	4.19	1.46	1.34
23	D	403[A]	CLA	O2A-CGA	4.18	1.45	1.33
23	b	608	CLA	C3D-C2D	4.18	1.50	1.39
33	E	101[B]	LHG	O7-C7	4.18	1.46	1.34
34	Z	101	LMG	O7-C10	4.18	1.46	1.34
23	c	507	CLA	CHC-C1C	4.18	1.47	1.38
23	b	610	CLA	CHB-C1B	4.18	1.48	1.39
23	C	510	CLA	OBD-CAD	4.18	1.29	1.22
33	d	408[B]	LHG	O8-C23	4.18	1.45	1.33
23	d	402[B]	CLA	CHD-C1D	4.18	1.46	1.38
23	c	503	CLA	C3D-C2D	4.17	1.50	1.39
23	C	509	CLA	C3D-C2D	4.17	1.50	1.39
23	d	404	CLA	CHD-C1D	4.17	1.46	1.38
23	c	509	CLA	O2A-CGA	4.16	1.45	1.33
23	D	404	CLA	CHC-C4B	4.16	1.48	1.39
23	C	514	CLA	CHD-C1D	4.15	1.46	1.38
33	L	101[B]	LHG	O8-C23	4.15	1.45	1.33
23	c	505	CLA	CHC-C1C	4.15	1.47	1.38
23	B	607	CLA	CHD-C1D	4.15	1.46	1.38
23	a	404[B]	CLA	CHD-C4C	4.14	1.48	1.39
23	c	507	CLA	C3D-C2D	4.14	1.50	1.39
23	b	611	CLA	CHC-C1C	4.14	1.46	1.38
23	b	608	CLA	O2A-CGA	4.14	1.45	1.33
23	c	503	CLA	O2A-CGA	4.14	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CHD-C4C	4.13	1.48	1.39
23	C	502	CLA	CHD-C1D	4.13	1.46	1.38
36	C	517[B]	DGD	O2G-C1B	4.13	1.46	1.34
36	C	517[A]	DGD	O2G-C1B	4.13	1.46	1.34
31	D	401[A]	PHO	OBD-CAD	4.13	1.28	1.22
25	l	101	SQD	O48-C23	4.13	1.45	1.33
23	c	503	CLA	CHD-C1D	4.13	1.46	1.38
23	D	404	CLA	CHB-C1B	4.13	1.48	1.39
23	b	607	CLA	C1B-NB	-4.13	1.32	1.37
23	d	403[B]	CLA	CHB-C1B	4.12	1.48	1.39
23	c	514	CLA	CHD-C4C	4.12	1.48	1.39
23	C	507	CLA	CHC-C1C	4.12	1.46	1.38
23	B	614	CLA	CHC-C1C	4.12	1.46	1.38
23	B	610	CLA	C3D-C2D	4.12	1.50	1.39
23	d	402[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	c	509	CLA	C3D-C2D	4.12	1.50	1.39
23	b	603	CLA	CHD-C1D	4.11	1.46	1.38
23	a	404[A]	CLA	CHD-C1D	4.11	1.46	1.38
23	B	609	CLA	C3D-C2D	4.11	1.50	1.39
23	b	609	CLA	CHD-C1D	4.11	1.46	1.38
23	d	402[A]	CLA	C1B-NB	-4.11	1.32	1.37
23	b	608	CLA	OBD-CAD	4.11	1.29	1.22
23	B	603	CLA	C1B-NB	-4.11	1.32	1.37
23	A	406[A]	CLA	CHD-C1D	4.10	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.10	1.50	1.39
36	c	519	DGD	O1G-C1A	4.10	1.45	1.33
23	D	403[B]	CLA	CHC-C1C	4.10	1.46	1.38
23	a	404[A]	CLA	CHD-C4C	4.10	1.48	1.39
23	c	502	CLA	CHD-C4C	4.10	1.48	1.39
36	c	518[B]	DGD	O1G-C1A	4.09	1.45	1.33
23	b	613	CLA	C3D-C2D	4.09	1.50	1.39
25	a	409[B]	SQD	O48-C23	4.09	1.45	1.33
23	c	509	CLA	CHD-C1D	4.09	1.46	1.38
23	A	406[A]	CLA	C1D-ND	4.09	1.42	1.37
34	C	501	LMG	O7-C10	4.09	1.45	1.34
23	B	601	CLA	CHC-C4B	4.09	1.48	1.39
23	b	610	CLA	CHD-C1D	4.09	1.46	1.38
23	B	607	CLA	O2D-CGD	4.09	1.43	1.33
23	B	604	CLA	CHC-C1C	4.09	1.46	1.38
23	C	514	CLA	CHD-C4C	4.09	1.48	1.39
23	A	405[B]	CLA	C3D-C2D	4.08	1.50	1.39
34	z	101	LMG	O7-C10	4.08	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	CHD-C1D	4.08	1.46	1.38
23	b	616	CLA	O2A-CGA	4.08	1.45	1.33
23	b	606	CLA	CHD-C1D	4.08	1.46	1.38
23	a	405[B]	CLA	C3D-C2D	4.08	1.50	1.39
23	b	608	CLA	CHD-C1D	4.07	1.46	1.38
23	a	404[B]	CLA	O2A-CGA	4.07	1.45	1.33
23	A	405[A]	CLA	O2A-CGA	4.07	1.45	1.33
23	B	612	CLA	CHD-C1D	4.07	1.46	1.38
23	C	513	CLA	CHD-C1D	4.07	1.46	1.38
23	c	512	CLA	CHD-C4C	4.07	1.48	1.39
23	b	606	CLA	CHD-C4C	4.07	1.48	1.39
34	C	520	LMG	O7-C10	4.07	1.45	1.34
23	b	615	CLA	O2A-CGA	4.07	1.45	1.33
23	B	607	CLA	CHB-C1B	4.07	1.48	1.39
33	D	408[B]	LHG	O7-C7	4.07	1.45	1.34
23	c	506	CLA	CHC-C4B	4.06	1.48	1.39
23	c	506	CLA	OBD-CAD	4.06	1.29	1.22
23	B	614	CLA	C4B-NB	-4.06	1.32	1.37
23	b	605	CLA	CHC-C1C	4.06	1.46	1.38
23	C	505	CLA	C1D-ND	4.06	1.42	1.37
23	b	610	CLA	CHD-C4C	4.06	1.48	1.39
23	c	511	CLA	CHB-C1B	4.06	1.48	1.39
23	b	607	CLA	CHD-C1D	4.06	1.46	1.38
23	B	610	CLA	OBD-CAD	4.06	1.29	1.22
23	C	506	CLA	CHC-C4B	4.05	1.48	1.39
23	C	504	CLA	CHC-C4B	4.05	1.48	1.39
23	D	403[B]	CLA	CHD-C1D	4.05	1.46	1.38
34	c	501	LMG	O8-C28	4.05	1.45	1.33
23	b	612	CLA	CHC-C1C	4.05	1.46	1.38
23	C	508	CLA	C1D-ND	4.05	1.42	1.37
25	a	409[A]	SQD	O47-C7	4.05	1.45	1.34
23	c	508	CLA	CHD-C4C	4.05	1.48	1.39
23	c	511	CLA	CHD-C4C	4.05	1.48	1.39
23	c	513	CLA	CHD-C4C	4.04	1.48	1.39
23	A	407	CLA	C1D-ND	4.04	1.42	1.37
23	C	512	CLA	CHD-C1D	4.04	1.46	1.38
23	C	509	CLA	O2A-CGA	4.04	1.45	1.33
23	C	513	CLA	O2A-CGA	4.04	1.45	1.33
34	c	520	LMG	O7-C10	4.04	1.45	1.34
23	B	615	CLA	CHB-C1B	4.04	1.48	1.39
23	b	605	CLA	CHD-C1D	4.03	1.46	1.38
23	b	611	CLA	CHB-C1B	4.03	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	CHD-C4C	4.03	1.48	1.39
33	d	414[B]	LHG	O8-C23	4.03	1.45	1.33
23	a	404[B]	CLA	CHD-C1D	4.03	1.46	1.38
23	B	615	CLA	O2A-CGA	4.03	1.45	1.33
23	C	510	CLA	CHC-C1C	4.03	1.46	1.38
36	C	519	DGD	O1G-C1A	4.03	1.45	1.33
23	c	507	CLA	CHD-C4C	4.03	1.48	1.39
23	b	616	CLA	CHD-C1D	4.03	1.46	1.38
23	B	612	CLA	CHB-C1B	4.03	1.48	1.39
23	b	614	CLA	CHC-C4B	4.03	1.48	1.39
23	b	609	CLA	CHB-C1B	4.02	1.48	1.39
23	D	403[A]	CLA	CHB-C1B	4.02	1.48	1.39
23	b	603	CLA	CHC-C4B	4.02	1.48	1.39
23	c	504	CLA	CHB-C1B	4.02	1.48	1.39
31	A	416[A]	PHO	O2A-CGA	4.02	1.45	1.33
25	X	101	SQD	O48-C23	4.02	1.45	1.33
23	B	615	CLA	CHD-C4C	4.01	1.48	1.39
23	C	514	CLA	C3D-C2D	4.01	1.50	1.39
38	F	102	HEM	FE-NC	4.01	2.08	1.95
23	a	404[A]	CLA	CHB-C1B	4.01	1.48	1.39
23	c	504	CLA	CHC-C4B	4.01	1.48	1.39
23	b	614	CLA	CHB-C1B	4.01	1.48	1.39
23	D	403[B]	CLA	C1D-ND	4.01	1.42	1.37
23	d	403[B]	CLA	CHC-C1C	4.01	1.46	1.38
23	B	601	CLA	CHD-C1D	4.00	1.46	1.38
36	c	518[A]	DGD	O1G-C1A	4.00	1.45	1.33
34	c	520	LMG	O8-C28	4.00	1.45	1.33
23	a	405[B]	CLA	CHD-C1D	4.00	1.46	1.38
23	A	406[B]	CLA	CHC-C4B	4.00	1.48	1.39
23	B	602	CLA	CHC-C4B	4.00	1.48	1.39
23	b	609	CLA	C1D-ND	3.99	1.42	1.37
23	B	614	CLA	CHD-C4C	3.99	1.48	1.39
23	B	611	CLA	C3B-C2B	3.99	1.54	1.41
23	b	613	CLA	CHB-C1B	3.99	1.48	1.39
23	d	403[A]	CLA	CHB-C1B	3.99	1.48	1.39
23	d	403[B]	CLA	CHD-C4C	3.99	1.48	1.39
31	D	401[B]	PHO	O2A-CGA	3.98	1.45	1.33
23	C	510	CLA	CHB-C1B	3.98	1.48	1.39
23	C	507	CLA	O2A-CGA	3.98	1.45	1.33
23	B	611	CLA	CHB-C1B	3.98	1.48	1.39
34	d	412	LMG	O7-C10	3.98	1.45	1.34
23	A	405[B]	CLA	CHD-C4C	3.98	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409[B]	SQD	O48-C23	3.98	1.45	1.33
23	b	601	CLA	CHD-C4C	3.97	1.48	1.39
23	A	405[A]	CLA	CHD-C1D	3.97	1.46	1.38
23	a	407	CLA	CHB-C1B	3.97	1.48	1.39
25	a	409[A]	SQD	O48-C23	3.97	1.44	1.33
25	a	409[B]	SQD	O47-C7	3.97	1.45	1.34
23	B	615	CLA	CHC-C4B	3.97	1.48	1.39
23	B	611	CLA	CHD-C1D	3.97	1.46	1.38
34	B	620	LMG	O7-C10	3.97	1.45	1.34
23	B	610	CLA	CHB-C1B	3.97	1.48	1.39
23	C	513	CLA	C3D-C2D	3.97	1.50	1.39
23	c	506	CLA	CHB-C1B	3.97	1.48	1.39
23	c	514	CLA	C3D-C2D	3.97	1.50	1.39
23	c	509	CLA	OBD-CAD	3.97	1.29	1.22
23	c	508	CLA	CHC-C4B	3.96	1.48	1.39
23	c	510	CLA	CHD-C1D	3.96	1.46	1.38
23	b	612	CLA	OBD-CAD	3.96	1.29	1.22
23	b	615	CLA	C3D-C2D	3.96	1.49	1.39
23	C	509	CLA	CHB-C1B	3.96	1.48	1.39
23	a	405[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	a	405[A]	CLA	C3D-C2D	3.96	1.49	1.39
23	B	612	CLA	C1D-ND	3.96	1.42	1.37
23	A	406[B]	CLA	O2A-CGA	3.96	1.44	1.33
23	d	403[A]	CLA	O2A-CGA	3.96	1.44	1.33
24	B	618	BCR	C23-C22	-3.95	1.37	1.45
34	c	501	LMG	O7-C10	3.95	1.45	1.34
23	c	511	CLA	CHD-C1D	3.95	1.46	1.38
23	C	512	CLA	C3D-C2D	3.95	1.49	1.39
23	d	404	CLA	C3D-C2D	3.95	1.49	1.39
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	c	504	CLA	CHD-C4C	3.95	1.48	1.39
23	A	406[A]	CLA	C3D-C2D	3.95	1.49	1.39
23	c	506	CLA	O2A-CGA	3.95	1.44	1.33
23	C	503	CLA	CHD-C4C	3.95	1.48	1.39
23	B	608	CLA	CHC-C1C	3.94	1.46	1.38
23	B	603	CLA	O2A-CGA	3.94	1.44	1.33
34	C	501	LMG	O8-C28	3.94	1.44	1.33
23	B	605	CLA	CHD-C4C	3.94	1.48	1.39
23	B	614	CLA	O2A-CGA	3.94	1.44	1.33
23	C	507	CLA	CHD-C4C	3.93	1.48	1.39
23	D	404	CLA	C3D-C2D	3.93	1.49	1.39
23	b	604	CLA	CHC-C4B	3.93	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	CHB-C1B	3.93	1.48	1.39
23	B	614	CLA	CHB-C1B	3.93	1.48	1.39
33	b	629[B]	LHG	O7-C7	3.93	1.45	1.34
23	B	602	CLA	C3D-C2D	3.93	1.49	1.39
33	b	629[B]	LHG	O8-C23	3.93	1.44	1.33
36	c	517[B]	DGD	O1G-C1A	3.93	1.44	1.33
23	d	403[A]	CLA	CHD-C1D	3.93	1.46	1.38
31	a	415[B]	PHO	O2A-CGA	3.92	1.44	1.33
23	C	503	CLA	O2A-CGA	3.92	1.44	1.33
23	C	504	CLA	CHD-C1D	3.92	1.46	1.38
23	b	605	CLA	CHD-C4C	3.92	1.48	1.39
23	c	513	CLA	CHC-C4B	3.92	1.48	1.39
23	B	604	CLA	C1D-ND	3.92	1.42	1.37
23	C	503	CLA	CHB-C1B	3.92	1.48	1.39
33	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
23	B	602	CLA	CHD-C1D	3.91	1.46	1.38
23	B	609	CLA	CHC-C4B	3.91	1.48	1.39
40	v	201	HEC	FE-NB	3.91	2.07	1.94
33	L	101[B]	LHG	O7-C7	3.91	1.45	1.34
33	D	408[A]	LHG	O8-C23	3.91	1.44	1.33
36	C	518[B]	DGD	O1G-C1A	3.91	1.44	1.33
36	C	518[B]	DGD	O2G-C1B	3.90	1.45	1.34
23	B	605	CLA	CHD-C1D	3.90	1.46	1.38
33	d	407[A]	LHG	O7-C7	3.90	1.45	1.34
23	b	614	CLA	C3D-C2D	3.90	1.49	1.39
23	B	604	CLA	CHB-C1B	3.90	1.48	1.39
36	h	102	DGD	O2G-C1B	3.90	1.45	1.34
31	A	416[B]	PHO	O2A-CGA	3.89	1.44	1.33
33	D	408[A]	LHG	O7-C7	3.89	1.45	1.34
23	C	506	CLA	CHD-C4C	3.89	1.48	1.39
23	B	608	CLA	C3D-C2D	3.89	1.49	1.39
36	c	518[B]	DGD	O2G-C1B	3.89	1.45	1.34
23	c	511	CLA	C3D-C2D	3.89	1.49	1.39
23	B	613	CLA	CHD-C1D	3.88	1.45	1.38
23	C	510	CLA	O2A-CGA	3.88	1.44	1.33
23	A	406[B]	CLA	OBD-CAD	3.88	1.29	1.22
23	C	511	CLA	CHB-C1B	3.88	1.48	1.39
23	b	611	CLA	CHD-C1D	3.88	1.45	1.38
23	A	406[B]	CLA	C3D-C2D	3.88	1.49	1.39
23	C	511	CLA	CHD-C4C	3.88	1.48	1.39
31	a	406[A]	PHO	OBD-CAD	3.87	1.27	1.22
23	b	607	CLA	C1D-ND	3.87	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C1B-NB	-3.87	1.33	1.37
23	c	510	CLA	CHC-C1C	3.86	1.46	1.38
23	B	603	CLA	CHC-C4B	3.86	1.48	1.39
23	B	606	CLA	CHD-C1D	3.86	1.45	1.38
23	C	504	CLA	CHB-C1B	3.86	1.48	1.39
35	b	622	HTG	C1'-S1	-3.86	1.76	1.81
23	b	606	CLA	O2A-CGA	3.85	1.44	1.33
23	D	404	CLA	OBD-CAD	3.85	1.29	1.22
23	d	402[B]	CLA	CHD-C4C	3.85	1.48	1.39
23	c	510	CLA	CHB-C1B	3.85	1.48	1.39
25	a	411	SQD	O47-C7	3.85	1.45	1.34
23	c	503	CLA	CHD-C4C	3.85	1.48	1.39
23	B	616	CLA	CHD-C1D	3.85	1.45	1.38
23	B	611	CLA	C1C-C2C	3.85	1.52	1.44
23	c	510	CLA	CHD-C4C	3.85	1.48	1.39
23	B	611	CLA	O2A-CGA	3.85	1.44	1.33
23	C	510	CLA	CHD-C4C	3.85	1.48	1.39
23	b	603	CLA	C3D-C2D	3.85	1.49	1.39
23	b	609	CLA	O2A-CGA	3.85	1.44	1.33
23	B	603	CLA	CHB-C1B	3.85	1.48	1.39
23	C	503	CLA	CHC-C4B	3.84	1.48	1.39
23	a	407	CLA	CHC-C4B	3.84	1.48	1.39
31	a	415[A]	PHO	O2A-CGA	3.84	1.44	1.33
34	d	412	LMG	O8-C28	3.84	1.44	1.33
36	C	518[A]	DGD	O2G-C1B	3.84	1.45	1.34
23	d	402[A]	CLA	OBD-CAD	3.84	1.29	1.22
23	B	609	CLA	CHD-C4C	3.84	1.48	1.39
23	A	404[B]	CLA	O2A-CGA	3.84	1.44	1.33
23	A	404[B]	CLA	OBD-CAD	3.84	1.29	1.22
33	d	407[B]	LHG	O7-C7	3.84	1.45	1.34
23	a	405[B]	CLA	CHD-C4C	3.84	1.48	1.39
23	B	608	CLA	CHB-C1B	3.83	1.48	1.39
23	c	502	CLA	O2A-CGA	3.83	1.44	1.33
23	b	606	CLA	OBD-CAD	3.83	1.29	1.22
23	c	508	CLA	CHB-C1B	3.83	1.48	1.39
23	C	509	CLA	CHD-C1D	3.83	1.45	1.38
23	c	504	CLA	O2A-CGA	3.83	1.44	1.33
23	b	610	CLA	OBD-CAD	3.83	1.29	1.22
23	c	505	CLA	O2A-CGA	3.83	1.44	1.33
23	b	605	CLA	C1B-NB	-3.83	1.33	1.37
23	d	402[B]	CLA	OBD-CAD	3.83	1.29	1.22
23	C	510	CLA	C4B-NB	-3.82	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C3D-C2D	3.82	1.49	1.39
23	C	505	CLA	C3D-C2D	3.82	1.49	1.39
23	b	607	CLA	C3D-C2D	3.82	1.49	1.39
23	c	507	CLA	CHB-C1B	3.82	1.48	1.39
23	b	616	CLA	C3D-C2D	3.82	1.49	1.39
23	D	403[B]	CLA	CHD-C4C	3.82	1.48	1.39
23	B	616	CLA	O2A-CGA	3.82	1.44	1.33
23	B	607	CLA	C1B-NB	-3.82	1.33	1.37
23	D	403[B]	CLA	CHB-C1B	3.82	1.48	1.39
23	b	612	CLA	O2A-CGA	3.82	1.44	1.33
23	c	510	CLA	O2A-CGA	3.82	1.44	1.33
23	C	509	CLA	OBD-CAD	3.81	1.29	1.22
23	c	513	CLA	CHB-C1B	3.81	1.48	1.39
36	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34
23	b	609	CLA	CHD-C4C	3.81	1.47	1.39
33	A	418[B]	LHG	O8-C23	3.81	1.44	1.33
23	b	608	CLA	CHD-C4C	3.81	1.47	1.39
23	C	504	CLA	CHD-C4C	3.81	1.47	1.39
23	A	404[A]	CLA	C3D-C2D	3.81	1.49	1.39
23	b	615	CLA	CHC-C4B	3.80	1.47	1.39
23	C	511	CLA	C3D-C2D	3.80	1.49	1.39
23	B	610	CLA	CHD-C1D	3.80	1.45	1.38
23	D	403[B]	CLA	C3D-C2D	3.80	1.49	1.39
23	c	502	CLA	CHC-C4B	3.80	1.47	1.39
23	b	604	CLA	C3D-C2D	3.80	1.49	1.39
33	D	408[B]	LHG	O8-C23	3.80	1.44	1.33
23	A	404[A]	CLA	CHB-C1B	3.80	1.47	1.39
23	B	602	CLA	CHB-C1B	3.80	1.47	1.39
23	b	612	CLA	CHD-C1D	3.79	1.45	1.38
23	c	504	CLA	O2D-CGD	3.79	1.42	1.33
36	C	517[B]	DGD	O1G-C1A	3.79	1.44	1.33
33	d	414[B]	LHG	O7-C7	3.79	1.45	1.34
36	C	518[A]	DGD	O1G-C1A	3.79	1.44	1.33
23	A	405[A]	CLA	CHD-C4C	3.79	1.47	1.39
23	c	512	CLA	C3D-C2D	3.79	1.49	1.39
23	c	509	CLA	CHB-C1B	3.79	1.47	1.39
23	D	404	CLA	CHD-C4C	3.79	1.47	1.39
23	a	405[A]	CLA	CHD-C4C	3.79	1.47	1.39
23	c	502	CLA	CHB-C1B	3.78	1.47	1.39
23	b	604	CLA	C1B-NB	-3.78	1.33	1.37
33	d	408[B]	LHG	O7-C7	3.78	1.45	1.34
23	C	505	CLA	O2A-CGA	3.78	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	CHD-C4C	3.78	1.47	1.39
23	c	510	CLA	C3D-C2D	3.78	1.49	1.39
23	C	506	CLA	CHB-C1B	3.78	1.47	1.39
36	c	517[A]	DGD	O1G-C1A	3.78	1.44	1.33
23	c	502	CLA	C3D-C2D	3.78	1.49	1.39
23	b	602	CLA	C3B-C4B	3.77	1.51	1.42
35	B	623	HTG	C1'-S1	-3.77	1.76	1.81
23	B	605	CLA	O2A-CGA	3.77	1.44	1.33
31	D	401[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	b	616	CLA	CHC-C4B	3.77	1.47	1.39
23	c	509	CLA	CHD-C4C	3.77	1.47	1.39
23	A	405[A]	CLA	CHC-C4B	3.76	1.47	1.39
23	B	602	CLA	O2A-CGA	3.76	1.44	1.33
23	C	502	CLA	O2A-CGA	3.76	1.44	1.33
25	A	409[A]	SQD	O48-C23	3.76	1.44	1.33
23	b	611	CLA	C3D-C2D	3.76	1.49	1.39
23	C	508	CLA	CHC-C4B	3.76	1.47	1.39
23	b	604	CLA	OBD-CAD	3.75	1.28	1.22
23	b	602	CLA	C3D-C2D	3.75	1.49	1.39
23	b	609	CLA	CHC-C4B	3.75	1.47	1.39
23	C	508	CLA	CHB-C1B	3.75	1.47	1.39
23	B	613	CLA	CHB-C1B	3.75	1.47	1.39
23	b	615	CLA	CHD-C1D	3.75	1.45	1.38
23	b	607	CLA	CHB-C1B	3.75	1.47	1.39
23	C	502	CLA	CHC-C4B	3.75	1.47	1.39
23	A	407	CLA	C3D-C2D	3.75	1.49	1.39
34	m	101	LMG	O7-C10	3.74	1.44	1.34
23	c	505	CLA	CHD-C4C	3.74	1.47	1.39
23	C	505	CLA	CHD-C1D	3.74	1.45	1.38
23	b	605	CLA	C3D-C2D	3.74	1.49	1.39
23	c	506	CLA	CHD-C4C	3.74	1.47	1.39
23	a	404[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	b	609	CLA	C3D-C2D	3.74	1.49	1.39
23	B	606	CLA	O2A-CGA	3.73	1.44	1.33
23	B	603	CLA	CHC-C1C	3.73	1.46	1.38
23	b	612	CLA	C1B-NB	-3.73	1.33	1.37
23	A	406[A]	CLA	O2A-CGA	3.73	1.44	1.33
33	D	407[B]	LHG	O7-C7	3.73	1.44	1.34
23	C	511	CLA	CHD-C1D	3.73	1.45	1.38
23	c	508	CLA	C3D-C2D	3.73	1.49	1.39
23	B	601	CLA	C3D-C2D	3.73	1.49	1.39
23	c	513	CLA	C3D-C2D	3.73	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	OBD-CAD	3.73	1.28	1.22
23	B	613	CLA	C3D-C2D	3.72	1.49	1.39
23	b	602	CLA	OBD-CAD	3.72	1.28	1.22
23	b	615	CLA	OBD-CAD	3.72	1.28	1.22
23	d	402[B]	CLA	CHC-C4B	3.72	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.72	1.49	1.39
23	b	610	CLA	C3D-C2D	3.72	1.49	1.39
36	h	102	DGD	O1G-C1A	3.72	1.44	1.33
23	a	404[B]	CLA	CHB-C1B	3.72	1.47	1.39
23	C	514	CLA	CHB-C1B	3.72	1.47	1.39
23	C	514	CLA	OBD-CAD	3.71	1.28	1.22
38	f	101	HEM	C4D-ND	-3.71	1.33	1.40
36	H	102	DGD	O1G-C1A	3.71	1.44	1.33
23	B	615	CLA	C3D-C2D	3.71	1.49	1.39
33	D	407[B]	LHG	O8-C23	3.71	1.44	1.33
35	o	301	HTG	C1'-S1	-3.71	1.76	1.81
33	A	418[B]	LHG	O7-C7	3.71	1.44	1.34
23	A	406[A]	CLA	CHD-C4C	3.70	1.47	1.39
23	C	508	CLA	C3D-C2D	3.70	1.49	1.39
23	c	513	CLA	OBD-CAD	3.70	1.28	1.22
33	d	407[B]	LHG	O8-C23	3.70	1.44	1.33
23	b	604	CLA	O2A-CGA	3.70	1.44	1.33
23	b	608	CLA	CHB-C1B	3.70	1.47	1.39
23	c	514	CLA	CHB-C1B	3.70	1.47	1.39
23	A	404[A]	CLA	CHD-C1D	3.70	1.45	1.38
23	c	508	CLA	OBD-CAD	3.69	1.28	1.22
23	b	613	CLA	CHC-C4B	3.69	1.47	1.39
23	b	605	CLA	OBD-CAD	3.69	1.28	1.22
23	C	512	CLA	C4B-NB	-3.69	1.33	1.37
31	a	406[B]	PHO	O2A-CGA	3.69	1.44	1.33
23	B	607	CLA	CHD-C4C	3.69	1.47	1.39
23	d	404	CLA	OBD-CAD	3.69	1.28	1.22
23	C	503	CLA	OBD-CAD	3.68	1.28	1.22
23	B	604	CLA	OBD-CAD	3.68	1.28	1.22
23	B	614	CLA	CHC-C4B	3.68	1.47	1.39
23	c	514	CLA	CHC-C4B	3.68	1.47	1.39
23	b	602	CLA	O2A-CGA	3.68	1.44	1.33
23	C	512	CLA	CHB-C1B	3.68	1.47	1.39
23	B	612	CLA	C1B-NB	-3.68	1.33	1.37
33	L	101[A]	LHG	O7-C7	3.68	1.44	1.34
25	A	409[A]	SQD	O47-C7	3.68	1.44	1.34
23	A	405[B]	CLA	CHB-C1B	3.68	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	c	519	DGD	O2G-C1B	3.68	1.44	1.34
23	B	612	CLA	C4B-NB	-3.68	1.33	1.37
23	A	407	CLA	CHC-C1C	3.68	1.46	1.38
23	B	606	CLA	CHC-C4B	3.68	1.47	1.39
23	a	404[B]	CLA	OBD-CAD	3.68	1.28	1.22
23	C	513	CLA	CHD-C4C	3.68	1.47	1.39
23	A	404[B]	CLA	CHB-C1B	3.68	1.47	1.39
33	d	408[A]	LHG	O7-C7	3.68	1.44	1.34
23	b	615	CLA	CHD-C4C	3.67	1.47	1.39
23	b	606	CLA	C3D-C2D	3.67	1.49	1.39
23	b	603	CLA	CHB-C1B	3.67	1.47	1.39
23	a	404[A]	CLA	C3D-C2D	3.67	1.49	1.39
23	B	603	CLA	OBD-CAD	3.67	1.28	1.22
23	A	405[B]	CLA	CHC-C4B	3.67	1.47	1.39
23	c	511	CLA	O2A-CGA	3.67	1.44	1.33
23	A	404[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	B	604	CLA	CHD-C4C	3.67	1.47	1.39
33	D	407[A]	LHG	O7-C7	3.66	1.44	1.34
23	c	505	CLA	OBD-CAD	3.66	1.28	1.22
23	B	612	CLA	O2A-CGA	3.66	1.44	1.33
23	b	613	CLA	CHD-C4C	3.66	1.47	1.39
23	C	511	CLA	O2A-CGA	3.66	1.44	1.33
36	C	517[A]	DGD	O1G-C1A	3.65	1.44	1.33
23	A	405[A]	CLA	CHB-C1B	3.65	1.47	1.39
23	C	509	CLA	CHD-C4C	3.65	1.47	1.39
23	B	609	CLA	C1B-NB	-3.65	1.33	1.37
23	C	514	CLA	C4B-NB	-3.65	1.33	1.37
23	d	402[A]	CLA	CHD-C1D	3.65	1.45	1.38
23	b	604	CLA	CHD-C4C	3.65	1.47	1.39
23	b	612	CLA	C3D-C2D	3.65	1.49	1.39
33	d	414[A]	LHG	O8-C23	3.64	1.44	1.33
23	D	403[A]	CLA	CHD-C4C	3.64	1.47	1.39
23	b	608	CLA	C1B-NB	-3.64	1.33	1.37
23	A	406[A]	CLA	CHC-C4B	3.64	1.47	1.39
23	B	608	CLA	O2A-CGA	3.64	1.44	1.33
23	a	405[B]	CLA	OBD-CAD	3.64	1.28	1.22
23	C	502	CLA	CHD-C4C	3.64	1.47	1.39
23	B	609	CLA	OBD-CAD	3.63	1.28	1.22
23	B	605	CLA	CHB-C1B	3.63	1.47	1.39
23	b	614	CLA	O2A-CGA	3.63	1.44	1.33
23	d	403[B]	CLA	C4B-NB	-3.63	1.33	1.37
31	A	416[A]	PHO	CHA-CBD	-3.63	1.47	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	CHD-C4C	3.63	1.47	1.39
23	b	613	CLA	CHD-C1D	3.63	1.45	1.38
23	a	404[B]	CLA	C3D-C2D	3.62	1.49	1.39
23	B	612	CLA	CHC-C4B	3.62	1.47	1.39
23	b	601	CLA	CHB-C1B	3.62	1.47	1.39
23	a	407	CLA	CHD-C1D	3.62	1.45	1.38
23	B	609	CLA	CHB-C1B	3.62	1.47	1.39
23	B	611	CLA	CHD-C4C	3.62	1.47	1.39
23	c	503	CLA	CHB-C1B	3.62	1.47	1.39
23	d	403[A]	CLA	C1D-ND	3.61	1.42	1.37
23	c	506	CLA	C3D-C2D	3.61	1.49	1.39
23	A	407	CLA	CHB-C1B	3.61	1.47	1.39
23	B	613	CLA	OBD-CAD	3.61	1.28	1.22
23	a	405[A]	CLA	CHD-C1D	3.61	1.45	1.38
23	b	614	CLA	CHD-C4C	3.61	1.47	1.39
23	b	603	CLA	CHD-C4C	3.61	1.47	1.39
23	d	403[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	615	CLA	CHB-C1B	3.61	1.47	1.39
23	B	612	CLA	C3D-C2D	3.61	1.49	1.39
33	b	629[A]	LHG	O7-C7	3.60	1.44	1.34
35	b	623	HTG	C1'-S1	-3.60	1.76	1.81
23	A	406[A]	CLA	CHB-C1B	3.60	1.47	1.39
33	D	407[A]	LHG	O8-C23	3.60	1.43	1.33
23	D	403[B]	CLA	CHC-C4B	3.60	1.47	1.39
23	b	611	CLA	CHC-C4B	3.60	1.47	1.39
23	d	403[A]	CLA	CHD-C4C	3.60	1.47	1.39
23	A	405[B]	CLA	OBD-CAD	3.60	1.28	1.22
33	A	418[A]	LHG	O7-C7	3.60	1.44	1.34
23	B	607	CLA	CHC-C4B	3.59	1.47	1.39
23	C	508	CLA	CHD-C4C	3.59	1.47	1.39
23	C	506	CLA	C3D-C2D	3.59	1.48	1.39
23	B	603	CLA	CHD-C4C	3.59	1.47	1.39
23	b	604	CLA	CHB-C1B	3.59	1.47	1.39
23	B	605	CLA	C3D-C2D	3.59	1.48	1.39
23	c	512	CLA	OBD-CAD	3.58	1.28	1.22
23	a	407	CLA	CHD-C4C	3.58	1.47	1.39
23	B	607	CLA	C1D-ND	3.58	1.42	1.37
23	d	403[B]	CLA	C3D-C2D	3.58	1.48	1.39
23	b	613	CLA	O2A-CGA	3.58	1.43	1.33
33	d	407[A]	LHG	O8-C23	3.58	1.43	1.33
23	C	507	CLA	CHB-C1B	3.58	1.47	1.39
23	d	404	CLA	CHC-C4B	3.57	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	H	102	DGD	O2G-C1B	3.57	1.44	1.34
23	c	511	CLA	CHC-C4B	3.57	1.47	1.39
23	C	507	CLA	C3D-C2D	3.57	1.48	1.39
25	A	409[B]	SQD	O47-C7	3.57	1.44	1.34
23	A	404[B]	CLA	C1B-NB	-3.57	1.33	1.37
23	B	606	CLA	C3D-C2D	3.57	1.48	1.39
23	c	507	CLA	OBD-CAD	3.56	1.28	1.22
23	A	404[A]	CLA	C4B-NB	-3.56	1.33	1.37
23	C	503	CLA	C4B-NB	-3.56	1.33	1.37
23	A	407	CLA	C1B-NB	-3.56	1.33	1.37
23	c	509	CLA	CHC-C4B	3.56	1.47	1.39
23	C	505	CLA	CHC-C4B	3.56	1.47	1.39
23	a	404[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	C	506	CLA	O2A-CGA	3.55	1.43	1.33
23	a	405[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	D	403[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	b	606	CLA	CHC-C4B	3.54	1.47	1.39
36	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	B	601	CLA	CHD-C4C	3.53	1.47	1.39
23	d	403[A]	CLA	C3D-C2D	3.53	1.48	1.39
23	B	615	CLA	OBD-CAD	3.53	1.28	1.22
23	c	503	CLA	C4B-NB	-3.53	1.33	1.37
23	B	609	CLA	C3B-C4B	3.53	1.51	1.42
23	A	406[B]	CLA	C1B-NB	-3.53	1.33	1.37
23	C	512	CLA	CHC-C4B	3.53	1.47	1.39
23	C	505	CLA	CHD-C4C	3.52	1.47	1.39
23	d	402[A]	CLA	CHD-C4C	3.52	1.47	1.39
23	b	603	CLA	OBD-CAD	3.52	1.28	1.22
23	b	601	CLA	CHC-C4B	3.52	1.47	1.39
23	B	607	CLA	O2A-CGA	3.51	1.43	1.33
23	d	402[B]	CLA	C1B-NB	-3.51	1.33	1.37
23	C	504	CLA	O2A-CGA	3.51	1.43	1.33
23	A	406[B]	CLA	C3B-C4B	3.51	1.51	1.42
33	d	414[A]	LHG	O7-C7	3.50	1.44	1.34
23	D	403[A]	CLA	CHC-C4B	3.50	1.47	1.39
23	a	405[A]	CLA	OBD-CAD	3.50	1.28	1.22
23	b	604	CLA	C4B-NB	-3.50	1.33	1.37
33	A	418[A]	LHG	O8-C23	3.49	1.43	1.33
23	b	607	CLA	CHC-C4B	3.49	1.47	1.39
23	a	405[B]	CLA	CHC-C4B	3.49	1.47	1.39
23	B	601	CLA	C3B-C4B	3.49	1.50	1.42
23	B	613	CLA	C1D-ND	3.49	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	OBD-CAD	3.49	1.28	1.22
23	d	404	CLA	CHD-C4C	3.48	1.47	1.39
23	B	607	CLA	OBD-CAD	3.48	1.28	1.22
23	B	614	CLA	CHD-C1D	3.48	1.45	1.38
23	A	405[A]	CLA	C1B-NB	-3.48	1.33	1.37
23	B	602	CLA	CHD-C4C	3.48	1.47	1.39
23	B	616	CLA	C4B-NB	-3.48	1.33	1.37
23	a	407	CLA	OBD-CAD	3.48	1.28	1.22
23	d	402[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	d	404	CLA	CHB-C1B	3.48	1.47	1.39
23	b	611	CLA	C1B-NB	-3.48	1.33	1.37
34	D	412	LMG	O8-C28	3.47	1.43	1.33
23	c	502	CLA	OBD-CAD	3.47	1.28	1.22
36	C	519	DGD	O2G-C1B	3.47	1.44	1.34
23	B	608	CLA	CHD-C4C	3.47	1.47	1.39
23	b	616	CLA	CHB-C1B	3.47	1.47	1.39
23	c	507	CLA	CHC-C4B	3.46	1.47	1.39
23	C	507	CLA	OBD-CAD	3.46	1.28	1.22
23	B	610	CLA	CHC-C4B	3.46	1.47	1.39
23	B	603	CLA	CHD-C1D	3.46	1.45	1.38
23	b	605	CLA	O2A-CGA	3.45	1.43	1.33
23	B	607	CLA	C3D-C2D	3.45	1.48	1.39
23	c	510	CLA	OBD-CAD	3.45	1.28	1.22
23	b	603	CLA	O2A-CGA	3.45	1.43	1.33
23	C	511	CLA	C4B-NB	-3.44	1.33	1.37
23	C	502	CLA	CHB-C1B	3.44	1.47	1.39
23	b	616	CLA	OBD-CAD	3.44	1.28	1.22
23	C	513	CLA	OBD-CAD	3.44	1.28	1.22
23	C	502	CLA	C3D-C2D	3.44	1.48	1.39
23	D	404	CLA	C3B-C4B	3.43	1.50	1.42
23	B	610	CLA	O2A-CGA	3.43	1.43	1.33
23	a	404[B]	CLA	CHC-C4B	3.42	1.47	1.39
23	c	514	CLA	C4B-NB	-3.42	1.33	1.37
23	a	405[B]	CLA	CHB-C1B	3.42	1.47	1.39
23	B	604	CLA	CHC-C4B	3.41	1.47	1.39
23	C	513	CLA	C3B-C4B	3.41	1.50	1.42
23	d	403[A]	CLA	C1B-NB	-3.41	1.33	1.37
23	C	504	CLA	OBD-CAD	3.40	1.28	1.22
23	b	612	CLA	CHD-C4C	3.40	1.47	1.39
23	d	402[B]	CLA	CHB-C1B	3.39	1.47	1.39
23	C	509	CLA	CHC-C4B	3.39	1.47	1.39
33	b	629[A]	LHG	O8-C23	3.39	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C1C-C2C	3.39	1.51	1.44
23	C	504	CLA	C3D-C2D	3.39	1.48	1.39
23	B	601	CLA	CHB-C1B	3.39	1.47	1.39
23	A	404[B]	CLA	C3B-C4B	3.38	1.50	1.42
23	c	505	CLA	C1B-NB	-3.38	1.33	1.37
23	b	615	CLA	C1B-NB	-3.38	1.33	1.37
38	F	102	HEM	C1B-NB	-3.38	1.34	1.40
23	C	514	CLA	CHC-C4B	3.38	1.47	1.39
23	d	403[A]	CLA	CHC-C4B	3.38	1.47	1.39
23	B	602	CLA	OBD-CAD	3.38	1.28	1.22
23	C	507	CLA	C4B-NB	-3.38	1.33	1.37
23	d	403[B]	CLA	OBD-CAD	3.37	1.28	1.22
23	B	610	CLA	CHD-C4C	3.37	1.46	1.39
23	B	613	CLA	CHC-C4B	3.37	1.47	1.39
23	A	406[A]	CLA	C3B-C4B	3.36	1.50	1.42
23	b	616	CLA	C3B-C4B	3.36	1.50	1.42
23	B	613	CLA	CHD-C4C	3.36	1.46	1.39
23	b	606	CLA	CHB-C1B	3.36	1.46	1.39
23	b	616	CLA	CHD-C4C	3.36	1.46	1.39
23	D	403[B]	CLA	OBD-CAD	3.36	1.28	1.22
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22
31	a	406[A]	PHO	O2A-CGA	3.35	1.43	1.33
23	C	506	CLA	C1B-NB	-3.35	1.33	1.37
23	c	513	CLA	C3B-C4B	3.35	1.50	1.42
23	b	607	CLA	CHD-C4C	3.35	1.46	1.39
23	C	513	CLA	CHB-C1B	3.34	1.46	1.39
23	C	507	CLA	CHC-C4B	3.34	1.46	1.39
23	b	601	CLA	C1B-NB	-3.34	1.33	1.37
23	B	614	CLA	C3D-C2D	3.34	1.48	1.39
23	B	613	CLA	O2A-CGA	3.33	1.43	1.33
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
23	A	406[B]	CLA	CHB-C1B	3.33	1.46	1.39
23	c	505	CLA	CHC-C4B	3.33	1.46	1.39
23	c	503	CLA	OBD-CAD	3.32	1.28	1.22
34	D	412	LMG	O7-C10	3.32	1.43	1.34
23	B	610	CLA	C1B-NB	-3.32	1.33	1.37
23	a	404[B]	CLA	C1B-NB	-3.32	1.33	1.37
23	D	404	CLA	O2A-CGA	3.32	1.43	1.33
23	D	404	CLA	C1C-C2C	3.32	1.51	1.44
23	b	606	CLA	C1B-NB	-3.31	1.33	1.37
23	A	407	CLA	OBD-CAD	3.31	1.28	1.22
23	c	503	CLA	CHC-C4B	3.31	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3B-C4B	3.31	1.50	1.42
23	B	616	CLA	OBD-CAD	3.31	1.28	1.22
23	B	616	CLA	CHD-C4C	3.31	1.46	1.39
23	B	611	CLA	C3B-C4B	3.31	1.50	1.42
23	B	608	CLA	OBD-CAD	3.30	1.28	1.22
23	b	602	CLA	C1B-NB	-3.30	1.33	1.37
23	B	612	CLA	OBD-CAD	3.30	1.28	1.22
23	C	511	CLA	OBD-CAD	3.29	1.28	1.22
23	C	506	CLA	C3B-C4B	3.28	1.50	1.42
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	B	615	CLA	C1C-C2C	3.28	1.50	1.44
23	a	407	CLA	C3D-C2D	3.28	1.48	1.39
23	b	612	CLA	CHC-C4B	3.27	1.46	1.39
23	b	614	CLA	C1B-NB	-3.27	1.33	1.37
23	A	407	CLA	CHC-C4B	3.27	1.46	1.39
23	B	605	CLA	C1B-NB	-3.27	1.33	1.37
23	a	405[A]	CLA	CHC-C4B	3.27	1.46	1.39
23	b	605	CLA	CHB-C1B	3.26	1.46	1.39
23	c	505	CLA	CHB-C1B	3.26	1.46	1.39
23	B	613	CLA	C1C-C2C	3.26	1.50	1.44
23	B	605	CLA	C3B-C4B	3.26	1.50	1.42
35	D	411	HTG	C1'-S1	-3.26	1.77	1.81
23	c	504	CLA	C3B-C4B	3.26	1.50	1.42
23	b	605	CLA	CHC-C4B	3.26	1.46	1.39
23	B	604	CLA	C3D-C2D	3.25	1.48	1.39
23	C	510	CLA	C1B-NB	-3.25	1.33	1.37
23	A	407	CLA	CHD-C4C	3.25	1.46	1.39
23	c	507	CLA	C1B-NB	-3.24	1.33	1.37
23	D	403[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	c	514	CLA	OBD-CAD	3.24	1.28	1.22
23	c	506	CLA	C3B-C4B	3.24	1.50	1.42
23	c	507	CLA	C4B-NB	-3.23	1.33	1.37
23	b	608	CLA	C4B-NB	-3.23	1.33	1.37
23	d	402[A]	CLA	CHC-C4B	3.23	1.46	1.39
23	c	504	CLA	OBD-CAD	3.23	1.28	1.22
23	C	502	CLA	C1B-NB	-3.23	1.33	1.37
23	D	404	CLA	C1B-NB	-3.22	1.33	1.37
23	b	616	CLA	C1B-NB	-3.22	1.33	1.37
23	c	505	CLA	C4B-NB	-3.22	1.33	1.37
35	b	625	HTG	C1'-S1	-3.21	1.77	1.81
23	b	610	CLA	O2A-CGA	3.21	1.42	1.33
23	c	510	CLA	C1B-C2B	3.20	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	CHB-C1B	3.20	1.46	1.39
23	b	610	CLA	C3B-C4B	3.20	1.50	1.42
23	B	603	CLA	C4B-NB	-3.20	1.33	1.37
23	A	405[B]	CLA	C1B-NB	-3.20	1.33	1.37
23	B	602	CLA	C1B-NB	-3.20	1.33	1.37
23	D	403[A]	CLA	C1B-NB	-3.20	1.33	1.37
23	C	514	CLA	C1B-NB	-3.19	1.33	1.37
23	B	616	CLA	CHC-C4B	3.19	1.46	1.39
23	a	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	B	604	CLA	C1B-C2B	3.18	1.50	1.43
23	c	514	CLA	C1B-NB	-3.18	1.33	1.37
23	C	505	CLA	C1B-NB	-3.18	1.33	1.37
23	a	405[B]	CLA	C4B-NB	-3.18	1.33	1.37
23	C	506	CLA	OBD-CAD	3.18	1.28	1.22
23	A	405[A]	CLA	C3B-C4B	3.17	1.50	1.42
23	C	511	CLA	C1B-NB	-3.17	1.33	1.37
23	c	512	CLA	CHC-C4B	3.17	1.46	1.39
23	A	404[B]	CLA	CHC-C4B	3.17	1.46	1.39
23	c	508	CLA	C1B-NB	-3.16	1.33	1.37
23	C	511	CLA	CHC-C4B	3.16	1.46	1.39
23	c	510	CLA	C4B-NB	-3.16	1.33	1.37
23	C	508	CLA	C1B-NB	-3.15	1.33	1.37
38	F	102	HEM	C4D-ND	-3.15	1.34	1.40
23	B	612	CLA	CHD-C4C	3.15	1.46	1.39
23	c	506	CLA	C1B-NB	-3.15	1.33	1.37
23	b	608	CLA	CHC-C4B	3.15	1.46	1.39
23	c	511	CLA	OBD-CAD	3.14	1.27	1.22
23	c	512	CLA	C1B-C2B	3.14	1.50	1.43
23	a	407	CLA	C1D-ND	3.14	1.41	1.37
35	c	522	HTG	C1'-S1	-3.14	1.77	1.81
23	D	403[B]	CLA	C4B-NB	-3.13	1.33	1.37
23	d	403[B]	CLA	CHC-C4B	3.13	1.46	1.39
23	B	604	CLA	O2A-CGA	3.12	1.42	1.33
23	d	402[B]	CLA	C3B-C4B	3.12	1.50	1.42
38	f	101	HEM	C1B-NB	-3.11	1.34	1.40
23	b	614	CLA	C3B-C4B	3.11	1.50	1.42
23	C	504	CLA	C1B-NB	-3.10	1.34	1.37
23	b	601	CLA	C3B-C4B	3.10	1.50	1.42
23	A	404[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	c	504	CLA	C3D-C2D	3.09	1.47	1.39
35	d	411	HTG	C1'-S1	-3.09	1.77	1.81
23	d	403[A]	CLA	C4B-NB	-3.09	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	C4B-NB	-3.09	1.34	1.37
23	C	503	CLA	C1B-NB	-3.07	1.34	1.37
23	C	507	CLA	C1B-NB	-3.07	1.34	1.37
23	D	403[B]	CLA	C1B-NB	-3.06	1.34	1.37
31	A	416[B]	PHO	CHA-CBD	-3.06	1.47	1.51
23	b	609	CLA	C3B-C4B	3.06	1.49	1.42
23	B	615	CLA	C3B-C4B	3.06	1.49	1.42
23	a	404[A]	CLA	C1B-NB	-3.06	1.34	1.37
23	a	405[B]	CLA	C3B-C4B	3.05	1.49	1.42
23	B	601	CLA	C1C-C2C	3.05	1.50	1.44
23	a	404[A]	CLA	C4B-NB	-3.05	1.34	1.37
23	b	614	CLA	OBD-CAD	3.04	1.27	1.22
23	a	405[A]	CLA	C1B-NB	-3.04	1.34	1.37
23	c	504	CLA	C1B-NB	-3.04	1.34	1.37
23	b	604	CLA	C1B-C2B	3.04	1.50	1.43
23	C	514	CLA	C1B-C2B	3.04	1.50	1.43
23	C	512	CLA	C4D-CHA	3.03	1.49	1.38
23	c	511	CLA	C3B-C4B	3.03	1.49	1.42
23	a	407	CLA	C1C-C2C	3.03	1.50	1.44
23	c	502	CLA	C1B-NB	-3.03	1.34	1.37
23	b	614	CLA	C1B-C2B	3.03	1.50	1.43
23	B	616	CLA	C1C-C2C	3.02	1.50	1.44
23	c	512	CLA	C4B-NB	-3.02	1.34	1.37
23	b	613	CLA	C4B-NB	-3.02	1.34	1.37
23	B	605	CLA	C1C-C2C	3.01	1.50	1.44
23	C	510	CLA	CHC-C4B	3.01	1.46	1.39
23	A	404[A]	CLA	CHC-C4B	3.01	1.46	1.39
23	b	612	CLA	C1B-C2B	3.01	1.50	1.43
23	C	509	CLA	C4B-NB	-3.01	1.34	1.37
35	b	625	HTG	C1-S1	-3.01	1.76	1.80
23	d	404	CLA	C3B-C4B	3.00	1.49	1.42
23	c	502	CLA	C3B-C4B	3.00	1.49	1.42
23	a	405[B]	CLA	C1B-NB	-3.00	1.34	1.37
23	C	505	CLA	OBD-CAD	3.00	1.27	1.22
23	B	610	CLA	C4B-NB	-3.00	1.34	1.37
23	c	504	CLA	C4B-NB	-2.99	1.34	1.37
23	C	504	CLA	C3B-C4B	2.99	1.49	1.42
23	a	404[B]	CLA	C3B-C4B	2.99	1.49	1.42
23	C	505	CLA	C4B-NB	-2.99	1.34	1.37
23	a	405[A]	CLA	C3B-C4B	2.98	1.49	1.42
23	a	407	CLA	C3B-C4B	2.98	1.49	1.42
23	c	508	CLA	C4B-NB	-2.97	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C4B-NB	-2.97	1.34	1.37
23	d	403[B]	CLA	C1B-C2B	2.97	1.50	1.43
23	d	403[B]	CLA	C1B-NB	-2.97	1.34	1.37
23	c	506	CLA	C1B-C2B	2.97	1.50	1.43
23	A	406[A]	CLA	C1B-C2B	2.96	1.50	1.43
23	c	503	CLA	C1B-C2B	2.96	1.50	1.43
23	C	506	CLA	C1B-C2B	2.95	1.50	1.43
23	b	607	CLA	C1B-C2B	2.95	1.50	1.43
23	c	505	CLA	C1B-C2B	2.94	1.50	1.43
23	b	613	CLA	C4D-CHA	2.94	1.48	1.38
23	C	513	CLA	C1C-C2C	2.93	1.50	1.44
23	C	511	CLA	C1B-C2B	2.93	1.50	1.43
23	B	605	CLA	C1B-C2B	2.92	1.50	1.43
23	D	404	CLA	C1B-C2B	2.92	1.50	1.43
23	b	604	CLA	C4D-CHA	2.92	1.48	1.38
23	c	508	CLA	C1C-C2C	2.92	1.50	1.44
23	c	504	CLA	C1C-C2C	2.92	1.50	1.44
23	A	405[B]	CLA	C3B-C4B	2.92	1.49	1.42
23	C	509	CLA	C1B-C2B	2.92	1.50	1.43
23	C	509	CLA	C1B-NB	-2.92	1.34	1.37
40	v	201	HEC	FE-NC	2.91	2.05	1.95
23	b	602	CLA	C1C-C2C	2.91	1.50	1.44
23	B	608	CLA	C1B-C2B	2.91	1.50	1.43
23	B	616	CLA	C4D-CHA	2.91	1.48	1.38
23	a	405[A]	CLA	C1C-C2C	2.91	1.50	1.44
23	b	616	CLA	C4B-NB	-2.90	1.34	1.37
23	C	502	CLA	C1C-C2C	2.90	1.50	1.44
23	b	607	CLA	O2A-CGA	2.90	1.41	1.33
23	c	510	CLA	CHC-C4B	2.90	1.45	1.39
23	b	611	CLA	C4B-NB	-2.89	1.34	1.37
23	c	513	CLA	C1B-NB	-2.89	1.34	1.37
23	B	610	CLA	C3B-C4B	2.88	1.49	1.42
23	b	603	CLA	C3B-C4B	2.88	1.49	1.42
23	B	614	CLA	C1B-NB	-2.88	1.34	1.37
23	b	612	CLA	C4B-NB	-2.88	1.34	1.37
23	c	511	CLA	C1B-C2B	2.88	1.50	1.43
23	a	407	CLA	C1B-NB	-2.88	1.34	1.37
23	C	502	CLA	C1B-C2B	2.87	1.50	1.43
32	M	101	LMT	O2'-C2'	-2.87	1.36	1.43
23	c	514	CLA	C3B-C4B	2.86	1.49	1.42
23	D	403[A]	CLA	C4B-NB	-2.86	1.34	1.37
23	B	614	CLA	OBD-CAD	2.86	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C4C-C3C	2.86	1.50	1.45
23	a	407	CLA	C1B-C2B	2.86	1.50	1.43
35	C	522	HTG	C1'-S1	-2.86	1.77	1.81
23	C	505	CLA	C1B-C2B	2.85	1.50	1.43
23	b	610	CLA	C1B-NB	-2.85	1.34	1.37
23	c	509	CLA	C1B-C2B	2.84	1.50	1.43
23	C	508	CLA	C4D-CHA	2.84	1.48	1.38
23	A	404[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	B	604	CLA	C1B-NB	-2.84	1.34	1.37
23	d	402[A]	CLA	C3B-C4B	2.84	1.49	1.42
23	b	601	CLA	C4B-NB	-2.84	1.34	1.37
23	C	505	CLA	C4D-CHA	2.83	1.48	1.38
23	b	606	CLA	C4B-NB	-2.83	1.34	1.37
23	b	606	CLA	C3B-C4B	2.83	1.49	1.42
23	B	602	CLA	C3B-C4B	2.83	1.49	1.42
23	b	608	CLA	C1C-C2C	2.82	1.50	1.44
23	c	509	CLA	C4D-CHA	2.81	1.48	1.38
23	b	611	CLA	OBD-CAD	2.81	1.27	1.22
23	b	614	CLA	C4B-NB	-2.81	1.34	1.37
23	b	609	CLA	C1B-NB	-2.81	1.34	1.37
28	A	413[A]	PL9	C6-C5	2.81	1.49	1.35
23	B	616	CLA	C1B-NB	-2.81	1.34	1.37
23	D	403[B]	CLA	C1B-C2B	2.80	1.49	1.43
23	c	507	CLA	C1B-C2B	2.80	1.49	1.43
25	a	409[B]	SQD	C6-S	-2.80	1.67	1.77
23	b	614	CLA	C1C-C2C	2.80	1.50	1.44
23	C	503	CLA	C3B-C4B	2.80	1.49	1.42
23	c	510	CLA	C4C-C3C	2.80	1.49	1.45
23	B	607	CLA	C4D-CHA	2.80	1.48	1.38
23	A	405[B]	CLA	C1B-C2B	2.80	1.49	1.43
23	B	606	CLA	OBD-CAD	2.80	1.27	1.22
23	B	612	CLA	C3B-C2B	2.80	1.50	1.41
23	C	512	CLA	OBD-CAD	2.79	1.27	1.22
23	B	614	CLA	C1B-C2B	2.79	1.49	1.43
23	D	403[A]	CLA	C1B-C2B	2.79	1.49	1.43
23	d	403[A]	CLA	C4C-C3C	2.79	1.49	1.45
23	b	615	CLA	C3B-C4B	2.79	1.49	1.42
23	c	509	CLA	C3B-C4B	2.79	1.49	1.42
23	B	612	CLA	C1C-C2C	2.79	1.50	1.44
23	b	607	CLA	OBD-CAD	2.79	1.27	1.22
23	c	511	CLA	C4D-CHA	2.78	1.48	1.38
23	B	606	CLA	C3B-C4B	2.78	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	407	CLA	C1B-C2B	2.77	1.49	1.43
23	B	610	CLA	C1C-C2C	2.77	1.49	1.44
23	c	505	CLA	C1C-C2C	2.77	1.49	1.44
23	b	603	CLA	C4D-CHA	2.77	1.48	1.38
40	V	201	HEC	FE-NC	2.77	2.04	1.95
23	b	613	CLA	C1C-C2C	2.77	1.49	1.44
23	B	604	CLA	C4D-CHA	2.77	1.48	1.38
23	A	404[A]	CLA	C1B-C2B	2.76	1.49	1.43
31	D	401[A]	PHO	CBD-CGD	-2.76	1.48	1.52
23	D	404	CLA	C4C-C3C	2.76	1.49	1.45
23	B	608	CLA	CHC-C4B	2.76	1.45	1.39
25	A	409[A]	SQD	C6-S	-2.76	1.67	1.77
28	a	413[B]	PL9	C6-C5	2.75	1.49	1.35
23	C	506	CLA	C4D-CHA	2.75	1.48	1.38
23	B	602	CLA	C4B-NB	-2.74	1.34	1.37
23	a	405[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	B	608	CLA	C4D-CHA	2.74	1.48	1.38
28	a	413[A]	PL9	C6-C5	2.74	1.49	1.35
25	A	409[B]	SQD	C6-S	-2.74	1.67	1.77
23	B	612	CLA	C4C-C3C	2.74	1.49	1.45
23	B	608	CLA	C1B-NB	-2.74	1.34	1.37
23	B	613	CLA	C1B-C2B	2.74	1.49	1.43
25	a	409[A]	SQD	C6-S	-2.73	1.67	1.77
23	B	612	CLA	C4D-CHA	2.73	1.48	1.38
23	c	509	CLA	C1B-NB	-2.73	1.34	1.37
23	d	403[B]	CLA	C4C-C3C	2.73	1.49	1.45
23	d	402[A]	CLA	C4B-NB	-2.73	1.34	1.37
23	A	405[A]	CLA	C1C-C2C	2.73	1.49	1.44
23	C	511	CLA	C4C-C3C	2.73	1.49	1.45
23	C	502	CLA	C4D-CHA	2.72	1.48	1.38
23	b	605	CLA	C4D-CHA	2.72	1.48	1.38
23	b	610	CLA	C4C-C3C	2.72	1.49	1.45
23	B	608	CLA	C3B-C4B	2.72	1.49	1.42
23	C	502	CLA	OBD-CAD	2.72	1.27	1.22
23	A	405[A]	CLA	C4B-NB	-2.72	1.34	1.37
23	C	504	CLA	C4B-NB	-2.71	1.34	1.37
40	V	201	HEC	FE-NB	2.71	2.03	1.94
23	b	603	CLA	C1B-C2B	2.71	1.49	1.43
23	c	514	CLA	C1C-C2C	2.70	1.49	1.44
23	b	608	CLA	C3B-C4B	2.70	1.49	1.42
23	c	508	CLA	C4D-CHA	2.70	1.48	1.38
23	c	510	CLA	C4D-CHA	2.70	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C1C-C2C	2.70	1.49	1.44
23	C	512	CLA	C1B-NB	-2.70	1.34	1.37
23	b	609	CLA	C4D-CHA	2.70	1.48	1.38
28	A	413[B]	PL9	C6-C5	2.70	1.49	1.35
32	t	101	LMT	O3'-C3'	-2.70	1.36	1.43
23	b	611	CLA	C1C-C2C	2.70	1.49	1.44
23	b	602	CLA	C4B-NB	-2.69	1.34	1.37
23	b	603	CLA	C1C-C2C	2.69	1.49	1.44
23	c	505	CLA	C4D-CHA	2.69	1.48	1.38
23	B	611	CLA	MG-NB	2.69	2.11	2.05
23	A	405[A]	CLA	C1B-C2B	2.69	1.49	1.43
34	Z	101	LMG	O8-C28	2.69	1.46	1.33
23	b	604	CLA	C3B-C4B	2.69	1.49	1.42
23	c	504	CLA	C4D-CHA	2.69	1.48	1.38
23	B	615	CLA	C1B-C2B	2.69	1.49	1.43
23	A	405[A]	CLA	C4D-CHA	2.69	1.48	1.38
23	c	511	CLA	C1C-C2C	2.69	1.49	1.44
23	C	503	CLA	C1C-C2C	2.69	1.49	1.44
23	C	512	CLA	C1C-C2C	2.68	1.49	1.44
23	B	614	CLA	C4D-CHA	2.68	1.47	1.38
23	B	616	CLA	C3B-C2B	2.68	1.50	1.41
23	b	604	CLA	C1C-C2C	2.67	1.49	1.44
23	B	613	CLA	C4C-C3C	2.67	1.49	1.45
23	a	405[A]	CLA	C4D-CHA	2.67	1.47	1.38
23	C	508	CLA	OBD-CAD	2.67	1.27	1.22
23	a	407	CLA	C4B-NB	-2.67	1.34	1.37
32	B	626	LMT	C3'-C2'	2.67	1.59	1.52
23	a	405[A]	CLA	C1B-C2B	2.67	1.49	1.43
23	C	507	CLA	C4C-C3C	2.67	1.49	1.45
23	c	513	CLA	C1B-C2B	2.67	1.49	1.43
23	b	603	CLA	C4B-NB	-2.67	1.34	1.37
23	C	506	CLA	C4C-C3C	2.67	1.49	1.45
23	b	615	CLA	C1B-C2B	2.67	1.49	1.43
23	B	602	CLA	C1B-C2B	2.66	1.49	1.43
23	C	514	CLA	C3B-C4B	2.66	1.49	1.42
23	d	402[A]	CLA	C1B-C2B	2.66	1.49	1.43
31	a	415[B]	PHO	C3A-C2A	-2.66	1.52	1.54
25	A	411	SQD	C6-S	-2.66	1.67	1.77
23	d	404	CLA	C4B-NB	-2.65	1.34	1.37
23	c	514	CLA	C1B-C2B	2.65	1.49	1.43
23	B	609	CLA	C1B-C2B	2.65	1.49	1.43
23	a	404[B]	CLA	C1B-C2B	2.65	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C3B-C4B	2.65	1.49	1.42
23	B	616	CLA	C1B-C2B	2.65	1.49	1.43
23	C	508	CLA	C1B-C2B	2.65	1.49	1.43
23	B	615	CLA	C1B-NB	-2.65	1.34	1.37
23	c	506	CLA	C4D-CHA	2.65	1.47	1.38
23	d	404	CLA	C1C-C2C	2.64	1.49	1.44
32	A	419	LMT	O3'-C3'	-2.64	1.36	1.43
23	B	614	CLA	C3D-C4D	-2.64	1.38	1.44
23	B	608	CLA	C3D-C4D	-2.64	1.38	1.44
23	b	615	CLA	C4D-CHA	2.64	1.47	1.38
25	f	102	SQD	C6-S	-2.64	1.67	1.77
23	d	402[B]	CLA	C4B-NB	-2.63	1.34	1.37
23	c	508	CLA	C1B-C2B	2.63	1.49	1.43
23	b	607	CLA	C1C-C2C	2.63	1.49	1.44
23	b	610	CLA	C1C-C2C	2.63	1.49	1.44
23	B	613	CLA	C4D-CHA	2.63	1.47	1.38
23	B	603	CLA	C4D-CHA	2.63	1.47	1.38
23	C	510	CLA	C1B-C2B	2.62	1.49	1.43
23	b	610	CLA	C4B-NB	-2.62	1.34	1.37
25	a	411	SQD	C6-S	-2.62	1.67	1.77
23	D	403[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	C	512	CLA	C3B-C4B	2.61	1.48	1.42
23	B	614	CLA	C3B-C4B	2.61	1.48	1.42
23	B	612	CLA	C1B-C2B	2.61	1.49	1.43
40	V	201	HEC	CAC-C3C	2.61	1.57	1.51
23	b	608	CLA	C3B-C2B	2.61	1.50	1.41
23	C	509	CLA	C4C-C3C	2.61	1.49	1.45
23	c	512	CLA	C4D-CHA	2.61	1.47	1.38
23	C	514	CLA	C1C-C2C	2.60	1.49	1.44
23	B	601	CLA	C1B-NB	-2.60	1.34	1.37
23	C	507	CLA	C1B-C2B	2.60	1.49	1.43
23	d	403[A]	CLA	C4D-CHA	2.60	1.47	1.38
23	B	611	CLA	C4D-CHA	2.60	1.47	1.38
23	c	511	CLA	C1B-NB	-2.59	1.34	1.37
23	c	504	CLA	C3D-C4D	-2.59	1.38	1.44
23	B	610	CLA	C4C-C3C	2.59	1.49	1.45
23	b	607	CLA	C4B-NB	-2.59	1.34	1.37
23	c	503	CLA	C1B-NB	-2.59	1.34	1.37
23	c	503	CLA	C3B-C4B	2.59	1.48	1.42
23	c	502	CLA	C1B-C2B	2.59	1.49	1.43
23	A	406[B]	CLA	C4B-NB	-2.59	1.34	1.37
23	B	615	CLA	C4D-CHA	2.59	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C4D-CHA	2.58	1.47	1.38
23	A	404[B]	CLA	C1B-C2B	2.58	1.49	1.43
35	B	621	HTG	C1'-S1	-2.58	1.78	1.81
23	B	601	CLA	C4B-NB	-2.58	1.34	1.37
23	A	406[A]	CLA	C4D-CHA	2.58	1.47	1.38
31	a	406[A]	PHO	CBD-CGD	-2.58	1.49	1.52
23	c	504	CLA	C1B-C2B	2.58	1.49	1.43
23	C	509	CLA	C1C-C2C	2.57	1.49	1.44
23	b	610	CLA	C1B-C2B	2.57	1.49	1.43
38	f	101	HEM	C1D-ND	-2.57	1.33	1.38
23	b	609	CLA	C3D-C4D	-2.57	1.38	1.44
23	c	512	CLA	C1B-NB	-2.56	1.34	1.37
23	c	502	CLA	C4D-CHA	2.56	1.47	1.38
23	C	509	CLA	C4D-CHA	2.56	1.47	1.38
23	C	510	CLA	C4D-CHA	2.56	1.47	1.38
36	C	519	DGD	O2G-C2G	-2.56	1.40	1.46
23	A	407	CLA	C4D-CHA	2.56	1.47	1.38
23	d	402[B]	CLA	C1B-C2B	2.56	1.49	1.43
23	C	509	CLA	C3B-C2B	2.56	1.49	1.41
23	B	607	CLA	C1B-C2B	2.56	1.49	1.43
23	A	404[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	a	404[A]	CLA	C4D-CHA	2.55	1.47	1.38
23	a	405[B]	CLA	C1C-C2C	2.55	1.49	1.44
23	B	602	CLA	C4D-CHA	2.55	1.47	1.38
23	C	510	CLA	C1C-NC	-2.55	1.34	1.37
23	d	403[A]	CLA	C1C-C2C	2.55	1.49	1.44
23	C	506	CLA	C4B-NB	-2.55	1.34	1.37
23	c	502	CLA	C4C-C3C	2.55	1.49	1.45
23	A	406[A]	CLA	C4B-NB	-2.55	1.34	1.37
23	C	504	CLA	C4D-CHA	2.55	1.47	1.38
23	C	514	CLA	C4D-CHA	2.55	1.47	1.38
23	C	507	CLA	C3B-C4B	2.54	1.48	1.42
23	C	512	CLA	C3B-C2B	2.54	1.49	1.41
23	b	606	CLA	C1B-C2B	2.54	1.49	1.43
23	A	404[A]	CLA	C4D-CHA	2.54	1.47	1.38
23	C	508	CLA	C1C-C2C	2.54	1.49	1.44
23	b	606	CLA	C4D-CHA	2.54	1.47	1.38
23	A	406[B]	CLA	C1C-C2C	2.54	1.49	1.44
23	b	601	CLA	C4D-CHA	2.54	1.47	1.38
23	B	604	CLA	C4C-C3C	2.54	1.49	1.45
23	C	513	CLA	C1B-NB	-2.53	1.34	1.37
23	b	607	CLA	C4D-CHA	2.53	1.47	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	C4D-CHA	2.53	1.47	1.38
23	c	502	CLA	C3D-C4D	-2.53	1.38	1.44
25	b	620	SQD	C6-S	-2.53	1.68	1.77
23	b	613	CLA	C1B-C2B	2.53	1.49	1.43
23	d	404	CLA	C4D-CHA	2.53	1.47	1.38
34	C	521	LMG	O1-C1	2.53	1.44	1.40
23	A	405[B]	CLA	C4B-NB	-2.53	1.34	1.37
23	c	505	CLA	C4C-C3C	2.52	1.49	1.45
23	B	602	CLA	C3D-C4D	-2.52	1.38	1.44
23	C	507	CLA	C4D-CHA	2.52	1.47	1.38
23	c	514	CLA	C4D-CHA	2.52	1.47	1.38
23	d	402[A]	CLA	C4D-CHA	2.52	1.47	1.38
23	a	405[B]	CLA	C1B-C2B	2.52	1.49	1.43
23	b	613	CLA	OBD-CAD	2.52	1.26	1.22
23	c	506	CLA	C1C-C2C	2.52	1.49	1.44
23	C	510	CLA	C3B-C4B	2.52	1.48	1.42
31	a	415[A]	PHO	C3A-C2A	-2.52	1.52	1.54
23	C	506	CLA	C1C-C2C	2.52	1.49	1.44
23	C	507	CLA	C1C-C2C	2.52	1.49	1.44
23	b	612	CLA	C1C-C2C	2.52	1.49	1.44
23	a	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
23	B	609	CLA	C4D-CHA	2.51	1.47	1.38
23	B	610	CLA	C4D-CHA	2.51	1.47	1.38
23	b	612	CLA	C3B-C4B	2.51	1.48	1.42
23	C	504	CLA	C1C-C2C	2.51	1.49	1.44
23	d	403[A]	CLA	C1B-C2B	2.51	1.49	1.43
28	d	406[B]	PL9	C6-C5	2.51	1.48	1.35
23	d	404	CLA	C1B-NB	-2.51	1.34	1.37
23	B	606	CLA	C4D-CHA	2.50	1.47	1.38
23	b	614	CLA	C4D-CHA	2.50	1.47	1.38
23	c	510	CLA	C3B-C4B	2.50	1.48	1.42
23	B	606	CLA	C1C-C2C	2.50	1.49	1.44
23	b	609	CLA	C1C-C2C	2.50	1.49	1.44
23	c	509	CLA	C4C-C3C	2.50	1.49	1.45
40	v	201	HEC	CMC-C2C	2.50	1.56	1.50
23	b	603	CLA	C1B-NB	-2.50	1.34	1.37
23	b	611	CLA	C1B-C2B	2.50	1.49	1.43
23	C	513	CLA	C4D-CHA	2.50	1.47	1.38
28	D	406[A]	PL9	C6-C5	2.50	1.48	1.35
23	c	502	CLA	C1C-C2C	2.49	1.49	1.44
23	b	611	CLA	C4C-C3C	2.49	1.49	1.45
32	b	621	LMT	C3'-C2'	2.49	1.58	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	C4D-CHA	2.49	1.47	1.38
23	A	405[B]	CLA	C4D-CHA	2.49	1.47	1.38
23	C	510	CLA	C1C-C2C	2.49	1.49	1.44
23	c	509	CLA	C1C-C2C	2.49	1.49	1.44
23	b	616	CLA	C3D-C4D	-2.49	1.38	1.44
23	D	403[B]	CLA	C4D-CHA	2.49	1.47	1.38
23	a	404[B]	CLA	C1C-C2C	2.48	1.49	1.44
23	a	404[B]	CLA	C4B-NB	-2.48	1.34	1.37
23	c	507	CLA	C3B-C4B	2.48	1.48	1.42
23	a	405[B]	CLA	C4D-CHA	2.48	1.47	1.38
36	H	102	DGD	O5D-C1E	2.48	1.44	1.40
23	b	612	CLA	C4D-CHA	2.48	1.47	1.38
31	A	416[A]	PHO	C3D-C4D	-2.48	1.37	1.41
28	D	406[B]	PL9	C6-C5	2.47	1.48	1.35
23	D	403[B]	CLA	C3B-C2B	2.47	1.49	1.41
23	a	404[A]	CLA	C1C-C2C	2.47	1.49	1.44
23	a	404[A]	CLA	C1B-C2B	2.47	1.49	1.43
35	B	623	HTG	C1-S1	-2.47	1.76	1.80
23	D	403[B]	CLA	C4C-C3C	2.47	1.49	1.45
23	B	605	CLA	C3D-C4D	-2.47	1.38	1.44
23	C	512	CLA	C1B-C2B	2.47	1.49	1.43
23	B	607	CLA	C3D-C4D	-2.46	1.38	1.44
23	D	403[A]	CLA	C1C-C2C	2.46	1.49	1.44
23	D	403[B]	CLA	C3D-C4D	-2.46	1.38	1.44
23	c	507	CLA	C4C-C3C	2.46	1.49	1.45
23	B	607	CLA	C1C-C2C	2.46	1.49	1.44
23	B	607	CLA	C3B-C4B	2.46	1.48	1.42
23	C	502	CLA	C3D-C4D	-2.46	1.38	1.44
32	T	101	LMT	O3'-C3'	-2.46	1.37	1.43
23	C	508	CLA	C3D-C4D	-2.46	1.38	1.44
32	B	626	LMT	O3'-C3'	-2.46	1.37	1.43
25	X	101	SQD	C6-S	-2.45	1.68	1.77
23	c	511	CLA	C3B-C2B	2.45	1.49	1.41
23	a	404[B]	CLA	C4D-CHA	2.45	1.47	1.38
23	B	610	CLA	C1B-C2B	2.45	1.49	1.43
23	B	601	CLA	C4D-CHA	2.45	1.47	1.38
23	B	601	CLA	C1B-C2B	2.45	1.49	1.43
38	F	102	HEM	C3C-C4C	-2.45	1.41	1.46
23	b	604	CLA	C4C-C3C	2.45	1.49	1.45
23	d	403[A]	CLA	C3D-C4D	-2.45	1.38	1.44
23	A	404[B]	CLA	C4C-C3C	2.45	1.49	1.45
23	C	511	CLA	C1C-C2C	2.45	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	416[B]	PHO	C1D-ND	-2.44	1.34	1.38
38	f	101	HEM	C1C-C2C	-2.44	1.40	1.45
23	B	605	CLA	C4B-NB	-2.44	1.34	1.37
23	b	603	CLA	C3B-C2B	2.44	1.49	1.41
31	a	406[B]	PHO	C4B-NB	-2.44	1.34	1.38
23	B	603	CLA	C3B-C2B	2.44	1.49	1.41
23	b	605	CLA	C4B-NB	-2.43	1.34	1.37
23	b	601	CLA	C1C-C2C	2.43	1.49	1.44
40	v	201	HEC	CAC-C3C	2.43	1.57	1.51
25	X	101	SQD	O6-C1	2.43	1.44	1.40
23	B	605	CLA	C4D-CHA	2.43	1.47	1.38
23	C	511	CLA	C3D-C4D	-2.43	1.38	1.44
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42
23	D	403[A]	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	605	CLA	OBD-CAD	2.43	1.26	1.22
23	c	514	CLA	C4C-C3C	2.43	1.49	1.45
23	d	404	CLA	C1B-C2B	2.43	1.49	1.43
23	B	603	CLA	C4C-C3C	2.42	1.49	1.45
23	C	505	CLA	C3B-C2B	2.42	1.49	1.41
32	e	101	LMT	O3'-C3'	-2.42	1.37	1.43
32	B	629	LMT	O3'-C3'	-2.42	1.37	1.43
35	b	622	HTG	O5-C1	2.42	1.46	1.42
23	B	604	CLA	C1C-C2C	2.42	1.49	1.44
23	B	606	CLA	C1B-C2B	2.42	1.49	1.43
23	A	404[A]	CLA	C1C-C2C	2.42	1.49	1.44
23	b	616	CLA	C4D-CHA	2.42	1.47	1.38
23	C	504	CLA	C1B-C2B	2.41	1.48	1.43
23	d	403[A]	CLA	C3B-C4B	2.41	1.48	1.42
26	D	413	GOL	C3-C2	2.41	1.61	1.51
23	c	507	CLA	C4D-CHA	2.41	1.47	1.38
23	b	608	CLA	C1B-C2B	2.40	1.48	1.43
23	C	504	CLA	C3D-C4D	-2.40	1.38	1.44
31	a	415[A]	PHO	C4B-NB	-2.40	1.34	1.38
23	C	510	CLA	C3B-C2B	2.40	1.49	1.41
23	C	507	CLA	C3D-C4D	-2.40	1.38	1.44
23	b	605	CLA	C1B-C2B	2.40	1.48	1.43
23	b	612	CLA	C3B-C2B	2.40	1.49	1.41
23	B	604	CLA	C4B-NB	-2.40	1.34	1.37
23	c	510	CLA	C1C-C2C	2.40	1.49	1.44
23	B	602	CLA	C4C-C3C	2.39	1.49	1.45
23	d	403[B]	CLA	C3D-C4D	-2.39	1.38	1.44
25	l	101	SQD	C6-S	-2.39	1.68	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	611	CLA	C3D-C4D	-2.39	1.38	1.44
31	a	406[A]	PHO	C4B-NB	-2.39	1.34	1.38
23	d	403[B]	CLA	C3B-C2B	2.39	1.49	1.41
23	b	602	CLA	C4D-CHA	2.39	1.46	1.38
23	C	509	CLA	C3B-C4B	2.39	1.48	1.42
23	A	406[A]	CLA	C1C-C2C	2.39	1.49	1.44
23	A	407	CLA	C3B-C2B	2.39	1.49	1.41
23	c	503	CLA	C3B-C2B	2.39	1.49	1.41
23	C	511	CLA	C4D-CHA	2.38	1.46	1.38
23	D	403[B]	CLA	C1C-C2C	2.38	1.49	1.44
23	D	403[A]	CLA	C3B-C2B	2.38	1.49	1.41
23	C	502	CLA	C4C-C3C	2.38	1.49	1.45
31	A	416[A]	PHO	C4B-NB	-2.38	1.34	1.38
23	C	503	CLA	C1B-C2B	2.38	1.48	1.43
23	c	512	CLA	C3B-C2B	2.38	1.49	1.41
23	b	613	CLA	C3B-C2B	2.37	1.49	1.41
23	A	407	CLA	C1C-C2C	2.37	1.49	1.44
23	c	505	CLA	C3B-C4B	2.37	1.48	1.42
23	c	505	CLA	C3B-C2B	2.37	1.49	1.41
23	B	608	CLA	C4C-C3C	2.37	1.49	1.45
23	b	607	CLA	C3B-C4B	2.37	1.48	1.42
23	a	407	CLA	C4D-CHA	2.37	1.46	1.38
23	C	508	CLA	C4C-C3C	2.37	1.49	1.45
23	a	405[A]	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	607	CLA	C4C-C3C	2.36	1.49	1.45
23	b	609	CLA	C1B-C2B	2.36	1.48	1.43
31	A	416[A]	PHO	C3A-C2A	-2.36	1.52	1.54
23	b	610	CLA	C4D-CHA	2.36	1.46	1.38
31	A	416[B]	PHO	C4B-NB	-2.36	1.34	1.38
23	C	505	CLA	C3D-C4D	-2.36	1.38	1.44
23	a	404[A]	CLA	C4C-C3C	2.36	1.49	1.45
23	B	612	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	602	CLA	C3B-C2B	2.36	1.49	1.41
23	b	607	CLA	C3B-C2B	2.35	1.49	1.41
23	d	403[B]	CLA	C4D-CHA	2.35	1.46	1.38
23	b	611	CLA	C3B-C2B	2.35	1.49	1.41
23	c	510	CLA	C3B-C2B	2.35	1.49	1.41
23	A	405[B]	CLA	C1C-C2C	2.35	1.49	1.44
23	C	512	CLA	C3D-C4D	-2.34	1.38	1.44
23	a	405[B]	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	503	CLA	C3B-C2B	2.34	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	o	301	HTG	O5-C1	2.34	1.46	1.42
23	B	615	CLA	C4B-NB	-2.34	1.34	1.37
23	B	606	CLA	C1B-NB	-2.33	1.34	1.37
32	m	103	LMT	C3'-C2'	2.33	1.58	1.52
23	A	406[B]	CLA	C1B-C2B	2.33	1.48	1.43
23	c	513	CLA	C1C-C2C	2.33	1.49	1.44
38	F	102	HEM	C3B-C4B	2.33	1.49	1.44
23	b	614	CLA	C4C-C3C	2.33	1.49	1.45
23	b	603	CLA	C3D-C4D	-2.33	1.38	1.44
23	B	609	CLA	C1C-C2C	2.33	1.49	1.44
23	B	604	CLA	C3D-C4D	-2.33	1.38	1.44
32	T	101	LMT	O2'-C2'	-2.33	1.37	1.43
28	d	406[A]	PL9	C6-C5	2.33	1.47	1.35
23	B	610	CLA	C3D-C4D	-2.32	1.38	1.44
32	a	416	LMT	O3'-C3'	-2.32	1.37	1.43
23	B	603	CLA	C3B-C4B	2.32	1.48	1.42
23	B	606	CLA	C3D-C4D	-2.32	1.38	1.44
32	F	101	LMT	O3'-C3'	-2.32	1.37	1.43
23	b	606	CLA	C3D-C4D	-2.32	1.38	1.44
23	C	505	CLA	C3B-C4B	2.32	1.48	1.42
23	c	514	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	612	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	611	CLA	C4D-CHA	2.31	1.46	1.38
23	b	605	CLA	C1C-C2C	2.31	1.49	1.44
23	b	613	CLA	C3B-C4B	2.30	1.48	1.42
26	a	418	GOL	C1-C2	2.30	1.61	1.51
31	D	401[B]	PHO	CBD-CGD	-2.30	1.49	1.52
32	B	627	LMT	O2'-C2'	-2.30	1.37	1.43
23	b	605	CLA	C1D-C2D	2.30	1.49	1.45
23	c	509	CLA	C3B-C2B	2.30	1.49	1.41
23	A	405[B]	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	616	CLA	C1B-C2B	2.30	1.48	1.43
23	c	512	CLA	C1C-C2C	2.29	1.49	1.44
23	c	502	CLA	C4B-NB	-2.29	1.35	1.37
23	c	503	CLA	C4D-CHA	2.29	1.46	1.38
23	b	615	CLA	C4B-NB	-2.29	1.35	1.37
23	b	611	CLA	C3B-C4B	2.27	1.48	1.42
32	m	103	LMT	O2B-C2B	-2.27	1.37	1.43
23	B	604	CLA	C3B-C4B	2.27	1.48	1.42
23	b	601	CLA	C1B-C2B	2.27	1.48	1.43
23	C	511	CLA	C3B-C2B	2.27	1.48	1.41
23	B	616	CLA	C3B-C4B	2.27	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C4D-CHA	2.26	1.46	1.38
23	b	601	CLA	C3B-C2B	2.26	1.48	1.41
23	B	614	CLA	C1C-C2C	2.26	1.48	1.44
23	d	402[B]	CLA	C1C-C2C	2.26	1.48	1.44
23	c	505	CLA	C3D-C4D	-2.25	1.39	1.44
23	B	604	CLA	C1A-CHA	2.25	1.52	1.43
23	B	606	CLA	MG-NA	2.25	2.11	2.06
23	A	405[A]	CLA	C3D-C4D	-2.25	1.39	1.44
23	c	512	CLA	C3B-C4B	2.25	1.48	1.42
31	a	406[A]	PHO	C1D-ND	-2.25	1.34	1.38
23	c	504	CLA	C4C-C3C	2.25	1.48	1.45
31	a	415[B]	PHO	C4B-NB	-2.25	1.34	1.38
23	C	514	CLA	C3D-C4D	-2.25	1.39	1.44
23	B	613	CLA	C3B-C2B	2.24	1.48	1.41
23	b	602	CLA	C4C-C3C	2.24	1.48	1.45
32	m	103	LMT	O3'-C3'	-2.24	1.37	1.43
23	c	509	CLA	C4B-NB	-2.24	1.35	1.37
23	A	407	CLA	C3D-C4D	-2.24	1.39	1.44
23	A	407	CLA	C4C-C3C	2.23	1.48	1.45
23	B	613	CLA	C3B-C4B	2.23	1.48	1.42
23	b	611	CLA	C3D-C4D	-2.23	1.39	1.44
31	D	401[B]	PHO	C1B-NB	-2.23	1.34	1.38
23	b	610	CLA	C3D-C4D	-2.23	1.39	1.44
32	A	419	LMT	O2'-C2'	-2.23	1.37	1.43
32	a	416	LMT	O2'-C2'	-2.23	1.37	1.43
31	D	401[B]	PHO	C1D-ND	-2.23	1.34	1.38
23	b	608	CLA	C4D-CHA	2.23	1.46	1.38
23	C	513	CLA	C1B-C2B	2.23	1.48	1.43
23	C	514	CLA	C3B-C2B	2.23	1.48	1.41
23	b	607	CLA	C3D-C4D	-2.23	1.39	1.44
23	c	506	CLA	C4B-NB	-2.22	1.35	1.37
36	C	518[A]	DGD	O5D-C1E	2.22	1.44	1.40
23	B	615	CLA	C4C-C3C	2.22	1.48	1.45
23	B	613	CLA	C4B-NB	-2.22	1.35	1.37
38	F	102	HEM	C1C-C2C	-2.22	1.40	1.45
23	A	407	CLA	C1C-NC	-2.22	1.34	1.37
32	B	627	LMT	O2B-C2B	-2.22	1.37	1.43
23	c	506	CLA	C3D-C4D	-2.22	1.39	1.44
23	C	503	CLA	C3D-C4D	-2.22	1.39	1.44
36	h	102	DGD	O5D-C1E	2.21	1.44	1.40
23	c	513	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	513	CLA	C4B-NB	-2.21	1.35	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	627	LMT	O3'-C3'	-2.21	1.37	1.43
32	t	101	LMT	O2'-C2'	-2.21	1.37	1.43
23	A	404[A]	CLA	C3B-C2B	2.20	1.48	1.41
23	A	405[B]	CLA	C3B-C2B	2.20	1.48	1.41
24	d	405	BCR	C30-C25	-2.20	1.50	1.53
23	A	406[B]	CLA	C4C-C3C	2.20	1.48	1.45
23	b	608	CLA	C3D-C4D	-2.20	1.39	1.44
23	D	403[B]	CLA	C3B-C4B	2.20	1.47	1.42
31	a	406[B]	PHO	CHA-CBD	-2.20	1.49	1.51
23	d	404	CLA	C4C-C3C	2.20	1.48	1.45
23	c	504	CLA	MG-NA	2.20	2.11	2.06
23	d	404	CLA	C1D-C2D	2.20	1.49	1.45
23	D	404	CLA	C3D-C4D	-2.19	1.39	1.44
23	b	605	CLA	C1C-NC	-2.19	1.34	1.37
23	a	404[A]	CLA	C3B-C4B	2.19	1.47	1.42
23	C	507	CLA	C3B-C2B	2.19	1.48	1.41
23	b	604	CLA	C3B-C2B	2.19	1.48	1.41
23	A	406[B]	CLA	C3D-C4D	-2.19	1.39	1.44
31	A	416[B]	PHO	C3A-C2A	-2.18	1.52	1.54
23	C	514	CLA	C1C-NC	-2.18	1.34	1.37
36	c	519	DGD	O5D-C1E	2.18	1.43	1.40
32	M	101	LMT	O3'-C3'	-2.18	1.37	1.43
23	C	504	CLA	C4C-C3C	2.18	1.48	1.45
31	A	416[A]	PHO	C1D-ND	-2.18	1.34	1.38
23	D	403[A]	CLA	C4C-C3C	2.18	1.48	1.45
23	c	510	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	614	CLA	C3B-C2B	2.17	1.48	1.41
23	B	603	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	604	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
26	b	624	GOL	C3-C2	2.17	1.60	1.51
23	A	404[B]	CLA	C4B-NB	-2.17	1.35	1.37
23	a	404[B]	CLA	C3B-C2B	2.17	1.48	1.41
23	C	505	CLA	C1C-C2C	2.16	1.48	1.44
32	B	626	LMT	O4'-C4B	-2.16	1.37	1.43
23	A	404[B]	CLA	C3B-C2B	2.16	1.48	1.41
23	a	404[A]	CLA	C3B-C2B	2.16	1.48	1.41
26	D	413	GOL	O2-C2	-2.16	1.36	1.43
23	D	403[A]	CLA	C3B-C4B	2.15	1.47	1.42
23	b	602	CLA	C1B-C2B	2.15	1.48	1.43
23	b	606	CLA	C1C-C2C	2.15	1.48	1.44
23	b	607	CLA	C1A-CHA	2.15	1.52	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	616	CLA	C1C-NC	-2.15	1.34	1.37
24	B	619	BCR	C30-C25	-2.15	1.50	1.53
23	c	508	CLA	C3D-C4D	-2.15	1.39	1.44
23	d	404	CLA	C3D-C4D	-2.15	1.39	1.44
23	C	512	CLA	C4C-C3C	2.15	1.48	1.45
36	c	519	DGD	O2G-C2G	-2.15	1.41	1.46
23	c	507	CLA	C1C-C2C	2.15	1.48	1.44
23	B	608	CLA	C3B-C2B	2.15	1.48	1.41
23	C	510	CLA	C4C-C3C	2.14	1.48	1.45
23	c	514	CLA	C3B-C2B	2.14	1.48	1.41
32	T	101	LMT	O3B-C3B	-2.14	1.37	1.43
23	B	606	CLA	C4B-NB	-2.14	1.35	1.37
23	C	505	CLA	C4C-C3C	2.13	1.48	1.45
23	A	406[B]	CLA	C1D-C2D	2.13	1.49	1.45
26	a	417	GOL	C3-C2	2.13	1.60	1.51
23	A	405[B]	CLA	C4C-C3C	2.13	1.48	1.45
23	C	513	CLA	C3D-C4D	-2.13	1.39	1.44
25	l	101	SQD	O6-C1	2.13	1.43	1.40
23	b	615	CLA	C3D-C4D	-2.13	1.39	1.44
23	d	402[B]	CLA	C3D-C4D	-2.13	1.39	1.44
23	C	506	CLA	C3D-C4D	-2.12	1.39	1.44
28	a	413[A]	PL9	C2-C3	2.12	1.40	1.34
23	B	601	CLA	C3B-C2B	2.12	1.48	1.41
23	c	511	CLA	C4C-C3C	2.12	1.48	1.45
23	C	507	CLA	C1D-C2D	2.12	1.49	1.45
23	d	402[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	A	406[A]	CLA	C1C-NC	-2.12	1.34	1.37
31	D	401[B]	PHO	CHA-CBD	-2.11	1.49	1.51
31	a	415[B]	PHO	C1B-NB	-2.11	1.34	1.38
23	b	602	CLA	C1D-C2D	2.11	1.49	1.45
23	A	406[A]	CLA	C3D-C4D	-2.11	1.39	1.44
23	b	609	CLA	C3B-C2B	2.11	1.48	1.41
23	c	503	CLA	C1C-C2C	2.11	1.48	1.44
23	c	503	CLA	C4C-C3C	2.11	1.48	1.45
23	C	513	CLA	C3B-C2B	2.11	1.48	1.41
23	c	514	CLA	C1D-C2D	2.10	1.49	1.45
23	b	603	CLA	C4C-C3C	2.10	1.48	1.45
23	D	404	CLA	C4B-NB	-2.10	1.35	1.37
23	B	608	CLA	C1C-NC	-2.10	1.34	1.37
23	C	509	CLA	C3D-C4D	-2.10	1.39	1.44
23	A	404[B]	CLA	C3D-C4D	-2.10	1.39	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	B	626	LMT	O5'-C5'	-2.10	1.39	1.44
23	a	404[A]	CLA	C3D-C4D	-2.10	1.39	1.44
23	a	405[A]	CLA	C4C-C3C	2.10	1.48	1.45
23	a	404[B]	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	511	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	615	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	509	CLA	C3D-C4D	-2.09	1.39	1.44
23	B	603	CLA	C1B-C2B	2.09	1.48	1.43
26	o	304	GOL	C1-C2	2.09	1.60	1.51
26	O	303	GOL	O2-C2	-2.09	1.37	1.43
23	c	511	CLA	C4B-NB	-2.09	1.35	1.37
23	c	508	CLA	C3B-C4B	2.09	1.47	1.42
32	e	101	LMT	O2B-C2B	-2.09	1.38	1.43
23	A	404[B]	CLA	C1C-C2C	2.09	1.48	1.44
23	d	403[A]	CLA	C3B-C2B	2.09	1.48	1.41
23	b	613	CLA	C1C-NC	-2.09	1.34	1.37
23	B	601	CLA	C4C-C3C	2.08	1.48	1.45
31	a	415[A]	PHO	C1B-NB	-2.08	1.34	1.38
23	B	606	CLA	C3B-C2B	2.08	1.48	1.41
36	c	518[A]	DGD	O2G-C2G	-2.07	1.41	1.46
23	c	507	CLA	C3B-C2B	2.07	1.48	1.41
23	C	513	CLA	C4B-NB	-2.07	1.35	1.37
23	B	607	CLA	C4B-NB	-2.07	1.35	1.37
40	V	201	HEC	CMB-C2B	2.06	1.55	1.50
23	b	616	CLA	C3B-C2B	2.06	1.48	1.41
32	A	417	LMT	O4'-C4B	-2.06	1.38	1.43
23	c	507	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	601	CLA	C1C-NC	-2.06	1.34	1.37
23	a	405[B]	CLA	C3B-C2B	2.06	1.48	1.41
23	C	503	CLA	C4D-CHA	2.06	1.45	1.38
31	A	416[B]	PHO	C3D-C4D	-2.06	1.38	1.41
32	e	101	LMT	O2'-C2'	-2.05	1.38	1.43
23	C	503	CLA	C4C-C3C	2.05	1.48	1.45
23	d	402[B]	CLA	C3B-C2B	2.05	1.48	1.41
23	A	407	CLA	C3B-C4B	2.05	1.47	1.42
23	b	605	CLA	C4C-C3C	2.05	1.48	1.45
23	c	512	CLA	C4C-C3C	2.05	1.48	1.45
31	D	401[A]	PHO	C1B-NB	-2.05	1.34	1.38
26	D	402	GOL	O2-C2	-2.04	1.37	1.43
23	B	607	CLA	C3B-C2B	2.04	1.48	1.41
28	A	413[A]	PL9	C2-C1	-2.04	1.39	1.44
23	b	614	CLA	C3B-C2B	2.04	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	401[B]	PHO	C4B-NB	-2.04	1.34	1.38
26	D	402	GOL	C3-C2	2.03	1.60	1.51
23	B	607	CLA	C4C-C3C	2.03	1.48	1.45
23	b	609	CLA	C1C-NC	-2.03	1.34	1.37
23	c	502	CLA	C1D-C2D	2.03	1.49	1.45
23	A	404[A]	CLA	C3D-C4D	-2.03	1.39	1.44
40	v	201	HEC	CMD-C2D	2.03	1.55	1.50
32	B	629	LMT	O2'-C2'	-2.03	1.38	1.43
23	C	502	CLA	C3B-C2B	2.03	1.48	1.41
23	c	512	CLA	C1D-C2D	2.03	1.49	1.45
23	b	614	CLA	C3D-C4D	-2.03	1.39	1.44
23	b	615	CLA	C1C-C2C	2.03	1.48	1.44
40	V	201	HEC	CMC-C2C	2.02	1.55	1.50
23	b	610	CLA	C3B-C2B	2.02	1.48	1.41
24	B	618	BCR	C19-C18	2.02	1.50	1.45
23	c	510	CLA	C1C-NC	-2.02	1.34	1.37
32	A	417	LMT	O3'-C3'	-2.02	1.38	1.43
23	C	511	CLA	C3B-C4B	2.02	1.47	1.42
28	D	406[B]	PL9	C2-C3	2.02	1.39	1.34
23	b	601	CLA	C4C-C3C	2.02	1.48	1.45
32	e	101	LMT	O3B-C3B	-2.01	1.38	1.43
32	A	417	LMT	O2'-C2'	-2.01	1.38	1.43
23	C	508	CLA	C3B-C2B	2.01	1.48	1.41
31	a	415[B]	PHO	CHA-CBD	-2.01	1.49	1.51
40	V	201	HEC	CMD-C2D	2.01	1.55	1.50
23	b	608	CLA	C4C-C3C	2.01	1.48	1.45
23	C	512	CLA	MG-NA	2.01	2.11	2.06
23	d	403[B]	CLA	C3B-C4B	2.01	1.47	1.42
23	a	407	CLA	C3B-C2B	2.00	1.48	1.41
28	A	413[B]	PL9	C2-C3	2.00	1.39	1.34
23	b	606	CLA	C3B-C2B	2.00	1.48	1.41

