Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 02:57 PM JST

PDB ID	:	8IR9 / pdb_00008ir9
Title	:	XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 30-microsecond delay
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.20 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:

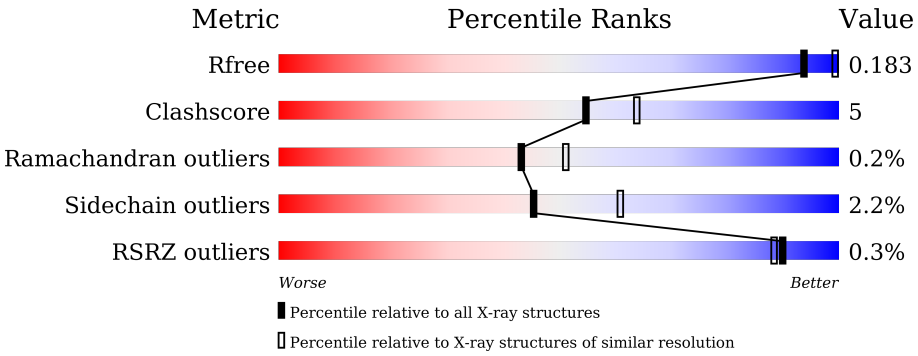
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.20 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.



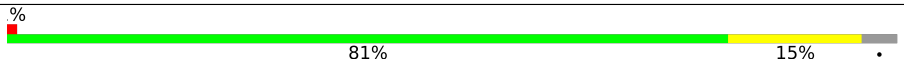
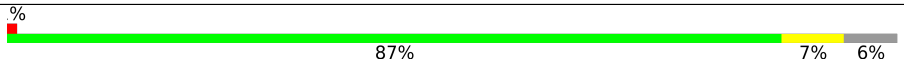
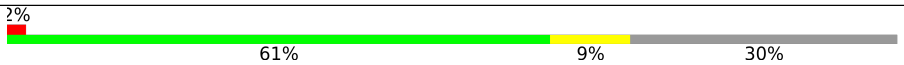