All (3357) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	611	CLA	C2B-C1B-NB	15.94	120.92	110.23
23	B	611	CLA	C3B-C2B-C1B	-12.94	91.54	107.16
31	a	415[B]	PHO	C2D-C1D-ND	12.41	118.09	109.53
31	D	401[A]	PHO	C2D-C1D-ND	11.89	117.73	109.53
31	A	416[B]	PHO	C2D-C1D-ND	11.76	117.65	109.53
31	a	415[A]	PHO	C2D-C1D-ND	11.37	117.38	109.53
31	a	406[A]	PHO	C2D-C1D-ND	11.17	117.24	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	401[B]	PHO	C2D-C1D-ND	11.10	117.19	109.53
31	a	406[B]	PHO	C2D-C1D-ND	11.02	117.13	109.53
31	A	416[A]	PHO	C2D-C1D-ND	10.94	117.08	109.53
23	a	407	CLA	C1D-ND-C4D	-10.89	98.60	106.33
23	B	611	CLA	C1D-ND-C4D	-10.78	98.68	106.33
23	a	404[B]	CLA	C1D-ND-C4D	-10.23	99.07	106.33
23	B	615	CLA	C1D-ND-C4D	-10.14	99.13	106.33
23	B	611	CLA	CHB-C1B-NB	-9.99	113.68	124.26
23	b	610	CLA	C1D-ND-C4D	-9.93	99.28	106.33
23	d	404	CLA	C1D-ND-C4D	-9.92	99.29	106.33
23	c	502	CLA	C1D-ND-C4D	-9.92	99.29	106.33
23	b	605	CLA	C1D-ND-C4D	-9.82	99.36	106.33
23	C	504	CLA	C1D-ND-C4D	-9.81	99.36	106.33
23	B	601	CLA	C1D-ND-C4D	-9.81	99.37	106.33
23	B	606	CLA	C1D-ND-C4D	-9.77	99.40	106.33
23	b	602	CLA	C1D-ND-C4D	-9.75	99.41	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-9.73	99.42	106.33
23	B	607	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	D	404	CLA	C1D-ND-C4D	-9.70	99.44	106.33
23	C	505	CLA	C2D-C1D-ND	9.69	117.25	110.10
23	c	512	CLA	C1D-ND-C4D	-9.66	99.47	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	C	514	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	B	613	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	C	502	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	b	607	CLA	C1D-ND-C4D	-9.61	99.51	106.33
23	B	614	CLA	C1D-ND-C4D	-9.51	99.58	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-9.46	99.61	106.33
23	a	407	CLA	C2D-C1D-ND	9.46	117.08	110.10
23	B	607	CLA	C2D-C1D-ND	9.45	117.06	110.10
23	c	506	CLA	C1D-ND-C4D	-9.44	99.63	106.33
23	C	505	CLA	C1D-ND-C4D	-9.44	99.63	106.33
23	c	504	CLA	C1D-ND-C4D	-9.40	99.66	106.33
23	B	605	CLA	C1D-ND-C4D	-9.39	99.66	106.33
23	A	407	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	C	511	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	C	513	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	B	613	CLA	C2D-C1D-ND	9.37	117.01	110.10
23	B	616	CLA	C2D-C1D-ND	9.36	117.00	110.10
23	b	614	CLA	C2D-C1D-ND	9.35	116.99	110.10
23	c	513	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	c	514	CLA	C1D-ND-C4D	-9.34	99.70	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	B	614	CLA	C2D-C1D-ND	9.27	116.93	110.10
23	b	614	CLA	C1D-ND-C4D	-9.25	99.76	106.33
23	B	606	CLA	C2D-C1D-ND	9.24	116.91	110.10
23	c	508	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	c	507	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	C	506	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	c	511	CLA	C1D-ND-C4D	-9.19	99.80	106.33
23	b	601	CLA	C1D-ND-C4D	-9.19	99.80	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	b	613	CLA	C2D-C1D-ND	9.16	116.86	110.10
23	D	403[A]	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	b	602	CLA	C2B-C1B-NB	9.16	116.37	110.23
23	b	615	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	c	510	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	A	407	CLA	C2D-C1D-ND	9.13	116.83	110.10
23	d	403[A]	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	B	611	CLA	C2D-C1D-ND	9.09	116.80	110.10
23	A	405[B]	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	C	504	CLA	C2D-C1D-ND	9.08	116.80	110.10
23	A	406[A]	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	B	615	CLA	C2D-C1D-ND	9.07	116.79	110.10
23	d	402[A]	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	D	403[B]	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	d	402[B]	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	C	510	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	d	404	CLA	C2D-C1D-ND	8.96	116.71	110.10
23	b	606	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	C	509	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	A	405[A]	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	b	607	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	b	609	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	a	404[A]	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	B	603	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	b	611	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	B	605	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	b	603	CLA	C1D-ND-C4D	-8.78	100.10	106.33
23	d	402[A]	CLA	C2D-C1D-ND	8.75	116.56	110.10
23	B	610	CLA	C2D-C1D-ND	8.73	116.54	110.10
23	C	507	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	B	608	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	b	608	CLA	C1D-ND-C4D	-8.65	100.19	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C1D-ND-C4D	-8.65	100.19	106.33
23	a	405[A]	CLA	C2D-C1D-ND	8.65	116.48	110.10
23	B	601	CLA	C2D-C1D-ND	8.64	116.47	110.10
23	B	616	CLA	C1D-ND-C4D	-8.64	100.20	106.33
23	c	513	CLA	C2B-C1B-NB	8.63	116.02	110.23
23	C	503	CLA	C1D-ND-C4D	-8.63	100.20	106.33
23	b	605	CLA	C2D-C1D-ND	8.62	116.45	110.10
23	b	606	CLA	C2B-C1B-NB	8.61	116.01	110.23
23	c	510	CLA	C2D-C1D-ND	8.59	116.43	110.10
23	b	610	CLA	C2D-C1D-ND	8.58	116.42	110.10
23	d	403[B]	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	c	509	CLA	C1D-ND-C4D	-8.51	100.29	106.33
23	B	610	CLA	C1D-ND-C4D	-8.51	100.29	106.33
23	C	514	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	b	602	CLA	C4A-NA-C1A	-8.50	102.89	106.71
23	D	403[A]	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-8.50	100.30	106.33
23	C	509	CLA	C2D-C1D-ND	8.49	116.36	110.10
23	B	609	CLA	C1D-ND-C4D	-8.48	100.31	106.33
23	B	603	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	505	CLA	C1D-ND-C4D	-8.45	100.33	106.33
23	b	611	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	b	615	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	c	503	CLA	C1D-ND-C4D	-8.42	100.36	106.33
23	c	508	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	a	405[B]	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	B	602	CLA	C1D-ND-C4D	-8.40	100.37	106.33
23	A	406[B]	CLA	C2B-C1B-NB	8.37	115.84	110.23
23	C	513	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	a	404[B]	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	A	405[B]	CLA	C2D-C1D-ND	8.30	116.22	110.10
23	B	612	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	C	510	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	A	405[A]	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	b	616	CLA	C1D-ND-C4D	-8.25	100.48	106.33
23	C	502	CLA	C2D-C1D-ND	8.23	116.17	110.10
23	D	403[B]	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	B	608	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	b	613	CLA	C1D-ND-C4D	-8.18	100.52	106.33
23	c	507	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	c	509	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	c	502	CLA	C2D-C1D-ND	8.16	116.12	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[A]	CLA	C2D-C1D-ND	8.15	116.11	110.10
31	a	406[A]	PHO	O2D-CGD-CBD	8.14	121.31	111.00
23	D	403[B]	CLA	C4A-NA-C1A	-8.14	103.05	106.71
23	d	402[B]	CLA	C2D-C1D-ND	8.13	116.10	110.10
23	b	614	CLA	C2B-C1B-NB	8.13	115.68	110.23
23	C	512	CLA	C1D-ND-C4D	-8.11	100.57	106.33
23	d	404	CLA	C2B-C1B-NB	8.10	115.66	110.23
23	b	616	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	512	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	b	601	CLA	C2D-C1D-ND	8.04	116.03	110.10
31	a	406[B]	PHO	O2D-CGD-CBD	8.04	121.18	111.00
23	b	604	CLA	C1D-ND-C4D	-8.01	100.64	106.33
23	c	511	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	513	CLA	C2D-C1D-ND	7.95	115.97	110.10
31	D	401[B]	PHO	O2D-CGD-CBD	7.95	121.06	111.00
23	C	513	CLA	C2B-C1B-NB	7.93	115.55	110.23
23	d	402[B]	CLA	C2B-C1B-NB	7.93	115.55	110.23
23	D	404	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	B	601	CLA	C2B-C1B-NB	7.92	115.54	110.23
23	b	609	CLA	C2D-C1D-ND	7.90	115.92	110.10
23	A	406[B]	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	c	503	CLA	C2D-C1D-ND	7.84	115.88	110.10
23	B	602	CLA	C2D-C1D-ND	7.83	115.88	110.10
23	a	405[B]	CLA	C2B-C1B-NB	7.83	115.48	110.23
31	a	415[A]	PHO	O2D-CGD-CBD	7.83	120.91	111.00
23	d	403[A]	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	c	514	CLA	C2B-C1B-NB	7.80	115.46	110.23
23	c	505	CLA	C2B-C1B-NB	7.79	115.45	110.23
23	b	602	CLA	C2D-C1D-ND	7.78	115.84	110.10
23	C	512	CLA	C2D-C1D-ND	7.76	115.82	110.10
23	c	514	CLA	C2D-C1D-ND	7.75	115.81	110.10
23	C	506	CLA	C2D-C1D-ND	7.72	115.79	110.10
23	c	506	CLA	C2D-C1D-ND	7.71	115.78	110.10
23	C	503	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	b	616	CLA	C2B-C1B-NB	7.67	115.37	110.23
23	A	404[B]	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	A	404[A]	CLA	C2D-C1D-ND	7.64	115.73	110.10
35	b	623	HTG	C1'-S1-C1	7.64	114.38	100.09
23	b	606	CLA	C2D-C1D-ND	7.62	115.72	110.10
23	b	603	CLA	C2D-C1D-ND	7.60	115.71	110.10
23	c	504	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	C	508	CLA	C2D-C1D-ND	7.58	115.69	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C1D-ND-C4D	-7.57	100.96	106.33
23	B	604	CLA	C1D-ND-C4D	-7.52	100.99	106.33
23	A	406[A]	CLA	C2B-C1B-NB	7.52	115.27	110.23
23	B	611	CLA	CHD-C4C-C3C	-7.51	113.80	124.84
23	C	511	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	c	505	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	B	605	CLA	CHD-C4C-C3C	-7.51	113.81	124.84
23	B	605	CLA	CMD-C2D-C1D	7.50	137.93	124.71
23	C	514	CLA	C2B-C1B-NB	7.48	115.25	110.23
23	c	502	CLA	CMD-C2D-C1D	7.46	137.86	124.71
31	A	416[A]	PHO	C2B-C1B-NB	7.46	114.68	109.53
31	A	416[A]	PHO	O2D-CGD-CBD	7.46	120.44	111.00
23	B	615	CLA	C4A-NA-C1A	-7.44	103.36	106.71
23	B	609	CLA	C2D-C1D-ND	7.44	115.59	110.10
23	c	502	CLA	CHD-C1D-ND	-7.44	117.62	124.45
23	b	608	CLA	C2D-C1D-ND	7.43	115.58	110.10
23	B	606	CLA	CMD-C2D-C1D	7.43	137.81	124.71
23	C	507	CLA	C2D-C1D-ND	7.42	115.57	110.10
23	B	606	CLA	C4A-NA-C1A	-7.40	103.38	106.71
23	b	611	CLA	C2B-C1B-NB	7.38	115.18	110.23
23	a	404[B]	CLA	C2B-C1B-NB	7.37	115.17	110.23
23	b	601	CLA	C2B-C1B-NB	7.37	115.17	110.23
31	D	401[A]	PHO	C4D-ND-C1D	-7.35	101.35	108.83
23	C	512	CLA	C2B-C1B-NB	7.34	115.15	110.23
23	a	404[A]	CLA	C2D-C1D-ND	7.32	115.50	110.10
31	a	415[B]	PHO	C4D-ND-C1D	-7.32	101.39	108.83
23	c	511	CLA	C2B-C1B-NB	7.31	115.14	110.23
23	b	615	CLA	C2B-C1B-NB	7.30	115.13	110.23
23	c	504	CLA	CMD-C2D-C1D	7.30	137.58	124.71
25	X	101	SQD	O6-C1-C2	7.27	119.65	108.30
31	a	415[B]	PHO	O2D-CGD-CBD	7.26	120.20	111.00
23	b	612	CLA	C2D-C1D-ND	7.25	115.44	110.10
23	c	508	CLA	CHD-C1D-ND	-7.22	117.81	124.45
31	A	416[B]	PHO	O2D-CGD-CBD	7.22	120.15	111.00
23	A	404[B]	CLA	C2B-C1B-NB	7.22	115.07	110.23
23	D	403[A]	CLA	C4A-NA-C1A	-7.21	103.46	106.71
23	b	616	CLA	O2D-CGD-CBD	7.20	124.06	111.27
23	b	604	CLA	C2D-C1D-ND	7.19	115.41	110.10
23	b	603	CLA	C4A-NA-C1A	-7.16	103.49	106.71
23	B	608	CLA	C2B-C1B-NB	7.16	115.03	110.23
23	B	616	CLA	CHD-C4C-C3C	-7.16	114.32	124.84
23	A	405[A]	CLA	C2B-C1B-NB	7.15	115.03	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C4A-NA-C1A	-7.14	103.50	106.71
23	C	506	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	C	507	CLA	CMD-C2D-C1D	7.13	137.28	124.71
23	a	407	CLA	C2B-C1B-NB	7.12	115.01	110.23
23	d	403[B]	CLA	C2D-C1D-ND	7.12	115.35	110.10
23	c	504	CLA	C4A-NA-C1A	-7.08	103.52	106.71
23	B	611	CLA	CMB-C2B-C1B	7.07	136.14	125.37
23	C	504	CLA	C4A-NA-C1A	-7.07	103.53	106.71
23	C	511	CLA	CMD-C2D-C1D	7.07	137.17	124.71
23	C	504	CLA	C2B-C1B-NB	7.07	114.97	110.23
23	b	615	CLA	C4A-NA-C1A	-7.06	103.53	106.71
23	b	602	CLA	CHD-C1D-ND	-7.06	117.97	124.45
23	b	603	CLA	C2B-C1B-NB	7.04	114.95	110.23
23	c	508	CLA	CMD-C2D-C1D	7.04	137.12	124.71
23	C	507	CLA	C2B-C1B-NB	7.01	114.93	110.23
23	B	606	CLA	CHD-C1D-ND	-7.01	118.01	124.45
23	B	610	CLA	O2D-CGD-CBD	6.99	123.69	111.27
23	b	606	CLA	C4A-NA-C1A	-6.99	103.56	106.71
31	A	416[B]	PHO	C2B-C1B-NB	6.98	114.35	109.53
23	c	504	CLA	C2B-C1B-NB	6.97	114.91	110.23
23	B	614	CLA	CMD-C2D-C1D	6.95	136.96	124.71
23	a	405[A]	CLA	C2B-C1B-NB	6.94	114.89	110.23
23	d	402[A]	CLA	C2B-C1B-NB	6.94	114.88	110.23
31	a	415[A]	PHO	C2B-C1B-NB	6.92	114.30	109.53
23	B	611	CLA	CMD-C2D-C1D	6.91	136.88	124.71
23	c	506	CLA	C2B-C1B-NB	6.90	114.86	110.23
23	b	605	CLA	C2B-C1B-NB	6.90	114.86	110.23
23	c	502	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	B	610	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	C	510	CLA	C2B-C1B-NB	6.85	114.83	110.23
23	B	603	CLA	O2D-CGD-CBD	6.82	123.39	111.27
23	b	613	CLA	CHD-C4C-C3C	-6.82	114.82	124.84
23	D	404	CLA	C2B-C1B-NB	6.81	114.80	110.23
23	C	513	CLA	CHD-C4C-C3C	-6.81	114.83	124.84
23	B	602	CLA	C2B-C1B-NB	6.81	114.80	110.23
23	d	404	CLA	CHD-C1D-ND	-6.81	118.20	124.45
23	d	403[B]	CLA	C2C-C1C-NC	6.80	116.34	109.97
23	B	615	CLA	C2B-C1B-NB	6.79	114.78	110.23
31	A	416[B]	PHO	C4D-ND-C1D	-6.77	101.94	108.83
23	b	610	CLA	C2B-C1B-NB	6.77	114.77	110.23
23	C	502	CLA	C2B-C1B-NB	6.76	114.76	110.23
23	c	503	CLA	C2B-C1B-NB	6.76	114.76	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	C4A-NA-C1A	-6.76	103.67	106.71
23	b	604	CLA	C2B-C1B-NB	6.75	114.76	110.23
23	b	601	CLA	O2D-CGD-CBD	6.75	123.26	111.27
23	A	405[B]	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	a	404[A]	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	b	605	CLA	CHD-C1D-ND	-6.74	118.26	124.45
31	D	401[B]	PHO	C4D-ND-C1D	-6.73	101.98	108.83
23	B	605	CLA	C2B-C1B-NB	6.73	114.74	110.23
23	b	610	CLA	CHD-C4C-C3C	-6.73	114.95	124.84
23	C	509	CLA	C2B-C1B-NB	6.72	114.74	110.23
31	a	415[A]	PHO	C4D-ND-C1D	-6.72	101.99	108.83
35	c	522	HTG	C1'-S1-C1	6.72	112.66	100.09
23	d	404	CLA	CMD-C2D-C1D	6.71	136.53	124.71
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.71
23	B	616	CLA	O2D-CGD-CBD	6.69	123.15	111.27
23	d	403[B]	CLA	CMD-C2D-C1D	6.65	136.44	124.71
23	A	404[A]	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	A	404[B]	CLA	CMD-C2D-C1D	6.64	136.42	124.71
23	b	616	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
23	C	504	CLA	CHD-C4C-C3C	-6.63	115.09	124.84
23	b	609	CLA	C4A-NA-C1A	-6.62	103.73	106.71
25	X	101	SQD	O47-C7-C8	6.62	125.76	111.50
23	c	510	CLA	C2B-C1B-NB	6.61	114.67	110.23
23	d	402[A]	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	B	609	CLA	C2B-C1B-NB	6.60	114.66	110.23
23	C	503	CLA	C2B-C1B-NB	6.60	114.66	110.23
31	a	415[B]	PHO	C1C-C2C-C3C	-6.59	103.13	108.61
23	B	604	CLA	C2D-C1D-ND	6.57	114.95	110.10
23	c	514	CLA	CHD-C1D-ND	-6.57	118.42	124.45
23	B	604	CLA	C2C-C1C-NC	6.57	116.12	109.97
23	C	507	CLA	CHD-C1D-ND	-6.56	118.42	124.45
23	C	508	CLA	O2D-CGD-CBD	6.55	122.92	111.27
23	B	602	CLA	CHD-C4C-C3C	-6.54	115.22	124.84
23	B	613	CLA	C2B-C1B-NB	6.54	114.62	110.23
23	B	603	CLA	C2B-C1B-NB	6.54	114.62	110.23
23	b	616	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	b	601	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	a	407	CLA	CHD-C4C-C3C	-6.53	115.25	124.84
23	D	403[B]	CLA	C2B-C1B-NB	6.52	114.60	110.23
23	A	406[B]	CLA	CMD-C2D-C1D	6.50	136.17	124.71
23	B	614	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	c	503	CLA	C2C-C1C-NC	6.49	116.05	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403[A]	CLA	C2C-C1C-NC	6.49	116.05	109.97
31	a	406[A]	PHO	C2B-C1B-NB	6.49	114.01	109.53
23	A	407	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	b	605	CLA	CMD-C2D-C1D	6.49	136.15	124.71
23	c	507	CLA	C2B-C1B-NB	6.49	114.58	110.23
23	b	612	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
23	c	509	CLA	C2B-C1B-NB	6.48	114.58	110.23
23	c	514	CLA	CMD-C2D-C1D	6.48	136.14	124.71
23	B	615	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
31	a	406[A]	PHO	C1C-C2C-C3C	-6.48	103.22	108.61
23	b	608	CLA	C2B-C1B-NB	6.46	114.56	110.23
23	a	405[B]	CLA	CHD-C1D-ND	-6.46	118.52	124.45
23	B	606	CLA	O2D-CGD-CBD	6.45	122.73	111.27
23	b	605	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
23	A	404[A]	CLA	C4A-NA-C1A	-6.44	103.81	106.71
25	A	409[A]	SQD	O6-C1-C2	6.44	118.36	108.30
31	A	416[A]	PHO	C1C-C2C-C3C	-6.44	103.26	108.61
23	b	616	CLA	CMD-C2D-C1D	6.43	136.05	124.71
23	C	509	CLA	C2C-C1C-NC	6.43	116.00	109.97
31	A	416[A]	PHO	C4D-ND-C1D	-6.43	102.29	108.83
31	a	415[B]	PHO	C2B-C1B-NB	6.40	113.95	109.53
23	a	405[A]	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	C	508	CLA	CMD-C2D-C1D	6.39	135.98	124.71
31	a	406[B]	PHO	C4D-ND-C1D	-6.39	102.33	108.83
23	b	609	CLA	C2B-C1B-NB	6.39	114.52	110.23
23	a	405[B]	CLA	CMD-C2D-C1D	6.39	135.97	124.71
23	B	601	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	b	611	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
23	a	404[B]	CLA	CMD-C2D-C1D	6.36	135.92	124.71
23	b	606	CLA	CMD-C2D-C1D	6.36	135.92	124.71
23	c	514	CLA	C4A-NA-C1A	-6.34	103.86	106.71
23	b	609	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
23	C	513	CLA	C4A-NA-C1A	-6.32	103.86	106.71
23	B	602	CLA	O2D-CGD-CBD	6.32	122.50	111.27
31	a	415[A]	PHO	C1C-C2C-C3C	-6.32	103.36	108.61
23	C	506	CLA	C4A-NA-C1A	-6.31	103.87	106.71
35	D	411	HTG	C1'-S1-C1	6.31	111.89	100.09
23	B	612	CLA	O2D-CGD-CBD	6.30	122.46	111.27
23	c	510	CLA	C1-C2-C3	-6.29	115.16	126.04
23	B	613	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	c	505	CLA	CHD-C1D-ND	-6.28	118.68	124.45
23	C	514	CLA	CHD-C1D-ND	-6.27	118.69	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	C	510	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	b	614	CLA	CMD-C2D-C1D	6.26	135.74	124.71
31	a	406[B]	PHO	C1C-C2C-C3C	-6.26	103.41	108.61
23	a	405[B]	CLA	CHD-C4C-C3C	-6.25	115.65	124.84
23	C	511	CLA	C2C-C1C-NC	6.24	115.82	109.97
23	b	603	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	B	605	CLA	CHD-C1D-ND	-6.23	118.73	124.45
31	D	401[A]	PHO	O2D-CGD-CBD	6.23	118.89	111.00
23	A	407	CLA	C2C-C1C-NC	6.22	115.80	109.97
23	B	609	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
31	D	401[A]	PHO	C1C-C2C-C3C	-6.21	103.45	108.61
23	a	404[A]	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	B	604	CLA	C2B-C1B-NB	6.19	114.38	110.23
23	c	511	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	c	512	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	a	404[A]	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	c	508	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	c	508	CLA	O2D-CGD-CBD	6.18	122.25	111.27
23	a	405[A]	CLA	C4A-NA-C1A	-6.17	103.93	106.71
24	Y	101	BCR	C33-C5-C6	-6.16	117.61	124.53
23	b	614	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	C	507	CLA	C2C-C1C-NC	6.16	115.74	109.97
25	l	101	SQD	O6-C1-C2	6.16	117.92	108.30
23	D	403[B]	CLA	CHD-C1D-ND	-6.16	118.80	124.45
23	C	509	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	b	601	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	A	406[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
31	D	401[A]	PHO	C2B-C1B-NB	6.14	113.77	109.53
23	b	606	CLA	CHD-C4C-C3C	-6.14	115.82	124.84
23	a	405[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	b	611	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	A	404[A]	CLA	CHD-C1D-ND	-6.11	118.83	124.45
23	B	606	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	B	601	CLA	O2D-CGD-CBD	6.11	122.12	111.27
23	D	403[B]	CLA	C2C-C1C-NC	6.10	115.69	109.97
23	c	507	CLA	CHD-C1D-ND	-6.10	118.84	124.45
23	D	403[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	B	616	CLA	C2B-C1B-NB	6.10	114.32	110.23
23	D	404	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	d	402[B]	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	b	601	CLA	CHD-C4C-C3C	-6.09	115.89	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	O2D-CGD-CBD	6.09	122.09	111.27
23	b	606	CLA	CHD-C1D-ND	-6.09	118.86	124.45
23	b	602	CLA	O2D-CGD-CBD	6.09	122.08	111.27
23	C	506	CLA	O2D-CGD-CBD	6.09	122.08	111.27
23	A	406[B]	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	B	610	CLA	CMD-C2D-C1D	6.08	135.42	124.71
23	b	615	CLA	CHD-C4C-C3C	-6.08	115.91	124.84
23	c	504	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	a	404[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	B	601	CLA	CHD-C1D-ND	-6.07	118.88	124.45
23	b	613	CLA	C2B-C1B-NB	6.07	114.30	110.23
23	D	404	CLA	CMD-C2D-C1D	6.06	135.40	124.71
23	b	612	CLA	C2B-C1B-NB	6.06	114.30	110.23
23	B	616	CLA	C2C-C1C-NC	6.06	115.65	109.97
23	b	608	CLA	CHD-C4C-C3C	-6.06	115.94	124.84
23	B	606	CLA	C2B-C1B-NB	6.05	114.29	110.23
40	V	201	HEC	C1D-ND-C4D	6.05	111.32	105.07
23	C	502	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
31	a	406[A]	PHO	C4D-ND-C1D	-6.05	102.68	108.83
31	A	416[B]	PHO	C1C-C2C-C3C	-6.04	103.59	108.61
23	b	607	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	C	502	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	C	514	CLA	CHD-C4C-C3C	-6.02	115.98	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.02	115.99	124.84
23	c	512	CLA	CMD-C2D-C1D	6.02	135.32	124.71
23	c	513	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
23	d	403[A]	CLA	C2B-C1B-NB	6.01	114.26	110.23
23	B	601	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	B	607	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	C	510	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
35	d	411	HTG	C1'-S1-C1	6.00	111.31	100.09
40	v	201	HEC	C1D-ND-C4D	5.99	111.26	105.07
23	c	504	CLA	CHD-C1D-ND	-5.99	118.95	124.45
23	B	608	CLA	C2C-C1C-NC	5.97	115.57	109.97
23	B	614	CLA	C2B-C1B-NB	5.97	114.23	110.23
23	D	404	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
23	c	510	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	c	503	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	B	605	CLA	O2D-CGD-CBD	5.95	121.84	111.27
23	c	507	CLA	CMD-C2D-C1D	5.94	135.18	124.71
23	B	616	CLA	C3C-C4C-NC	5.93	117.22	110.57
23	d	402[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	C	506	CLA	CHD-C1D-ND	-5.93	119.01	124.45
23	C	503	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
23	B	603	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	c	507	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	A	407	CLA	C2B-C1B-NB	5.92	114.20	110.23
23	C	506	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
23	b	610	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	b	611	CLA	O2D-CGD-CBD	5.92	121.79	111.27
23	c	505	CLA	C4A-NA-C1A	-5.92	104.05	106.71
23	A	406[A]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	D	403[A]	CLA	CHD-C1D-ND	-5.91	119.02	124.45
23	c	505	CLA	CMD-C2D-C1D	5.91	135.13	124.71
23	b	614	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	B	614	CLA	CHD-C1D-ND	-5.91	119.03	124.45
23	c	510	CLA	CHD-C4C-C3C	-5.91	116.16	124.84
24	D	405	BCR	C7-C8-C9	-5.90	117.32	126.23
23	C	512	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	C	511	CLA	C2B-C1B-NB	5.89	114.18	110.23
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.71
31	a	406[B]	PHO	C2B-C1B-NB	5.89	113.59	109.53
23	c	510	CLA	CMD-C2D-C1D	5.89	135.09	124.71
23	A	404[B]	CLA	CHD-C1D-ND	-5.89	119.04	124.45
23	b	604	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
31	D	401[B]	PHO	C1C-C2C-C3C	-5.88	103.72	108.61
23	B	610	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
23	D	403[A]	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	C	503	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	b	602	CLA	CMD-C2D-C1D	5.87	135.06	124.71
38	F	102	HEM	CAD-CBD-CGD	5.87	126.24	113.60
23	b	601	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	b	604	CLA	O2D-CGD-CBD	5.87	121.70	111.27
23	d	402[B]	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	b	607	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	A	405[B]	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	D	403[B]	CLA	CMD-C2D-C1D	5.87	135.05	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-5.86	104.07	106.71
23	A	406[B]	CLA	C4A-NA-C1A	-5.86	104.07	106.71
23	B	609	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	b	611	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	c	513	CLA	CMD-C2D-C1D	5.84	135.00	124.71
23	A	404[A]	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	c	506	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	b	605	CLA	O2D-CGD-CBD	5.83	121.63	111.27
23	c	512	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	B	608	CLA	CMD-C2D-C1D	5.83	134.98	124.71
23	b	614	CLA	O2D-CGD-CBD	5.83	121.62	111.27
23	c	506	CLA	O2D-CGD-CBD	5.83	121.62	111.27
23	B	614	CLA	C4A-NA-C1A	-5.83	104.09	106.71
23	B	614	CLA	C3D-C2D-C1D	-5.82	97.88	105.83
23	C	504	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	b	613	CLA	C2C-C1C-NC	5.82	115.42	109.97
23	B	609	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	C	505	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	C	502	CLA	CMD-C2D-C1D	5.81	134.96	124.71
23	c	512	CLA	C2B-C1B-NB	5.81	114.13	110.23
23	a	404[B]	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
23	C	508	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	D	404	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	a	404[B]	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	C	508	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	C	513	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	B	611	CLA	O2D-CGD-CBD	5.77	121.53	111.27
23	b	604	CLA	CMD-C2D-C1D	5.77	134.89	124.71
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	C	505	CLA	CMD-C2D-C1D	5.77	134.87	124.71
25	A	409[B]	SQD	O6-C1-C2	5.77	117.30	108.30
23	b	613	CLA	CMD-C2D-C1D	5.76	134.87	124.71
23	C	514	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	C	510	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	b	615	CLA	CMD-C2D-C1D	5.75	134.85	124.71
23	c	508	CLA	C2B-C1B-NB	5.75	114.09	110.23
23	B	607	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	c	502	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
23	C	510	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	c	513	CLA	C4A-NA-C1A	-5.72	104.14	106.71
23	B	603	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	C	505	CLA	C2B-C1B-NB	5.71	114.06	110.23
23	c	509	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
25	l	101	SQD	O47-C7-C8	5.71	123.80	111.50
23	c	511	CLA	CHD-C1D-ND	-5.70	119.21	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	614	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	B	607	CLA	CMD-C2D-C1D	5.70	134.75	124.71
25	a	409[A]	SQD	O6-C1-C2	5.69	117.19	108.30
23	b	603	CLA	CMD-C2D-C1D	5.69	134.75	124.71
23	C	506	CLA	C2C-C1C-NC	5.69	115.30	109.97
23	B	602	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	A	407	CLA	CMD-C2D-C1D	5.69	134.74	124.71
23	b	604	CLA	C1-C2-C3	-5.69	116.21	126.04
23	C	512	CLA	O2D-CGD-CBD	5.68	121.37	111.27
23	A	405[B]	CLA	C2C-C1C-NC	5.68	115.29	109.97
23	b	607	CLA	C2B-C1B-NB	5.68	114.04	110.23
23	A	405[B]	CLA	CMD-C2D-C1D	5.66	134.69	124.71
23	d	404	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
25	A	409[A]	SQD	C1-O5-C5	-5.64	102.61	113.69
23	c	513	CLA	O2D-CGD-CBD	5.64	121.29	111.27
23	D	403[B]	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	C	506	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	A	405[B]	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
23	b	614	CLA	C3D-C2D-C1D	-5.63	98.15	105.83
23	B	611	CLA	C3D-C2D-C1D	-5.62	98.16	105.83
23	B	605	CLA	C4A-NA-C1A	-5.62	104.18	106.71
23	C	511	CLA	CHD-C1D-ND	-5.61	119.30	124.45
23	C	502	CLA	CHD-C1D-ND	-5.61	119.30	124.45
31	D	401[B]	PHO	C2B-C1B-NB	5.61	113.40	109.53
23	c	506	CLA	CMD-C2D-C1D	5.60	134.58	124.71
23	B	601	CLA	C4A-NA-C1A	-5.59	104.19	106.71
23	C	512	CLA	CMD-C2D-C1D	5.59	134.57	124.71
23	a	407	CLA	O2D-CGD-CBD	5.59	121.21	111.27
23	b	613	CLA	C3D-C2D-C1D	-5.59	98.20	105.83
35	B	621	HTG	C1'-S1-C1	5.59	110.55	100.09
23	b	602	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
23	d	403[B]	CLA	C2B-C1B-NB	5.59	113.98	110.23
23	b	607	CLA	CMD-C2D-C1D	5.58	134.56	124.71
25	b	620	SQD	O6-C1-C2	5.58	117.01	108.30
23	B	612	CLA	CMD-C2D-C1D	5.57	134.53	124.71
23	c	505	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	b	603	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	A	406[B]	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
23	B	612	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
23	b	612	CLA	CMD-C2D-C1D	5.55	134.50	124.71
23	c	511	CLA	CMD-C2D-C1D	5.55	134.49	124.71
23	A	405[A]	CLA	C2C-C1C-NC	5.54	115.17	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	c	509	CLA	C2C-C1C-NC	5.53	115.16	109.97
23	b	608	CLA	O2D-CGD-CBD	5.53	121.10	111.27
23	b	609	CLA	CMD-C2D-C1D	5.53	134.47	124.71
23	B	607	CLA	O2D-CGD-CBD	5.53	121.10	111.27
23	B	614	CLA	O2D-CGD-CBD	5.53	121.09	111.27
23	B	608	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
23	B	613	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	b	608	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	d	403[B]	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	c	513	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	B	605	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
23	C	508	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	a	404[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	c	506	CLA	C2C-C1C-NC	5.51	115.13	109.97
23	d	402[A]	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	b	611	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	C	505	CLA	C3D-C2D-C1D	-5.50	98.32	105.83
23	d	403[A]	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
34	C	501	LMG	C7-O1-C1	-5.49	103.01	113.74
23	d	402[B]	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	c	508	CLA	C2C-C1C-NC	5.49	115.11	109.97
23	d	402[A]	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	c	506	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	a	405[A]	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	b	610	CLA	O2D-CGD-CBD	5.48	121.01	111.27
23	B	616	CLA	C3D-C2D-C1D	-5.48	98.36	105.83
23	C	513	CLA	CMD-C2D-C1D	5.48	134.36	124.71
23	c	510	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	B	613	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	D	403[A]	CLA	C2B-C1B-NB	5.47	113.90	110.23
23	b	612	CLA	C2C-C1C-NC	5.46	115.09	109.97
23	c	505	CLA	O2D-CGD-CBD	5.46	120.97	111.27
23	b	607	CLA	CHD-C1D-ND	-5.46	119.44	124.45
23	c	502	CLA	O2D-CGD-CBD	5.45	120.96	111.27
23	b	613	CLA	CHD-C1D-ND	-5.45	119.44	124.45
23	d	403[B]	CLA	C4A-NA-C1A	-5.45	104.26	106.71
23	d	403[A]	CLA	CMD-C2D-C1D	5.44	134.30	124.71
23	C	514	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	A	404[B]	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
23	c	507	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
23	c	514	CLA	CHD-C4C-C3C	-5.42	116.88	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	O2D-CGD-CBD	5.41	120.88	111.27
23	A	405[A]	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	a	405[B]	CLA	O2D-CGD-CBD	5.41	120.88	111.27
23	A	407	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	B	607	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	c	505	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
31	a	415[A]	PHO	C1-C2-C3	-5.39	116.72	126.04
23	b	610	CLA	CHD-C1D-ND	-5.39	119.50	124.45
23	c	512	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	A	405[A]	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	B	608	CLA	O2D-CGD-CBD	5.37	120.82	111.27
23	b	606	CLA	C2C-C1C-NC	5.37	115.00	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.37	116.95	124.84
23	b	604	CLA	CHD-C4C-C3C	-5.36	116.96	124.84
23	b	608	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	B	607	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	C	504	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	B	606	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
23	B	604	CLA	CMD-C2D-C1D	5.35	134.14	124.71
25	A	409[A]	SQD	C1-C2-C3	-5.35	98.86	110.00
23	c	514	CLA	C2C-C1C-NC	5.34	114.98	109.97
23	a	404[A]	CLA	CHD-C1D-ND	-5.34	119.55	124.45
31	D	401[A]	PHO	C3D-C4D-ND	5.34	115.00	107.72
23	B	607	CLA	C3D-C2D-C1D	-5.34	98.55	105.83
23	C	503	CLA	CMD-C2D-C1D	5.32	134.10	124.71
23	b	608	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	B	604	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
23	B	610	CLA	C3D-C2D-C1D	-5.31	98.59	105.83
23	B	615	CLA	C2C-C1C-NC	5.31	114.94	109.97
23	c	505	CLA	C3B-C2B-C1B	-5.30	100.76	107.16
23	C	511	CLA	O2D-CGD-CBD	5.30	120.68	111.27
31	a	415[B]	PHO	C3D-C4D-ND	5.30	114.94	107.72
23	b	613	CLA	C3C-C4C-NC	5.29	116.51	110.57
23	b	614	CLA	C4A-NA-C1A	-5.29	104.33	106.71
23	a	407	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	B	602	CLA	CMD-C2D-C1D	5.29	134.03	124.71
23	B	604	CLA	O2D-CGD-CBD	5.28	120.66	111.27
23	b	611	CLA	C4A-NA-C1A	-5.28	104.33	106.71
35	C	522	HTG	C1'-S1-C1	5.28	109.96	100.09
23	B	615	CLA	CHD-C1D-ND	-5.27	119.61	124.45
23	C	512	CLA	C3B-C2B-C1B	-5.26	100.81	107.16
23	B	611	CLA	CHD-C1D-ND	-5.26	119.62	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	c	508	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	b	605	CLA	C2C-C1C-NC	5.25	114.89	109.97
24	t	102	BCR	C33-C5-C6	-5.24	118.64	124.53
23	d	404	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
23	C	514	CLA	C3B-C2B-C1B	-5.24	100.84	107.16
23	c	506	CLA	CHD-C1D-ND	-5.23	119.64	124.45
23	c	512	CLA	O2D-CGD-CBD	5.23	120.56	111.27
23	C	508	CLA	C2B-C1B-NB	5.23	113.74	110.23
23	a	405[B]	CLA	C4A-NA-C1A	-5.22	104.36	106.71
23	b	609	CLA	CHD-C1D-ND	-5.22	119.66	124.45
23	c	503	CLA	C3B-C2B-C1B	-5.21	100.87	107.16
23	B	602	CLA	C2C-C1C-NC	5.21	114.86	109.97
23	C	512	CLA	C2C-C1C-NC	5.20	114.84	109.97
25	b	620	SQD	O47-C7-C8	5.20	122.70	111.50
23	b	616	CLA	C3D-C2D-C1D	-5.19	98.74	105.83
24	H	101	BCR	C38-C26-C25	-5.19	118.70	124.53
23	d	404	CLA	O2D-CGD-CBD	5.19	120.49	111.27
31	a	415[A]	PHO	C3D-C4D-ND	5.19	114.79	107.72
23	B	608	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	B	603	CLA	CHD-C1D-ND	-5.19	119.69	124.45
23	c	509	CLA	O2D-CGD-CBD	5.18	120.48	111.27
23	d	403[A]	CLA	CHD-C1D-ND	-5.18	119.69	124.45
23	B	602	CLA	C3C-C4C-NC	5.18	116.38	110.57
23	a	407	CLA	C4A-NA-C1A	-5.17	104.38	106.71
23	B	608	CLA	CHD-C1D-ND	-5.17	119.71	124.45
23	b	611	CLA	C3D-C2D-C1D	-5.16	98.78	105.83
23	c	509	CLA	C4A-NA-C1A	-5.16	104.39	106.71
23	C	509	CLA	O2D-CGD-CBD	5.16	120.44	111.27
23	A	404[B]	CLA	C2C-C1C-NC	5.16	114.80	109.97
23	C	503	CLA	C2C-C1C-NC	5.15	114.80	109.97
23	C	509	CLA	C3C-C4C-NC	5.15	116.35	110.57
23	B	604	CLA	C3C-C4C-NC	5.14	116.33	110.57
31	D	401[B]	PHO	C3D-C4D-ND	5.14	114.72	107.72
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	a	404[B]	CLA	C2C-C1C-NC	5.12	114.77	109.97
23	B	605	CLA	C3C-C4C-NC	5.12	116.31	110.57
23	B	612	CLA	CAC-C3C-C4C	5.11	131.44	124.81
23	B	615	CLA	CMD-C2D-C1D	5.11	133.72	124.71
23	b	602	CLA	C3B-C2B-C1B	-5.11	100.99	107.16
23	b	606	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
23	c	511	CLA	C2C-C1C-NC	5.10	114.75	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C3C-C4C-NC	5.10	116.29	110.57
31	A	416[B]	PHO	C3D-C4D-ND	5.10	114.67	107.72
23	A	407	CLA	C3D-C2D-C1D	-5.09	98.88	105.83
23	B	612	CLA	CHD-C1D-ND	-5.09	119.78	124.45
23	b	614	CLA	C3B-C2B-C1B	-5.09	101.02	107.16
23	B	609	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	b	615	CLA	CHD-C1D-ND	-5.08	119.78	124.45
23	d	403[B]	CLA	CHD-C4C-C3C	-5.08	117.37	124.84
25	a	409[A]	SQD	O47-C7-C8	5.08	122.45	111.50
23	d	402[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	B	608	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
23	C	509	CLA	CMD-C2D-C1D	5.07	133.66	124.71
23	b	603	CLA	CHD-C1D-ND	-5.07	119.80	124.45
23	b	614	CLA	C2C-C1C-NC	5.07	114.72	109.97
23	c	503	CLA	O2D-CGD-CBD	5.07	120.27	111.27
23	D	403[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	B	616	CLA	C4A-NA-C1A	-5.06	104.43	106.71
23	B	613	CLA	C1-C2-C3	-5.06	117.30	126.04
23	b	610	CLA	C4A-NA-C1A	-5.05	104.44	106.71
23	D	403[B]	CLA	C3B-C2B-C1B	-5.05	101.07	107.16
23	C	504	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
24	d	405	BCR	C15-C14-C13	-5.04	120.11	127.31
23	b	607	CLA	C3C-C4C-NC	5.04	116.22	110.57
31	a	415[B]	PHO	C1-C2-C3	-5.04	117.33	126.04
23	A	407	CLA	C3C-C4C-NC	5.04	116.22	110.57
23	B	610	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	C	507	CLA	C4A-NA-C1A	-5.03	104.44	106.71
23	B	615	CLA	C3D-C2D-C1D	-5.02	98.99	105.83
23	B	612	CLA	C2B-C1B-NB	5.01	113.59	110.23
23	A	405[A]	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	D	403[A]	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	C	505	CLA	O2D-CGD-CBD	5.00	120.15	111.27
23	c	502	CLA	C4A-NA-C1A	-5.00	104.46	106.71
23	b	606	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	B	612	CLA	C3C-C4C-NC	4.99	116.17	110.57
38	f	101	HEM	CHC-C4B-NB	4.99	129.84	124.42
23	B	613	CLA	CMD-C2D-C1D	4.99	133.50	124.71
23	C	508	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	b	607	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
28	a	413[A]	PL9	C7-C8-C9	-4.98	118.50	126.79
23	c	513	CLA	C3B-C2B-C1B	-4.98	101.16	107.16
23	C	510	CLA	C4A-NA-C1A	-4.97	104.47	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	510	CLA	O2D-CGD-CBD	4.97	120.10	111.27
23	B	607	CLA	C2B-C1B-NB	4.97	113.56	110.23
23	a	405[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	b	605	CLA	O2D-CGD-O1D	-4.96	114.14	123.84
31	A	416[A]	PHO	C3D-C4D-ND	4.96	114.48	107.72
23	b	612	CLA	O2D-CGD-CBD	4.95	120.07	111.27
23	B	610	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	b	611	CLA	C3C-C4C-NC	4.95	116.12	110.57
23	c	509	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
28	A	413[A]	PL9	C7-C8-C9	-4.94	118.56	126.79
23	b	610	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	b	615	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	C	512	CLA	C4A-NA-C1A	-4.94	104.49	106.71
23	B	606	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	c	507	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	C	512	CLA	CHD-C1D-ND	-4.91	119.94	124.45
23	c	509	CLA	CMD-C2D-C1D	4.91	133.37	124.71
23	b	608	CLA	CMD-C2D-C1D	4.91	133.37	124.71
25	a	409[A]	SQD	C1-O5-C5	-4.91	104.05	113.69
23	C	508	CLA	C3C-C4C-NC	4.90	116.07	110.57
23	c	506	CLA	C3C-C4C-NC	4.90	116.07	110.57
23	C	507	CLA	O2D-CGD-CBD	4.90	119.98	111.27
25	a	409[B]	SQD	O47-C7-C8	4.90	122.05	111.50
23	c	514	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
23	d	403[A]	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	B	614	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
23	a	405[B]	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
23	B	612	CLA	O2D-CGD-O1D	-4.88	114.29	123.84
23	D	404	CLA	O2D-CGD-CBD	4.88	119.94	111.27
23	c	511	CLA	O2D-CGD-CBD	4.88	119.94	111.27
23	B	603	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	b	602	CLA	O2D-CGD-O1D	-4.87	114.31	123.84
28	A	413[B]	PL9	C7-C8-C9	-4.87	118.68	126.79
23	C	513	CLA	C3B-C2B-C1B	-4.87	101.29	107.16
23	c	504	CLA	O2D-CGD-CBD	4.87	119.91	111.27
23	d	402[B]	CLA	O2D-CGD-CBD	4.86	119.90	111.27
23	c	502	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	a	407	CLA	C3C-C4C-NC	4.86	116.02	110.57
23	c	511	CLA	C1-C2-C3	-4.86	117.64	126.04
23	d	402[B]	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
23	a	407	CLA	C3D-C4D-ND	4.85	118.08	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	402[B]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	B	610	CLA	O2A-CGA-CBA	4.84	127.11	111.91
23	A	405[B]	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	C	509	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	c	502	CLA	C2C-C1C-NC	4.84	114.50	109.97
23	A	406[B]	CLA	C3D-C4D-ND	4.83	118.05	110.24
23	A	406[A]	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	b	605	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
25	X	101	SQD	O8-S-C6	4.82	113.43	105.74
23	a	405[A]	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	C	502	CLA	C2C-C1C-NC	4.81	114.48	109.97
23	B	608	CLA	C4A-NA-C1A	-4.81	104.54	106.71
23	C	505	CLA	C4A-NA-C1A	-4.81	104.54	106.71
23	A	406[B]	CLA	C2C-C1C-NC	4.81	114.48	109.97
23	b	616	CLA	CHD-C1D-ND	-4.81	120.04	124.45
23	d	404	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
25	f	102	SQD	O47-C7-C8	4.80	121.85	111.50
23	C	514	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	603	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	C	504	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	B	604	CLA	C1-C2-C3	-4.79	117.77	126.04
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	a	405[B]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	a	407	CLA	C2C-C1C-NC	4.78	114.45	109.97
23	b	615	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
31	a	406[B]	PHO	C3D-C4D-ND	4.78	114.23	107.72
23	B	612	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
23	b	602	CLA	C3D-C4D-ND	4.78	117.96	110.24
23	C	504	CLA	C3C-C4C-NC	4.77	115.92	110.57
23	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	a	404[B]	CLA	C3D-C4D-ND	4.77	117.95	110.24
23	C	511	CLA	C3B-C2B-C1B	-4.77	101.41	107.16
23	c	504	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	c	508	CLA	C3B-C2B-C1B	-4.76	101.41	107.16
23	c	503	CLA	C1C-C2C-C3C	-4.76	101.95	106.96
23	a	407	CLA	CMD-C2D-C1D	4.76	133.10	124.71
23	b	604	CLA	CHD-C1D-ND	-4.76	120.08	124.45
23	c	504	CLA	C3D-C2D-C1D	-4.75	99.34	105.83
23	b	609	CLA	C3C-C4C-NC	4.75	115.90	110.57
35	b	622	HTG	C1-O5-C5	4.75	121.33	112.58
23	c	510	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
25	f	102	SQD	C1-O5-C5	4.73	122.98	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C3C-C4C-NC	4.73	115.88	110.57
34	B	620	LMG	O7-C10-C11	4.73	121.69	111.50
23	b	611	CLA	C3B-C2B-C1B	-4.73	101.46	107.16
23	d	403[B]	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
23	D	403[B]	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	C	509	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
23	B	601	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	C	503	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	C	507	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	a	404[A]	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	B	615	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	B	601	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
23	a	404[B]	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	D	403[B]	CLA	O2D-CGD-CBD	4.70	119.62	111.27
23	b	613	CLA	C4A-NA-C1A	-4.70	104.59	106.71
23	C	508	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	C	508	CLA	C4A-NA-C1A	-4.69	104.60	106.71
23	c	505	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	b	612	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	C	506	CLA	C3C-C4C-NC	4.68	115.82	110.57
23	B	605	CLA	C2C-C1C-NC	4.68	114.36	109.97
23	c	503	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	B	611	CLA	CMC-C2C-C1C	4.68	132.16	125.04
24	b	617	BCR	C33-C5-C6	-4.67	119.28	124.53
23	B	613	CLA	C4A-NA-C1A	-4.67	104.61	106.71
23	c	514	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	B	613	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	b	603	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
23	B	607	CLA	O2D-CGD-O1D	-4.66	114.73	123.84
23	c	508	CLA	C1C-C2C-C3C	-4.65	102.07	106.96
23	b	616	CLA	C3C-C4C-NC	4.65	115.78	110.57
31	A	416[B]	PHO	C1-C2-C3	-4.65	118.01	126.04
23	b	610	CLA	C3C-C4C-NC	4.64	115.78	110.57
23	C	510	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
31	a	406[A]	PHO	C3D-C4D-ND	4.64	114.04	107.72
23	C	502	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	C	513	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	B	602	CLA	C3B-C2B-C1B	-4.63	101.57	107.16
23	d	402[A]	CLA	O2D-CGD-CBD	4.63	119.49	111.27
25	a	409[B]	SQD	O6-C1-C2	4.63	115.53	108.30
23	D	404	CLA	C3D-C4D-ND	4.63	117.72	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	509	CLA	CHD-C1D-ND	-4.62	120.20	124.45
23	C	507	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	b	615	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
23	b	607	CLA	C3D-C4D-ND	4.61	117.70	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.61	116.12	126.06
23	a	405[B]	CLA	C3D-C4D-ND	4.60	117.68	110.24
23	c	502	CLA	C3D-C4D-ND	4.60	117.68	110.24
23	b	604	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	b	610	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
23	b	601	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	b	603	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	c	507	CLA	O2D-CGD-CBD	4.59	119.43	111.27
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	B	604	CLA	C3B-C2B-C1B	-4.59	101.63	107.16
23	b	605	CLA	C3D-C4D-ND	4.58	117.65	110.24
23	a	407	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	A	404[A]	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	C	510	CLA	O2D-CGD-CBD	4.57	119.39	111.27
23	A	405[A]	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
23	B	607	CLA	C3C-C4C-NC	4.57	115.70	110.57
23	C	511	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	c	512	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
23	C	507	CLA	C1C-C2C-C3C	-4.57	102.16	106.96
23	b	606	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
23	B	616	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
23	C	503	CLA	O2D-CGD-CBD	4.56	119.37	111.27
23	D	404	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	D	403[B]	CLA	C1-C2-C3	-4.55	118.17	126.04
23	B	603	CLA	CMD-C2D-C1D	4.55	132.73	124.71
28	a	413[B]	PL9	C7-C3-C4	4.55	120.58	116.88
23	B	601	CLA	C3C-C4C-NC	4.55	115.67	110.57
23	b	601	CLA	C2C-C1C-NC	4.55	114.23	109.97
23	B	609	CLA	C3C-C4C-NC	4.55	115.67	110.57
23	b	616	CLA	C2C-C1C-NC	4.55	114.23	109.97
23	c	504	CLA	C3C-C4C-NC	4.54	115.67	110.57
23	C	504	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
23	C	504	CLA	C2C-C1C-NC	4.54	114.23	109.97
23	c	507	CLA	C3D-C4D-ND	4.54	117.58	110.24
23	d	403[A]	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	A	406[B]	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	A	406[A]	CLA	CMB-C2B-C1B	4.53	132.27	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C1-C2-C3	-4.53	118.20	126.04
23	b	612	CLA	C1-C2-C3	-4.53	118.20	126.04
23	c	510	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
23	A	406[A]	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	d	402[B]	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
23	c	506	CLA	C3D-C4D-ND	4.52	117.56	110.24
23	B	602	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	c	508	CLA	CMB-C2B-C1B	4.52	132.25	125.37
23	c	513	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	b	612	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	c	502	CLA	O2D-CGD-O1D	-4.52	115.00	123.84
23	b	616	CLA	C1D-CHD-C4C	-4.52	116.31	126.06
23	c	511	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
23	d	404	CLA	C2C-C1C-NC	4.52	114.20	109.97
23	A	406[A]	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	b	610	CLA	O2A-CGA-CBA	4.51	126.06	111.91
23	b	612	CLA	C3B-C4B-NB	4.51	114.70	110.52
23	B	612	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	b	604	CLA	C3C-C4C-NC	4.51	115.62	110.57
23	b	605	CLA	C4A-NA-C1A	-4.51	104.68	106.71
23	D	404	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	d	402[B]	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
23	C	506	CLA	C1-C2-C3	-4.49	118.28	126.04
23	d	403[A]	CLA	C3D-C4D-ND	4.49	117.50	110.24
24	K	102	BCR	C7-C8-C9	-4.49	119.45	126.23
23	b	609	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
23	A	404[B]	CLA	C1D-CHD-C4C	-4.48	116.39	126.06
23	B	615	CLA	C3D-C4D-ND	4.48	117.49	110.24
23	B	604	CLA	C4A-NA-C1A	-4.48	104.69	106.71
23	B	601	CLA	C3D-C4D-ND	4.47	117.48	110.24
23	c	514	CLA	C3D-C4D-ND	4.47	117.47	110.24
23	C	513	CLA	C3C-C4C-NC	4.47	115.58	110.57
28	A	413[B]	PL9	C32-C33-C34	-4.47	116.90	127.66
25	b	620	SQD	C1-O5-C5	-4.47	104.92	113.69
23	C	510	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	a	404[B]	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
23	C	502	CLA	O2D-CGD-O1D	-4.46	115.11	123.84
23	A	404[B]	CLA	C3B-C4B-NB	4.46	114.65	110.52
23	b	610	CLA	C3D-C4D-ND	4.46	117.45	110.24
38	F	102	HEM	C4C-NC-C1C	4.46	109.72	105.35
23	B	610	CLA	C3C-C4C-NC	4.45	115.57	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406[B]	CLA	O2D-CGD-CBD	4.45	119.18	111.27
23	A	407	CLA	C4A-NA-C1A	-4.45	104.71	106.71
23	d	404	CLA	C4A-NA-C1A	-4.45	104.71	106.71
38	F	102	HEM	CHD-C4C-NC	4.45	129.25	124.44
23	C	505	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	b	604	CLA	C3B-C2B-C1B	-4.45	101.80	107.16
23	C	503	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	a	405[A]	CLA	O2D-CGD-CBD	4.44	119.17	111.27
23	B	602	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	b	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	d	404	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	B	615	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	c	514	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	D	403[B]	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	b	601	CLA	C3D-C4D-ND	4.43	117.41	110.24
34	C	501	LMG	O1-C1-C2	4.43	115.22	108.30
23	C	512	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
23	C	503	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	b	616	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
23	b	608	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	b	609	CLA	C1-C2-C3	-4.42	118.40	126.04
23	C	510	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	B	609	CLA	C3D-C4D-ND	4.41	117.38	110.24
23	A	404[B]	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	b	601	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
23	C	511	CLA	C3D-C4D-ND	4.40	117.36	110.24
23	c	511	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
23	a	404[B]	CLA	C1D-CHD-C4C	-4.40	116.56	126.06
23	a	407	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
23	a	404[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	C	510	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	c	508	CLA	CMC-C2C-C1C	4.39	131.73	125.04
23	d	402[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	c	509	CLA	CHD-C1D-ND	-4.39	120.42	124.45
23	B	603	CLA	C3C-C4C-NC	4.39	115.49	110.57
23	C	511	CLA	C1-C2-C3	-4.38	118.46	126.04
23	B	610	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
23	B	616	CLA	CMD-C2D-C1D	4.38	132.43	124.71
23	D	404	CLA	C3C-C4C-NC	4.38	115.48	110.57
23	d	402[A]	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	C	506	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
24	d	405	BCR	C7-C8-C9	-4.37	119.63	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	B	605	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	A	405[B]	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
25	X	101	SQD	C1-O5-C5	-4.37	105.12	113.69
23	A	406[B]	CLA	C3B-C2B-C1B	-4.36	101.89	107.16
23	A	405[A]	CLA	C3D-C4D-ND	4.36	117.30	110.24
33	E	101[A]	LHG	O7-C7-C8	4.36	120.90	111.50
23	b	604	CLA	C3B-C4B-NB	4.36	114.56	110.52
23	a	405[A]	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
23	a	405[A]	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	c	508	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	c	513	CLA	C3D-C4D-ND	4.35	117.28	110.24
34	C	501	LMG	O7-C10-C11	4.35	120.88	111.50
23	A	404[B]	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
23	c	510	CLA	C3B-C4B-NB	4.35	114.55	110.52
23	B	607	CLA	C3D-C4D-ND	4.34	117.27	110.24
23	C	513	CLA	C3D-C4D-ND	4.34	117.26	110.24
23	B	609	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
23	d	403[A]	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	C	503	CLA	C3C-C4C-NC	4.34	115.44	110.57
23	b	603	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
23	b	609	CLA	C2C-C1C-NC	4.34	114.03	109.97
23	b	608	CLA	C3B-C2B-C1B	-4.34	101.93	107.16
23	d	403[B]	CLA	C1C-C2C-C3C	-4.33	102.40	106.96
23	b	616	CLA	O2D-CGD-O1D	-4.33	115.38	123.84
28	D	406[B]	PL9	C42-C43-C44	-4.33	117.25	127.66
33	E	101[B]	LHG	O7-C7-C8	4.33	120.82	111.50
23	C	514	CLA	O2D-CGD-CBD	4.33	118.95	111.27
23	D	403[B]	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	a	404[B]	CLA	C3B-C4B-NB	4.32	114.52	110.52
23	c	509	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
38	F	102	HEM	C1B-NB-C4B	4.32	109.53	105.07
23	c	507	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	b	614	CLA	C3C-C4C-NC	4.31	115.41	110.57
32	t	101	LMT	C3'-C4'-C5'	-4.31	101.04	110.93
23	C	511	CLA	C1C-C2C-C3C	-4.31	102.42	106.96
23	C	503	CLA	C4A-NA-C1A	-4.31	104.77	106.71
23	A	407	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
25	a	409[A]	SQD	C1-C2-C3	-4.31	101.02	110.00
23	B	603	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	C	504	CLA	C1D-CHD-C4C	-4.31	116.77	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	612	CLA	C4A-NA-C1A	-4.31	104.77	106.71
23	D	404	CLA	CMB-C2B-C1B	4.31	131.93	125.37
23	C	506	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	d	403[B]	CLA	C3D-C4D-ND	4.30	117.19	110.24
28	A	413[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	A	405[B]	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	b	603	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	B	603	CLA	O2D-CGD-O1D	-4.30	115.44	123.84
23	B	611	CLA	C3D-C4D-ND	4.29	117.19	110.24
23	b	603	CLA	C1D-CHD-C4C	-4.29	116.79	126.06
23	A	405[B]	CLA	O2D-CGD-CBD	4.29	118.89	111.27
23	a	405[A]	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	b	605	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
23	C	507	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	a	404[A]	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	A	405[B]	CLA	C4A-NA-C1A	-4.28	104.78	106.71
24	d	405	BCR	C29-C30-C25	4.28	117.07	110.48
23	A	405[A]	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
23	c	504	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
23	c	506	CLA	C3B-C2B-C1B	-4.27	102.00	107.16
23	C	512	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	b	615	CLA	C3C-C4C-NC	4.27	115.36	110.57
25	a	409[A]	SQD	O9-S-C6	4.27	112.01	106.94
34	Z	101	LMG	O7-C10-C11	4.27	120.69	111.50
23	a	404[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	c	503	CLA	CMD-C2D-C1D	4.26	132.22	124.71
23	C	502	CLA	C3D-C4D-ND	4.26	117.13	110.24
23	B	615	CLA	CMB-C2B-C1B	4.26	131.85	125.37
23	d	402[B]	CLA	C3D-C4D-ND	4.25	117.12	110.24
34	c	501	LMG	O7-C10-C11	4.25	120.67	111.50
23	c	512	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	C	512	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
23	c	504	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
24	y	101	BCR	C33-C5-C6	-4.24	119.76	124.53
23	C	514	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	B	613	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	B	611	CLA	CHD-C4C-NC	4.24	130.88	124.20
23	c	503	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	B	611	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	c	513	CLA	C2C-C1C-NC	4.23	113.94	109.97
24	C	516	BCR	C7-C8-C9	-4.23	119.84	126.23
23	b	605	CLA	C3C-C4C-NC	4.23	115.31	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	405[B]	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
24	B	617	BCR	C7-C8-C9	-4.22	119.85	126.23
23	B	612	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	d	403[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	B	615	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
23	B	603	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	d	403[B]	CLA	C3C-C4C-NC	4.22	115.30	110.57
23	B	602	CLA	O2D-CGD-O1D	-4.22	115.60	123.84
23	b	613	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
23	A	407	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	d	403[B]	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	b	614	CLA	O2D-CGD-O1D	-4.21	115.60	123.84
23	C	505	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
23	c	509	CLA	C3C-C4C-NC	4.21	115.30	110.57
23	d	402[A]	CLA	C3C-C4C-NC	4.21	115.29	110.57
36	C	518[B]	DGD	O2G-C1B-C2B	4.20	120.56	111.50
23	D	404	CLA	C4-C3-C5	4.20	122.33	115.27
23	c	511	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	B	606	CLA	C3C-C4C-NC	4.19	115.27	110.57
32	B	626	LMT	C1'-O5'-C5'	-4.18	105.47	113.69
34	c	521	LMG	O7-C10-C11	4.18	120.52	111.50
33	A	418[A]	LHG	O8-C23-O10	-4.18	113.04	123.59
31	D	401[B]	PHO	C1A-C2A-C3A	-4.18	98.86	102.84
23	a	405[B]	CLA	C2C-C1C-NC	4.18	113.89	109.97
24	B	618	BCR	C29-C30-C25	4.18	116.91	110.48
23	b	614	CLA	C3D-C4D-ND	4.17	116.99	110.24
24	d	405	BCR	C40-C30-C25	-4.17	103.53	110.30
34	m	101	LMG	O7-C10-C11	4.17	120.49	111.50
23	C	502	CLA	C3C-C4C-NC	4.17	115.25	110.57
23	A	404[A]	CLA	C3B-C4B-NB	4.17	114.38	110.52
23	b	608	CLA	CMC-C2C-C1C	4.16	131.38	125.04
23	b	607	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
23	b	615	CLA	C3D-C4D-ND	4.16	116.97	110.24
23	B	613	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
33	d	408[B]	LHG	O7-C7-C8	4.16	120.46	111.50
23	C	504	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	C	514	CLA	C4A-NA-C1A	-4.15	104.84	106.71
23	C	514	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	c	512	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
23	A	406[A]	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	b	615	CLA	C1D-CHD-C4C	-4.15	117.11	126.06
23	B	607	CLA	C1C-C2C-C3C	-4.15	102.59	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403[A]	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
23	a	404[A]	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
23	b	602	CLA	C2C-C1C-NC	4.14	113.85	109.97
23	B	606	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	B	608	CLA	O2D-CGD-O1D	-4.14	115.75	123.84
23	c	503	CLA	CHD-C1D-ND	-4.14	120.65	124.45
25	A	409[B]	SQD	C1-C2-C3	-4.13	101.39	110.00
23	B	604	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
23	A	407	CLA	C3B-C4B-NB	4.13	114.35	110.52
23	c	507	CLA	C3B-C4B-NB	4.13	114.35	110.52
28	a	413[A]	PL9	C7-C3-C4	4.13	120.24	116.88
24	c	515	BCR	C11-C10-C9	-4.13	121.41	127.31
23	c	504	CLA	C3D-C4D-ND	4.13	116.92	110.24
24	T	102	BCR	C15-C16-C17	-4.13	115.02	123.47
23	b	608	CLA	C1-C2-C3	-4.13	118.91	126.04
23	b	606	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	B	614	CLA	C1C-C2C-C3C	-4.12	102.62	106.96
23	d	402[A]	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	B	613	CLA	O2D-CGD-CBD	4.12	118.59	111.27
23	C	510	CLA	C3B-C4B-NB	4.12	114.33	110.52
23	c	507	CLA	C1-C2-C3	-4.12	118.92	126.04
23	B	614	CLA	C1D-CHD-C4C	-4.11	117.18	126.06
23	B	616	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
23	c	502	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
23	C	508	CLA	O2D-CGD-O1D	-4.11	115.80	123.84
23	B	606	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
23	B	613	CLA	CMC-C2C-C1C	4.11	131.29	125.04
23	b	608	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	B	610	CLA	CAA-C2A-C3A	-4.10	101.54	112.78
23	c	505	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	C	509	CLA	C3B-C4B-NB	4.10	114.32	110.52
23	B	605	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
23	c	503	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	C	506	CLA	C3D-C2D-C1D	-4.10	100.24	105.83
23	b	606	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
34	C	521	LMG	O6-C5-C4	4.09	117.13	109.69
23	c	512	CLA	O2D-CGD-O1D	-4.09	115.84	123.84
23	d	402[A]	CLA	CMB-C2B-C1B	4.09	131.60	125.37
23	d	403[A]	CLA	O2D-CGD-CBD	4.09	118.53	111.27
23	c	513	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
33	D	408[B]	LHG	O7-C7-C8	4.09	120.31	111.50
23	d	403[A]	CLA	C3B-C2B-C1B	-4.09	102.23	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	521	LMG	O6-C5-C4	4.09	117.12	109.69
23	d	402[A]	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
35	V	202	HTG	C1-O5-C5	4.09	117.73	112.19
23	b	613	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
23	C	509	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	B	615	CLA	O2D-CGD-CBD	4.08	118.52	111.27
23	c	510	CLA	C3D-C4D-ND	4.08	116.83	110.24
31	D	401[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	b	609	CLA	C3D-C4D-ND	4.08	116.83	110.24
23	D	403[B]	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	c	506	CLA	CMB-C2B-C1B	4.07	131.57	125.37
23	D	403[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
24	y	101	BCR	C15-C14-C13	-4.07	121.50	127.31
23	B	606	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
31	A	416[A]	PHO	C1-C2-C3	-4.07	119.00	126.04
23	b	608	CLA	C1C-C2C-C3C	-4.06	102.68	106.96
23	D	403[A]	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	a	404[A]	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
23	d	402[A]	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	d	402[A]	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
23	c	505	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	C	502	CLA	C1D-CHD-C4C	-4.06	117.31	126.06
23	c	511	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	B	614	CLA	CMC-C2C-C1C	4.05	131.21	125.04
23	D	404	CLA	C3B-C2B-C1B	-4.05	102.28	107.16
23	C	509	CLA	O2D-CGD-O1D	-4.04	115.93	123.84
25	a	409[A]	SQD	C44-O6-C1	-4.04	105.84	113.74
23	C	511	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
23	c	510	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
38	F	102	HEM	CHC-C4B-NB	4.04	128.81	124.42
34	C	521	LMG	O7-C10-C11	4.04	120.20	111.50
23	d	402[B]	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
23	C	512	CLA	O2D-CGD-O1D	-4.03	115.96	123.84
23	A	404[A]	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	a	404[A]	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	B	608	CLA	C3D-C4D-ND	4.03	116.75	110.24
28	a	413[A]	PL9	C32-C33-C34	-4.03	117.96	127.66
23	c	506	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
38	f	101	HEM	CAD-CBD-CGD	4.02	122.26	113.60
23	B	610	CLA	C4A-NA-C1A	-4.02	104.90	106.71
23	c	510	CLA	C3C-C4C-NC	4.02	115.08	110.57
23	B	609	CLA	CMB-C2B-C1B	4.02	131.49	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	602	CLA	C3D-C2D-C1D	-4.02	100.35	105.83
23	c	510	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
23	d	403[B]	CLA	O2D-CGD-CBD	4.02	118.41	111.27
23	b	601	CLA	C1D-CHD-C4C	-4.01	117.40	126.06
23	b	611	CLA	C3D-C4D-ND	4.01	116.73	110.24
23	B	605	CLA	C3D-C4D-ND	4.01	116.73	110.24
23	b	610	CLA	C1-C2-C3	-4.01	119.11	126.04
23	a	404[B]	CLA	C3B-C2B-C1B	-4.01	102.32	107.16
23	A	404[A]	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	B	614	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
23	b	610	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
23	b	612	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
23	c	508	CLA	C3D-C4D-ND	4.00	116.71	110.24
23	B	615	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
36	C	518[A]	DGD	O2G-C1B-C2B	4.00	120.12	111.50
23	b	604	CLA	CAC-C3C-C4C	4.00	130.00	124.81
23	c	503	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
23	C	505	CLA	C3D-C4D-ND	4.00	116.70	110.24
35	o	301	HTG	O5-C1-C2	4.00	115.34	110.31
23	A	404[B]	CLA	O2D-CGD-CBD	3.99	118.37	111.27
23	c	514	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	b	610	CLA	O2A-CGA-O1A	-3.99	113.52	123.59
25	A	411	SQD	O47-C7-C8	3.98	120.09	111.50
23	B	616	CLA	O2D-CGD-O1D	-3.98	116.05	123.84
23	b	612	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
25	A	409[B]	SQD	C1-O5-C5	-3.98	105.88	113.69
23	b	603	CLA	CAA-C2A-C3A	-3.98	101.89	112.78
28	a	413[B]	PL9	C32-C33-C34	-3.98	118.08	127.66
23	A	407	CLA	C1C-C2C-C3C	-3.98	102.78	106.96
23	B	603	CLA	CAC-C3C-C4C	3.98	129.97	124.81
23	c	512	CLA	C3B-C4B-NB	3.97	114.20	110.52
23	c	513	CLA	C1-C2-C3	-3.97	119.17	126.04
23	C	506	CLA	CMB-C2B-C1B	3.97	131.42	125.37
23	b	612	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
23	B	616	CLA	CHD-C1D-ND	-3.97	120.81	124.45
36	C	517[A]	DGD	O2G-C1B-C2B	3.97	120.05	111.50
23	A	406[A]	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	b	612	CLA	C3D-C4D-ND	3.96	116.65	110.24
23	c	505	CLA	C1-O2A-CGA	3.96	126.84	116.44
23	B	606	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
23	B	608	CLA	C3C-C4C-NC	3.96	115.01	110.57
23	B	614	CLA	C3C-C4C-NC	3.96	115.01	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	b	625	HTG	C1-O5-C5	3.96	119.88	112.58
25	A	409[A]	SQD	O9-S-C6	3.96	111.64	106.94
23	c	507	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	b	607	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
25	A	409[B]	SQD	O47-C7-C8	3.95	120.02	111.50
23	c	503	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	604	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	d	404	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	A	405[A]	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	A	407	CLA	C1-C2-C3	-3.94	119.23	126.04
23	b	616	CLA	O2A-CGA-CBA	3.94	124.27	111.91
23	c	509	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	b	608	CLA	C3D-C2D-C1D	-3.94	100.46	105.83
23	B	601	CLA	C2C-C1C-NC	3.94	113.66	109.97
23	c	511	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
23	B	603	CLA	C1D-CHD-C4C	-3.93	117.57	126.06
38	f	101	HEM	C4C-NC-C1C	3.93	109.20	105.35
23	C	507	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
23	B	616	CLA	C3B-C4B-NB	3.93	114.16	110.52
23	A	404[A]	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	C	509	CLA	C1C-C2C-C3C	-3.92	102.84	106.96
23	b	601	CLA	C3C-C4C-NC	3.91	114.95	110.57
25	a	411	SQD	O47-C7-C8	3.91	119.92	111.50
34	d	412	LMG	O7-C10-C11	3.91	119.92	111.50
23	c	514	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	B	602	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	B	608	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	A	406[B]	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
23	a	407	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
23	c	505	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	C	510	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
23	B	615	CLA	CMC-C2C-C1C	3.90	130.97	125.04
23	B	609	CLA	O2D-CGD-CBD	3.90	118.19	111.27
23	c	510	CLA	CAC-C3C-C4C	3.90	129.87	124.81
23	C	505	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	B	604	CLA	CMB-C2B-C1B	3.89	131.30	125.37
23	C	513	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
34	Z	101	LMG	C1-C2-C3	3.89	118.10	110.00
23	A	406[A]	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	b	615	CLA	O2D-CGD-CBD	3.89	118.17	111.27
23	C	508	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
23	B	615	CLA	C4-C3-C5	3.88	121.80	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404[A]	CLA	O2D-CGD-CBD	3.88	118.16	111.27
23	c	512	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
24	b	617	BCR	C7-C8-C9	-3.86	120.40	126.23
25	l	101	SQD	O7-S-C6	3.86	111.53	106.94
23	A	407	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
23	b	604	CLA	C1C-C2C-C3C	-3.86	102.90	106.96
23	b	606	CLA	C3C-C4C-NC	3.86	114.89	110.57
34	c	520	LMG	O7-C10-C11	3.85	119.81	111.50
23	c	504	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
23	a	404[B]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	c	505	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	b	606	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	B	610	CLA	C3D-C4D-ND	3.84	116.45	110.24
23	A	407	CLA	O2D-CGD-CBD	3.84	118.09	111.27
23	B	611	CLA	CHB-C4A-NA	3.83	129.81	124.51
34	c	521	LMG	C3-C4-C5	3.83	117.07	110.24
23	B	608	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
28	A	413[A]	PL9	C7-C3-C4	3.83	119.99	116.88
23	A	404[A]	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
23	A	405[A]	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	c	509	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
28	a	413[B]	PL9	C7-C8-C9	-3.82	120.44	126.79
23	C	513	CLA	C2C-C1C-NC	3.82	113.55	109.97
28	a	413[B]	PL9	C7-C3-C2	-3.82	118.28	123.30
23	B	608	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	c	510	CLA	C4A-NA-C1A	-3.81	104.99	106.71
25	A	409[B]	SQD	C44-O6-C1	-3.81	106.30	113.74
23	b	609	CLA	O2D-CGD-CBD	3.81	118.03	111.27
23	B	616	CLA	C3D-C4D-ND	3.81	116.40	110.24
23	b	611	CLA	C3B-C4B-NB	3.81	114.05	110.52
23	b	613	CLA	C1-C2-C3	-3.80	119.46	126.04
23	C	512	CLA	C3D-C4D-ND	3.80	116.39	110.24
23	B	606	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
23	A	404[A]	CLA	O2A-CGA-CBA	3.79	123.81	111.91
23	b	605	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
25	A	411	SQD	O8-S-C6	3.79	111.78	105.74
23	C	502	CLA	C3B-C2B-C1B	-3.79	102.59	107.16
23	d	403[B]	CLA	C3B-C4B-NB	3.79	114.03	110.52
23	B	613	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	b	602	CLA	C3C-C4C-NC	3.78	114.81	110.57
23	A	404[A]	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
28	d	406[B]	PL9	C42-C43-C44	-3.77	118.58	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	405[B]	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	c	502	CLA	CMB-C2B-C1B	3.77	131.11	125.37
23	D	403[A]	CLA	C3B-C4B-NB	3.77	114.01	110.52
23	A	405[B]	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	C	511	CLA	C4A-NA-C1A	-3.77	105.01	106.71
23	c	506	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
28	a	413[A]	PL9	C15-C14-C16	3.76	121.60	115.27
23	D	403[A]	CLA	C1-C2-C3	-3.76	119.54	126.04
23	C	509	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
23	b	603	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	B	611	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
23	a	407	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
23	B	602	CLA	CMC-C2C-C1C	3.75	130.75	125.04
23	C	507	CLA	C1-C2-C3	-3.75	119.56	126.04
23	A	406[B]	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	c	505	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	a	405[B]	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	b	615	CLA	CMB-C2B-C1B	3.75	131.08	125.37
23	B	616	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	b	604	CLA	C3D-C4D-ND	3.75	116.30	110.24
23	A	405[A]	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
23	C	513	CLA	C1-C2-C3	-3.75	119.56	126.04
23	c	512	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	c	507	CLA	C3C-C4C-NC	3.74	114.77	110.57
23	b	607	CLA	C4A-NA-C1A	-3.74	105.02	106.71
33	d	414[B]	LHG	O7-C7-C8	3.74	119.56	111.50
24	K	102	BCR	C38-C26-C25	-3.73	120.33	124.53
33	d	414[A]	LHG	O8-C23-O10	-3.73	114.17	123.59
23	c	512	CLA	C4A-NA-C1A	-3.73	105.03	106.71
23	b	602	CLA	CAA-C2A-C3A	-3.72	102.58	112.78
23	B	602	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
33	b	629[B]	LHG	O7-C7-C8	3.72	119.52	111.50
23	c	502	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
24	T	102	BCR	C11-C10-C9	-3.72	122.00	127.31
23	A	404[A]	CLA	O2D-CGD-CBD	3.72	117.88	111.27
23	b	614	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
25	l	101	SQD	C1-O5-C5	-3.71	106.40	113.69
33	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.50
23	d	404	CLA	CMB-C2B-C1B	3.71	131.02	125.37
23	D	404	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
28	a	413[A]	PL9	C7-C3-C2	-3.71	118.42	123.30
24	d	405	BCR	C38-C26-C25	-3.71	120.37	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	514	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
23	C	511	CLA	C3C-C4C-NC	3.70	114.72	110.57
23	c	514	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
33	d	407[B]	LHG	O7-C7-C8	3.70	119.47	111.50
23	B	609	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
23	A	405[B]	CLA	CMB-C2B-C1B	3.70	131.00	125.37
23	b	616	CLA	C3D-C4D-ND	3.70	116.22	110.24
23	b	613	CLA	O2A-CGA-O1A	-3.69	114.27	123.59
23	b	606	CLA	C4-C3-C5	3.69	121.48	115.27
23	b	612	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	b	603	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	c	511	CLA	CMC-C2C-C1C	3.69	130.66	125.04
23	C	514	CLA	C3B-C4B-NB	3.69	113.94	110.52
23	B	614	CLA	C3D-C4D-ND	3.69	116.20	110.24
23	a	407	CLA	CMC-C2C-C1C	3.69	130.65	125.04
23	b	611	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
23	c	503	CLA	CMB-C2B-C1B	3.68	130.97	125.37
23	c	502	CLA	C3C-C4C-NC	3.68	114.69	110.57
23	B	603	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
23	C	508	CLA	CMB-C2B-C1B	3.67	130.96	125.37
23	B	601	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
25	A	409[A]	SQD	C44-O6-C1	-3.67	106.57	113.74
28	a	413[A]	PL9	C30-C29-C31	3.67	121.44	115.27
23	d	403[B]	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
24	b	618	BCR	C37-C22-C21	-3.67	117.78	122.92
28	D	406[A]	PL9	C42-C43-C44	-3.67	118.83	127.66
23	b	608	CLA	C1D-CHD-C4C	-3.67	118.14	126.06
23	B	605	CLA	C1-C2-C3	-3.67	119.70	126.04
23	C	507	CLA	C3C-C4C-NC	3.67	114.68	110.57
23	B	604	CLA	C3D-C2D-C1D	-3.66	100.83	105.83
23	B	610	CLA	O2D-CGD-O1D	-3.66	116.68	123.84
23	D	403[A]	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
36	c	518[B]	DGD	O2G-C1B-C2B	3.66	119.39	111.50
23	B	613	CLA	C3B-C4B-NB	3.66	113.91	110.52
23	B	604	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
23	A	404[B]	CLA	C3C-C4C-NC	3.66	114.67	110.57
23	B	610	CLA	CAA-CBA-CGA	-3.66	102.57	113.25
25	l	101	SQD	C3-C4-C5	3.65	116.76	110.24
23	b	613	CLA	O2D-CGD-CBD	3.65	117.76	111.27
23	c	506	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
28	A	413[A]	PL9	C15-C14-C16	3.65	121.41	115.27
23	C	511	CLA	C3B-C4B-NB	3.65	113.90	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	L	101[B]	LHG	O7-C7-C8	3.65	119.37	111.50
23	B	616	CLA	C4C-C3C-C2C	-3.65	101.58	106.90
23	C	503	CLA	C1C-C2C-C3C	-3.64	103.12	106.96
23	B	602	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	a	405[A]	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
36	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.50
23	a	404[B]	CLA	O2D-CGD-CBD	3.63	117.72	111.27
23	b	614	CLA	O2A-CGA-O1A	-3.63	114.42	123.59
23	c	509	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	B	610	CLA	CMB-C2B-C1B	3.63	130.90	125.37
28	A	413[B]	PL9	C15-C14-C16	3.63	121.38	115.27
23	a	405[A]	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	B	612	CLA	C4C-C3C-C2C	-3.63	101.61	106.90
36	C	517[B]	DGD	O2G-C1B-C2B	3.63	119.32	111.50
23	b	601	CLA	O2D-CGD-O1D	-3.63	116.75	123.84
23	c	513	CLA	CMB-C2B-C1B	3.62	130.89	125.37
23	b	611	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	b	609	CLA	C3B-C2B-C1B	-3.62	102.80	107.16
23	d	404	CLA	C1C-C2C-C3C	-3.62	103.16	106.96
23	d	402[B]	CLA	C3C-C4C-NC	3.62	114.63	110.57
23	a	404[A]	CLA	O2A-CGA-O1A	-3.62	114.47	123.59
23	B	609	CLA	CBC-CAC-C3C	-3.61	102.47	112.43
23	C	506	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	c	506	CLA	CAC-C3C-C4C	3.61	129.50	124.81
23	C	504	CLA	C4C-C3C-C2C	-3.60	101.64	106.90
23	B	610	CLA	O2A-CGA-O1A	-3.60	114.50	123.59
23	b	604	CLA	O2D-CGD-O1D	-3.60	116.79	123.84
33	d	414[A]	LHG	O8-C23-C24	3.60	123.21	111.91
23	B	612	CLA	CMC-C2C-C1C	3.60	130.52	125.04
23	B	605	CLA	CHD-C4C-NC	3.60	129.87	124.20
28	d	406[A]	PL9	C42-C43-C44	-3.59	119.02	127.66
23	c	514	CLA	C3B-C4B-NB	3.59	113.84	110.52
23	A	405[B]	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
23	B	603	CLA	CMC-C2C-C1C	3.58	130.50	125.04
24	A	408	BCR	C24-C23-C22	-3.58	120.82	126.23
23	b	615	CLA	C4-C3-C5	3.58	121.29	115.27
23	C	507	CLA	C3B-C4B-NB	3.58	113.83	110.52
40	V	201	HEC	CBD-CAD-C3D	-3.58	102.69	112.63
28	A	413[A]	PL9	C22-C23-C24	-3.57	119.05	127.66
23	C	513	CLA	C4-C3-C5	3.57	121.28	115.27
23	D	404	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
23	C	506	CLA	C1D-CHD-C4C	-3.57	118.35	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406[A]	PL9	C40-C39-C41	3.57	121.28	115.27
36	c	518[A]	DGD	O2G-C1B-C2B	3.57	119.19	111.50
38	f	101	HEM	CHD-C1D-ND	3.57	128.29	124.42
33	A	418[B]	LHG	O7-C7-C8	3.57	119.19	111.50
23	B	604	CLA	CHD-C1D-ND	-3.57	121.18	124.45
23	A	405[B]	CLA	CAA-C2A-C3A	-3.56	103.02	112.78
28	a	413[B]	PL9	C15-C14-C16	3.56	121.27	115.27
23	A	406[B]	CLA	C3C-C4C-NC	3.56	114.57	110.57
23	B	604	CLA	C3B-C4B-NB	3.56	113.82	110.52
23	A	405[A]	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
23	B	605	CLA	C4-C3-C5	3.55	121.25	115.27
25	A	409[A]	SQD	O47-C7-C8	3.55	119.16	111.50
23	B	613	CLA	CAC-C3C-C4C	3.55	129.42	124.81
28	D	406[B]	PL9	C25-C24-C26	3.55	121.24	115.27
23	b	612	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
28	A	413[A]	PL9	C7-C3-C2	-3.55	118.63	123.30
23	c	507	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
23	C	505	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
38	f	101	HEM	C1B-NB-C4B	3.55	108.74	105.07
24	B	617	BCR	C16-C17-C18	-3.54	122.25	127.31
23	b	612	CLA	C4-C3-C5	3.54	121.23	115.27
23	B	604	CLA	C3D-C4D-ND	3.54	115.97	110.24
23	A	406[A]	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
24	t	102	BCR	C11-C10-C9	-3.54	122.26	127.31
34	c	501	LMG	C7-O1-C1	-3.54	106.83	113.74
23	c	513	CLA	C3C-C4C-NC	3.54	114.54	110.57
25	X	101	SQD	C44-O6-C1	-3.53	106.84	113.74
23	B	607	CLA	C4-C3-C5	3.53	121.21	115.27
23	b	608	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
23	b	602	CLA	CMC-C2C-C1C	3.53	130.41	125.04
23	B	610	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	A	405[A]	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
23	B	601	CLA	C4C-C3C-C2C	-3.52	101.77	106.90
38	f	101	HEM	C4D-ND-C1D	3.52	108.71	105.07
23	b	609	CLA	CBC-CAC-C3C	-3.52	102.73	112.43
23	c	507	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
28	A	413[B]	PL9	C22-C23-C24	-3.52	119.19	127.66
24	Y	101	BCR	C16-C17-C18	-3.51	122.31	127.31
23	b	613	CLA	C1D-CHD-C4C	-3.51	118.50	126.06
28	a	413[B]	PL9	C27-C28-C29	-3.50	119.22	127.66
23	B	607	CLA	C3B-C2B-C1B	-3.50	102.93	107.16
23	C	512	CLA	C1C-C2C-C3C	-3.50	103.27	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	416[B]	PHO	C1A-C2A-C3A	-3.50	99.51	102.84
23	b	614	CLA	C1D-CHD-C4C	-3.50	118.51	126.06
24	h	101	BCR	C38-C26-C25	-3.50	120.60	124.53
33	A	418[A]	LHG	O7-C7-C8	3.50	119.04	111.50
23	b	609	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
23	B	610	CLA	C1D-CHD-C4C	-3.49	118.52	126.06
23	C	507	CLA	CBC-CAC-C3C	-3.49	102.81	112.43
24	C	515	BCR	C15-C14-C13	-3.49	122.33	127.31
23	C	504	CLA	C4-C3-C5	3.49	121.14	115.27
23	b	614	CLA	C1-C2-C3	-3.49	120.01	126.04
23	b	613	CLA	C3B-C4B-NB	3.49	113.75	110.52
28	d	406[B]	PL9	C7-C3-C4	3.48	119.71	116.88
23	C	508	CLA	C3D-C4D-ND	3.48	115.87	110.24
23	c	511	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
23	C	506	CLA	C4-C3-C5	3.48	121.13	115.27
23	d	403[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
25	a	409[B]	SQD	C1-O5-C5	-3.48	106.86	113.69
23	C	508	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
24	h	101	BCR	C7-C8-C9	-3.48	120.98	126.23
23	C	503	CLA	C1-C2-C3	-3.48	120.03	126.04
23	b	611	CLA	C1-C2-C3	-3.47	120.03	126.04
23	B	614	CLA	CHD-C4C-NC	3.47	129.67	124.20
36	c	517[B]	DGD	O2G-C1B-C2B	3.47	118.98	111.50
23	d	403[A]	CLA	C3B-C4B-NB	3.47	113.73	110.52
23	c	511	CLA	C3B-C4B-NB	3.46	113.73	110.52
34	C	520	LMG	O7-C10-C11	3.46	118.97	111.50
31	A	416[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
34	C	521	LMG	C3-C4-C5	3.46	116.42	110.24
33	d	414[B]	LHG	O8-C23-C24	3.46	122.77	111.91
28	d	406[A]	PL9	C37-C38-C39	-3.46	119.33	127.66
23	B	609	CLA	C3B-C2B-C1B	-3.46	102.98	107.16
23	b	604	CLA	CMC-C2C-C1C	3.46	130.30	125.04
23	C	509	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
23	b	607	CLA	C3B-C4B-NB	3.45	113.72	110.52
23	C	502	CLA	CMB-C2B-C1B	3.45	130.62	125.37
23	b	606	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
23	A	404[A]	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
23	C	509	CLA	C4A-NA-C1A	-3.45	105.16	106.71
23	B	609	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
25	a	411	SQD	O48-C23-C24	3.45	122.72	111.91
23	B	601	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
33	D	407[B]	LHG	O7-C7-C8	3.44	118.91	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CMC-C2C-C1C	3.43	130.27	125.04
23	b	610	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
38	F	102	HEM	CHB-C1B-NB	3.43	128.60	124.37
23	d	402[B]	CLA	CBC-CAC-C3C	-3.43	102.98	112.43
23	a	404[B]	CLA	CAA-C2A-C3A	-3.43	103.39	112.78
31	a	406[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
23	B	605	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
23	C	513	CLA	CHD-C4C-NC	3.42	129.59	124.20
33	d	408[A]	LHG	O7-C7-C8	3.42	118.86	111.50
38	F	102	HEM	CBD-CAD-C3D	-3.41	103.14	112.63
23	d	402[A]	CLA	CHD-C4C-NC	3.41	129.58	124.20
38	f	101	HEM	CHA-C4D-ND	3.41	128.58	124.37
34	C	520	LMG	O8-C28-C29	3.41	122.61	111.91
23	A	404[B]	CLA	C3B-C2B-C1B	-3.41	103.05	107.16
23	b	605	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
31	a	406[A]	PHO	O1D-CGD-CBD	-3.41	119.07	124.74
23	b	607	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
24	C	515	BCR	C7-C8-C9	-3.40	121.09	126.23
23	A	404[B]	CLA	CAA-C2A-C3A	-3.40	103.46	112.78
23	B	605	CLA	CMB-C2B-C1B	3.40	130.55	125.37
23	C	508	CLA	C4C-C3C-C2C	-3.40	101.94	106.90
23	C	505	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
23	B	603	CLA	CAA-C2A-C3A	-3.40	103.48	112.78
24	C	515	BCR	C33-C5-C6	-3.40	120.72	124.53
23	a	405[B]	CLA	CHD-C4C-NC	3.39	129.55	124.20
25	X	101	SQD	C1-C2-C3	-3.39	102.93	110.00
23	b	602	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	B	607	CLA	C1D-CHD-C4C	-3.39	118.75	126.06
23	B	616	CLA	CAC-C3C-C4C	3.39	129.20	124.81
28	A	413[B]	PL9	C17-C18-C19	-3.39	119.51	127.66
24	B	617	BCR	C33-C5-C6	-3.38	120.73	124.53
23	C	506	CLA	CAC-C3C-C4C	3.38	129.20	124.81
23	d	402[A]	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	A	404[B]	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
28	a	413[A]	PL9	C27-C28-C29	-3.38	119.53	127.66
23	C	503	CLA	O2D-CGD-O1D	-3.38	117.24	123.84
23	b	611	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
28	A	413[A]	PL9	C37-C38-C39	-3.37	119.54	127.66
23	C	510	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
23	C	503	CLA	C4-C3-C5	3.37	120.94	115.27
23	D	404	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
28	d	406[B]	PL9	C40-C39-C41	3.37	120.94	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	CAC-C3C-C4C	3.37	129.18	124.81
23	b	613	CLA	O2A-CGA-CBA	3.37	122.47	111.91
28	A	413[A]	PL9	C27-C28-C29	-3.36	119.56	127.66
23	B	605	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
23	a	404[B]	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	A	406[B]	CLA	CMB-C2B-C1B	3.36	130.49	125.37
23	a	404[A]	CLA	O2A-CGA-CBA	3.36	122.45	111.91
23	d	402[B]	CLA	CHD-C4C-NC	3.36	129.49	124.20
23	D	403[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
36	h	102	DGD	O2G-C1B-C2B	3.35	118.73	111.50
23	B	609	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
23	d	402[B]	CLA	CAA-C2A-C3A	-3.35	103.59	112.78
24	y	101	BCR	C38-C26-C25	-3.35	120.76	124.53
24	K	102	BCR	C24-C23-C22	-3.35	121.17	126.23
23	c	513	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.81
33	b	629[A]	LHG	O7-C7-C8	3.35	118.72	111.50
31	a	415[A]	PHO	C4-C3-C5	3.35	120.90	115.27
28	d	406[B]	PL9	C10-C9-C11	3.34	120.90	115.27
23	c	512	CLA	CHD-C4C-NC	3.34	129.47	124.20
23	b	609	CLA	CMC-C2C-C1C	3.34	130.13	125.04
23	C	509	CLA	C1-C2-C3	-3.34	120.26	126.04
23	c	513	CLA	C1C-C2C-C3C	-3.34	103.44	106.96
23	C	507	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	d	403[A]	CLA	C4-C3-C5	3.34	120.89	115.27
23	c	509	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
24	k	101	BCR	C7-C8-C9	-3.34	121.19	126.23
23	c	513	CLA	CHD-C4C-NC	3.34	129.46	124.20
34	c	521	LMG	C9-C8-C7	-3.34	103.89	111.79
23	b	609	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	B	603	CLA	O2A-CGA-CBA	3.34	122.38	111.91
23	a	404[A]	CLA	C1-C2-C3	-3.33	120.28	126.04
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
23	a	405[B]	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	b	611	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
23	B	614	CLA	C1-C2-C3	-3.33	120.28	126.04
28	A	413[B]	PL9	C37-C38-C39	-3.33	119.65	127.66
23	a	405[B]	CLA	C1C-C2C-C3C	-3.33	103.46	106.96
23	B	610	CLA	C4C-C3C-C2C	-3.32	102.05	106.90
23	B	615	CLA	CED-O2D-CGD	3.32	123.46	115.94
23	C	511	CLA	C4-C3-C5	3.32	120.86	115.27
24	D	405	BCR	C28-C27-C26	-3.32	108.14	114.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	506	CLA	C1D-CHD-C4C	-3.32	118.89	126.06
23	b	612	CLA	CHB-C1B-NB	-3.32	120.74	124.26
23	d	403[B]	CLA	CHC-C1C-C2C	-3.32	117.50	126.73
23	A	407	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
23	a	404[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	c	512	CLA	CBC-CAC-C3C	-3.32	103.28	112.43
23	b	613	CLA	C3D-C4D-ND	3.32	115.60	110.24
23	C	502	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
23	B	602	CLA	CAA-C2A-C3A	-3.32	103.70	112.78
23	B	613	CLA	O2A-CGA-O1A	-3.31	115.23	123.59
28	A	413[B]	PL9	C27-C28-C29	-3.31	119.68	127.66
23	b	616	CLA	CMB-C2B-C1B	3.31	130.41	125.37
23	C	513	CLA	CMC-C2C-C1C	3.31	130.08	125.04
24	t	102	BCR	C21-C20-C19	-3.31	112.89	123.22
23	b	609	CLA	CAC-C3C-C4C	3.31	129.10	124.81
23	c	511	CLA	C4-C3-C5	3.31	120.84	115.27
23	C	506	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
23	A	407	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
23	b	614	CLA	C3B-C4B-NB	3.30	113.58	110.52
34	c	520	LMG	O1-C7-C8	-3.30	102.92	110.90
33	A	418[A]	LHG	O8-C23-C24	3.30	122.28	111.91
33	A	418[B]	LHG	C5-O7-C7	-3.30	109.66	117.79
28	a	413[A]	PL9	C37-C38-C39	-3.30	119.71	127.66
32	A	417	LMT	O5B-C5B-C4B	3.30	115.69	109.69
23	C	507	CLA	CMC-C2C-C1C	3.30	130.07	125.04
35	b	622	HTG	O2-C2-C1	3.30	116.33	110.27
23	a	404[A]	CLA	C3B-C4B-NB	3.30	113.58	110.52
23	B	605	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	B	603	CLA	O2A-CGA-O1A	-3.30	115.27	123.59
23	B	616	CLA	CMC-C2C-C1C	3.30	130.06	125.04
23	d	402[B]	CLA	C3B-C4B-NB	3.30	113.57	110.52
23	d	403[A]	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
35	b	622	HTG	C1'-S1-C1	3.29	106.25	100.09
35	b	625	HTG	O5-C5-C4	3.29	115.67	109.69
28	D	406[A]	PL9	C25-C24-C26	3.29	120.81	115.27
23	A	406[A]	CLA	C3B-C4B-NB	3.29	113.56	110.52
23	A	406[A]	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	B	614	CLA	O2A-CGA-O1A	-3.28	115.31	123.59
23	c	503	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	c	513	CLA	C4-C3-C5	3.28	120.79	115.27
23	a	404[A]	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
23	C	506	CLA	O2D-CGD-O1D	-3.28	117.43	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	606	CLA	C3B-C4B-NB	3.28	113.55	110.52
24	c	515	BCR	C15-C14-C13	-3.28	122.64	127.31
23	C	502	CLA	CAC-C3C-C4C	3.27	129.06	124.81
23	C	511	CLA	CMB-C2B-C1B	3.27	130.35	125.37
23	c	510	CLA	O2A-CGA-CBA	3.27	122.16	111.91
23	b	607	CLA	O2D-CGD-CBD	3.27	117.07	111.27
25	b	620	SQD	O8-S-C6	3.27	110.94	105.74
23	b	615	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
23	b	607	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
35	B	623	HTG	C1'-S1-C1	3.26	106.19	100.09
23	c	502	CLA	C1-C2-C3	-3.26	120.40	126.04
23	c	504	CLA	CMB-C2B-C1B	3.26	130.34	125.37
23	c	512	CLA	C4-C3-C5	3.26	120.75	115.27
23	A	404[B]	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
23	b	612	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	b	612	CLA	O2A-CGA-CBA	3.25	122.12	111.91
23	b	605	CLA	C4-C3-C5	3.25	120.74	115.27
23	D	403[B]	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
23	c	510	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
31	a	406[B]	PHO	C1-C2-C3	-3.25	120.43	126.04
23	c	507	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
23	C	507	CLA	CAC-C3C-C4C	3.25	129.02	124.81
23	d	403[A]	CLA	C1-C2-C3	-3.24	120.43	126.04
23	b	605	CLA	CHD-C4C-NC	3.24	129.32	124.20
31	D	401[B]	PHO	O1D-CGD-CBD	-3.24	119.34	124.74
23	B	602	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
23	b	616	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
34	Z	101	LMG	O6-C1-C2	3.24	117.21	110.35
28	D	406[B]	PL9	C27-C28-C29	-3.24	119.86	127.66
25	A	409[B]	SQD	O7-S-C6	3.24	110.78	106.94
23	C	510	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	B	607	CLA	CBC-CAC-C3C	-3.23	103.52	112.43
23	b	608	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	A	406[A]	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
23	d	403[B]	CLA	O2A-CGA-CBA	3.23	122.03	111.91
23	b	606	CLA	CHD-C4C-NC	3.23	129.29	124.20
24	Y	101	BCR	C15-C14-C13	-3.22	122.71	127.31
23	c	504	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	b	612	CLA	CMC-C2C-C1C	3.22	129.95	125.04
23	B	613	CLA	C4-C3-C5	3.22	120.69	115.27
25	f	102	SQD	O7-S-C6	3.22	110.77	106.94
23	c	506	CLA	C1C-C2C-C3C	-3.22	103.57	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	409[A]	SQD	C45-O47-C7	-3.21	109.88	117.79
23	b	613	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
23	b	608	CLA	CAC-C3C-C4C	3.21	128.98	124.81
23	b	610	CLA	CHD-C4C-NC	3.21	129.26	124.20
23	c	509	CLA	C3B-C4B-NB	3.21	113.49	110.52
23	C	510	CLA	CAC-C3C-C4C	3.21	128.98	124.81
23	b	603	CLA	C3B-C4B-NB	3.21	113.49	110.52
28	a	413[A]	PL9	C17-C18-C19	-3.21	119.94	127.66
23	d	404	CLA	O2D-CGD-O1D	-3.21	117.57	123.84
23	d	403[B]	CLA	C1-C2-C3	-3.20	120.50	126.04
34	z	101	LMG	O7-C10-C11	3.20	118.41	111.50
23	b	616	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
31	a	406[A]	PHO	O2A-CGA-O1A	-3.20	115.51	123.59
23	B	611	CLA	C1-C2-C3	-3.20	120.51	126.04
28	a	413[A]	PL9	C25-C24-C26	3.20	120.65	115.27
23	B	612	CLA	C11-C12-C13	-3.20	105.58	115.92
23	b	610	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
28	D	406[A]	PL9	C17-C18-C19	-3.20	119.96	127.66
23	b	602	CLA	CMB-C2B-C1B	3.19	130.23	125.37
23	a	407	CLA	O2A-CGA-CBA	3.19	121.93	111.91
31	A	416[A]	PHO	C4-C3-C5	3.19	120.64	115.27
23	c	504	CLA	C1-C2-C3	-3.19	120.53	126.04
23	b	605	CLA	CMB-C2B-C1B	3.19	130.22	125.37
23	B	616	CLA	O2A-CGA-CBA	3.19	121.91	111.91
23	A	406[B]	CLA	O2A-CGA-O1A	-3.18	115.55	123.59
23	c	508	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	a	404[B]	CLA	CHC-C1C-C2C	-3.18	117.90	126.73
23	d	403[A]	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	d	404	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
23	A	405[B]	CLA	C3B-C4B-NB	3.17	113.46	110.52
23	c	507	CLA	CAC-C3C-C4C	3.17	128.93	124.81
34	m	101	LMG	O8-C28-C29	3.17	121.85	111.91
28	d	406[B]	PL9	C7-C8-C9	-3.17	121.52	126.79
23	a	407	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
23	b	614	CLA	CMC-C2C-C1C	3.16	129.86	125.04
23	b	601	CLA	C4-C3-C5	3.16	120.59	115.27
23	A	405[A]	CLA	CMB-C2B-C1B	3.16	130.18	125.37
34	C	521	LMG	O8-C28-C29	3.16	121.82	111.91
23	B	604	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
24	B	617	BCR	C37-C22-C21	-3.16	118.50	122.92
23	B	612	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
23	a	404[A]	CLA	C4-C3-C5	3.15	120.57	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	C4-C3-C5	3.15	120.56	115.27
23	c	502	CLA	C1D-CHD-C4C	-3.14	119.27	126.06
23	b	601	CLA	CHD-C4C-NC	3.14	129.16	124.20
23	b	602	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
23	C	510	CLA	O2A-CGA-CBA	3.14	121.77	111.91
23	C	507	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
24	c	515	BCR	C37-C22-C21	-3.14	118.53	122.92
23	c	505	CLA	CAC-C3C-C4C	3.14	128.88	124.81
25	b	620	SQD	C3-C4-C5	3.14	115.83	110.24
25	X	101	SQD	O48-C23-C24	3.13	121.75	111.91
23	a	407	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	b	605	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
33	d	414[B]	LHG	O8-C23-O10	-3.13	115.69	123.59
23	b	616	CLA	CHD-C4C-NC	3.13	129.14	124.20
23	D	404	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	c	514	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	C	503	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	a	405[B]	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
23	A	404[A]	CLA	C1-C2-C3	-3.13	120.63	126.04
28	a	413[B]	PL9	C30-C29-C31	3.13	120.53	115.27
23	B	606	CLA	CMC-C2C-C1C	3.13	129.80	125.04
23	C	507	CLA	C4-C3-C5	3.13	120.53	115.27
23	B	611	CLA	C4C-C3C-C2C	-3.12	102.34	106.90
23	C	514	CLA	CBC-CAC-C3C	-3.12	103.82	112.43
23	a	405[A]	CLA	CMB-C2B-C1B	3.12	130.12	125.37
25	a	409[B]	SQD	C44-O6-C1	-3.12	107.64	113.74
23	A	405[A]	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	D	403[B]	CLA	C3B-C4B-NB	3.12	113.41	110.52
23	a	405[A]	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	B	613	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	d	402[B]	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	c	509	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
23	b	601	CLA	C1C-C2C-C3C	-3.11	103.68	106.96
23	A	407	CLA	CBC-CAC-C3C	-3.11	103.85	112.43
23	C	513	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
28	a	413[B]	PL9	C17-C18-C19	-3.11	120.17	127.66
25	a	409[B]	SQD	C45-O47-C7	-3.11	110.14	117.79
23	B	603	CLA	C3B-C4B-NB	3.11	113.40	110.52
25	f	102	SQD	O5-C1-C2	3.11	116.93	110.35
23	C	510	CLA	O2A-CGA-O1A	-3.11	115.75	123.59
23	c	508	CLA	C4-C3-C5	3.11	120.50	115.27
23	D	403[A]	CLA	C1D-CHD-C4C	-3.11	119.36	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	413[A]	PL9	C35-C34-C36	3.10	120.49	115.27
31	a	415[B]	PHO	C4-C3-C5	3.10	120.49	115.27
33	D	408[A]	LHG	O7-C7-C8	3.10	118.19	111.50
23	B	613	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
28	A	413[B]	PL9	C20-C19-C21	3.10	120.49	115.27
23	b	601	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
32	B	626	LMT	O1'-C1'-C2'	3.10	113.14	108.30
24	k	101	BCR	C24-C23-C22	-3.10	121.55	126.23
31	a	406[A]	PHO	O2A-CGA-CBA	3.10	121.63	111.91
38	f	101	HEM	CBD-CAD-C3D	-3.10	104.02	112.63
23	D	404	CLA	CMC-C2C-C1C	3.10	129.75	125.04
23	b	612	CLA	CAC-C3C-C4C	3.10	128.83	124.81
24	D	405	BCR	C29-C30-C25	3.10	115.25	110.48
23	B	607	CLA	C2A-C1A-CHA	-3.10	118.45	123.86
23	C	511	CLA	CHD-C4C-NC	3.09	129.08	124.20
23	a	405[A]	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
23	b	606	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
32	B	626	LMT	C4B-C3B-C2B	3.08	116.21	110.82
28	a	413[B]	PL9	C25-C24-C26	3.08	120.46	115.27
23	c	509	CLA	C1-C2-C3	-3.08	120.71	126.04
23	c	512	CLA	CHC-C1C-C2C	-3.08	118.17	126.73
33	D	407[A]	LHG	O8-C23-O10	-3.08	115.82	123.59
23	B	613	CLA	C1D-CHD-C4C	-3.08	119.41	126.06
24	c	516	BCR	C11-C10-C9	-3.08	122.92	127.31
23	b	602	CLA	C1-C2-C3	-3.08	120.72	126.04
24	a	408	BCR	C38-C26-C25	-3.08	121.07	124.53
23	a	404[B]	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	d	403[B]	CLA	C4-C3-C5	3.08	120.44	115.27
23	C	509	CLA	CHC-C1C-C2C	-3.08	118.19	126.73
23	c	510	CLA	CMC-C2C-C1C	3.08	129.72	125.04
23	a	405[A]	CLA	C3B-C4B-NB	3.07	113.37	110.52
23	c	503	CLA	C3B-C4B-NB	3.07	113.37	110.52
24	B	617	BCR	C15-C14-C13	-3.07	122.93	127.31
23	b	602	CLA	C2A-C1A-CHA	-3.07	118.49	123.86
23	B	603	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
32	A	419	LMT	O5B-C5B-C4B	3.07	115.26	109.69
23	b	602	CLA	CMA-C3A-C4A	-3.07	103.53	111.77
23	B	606	CLA	CBC-CAC-C3C	-3.06	103.98	112.43
23	d	403[B]	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
24	y	101	BCR	C24-C23-C22	-3.06	121.61	126.23
23	B	608	CLA	CHC-C1C-C2C	-3.06	118.24	126.73
33	a	419[A]	LHG	O7-C7-C8	3.05	118.08	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	B	627	LMT	O1'-C1'-C2'	3.05	113.07	108.30
36	c	519	DGD	O2G-C1B-C2B	3.05	118.08	111.50
23	c	503	CLA	CBC-CAC-C3C	-3.05	104.02	112.43
25	a	409[B]	SQD	C1-C2-C3	-3.05	103.64	110.00
25	a	409[B]	SQD	O8-S-C6	3.05	110.60	105.74
23	c	504	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
23	B	612	CLA	C1D-CHD-C4C	-3.05	119.48	126.06
34	B	620	LMG	O8-C28-C29	3.05	121.47	111.91
23	A	404[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
24	D	405	BCR	C10-C11-C12	-3.05	113.71	123.22
33	D	408[A]	LHG	O8-C23-C24	3.05	121.46	111.91
28	A	413[A]	PL9	O1-C4-C3	-3.05	117.37	120.72
23	C	511	CLA	O2A-CGA-O1A	-3.04	115.91	123.59
23	C	512	CLA	C4-C3-C5	3.04	120.39	115.27
28	a	413[A]	PL9	C10-C9-C11	3.04	120.39	115.27
23	b	609	CLA	C3B-C4B-NB	3.04	113.34	110.52
23	D	404	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
25	A	409[B]	SQD	O9-S-C6	3.04	110.55	106.94
23	C	506	CLA	CMC-C2C-C1C	3.04	129.67	125.04
23	D	403[B]	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
38	F	102	HEM	CHD-C1D-ND	3.04	127.72	124.42
28	A	413[A]	PL9	C20-C19-C21	3.04	120.38	115.27
24	k	101	BCR	C29-C30-C25	3.04	115.16	110.48
23	C	514	CLA	CMC-C2C-C1C	3.04	129.66	125.04
23	b	607	CLA	CBC-CAC-C3C	-3.03	104.07	112.43
33	d	414[A]	LHG	O7-C7-C8	3.03	118.04	111.50
23	b	615	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	C	504	CLA	CHD-C4C-NC	3.03	128.98	124.20
33	a	419[B]	LHG	O7-C7-C8	3.03	118.04	111.50
24	B	619	BCR	C38-C26-C25	-3.03	121.12	124.53
23	b	612	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
25	l	101	SQD	O48-C23-C24	3.03	121.42	111.91
23	A	407	CLA	CMA-C3A-C2A	-3.03	101.61	113.83
23	b	605	CLA	O2A-CGA-O1A	-3.03	115.95	123.59
23	B	613	CLA	O2A-CGA-CBA	3.02	121.39	111.91
24	d	405	BCR	C16-C17-C18	-3.02	123.00	127.31
23	C	513	CLA	O2A-CGA-CBA	3.02	121.39	111.91
23	A	405[A]	CLA	C3B-C4B-NB	3.02	113.32	110.52
23	b	614	CLA	CAC-C3C-C4C	3.02	128.73	124.81
34	Z	101	LMG	C4-C3-C2	3.02	116.09	110.82
23	c	511	CLA	CAC-C3C-C4C	3.02	128.73	124.81
23	c	509	CLA	CMB-C2B-C1B	3.02	129.96	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C4-C3-C5	3.02	120.35	115.27
23	C	511	CLA	CMC-C2C-C1C	3.02	129.63	125.04
23	C	502	CLA	C4-C3-C5	3.02	120.34	115.27
31	a	415[A]	PHO	CBA-CAA-C2A	-3.02	105.00	113.81
23	A	405[B]	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
23	A	406[A]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	B	615	CLA	C11-C10-C8	-3.01	106.19	115.92
33	D	408[A]	LHG	O8-C23-O10	-3.01	115.99	123.59
24	D	405	BCR	C37-C22-C23	3.01	122.82	118.08
23	C	513	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
28	a	413[B]	PL9	C42-C43-C44	-3.01	120.42	127.66
31	a	415[A]	PHO	CMB-C2B-C3B	3.01	130.30	124.68
23	b	615	CLA	C11-C10-C8	-3.01	106.20	115.92
23	b	616	CLA	CMC-C2C-C1C	3.00	129.62	125.04
25	A	411	SQD	O48-C23-C24	3.00	121.33	111.91
28	D	406[A]	PL9	C53-C6-C1	3.00	121.13	114.99
23	A	406[B]	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	a	406[B]	PHO	O1D-CGD-CBD	-3.00	119.74	124.74
23	c	510	CLA	CHB-C1B-NB	-3.00	121.08	124.26
28	d	406[A]	PL9	C22-C23-C24	-3.00	120.44	127.66
28	d	406[A]	PL9	C36-C34-C33	-3.00	115.05	121.12
23	a	405[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	d	404	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
33	A	418[B]	LHG	O8-C23-O10	-3.00	116.03	123.59
23	c	513	CLA	O2A-CGA-CBA	3.00	121.31	111.91
23	C	502	CLA	C3B-C4B-NB	2.99	113.29	110.52
23	b	603	CLA	C2A-C1A-CHA	-2.99	118.62	123.86
35	o	301	HTG	C1'-S1-C1	2.99	105.69	100.09
23	C	511	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
28	A	413[A]	PL9	C17-C18-C19	-2.99	120.45	127.66
23	C	505	CLA	CMC-C2C-C1C	2.99	129.60	125.04
28	a	413[B]	PL9	C37-C38-C39	-2.99	120.46	127.66
23	B	608	CLA	CHB-C4A-NA	2.99	128.65	124.51
23	a	404[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
36	h	102	DGD	O1G-C1A-C2A	2.99	121.29	111.91
23	d	404	CLA	C4-C3-C5	2.99	120.30	115.27
23	C	511	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	B	604	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	B	603	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
25	f	102	SQD	C4-C3-C2	-2.99	105.61	110.82
23	c	503	CLA	CHD-C4C-NC	2.99	128.91	124.20
23	c	510	CLA	C4C-C3C-C2C	-2.98	102.55	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	f	102	SQD	O5-C5-C4	2.98	115.11	109.69
23	B	606	CLA	O2A-CGA-CBA	2.98	121.27	111.91
23	d	403[A]	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
35	b	622	HTG	O5-C5-C4	2.98	115.11	109.69
28	d	406[B]	PL9	C15-C14-C16	2.98	120.28	115.27
23	c	502	CLA	CHD-C4C-NC	2.98	128.90	124.20
25	l	101	SQD	C4-C3-C2	2.98	116.02	110.82
23	a	404[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
23	b	605	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
23	d	404	CLA	C3B-C4B-NB	2.98	113.28	110.52
23	A	405[B]	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
23	A	406[A]	CLA	CMC-C2C-C1C	2.98	129.57	125.04
28	D	406[B]	PL9	C17-C18-C19	-2.98	120.50	127.66
34	C	521	LMG	O1-C1-C2	2.97	112.95	108.30
36	C	517[A]	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
23	d	403[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
28	a	413[A]	PL9	C42-C43-C44	-2.97	120.50	127.66
23	C	504	CLA	C1-C2-C3	-2.97	120.90	126.04
23	a	404[A]	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	b	608	CLA	CHD-C4C-NC	2.97	128.88	124.20
28	d	406[A]	PL9	C10-C9-C11	2.97	120.27	115.27
34	D	412	LMG	O7-C10-C11	2.97	117.89	111.50
25	A	409[A]	SQD	O8-S-C6	2.96	110.46	105.74
24	B	619	BCR	C7-C8-C9	-2.96	121.76	126.23
23	D	403[B]	CLA	O2A-CGA-CBA	2.96	121.21	111.91
23	a	407	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
24	c	515	BCR	C28-C27-C26	-2.96	108.79	114.08
31	a	415[A]	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
23	B	611	CLA	C2A-C1A-CHA	-2.96	118.68	123.86
23	D	403[B]	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
24	H	101	BCR	C16-C17-C18	-2.96	123.08	127.31
23	B	605	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
23	c	511	CLA	CHD-C4C-NC	2.96	128.87	124.20
23	C	512	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	c	511	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
35	b	622	HTG	O5-C1-C2	2.96	114.03	110.31
23	c	503	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
23	b	612	CLA	CHD-C4C-NC	2.96	128.86	124.20
23	B	606	CLA	CHD-C4C-NC	2.96	128.86	124.20
23	b	614	CLA	O2A-CGA-CBA	2.96	121.19	111.91
23	B	614	CLA	C2A-C1A-CHA	-2.96	118.69	123.86
23	B	601	CLA	CHD-C4C-NC	2.96	128.86	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
23	c	514	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
23	C	506	CLA	C3B-C4B-NB	2.95	113.26	110.52
23	b	610	CLA	CMB-C2B-C1B	2.95	129.87	125.37
23	c	505	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	A	404[B]	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
23	B	607	CLA	O2A-CGA-O1A	-2.95	116.14	123.59
23	B	614	CLA	O2A-CGA-CBA	2.95	121.17	111.91
23	A	407	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
23	B	615	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	D	403[A]	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	b	603	CLA	O2A-CGA-CBA	2.95	121.17	111.91
23	C	512	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
31	A	416[B]	PHO	C4-C3-C5	2.95	120.23	115.27
24	a	408	BCR	C29-C30-C25	2.95	115.02	110.48
23	C	510	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
23	c	505	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	b	609	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
23	B	602	CLA	C11-C12-C13	-2.94	106.41	115.92
23	B	608	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
36	h	102	DGD	O1G-C1A-O1A	-2.94	116.17	123.59
23	B	608	CLA	CAC-C3C-C4C	2.94	128.62	124.81
23	a	405[B]	CLA	CAC-C3C-C4C	2.94	128.62	124.81
23	b	610	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
23	B	615	CLA	CHD-C4C-NC	2.94	128.83	124.20
34	c	501	LMG	C8-O7-C10	-2.94	110.56	117.79
23	c	502	CLA	C3B-C4B-NB	2.94	113.24	110.52
34	c	520	LMG	O8-C28-C29	2.94	121.12	111.91
24	y	101	BCR	C10-C11-C12	-2.93	114.06	123.22
36	c	517[B]	DGD	O3G-C3G-C2G	-2.93	103.82	110.90
23	b	606	CLA	CMB-C2B-C1B	2.93	129.84	125.37
23	c	514	CLA	O2A-CGA-CBA	2.93	121.11	111.91
28	D	406[A]	PL9	C10-C9-C11	2.93	120.20	115.27
38	f	101	HEM	CHB-C1B-NB	2.93	127.99	124.37
23	B	606	CLA	O2A-CGA-O1A	-2.93	116.20	123.59
23	d	402[B]	CLA	CMB-C2B-C1B	2.93	129.83	125.37
24	D	405	BCR	C38-C26-C25	-2.93	121.24	124.53
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	B	614	CLA	CAC-C3C-C4C	2.93	128.61	124.81
23	c	503	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	c	502	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
24	B	619	BCR	C21-C20-C19	-2.93	114.09	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CMB-C2B-C1B	2.92	129.82	125.37
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	d	402[A]	CLA	CMA-C3A-C2A	-2.92	102.03	113.83
23	b	610	CLA	CMC-C2C-C1C	2.92	129.49	125.04
23	a	404[B]	CLA	CHD-C4C-NC	2.92	128.81	124.20
28	d	406[B]	PL9	C53-C6-C1	2.92	120.96	114.99
23	a	405[B]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	c	514	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	C	502	CLA	CHD-C4C-NC	2.92	128.80	124.20
23	c	509	CLA	C4-C3-C5	2.92	120.18	115.27
33	E	101[A]	LHG	O8-C23-C24	2.92	121.06	111.91
23	C	512	CLA	C3B-C4B-NB	2.92	113.22	110.52
23	b	611	CLA	CHC-C1C-C2C	-2.91	118.63	126.73
23	C	502	CLA	CMC-C2C-C1C	2.91	129.48	125.04
23	D	403[A]	CLA	C4-C3-C5	2.91	120.17	115.27
23	c	509	CLA	CHC-C1C-C2C	-2.91	118.64	126.73
23	b	616	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
23	A	404[A]	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
23	C	508	CLA	C1-C2-C3	-2.91	121.01	126.04
23	a	405[B]	CLA	C3B-C4B-NB	2.91	113.21	110.52
23	D	404	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
33	E	101[B]	LHG	O8-C23-C24	2.91	121.03	111.91
24	c	516	BCR	C37-C22-C21	-2.91	118.85	122.92
23	C	504	CLA	O2A-CGA-O1A	-2.91	116.26	123.59
23	A	404[B]	CLA	CAC-C3C-C4C	2.91	128.58	124.81
23	c	508	CLA	CHD-C4C-NC	2.91	128.78	124.20
23	a	404[B]	CLA	O2A-CGA-CBA	2.90	121.02	111.91
23	B	607	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
23	C	502	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	b	603	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	c	515	BCR	C16-C17-C18	-2.90	123.17	127.31
23	c	510	CLA	C4-C3-C5	2.90	120.15	115.27
23	A	405[A]	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	b	603	CLA	CBC-CAC-C3C	-2.90	104.44	112.43
34	z	101	LMG	O8-C28-C29	2.90	121.01	111.91
23	B	601	CLA	C1-O2A-CGA	2.90	124.05	116.44
23	D	403[A]	CLA	O2A-CGA-CBA	2.90	121.00	111.91
23	b	614	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	c	508	CLA	O2A-CGA-CBA	2.90	121.00	111.91
32	M	101	LMT	C3'-C4'-C5'	-2.90	104.28	110.93
25	A	409[B]	SQD	O48-C23-C24	2.90	121.00	111.91
23	A	406[B]	CLA	CHD-C4C-NC	2.90	128.77	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	604	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	A	406[B]	CLA	C3B-C4B-NB	2.89	113.20	110.52
23	c	510	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	B	609	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	B	608	CLA	CMA-C3A-C4A	-2.89	104.00	111.77
33	D	408[B]	LHG	O8-C23-C24	2.89	120.98	111.91
24	C	516	BCR	C32-C1-C6	-2.89	105.61	110.30
23	B	605	CLA	CMC-C2C-C1C	2.89	129.44	125.04
24	H	101	BCR	C24-C23-C22	-2.89	121.87	126.23
23	d	403[A]	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
23	a	407	CLA	CMA-C3A-C2A	-2.89	102.18	113.83
24	A	408	BCR	C40-C30-C25	-2.89	105.62	110.30
23	B	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
36	C	519	DGD	O1G-C1A-C2A	2.88	120.96	111.91
23	A	404[B]	CLA	O2A-CGA-CBA	2.88	120.96	111.91
33	d	407[A]	LHG	O7-C7-C8	2.88	117.71	111.50
23	D	403[A]	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
23	d	402[B]	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
28	a	413[B]	PL9	C35-C34-C36	2.88	120.12	115.27
24	y	101	BCR	C21-C20-C19	-2.88	114.23	123.22
23	C	508	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
28	A	413[B]	PL9	C35-C34-C36	2.88	120.11	115.27
28	a	413[B]	PL9	C22-C23-C24	-2.88	120.73	127.66
23	c	509	CLA	CAA-C2A-C3A	-2.88	104.90	112.78
31	a	415[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	C	504	CLA	CMB-C2B-C1B	2.88	129.75	125.37
23	a	405[B]	CLA	CMB-C2B-C1B	2.88	129.75	125.37
23	A	406[A]	CLA	CHD-C4C-NC	2.88	128.73	124.20
23	d	404	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
25	a	409[A]	SQD	O47-C7-O49	-2.87	116.75	123.70
23	a	407	CLA	CHD-C4C-NC	2.87	128.73	124.20
23	A	406[B]	CLA	C2A-C1A-CHA	-2.87	118.83	123.86
23	D	404	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
31	A	416[A]	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
32	B	626	LMT	C2'-C3'-C4'	2.87	116.24	109.68
23	b	615	CLA	CHD-C4C-NC	2.87	128.73	124.20
28	D	406[B]	PL9	C53-C6-C1	2.87	120.86	114.99
23	D	403[B]	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
23	a	404[A]	CLA	CAC-C3C-C4C	2.87	128.53	124.81
33	A	418[A]	LHG	C5-O7-C7	-2.87	110.73	117.79
23	C	511	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	B	604	CLA	CHC-C1C-C2C	-2.86	118.78	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	F	102	HEM	CBA-CAA-C2A	-2.86	104.68	112.63
23	D	403[B]	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
23	B	601	CLA	CMB-C2B-C1B	2.86	129.73	125.37
25	b	620	SQD	O7-S-C6	2.86	110.34	106.94
28	D	406[A]	PL9	C51-C49-C50	2.86	120.92	114.60
23	c	506	CLA	C1-C2-C3	-2.86	121.10	126.04
23	A	406[B]	CLA	O2A-CGA-CBA	2.86	120.87	111.91
23	C	505	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
31	a	406[B]	PHO	C1A-C2A-C3A	-2.85	100.12	102.84
23	b	607	CLA	C4-C3-C5	2.85	120.07	115.27
23	c	509	CLA	O2A-CGA-CBA	2.85	120.86	111.91
23	b	613	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	B	601	CLA	CAC-C3C-C4C	2.85	128.51	124.81
23	d	402[A]	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
28	a	413[A]	PL9	C53-C6-C1	2.85	120.82	114.99
35	o	301	HTG	C1-O5-C5	2.85	117.84	112.58
23	c	505	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
28	A	413[B]	PL9	C10-C9-C11	2.85	120.06	115.27
23	C	514	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	c	504	CLA	CMC-C2C-C1C	2.85	129.37	125.04
23	B	604	CLA	CMC-C2C-C1C	2.85	129.37	125.04
36	C	517[A]	DGD	O6D-C1D-O3G	-2.85	103.24	109.97
23	b	607	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
23	d	403[B]	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	B	607	CLA	CMC-C2C-C1C	2.84	129.37	125.04
23	B	601	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
25	A	409[A]	SQD	O48-C23-C24	2.84	120.82	111.91
23	d	402[B]	CLA	O2A-CGA-CBA	2.84	120.81	111.91
24	C	516	BCR	C33-C5-C6	-2.84	121.34	124.53
23	C	510	CLA	CMC-C2C-C1C	2.84	129.36	125.04
23	a	405[A]	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
23	b	613	CLA	CHD-C4C-NC	2.83	128.67	124.20
23	A	406[A]	CLA	O2A-CGA-CBA	2.83	120.80	111.91
23	A	404[B]	CLA	C2A-C1A-CHA	-2.83	118.91	123.86
23	C	506	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
23	a	407	CLA	CBC-CAC-C3C	-2.83	104.63	112.43
28	D	406[B]	PL9	C20-C19-C21	2.83	120.03	115.27
28	D	406[A]	PL9	C37-C38-C39	-2.83	120.85	127.66
36	c	518[B]	DGD	C2G-O2G-C1B	-2.82	110.84	117.79
23	a	407	CLA	CAA-C2A-C3A	-2.82	105.05	112.78
36	c	519	DGD	O3G-C1D-C2D	-2.82	103.90	108.30
23	c	508	CLA	C1D-CHD-C4C	-2.82	119.97	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	B	616	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
23	A	405[B]	CLA	CHD-C4C-NC	2.82	128.65	124.20
28	A	413[A]	PL9	C35-C34-C36	2.82	120.01	115.27
23	b	613	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
31	a	406[B]	PHO	O2A-CGA-CBA	2.82	120.75	111.91
23	A	406[B]	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
23	c	506	CLA	C3B-C4B-NB	2.82	113.13	110.52
23	C	512	CLA	CAC-C3C-C4C	2.82	128.47	124.81
23	B	611	CLA	C3B-C4B-NB	2.82	113.13	110.52
33	L	101[A]	LHG	O8-C23-C24	2.82	120.75	111.91
23	c	513	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	C	502	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
25	l	101	SQD	O9-S-C6	2.82	110.28	106.94
23	b	609	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
23	A	404[A]	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
23	b	603	CLA	CMA-C3A-C2A	-2.81	102.49	113.83
23	A	406[A]	CLA	C4-C3-C5	2.81	119.99	115.27
28	A	413[A]	PL9	C30-C29-C31	2.81	119.99	115.27
25	f	102	SQD	O48-C23-C24	2.80	120.71	111.91
24	D	405	BCR	C31-C1-C6	-2.80	105.75	110.30
23	A	407	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	B	609	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	c	502	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
31	A	416[B]	PHO	CED-O2D-CGD	2.80	122.27	115.94
28	a	413[A]	PL9	C22-C23-C24	-2.80	120.92	127.66
40	V	201	HEC	CAD-CBD-CGD	-2.80	107.58	113.60
23	B	615	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
28	D	406[B]	PL9	C10-C9-C11	2.80	119.98	115.27
38	f	101	HEM	CHD-C4C-NC	2.80	127.46	124.44
23	b	616	CLA	CBC-CAC-C3C	-2.80	104.72	112.43
23	c	506	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
23	B	603	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
34	c	520	LMG	C8-O7-C10	-2.79	110.91	117.79
23	A	405[A]	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
23	b	603	CLA	CHD-C4C-NC	2.79	128.60	124.20
23	B	608	CLA	C1-C2-C3	-2.79	121.22	126.04
23	b	612	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
23	a	405[A]	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
24	t	102	BCR	C1-C6-C7	2.79	123.67	115.78
23	b	602	CLA	C11-C12-C13	-2.78	106.92	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C29-C30-C25	2.78	114.76	110.48
23	A	407	CLA	O2A-CGA-CBA	2.78	120.63	111.91
23	c	511	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
23	b	606	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
28	A	413[B]	PL9	C30-C29-C31	2.78	119.94	115.27
23	C	514	CLA	CMB-C2B-C1B	2.78	129.60	125.37
23	b	601	CLA	C1-O2A-CGA	2.78	123.73	116.44
23	c	507	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	a	404[B]	CLA	C2A-C1A-CHA	-2.78	119.01	123.86
23	b	607	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
25	l	101	SQD	O48-C23-O10	-2.77	116.59	123.59
24	B	618	BCR	C37-C22-C21	-2.77	119.04	122.92
23	B	614	CLA	C3B-C4B-NB	2.77	113.09	110.52
23	A	405[A]	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	b	602	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
31	a	406[A]	PHO	CMB-C2B-C3B	2.77	129.86	124.68
23	b	602	CLA	CHD-C4C-NC	2.77	128.57	124.20
23	b	615	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
23	B	602	CLA	C3B-C4B-NB	2.77	113.08	110.52
24	a	408	BCR	C40-C30-C25	-2.77	105.81	110.30
23	b	614	CLA	CBC-CAC-C3C	-2.77	104.81	112.43
23	B	609	CLA	C16-C15-C13	-2.76	106.98	115.92
32	T	101	LMT	C1'-O5'-C5'	-2.76	108.26	113.69
23	d	402[A]	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	B	608	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
23	a	405[B]	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
31	a	415[B]	PHO	CMB-C2B-C3B	2.76	129.84	124.68
23	a	405[A]	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
23	c	510	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
23	C	503	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
23	b	609	CLA	CHD-C4C-NC	2.76	128.55	124.20
28	D	406[B]	PL9	C51-C49-C50	2.76	120.69	114.60
23	B	604	CLA	CHB-C1B-NB	-2.76	121.34	124.26
23	c	505	CLA	C4C-C3C-C2C	-2.75	102.88	106.90
28	a	413[B]	PL9	C10-C9-C11	2.75	119.91	115.27
33	D	407[A]	LHG	O7-C7-C8	2.75	117.44	111.50
23	C	511	CLA	O2A-CGA-CBA	2.75	120.55	111.91
35	b	623	HTG	O5-C1-C2	2.75	113.78	110.31
28	d	406[B]	PL9	C27-C28-C29	-2.75	121.03	127.66
24	T	102	BCR	C2-C1-C6	2.75	114.72	110.48
23	A	405[B]	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
23	b	614	CLA	CHC-C1C-C2C	-2.75	119.09	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	407[B]	LHG	O8-C23-C24	2.75	120.54	111.91
23	C	505	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
23	B	606	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
28	a	413[B]	PL9	C40-C39-C41	2.75	119.89	115.27
24	d	405	BCR	C37-C22-C23	2.75	122.41	118.08
23	b	603	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
28	d	406[A]	PL9	C36-C37-C38	-2.74	102.86	111.88
23	B	609	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
23	C	504	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
23	c	511	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
35	B	623	HTG	C3-C4-C5	2.74	115.13	110.24
23	B	604	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	C	514	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
23	b	604	CLA	C4-C3-C5	2.74	119.88	115.27
23	b	612	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
24	B	618	BCR	C38-C26-C25	-2.74	121.45	124.53
24	A	408	BCR	C33-C5-C6	-2.74	121.45	124.53
33	d	407[B]	LHG	C5-O7-C7	-2.74	111.06	117.79
23	D	404	CLA	C1-C2-C3	-2.73	121.31	126.04
23	C	512	CLA	C1-O2A-CGA	2.73	123.62	116.44
24	T	102	BCR	C15-C14-C13	2.73	131.21	127.31
33	D	408[B]	LHG	O8-C23-O10	-2.73	116.69	123.59
25	X	101	SQD	O47-C7-O49	-2.73	117.10	123.70
23	c	510	CLA	O2A-C1-C2	2.73	115.81	108.64
23	B	607	CLA	C3B-C4B-NB	2.73	113.05	110.52
23	b	615	CLA	C3B-C4B-NB	2.73	113.05	110.52
25	a	411	SQD	O7-S-C6	2.73	110.18	106.94
24	B	619	BCR	C24-C23-C22	-2.73	122.11	126.23
32	b	627	LMT	C3'-C4'-C5'	-2.73	104.67	110.93
23	B	603	CLA	C4-C3-C5	2.73	119.86	115.27
23	b	601	CLA	C3B-C4B-NB	2.73	113.05	110.52
23	C	505	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
23	c	504	CLA	C3B-C4B-NB	2.72	113.04	110.52
28	A	413[B]	PL9	C53-C6-C1	2.72	120.56	114.99
24	b	617	BCR	C24-C23-C22	-2.72	122.12	126.23
23	B	605	CLA	CED-O2D-CGD	2.72	122.09	115.94
28	d	406[A]	PL9	C27-C28-C29	-2.72	121.11	127.66
24	t	102	BCR	C7-C6-C5	-2.72	114.88	121.46
23	c	504	CLA	CAC-C3C-C4C	2.72	128.33	124.81
24	T	102	BCR	C21-C20-C19	-2.71	114.75	123.22
23	C	507	CLA	C2A-C1A-CHA	-2.71	119.11	123.86
24	c	516	BCR	C37-C22-C23	2.71	122.35	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C3B-C4B-NB	2.71	113.03	110.52
23	A	407	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	C	514	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
24	a	408	BCR	C37-C22-C21	-2.71	119.13	122.92
23	C	503	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
23	C	514	CLA	O2A-CGA-CBA	2.71	120.40	111.91
23	c	512	CLA	O2A-CGA-CBA	2.71	120.40	111.91
23	C	514	CLA	C1-C2-C3	-2.71	121.36	126.04
23	d	404	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	b	604	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
23	B	611	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
23	b	606	CLA	C1-O2A-CGA	2.70	123.54	116.44
23	b	606	CLA	C4C-C3C-C2C	-2.70	102.96	106.90
23	C	512	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	D	404	CLA	C3B-C4B-NB	2.70	113.02	110.52
24	k	101	BCR	C15-C14-C13	-2.70	123.45	127.31
28	a	413[B]	PL9	C20-C19-C21	2.70	119.81	115.27
23	b	613	CLA	CAC-C3C-C4C	2.70	128.31	124.81
24	B	619	BCR	C31-C1-C6	-2.70	105.92	110.30
23	c	505	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
23	B	607	CLA	C1-C2-C3	-2.70	121.38	126.04
23	C	514	CLA	C2A-C1A-CHA	-2.70	119.14	123.86
28	d	406[B]	PL9	C37-C38-C39	-2.70	121.16	127.66
23	A	404[B]	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	B	616	CLA	CHD-C4C-NC	2.70	128.45	124.20
23	b	615	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
34	d	412	LMG	C7-O1-C1	-2.70	108.47	113.74
23	D	404	CLA	CHD-C4C-NC	2.70	128.45	124.20
33	A	418[B]	LHG	O8-C23-C24	2.69	120.36	111.91
23	A	406[B]	CLA	CAA-C2A-C3A	-2.69	105.40	112.78
23	a	404[A]	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
33	d	407[B]	LHG	O8-C23-O10	-2.69	116.79	123.59
23	b	603	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
40	V	201	HEC	C4B-NB-C1B	2.69	107.85	105.07
23	C	503	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
33	L	101[A]	LHG	O8-C23-O10	-2.69	116.80	123.59
23	c	512	CLA	CMB-C2B-C1B	2.69	129.47	125.37
23	D	403[A]	CLA	CAC-C3C-C4C	2.69	128.30	124.81
23	B	609	CLA	O2A-CGA-CBA	2.69	120.34	111.91
24	C	515	BCR	C16-C17-C18	-2.69	123.48	127.31
31	a	406[B]	PHO	CMB-C2B-C3B	2.69	129.70	124.68
23	b	614	CLA	CHD-C4C-NC	2.68	128.43	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
23	C	513	CLA	CMB-C2B-C1B	2.68	129.46	125.37
23	c	514	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
23	A	405[B]	CLA	C4-C3-C5	2.68	119.78	115.27
23	D	404	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
23	c	513	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
24	h	101	BCR	C36-C18-C17	-2.68	119.17	122.92
33	b	629[A]	LHG	O8-C23-C24	2.68	120.32	111.91
24	d	405	BCR	C10-C11-C12	-2.68	114.85	123.22
23	C	503	CLA	CHD-C4C-NC	2.68	128.42	124.20
23	b	616	CLA	CAC-C3C-C4C	2.68	128.28	124.81
32	M	101	LMT	C1'-O5'-C5'	-2.68	108.44	113.69
32	T	101	LMT	C3'-C4'-C5'	-2.67	104.80	110.93
24	B	618	BCR	C7-C8-C9	-2.67	122.19	126.23
23	A	404[A]	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
34	c	521	LMG	O8-C28-C29	2.67	120.29	111.91
23	b	611	CLA	CHD-C4C-NC	2.67	128.41	124.20
24	y	101	BCR	C16-C17-C18	-2.67	123.50	127.31
23	b	611	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	B	610	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
23	d	403[B]	CLA	CAC-C3C-C4C	2.67	128.27	124.81
23	C	514	CLA	CHB-C1B-NB	-2.67	121.43	124.26
24	h	101	BCR	C33-C5-C6	-2.67	121.53	124.53
23	d	404	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
23	c	514	CLA	CMC-C2C-C1C	2.67	129.10	125.04
34	C	520	LMG	O8-C28-O10	-2.67	116.86	123.59
24	B	617	BCR	C37-C22-C23	2.67	122.28	118.08
23	b	608	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
24	k	101	BCR	C36-C18-C19	2.67	122.28	118.08
23	b	603	CLA	C4-C3-C5	2.67	119.76	115.27
24	Y	101	BCR	C28-C27-C26	-2.67	109.32	114.08
23	d	404	CLA	O2A-CGA-CBA	2.67	120.28	111.91
23	C	504	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
23	d	402[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	b	610	CLA	CAA-CBA-CGA	-2.67	105.46	113.25
23	c	503	CLA	O2A-CGA-CBA	2.66	120.27	111.91
23	C	510	CLA	CHD-C4C-NC	2.66	128.40	124.20
23	c	504	CLA	CHD-C4C-NC	2.66	128.40	124.20
23	C	502	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
24	c	516	BCR	C32-C1-C6	-2.66	105.98	110.30
25	X	101	SQD	O48-C23-O10	-2.66	116.88	123.59
31	D	401[B]	PHO	CMA-C3A-C4A	-2.66	108.55	114.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	CAC-C3C-C4C	2.66	128.26	124.81
33	a	419[A]	LHG	O8-C23-C24	2.66	120.25	111.91
23	C	511	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
33	a	419[B]	LHG	O8-C23-C24	2.66	120.25	111.91
23	B	602	CLA	CHD-C4C-NC	2.66	128.39	124.20
31	D	401[A]	PHO	C1-C2-C3	-2.66	121.45	126.04
36	H	102	DGD	O1G-C1A-C2A	2.66	120.24	111.91
23	B	612	CLA	C1-C2-C3	-2.66	121.45	126.04
24	b	618	BCR	C37-C22-C23	2.65	122.26	118.08
23	D	403[A]	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
23	c	512	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	d	402[A]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	d	403[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
36	C	518[A]	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
23	d	403[A]	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	A	405[A]	CLA	C4-C3-C5	2.65	119.73	115.27
28	a	413[A]	PL9	C40-C39-C41	2.65	119.72	115.27
28	A	413[B]	PL9	C40-C39-C41	2.65	119.72	115.27
34	C	501	LMG	O6-C1-O1	-2.65	103.71	109.97
23	B	614	CLA	CHC-C1C-C2C	-2.64	119.38	126.73
31	D	401[B]	PHO	C1-C2-C3	-2.64	121.47	126.04
36	c	519	DGD	O1G-C1A-C2A	2.64	120.21	111.91
23	D	403[A]	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
33	D	407[A]	LHG	O8-C23-C24	2.64	120.20	111.91
34	C	501	LMG	C6-C5-C4	2.64	119.19	113.00
23	A	406[B]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	C	507	CLA	CHD-C4C-NC	2.64	128.37	124.20
23	b	605	CLA	C3B-C4B-NB	2.64	112.96	110.52
23	c	512	CLA	CMA-C3A-C4A	2.64	118.87	111.77
23	a	404[B]	CLA	CAA-C2A-C1A	-2.64	103.33	111.97
23	d	403[B]	CLA	CMB-C2B-C1B	2.64	129.39	125.37
32	B	629	LMT	C3'-C4'-C5'	-2.64	104.88	110.93
23	B	611	CLA	C2C-C1C-NC	2.64	112.44	109.97
23	b	609	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	c	507	CLA	CHD-C4C-NC	2.64	128.36	124.20
24	d	405	BCR	C36-C18-C17	-2.63	119.23	122.92
23	C	502	CLA	C11-C12-C13	-2.63	107.40	115.92
23	b	609	CLA	C7-C6-C5	-2.63	106.20	113.36
23	d	404	CLA	C2A-C1A-CHA	-2.63	119.25	123.86
33	d	408[B]	LHG	O8-C23-C24	2.63	120.17	111.91
36	C	517[B]	DGD	C3G-C2G-C1G	-2.63	105.56	111.79
28	A	413[A]	PL9	C40-C39-C41	2.63	119.70	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	610	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	b	609	CLA	O2A-CGA-O1A	-2.63	116.95	123.59
31	D	401[B]	PHO	O2A-CGA-CBA	2.63	120.17	111.91
23	C	510	CLA	C16-C15-C13	-2.63	107.41	115.92
24	c	516	BCR	C21-C20-C19	-2.63	115.01	123.22
23	d	404	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	B	612	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	b	601	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
24	k	101	BCR	C2-C1-C6	2.63	114.53	110.48
28	d	406[B]	PL9	C35-C34-C36	2.63	119.69	115.27
23	b	608	CLA	O2A-CGA-O1A	-2.63	116.96	123.59
23	B	610	CLA	C3B-C4B-NB	2.62	112.95	110.52
32	A	419	LMT	O5'-C5'-C6'	2.62	112.96	106.44
28	A	413[B]	PL9	C42-C43-C44	-2.62	121.34	127.66
38	F	102	HEM	O2A-CGA-CBA	2.62	122.45	114.03
23	A	404[B]	CLA	O2A-CGA-O1A	-2.62	116.97	123.59
23	B	612	CLA	C4-C3-C5	2.62	119.68	115.27
23	C	511	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	c	507	CLA	C4-C3-C5	2.62	119.68	115.27
23	C	502	CLA	C1-C2-C3	-2.62	121.51	126.04
23	c	503	CLA	C1-C2-C3	-2.62	121.51	126.04
23	A	406[B]	CLA	CBC-CAC-C3C	-2.62	105.22	112.43
23	A	407	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	b	611	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	b	616	CLA	C3B-C4B-NB	2.62	112.94	110.52
23	c	506	CLA	O2A-CGA-CBA	2.61	120.11	111.91
23	a	405[B]	CLA	C4-C3-C5	2.61	119.67	115.27
24	T	102	BCR	C12-C13-C14	-2.61	114.93	118.94
23	d	402[B]	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
25	a	409[B]	SQD	O47-C7-O49	-2.61	117.39	123.70
28	a	413[A]	PL9	C47-C48-C49	-2.61	118.83	127.75
23	a	405[A]	CLA	O2A-CGA-CBA	2.61	120.10	111.91
33	d	408[A]	LHG	O8-C23-C24	2.61	120.09	111.91
40	v	201	HEC	CHA-C4D-ND	2.61	127.25	124.42
23	D	403[B]	CLA	C2A-C1A-CHA	-2.60	119.30	123.86
33	b	629[B]	LHG	O8-C23-C24	2.60	120.08	111.91
23	b	608	CLA	C11-C12-C13	-2.60	107.50	115.92
23	c	511	CLA	O2A-CGA-CBA	2.60	120.08	111.91
23	B	612	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
23	A	405[A]	CLA	CMA-C3A-C2A	-2.60	103.33	113.83
28	a	413[A]	PL9	C10-C9-C8	-2.60	117.01	123.68
23	A	407	CLA	C4-C3-C5	2.60	119.64	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	406[B]	PHO	O2A-CGA-O1A	-2.60	117.03	123.59
24	D	405	BCR	C40-C30-C25	-2.60	106.08	110.30
23	C	513	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	B	611	CLA	OBD-CAD-C3D	-2.60	122.27	128.52
23	a	405[A]	CLA	CMC-C2C-C1C	2.60	128.99	125.04
23	B	606	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
23	B	607	CLA	CHD-C4C-NC	2.60	128.29	124.20
24	B	618	BCR	C2-C1-C6	2.60	114.48	110.48
23	b	608	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	c	505	CLA	CBC-CAC-C3C	-2.60	105.28	112.43
32	a	416	LMT	C3'-C4'-C5'	-2.60	104.98	110.93
31	D	401[A]	PHO	O2A-CGA-CBA	2.59	120.05	111.91
23	b	602	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	B	601	CLA	O2A-CGA-CBA	2.59	120.04	111.91
28	d	406[B]	PL9	C12-C13-C14	-2.59	121.42	127.66
40	v	201	HEC	CHA-C1A-NA	2.59	127.24	124.44
25	a	411	SQD	C1-O5-C5	2.59	118.77	113.69
23	B	611	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	c	513	CLA	C3B-C4B-NB	2.59	112.92	110.52
23	d	402[A]	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
24	b	617	BCR	C16-C15-C14	-2.59	118.18	123.47
23	B	602	CLA	C2A-C1A-CHA	-2.58	119.34	123.86
23	C	503	CLA	O2A-CGA-CBA	2.58	120.02	111.91
23	c	503	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
36	H	102	DGD	O6E-C5E-C6E	2.58	112.85	106.44
23	C	514	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
23	b	602	CLA	CHB-C1B-C2B	-2.58	119.95	127.24
28	A	413[B]	PL9	C7-C3-C2	-2.58	119.91	123.30
36	c	518[B]	DGD	C1D-O6D-C5D	2.58	118.75	113.69
23	A	406[A]	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
23	b	608	CLA	O2A-CGA-CBA	2.58	119.99	111.91
23	A	405[A]	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	b	605	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	B	614	CLA	CBC-CAC-C3C	-2.58	105.33	112.43
23	B	608	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	D	403[A]	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
23	B	606	CLA	C4-C3-C5	2.57	119.60	115.27
31	D	401[A]	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
23	A	404[B]	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
25	A	409[A]	SQD	O48-C23-O10	-2.57	117.11	123.59
23	c	509	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	a	404[B]	CLA	C1-C2-C3	-2.57	121.60	126.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	401[A]	PHO	O2A-CGA-O1A	-2.57	117.12	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.56	119.37	123.86
28	D	406[B]	PL9	C40-C39-C41	2.56	119.58	115.27
25	b	620	SQD	O48-C23-C24	2.56	119.95	111.91
34	D	412	LMG	O8-C28-C29	2.56	119.95	111.91
24	a	408	BCR	C7-C8-C9	-2.56	122.36	126.23
23	B	616	CLA	CBC-CAC-C3C	-2.56	105.36	112.43
23	A	405[B]	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
24	b	619	BCR	C38-C26-C25	-2.56	121.65	124.53
23	c	514	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
40	V	201	HEC	C1D-C2D-C3D	-2.56	104.26	106.96
23	C	510	CLA	CHB-C1B-NB	-2.56	121.55	124.26
36	c	518[B]	DGD	O1G-C1A-C2A	2.56	119.95	111.91
23	B	607	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
28	A	413[A]	PL9	C10-C9-C8	-2.56	117.11	123.68
36	C	518[B]	DGD	C2G-O2G-C1B	-2.56	111.49	117.79
23	a	405[B]	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
23	c	513	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
23	b	613	CLA	CED-O2D-CGD	2.56	121.72	115.94
23	B	604	CLA	C6-C5-C3	-2.56	106.75	113.45
24	Y	101	BCR	C10-C11-C12	-2.56	115.24	123.22
36	h	102	DGD	O3G-C1D-C2D	2.56	112.29	108.30
26	b	628	GOL	C3-C2-C1	-2.56	101.77	111.70
23	C	502	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	B	614	CLA	C4C-C3C-C2C	-2.55	103.17	106.90
24	d	405	BCR	C40-C30-C39	2.55	116.37	108.53
28	a	413[B]	PL9	C53-C6-C1	2.55	120.21	114.99
23	B	610	CLA	CHD-C4C-NC	2.55	128.23	124.20
23	c	507	CLA	CMB-C2B-C1B	2.55	129.26	125.37
32	b	621	LMT	C1'-O5'-C5'	-2.55	108.68	113.69
23	B	612	CLA	C3B-C4B-NB	2.55	112.88	110.52
23	c	514	CLA	CMB-C2B-C1B	2.55	129.25	125.37
31	a	415[B]	PHO	O2D-CGD-O1D	-2.55	118.85	123.84
23	B	603	CLA	CMA-C3A-C2A	-2.55	103.55	113.83
33	d	408[B]	LHG	C5-O7-C7	-2.55	111.52	117.79
31	A	416[B]	PHO	C6-C5-C3	-2.55	106.78	113.45
23	A	405[A]	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
23	d	403[A]	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
28	A	413[A]	PL9	C47-C48-C49	-2.54	119.05	127.75
24	K	102	BCR	C2-C1-C6	2.54	114.40	110.48
23	a	405[B]	CLA	C2A-C1A-CHA	-2.54	119.41	123.86
23	C	512	CLA	CHC-C1C-C2C	-2.54	119.67	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	511	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
23	C	513	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
23	C	504	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
23	d	403[B]	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
23	B	608	CLA	CMC-C2C-C1C	2.54	128.90	125.04
23	b	616	CLA	OBD-CAD-C3D	-2.54	122.42	128.52
31	A	416[B]	PHO	O2D-CGD-O1D	-2.54	118.88	123.84
23	c	505	CLA	CHD-C4C-NC	2.54	128.20	124.20
36	c	517[B]	DGD	C2G-O2G-C1B	-2.53	111.55	117.79
23	b	607	CLA	C2A-C1A-CHA	-2.53	119.43	123.86
23	c	502	CLA	O2A-CGA-CBA	2.53	119.85	111.91
24	H	101	BCR	C36-C18-C17	-2.53	119.38	122.92
23	d	402[B]	CLA	C4-C3-C5	2.53	119.53	115.27
23	b	607	CLA	O2A-CGA-O1A	-2.53	117.21	123.59
24	D	405	BCR	C3-C4-C5	-2.53	109.56	114.08
23	D	403[B]	CLA	CMB-C2B-C1B	2.53	129.22	125.37
23	C	505	CLA	CBC-CAC-C3C	-2.53	105.46	112.43
36	C	518[B]	DGD	O1G-C1A-O1A	-2.53	117.22	123.59
32	m	103	LMT	C3B-C4B-C5B	-2.53	105.73	110.24
25	b	620	SQD	C1-C2-C3	-2.52	104.74	110.00
38	F	102	HEM	CMD-C2D-C1D	2.52	128.88	125.04
28	a	413[B]	PL9	C47-C48-C49	-2.52	119.12	127.75
23	B	605	CLA	C7-C6-C5	-2.52	106.51	113.36
40	V	201	HEC	CHA-C4D-ND	2.52	127.16	124.42
23	C	513	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
23	B	616	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
25	X	101	SQD	O8-S-O7	-2.52	105.12	111.27
23	c	513	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	b	605	CLA	C1-C2-C3	-2.52	121.69	126.04
28	d	406[B]	PL9	C20-C19-C21	2.52	119.50	115.27
23	D	403[B]	CLA	CAC-C3C-C4C	2.51	128.07	124.81
23	B	606	CLA	C4C-C3C-C2C	-2.51	103.23	106.90
23	d	402[A]	CLA	CAA-CBA-CGA	2.51	120.59	113.25
28	A	413[B]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	c	514	CLA	C1-C2-C3	-2.51	121.70	126.04
23	d	403[B]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	D	404	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
23	a	407	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	d	403[A]	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	A	406[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	a	404[A]	CLA	CHD-C4C-NC	2.51	128.15	124.20
24	Y	101	BCR	C15-C16-C17	-2.51	118.34	123.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C6-C7-C8	-2.50	107.82	115.92
23	a	404[B]	CLA	CMB-C2B-C1B	2.50	129.18	125.37
23	C	512	CLA	C1-C2-C3	-2.50	121.72	126.04
28	D	406[A]	PL9	C42-C41-C39	-2.50	104.75	112.98
24	d	405	BCR	C39-C30-C25	-2.50	106.25	110.30
36	c	518[A]	DGD	O1G-C1A-C2A	2.50	119.74	111.91
28	A	413[B]	PL9	C12-C13-C14	-2.50	121.65	127.66
23	b	609	CLA	CHC-C1C-C2C	-2.50	119.80	126.73
23	c	502	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	b	605	CLA	CMC-C2C-C1C	2.49	128.84	125.04
23	C	508	CLA	O2A-CGA-CBA	2.49	119.73	111.91
23	a	404[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
23	B	611	CLA	C4A-NA-C1A	-2.49	105.59	106.71
23	C	503	CLA	C3B-C4B-NB	2.49	112.83	110.52
24	Y	101	BCR	C38-C26-C25	-2.49	121.73	124.53
34	D	412	LMG	O8-C28-O10	-2.49	117.31	123.59
23	C	503	CLA	CBC-CAC-C3C	-2.49	105.57	112.43
23	c	504	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
24	D	405	BCR	C16-C17-C18	-2.49	123.76	127.31
23	C	508	CLA	C4-C3-C5	2.49	119.45	115.27
24	T	102	BCR	C16-C17-C18	-2.49	123.76	127.31
25	a	409[A]	SQD	O8-S-C6	2.49	109.70	105.74
23	B	616	CLA	C1-O2A-CGA	2.48	122.96	116.44
23	d	402[A]	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
23	C	510	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
23	C	502	CLA	C1-O2A-CGA	2.48	122.96	116.44
23	b	606	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
23	b	611	CLA	CMC-C2C-C1C	2.48	128.82	125.04
23	B	604	CLA	C11-C12-C13	-2.48	107.90	115.92
34	C	501	LMG	C8-O7-C10	-2.48	111.69	117.79
38	F	102	HEM	CHA-C4D-ND	2.48	127.43	124.37
23	c	504	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	511	CLA	CHB-C1B-NB	-2.48	121.64	124.26
24	h	101	BCR	C11-C10-C9	-2.48	123.78	127.31
23	B	606	CLA	CMB-C2B-C1B	2.48	129.14	125.37
23	B	601	CLA	CMC-C2C-C1C	2.48	128.81	125.04
28	D	406[A]	PL9	C20-C19-C21	2.47	119.43	115.27
23	B	613	CLA	CHD-C4C-NC	2.47	128.10	124.20
36	c	517[A]	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
23	A	407	CLA	CHB-C1B-NB	-2.47	121.64	124.26
24	Y	101	BCR	C36-C18-C17	-2.47	119.46	122.92
23	D	404	CLA	O2A-CGA-CBA	2.47	119.66	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C1-O2A-CGA	2.47	122.92	116.44
24	a	408	BCR	C8-C7-C6	-2.47	120.27	127.20
34	m	101	LMG	C8-O7-C10	-2.47	111.72	117.79
36	C	518[B]	DGD	O1G-C1A-C2A	2.47	119.64	111.91
24	K	102	BCR	C3-C4-C5	-2.47	109.67	114.08
24	c	515	BCR	C20-C21-C22	-2.47	123.79	127.31
23	c	502	CLA	C4-C3-C5	2.46	119.42	115.27
24	B	619	BCR	C39-C30-C25	-2.46	106.30	110.30
31	D	401[A]	PHO	CMB-C2B-C3B	2.46	129.29	124.68
23	b	608	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
23	B	615	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
35	b	622	HTG	C6-C5-C4	-2.46	107.24	113.00
23	c	510	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
23	B	609	CLA	CMC-C2C-C1C	2.46	128.78	125.04
34	d	412	LMG	O8-C28-O10	-2.46	117.39	123.59
23	b	613	CLA	C4-C3-C5	2.46	119.40	115.27
23	A	407	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
23	c	514	CLA	CHD-C4C-NC	2.45	128.07	124.20
23	A	404[B]	CLA	C1-C2-C3	-2.45	121.80	126.04
23	B	613	CLA	C4-C3-C2	-2.45	117.39	123.68
24	k	101	BCR	C20-C21-C22	-2.45	123.81	127.31
23	B	603	CLA	CHD-C4C-NC	2.45	128.07	124.20
24	k	101	BCR	C16-C17-C18	-2.45	123.81	127.31
23	B	608	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
23	A	404[A]	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
23	B	605	CLA	CHC-C1C-C2C	-2.45	119.93	126.73
23	c	512	CLA	CMC-C2C-C1C	2.45	128.77	125.04
28	D	406[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	B	604	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
40	v	201	HEC	CAD-CBD-CGD	-2.45	108.34	113.60
23	b	604	CLA	CMB-C2B-C1B	2.45	129.09	125.37
35	o	301	HTG	O2-C2-C3	-2.44	104.70	110.35
25	a	409[B]	SQD	O48-C23-C24	2.44	119.57	111.91
23	D	404	CLA	CMA-C3A-C2A	-2.44	103.99	113.83
24	c	515	BCR	C33-C5-C6	-2.44	121.79	124.53
33	A	418[B]	LHG	O7-C7-O9	-2.44	117.81	123.70
31	a	406[B]	PHO	O2D-CGD-O1D	-2.44	119.08	123.84
23	C	504	CLA	O2A-CGA-CBA	2.43	119.55	111.91
23	B	615	CLA	C6-C7-C8	-2.43	108.06	115.92
36	H	102	DGD	O1G-C1A-O1A	-2.43	117.45	123.59
23	c	511	CLA	C11-C10-C8	-2.43	108.06	115.92
23	b	615	CLA	O2A-CGA-O1A	-2.43	117.46	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	614	CLA	CHB-C1B-NB	-2.43	121.68	124.26
31	D	401[B]	PHO	CMB-C2B-C3B	2.43	129.22	124.68
23	B	608	CLA	O2A-CGA-CBA	2.43	119.52	111.91
23	C	506	CLA	CHD-C4C-NC	2.43	128.03	124.20
38	F	102	HEM	C4A-NA-C1A	2.42	107.72	105.35
23	A	405[A]	CLA	CAA-CBA-CGA	2.42	120.34	113.25
23	B	615	CLA	O2A-CGA-CBA	2.42	119.51	111.91
23	B	607	CLA	CMB-C2B-C1B	2.42	129.06	125.37
24	A	408	BCR	C38-C26-C25	-2.42	121.81	124.53
23	A	406[A]	CLA	C1-C2-C3	-2.42	121.86	126.04
23	d	402[B]	CLA	C4C-C3C-C2C	-2.42	103.37	106.90
23	c	505	CLA	CAA-C2A-C3A	-2.42	106.16	112.78
24	c	516	BCR	C16-C17-C18	-2.42	123.86	127.31
28	D	406[A]	PL9	C7-C8-C9	-2.41	122.77	126.79
25	A	411	SQD	O48-C23-O10	-2.41	117.50	123.59
33	A	418[A]	LHG	O7-C7-O9	-2.41	117.87	123.70
23	b	602	CLA	C4-C3-C5	2.41	119.33	115.27
23	c	513	CLA	CMC-C2C-C1C	2.41	128.71	125.04
24	c	515	BCR	C37-C22-C23	2.41	121.88	118.08
23	B	614	CLA	CMA-C3A-C2A	-2.41	104.11	113.83
23	A	407	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
23	C	510	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
31	D	401[A]	PHO	CMA-C3A-C4A	-2.41	109.11	114.38
23	B	606	CLA	CAC-C3C-C4C	2.41	127.93	124.81
24	Y	101	BCR	C37-C22-C23	2.41	121.87	118.08
23	b	616	CLA	CHC-C1C-C2C	-2.41	120.05	126.73
23	c	508	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
23	B	609	CLA	C1-C2-C3	-2.40	121.89	126.04
23	c	507	CLA	CMC-C2C-C1C	2.40	128.70	125.04
23	b	615	CLA	CBC-CAC-C3C	-2.40	105.81	112.43
33	b	629[A]	LHG	O8-C23-O10	-2.40	117.53	123.59
28	D	406[B]	PL9	C22-C23-C24	-2.40	121.88	127.66
23	b	605	CLA	C1-O2A-CGA	2.40	122.74	116.44
33	d	408[A]	LHG	O8-C23-O10	-2.40	117.54	123.59
31	A	416[B]	PHO	O2A-CGA-CBA	2.40	119.43	111.91
28	d	406[A]	PL9	C17-C18-C19	-2.40	121.89	127.66
23	B	613	CLA	CHC-C1C-C2C	-2.40	120.08	126.73
23	b	616	CLA	C4-C3-C5	2.40	119.30	115.27
23	c	512	CLA	C1-C2-C3	-2.39	121.90	126.04
23	a	405[B]	CLA	O2A-CGA-CBA	2.39	119.42	111.91
23	C	503	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
23	C	506	CLA	O2A-CGA-CBA	2.39	119.42	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	406[A]	PL9	C7-C8-C9	-2.39	122.81	126.79
23	C	507	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
40	v	201	HEC	C4B-NB-C1B	2.39	107.54	105.07
23	B	608	CLA	CMA-C3A-C2A	-2.39	104.19	113.83
23	c	507	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
23	B	615	CLA	C3B-C4B-NB	2.39	112.73	110.52
24	c	515	BCR	C34-C9-C10	-2.39	119.58	122.92
23	c	514	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	C	513	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	c	510	CLA	C1-O2A-CGA	2.39	122.71	116.44
32	m	103	LMT	C3'-C4'-C5'	-2.39	105.45	110.93
28	d	406[B]	PL9	C22-C23-C24	-2.39	121.91	127.66
32	B	627	LMT	O5'-C5'-C6'	2.39	112.37	106.44
23	B	611	CLA	O2A-CGA-CBA	2.39	119.40	111.91
23	B	612	CLA	C4A-NA-C1A	-2.39	105.63	106.71
23	A	405[B]	CLA	CMC-C2C-C1C	2.39	128.67	125.04
23	D	403[B]	CLA	CMC-C2C-C1C	2.39	128.67	125.04
31	a	415[B]	PHO	C1A-C2A-C3A	-2.39	100.57	102.84
36	c	517[B]	DGD	O6D-C1D-O3G	-2.39	104.33	109.97
23	b	615	CLA	O2A-CGA-CBA	2.39	119.39	111.91
23	C	510	CLA	C11-C12-C13	-2.38	108.21	115.92
23	c	502	CLA	CAC-C3C-C4C	2.38	127.90	124.81
23	C	514	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
28	A	413[B]	PL9	C45-C44-C46	2.38	119.28	115.27
23	D	403[A]	CLA	CMC-C2C-C1C	2.38	128.67	125.04
33	D	407[B]	LHG	O8-C23-O10	-2.38	117.58	123.59
23	d	403[A]	CLA	CMB-C2B-C1B	2.38	129.00	125.37
24	H	101	BCR	C16-C15-C14	-2.38	118.59	123.47
23	a	404[A]	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
23	C	505	CLA	CMB-C2B-C1B	2.38	129.00	125.37
28	a	413[A]	PL9	C20-C19-C21	2.38	119.28	115.27
23	B	605	CLA	O2A-CGA-CBA	2.38	119.38	111.91
23	C	507	CLA	O2A-CGA-CBA	2.38	119.38	111.91
24	y	101	BCR	C35-C13-C14	-2.38	119.59	122.92
24	b	617	BCR	C29-C30-C25	2.38	114.14	110.48
23	B	612	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
31	A	416[B]	PHO	CMA-C3A-C4A	-2.38	109.17	114.38
23	B	608	CLA	C11-C12-C13	-2.38	108.23	115.92
23	B	610	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
28	D	406[A]	PL9	C36-C37-C38	-2.38	104.07	111.88
23	B	605	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
24	H	101	BCR	C10-C11-C12	-2.38	115.80	123.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	512	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
32	A	419	LMT	O1'-C1'-C2'	2.37	112.01	108.30
23	A	407	CLA	C1-O2A-CGA	2.37	122.67	116.44
23	c	505	CLA	CMB-C2B-C1B	2.37	128.98	125.37
23	C	508	CLA	CBC-CAC-C3C	-2.37	105.89	112.43
23	b	607	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	A	406[A]	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	C	505	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
23	C	507	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
36	c	517[B]	DGD	C3G-C2G-C1G	-2.37	106.18	111.79
32	b	627	LMT	C1'-O5'-C5'	-2.37	109.04	113.69
32	b	621	LMT	C2'-C3'-C4'	2.37	115.09	109.68
24	D	405	BCR	C29-C28-C27	-2.37	106.08	111.38
23	C	507	CLA	C4C-C3C-C2C	-2.37	103.45	106.90
23	A	405[B]	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
32	B	629	LMT	O5'-C5'-C4'	2.37	114.74	109.75
23	b	601	CLA	C2A-C1A-CHA	-2.37	119.72	123.86
31	A	416[A]	PHO	C4D-CHA-CBD	2.37	109.59	108.52
34	C	521	LMG	C1-C2-C3	-2.37	105.07	110.00
23	B	612	CLA	C2A-C1A-CHA	-2.36	119.72	123.86
23	b	609	CLA	CMA-C3A-C4A	-2.36	105.42	111.77
23	c	509	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	B	607	CLA	CMA-C3A-C2A	-2.36	104.30	113.83
24	b	619	BCR	C39-C30-C25	-2.36	106.47	110.30
31	a	415[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	C	506	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	B	605	CLA	C3B-C4B-NB	2.36	112.70	110.52
36	c	517[A]	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	c	511	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
34	B	620	LMG	C12-C11-C10	-2.36	105.04	113.62
23	C	512	CLA	O2A-CGA-CBA	2.36	119.31	111.91
36	C	517[B]	DGD	O1G-C1A-O1A	-2.36	117.64	123.59
23	C	510	CLA	O2A-C1-C2	2.36	114.83	108.64
23	a	404[B]	CLA	C4-C3-C5	2.36	119.24	115.27
23	b	611	CLA	O2A-CGA-CBA	2.36	119.30	111.91
28	d	406[B]	PL9	C36-C37-C38	-2.36	104.14	111.88
24	Y	101	BCR	C36-C18-C19	2.36	121.79	118.08
28	d	406[A]	PL9	C12-C13-C14	-2.36	121.99	127.66
23	a	405[A]	CLA	C1-C2-C3	-2.35	121.98	126.04
25	A	409[B]	SQD	O9-S-O7	-2.35	105.81	113.95
24	b	619	BCR	C16-C15-C14	-2.35	118.66	123.47
23	c	511	CLA	C11-C12-C13	-2.35	108.32	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	413[A]	PL9	C45-C44-C46	2.35	119.22	115.27
24	A	408	BCR	C8-C7-C6	-2.35	120.61	127.20
32	B	629	LMT	O1'-C1'-C2'	2.35	111.97	108.30
23	c	502	CLA	CMC-C2C-C1C	2.34	128.61	125.04
23	B	611	CLA	CMB-C2B-C3B	2.34	132.26	126.59
23	B	608	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
23	A	406[A]	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
24	c	516	BCR	C33-C5-C6	-2.34	121.90	124.53
23	c	507	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	D	403[B]	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	c	506	CLA	CHB-C1B-NB	-2.34	121.78	124.26
28	A	413[A]	PL9	C42-C43-C44	-2.34	122.03	127.66
23	c	505	CLA	O2A-CGA-CBA	2.34	119.24	111.91
23	C	505	CLA	CAC-C3C-C4C	2.34	127.84	124.81
23	b	603	CLA	CMC-C2C-C1C	2.34	128.59	125.04
23	B	608	CLA	CMB-C2B-C1B	2.33	128.92	125.37
23	D	404	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
33	d	407[A]	LHG	C6-C5-C4	-2.33	106.27	111.79
28	d	406[A]	PL9	C20-C19-C21	2.33	119.20	115.27
23	C	504	CLA	CBC-CAC-C3C	-2.33	106.00	112.43
23	a	404[B]	CLA	CMA-C3A-C2A	-2.33	104.43	113.83
33	d	408[B]	LHG	O7-C7-O9	-2.33	118.07	123.70
24	b	619	BCR	C15-C14-C13	-2.33	123.98	127.31
23	D	403[A]	CLA	CMB-C2B-C1B	2.33	128.92	125.37
23	c	504	CLA	OBD-CAD-C3D	-2.33	122.92	128.52
24	C	515	BCR	C38-C26-C25	-2.33	121.91	124.53
23	C	509	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
31	a	406[B]	PHO	CMA-C3A-C4A	-2.33	109.28	114.38
38	F	102	HEM	O2D-CGD-CBD	2.33	121.50	114.03
24	K	102	BCR	C36-C18-C19	2.32	121.74	118.08
23	B	614	CLA	OBD-CAD-C3D	-2.32	122.93	128.52
25	a	409[B]	SQD	O9-S-C6	2.32	109.70	106.94
23	c	504	CLA	CHC-C1C-C2C	-2.32	120.28	126.73
23	C	513	CLA	CHB-C1B-C2B	-2.32	120.68	127.24
33	L	101[B]	LHG	O8-C23-C24	2.32	119.19	111.91
28	D	406[B]	PL9	C30-C29-C31	2.32	119.18	115.27
23	C	508	CLA	C3B-C4B-NB	2.32	112.67	110.52
23	c	507	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
28	A	413[B]	PL9	C25-C24-C26	2.32	119.17	115.27
23	b	614	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	B	604	CLA	C4-C3-C5	2.32	119.17	115.27
23	B	610	CLA	CAC-C3C-C4C	2.32	127.82	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	613	CLA	C16-C15-C13	-2.32	108.42	115.92
23	b	601	CLA	O2A-CGA-CBA	2.32	119.19	111.91
24	d	405	BCR	C33-C5-C6	-2.32	121.92	124.53
23	c	506	CLA	CMC-C2C-C1C	2.32	128.57	125.04
23	B	601	CLA	CHC-C1C-C2C	-2.32	120.29	126.73
23	b	611	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
36	C	519	DGD	O2G-C1B-C2B	2.32	116.50	111.50
23	c	510	CLA	C4-C3-C2	-2.32	117.73	123.68
23	B	615	CLA	CHC-C1C-C2C	-2.32	120.29	126.73
23	b	610	CLA	C4-C3-C2	-2.32	117.73	123.68
24	T	102	BCR	C35-C13-C12	2.32	121.73	118.08
25	a	411	SQD	O48-C23-O10	-2.32	117.75	123.59
23	d	402[B]	CLA	C1-C2-C3	-2.32	122.04	126.04
24	A	408	BCR	C15-C14-C13	-2.32	124.00	127.31
23	C	509	CLA	CHD-C4C-NC	2.31	127.85	124.20
34	d	412	LMG	O8-C28-C29	2.31	119.17	111.91
28	d	406[B]	PL9	C17-C18-C19	-2.31	122.09	127.66
23	b	606	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
23	C	502	CLA	C2A-C1A-CHA	-2.31	119.82	123.86
25	a	411	SQD	C3-C4-C5	2.31	114.36	110.24
40	V	201	HEC	CBC-CAC-C3C	2.31	118.80	112.43
23	d	402[A]	CLA	CMC-C2C-C1C	2.31	128.56	125.04
23	c	510	CLA	CMB-C2B-C1B	2.31	128.89	125.37
23	b	608	CLA	CMB-C2B-C3B	2.31	132.18	126.59
24	h	101	BCR	C24-C23-C22	-2.31	122.74	126.23
23	b	602	CLA	C1-O2A-CGA	2.31	122.50	116.44
23	b	610	CLA	CHC-C1C-C2C	-2.31	120.31	126.73
31	A	416[B]	PHO	CMB-C2B-C3B	2.31	129.00	124.68
23	b	615	CLA	C6-C7-C8	-2.31	108.46	115.92
23	B	603	CLA	CBC-CAC-C3C	-2.31	106.07	112.43
25	A	411	SQD	C4-C3-C2	-2.31	106.79	110.82
24	d	405	BCR	C11-C10-C9	-2.31	124.02	127.31
23	B	601	CLA	C3B-C4B-NB	2.31	112.66	110.52
25	a	411	SQD	O8-S-C6	2.31	109.42	105.74
36	C	518[A]	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
23	B	606	CLA	C3B-C4B-NB	2.31	112.66	110.52
35	B	623	HTG	O5-C5-C4	2.31	113.88	109.69
24	a	408	BCR	C33-C5-C6	-2.31	121.94	124.53
23	B	602	CLA	CHC-C1C-C2C	-2.31	120.33	126.73
32	M	101	LMT	C1-O1'-C1'	2.30	117.66	113.84
24	K	102	BCR	C29-C30-C25	2.30	114.03	110.48
23	b	604	CLA	CHB-C4A-NA	2.30	127.70	124.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	413[B]	PL9	C51-C49-C50	2.30	119.69	114.60
23	c	508	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
36	C	517[A]	DGD	O6E-C5E-C4E	2.30	113.88	109.69
40	v	201	HEC	CBA-CAA-C2A	-2.30	106.23	112.63
25	l	101	SQD	C44-O6-C1	-2.30	109.25	113.74
24	B	618	BCR	C37-C22-C23	2.30	121.70	118.08
23	b	613	CLA	CBC-CAC-C3C	-2.30	106.09	112.43
24	b	618	BCR	C28-C27-C26	-2.30	109.97	114.08
24	B	617	BCR	C21-C20-C19	-2.30	116.05	123.22
23	c	513	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
24	h	101	BCR	C16-C17-C18	-2.30	124.03	127.31
23	c	508	CLA	C4C-C3C-C2C	-2.30	103.55	106.90
23	D	404	CLA	CHB-C1B-NB	-2.30	121.83	124.26
25	a	409[A]	SQD	O48-C23-C24	2.30	119.11	111.91
34	c	521	LMG	O8-C28-O10	-2.29	117.80	123.59
24	B	617	BCR	C31-C1-C6	-2.29	106.58	110.30
23	C	505	CLA	CHD-C4C-NC	2.29	127.82	124.20
23	C	506	CLA	C11-C10-C8	-2.29	108.51	115.92
23	A	405[B]	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
23	C	502	CLA	OBD-CAD-C3D	-2.29	123.00	128.52
23	b	606	CLA	CHB-C1B-C2B	-2.29	120.76	127.24
32	e	101	LMT	O1'-C1'-C2'	2.29	111.88	108.30
23	b	607	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
23	C	514	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
31	a	415[B]	PHO	O2A-CGA-CBA	2.29	119.09	111.91
23	C	508	CLA	CHC-C4B-NB	2.29	126.68	124.26
23	c	505	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
28	D	406[B]	PL9	C36-C37-C38	-2.29	104.36	111.88
23	B	605	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	c	508	CLA	CBC-CAC-C3C	-2.29	106.13	112.43
31	a	415[B]	PHO	CBA-CAA-C2A	-2.29	107.13	113.81
36	C	517[A]	DGD	C3G-C2G-C1G	-2.29	106.38	111.79
23	C	504	CLA	CAC-C3C-C4C	2.29	127.78	124.81
23	b	610	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	C	514	CLA	C4-C3-C5	2.29	119.11	115.27
24	K	102	BCR	C39-C30-C25	-2.28	106.60	110.30
23	b	607	CLA	CHD-C4C-NC	2.28	127.80	124.20
25	A	411	SQD	O6-C44-C45	-2.28	105.40	110.90
23	A	406[B]	CLA	C4-C3-C5	2.28	119.11	115.27
25	f	102	SQD	O47-C7-O49	-2.28	118.19	123.70
36	c	518[B]	DGD	O1G-C1A-O1A	-2.28	117.84	123.59
32	b	621	LMT	C1-O1'-C1'	2.28	117.62	113.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	619	BCR	C2-C1-C6	2.28	113.99	110.48
31	a	415[B]	PHO	O1D-CGD-CBD	-2.28	120.95	124.74
28	d	406[A]	PL9	C51-C49-C50	2.28	119.63	114.60
36	C	519	DGD	O3G-C3G-C2G	-2.28	105.41	110.90
23	A	404[B]	CLA	CHB-C1B-C2B	-2.28	120.81	127.24
23	C	509	CLA	CHB-C1B-NB	-2.27	121.85	124.26
23	B	610	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
24	c	515	BCR	C36-C18-C17	-2.27	119.74	122.92
24	A	408	BCR	C31-C1-C6	-2.27	106.61	110.30
23	B	605	CLA	CHA-C1A-NA	-2.27	121.20	126.40
25	A	409[B]	SQD	O48-C23-O10	-2.27	117.86	123.59
23	C	511	CLA	CBC-CAC-C3C	-2.27	106.17	112.43
28	a	413[B]	PL9	C51-C49-C50	2.27	119.61	114.60
23	C	509	CLA	CAC-C3C-C4C	2.27	127.75	124.81
31	a	415[A]	PHO	O2A-CGA-CBA	2.27	119.03	111.91
23	C	505	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
31	A	416[B]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
24	B	619	BCR	C3-C4-C5	-2.27	110.03	114.08
36	C	517[B]	DGD	O1G-C1A-C2A	2.27	119.02	111.91
28	A	413[A]	PL9	C35-C34-C33	-2.27	117.86	123.68
32	A	419	LMT	O5'-C5'-C4'	2.27	114.53	109.75
23	a	404[A]	CLA	C7-C6-C5	-2.27	107.20	113.36
23	c	511	CLA	C4-C3-C2	-2.27	117.87	123.68
23	A	407	CLA	CMB-C2B-C1B	2.27	128.82	125.37
23	D	403[B]	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
28	a	413[B]	PL9	C45-C44-C46	2.26	119.08	115.27
23	c	508	CLA	CHC-C1C-C2C	-2.26	120.44	126.73
23	c	505	CLA	CED-O2D-CGD	2.26	121.05	115.94
36	C	518[A]	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
23	b	607	CLA	C1-O2A-CGA	2.26	122.37	116.44
23	d	404	CLA	CHB-C1B-NB	-2.26	121.87	124.26
25	X	101	SQD	O5-C1-C2	-2.26	105.58	110.35
23	B	601	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	C	502	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
24	y	101	BCR	C34-C9-C10	-2.25	119.77	122.92
31	D	401[A]	PHO	C4-C3-C5	2.25	119.06	115.27
31	a	415[B]	PHO	C4A-C3A-C2A	-2.25	100.70	102.84
23	D	403[A]	CLA	CED-O2D-CGD	2.25	121.03	115.94
25	a	411	SQD	O5-C5-C4	2.25	113.78	109.69
31	a	406[A]	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
23	b	605	CLA	CAC-C3C-C4C	2.25	127.73	124.81
28	D	406[B]	PL9	C47-C48-C49	-2.25	120.06	127.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	408	BCR	C11-C10-C9	-2.25	124.10	127.31
23	d	402[A]	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
24	y	101	BCR	C28-C27-C26	-2.25	110.06	114.08
23	c	505	CLA	C4-C3-C5	2.25	119.05	115.27
23	b	616	CLA	C11-C12-C13	-2.25	108.66	115.92
23	B	602	CLA	O2A-CGA-CBA	2.25	118.95	111.91
32	B	627	LMT	O5'-C5'-C4'	2.25	114.49	109.75
23	b	612	CLA	CMB-C2B-C1B	2.24	128.79	125.37
36	c	517[A]	DGD	O3G-C3G-C2G	-2.24	105.48	110.90
23	c	513	CLA	CBA-CAA-C2A	-2.24	107.24	113.86
23	B	608	CLA	C11-C10-C8	-2.24	108.67	115.92
28	d	406[A]	PL9	C47-C48-C49	-2.24	120.08	127.75
23	B	605	CLA	OBD-CAD-C3D	-2.24	123.12	128.52
24	C	516	BCR	C29-C30-C25	2.24	113.93	110.48
23	A	405[B]	CLA	CHB-C1B-NB	-2.24	121.88	124.26
28	d	406[B]	PL9	C51-C49-C50	2.24	119.56	114.60
35	b	622	HTG	O2-C2-C3	-2.24	105.17	110.35
24	D	405	BCR	C21-C20-C19	-2.24	116.22	123.22
23	B	610	CLA	CMC-C2C-C1C	2.24	128.45	125.04
32	a	416	LMT	O5B-C1B-C2B	2.24	115.09	110.35
23	c	502	CLA	CBC-CAC-C3C	-2.24	106.26	112.43
23	A	404[B]	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
23	b	609	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
24	Y	101	BCR	C1-C6-C7	2.24	122.11	115.78
23	D	403[B]	CLA	C4-C3-C5	2.24	119.03	115.27
23	c	506	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	a	404[B]	CLA	CAC-C3C-C4C	2.24	127.71	124.81
23	B	614	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
33	D	407[B]	LHG	O8-C23-C24	2.24	118.92	111.91
36	c	519	DGD	O6D-C5D-C6D	2.24	111.18	106.67
23	B	613	CLA	CAA-C2A-C3A	-2.23	106.66	112.78
24	t	102	BCR	C37-C22-C23	2.23	121.59	118.08
25	b	620	SQD	O5-C1-C2	-2.23	105.62	110.35
23	b	613	CLA	CMA-C3A-C4A	-2.23	105.78	111.77
28	a	413[A]	PL9	C35-C34-C33	-2.23	117.95	123.68
23	b	612	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
28	A	413[A]	PL9	C25-C24-C26	2.23	119.02	115.27
24	T	102	BCR	C1-C6-C7	2.23	122.08	115.78
38	F	102	HEM	CHA-C1A-NA	2.23	127.94	123.85
23	b	601	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
25	a	409[B]	SQD	C3-C4-C5	2.23	114.21	110.24
23	C	513	CLA	CBC-CAC-C3C	-2.23	106.30	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	A	413[A]	PL9	C12-C13-C14	-2.23	122.30	127.66
23	B	604	CLA	O2A-CGA-CBA	2.22	118.89	111.91
31	A	416[A]	PHO	CED-O2D-CGD	2.22	120.97	115.94
28	A	413[A]	PL9	C53-C6-C1	2.22	119.54	114.99
25	A	409[A]	SQD	O9-S-O7	-2.22	106.25	113.95
23	A	404[A]	CLA	CHD-C4C-NC	2.22	127.71	124.20
23	b	609	CLA	OBD-CAD-C3D	-2.22	123.17	128.52
23	d	402[B]	CLA	CHB-C4A-NA	2.22	127.59	124.51
24	b	618	BCR	C2-C1-C6	2.22	113.90	110.48
24	C	516	BCR	C2-C1-C6	2.22	113.90	110.48
31	a	415[A]	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
23	B	602	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
33	d	407[A]	LHG	O8-C23-O10	-2.22	117.99	123.59
23	D	403[B]	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
23	c	510	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
23	b	604	CLA	C6-C5-C3	-2.22	107.64	113.45
36	H	102	DGD	C1E-O6E-C5E	-2.22	109.34	113.69
24	C	516	BCR	C11-C10-C9	-2.22	124.15	127.31
23	C	513	CLA	CBA-CAA-C2A	-2.22	107.32	113.86
23	D	403[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
23	C	503	CLA	CMB-C2B-C1B	2.21	128.74	125.37
25	X	101	SQD	C46-C45-C44	-2.21	106.55	111.79
23	B	601	CLA	CHB-C4A-NA	2.21	127.57	124.51
24	c	515	BCR	C36-C18-C19	2.21	121.56	118.08
23	c	508	CLA	C1-C2-C3	-2.21	122.22	126.04
24	B	619	BCR	C2-C3-C4	-2.21	106.44	111.38
23	d	404	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	a	405[B]	CLA	CBC-CAC-C3C	-2.21	106.33	112.43
23	c	509	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
33	D	407[B]	LHG	C5-O7-C7	-2.21	112.35	117.79
25	b	620	SQD	O47-C7-O49	-2.21	118.36	123.70
23	C	506	CLA	CHA-C1A-NA	-2.21	121.34	126.40
25	A	409[B]	SQD	O8-S-C6	2.21	109.26	105.74
24	h	101	BCR	C37-C22-C21	-2.21	119.83	122.92
23	B	609	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	c	504	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
23	b	602	CLA	CHC-C1C-C2C	-2.21	120.60	126.73
24	k	101	BCR	C34-C9-C8	2.21	121.55	118.08
23	C	505	CLA	O2A-CGA-CBA	2.21	118.83	111.91
23	d	402[B]	CLA	C1-O2A-CGA	2.21	122.23	116.44
33	E	101[A]	LHG	O7-C7-O9	-2.21	118.37	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CAA-C2A-C3A	-2.21	106.74	112.78
33	d	407[B]	LHG	O7-C7-O9	-2.21	118.37	123.70
25	f	102	SQD	O48-C23-O10	-2.20	118.03	123.59
23	c	514	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
24	C	515	BCR	C40-C30-C25	-2.20	106.73	110.30
23	B	602	CLA	C11-C10-C8	-2.20	108.80	115.92
25	l	101	SQD	C9-C8-C7	-2.20	105.61	113.62
36	C	517[A]	DGD	O3G-C3G-C2G	-2.20	105.59	110.90
25	f	102	SQD	O8-S-C6	2.20	109.25	105.74
24	T	102	BCR	C33-C5-C6	-2.20	122.06	124.53
25	a	409[A]	SQD	O9-S-O7	-2.20	106.34	113.95
23	B	606	CLA	CHB-C1B-C2B	-2.20	121.03	127.24
36	C	517[B]	DGD	O3G-C3G-C2G	-2.20	105.60	110.90
28	d	406[B]	PL9	C45-C44-C46	2.20	118.97	115.27
23	b	601	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
23	c	506	CLA	CHD-C4C-NC	2.20	127.66	124.20
24	b	618	BCR	C29-C30-C25	2.19	113.86	110.48
24	b	619	BCR	C11-C10-C9	-2.19	124.18	127.31
36	c	518[A]	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
23	B	612	CLA	CMB-C2B-C3B	2.19	131.90	126.59
23	c	507	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	C	508	CLA	CAC-C3C-C4C	2.19	127.65	124.81
24	b	617	BCR	C32-C1-C6	-2.19	106.75	110.30
24	h	101	BCR	C16-C15-C14	-2.19	118.99	123.47
24	h	101	BCR	C10-C11-C12	-2.19	116.39	123.22
31	a	415[A]	PHO	C4-C3-C2	-2.19	118.07	123.68
23	b	614	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
24	c	516	BCR	C38-C26-C25	-2.19	122.07	124.53
28	A	413[B]	PL9	C35-C34-C33	-2.18	118.07	123.68
23	A	404[B]	CLA	CHC-C1C-NC	2.18	127.52	124.20
23	b	613	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
23	C	504	CLA	C3B-C4B-NB	2.18	112.54	110.52
25	A	409[B]	SQD	O47-C7-O49	-2.18	118.43	123.70
31	D	401[B]	PHO	O2A-CGA-O1A	-2.18	118.08	123.59
23	A	406[B]	CLA	C1-C2-C3	-2.18	122.27	126.04
23	B	604	CLA	CHC-C4B-NB	2.18	126.57	124.26
23	c	509	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	A	407	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	b	611	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
23	b	606	CLA	CMC-C2C-C1C	2.18	128.36	125.04
24	C	515	BCR	C29-C30-C25	2.18	113.83	110.48
32	A	417	LMT	O1'-C1'-C2'	2.18	111.70	108.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	404	CLA	C1-O2A-CGA	2.18	122.16	116.44
23	B	605	CLA	CAC-C3C-C2C	2.18	131.25	127.53
23	c	514	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
24	d	405	BCR	C35-C13-C14	-2.18	119.88	122.92
24	b	618	BCR	C8-C7-C6	-2.18	121.09	127.20
23	B	614	CLA	C4-C3-C5	2.18	118.93	115.27
28	D	406[B]	PL9	C45-C44-C46	2.18	118.93	115.27
25	X	101	SQD	O5-C1-O6	2.18	115.12	109.97
23	a	405[A]	CLA	C4-C3-C5	2.17	118.92	115.27
23	C	505	CLA	C1-C2-C3	-2.17	122.29	126.04
24	Y	101	BCR	C7-C6-C5	-2.17	116.20	121.46
23	a	405[B]	CLA	C1-C2-C3	-2.17	122.29	126.04
34	m	101	LMG	O8-C28-O10	-2.17	118.12	123.59
35	b	623	HTG	C1-C2-C3	2.17	114.87	110.59
33	A	418[A]	LHG	O4-P-O5	2.17	122.96	112.24
23	C	511	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	b	611	CLA	C7-C6-C5	-2.17	107.47	113.36
31	D	401[B]	PHO	O2D-CGD-O1D	-2.17	119.60	123.84
23	b	604	CLA	C4-C3-C2	-2.17	118.12	123.68
23	C	509	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	A	405[B]	CLA	CAC-C3C-C4C	2.17	127.62	124.81
38	F	102	HEM	C4B-C3B-C2B	-2.17	105.39	107.11
23	c	503	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
24	T	102	BCR	C7-C8-C9	-2.16	122.96	126.23
23	c	507	CLA	C1-O2A-CGA	2.16	122.12	116.44
28	a	413[A]	PL9	C45-C44-C46	2.16	118.91	115.27
40	v	201	HEC	CMD-C2D-C1D	2.16	128.33	125.04
34	C	501	LMG	O8-C28-C29	2.16	118.69	111.91
23	C	512	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
23	B	607	CLA	C11-C10-C8	-2.16	108.94	115.92
24	T	102	BCR	C34-C9-C10	-2.16	119.90	122.92
23	a	407	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	A	405[A]	CLA	O2A-CGA-CBA	2.16	118.68	111.91
23	b	603	CLA	CAC-C3C-C4C	2.16	127.61	124.81
31	a	406[A]	PHO	O2D-CGD-O1D	-2.16	119.62	123.84
36	H	102	DGD	C3E-C4E-C5E	-2.16	106.39	110.24
23	a	407	CLA	CMB-C2B-C1B	2.16	128.66	125.37
23	C	508	CLA	CHD-C4C-NC	2.16	127.60	124.20
23	B	615	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
23	b	614	CLA	C4-C3-C5	2.16	118.90	115.27
23	b	615	CLA	C2A-C1A-CHA	-2.16	120.09	123.86
23	c	512	CLA	O2A-CGA-O1A	-2.16	118.15	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	CGD-CBD-CAD	-2.16	103.75	110.73
32	M	101	LMT	C3B-C4B-C5B	-2.15	106.40	110.24
23	d	403[B]	CLA	CAA-C2A-C3A	-2.15	106.88	112.78
24	h	101	BCR	C34-C9-C8	2.15	121.47	118.08
28	D	406[A]	PL9	C12-C13-C14	-2.15	122.48	127.66
24	c	516	BCR	C7-C8-C9	-2.15	122.99	126.23
24	d	405	BCR	C38-C26-C27	2.15	117.75	113.62
25	b	620	SQD	C44-O6-C1	-2.15	109.54	113.74
33	d	414[A]	LHG	O7-C7-O9	-2.15	118.51	123.70
23	C	509	CLA	C4-C3-C5	2.15	118.89	115.27
34	C	520	LMG	C8-O7-C10	-2.15	112.50	117.79
23	C	508	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	B	612	CLA	CMA-C3A-C2A	-2.15	105.17	113.83
23	B	616	CLA	CHA-C1A-NA	-2.15	121.48	126.40
25	b	620	SQD	O9-S-C6	2.15	109.49	106.94
34	d	412	LMG	O8-C9-C8	-2.15	102.19	108.43
25	f	102	SQD	O6-C1-C2	2.15	111.65	108.30
23	c	508	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
31	a	406[B]	PHO	C4-C3-C5	2.14	118.88	115.27
23	C	509	CLA	O2A-CGA-CBA	2.14	118.64	111.91
23	B	609	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
23	c	506	CLA	C4-C3-C5	2.14	118.88	115.27
36	H	102	DGD	O2G-C1B-C2B	2.14	116.12	111.50
24	b	619	BCR	C31-C1-C6	-2.14	106.82	110.30
35	C	522	HTG	C1-O5-C5	2.14	116.53	112.58
24	b	617	BCR	C21-C20-C19	-2.14	116.53	123.22
28	d	406[A]	PL9	C45-C44-C46	2.14	118.87	115.27
23	B	607	CLA	O2A-CGA-CBA	2.14	118.63	111.91
24	d	405	BCR	C21-C20-C19	-2.14	116.53	123.22
23	b	616	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
24	H	101	BCR	C37-C22-C21	-2.14	119.92	122.92
28	d	406[B]	PL9	C7-C3-C2	-2.14	120.48	123.30
23	D	403[A]	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
23	b	604	CLA	O2A-CGA-CBA	2.14	118.63	111.91
23	b	611	CLA	CHB-C4A-NA	2.14	127.47	124.51
28	A	413[B]	PL9	C32-C31-C29	-2.14	105.94	112.98
24	h	101	BCR	C36-C18-C19	2.14	121.45	118.08
34	m	101	LMG	O7-C10-O9	-2.14	118.53	123.70
23	b	607	CLA	CAA-CBA-CGA	2.14	119.50	113.25
23	b	602	CLA	CHB-C4A-NA	2.14	127.47	124.51
34	c	501	LMG	O6-C5-C4	2.14	113.58	109.69
23	A	406[B]	CLA	CHB-C1B-C2B	-2.14	121.20	127.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	612	CLA	C7-C6-C5	-2.14	107.56	113.36
23	D	404	CLA	C4-C3-C2	-2.13	118.20	123.68
23	c	502	CLA	C1-O2A-CGA	2.13	122.04	116.44
23	a	407	CLA	CHC-C1C-C2C	-2.13	120.81	126.73
24	Y	101	BCR	C40-C30-C25	-2.13	106.84	110.30
24	t	102	BCR	C36-C18-C19	2.13	121.44	118.08
32	t	101	LMT	O5'-C5'-C6'	2.13	111.73	106.44
24	y	101	BCR	C35-C13-C12	2.13	121.43	118.08
23	C	505	CLA	C4-C3-C5	2.13	118.86	115.27
23	b	603	CLA	C7-C6-C5	-2.13	107.57	113.36
36	c	517[A]	DGD	O6D-C1D-O3G	-2.13	104.93	109.97
23	A	406[A]	CLA	CHB-C4A-NA	2.13	127.46	124.51
36	C	517[A]	DGD	O5D-C6D-C5D	-2.13	105.11	109.05
23	C	504	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
25	l	101	SQD	O5-C1-C2	-2.13	105.84	110.35
33	d	407[A]	LHG	O8-C23-C24	2.13	118.59	111.91
23	c	502	CLA	C2A-C1A-CHA	-2.13	120.14	123.86
24	H	101	BCR	C38-C26-C27	2.13	117.70	113.62
24	Y	101	BCR	C35-C13-C12	2.13	121.43	118.08
23	a	405[A]	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
35	c	522	HTG	O5-C1-C2	2.12	112.99	110.31
23	B	602	CLA	CMB-C2B-C1B	2.12	128.60	125.37
23	d	403[A]	CLA	CHD-C4C-NC	2.12	127.55	124.20
23	C	508	CLA	CHA-C1A-NA	-2.12	121.53	126.40
23	B	608	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
23	B	603	CLA	C7-C6-C5	-2.12	107.59	113.36
23	B	609	CLA	C7-C6-C5	-2.12	107.59	113.36
23	A	405[A]	CLA	CHB-C4A-NA	2.12	127.44	124.51
23	A	404[B]	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
23	A	404[B]	CLA	C7-C6-C5	-2.12	107.60	113.36
23	d	404	CLA	CMA-C3A-C2A	-2.12	105.28	113.83
34	Z	101	LMG	C1-O6-C5	2.12	117.85	113.69
23	d	404	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
33	d	414[B]	LHG	O7-C7-O9	-2.12	118.58	123.70
23	B	613	CLA	C2A-C1A-CHA	-2.12	120.16	123.86
23	C	511	CLA	C4-C3-C2	-2.12	118.25	123.68
23	C	509	CLA	CMB-C2B-C1B	2.12	128.59	125.37
23	b	611	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
36	c	517[A]	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
23	d	402[A]	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	d	403[A]	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
23	A	406[B]	CLA	CAC-C3C-C4C	2.11	127.55	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	C	518[A]	DGD	O1G-C1A-C2A	2.11	118.53	111.91
25	a	409[A]	SQD	C3-C4-C5	2.11	114.00	110.24
33	L	101[B]	LHG	O8-C23-O10	-2.11	118.28	123.59
24	t	102	BCR	C20-C21-C22	-2.11	124.31	127.31
24	B	619	BCR	C16-C15-C14	-2.11	119.16	123.47
23	C	504	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	B	609	CLA	CHA-C1A-NA	-2.10	121.58	126.40
28	d	406[A]	PL9	C31-C32-C33	-2.10	104.97	111.88
23	d	402[A]	CLA	CAC-C3C-C2C	2.10	131.13	127.53
25	X	101	SQD	O7-S-C6	2.10	109.44	106.94
23	c	511	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
23	A	405[B]	CLA	C1-C2-C3	-2.10	122.41	126.04
26	B	625	GOL	C3-C2-C1	-2.10	103.53	111.70
23	b	608	CLA	C4-C3-C5	2.10	118.81	115.27
28	a	413[A]	PL9	C51-C49-C50	2.10	119.25	114.60
23	C	513	CLA	CHC-C1C-C2C	-2.10	120.89	126.73
33	E	101[B]	LHG	O7-C7-O9	-2.10	118.62	123.70
23	A	404[A]	CLA	C7-C6-C5	-2.10	107.65	113.36
23	b	616	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
23	C	505	CLA	CHB-C1B-NB	-2.10	122.03	124.26
32	M	101	LMT	O6'-C6'-C5'	-2.10	104.09	111.29
34	m	101	LMG	C7-O1-C1	-2.10	109.64	113.74
23	b	601	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
24	b	619	BCR	C24-C23-C22	-2.10	123.06	126.23
40	V	201	HEC	C3D-C4D-ND	-2.10	108.32	110.36
35	o	301	HTG	C2'-C1'-S1	-2.10	105.63	112.40
24	b	619	BCR	C37-C22-C21	-2.09	119.99	122.92
23	c	514	CLA	C4-C3-C5	2.09	118.79	115.27
23	B	610	CLA	C1-C2-C3	-2.09	122.42	126.04
24	t	102	BCR	C29-C30-C25	2.09	113.70	110.48
23	C	505	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
34	m	101	LMG	C3-C4-C5	2.09	113.97	110.24
28	A	413[A]	PL9	C51-C49-C50	2.09	119.22	114.60
24	b	619	BCR	C21-C20-C19	-2.09	116.69	123.22
23	d	402[B]	CLA	CAC-C3C-C2C	2.09	131.11	127.53
34	C	521	LMG	C9-C8-C7	-2.09	106.84	111.79
24	d	405	BCR	C28-C27-C26	-2.09	110.34	114.08
28	D	406[B]	PL9	C7-C3-C4	2.09	118.58	116.88
23	A	405[B]	CLA	CAA-CBA-CGA	2.09	119.36	113.25
23	B	607	CLA	OBD-CAD-C3D	-2.09	123.49	128.52
23	b	602	CLA	O2A-CGA-CBA	2.09	118.47	111.91
24	b	617	BCR	C8-C7-C6	-2.09	121.33	127.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	405	BCR	C30-C25-C24	2.09	121.69	115.78
38	F	102	HEM	C4C-CHD-C1D	-2.09	121.55	126.06
35	b	625	HTG	O5-C1-C2	2.09	112.94	110.31
40	V	201	HEC	C3B-C4B-NB	-2.09	107.84	110.17
28	d	406[B]	PL9	C36-C34-C33	-2.09	116.89	121.12
24	y	101	BCR	C11-C10-C9	-2.09	124.33	127.31
23	B	604	CLA	CED-O2D-CGD	2.09	120.66	115.94
36	C	518[B]	DGD	O2G-C1B-O1B	-2.09	118.66	123.70
28	D	406[B]	PL9	C37-C38-C39	-2.09	122.64	127.66
31	A	416[A]	PHO	OBD-CAD-C3D	-2.09	124.52	127.98
24	A	408	BCR	C11-C10-C9	-2.09	124.33	127.31
23	a	405[A]	CLA	CAC-C3C-C4C	2.08	127.52	124.81
23	b	611	CLA	OBD-CAD-C3D	-2.08	123.50	128.52
23	d	402[A]	CLA	CHB-C1B-NB	-2.08	122.05	124.26
23	b	602	CLA	C11-C10-C8	-2.08	109.19	115.92
23	b	615	CLA	CHA-C1A-NA	-2.08	121.63	126.40
32	B	626	LMT	C1B-C2B-C3B	2.08	114.33	110.00
23	A	406[B]	CLA	CHC-C4B-NB	-2.08	122.05	124.26
23	C	505	CLA	C1-O2A-CGA	2.08	121.91	116.44
24	H	101	BCR	C11-C10-C9	-2.08	124.34	127.31
23	C	507	CLA	CMB-C2B-C1B	2.08	128.54	125.37
24	K	102	BCR	C33-C5-C6	-2.08	122.19	124.53
28	A	413[A]	PL9	C10-C9-C11	2.08	118.77	115.27
25	A	411	SQD	C9-C8-C7	-2.08	106.07	113.62
28	A	413[B]	PL9	C7-C3-C4	2.08	118.56	116.88
23	c	513	CLA	CAC-C3C-C4C	2.08	127.50	124.81
23	D	403[A]	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
40	v	201	HEC	CBD-CAD-C3D	-2.07	106.86	112.63
33	b	629[B]	LHG	C5-O7-C7	-2.07	112.68	117.79
23	b	605	CLA	OBD-CAD-C3D	-2.07	123.53	128.52
23	B	605	CLA	CHB-C1B-NB	-2.07	122.06	124.26
23	d	402[B]	CLA	CMA-C3A-C2A	-2.07	105.46	113.83
34	C	501	LMG	C9-C8-C7	-2.07	106.89	111.79
32	B	627	LMT	O5B-C5B-C4B	2.07	113.46	109.69
23	a	404[B]	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	c	503	CLA	CHB-C1B-NB	-2.07	122.06	124.26
28	d	406[A]	PL9	C40-C39-C38	-2.07	118.37	123.68
23	b	601	CLA	CAC-C3C-C4C	2.07	127.50	124.81
23	d	403[A]	CLA	CBB-CAB-C3B	-2.07	117.32	127.62
36	c	518[B]	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
23	B	614	CLA	CMB-C2B-C1B	2.07	128.52	125.37
24	c	515	BCR	C7-C8-C9	-2.07	123.11	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
23	B	603	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
23	A	406[B]	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	k	101	BCR	C3-C4-C5	-2.07	110.39	114.08
34	c	521	LMG	C13-C12-C11	-2.07	105.77	113.19
23	D	404	CLA	CHB-C4A-NA	2.07	127.37	124.51
24	T	102	BCR	C3-C4-C5	-2.06	110.39	114.08
28	A	413[B]	PL9	C10-C9-C8	-2.06	118.39	123.68
23	A	406[B]	CLA	CMC-C2C-C1C	2.06	128.18	125.04
23	b	601	CLA	CMC-C2C-C1C	2.06	128.18	125.04
23	A	405[B]	CLA	CED-O2D-CGD	2.06	120.60	115.94
23	d	404	CLA	CGD-CBD-CAD	-2.06	104.06	110.73
23	A	407	CLA	C11-C12-C13	-2.06	109.26	115.92
23	c	508	CLA	C3B-C4B-NB	2.06	112.43	110.52
23	b	602	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	a	404[B]	CLA	CHC-C1C-NC	2.06	127.33	124.20
23	d	403[A]	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
24	C	516	BCR	C3-C4-C5	-2.06	110.40	114.08
23	B	604	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
23	B	615	CLA	C1-O2A-CGA	2.06	121.84	116.44
28	D	406[A]	PL9	C27-C28-C29	-2.06	122.71	127.66
23	b	606	CLA	O2A-CGA-CBA	2.06	118.36	111.91
23	C	503	CLA	CHB-C1B-C2B	-2.05	121.43	127.24
32	m	103	LMT	C1'-O5'-C5'	-2.05	109.66	113.69
23	c	506	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
24	t	102	BCR	C29-C28-C27	-2.05	106.79	111.38
23	B	604	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
28	d	406[A]	PL9	O2-C1-C6	-2.05	117.04	120.59
24	b	617	BCR	C35-C13-C12	2.05	121.31	118.08
23	c	511	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
31	A	416[A]	PHO	O1D-CGD-CBD	-2.05	121.33	124.74
23	c	512	CLA	CAC-C3C-C4C	2.05	127.47	124.81
28	D	406[A]	PL9	C45-C44-C46	2.05	118.72	115.27
33	E	101[B]	LHG	C5-O7-C7	-2.05	112.75	117.79
23	b	605	CLA	O2A-CGA-CBA	2.05	118.33	111.91
36	H	102	DGD	C2G-O2G-C1B	-2.05	112.75	117.79
33	L	101[A]	LHG	O4-P-O5	2.05	122.36	112.24
24	K	102	BCR	C20-C21-C22	-2.05	124.39	127.31
23	B	610	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	a	404[A]	CLA	CMB-C2B-C3B	2.05	131.54	126.59
23	b	610	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
23	A	406[A]	CLA	CBC-CAC-C3C	-2.04	106.79	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	513	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
34	C	521	LMG	O6-C1-C2	-2.04	106.02	110.35
23	A	405[B]	CLA	CHB-C4A-NA	2.04	127.34	124.51
23	b	603	CLA	CMB-C2B-C1B	2.04	128.48	125.37
28	D	406[B]	PL9	O2-C1-C6	-2.04	117.06	120.59
31	a	415[A]	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
31	a	406[A]	PHO	C1-C2-C3	-2.04	122.51	126.04
23	B	610	CLA	CHB-C1B-NB	-2.04	122.10	124.26
23	C	506	CLA	C4-C3-C2	-2.04	118.44	123.68
23	A	405[B]	CLA	O2A-CGA-CBA	2.04	118.31	111.91
23	b	601	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
23	c	507	CLA	O2A-CGA-CBA	2.04	118.31	111.91
23	b	604	CLA	CHD-C4C-NC	2.04	127.42	124.20
33	b	629[A]	LHG	O7-C7-O9	-2.04	118.77	123.70
23	a	405[B]	CLA	CHB-C4A-NA	2.04	127.33	124.51
34	B	620	LMG	O6-C5-C4	2.04	113.39	109.69
23	c	505	CLA	CHB-C1B-NB	-2.04	122.10	124.26
23	A	407	CLA	OBD-CAD-C3D	-2.04	123.62	128.52
25	a	409[B]	SQD	O7-S-C6	2.04	109.36	106.94
24	d	405	BCR	C30-C25-C24	2.04	121.54	115.78
23	B	615	CLA	CAC-C3C-C4C	2.04	127.45	124.81
23	b	608	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
26	B	622	GOL	C3-C2-C1	-2.03	103.80	111.70
23	B	607	CLA	C6-C7-C8	-2.03	109.34	115.92
23	b	607	CLA	C6-C7-C8	-2.03	109.34	115.92
23	B	615	CLA	CHA-C1A-NA	-2.03	121.74	126.40
33	d	408[B]	LHG	O8-C23-O10	-2.03	118.46	123.59
23	c	508	CLA	CBB-CAB-C3B	-2.03	117.50	127.62
23	c	502	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
28	D	406[A]	PL9	C47-C48-C49	-2.03	120.81	127.75
23	a	404[B]	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
28	D	406[A]	PL9	C21-C22-C23	-2.03	105.21	111.88
24	y	101	BCR	C1-C6-C7	2.03	121.52	115.78
24	H	101	BCR	C7-C8-C9	-2.03	123.17	126.23
23	c	512	CLA	CHB-C1B-NB	-2.03	122.11	124.26
24	D	405	BCR	C39-C30-C25	-2.03	107.01	110.30
23	B	603	CLA	CMB-C2B-C3B	2.03	131.50	126.59
23	B	606	CLA	C1-O2A-CGA	2.03	121.76	116.44
35	b	625	HTG	C4-C3-C2	-2.03	107.28	110.82
24	y	101	BCR	C40-C30-C25	-2.03	107.01	110.30
23	b	616	CLA	CHA-C1A-NA	-2.03	121.76	126.40
24	t	102	BCR	C15-C14-C13	-2.02	124.42	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	504	CLA	O2A-CGA-CBA	2.02	118.26	111.91
32	M	101	LMT	O5B-C5B-C6B	2.02	111.47	106.44
23	b	610	CLA	CAC-C3C-C2C	2.02	130.99	127.53
23	a	405[A]	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	d	402[B]	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	a	405[B]	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	b	613	CLA	OBD-CAD-C3D	-2.02	123.66	128.52
38	F	102	HEM	C4D-ND-C1D	2.02	107.16	105.07
38	f	101	HEM	O2D-CGD-CBD	2.02	120.52	114.03
23	b	607	CLA	C1-C2-C3	-2.02	122.55	126.04
25	a	409[A]	SQD	O4-C4-C3	-2.02	105.68	110.35
23	B	612	CLA	CHB-C4A-NA	2.02	127.30	124.51
36	h	102	DGD	C2G-O2G-C1B	-2.02	112.83	117.79
23	b	615	CLA	CMC-C2C-C1C	2.02	128.11	125.04
23	A	404[B]	CLA	CED-O2D-CGD	2.02	120.50	115.94
36	c	517[A]	DGD	O1G-C1A-C2A	2.01	118.23	111.91
24	C	516	BCR	C39-C30-C25	-2.01	107.03	110.30
32	F	101	LMT	C1'-O5'-C5'	-2.01	109.74	113.69
23	B	606	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
23	B	604	CLA	CHA-C1A-NA	-2.01	121.79	126.40
23	c	512	CLA	C4-C3-C2	-2.01	118.52	123.68
23	a	404[B]	CLA	CHB-C4A-NA	2.01	127.29	124.51
36	H	102	DGD	O3G-C3G-C2G	-2.01	106.06	110.90
23	d	404	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
34	c	520	LMG	O8-C28-O10	-2.01	118.53	123.59
24	D	405	BCR	C2-C1-C6	2.01	113.57	110.48
31	A	416[A]	PHO	CMB-C2B-C3B	2.00	128.43	124.68
23	b	613	CLA	CHB-C4A-NA	2.00	127.28	124.51
36	C	517[A]	DGD	C4E-C3E-C2E	-2.00	107.33	110.82
36	c	519	DGD	O3G-C3G-C2G	-2.00	106.07	110.90
34	c	520	LMG	O6-C5-C4	2.00	113.33	109.69
23	b	602	CLA	CAA-CBA-CGA	-2.00	107.41	113.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	201	HEC	NA
40	v	201	HEC	NA

All (1701) 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	A	407	CLA	C4-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
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	C2B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	a	404[B]	CLA	C2B-C3B-CAB-CBB
23	a	404[B]	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C2-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
23	b	606	CLA	C12-C13-C15-C16
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
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	C2B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
23	d	404	CLA	C2-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
24	H	101	BCR	C23-C24-C25-C30
24	T	102	BCR	C13-C14-C15-C16
24	Y	101	BCR	C1-C6-C7-C8
24	Y	101	BCR	C5-C6-C7-C8
24	c	516	BCR	C7-C8-C9-C34
24	d	405	BCR	C21-C22-C23-C24
24	y	101	BCR	C1-C6-C7-C8
24	y	101	BCR	C5-C6-C7-C8
25	A	409[B]	SQD	C8-C7-O47-C45
25	A	411	SQD	O6-C44-C45-O47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	X	101	SQD	C2-C1-O6-C44
25	X	101	SQD	O49-C7-O47-C45
25	X	101	SQD	C8-C7-O47-C45
25	a	411	SQD	O6-C44-C45-O47
25	a	411	SQD	C5-C6-S-O7
25	a	411	SQD	C5-C6-S-O8
25	a	411	SQD	C5-C6-S-O9
25	b	620	SQD	C8-C7-O47-C45
25	f	102	SQD	O6-C44-C45-O47
25	f	102	SQD	O49-C7-O47-C45
25	f	102	SQD	C8-C7-O47-C45
25	l	101	SQD	O49-C7-O47-C45
26	A	410	GOL	O1-C1-C2-C3
26	B	622	GOL	C1-C2-C3-O3
26	D	402	GOL	O1-C1-C2-C3
26	D	413	GOL	C1-C2-C3-O3
26	O	303	GOL	O1-C1-C2-C3
26	V	203[A]	GOL	C1-C2-C3-O3
26	V	203[B]	GOL	C1-C2-C3-O3
26	V	203[B]	GOL	O2-C2-C3-O3
26	a	410	GOL	O1-C1-C2-C3
26	a	418	GOL	C1-C2-C3-O3
26	b	624	GOL	C1-C2-C3-O3
26	c	527	GOL	C1-C2-C3-O3
26	o	303	GOL	C1-C2-C3-O3
26	o	304	GOL	O1-C1-C2-C3
26	o	304	GOL	C1-C2-C3-O3
28	A	413[A]	PL9	C9-C11-C12-C13
28	A	413[A]	PL9	C15-C14-C16-C17
28	A	413[A]	PL9	C14-C16-C17-C18
28	A	413[B]	PL9	C9-C11-C12-C13
28	A	413[B]	PL9	C14-C16-C17-C18
28	A	413[B]	PL9	C30-C29-C31-C32
28	a	413[A]	PL9	C9-C11-C12-C13
28	a	413[A]	PL9	C14-C16-C17-C18
28	a	413[A]	PL9	C23-C24-C26-C27
28	a	413[A]	PL9	C25-C24-C26-C27
28	a	413[B]	PL9	C9-C11-C12-C13
28	a	413[B]	PL9	C14-C16-C17-C18
32	A	417	LMT	C2'-C1'-O1'-C1
32	A	417	LMT	O5'-C1'-O1'-C1
32	A	419	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	419	LMT	O5'-C1'-O1'-C1
32	A	419	LMT	C2-C1-O1'-C1'
32	B	627	LMT	C2'-C1'-O1'-C1
32	B	629	LMT	O5'-C1'-O1'-C1
32	B	629	LMT	C2-C1-O1'-C1'
32	F	101	LMT	C2'-C1'-O1'-C1
32	F	101	LMT	O5'-C1'-O1'-C1
32	T	101	LMT	C2-C1-O1'-C1'
32	b	621	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2-C1-O1'-C1'
33	D	407[A]	LHG	O2-C2-C3-O3
33	D	407[A]	LHG	C3-O3-P-O4
33	D	407[A]	LHG	C3-O3-P-O5
33	D	407[A]	LHG	C3-O3-P-O6
33	D	407[A]	LHG	C4-O6-P-O4
33	D	407[B]	LHG	O2-C2-C3-O3
33	D	407[B]	LHG	C3-O3-P-O4
33	D	407[B]	LHG	C3-O3-P-O5
33	D	407[B]	LHG	C3-O3-P-O6
33	D	407[B]	LHG	C4-O6-P-O3
33	D	407[B]	LHG	C4-O6-P-O4
33	D	407[B]	LHG	C4-O6-P-O5
33	E	101[A]	LHG	C3-O3-P-O4
33	E	101[A]	LHG	C3-O3-P-O5
33	E	101[A]	LHG	O10-C23-O8-C6
33	E	101[A]	LHG	C24-C23-O8-C6
33	E	101[B]	LHG	C3-O3-P-O4
33	E	101[B]	LHG	C3-O3-P-O5
33	E	101[B]	LHG	C3-O3-P-O6
33	E	101[B]	LHG	O10-C23-O8-C6
33	E	101[B]	LHG	C24-C23-O8-C6
33	L	101[A]	LHG	C4-O6-P-O4
33	L	101[A]	LHG	C4-O6-P-O5
33	L	101[B]	LHG	C4-O6-P-O4
33	L	101[B]	LHG	C4-O6-P-O5
33	a	419[A]	LHG	C3-O3-P-O4
33	a	419[A]	LHG	C4-O6-P-O5
33	a	419[A]	LHG	O10-C23-O8-C6
33	a	419[A]	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	419[B]	LHG	C3-O3-P-O4
33	a	419[B]	LHG	C4-O6-P-O5
33	a	419[B]	LHG	O10-C23-O8-C6
33	a	419[B]	LHG	C24-C23-O8-C6
33	b	629[A]	LHG	C4-O6-P-O4
33	b	629[A]	LHG	C4-O6-P-O5
33	b	629[B]	LHG	C4-O6-P-O3
33	b	629[B]	LHG	C4-O6-P-O4
33	b	629[B]	LHG	C4-O6-P-O5
33	d	407[A]	LHG	C3-O3-P-O4
33	d	407[A]	LHG	C3-O3-P-O5
33	d	407[A]	LHG	C4-O6-P-O4
33	d	407[B]	LHG	O2-C2-C3-O3
33	d	407[B]	LHG	C3-O3-P-O4
33	d	407[B]	LHG	C4-O6-P-O4
33	d	407[B]	LHG	C4-O6-P-O5
33	d	414[A]	LHG	C3-O3-P-O5
34	C	521	LMG	C11-C10-O7-C8
34	c	521	LMG	O9-C10-O7-C8
34	c	521	LMG	C11-C10-O7-C8
34	Z	101	LMG	O9-C10-O7-C8
34	Z	101	LMG	C11-C10-O7-C8
34	z	101	LMG	O6-C1-O1-C7
34	z	101	LMG	O9-C10-O7-C8
35	o	301	HTG	C2'-C1'-S1-C1
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
32	A	419	LMT	O5B-C1B-O1B-C4'
32	B	627	LMT	C4'-C5'-C6'-O6'
23	c	514	CLA	CBD-CGD-O2D-CED
32	T	101	LMT	O5'-C5'-C6'-O6'
25	A	409[A]	SQD	O49-C7-O47-C45
25	A	409[B]	SQD	O49-C7-O47-C45
25	b	620	SQD	O49-C7-O47-C45
34	C	521	LMG	O9-C10-O7-C8
23	B	614	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	404	CLA	C3-C5-C6-C7
32	a	416	LMT	O5B-C5B-C6B-O6B
25	l	101	SQD	C8-C7-O47-C45
34	z	101	LMG	C11-C10-O7-C8
32	T	101	LMT	C4B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	A	413[A]	PL9	C20-C19-C21-C22
32	B	626	LMT	C4'-C5'-C6'-O6'
32	m	103	LMT	C4B-C5B-C6B-O6B
23	A	407	CLA	C2-C3-C5-C6
28	A	413[A]	PL9	C18-C19-C21-C22
28	A	413[B]	PL9	C18-C19-C21-C22
23	D	404	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C3-C5-C6-C7
32	F	101	LMT	O5'-C5'-C6'-O6'
35	D	411	HTG	S1-C1'-C2'-C3'
35	b	625	HTG	S1-C1'-C2'-C3'
35	D	411	HTG	O5-C5-C6-O6
32	B	626	LMT	O5'-C5'-C6'-O6'
32	B	627	LMT	O5B-C5B-C6B-O6B
32	b	627	LMT	O5'-C5'-C6'-O6'
23	C	510	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
23	c	512	CLA	CBD-CGD-O2D-CED
33	d	407[A]	LHG	O2-C2-C3-O3
34	C	521	LMG	O6-C5-C6-O5
32	e	101	LMT	C4'-C5'-C6'-O6'
25	A	409[A]	SQD	C8-C7-O47-C45
23	C	514	CLA	CBD-CGD-O2D-CED
35	B	623	HTG	O5-C5-C6-O6
32	T	101	LMT	C4'-C5'-C6'-O6'
32	a	416	LMT	C4B-C5B-C6B-O6B
32	B	626	LMT	O5B-C5B-C6B-O6B
32	B	629	LMT	O5'-C5'-C6'-O6'
32	m	103	LMT	O5B-C5B-C6B-O6B
34	c	521	LMG	C4-C5-C6-O5
35	D	411	HTG	C4-C5-C6-O6
35	b	625	HTG	O5-C5-C6-O6
32	F	101	LMT	C4'-C5'-C6'-O6'
32	A	419	LMT	O5B-C5B-C6B-O6B
32	A	419	LMT	O5'-C5'-C6'-O6'
32	B	627	LMT	O5'-C5'-C6'-O6'
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
28	A	413[B]	PL9	C15-C14-C16-C17
28	A	413[B]	PL9	C20-C19-C21-C22
28	a	413[A]	PL9	C15-C14-C16-C17
28	a	413[A]	PL9	C30-C29-C31-C32
28	a	413[B]	PL9	C15-C14-C16-C17
28	a	413[B]	PL9	C30-C29-C31-C32
23	B	605	CLA	C2-C3-C5-C6
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
28	A	413[A]	PL9	C13-C14-C16-C17
28	A	413[B]	PL9	C13-C14-C16-C17
28	a	413[A]	PL9	C13-C14-C16-C17
28	a	413[A]	PL9	C28-C29-C31-C32
28	a	413[B]	PL9	C13-C14-C16-C17
28	a	413[B]	PL9	C28-C29-C31-C32
32	T	101	LMT	O5B-C5B-C6B-O6B
32	b	621	LMT	O5'-C1'-O1'-C1
32	e	101	LMT	O5'-C1'-O1'-C1
28	A	413[A]	PL9	C44-C46-C47-C48
28	A	413[B]	PL9	C44-C46-C47-C48
28	D	406[A]	PL9	C39-C41-C42-C43
28	D	406[B]	PL9	C39-C41-C42-C43
28	d	406[B]	PL9	C39-C41-C42-C43
23	c	510	CLA	CBA-CGA-O2A-C1
23	c	502	CLA	CBD-CGD-O2D-CED
32	b	621	LMT	O5'-C5'-C6'-O6'
32	B	627	LMT	C4B-C5B-C6B-O6B
34	c	520	LMG	C4-C5-C6-O5
33	D	407[B]	LHG	C1-C2-C3-O3
33	d	407[A]	LHG	C1-C2-C3-O3
23	a	407	CLA	CBA-CGA-O2A-C1
25	X	101	SQD	C23-C24-C25-C26
35	b	623	HTG	C1'-C2'-C3'-C4'
32	B	629	LMT	C4'-C5'-C6'-O6'
32	e	101	LMT	O5B-C5B-C6B-O6B
32	b	627	LMT	C4'-C5'-C6'-O6'
23	C	508	CLA	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	B	629	LMT	C2'-C1'-O1'-C1
32	e	101	LMT	C2'-C1'-O1'-C1
32	t	101	LMT	C2'-C1'-O1'-C1
40	V	201	HEC	C2C-C3C-CAC-CBC
28	A	413[A]	PL9	C30-C29-C31-C32
28	a	413[B]	PL9	C25-C24-C26-C27
23	C	503	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
24	D	405	BCR	C37-C22-C23-C24
24	Y	101	BCR	C37-C22-C23-C24
24	b	619	BCR	C7-C8-C9-C34
24	d	405	BCR	C37-C22-C23-C24
24	b	619	BCR	C7-C8-C9-C10
32	e	101	LMT	O5'-C5'-C6'-O6'
33	E	101[A]	LHG	C23-C24-C25-C26
36	c	518[B]	DGD	C1B-C2B-C3B-C4B
23	a	407	CLA	O1A-CGA-O2A-C1
23	A	407	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	A	407	CLA	C3-C5-C6-C7
32	A	419	LMT	C5'-C4'-O1B-C1B
32	B	626	LMT	C5'-C4'-O1B-C1B
23	B	601	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
23	C	509	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
34	B	620	LMG	C39-C40-C41-C42
26	B	622	GOL	O2-C2-C3-O3
26	a	410	GOL	O1-C1-C2-O2
36	c	518[A]	DGD	C1B-C2B-C3B-C4B
32	A	419	LMT	C4B-C5B-C6B-O6B
23	D	404	CLA	C10-C11-C12-C13
23	c	510	CLA	C3-C5-C6-C7
25	l	101	SQD	C30-C31-C32-C33
32	t	101	LMT	O5'-C5'-C6'-O6'
34	c	521	LMG	O6-C5-C6-O5
33	D	408[A]	LHG	C33-C34-C35-C36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	C	519	DGD	C6B-C7B-C8B-C9B
23	c	514	CLA	C10-C11-C12-C13
25	l	101	SQD	C7-C8-C9-C10
34	Z	101	LMG	C10-C11-C12-C13
33	D	408[B]	LHG	C33-C34-C35-C36
36	h	102	DGD	C6B-C7B-C8B-C9B
23	b	604	CLA	C8-C10-C11-C12
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	C	511	CLA	C11-C12-C13-C15
23	c	505	CLA	C12-C13-C15-C16
23	C	512	CLA	C3-C5-C6-C7
23	c	514	CLA	O1D-CGD-O2D-CED
23	B	606	CLA	C10-C11-C12-C13
23	c	513	CLA	C15-C16-C17-C18
32	B	626	LMT	C6-C7-C8-C9
32	a	416	LMT	O1'-C1-C2-C3
25	X	101	SQD	O5-C1-O6-C44
25	l	101	SQD	O5-C1-O6-C44
32	B	627	LMT	O5'-C1'-O1'-C1
23	B	614	CLA	C8-C10-C11-C12
23	a	404[A]	CLA	C15-C16-C17-C18
28	a	413[B]	PL9	C24-C26-C27-C28
28	d	406[A]	PL9	C39-C41-C42-C43
35	b	622	HTG	S1-C1'-C2'-C3'
32	A	419	LMT	O1'-C1-C2-C3
23	C	512	CLA	C8-C10-C11-C12
23	b	614	CLA	C8-C10-C11-C12
23	c	508	CLA	C5-C6-C7-C8
23	c	510	CLA	O1A-CGA-O2A-C1
23	B	614	CLA	C10-C11-C12-C13
23	a	404[B]	CLA	C15-C16-C17-C18
23	b	604	CLA	C5-C6-C7-C8
23	b	611	CLA	C8-C10-C11-C12
23	b	611	CLA	C15-C16-C17-C18
33	E	101[A]	LHG	C3-O3-P-O6
33	E	101[A]	LHG	C4-O6-P-O3
33	E	101[B]	LHG	C4-O6-P-O3
33	L	101[A]	LHG	C4-O6-P-O3
33	L	101[B]	LHG	C4-O6-P-O3
33	a	419[A]	LHG	C3-O3-P-O6
33	a	419[A]	LHG	C4-O6-P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	419[B]	LHG	C3-O3-P-O6
33	a	419[B]	LHG	C4-O6-P-O3
33	b	629[A]	LHG	C4-O6-P-O3
33	d	407[A]	LHG	C3-O3-P-O6
33	d	407[B]	LHG	C3-O3-P-O6
33	d	407[B]	LHG	C4-O6-P-O3
25	A	409[A]	SQD	C7-C8-C9-C10
23	D	404	CLA	C3-C5-C6-C7
25	A	409[B]	SQD	C7-C8-C9-C10
33	D	407[A]	LHG	C1-C2-C3-O3
33	d	407[B]	LHG	C1-C2-C3-O3
34	B	620	LMG	O9-C10-O7-C8
25	A	409[A]	SQD	C12-C13-C14-C15
25	b	620	SQD	C18-C19-C20-C21
23	b	614	CLA	C10-C11-C12-C13
23	b	610	CLA	C2A-CAA-CBA-CGA
23	c	510	CLA	C16-C17-C18-C20
36	c	517[B]	DGD	O6D-C5D-C6D-O5D
34	B	620	LMG	C11-C10-O7-C8
36	C	517[B]	DGD	O6D-C5D-C6D-O5D
35	o	301	HTG	C1'-C2'-C3'-C4'
25	X	101	SQD	C30-C31-C32-C33
25	a	411	SQD	C25-C26-C27-C28
32	t	101	LMT	C4-C5-C6-C7
33	L	101[A]	LHG	C15-C16-C17-C18
33	L	101[A]	LHG	C17-C18-C19-C20
33	L	101[B]	LHG	C13-C14-C15-C16
33	b	629[B]	LHG	C27-C28-C29-C30
34	D	412	LMG	C19-C20-C21-C22
35	B	621	HTG	C3'-C4'-C5'-C6'
36	c	517[A]	DGD	C9A-CAA-CBA-CCA
36	c	517[B]	DGD	C2B-C3B-C4B-C5B
36	c	518[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[B]	DGD	C9A-CAA-CBA-CCA
32	A	419	LMT	C4'-C5'-C6'-O6'
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
35	B	623	HTG	S1-C1'-C2'-C3'
25	A	409[B]	SQD	C15-C16-C17-C18
32	b	627	LMT	C7-C8-C9-C10
33	D	408[B]	LHG	C32-C33-C34-C35
33	L	101[B]	LHG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	414[A]	LHG	C16-C17-C18-C19
34	B	620	LMG	C17-C18-C19-C20
35	b	622	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	C2B-C3B-C4B-C5B
23	c	513	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	C15-C16-C17-C18
33	d	408[B]	LHG	C27-C28-C29-C30
36	h	102	DGD	CAA-CBA-CCA-CDA
25	f	102	SQD	C32-C33-C34-C35
32	M	101	LMT	C3-C4-C5-C6
33	D	407[A]	LHG	C16-C17-C18-C19
33	d	414[A]	LHG	C32-C33-C34-C35
34	c	501	LMG	C30-C31-C32-C33
36	C	517[A]	DGD	C5B-C6B-C7B-C8B
36	c	518[B]	DGD	CBA-CCA-CDA-CEA
32	e	101	LMT	C5-C6-C7-C8
33	a	419[A]	LHG	C26-C27-C28-C29
33	b	629[B]	LHG	C16-C17-C18-C19
33	d	414[B]	LHG	C16-C17-C18-C19
36	c	517[A]	DGD	C5A-C6A-C7A-C8A
36	c	518[A]	DGD	CBA-CCA-CDA-CEA
23	B	616	CLA	C3-C5-C6-C7
25	A	411	SQD	C2-C1-O6-C44
36	C	518[A]	DGD	C2E-C1E-O5D-C6D
36	C	518[B]	DGD	C2E-C1E-O5D-C6D
32	A	417	LMT	O1'-C1-C2-C3
32	B	629	LMT	C3-C4-C5-C6
33	a	419[B]	LHG	C26-C27-C28-C29
36	C	517[A]	DGD	C4B-C5B-C6B-C7B
36	C	518[B]	DGD	CCB-CDB-CEB-CFB
36	H	102	DGD	C5B-C6B-C7B-C8B
36	c	517[A]	DGD	C2B-C3B-C4B-C5B
36	c	517[B]	DGD	C9A-CAA-CBA-CCA
36	c	518[A]	DGD	CAA-CBA-CCA-CDA
23	B	603	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C20
23	c	506	CLA	C4-C3-C5-C6
28	D	406[B]	PL9	C15-C14-C16-C17
28	d	406[B]	PL9	C15-C14-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	L	101[A]	LHG	C13-C14-C15-C16
34	B	620	LMG	C34-C35-C36-C37
36	c	519	DGD	C2B-C3B-C4B-C5B
23	B	602	CLA	C6-C7-C8-C9
23	C	512	CLA	C11-C12-C13-C14
23	a	405[A]	CLA	C11-C12-C13-C14
23	a	405[B]	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	c	514	CLA	C6-C7-C8-C9
23	D	404	CLA	O1D-CGD-O2D-CED
25	A	409[A]	SQD	C15-C16-C17-C18
25	l	101	SQD	C11-C10-C9-C8
32	A	419	LMT	C3-C4-C5-C6
32	e	101	LMT	C4-C5-C6-C7
33	d	407[B]	LHG	C34-C35-C36-C37
34	C	521	LMG	C19-C20-C21-C22
34	D	412	LMG	C35-C36-C37-C38
36	C	518[A]	DGD	CCB-CDB-CEB-CFB
23	C	507	CLA	C15-C16-C17-C18
23	B	610	CLA	C2A-CAA-CBA-CGA
35	B	623	HTG	C4-C5-C6-O6
36	c	517[B]	DGD	C4D-C5D-C6D-O5D
26	B	622	GOL	O1-C1-C2-C3
26	B	625	GOL	C1-C2-C3-O3
26	D	413	GOL	O1-C1-C2-C3
26	O	302	GOL	O1-C1-C2-C3
26	a	410	GOL	C1-C2-C3-O3
26	a	417	GOL	O1-C1-C2-C3
26	d	413	GOL	O1-C1-C2-C3
26	v	202[A]	GOL	O1-C1-C2-C3
26	v	202[B]	GOL	O1-C1-C2-C3
33	A	418[B]	LHG	O1-C1-C2-C3
24	Y	101	BCR	C21-C22-C23-C24
25	b	620	SQD	C13-C14-C15-C16
32	T	101	LMT	C7-C8-C9-C10
33	D	408[A]	LHG	C32-C33-C34-C35
33	b	629[A]	LHG	C14-C15-C16-C17
33	b	629[B]	LHG	C14-C15-C16-C17
40	v	201	HEC	C2C-C3C-CAC-CBC
34	C	501	LMG	C10-C11-C12-C13
34	c	501	LMG	C10-C11-C12-C13
32	B	627	LMT	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	m	103	LMT	C7-C8-C9-C10
33	D	407[B]	LHG	C16-C17-C18-C19
33	E	101[B]	LHG	C24-C25-C26-C27
33	L	101[A]	LHG	C12-C13-C14-C15
33	L	101[B]	LHG	C17-C18-C19-C20
33	L	101[B]	LHG	C25-C26-C27-C28
33	d	414[A]	LHG	C29-C30-C31-C32
34	C	501	LMG	C17-C18-C19-C20
36	C	517[B]	DGD	C5B-C6B-C7B-C8B
36	c	518[B]	DGD	CAA-CBA-CCA-CDA
36	c	519	DGD	CBA-CCA-CDA-CEA
36	c	519	DGD	CBB-CCB-CDB-CEB
36	h	102	DGD	C7B-C8B-C9B-CAB
40	V	201	HEC	C4C-C3C-CAC-CBC
23	b	602	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
23	d	403[A]	CLA	C16-C17-C18-C20
25	A	411	SQD	O5-C1-O6-C44
23	A	405[A]	CLA	C15-C16-C17-C18
23	B	615	CLA	C5-C6-C7-C8
33	b	629[A]	LHG	C16-C17-C18-C19
34	C	501	LMG	C12-C13-C14-C15
34	C	501	LMG	C36-C37-C38-C39
34	D	412	LMG	C30-C31-C32-C33
36	C	517[B]	DGD	C4B-C5B-C6B-C7B
25	A	411	SQD	C17-C18-C19-C20
32	B	629	LMT	C11-C10-C9-C8
34	C	501	LMG	C19-C20-C21-C22
34	C	520	LMG	C34-C35-C36-C37
34	C	521	LMG	C18-C19-C20-C21
34	c	520	LMG	C31-C32-C33-C34
34	c	501	LMG	C4-C5-C6-O5
23	B	614	CLA	C5-C6-C7-C8
25	X	101	SQD	C29-C30-C31-C32
34	d	412	LMG	C29-C30-C31-C32
33	d	408[A]	LHG	C27-C28-C29-C30
34	C	520	LMG	C16-C17-C18-C19
36	C	517[A]	DGD	C9A-CAA-CBA-CCA
23	c	512	CLA	O1D-CGD-O2D-CED
23	C	507	CLA	C3A-C2A-CAA-CBA
32	a	416	LMT	C1-C2-C3-C4
32	F	101	LMT	C2-C1-O1'-C1'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	e	101	LMT	C2-C1-O1'-C1'
32	m	103	LMT	C2-C1-O1'-C1'
25	b	620	SQD	C27-C28-C29-C30
33	E	101[A]	LHG	C24-C25-C26-C27
36	H	102	DGD	CCB-CDB-CEB-CFB
36	h	102	DGD	C9A-CAA-CBA-CCA
23	b	615	CLA	C16-C17-C18-C20
33	L	101[A]	LHG	C25-C26-C27-C28
31	a	415[B]	PHO	C2C-C3C-CAC-CBC
33	b	629[A]	LHG	C27-C28-C29-C30
34	m	101	LMG	C39-C40-C41-C42
36	c	517[B]	DGD	C5A-C6A-C7A-C8A
36	c	517[A]	DGD	O6D-C5D-C6D-O5D
33	E	101[B]	LHG	C23-C24-C25-C26
32	A	419	LMT	C1-C2-C3-C4
23	D	404	CLA	C4-C3-C5-C6
31	a	406[B]	PHO	C4-C3-C5-C6
23	c	506	CLA	C2-C3-C5-C6
28	A	413[A]	PL9	C12-C11-C9-C8
28	D	406[A]	PL9	C13-C14-C16-C17
25	b	620	SQD	C31-C32-C33-C34
33	d	414[B]	LHG	C32-C33-C34-C35
34	c	520	LMG	O6-C5-C6-O5
26	A	410	GOL	O1-C1-C2-O2
26	D	402	GOL	O1-C1-C2-O2
26	D	413	GOL	O2-C2-C3-O3
26	O	302	GOL	O1-C1-C2-O2
26	V	203[A]	GOL	O2-C2-C3-O3
26	b	624	GOL	O2-C2-C3-O3
26	c	527	GOL	O2-C2-C3-O3
26	o	304	GOL	O1-C1-C2-O2
32	A	419	LMT	C5-C6-C7-C8
33	d	414[A]	LHG	C24-C25-C26-C27
34	c	501	LMG	C34-C35-C36-C37
23	B	603	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
32	b	627	LMT	C3-C4-C5-C6
34	C	501	LMG	C39-C40-C41-C42
33	E	101[A]	LHG	O2-C2-C3-O3
32	b	621	LMT	C3'-C4'-O1B-C1B
25	b	620	SQD	C26-C27-C28-C29
33	D	407[A]	LHG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	414[B]	LHG	C25-C26-C27-C28
23	c	512	CLA	C3-C5-C6-C7
36	C	517[B]	DGD	C4D-C5D-C6D-O5D
25	a	411	SQD	C31-C32-C33-C34
32	B	626	LMT	C5-C6-C7-C8
32	B	626	LMT	C7-C8-C9-C10
33	L	101[B]	LHG	C27-C28-C29-C30
34	m	101	LMG	C35-C36-C37-C38
34	c	520	LMG	C34-C35-C36-C37
23	B	616	CLA	C2-C1-O2A-CGA
36	C	517[A]	DGD	O6D-C5D-C6D-O5D
32	B	626	LMT	C4B-C5B-C6B-O6B
25	X	101	SQD	C24-C25-C26-C27
25	b	620	SQD	C14-C15-C16-C17
33	d	408[B]	LHG	C25-C26-C27-C28
23	C	511	CLA	C10-C11-C12-C13
32	b	621	LMT	C4'-C5'-C6'-O6'
32	B	627	LMT	C5-C6-C7-C8
32	b	627	LMT	C5-C6-C7-C8
33	A	418[A]	LHG	C34-C35-C36-C37
33	L	101[B]	LHG	C15-C16-C17-C18
36	C	517[B]	DGD	C8A-C9A-CAA-CBA
24	H	101	BCR	C23-C24-C25-C26
24	b	617	BCR	C1-C6-C7-C8
24	b	617	BCR	C5-C6-C7-C8
36	c	517[A]	DGD	C7A-C8A-C9A-CAA
23	B	615	CLA	C10-C11-C12-C13
33	d	408[A]	LHG	C29-C30-C31-C32
33	d	407[A]	LHG	C34-C35-C36-C37
36	c	518[A]	DGD	C6A-C7A-C8A-C9A
34	C	521	LMG	C13-C14-C15-C16
34	c	501	LMG	C29-C30-C31-C32
36	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	C	507	CLA	C4-C3-C5-C6
28	A	413[A]	PL9	C45-C44-C46-C47
28	a	413[A]	PL9	C12-C11-C9-C10
23	A	407	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	506	CLA	C2-C3-C5-C6
23	C	512	CLA	C11-C12-C13-C15
23	D	404	CLA	C11-C10-C8-C7
23	a	405[A]	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
28	A	413[B]	PL9	C12-C11-C9-C8
28	d	406[A]	PL9	C13-C14-C16-C17
31	a	406[B]	PHO	C2-C3-C5-C6
32	A	419	LMT	C3'-C4'-O1B-C1B
32	B	626	LMT	C3'-C4'-O1B-C1B
33	A	418[A]	LHG	C12-C13-C14-C15
36	c	518[A]	DGD	C4A-C5A-C6A-C7A
23	C	504	CLA	CBD-CGD-O2D-CED
23	a	407	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C19
23	c	513	CLA	CBA-CGA-O2A-C1
33	D	408[B]	LHG	C15-C16-C17-C18
34	c	520	LMG	C33-C34-C35-C36
32	B	629	LMT	C4-C5-C6-C7
33	d	408[B]	LHG	C34-C35-C36-C37
35	b	622	HTG	C1'-C2'-C3'-C4'
33	A	418[B]	LHG	C12-C13-C14-C15
33	d	408[A]	LHG	C25-C26-C27-C28
33	D	408[A]	LHG	C13-C14-C15-C16
34	C	501	LMG	C20-C21-C22-C23
34	m	101	LMG	C38-C39-C40-C41
36	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	b	607	CLA	C3-C5-C6-C7
25	f	102	SQD	C25-C26-C27-C28
34	m	101	LMG	C14-C15-C16-C17
36	C	519	DGD	C2B-C3B-C4B-C5B
23	B	610	CLA	C16-C17-C18-C19
36	C	518[A]	DGD	O6E-C1E-O5D-C6D
36	C	518[B]	DGD	O6E-C1E-O5D-C6D
36	c	517[B]	DGD	O6E-C1E-O5D-C6D
23	A	405[B]	CLA	C15-C16-C17-C18
23	C	513	CLA	C10-C11-C12-C13
32	e	101	LMT	C1-C2-C3-C4
33	D	408[A]	LHG	C15-C16-C17-C18
34	C	520	LMG	C11-C12-C13-C14
34	C	521	LMG	C17-C18-C19-C20
35	b	622	HTG	C3'-C4'-C5'-C6'
34	m	101	LMG	C11-C10-O7-C8
36	c	517[B]	DGD	C7A-C8A-C9A-CAA
23	A	406[B]	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	CBD-CGD-O2D-CED
32	a	416	LMT	C3-C4-C5-C6
34	C	520	LMG	C37-C38-C39-C40
23	C	510	CLA	O1D-CGD-O2D-CED
34	m	101	LMG	O9-C10-O7-C8
36	c	518[B]	DGD	C2B-C3B-C4B-C5B
25	A	409[A]	SQD	O6-C44-C45-O47
25	A	409[B]	SQD	O6-C44-C45-O47
25	X	101	SQD	O47-C45-C46-O48
32	B	629	LMT	O1'-C1-C2-C3
33	d	408[A]	LHG	C34-C35-C36-C37
33	d	414[A]	LHG	C25-C26-C27-C28
33	d	414[B]	LHG	C24-C25-C26-C27
36	h	102	DGD	CAB-CBB-CCB-CDB
36	c	517[B]	DGD	CAA-CBA-CCA-CDA
34	Z	101	LMG	O6-C5-C6-O5
23	b	605	CLA	C5-C6-C7-C8
23	C	506	CLA	C4-C3-C5-C6
23	D	404	CLA	C2-C3-C5-C6
28	A	413[B]	PL9	C28-C29-C31-C32
28	a	413[B]	PL9	C4-C3-C7-C8
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
36	c	518[A]	DGD	C2B-C3B-C4B-C5B
36	c	518[B]	DGD	C4A-C5A-C6A-C7A
36	c	518[B]	DGD	C6A-C7A-C8A-C9A
25	b	620	SQD	C24-C23-O48-C46
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	608	CLA	C13-C15-C16-C17
23	b	605	CLA	C8-C10-C11-C12
24	D	405	BCR	C21-C22-C23-C24
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	507	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
32	M	101	LMT	O5'-C5'-C6'-O6'
23	B	610	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C16-C17-C18-C20
25	a	409[A]	SQD	C9-C10-C11-C12
25	a	409[B]	SQD	C9-C10-C11-C12
33	A	418[A]	LHG	C26-C27-C28-C29
33	D	407[B]	LHG	C12-C13-C14-C15
33	D	407[A]	LHG	C4-O6-P-O3
32	B	627	LMT	C6-C7-C8-C9
36	h	102	DGD	C9B-CAB-CBB-CCB
40	V	201	HEC	C2B-C3B-CAB-CBB
34	B	620	LMG	C37-C38-C39-C40
34	z	101	LMG	C20-C21-C22-C23
23	c	507	CLA	C15-C16-C17-C18
33	D	407[B]	LHG	O6-C4-C5-C6
34	D	412	LMG	C12-C13-C14-C15
23	C	514	CLA	O1D-CGD-O2D-CED
32	t	101	LMT	C7-C8-C9-C10
33	d	408[A]	LHG	C28-C29-C30-C31
23	b	601	CLA	C8-C10-C11-C12
23	B	608	CLA	C16-C17-C18-C20
32	e	101	LMT	C4B-C5B-C6B-O6B
34	z	101	LMG	C14-C15-C16-C17
36	C	517[A]	DGD	C8A-C9A-CAA-CBA
36	c	517[A]	DGD	C4D-C5D-C6D-O5D
33	D	408[B]	LHG	C29-C30-C31-C32
36	H	102	DGD	CAB-CBB-CCB-CDB
32	e	101	LMT	C9-C10-C11-C12
33	A	418[B]	LHG	C18-C19-C20-C21
33	D	407[A]	LHG	C10-C11-C12-C13
33	D	407[B]	LHG	C11-C10-C9-C8
23	d	403[A]	CLA	C16-C17-C18-C19
23	d	403[B]	CLA	C16-C17-C18-C20
32	a	416	LMT	O5'-C5'-C6'-O6'
23	b	605	CLA	C3-C5-C6-C7
25	A	411	SQD	O6-C44-C45-C46
25	a	409[A]	SQD	O6-C44-C45-C46
25	a	411	SQD	O6-C44-C45-C46
25	b	620	SQD	C44-C45-C46-O48
25	f	102	SQD	O6-C44-C45-C46
25	f	102	SQD	C44-C45-C46-O48
33	D	407[B]	LHG	C26-C27-C28-C29
33	E	101[A]	LHG	C4-C5-C6-O8
33	E	101[B]	LHG	C4-C5-C6-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	c	501	LMG	C7-C8-C9-O8
36	C	518[A]	DGD	CDA-CEA-CFA-CGA
36	c	517[B]	DGD	O6E-C5E-C6E-O5E
23	c	507	CLA	C10-C11-C12-C13
34	C	520	LMG	C17-C18-C19-C20
34	C	521	LMG	C20-C21-C22-C23
34	z	101	LMG	C19-C20-C21-C22
36	H	102	DGD	C9B-CAB-CBB-CCB
36	C	518[A]	DGD	C2G-C3G-O3G-C1D
36	C	518[B]	DGD	C5D-C6D-O5D-C1E
36	c	518[A]	DGD	C2G-C3G-O3G-C1D
36	c	518[A]	DGD	C5D-C6D-O5D-C1E
36	c	518[B]	DGD	C5D-C6D-O5D-C1E
25	A	409[B]	SQD	C11-C10-C9-C8
32	a	416	LMT	C9-C10-C11-C12
34	Z	101	LMG	C11-C12-C13-C14
25	l	101	SQD	C34-C35-C36-C37
33	D	408[B]	LHG	C13-C14-C15-C16
33	b	629[A]	LHG	C9-C10-C11-C12
23	c	502	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
25	A	411	SQD	C26-C27-C28-C29
33	A	418[B]	LHG	C26-C27-C28-C29
33	D	408[A]	LHG	C29-C30-C31-C32
34	m	101	LMG	C37-C38-C39-C40
28	A	413[B]	PL9	C39-C41-C42-C43
33	d	414[A]	LHG	C33-C34-C35-C36
36	C	518[B]	DGD	CDA-CEA-CFA-CGA
26	B	622	GOL	O1-C1-C2-O2
26	a	410	GOL	O2-C2-C3-O3
26	o	303	GOL	O2-C2-C3-O3
26	o	304	GOL	O2-C2-C3-O3
25	A	409[B]	SQD	C12-C13-C14-C15
33	b	629[B]	LHG	C9-C10-C11-C12
23	c	513	CLA	C10-C11-C12-C13
35	b	623	HTG	O5-C5-C6-O6
25	A	411	SQD	C27-C28-C29-C30
32	M	101	LMT	C2-C3-C4-C5
23	b	601	CLA	C13-C15-C16-C17
34	d	412	LMG	O6-C5-C6-O5
36	C	517[A]	DGD	O6E-C5E-C6E-O5E
36	C	517[B]	DGD	O6E-C5E-C6E-O5E

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	c	517[A]	DGD	O6E-C5E-C6E-O5E
28	a	413[B]	PL9	C12-C11-C9-C10
23	B	608	CLA	C16-C17-C18-C19
33	D	408[B]	LHG	C24-C23-O8-C6
35	o	301	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	CDB-CEB-CFB-CGB
23	C	507	CLA	C5-C6-C7-C8
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
25	b	620	SQD	C46-C45-O47-C7
25	l	101	SQD	C46-C45-O47-C7
34	D	412	LMG	O6-C5-C6-O5
23	b	601	CLA	C2-C1-O2A-CGA
25	a	409[A]	SQD	C12-C13-C14-C15
33	D	407[B]	LHG	C34-C35-C36-C37
32	a	416	LMT	C2-C3-C4-C5
23	B	601	CLA	CBA-CGA-O2A-C1
36	c	517[A]	DGD	C2A-C1A-O1G-C1G
36	c	519	DGD	C2A-C1A-O1G-C1G
33	D	408[B]	LHG	O10-C23-O8-C6
25	X	101	SQD	C34-C35-C36-C37
32	F	101	LMT	C6-C7-C8-C9
32	b	627	LMT	O1'-C1-C2-C3
33	D	408[A]	LHG	C17-C18-C19-C20
34	B	620	LMG	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
25	A	409[A]	SQD	C11-C10-C9-C8
32	F	101	LMT	C4-C5-C6-C7
33	A	418[A]	LHG	O2-C2-C3-O3
23	B	610	CLA	C13-C15-C16-C17
33	E	101[A]	LHG	C25-C26-C27-C28
33	d	408[A]	LHG	C33-C34-C35-C36
33	E	101[A]	LHG	C13-C14-C15-C16
34	D	412	LMG	C36-C37-C38-C39
23	A	404[A]	CLA	C13-C15-C16-C17
23	c	513	CLA	O1A-CGA-O2A-C1
25	b	620	SQD	O10-C23-O48-C46
36	C	519	DGD	CDB-CEB-CFB-CGB
34	c	520	LMG	C10-C11-C12-C13
23	C	511	CLA	C4-C3-C5-C6
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
23	C	506	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	D	404	CLA	C12-C13-C15-C16
23	a	407	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	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	c	506	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	c	511	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
28	D	406[B]	PL9	C13-C14-C16-C17
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	510	CLA	C6-C7-C8-C9
23	C	511	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
23	D	404	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
34	c	521	LMG	C29-C28-O8-C9
23	A	404[B]	CLA	C13-C15-C16-C17
23	B	612	CLA	C10-C11-C12-C13
23	c	513	CLA	C13-C15-C16-C17
33	A	418[B]	LHG	C32-C33-C34-C35
31	D	401[B]	PHO	C2C-C3C-CAC-CBC
23	d	403[B]	CLA	C16-C17-C18-C19
26	l	103[A]	GOL	O1-C1-C2-C3
33	A	418[B]	LHG	C1-C2-C3-O3
33	d	407[B]	LHG	C25-C26-C27-C28
23	C	511	CLA	CBA-CGA-O2A-C1
23	d	404	CLA	CBA-CGA-O2A-C1
33	D	407[B]	LHG	C13-C14-C15-C16
34	c	501	LMG	C35-C36-C37-C38
33	a	419[A]	LHG	C23-C24-C25-C26
23	B	603	CLA	C13-C15-C16-C17
23	b	604	CLA	C13-C15-C16-C17
23	c	510	CLA	C8-C10-C11-C12
25	a	409[B]	SQD	C12-C13-C14-C15
32	b	627	LMT	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
40	v	201	HEC	C2B-C3B-CAB-CBB
23	a	405[A]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
34	C	521	LMG	C4-C5-C6-O5
23	B	601	CLA	C15-C16-C17-C18
23	C	503	CLA	C13-C15-C16-C17
32	B	626	LMT	C1-C2-C3-C4
28	A	413[A]	PL9	C39-C41-C42-C43
23	C	513	CLA	CBA-CGA-O2A-C1
23	c	514	CLA	C4-C3-C5-C6
28	D	406[A]	PL9	C45-C44-C46-C47
28	d	406[B]	PL9	C45-C44-C46-C47
23	C	511	CLA	C2-C3-C5-C6
28	d	406[B]	PL9	C13-C14-C16-C17
28	d	406[B]	PL9	C28-C29-C31-C32
36	c	518[A]	DGD	CBB-CCB-CDB-CEB
23	a	404[B]	CLA	C2C-C3C-CAC-CBC
25	A	411	SQD	C24-C23-O48-C46
33	d	408[B]	LHG	C24-C23-O8-C6
33	a	419[B]	LHG	C23-C24-C25-C26
34	c	520	LMG	C28-C29-C30-C31
36	C	517[A]	DGD	CCA-CDA-CEA-CFA
23	c	507	CLA	C3A-C2A-CAA-CBA
32	B	627	LMT	C3-C4-C5-C6
33	a	419[A]	LHG	C10-C11-C12-C13
32	b	627	LMT	C2-C1-O1'-C1'
36	C	517[B]	DGD	C7A-C8A-C9A-CAA
40	v	201	HEC	C4C-C3C-CAC-CBC
23	b	608	CLA	C13-C15-C16-C17
36	C	518[B]	DGD	C7A-C8A-C9A-CAA
23	b	606	CLA	C16-C17-C18-C19
23	C	503	CLA	C15-C16-C17-C18
25	A	409[A]	SQD	O6-C44-C45-C46
25	A	409[B]	SQD	O6-C44-C45-C46
33	a	419[A]	LHG	C4-C5-C6-O8
33	a	419[B]	LHG	C4-C5-C6-O8
33	L	101[A]	LHG	C27-C28-C29-C30
33	d	408[B]	LHG	C9-C10-C11-C12
36	C	517[A]	DGD	C1B-C2B-C3B-C4B
36	c	519	DGD	O1A-C1A-O1G-C1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	620	SQD	C11-C10-C9-C8
23	b	616	CLA	C5-C6-C7-C8
33	L	101[B]	LHG	C26-C27-C28-C29
36	H	102	DGD	C7A-C8A-C9A-CAA
23	B	601	CLA	O1A-CGA-O2A-C1
36	c	517[A]	DGD	O1A-C1A-O1G-C1G
28	D	406[A]	PL9	C15-C14-C16-C17
36	c	517[B]	DGD	C2A-C1A-O1G-C1G
28	D	406[A]	PL9	C43-C44-C46-C47
36	C	517[A]	DGD	C4D-C5D-C6D-O5D
36	C	517[A]	DGD	C7A-C8A-C9A-CAA
33	d	414[A]	LHG	C3-O3-P-O6
26	D	413	GOL	O1-C1-C2-O2
26	O	303	GOL	O1-C1-C2-O2
26	v	202[A]	GOL	O1-C1-C2-O2
33	L	101[B]	LHG	C10-C11-C12-C13
36	C	517[A]	DGD	C3B-C4B-C5B-C6B
25	a	409[B]	SQD	C34-C35-C36-C37
33	d	414[B]	LHG	C33-C34-C35-C36
35	c	522	HTG	C4'-C5'-C6'-C7'
23	d	404	CLA	O1A-CGA-O2A-C1
23	A	406[A]	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C20
34	C	521	LMG	C38-C39-C40-C41
36	c	517[B]	DGD	C7B-C8B-C9B-CAB
23	a	405[A]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
36	c	518[B]	DGD	C9B-CAB-CBB-CCB
23	d	402[B]	CLA	C15-C16-C17-C18
34	Z	101	LMG	C19-C20-C21-C22
25	a	409[A]	SQD	O6-C44-C45-O47
25	a	409[B]	SQD	O6-C44-C45-O47
25	b	620	SQD	O47-C45-C46-O48
34	d	412	LMG	C10-C11-C12-C13
33	b	629[B]	LHG	C10-C11-C12-C13
36	c	517[A]	DGD	O6E-C1E-O5D-C6D
28	a	413[A]	PL9	C24-C26-C27-C28
33	A	418[A]	LHG	C1-C2-C3-O3
32	B	626	LMT	C9-C10-C11-C12
32	e	101	LMT	C3-C4-C5-C6
36	C	519	DGD	C8A-C9A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	C	519	DGD	CAB-CBB-CCB-CDB
23	A	407	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
32	a	416	LMT	C4'-C5'-C6'-O6'
23	B	610	CLA	C11-C12-C13-C14
23	B	614	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
36	C	519	DGD	C6A-C7A-C8A-C9A
34	c	521	LMG	O10-C28-O8-C9
33	D	408[A]	LHG	C27-C28-C29-C30
33	b	629[A]	LHG	C34-C35-C36-C37
23	C	502	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C16-C17-C18-C19
24	B	617	BCR	C1-C6-C7-C8
24	B	617	BCR	C5-C6-C7-C8
24	D	405	BCR	C23-C24-C25-C26
24	D	405	BCR	C23-C24-C25-C30
24	d	405	BCR	C23-C24-C25-C26
24	d	405	BCR	C23-C24-C25-C30
24	h	101	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C30
23	c	508	CLA	C8-C10-C11-C12
32	b	621	LMT	C11-C10-C9-C8
33	d	408[B]	LHG	C28-C29-C30-C31
34	C	501	LMG	C18-C19-C20-C21
33	E	101[B]	LHG	C13-C14-C15-C16
23	B	605	CLA	C5-C6-C7-C8
23	c	510	CLA	C13-C15-C16-C17
33	L	101[A]	LHG	C11-C10-C9-C8
36	C	519	DGD	CAA-CBA-CCA-CDA
33	E	101[B]	LHG	C25-C26-C27-C28
25	A	409[A]	SQD	C18-C19-C20-C21
33	a	419[A]	LHG	C7-C8-C9-C10
34	B	620	LMG	C14-C15-C16-C17
33	D	408[B]	LHG	C17-C18-C19-C20
36	C	518[A]	DGD	C5B-C6B-C7B-C8B
33	b	629[A]	LHG	C13-C14-C15-C16
23	c	510	CLA	C10-C11-C12-C13
33	L	101[A]	LHG	O6-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	b	629[B]	LHG	O6-C4-C5-C6
33	A	418[B]	LHG	O2-C2-C3-O3
35	B	623	HTG	C4'-C5'-C6'-C7'
36	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	b	607	CLA	C12-C13-C15-C16
23	c	505	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
23	d	403[B]	CLA	C11-C12-C13-C15
28	a	413[A]	PL9	C12-C11-C9-C8
33	D	407[A]	LHG	C11-C10-C9-C8
36	C	519	DGD	C4A-C5A-C6A-C7A
36	c	517[A]	DGD	CCB-CDB-CEB-CFB
25	a	409[A]	SQD	C27-C28-C29-C30
25	b	620	SQD	C28-C29-C30-C31
33	L	101[A]	LHG	C24-C25-C26-C27
23	c	512	CLA	CBA-CGA-O2A-C1
33	D	408[A]	LHG	C10-C11-C12-C13
33	a	419[B]	LHG	C10-C11-C12-C13
33	d	407[A]	LHG	C13-C14-C15-C16
23	C	504	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	O1A-CGA-O2A-C1
23	B	601	CLA	C2A-CAA-CBA-CGA
36	C	518[A]	DGD	C7A-C8A-C9A-CAA
34	d	412	LMG	C11-C12-C13-C14
34	d	412	LMG	C35-C36-C37-C38
35	c	522	HTG	C2'-C1'-S1-C1
34	c	501	LMG	C21-C22-C23-C24
23	b	601	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
36	C	517[B]	DGD	CCA-CDA-CEA-CFA
23	C	508	CLA	C13-C15-C16-C17
23	A	404[B]	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	C	502	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	504	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
31	a	406[A]	PHO	CAD-CBD-CGD-O2D
31	a	406[B]	PHO	CAD-CBD-CGD-O2D
31	a	415[B]	PHO	CAD-CBD-CGD-O2D
38	f	101	HEM	C2B-C3B-CAB-CBB
33	D	408[B]	LHG	C10-C11-C12-C13
33	b	629[B]	LHG	C13-C14-C15-C16
36	C	519	DGD	CDA-CEA-CFA-CGA
28	d	406[A]	PL9	C45-C44-C46-C47
25	a	409[A]	SQD	C34-C35-C36-C37
36	C	517[B]	DGD	C6A-C7A-C8A-C9A
36	c	518[A]	DGD	O6E-C1E-O5D-C6D
36	C	518[B]	DGD	C1A-C2A-C3A-C4A
25	a	409[B]	SQD	O6-C44-C45-C46
25	l	101	SQD	C44-C45-C46-O48
33	D	408[B]	LHG	C2-C3-O3-P
23	C	502	CLA	CBD-CGD-O2D-CED
33	E	101[A]	LHG	O6-C4-C5-O7
33	L	101[A]	LHG	O6-C4-C5-O7
33	b	629[B]	LHG	O6-C4-C5-O7
33	D	408[B]	LHG	C27-C28-C29-C30
34	d	412	LMG	C18-C19-C20-C21
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
25	A	411	SQD	O10-C23-O48-C46
33	d	408[B]	LHG	O10-C23-O8-C6
36	C	517[B]	DGD	C2E-C1E-O5D-C6D
36	c	517[A]	DGD	C2E-C1E-O5D-C6D
36	c	518[A]	DGD	C2E-C1E-O5D-C6D
25	X	101	SQD	C32-C33-C34-C35
33	A	418[A]	LHG	C32-C33-C34-C35
33	A	418[B]	LHG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	f	102	SQD	O47-C45-C46-O48
25	l	101	SQD	O47-C45-C46-O48
33	a	419[A]	LHG	O7-C5-C6-O8
34	c	501	LMG	O7-C8-C9-O8
25	A	409[A]	SQD	C34-C35-C36-C37
23	b	601	CLA	O1A-CGA-O2A-C1
36	c	517[B]	DGD	O1A-C1A-O1G-C1G
25	a	411	SQD	C16-C17-C18-C19
23	A	406[B]	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
26	B	625	GOL	O1-C1-C2-O2
26	a	418	GOL	O2-C2-C3-O3
33	b	629[B]	LHG	C28-C29-C30-C31
33	d	407[A]	LHG	C11-C10-C9-C8
33	d	408[A]	LHG	C9-C10-C11-C12
23	B	613	CLA	C15-C16-C17-C18
34	C	520	LMG	C31-C32-C33-C34
28	D	406[B]	PL9	C28-C29-C31-C32
23	B	610	CLA	C14-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C14
23	b	616	CLA	O1A-CGA-O2A-C1
23	C	511	CLA	C8-C10-C11-C12
23	b	615	CLA	C5-C6-C7-C8
24	K	102	BCR	C7-C8-C9-C34
26	l	103[B]	GOL	O1-C1-C2-C3
23	b	604	CLA	C15-C16-C17-C18
24	K	102	BCR	C7-C8-C9-C10
24	c	516	BCR	C7-C8-C9-C10
32	b	627	LMT	C1-C2-C3-C4
33	d	414[A]	LHG	C18-C19-C20-C21
36	h	102	DGD	CDA-CEA-CFA-CGA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	d	402[A]	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C13-C15-C16-C17
33	d	407[A]	LHG	C16-C17-C18-C19
23	C	510	CLA	C2-C1-O2A-CGA
33	d	407[B]	LHG	C13-C14-C15-C16
34	z	101	LMG	C10-C11-C12-C13
25	a	409[A]	SQD	C35-C36-C37-C38
34	C	521	LMG	C35-C36-C37-C38
36	C	519	DGD	C7B-C8B-C9B-CAB
36	c	518[B]	DGD	C5A-C6A-C7A-C8A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	D	408[A]	LHG	C2-C3-O3-P
33	d	408[B]	LHG	C2-C3-O3-P
23	C	507	CLA	C2-C3-C5-C6
28	a	413[B]	PL9	C23-C24-C26-C27
23	a	405[B]	CLA	C4B-C3B-CAB-CBB
33	D	407[A]	LHG	C4-O6-P-O5
33	E	101[A]	LHG	C4-O6-P-O5
33	E	101[B]	LHG	C4-O6-P-O5
33	a	419[A]	LHG	C4-O6-P-O4
33	a	419[B]	LHG	C4-O6-P-O4
23	C	503	CLA	C16-C17-C18-C19
34	c	520	LMG	C30-C31-C32-C33
36	C	517[B]	DGD	O6E-C1E-O5D-C6D
23	B	611	CLA	C8-C10-C11-C12
33	E	101[A]	LHG	O6-C4-C5-C6
33	L	101[B]	LHG	O6-C4-C5-C6
33	L	101[B]	LHG	C11-C12-C13-C14
34	Z	101	LMG	C29-C28-O8-C9
23	b	601	CLA	CAA-CBA-CGA-O2A
34	B	620	LMG	O8-C28-C29-C30
33	d	408[B]	LHG	C11-C10-C9-C8
23	B	607	CLA	C3-C5-C6-C7
32	m	103	LMT	O5'-C5'-C6'-O6'
33	L	101[A]	LHG	C26-C27-C28-C29
34	B	620	LMG	C18-C19-C20-C21
25	l	101	SQD	C33-C34-C35-C36
36	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
36	C	517[A]	DGD	C6A-C7A-C8A-C9A
23	b	604	CLA	C10-C11-C12-C13
31	A	416[B]	PHO	C2C-C3C-CAC-CBC
34	z	101	LMG	C13-C14-C15-C16
33	L	101[B]	LHG	C24-C25-C26-C27
23	A	406[A]	CLA	C12-C13-C15-C16
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	508	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	d	403[A]	CLA	C11-C12-C13-C15
33	D	407[B]	LHG	O6-C4-C5-O7
25	A	409[A]	SQD	C13-C14-C15-C16
33	E	101[B]	LHG	C11-C10-C9-C8
36	c	519	DGD	CDA-CEA-CFA-CGA
33	D	407[A]	LHG	C34-C35-C36-C37
36	C	517[B]	DGD	C3B-C4B-C5B-C6B
25	a	409[B]	SQD	C35-C36-C37-C38
36	c	518[A]	DGD	C5A-C6A-C7A-C8A
34	c	501	LMG	C14-C15-C16-C17
32	B	629	LMT	C2-C3-C4-C5
33	A	418[B]	LHG	C29-C30-C31-C32
34	c	520	LMG	C32-C33-C34-C35
36	c	517[B]	DGD	C2E-C1E-O5D-C6D
33	E	101[A]	LHG	O7-C5-C6-O8
33	a	419[B]	LHG	O7-C5-C6-O8
23	a	404[B]	CLA	C4C-C3C-CAC-CBC
33	d	407[B]	LHG	C11-C10-C9-C8
33	d	408[A]	LHG	C32-C33-C34-C35
36	C	518[A]	DGD	C8A-C9A-CAA-CBA
36	H	102	DGD	C8A-C9A-CAA-CBA
33	d	414[B]	LHG	C29-C30-C31-C32
36	h	102	DGD	C3B-C4B-C5B-C6B
36	C	518[A]	DGD	C5D-C6D-O5D-C1E
36	C	518[B]	DGD	C2G-C3G-O3G-C1D
36	H	102	DGD	O2G-C1B-C2B-C3B
23	C	511	CLA	C13-C15-C16-C17
23	b	602	CLA	C10-C11-C12-C13
23	b	612	CLA	C10-C11-C12-C13
25	A	411	SQD	C30-C31-C32-C33
35	b	625	HTG	C4-C5-C6-O6
33	d	408[A]	LHG	C2-C3-O3-P
32	T	101	LMT	C3-C4-C5-C6
34	C	520	LMG	C30-C31-C32-C33
33	d	407[B]	LHG	C9-C10-C11-C12
34	C	501	LMG	C11-C12-C13-C14
36	C	518[B]	DGD	C5B-C6B-C7B-C8B
33	d	414[A]	LHG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C15-C16-C17-C18
23	B	603	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C12-C13-C14
23	B	611	CLA	C14-C13-C15-C16
23	C	514	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
34	C	520	LMG	C29-C30-C31-C32
36	C	519	DGD	C7A-C8A-C9A-CAA
36	c	517[B]	DGD	CBA-CCA-CDA-CEA
33	D	407[A]	LHG	C26-C27-C28-C29
32	m	103	LMT	C11-C10-C9-C8
26	a	417	GOL	O1-C1-C2-O2
33	A	418[B]	LHG	O1-C1-C2-O2
36	C	518[A]	DGD	C7B-C8B-C9B-CAB
33	d	414[A]	LHG	C11-C12-C13-C14
23	B	613	CLA	C13-C15-C16-C17
23	C	505	CLA	C2B-C3B-CAB-CBB
23	D	403[A]	CLA	C2B-C3B-CAB-CBB
23	D	403[B]	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
25	a	411	SQD	C18-C19-C20-C21
36	c	517[B]	DGD	CCB-CDB-CEB-CFB
28	a	413[A]	PL9	C43-C44-C46-C47
28	d	406[B]	PL9	C43-C44-C46-C47
33	L	101[A]	LHG	C23-C24-C25-C26
33	D	407[A]	LHG	C13-C14-C15-C16
33	d	414[B]	LHG	C17-C18-C19-C20
32	A	417	LMT	O5B-C5B-C6B-O6B
34	Z	101	LMG	C21-C22-C23-C24
23	D	404	CLA	C8-C10-C11-C12
33	b	629[A]	LHG	C28-C29-C30-C31
34	m	101	LMG	C30-C31-C32-C33
23	B	601	CLA	CAA-CBA-CGA-O2A
33	D	407[B]	LHG	C10-C11-C12-C13
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
36	c	519	DGD	O6D-C5D-C6D-O5D
36	H	102	DGD	CCA-CDA-CEA-CFA
25	A	411	SQD	C15-C16-C17-C18
23	c	511	CLA	O1A-CGA-O2A-C1
32	m	103	LMT	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	L	101[B]	LHG	O6-C4-C5-O7
28	A	413[A]	PL9	C28-C29-C31-C32
28	a	413[B]	PL9	C12-C11-C9-C8
36	C	519	DGD	C9A-CAA-CBA-CCA
32	t	101	LMT	C2-C3-C4-C5
33	d	408[A]	LHG	C10-C11-C12-C13
34	D	412	LMG	C18-C19-C20-C21
34	m	101	LMG	C2-C1-O1-C7
36	c	518[B]	DGD	C2E-C1E-O5D-C6D
33	E	101[B]	LHG	O7-C5-C6-O8
33	d	414[B]	LHG	C3-O3-P-O6
25	A	409[A]	SQD	C16-C17-C18-C19
25	X	101	SQD	C44-C45-C46-O48
23	B	603	CLA	C11-C12-C13-C15
23	B	605	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C10
23	C	513	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C12-C13-C15
25	a	411	SQD	C15-C16-C17-C18
23	d	402[A]	CLA	C4C-C3C-CAC-CBC
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C12-C13-C14
23	a	407	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
23	d	403[A]	CLA	C11-C12-C13-C14
33	D	407[A]	LHG	C28-C29-C30-C31
31	a	406[A]	PHO	C2C-C3C-CAC-CBC
23	c	510	CLA	C15-C16-C17-C18
32	b	621	LMT	C7-C8-C9-C10
23	C	503	CLA	C16-C17-C18-C20
33	A	418[A]	LHG	O1-C1-C2-C3
25	a	411	SQD	C26-C27-C28-C29
38	f	101	HEM	CAD-CBD-CGD-O1D
23	D	404	CLA	C15-C16-C17-C18
23	b	607	CLA	C8-C10-C11-C12
23	d	402[A]	CLA	C15-C16-C17-C18
33	d	408[B]	LHG	C33-C34-C35-C36
23	c	511	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	d	406[B]	PL9	C18-C19-C21-C22
23	c	511	CLA	CBA-CGA-O2A-C1
38	F	102	HEM	CAD-CBD-CGD-O1D
25	a	409[A]	SQD	C11-C12-C13-C14
33	D	407[B]	LHG	C28-C29-C30-C31
36	C	519	DGD	O6D-C5D-C6D-O5D
33	D	408[A]	LHG	O10-C23-O8-C6
33	D	408[A]	LHG	C24-C23-O8-C6
36	C	517[B]	DGD	C1B-C2B-C3B-C4B
23	B	602	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C4B-C3B-CAB-CBB
23	D	403[A]	CLA	C4B-C3B-CAB-CBB
23	D	403[B]	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C2A-CAA-CBA-CGA
32	M	101	LMT	O5'-C1'-O1'-C1
36	c	518[B]	DGD	O6E-C1E-O5D-C6D
25	b	620	SQD	C33-C34-C35-C36
34	c	501	LMG	C38-C39-C40-C41
32	F	101	LMT	C2-C3-C4-C5
23	b	611	CLA	C3-C5-C6-C7
23	B	614	CLA	C4-C3-C5-C6
31	a	406[A]	PHO	C4-C3-C5-C6
40	V	201	HEC	C4B-C3B-CAB-CBB
31	a	406[A]	PHO	C2-C3-C5-C6
25	l	101	SQD	C24-C25-C26-C27
33	d	408[B]	LHG	C29-C30-C31-C32
23	C	507	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
32	A	417	LMT	C9-C10-C11-C12
36	c	517[A]	DGD	C4B-C5B-C6B-C7B
34	c	501	LMG	O8-C28-C29-C30
32	t	101	LMT	O1'-C1-C2-C3
36	c	517[B]	DGD	C6B-C7B-C8B-C9B
23	b	608	CLA	C16-C17-C18-C20
25	a	409[B]	SQD	C27-C28-C29-C30
33	b	629[B]	LHG	C17-C18-C19-C20
33	d	407[A]	LHG	C9-C10-C11-C12
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
33	D	407[A]	LHG	C17-C18-C19-C20
40	V	201	HEC	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	601	CLA	C4-C3-C5-C6
33	E	101[B]	LHG	C12-C13-C14-C15
33	a	419[B]	LHG	C24-C25-C26-C27
33	d	408[B]	LHG	C32-C33-C34-C35
28	A	413[B]	PL9	C4-C3-C7-C8
28	a	413[A]	PL9	C4-C3-C7-C8
23	A	407	CLA	C11-C12-C13-C14
23	B	613	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14
23	C	506	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	a	405[A]	CLA	C14-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C9
35	d	411	HTG	S1-C1'-C2'-C3'
33	b	629[A]	LHG	C10-C11-C12-C13
23	b	610	CLA	C13-C15-C16-C17
33	d	414[A]	LHG	C1-C2-C3-O3
36	H	102	DGD	O1G-C1G-C2G-C3G
36	h	102	DGD	O1G-C1G-C2G-C3G
25	a	409[A]	SQD	C10-C11-C12-C13
32	e	101	LMT	C2-C3-C4-C5
33	E	101[A]	LHG	C12-C13-C14-C15
31	D	401[A]	PHO	O2A-C1-C2-C3
31	D	401[B]	PHO	O2A-C1-C2-C3
31	a	406[A]	PHO	O2A-C1-C2-C3
31	A	416[A]	PHO	C2C-C3C-CAC-CBC
34	B	620	LMG	O6-C1-O1-C7
36	c	517[A]	DGD	CBA-CCA-CDA-CEA
32	b	621	LMT	C3-C4-C5-C6
23	b	610	CLA	C3-C5-C6-C7
40	V	201	HEC	CAD-CBD-CGD-O1D
28	a	413[A]	PL9	C45-C44-C46-C47
23	a	405[A]	CLA	C1A-C2A-CAA-CBA
23	B	601	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C10-C8-C7
23	C	503	CLA	C12-C13-C15-C16
23	C	504	CLA	C6-C7-C8-C10
28	a	413[B]	PL9	C43-C44-C46-C47
34	C	521	LMG	C11-C12-C13-C14
23	B	615	CLA	C8-C10-C11-C12
33	A	418[A]	LHG	C29-C30-C31-C32
33	L	101[A]	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	d	412	LMG	C16-C17-C18-C19
36	C	519	DGD	C3B-C4B-C5B-C6B
35	b	622	HTG	O5-C5-C6-O6
23	a	404[B]	CLA	C2A-CAA-CBA-CGA
25	f	102	SQD	C26-C27-C28-C29
25	l	101	SQD	C29-C30-C31-C32
23	c	503	CLA	C16-C17-C18-C19
23	B	606	CLA	C8-C10-C11-C12
38	f	101	HEM	CAD-CBD-CGD-O2D
34	B	620	LMG	C20-C21-C22-C23
28	a	413[B]	PL9	C45-C44-C46-C47
33	a	419[B]	LHG	C7-C8-C9-C10
23	b	601	CLA	C2-C3-C5-C6
23	B	602	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C2B-C3B-CAB-CBB
23	a	407	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
38	F	102	HEM	CAD-CBD-CGD-O2D
23	a	407	CLA	C15-C16-C17-C18
23	B	612	CLA	O1A-CGA-O2A-C1
25	a	409[B]	SQD	C11-C12-C13-C14
36	C	518[B]	DGD	C8B-C9B-CAB-CBB
36	c	519	DGD	C1A-C2A-C3A-C4A
33	A	418[B]	LHG	C11-C12-C13-C14
36	h	102	DGD	CBA-CCA-CDA-CEA
23	B	612	CLA	CBA-CGA-O2A-C1
33	d	414[B]	LHG	C23-C24-C25-C26
32	e	101	LMT	O1'-C1-C2-C3
33	a	419[A]	LHG	C24-C25-C26-C27
33	d	414[A]	LHG	C27-C28-C29-C30
23	A	406[A]	CLA	C16-C17-C18-C19
33	d	414[A]	LHG	C17-C18-C19-C20
23	D	404	CLA	O1A-CGA-O2A-C1
33	A	418[B]	LHG	C17-C18-C19-C20
33	d	407[A]	LHG	C25-C26-C27-C28
23	C	513	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
23	a	404[A]	CLA	C2-C1-O2A-CGA
23	b	610	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C2-C3-C5-C6
28	d	406[A]	PL9	C43-C44-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	B	621	HTG	C4'-C5'-C6'-C7'
33	d	407[B]	LHG	O10-C23-O8-C6
32	e	101	LMT	C2B-C1B-O1B-C4'
23	B	614	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
34	c	521	LMG	C31-C32-C33-C34
25	A	411	SQD	C19-C20-C21-C22
36	C	518[B]	DGD	C8A-C9A-CAA-CBA
36	C	518[B]	DGD	C7B-C8B-C9B-CAB
23	B	605	CLA	CBD-CGD-O2D-CED
24	Y	101	BCR	C23-C24-C25-C30
24	a	408	BCR	C1-C6-C7-C8
24	y	101	BCR	C23-C24-C25-C30
33	d	407[B]	LHG	C24-C23-O8-C6
34	C	520	LMG	C36-C37-C38-C39
35	b	623	HTG	C4'-C5'-C6'-C7'
23	b	616	CLA	C4-C3-C5-C6
28	D	406[B]	PL9	C45-C44-C46-C47
33	d	414[A]	LHG	C9-C10-C11-C12
34	C	501	LMG	C13-C14-C15-C16
36	h	102	DGD	CCA-CDA-CEA-CFA
23	c	514	CLA	C2-C3-C5-C6
28	A	413[A]	PL9	C43-C44-C46-C47
36	c	517[B]	DGD	C5D-C6D-O5D-C1E
25	b	620	SQD	C30-C31-C32-C33
33	A	418[A]	LHG	C17-C18-C19-C20
32	B	629	LMT	C1-C2-C3-C4
36	c	517[A]	DGD	CDB-CEB-CFB-CGB
33	E	101[B]	LHG	O6-C4-C5-O7
32	t	101	LMT	C4'-C5'-C6'-O6'
38	f	101	HEM	CAA-CBA-CGA-O2A
34	z	101	LMG	O7-C10-C11-C12
23	b	603	CLA	C4B-C3B-CAB-CBB
23	B	616	CLA	C16-C17-C18-C20
36	c	518[A]	DGD	C1A-C2A-C3A-C4A
28	D	406[A]	PL9	C35-C34-C36-C37
28	d	406[B]	PL9	C20-C19-C21-C22
23	B	611	CLA	C12-C13-C15-C16
23	b	616	CLA	C2-C3-C5-C6
25	a	411	SQD	C27-C28-C29-C30
33	d	407[B]	LHG	C16-C17-C18-C19
34	d	412	LMG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	Z	101	LMG	C2-C1-O1-C7
33	b	629[A]	LHG	C25-C26-C27-C28
36	H	102	DGD	O1G-C1G-C2G-O2G
25	A	411	SQD	C7-C8-C9-C10
23	C	509	CLA	C13-C15-C16-C17
33	A	418[A]	LHG	O8-C23-C24-C25
33	L	101[B]	LHG	C11-C10-C9-C8
23	D	404	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	C8-C10-C11-C12
23	C	511	CLA	CAA-CBA-CGA-O2A
23	b	604	CLA	C4-C3-C5-C6
28	A	413[A]	PL9	C25-C24-C26-C27
33	A	418[B]	LHG	O8-C23-C24-C25
23	B	601	CLA	C11-C12-C13-C14
23	B	605	CLA	C6-C7-C8-C9
23	B	611	CLA	C11-C12-C13-C14
23	B	614	CLA	C11-C10-C8-C9
23	a	405[A]	CLA	C6-C7-C8-C9
23	b	601	CLA	C11-C12-C13-C14
23	b	607	CLA	C14-C13-C15-C16
33	E	101[B]	LHG	C17-C18-C19-C20
23	b	615	CLA	C3A-C2A-CAA-CBA
33	a	419[A]	LHG	O8-C23-C24-C25
34	Z	101	LMG	O7-C10-C11-C12
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
31	D	401[A]	PHO	CAD-CBD-CGD-O2D
31	D	401[B]	PHO	CAD-CBD-CGD-O2D
38	F	102	HEM	C2B-C3B-CAB-CBB
34	d	412	LMG	C28-C29-C30-C31
32	t	101	LMT	C11-C10-C9-C8
34	C	501	LMG	C31-C32-C33-C34
34	c	520	LMG	C14-C15-C16-C17
23	C	503	CLA	C3-C5-C6-C7
23	B	608	CLA	C2-C1-O2A-CGA
33	L	101[A]	LHG	C11-C12-C13-C14
33	L	101[A]	LHG	O7-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	416	LMT	C7-C8-C9-C10
23	B	605	CLA	O1D-CGD-O2D-CED
23	c	505	CLA	C4-C3-C5-C6
28	D	406[B]	PL9	C35-C34-C36-C37
40	v	201	HEC	CAD-CBD-CGD-O2D
34	m	101	LMG	O6-C1-O1-C7
23	B	614	CLA	C2-C3-C5-C6
28	D	406[B]	PL9	C43-C44-C46-C47
33	E	101[B]	LHG	O7-C7-C8-C9
33	b	629[A]	LHG	O7-C7-C8-C9
33	D	407[B]	LHG	C32-C33-C34-C35
34	B	620	LMG	O1-C7-C8-C9
40	v	201	HEC	C4B-C3B-CAB-CBB
36	c	519	DGD	C7B-C8B-C9B-CAB
34	m	101	LMG	C32-C33-C34-C35
23	B	602	CLA	O2A-C1-C2-C3
31	a	406[B]	PHO	O2A-C1-C2-C3
36	C	519	DGD	CCB-CDB-CEB-CFB
38	f	101	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	CAA-CBA-CGA-O1A
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
23	B	602	CLA	C8-C10-C11-C12
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
25	a	411	SQD	C28-C29-C30-C31
36	C	519	DGD	C2A-C3A-C4A-C5A
23	A	405[A]	CLA	CHA-CBD-CGD-O1D
23	A	405[A]	CLA	CHA-CBD-CGD-O2D
23	A	405[B]	CLA	CHA-CBD-CGD-O1D
23	A	405[B]	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	510	CLA	CHA-CBD-CGD-O1D
23	d	402[A]	CLA	CHA-CBD-CGD-O1D
23	d	402[A]	CLA	CHA-CBD-CGD-O2D
23	d	402[B]	CLA	CHA-CBD-CGD-O2D
40	v	201	HEC	CAD-CBD-CGD-O1D
33	a	419[B]	LHG	O8-C23-C24-C25
25	a	411	SQD	O48-C23-C24-C25
33	L	101[B]	LHG	O7-C7-C8-C9
25	l	101	SQD	C9-C10-C11-C12
34	c	521	LMG	O1-C7-C8-O7
36	h	102	DGD	O1G-C1G-C2G-O2G
25	b	620	SQD	C25-C26-C27-C28
23	B	613	CLA	CAA-CBA-CGA-O2A
23	c	508	CLA	C2A-CAA-CBA-CGA
26	l	103[B]	GOL	O1-C1-C2-O2
26	v	202[B]	GOL	O1-C1-C2-O2
31	D	401[A]	PHO	CHA-CBD-CGD-O2D
31	a	406[A]	PHO	CHA-CBD-CGD-O1D
33	A	418[A]	LHG	O1-C1-C2-O2
35	o	301	HTG	C4'-C5'-C6'-C7'
36	C	519	DGD	CBA-CCA-CDA-CEA
23	c	514	CLA	C12-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C15
34	Z	101	LMG	O10-C28-O8-C9
23	B	616	CLA	C16-C17-C18-C19
23	C	507	CLA	C16-C17-C18-C20
23	b	608	CLA	C16-C17-C18-C19
28	A	413[A]	PL9	C4-C3-C7-C8
31	a	415[A]	PHO	C2C-C3C-CAC-CBC
23	b	605	CLA	C13-C15-C16-C17
23	B	612	CLA	CAA-CBA-CGA-O2A
33	d	414[A]	LHG	C30-C31-C32-C33
23	B	615	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16
28	d	406[A]	PL9	C34-C36-C37-C38
36	c	517[B]	DGD	C8B-C9B-CAB-CBB
23	b	612	CLA	C13-C15-C16-C17
31	a	415[B]	PHO	C8-C10-C11-C12
23	B	612	CLA	C2B-C3B-CAB-CBB
34	B	620	LMG	C32-C33-C34-C35
23	C	513	CLA	CAA-CBA-CGA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	C	519	DGD	O1G-C1A-C2A-C3A
34	Z	101	LMG	O9-C10-C11-C12
32	A	417	LMT	C2B-C1B-O1B-C4'
23	b	610	CLA	C16-C17-C18-C19
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
36	C	519	DGD	C8B-C9B-CAB-CBB
33	b	629[B]	LHG	O7-C7-C8-C9
34	C	520	LMG	O7-C10-C11-C12
33	d	407[B]	LHG	C30-C31-C32-C33
26	B	625	GOL	O1-C1-C2-C3
33	E	101[B]	LHG	O9-C7-C8-C9
24	y	101	BCR	C21-C22-C23-C24
25	A	409[B]	SQD	C16-C17-C18-C19
36	c	517[B]	DGD	CDB-CEB-CFB-CGB
23	C	512	CLA	C1A-C2A-CAA-CBA
23	a	405[B]	CLA	C1A-C2A-CAA-CBA
23	c	507	CLA	C1A-C2A-CAA-CBA
33	A	418[B]	LHG	C9-C10-C11-C12
33	b	629[A]	LHG	O9-C7-C8-C9
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
23	C	511	CLA	CAA-CBA-CGA-O1A
33	A	418[A]	LHG	O10-C23-C24-C25
33	A	418[B]	LHG	O10-C23-C24-C25
33	L	101[A]	LHG	O9-C7-C8-C9
33	a	419[A]	LHG	O10-C23-C24-C25
33	a	419[B]	LHG	O10-C23-C24-C25
34	C	520	LMG	O9-C10-C11-C12
32	A	419	LMT	C7-C8-C9-C10
34	B	620	LMG	C36-C37-C38-C39
36	C	517[A]	DGD	C3A-C4A-C5A-C6A
34	C	520	LMG	O1-C7-C8-C9
33	E	101[A]	LHG	O7-C7-C8-C9
34	c	520	LMG	O7-C10-C11-C12
33	b	629[B]	LHG	C34-C35-C36-C37
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
36	c	518[B]	DGD	CBB-CCB-CDB-CEB
28	A	413[B]	PL9	C45-C44-C46-C47
33	L	101[B]	LHG	O9-C7-C8-C9
36	C	519	DGD	O1A-C1A-C2A-C3A
34	c	520	LMG	C29-C30-C31-C32
34	B	620	LMG	C2-C1-O1-C7
23	B	610	CLA	C4B-C3B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	407[A]	LHG	C4-O6-P-O5
33	d	408[B]	LHG	C4-O6-P-O5
25	a	411	SQD	O10-C23-C24-C25
33	b	629[B]	LHG	O9-C7-C8-C9
35	b	623	HTG	S1-C1'-C2'-C3'
24	C	515	BCR	C1-C6-C7-C8
23	b	611	CLA	C13-C15-C16-C17
23	b	615	CLA	C13-C15-C16-C17
23	C	513	CLA	CAA-CBA-CGA-O1A
23	b	613	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
23	b	610	CLA	C16-C17-C18-C20
32	m	103	LMT	C9-C10-C11-C12
33	d	408[A]	LHG	O10-C23-O8-C6
33	b	629[B]	LHG	C12-C13-C14-C15
33	A	418[A]	LHG	C18-C19-C20-C21
28	d	406[A]	PL9	C15-C14-C16-C17
33	d	408[A]	LHG	C30-C31-C32-C33
28	d	406[A]	PL9	C11-C12-C13-C14
36	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	B	611	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	a	405[B]	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	606	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
25	a	409[B]	SQD	C10-C11-C12-C13
33	A	418[B]	LHG	C16-C17-C18-C19
33	d	408[B]	LHG	C10-C11-C12-C13
33	E	101[A]	LHG	O8-C23-C24-C25
36	C	518[A]	DGD	O2G-C1B-C2B-C3B
23	B	612	CLA	C11-C10-C8-C9
23	C	504	CLA	C11-C10-C8-C9
23	a	405[B]	CLA	C6-C7-C8-C9
23	b	607	CLA	C6-C7-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	A	418[A]	LHG	C30-C31-C32-C33
26	B	625	GOL	O2-C2-C3-O3
33	D	408[A]	LHG	C28-C29-C30-C31
23	b	610	CLA	C5-C6-C7-C8
23	b	612	CLA	O1A-CGA-O2A-C1
23	C	506	CLA	CAA-CBA-CGA-O2A
34	D	412	LMG	O7-C10-C11-C12
36	C	518[B]	DGD	O2G-C1B-C2B-C3B
36	C	517[A]	DGD	CBA-CCA-CDA-CEA
33	L	101[A]	LHG	C32-C33-C34-C35
23	B	603	CLA	CBD-CGD-O2D-CED
33	D	408[A]	LHG	O8-C23-C24-C25
28	A	413[B]	PL9	C46-C47-C48-C49
34	C	521	LMG	C10-C11-C12-C13
23	B	613	CLA	CAA-CBA-CGA-O1A
34	D	412	LMG	O9-C10-C11-C12
23	B	602	CLA	C6-C7-C8-C10
23	B	615	CLA	C12-C13-C15-C16
23	C	509	CLA	C12-C13-C15-C16
23	a	405[A]	CLA	C6-C7-C8-C10
23	b	607	CLA	C6-C7-C8-C10
33	E	101[A]	LHG	O9-C7-C8-C9
33	E	101[A]	LHG	O10-C23-C24-C25
34	c	521	LMG	O9-C10-C11-C12
23	c	502	CLA	CAA-CBA-CGA-O2A
23	c	506	CLA	CAA-CBA-CGA-O2A
23	c	513	CLA	CAA-CBA-CGA-O2A
25	A	411	SQD	O48-C23-C24-C25
33	D	408[B]	LHG	O8-C23-C24-C25
33	d	408[B]	LHG	O8-C23-C24-C25
34	c	521	LMG	O7-C10-C11-C12
36	c	517[A]	DGD	O2G-C1B-C2B-C3B
34	c	521	LMG	C28-C29-C30-C31
24	d	405	BCR	C7-C8-C9-C10
23	B	612	CLA	CAA-CBA-CGA-O1A
33	D	408[A]	LHG	O10-C23-C24-C25
36	c	517[A]	DGD	O1B-C1B-C2B-C3B
24	H	101	BCR	C9-C10-C11-C12
36	h	102	DGD	C6A-C7A-C8A-C9A
32	B	626	LMT	C2-C1-O1'-C1'
33	E	101[B]	LHG	O8-C23-C24-C25
25	A	409[B]	SQD	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	d	412	LMG	C38-C39-C40-C41
32	a	416	LMT	O5'-C1'-O1'-C1
23	B	615	CLA	O1D-CGD-O2D-CED
23	b	604	CLA	O1A-CGA-O2A-C1
25	f	102	SQD	C11-C10-C9-C8
23	c	513	CLA	CAA-CBA-CGA-O1A
33	D	408[B]	LHG	O10-C23-C24-C25
33	d	408[B]	LHG	O10-C23-C24-C25
36	C	518[A]	DGD	O1B-C1B-C2B-C3B
23	b	612	CLA	C8-C10-C11-C12
33	d	414[A]	LHG	C31-C32-C33-C34
34	B	620	LMG	O6-C5-C6-O5
25	A	411	SQD	O10-C23-C24-C25
34	c	520	LMG	O9-C10-C11-C12
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
36	C	518[B]	DGD	O1B-C1B-C2B-C3B
23	b	614	CLA	O1D-CGD-O2D-CED
33	E	101[A]	LHG	C11-C10-C9-C8
33	d	408[A]	LHG	O8-C23-C24-C25
36	c	517[B]	DGD	O2G-C1B-C2B-C3B

There are no ring outliers.

181 monomers are involved in 372 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	T	102	BCR	5	0
32	a	416	LMT	1	0
23	B	606	CLA	2	0
23	c	503	CLA	2	0
23	B	605	CLA	3	0
23	A	407	CLA	3	0
23	A	404[A]	CLA	2	0
23	c	514	CLA	2	0
36	c	519	DGD	2	0
23	c	511	CLA	2	0
36	C	518[A]	DGD	1	0
31	A	416[B]	PHO	1	0
33	d	408[B]	LHG	7	0
23	c	504	CLA	4	0
23	b	610	CLA	1	0
24	H	101	BCR	1	0
23	C	504	CLA	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	k	101	BCR	1	0
26	D	413	GOL	3	0
24	d	405	BCR	2	0
23	b	616	CLA	3	0
38	F	102	HEM	1	0
23	B	614	CLA	2	0
23	b	605	CLA	4	0
31	A	416[A]	PHO	1	0
33	d	408[A]	LHG	11	0
24	B	619	BCR	2	0
23	a	404[A]	CLA	2	0
32	A	417	LMT	1	0
24	B	617	BCR	1	0
33	D	408[B]	LHG	3	0
34	C	521	LMG	3	0
23	C	510	CLA	2	0
23	b	606	CLA	2	0
34	d	412	LMG	3	0
33	D	407[B]	LHG	2	0
25	f	102	SQD	1	0
23	c	506	CLA	8	0
23	C	502	CLA	4	0
23	C	503	CLA	2	0
24	c	515	BCR	2	0
25	a	409[A]	SQD	5	0
23	b	601	CLA	1	0
36	C	517[B]	DGD	1	0
31	a	406[B]	PHO	2	0
26	v	202[B]	GOL	2	0
32	t	101	LMT	3	0
33	D	408[A]	LHG	4	0
28	D	406[B]	PL9	1	0
23	d	402[B]	CLA	4	0
24	h	101	BCR	5	0
24	c	516	BCR	1	0
23	A	406[B]	CLA	2	0
33	D	407[A]	LHG	2	0
34	c	520	LMG	1	0
28	A	413[B]	PL9	10	0
25	X	101	SQD	1	0
34	z	101	LMG	2	0
23	b	604	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	a	413[B]	PL9	4	0
36	C	517[A]	DGD	1	0
23	b	609	CLA	4	0
25	b	620	SQD	2	0
26	v	202[A]	GOL	1	0
24	a	408	BCR	1	0
23	c	507	CLA	4	0
31	a	415[B]	PHO	1	0
23	b	612	CLA	3	0
25	l	101	SQD	2	0
23	B	601	CLA	1	0
28	D	406[A]	PL9	1	0
26	b	628	GOL	2	0
23	d	402[A]	CLA	3	0
23	C	506	CLA	4	0
23	C	507	CLA	6	0
24	K	102	BCR	1	0
23	D	403[B]	CLA	5	0
33	E	101[B]	LHG	2	0
23	A	406[A]	CLA	1	0
32	B	629	LMT	1	0
23	a	407	CLA	4	0
24	t	102	BCR	7	0
28	A	413[A]	PL9	11	0
23	B	613	CLA	4	0
26	a	417	GOL	2	0
24	A	408	BCR	1	0
23	c	502	CLA	2	0
26	O	302	GOL	1	0
26	l	103[B]	GOL	1	0
28	a	413[A]	PL9	4	0
32	B	626	LMT	1	0
35	B	623	HTG	1	0
36	h	102	DGD	2	0
25	A	411	SQD	1	0
31	a	415[A]	PHO	1	0
23	C	505	CLA	1	0
23	B	612	CLA	3	0
23	B	604	CLA	1	0
23	C	513	CLA	2	0
23	B	609	CLA	3	0
23	D	403[A]	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	403[B]	CLA	5	0
32	b	621	LMT	1	0
33	A	418[A]	LHG	2	0
33	E	101[A]	LHG	4	0
23	B	616	CLA	3	0
36	H	102	DGD	1	0
24	y	101	BCR	1	0
26	l	103[A]	GOL	1	0
23	C	512	CLA	2	0
24	b	617	BCR	1	0
23	B	603	CLA	1	0
23	c	513	CLA	7	0
32	B	627	LMT	1	0
32	e	101	LMT	1	0
23	A	405[B]	CLA	5	0
23	d	403[A]	CLA	1	0
26	B	622	GOL	2	0
34	c	501	LMG	1	0
23	C	514	CLA	1	0
23	a	405[B]	CLA	4	0
35	B	621	HTG	1	0
34	c	521	LMG	1	0
25	A	409[B]	SQD	1	0
32	A	419	LMT	1	0
23	c	510	CLA	3	0
35	b	625	HTG	1	0
32	m	103	LMT	2	0
23	C	509	CLA	4	0
23	b	615	CLA	1	0
23	c	509	CLA	9	0
23	b	607	CLA	2	0
23	C	511	CLA	2	0
36	C	519	DGD	2	0
33	a	419[B]	LHG	3	0
23	B	602	CLA	1	0
23	A	405[A]	CLA	1	0
24	D	405	BCR	1	0
26	a	418	GOL	3	0
35	c	522	HTG	1	0
31	D	401[B]	PHO	2	0
36	C	518[B]	DGD	2	0
26	D	402	GOL	4	0

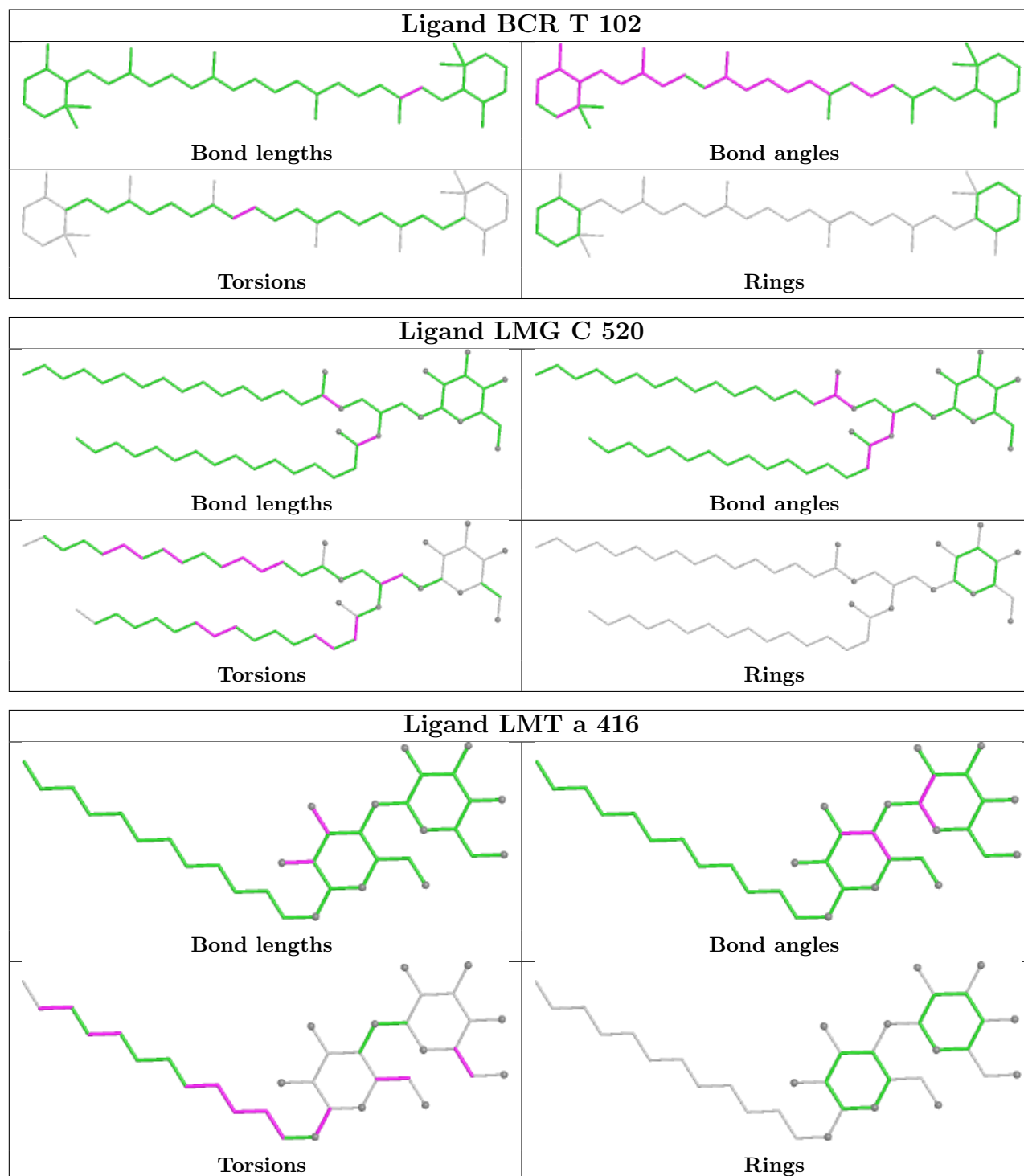
Continued on next page...

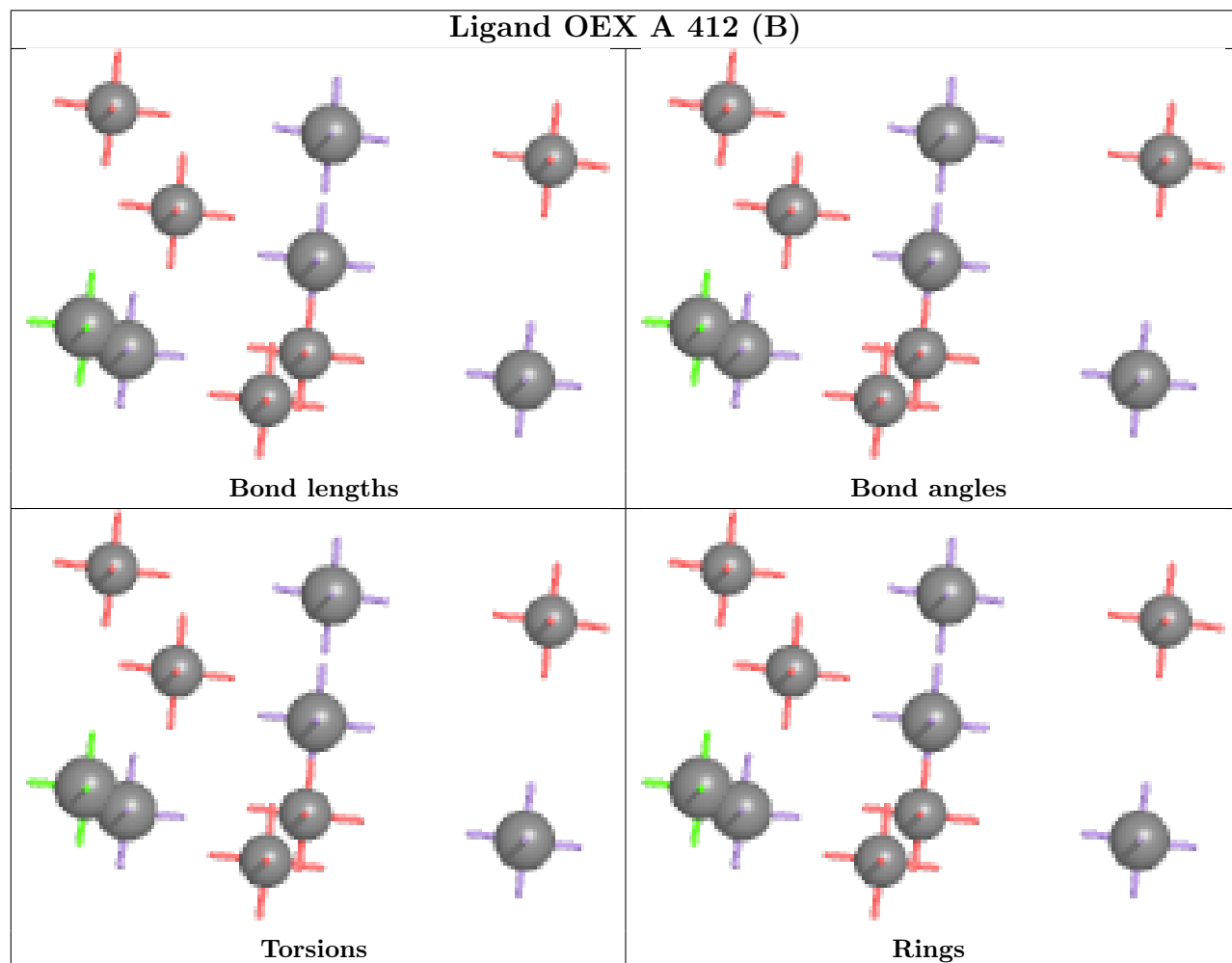
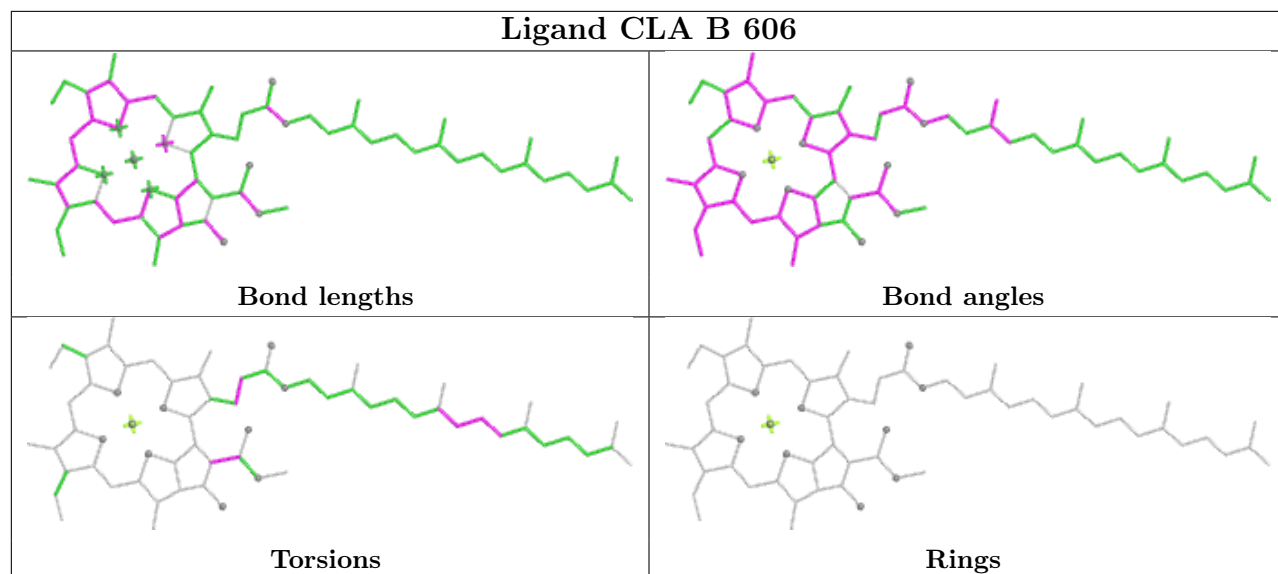
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	405[A]	CLA	2	0
23	B	615	CLA	5	0
25	A	409[A]	SQD	1	0
34	B	620	LMG	2	0
36	c	518[B]	DGD	2	0
24	b	619	BCR	4	0
33	a	419[A]	LHG	5	0
24	C	515	BCR	1	0
23	B	610	CLA	2	0
31	D	401[A]	PHO	1	0
34	Z	101	LMG	3	0
23	a	404[B]	CLA	10	0
23	c	508	CLA	2	0
35	b	622	HTG	2	0
36	c	517[B]	DGD	2	0
36	c	518[A]	DGD	3	0
33	L	101[B]	LHG	1	0
23	d	404	CLA	2	0
25	a	411	SQD	1	0
33	d	407[B]	LHG	2	0
32	M	101	LMT	2	0
23	D	404	CLA	1	0
23	c	512	CLA	6	0
25	a	409[B]	SQD	4	0
24	Y	101	BCR	2	0
35	o	301	HTG	1	0
23	b	613	CLA	4	0
23	A	404[B]	CLA	6	0
26	O	303	GOL	2	0
24	b	618	BCR	3	0
23	b	614	CLA	1	0
36	c	517[A]	DGD	1	0
24	B	618	BCR	2	0
23	b	608	CLA	1	0
35	d	411	HTG	1	0
23	c	505	CLA	2	0
23	C	508	CLA	2	0
33	d	407[A]	LHG	2	0

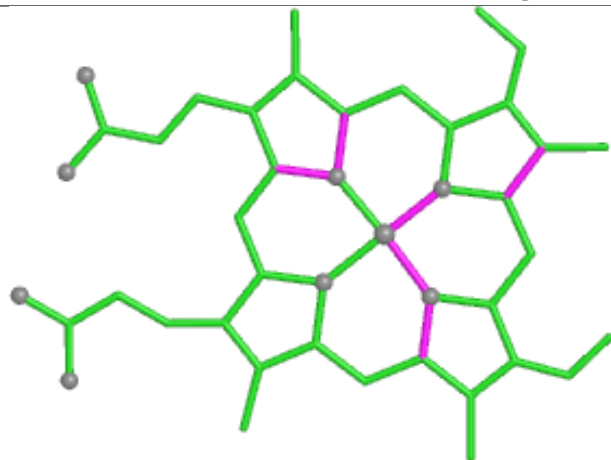
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

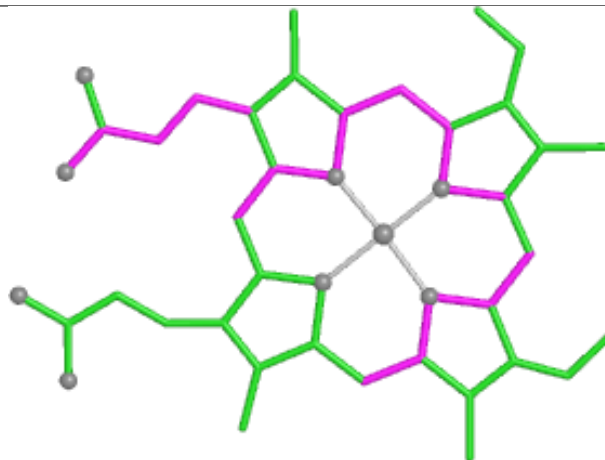




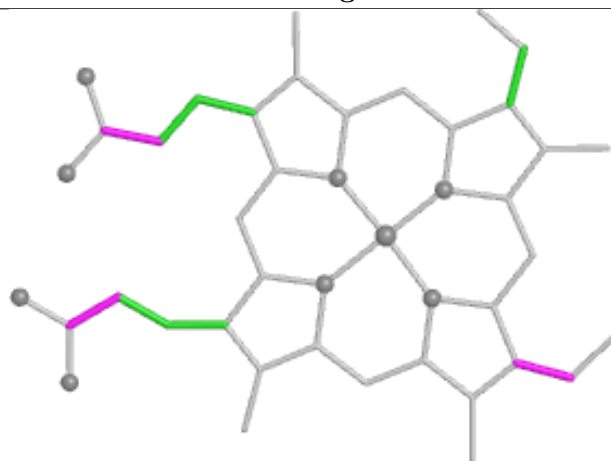
Ligand HEM f 101



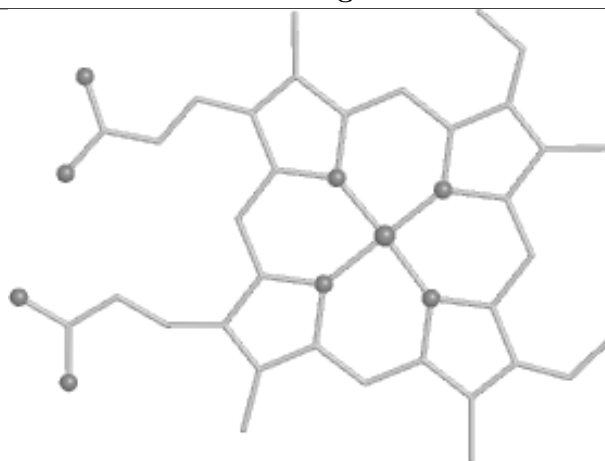
Bond lengths



Bond angles

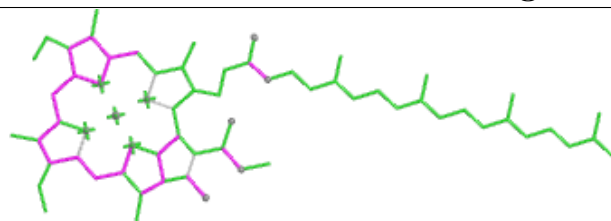


Torsions

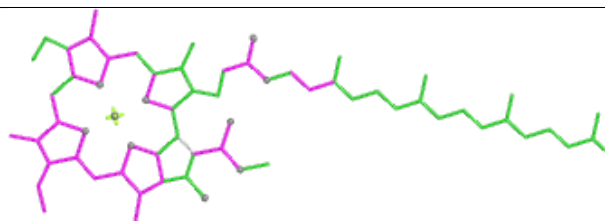


Rings

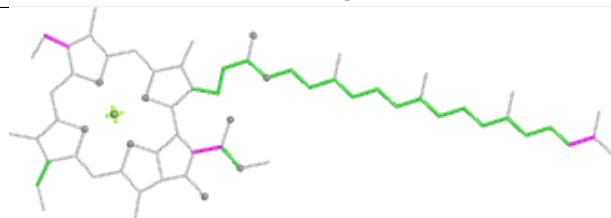
Ligand CLA c 503



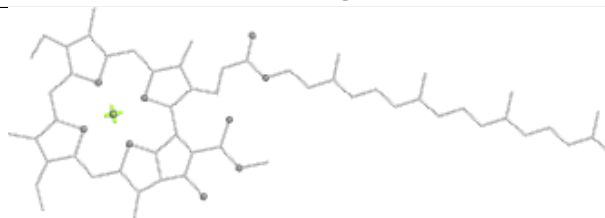
Bond lengths



Bond angles

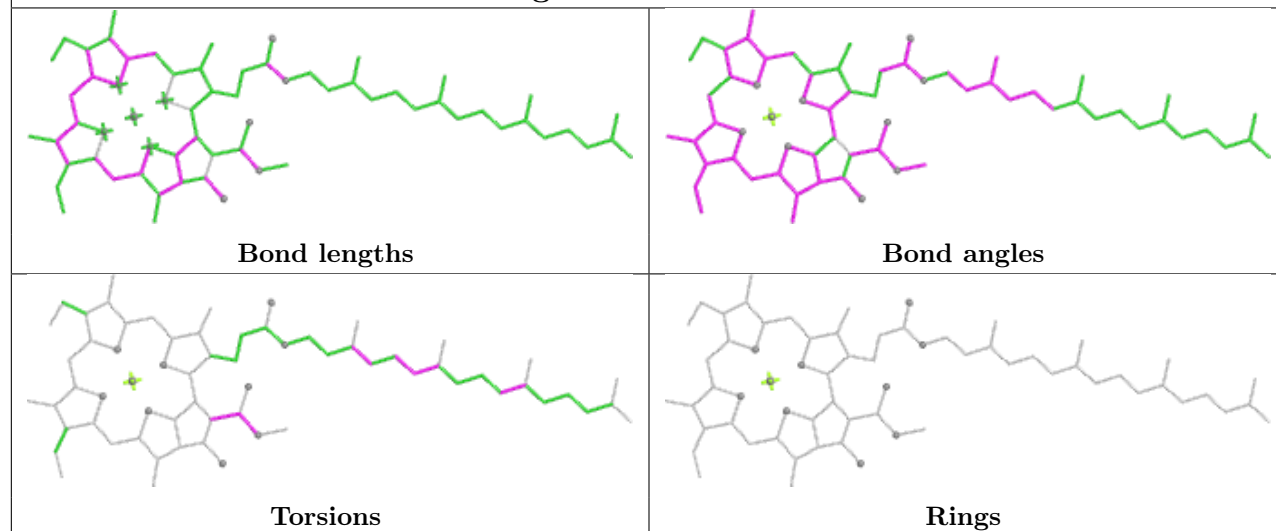


Torsions

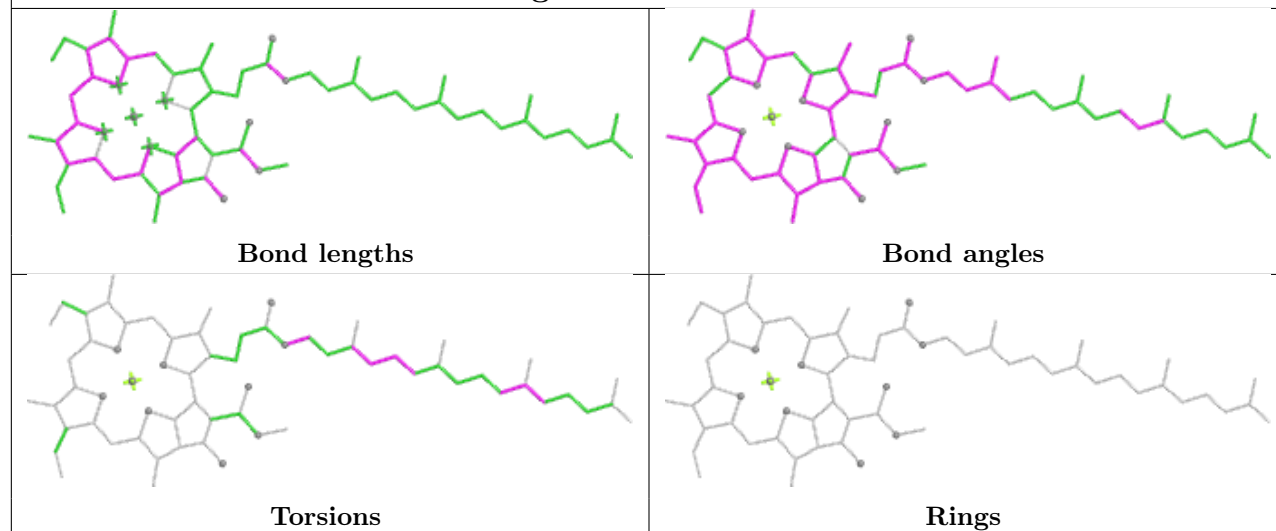


Rings

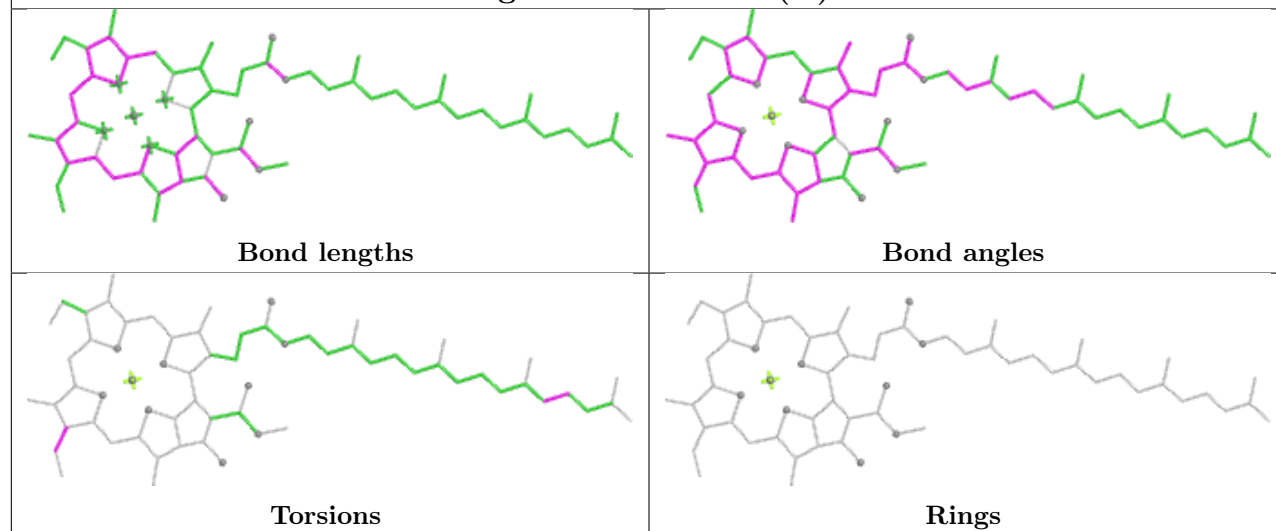
Ligand CLA B 605



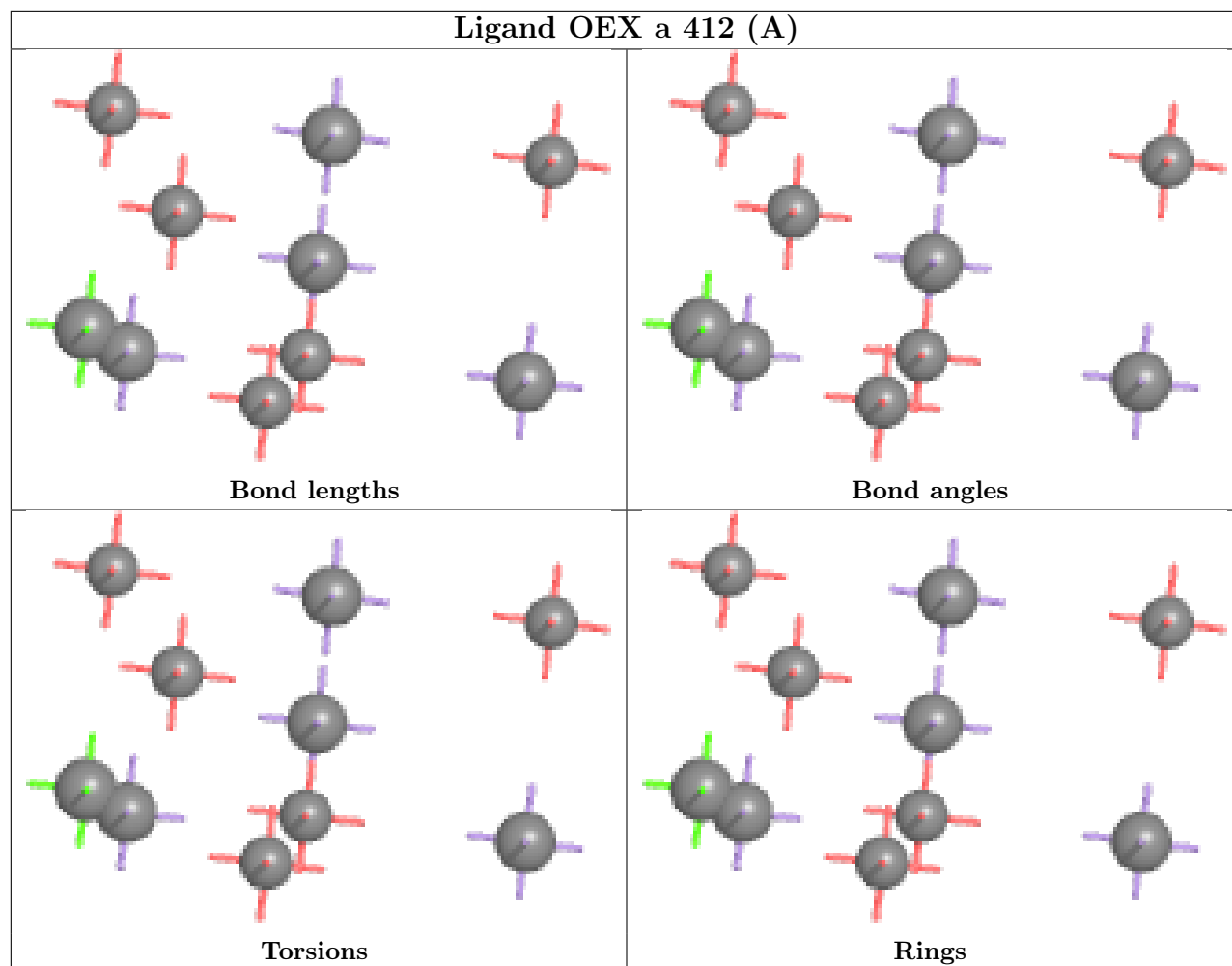
Ligand CLA A 407



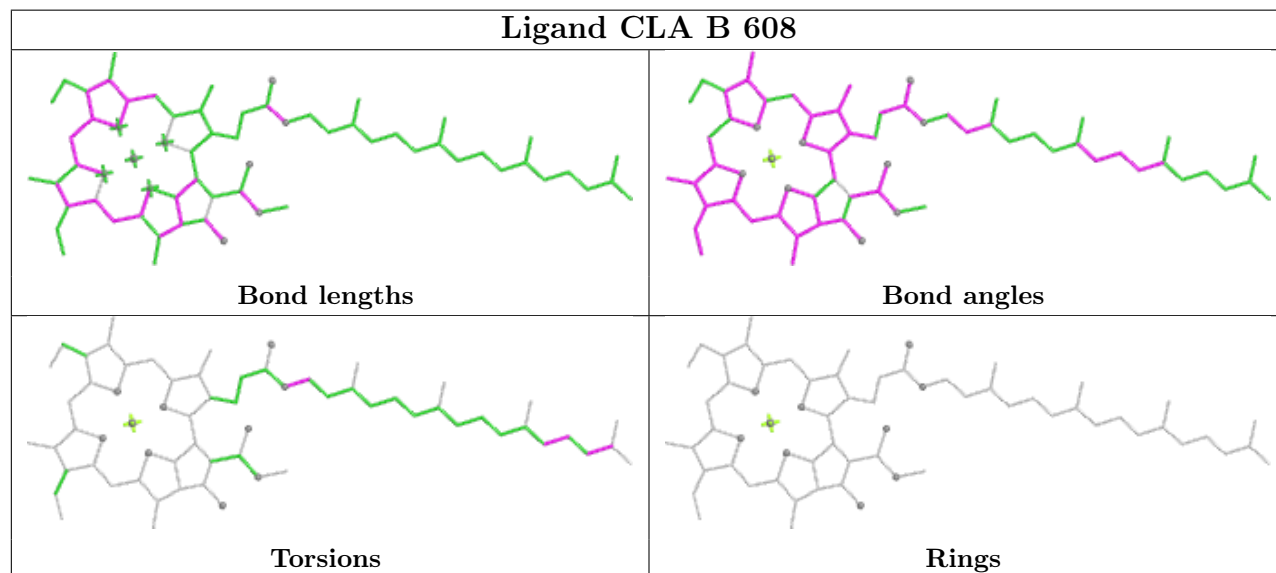
Ligand CLA A 404 (A)



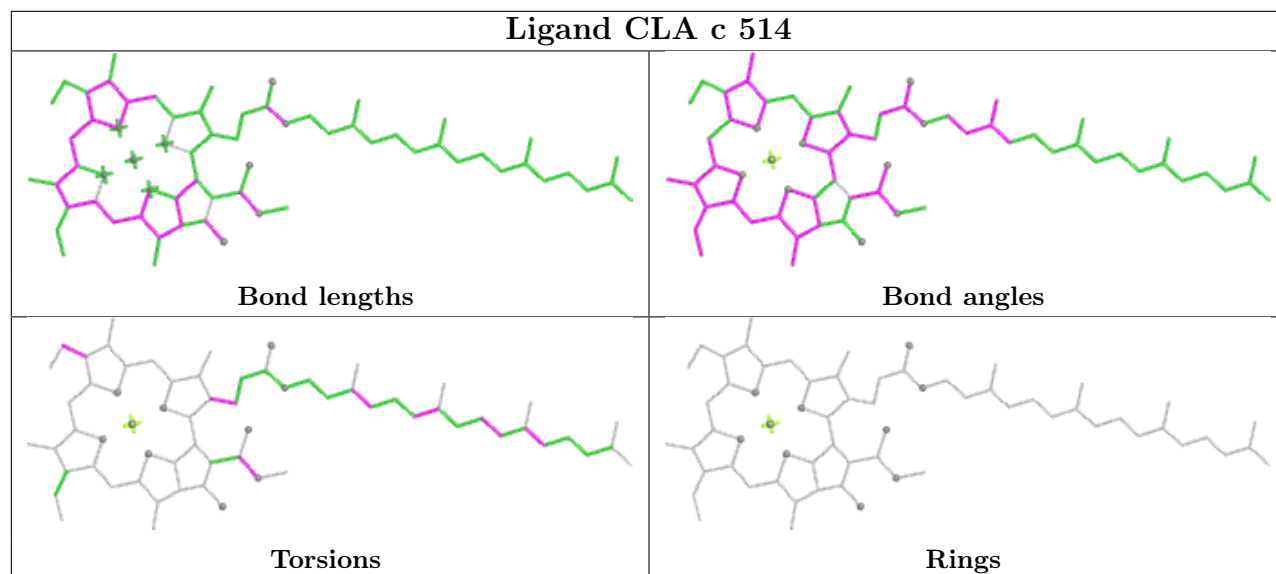
Ligand OEX a 412 (A)



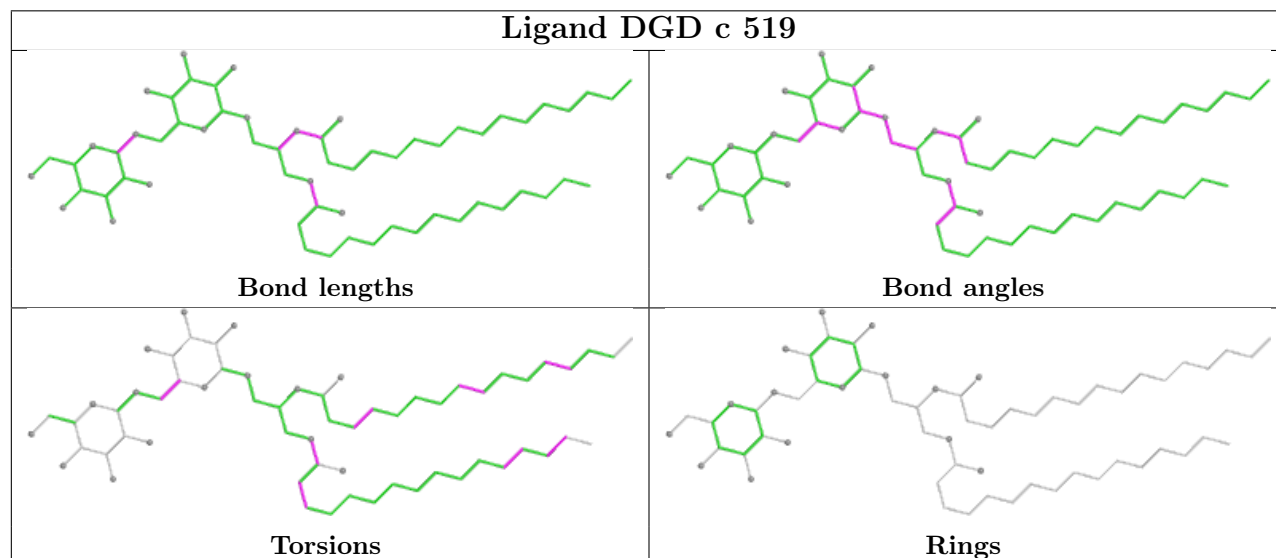
Ligand CLA B 608



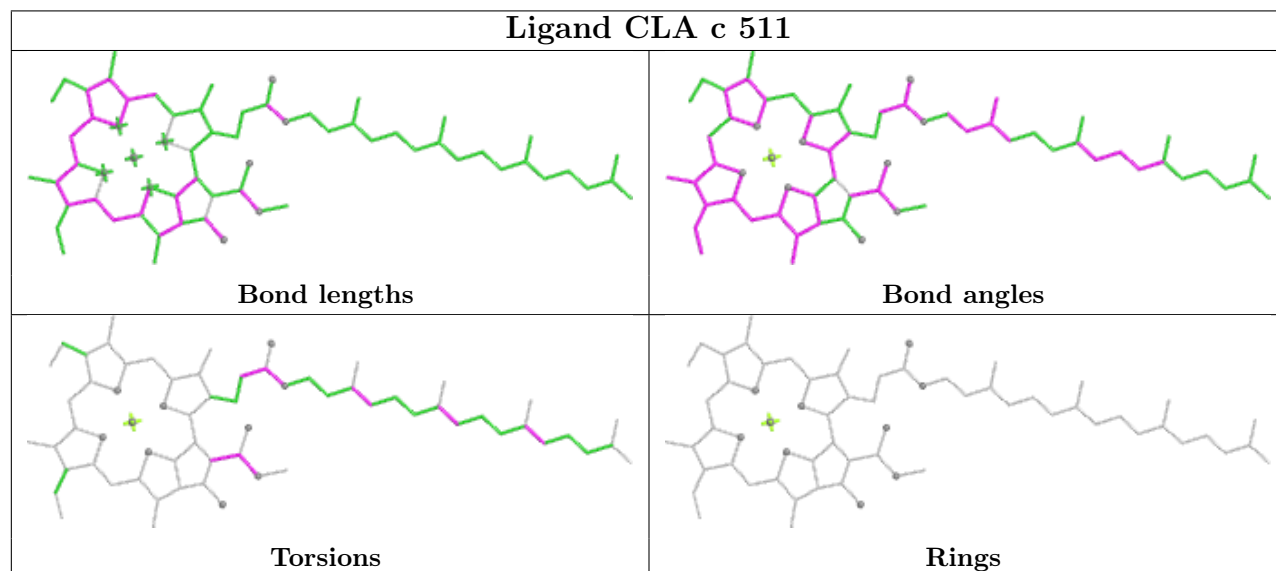
Ligand CLA c 514

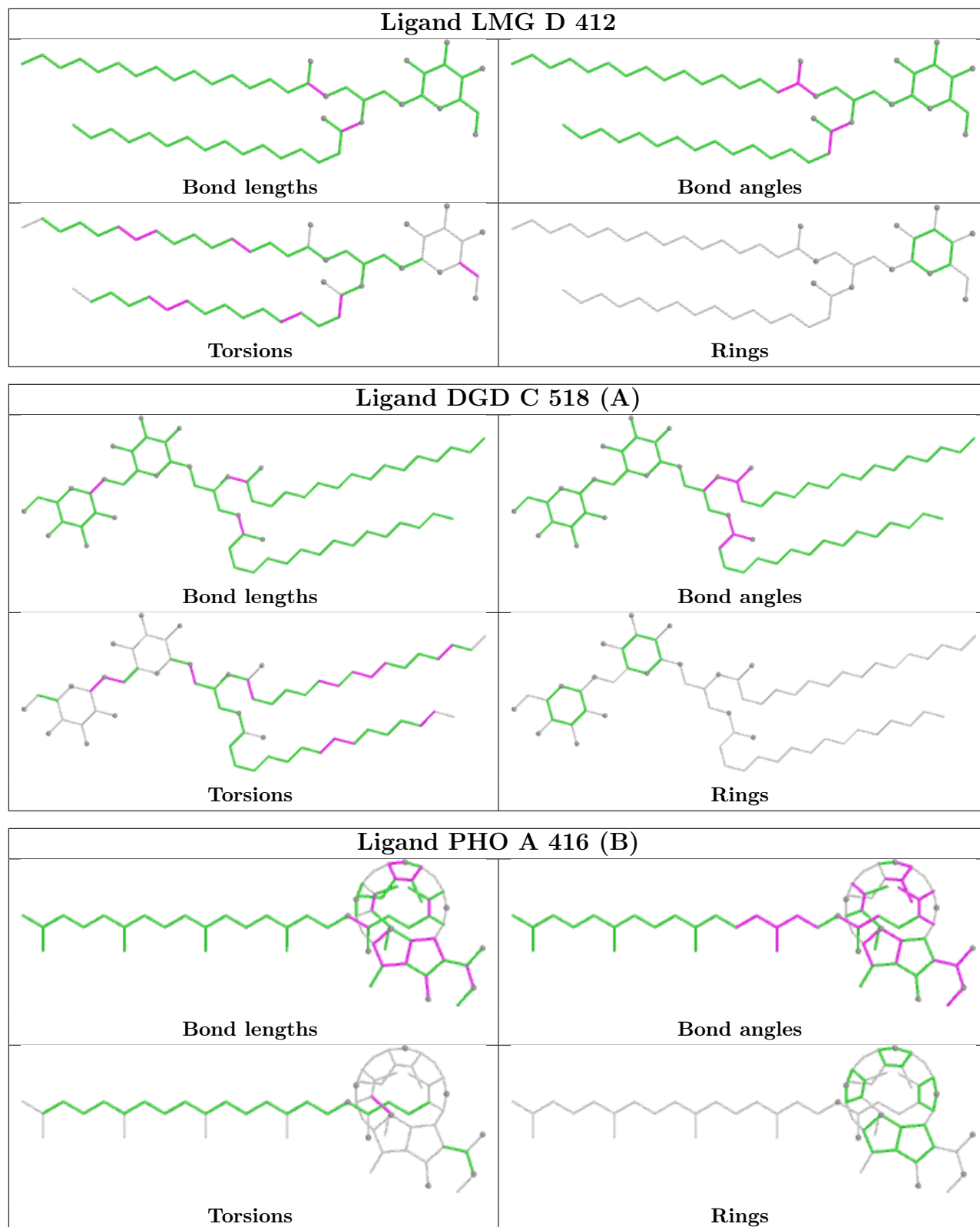


Ligand DGD c 519

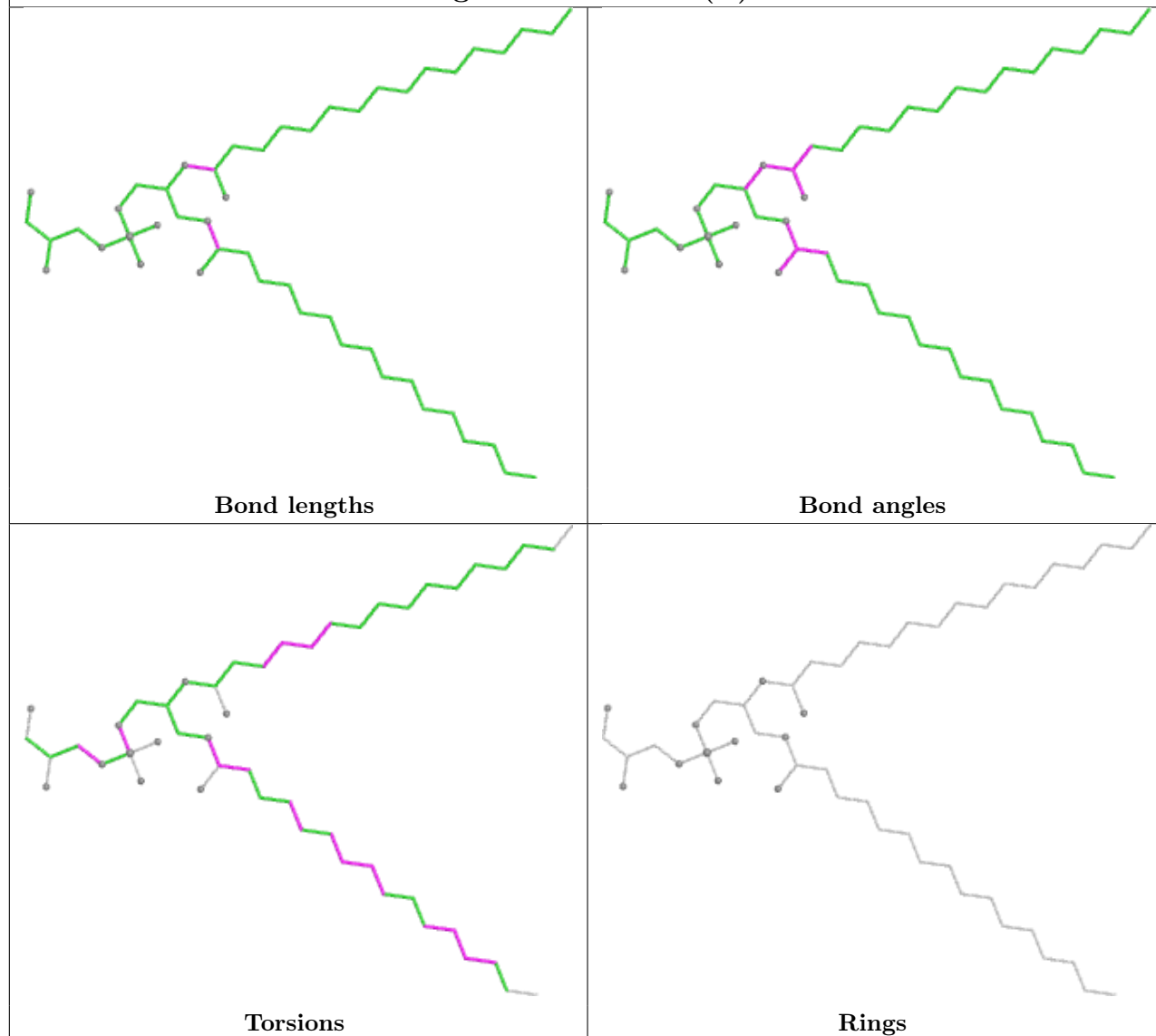


Ligand CLA c 511

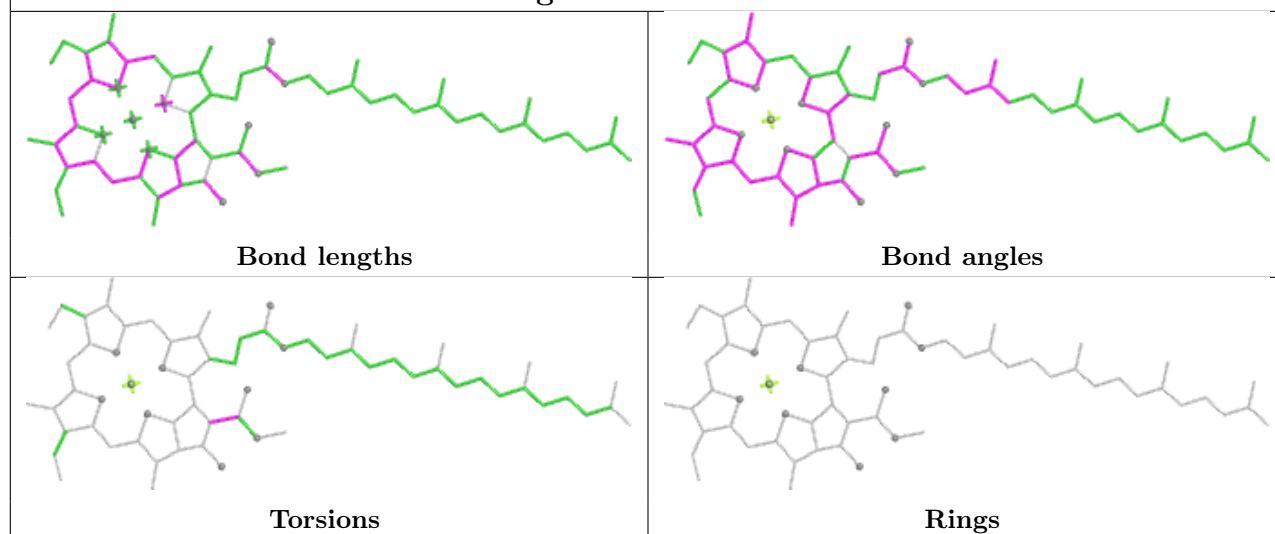


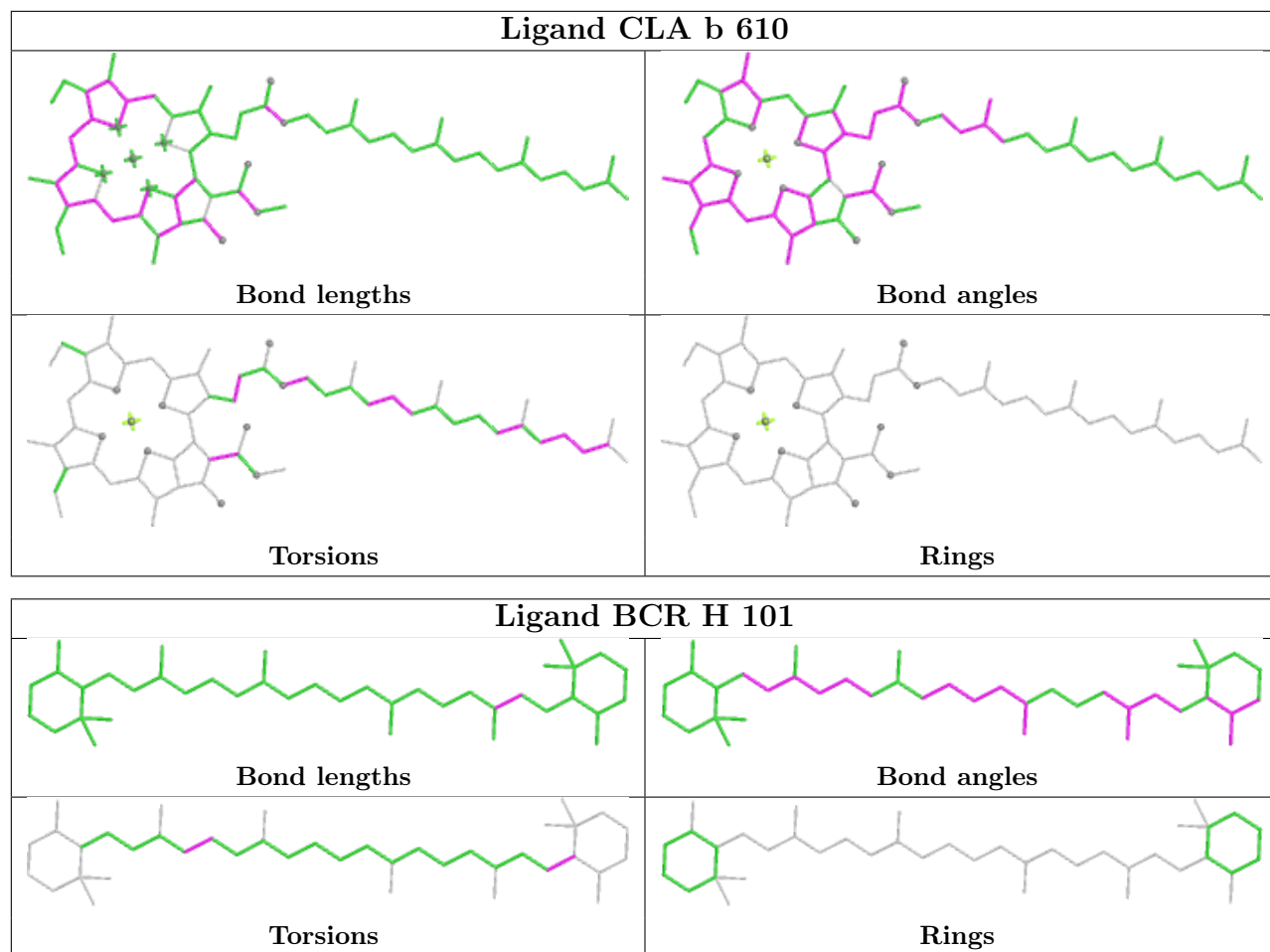


Ligand LHG d 408 (B)

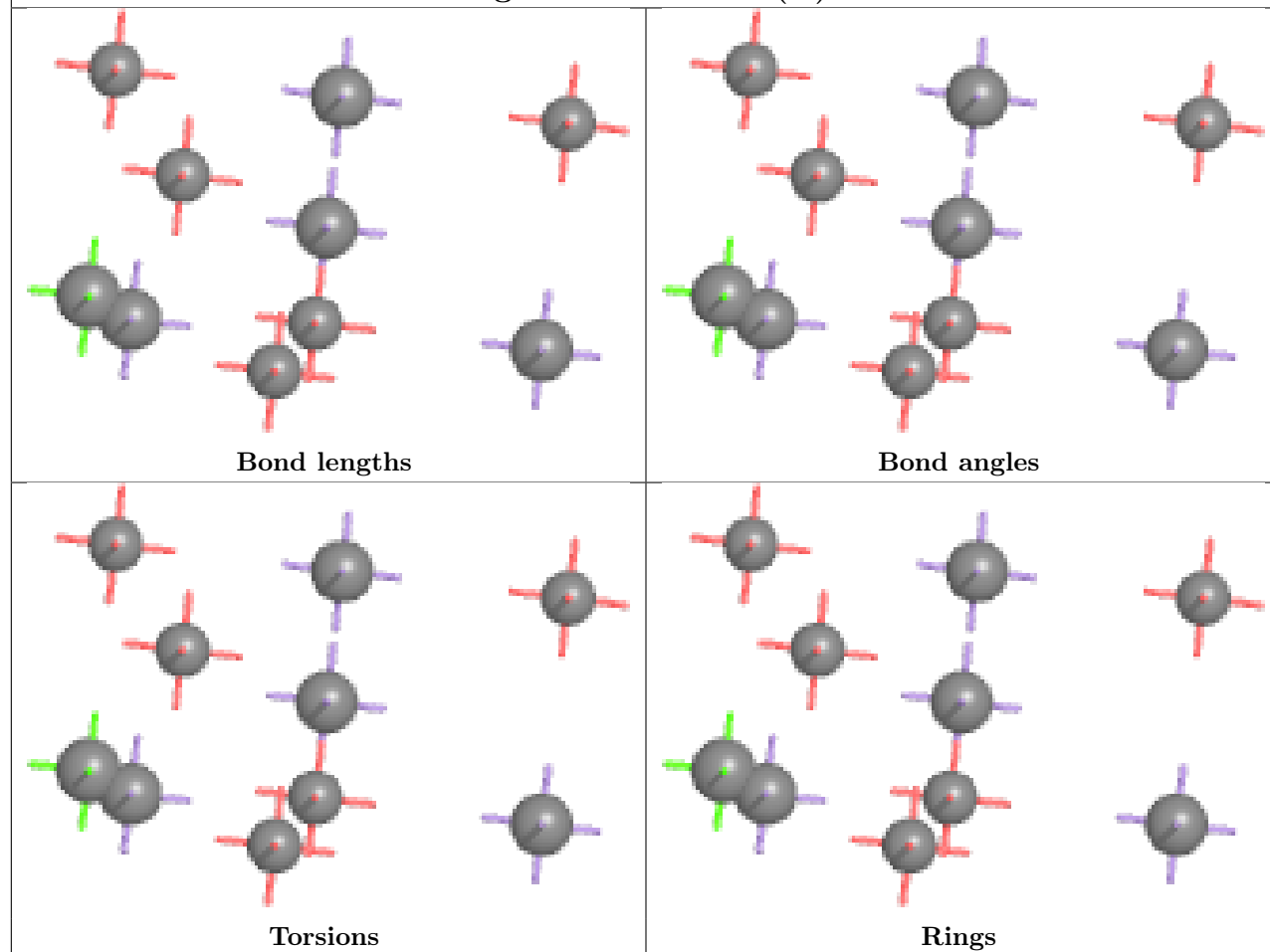


Ligand CLA c 504

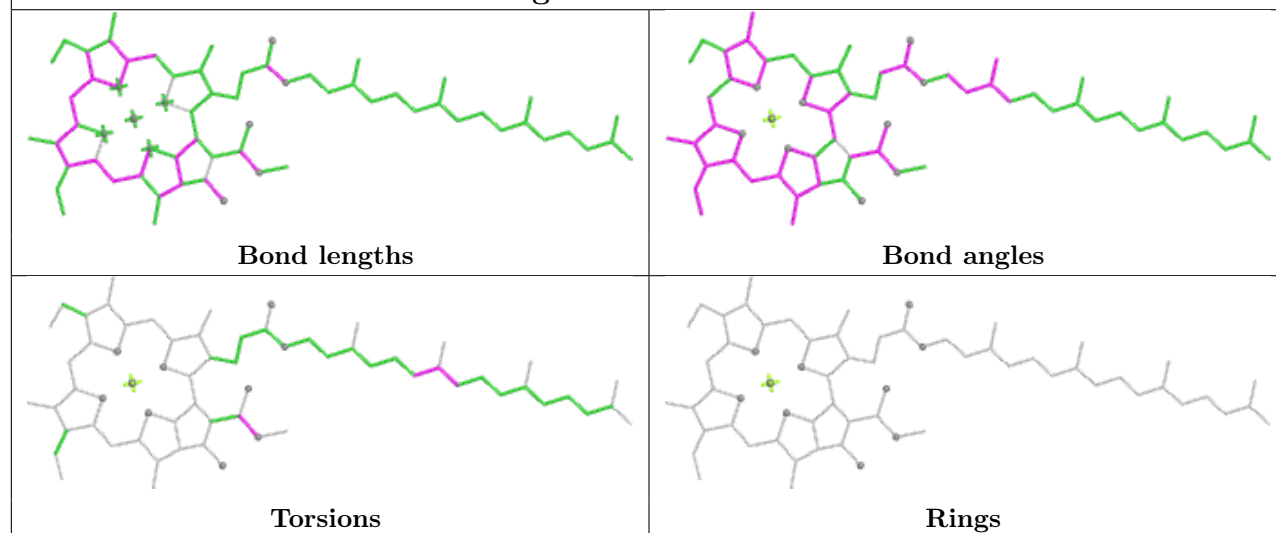


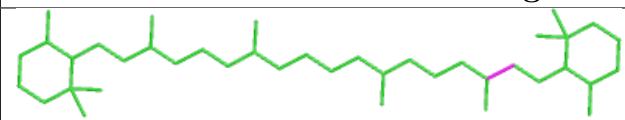
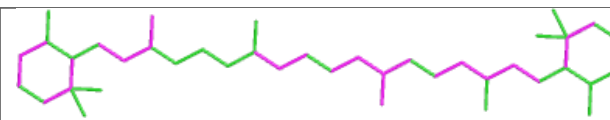
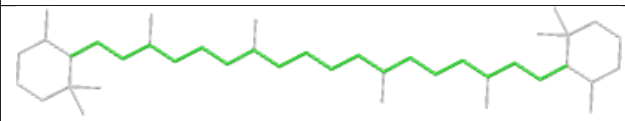
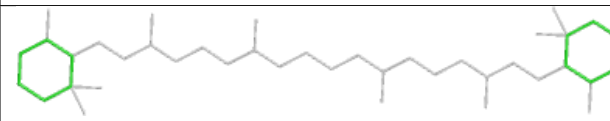


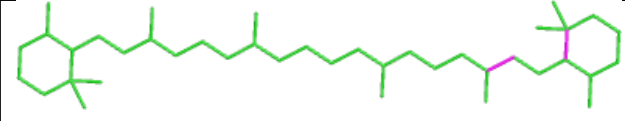
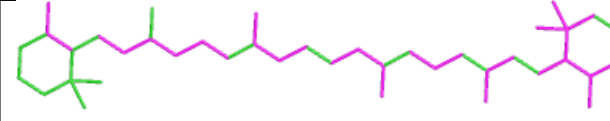
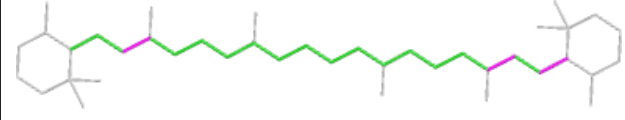
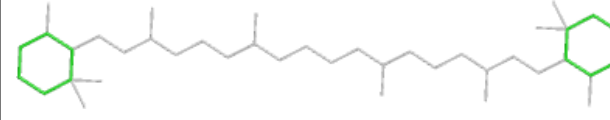
Ligand OEX A 412 (A)

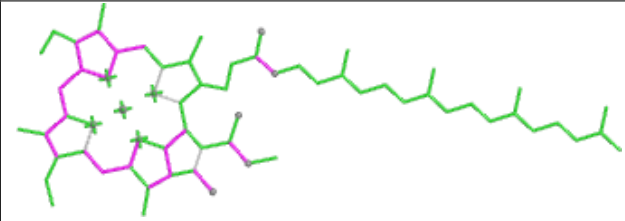
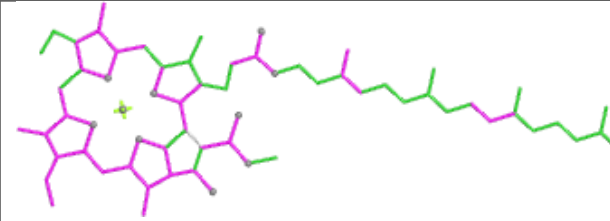
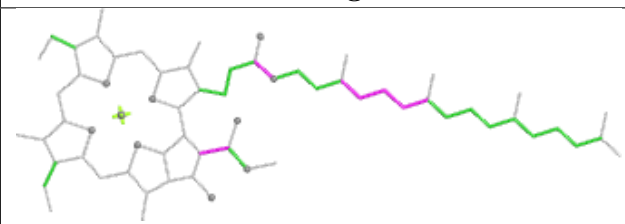
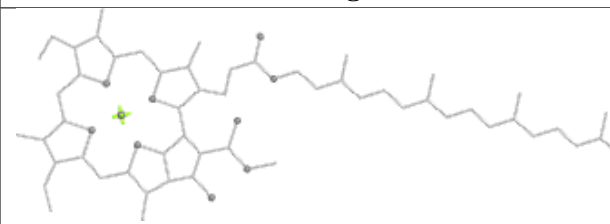


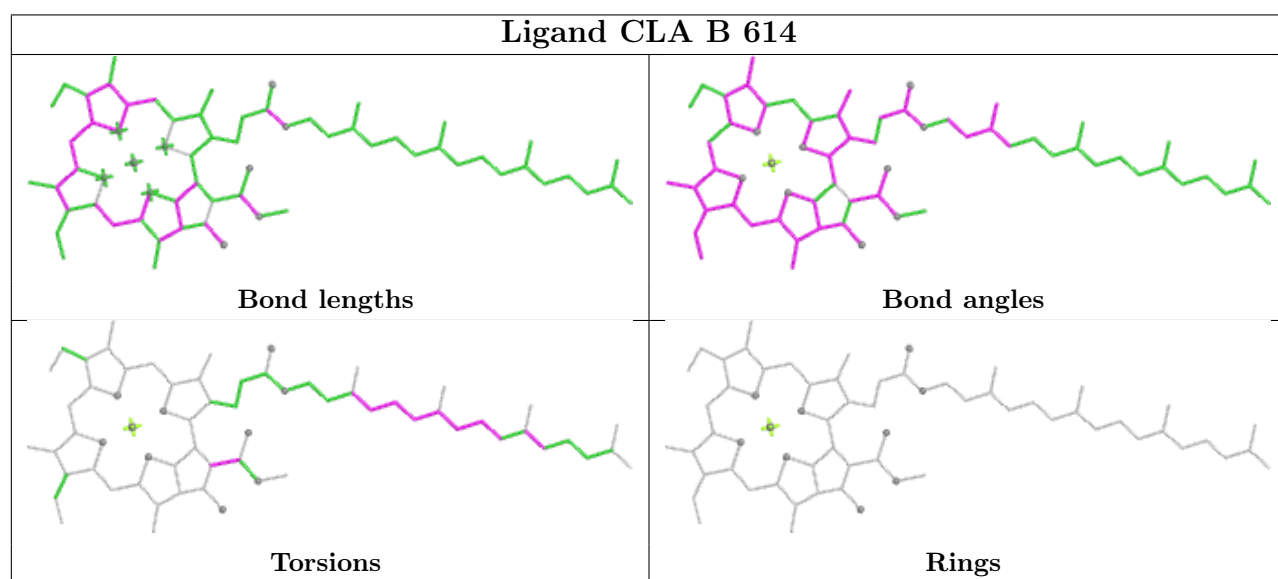
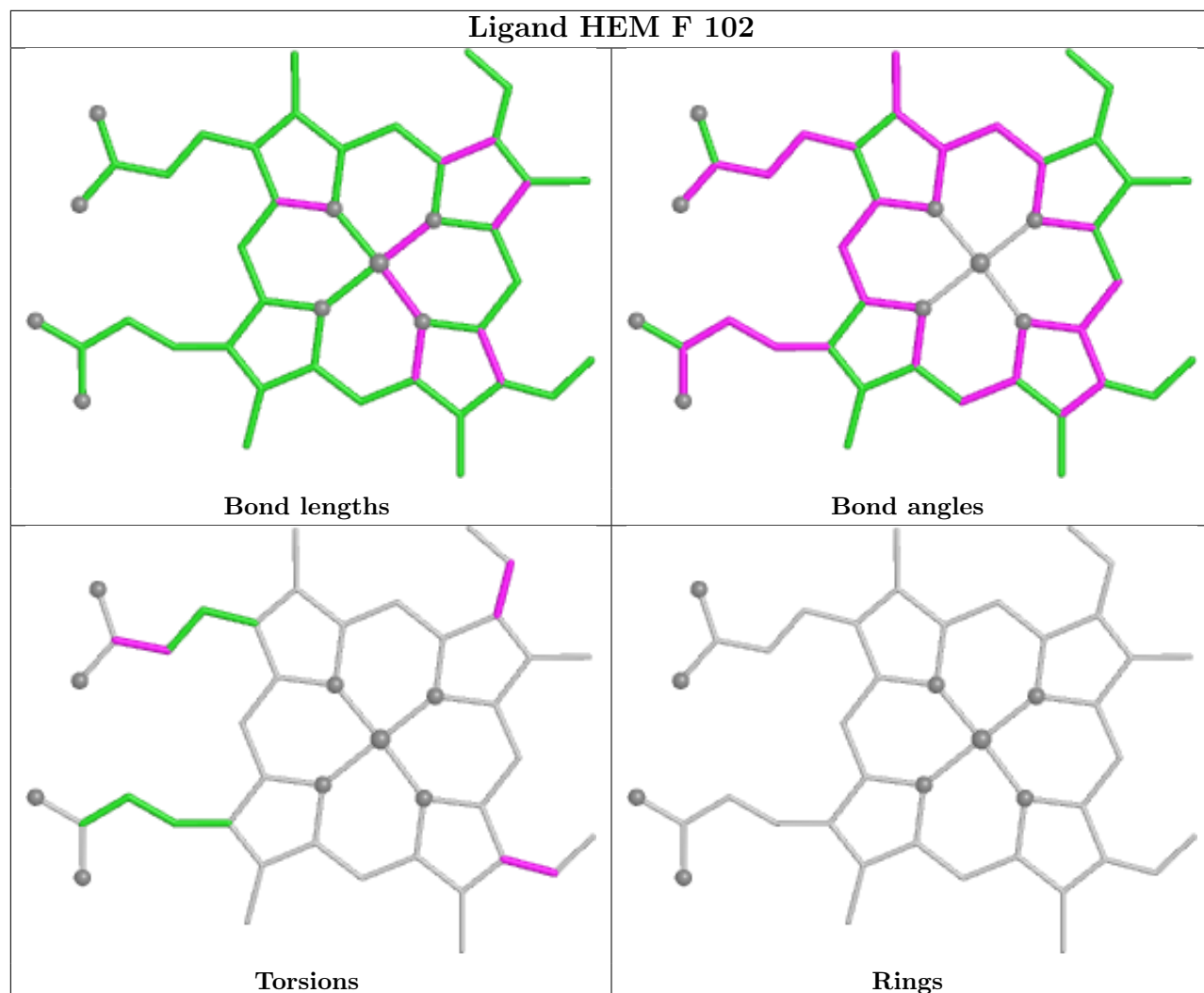
Ligand CLA C 504

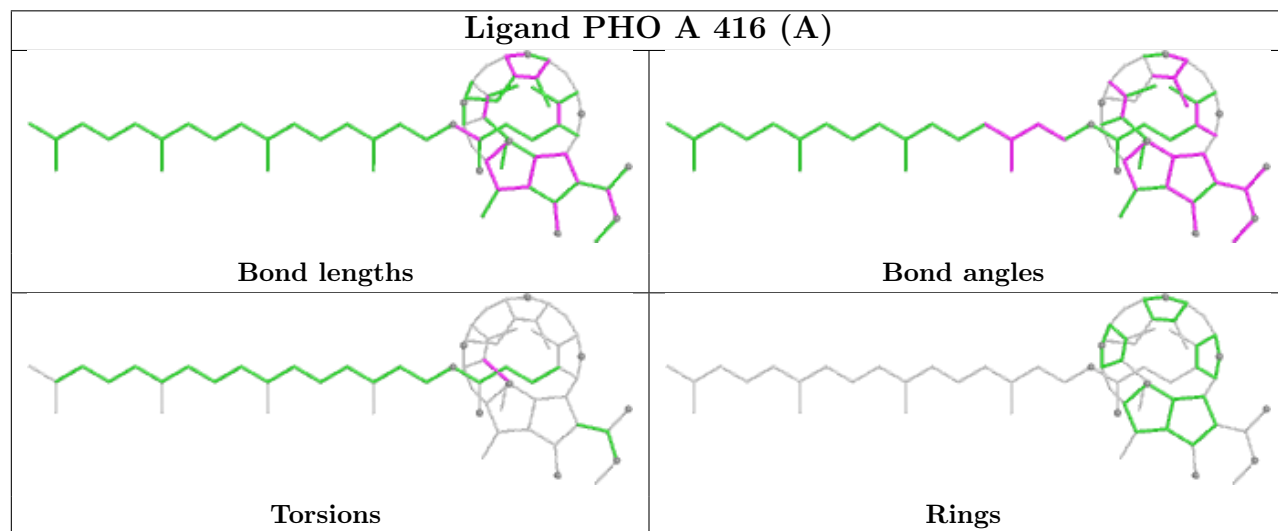
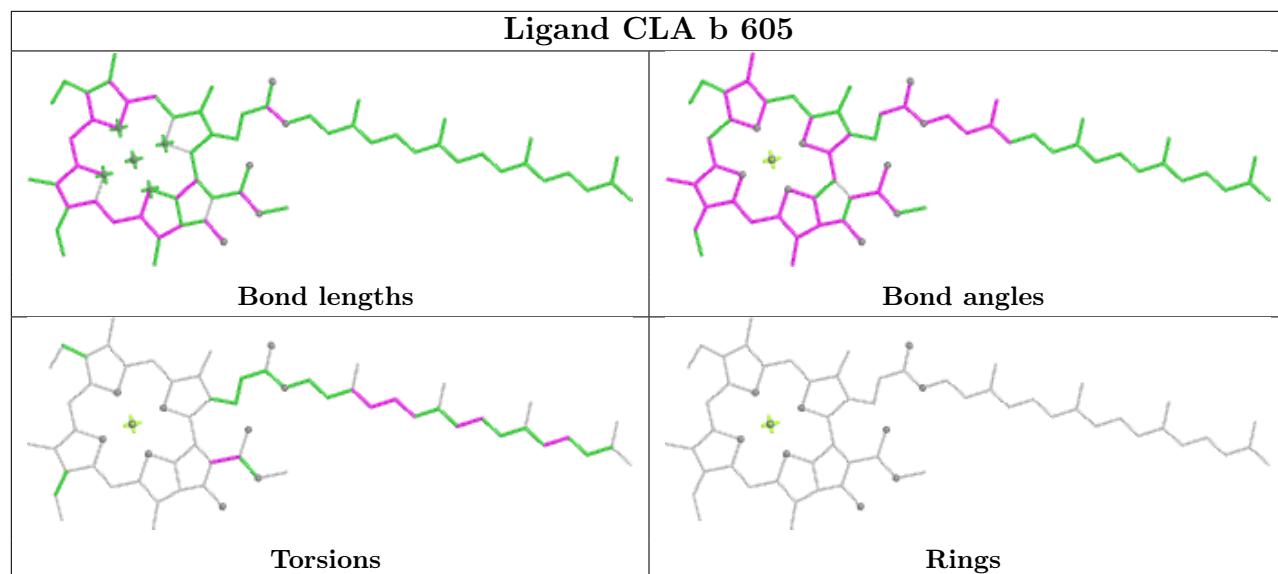


Ligand BCR k 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

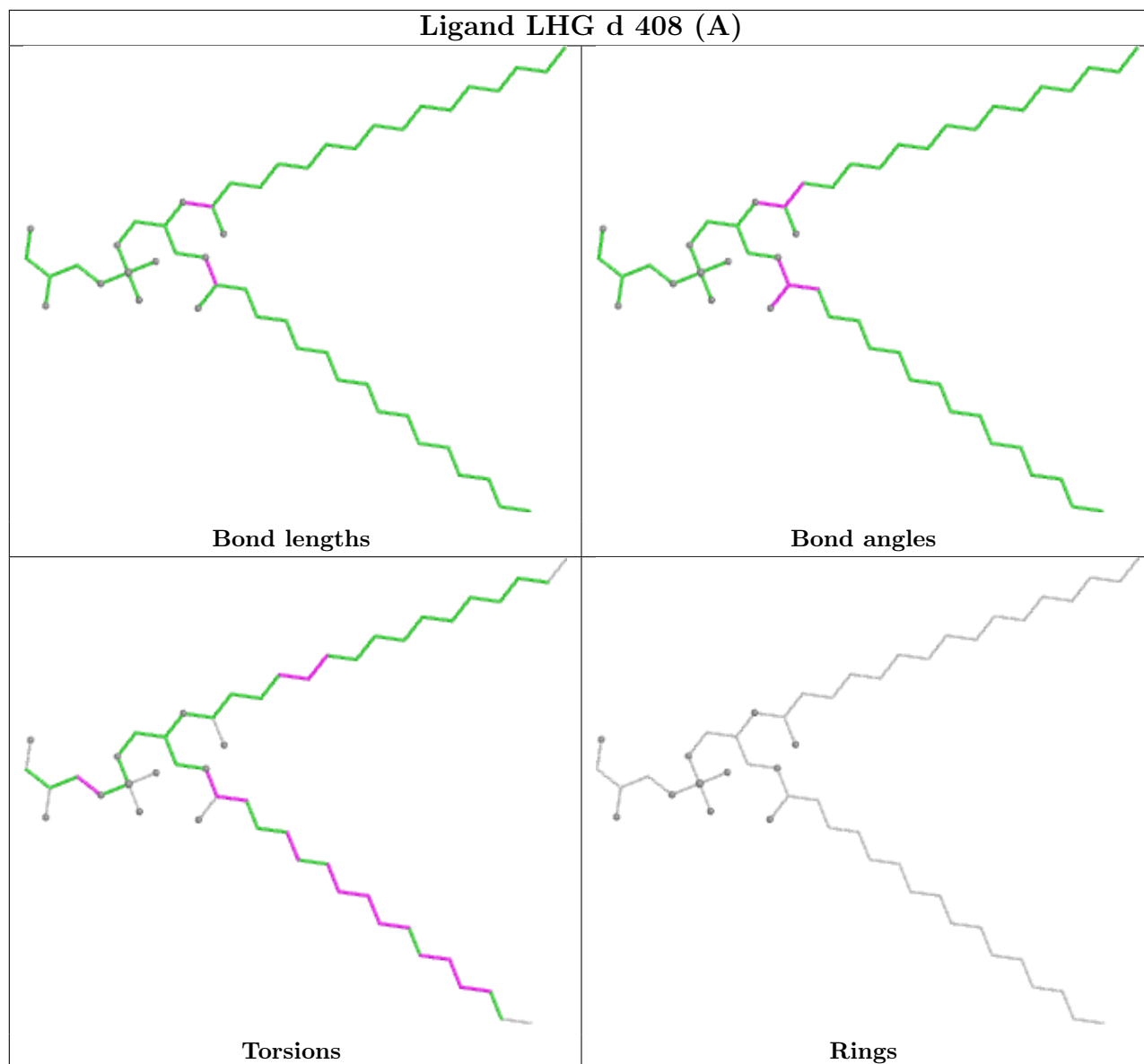
Ligand BCR d 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

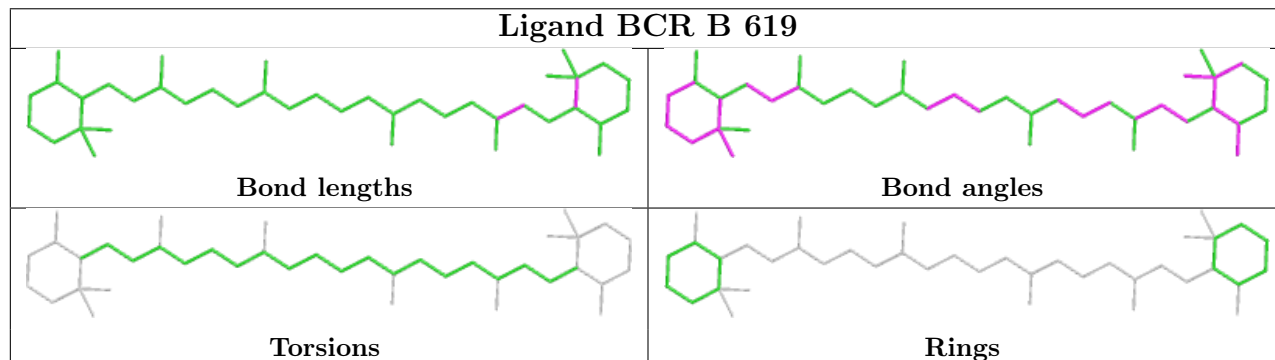


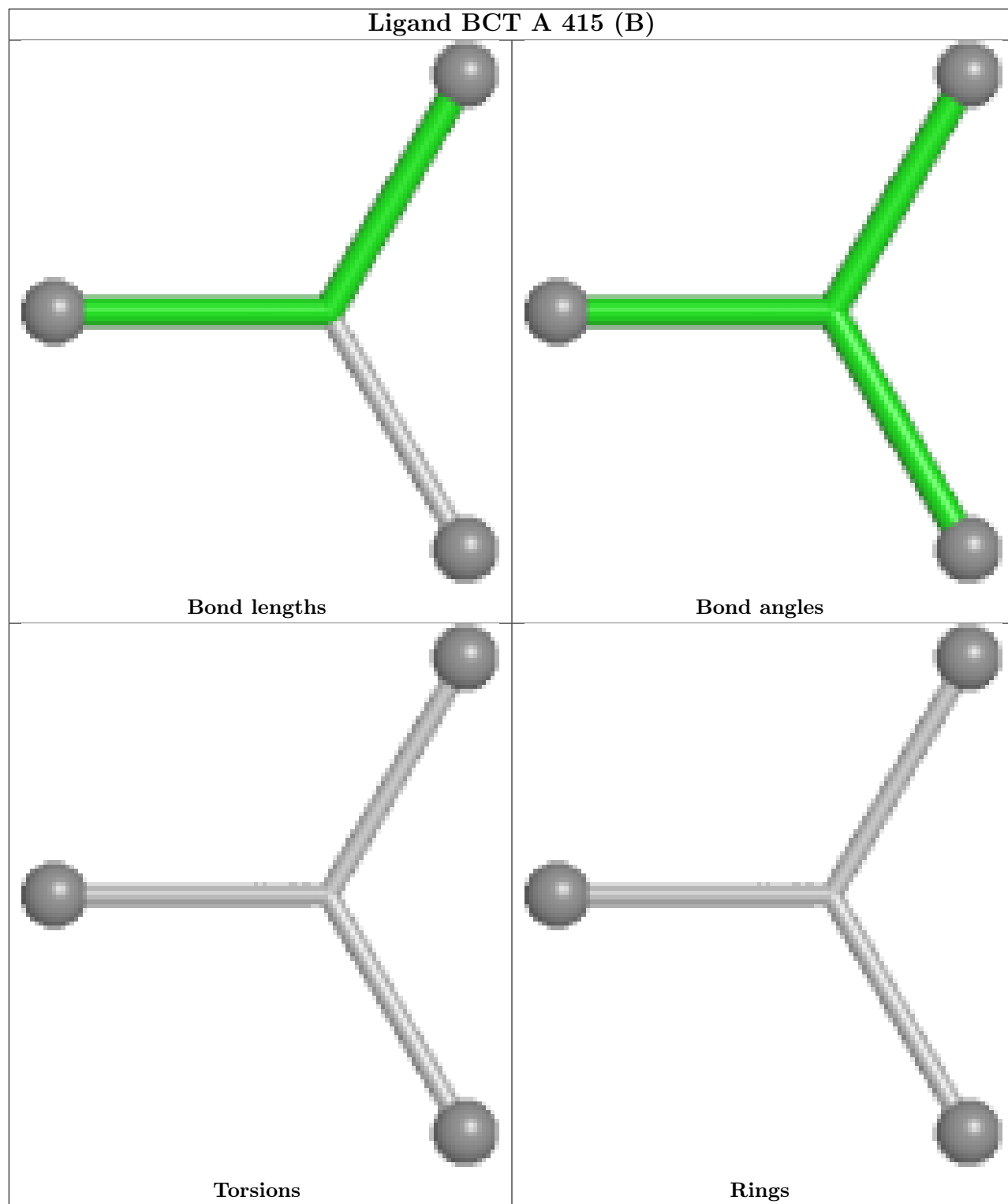


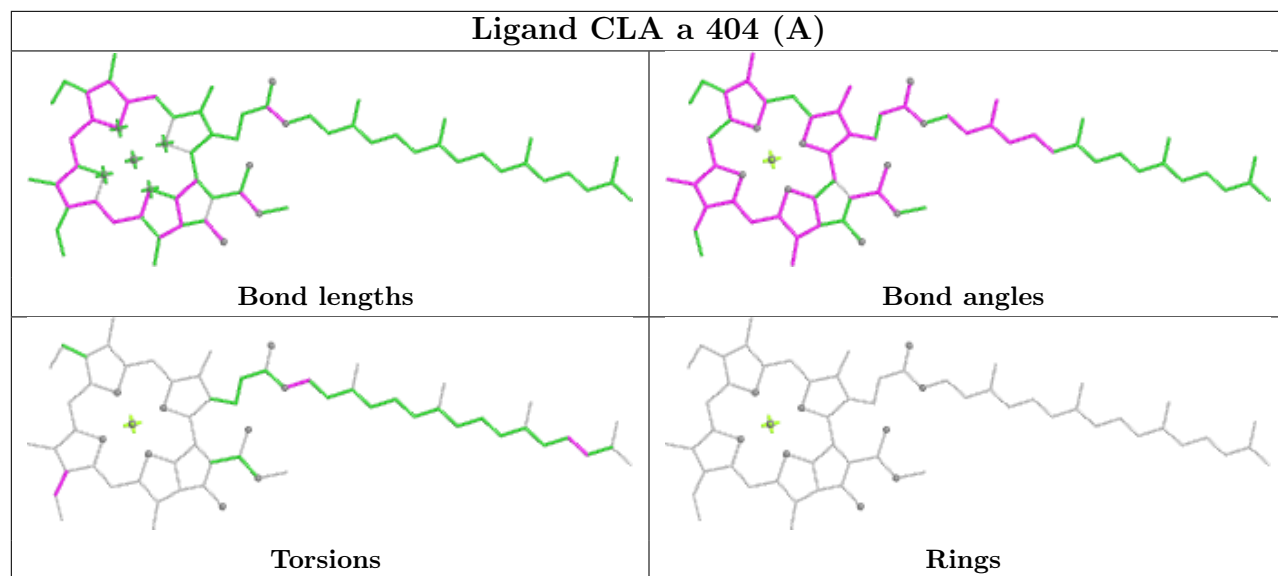
Ligand LHG d 408 (A)

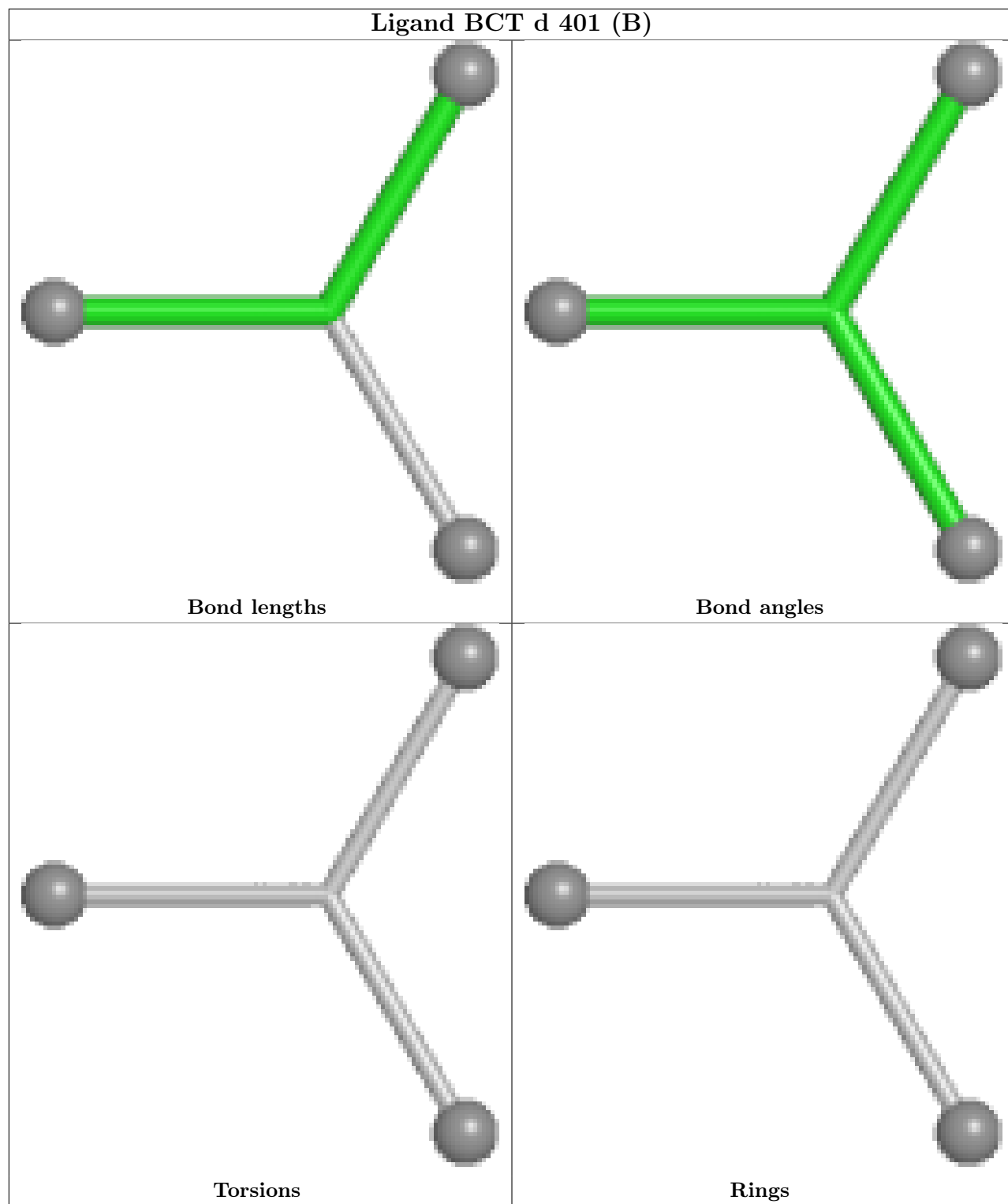


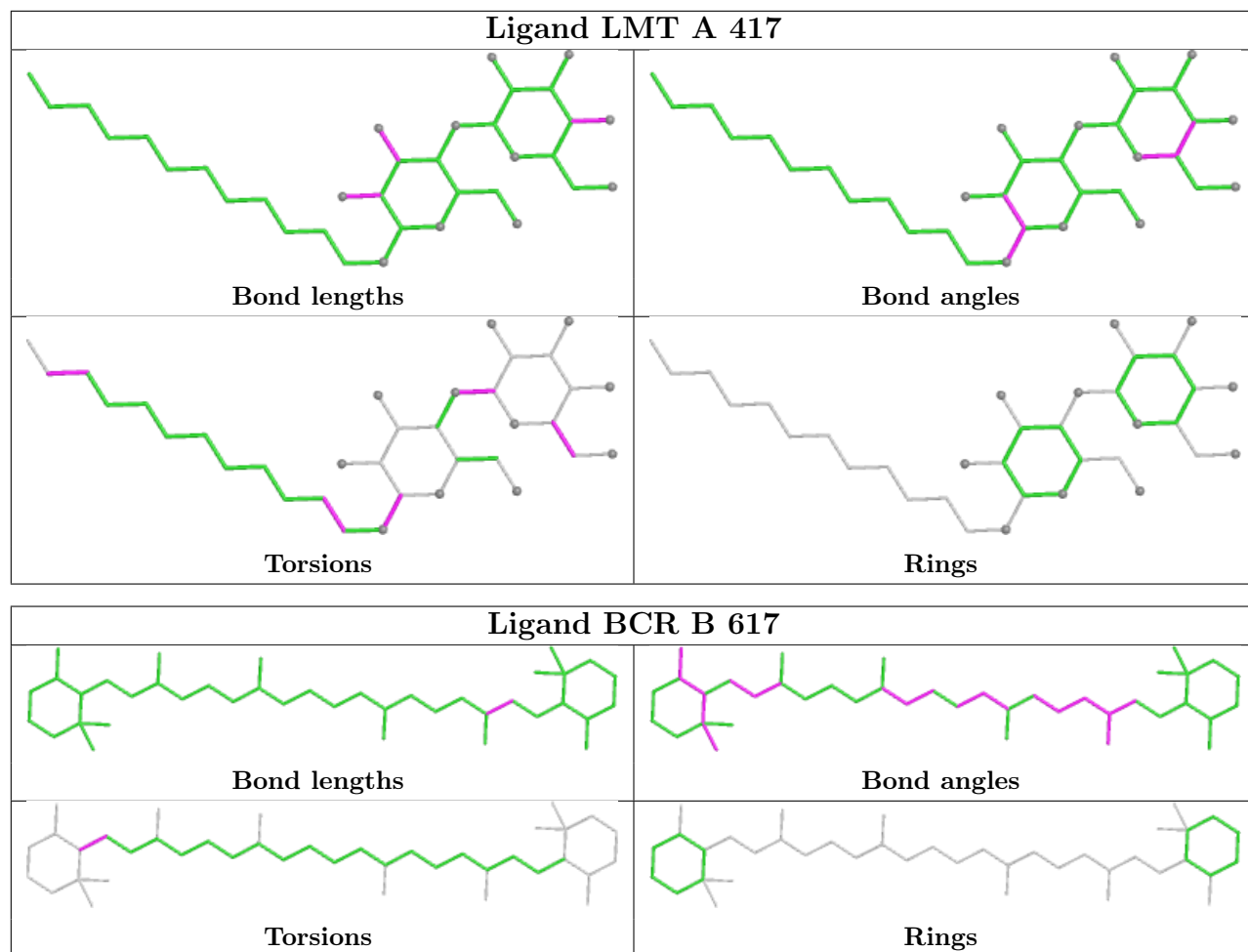
Ligand BCR B 619

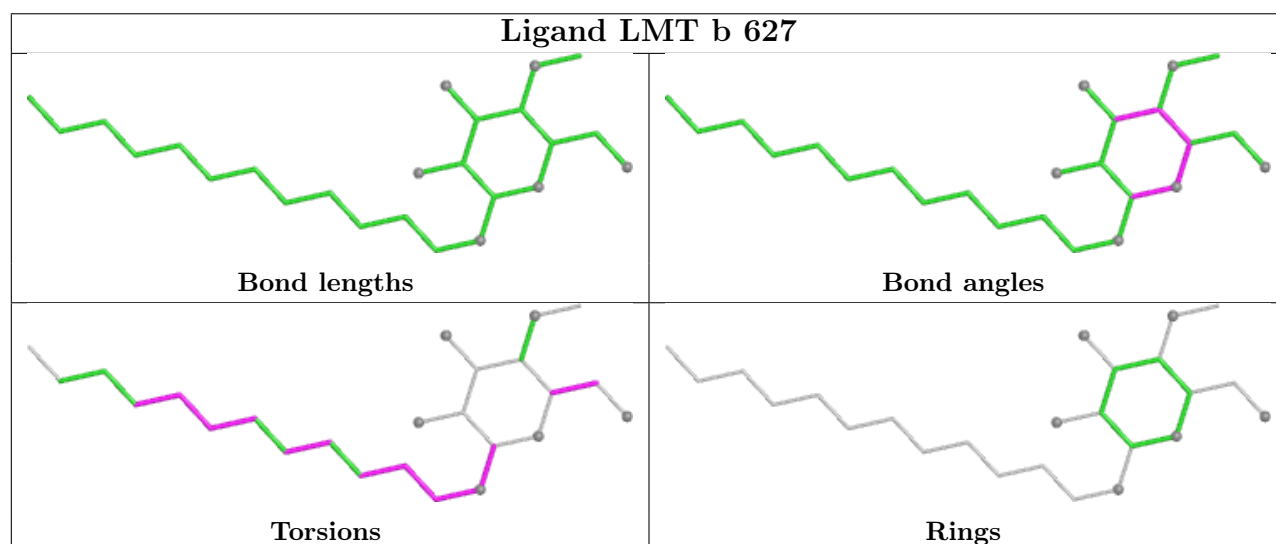
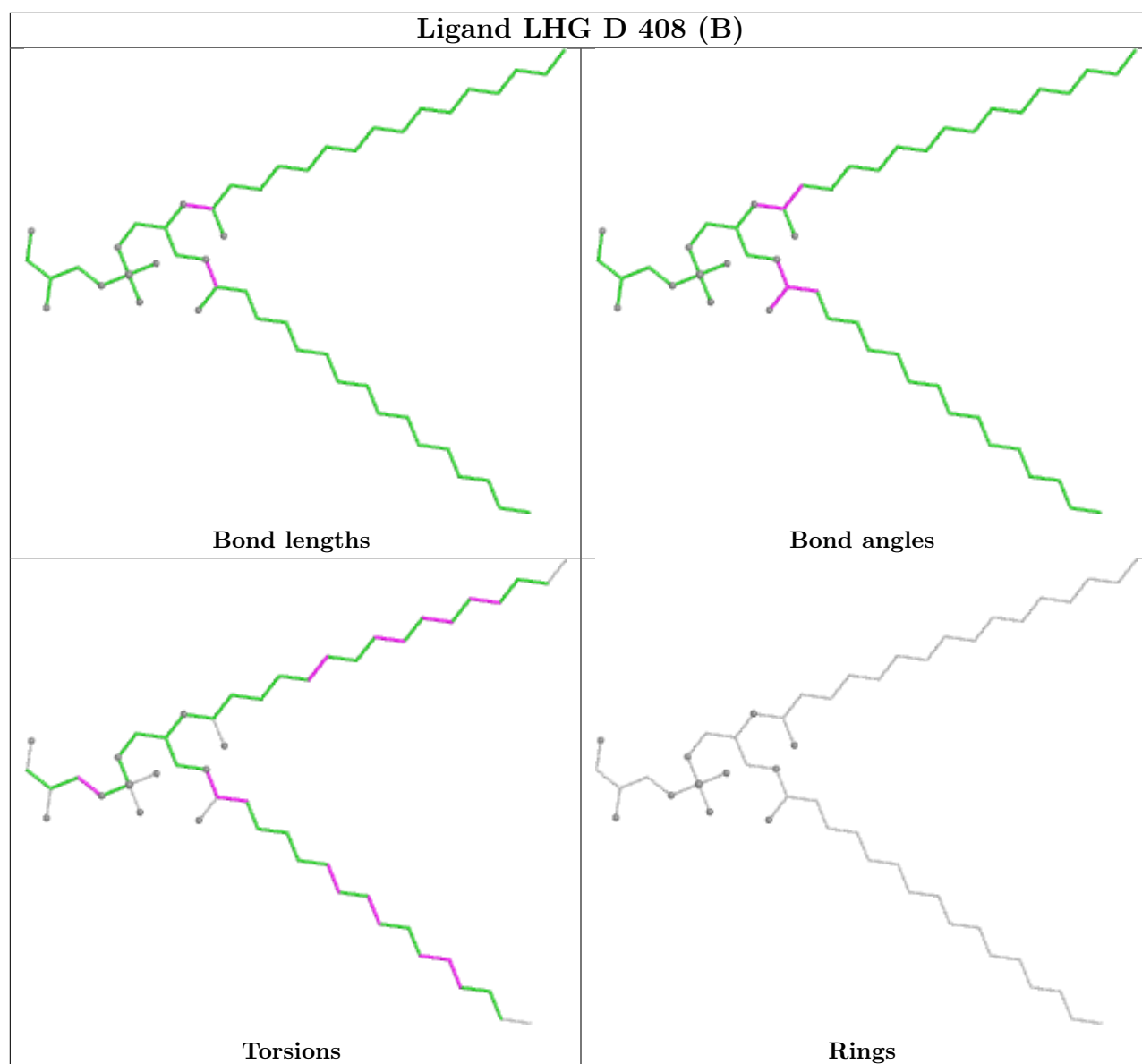


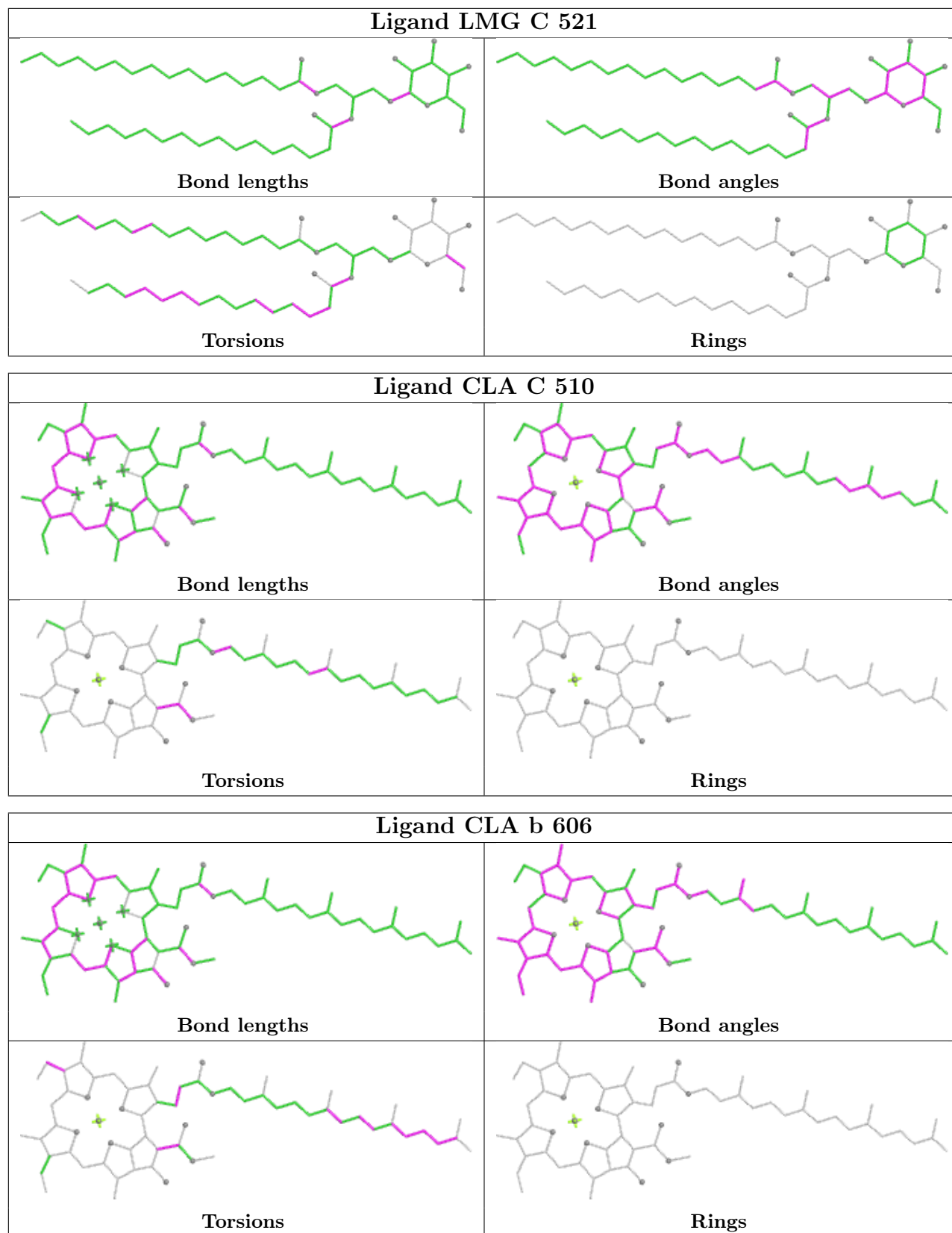


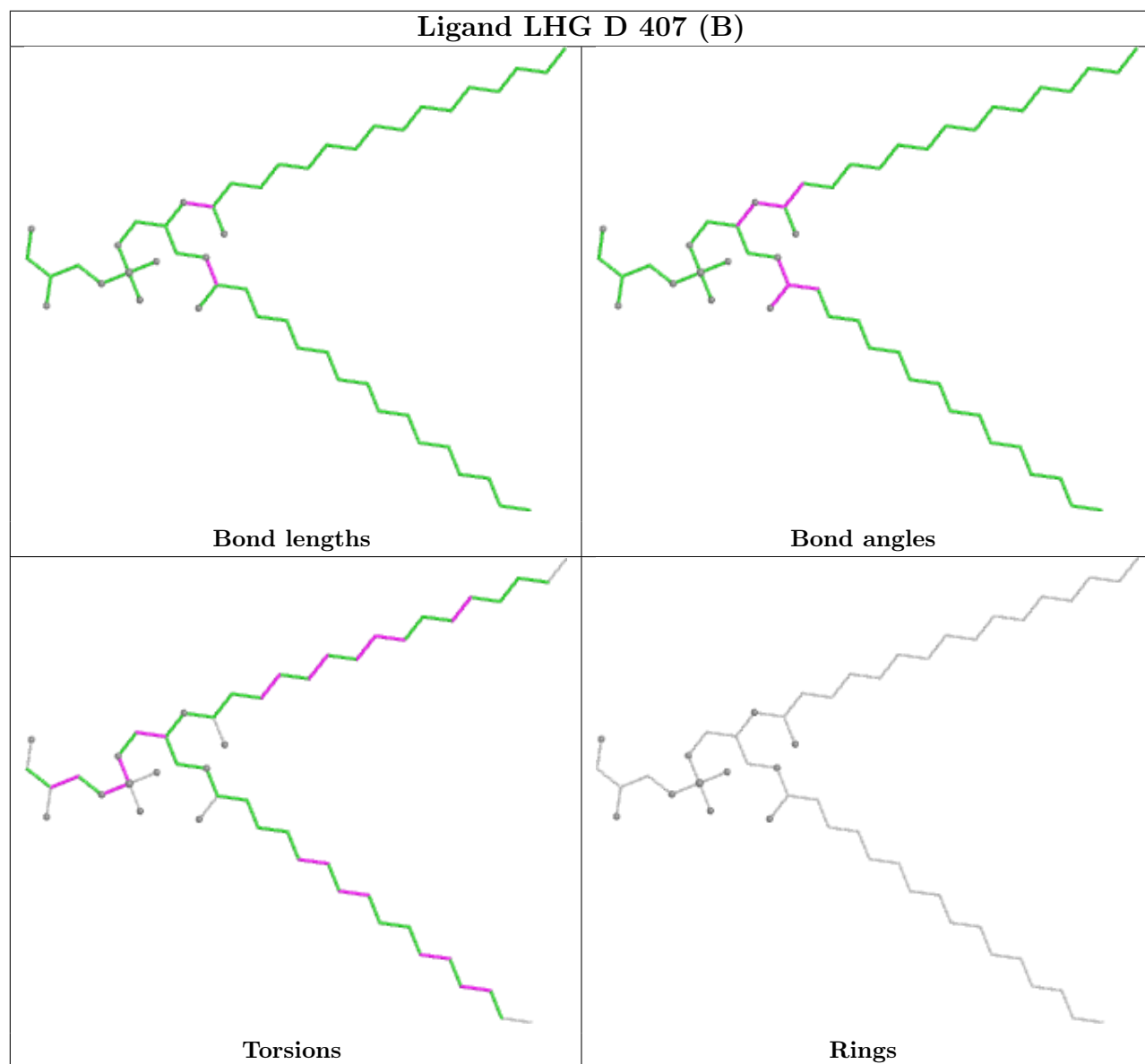
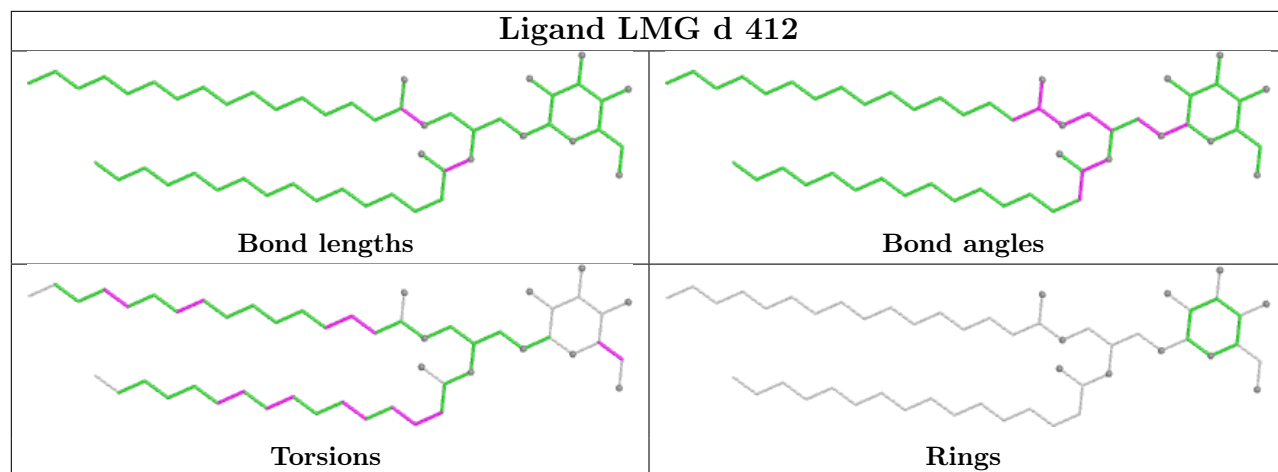


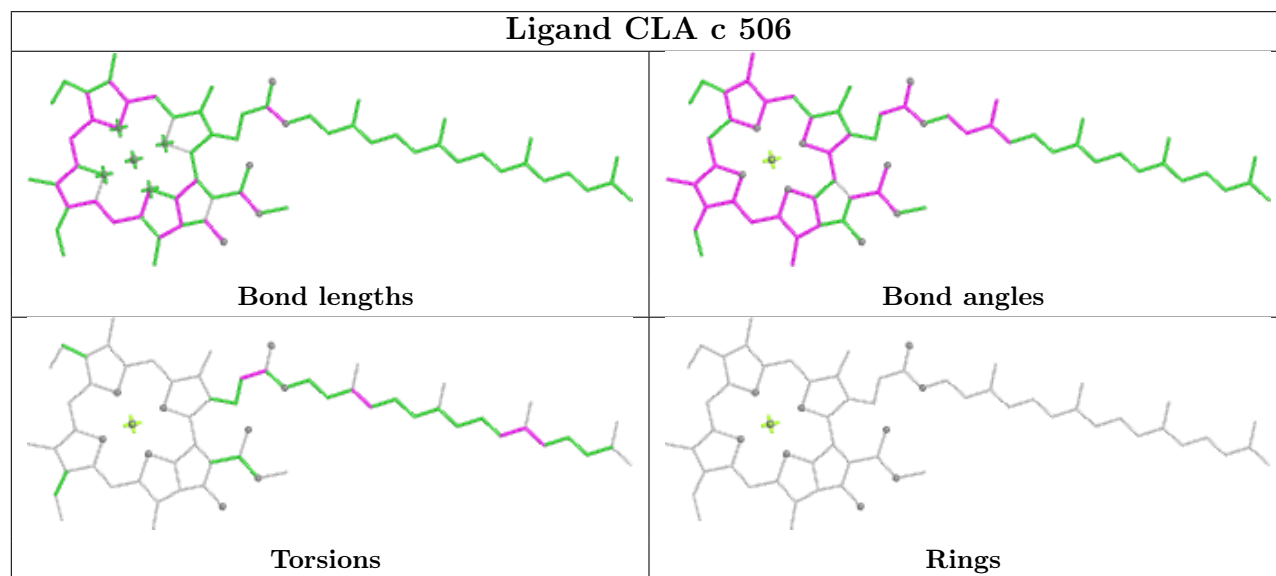
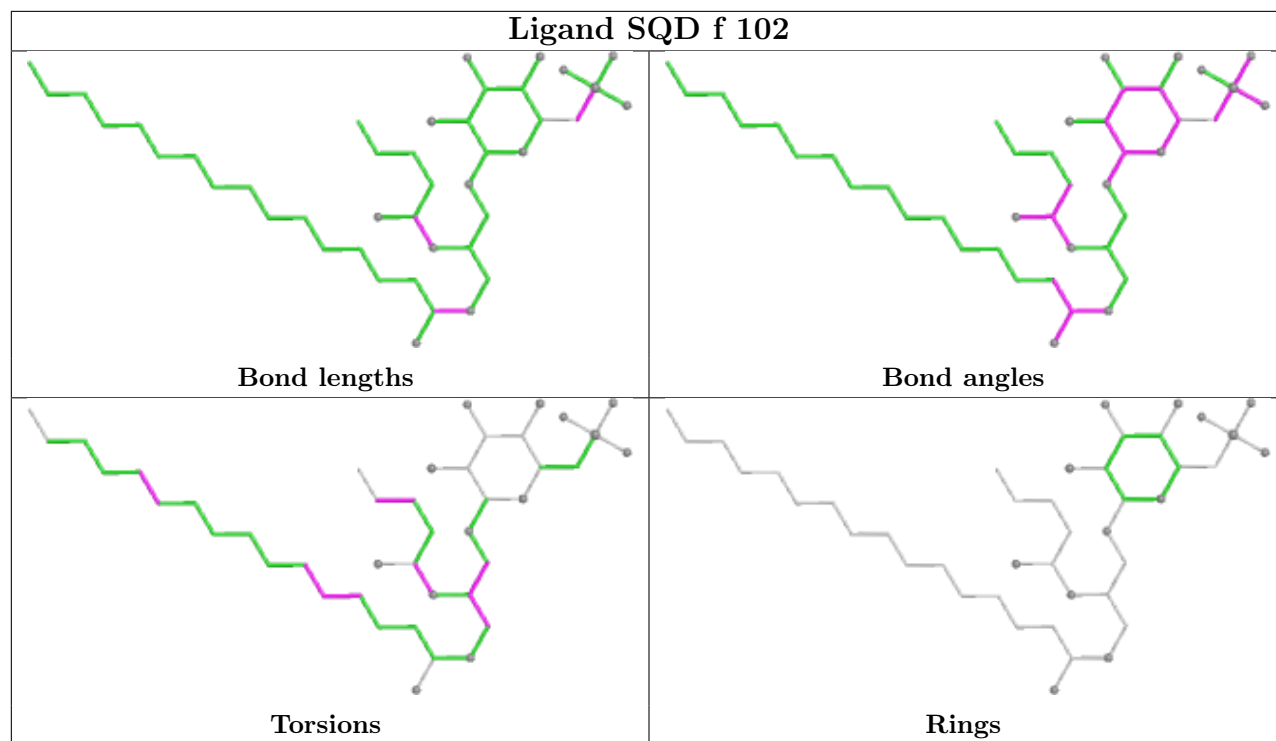


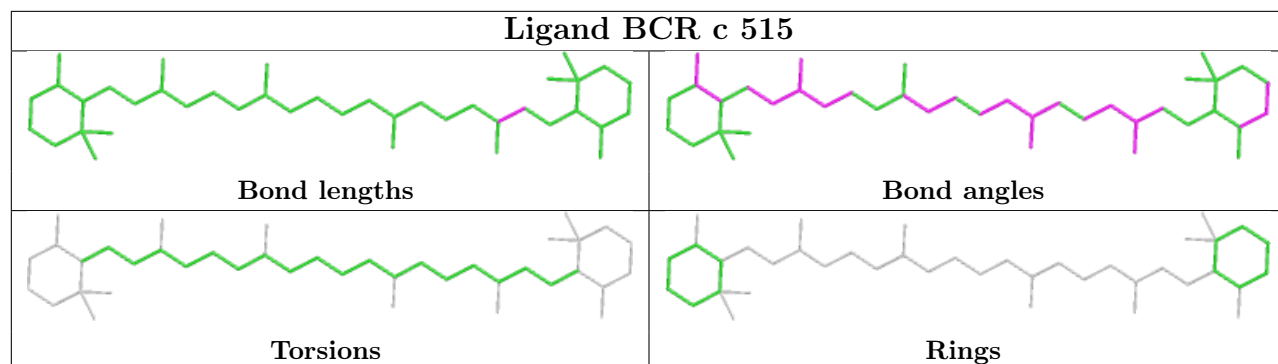
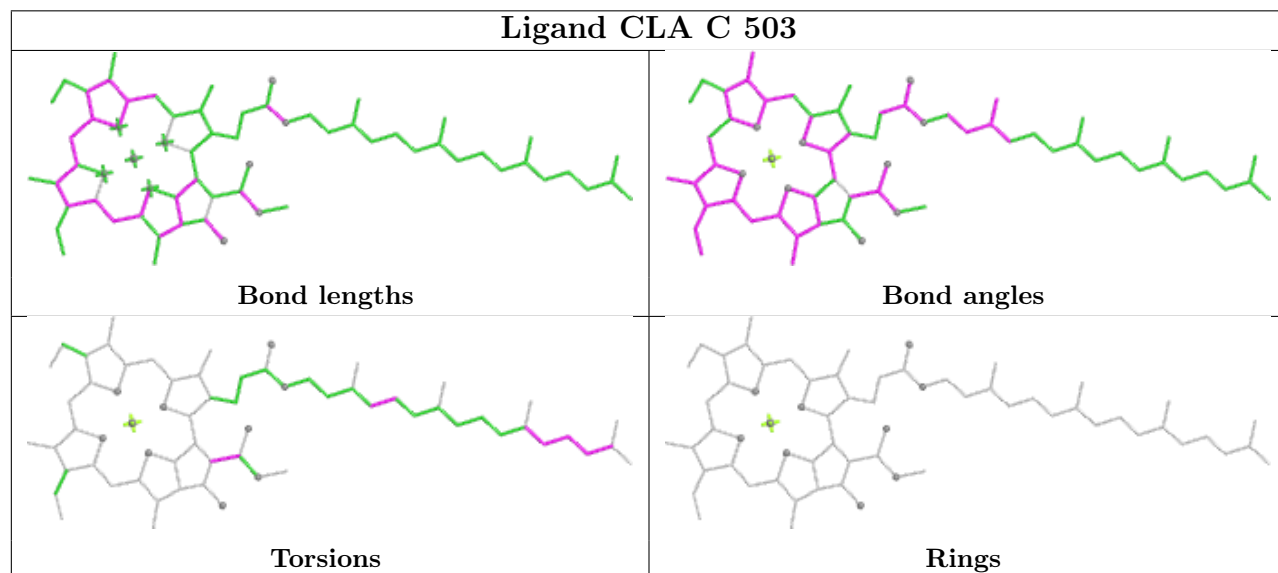
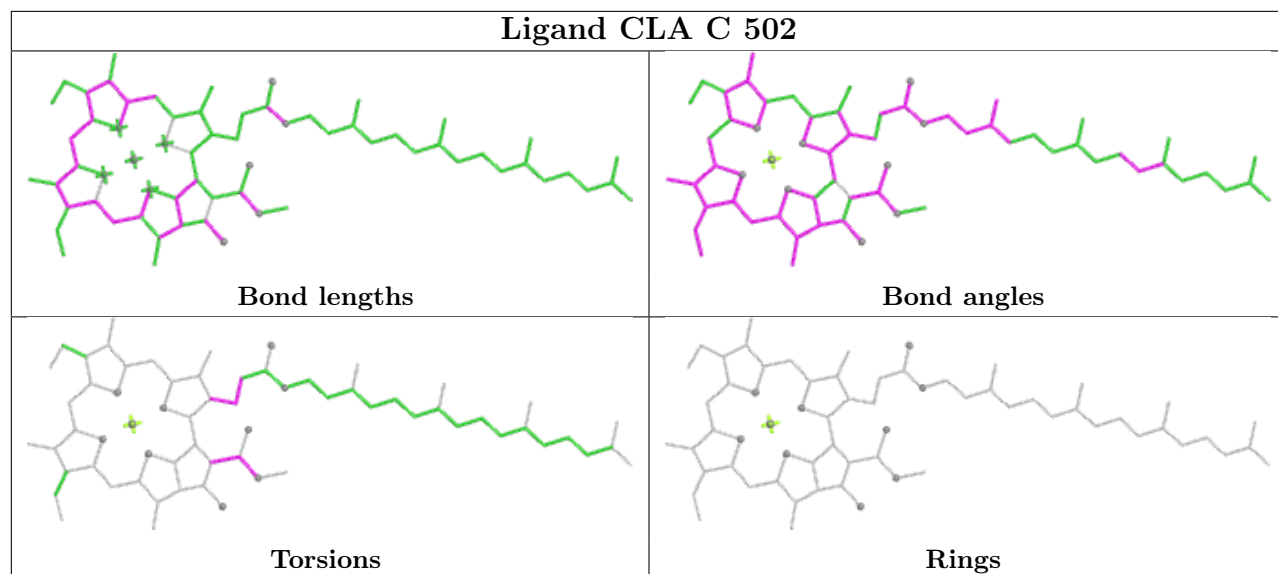


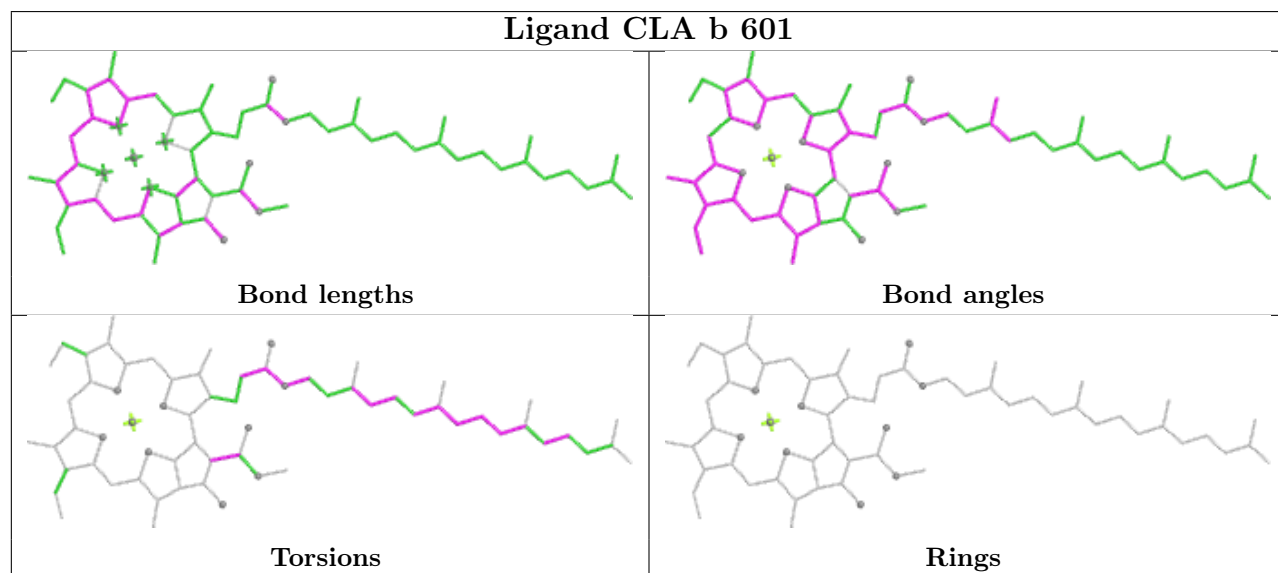
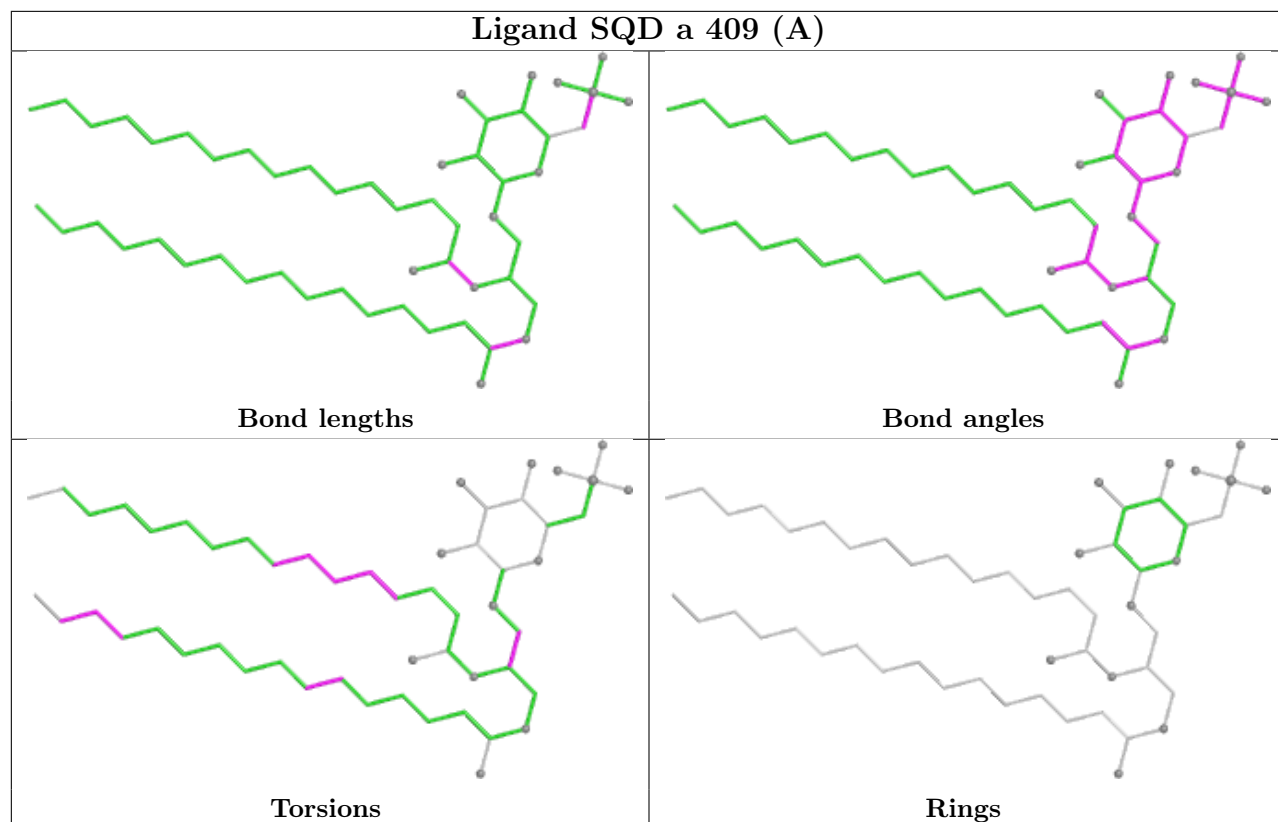




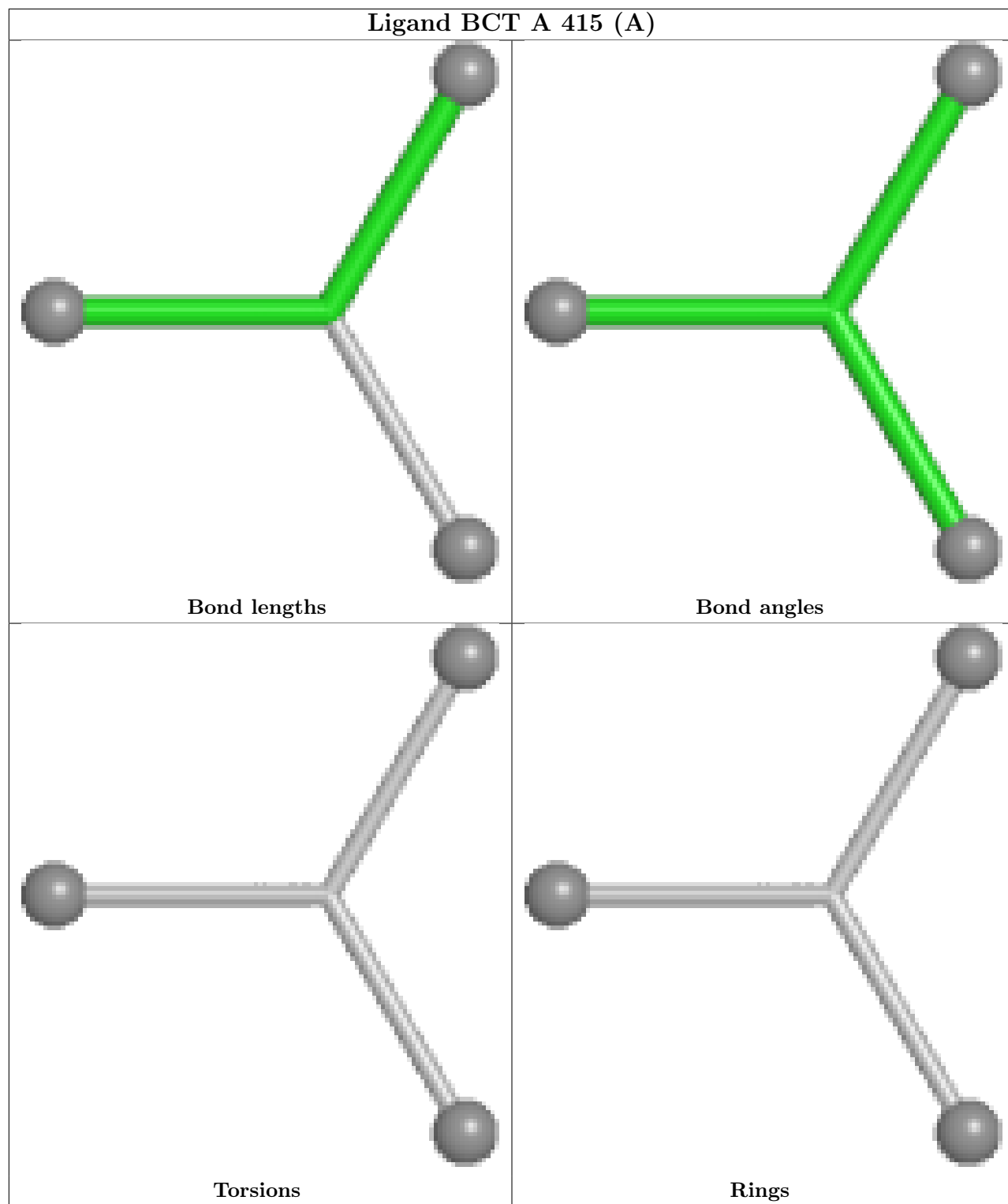


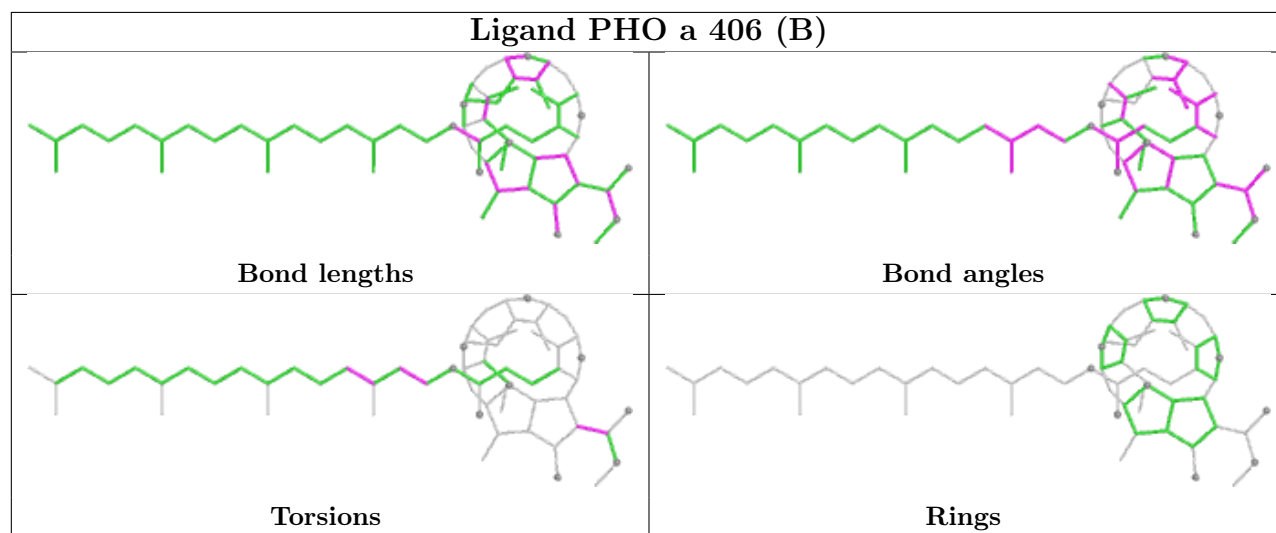
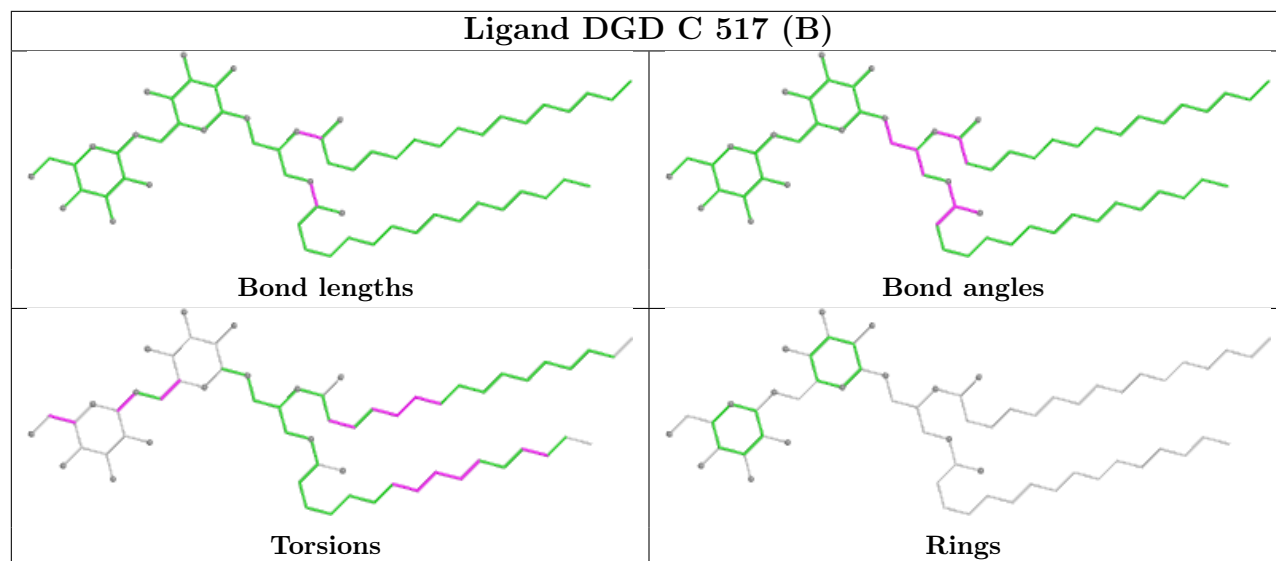


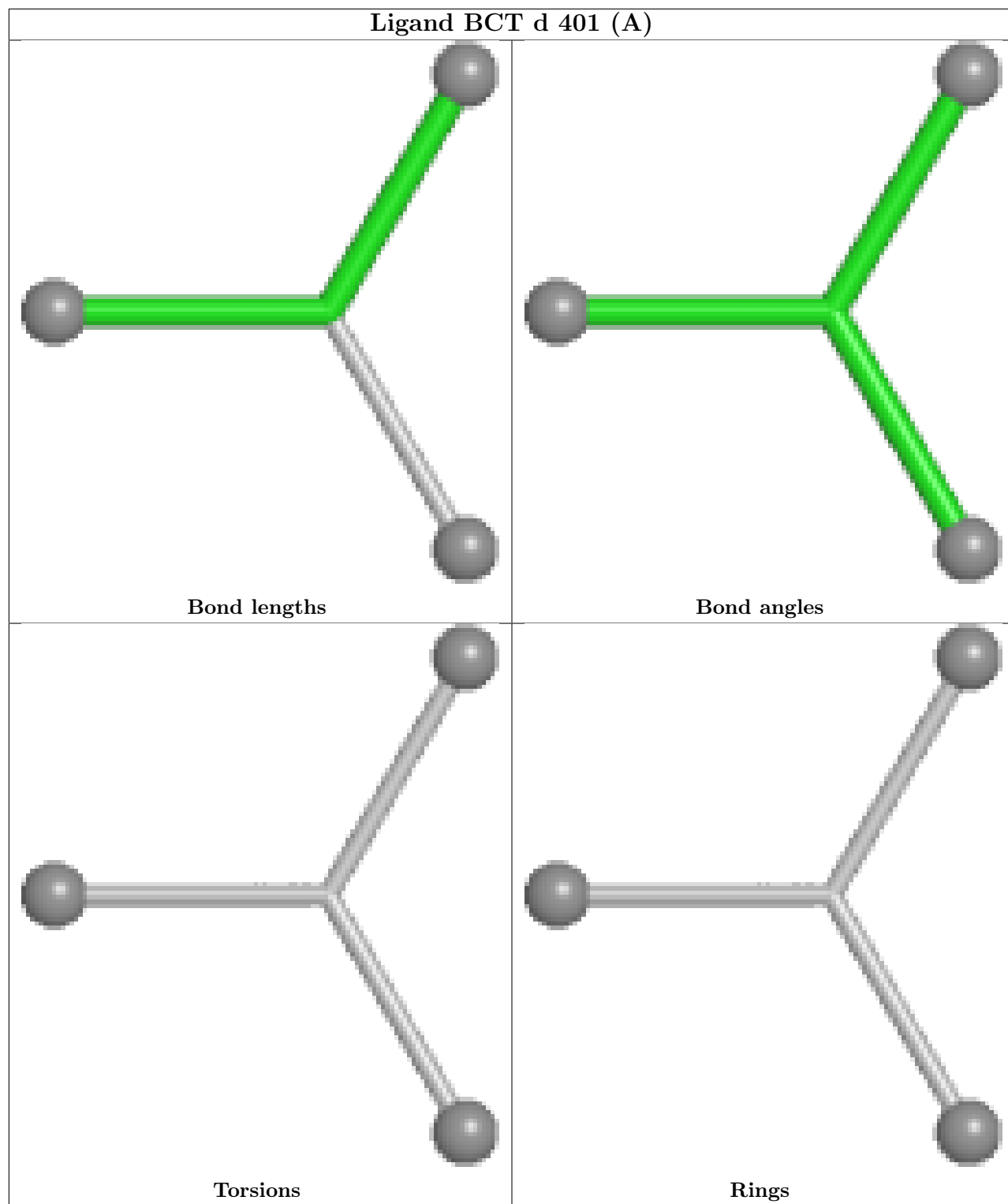




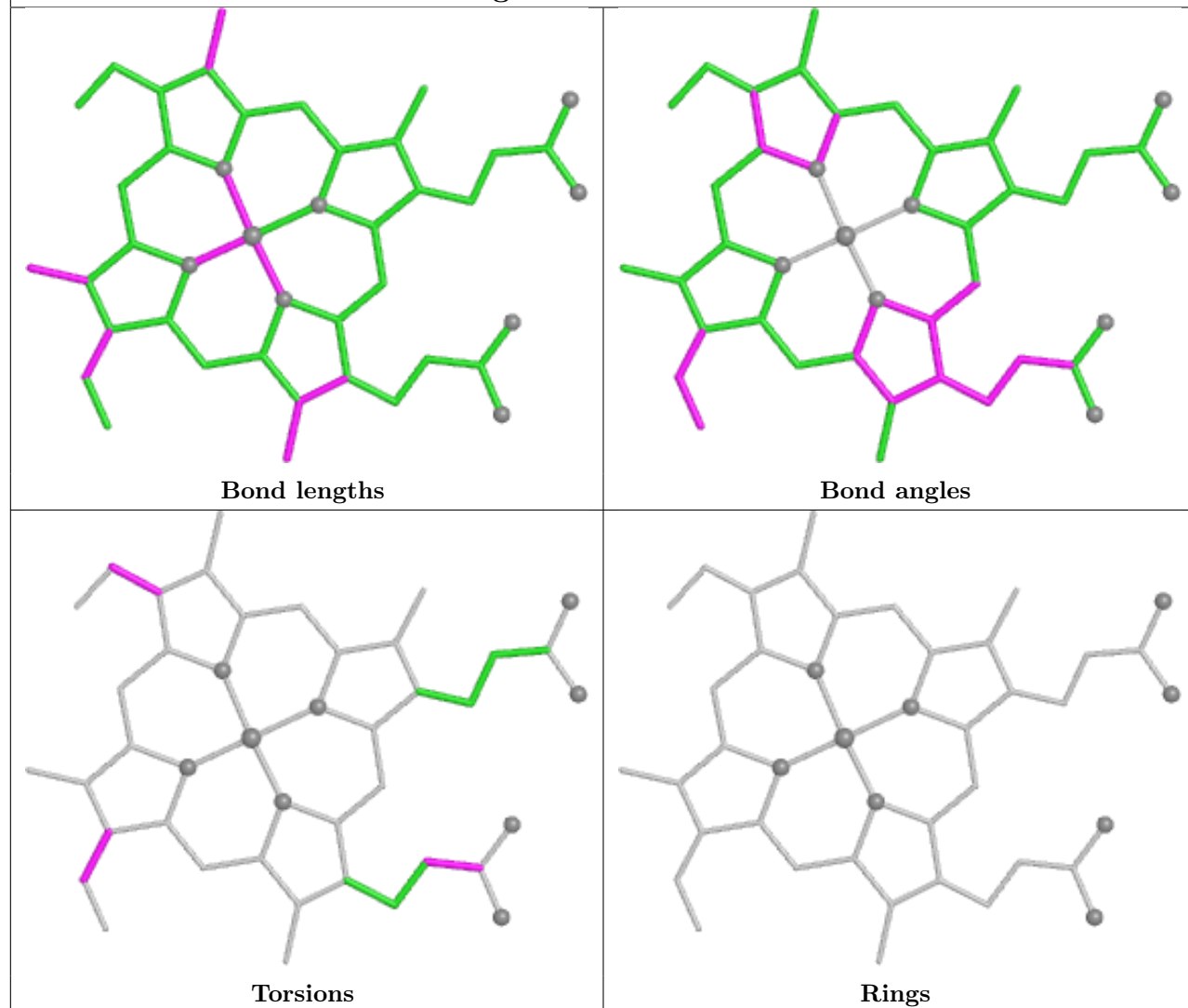
Ligand BCT A 415 (A)



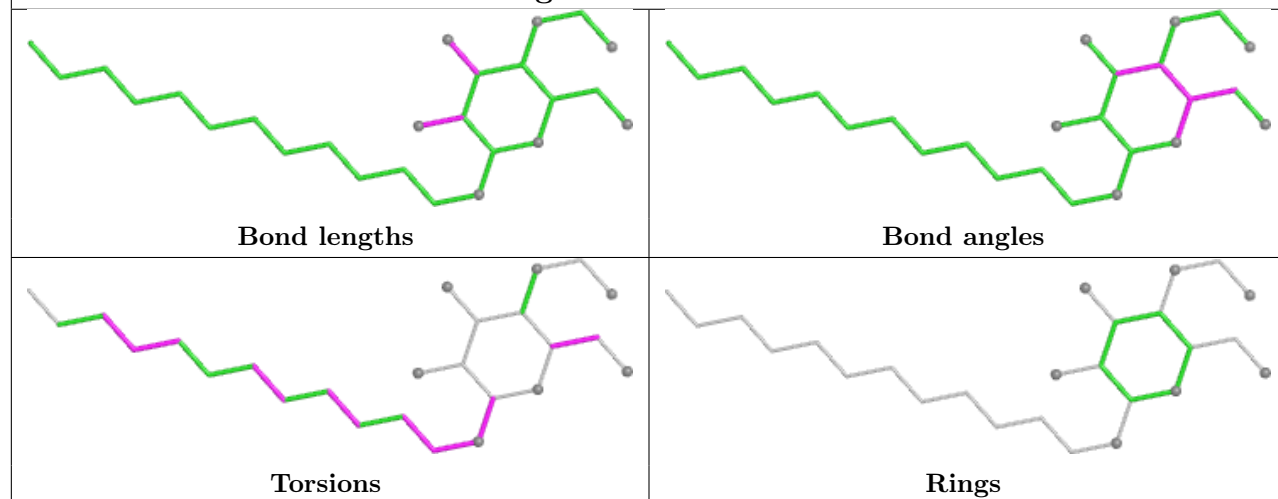


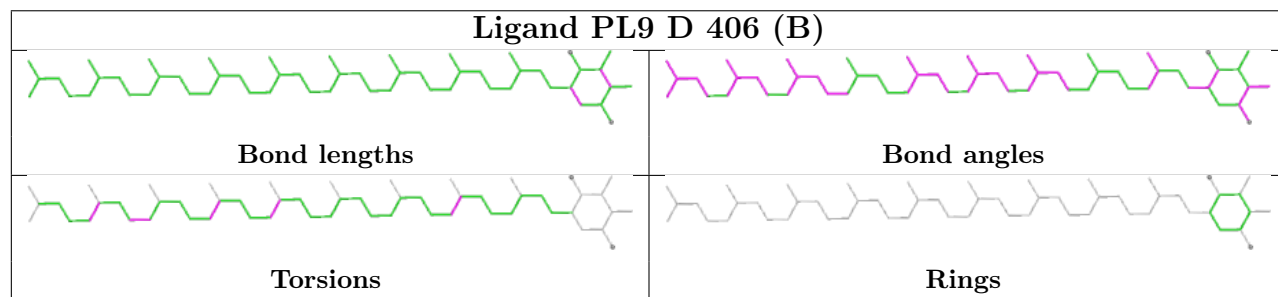
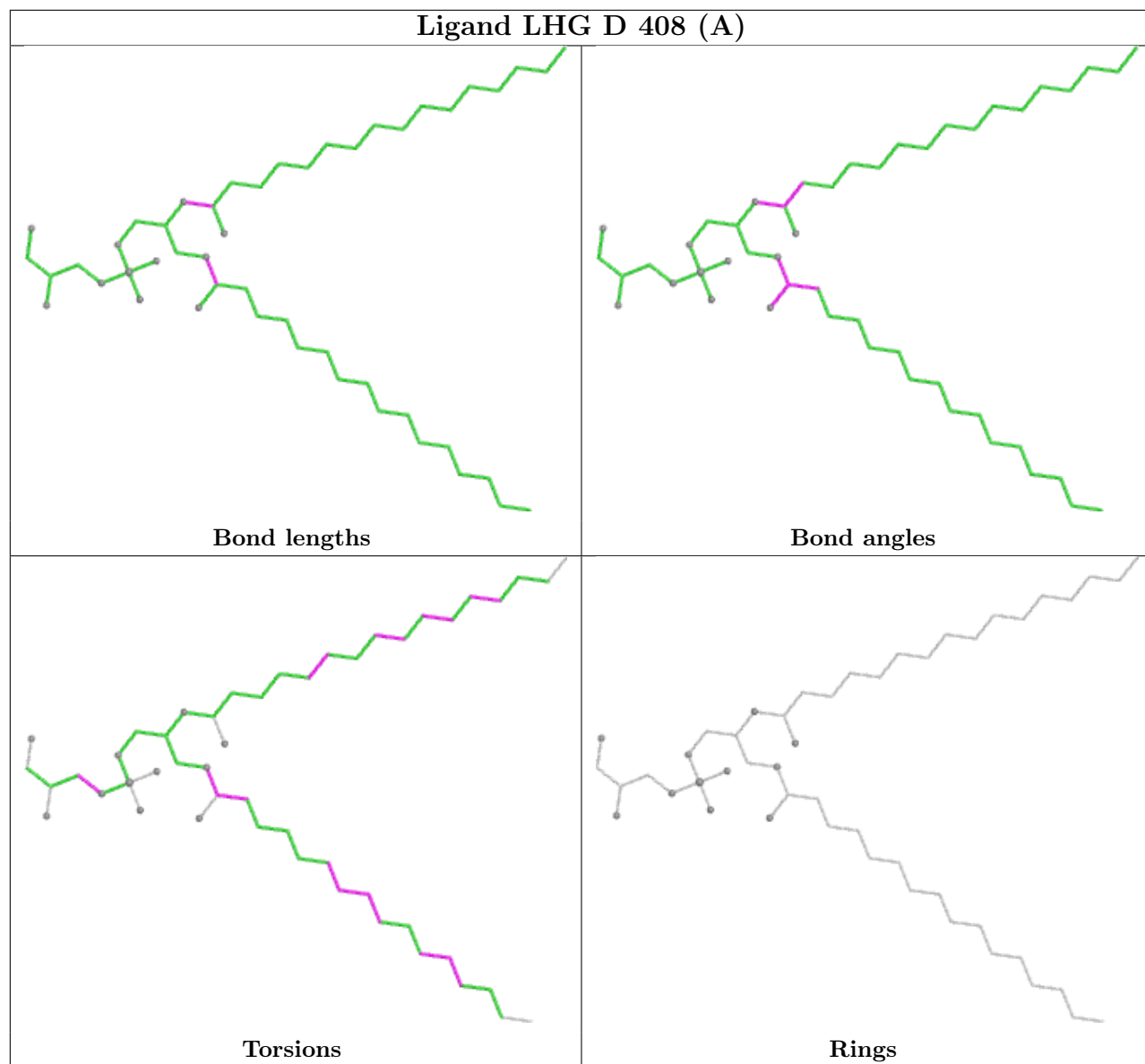


Ligand HEC V 201



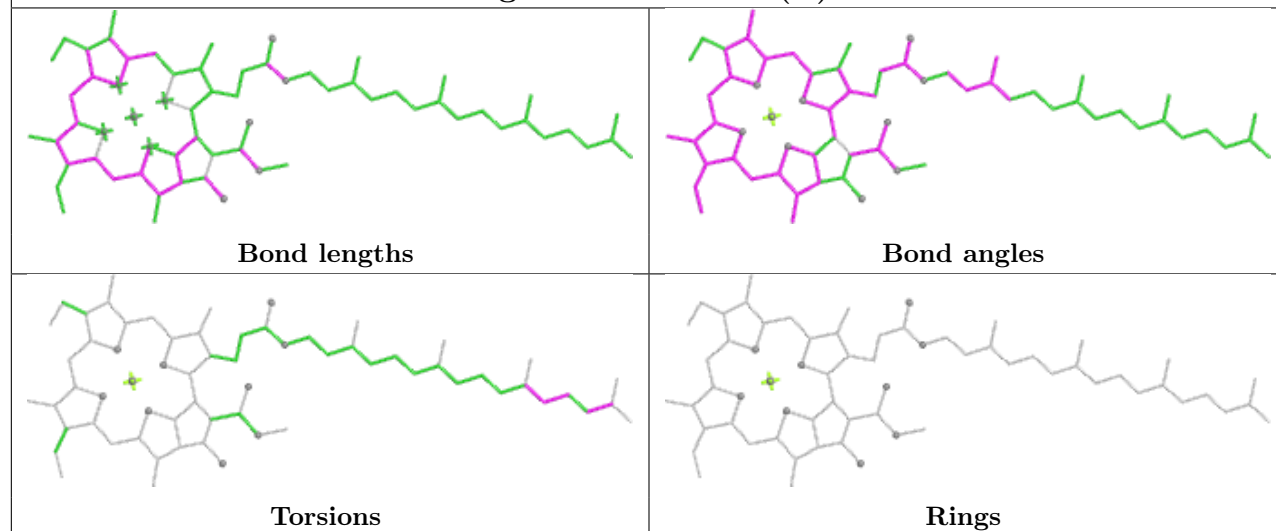
Ligand LMT t 101



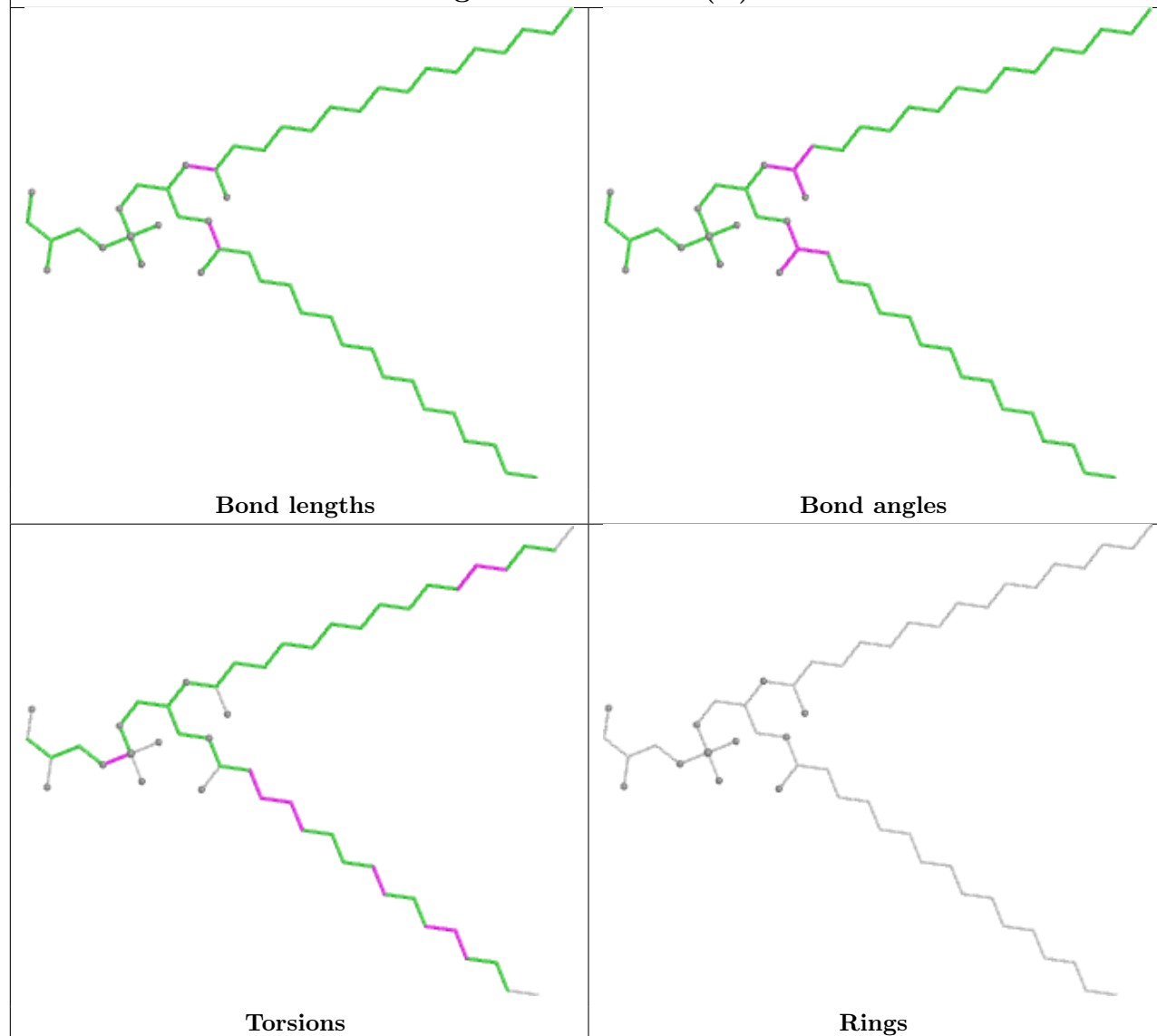


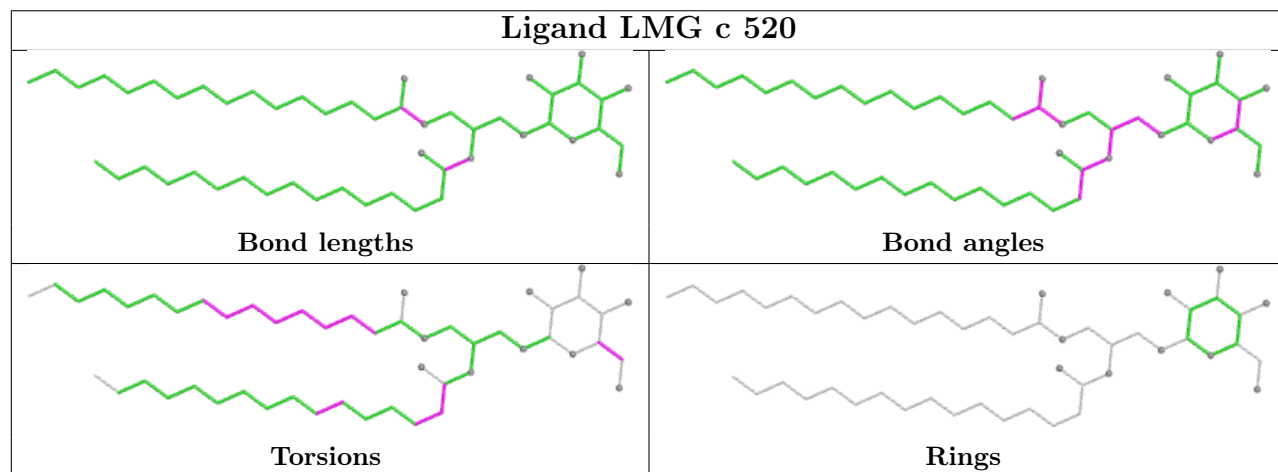
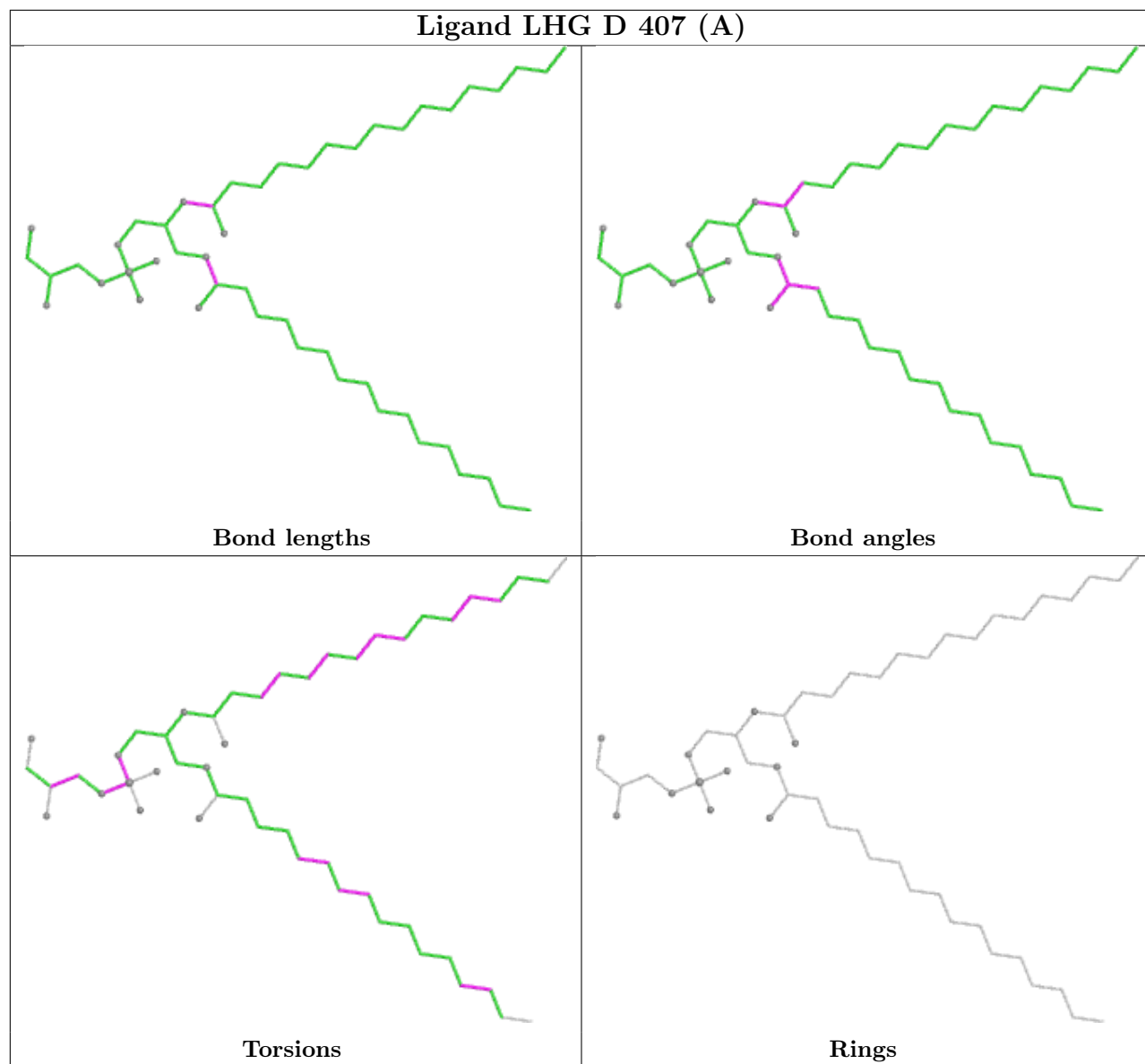
Ligand CLA d 402 (B)	
Bond lengths	Bond angles
Torsions	Rings
Ligand BCR h 101	
Bond lengths	Bond angles
Torsions	Rings
Ligand BCR c 516	
Bond lengths	Bond angles
Torsions	Rings

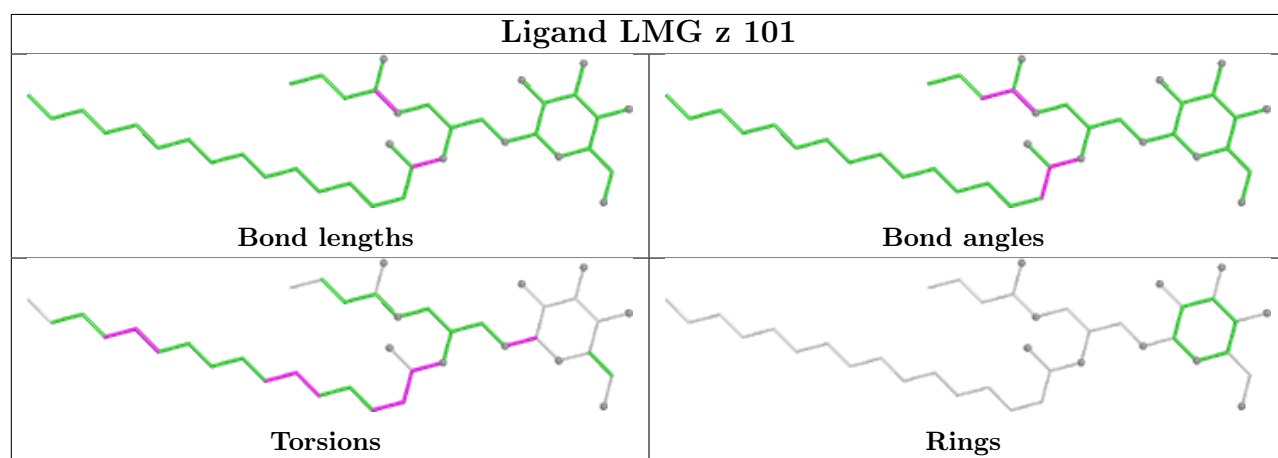
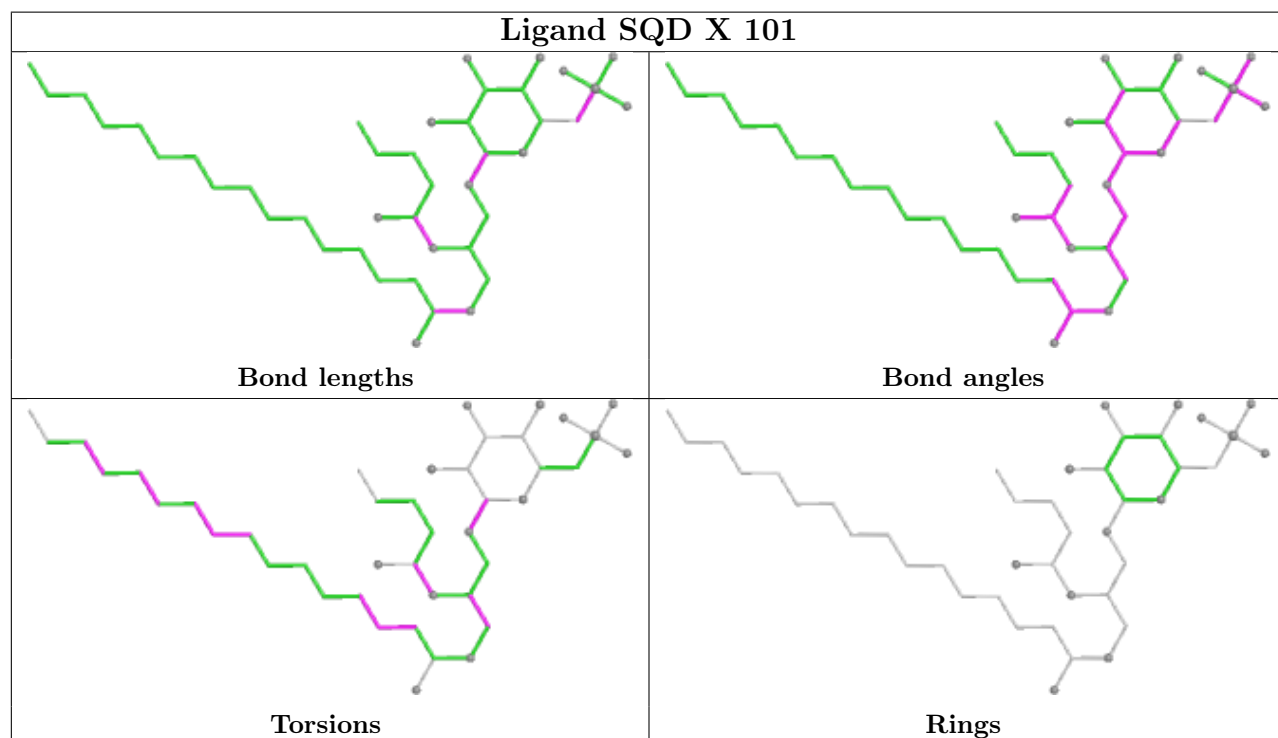
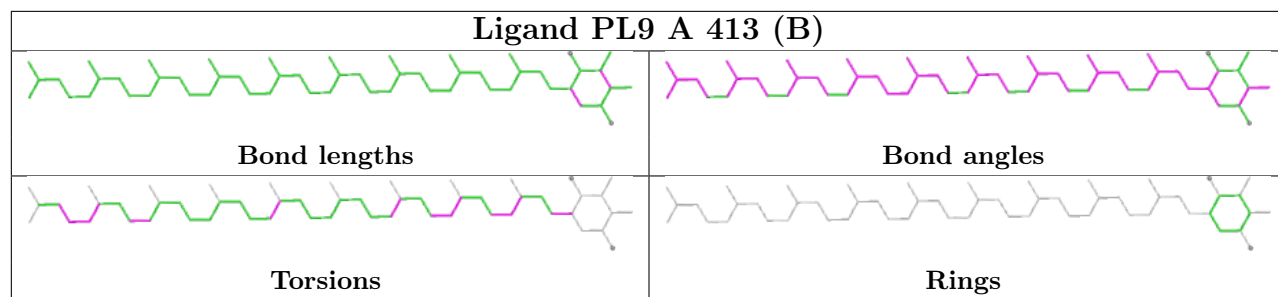
Ligand CLA A 406 (B)

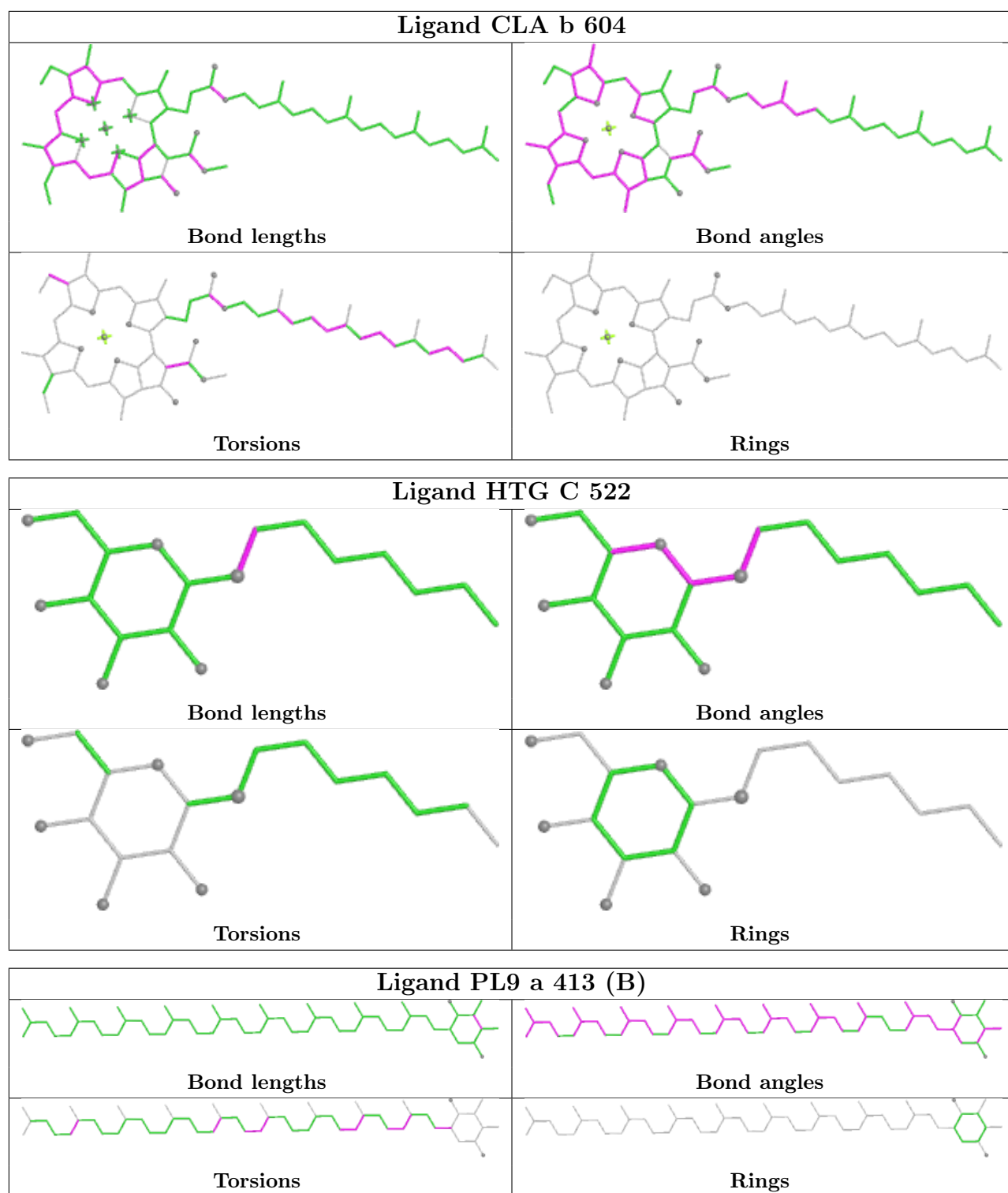


Ligand LHG d 414 (B)

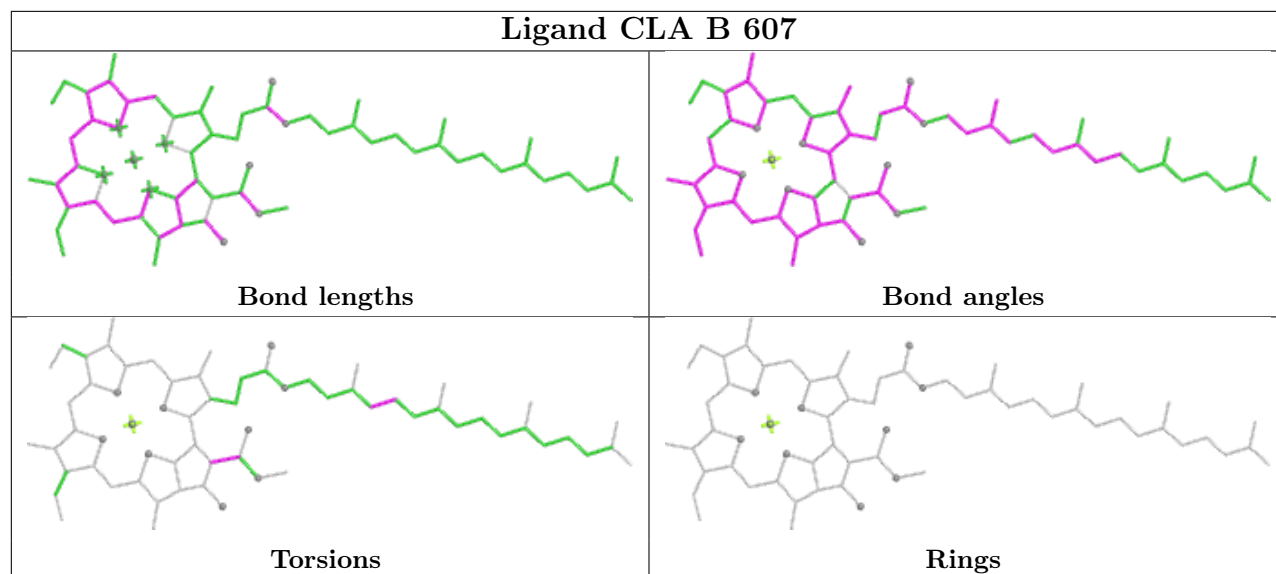




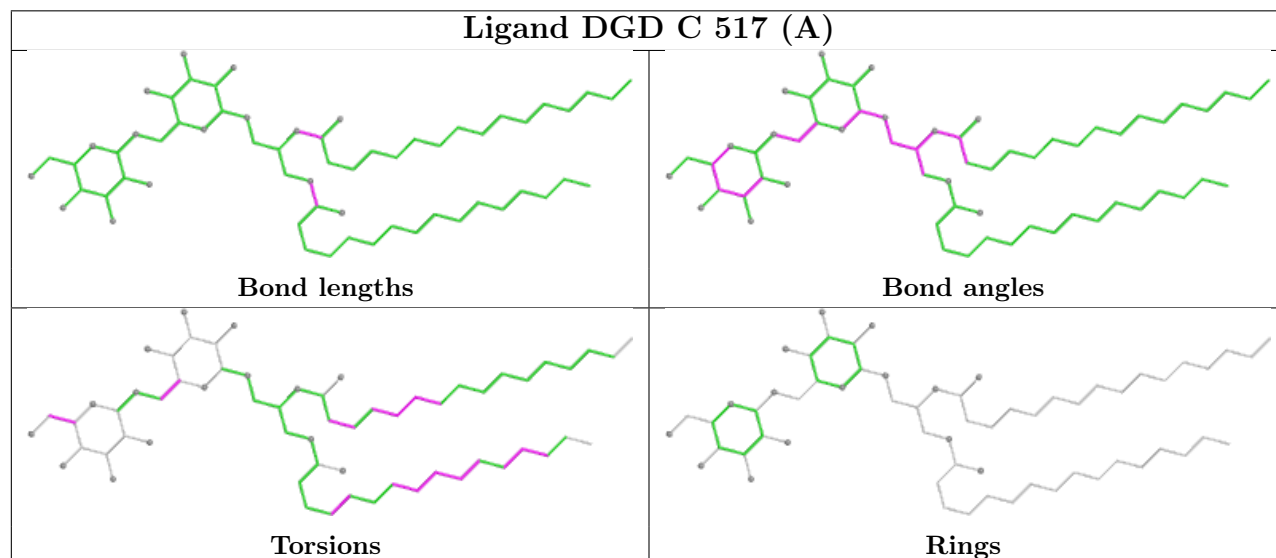




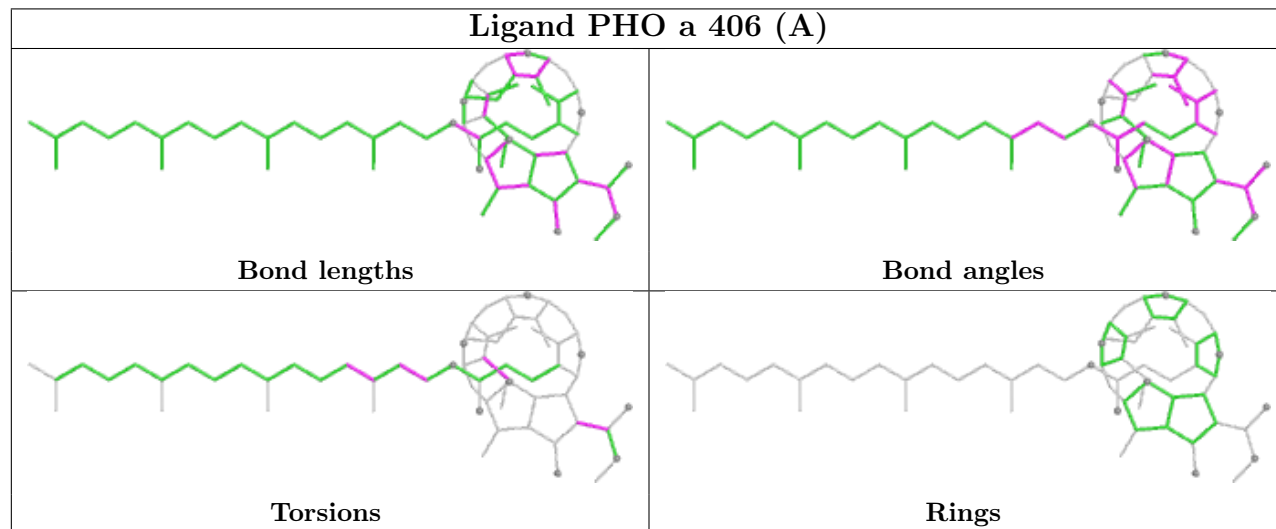
Ligand CLA B 607

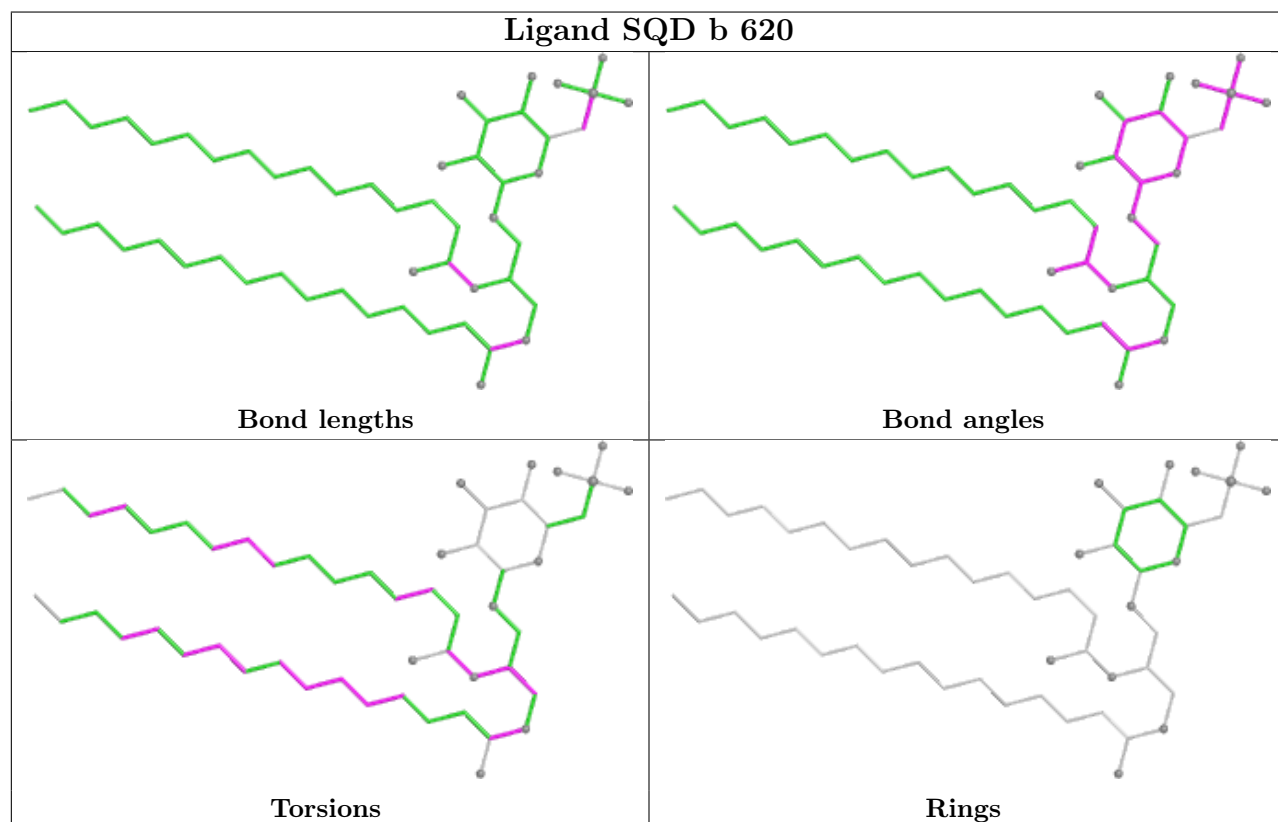
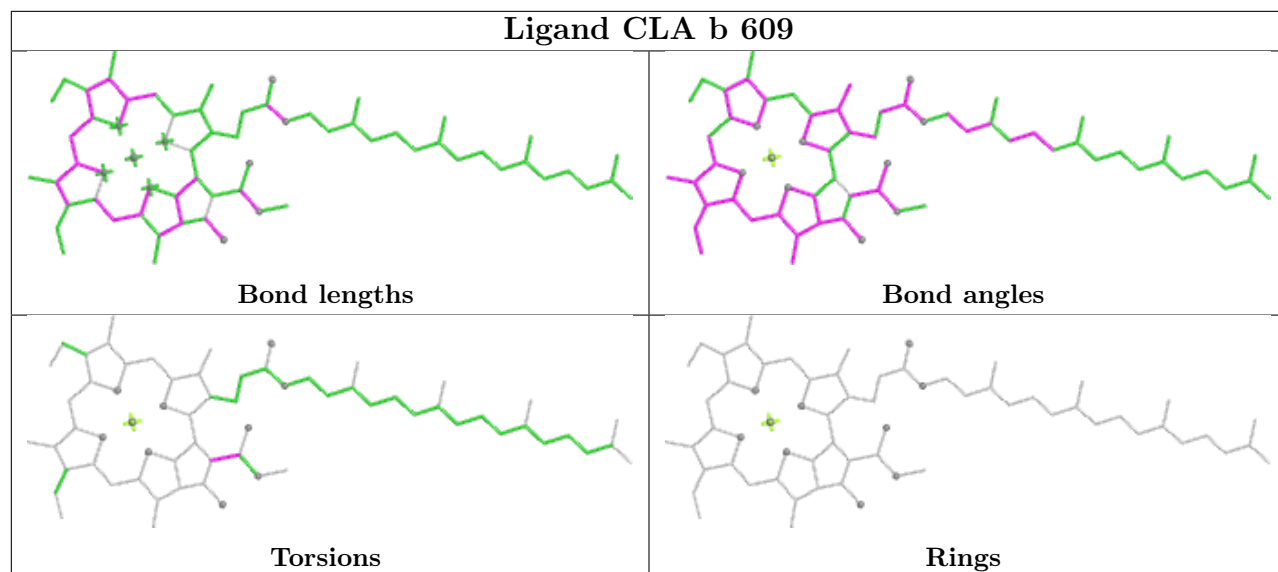


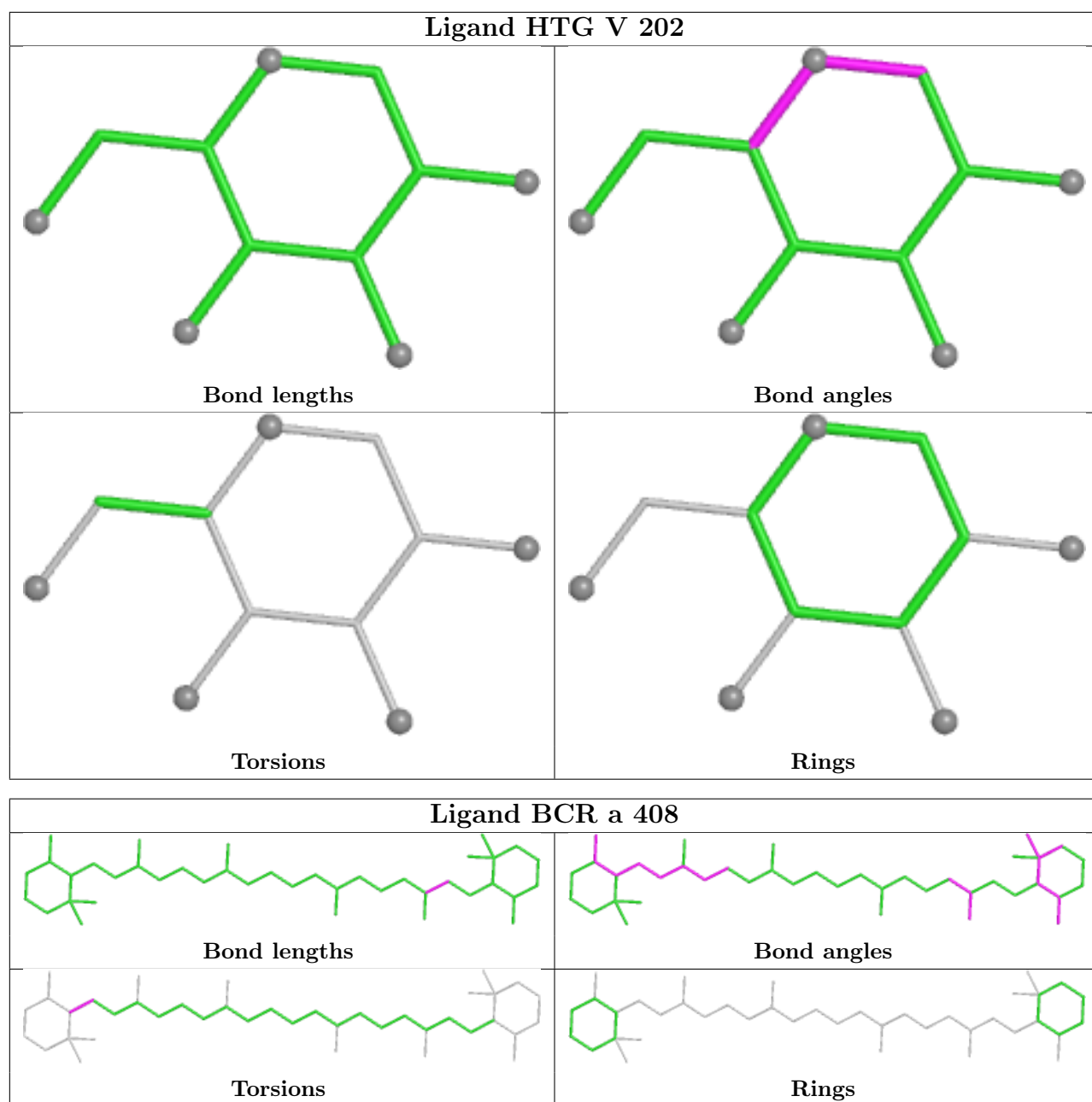
Ligand DGD C 517 (A)

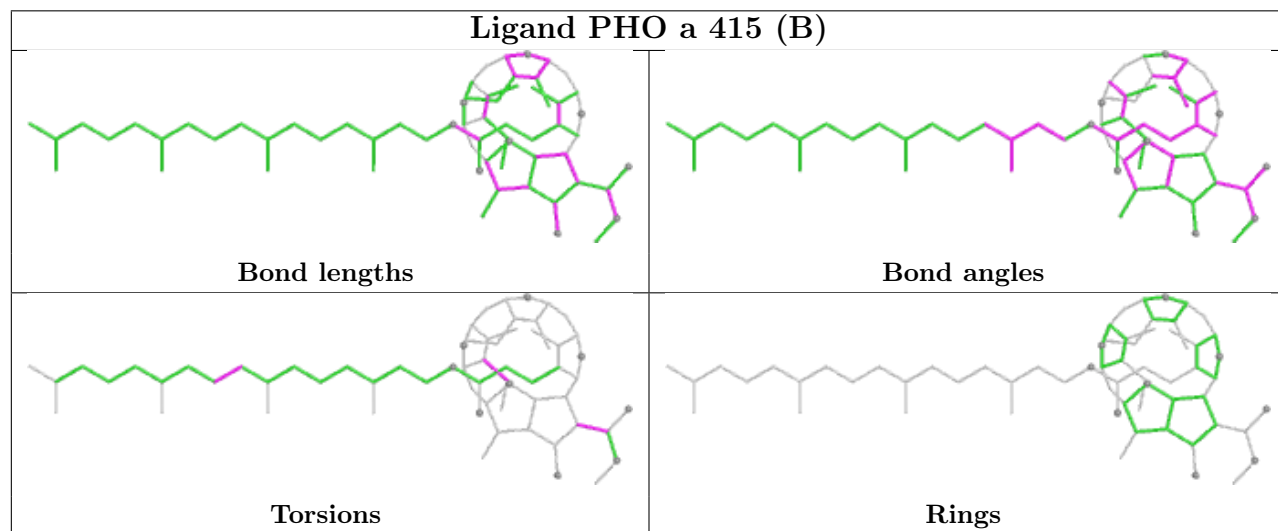
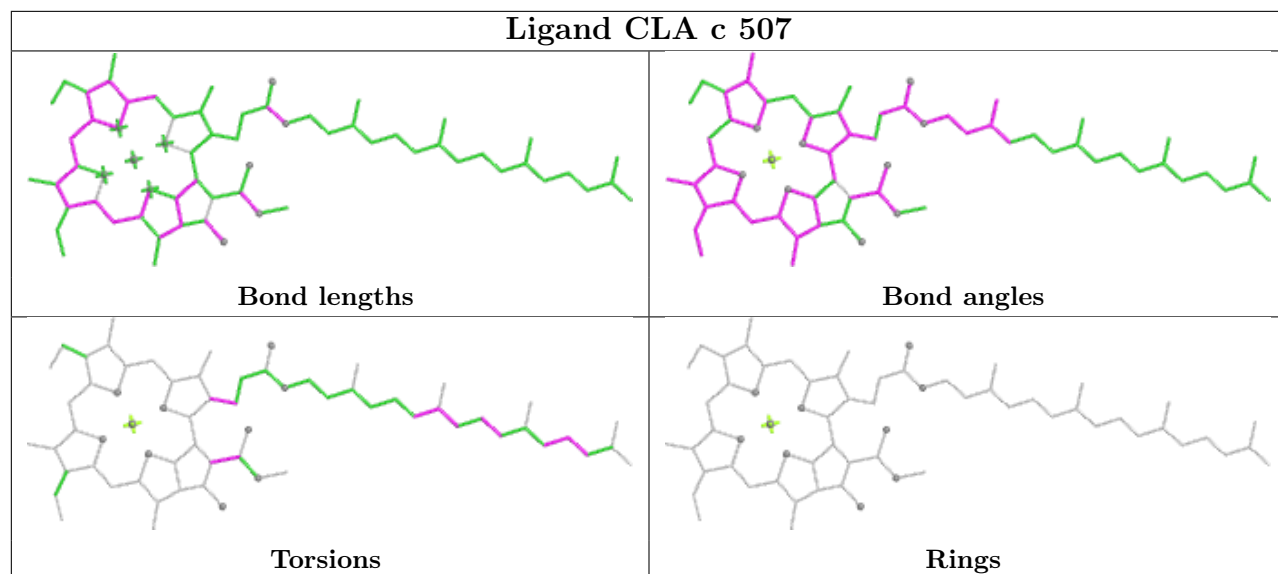


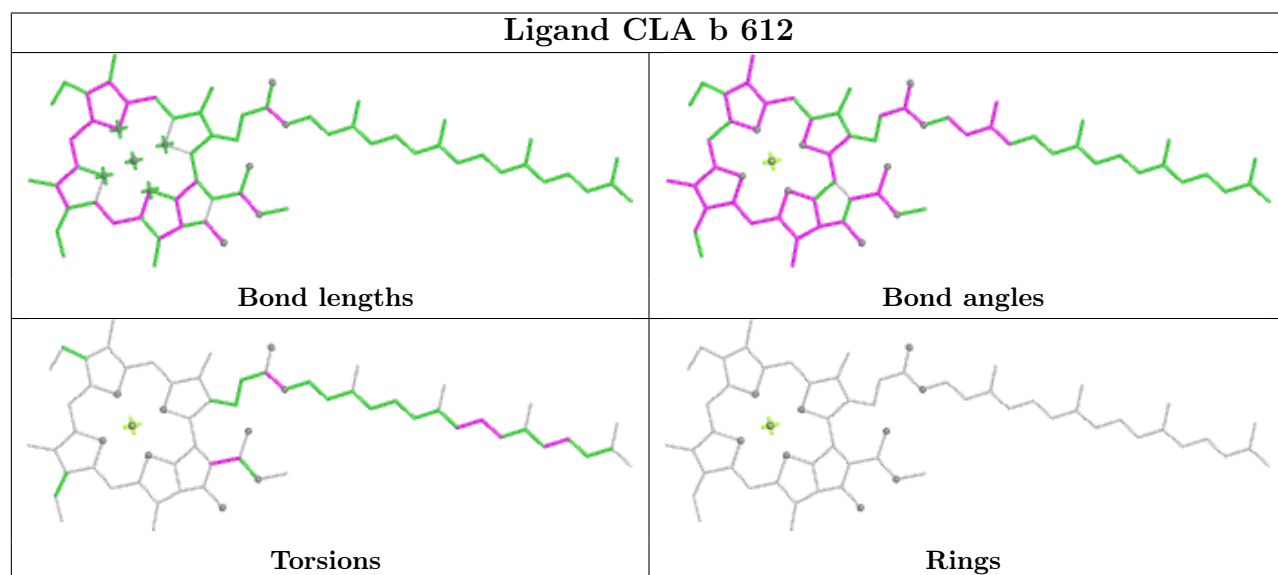
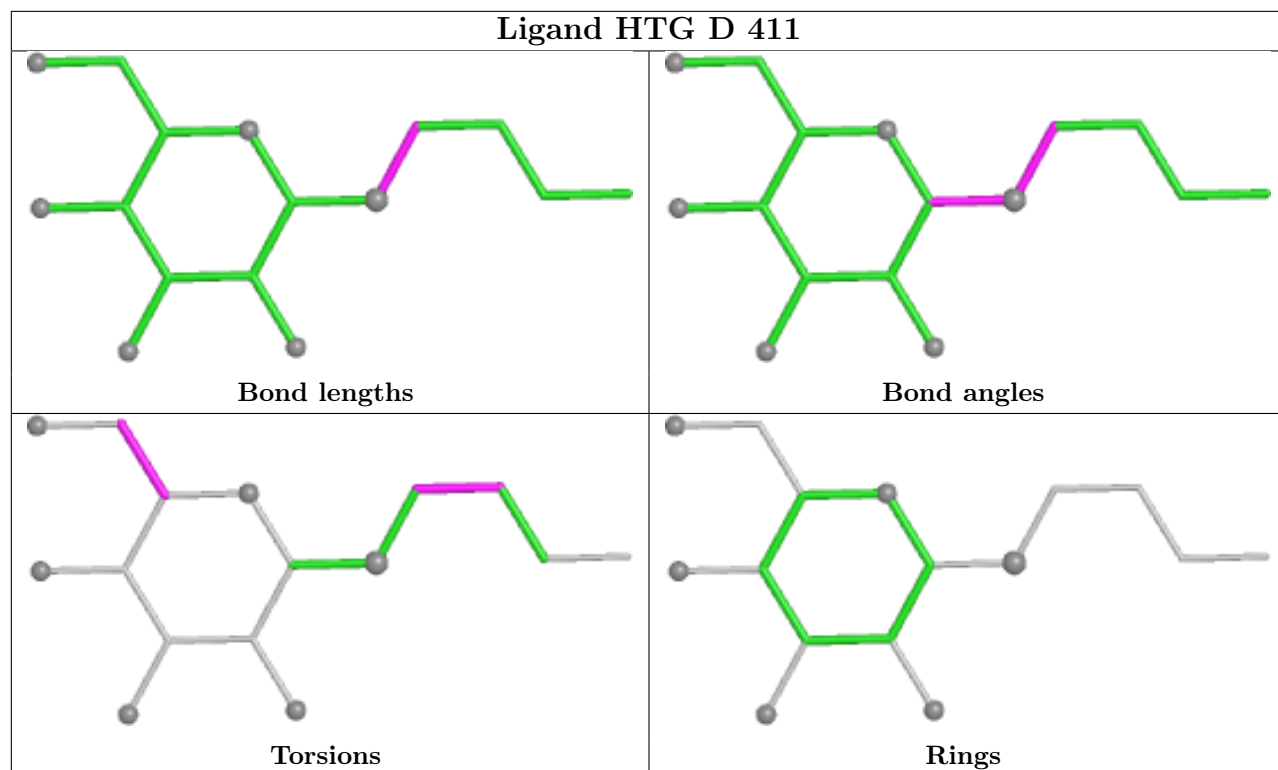
Ligand PHO a 406 (A)

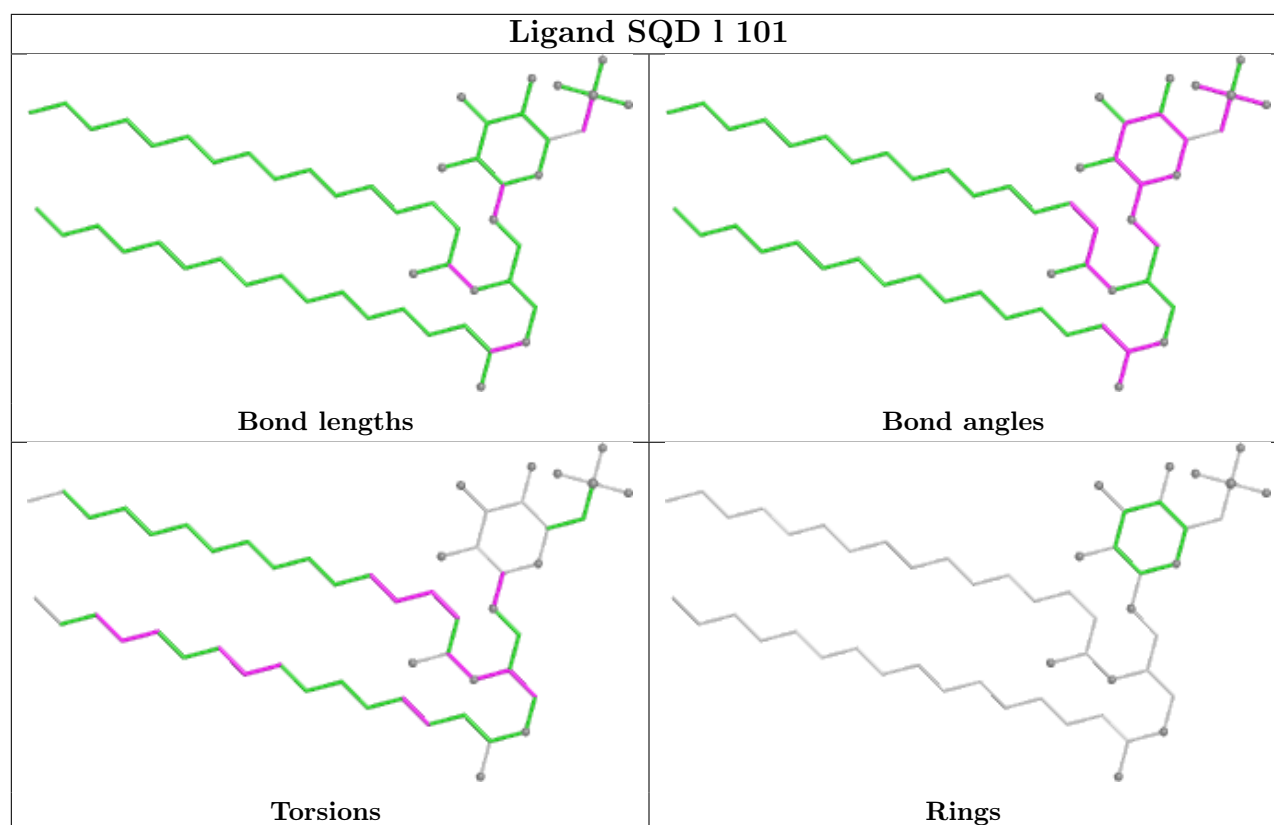




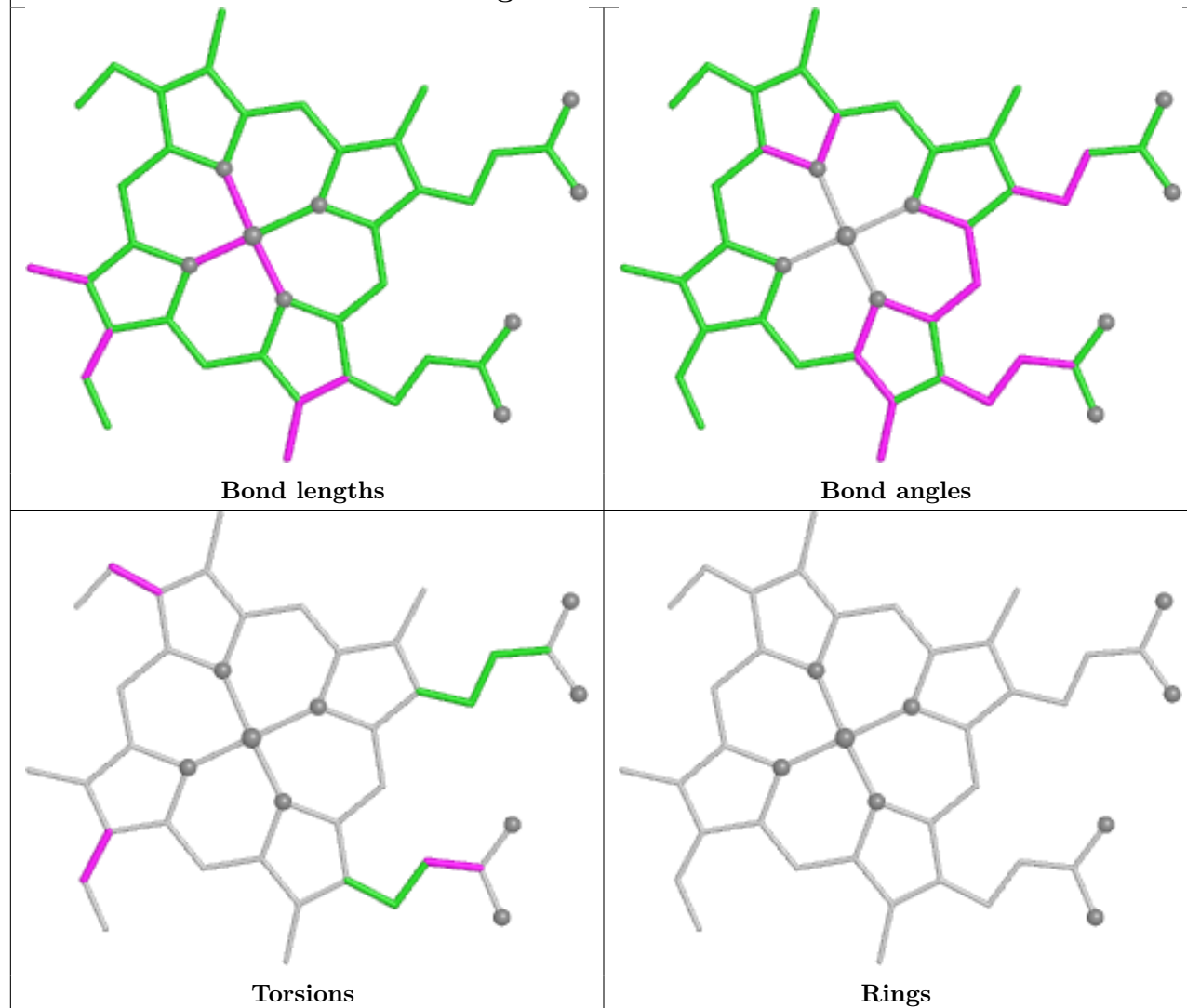




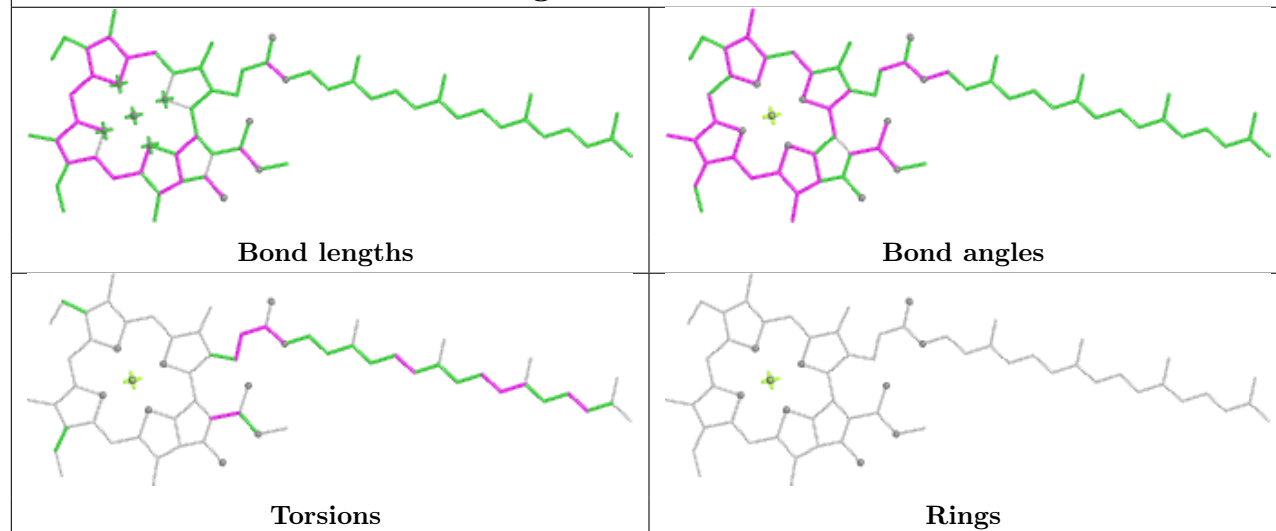


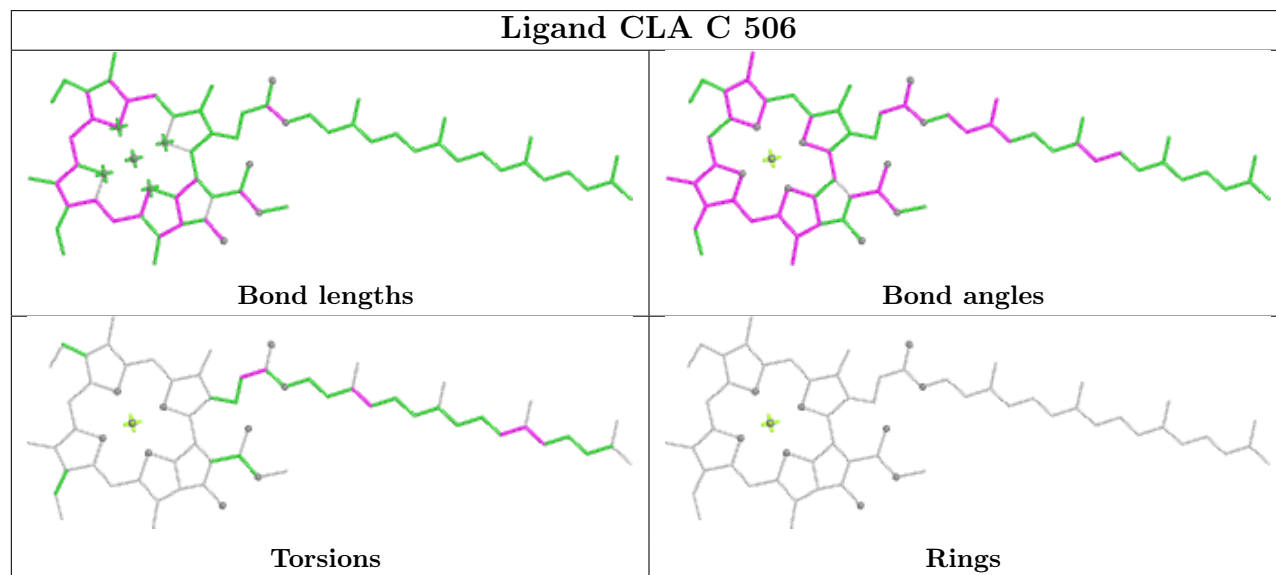
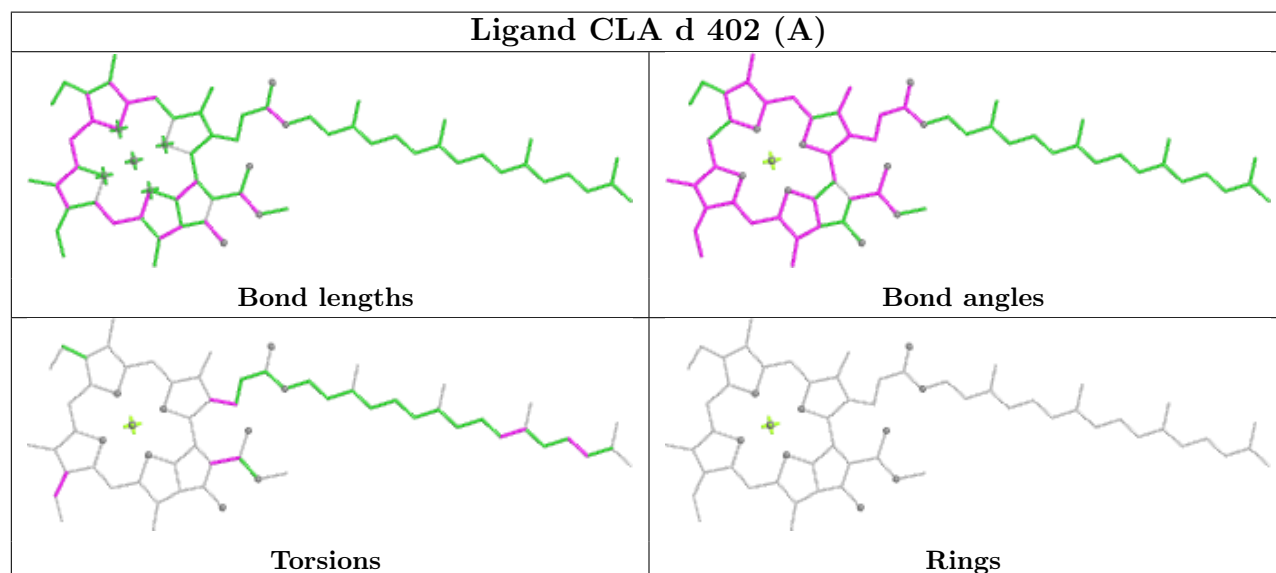
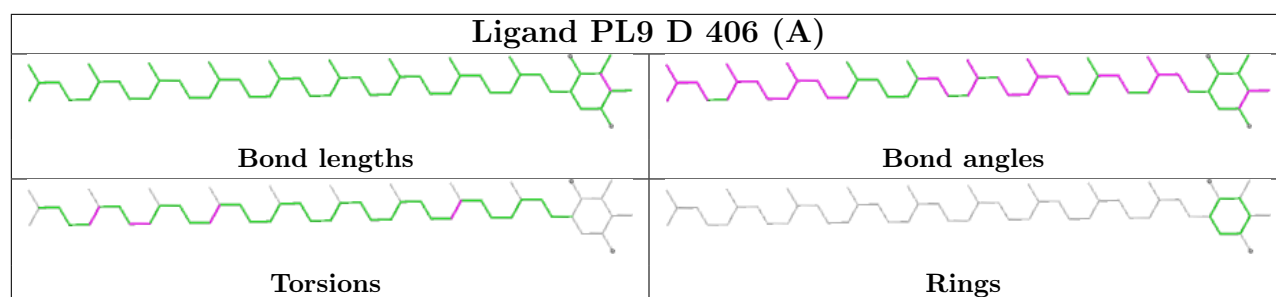


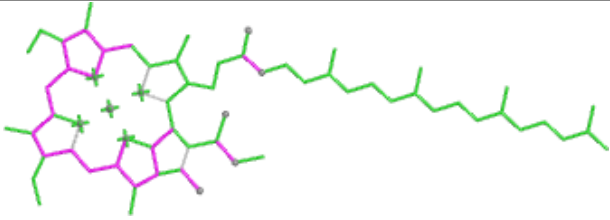
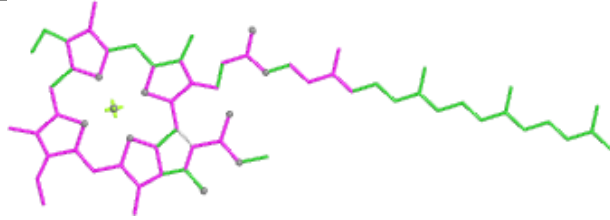
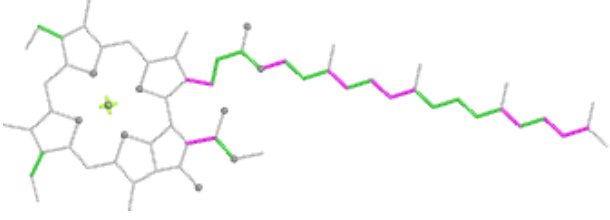
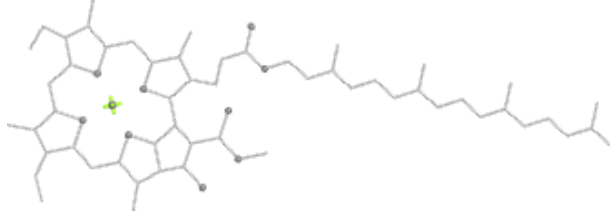
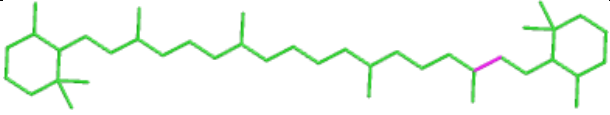
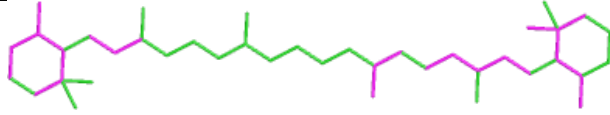
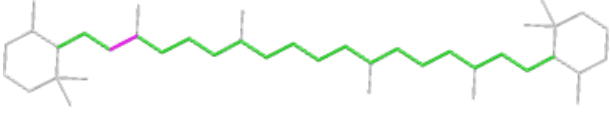
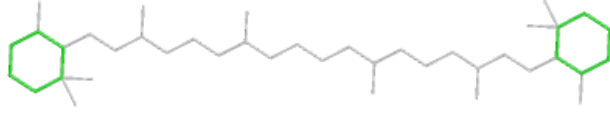
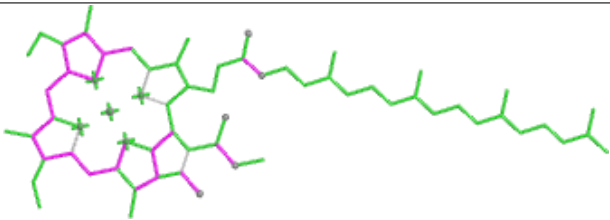
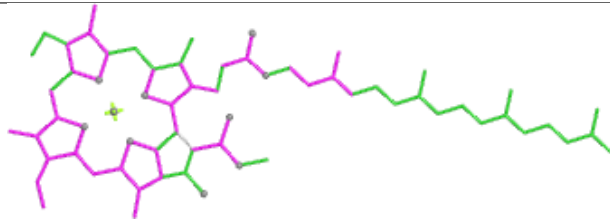
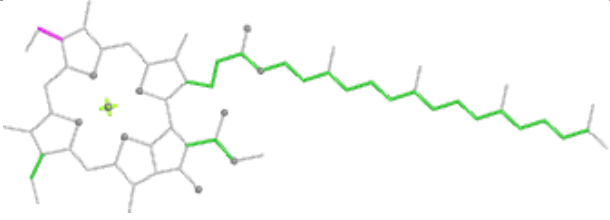
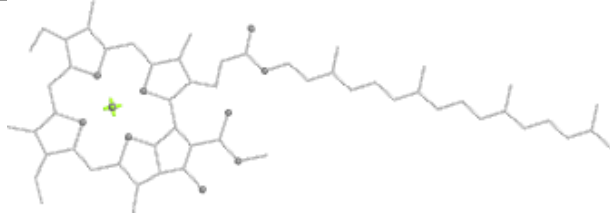
Ligand HEC v 201

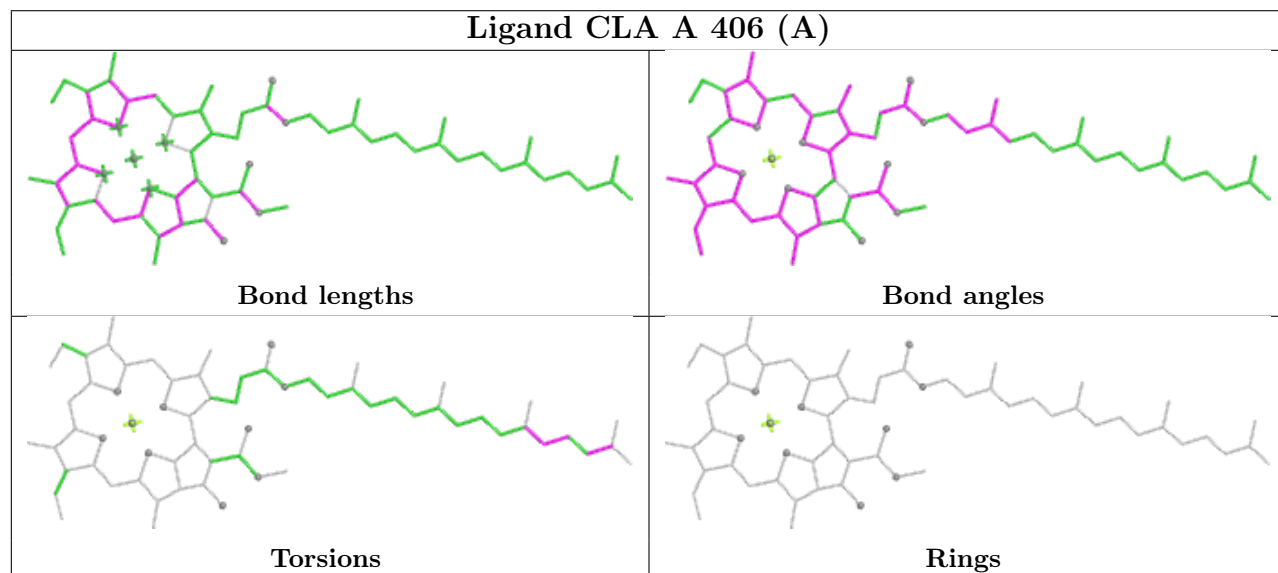
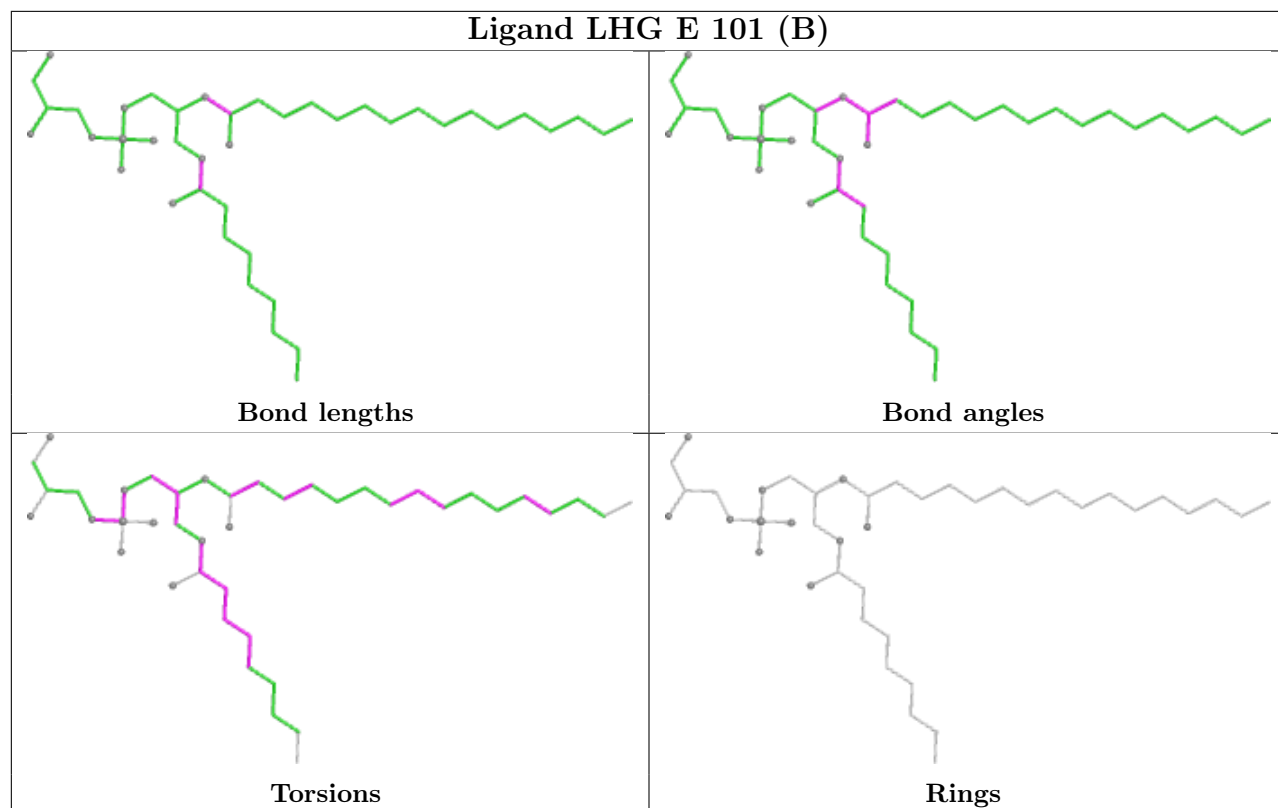


Ligand CLA B 601

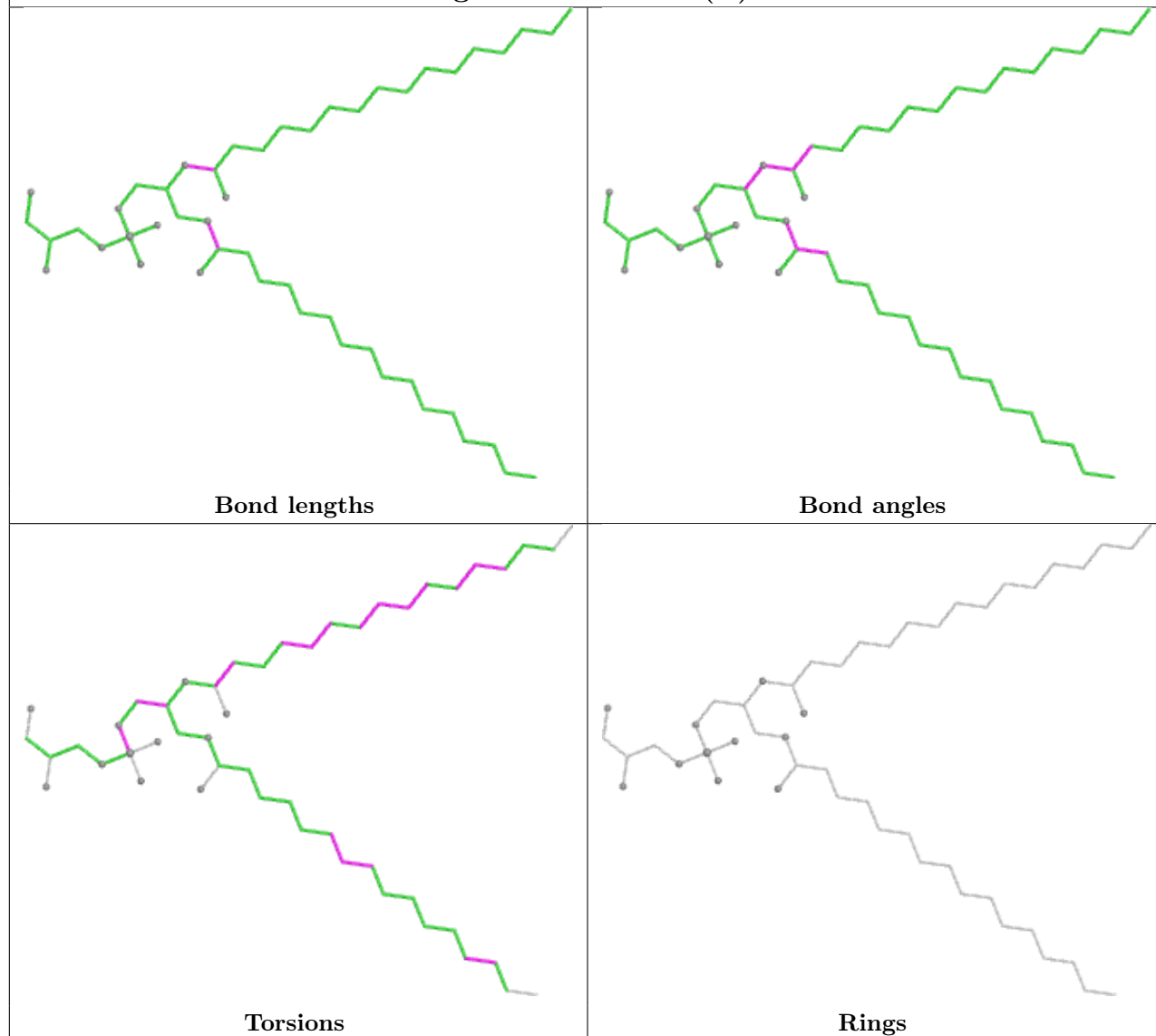




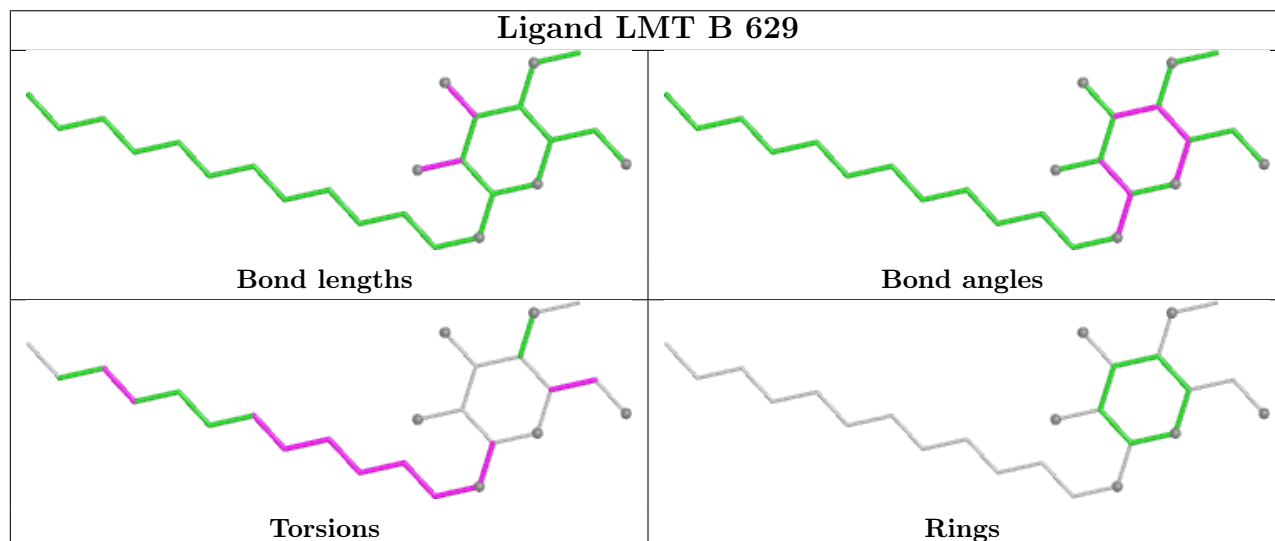
Ligand CLA C 507	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA D 403 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings

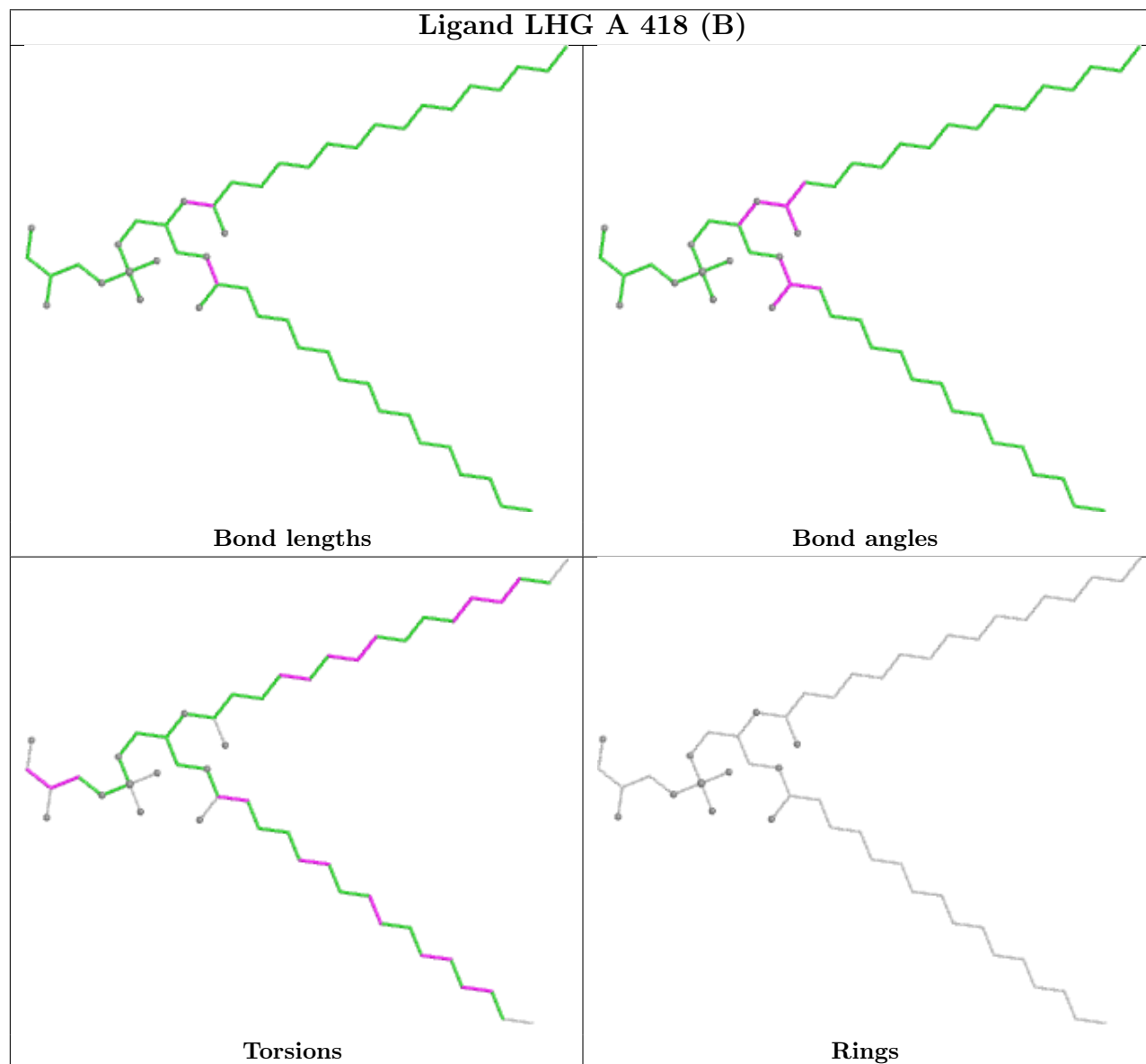
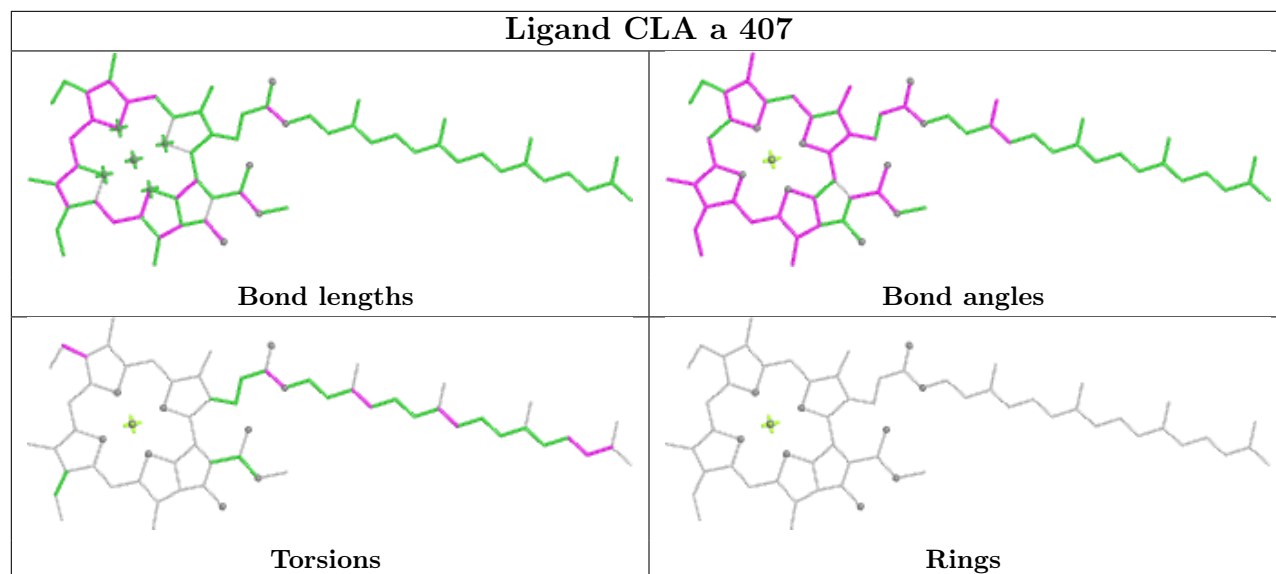


Ligand LHG b 629 (B)

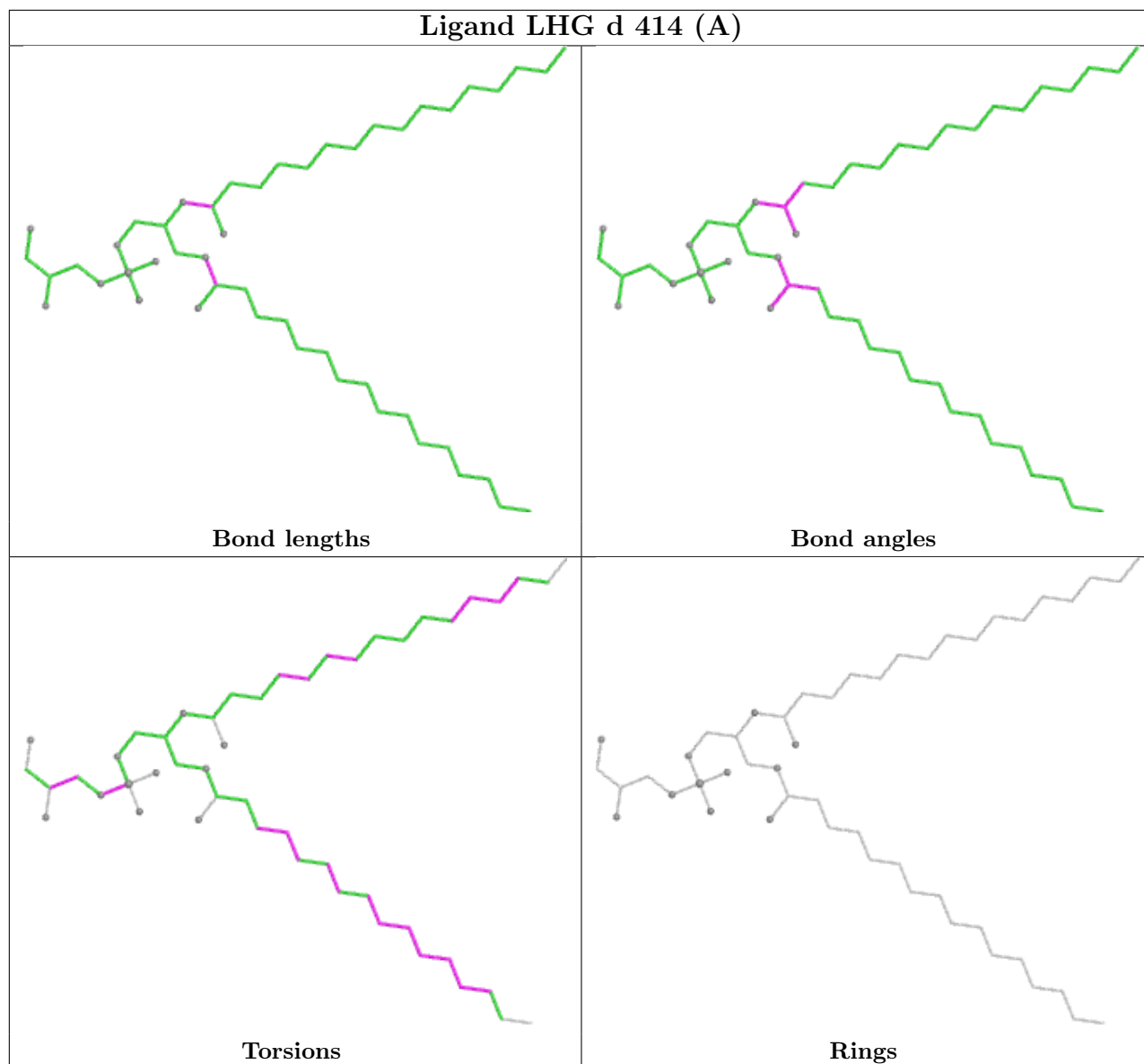


Ligand LMT B 629

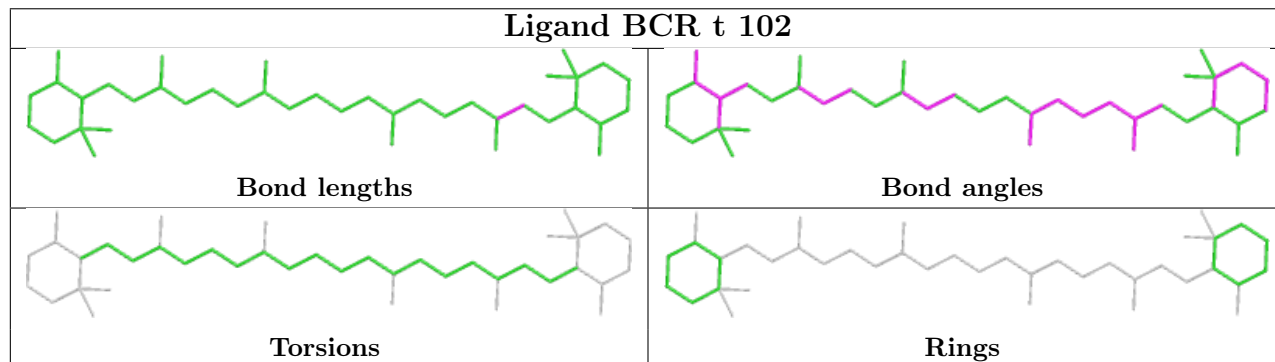


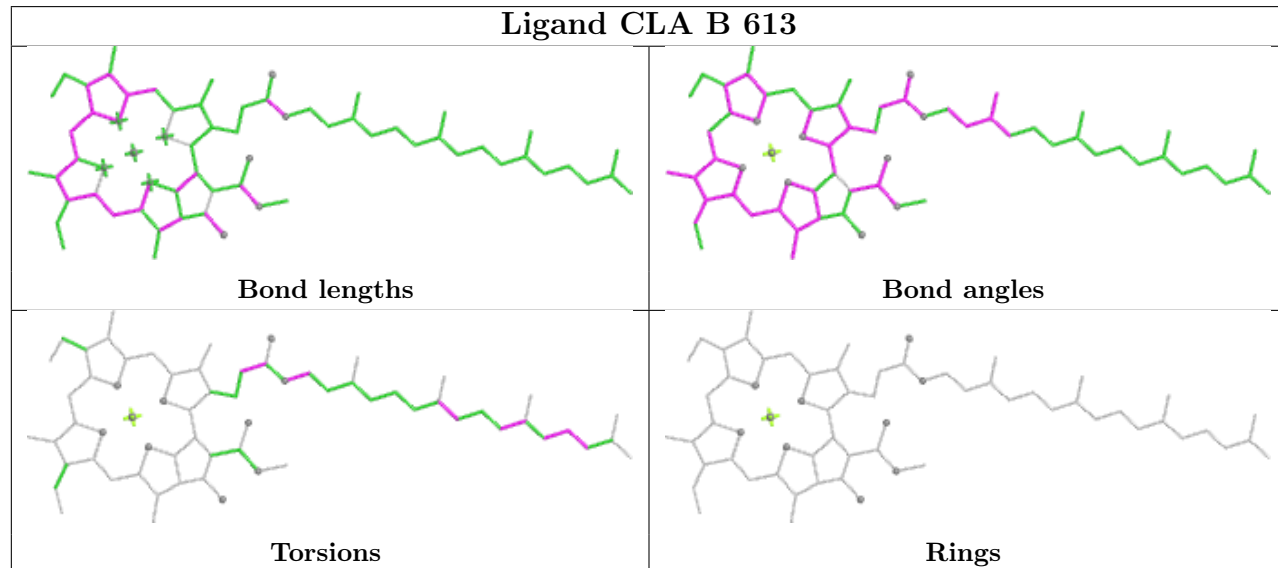
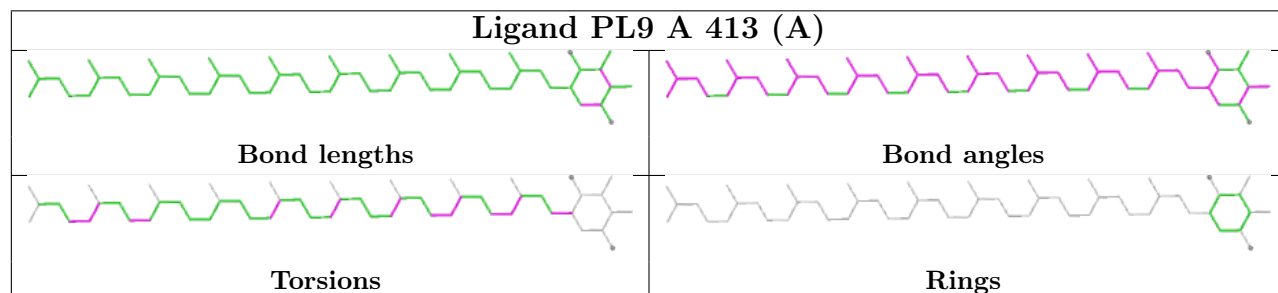
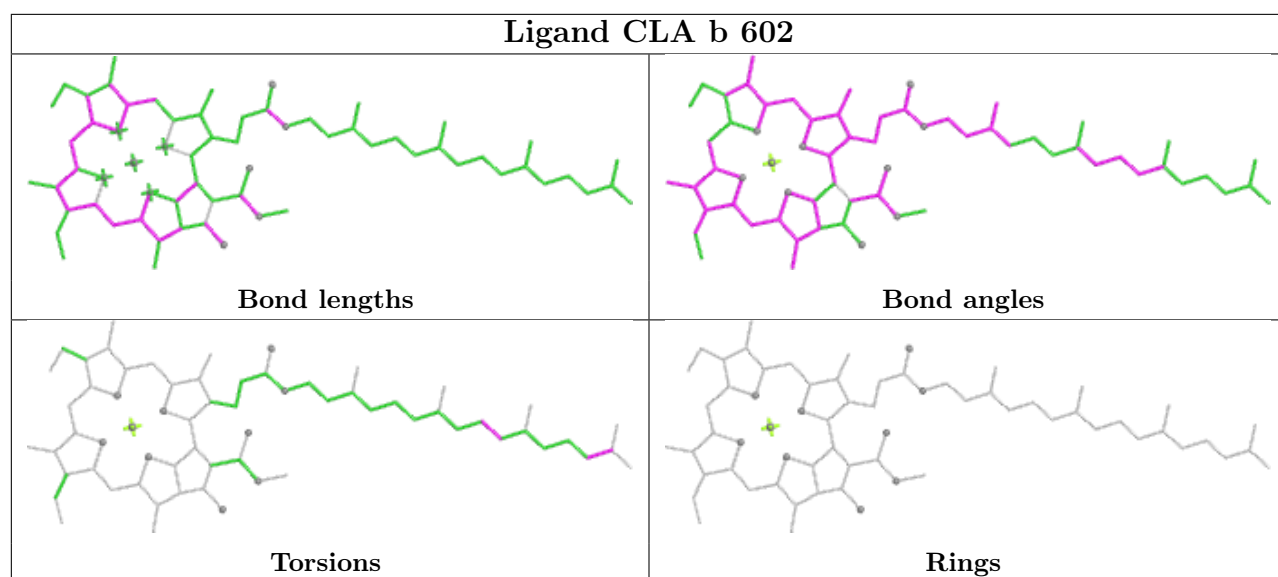


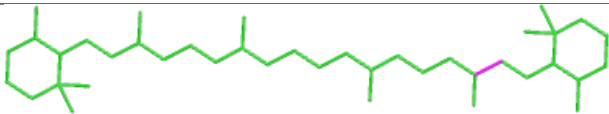
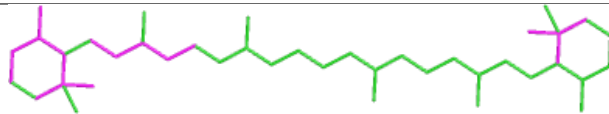
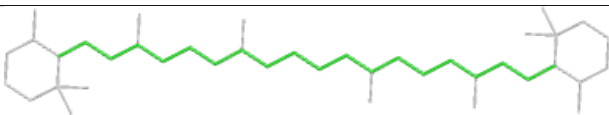
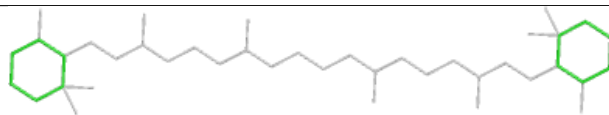
Ligand LHG d 414 (A)

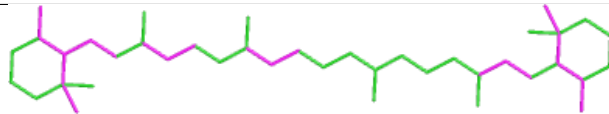
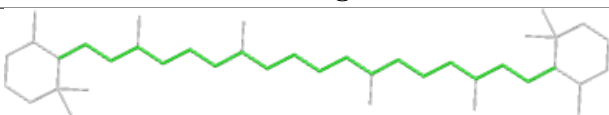
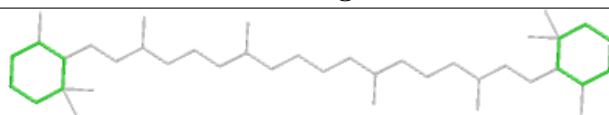


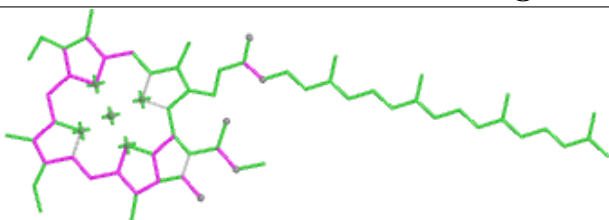
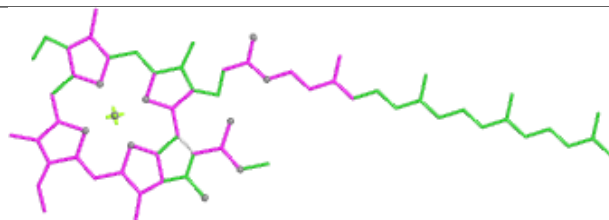
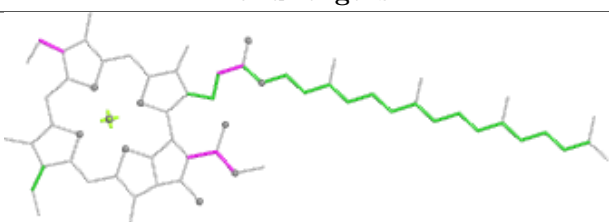
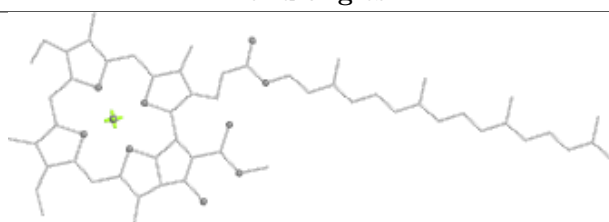
Ligand BCR t 102

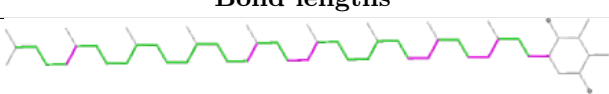
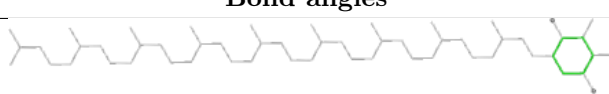


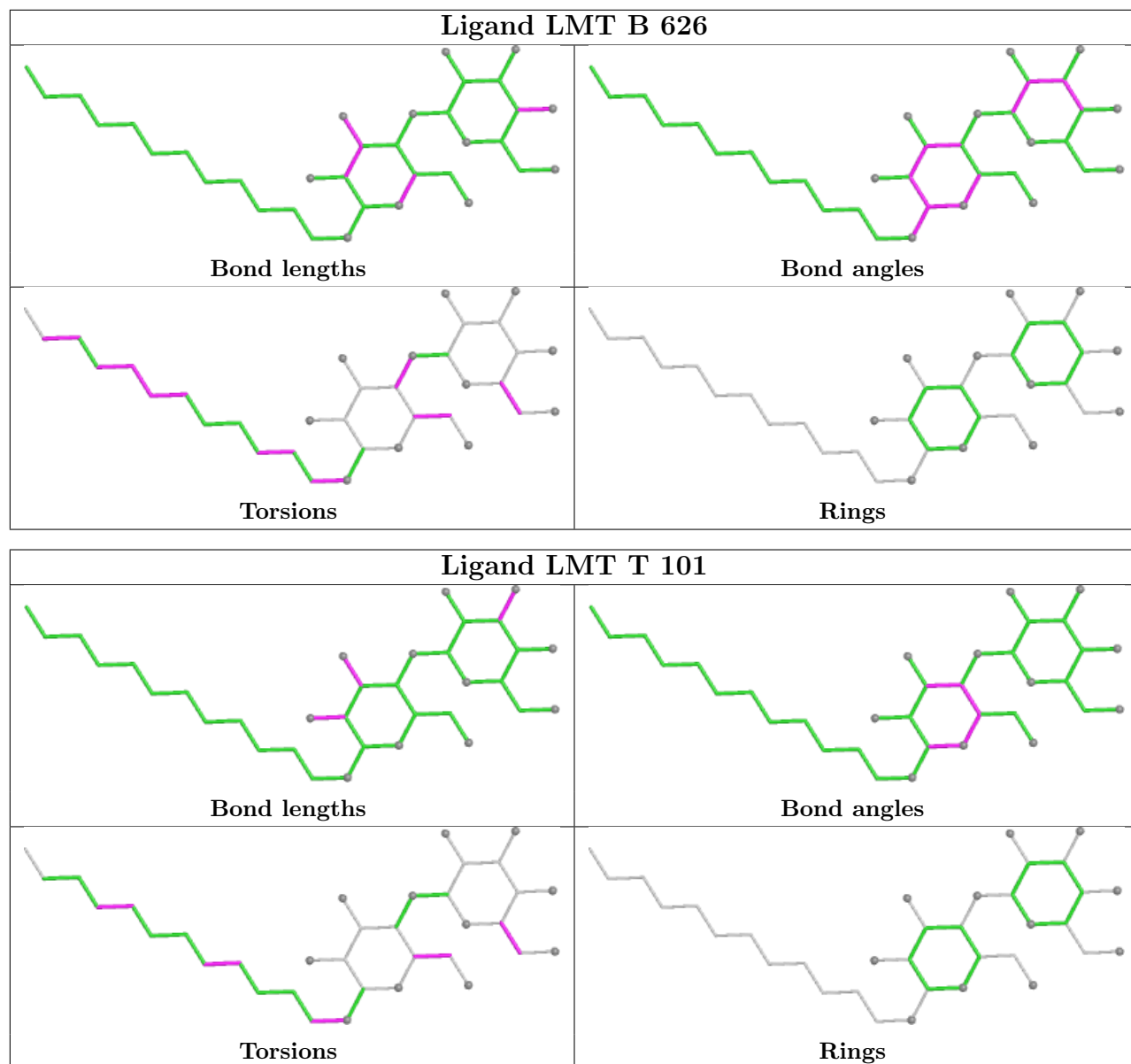


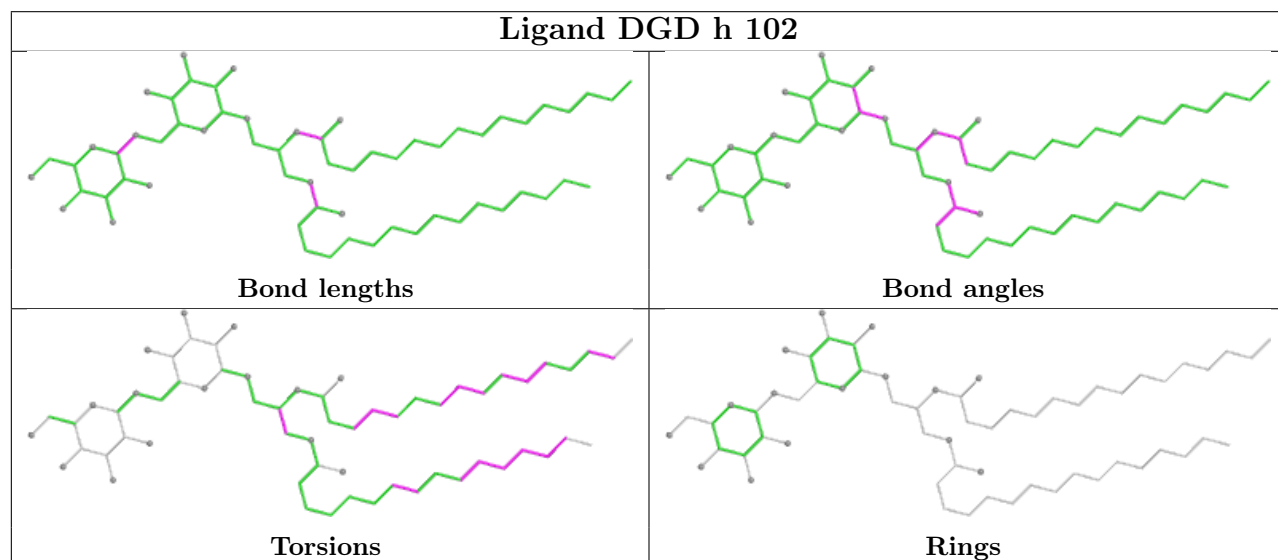
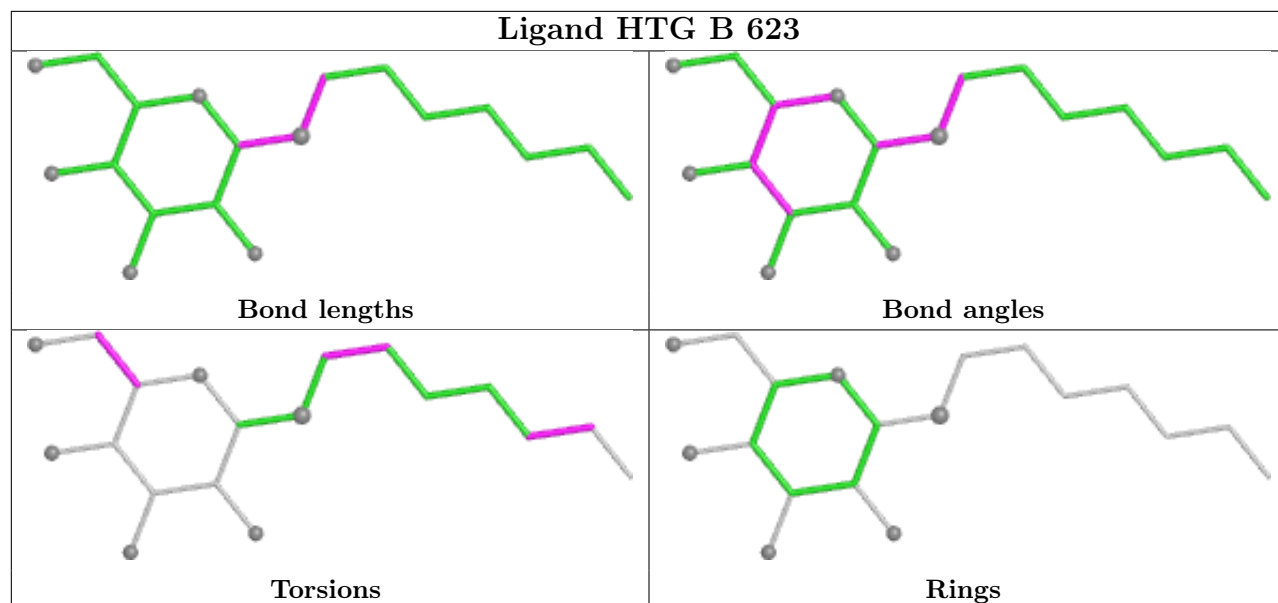
Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

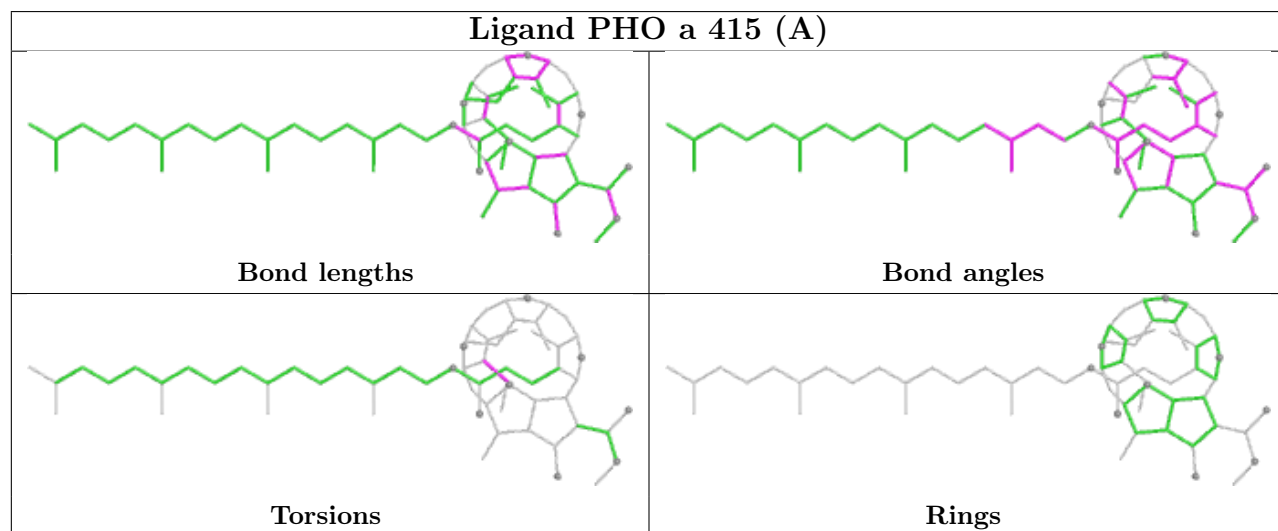
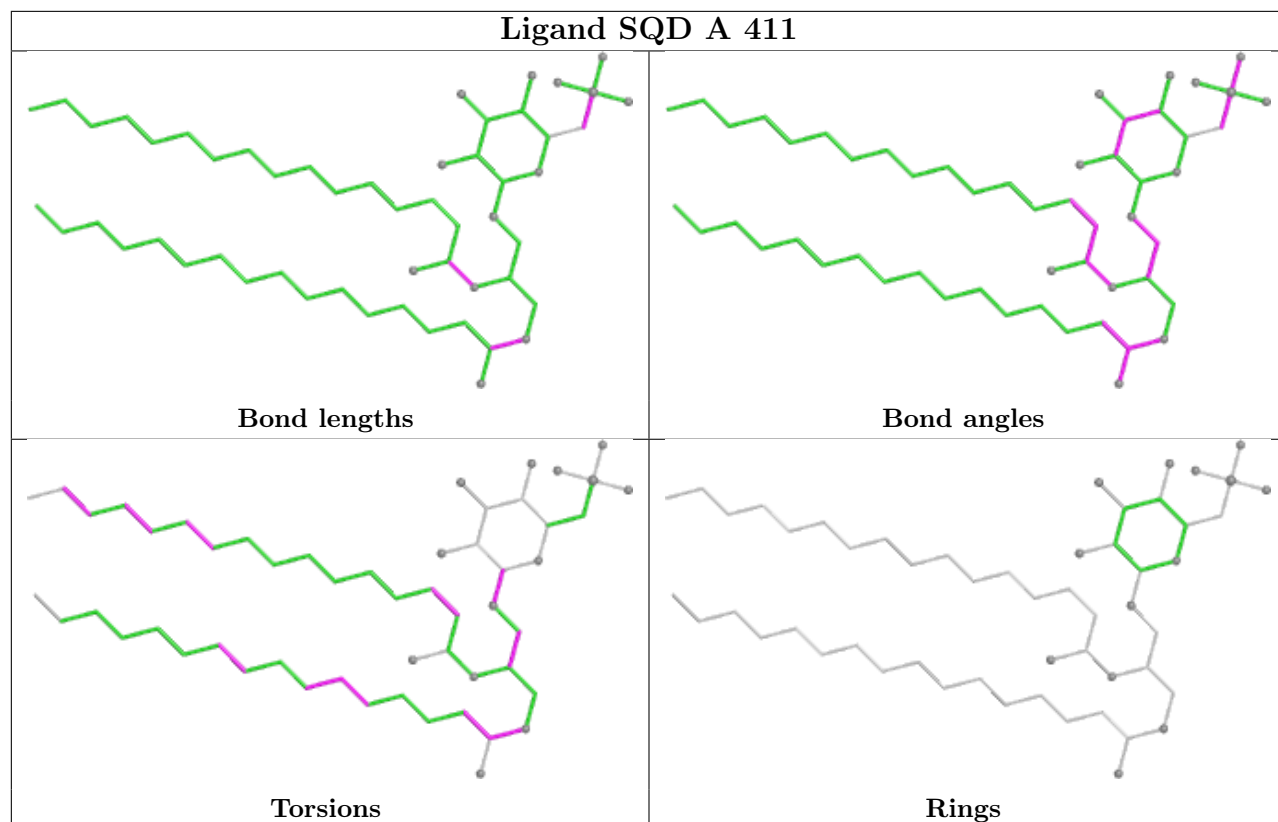
Ligand BCR A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

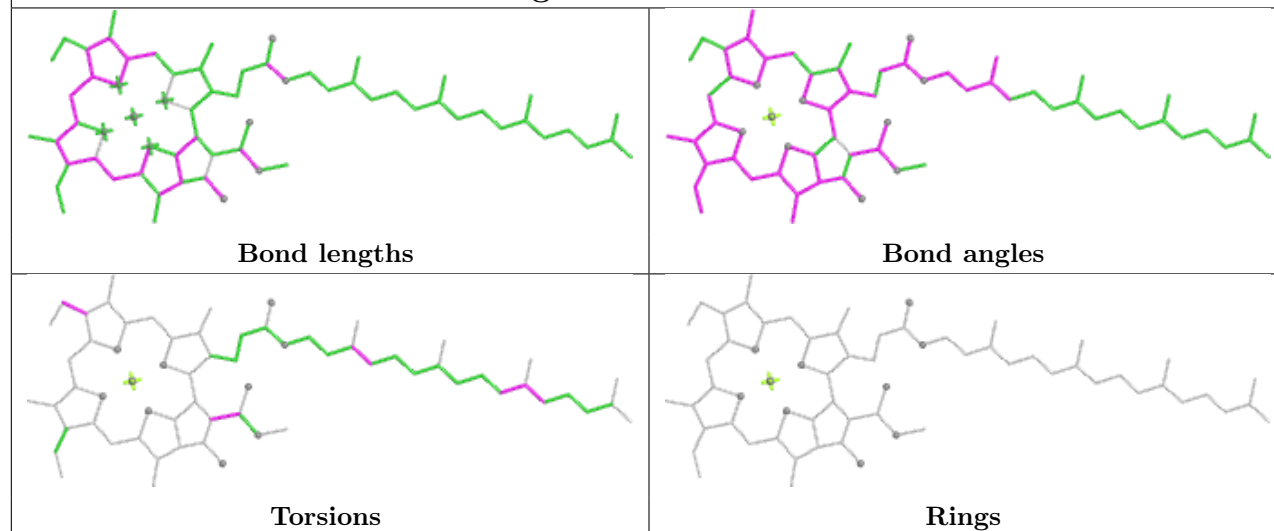
Ligand PL9 a 413 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings



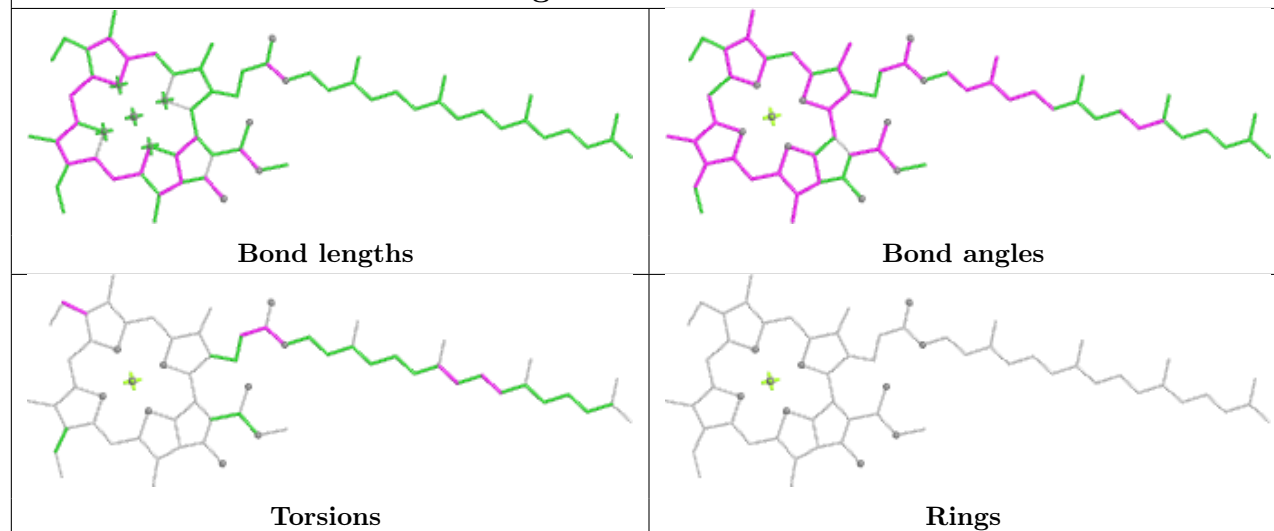




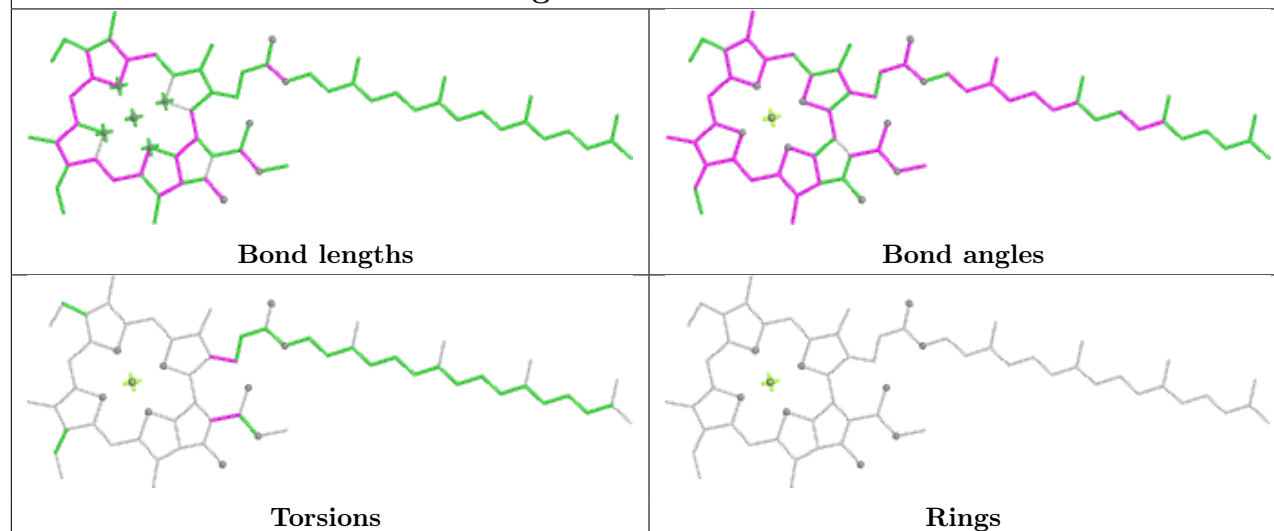
Ligand CLA C 505

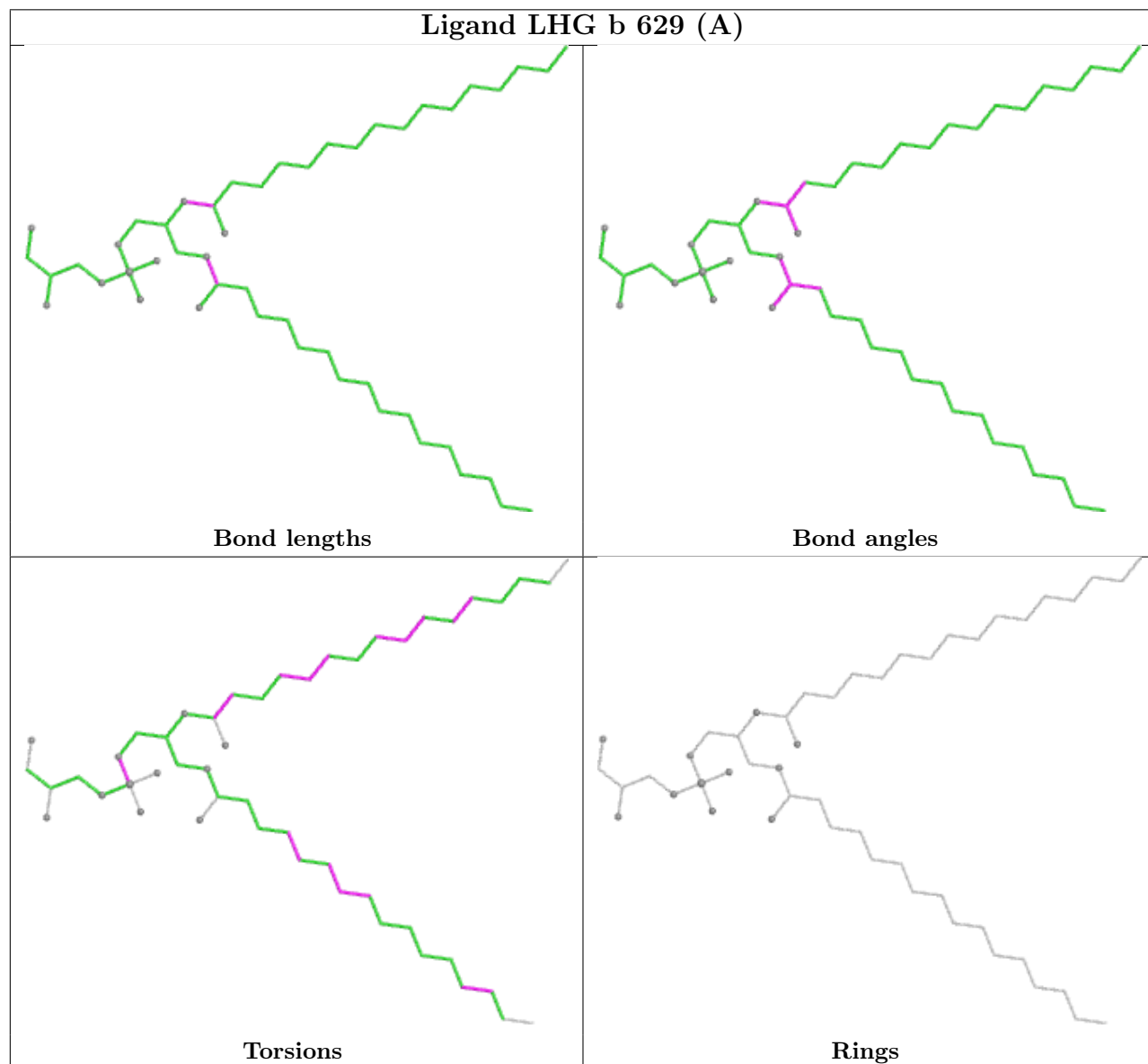
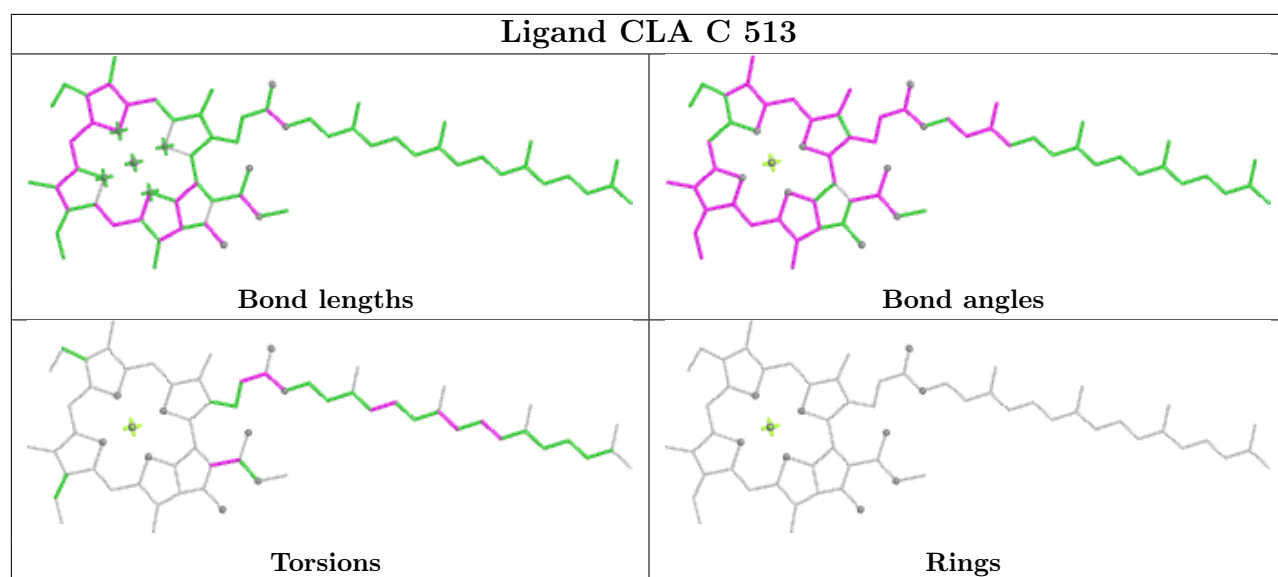


Ligand CLA B 612

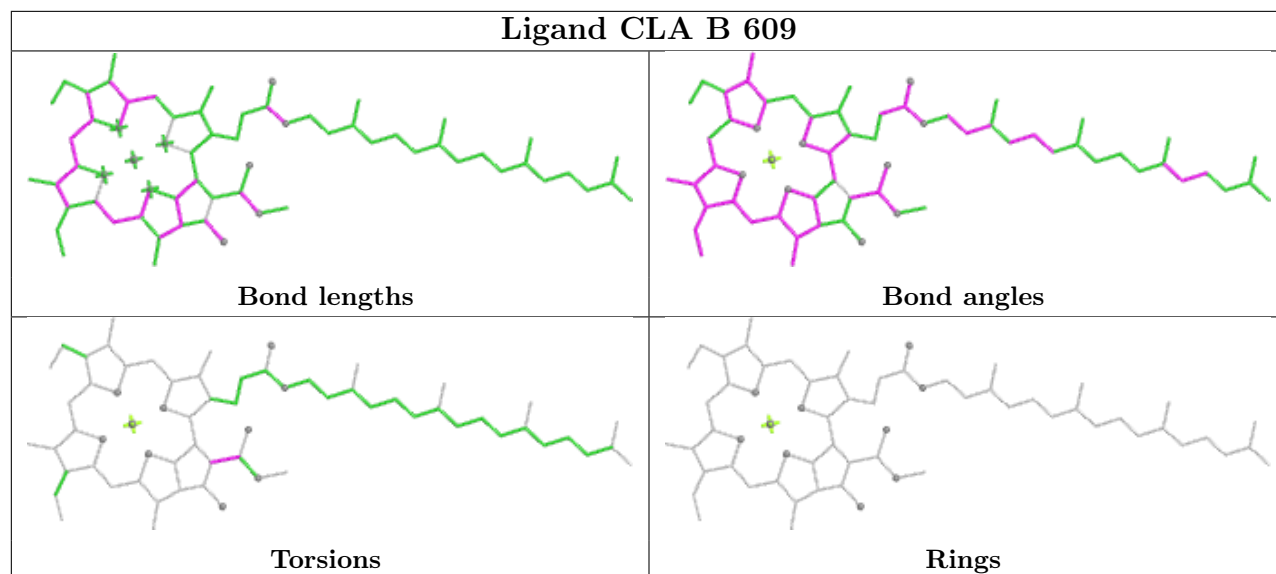


Ligand CLA B 604

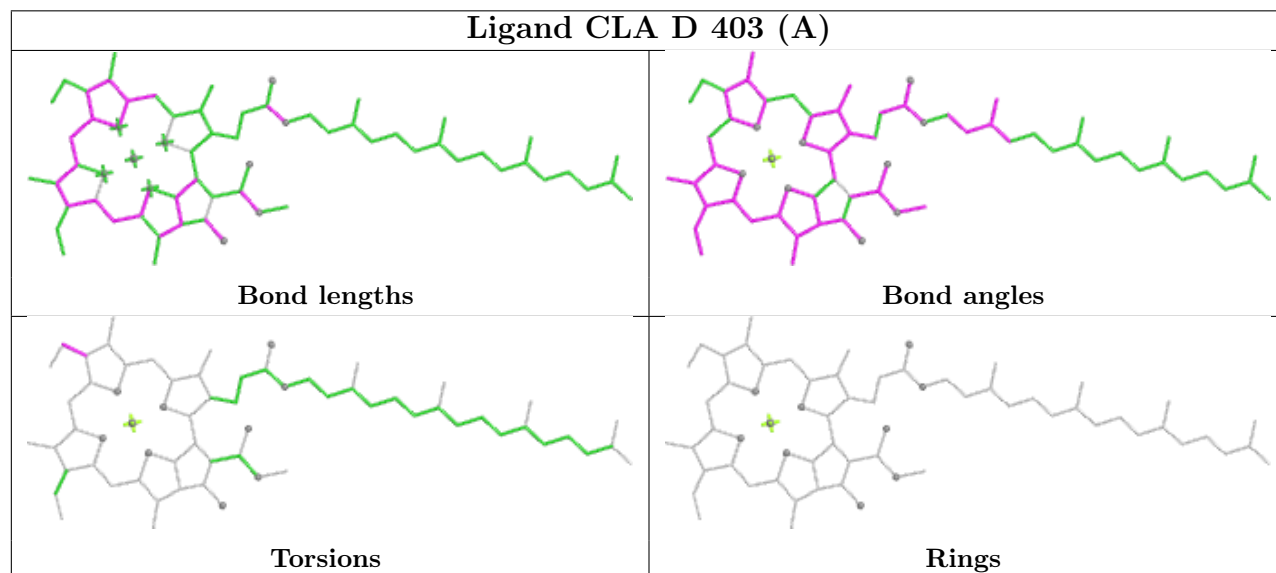




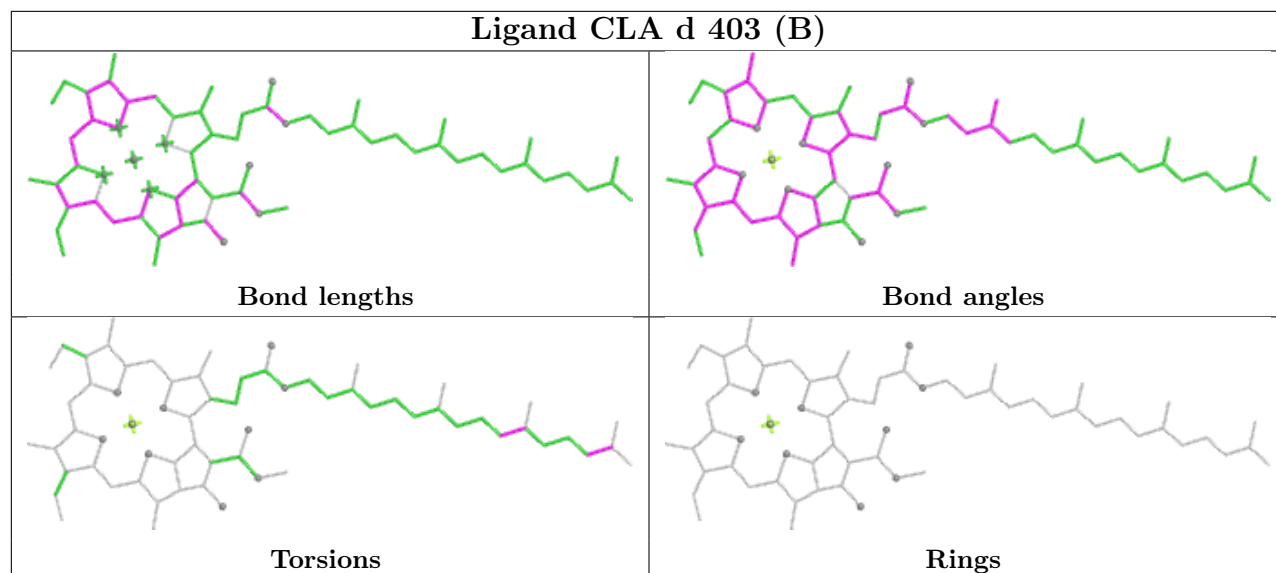
Ligand CLA B 609

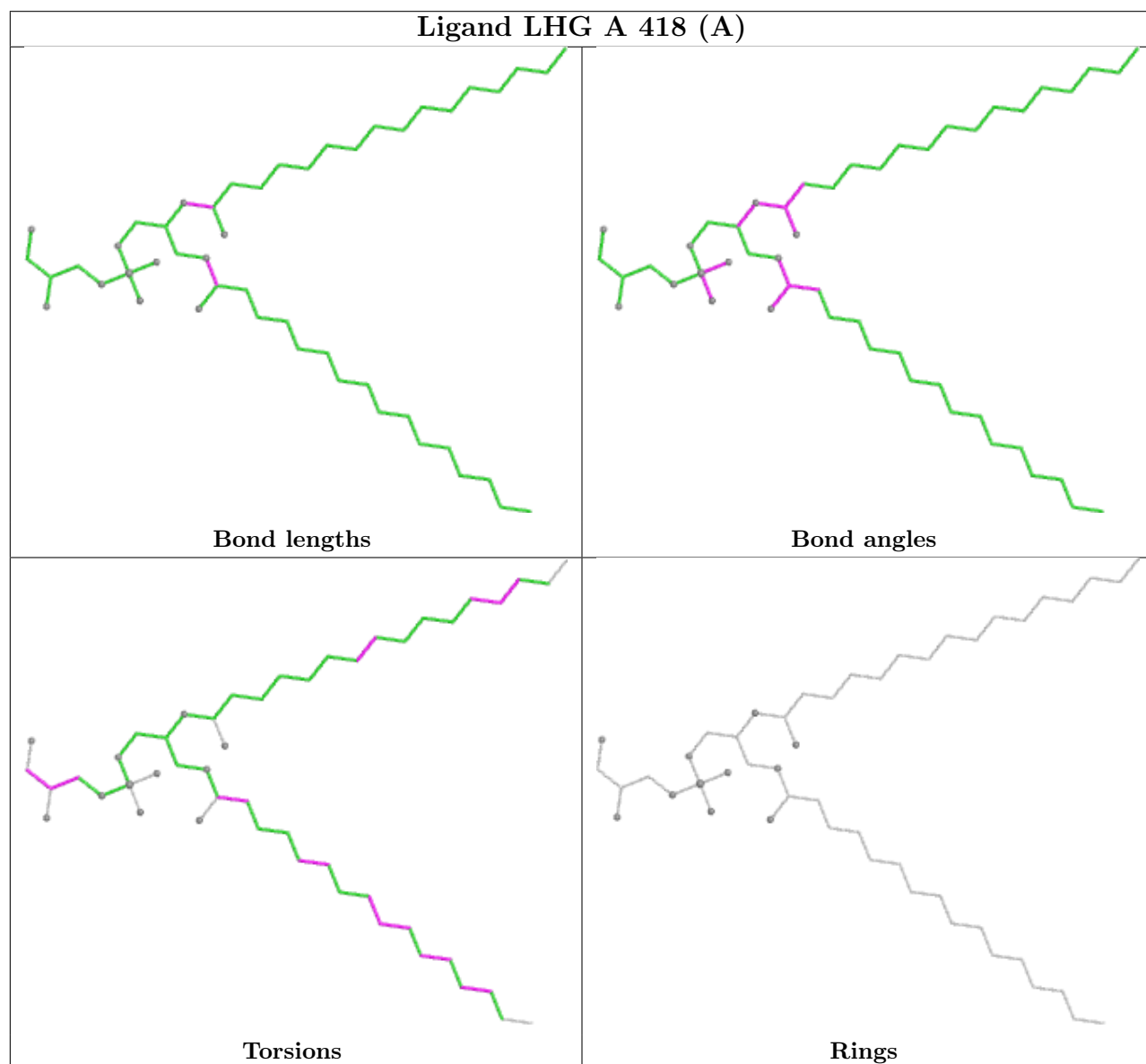
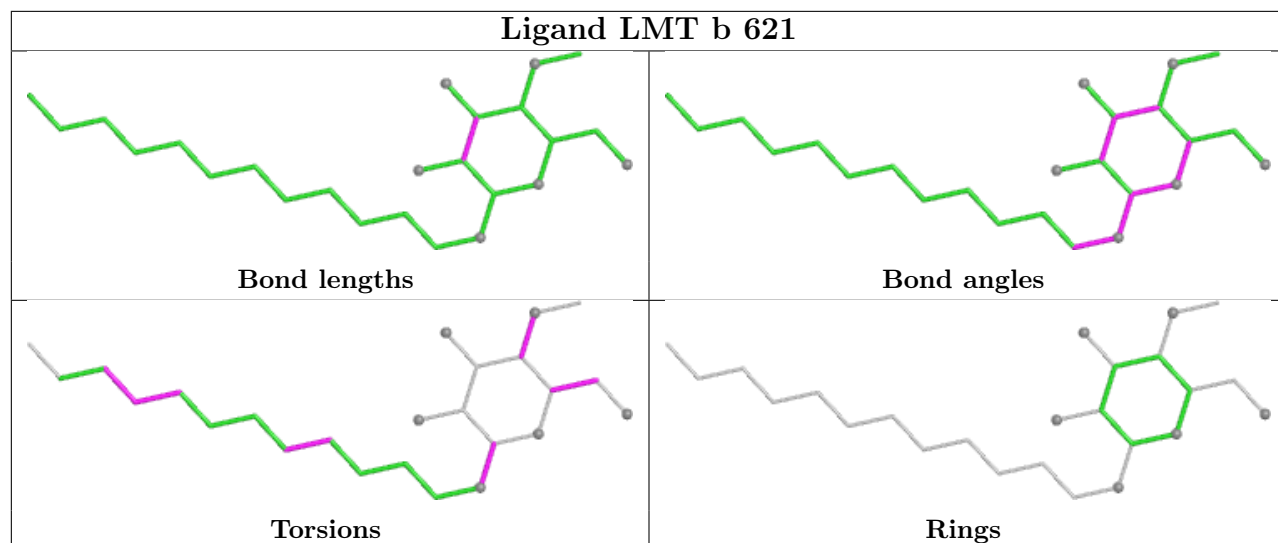


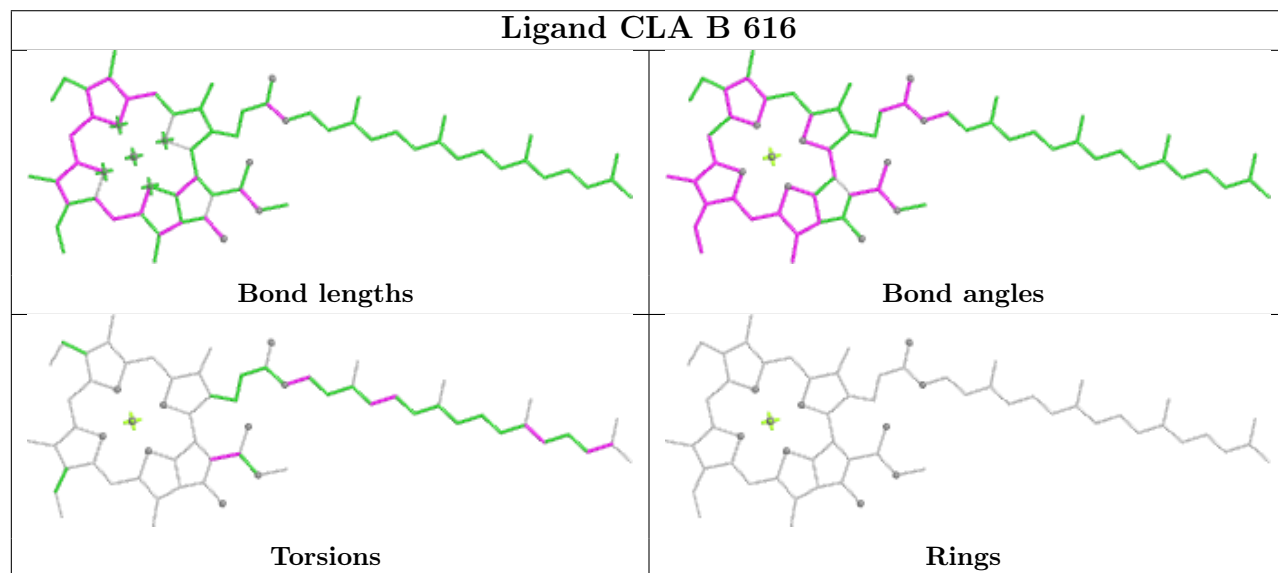
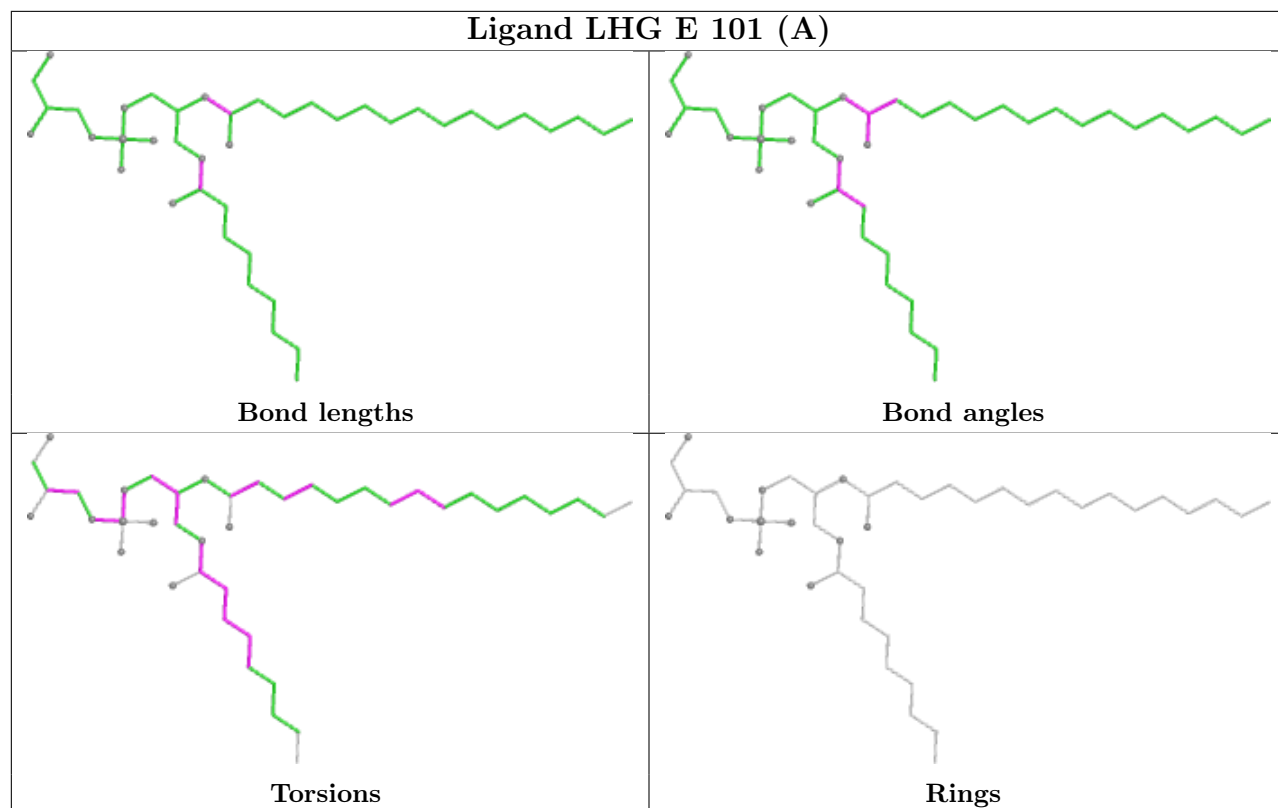
Ligand CLA D 403 (A)

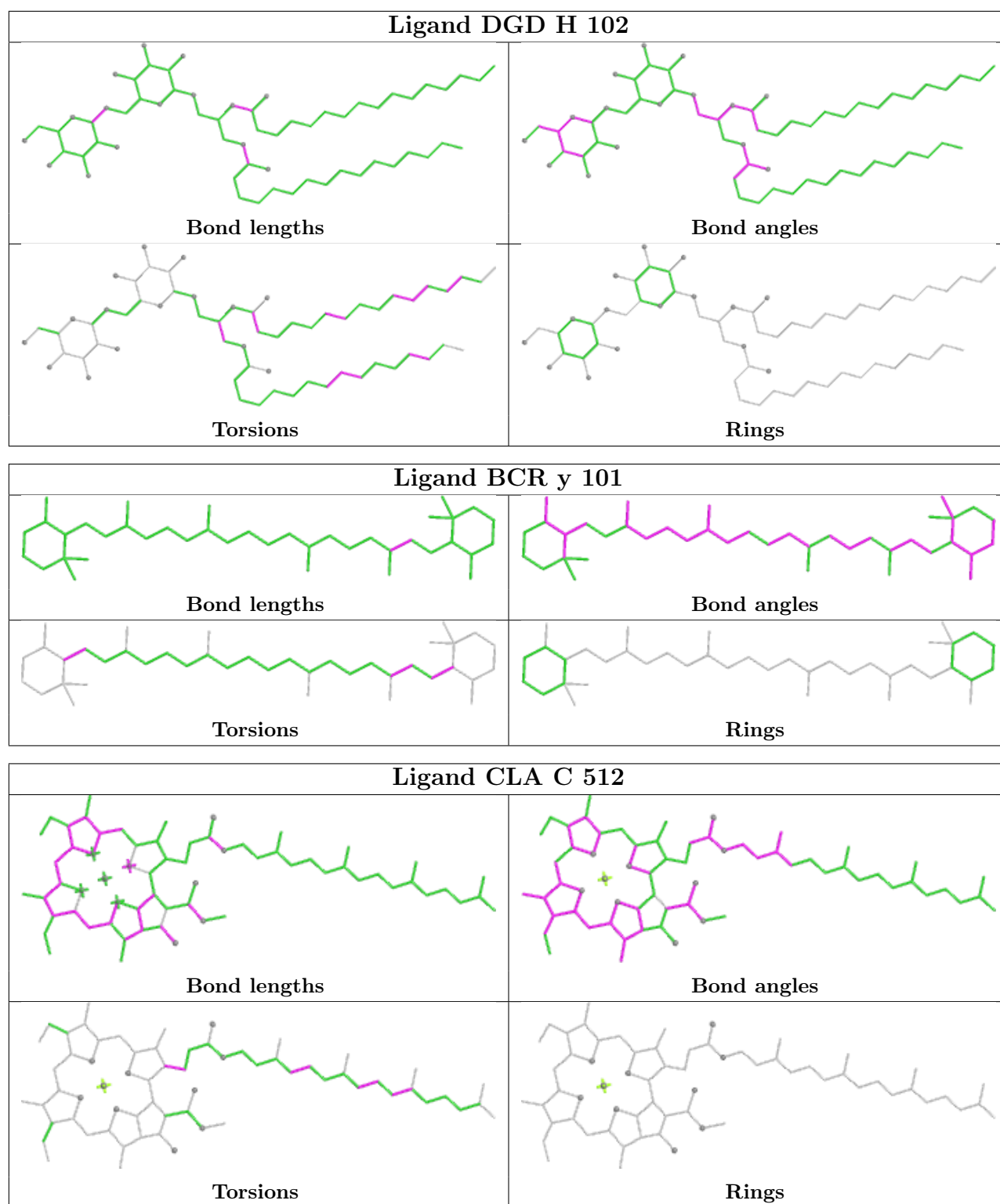


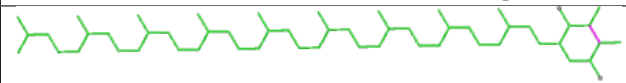
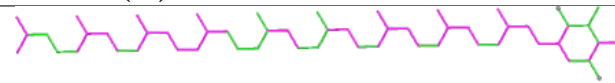
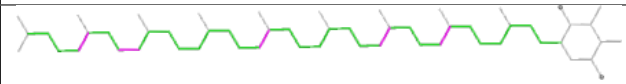
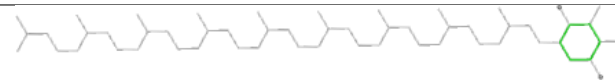
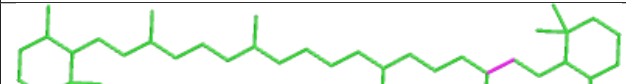
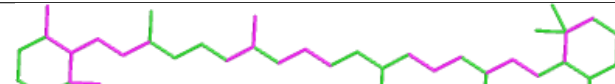
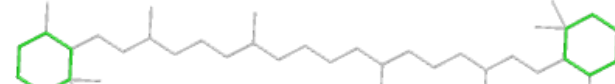
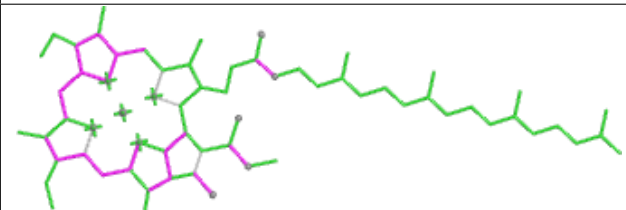
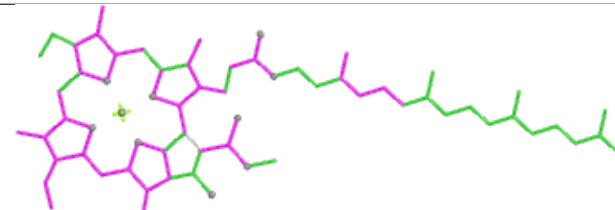
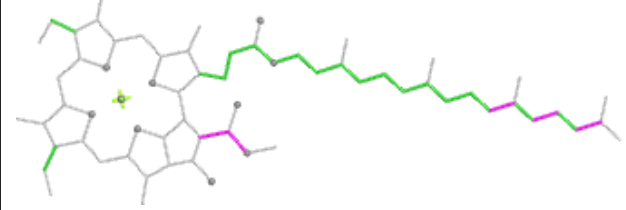
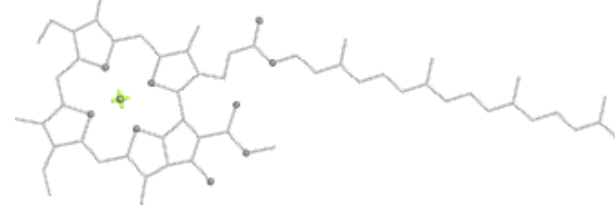
Ligand CLA d 403 (B)



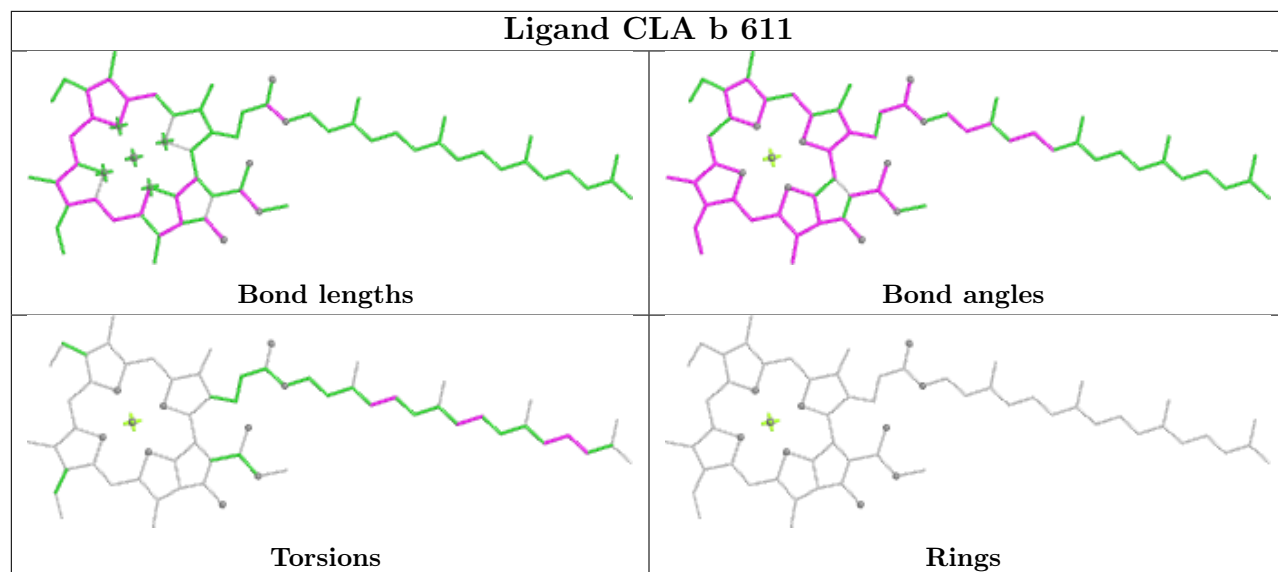




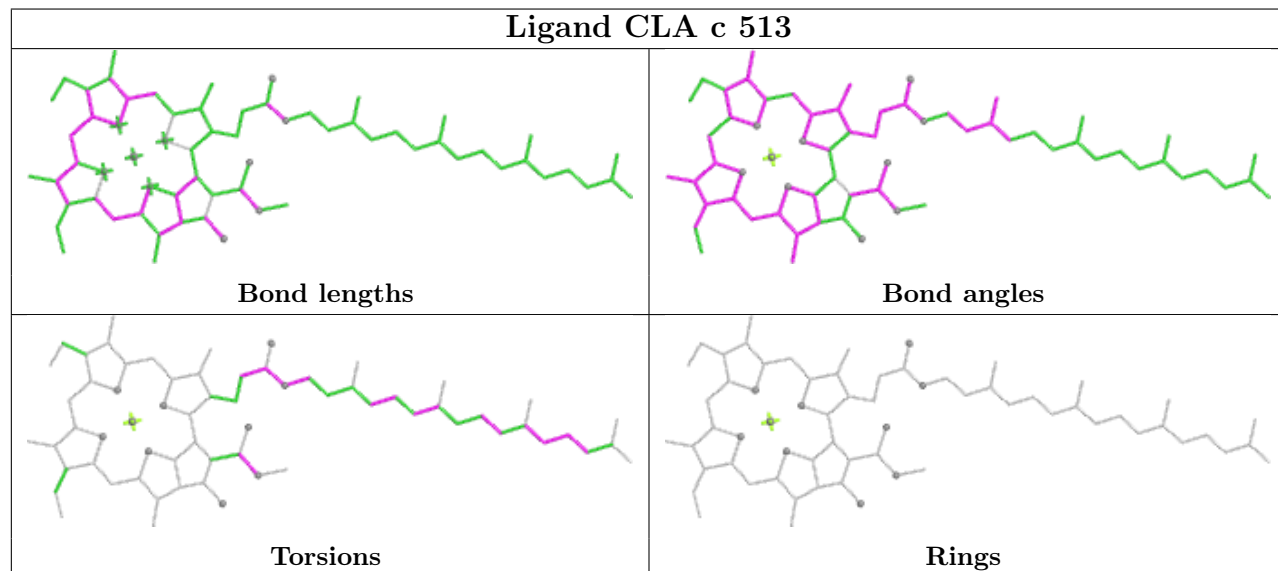


Ligand PL9 d 406 (B)	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 617	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

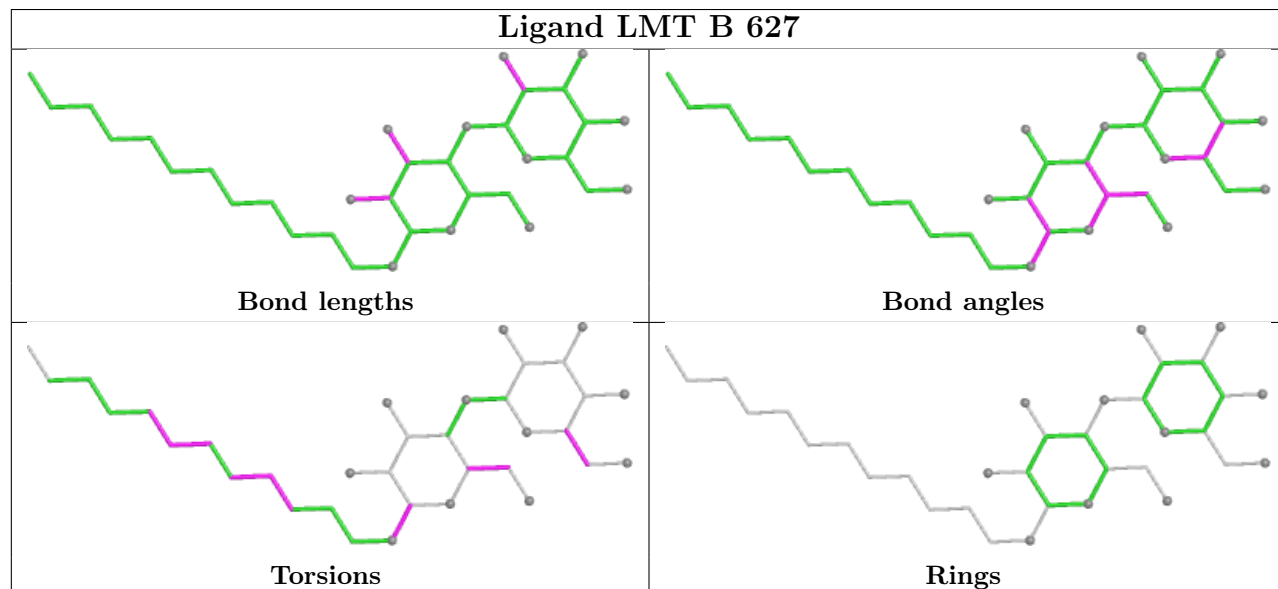
Ligand CLA b 611

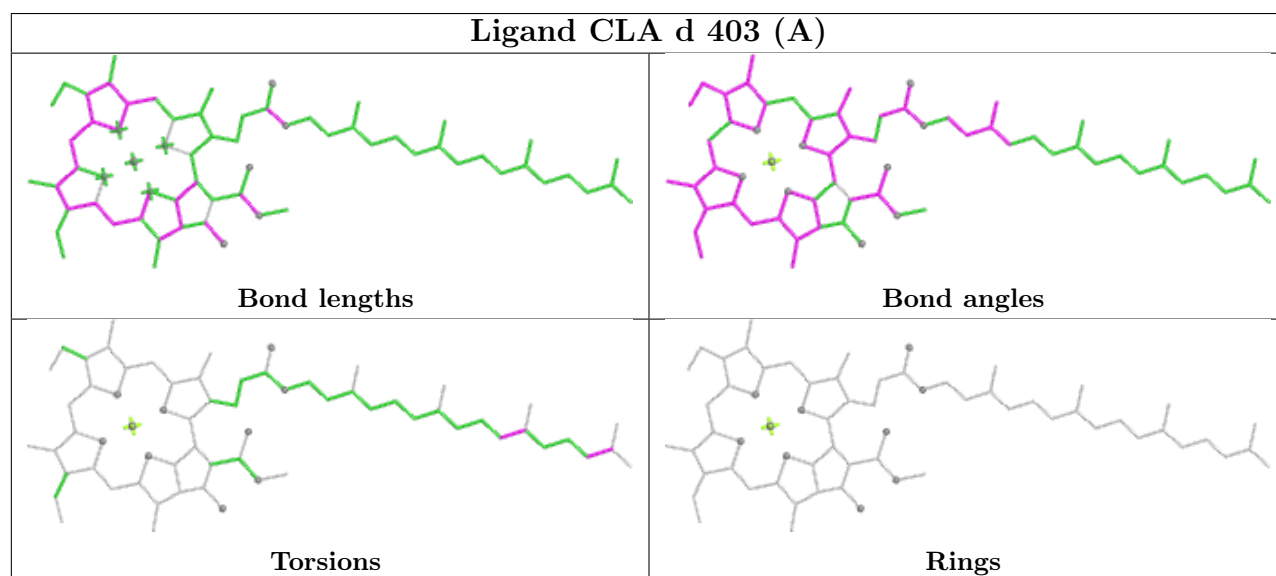
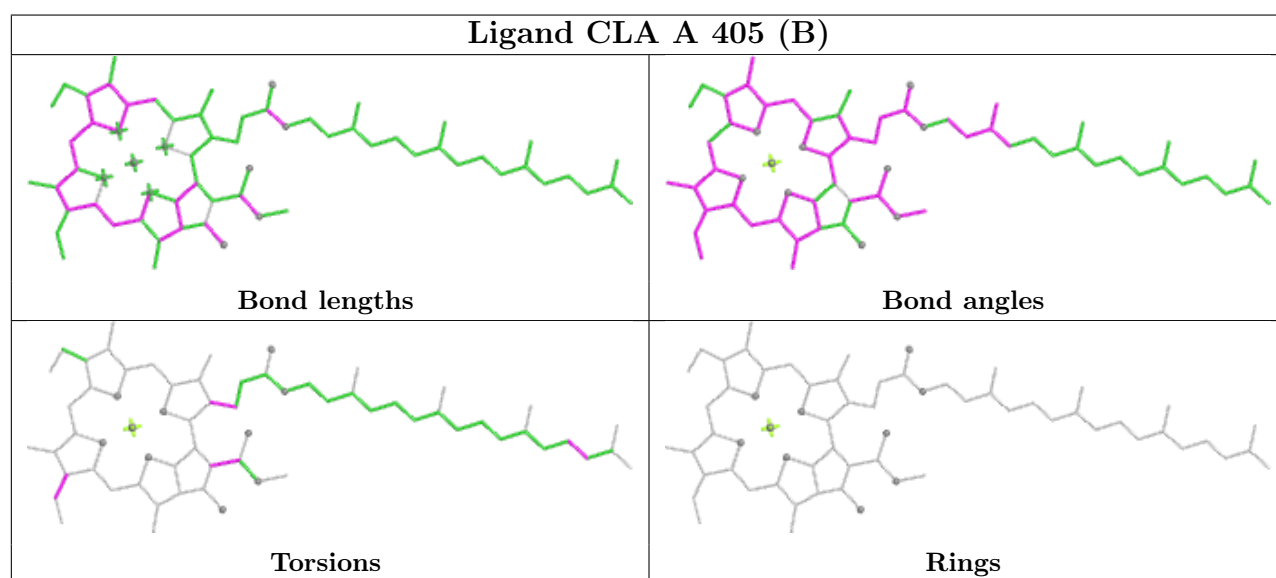
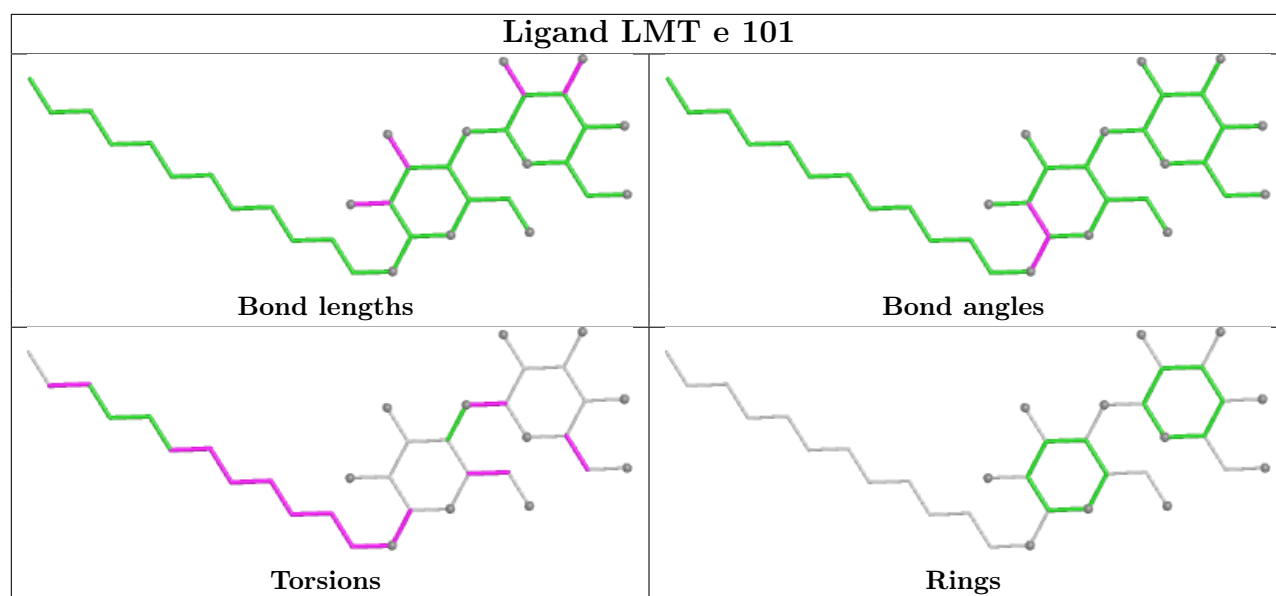


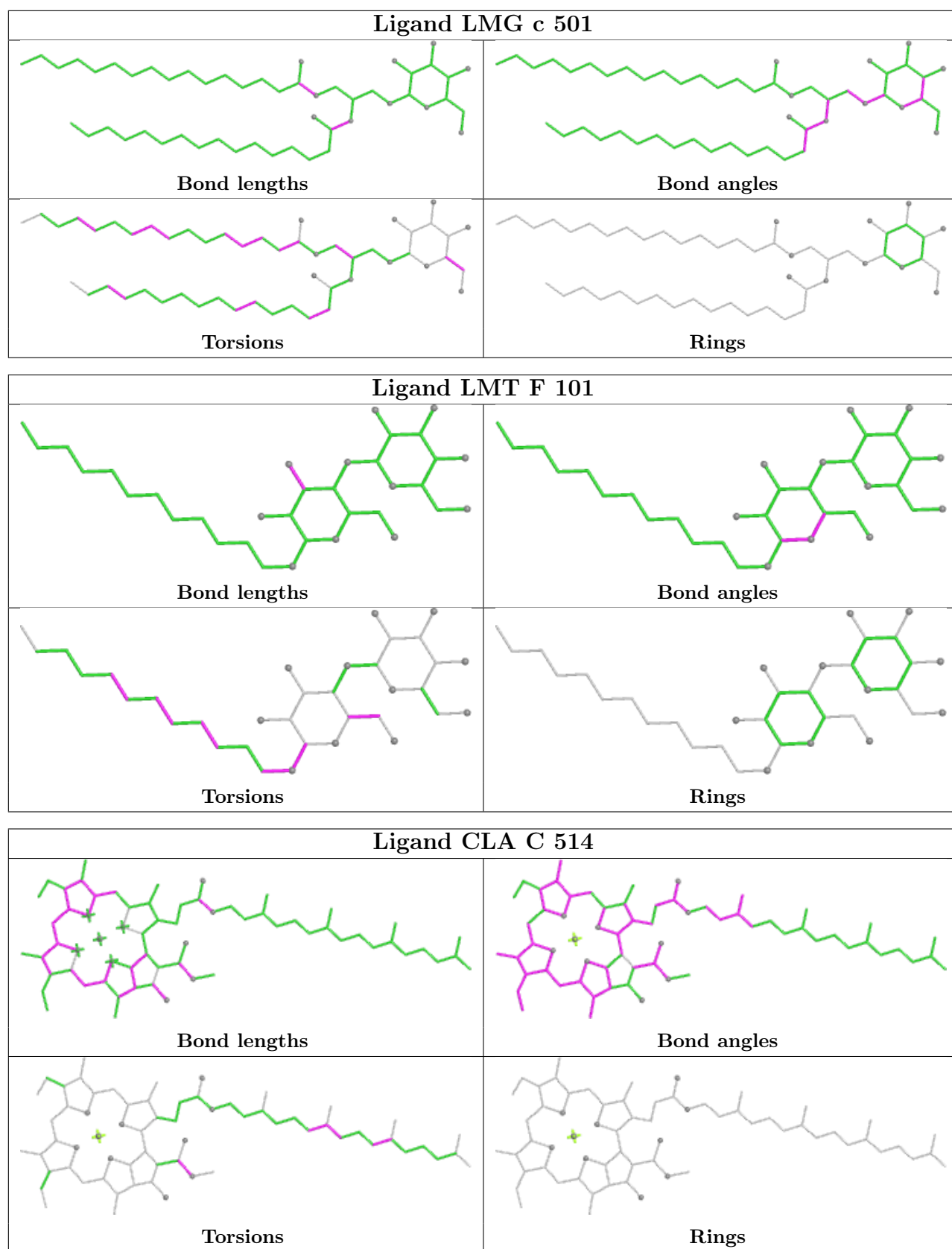
Ligand CLA c 513



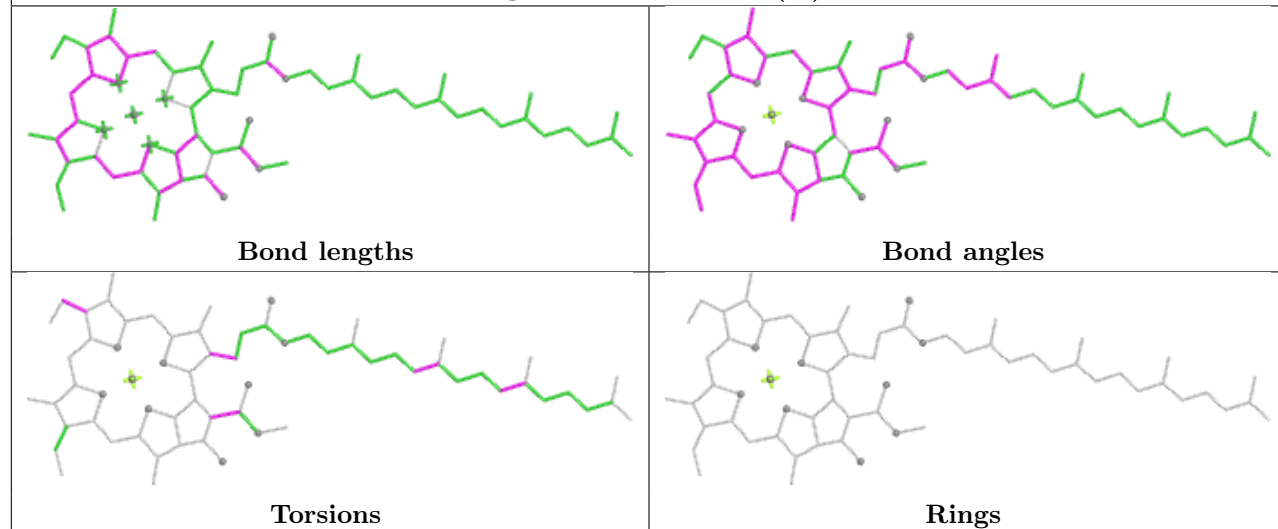
Ligand LMT B 627



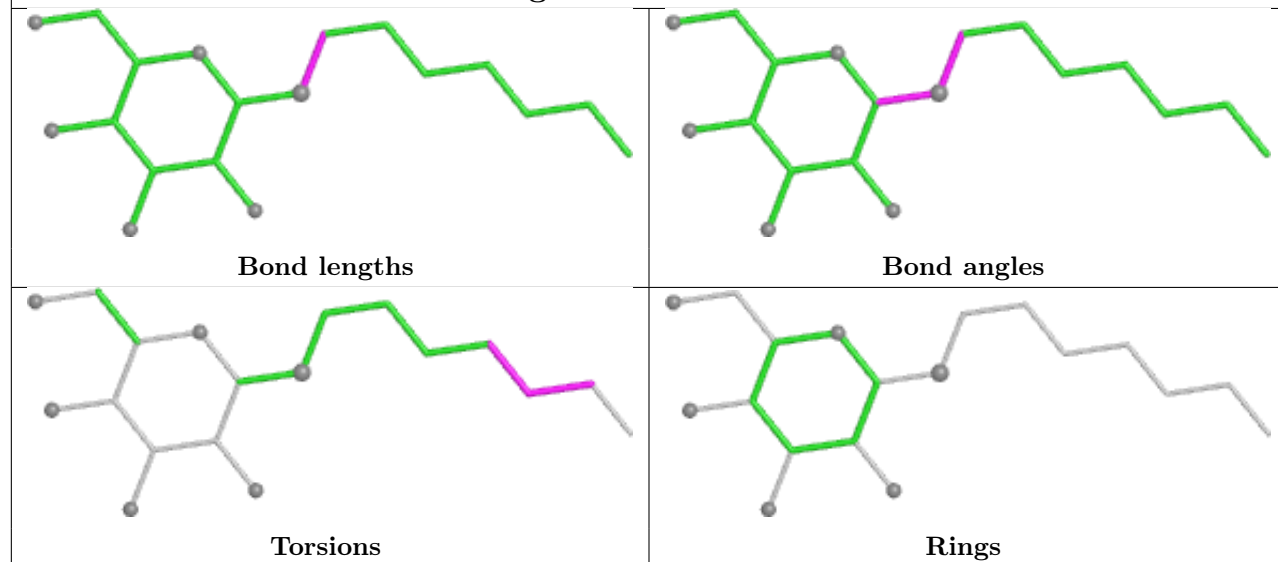




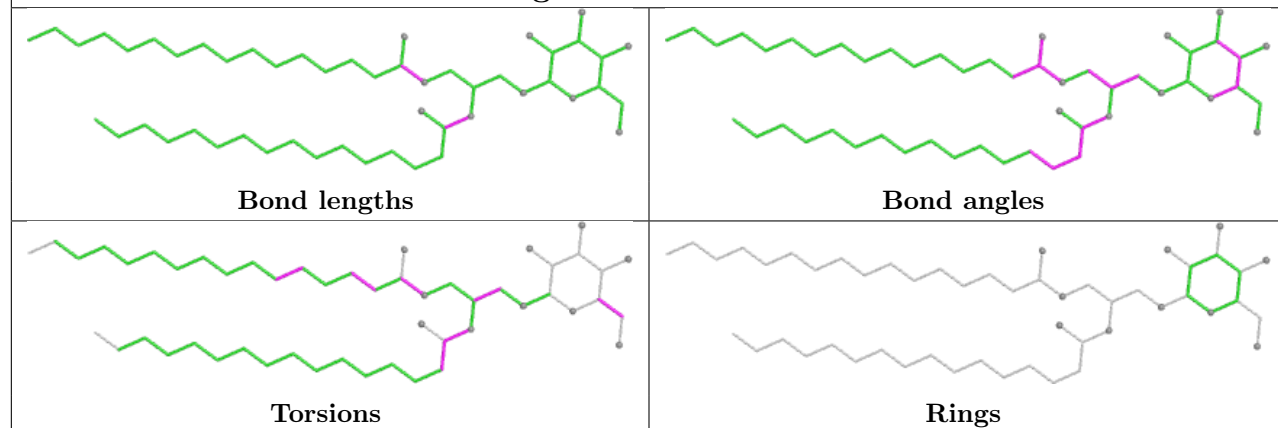
Ligand CLA a 405 (B)

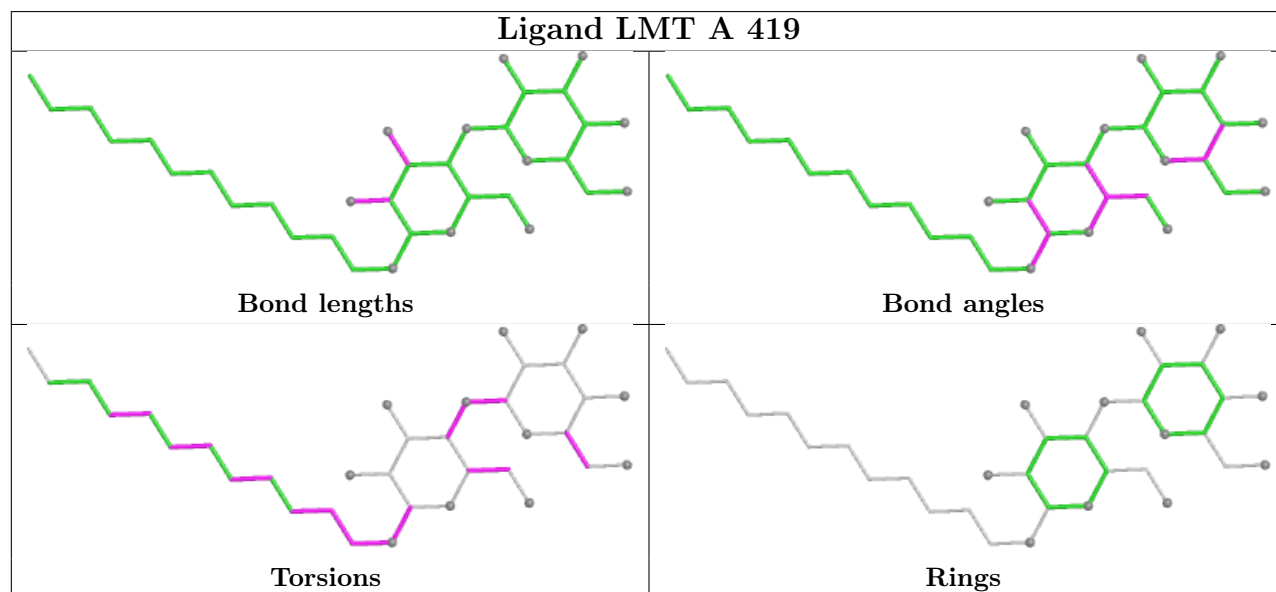
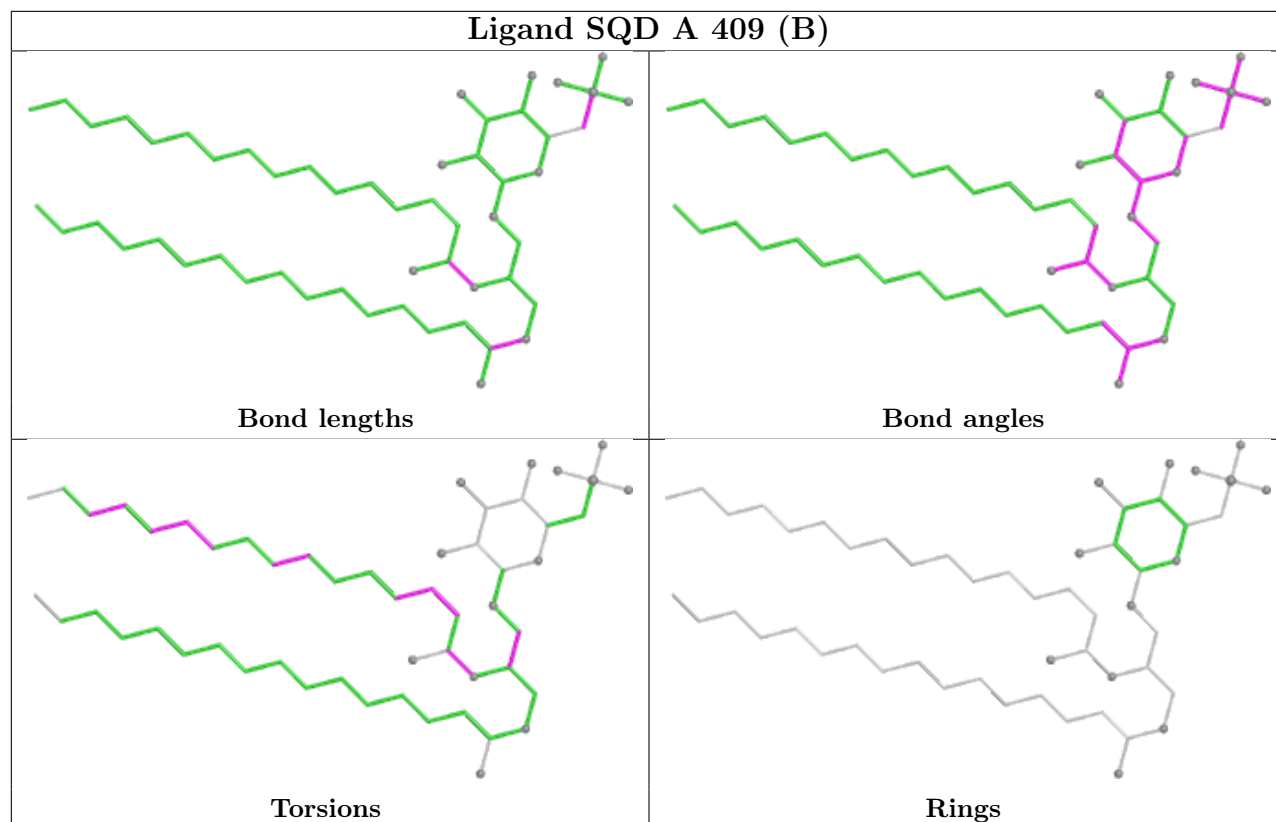


Ligand HTG B 621

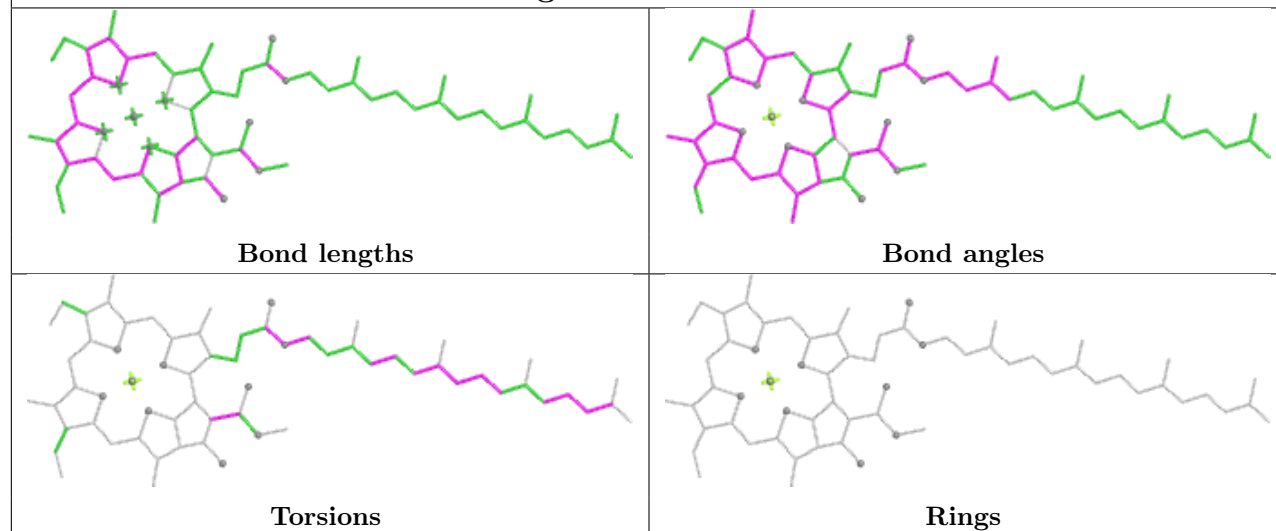


Ligand LMG c 521





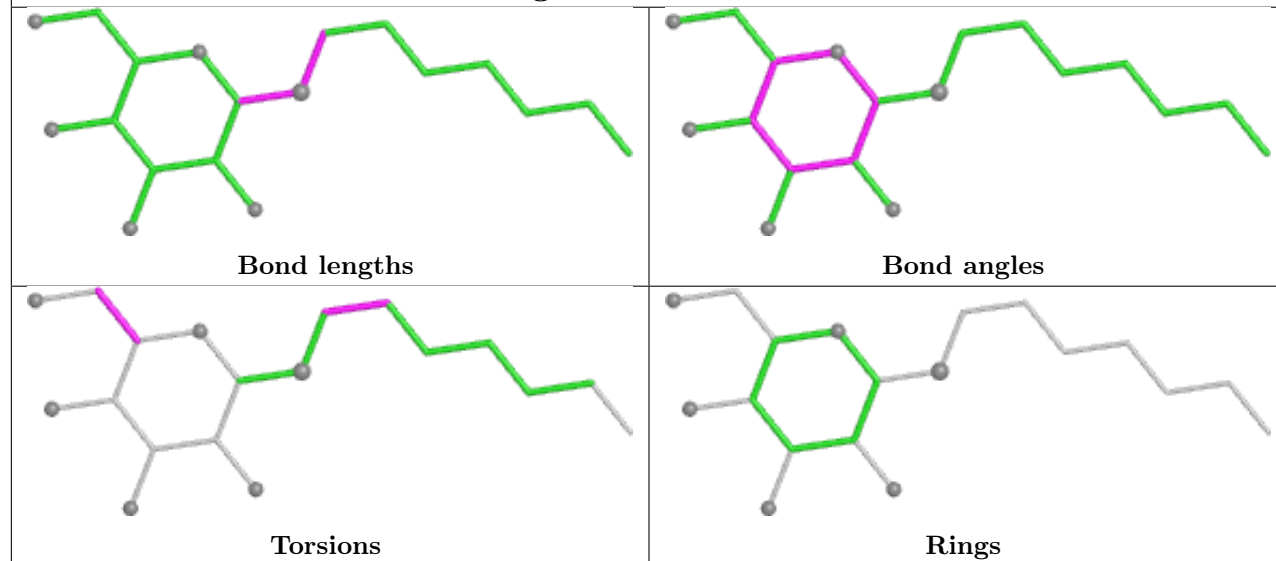
Ligand CLA c 510

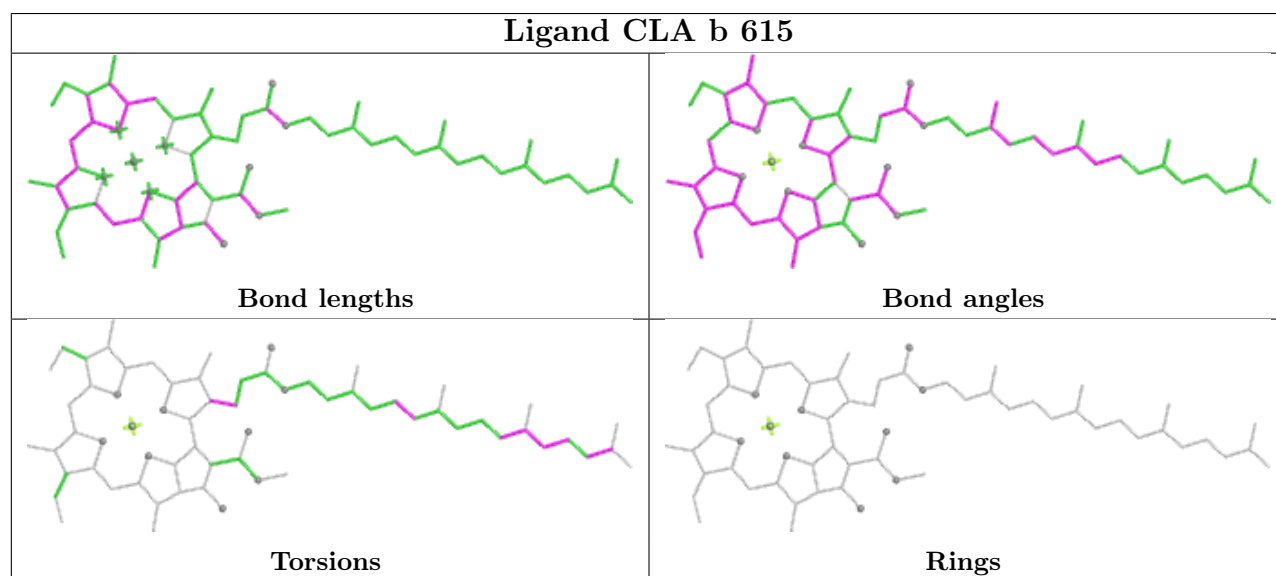
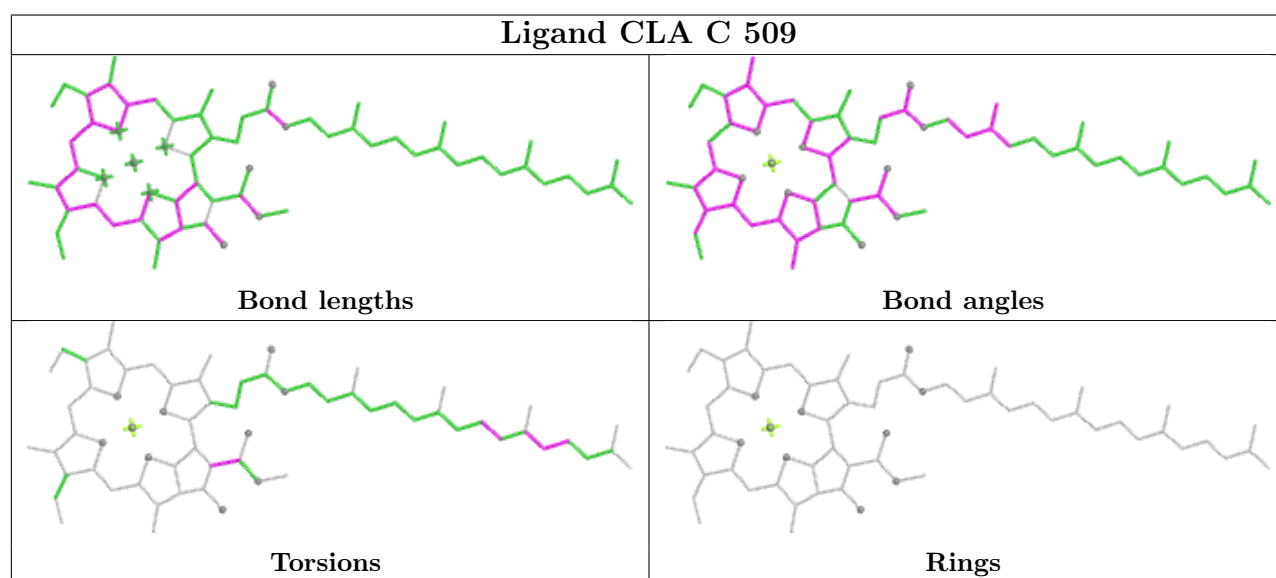
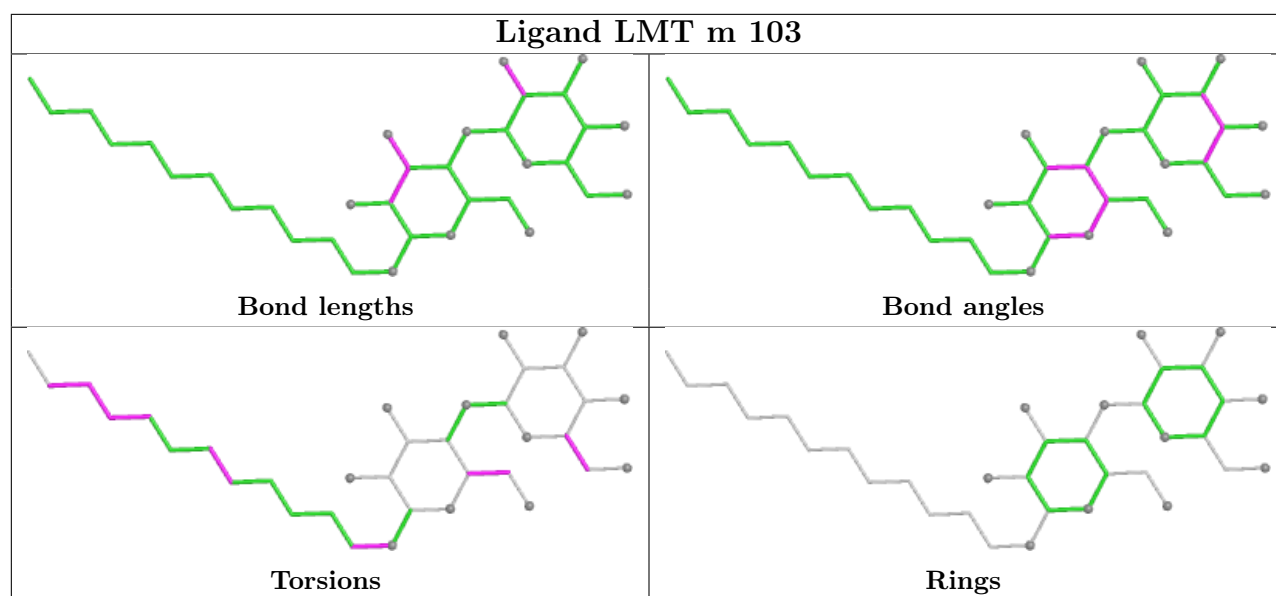


Ligand PL9 d 406 (A)

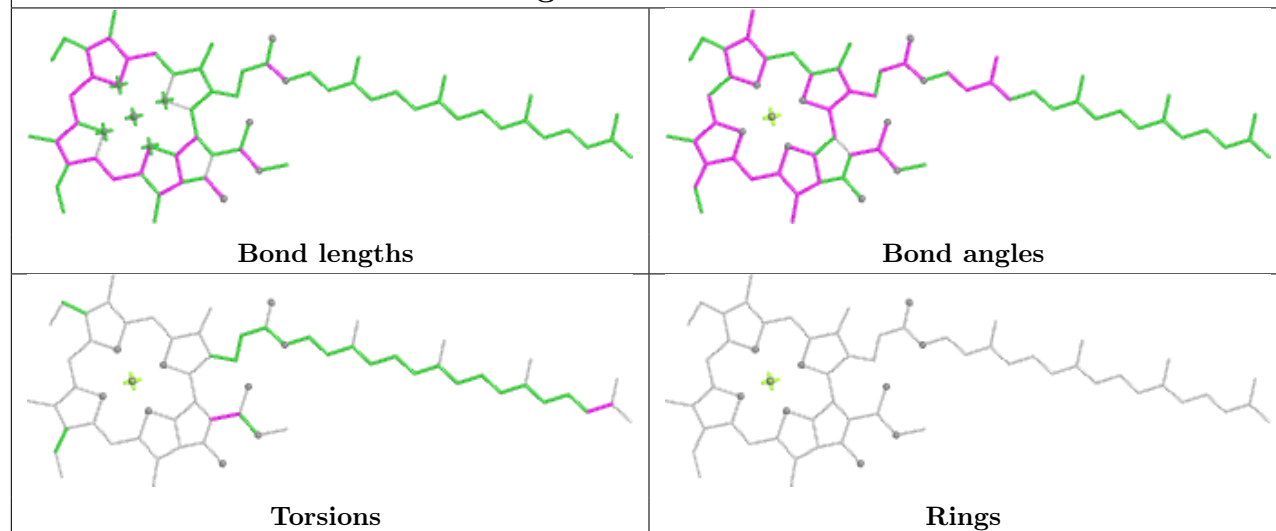


Ligand HTG b 625

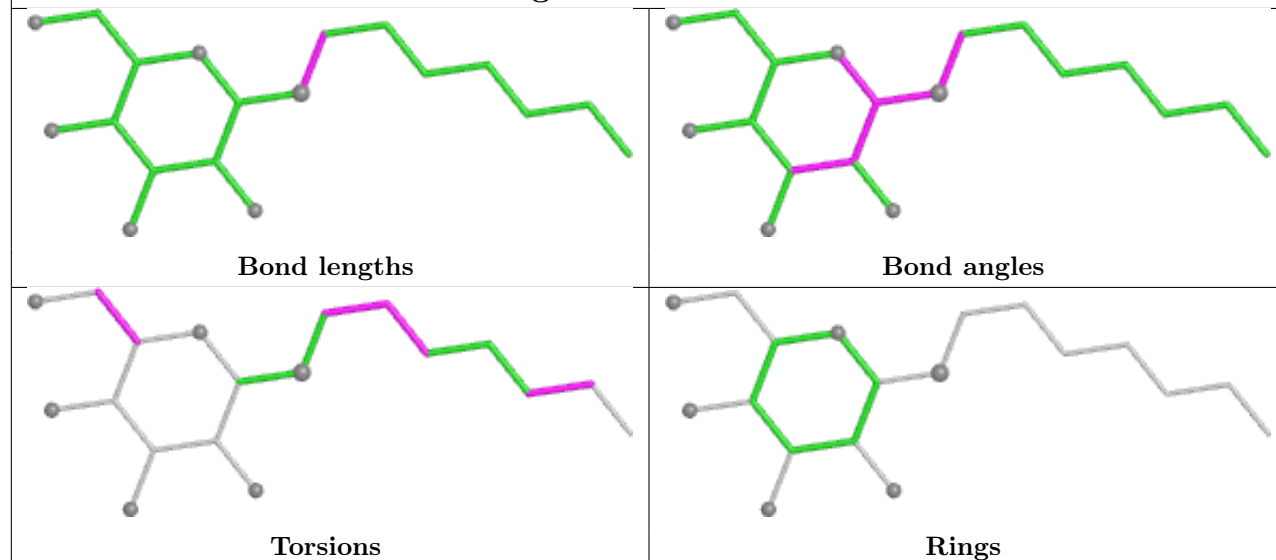




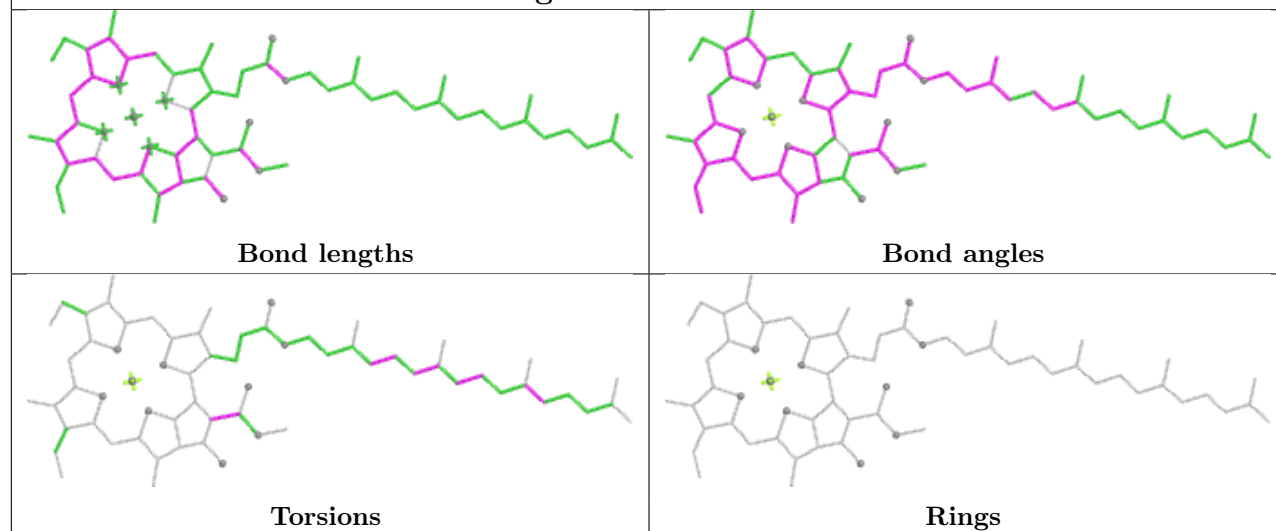
Ligand CLA c 509



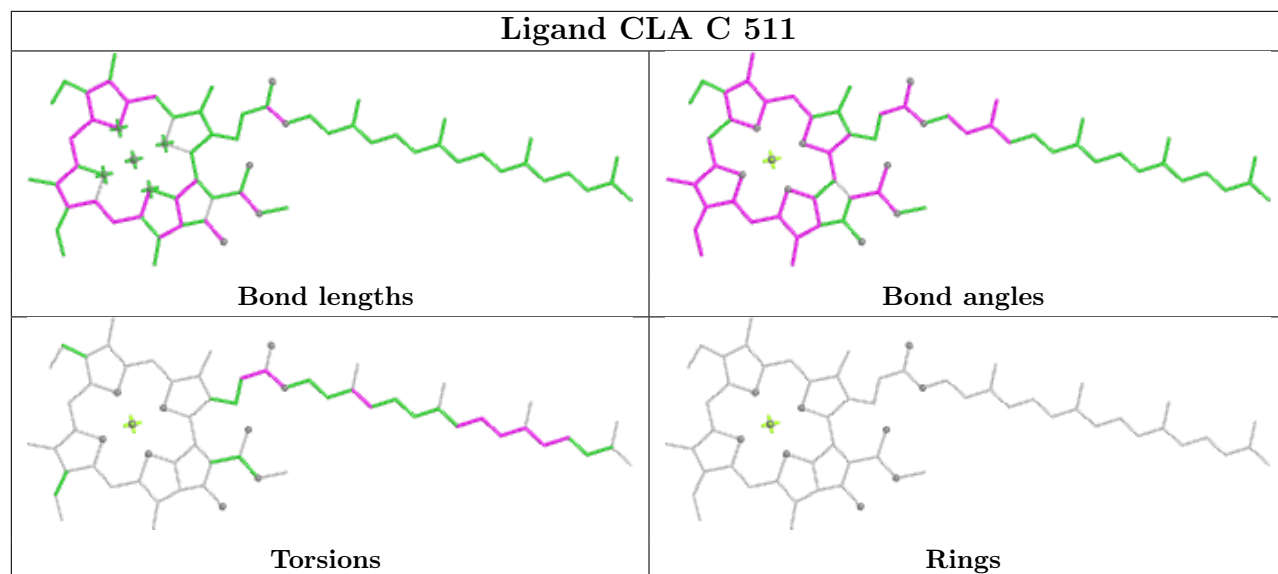
Ligand HTG b 623



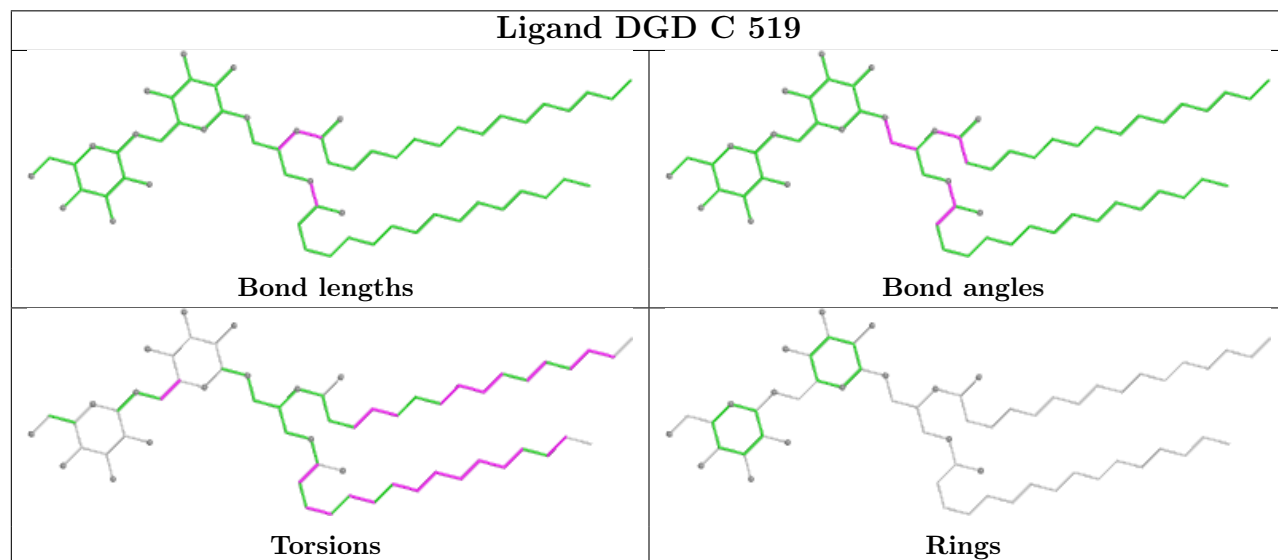
Ligand CLA b 607

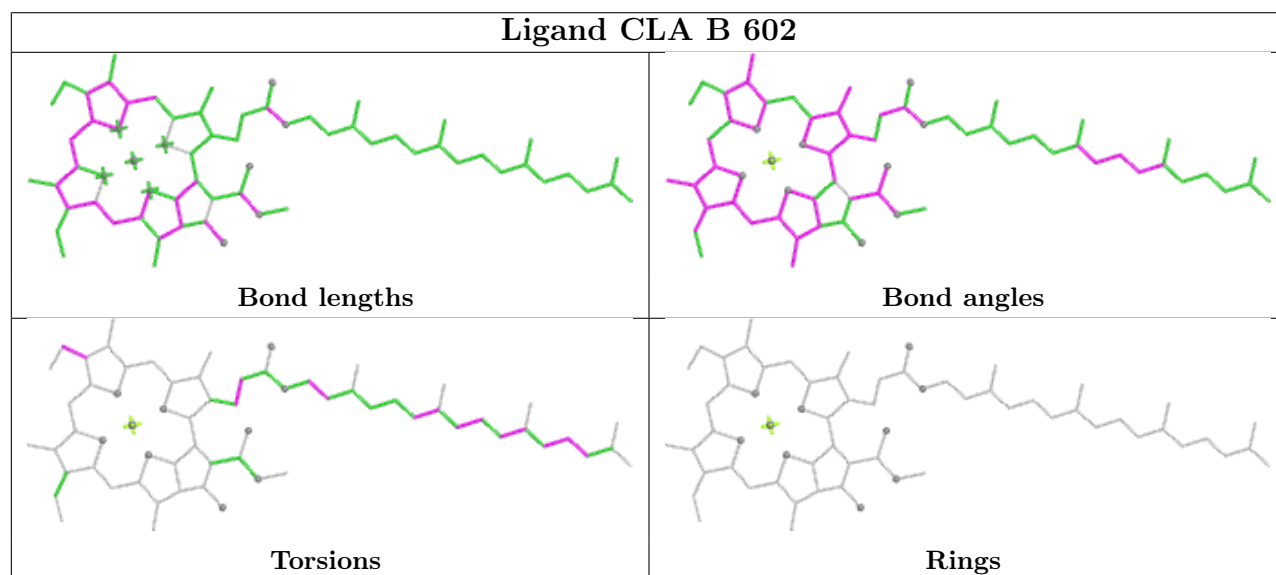
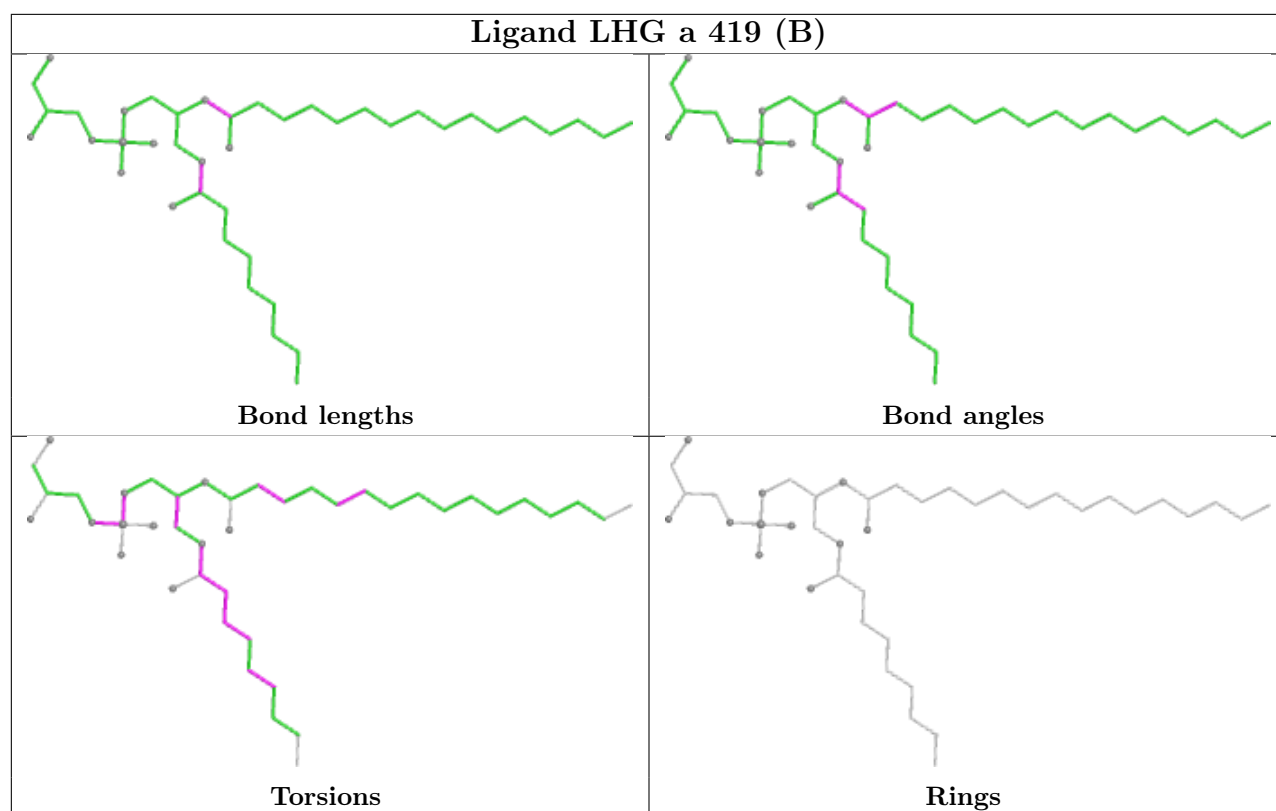


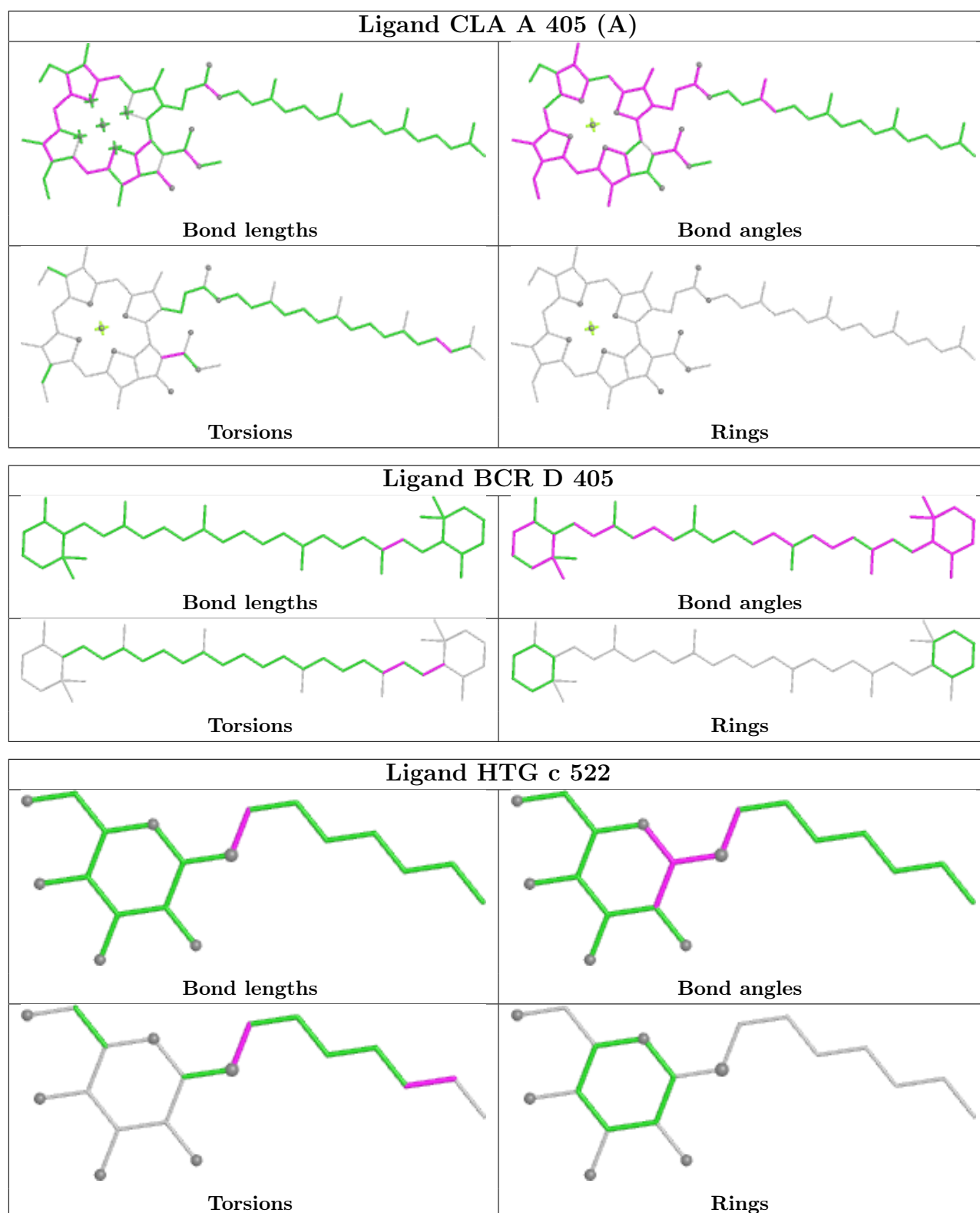
Ligand CLA C 511



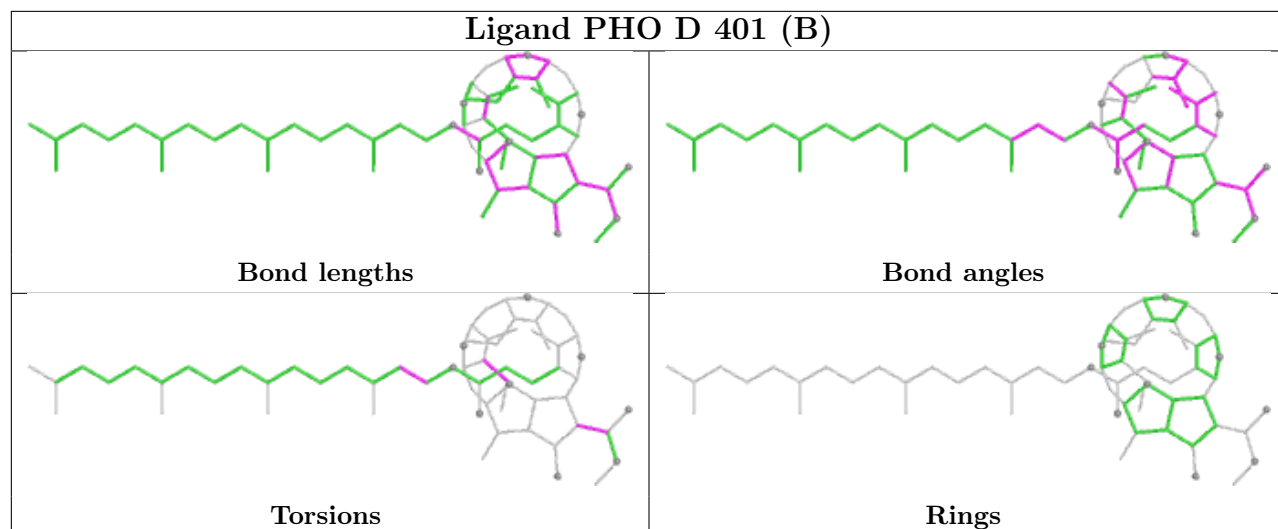
Ligand DGD C 519



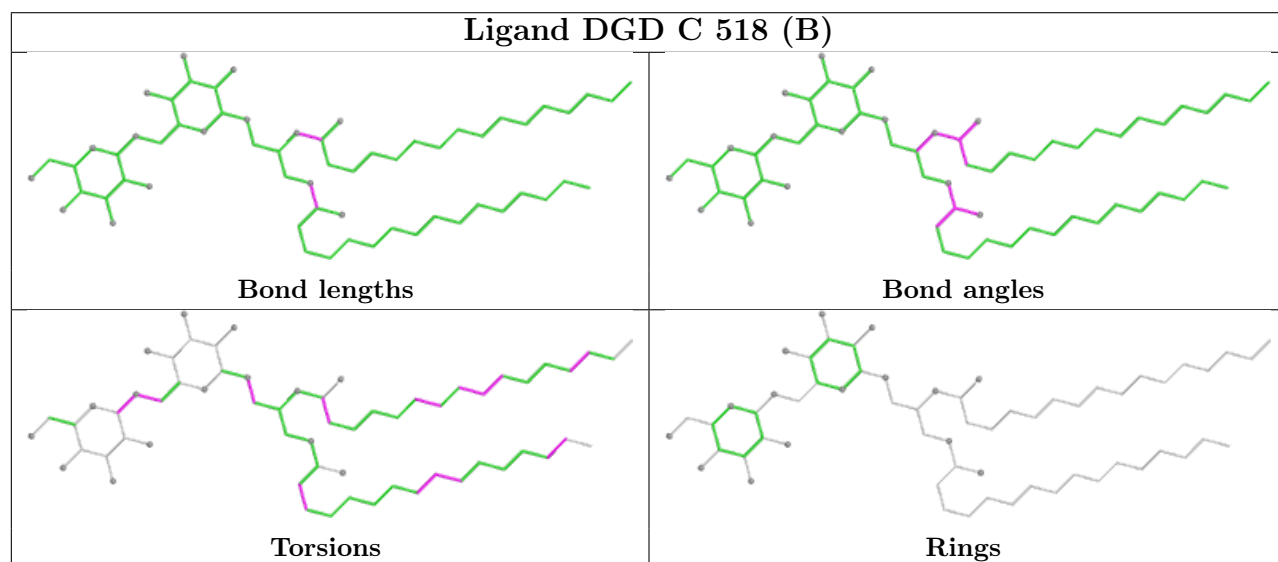




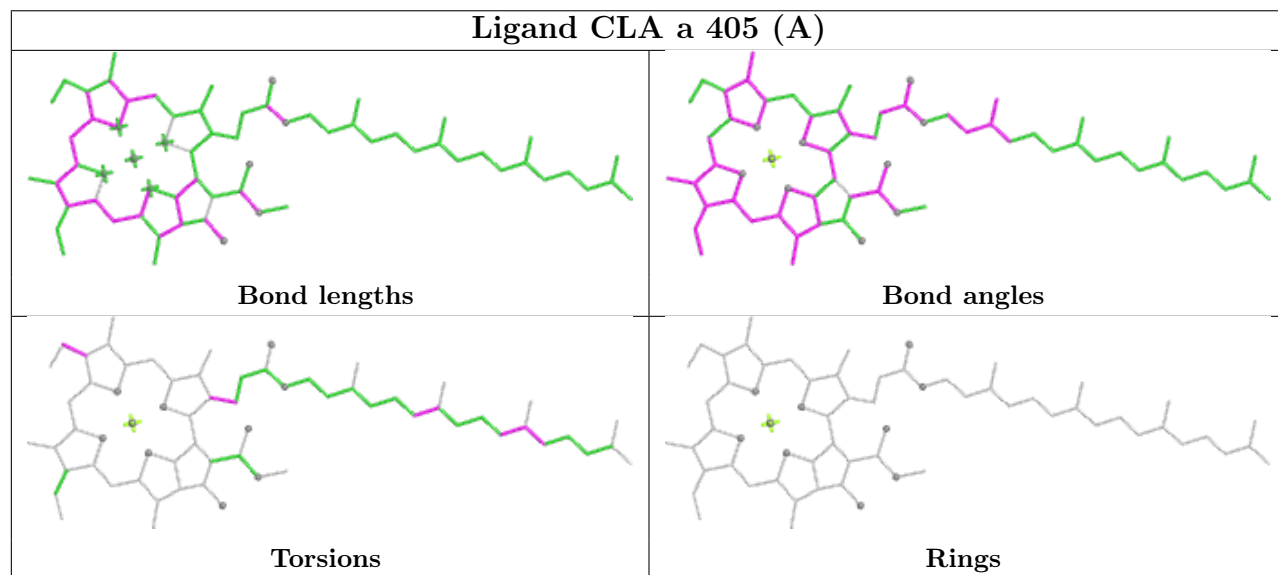
Ligand PHO D 401 (B)

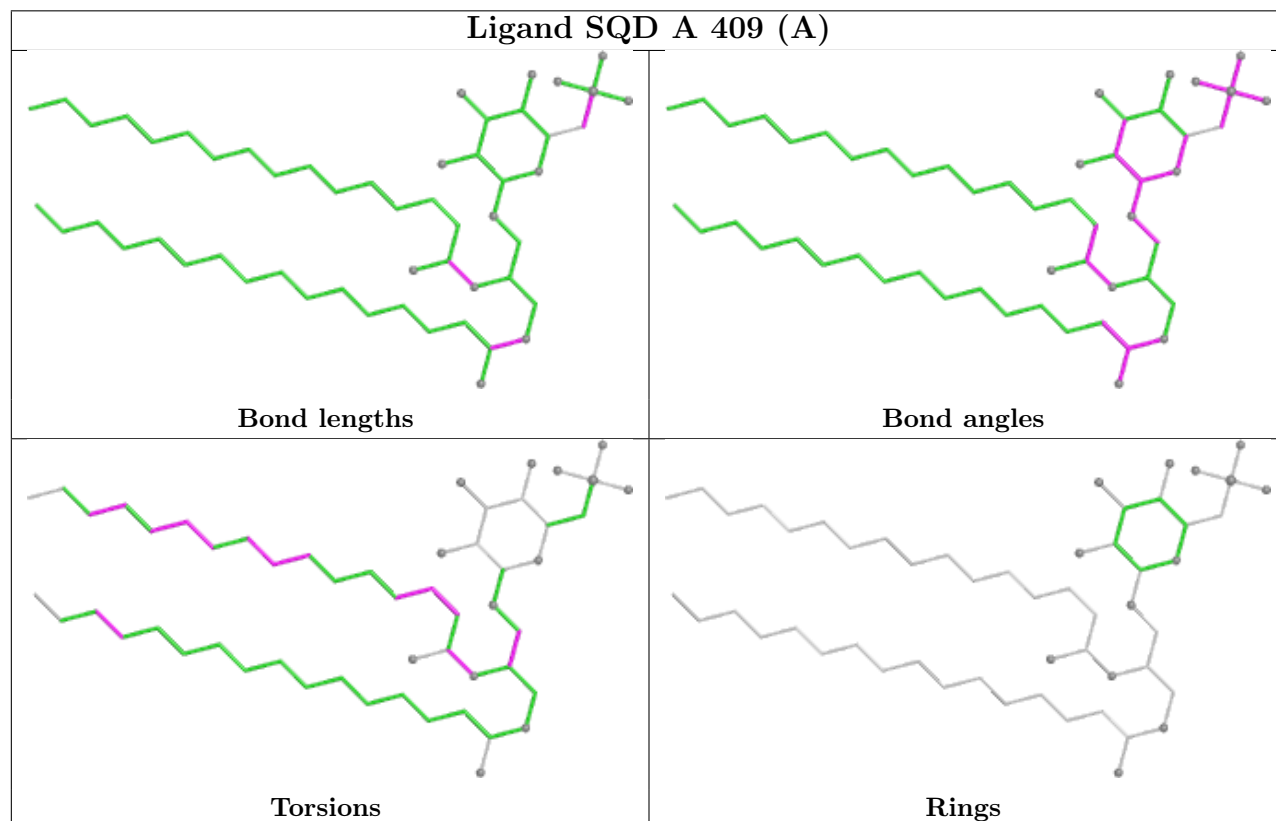
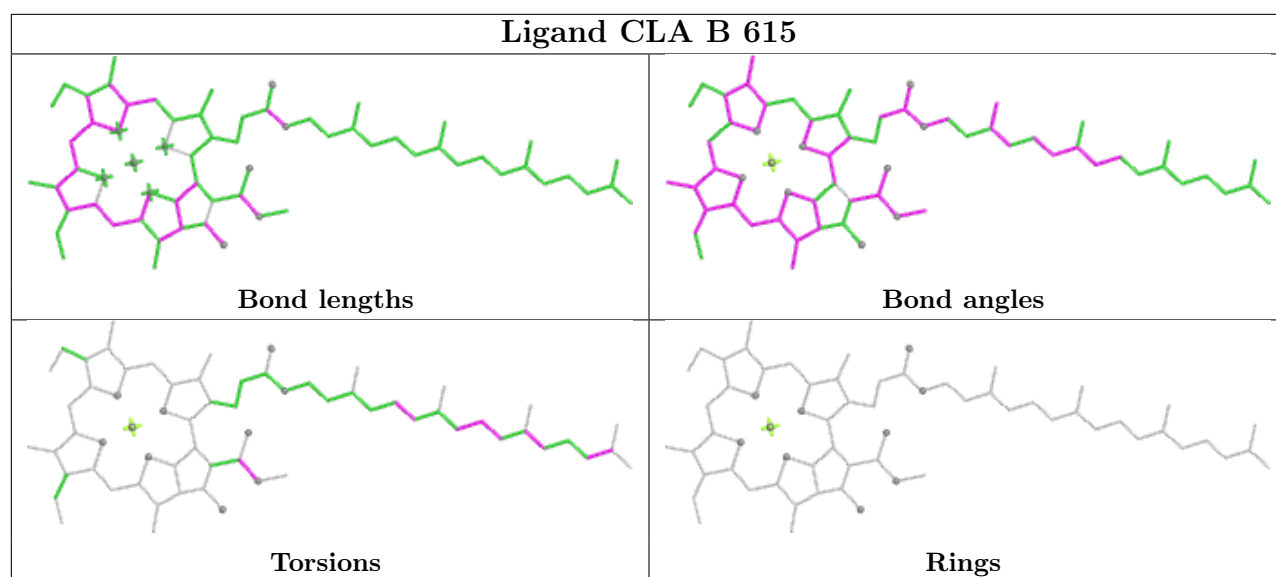


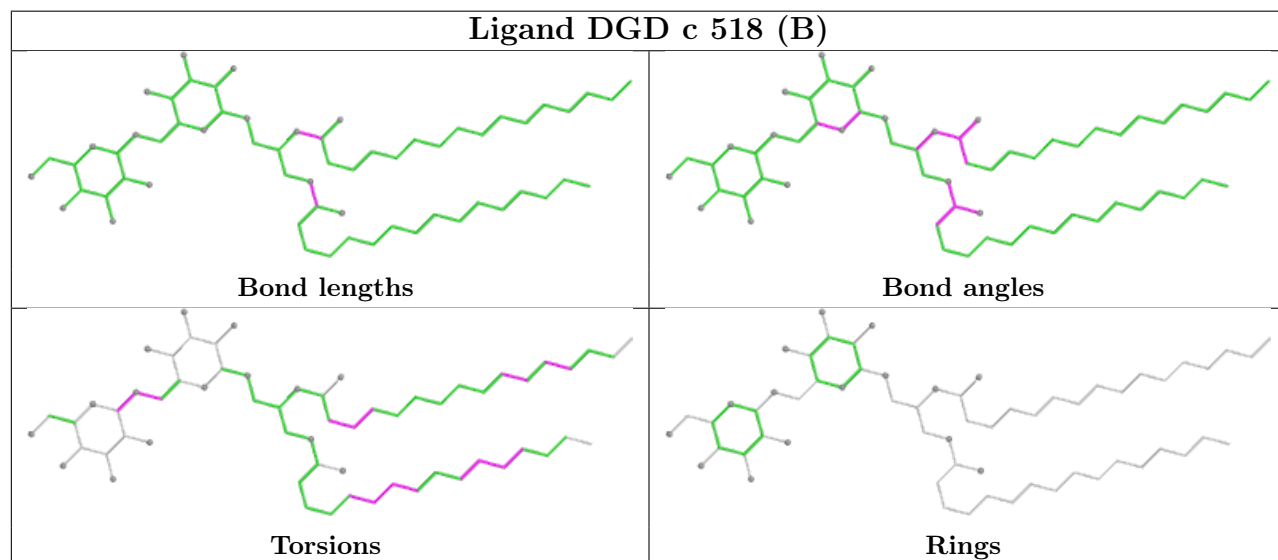
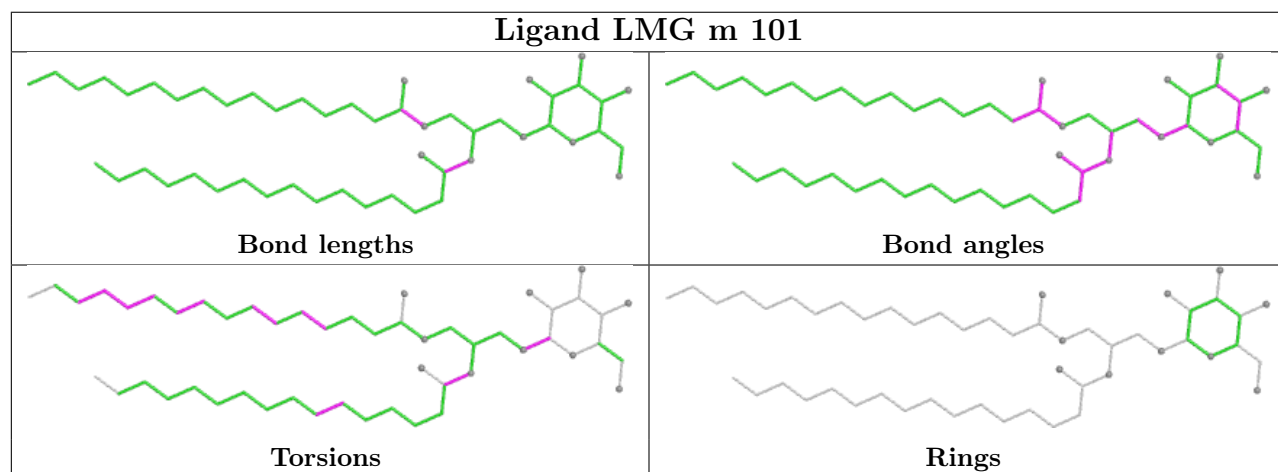
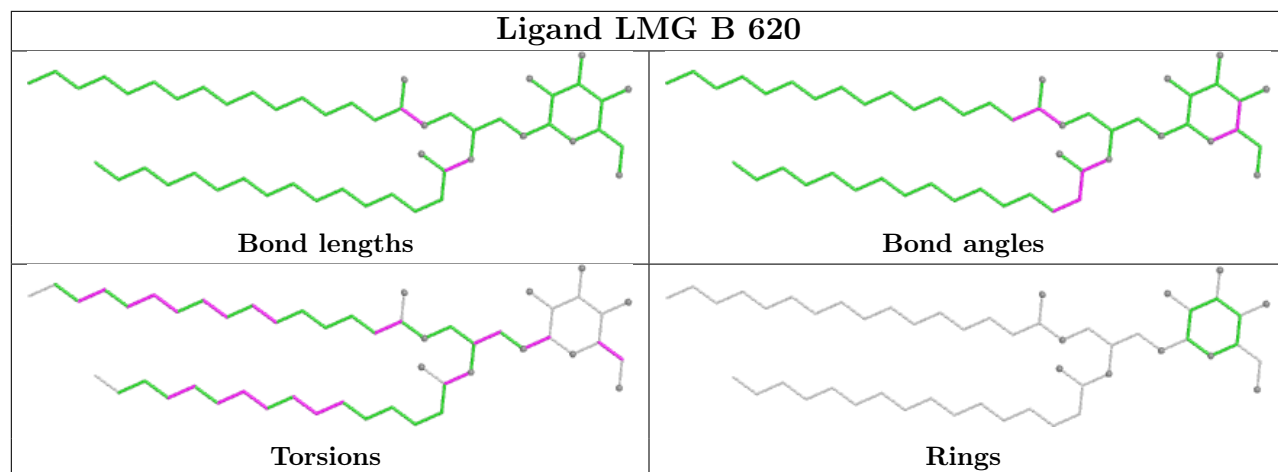
Ligand DGD C 518 (B)



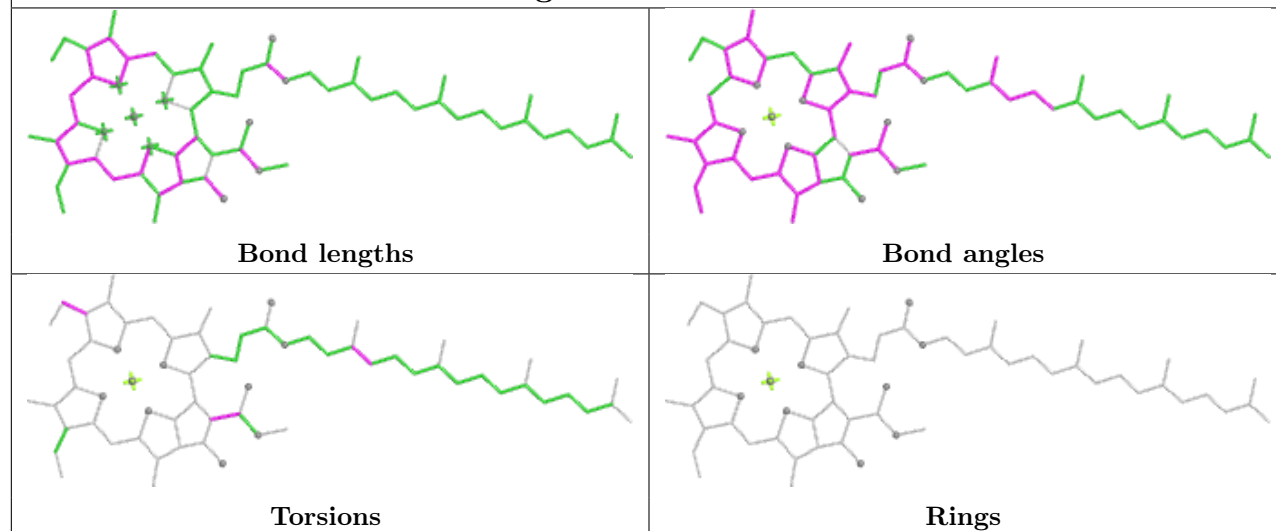
Ligand CLA a 405 (A)



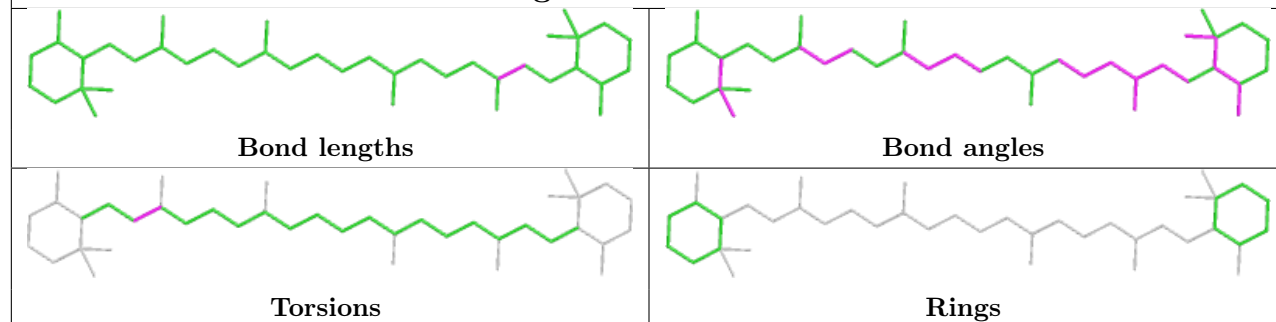




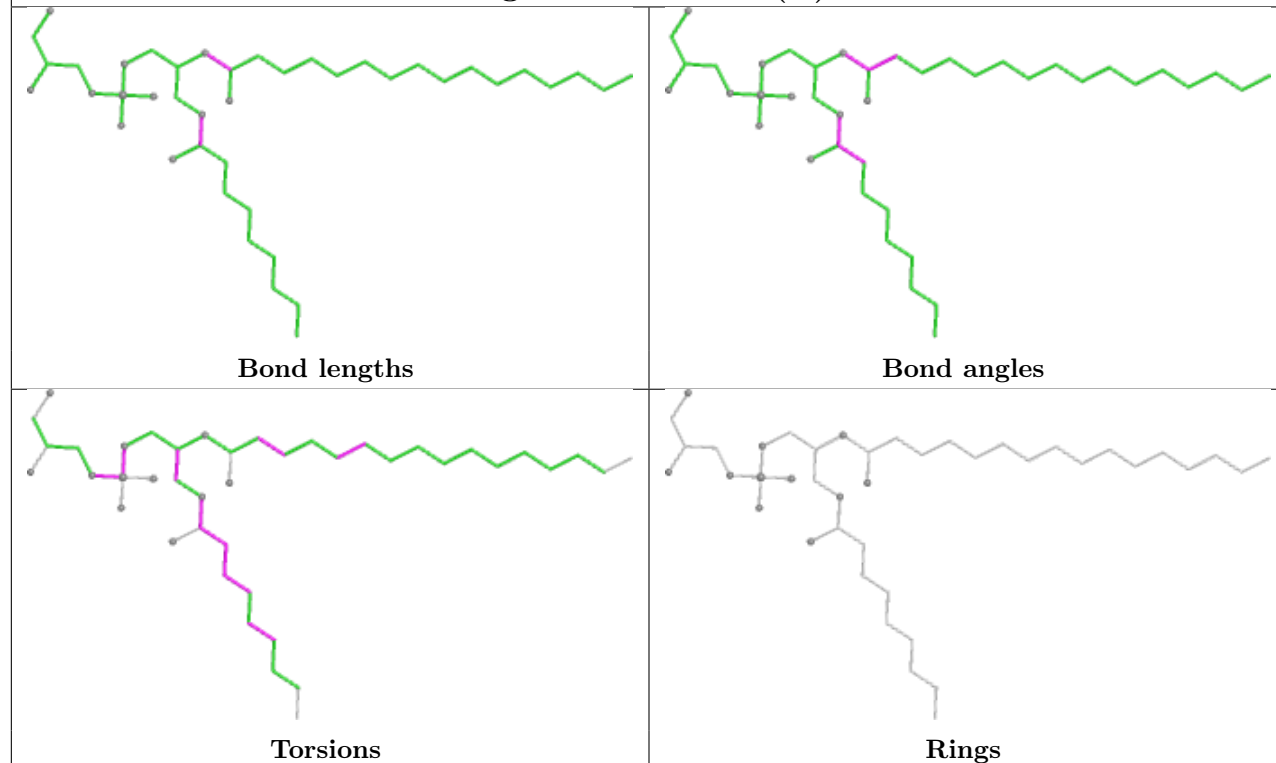
Ligand CLA b 603

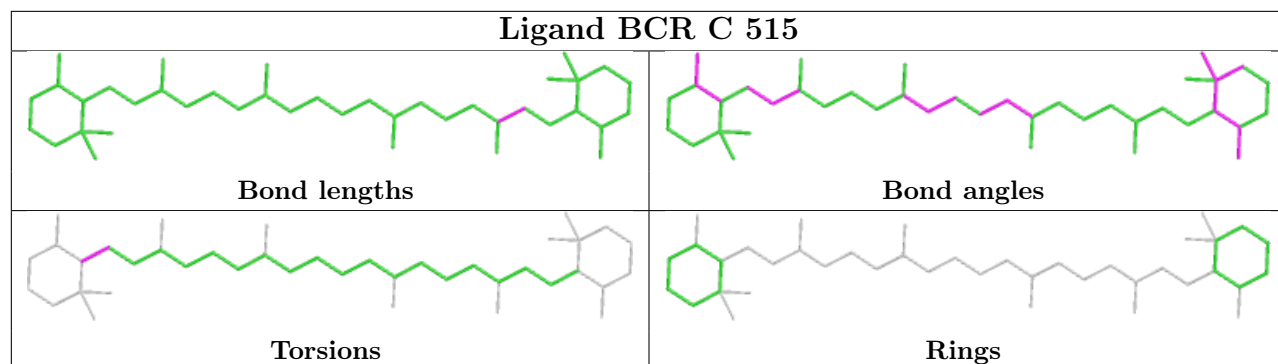
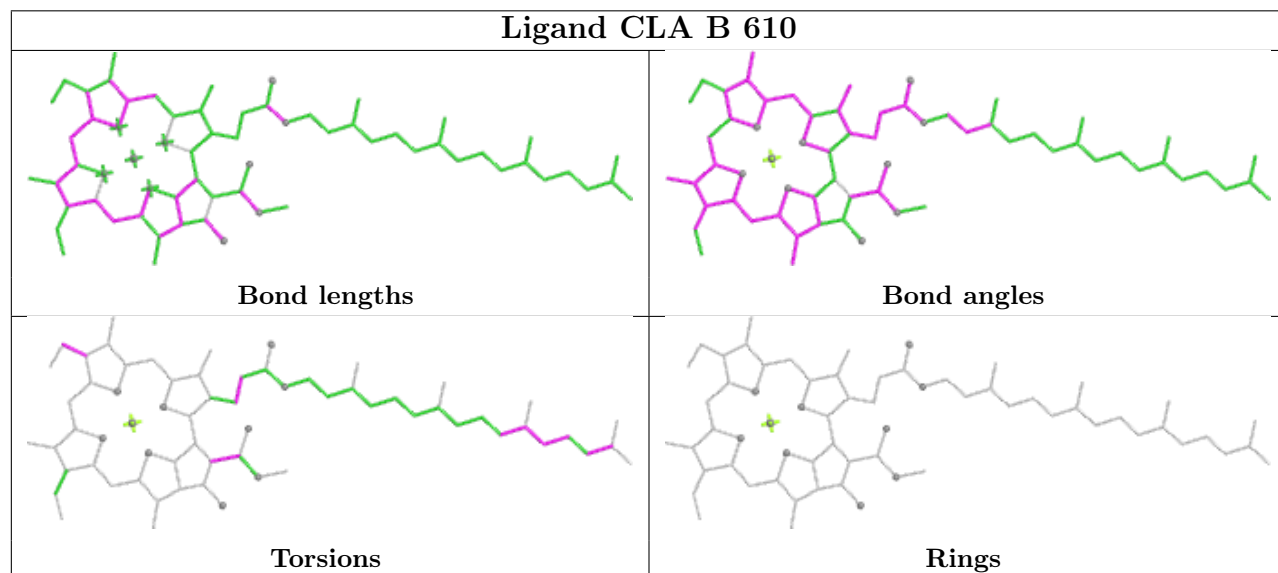
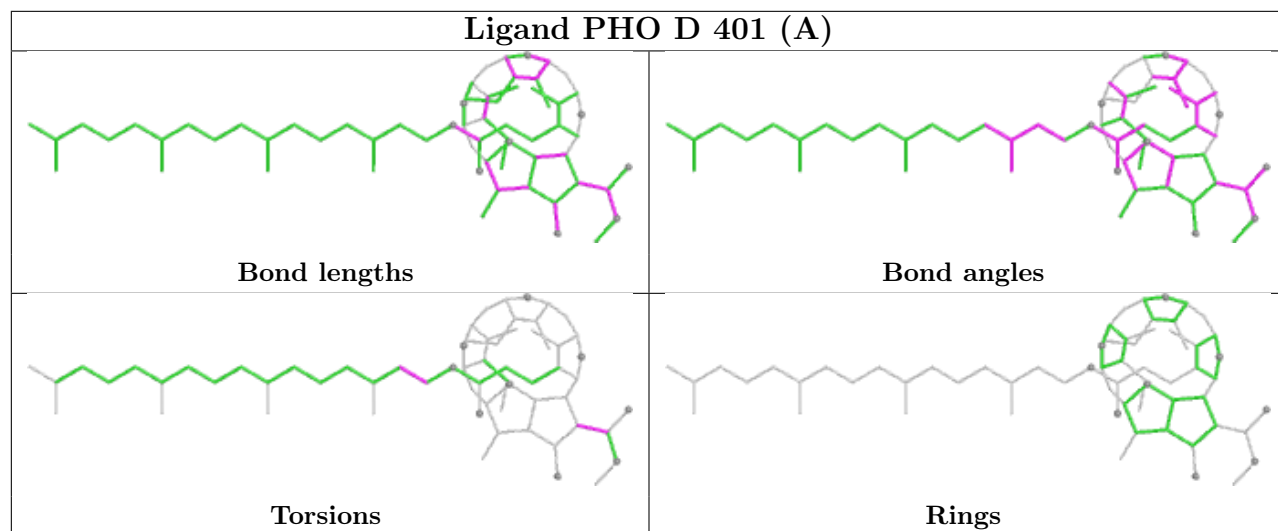


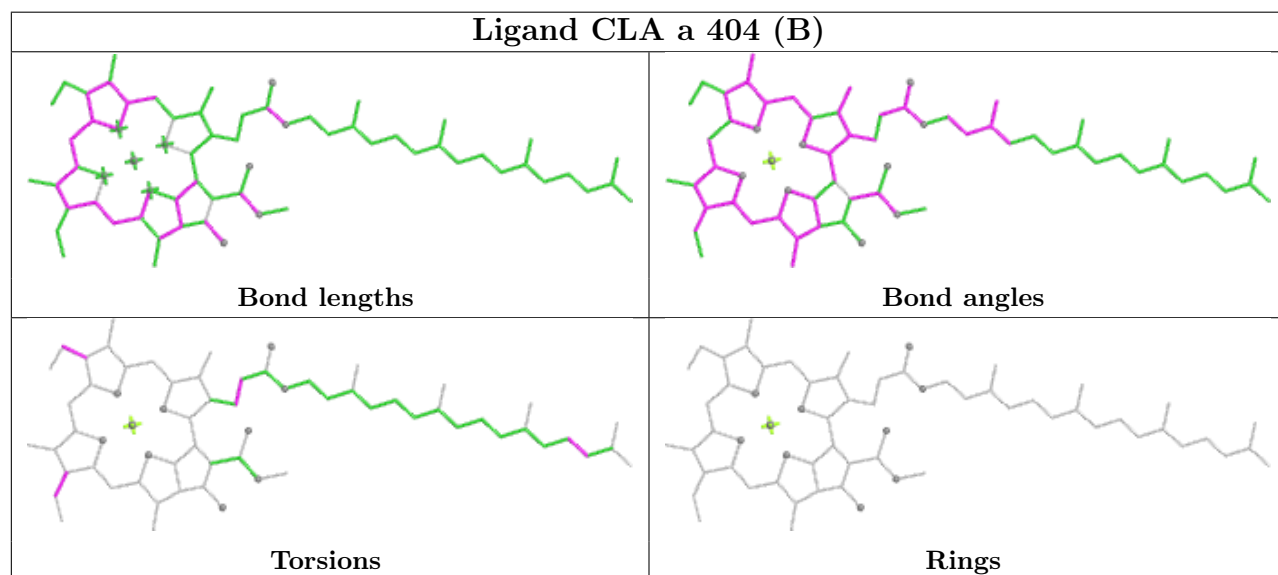
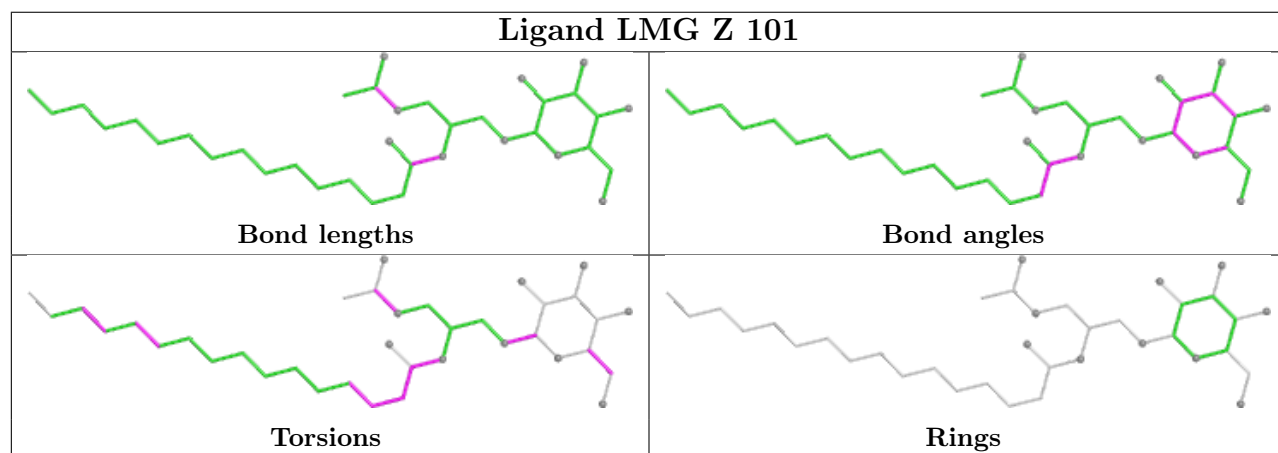
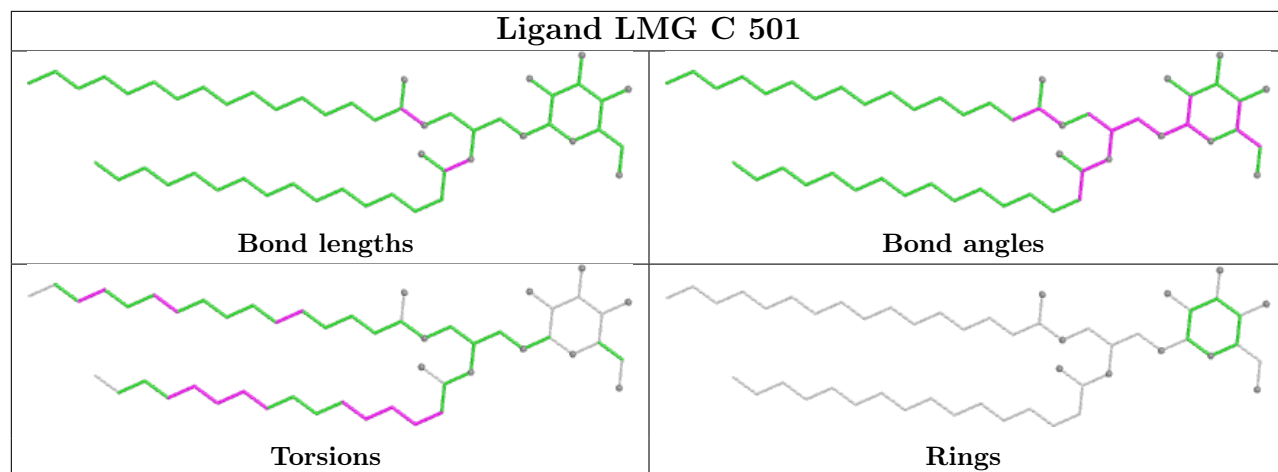
Ligand BCR b 619



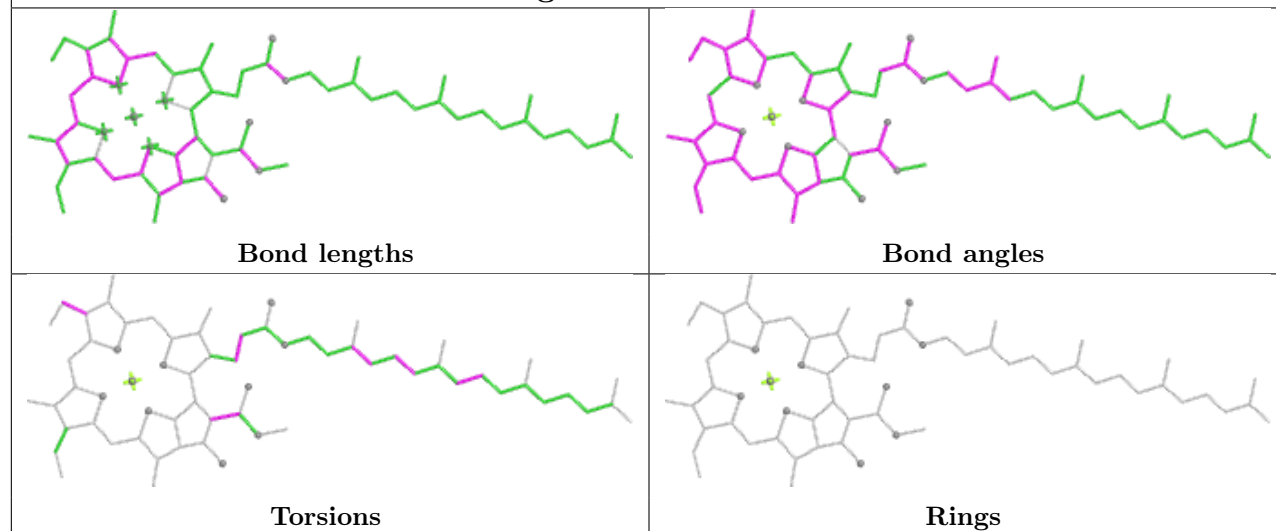
Ligand LHG a 419 (A)



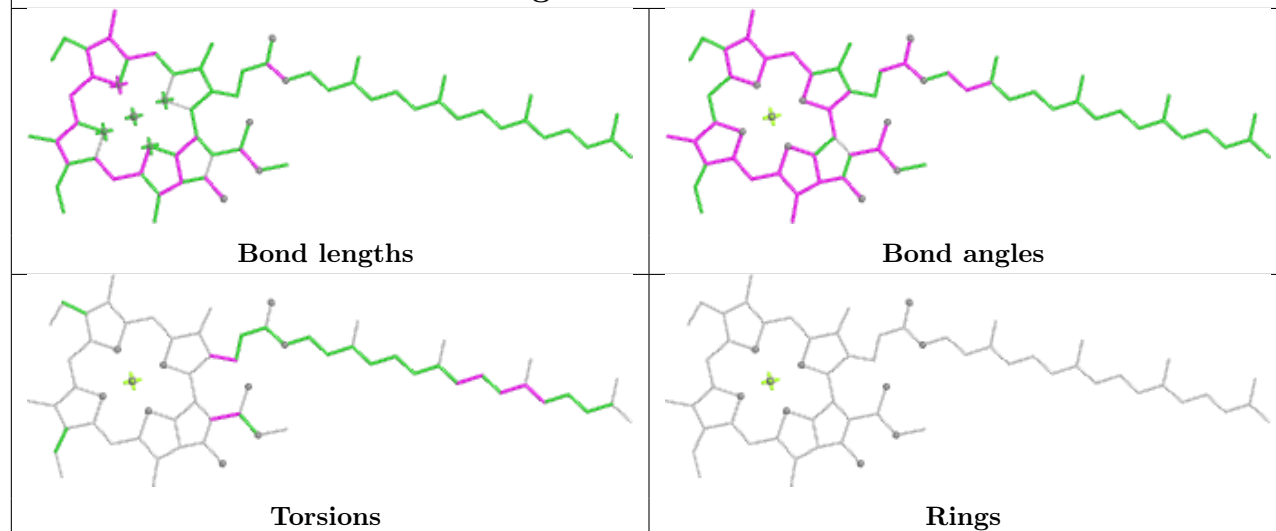
Ligand BCR C 515**Ligand CLA B 610****Ligand PHO D 401 (A)**



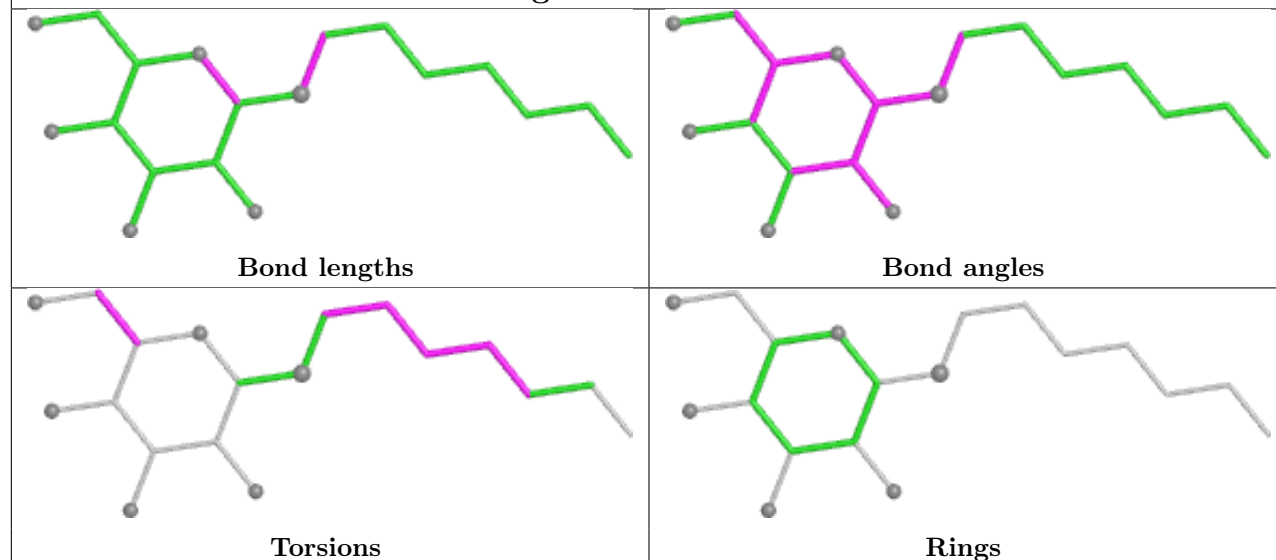
Ligand CLA c 508



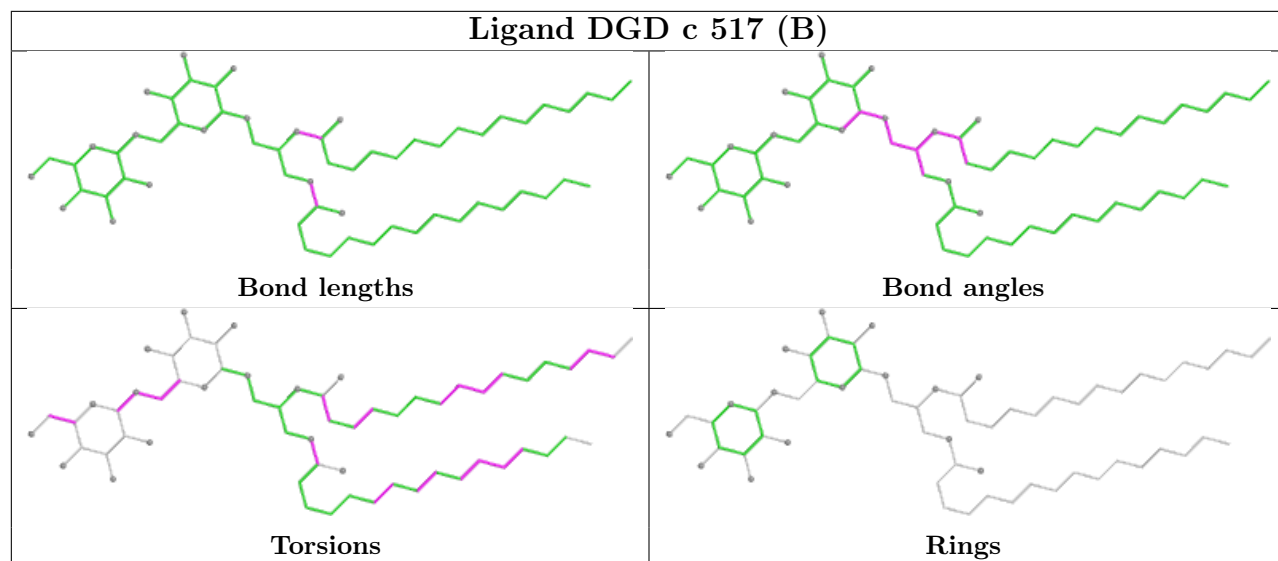
Ligand CLA B 611



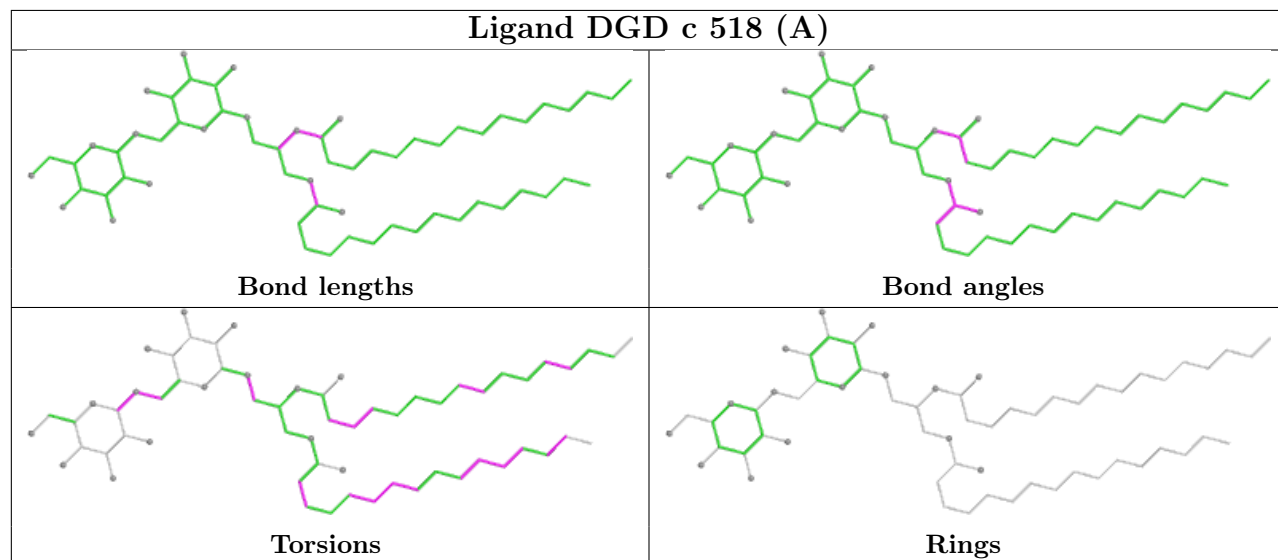
Ligand HTG b 622



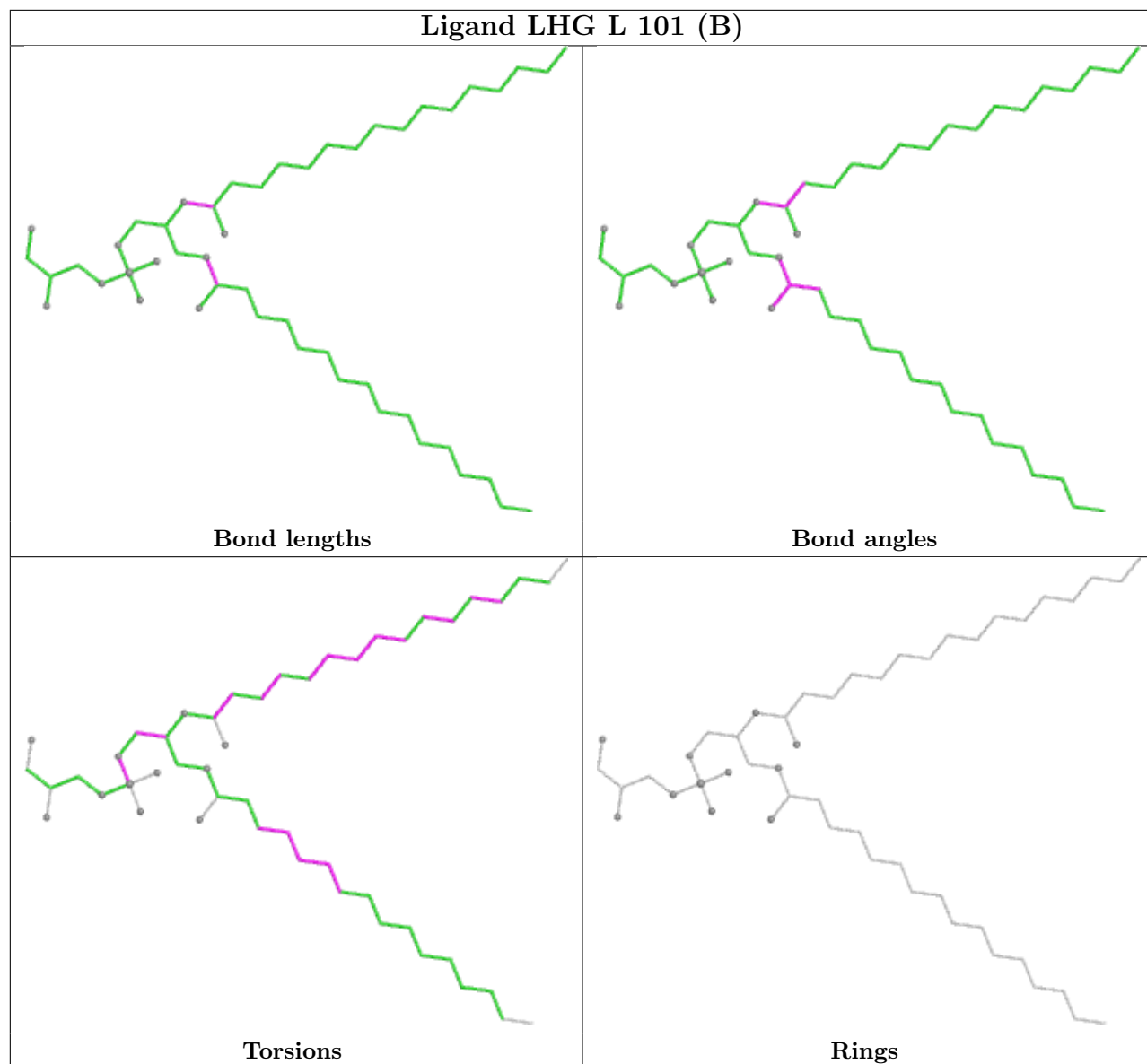
Ligand DGD c 517 (B)



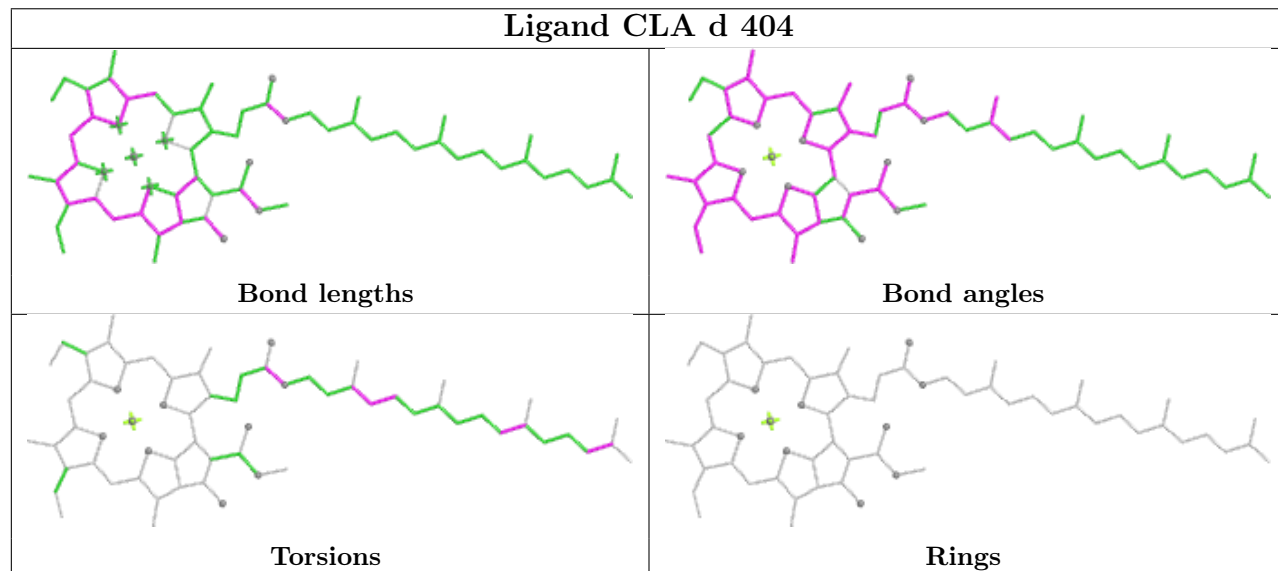
Ligand DGD c 518 (A)

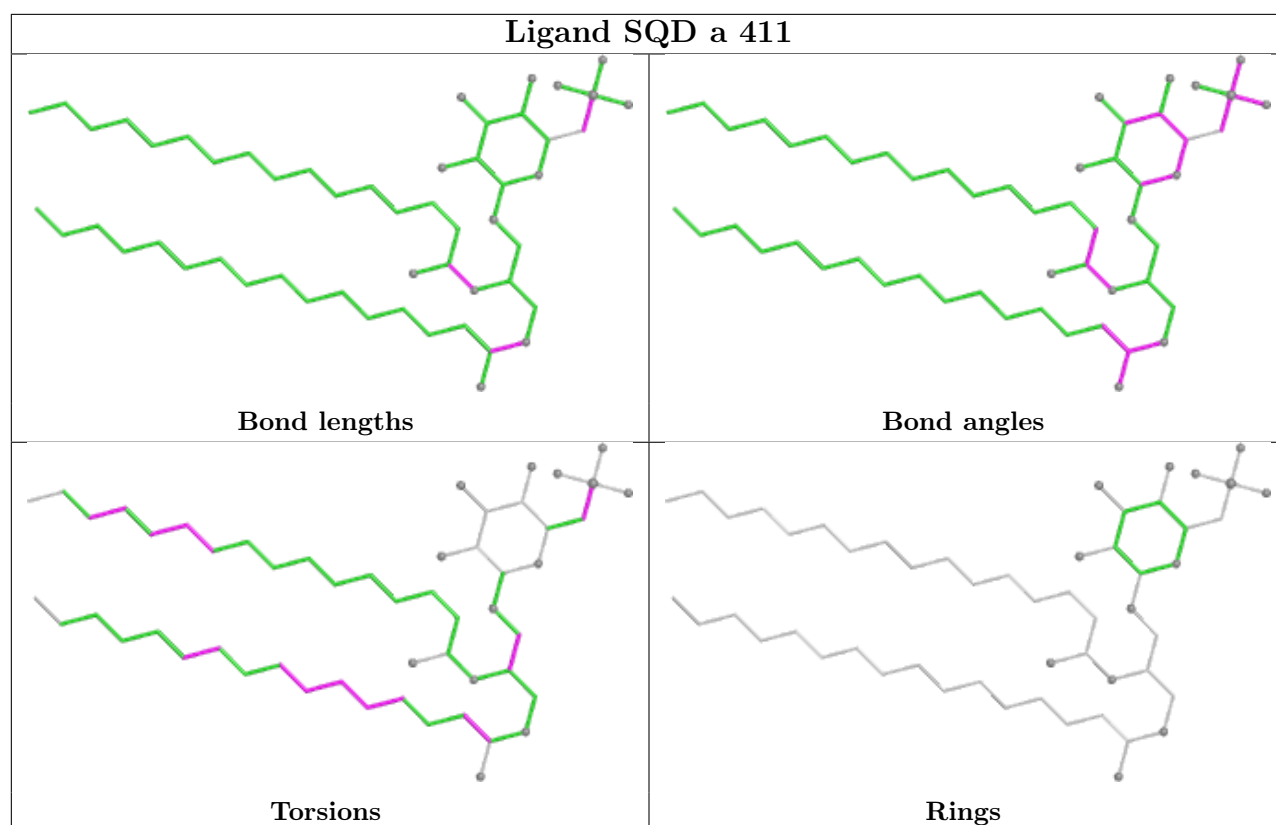


Ligand LHG L 101 (B)

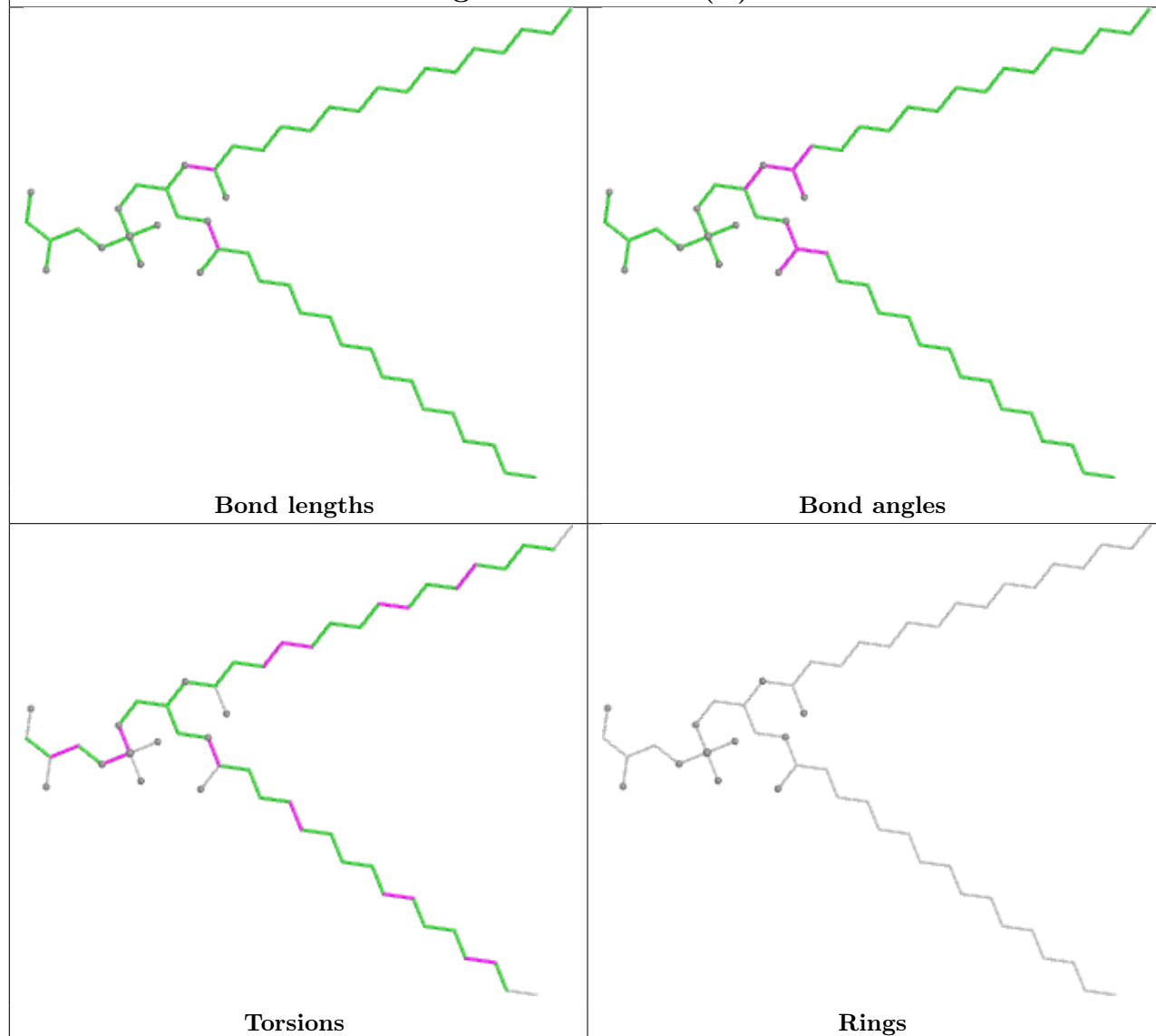


Ligand CLA d 404

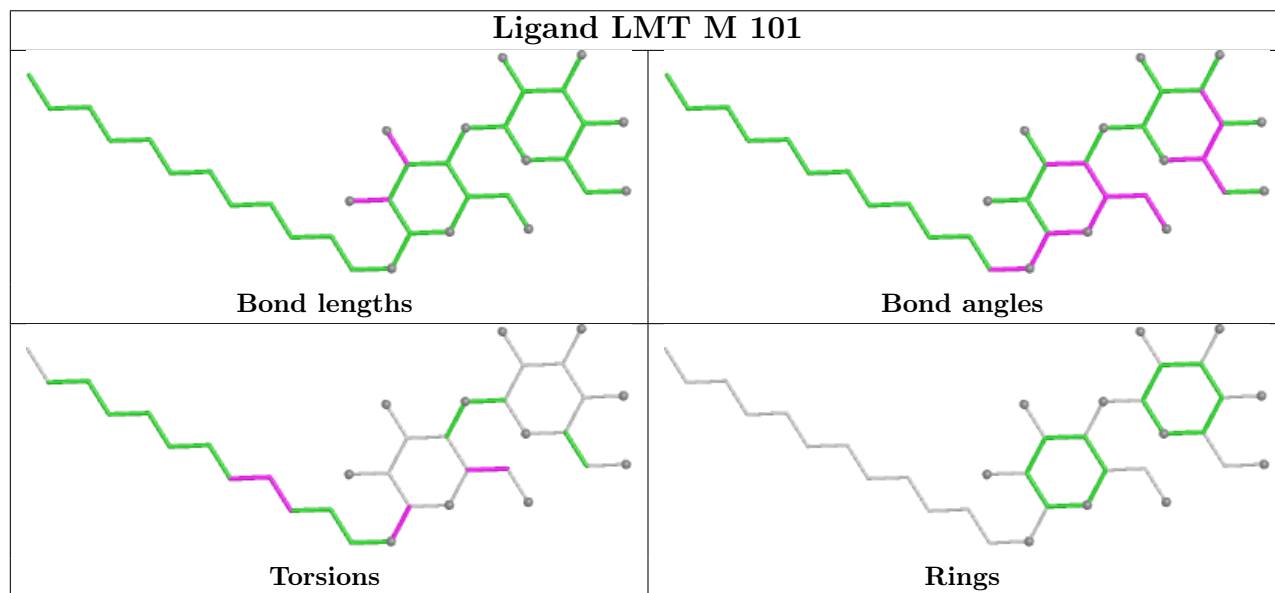




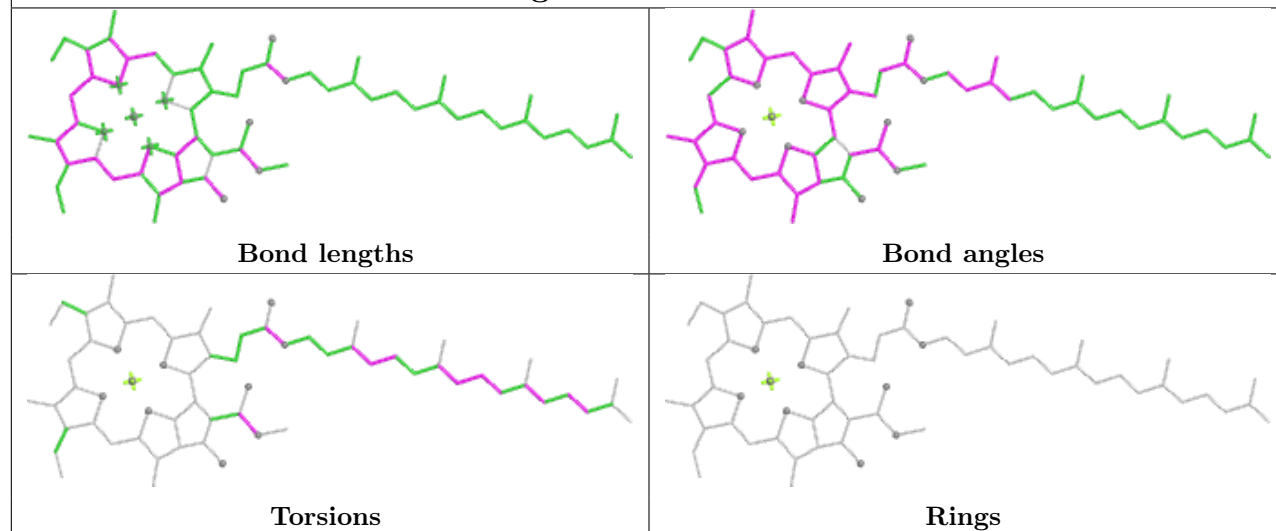
Ligand LHG d 407 (B)



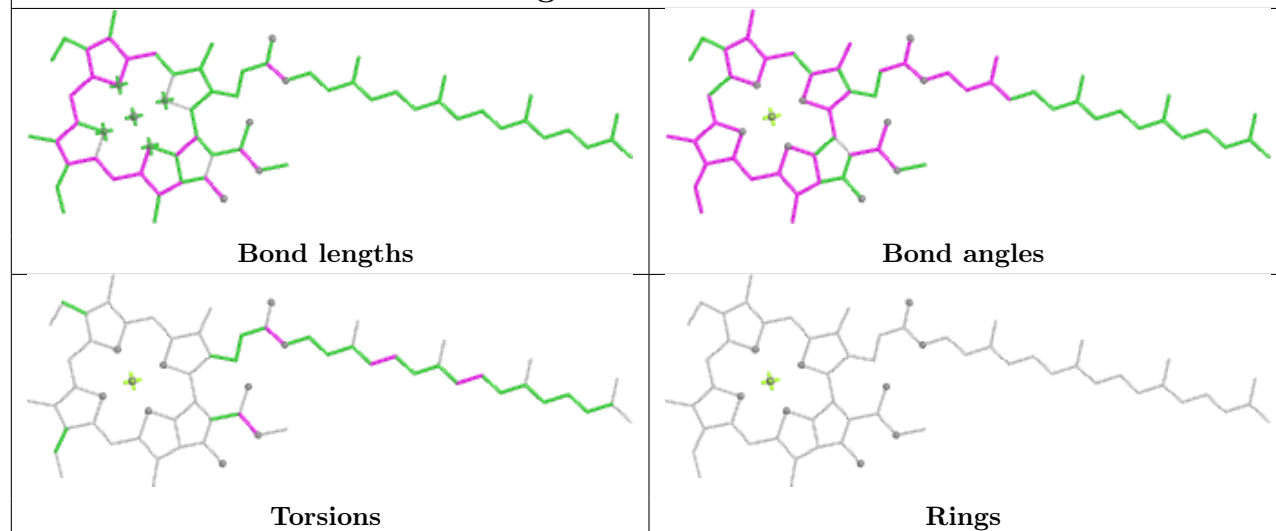
Ligand LMT M 101

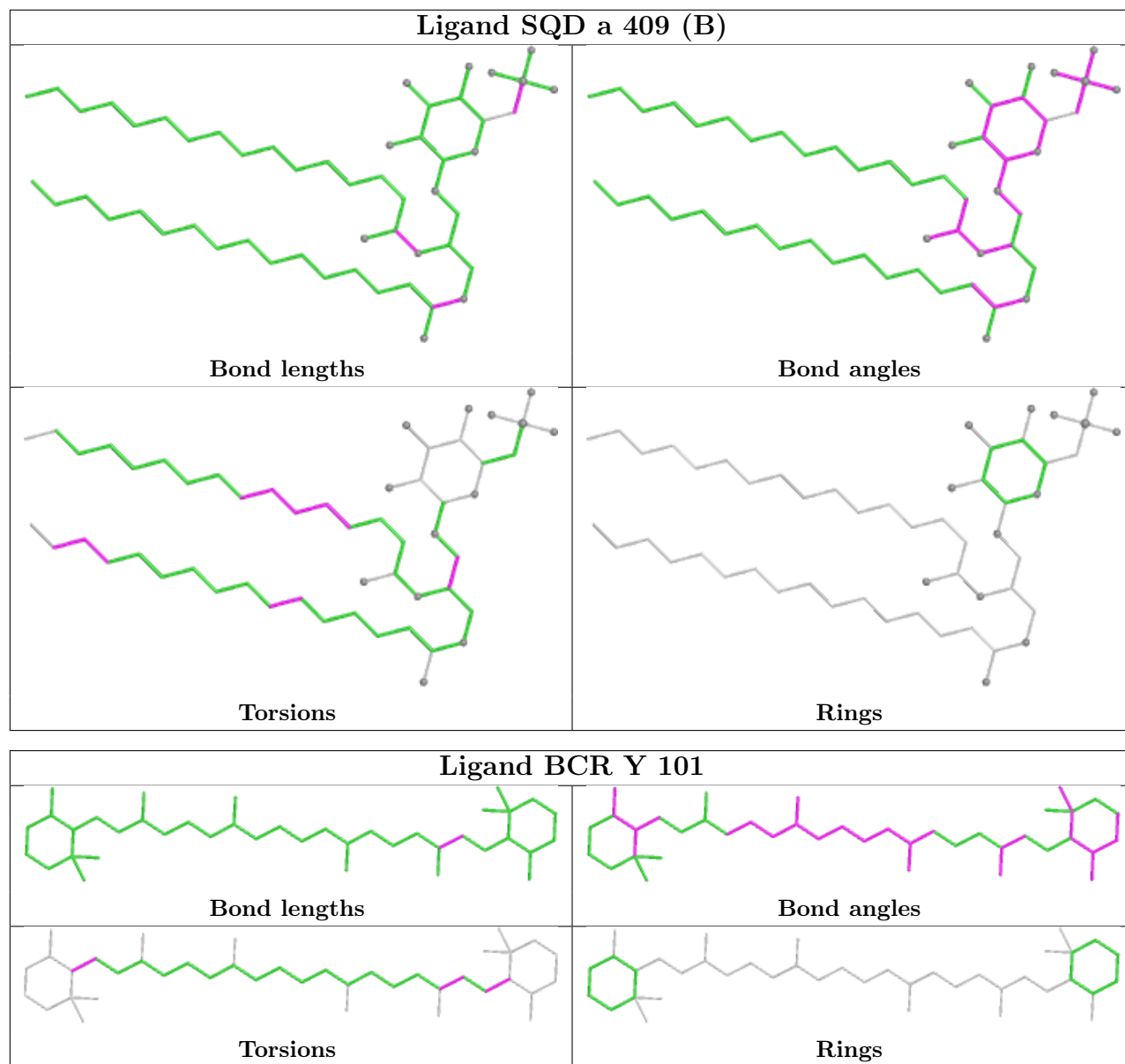


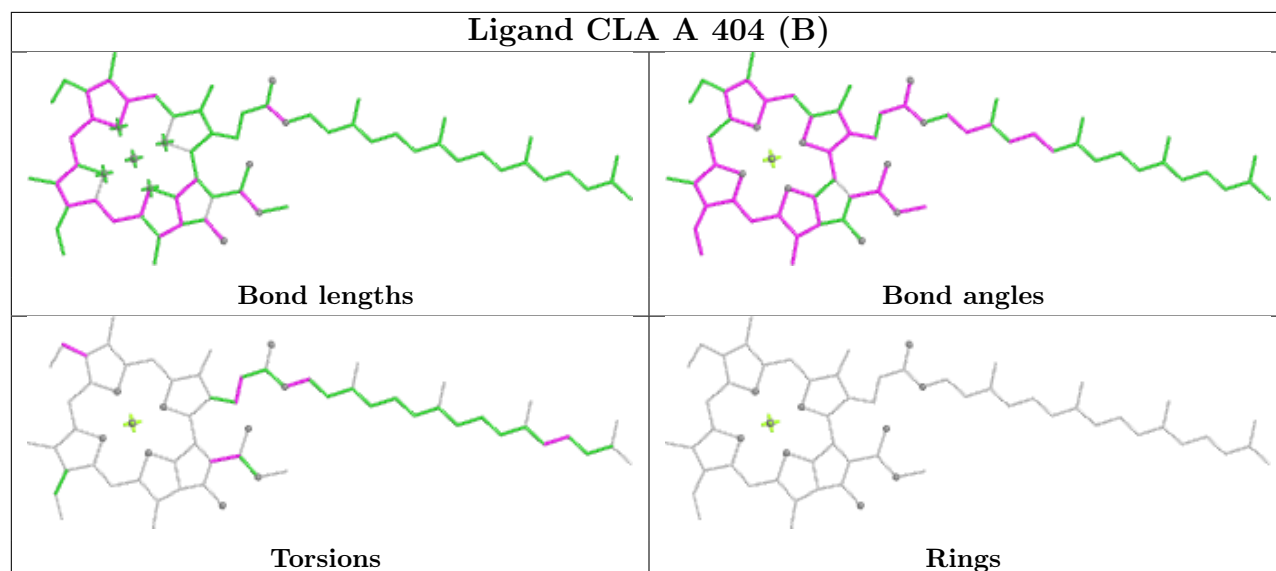
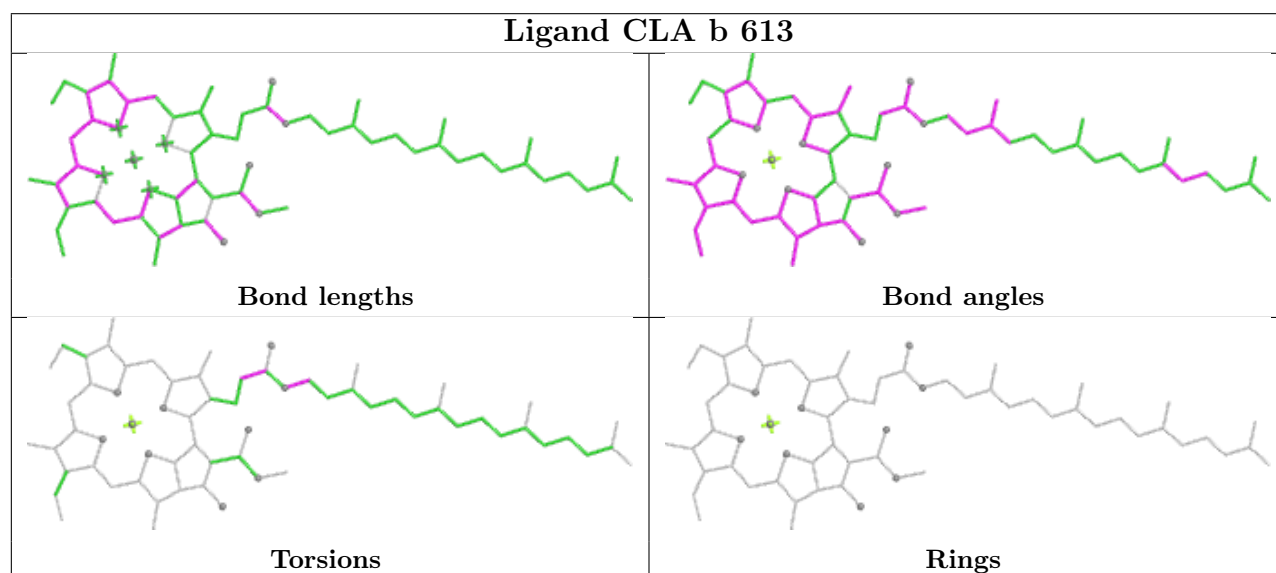
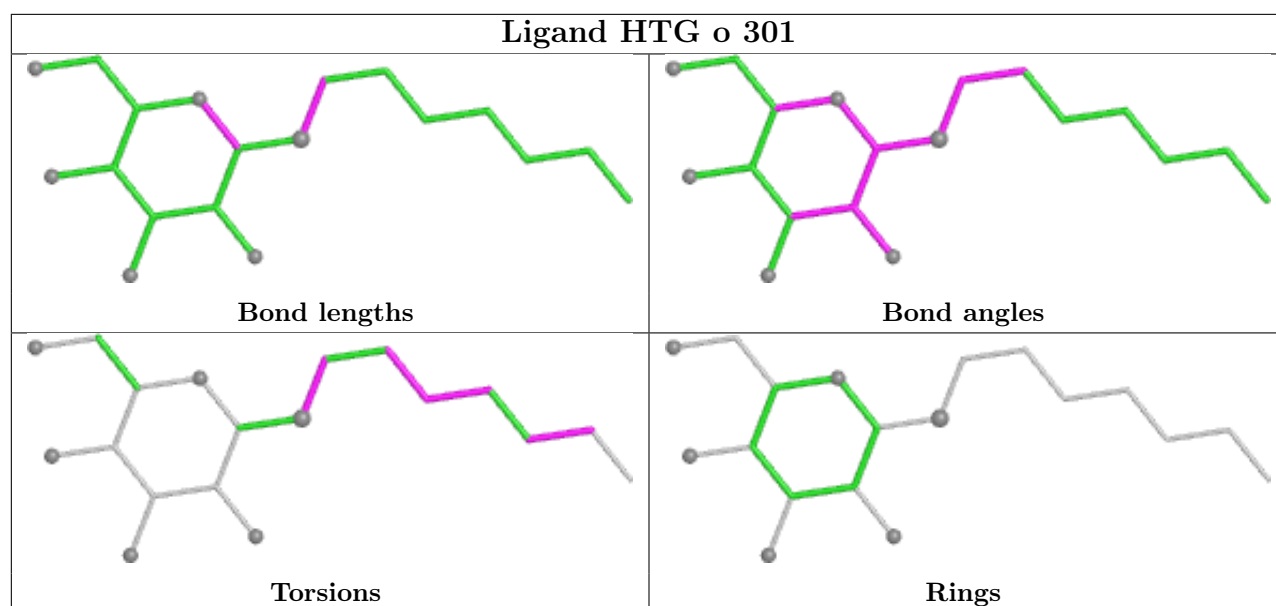
Ligand CLA D 404

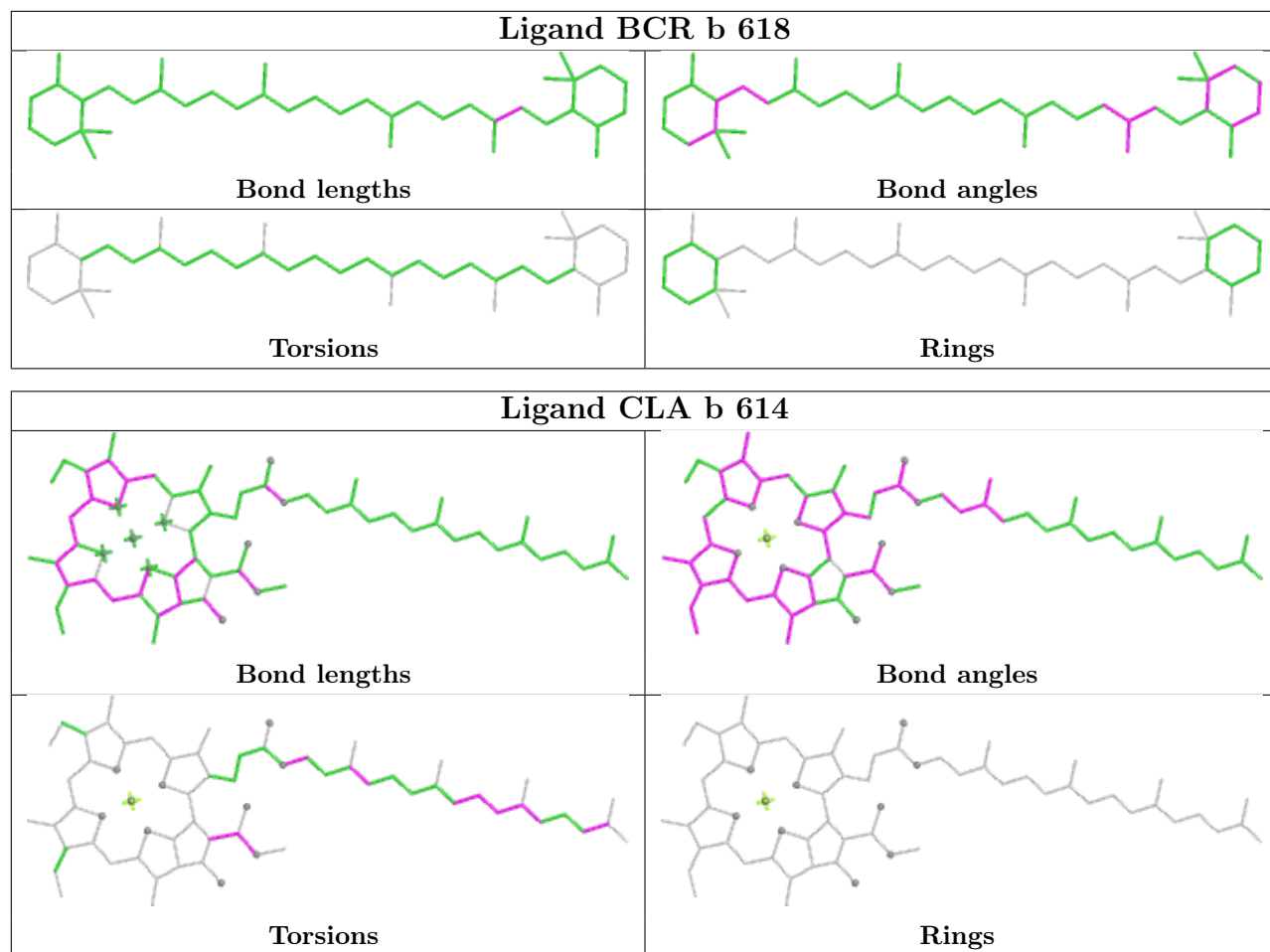


Ligand CLA c 512

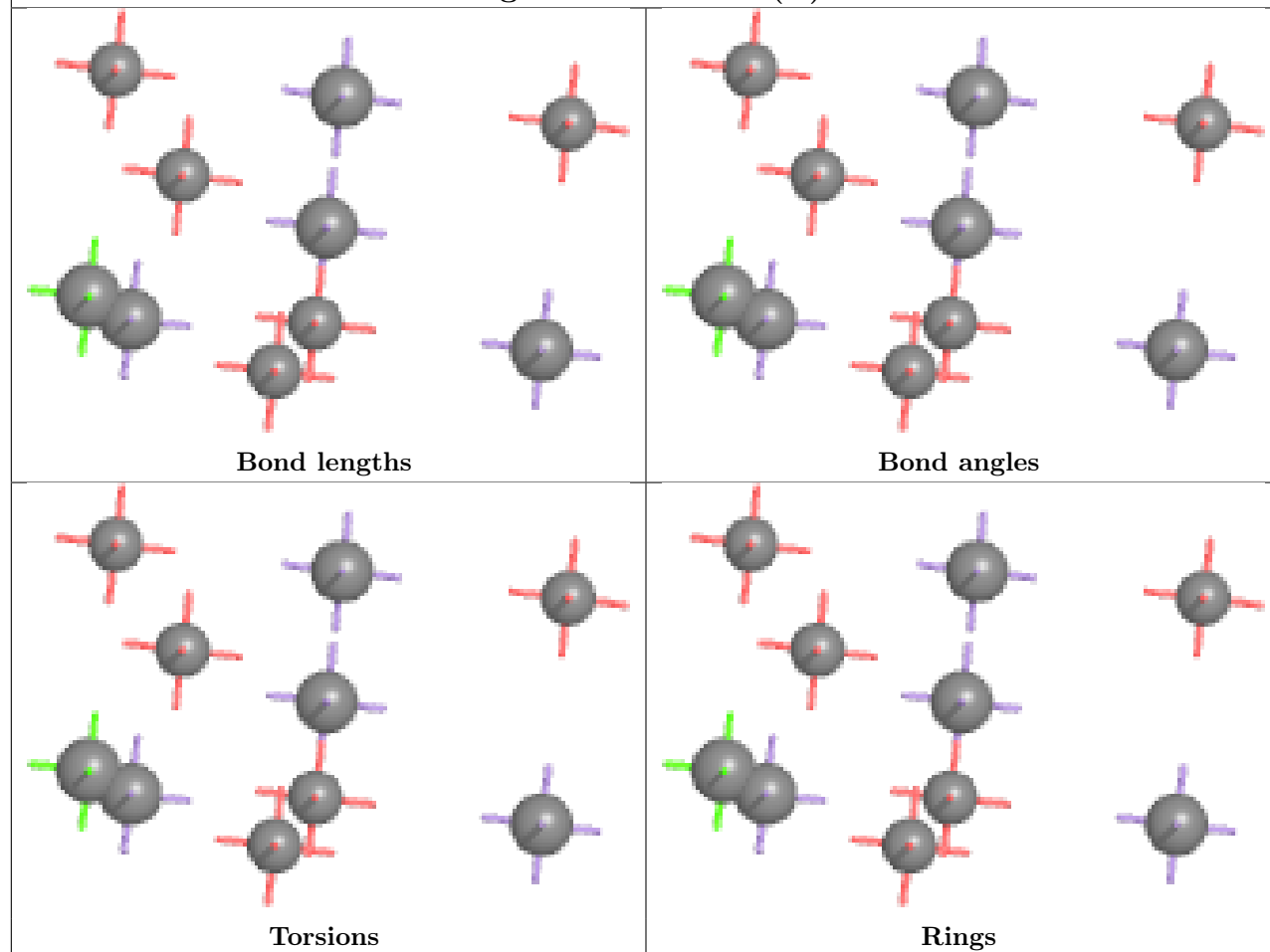




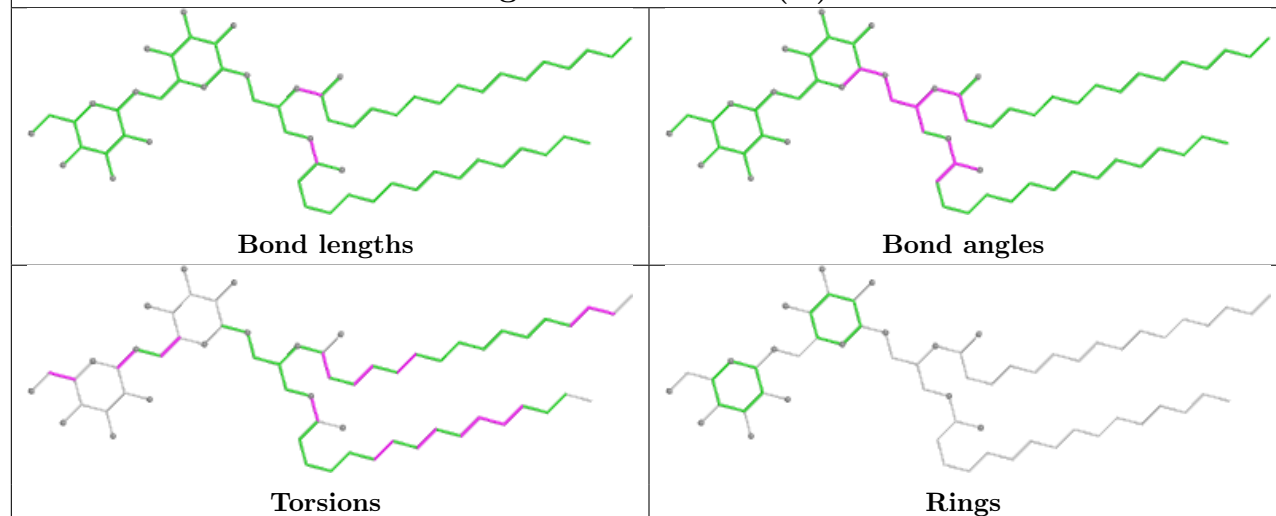


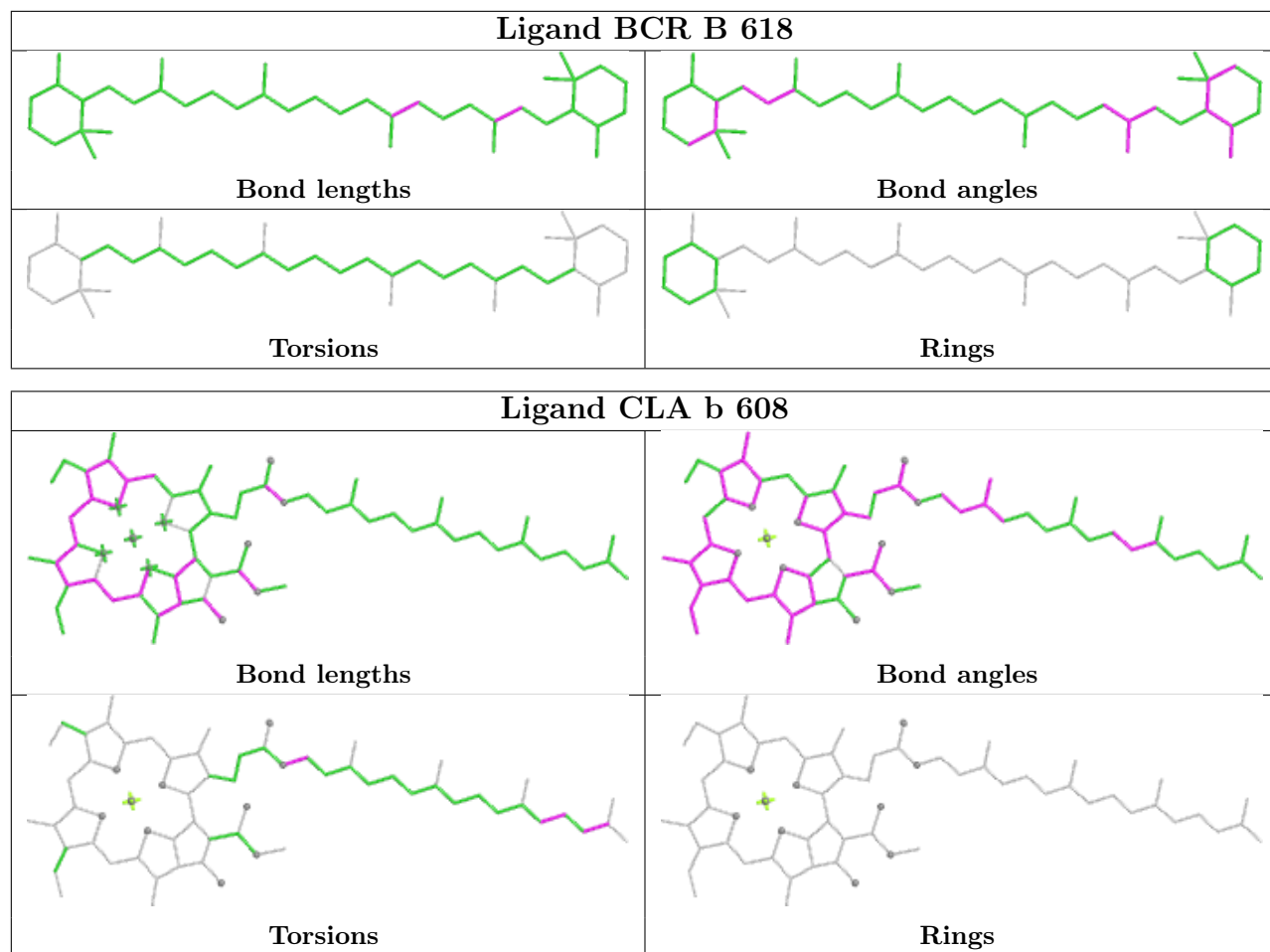


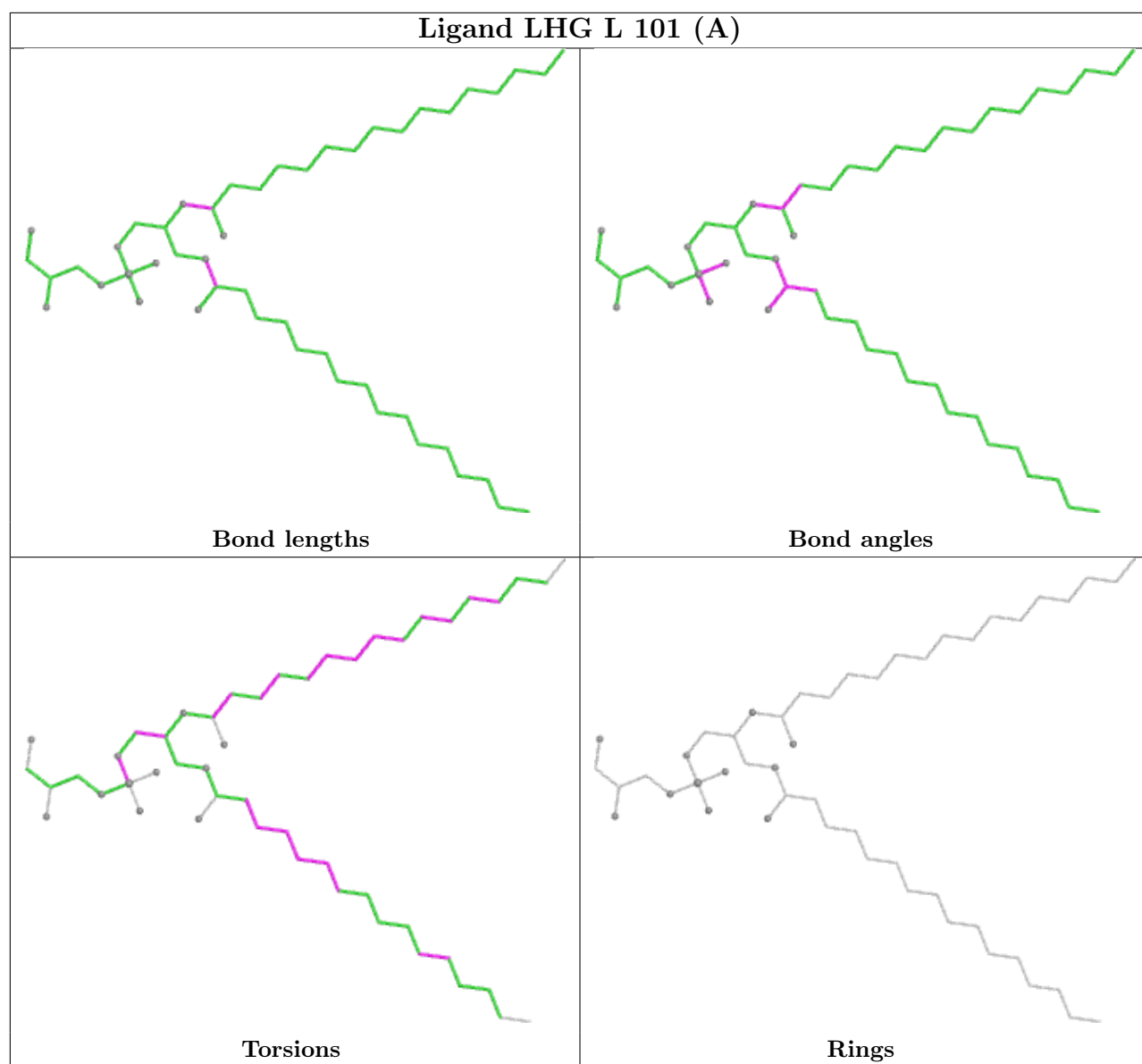
Ligand OEX a 412 (B)

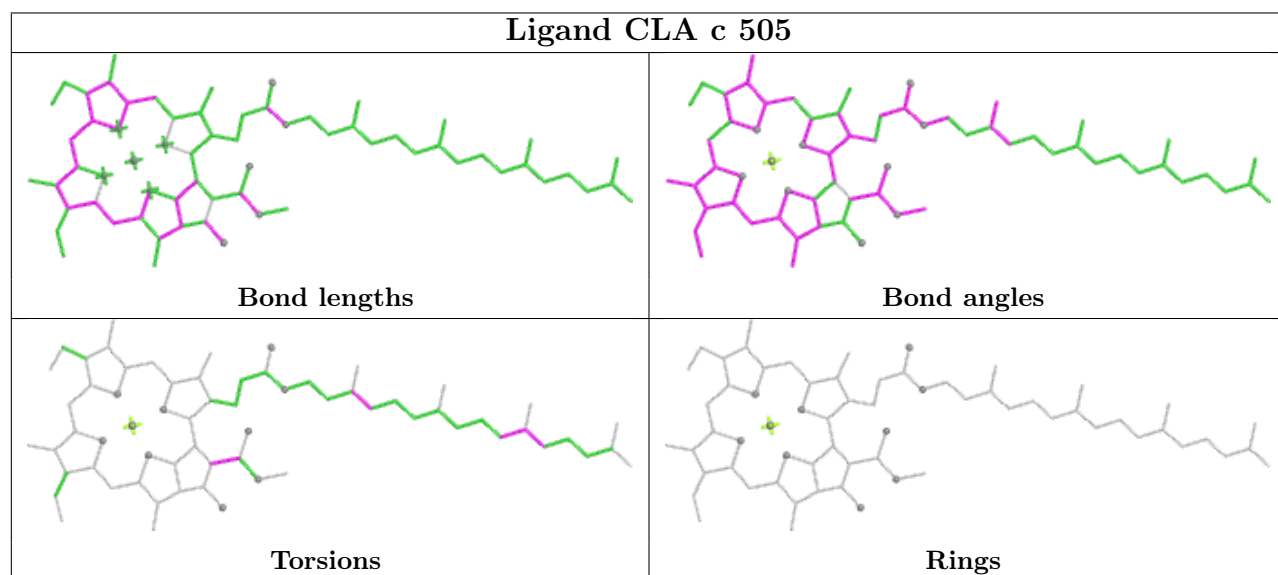
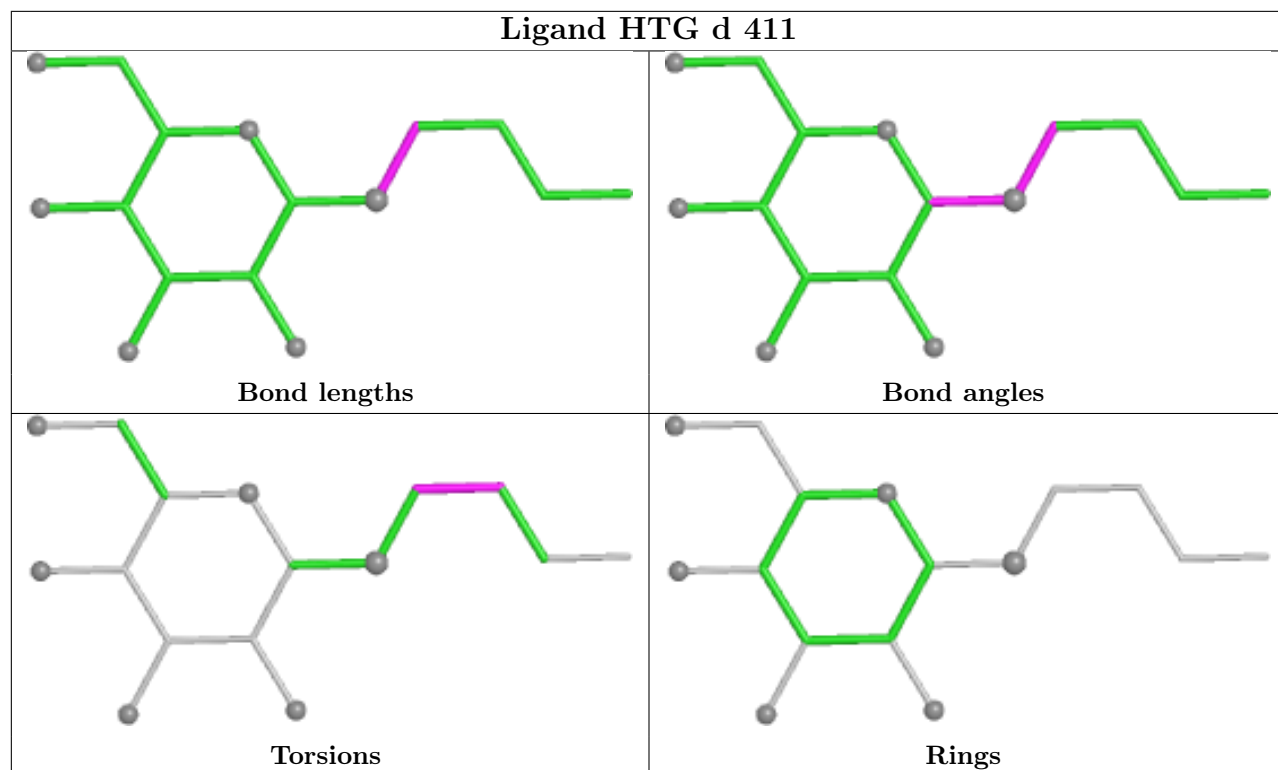


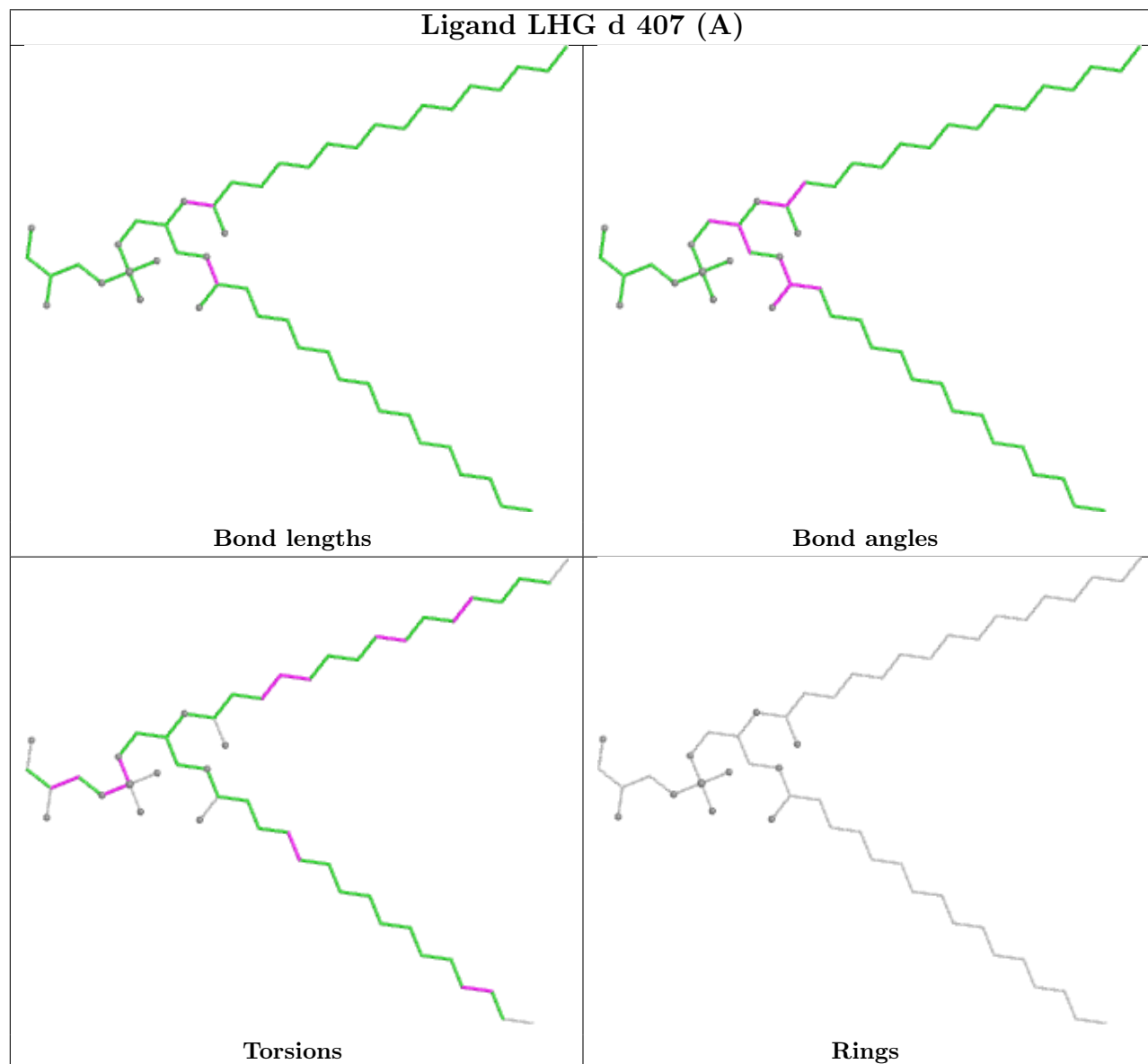
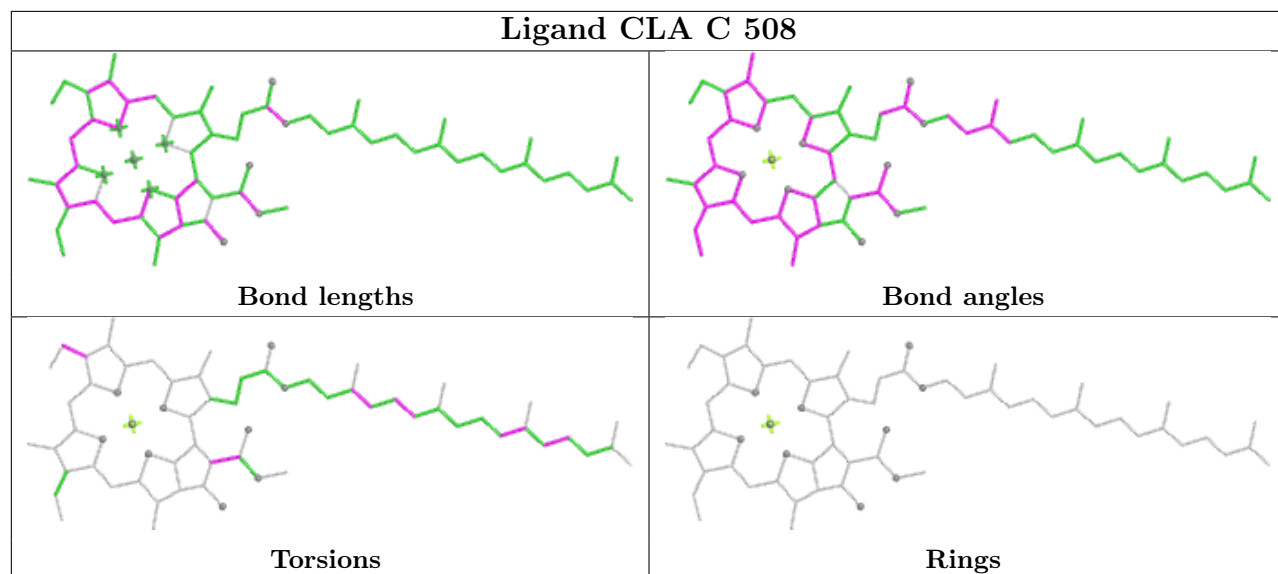
Ligand DGD c 517 (A)











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%)	-0.69	1 (0%) 90 90	19, 25, 59, 119	222 (66%)
1	a	334/344 (97%)	-0.63	1 (0%) 90 90	20, 28, 64, 128	221 (66%)
2	B	504/505 (99%)	-0.59	1 (0%) 91 91	21, 52, 82, 116	20 (3%)
2	b	504/505 (99%)	-0.51	0 100 100	23, 57, 98, 150	19 (3%)
3	C	451/455 (99%)	-0.59	0 100 100	21, 59, 82, 134	97 (21%)
3	c	455/455 (100%)	-0.49	1 (0%) 91 91	24, 65, 87, 128	100 (21%)
4	D	342/342 (100%)	-0.73	0 100 100	19, 44, 64, 127	114 (33%)
4	d	341/342 (99%)	-0.71	0 100 100	21, 49, 73, 128	116 (34%)
5	E	81/84 (96%)	-0.36	0 100 100	51, 69, 96, 147	0
5	e	79/84 (94%)	-0.38	1 (1%) 75 76	31, 74, 116, 142	2 (2%)
6	F	34/44 (77%)	-0.54	0 100 100	52, 59, 89, 110	0
6	f	31/44 (70%)	-0.29	1 (3%) 50 52	53, 66, 94, 132	1 (3%)
7	H	64/65 (98%)	-0.35	1 (1%) 70 72	53, 62, 88, 108	0
7	h	64/65 (98%)	-0.38	0 100 100	39, 72, 93, 105	1 (1%)
8	I	37/38 (97%)	-0.19	0 100 100	55, 65, 117, 143	0
8	i	37/38 (97%)	-0.36	0 100 100	53, 64, 111, 130	0
9	J	38/39 (97%)	-0.40	0 100 100	49, 67, 118, 153	0
9	j	39/39 (100%)	-0.31	0 100 100	56, 77, 124, 150	0
10	K	37/37 (100%)	-0.65	0 100 100	57, 66, 85, 105	0
10	k	37/37 (100%)	-0.51	0 100 100	67, 74, 95, 111	0
11	L	36/37 (97%)	-0.71	0 100 100	22, 45, 110, 128	2 (5%)
11	l	36/37 (97%)	-0.60	0 100 100	23, 46, 104, 118	2 (5%)
12	M	32/36 (88%)	-0.71	0 100 100	25, 47, 76, 125	1 (3%)
12	m	33/36 (91%)	-0.65	0 100 100	23, 48, 71, 137	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%)	-0.53	0 100 100	20, 64, 118, 161	10 (4%)
13	o	243/244 (99%)	-0.48	0 100 100	22, 68, 121, 153	8 (3%)
14	T	29/32 (90%)	-0.65	0 100 100	25, 45, 54, 65	6 (20%)
14	t	29/32 (90%)	-0.65	1 (3%) 48 50	26, 46, 59, 72	5 (17%)
15	U	96/104 (92%)	-0.62	0 100 100	24, 57, 87, 101	4 (4%)
15	u	97/104 (93%)	-0.69	0 100 100	28, 60, 80, 121	4 (4%)
16	V	137/137 (100%)	-0.73	0 100 100	23, 56, 81, 103	6 (4%)
16	v	137/137 (100%)	-0.57	0 100 100	26, 70, 99, 131	6 (4%)
17	X	38/40 (95%)	-0.24	0 100 100	34, 73, 92, 111	1 (2%)
17	x	38/40 (95%)	-0.10	0 100 100	67, 80, 118, 151	0
18	Y	29/30 (96%)	-0.15	1 (3%) 48 50	67, 81, 117, 120	0
18	y	29/30 (96%)	-0.23	0 100 100	77, 88, 110, 112	0
19	Z	62/62 (100%)	-0.33	0 100 100	67, 81, 130, 150	0
19	z	62/62 (100%)	0.09	0 100 100	80, 94, 137, 165	0
20	R	34/34 (100%)	0.52	1 (2%) 53 56	87, 110, 132, 143	0
All	All	5283/5384 (98%)	-0.55	10 (0%) 91 91	19, 57, 100, 165	970 (18%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.8
5	e	79[A]	PHE	3.5
6	f	16[A]	PHE	3.1
3	c	245[A]	ILE	2.3
1	A	11	ALA	2.2
1	a	11	ALA	2.2
20	R	28	VAL	2.2
14	t	30[A]	THR	2.1
2	B	494	GLY	2.1
18	Y	18	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	60,70,83,88	0
14	FME	T	1	10/11	0.96	0.07	43,53,70,79	0
14	FME	t	1	10/11	0.96	0.07	41,46,62,73	0
12	FME	m	1	10/11	0.97	0.07	50,61,88,116	0
8	FME	i	1	10/11	0.97	0.07	54,70,80,85	0
12	FME	M	1	10/11	0.98	0.06	43,55,88,98	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($\text{\AA}^2$)	Q<0.9
26	GOL	a	417	6/6	0.61	0.17	79,98,105,108	0
32	LMT	F	101	35/35	0.69	0.15	91,127,168,174	0
32	LMT	e	101	35/35	0.69	0.14	100,141,180,182	0
29	UNL	A	414	28/-	0.70	0.14	81,103,122,140	0
29	UNL	a	414	30/-	0.70	0.12	80,106,129,138	0
29	UNL	j	101	10/-	0.71	0.19	73,87,102,104	0
32	LMT	A	419	35/35	0.71	0.12	89,125,143,156	0
29	UNL	K	101[B]	34/-	0.72	0.14	72,97,111,114	34
32	LMT	B	627	35/35	0.72	0.14	62,116,137,153	0
29	UNL	I	101	40/-	0.72	0.15	73,100,150,155	0
29	UNL	K	101[A]	34/-	0.72	0.14	72,97,111,114	34
29	UNL	m	102	10/-	0.73	0.19	61,71,91,93	0
32	LMT	A	417	35/35	0.73	0.12	59,109,132,137	0
25	SQD	f	102	43/54	0.74	0.13	94,125,167,177	0
29	UNL	J	101	10/-	0.74	0.22	60,75,83,91	0
35	HTG	C	522	19/19	0.74	0.12	99,119,131,131	0
32	LMT	a	416	35/35	0.75	0.12	107,126,147,155	0
33	LHG	a	419[A]	42/49	0.76	0.11	85,125,144,152	42
33	LHG	a	419[B]	42/49	0.76	0.11	85,125,144,152	42
29	UNL	l	102	10/-	0.76	0.16	63,77,90,92	0
29	UNL	B	628	40/-	0.78	0.13	71,99,149,159	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	UNL	b	626	33/-	0.79	0.13	63,94,149,161	0
29	UNL	c	525[B]	32/-	0.80	0.14	86,104,116,126	32
26	GOL	B	625	6/6	0.80	0.14	68,88,99,112	0
29	UNL	c	525[A]	32/-	0.80	0.14	86,104,116,126	32
35	HTG	B	621	19/19	0.80	0.14	60,90,112,112	0
32	LMT	b	621	25/35	0.80	0.12	78,103,153,161	0
34	LMG	C	521	51/55	0.81	0.11	56,115,150,170	0
26	GOL	o	303	6/6	0.81	0.15	79,100,105,111	0
26	GOL	o	304	6/6	0.81	0.14	76,87,97,97	0
35	HTG	D	411	16/19	0.81	0.12	88,102,126,149	0
35	HTG	c	522	19/19	0.81	0.10	103,120,141,142	0
26	GOL	d	413	6/6	0.82	0.21	49,63,77,82	0
29	UNL	D	410	40/-	0.82	0.12	62,90,136,141	0
35	HTG	b	623	19/19	0.82	0.12	79,124,158,158	0
26	GOL	O	302	6/6	0.82	0.09	79,87,104,108	0
32	LMT	T	101	35/35	0.83	0.10	61,120,165,176	0
28	PL9	A	413[A]	55/55	0.83	0.14	61,85,102,106	55
28	PL9	A	413[B]	55/55	0.83	0.14	61,85,102,106	55
32	LMT	B	626	35/35	0.83	0.11	66,102,146,152	0
26	GOL	A	410	6/6	0.83	0.13	63,79,84,85	0
26	GOL	O	303	6/6	0.83	0.13	69,83,99,99	0
28	PL9	a	413[A]	55/55	0.84	0.13	72,95,109,116	55
32	LMT	B	629	25/35	0.84	0.12	56,84,135,159	0
29	UNL	d	410	36/-	0.84	0.10	65,96,131,136	0
28	PL9	a	413[B]	55/55	0.84	0.13	72,95,109,117	55
25	SQD	a	411	54/54	0.84	0.10	63,90,135,145	0
34	LMG	Z	101	37/55	0.85	0.13	66,115,142,163	0
29	UNL	B	624	33/-	0.85	0.13	54,104,138,148	0
32	LMT	m	103	35/35	0.85	0.10	54,88,104,115	0
26	GOL	v	202[B]	6/6	0.85	0.11	60,72,79,80	6
35	HTG	b	622	19/19	0.85	0.12	60,90,115,118	0
26	GOL	b	624	6/6	0.85	0.14	84,98,100,109	0
26	GOL	v	202[A]	6/6	0.85	0.11	60,72,80,80	6
35	HTG	d	411	16/19	0.85	0.11	89,124,140,154	0
34	LMG	z	101	39/55	0.86	0.12	72,125,150,157	0
25	SQD	A	411	54/54	0.86	0.10	57,86,128,153	0
34	LMG	c	521	51/55	0.86	0.10	74,126,157,185	0
32	LMT	t	101	26/35	0.86	0.11	64,98,139,140	0
37	CA	F	103	1/1	0.86	0.23	122,122,122,122	0
35	HTG	V	202	11/19	0.87	0.09	78,108,125,127	0
32	LMT	M	101	35/35	0.87	0.10	57,93,120,130	0
32	LMT	b	627	25/35	0.87	0.12	51,88,142,153	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
25	SQD	X	101	43/54	0.88	0.11	72,103,125,141	0
26	GOL	l	103[A]	6/6	0.88	0.15	61,91,98,100	6
26	GOL	l	103[B]	6/6	0.88	0.15	61,91,98,100	6
26	GOL	c	527	6/6	0.88	0.14	89,98,113,115	0
23	CLA	b	601	65/65	0.89	0.10	59,90,123,154	0
29	UNL	D	409	17/-	0.89	0.11	62,72,103,109	0
25	SQD	l	101	54/54	0.89	0.09	59,87,139,148	0
25	SQD	b	620	54/54	0.89	0.09	55,94,121,128	0
33	LHG	E	101[A]	42/49	0.89	0.10	71,96,111,117	42
33	LHG	E	101[B]	42/49	0.89	0.10	71,96,111,117	42
26	GOL	a	410	6/6	0.89	0.12	70,73,91,93	0
35	HTG	o	301	19/19	0.90	0.11	58,83,117,119	0
35	HTG	B	623	19/19	0.90	0.08	64,77,94,103	0
26	GOL	V	203[A]	6/6	0.91	0.11	56,65,67,73	6
26	GOL	V	203[B]	6/6	0.91	0.11	56,65,67,73	6
26	GOL	D	413	6/6	0.91	0.14	45,64,71,91	0
26	GOL	B	622	6/6	0.91	0.13	66,76,84,85	0
26	GOL	a	418	6/6	0.91	0.21	54,74,79,80	0
34	LMG	C	501	51/55	0.91	0.09	64,89,114,133	0
23	CLA	B	601	65/65	0.91	0.09	56,80,112,156	0
37	CA	f	103	1/1	0.91	0.10	117,117,117,117	0
23	CLA	c	514	65/65	0.92	0.09	68,96,126,148	0
34	LMG	C	520	51/55	0.92	0.09	54,81,114,130	0
26	GOL	D	402	6/6	0.92	0.24	47,72,77,80	0
34	LMG	c	501	51/55	0.92	0.08	69,91,107,113	0
34	LMG	c	520	51/55	0.92	0.09	59,90,127,156	0
34	LMG	B	620	51/55	0.92	0.07	49,66,89,112	0
34	LMG	m	101	51/55	0.92	0.08	48,72,97,107	0
25	SQD	A	409[A]	54/54	0.93	0.09	56,78,109,113	54
29	UNL	d	409	17/-	0.93	0.09	67,80,117,121	0
25	SQD	A	409[B]	54/54	0.93	0.09	56,78,109,113	54
23	CLA	c	513	65/65	0.93	0.09	59,80,117,144	0
23	CLA	C	514	65/65	0.93	0.08	63,87,112,119	0
24	BCR	C	515	40/40	0.93	0.08	55,73,87,93	0
24	BCR	D	405	40/40	0.93	0.08	41,56,98,102	0
24	BCR	T	102	40/40	0.93	0.07	43,58,70,78	0
34	LMG	D	412	51/55	0.93	0.08	46,67,120,132	0
24	BCR	d	405	40/40	0.93	0.08	48,64,98,104	0
24	BCR	t	102	40/40	0.93	0.07	40,58,79,85	0
33	LHG	A	418[A]	49/49	0.93	0.08	46,60,79,84	49
36	DGD	C	518[A]	62/66	0.93	0.08	50,63,110,114	62
36	DGD	C	518[B]	62/66	0.93	0.08	50,63,110,114	62

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	LMG	d	412	51/55	0.93	0.08	54,68,116,145	0
33	LHG	A	418[B]	49/49	0.93	0.08	46,60,79,84	49
24	BCR	c	515	40/40	0.94	0.08	66,82,95,96	0
23	CLA	C	507	65/65	0.94	0.08	54,70,117,136	0
26	GOL	b	628	6/6	0.94	0.08	75,79,82,86	0
23	CLA	B	614	65/65	0.94	0.07	35,49,100,116	0
33	LHG	D	408[A]	49/49	0.94	0.09	43,58,107,110	49
33	LHG	D	408[B]	49/49	0.94	0.09	43,58,107,110	49
23	CLA	d	404	65/65	0.94	0.09	54,68,124,147	0
26	GOL	C	523[A]	6/6	0.94	0.09	53,56,61,68	6
26	GOL	C	523[B]	6/6	0.94	0.09	54,58,61,68	6
24	BCR	B	619	40/40	0.94	0.08	46,58,90,104	0
33	LHG	d	414[A]	49/49	0.94	0.08	48,65,80,87	49
33	LHG	d	414[B]	49/49	0.94	0.08	48,66,80,87	49
35	HTG	b	625	19/19	0.94	0.07	61,79,95,108	0
23	CLA	C	505	65/65	0.94	0.07	40,56,98,131	0
23	CLA	b	616	65/65	0.94	0.08	50,63,122,134	0
25	SQD	a	409[A]	54/54	0.94	0.09	60,81,112,118	54
25	SQD	a	409[B]	54/54	0.94	0.09	60,80,112,118	54
24	BCR	K	102	40/40	0.94	0.09	54,65,80,91	0
36	DGD	c	517[A]	62/66	0.94	0.08	49,65,100,108	62
36	DGD	c	517[B]	62/66	0.94	0.08	49,65,100,108	62
36	DGD	c	518[A]	62/66	0.94	0.07	53,67,118,128	62
36	DGD	c	518[B]	62/66	0.94	0.07	53,68,118,128	62
36	DGD	c	519	62/66	0.94	0.07	48,63,100,128	0
23	CLA	c	507	65/65	0.94	0.08	47,70,117,134	0
24	BCR	Y	101	40/40	0.94	0.08	54,63,80,89	0
37	CA	o	302	1/1	0.94	0.07	113,113,113,113	0
26	GOL	c	526[B]	6/6	0.95	0.08	64,66,71,74	6
23	CLA	A	407	65/65	0.95	0.08	39,52,127,140	0
24	BCR	A	408	40/40	0.95	0.07	40,51,64,65	0
29	UNL	d	415	18/-	0.95	0.09	66,79,126,127	0
24	BCR	B	618	40/40	0.95	0.06	37,54,69,79	0
23	CLA	a	405[A]	65/65	0.95	0.07	38,52,118,133	65
23	CLA	a	405[B]	65/65	0.95	0.07	38,52,118,133	65
30	BCT	d	401[A]	4/4	0.95	0.07	53,60,61,76	4
30	BCT	d	401[B]	4/4	0.95	0.07	54,60,61,77	4
23	CLA	a	407	65/65	0.95	0.10	42,55,139,160	0
24	BCR	H	101	40/40	0.95	0.08	50,64,84,89	0
23	CLA	B	616	65/65	0.95	0.08	46,59,129,139	0
23	CLA	b	606	65/65	0.95	0.07	42,62,115,119	0
23	CLA	b	614	65/65	0.95	0.07	39,50,98,113	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
28	PL9	D	406[A]	55/55	0.95	0.07	35,47,55,65	55
28	PL9	D	406[B]	55/55	0.95	0.07	35,47,55,64	55
24	BCR	b	617	40/40	0.95	0.06	41,52,64,66	0
24	BCR	b	618	40/40	0.95	0.06	42,57,76,84	0
24	BCR	b	619	40/40	0.95	0.07	48,61,90,95	0
23	CLA	B	603	65/65	0.95	0.08	43,53,73,87	0
24	BCR	c	516	40/40	0.95	0.07	57,66,80,82	0
23	CLA	c	505	65/65	0.95	0.07	46,64,108,137	0
24	BCR	h	101	40/40	0.95	0.09	54,69,91,98	0
24	BCR	k	101	40/40	0.95	0.08	56,72,84,86	0
23	CLA	B	606	65/65	0.95	0.08	41,57,108,129	0
24	BCR	y	101	40/40	0.95	0.07	58,72,85,96	0
23	CLA	c	508	65/65	0.95	0.09	49,68,83,90	0
36	DGD	C	519	62/66	0.95	0.07	41,56,101,115	0
29	UNL	X	102	18/-	0.95	0.09	52,68,103,105	0
23	CLA	C	509	65/65	0.95	0.07	44,55,117,141	0
23	CLA	C	513	65/65	0.95	0.08	57,75,108,121	0
26	GOL	c	526[A]	6/6	0.95	0.08	65,66,71,74	6
33	LHG	b	629[A]	49/49	0.95	0.07	45,57,70,81	49
36	DGD	h	102	62/66	0.95	0.07	51,65,80,90	0
33	LHG	b	629[B]	49/49	0.95	0.07	45,57,70,82	49
33	LHG	d	408[A]	49/49	0.95	0.09	49,63,108,129	49
33	LHG	d	408[B]	49/49	0.95	0.09	49,63,108,129	49
23	CLA	c	504	65/65	0.96	0.06	51,71,85,88	0
28	PL9	d	406[A]	55/55	0.96	0.06	37,49,59,65	55
28	PL9	d	406[B]	55/55	0.96	0.06	37,49,59,65	55
23	CLA	C	508	65/65	0.96	0.07	52,64,85,95	0
23	CLA	c	506	65/65	0.96	0.07	47,65,92,105	0
23	CLA	A	406[B]	65/65	0.96	0.06	36,45,110,121	65
23	CLA	C	510	65/65	0.96	0.08	44,59,84,91	0
23	CLA	c	509	65/65	0.96	0.07	47,62,121,152	0
23	CLA	c	512	65/65	0.96	0.07	54,70,85,101	0
23	CLA	B	607	65/65	0.96	0.06	32,46,73,77	0
23	CLA	B	611	65/65	0.96	0.06	32,44,65,72	0
23	CLA	D	404	65/65	0.96	0.07	49,58,120,137	0
23	CLA	B	613	65/65	0.96	0.06	38,46,99,109	0
23	CLA	A	404[A]	65/65	0.96	0.06	35,41,54,66	65
23	CLA	A	404[B]	65/65	0.96	0.06	35,41,56,66	65
23	CLA	C	502	65/65	0.96	0.06	49,60,75,82	0
24	BCR	C	516	40/40	0.96	0.06	49,64,75,83	0
23	CLA	B	602	65/65	0.96	0.07	46,56,75,88	0
23	CLA	b	607	65/65	0.96	0.06	36,46,77,84	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	b	609	65/65	0.96	0.07	51,66,83,88	0
36	DGD	C	517[A]	62/66	0.96	0.06	46,59,101,106	62
36	DGD	C	517[B]	62/66	0.96	0.06	46,59,101,107	62
23	CLA	b	612	65/65	0.96	0.07	38,53,67,76	0
23	CLA	b	613	65/65	0.96	0.06	41,50,85,95	0
24	BCR	a	408	40/40	0.96	0.06	40,54,63,75	0
36	DGD	H	102	62/66	0.96	0.07	44,61,75,90	0
33	LHG	d	407[A]	49/49	0.96	0.07	47,54,69,75	49
33	LHG	d	407[B]	49/49	0.96	0.07	47,54,69,75	49
23	CLA	C	506	65/65	0.96	0.07	50,60,91,105	0
23	CLA	A	406[A]	65/65	0.96	0.06	36,46,110,121	65
31	PHO	A	416[A]	64/64	0.96	0.06	38,48,54,58	64
31	PHO	A	416[B]	64/64	0.96	0.06	38,48,54,57	64
37	CA	C	524	1/1	0.96	0.05	75,75,75,75	0
31	PHO	a	415[A]	64/64	0.96	0.06	45,55,62,66	64
37	CA	O	301	1/1	0.96	0.04	106,106,106,106	0
31	PHO	a	415[B]	64/64	0.96	0.06	45,55,62,67	64
23	CLA	c	502	65/65	0.96	0.07	56,67,81,88	0
23	CLA	A	405[A]	65/65	0.97	0.05	32,42,54,66	65
23	CLA	c	510	65/65	0.97	0.07	41,60,86,100	0
31	PHO	D	401[A]	64/64	0.97	0.04	38,44,51,55	64
31	PHO	D	401[B]	64/64	0.97	0.04	38,44,51,55	64
31	PHO	a	406[A]	64/64	0.97	0.05	40,46,53,60	64
31	PHO	a	406[B]	64/64	0.97	0.05	40,46,53,60	64
23	CLA	c	511	65/65	0.97	0.06	47,61,79,83	0
23	CLA	C	504	65/65	0.97	0.06	49,62,72,83	0
23	CLA	A	405[B]	65/65	0.97	0.05	32,42,54,66	65
23	CLA	B	609	65/65	0.97	0.06	45,59,72,76	0
23	CLA	d	402[A]	65/65	0.97	0.05	36,43,61,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	36,43,61,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	33,45,71,89	65
23	CLA	d	403[B]	65/65	0.97	0.06	33,45,71,89	65
23	CLA	b	602	65/65	0.97	0.07	51,61,81,87	0
23	CLA	b	603	65/65	0.97	0.06	44,57,75,91	0
24	BCR	B	617	40/40	0.97	0.05	39,51,60,67	0
23	CLA	b	604	65/65	0.97	0.06	42,52,94,121	0
23	CLA	b	605	65/65	0.97	0.06	38,50,74,80	0
23	CLA	B	610	65/65	0.97	0.07	41,52,68,84	0
22	CL	a	403[A]	1/1	0.97	0.07	52,52,52,52	1
23	CLA	b	608	65/65	0.97	0.05	37,56,78,98	0
23	CLA	B	612	65/65	0.97	0.06	35,49,60,75	0
23	CLA	b	610	65/65	0.97	0.07	47,59,71,75	0

Continued on next page...

Continued from previous page...

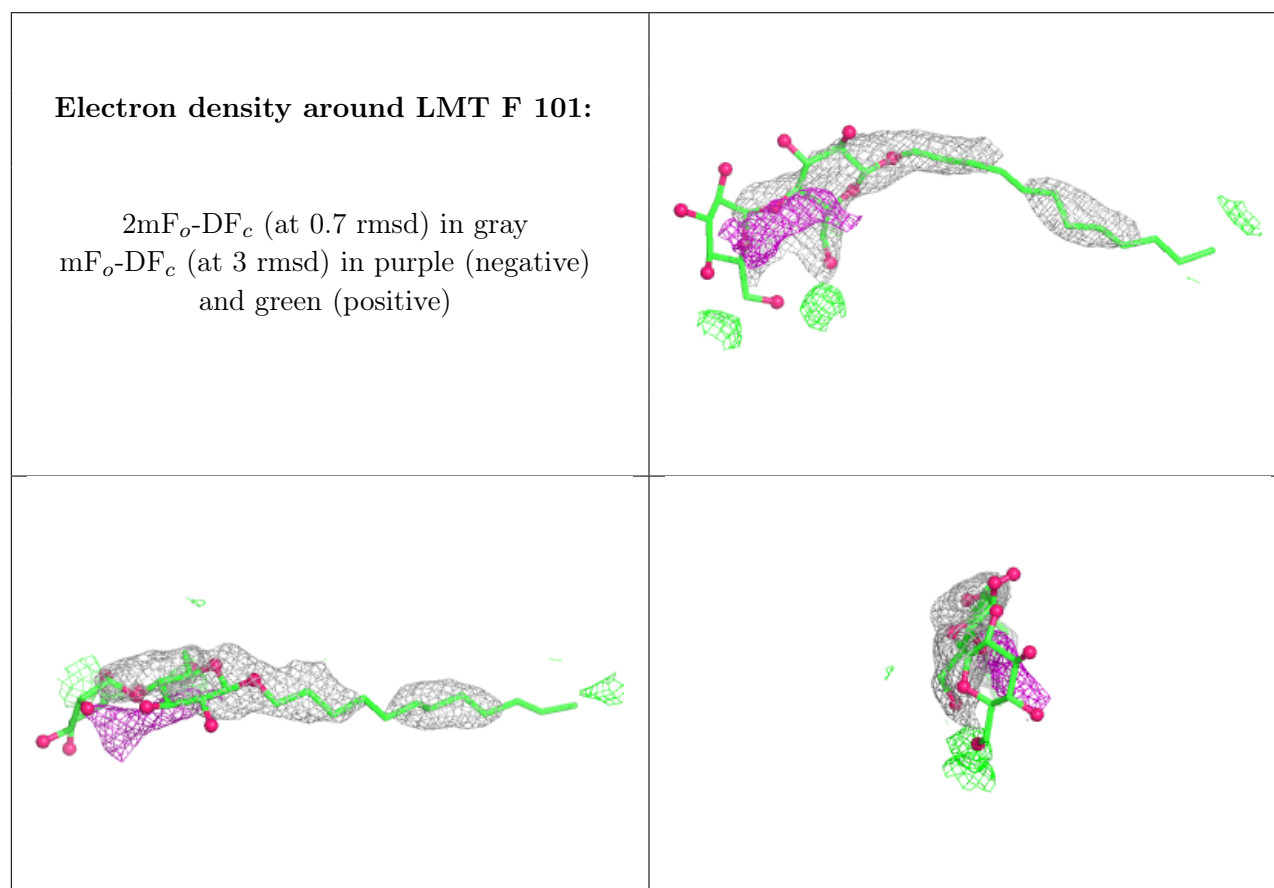
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	LHG	D	407[A]	49/49	0.97	0.06	45,53,65,73	49
33	LHG	D	407[B]	49/49	0.97	0.06	45,53,65,73	49
23	CLA	b	611	65/65	0.97	0.06	36,48,67,85	0
22	CL	a	403[B]	1/1	0.97	0.07	51,51,51,51	1
23	CLA	C	511	65/65	0.97	0.05	44,56,76,87	0
23	CLA	C	512	65/65	0.97	0.07	52,63,82,92	0
33	LHG	L	101[A]	49/49	0.97	0.06	46,54,64,85	49
33	LHG	L	101[B]	49/49	0.97	0.06	46,54,63,85	49
23	CLA	b	615	65/65	0.97	0.06	45,62,85,90	0
23	CLA	B	604	65/65	0.97	0.06	35,47,105,134	0
23	CLA	B	615	65/65	0.97	0.05	42,53,77,94	0
23	CLA	c	503	65/65	0.97	0.06	42,57,87,101	0
23	CLA	D	403[A]	65/65	0.97	0.06	32,42,67,73	65
23	CLA	D	403[B]	65/65	0.97	0.06	32,42,67,73	65
23	CLA	B	605	65/65	0.97	0.06	38,48,63,77	0
37	CA	c	523	1/1	0.97	0.06	78,78,78,78	0
23	CLA	a	404[A]	65/65	0.97	0.06	36,44,61,73	65
23	CLA	a	404[B]	65/65	0.97	0.06	37,44,61,73	65
23	CLA	B	608	65/65	0.98	0.05	35,48,69,73	0
30	BCT	A	415[A]	4/4	0.98	0.05	53,53,57,67	4
30	BCT	A	415[B]	4/4	0.98	0.05	53,53,57,67	4
23	CLA	C	503	65/65	0.98	0.06	38,55,79,86	0
38	HEM	f	101	43/43	0.98	0.07	60,84,110,124	0
40	HEC	V	201	43/43	0.98	0.06	39,52,68,71	0
40	HEC	v	201	43/43	0.98	0.07	50,61,70,75	0
27	OEX	A	412[A]	10/10	0.99	0.03	37,44,51,55	10
27	OEX	A	412[B]	10/10	0.99	0.03	37,44,51,55	10
22	CL	A	402[A]	1/1	0.99	0.07	40,40,40,40	1
37	CA	c	524	1/1	0.99	0.05	81,81,81,81	0
22	CL	A	402[B]	1/1	0.99	0.07	40,40,40,40	1
22	CL	A	403[A]	1/1	0.99	0.05	45,45,45,45	1
38	HEM	F	102	43/43	0.99	0.06	52,68,86,92	0
22	CL	A	403[B]	1/1	0.99	0.05	45,45,45,45	1
39	MG	J	102	1/1	0.99	0.04	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.04	64,64,64,64	0
22	CL	a	402[A]	1/1	0.99	0.07	47,47,47,47	1
22	CL	a	402[B]	1/1	0.99	0.07	47,47,47,47	1
21	FE2	A	401[A]	1/1	1.00	0.01	49,49,49,49	1
21	FE2	A	401[B]	1/1	1.00	0.01	50,50,50,50	1
27	OEX	a	412[A]	10/10	1.00	0.02	47,49,54,54	10
27	OEX	a	412[B]	10/10	1.00	0.02	46,49,53,54	10
21	FE2	a	401[A]	1/1	1.00	0.01	52,52,52,52	1

Continued on next page...

Continued from previous page...

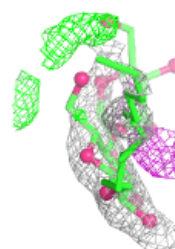
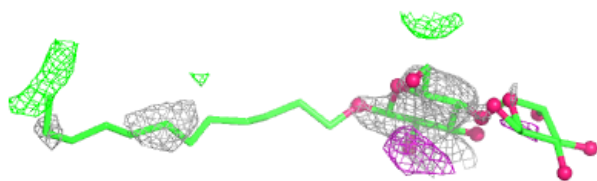
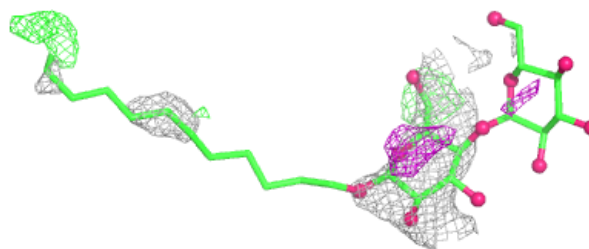
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
21	FE2	a	401[B]	1/1	1.00	0.01	52,52,52,52	1

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.

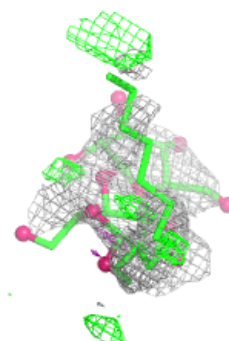
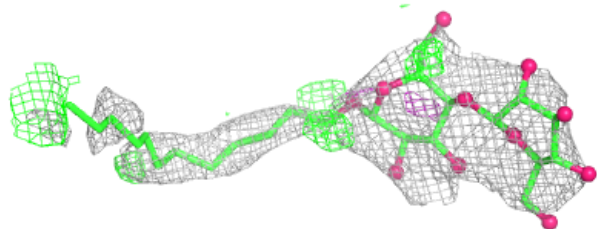
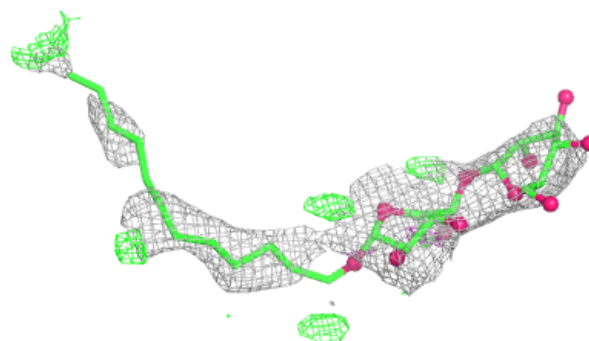


Electron density around LMT e 101:

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

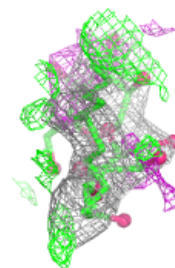
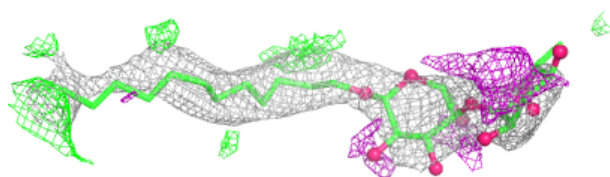
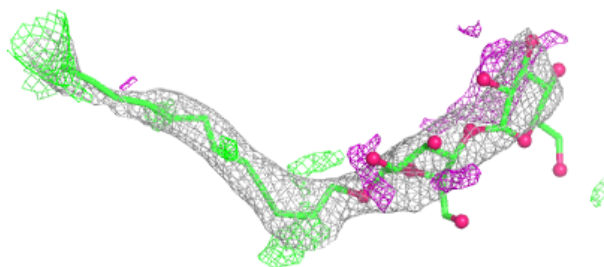
**Electron density around LMT A 419:**

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

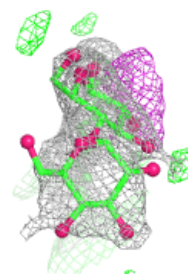
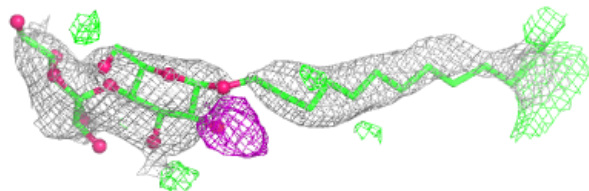
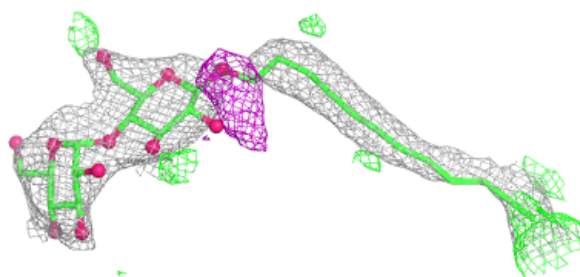


Electron density around LMT B 627:

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

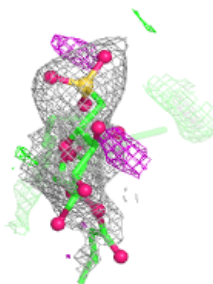
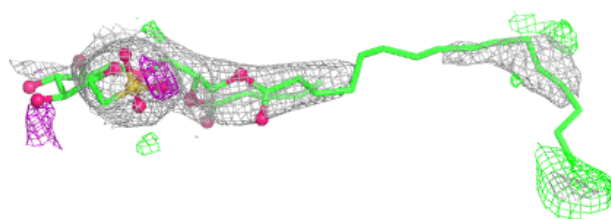
**Electron density around LMT A 417:**

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

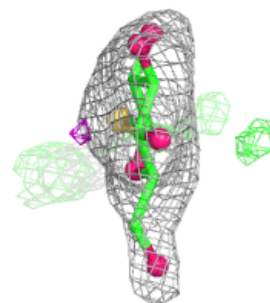
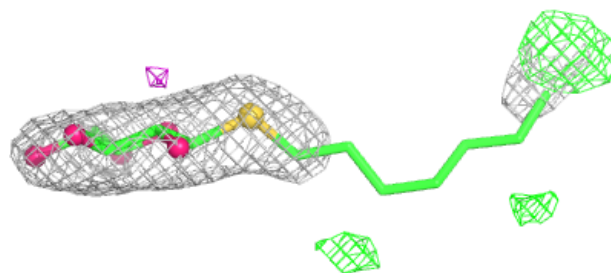
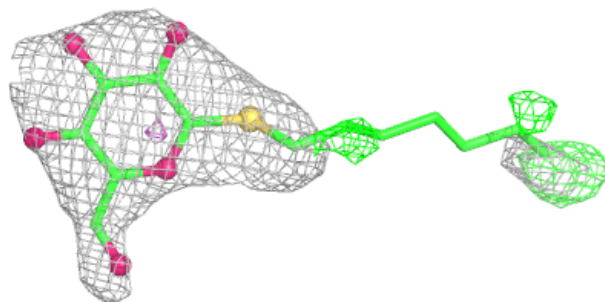


Electron density around SQD f 102:

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

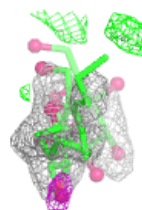
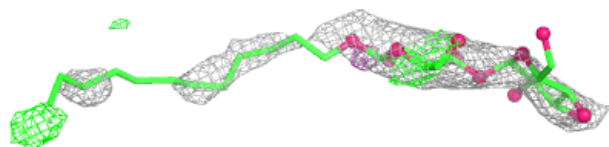
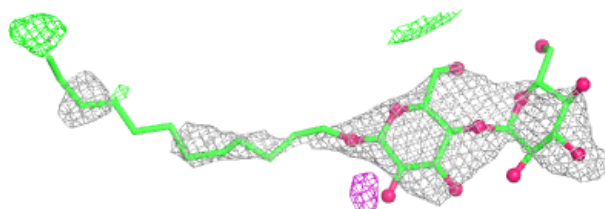
**Electron density around HTG C 522:**

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

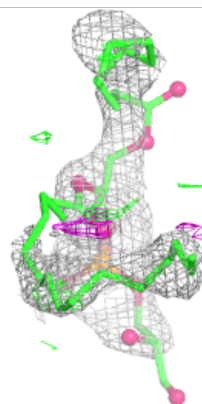
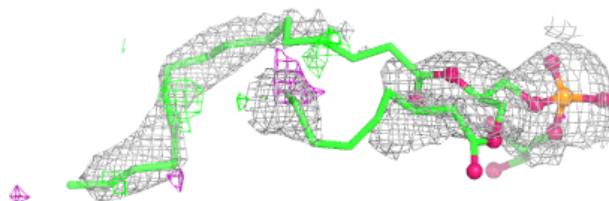
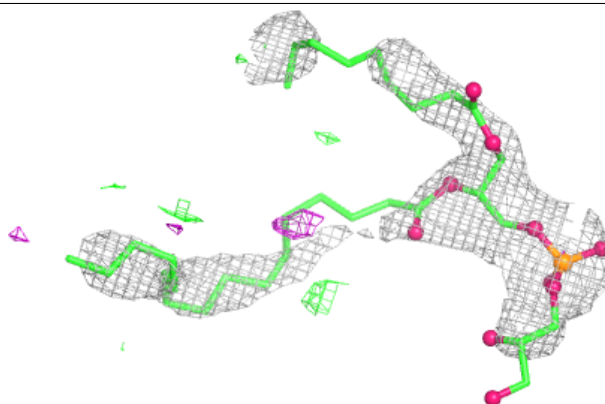


Electron density around LMT a 416:

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

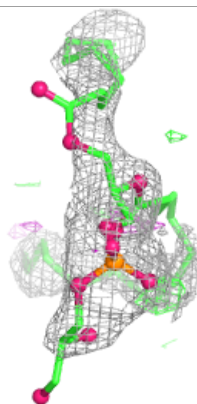
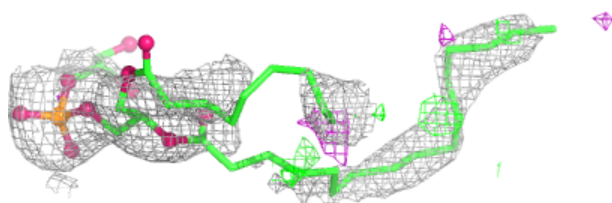
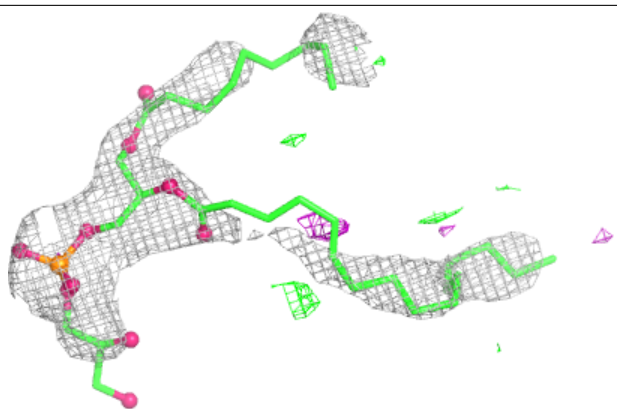
**Electron density around LHG a 419 (A):**

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

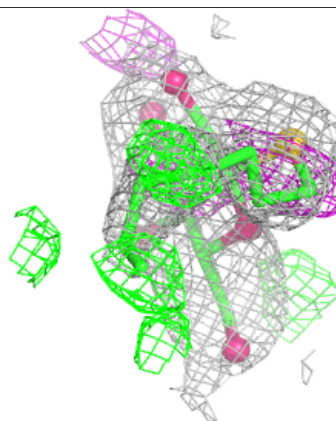
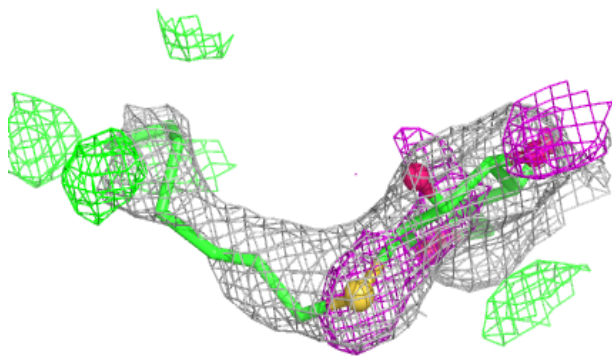
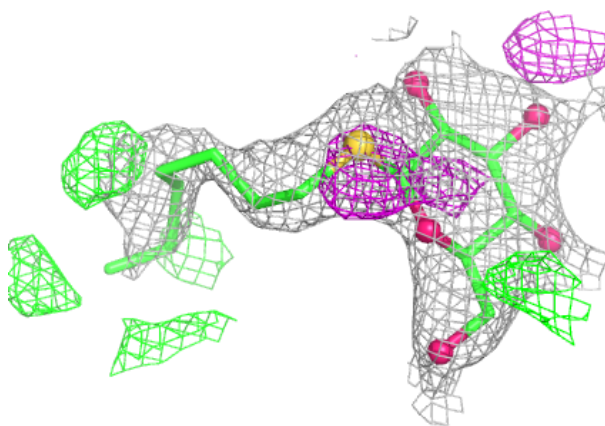


Electron density around LHG a 419 (B):

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

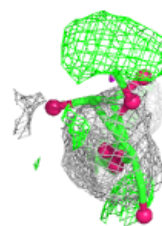
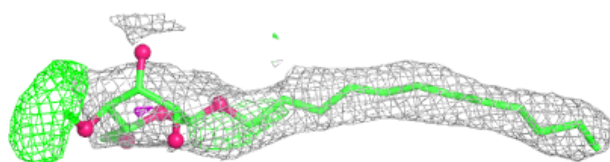
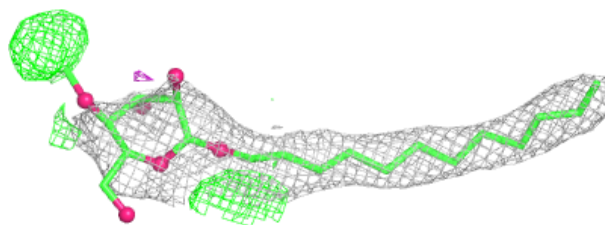
**Electron density around HTG B 621:**

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

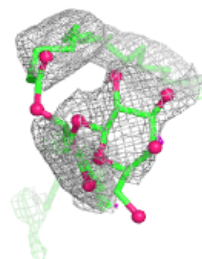
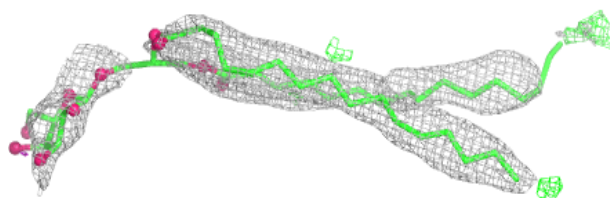
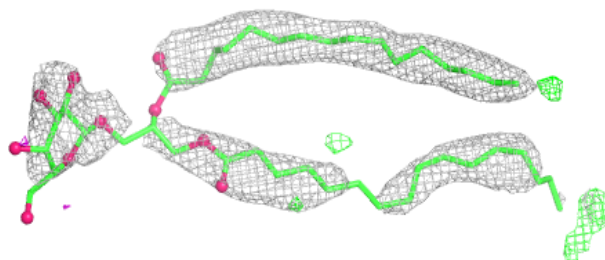


Electron density around LMT b 621:

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

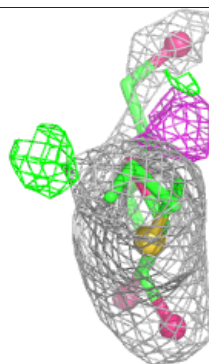
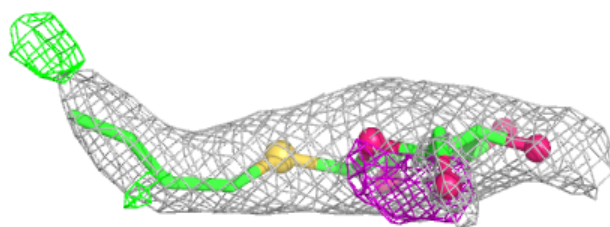
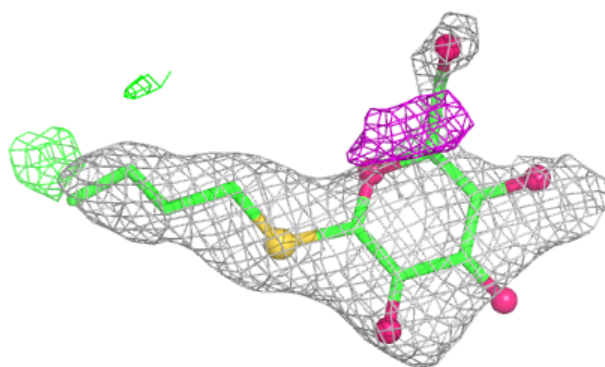
**Electron density around LMG C 521:**

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

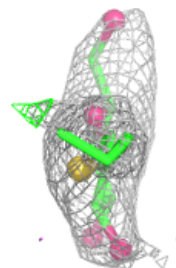
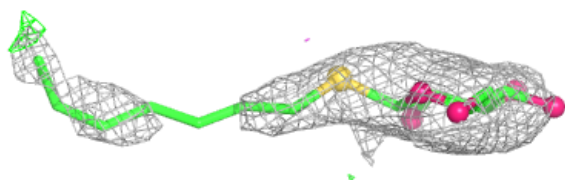
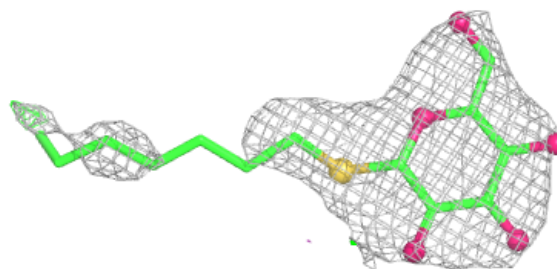


Electron density around HTG D 411:

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

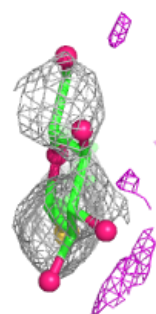
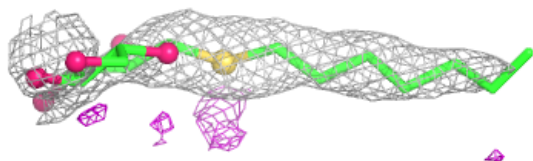
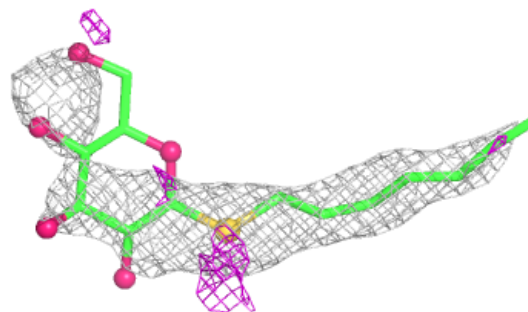
**Electron density around HTG c 522:**

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

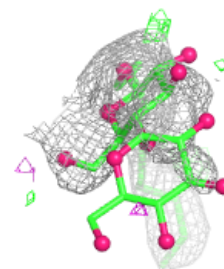
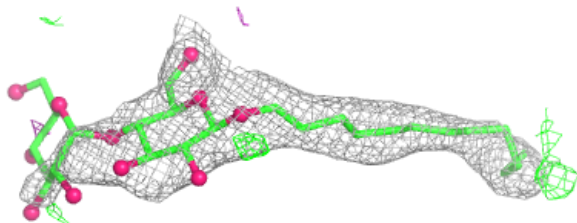
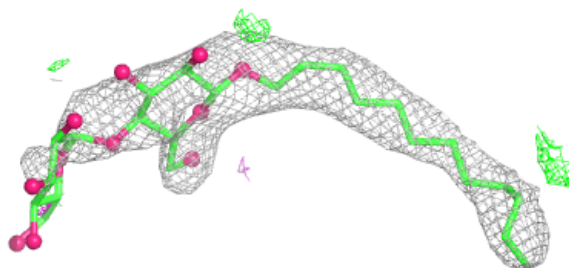


Electron density around HTG b 623:

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

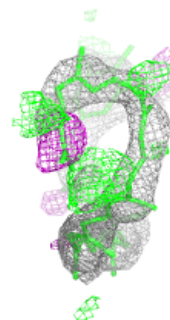
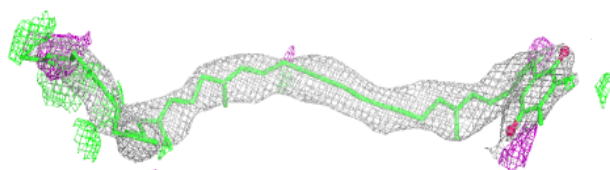
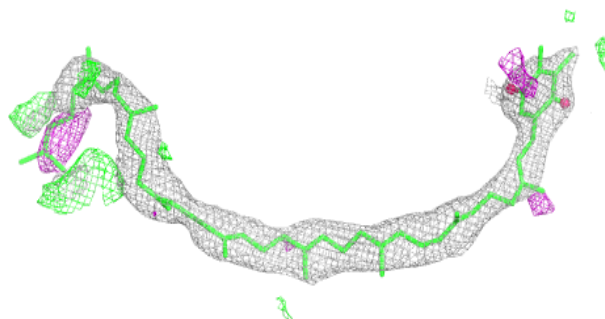
**Electron density around LMT T 101:**

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

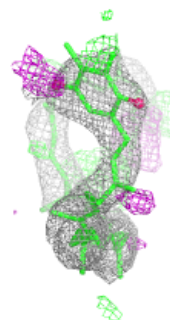
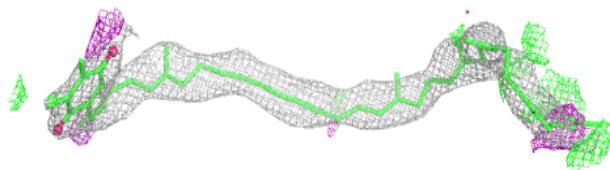
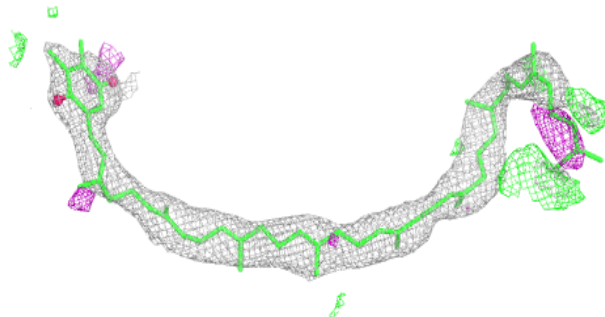


Electron density around PL9 A 413 (A):

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

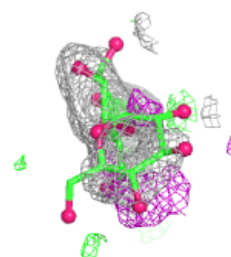
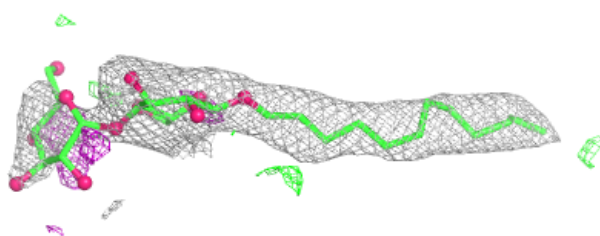
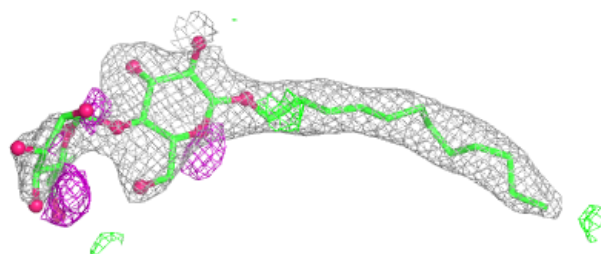
**Electron density around PL9 A 413 (B):**

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

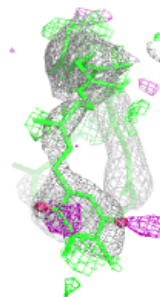
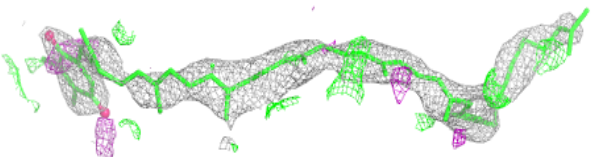
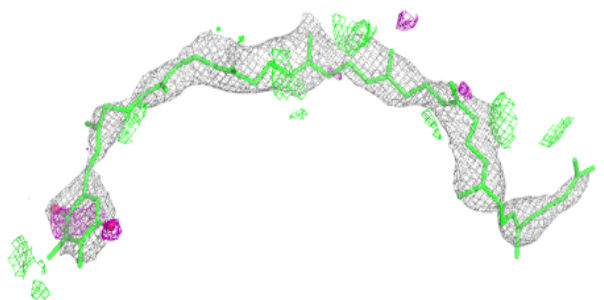


Electron density around LMT B 626:

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

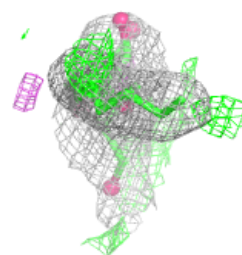
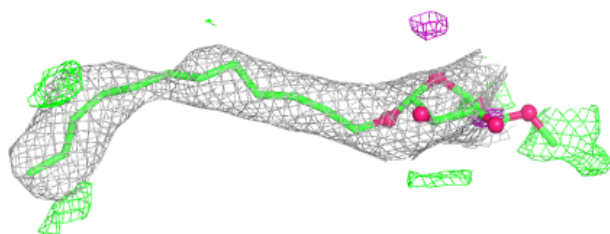
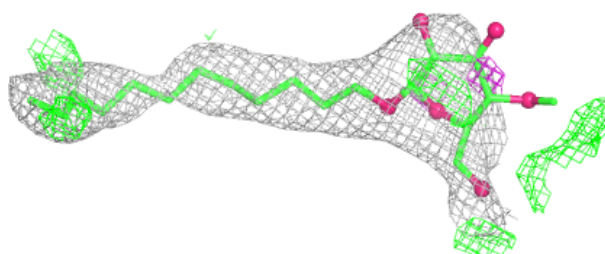
**Electron density around PL9 a 413 (A):**

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

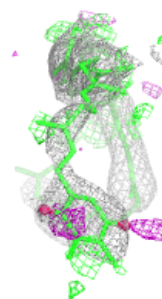
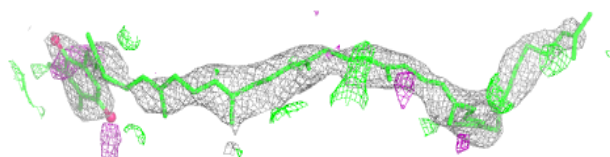
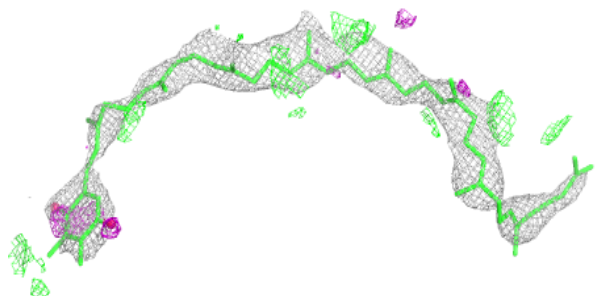


Electron density around LMT B 629:

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

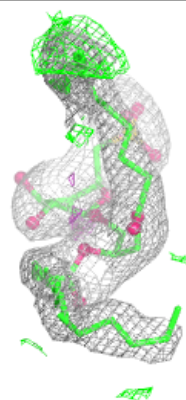
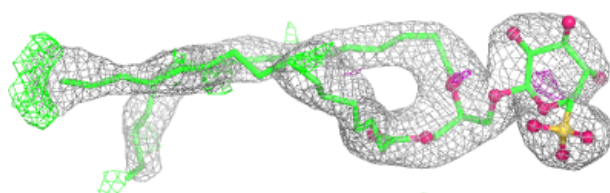
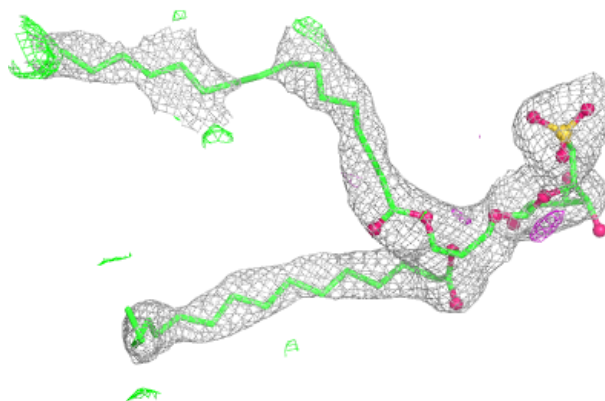
**Electron density around PL9 a 413 (B):**

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

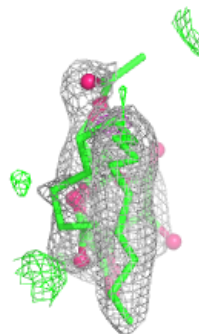
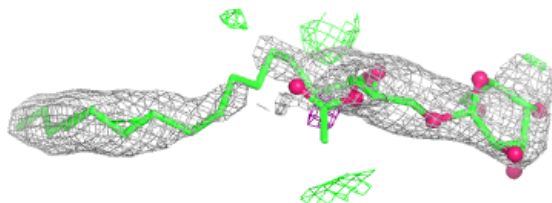
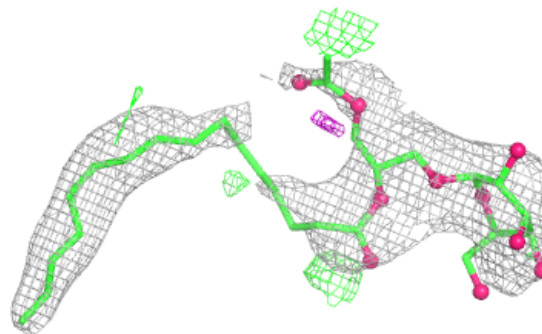


Electron density around SQD a 411:

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

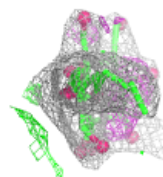
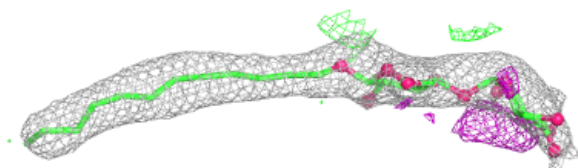
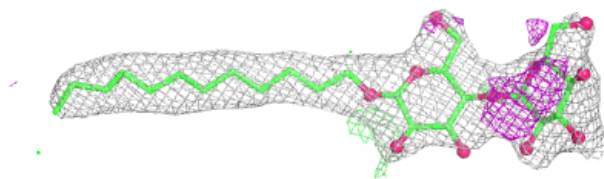
**Electron density around LMG Z 101:**

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

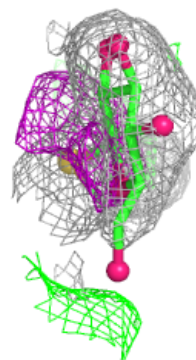
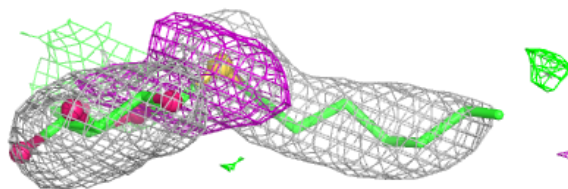
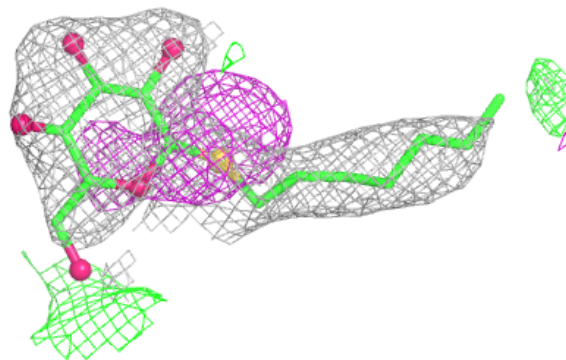


Electron density around LMT m 103:

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

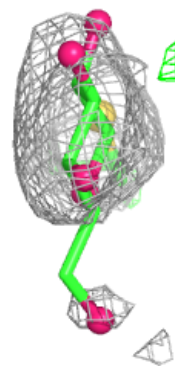
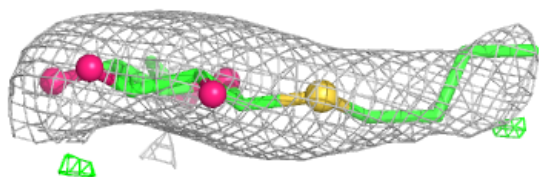
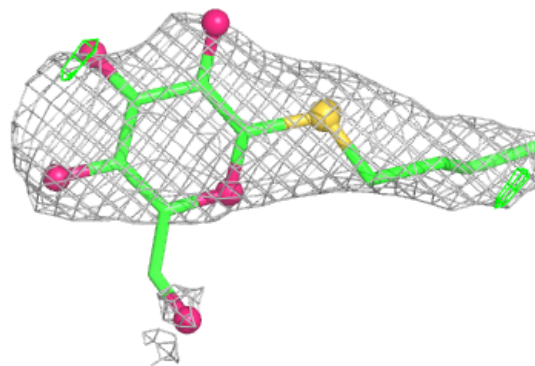
**Electron density around HTG b 622:**

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

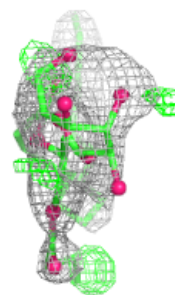
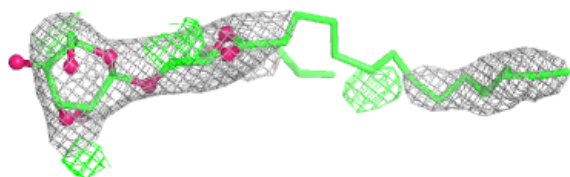
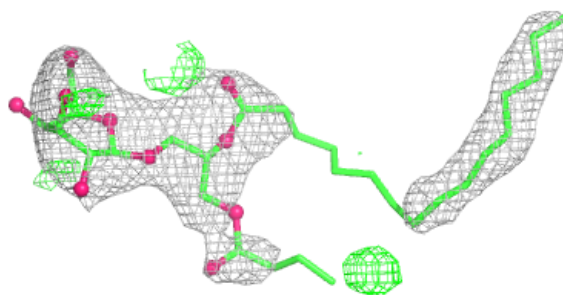


Electron density around HTG d 411:

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

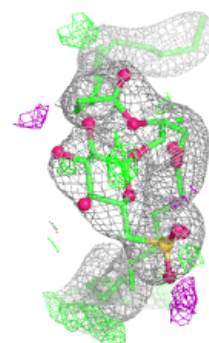
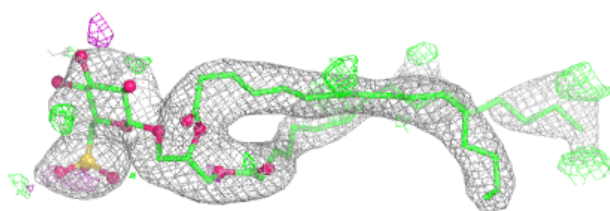
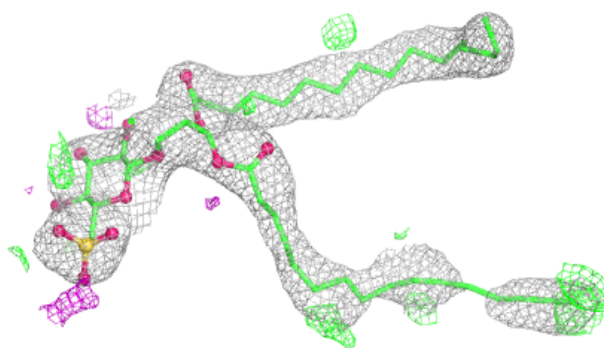
**Electron density around LMG z 101:**

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

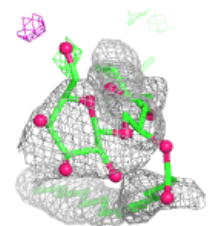
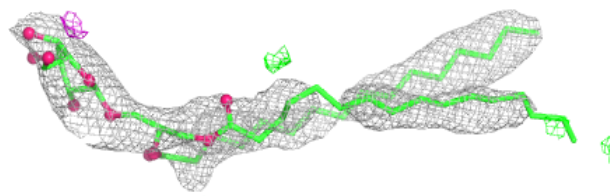
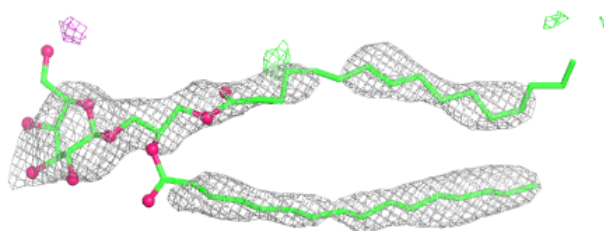


Electron density around SQD A 411:

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

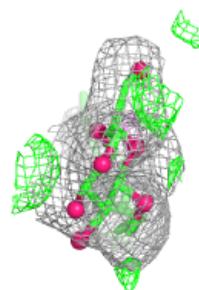
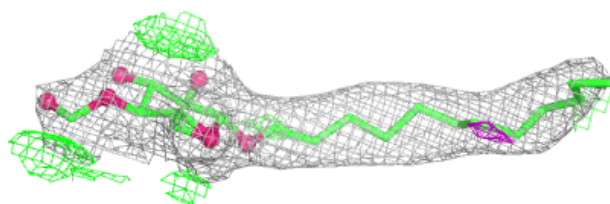
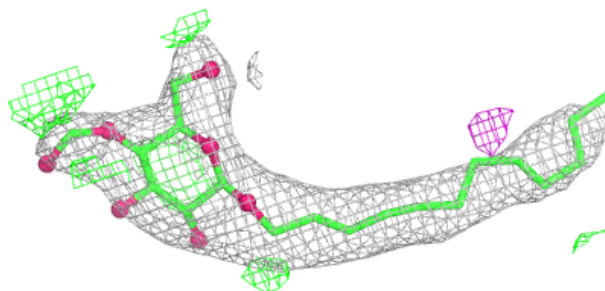
**Electron density around LMG c 521:**

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



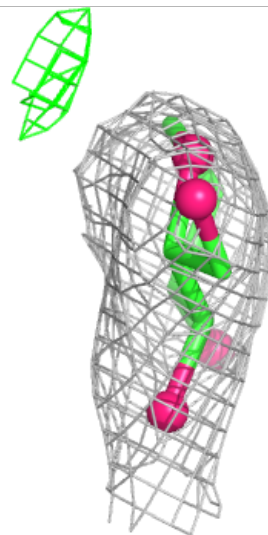
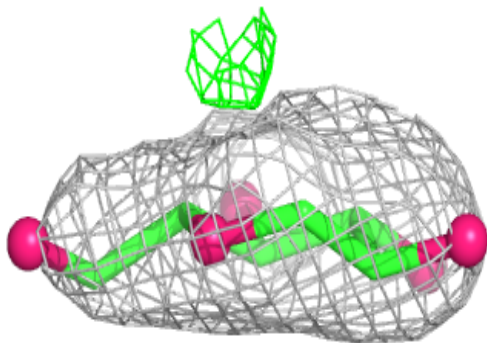
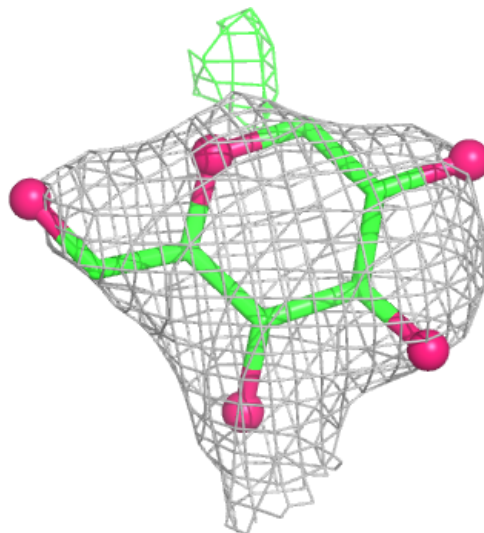
Electron density around LMT t 101:

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



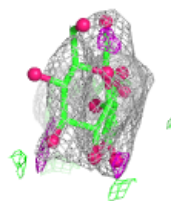
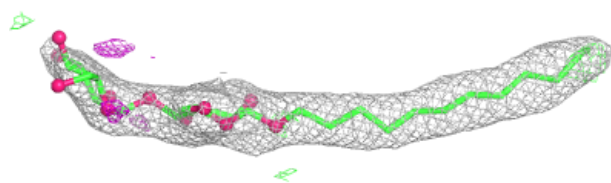
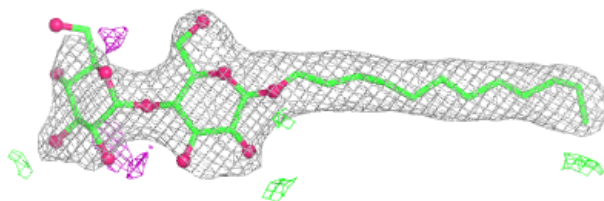
Electron density around HTG V 202:

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

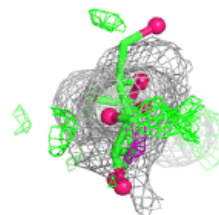
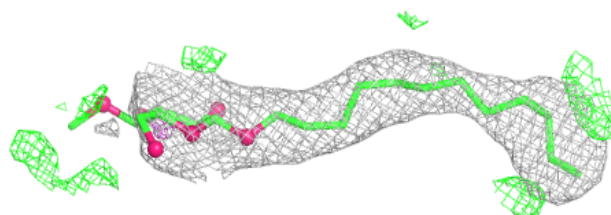
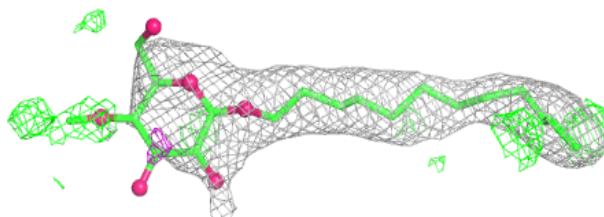


Electron density around LMT M 101:

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

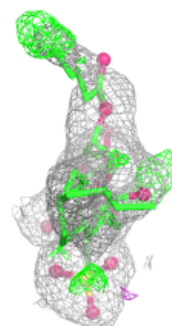
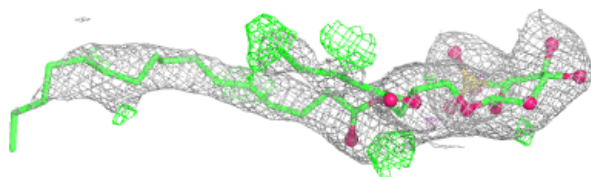
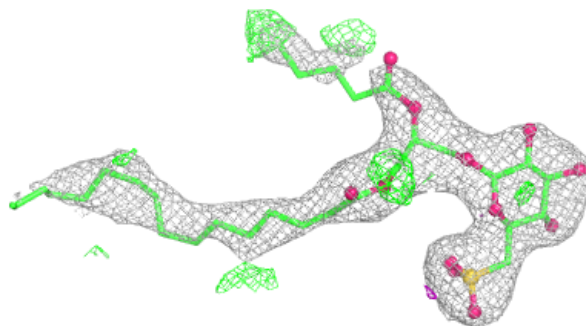
**Electron density around LMT b 627:**

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

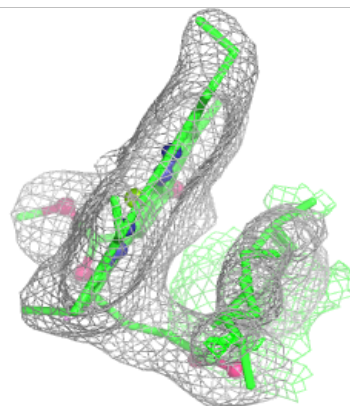
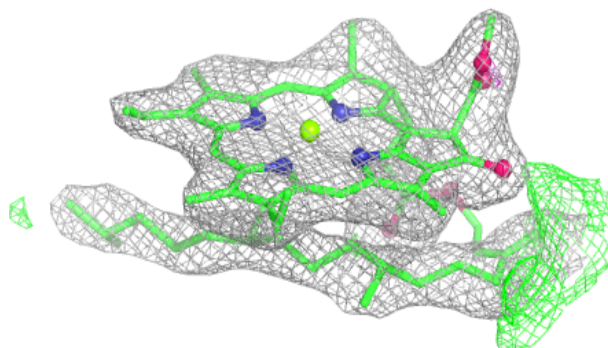
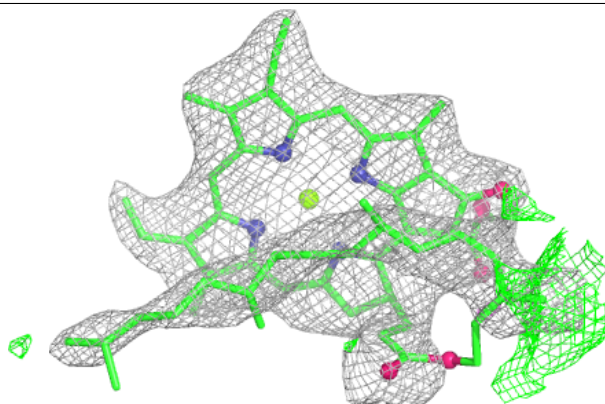


Electron density around SQD X 101:

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

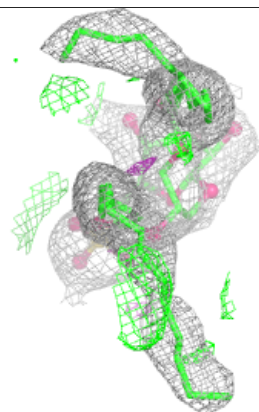
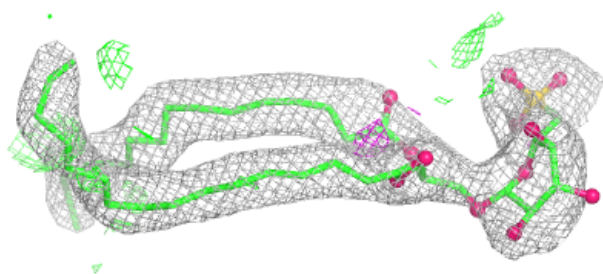
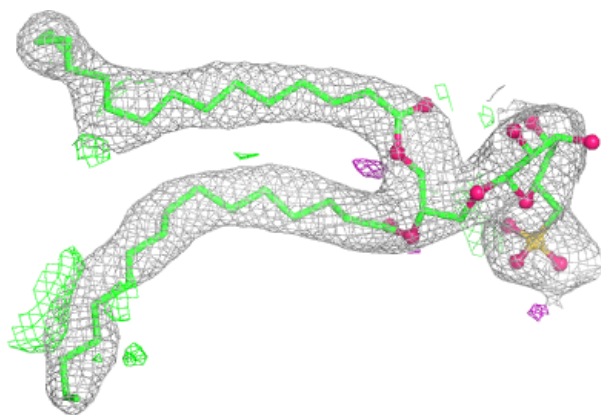
**Electron density around CLA b 601:**

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

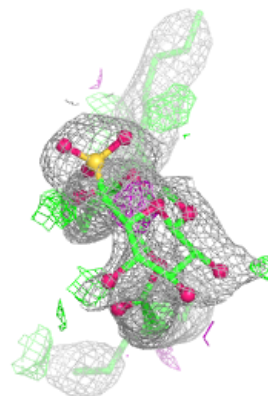
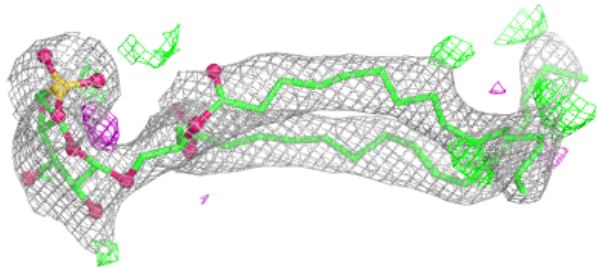
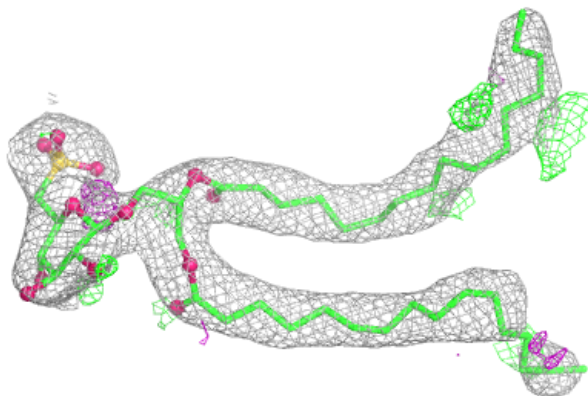


Electron density around SQD 1 101:

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

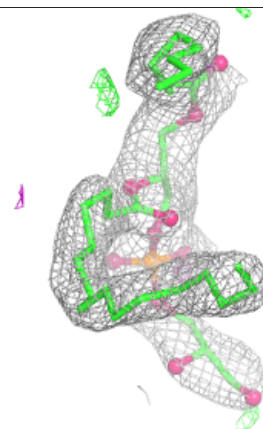
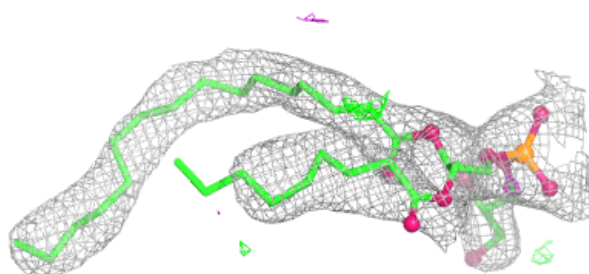
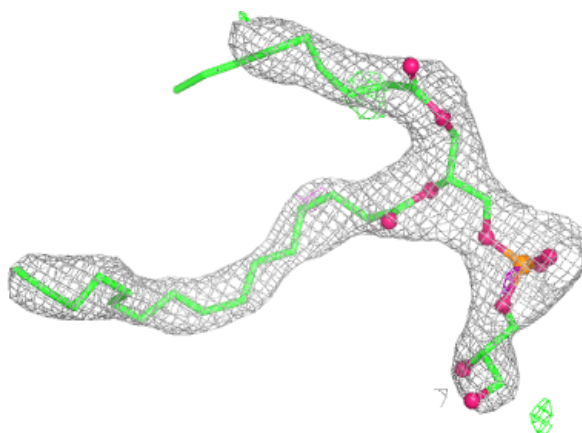
**Electron density around SQD b 620:**

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



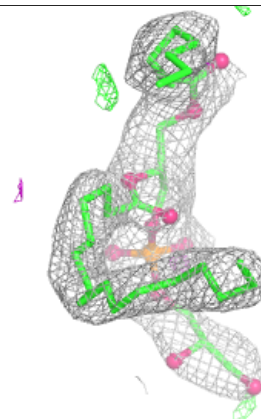
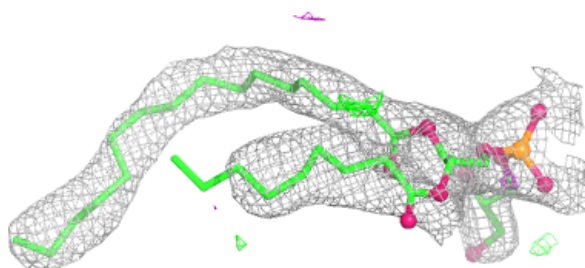
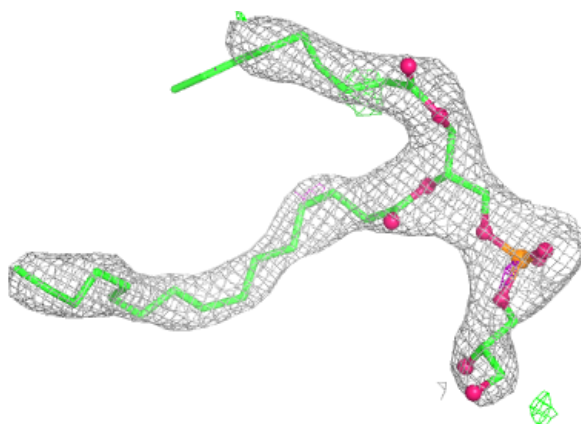
Electron density around LHG E 101 (A):

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

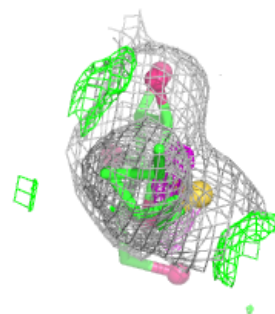
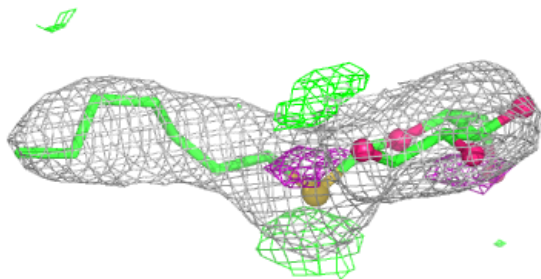
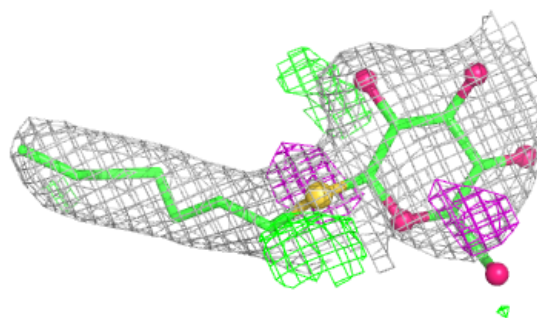


Electron density around LHG E 101 (B):

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

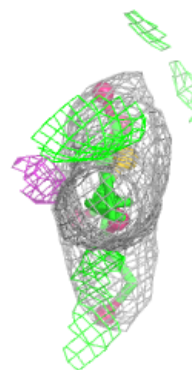
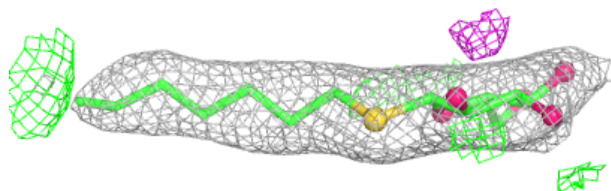
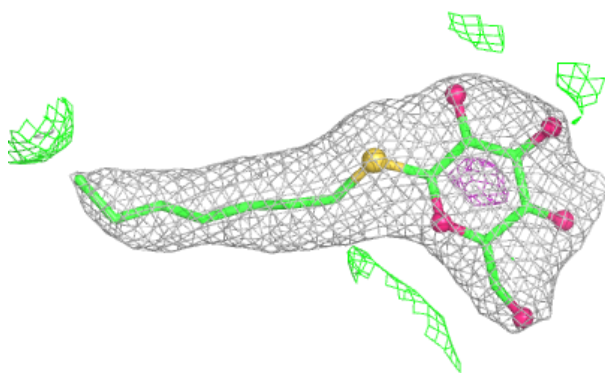
**Electron density around HTG o 301:**

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

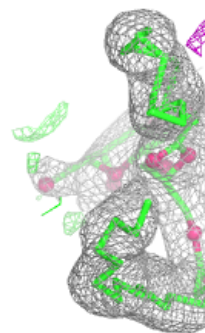
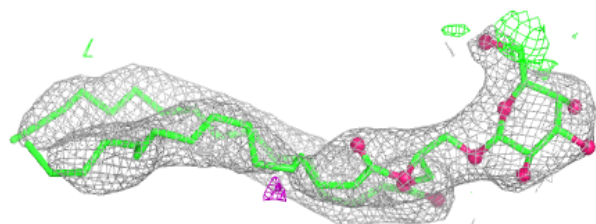
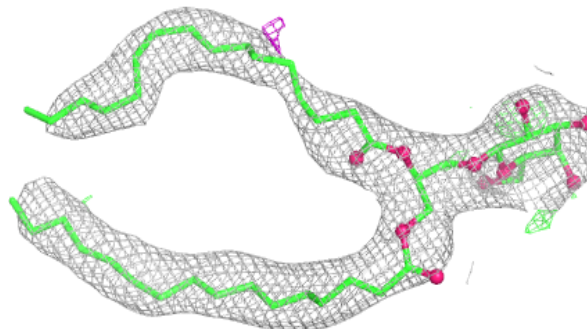


Electron density around HTG B 623:

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

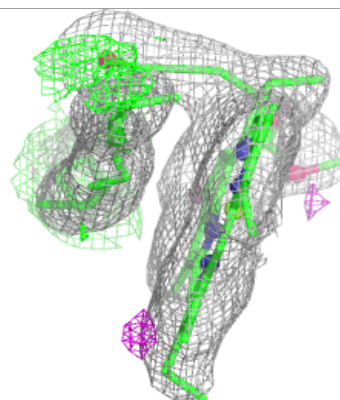
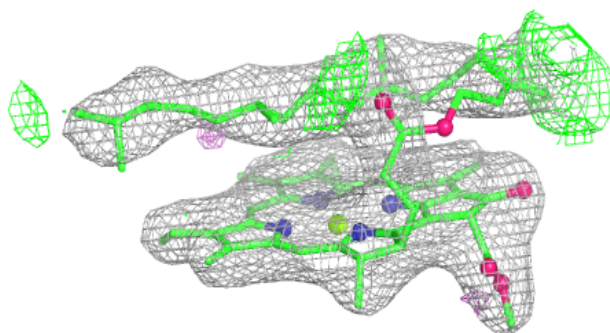
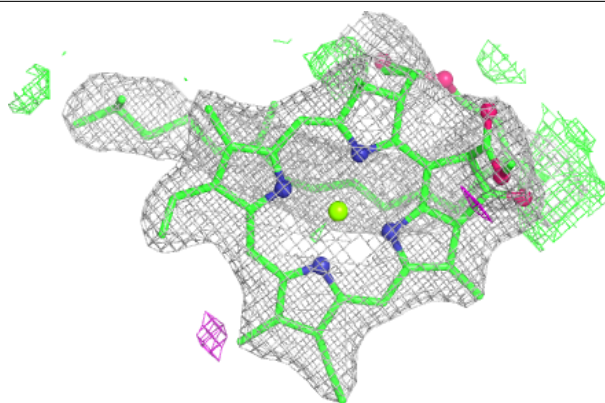
**Electron density around LMG C 501:**

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

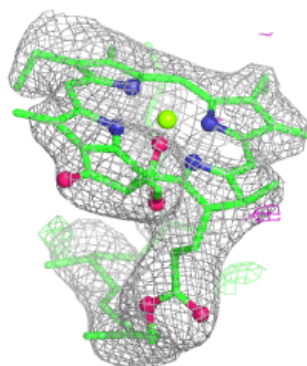
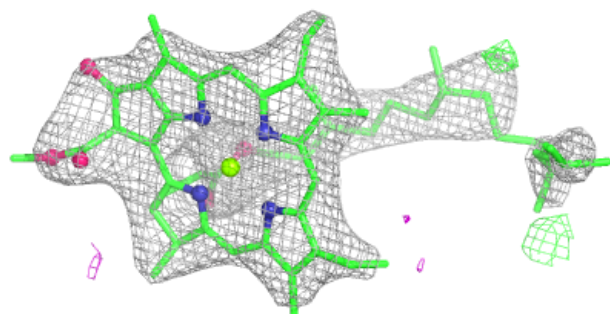
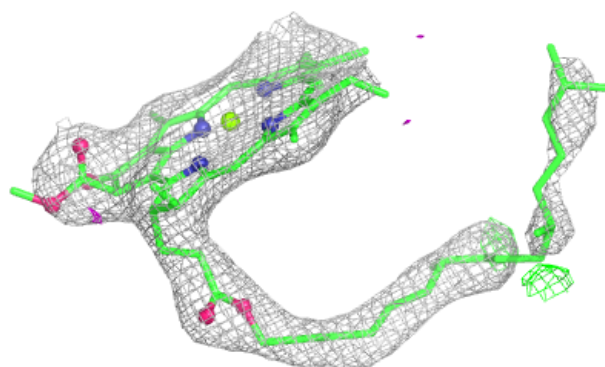


Electron density around CLA B 601:

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

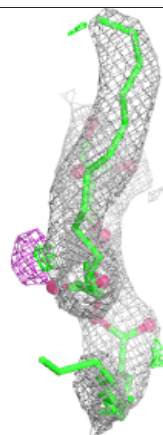
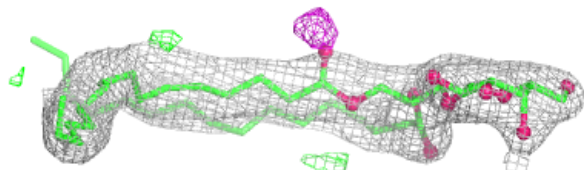
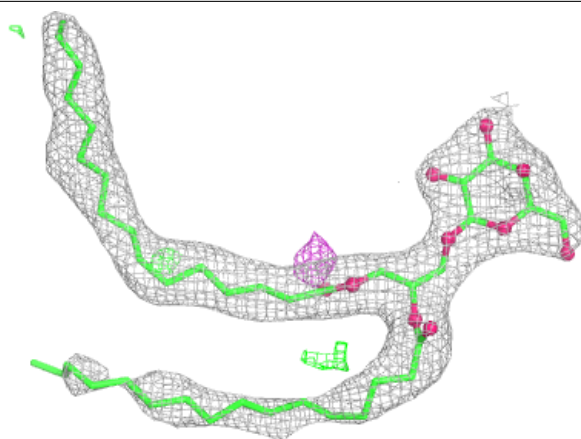
**Electron density around CLA c 514:**

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

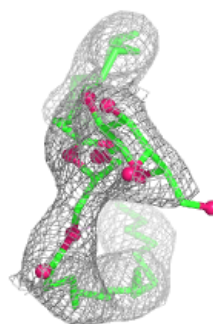
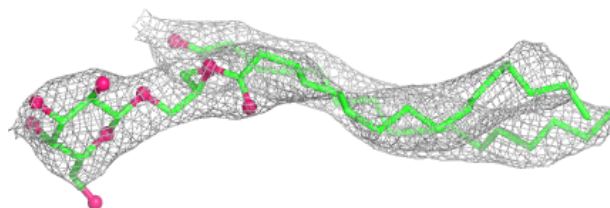
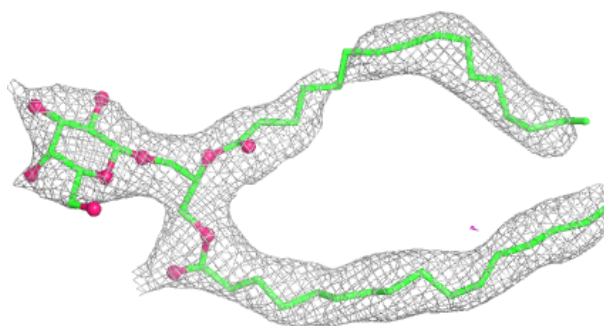


Electron density around LMG C 520:

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

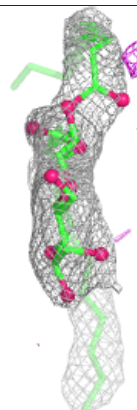
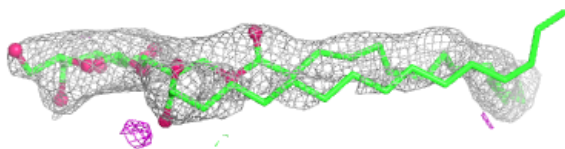
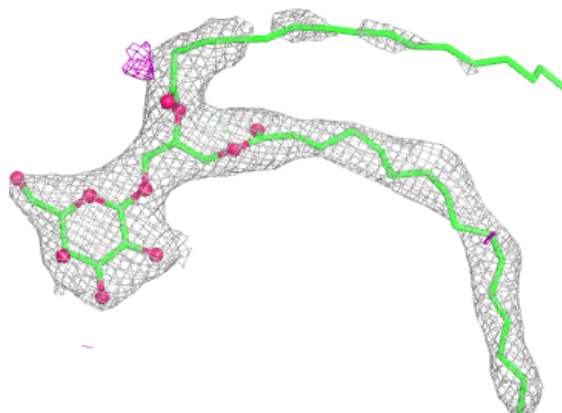
**Electron density around LMG c 501:**

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



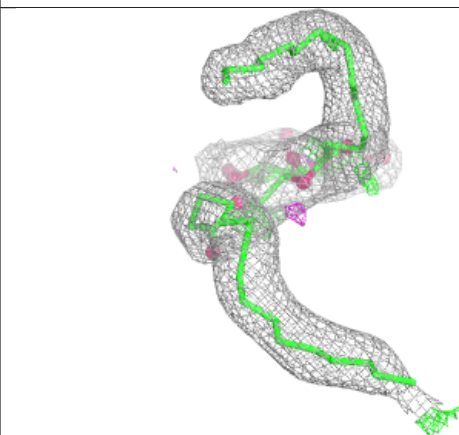
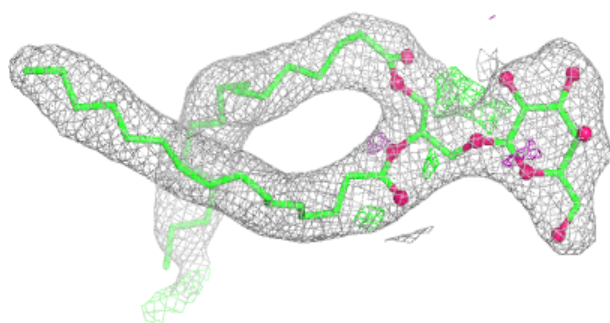
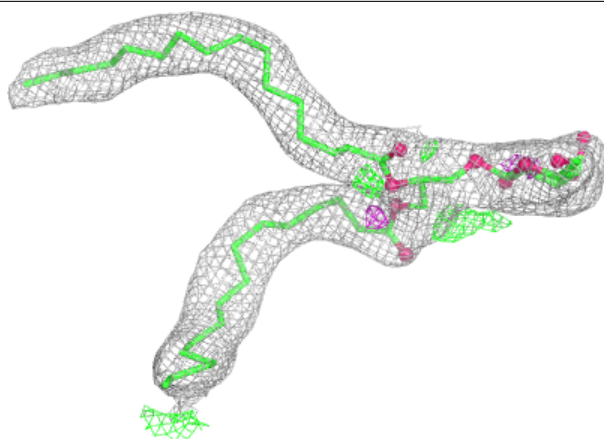
Electron density around LMG c 520:

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

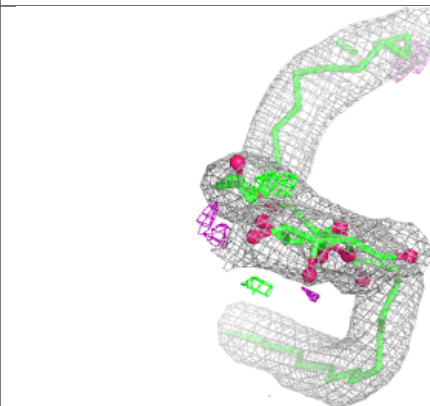
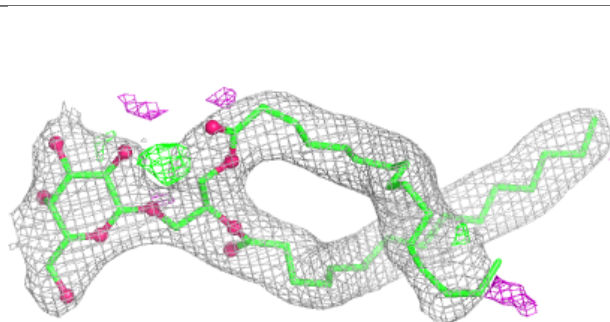
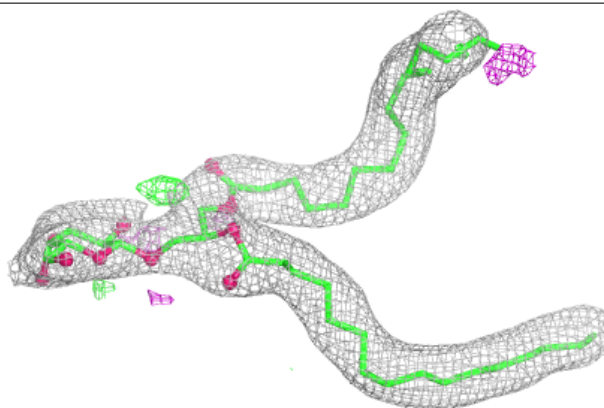


Electron density around LMG B 620:

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

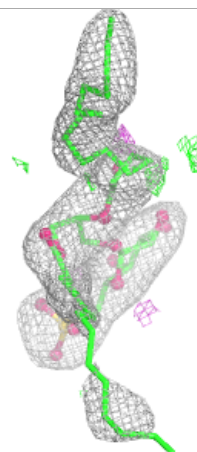
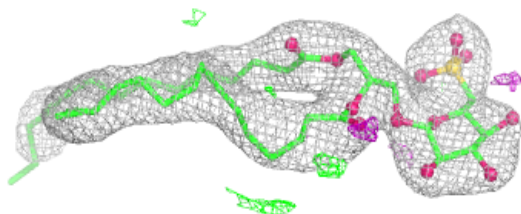
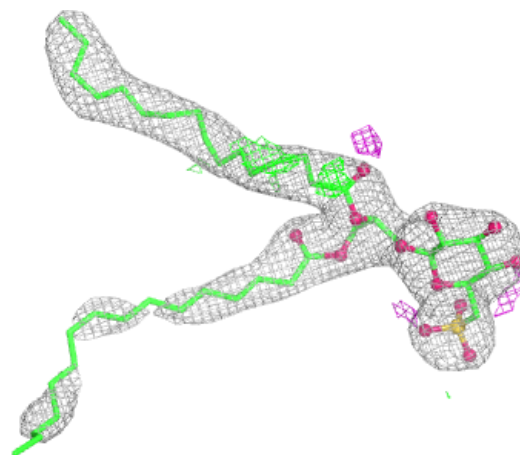
**Electron density around LMG m 101:**

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



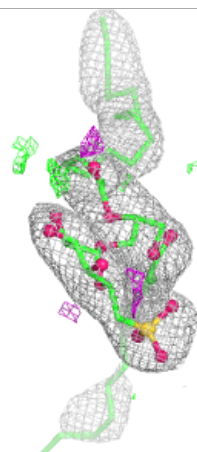
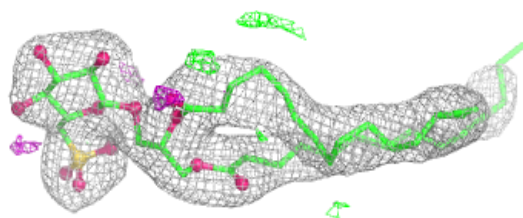
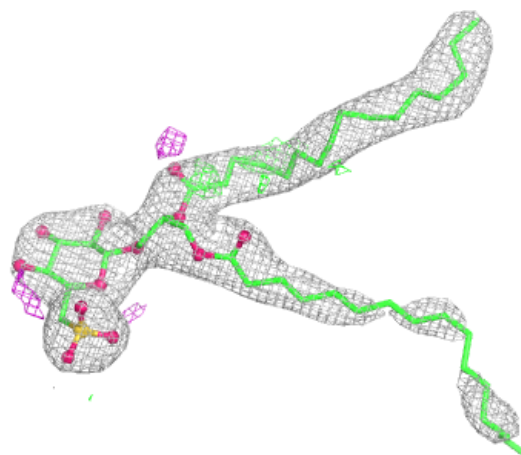
Electron density around SQD A 409 (A):

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



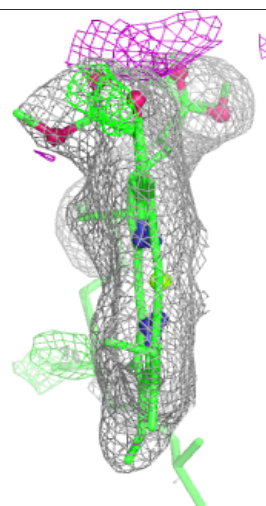
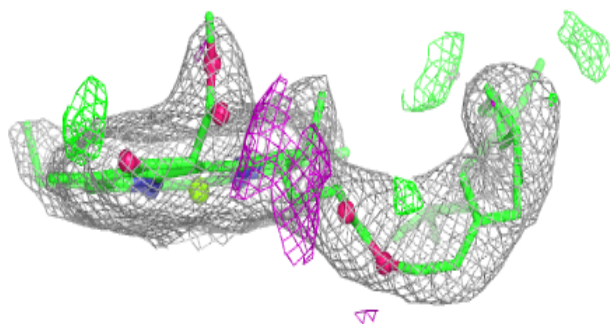
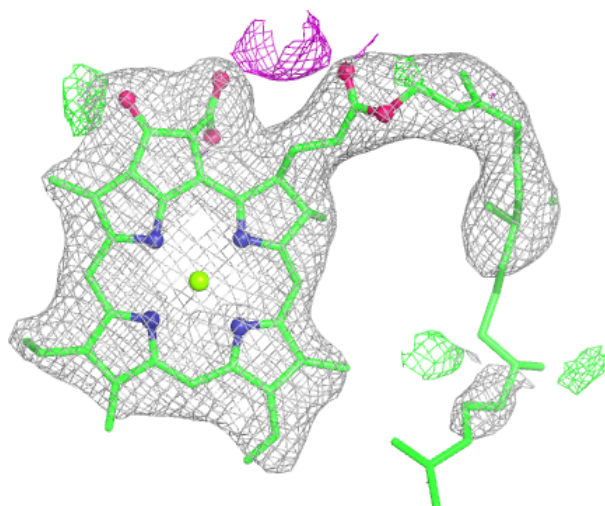
Electron density around SQD A 409 (B):

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



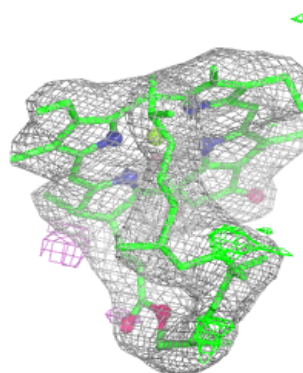
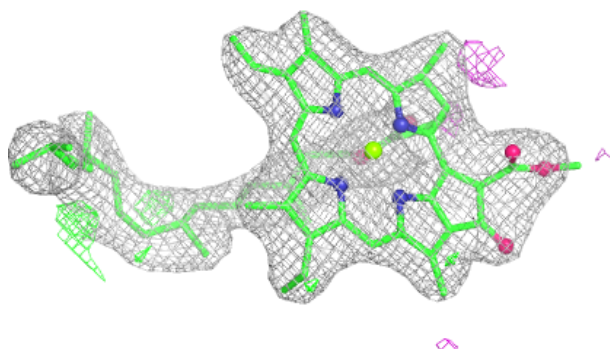
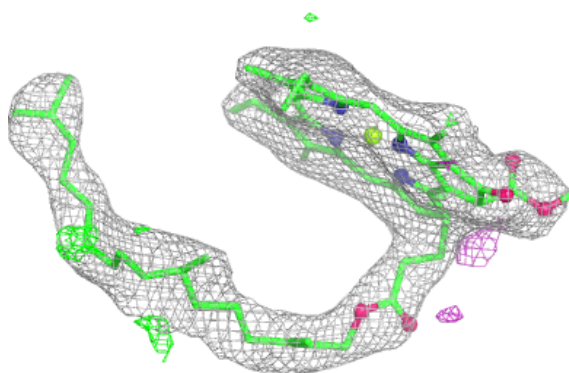
Electron density around CLA c 513:

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

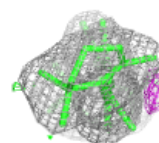
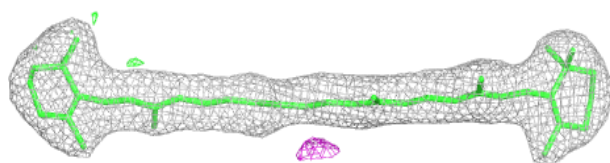
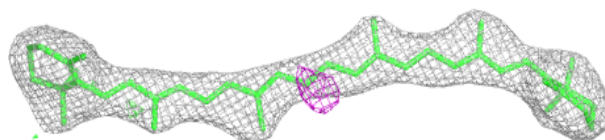


Electron density around CLA C 514:

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

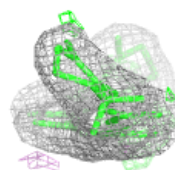
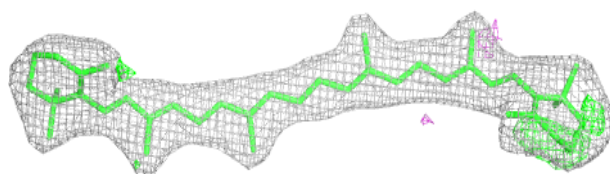
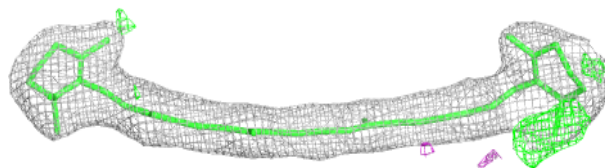
**Electron density around BCR C 515:**

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

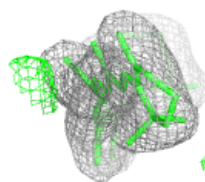
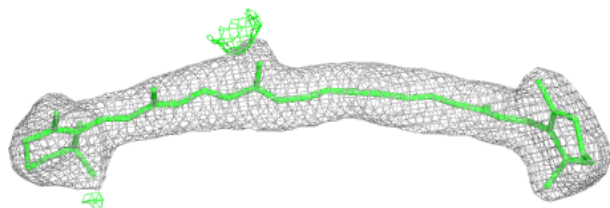
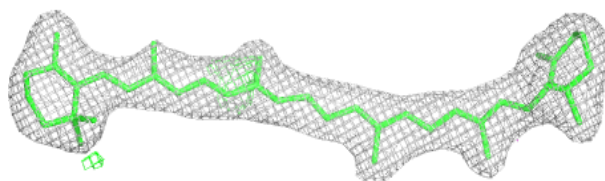


Electron density around BCR D 405:

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

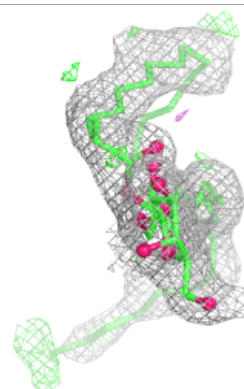
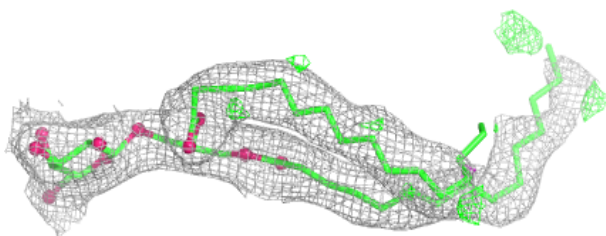
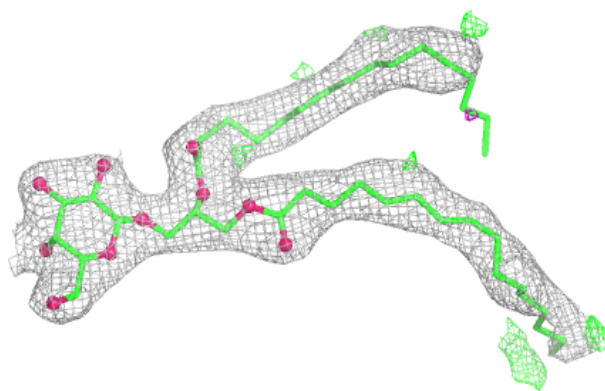
**Electron density around BCR T 102:**

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

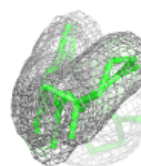
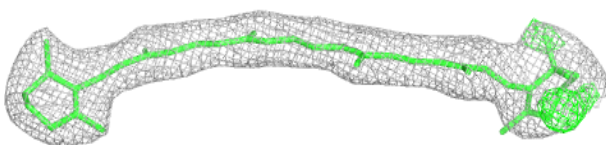
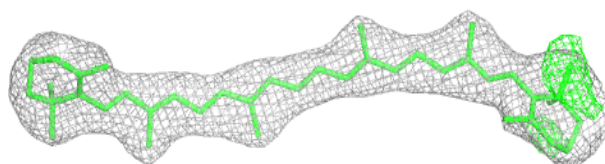


Electron density around LMG D 412:

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

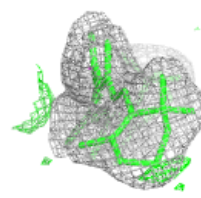
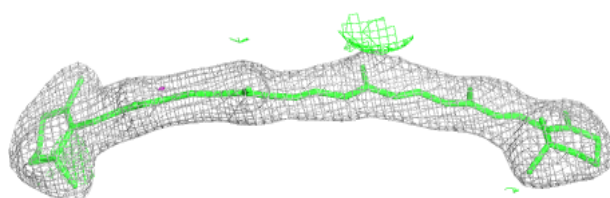
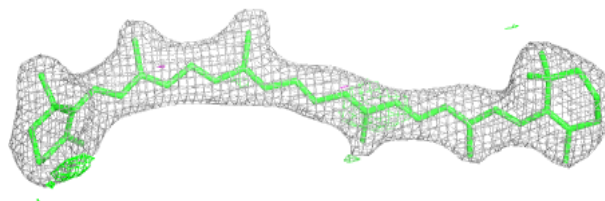
**Electron density around BCR d 405:**

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

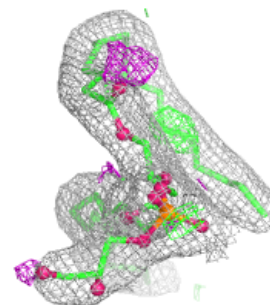
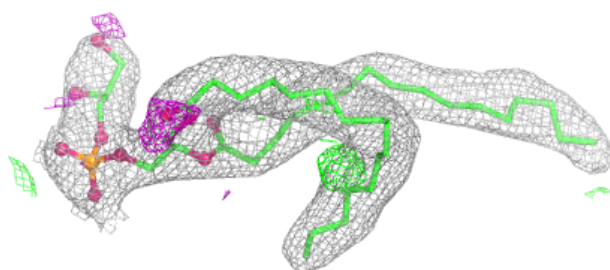
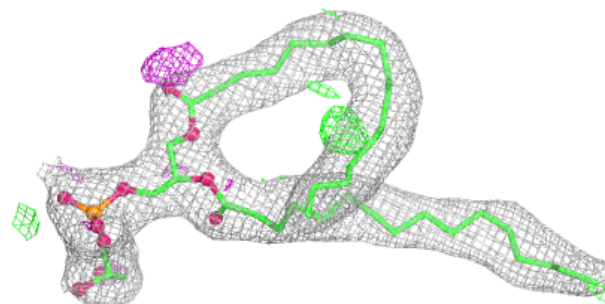


Electron density around BCR t 102:

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

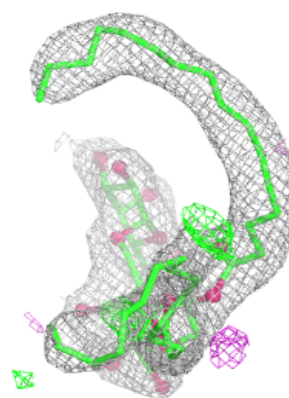
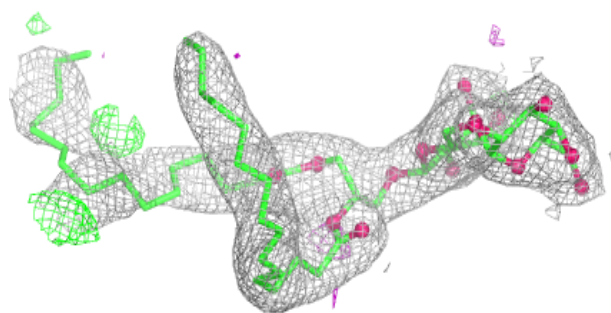
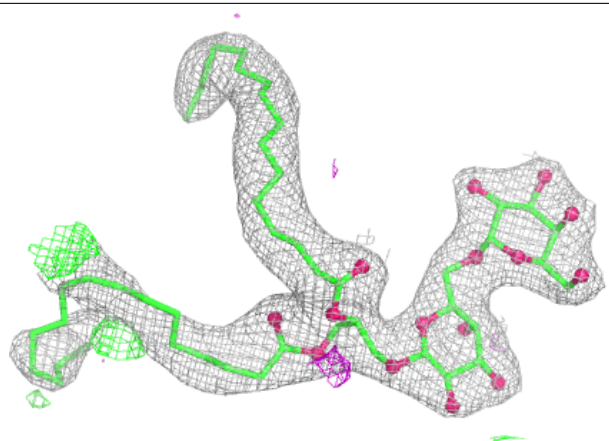
**Electron density around LHG A 418 (A):**

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



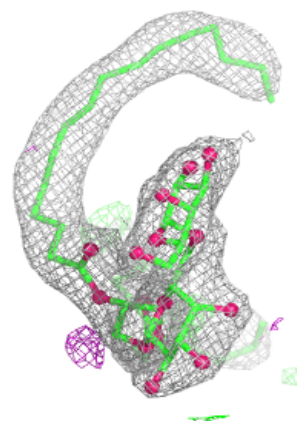
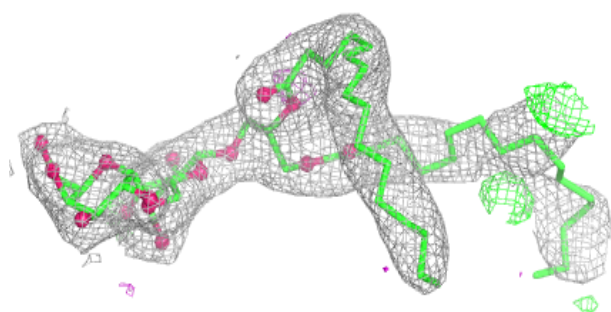
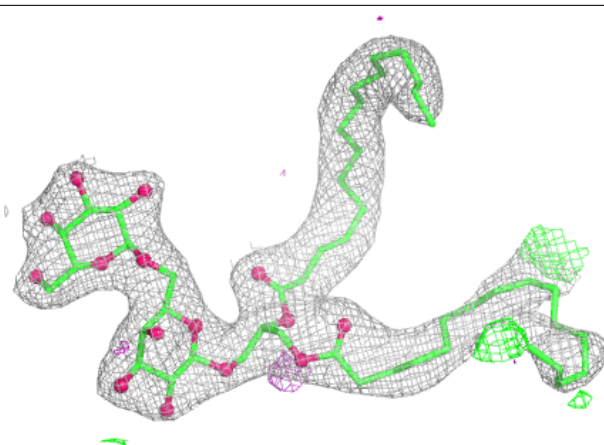
Electron density around DGD C 518 (A):

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



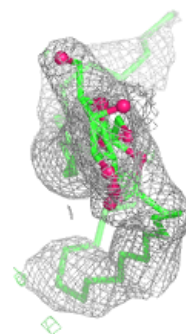
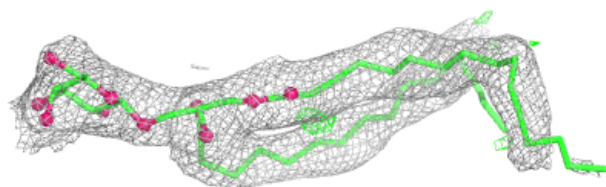
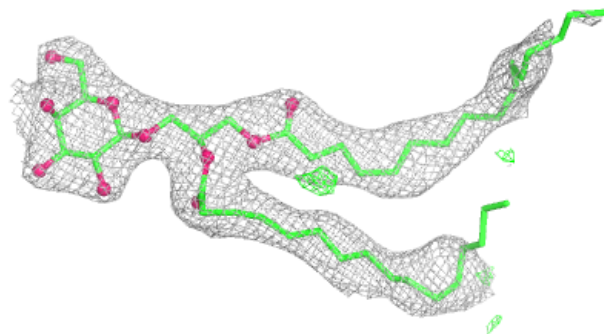
Electron density around DGD C 518 (B):

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

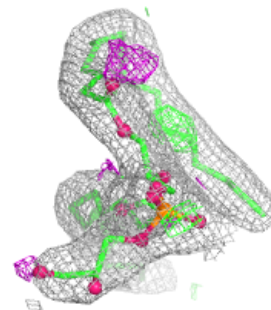
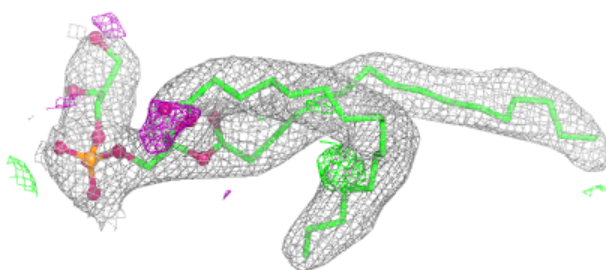
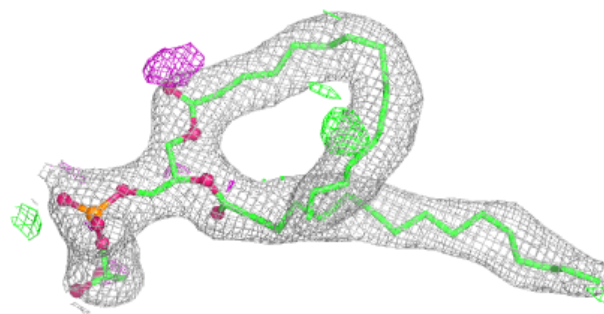


Electron density around LMG d 412:

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

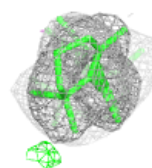
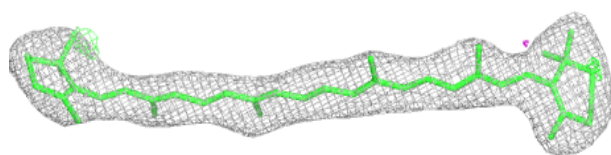
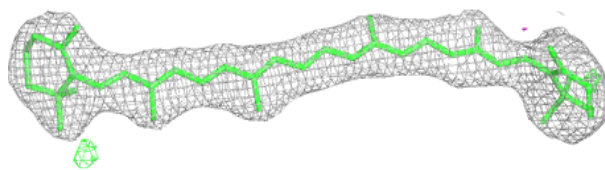
**Electron density around LHG A 418 (B):**

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

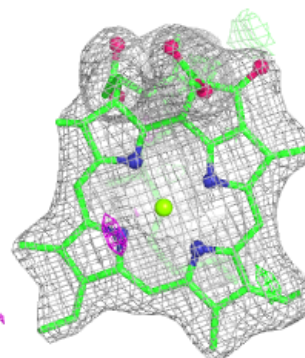
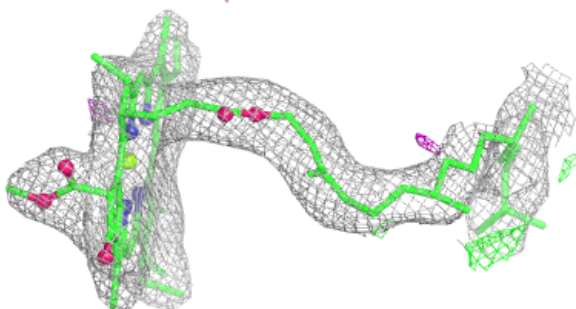
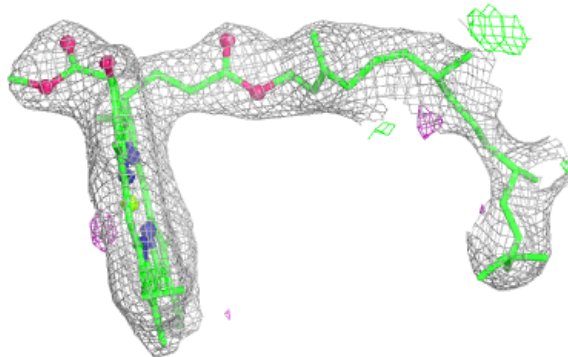


Electron density around BCR c 515:

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

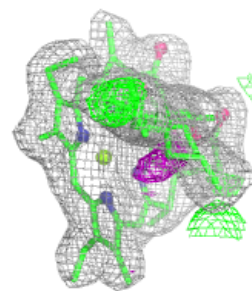
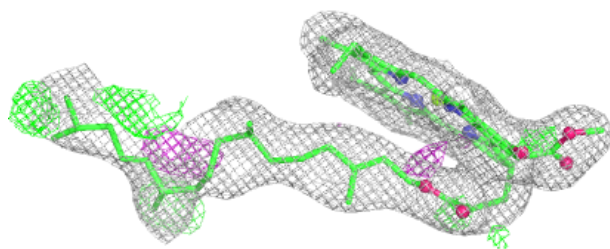
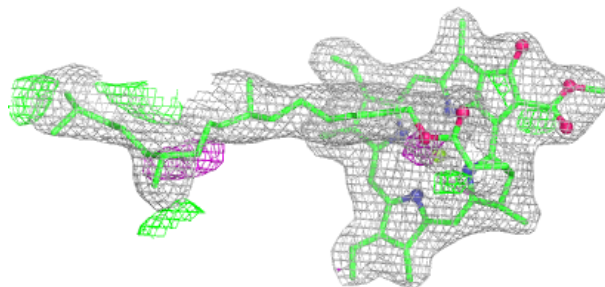
**Electron density around CLA C 507:**

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

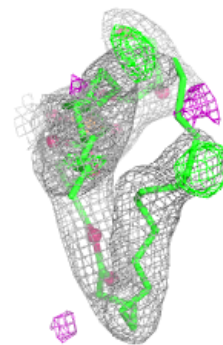
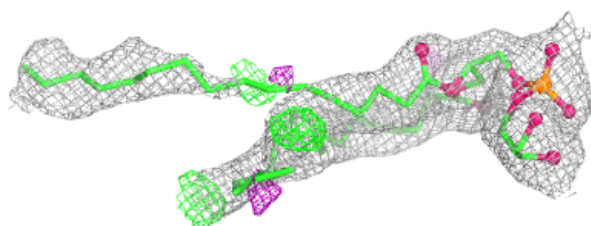
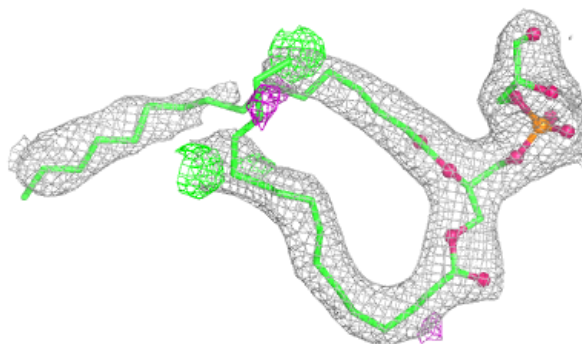


Electron density around CLA B 614:

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

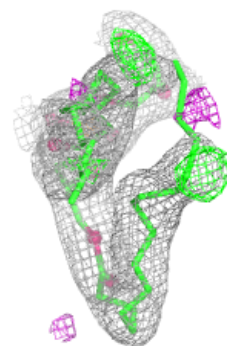
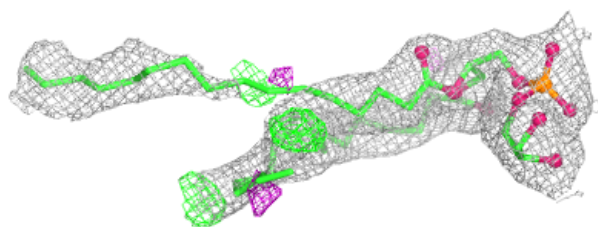
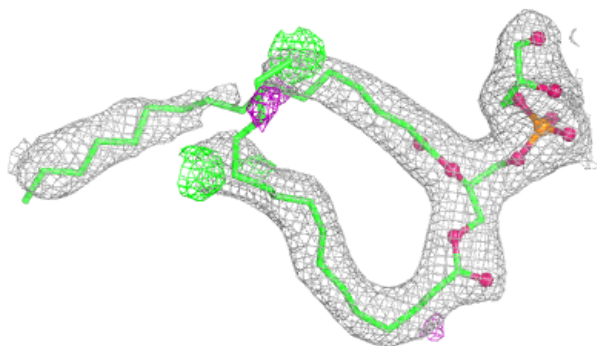
**Electron density around LHG D 408 (A):**

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

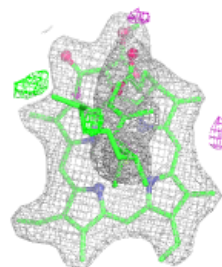
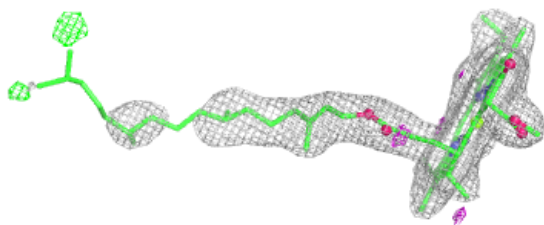
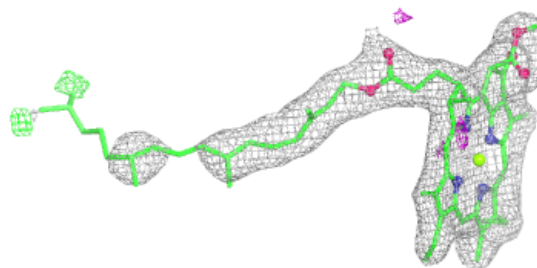


Electron density around LHG D 408 (B):

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

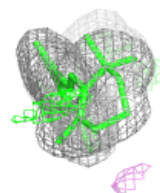
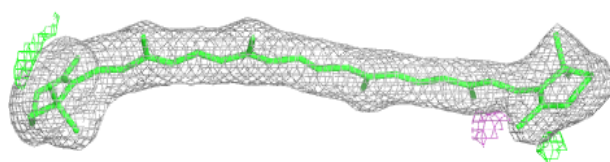
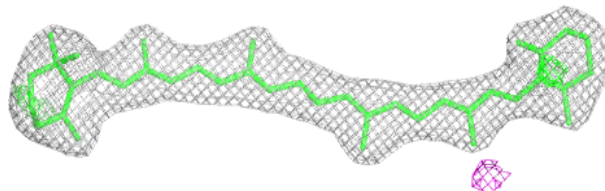
**Electron density around CLA d 404:**

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

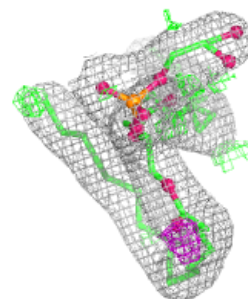
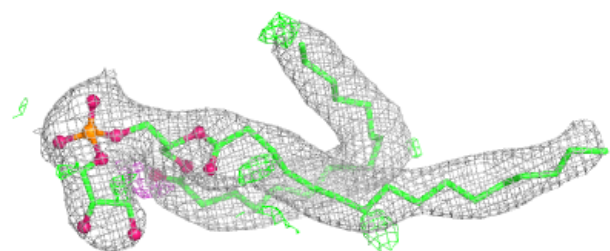
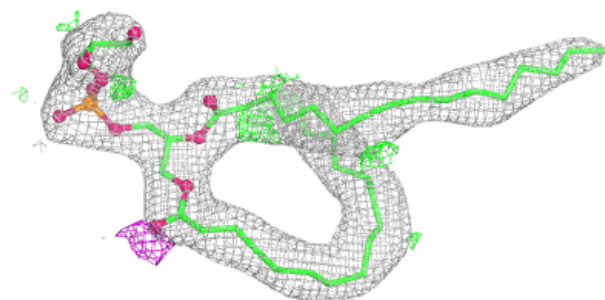


Electron density around BCR B 619:

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

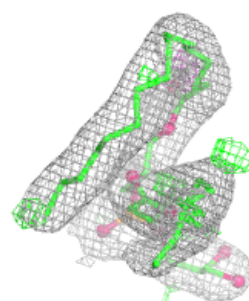
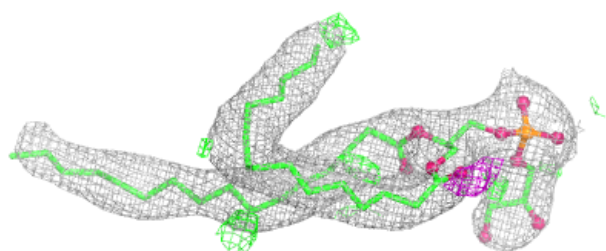
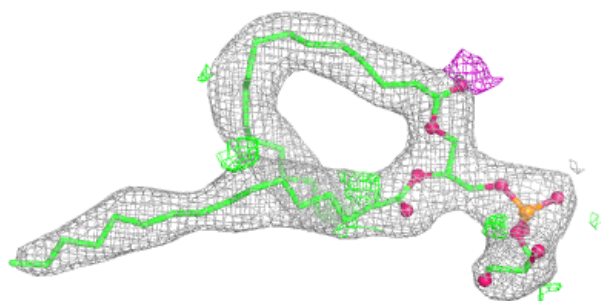
**Electron density around LHG d 414 (A):**

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

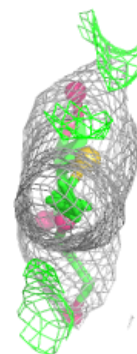
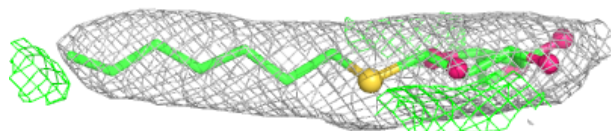
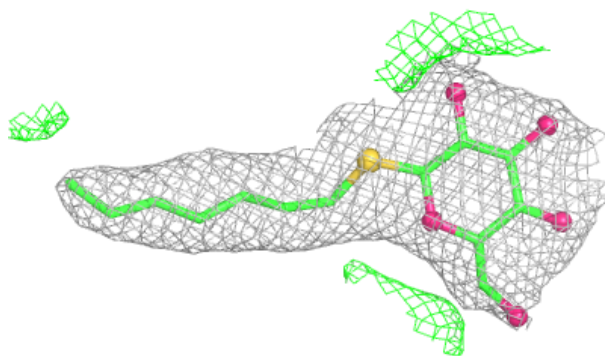


Electron density around LHG d 414 (B):

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

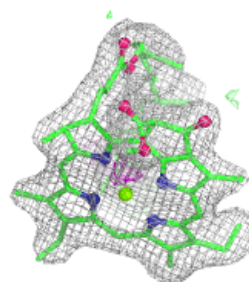
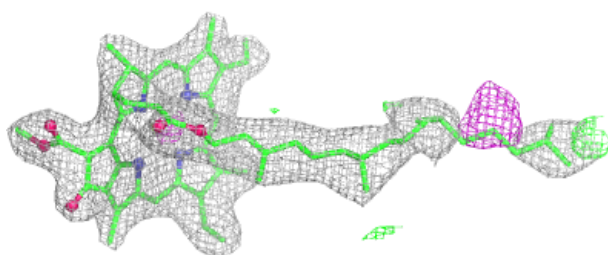
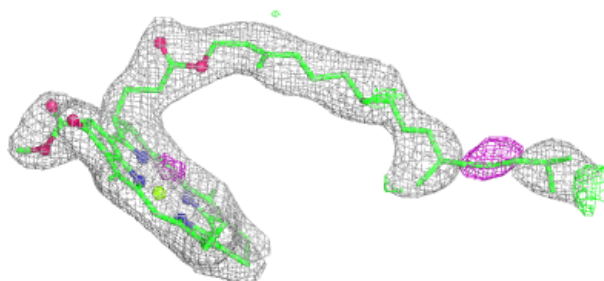
**Electron density around HTG b 625:**

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



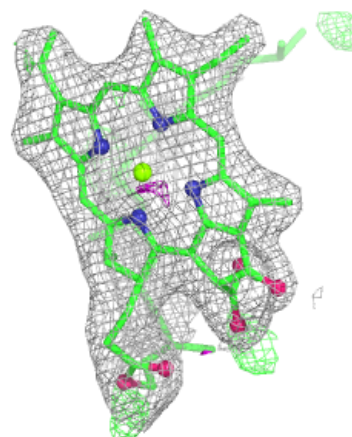
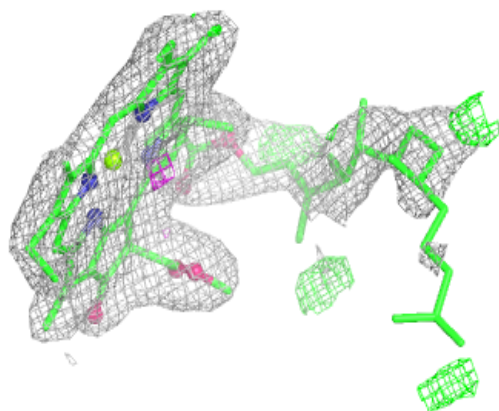
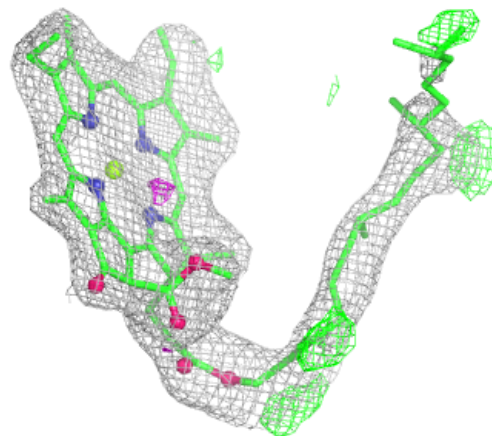
Electron density around CLA C 505:

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



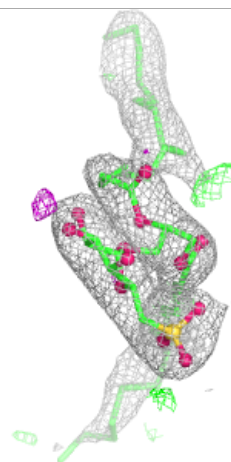
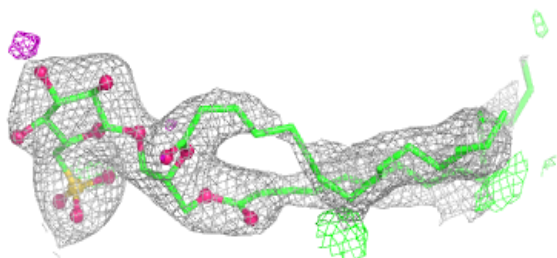
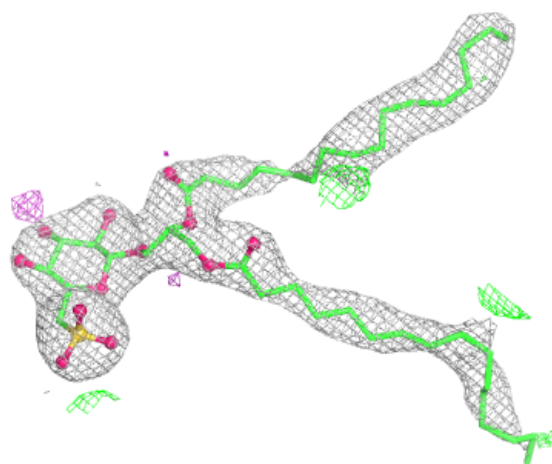
Electron density around CLA b 616:

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



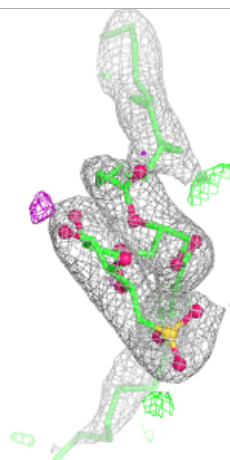
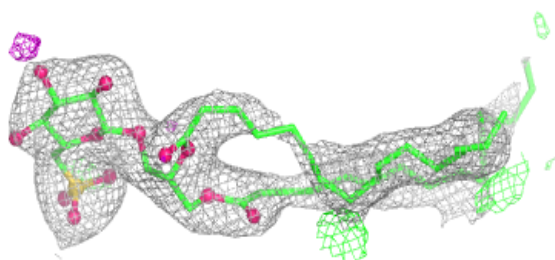
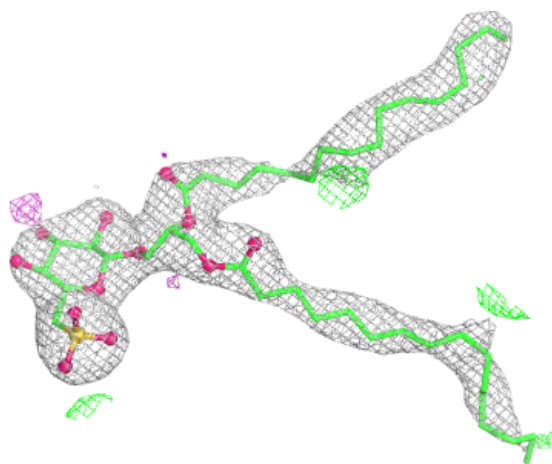
Electron density around SQD a 409 (A):

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



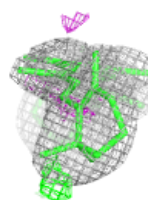
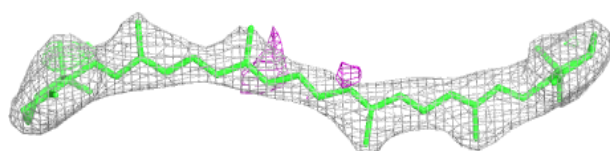
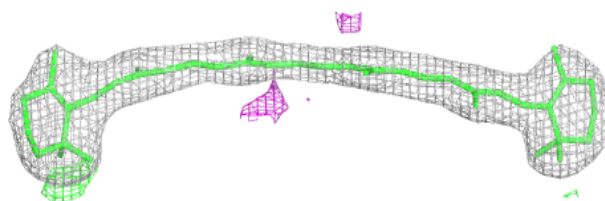
Electron density around SQD a 409 (B):

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

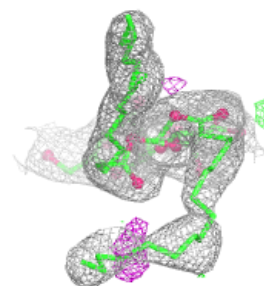
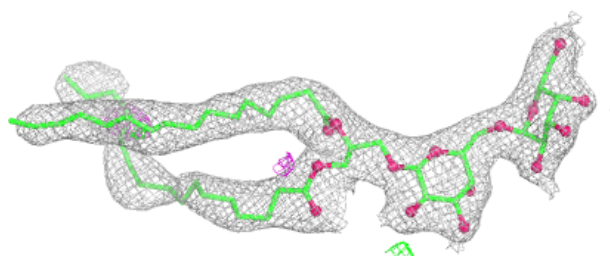
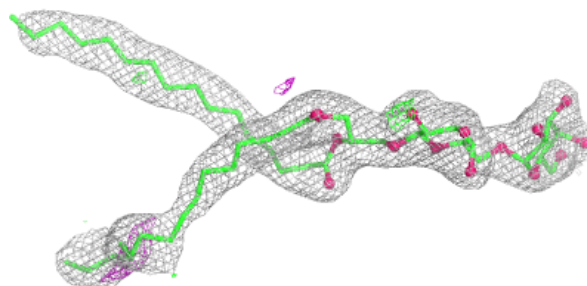


Electron density around BCR K 102:

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

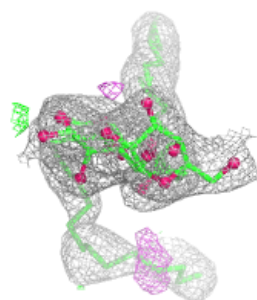
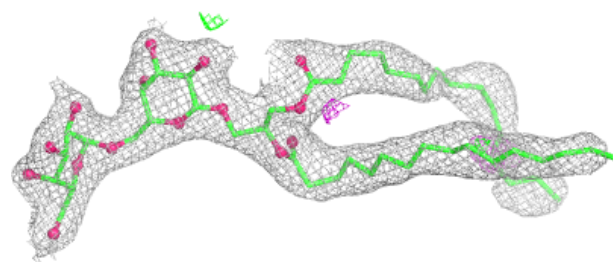
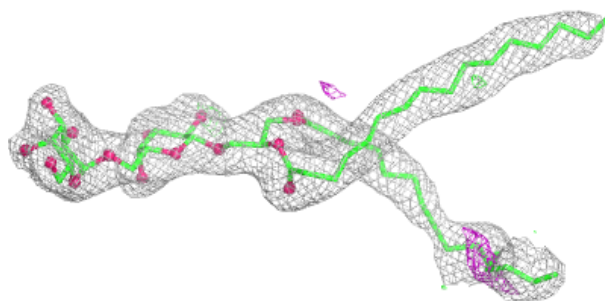
**Electron density around DGD c 517 (A):**

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

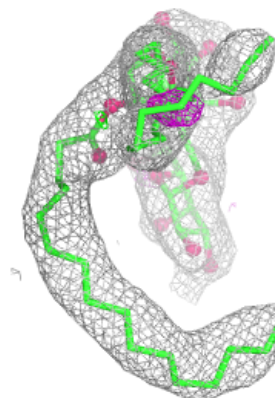
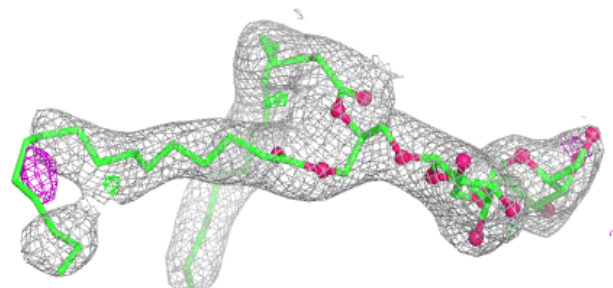
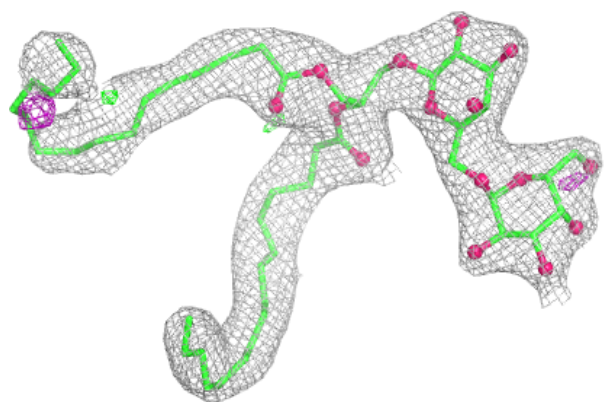


Electron density around DGD c 517 (B):

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

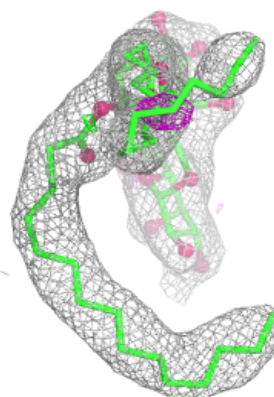
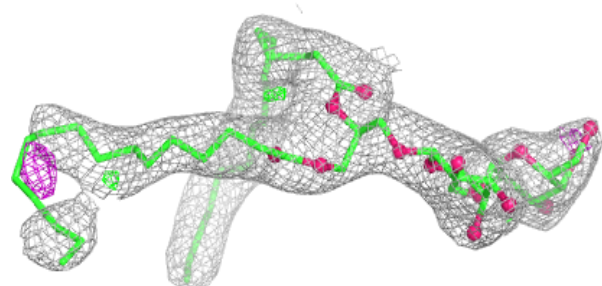
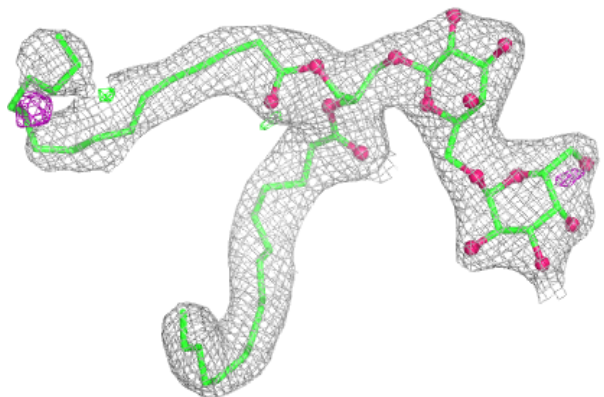
**Electron density around DGD c 518 (A):**

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

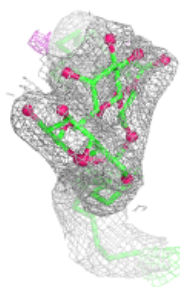
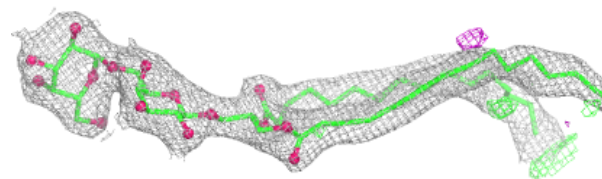
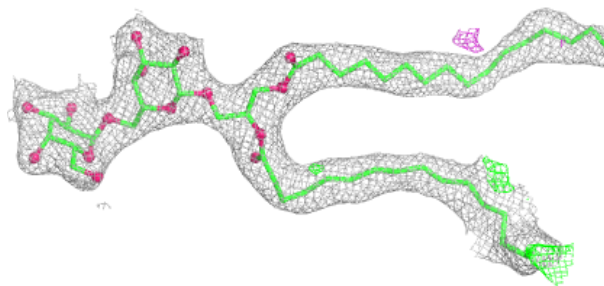


Electron density around DGD c 518 (B):

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

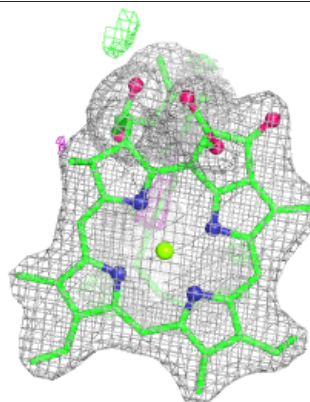
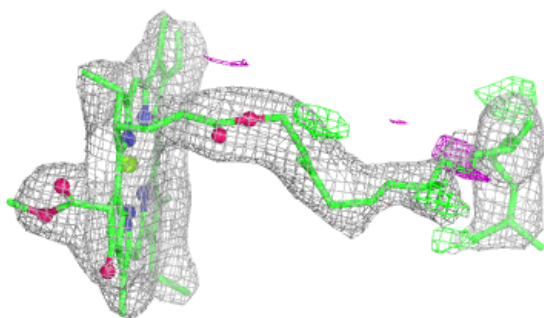
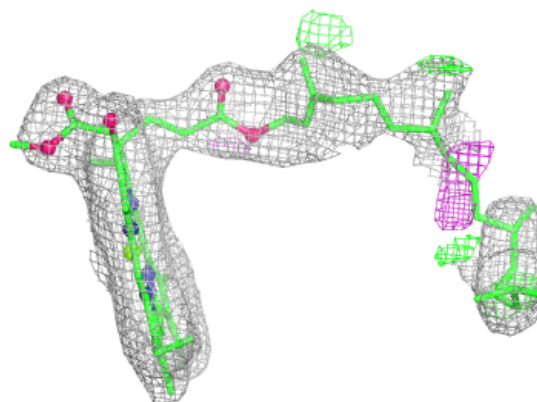
**Electron density around DGD c 519:**

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

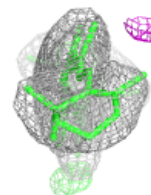
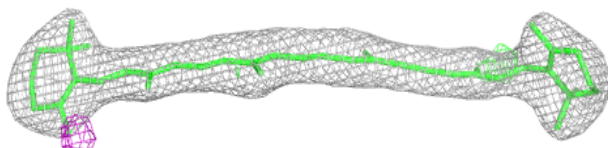
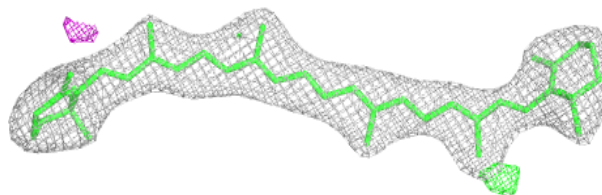


Electron density around CLA c 507:

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

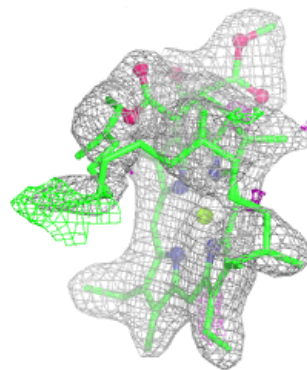
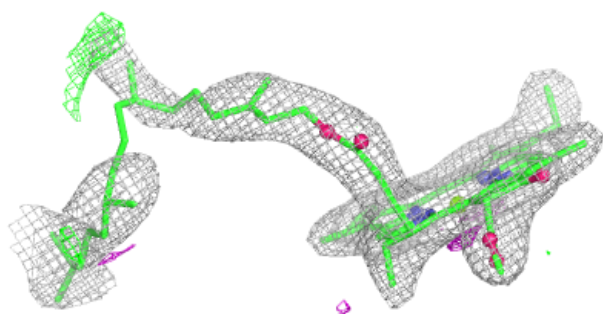
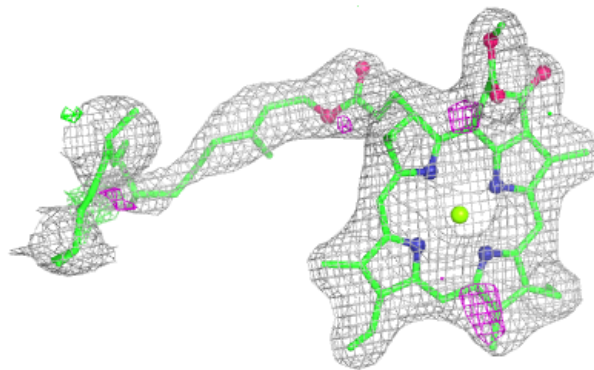
**Electron density around BCR Y 101:**

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

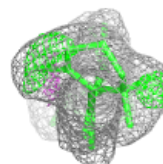
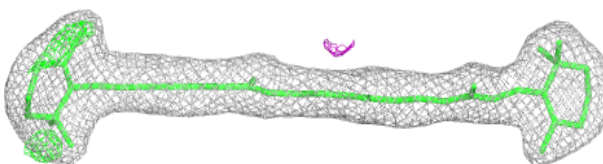
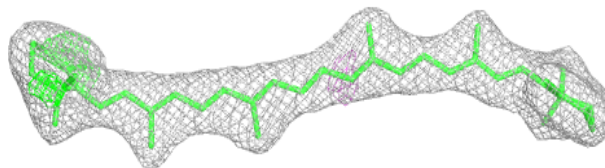


Electron density around CLA A 407:

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

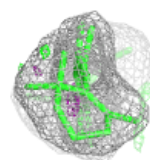
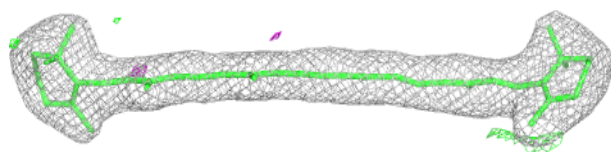
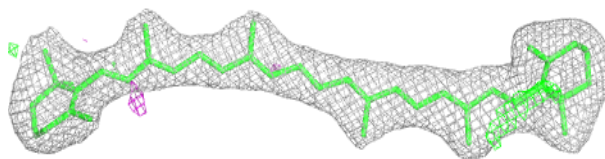
**Electron density around BCR A 408:**

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

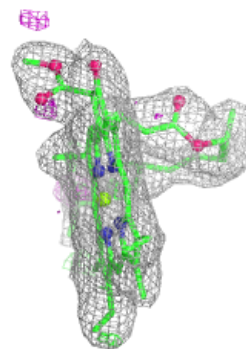
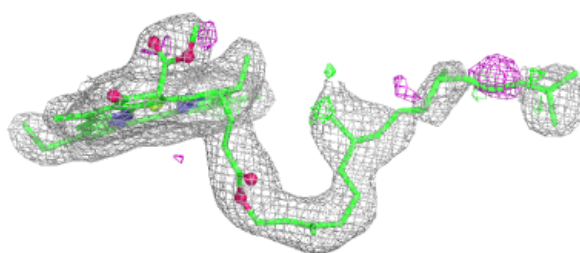
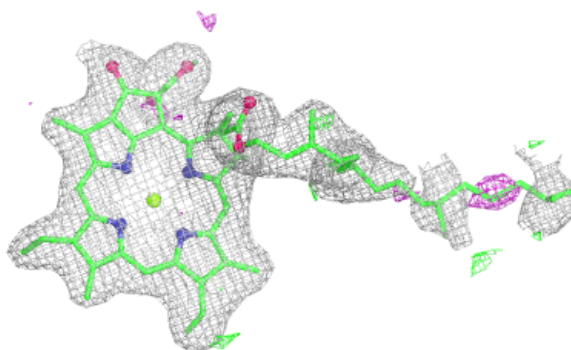


Electron density around BCR B 618:

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

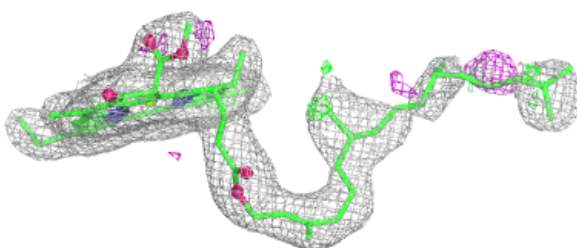
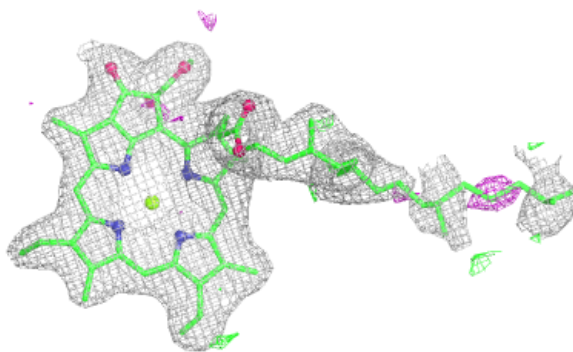
**Electron density around CLA a 405 (A):**

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



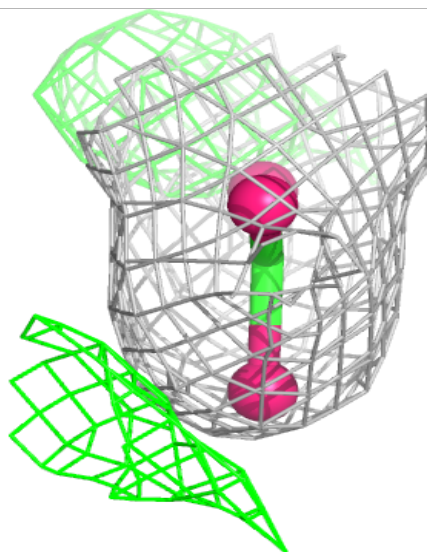
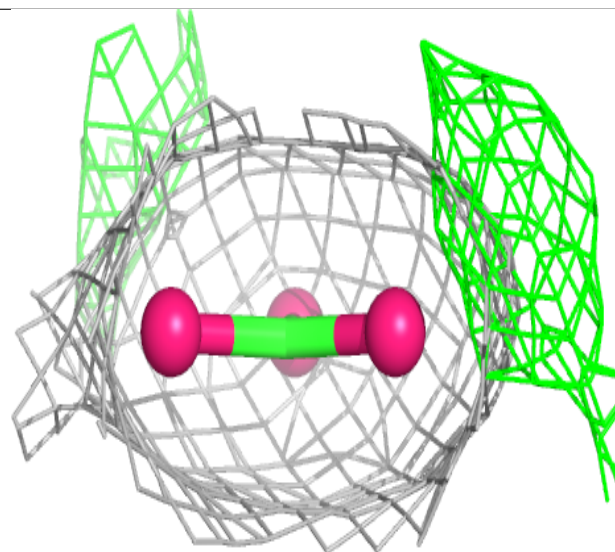
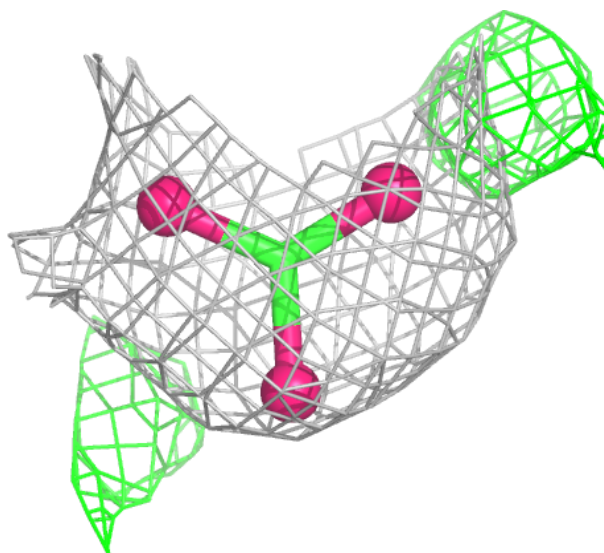
Electron density around CLA a 405 (B):

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



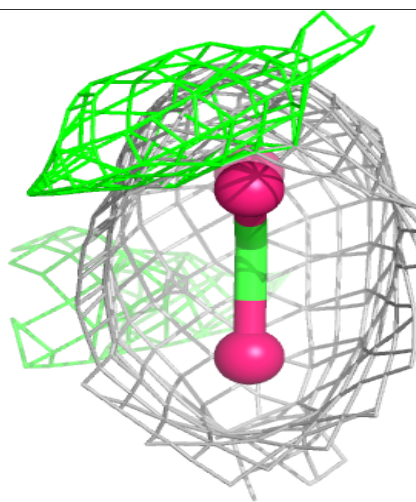
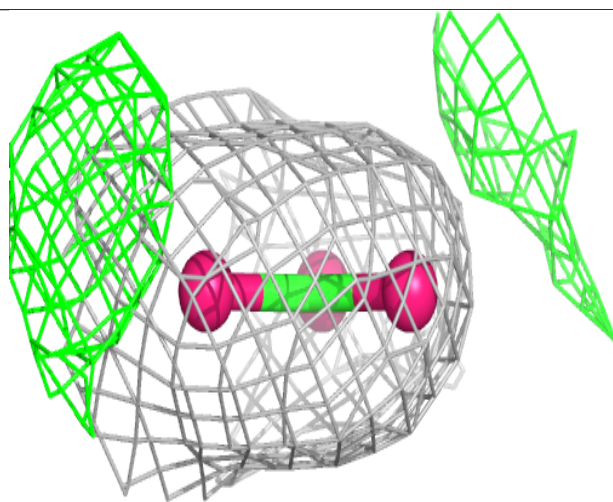
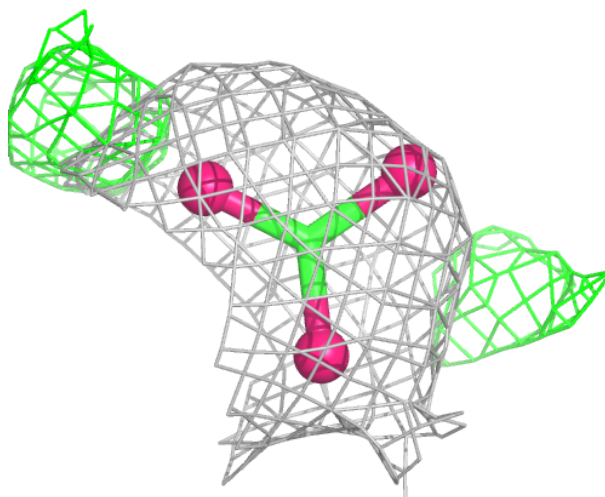
Electron density around BCT d 401 (A):

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



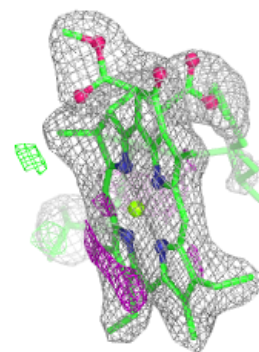
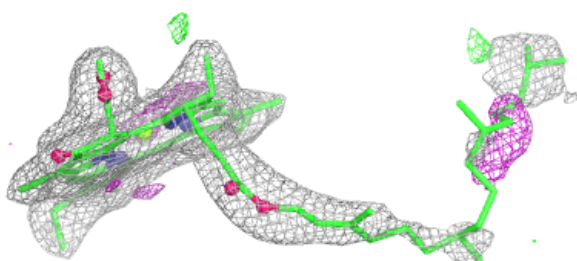
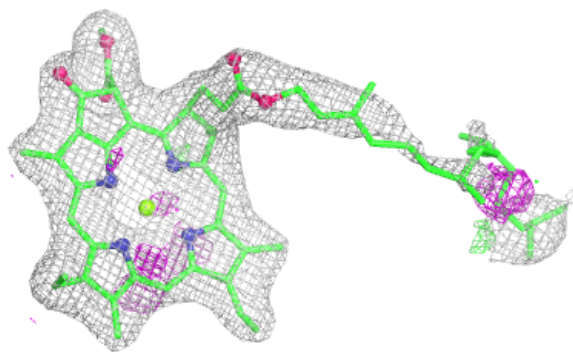
Electron density around BCT d 401 (B):

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

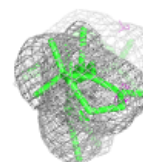
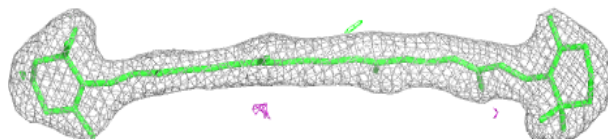
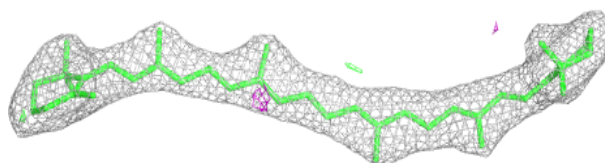


Electron density around CLA a 407:

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

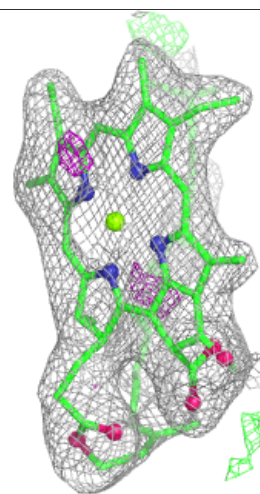
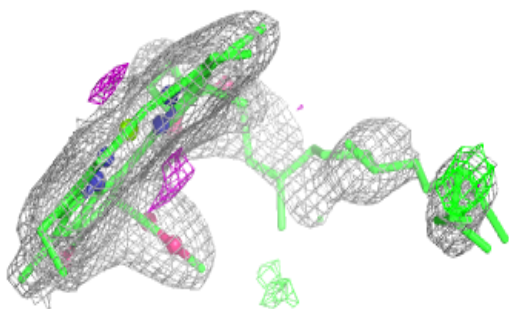
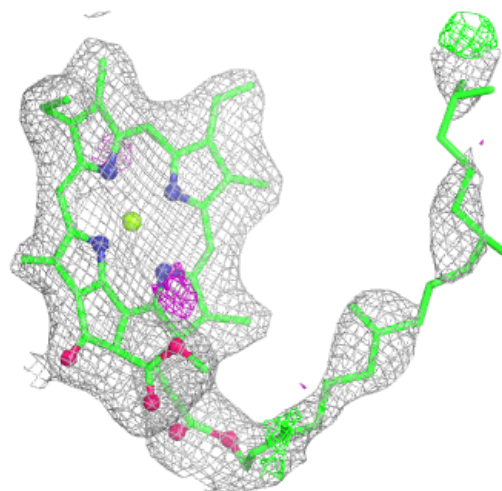
**Electron density around BCR H 101:**

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



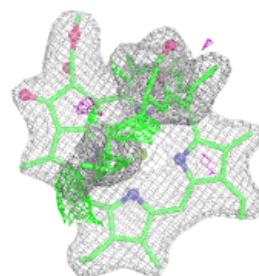
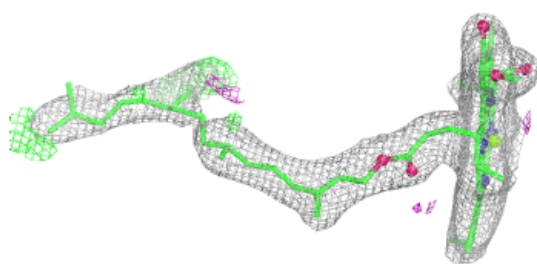
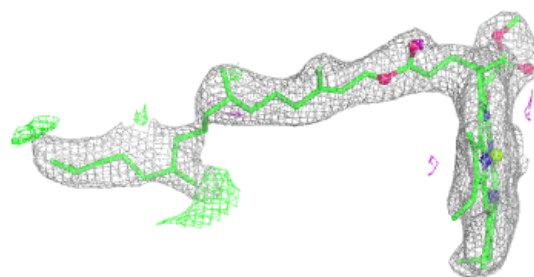
Electron density around CLA B 616:

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

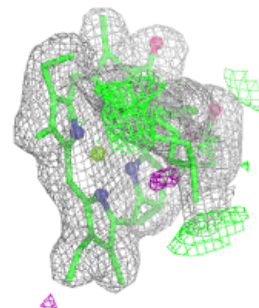
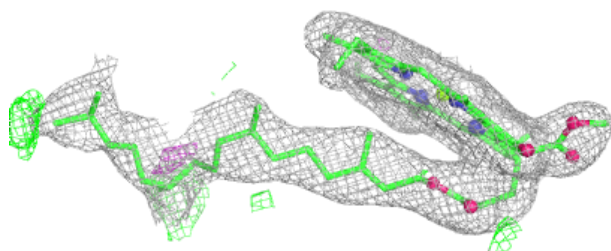
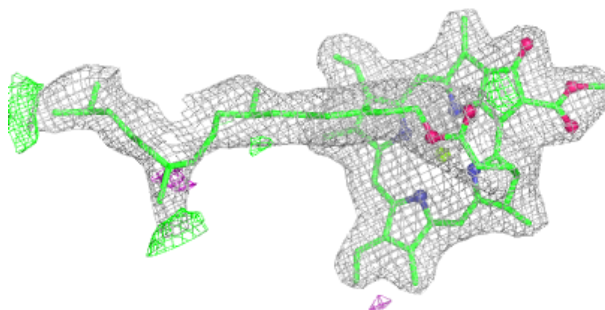


Electron density around CLA b 606:

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

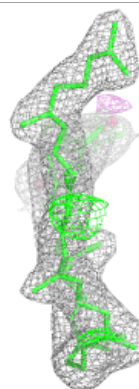
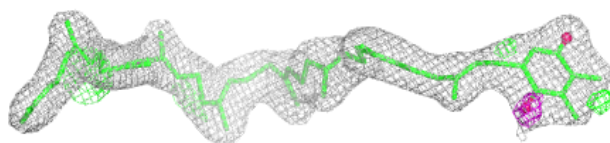
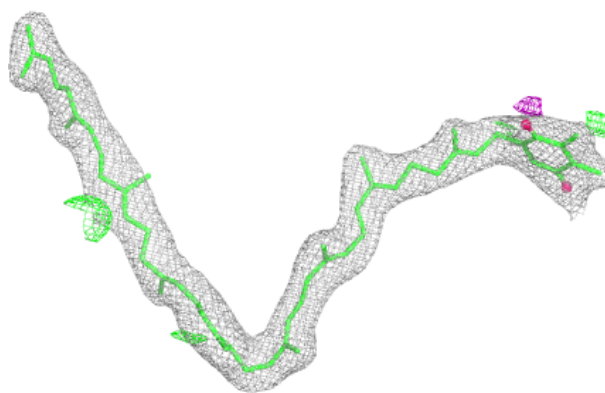
**Electron density around CLA b 614:**

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

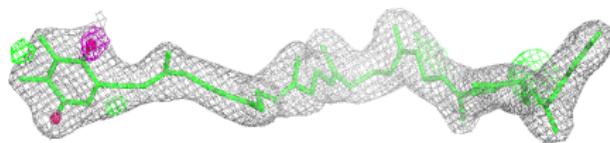
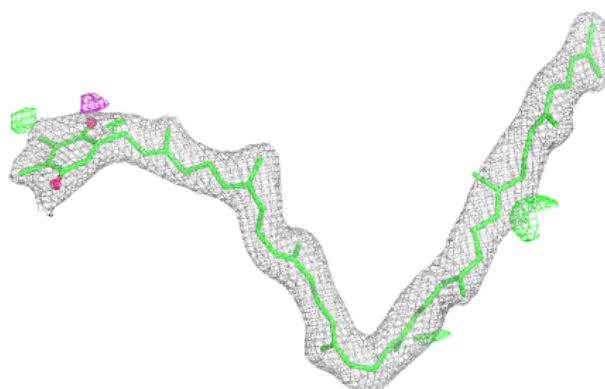


Electron density around PL9 D 406 (A):

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

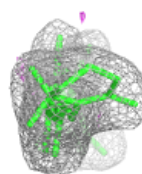
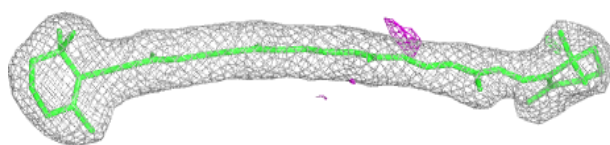
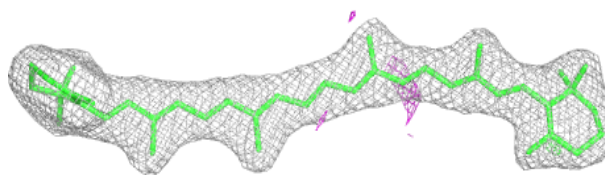
**Electron density around PL9 D 406 (B):**

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

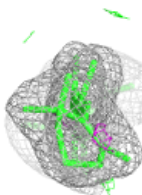
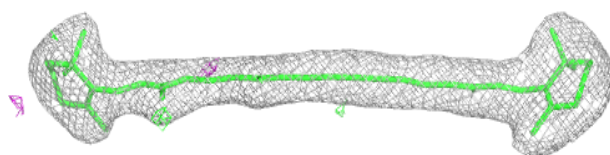
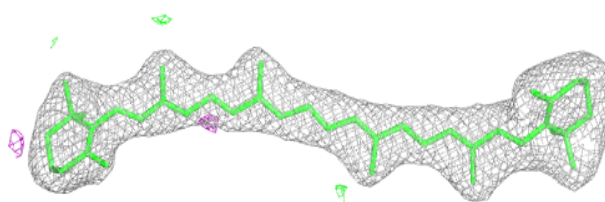


Electron density around BCR b 617:

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

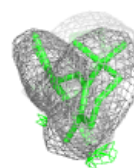
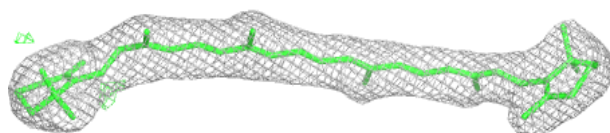
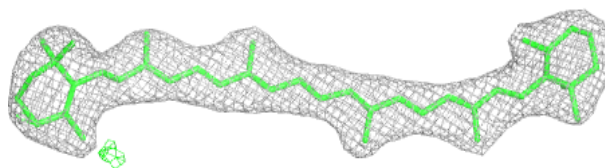
**Electron density around BCR b 618:**

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

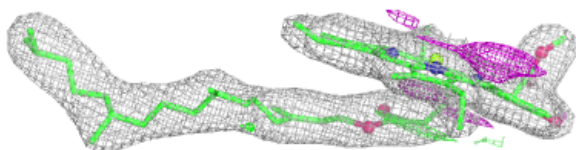
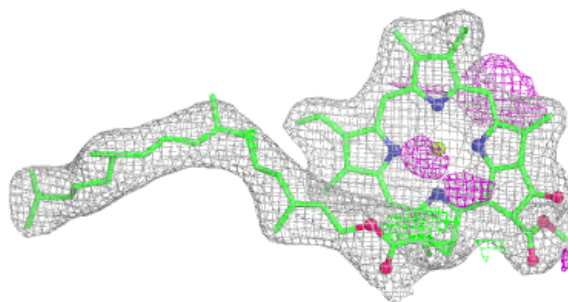


Electron density around BCR b 619:

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

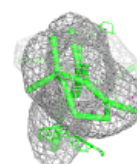
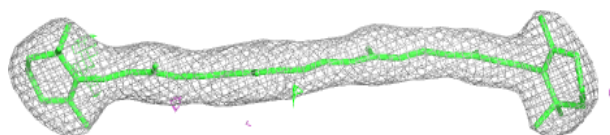
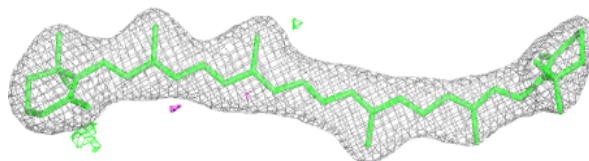
**Electron density around CLA B 603:**

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

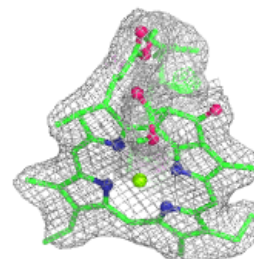
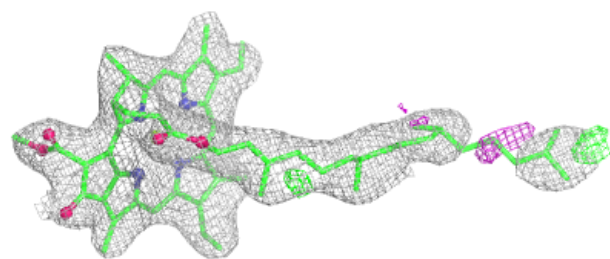
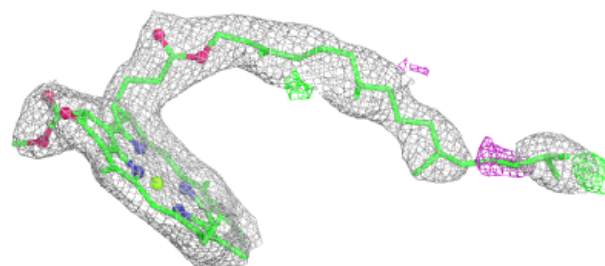


Electron density around BCR c 516:

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

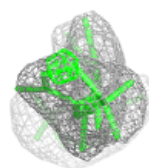
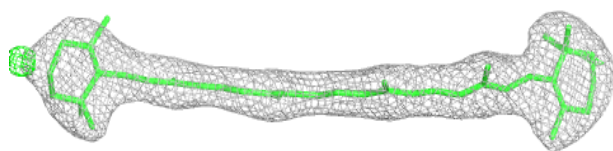
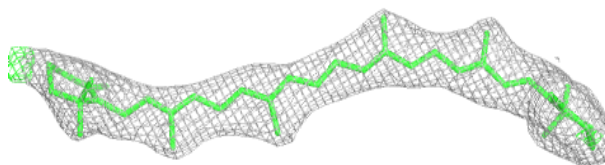
**Electron density around CLA c 505:**

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

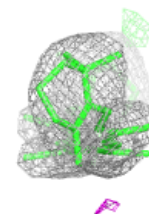
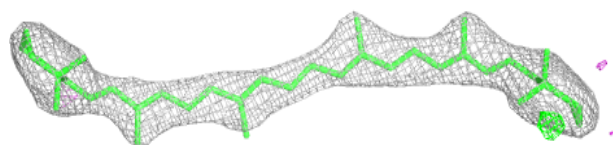
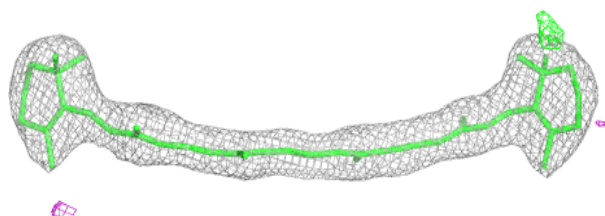


Electron density around BCR h 101:

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

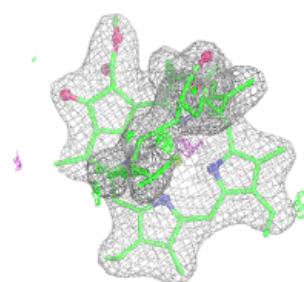
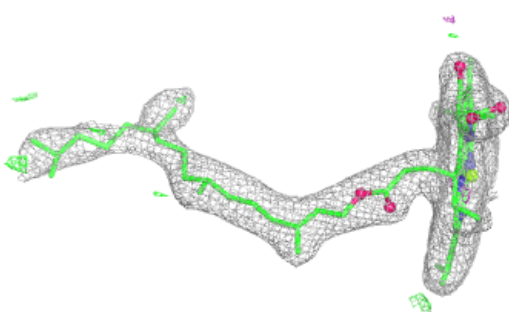
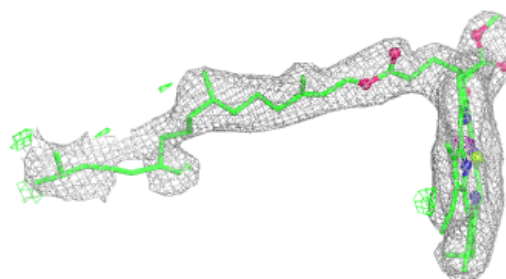
**Electron density around BCR k 101:**

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

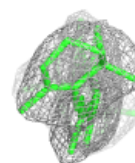
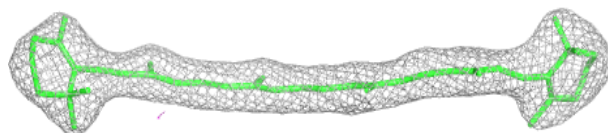
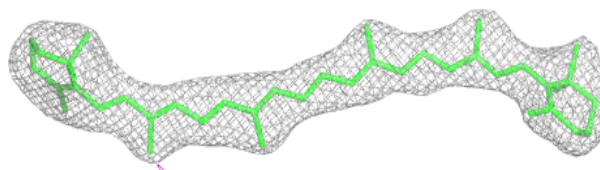


Electron density around CLA B 606:

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

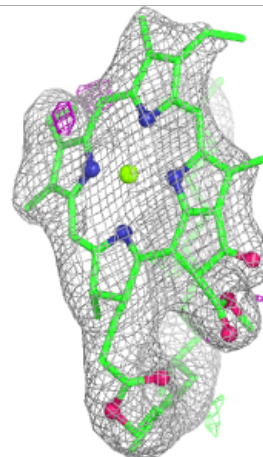
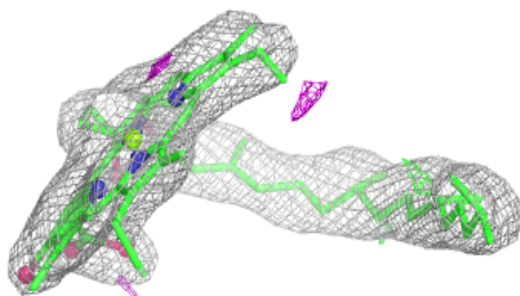
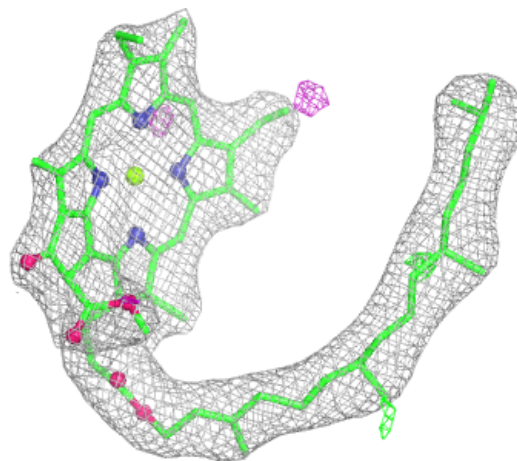
**Electron density around BCR y 101:**

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



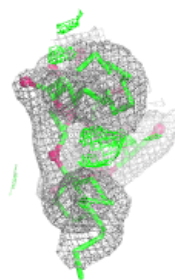
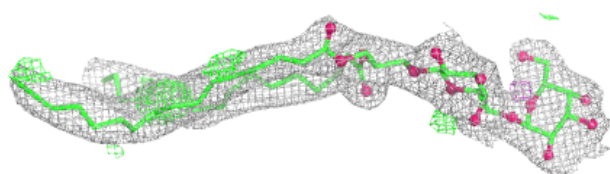
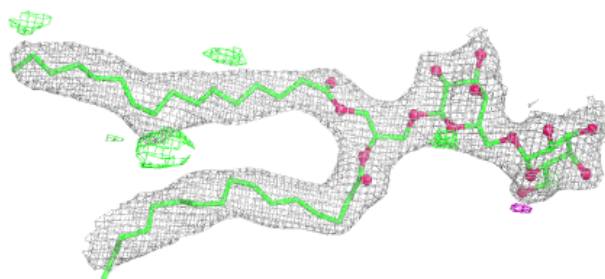
Electron density around CLA c 508:

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

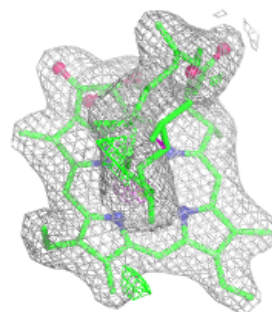
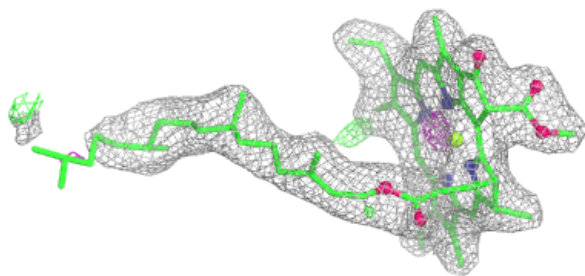
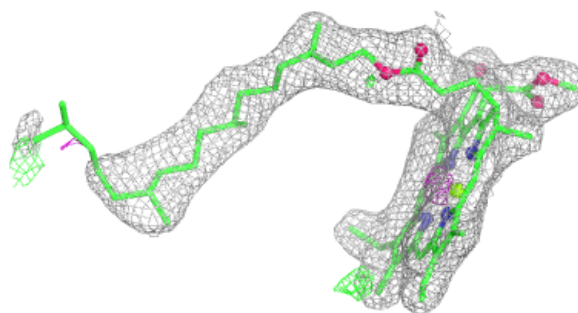


Electron density around DGD C 519:

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

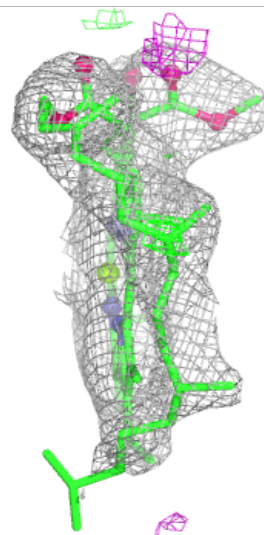
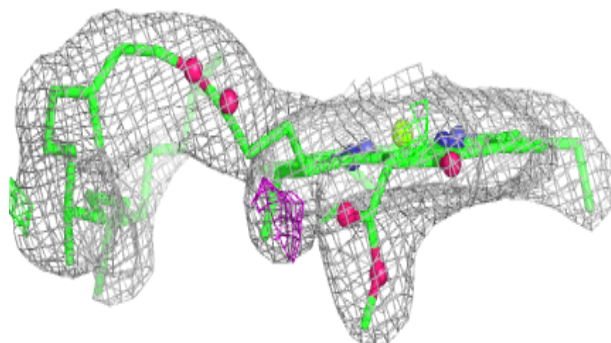
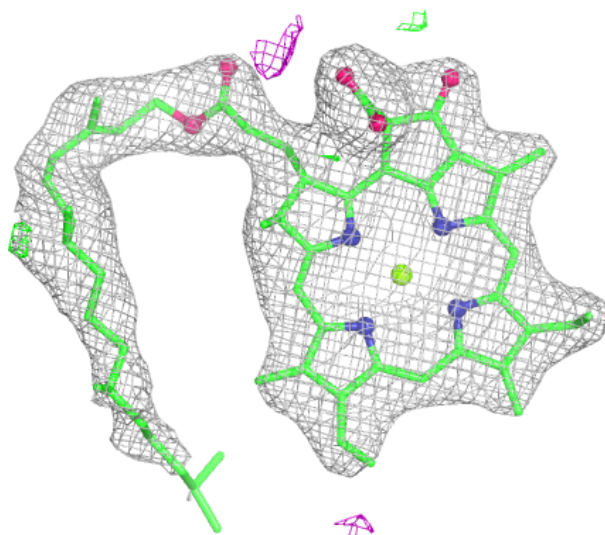
**Electron density around CLA C 509:**

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



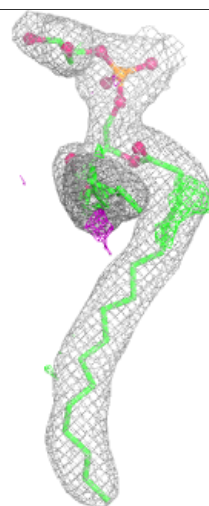
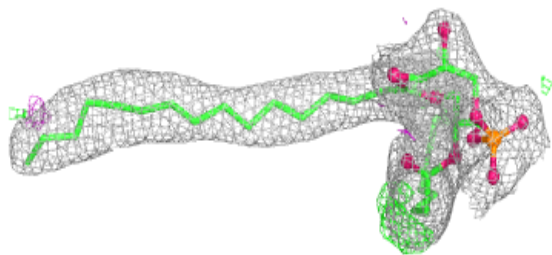
Electron density around CLA C 513:

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



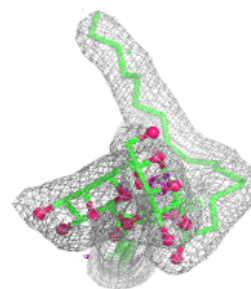
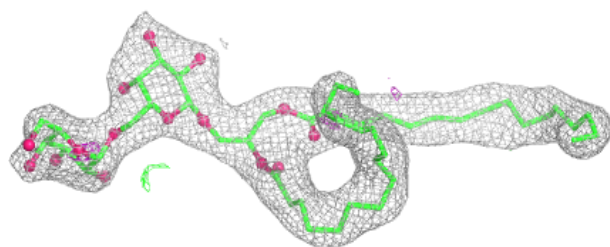
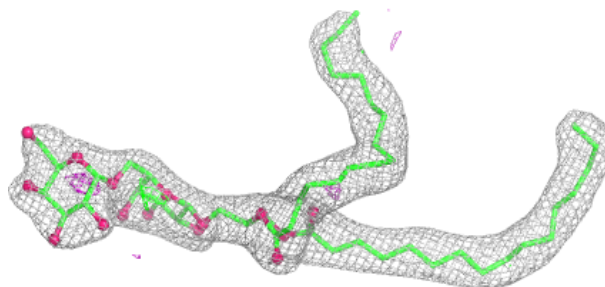
Electron density around LHG b 629 (A):

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



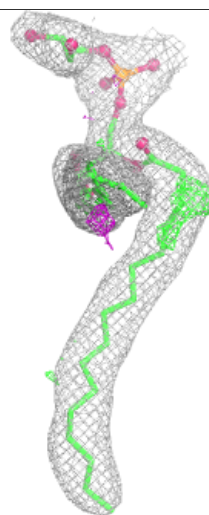
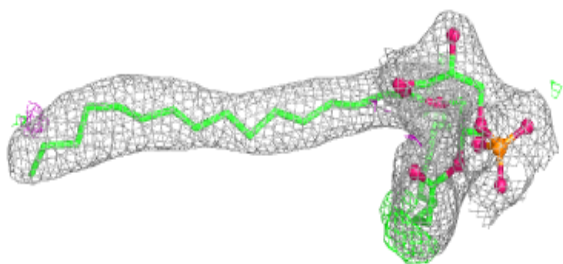
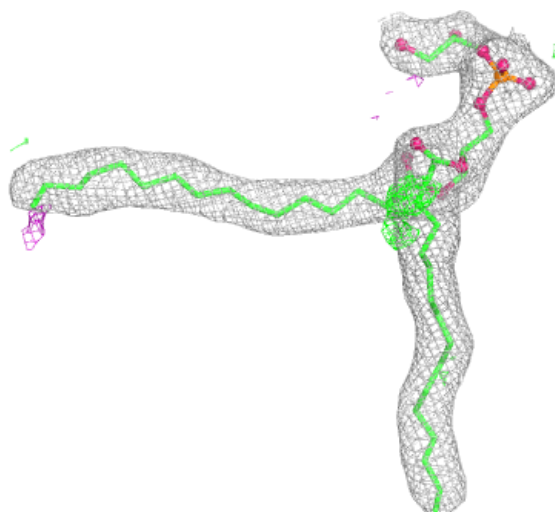
Electron density around DGD h 102:

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



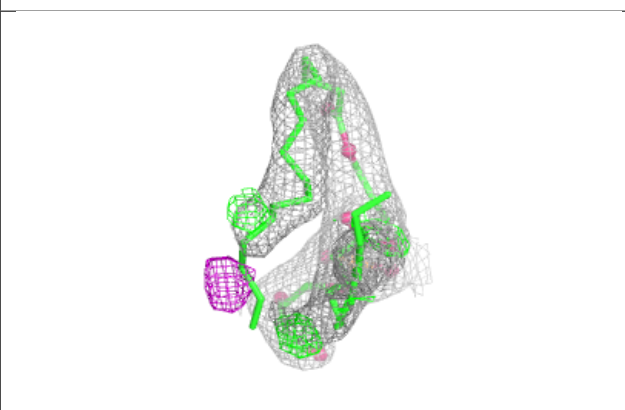
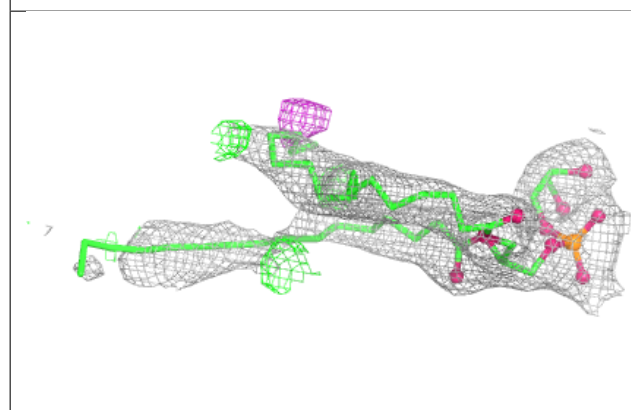
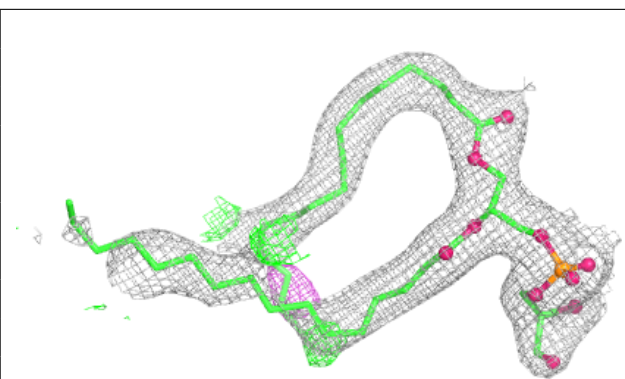
Electron density around LHG b 629 (B):

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

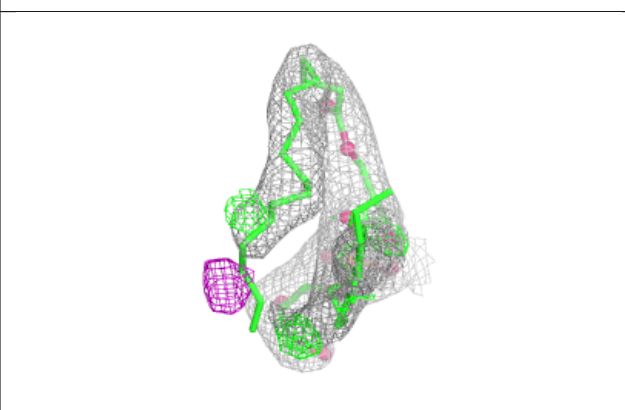
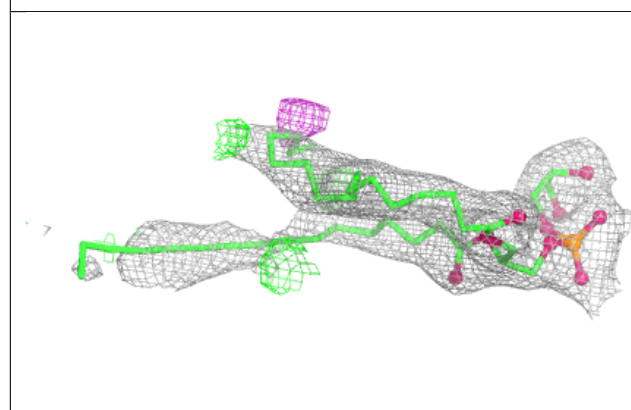
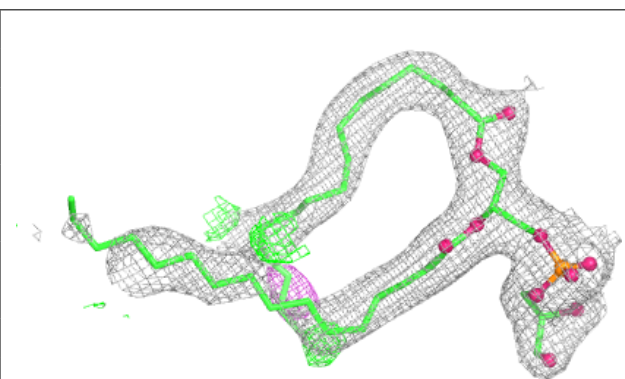


Electron density around LHG d 408 (A):

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

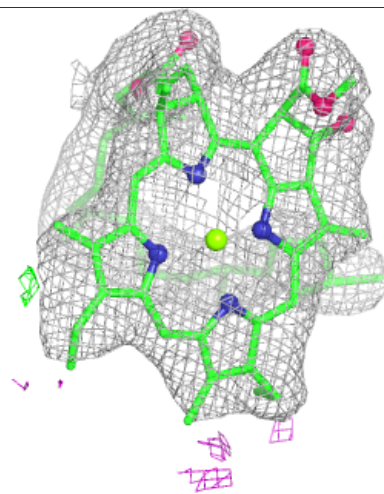
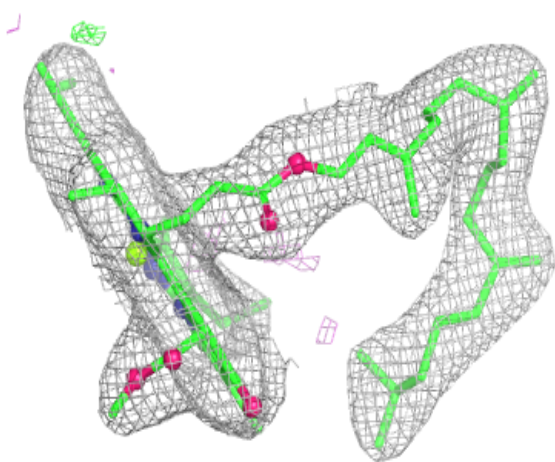
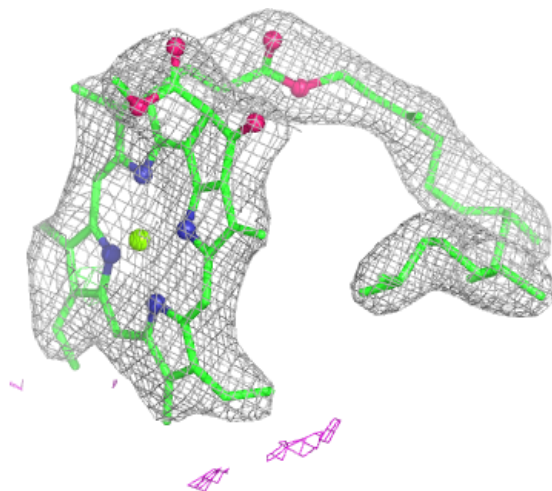
**Electron density around LHG d 408 (B):**

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



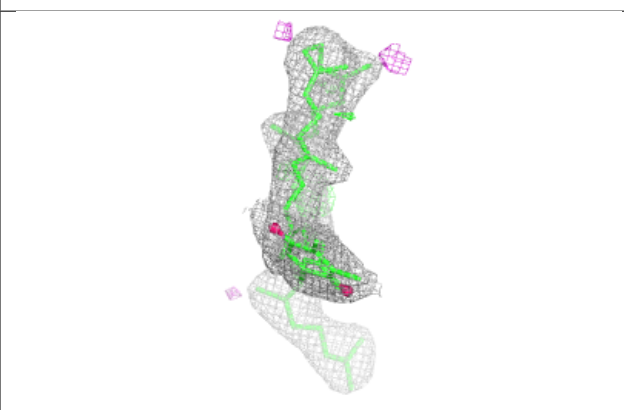
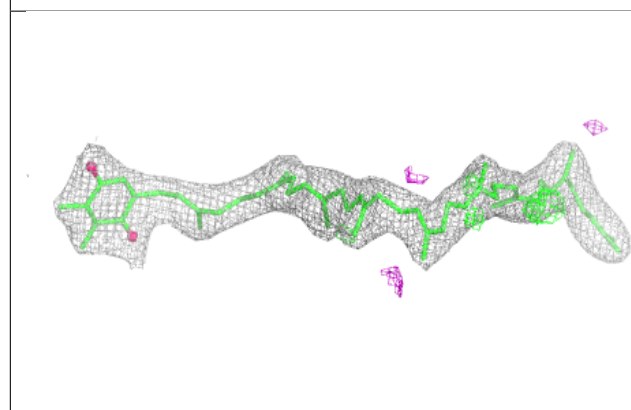
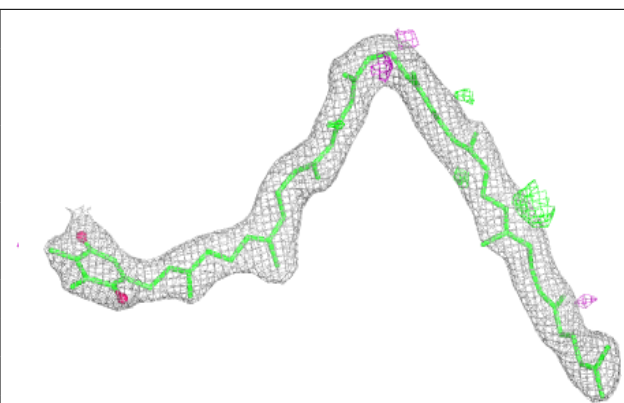
Electron density around CLA c 504:

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

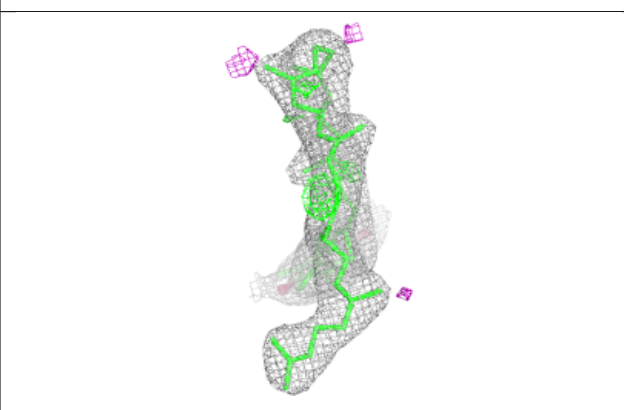
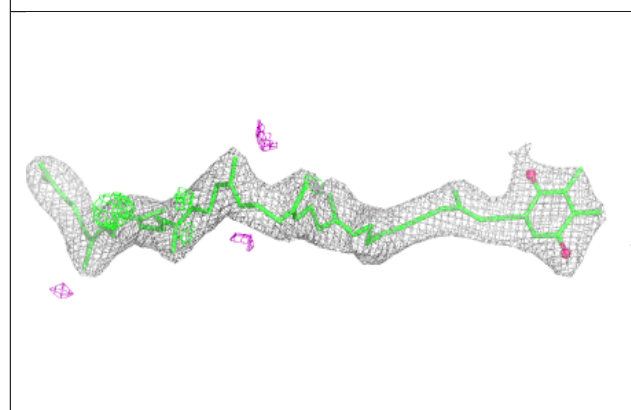
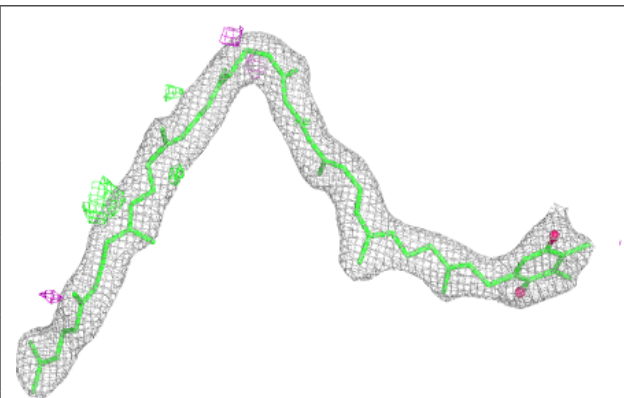


Electron density around PL9 d 406 (A):

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

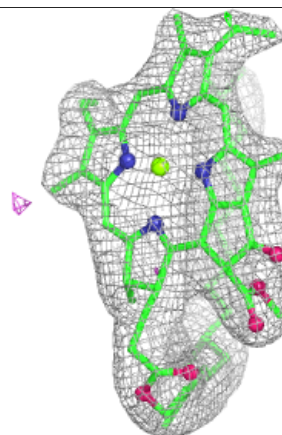
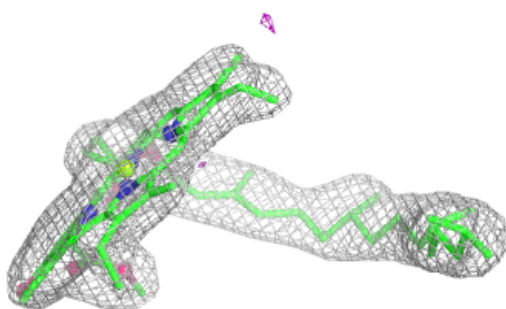
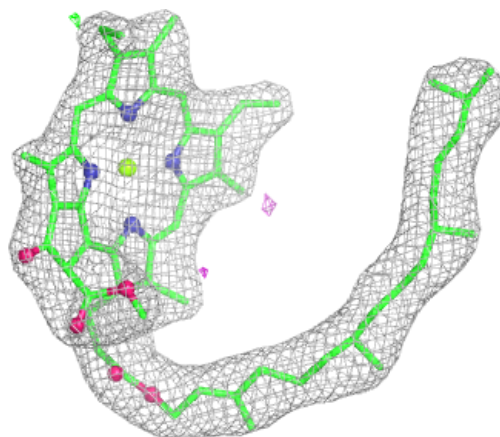
**Electron density around PL9 d 406 (B):**

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



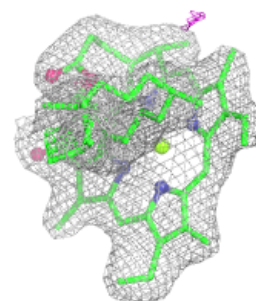
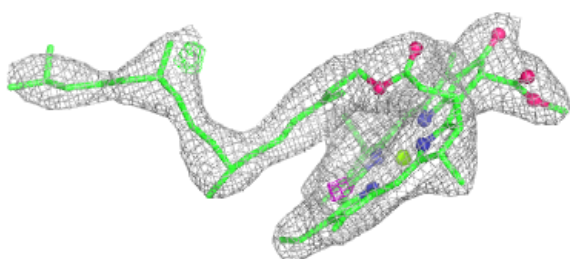
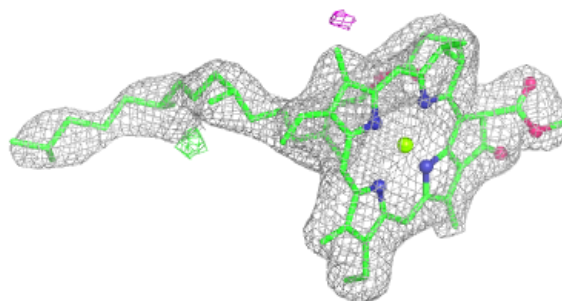
Electron density around CLA C 508:

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

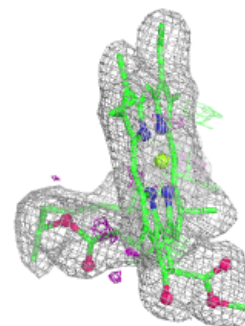
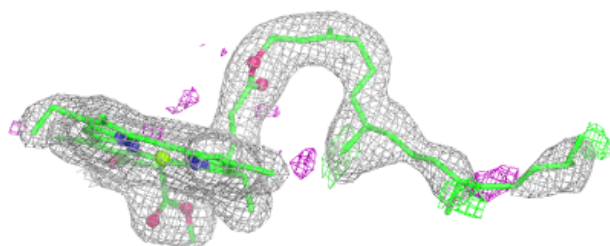
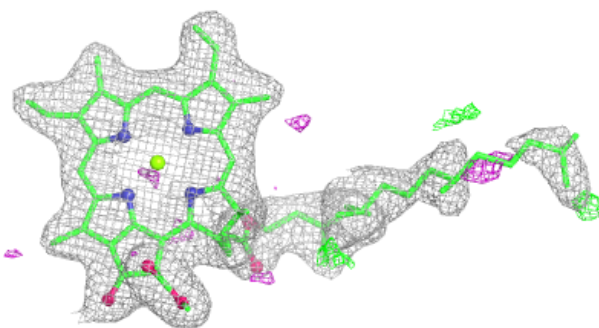


Electron density around CLA c 506:

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

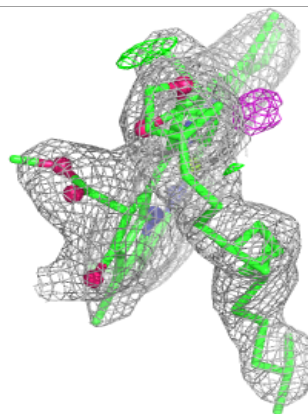
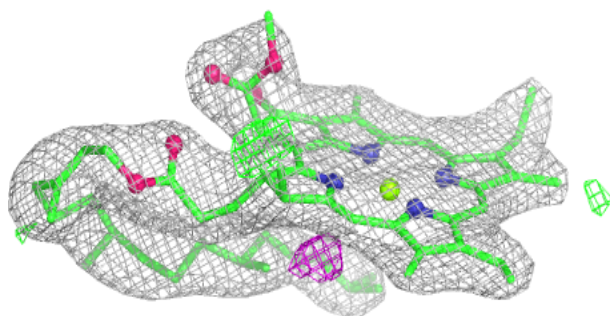
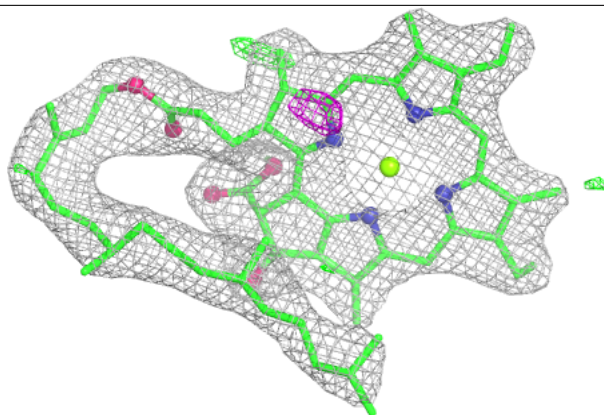
**Electron density around CLA A 406 (B):**

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

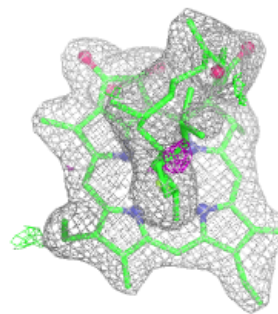
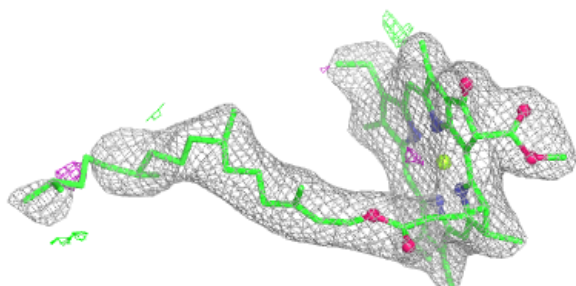
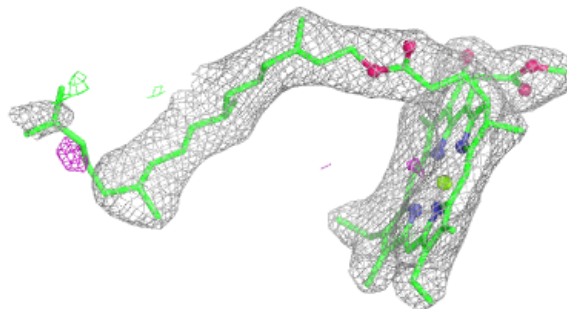


Electron density around CLA C 510:

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

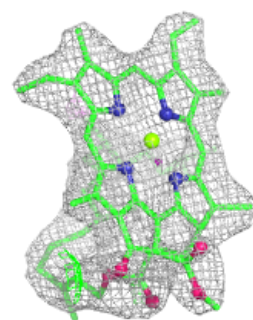
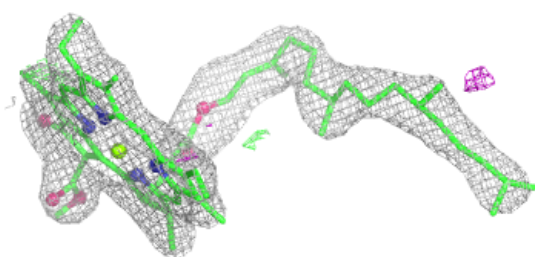
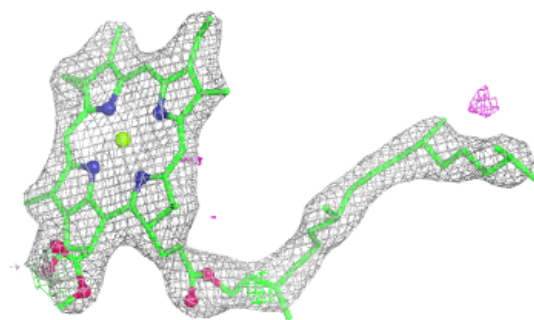
**Electron density around CLA c 509:**

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

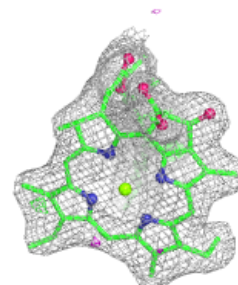
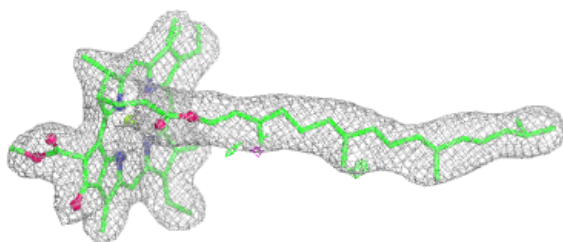
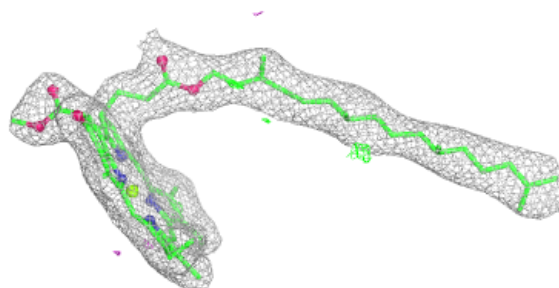


Electron density around CLA c 512:

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

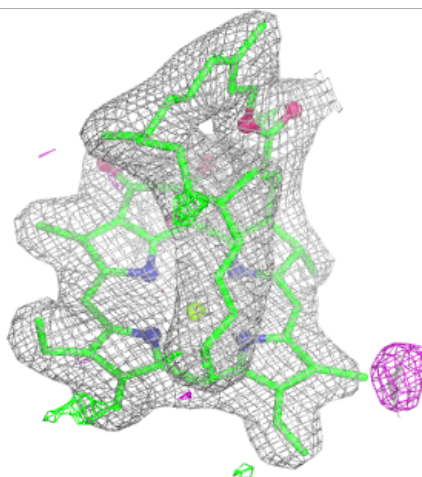
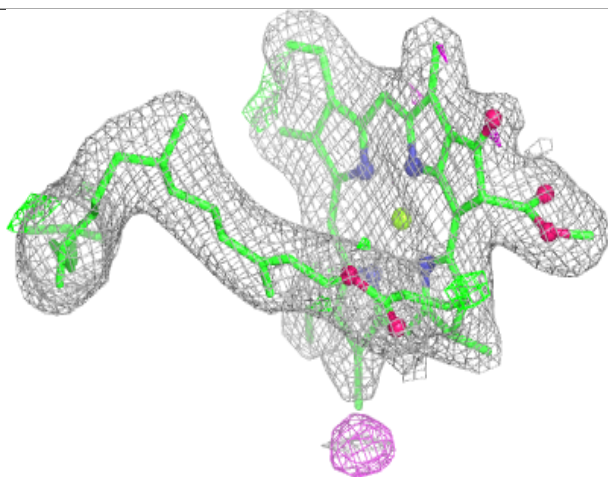
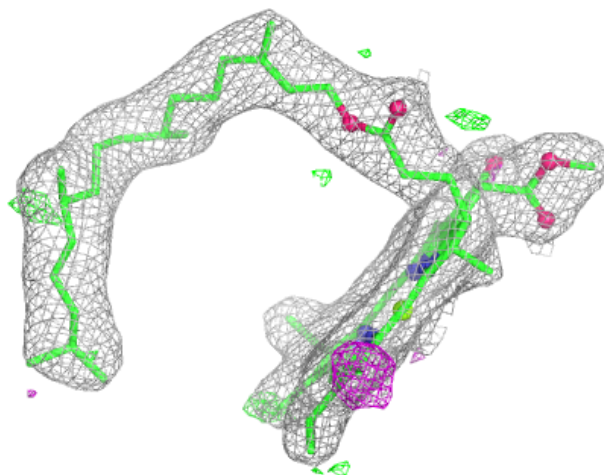
**Electron density around CLA B 607:**

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



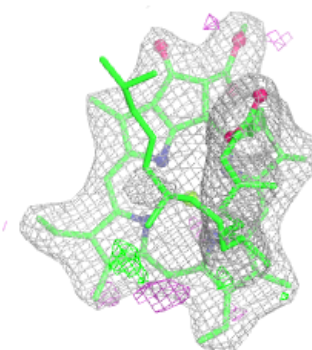
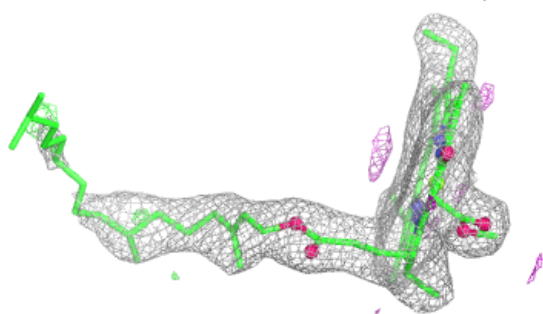
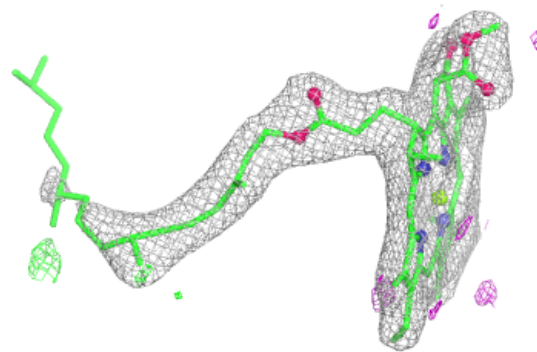
Electron density around CLA B 611:

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



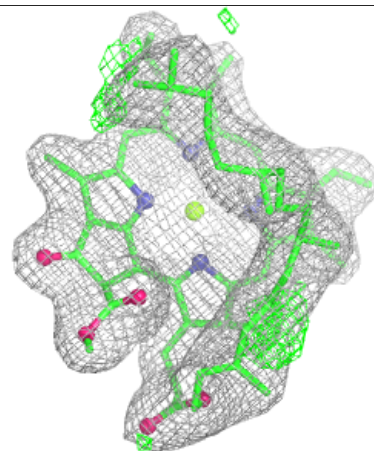
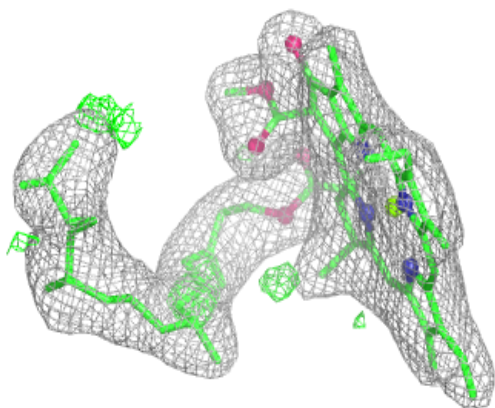
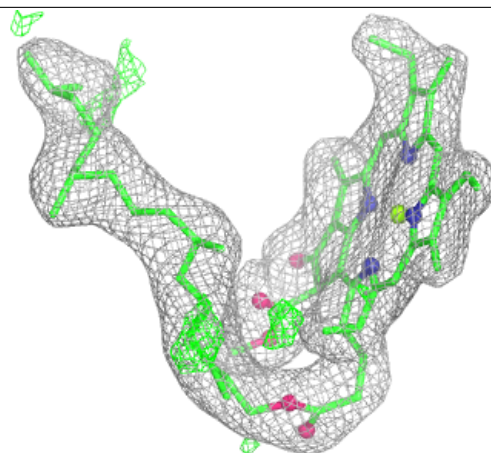
Electron density around CLA D 404:

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



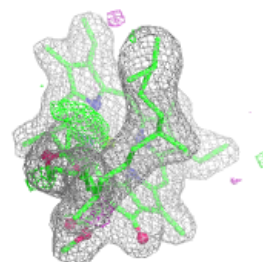
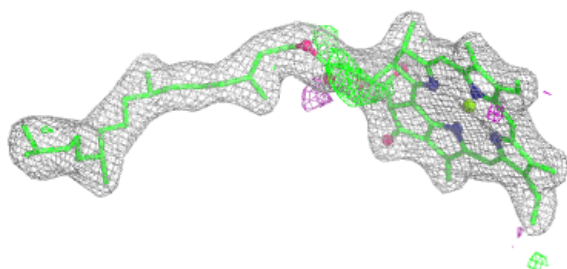
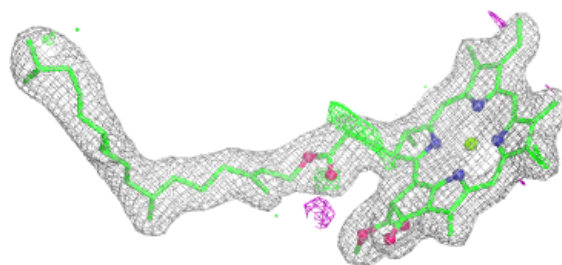
Electron density around CLA B 613:

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

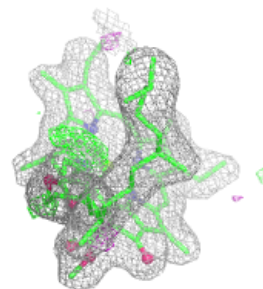
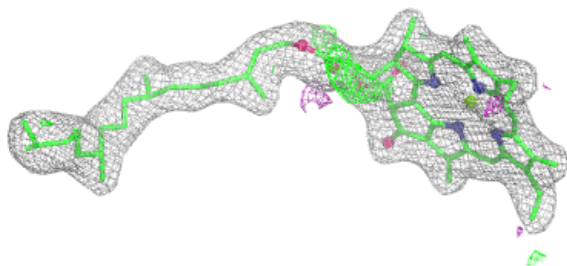
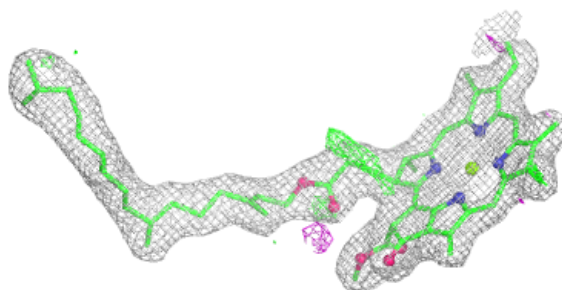


Electron density around CLA A 404 (A):

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

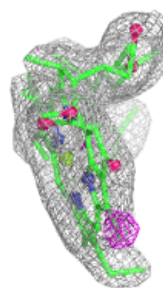
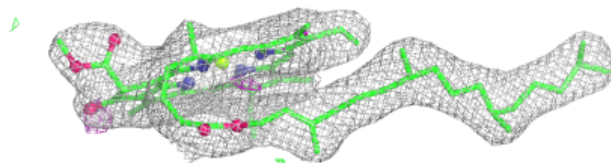
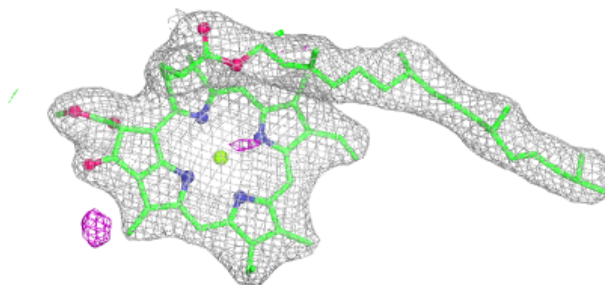
**Electron density around CLA A 404 (B):**

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

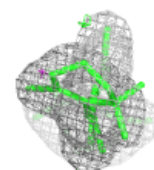
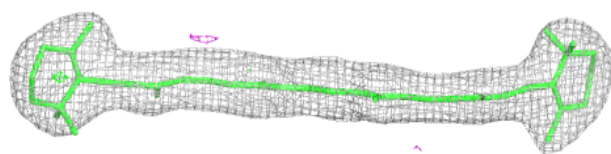
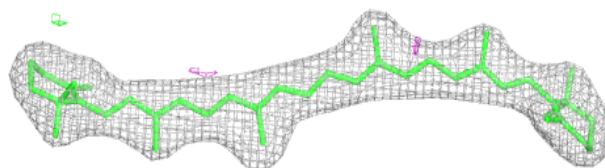


Electron density around CLA C 502:

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

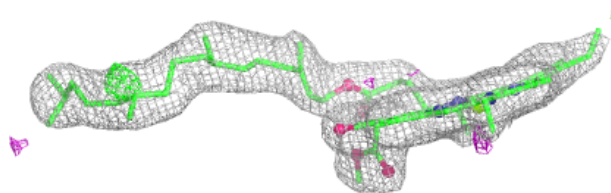
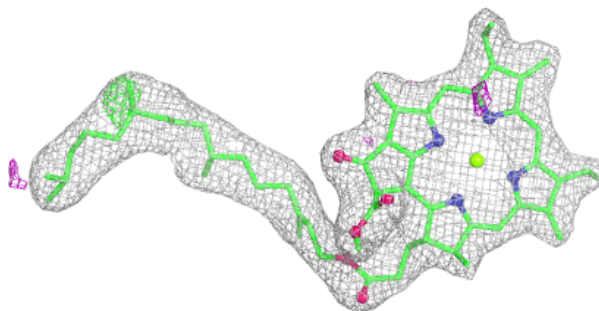
**Electron density around BCR C 516:**

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

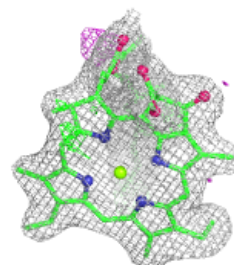
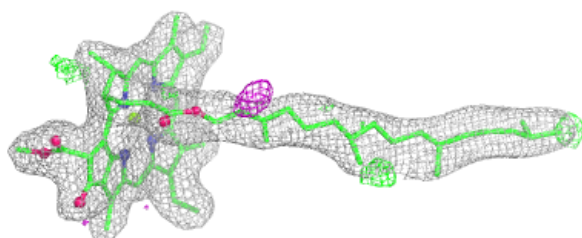
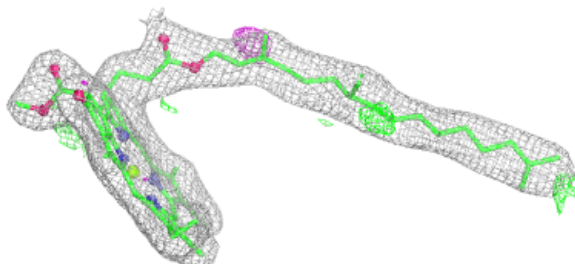


Electron density around CLA B 602:

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

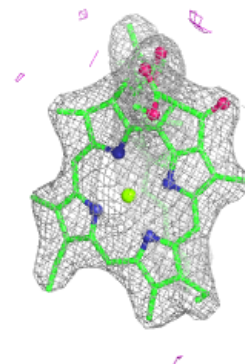
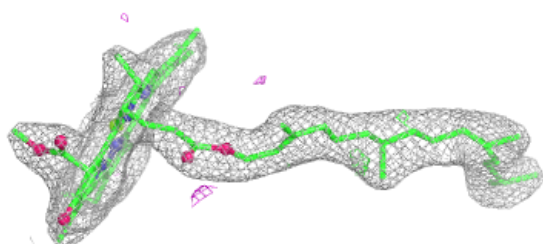
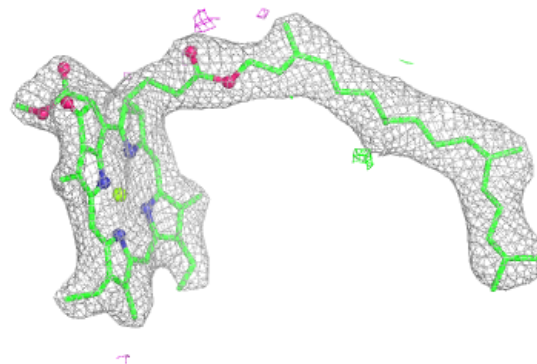
**Electron density around CLA b 607:**

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

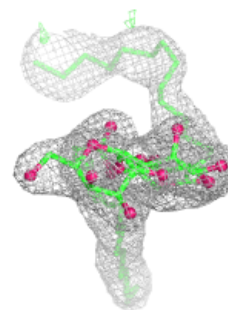
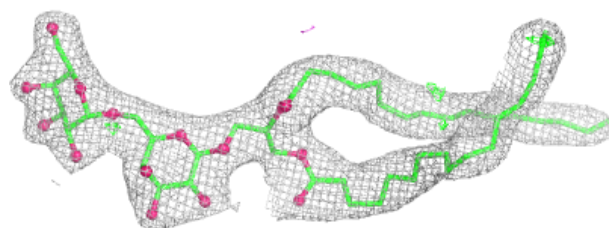
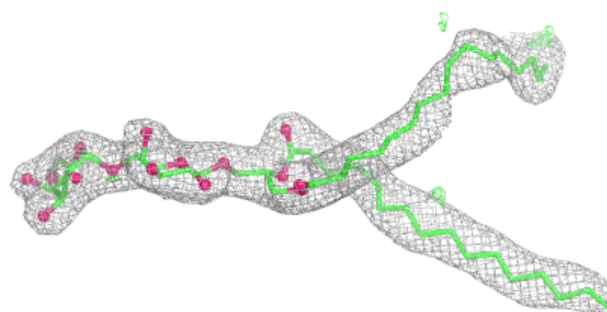


Electron density around CLA b 609:

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

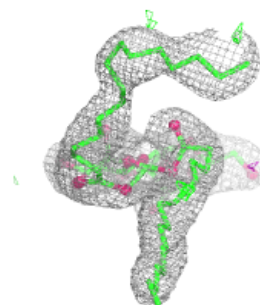
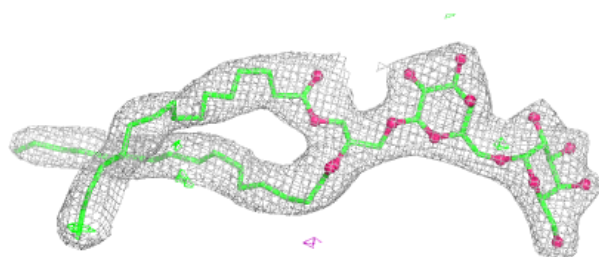
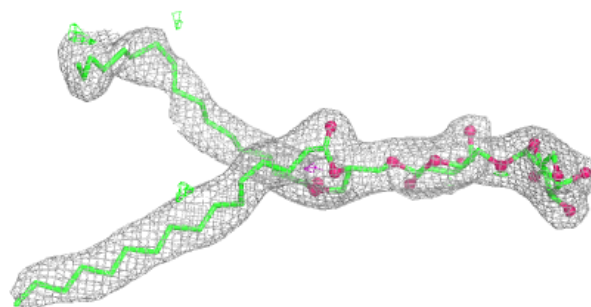
**Electron density around DGD C 517 (A):**

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

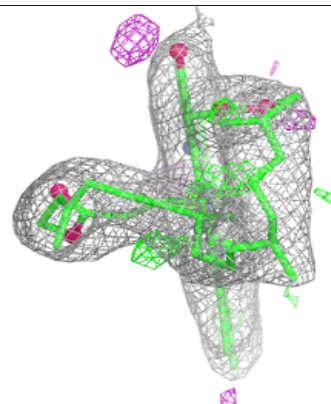
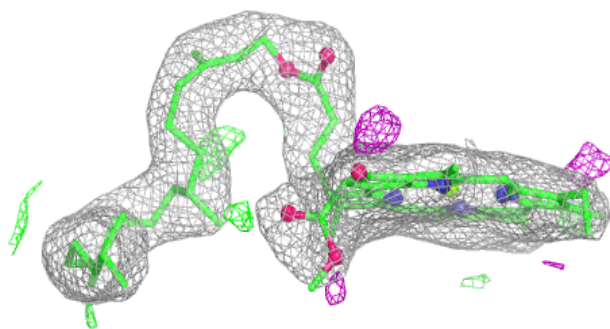
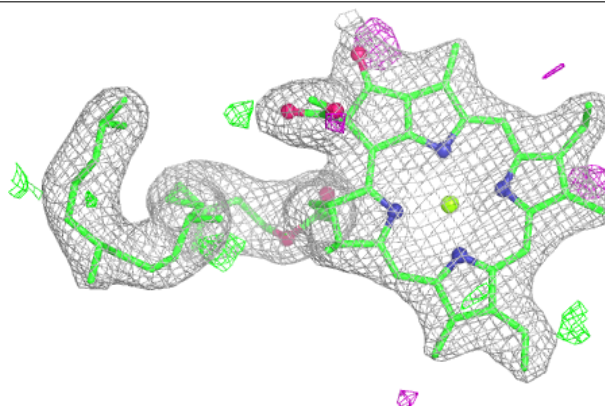


Electron density around DGD C 517 (B):

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

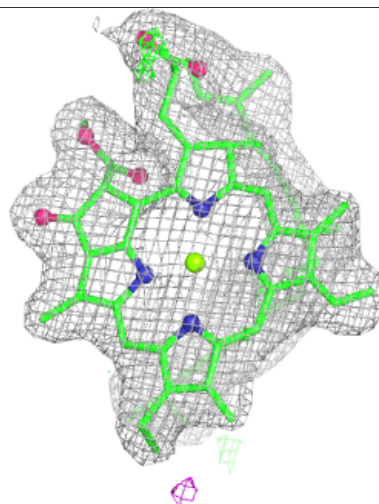
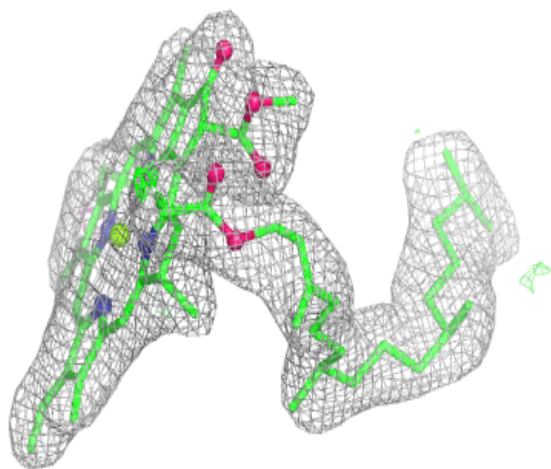
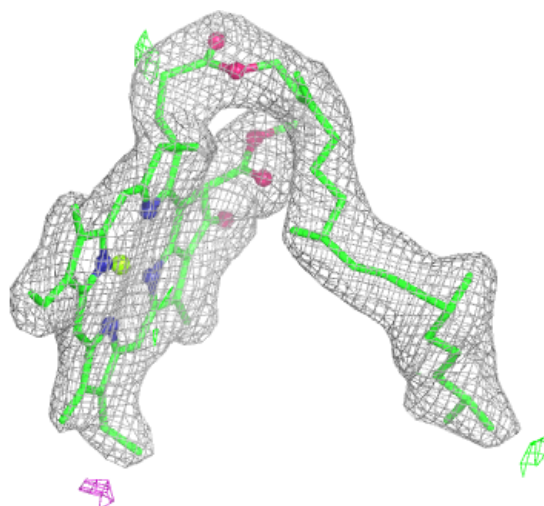
**Electron density around CLA b 612:**

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



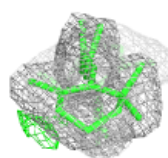
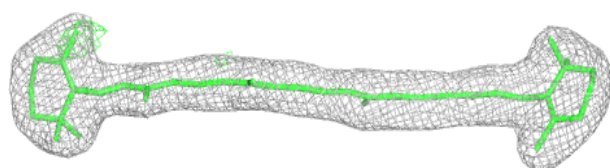
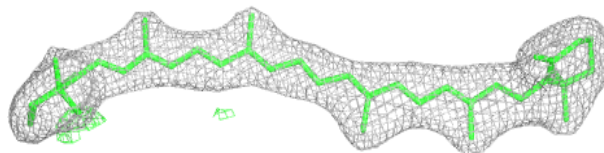
Electron density around CLA b 613:

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

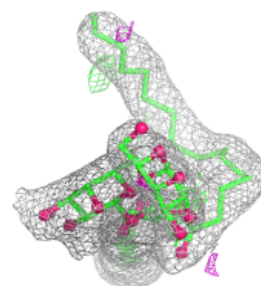
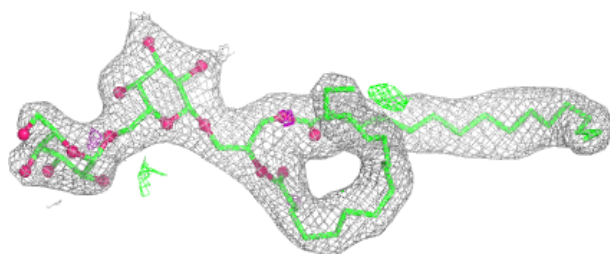
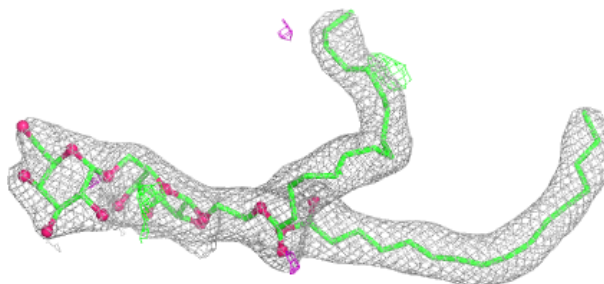


Electron density around BCR a 408:

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

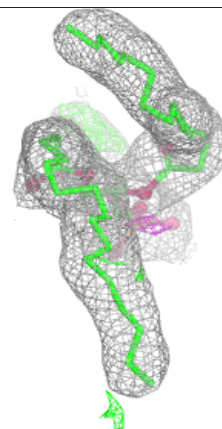
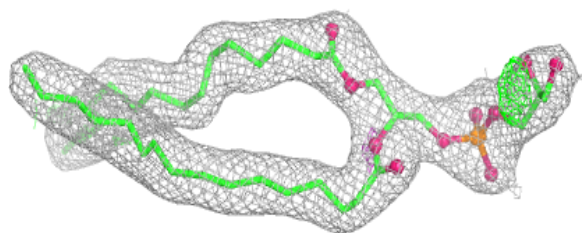
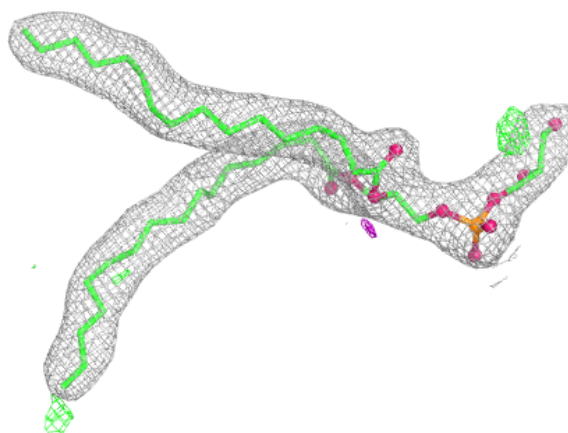
**Electron density around DGD H 102:**

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



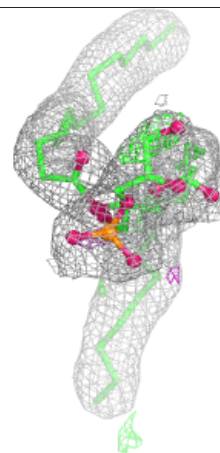
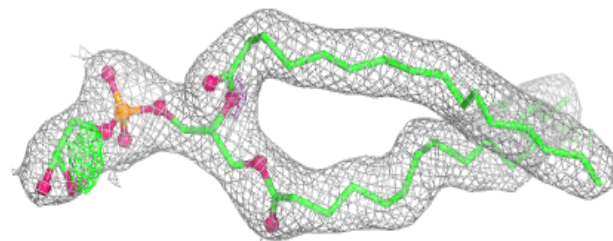
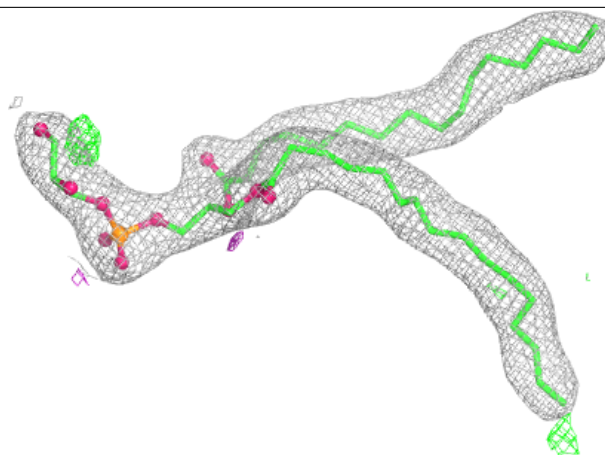
Electron density around LHG d 407 (A):

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



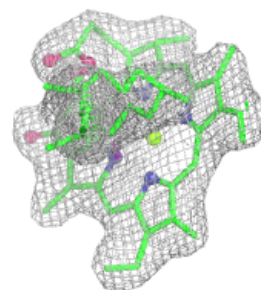
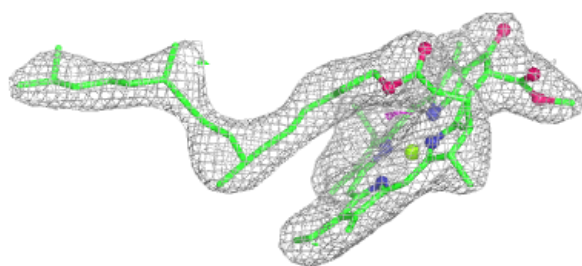
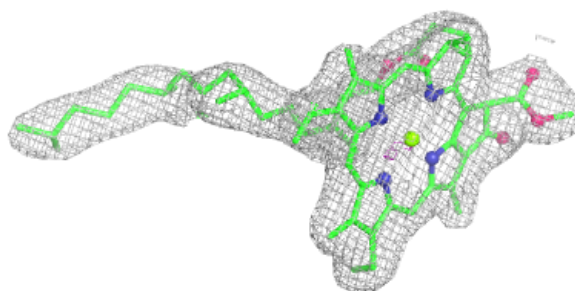
Electron density around LHG d 407 (B):

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

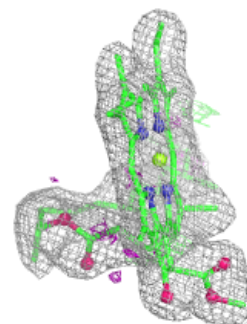
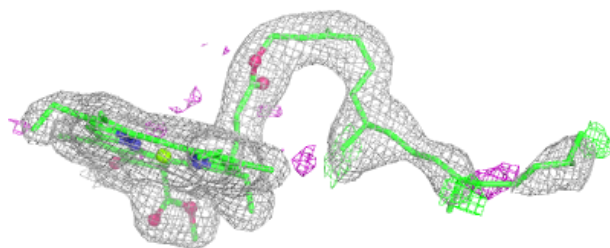
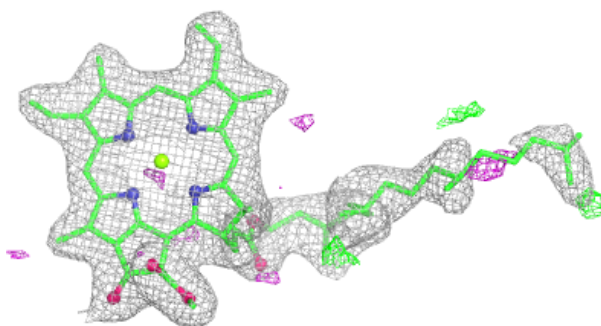


Electron density around CLA C 506:

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

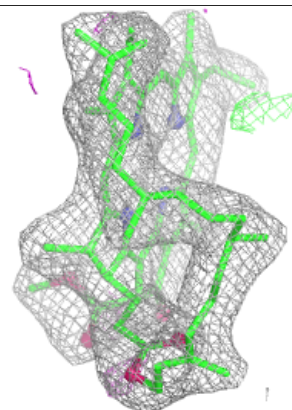
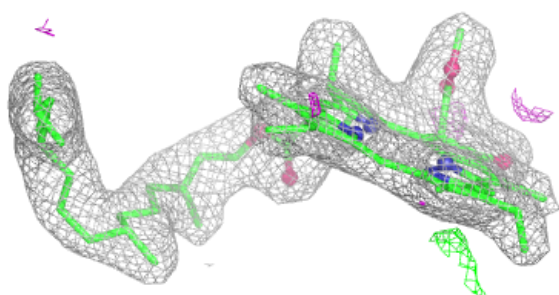
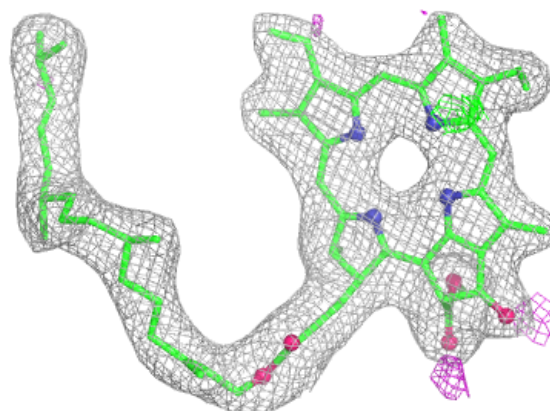
**Electron density around CLA A 406 (A):**

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

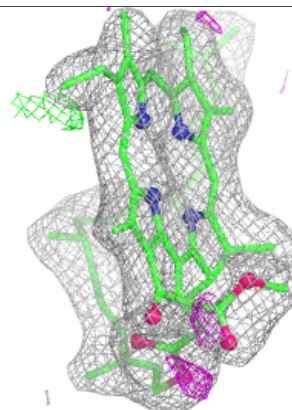
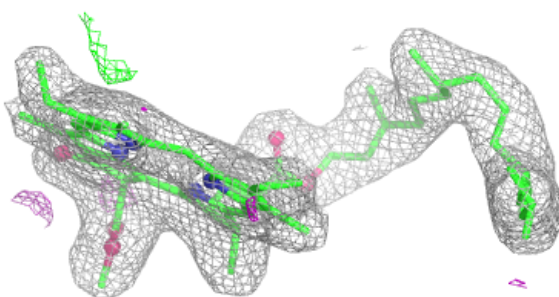
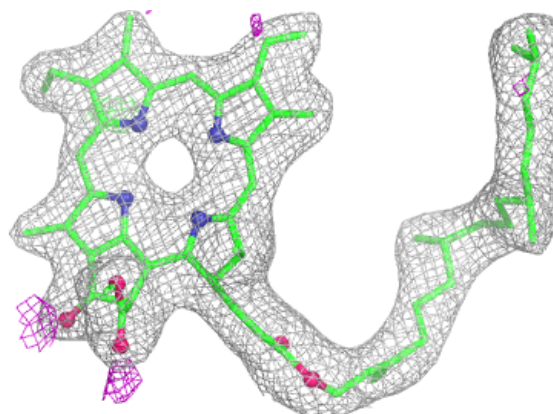


Electron density around PHO A 416 (A):

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

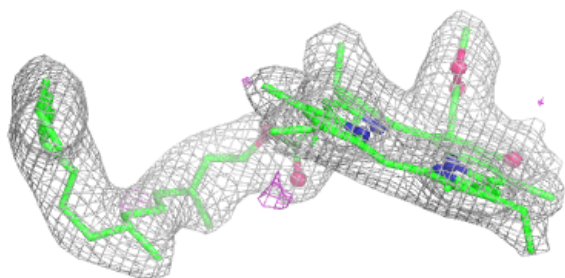
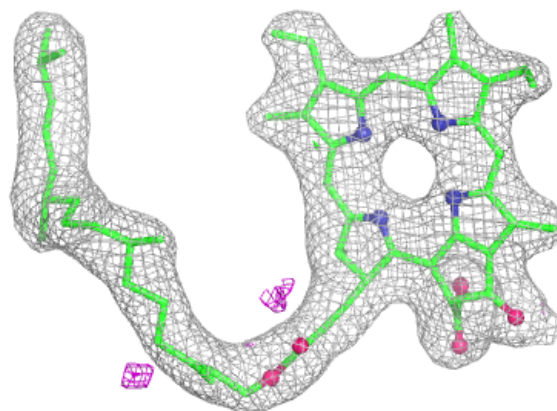
**Electron density around PHO A 416 (B):**

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

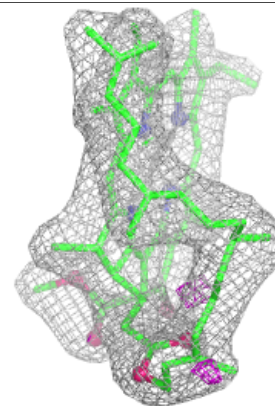
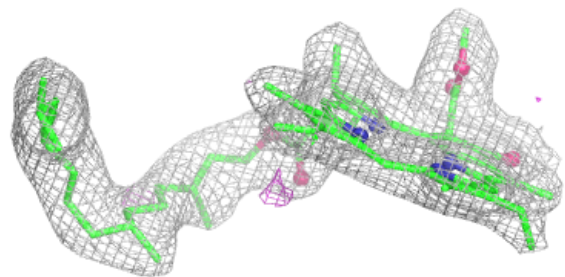
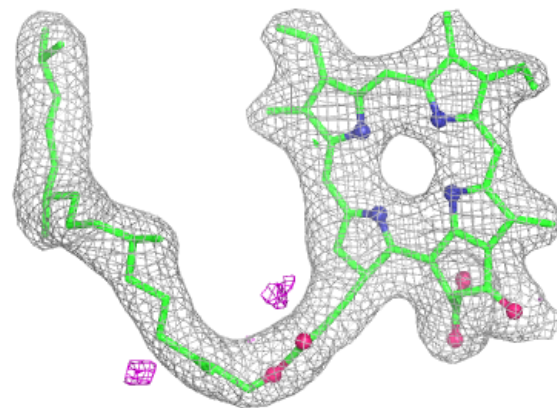


Electron density around PHO a 415 (A):

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

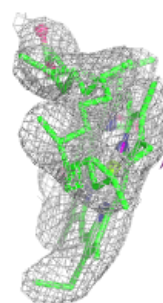
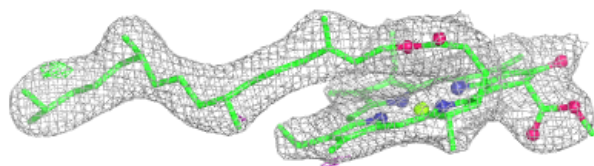
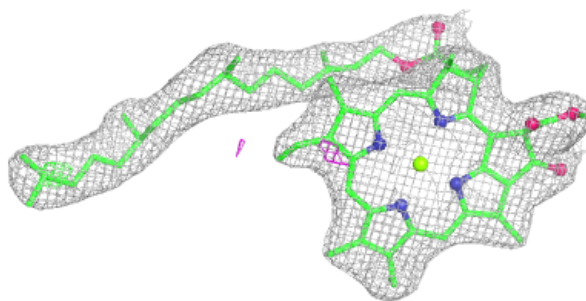
**Electron density around PHO a 415 (B):**

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

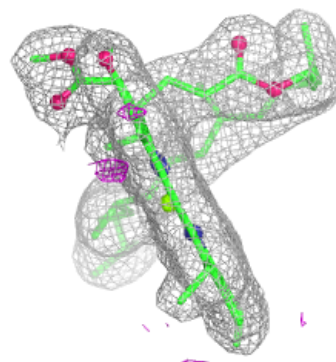
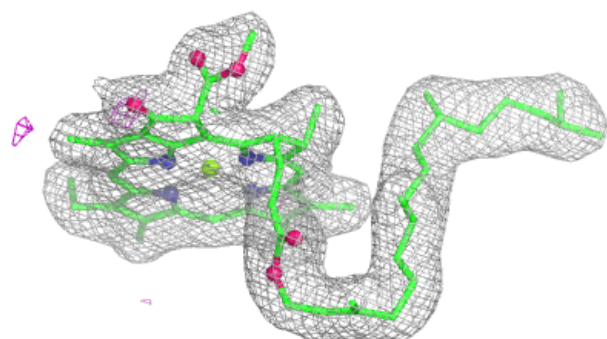
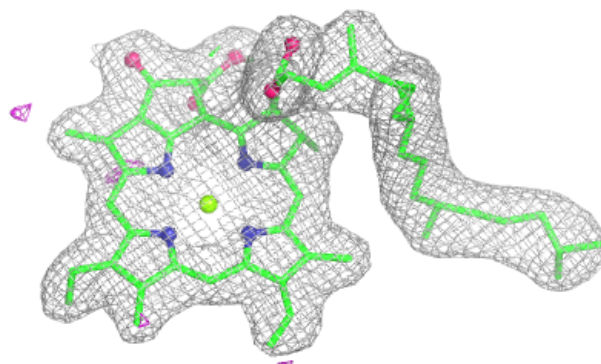


Electron density around CLA c 502:

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

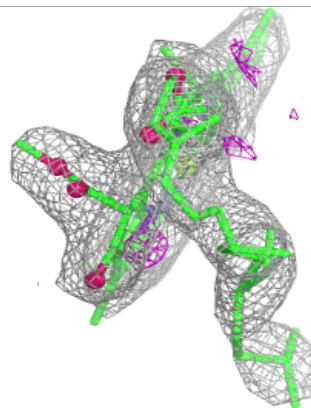
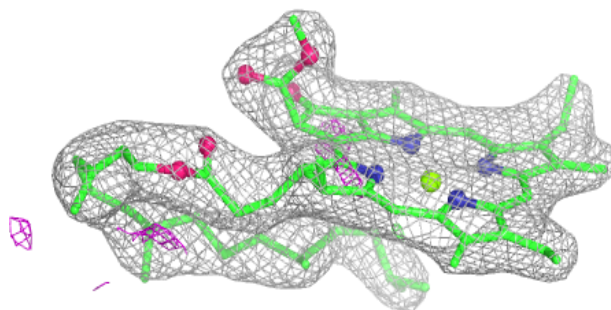
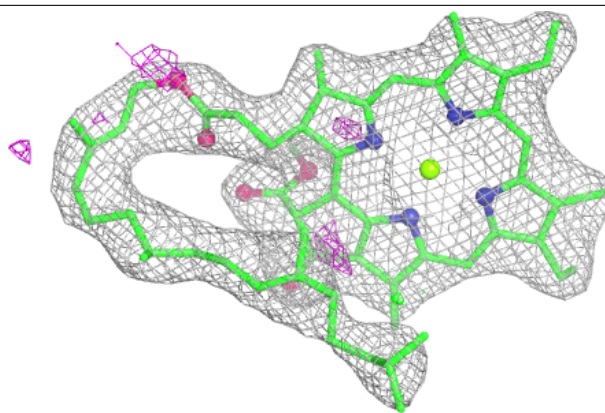
**Electron density around CLA A 405 (A):**

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



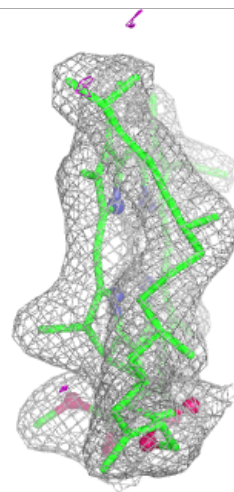
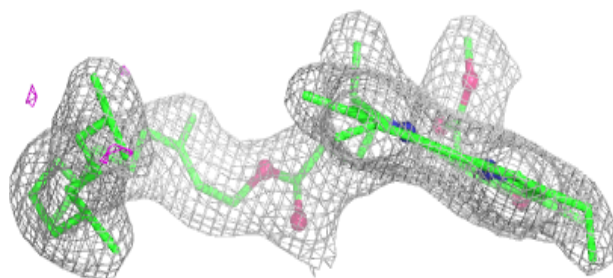
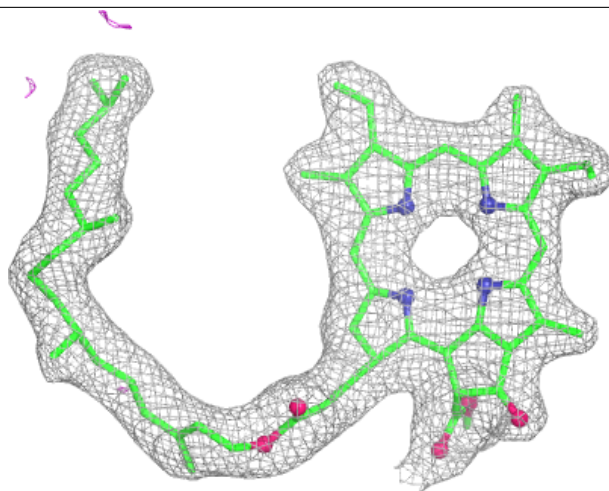
Electron density around CLA c 510:

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



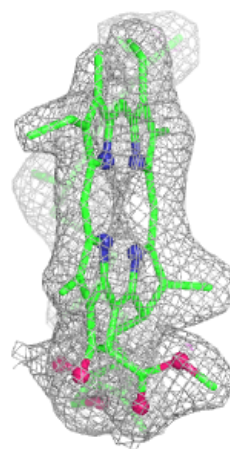
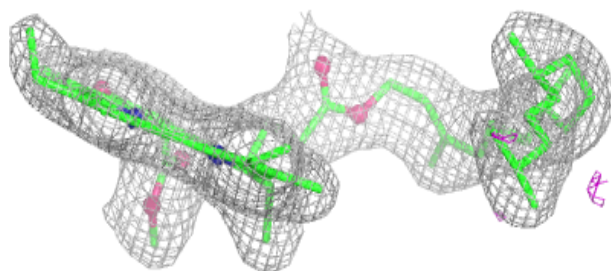
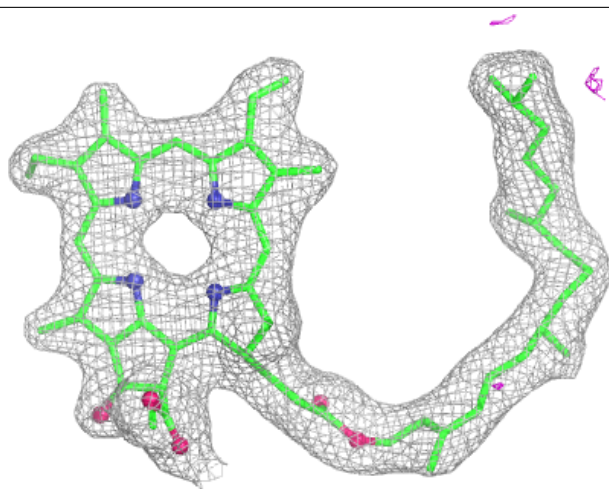
Electron density around PHO D 401 (A):

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



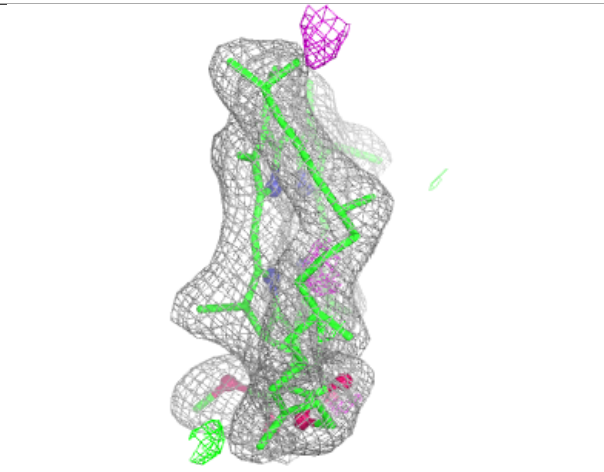
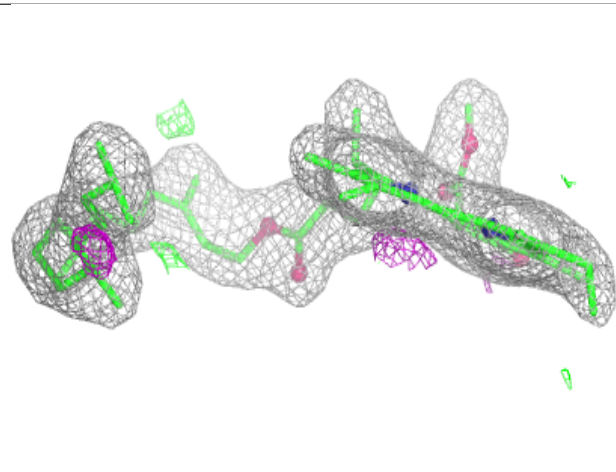
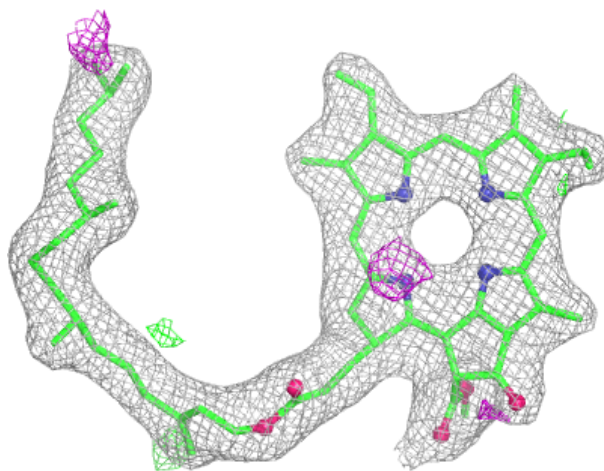
Electron density around PHO D 401 (B):

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



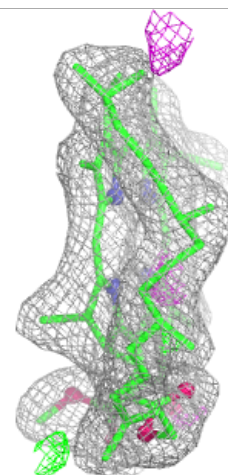
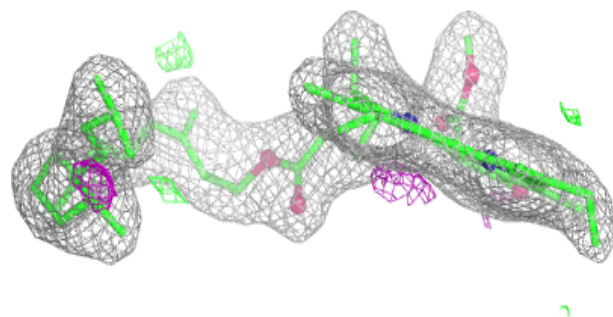
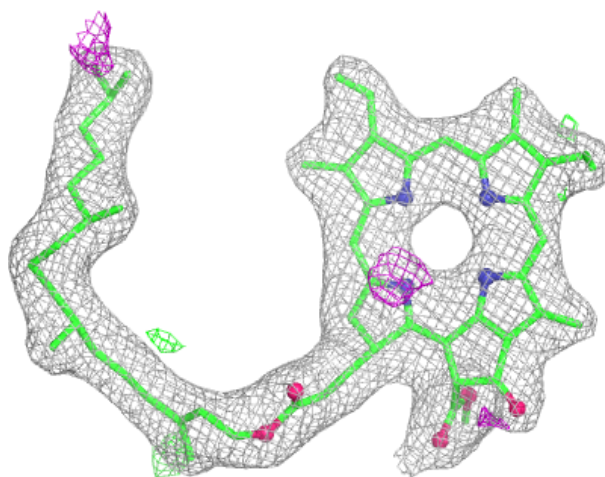
Electron density around PHO a 406 (A):

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



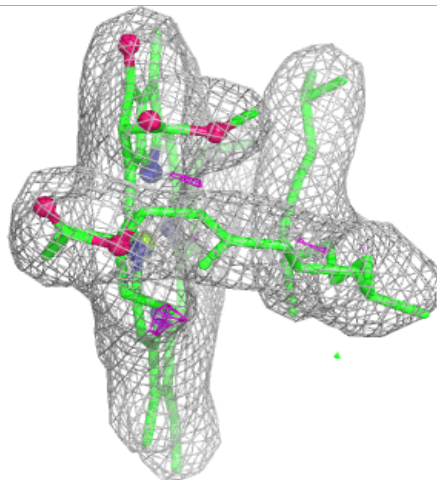
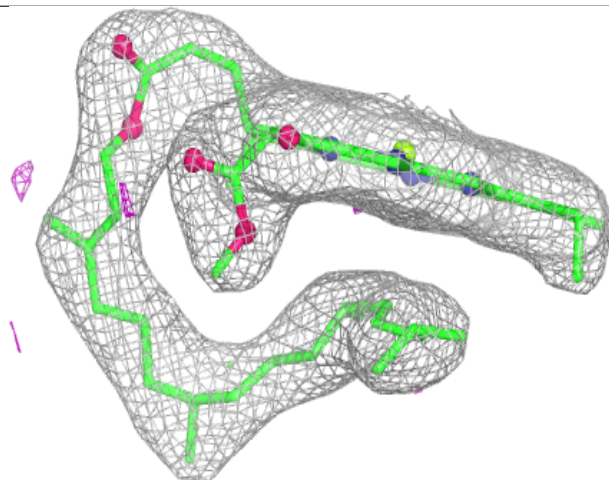
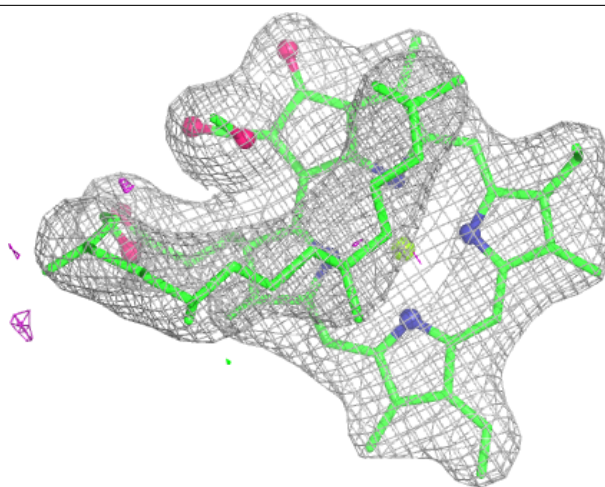
Electron density around PHO a 406 (B):

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



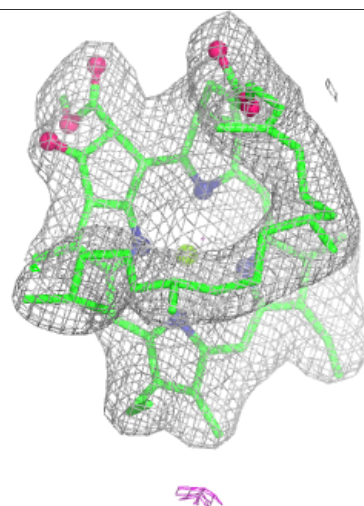
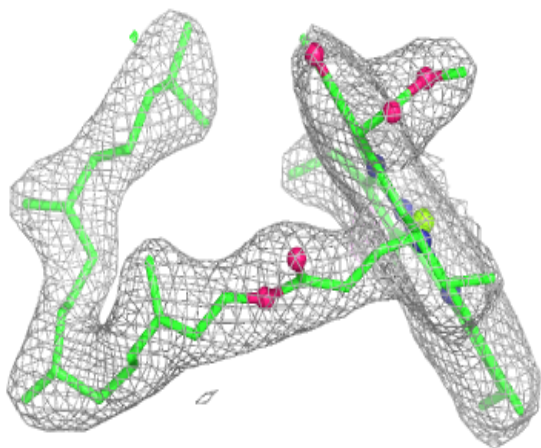
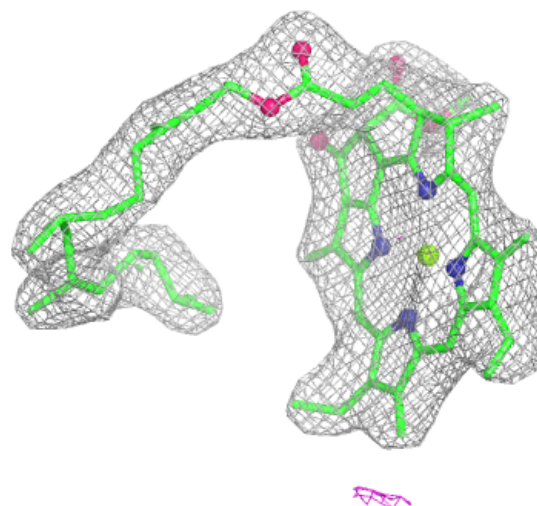
Electron density around CLA c 511:

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



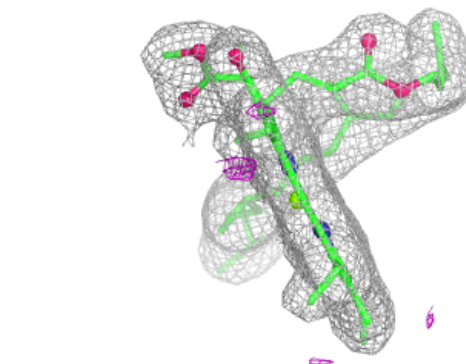
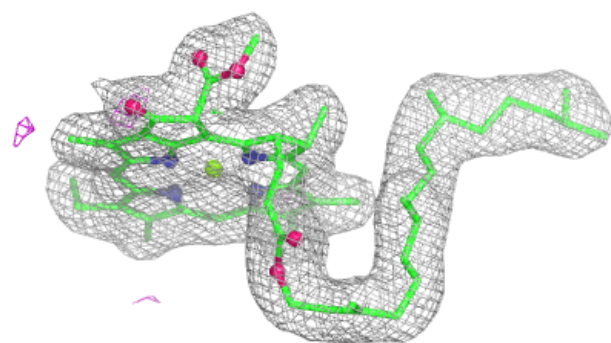
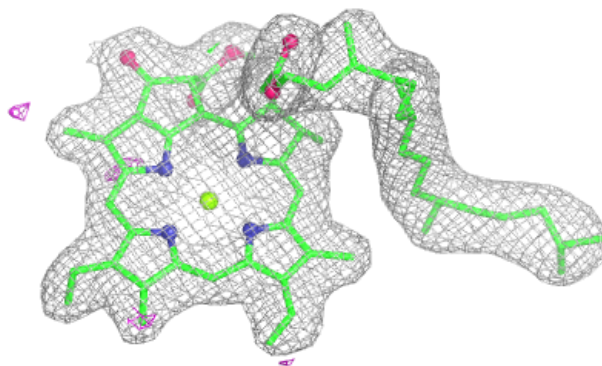
Electron density around CLA C 504:

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

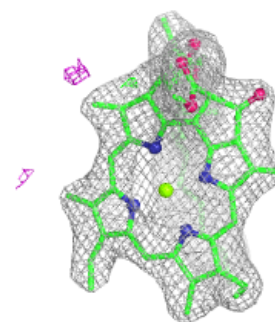
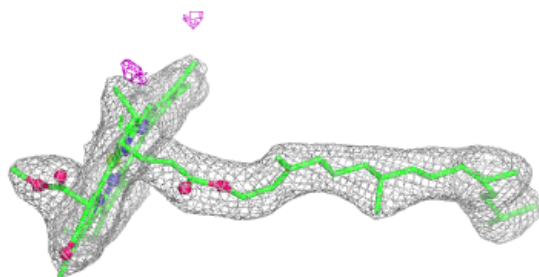
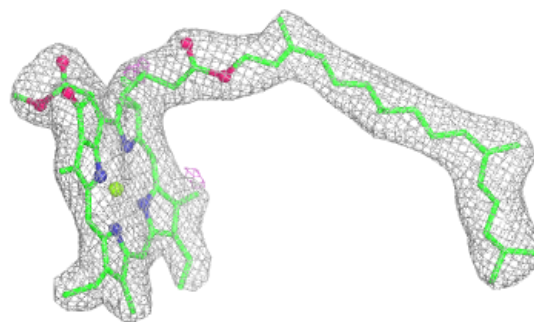


Electron density around CLA A 405 (B):

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

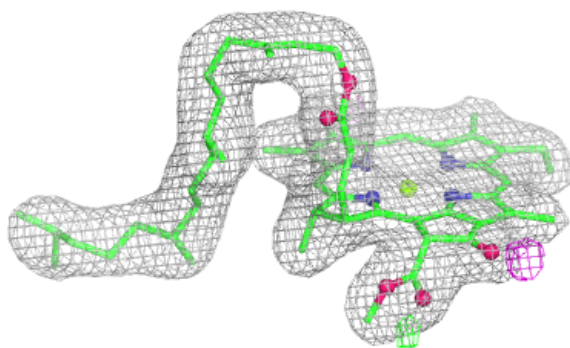
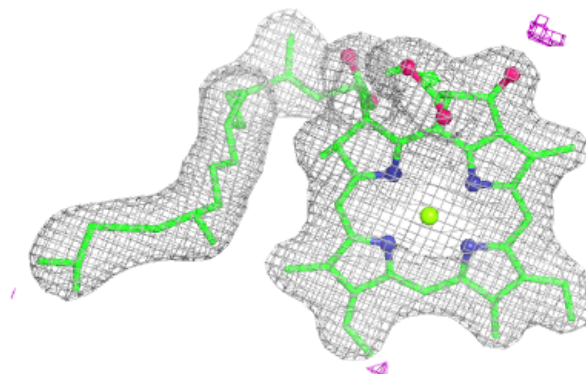
**Electron density around CLA B 609:**

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

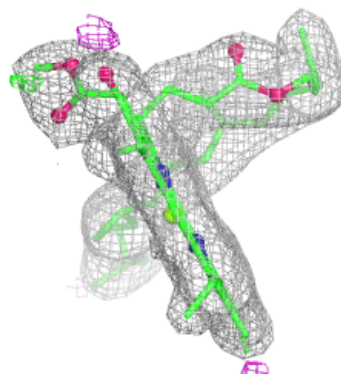
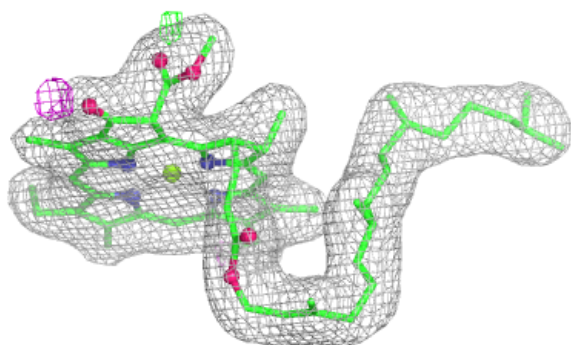
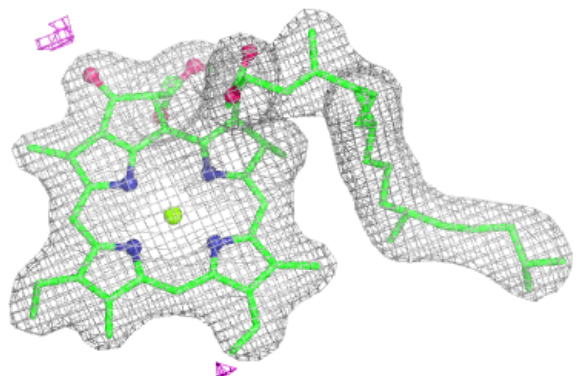


Electron density around CLA d 402 (A):

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

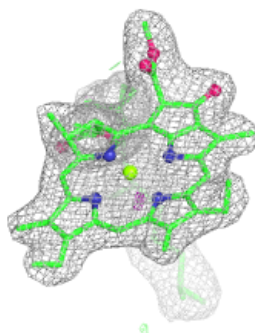
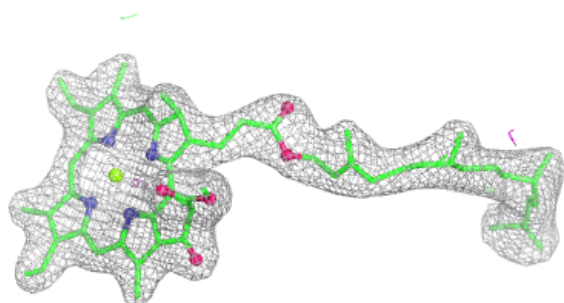
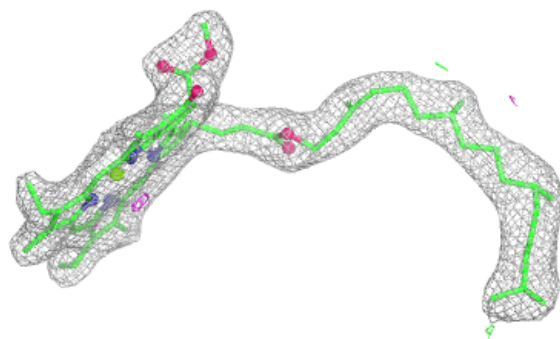
**Electron density around CLA d 402 (B):**

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

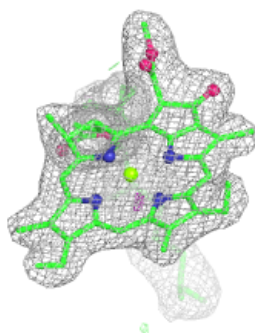
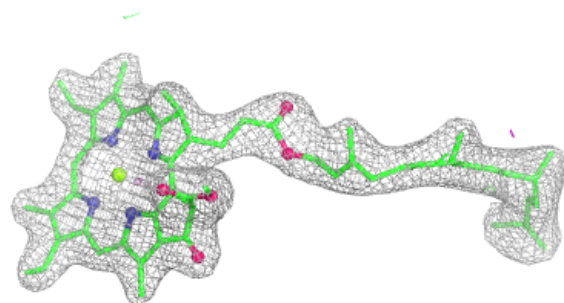
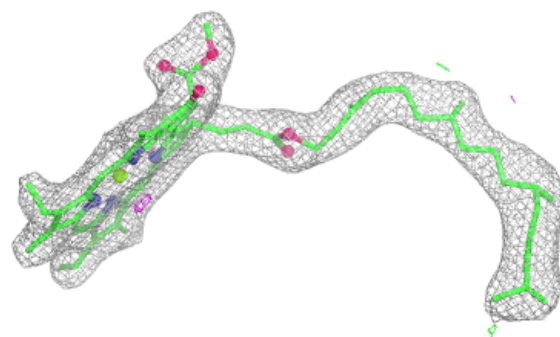


Electron density around CLA d 403 (A):

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

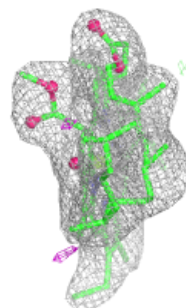
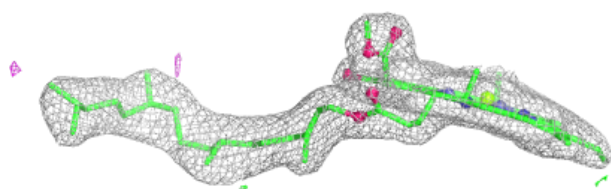
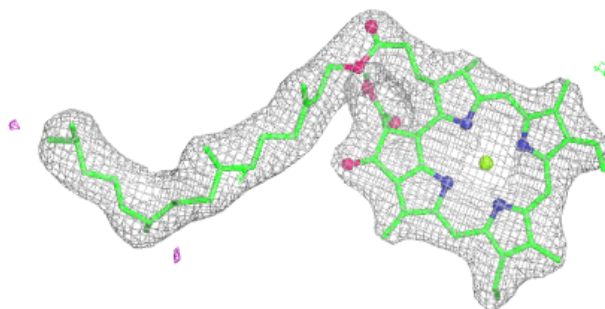
**Electron density around CLA d 403 (B):**

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

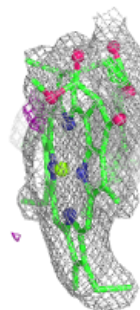
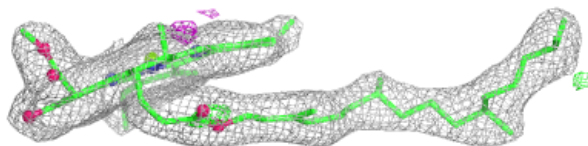
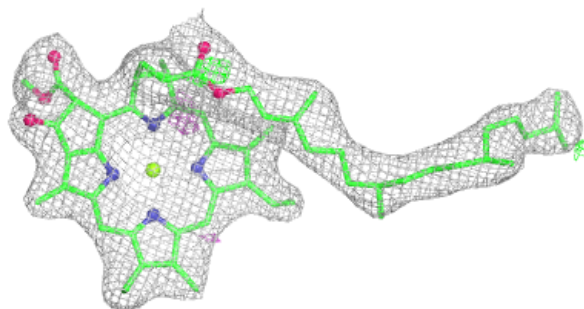


Electron density around CLA b 602:

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

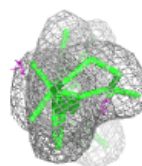
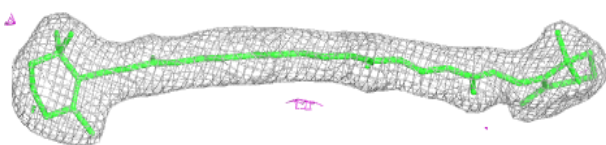
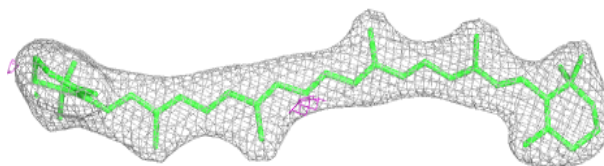
**Electron density around CLA b 603:**

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

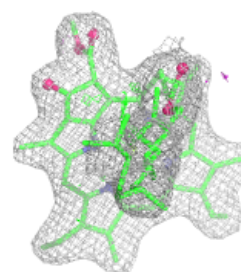
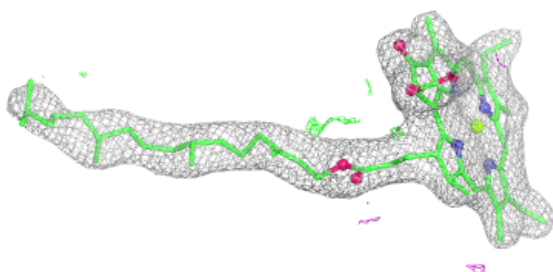
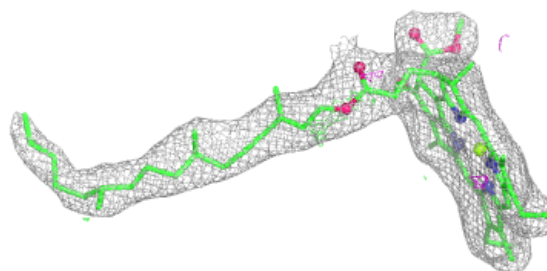


Electron density around BCR B 617:

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

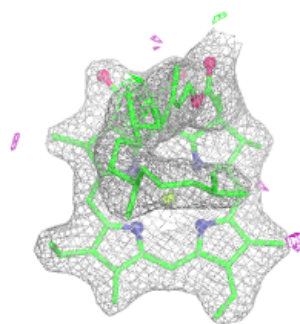
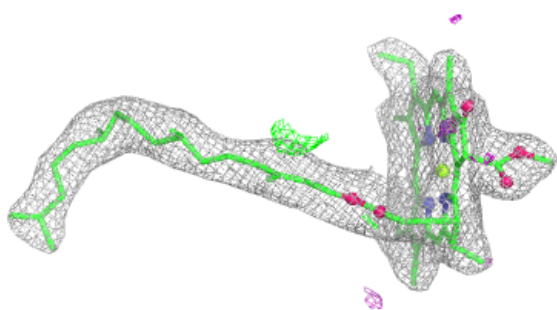
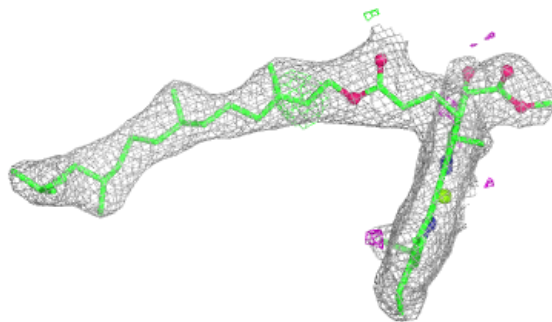
**Electron density around CLA b 604:**

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



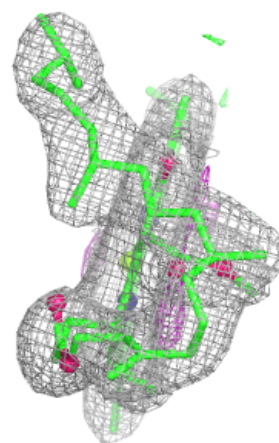
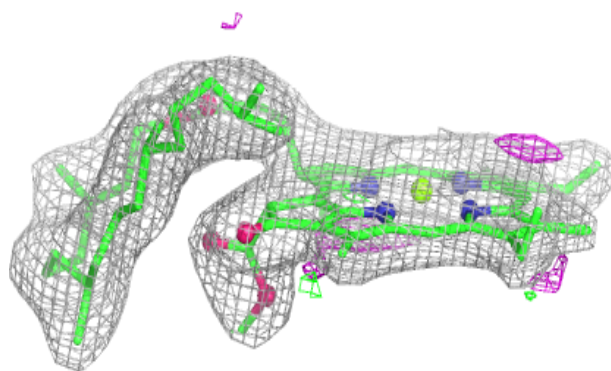
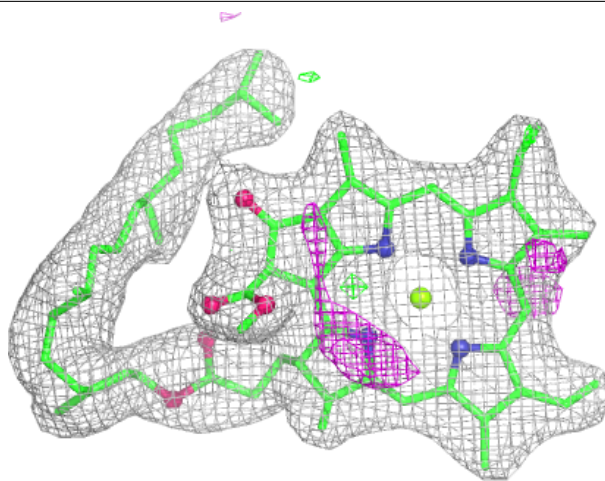
Electron density around CLA b 605:

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



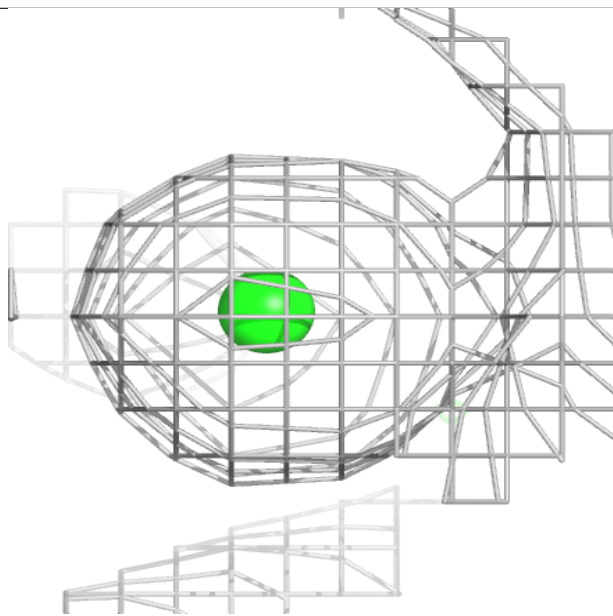
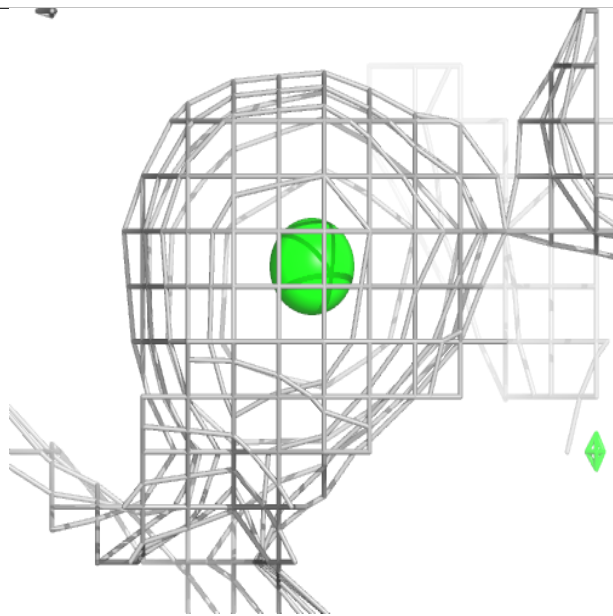
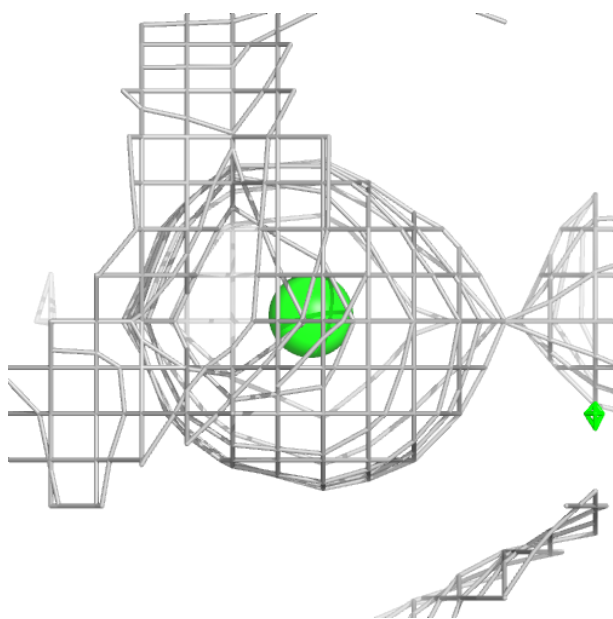
Electron density around CLA B 610:

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



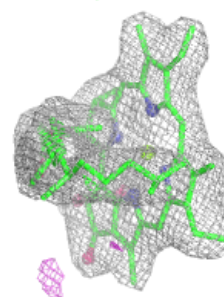
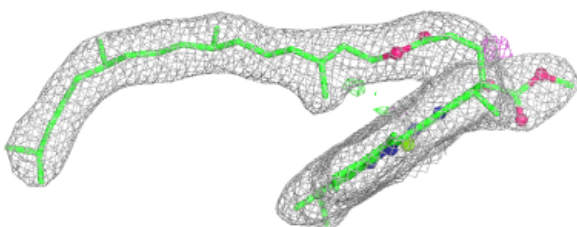
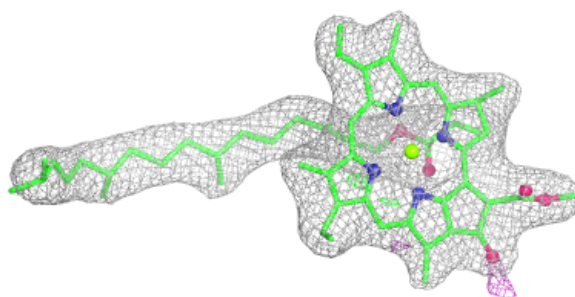
Electron density around CL a 403 (A):

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

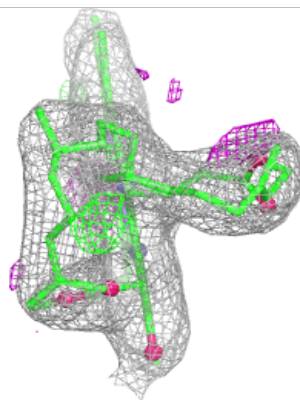
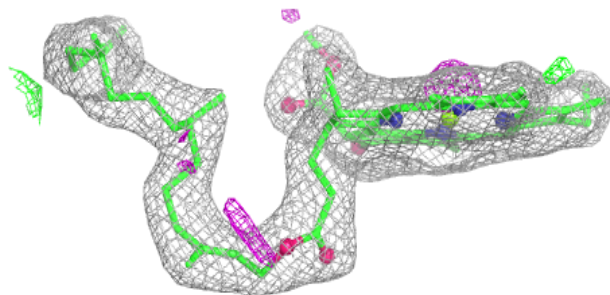
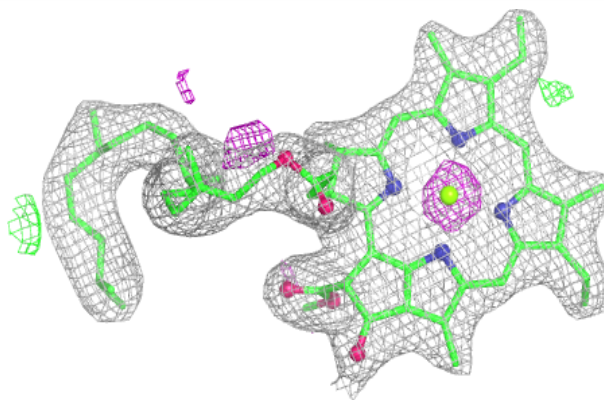


Electron density around CLA b 608:

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

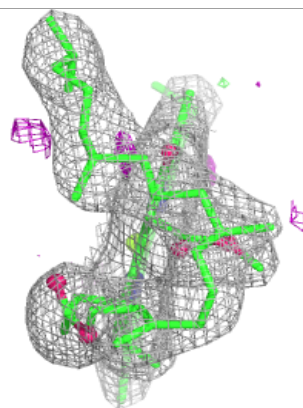
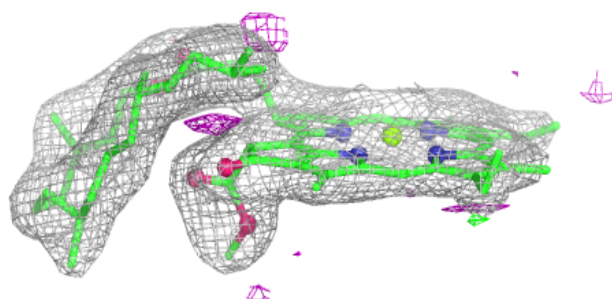
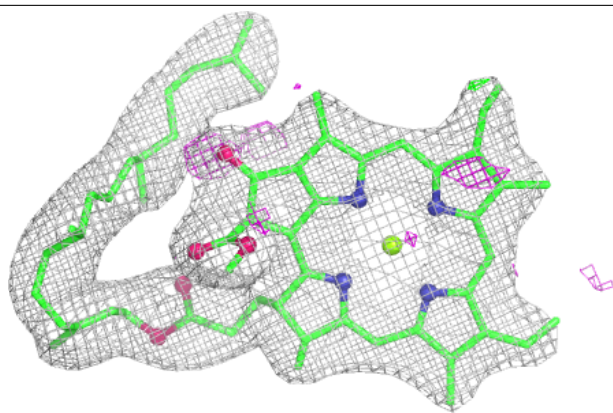
**Electron density around CLA B 612:**

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



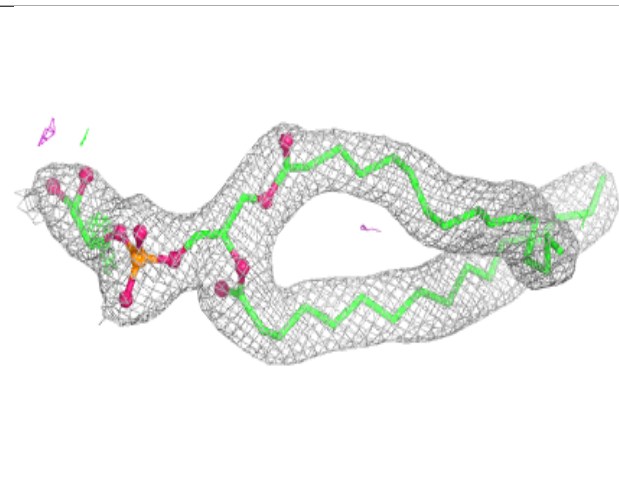
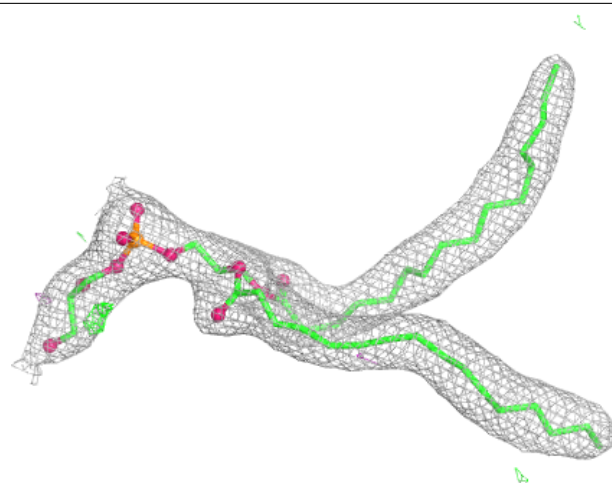
Electron density around CLA b 610:

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



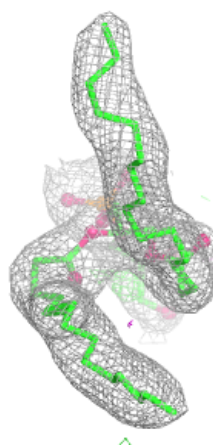
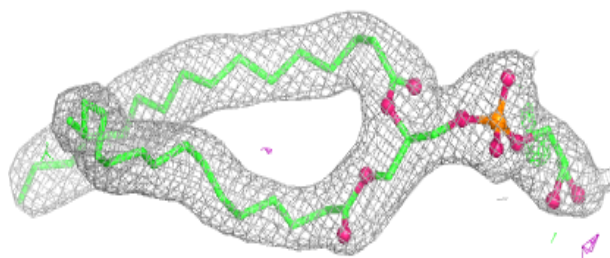
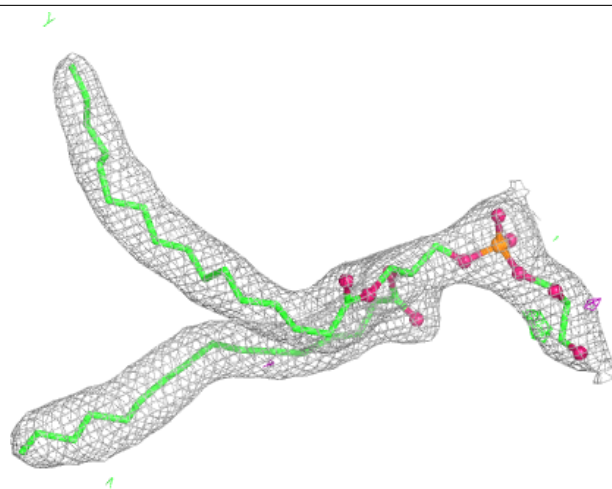
Electron density around LHG D 407 (A):

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



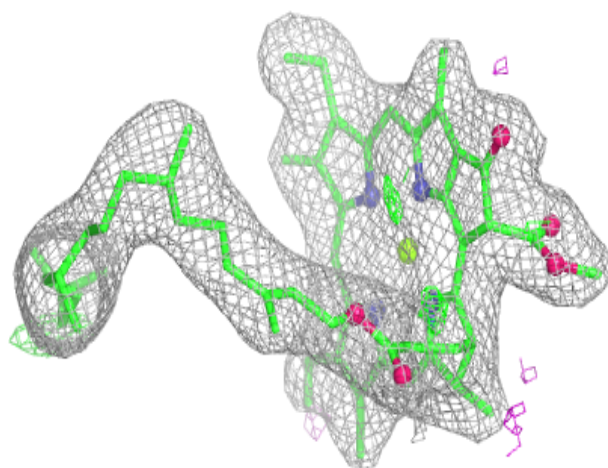
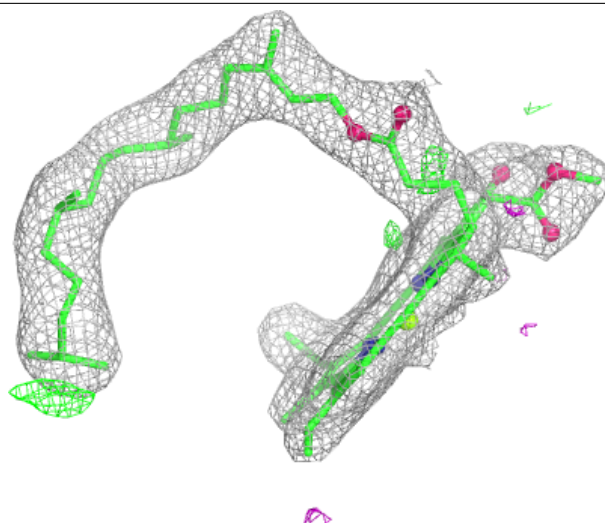
Electron density around LHG D 407 (B):

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



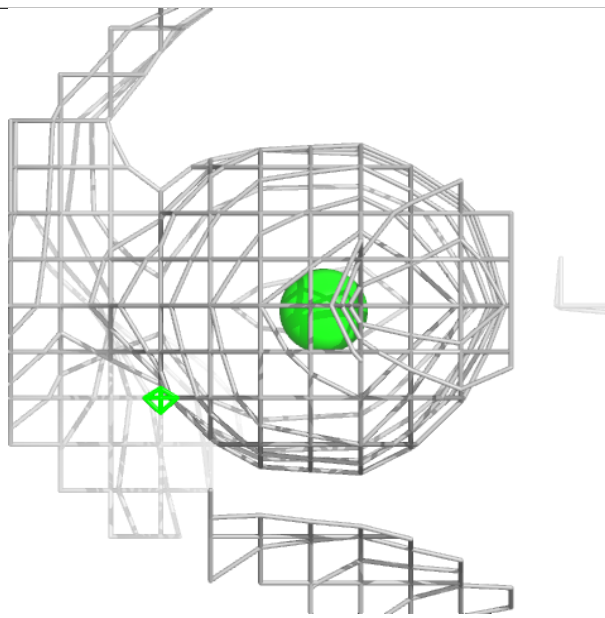
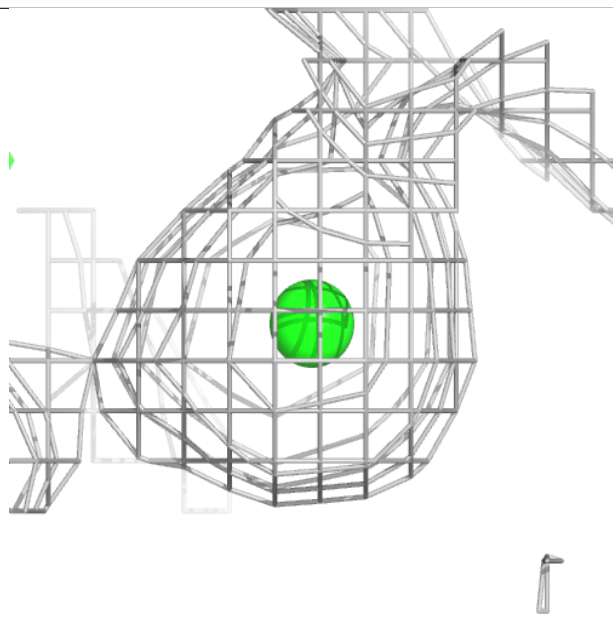
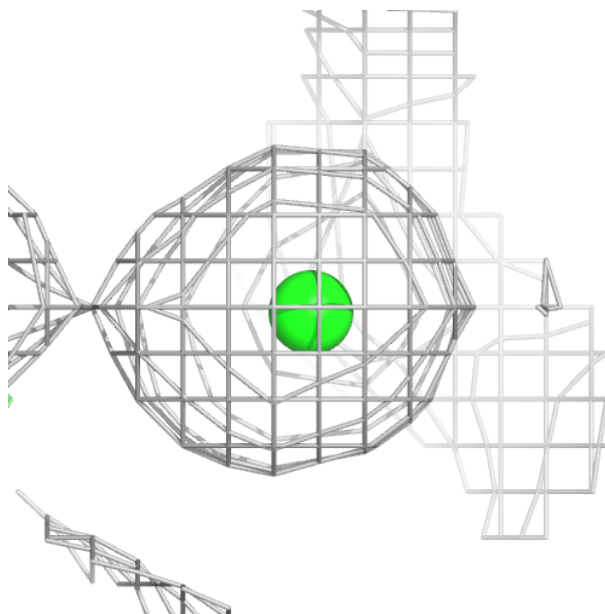
Electron density around CLA b 611:

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



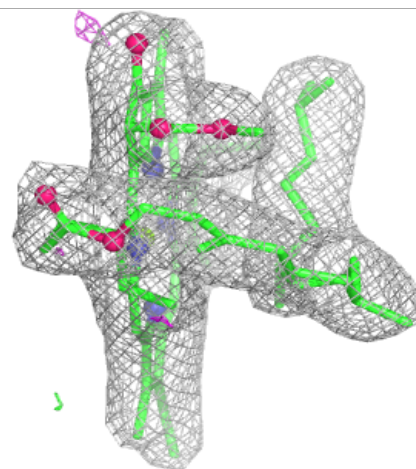
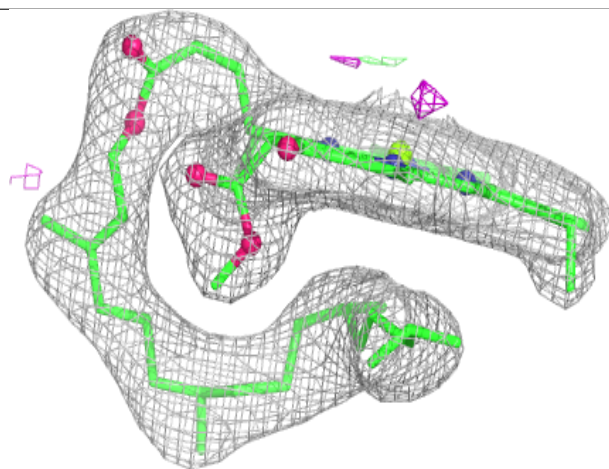
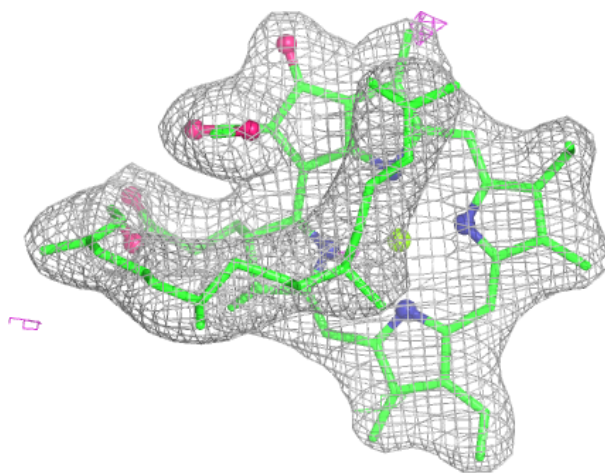
Electron density around CL a 403 (B):

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



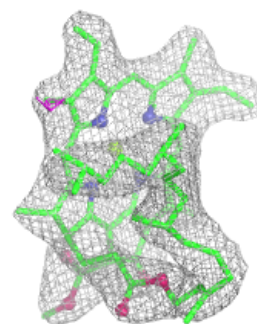
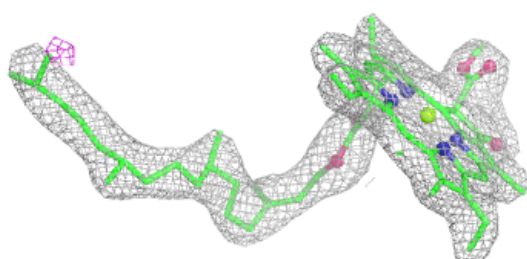
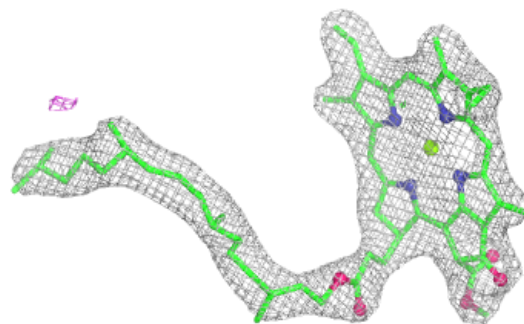
Electron density around CLA C 511:

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



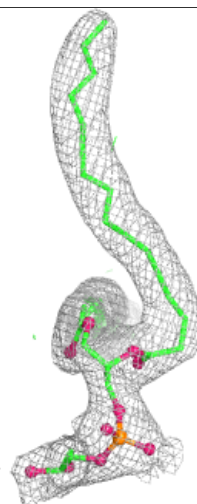
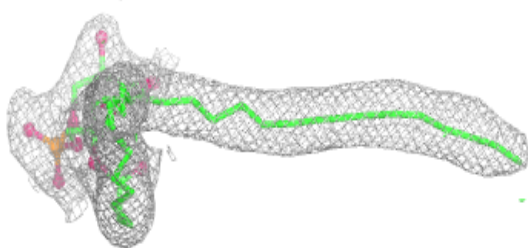
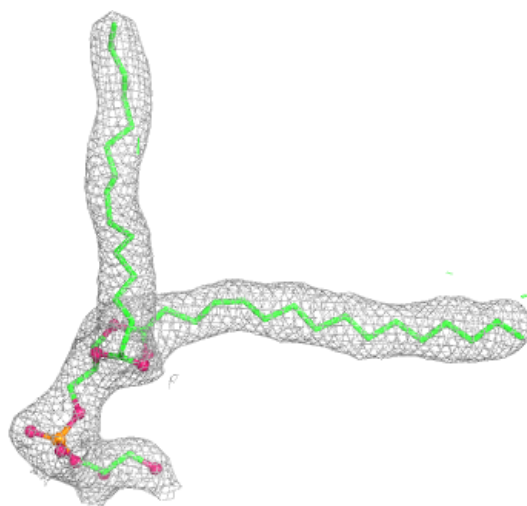
Electron density around CLA C 512:

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



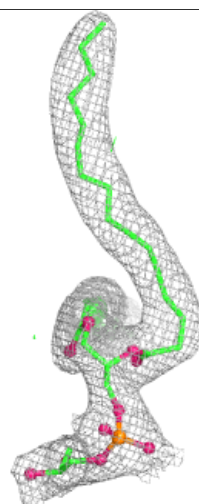
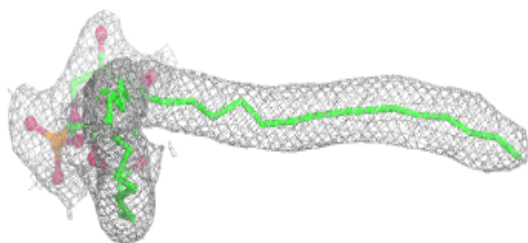
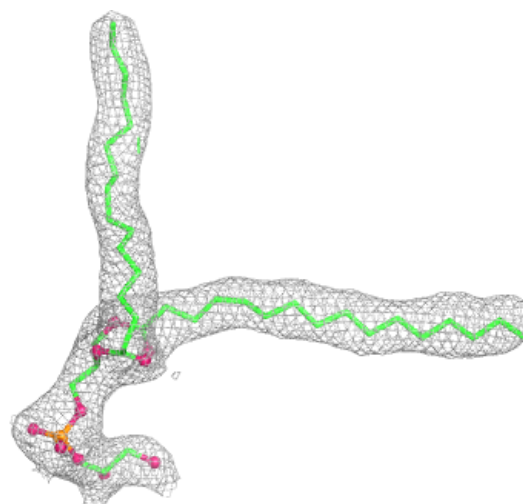
Electron density around LHG L 101 (A):

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



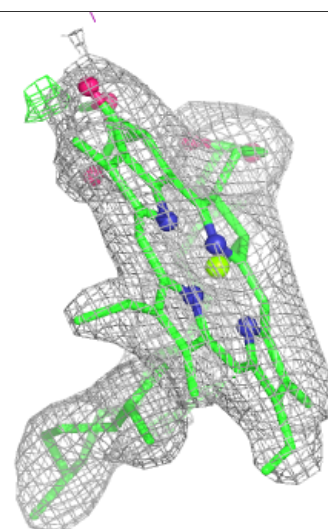
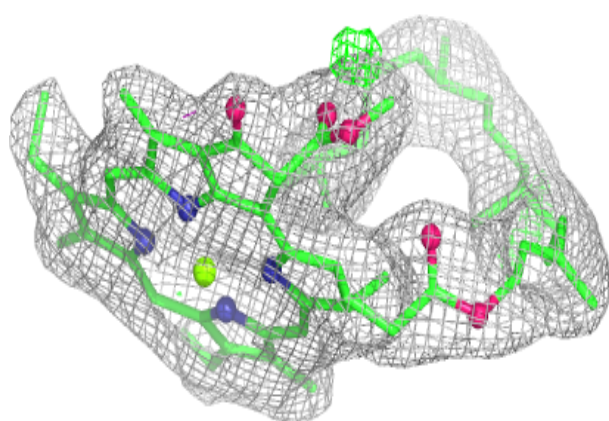
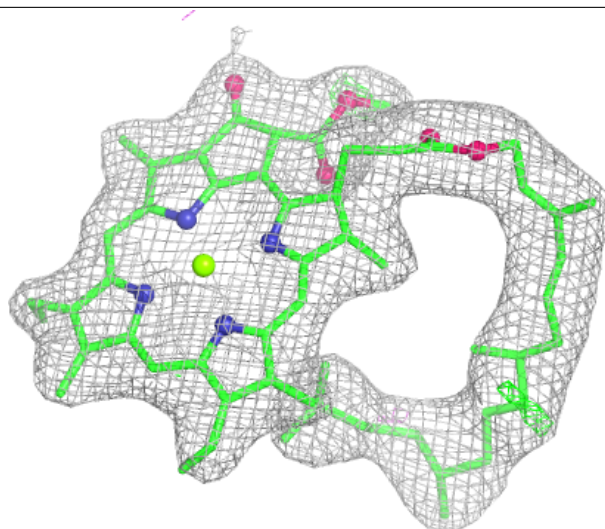
Electron density around LHG L 101 (B):

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



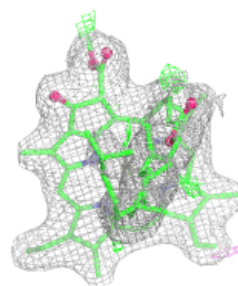
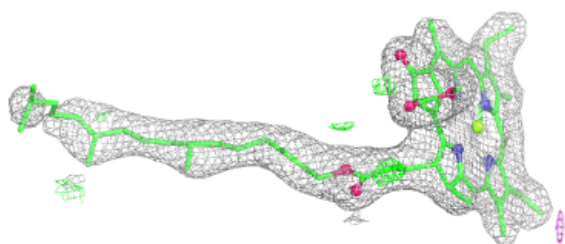
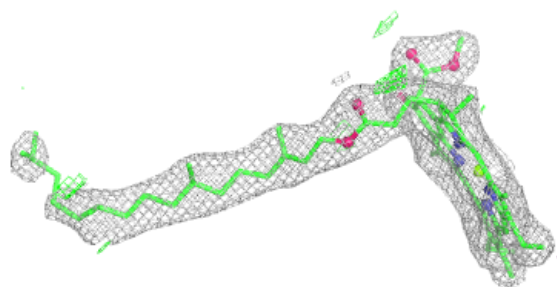
Electron density around CLA b 615:

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

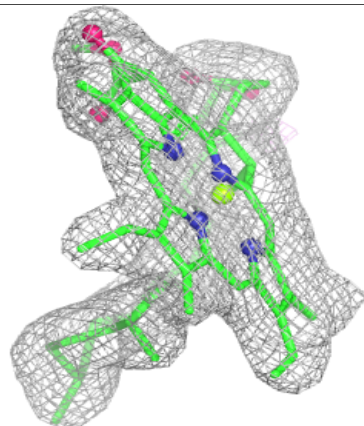
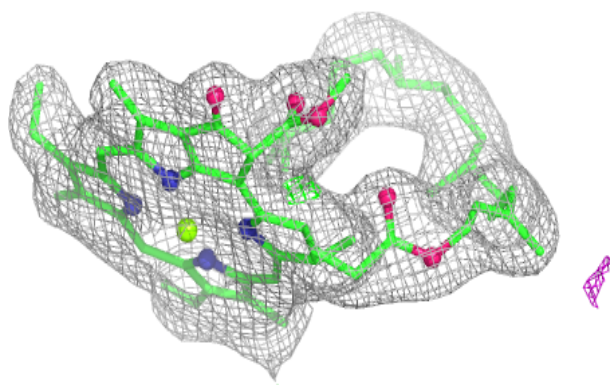
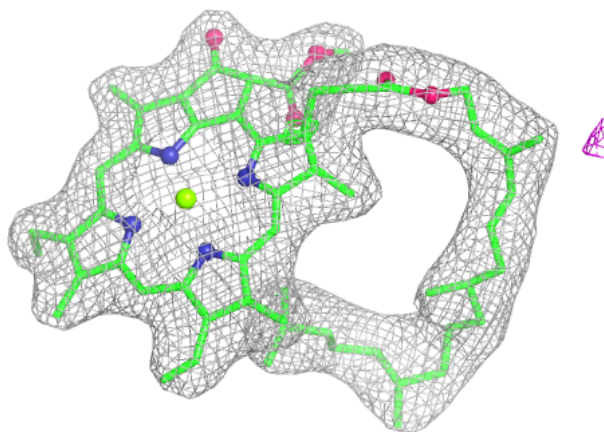


Electron density around CLA B 604:

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

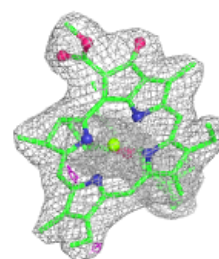
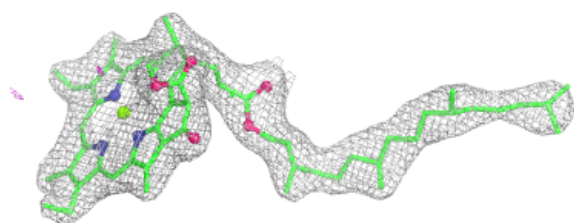
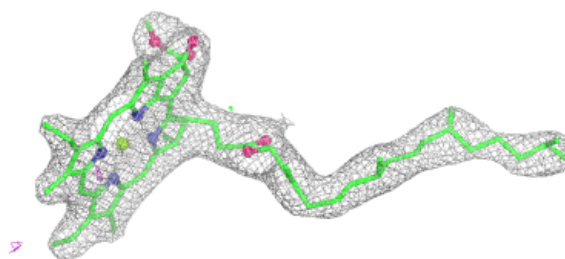
**Electron density around CLA B 615:**

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

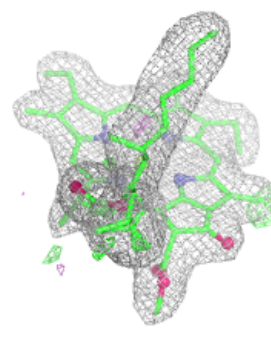
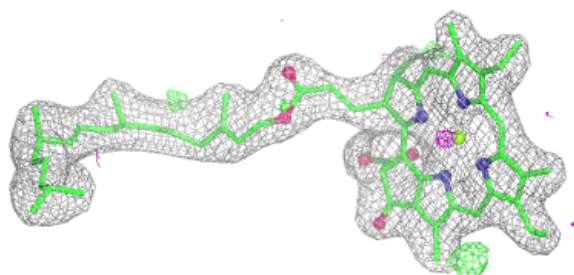
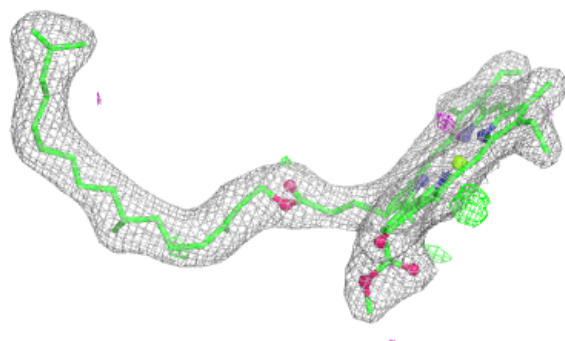


Electron density around CLA c 503:

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

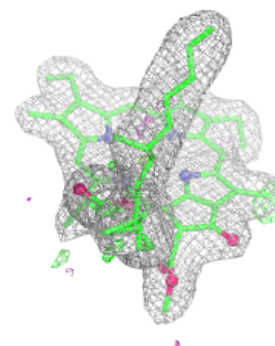
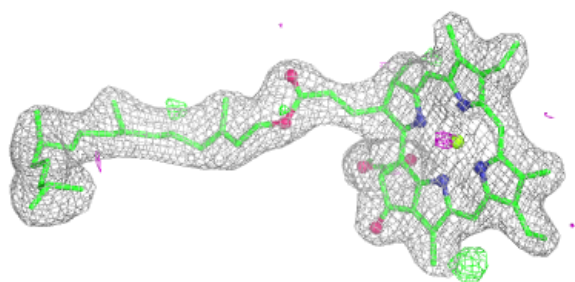
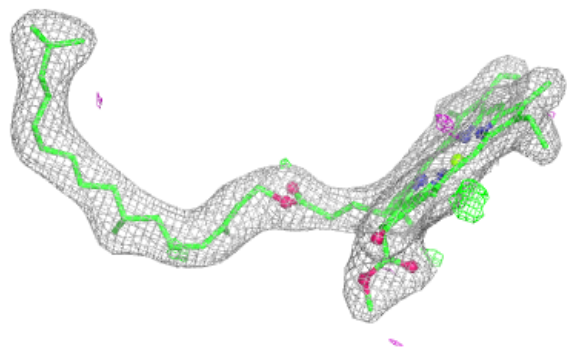
**Electron density around CLA D 403 (A):**

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

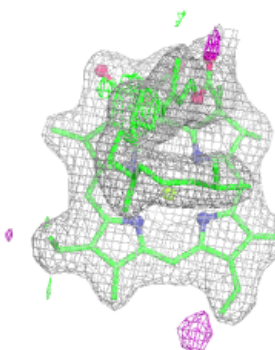
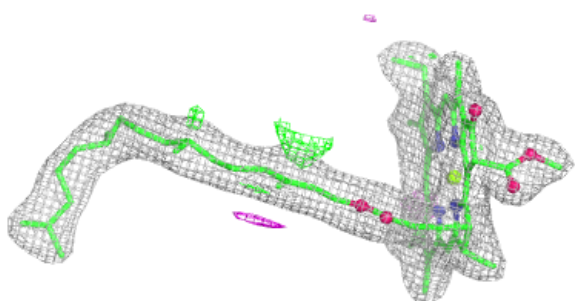
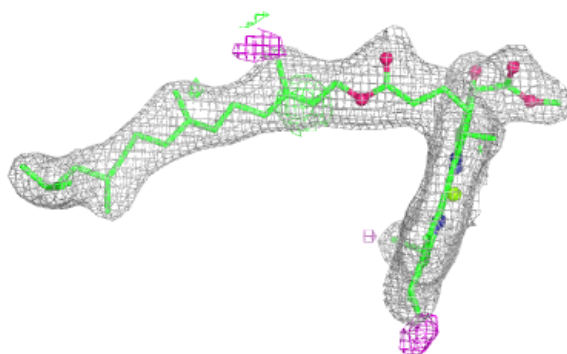


Electron density around CLA D 403 (B):

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

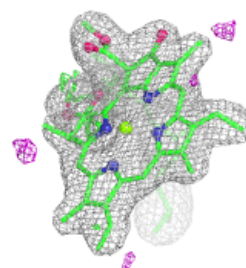
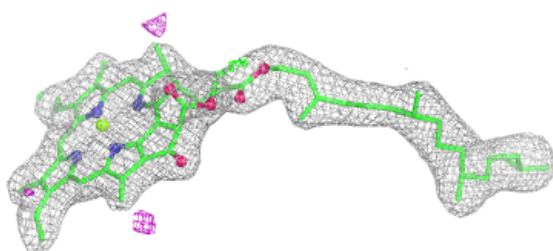
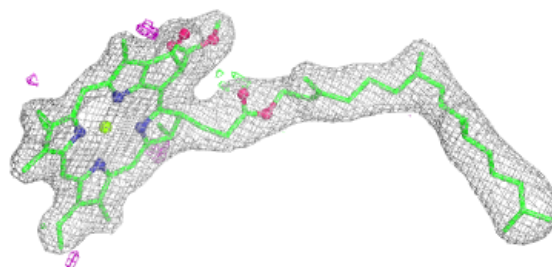
**Electron density around CLA B 605:**

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

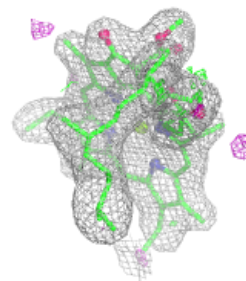
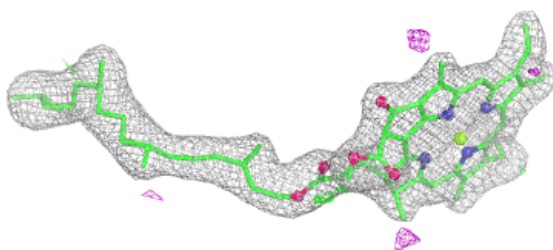
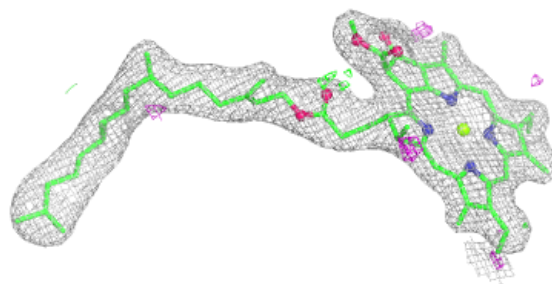


Electron density around CLA a 404 (A):

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

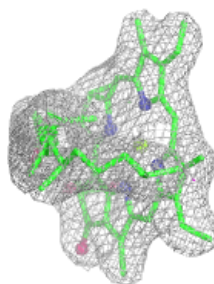
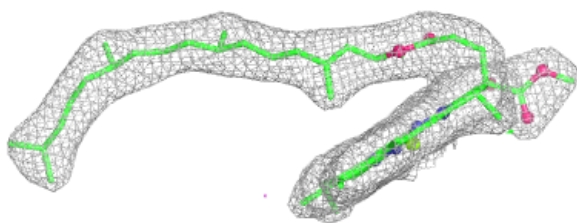
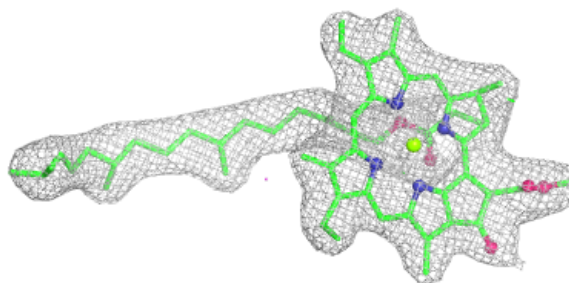
**Electron density around CLA a 404 (B):**

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



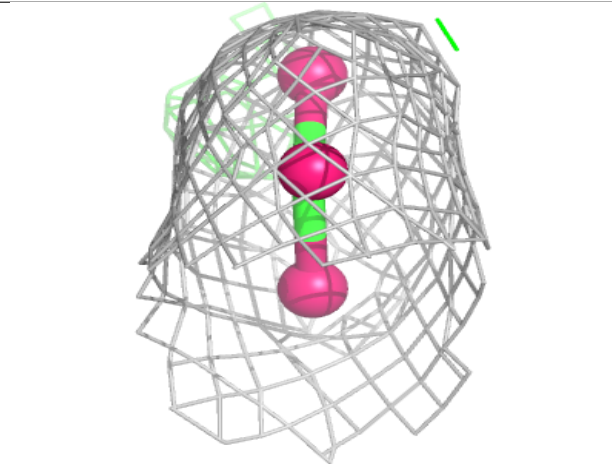
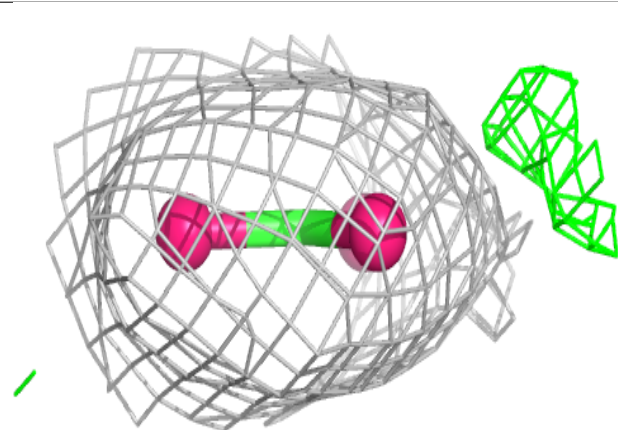
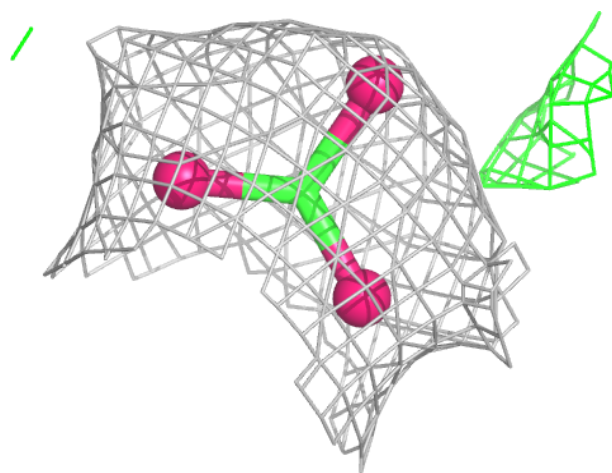
Electron density around CLA B 608:

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



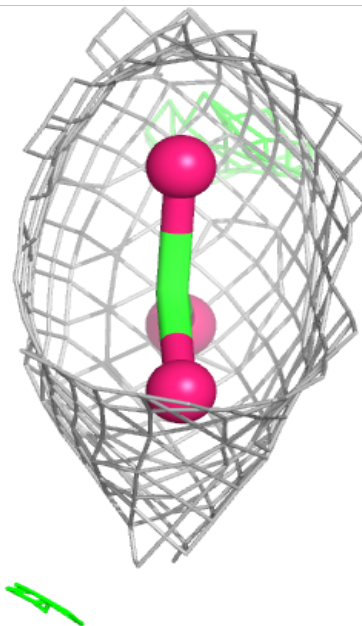
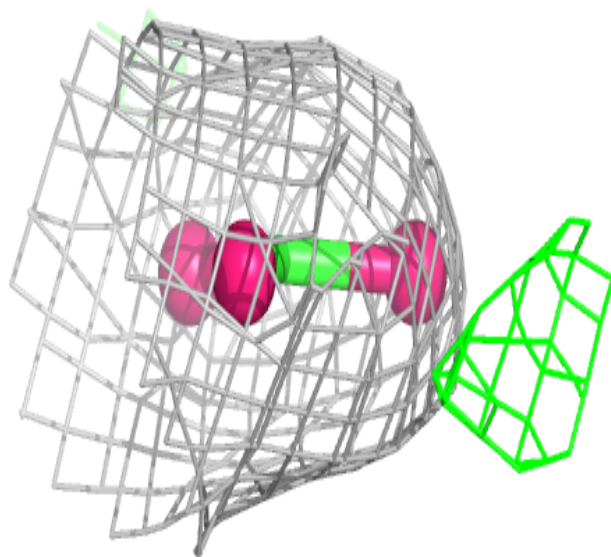
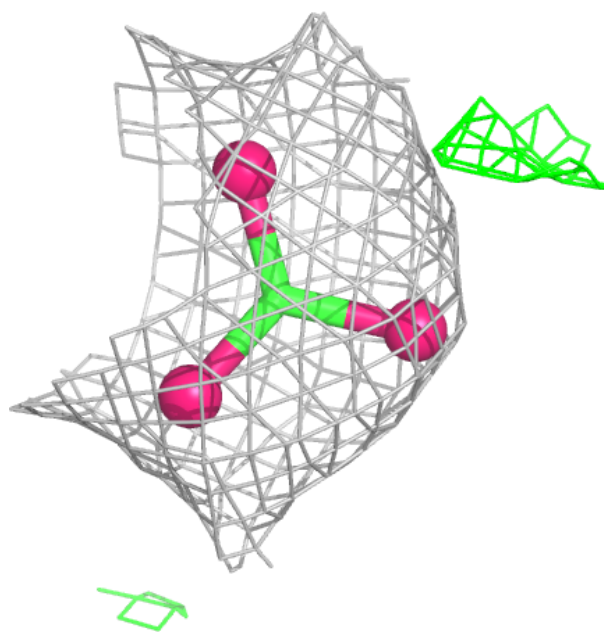
Electron density around BCT A 415 (A):

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



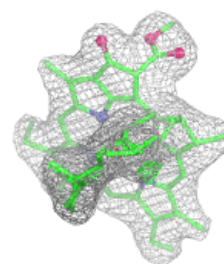
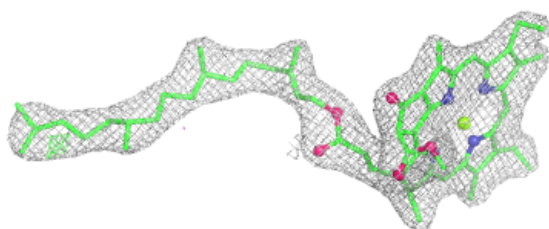
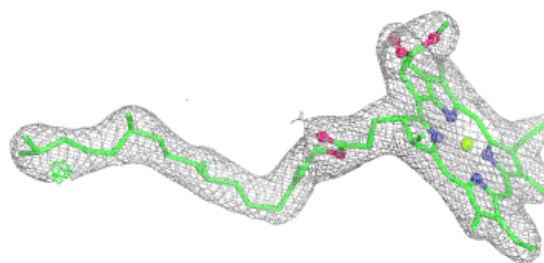
Electron density around BCT A 415 (B):

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



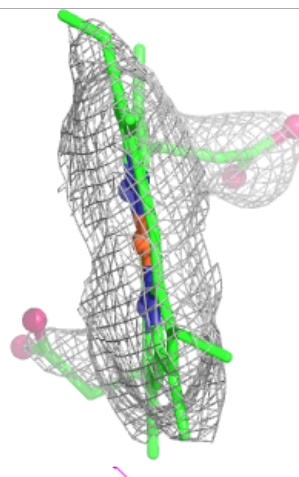
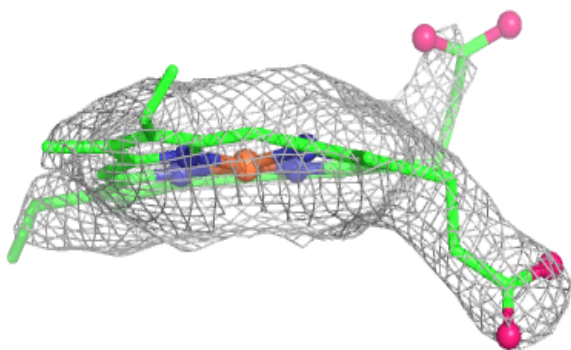
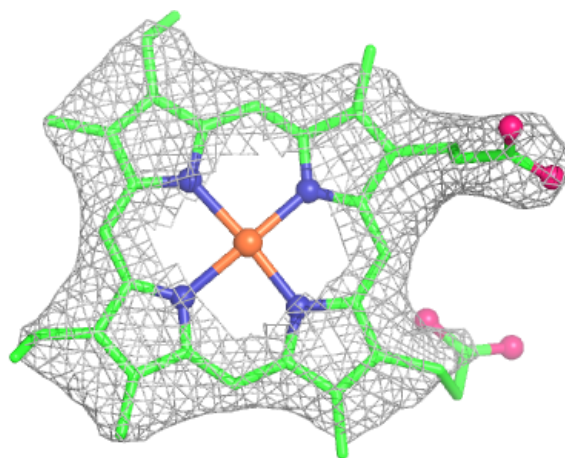
Electron density around CLA C 503:

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



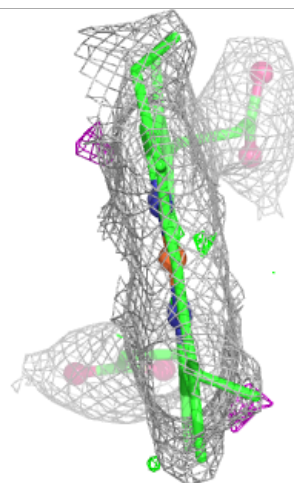
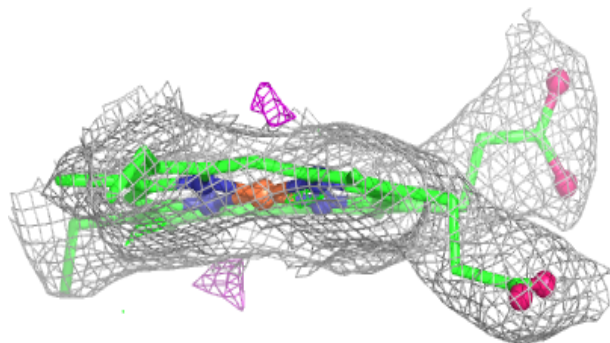
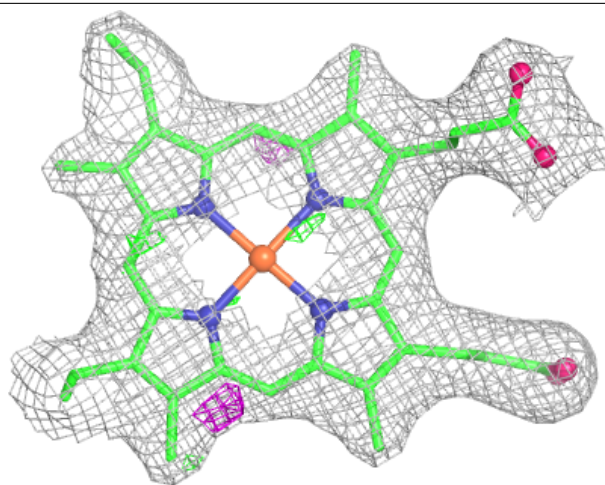
Electron density around HEM f 101:

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



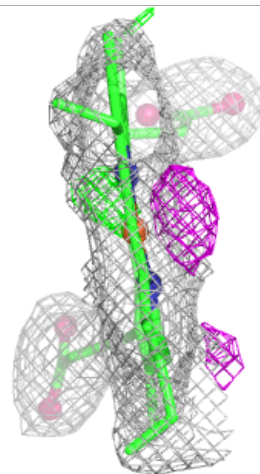
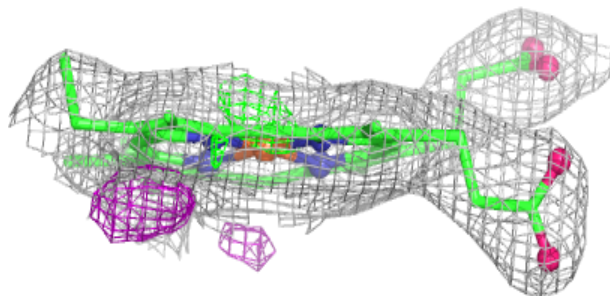
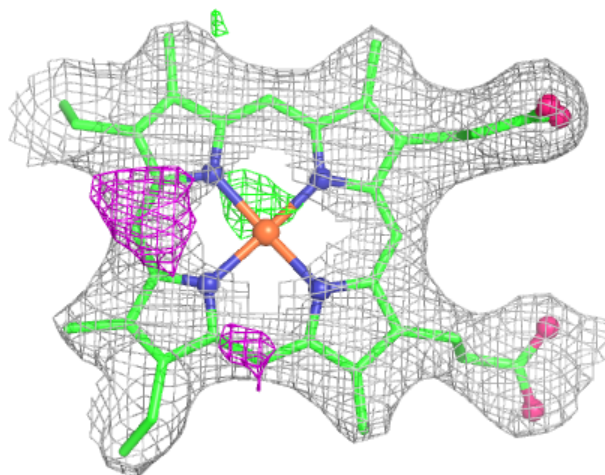
Electron density around HEC V 201:

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



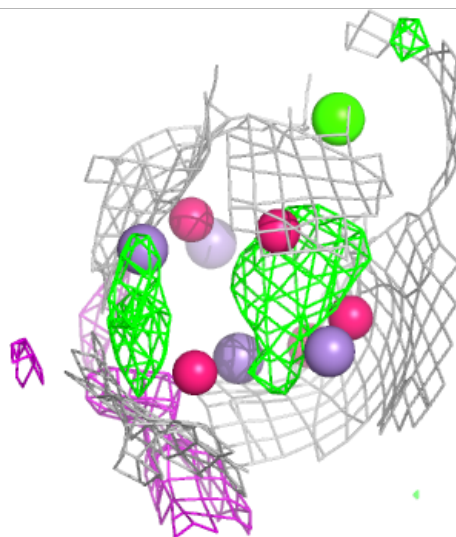
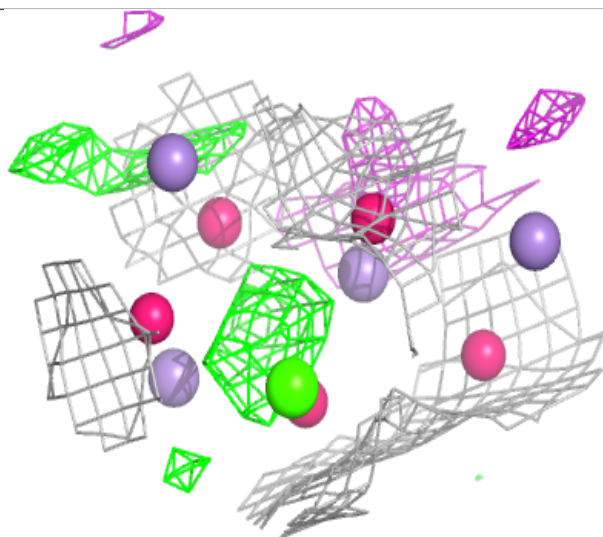
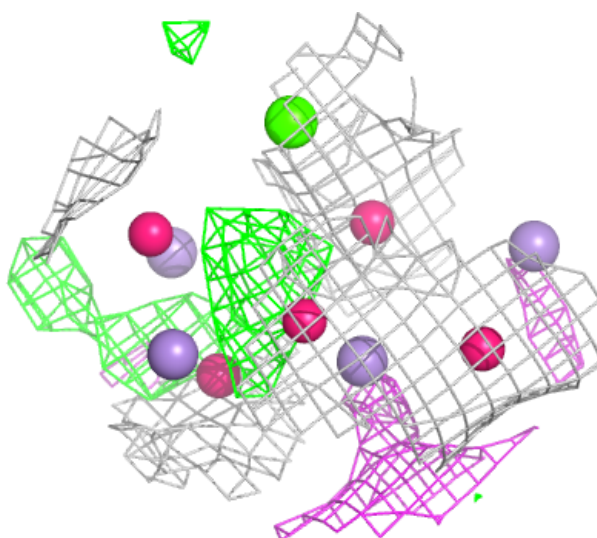
Electron density around HEC v 201:

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



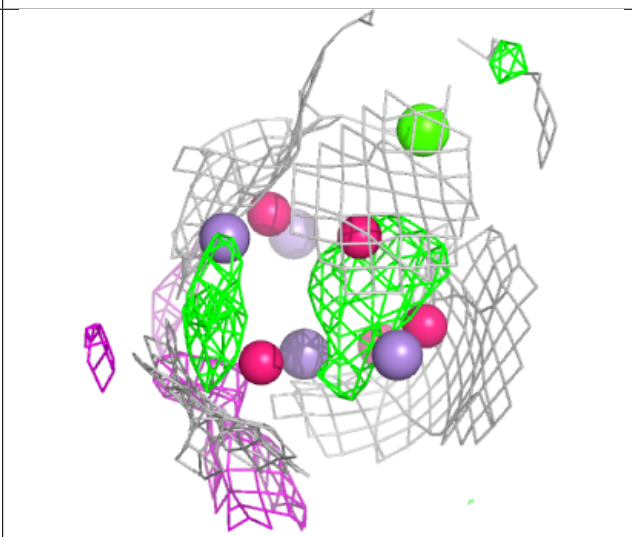
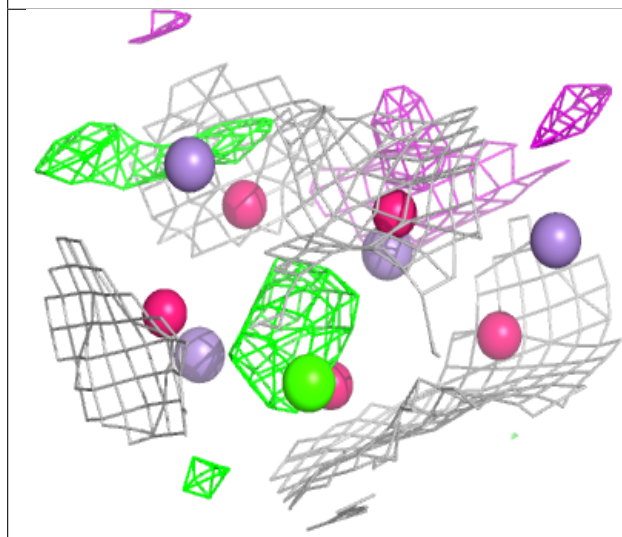
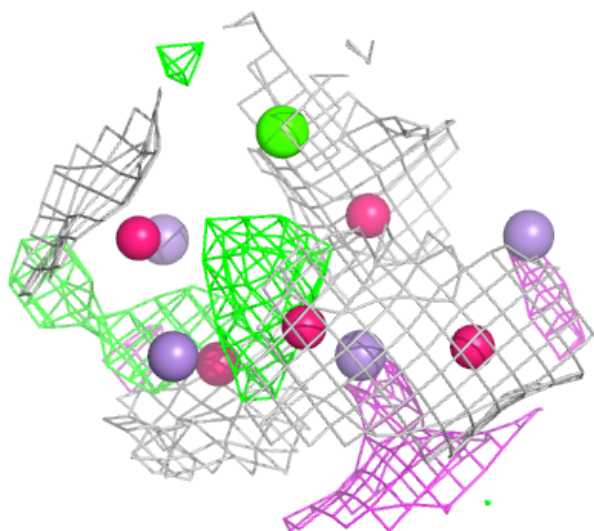
Electron density around OEX A 412 (A):

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



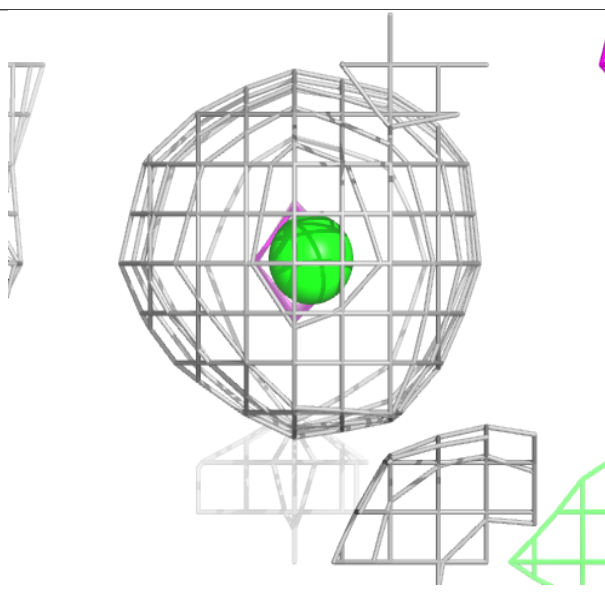
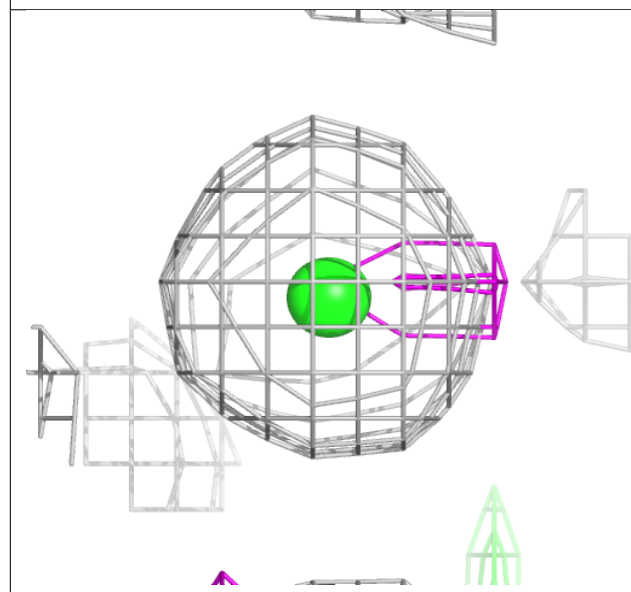
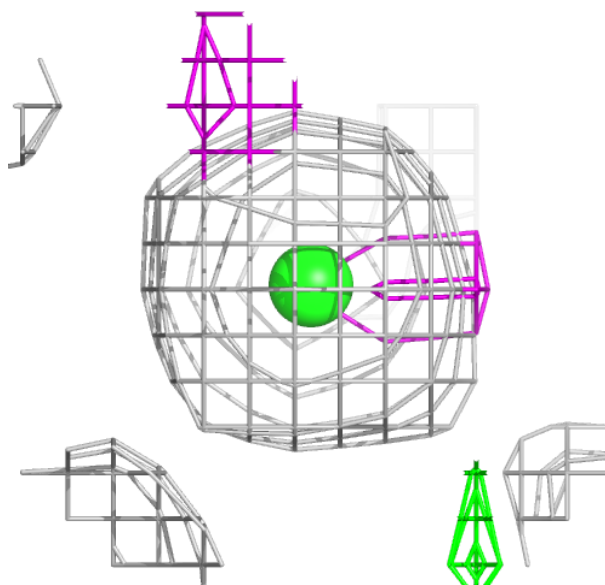
Electron density around OEX A 412 (B):

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



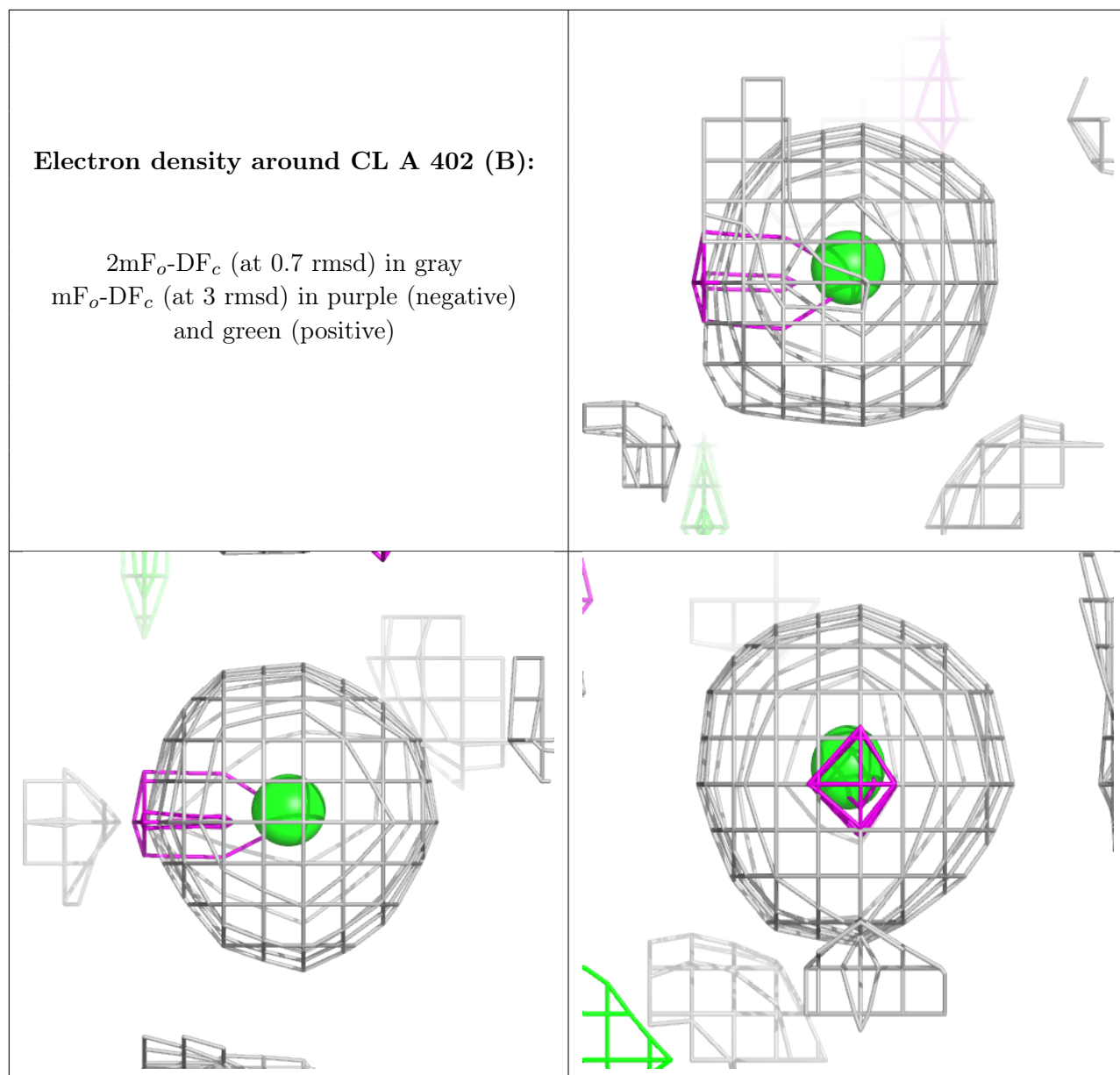
Electron density around CL A 402 (A):

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



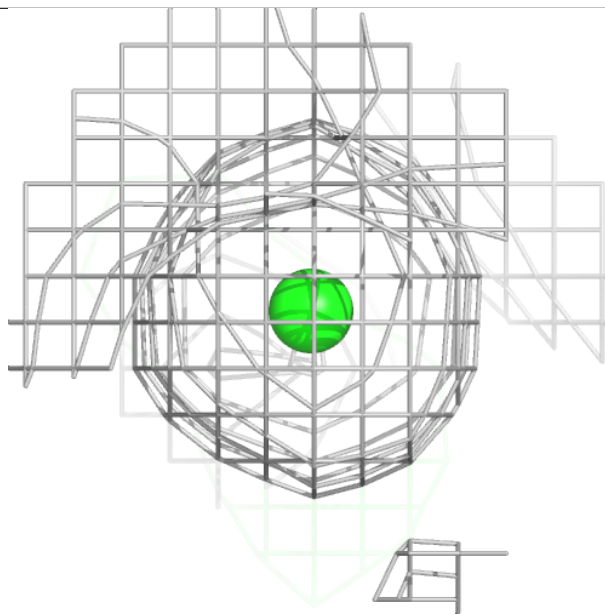
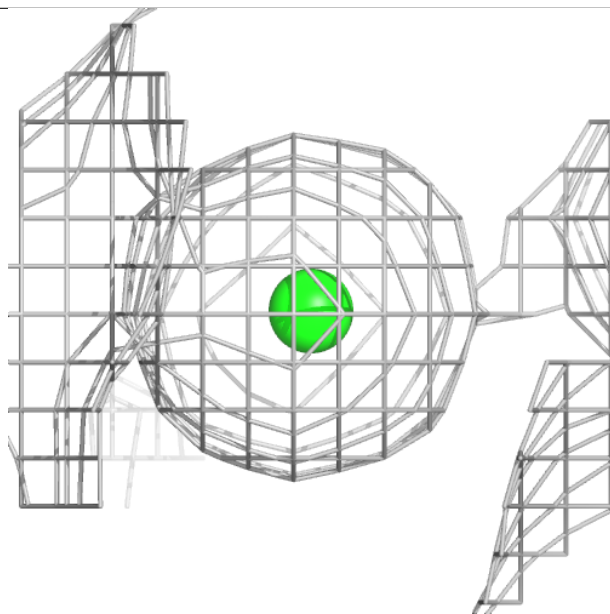
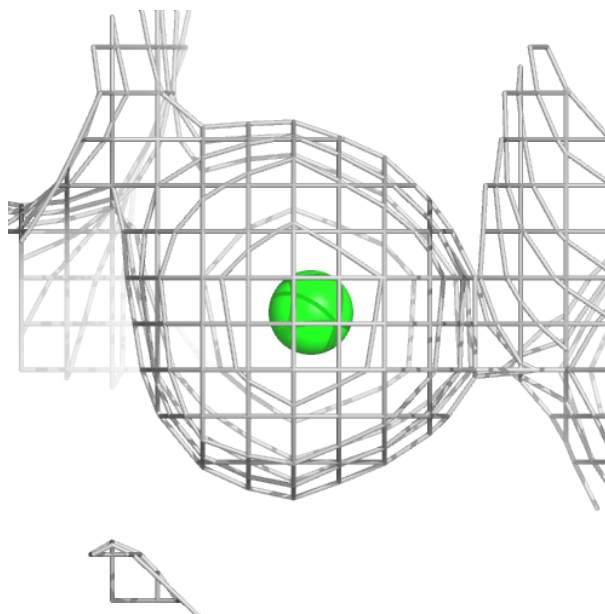
Electron density around CL A 402 (B):

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



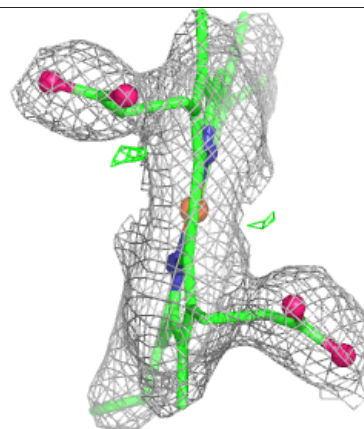
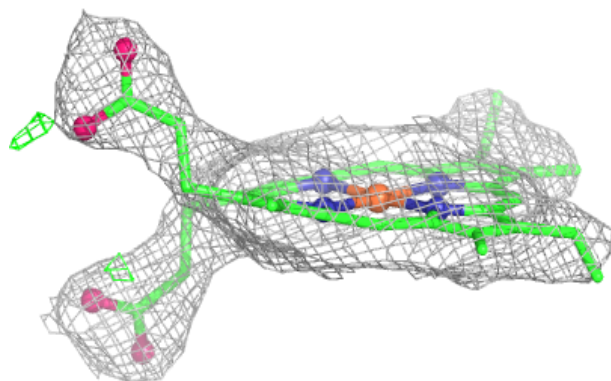
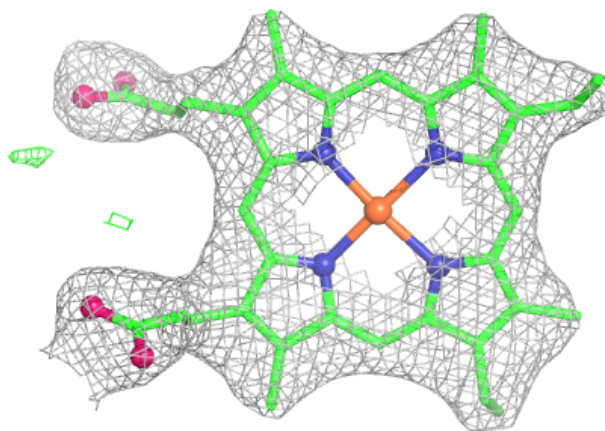
Electron density around CL A 403 (A):

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



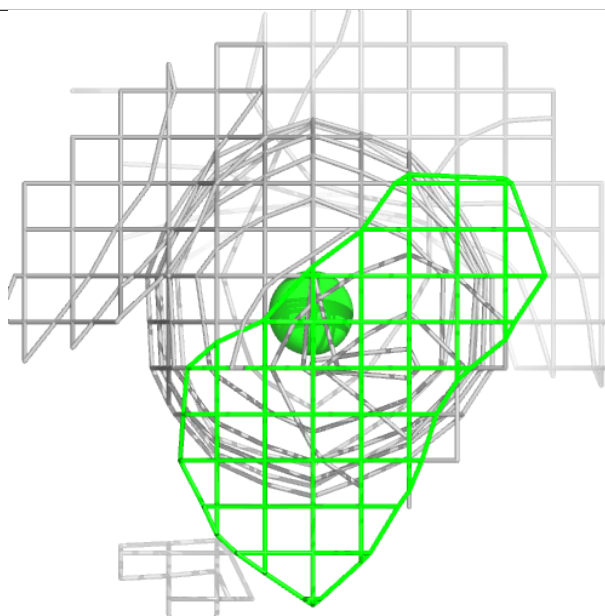
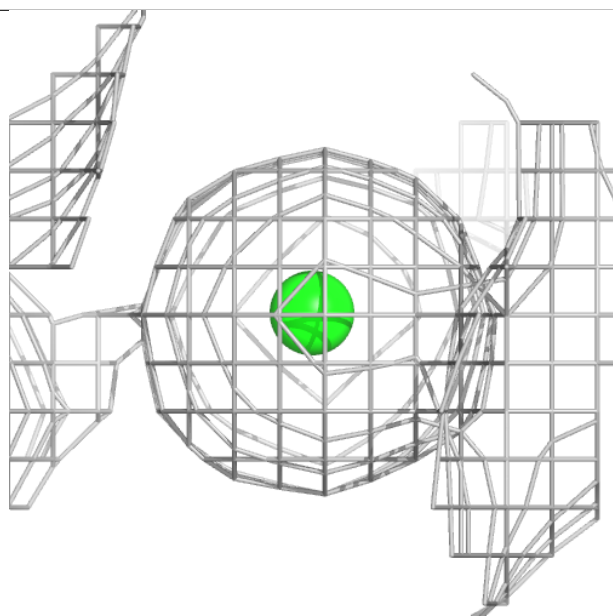
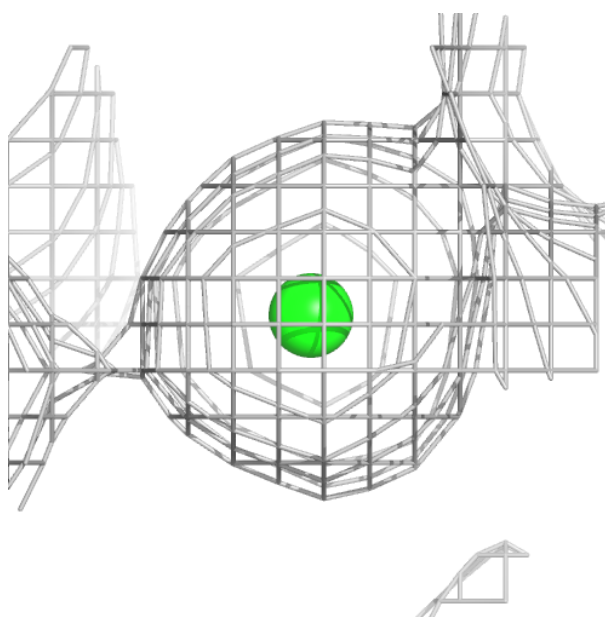
Electron density around HEM F 102:

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



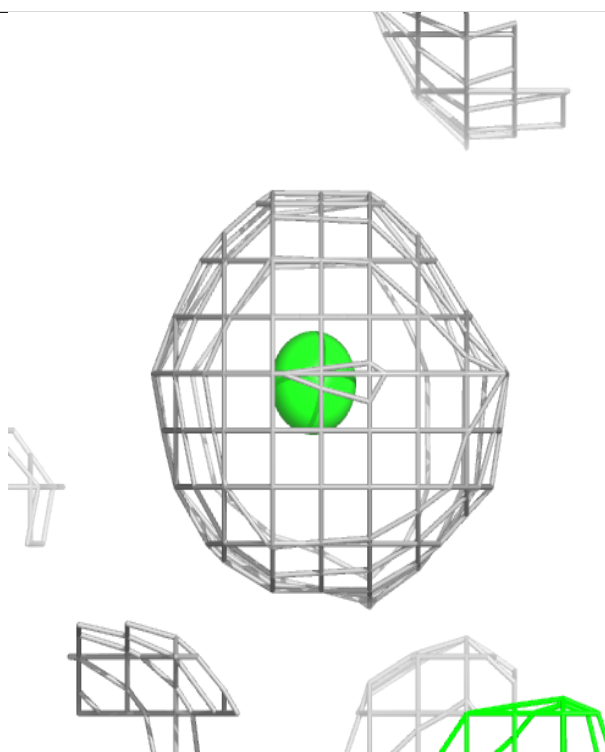
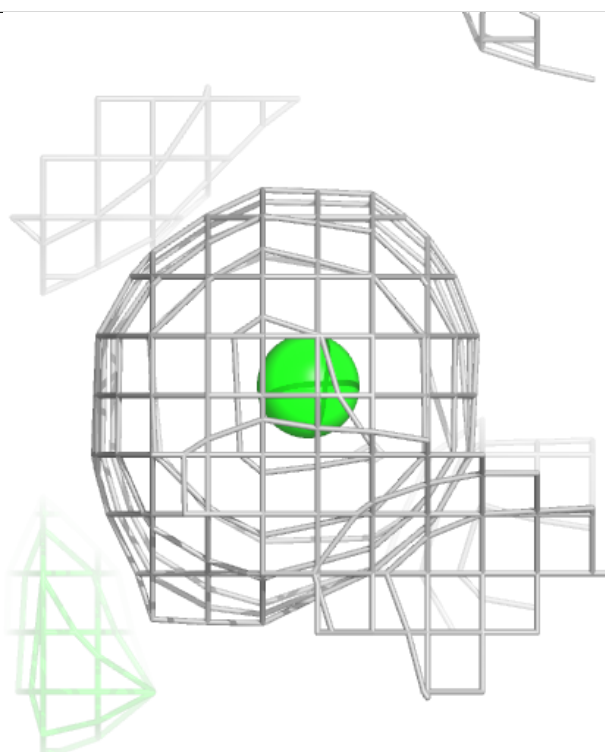
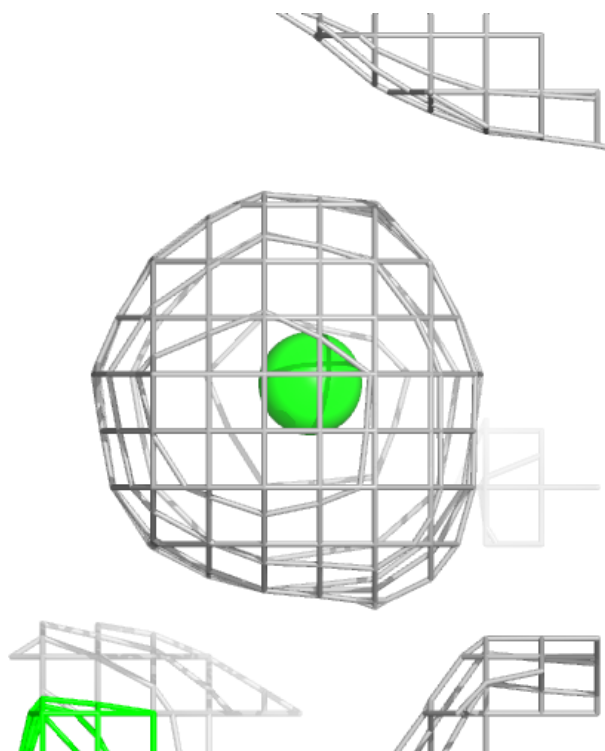
Electron density around CL A 403 (B):

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



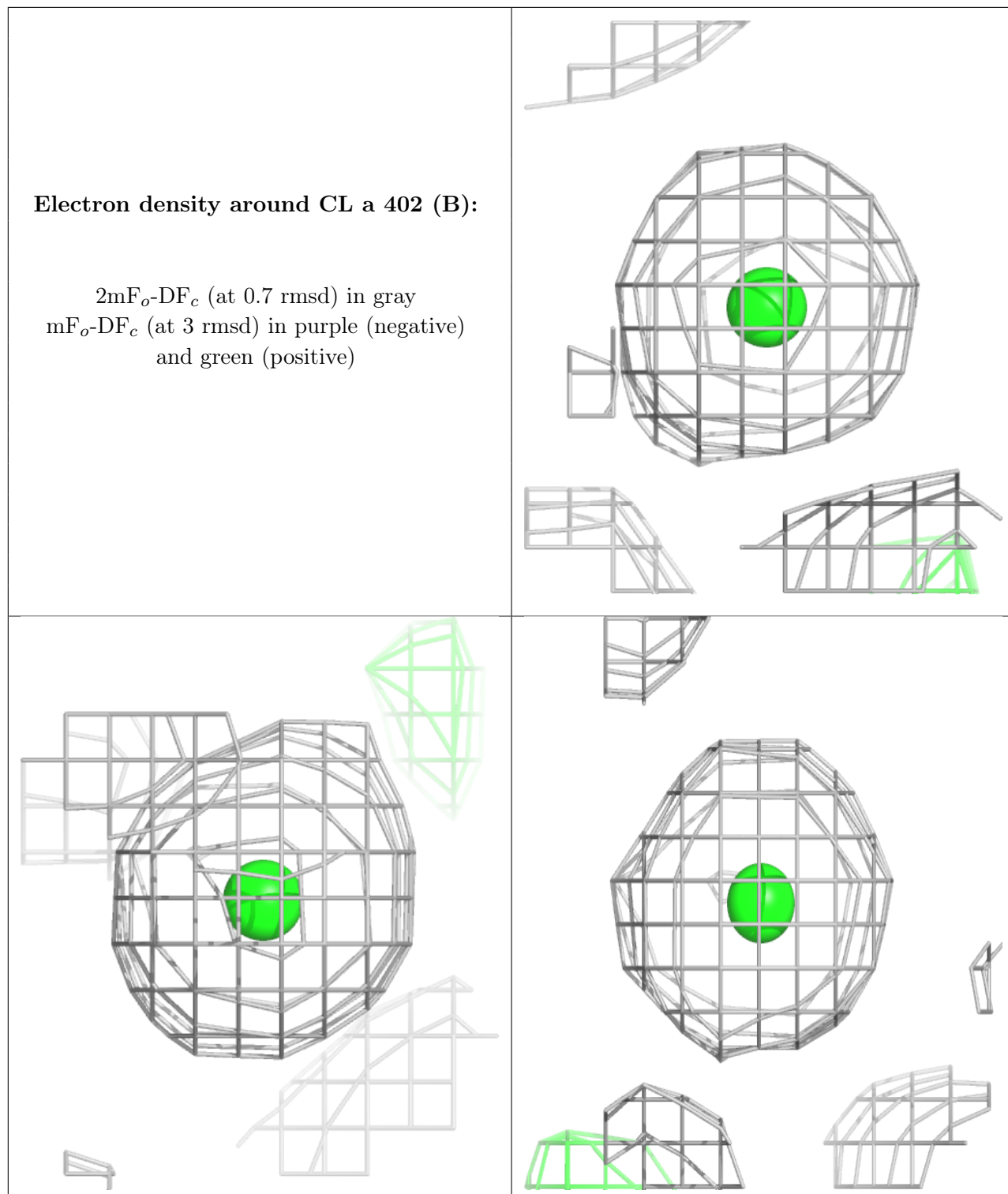
Electron density around CL a 402 (A):

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



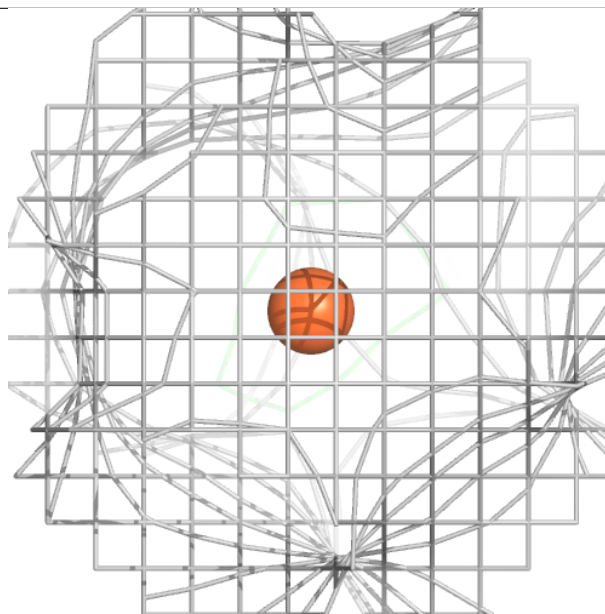
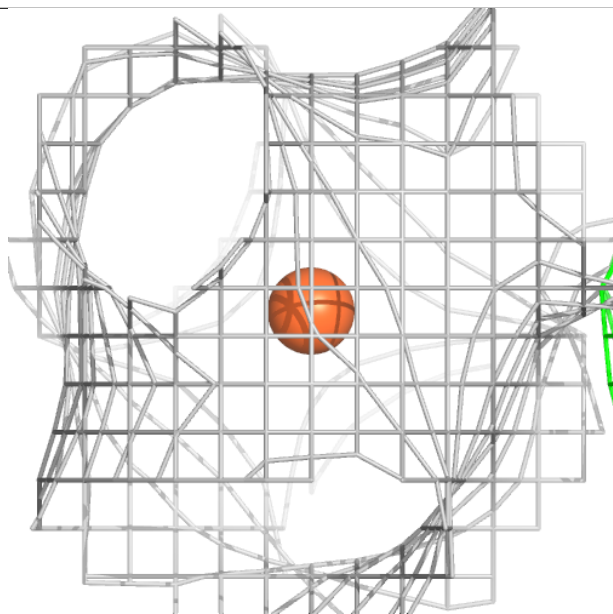
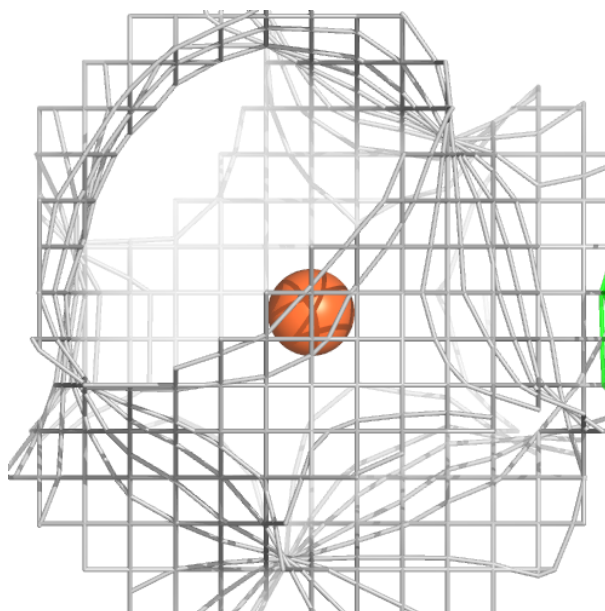
Electron density around CL a 402 (B):

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



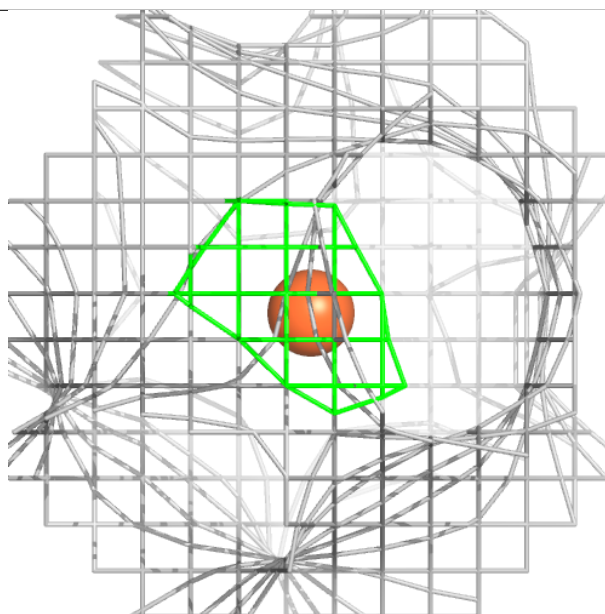
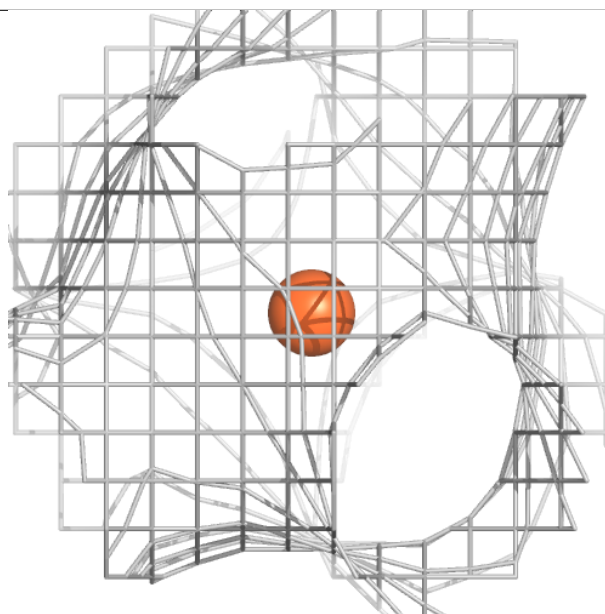
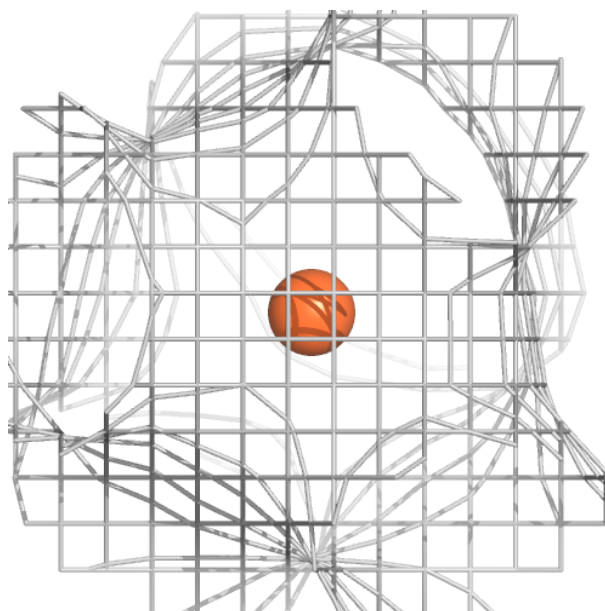
Electron density around FE2 A 401 (A):

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



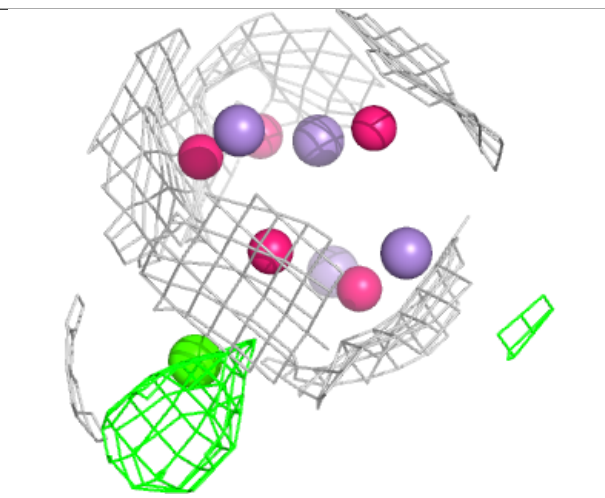
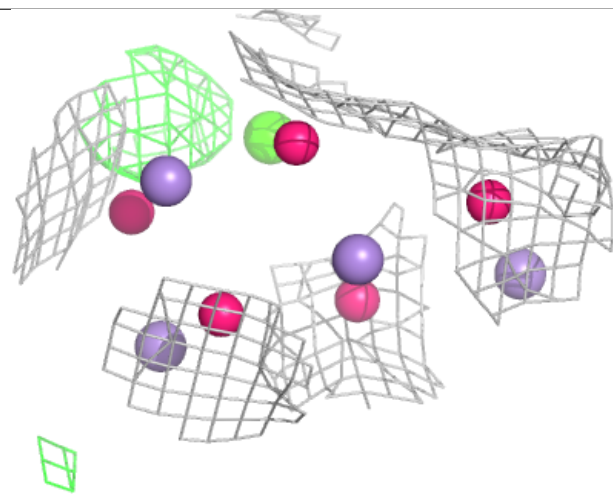
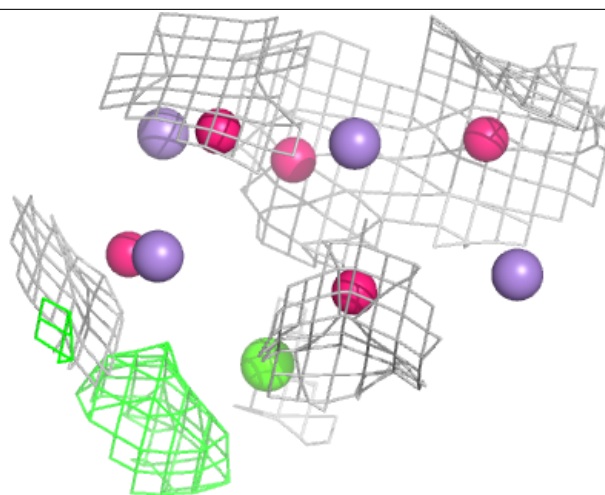
Electron density around FE2 A 401 (B):

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



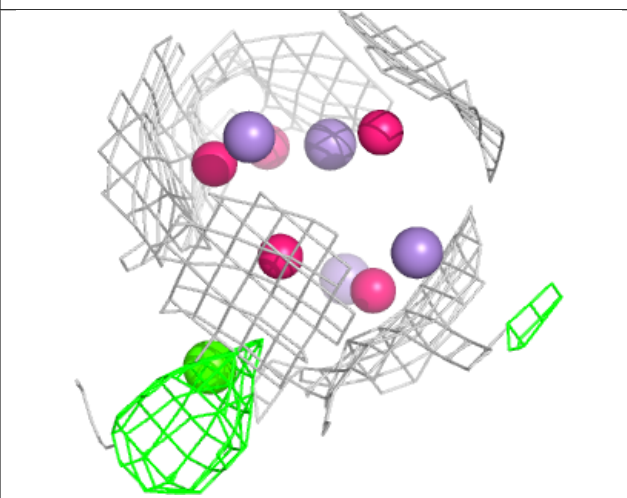
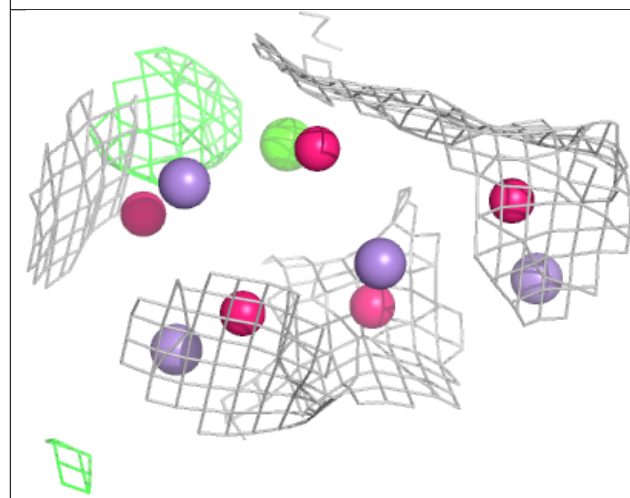
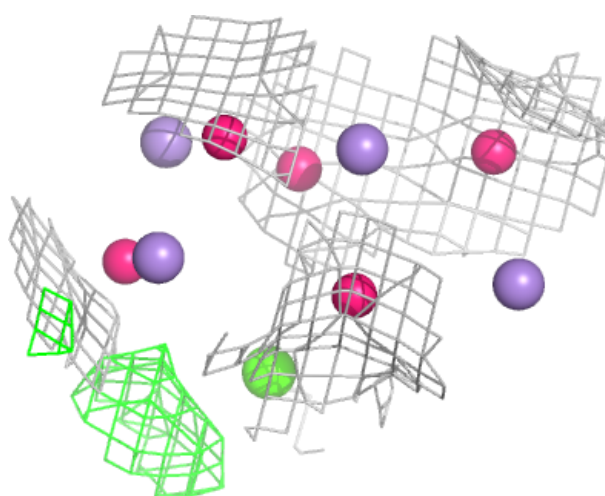
Electron density around OEX a 412 (A):

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



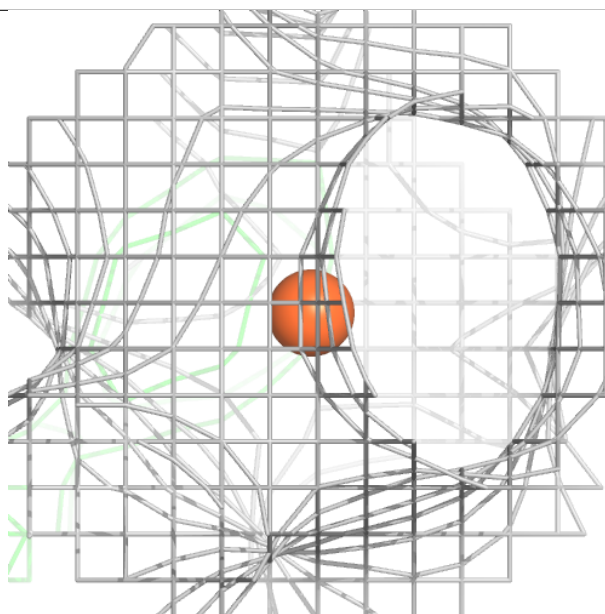
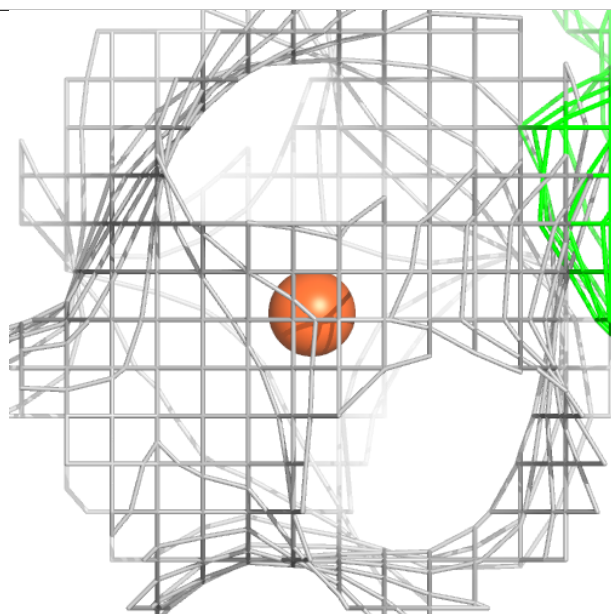
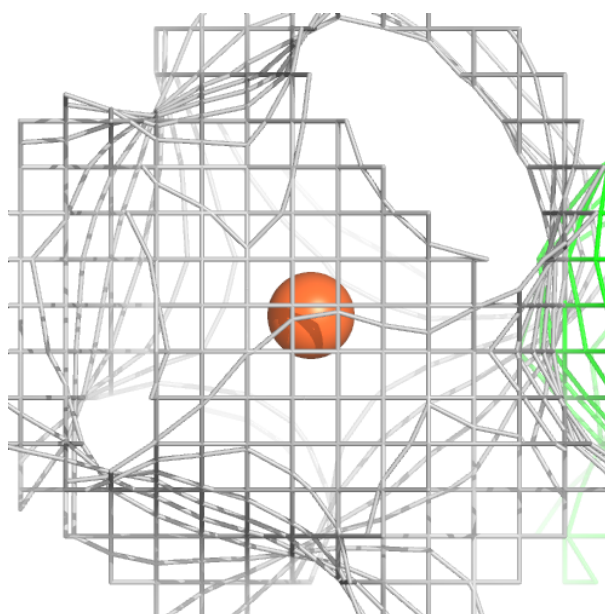
Electron density around OEX a 412 (B):

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



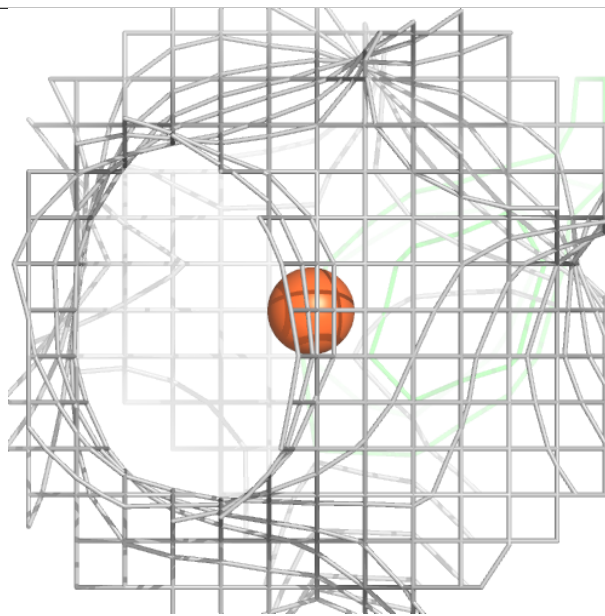
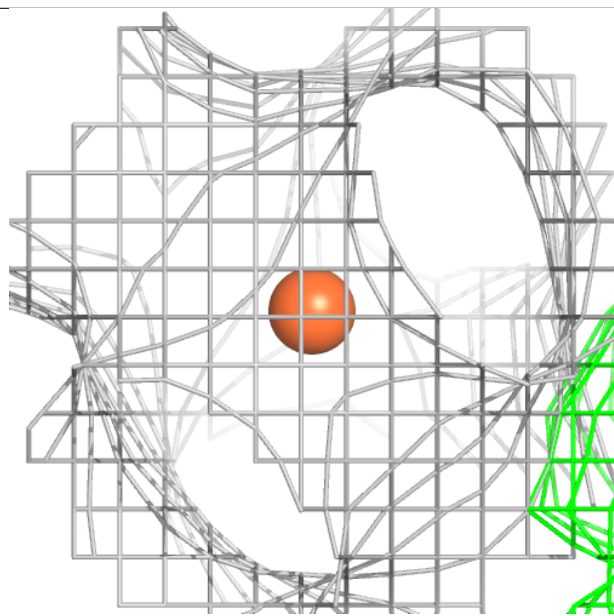
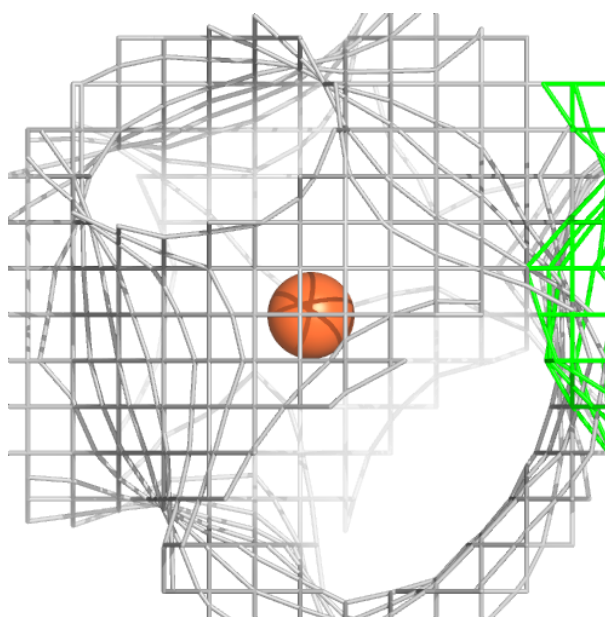
Electron density around FE2 a 401 (A):

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



Electron density around FE2 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.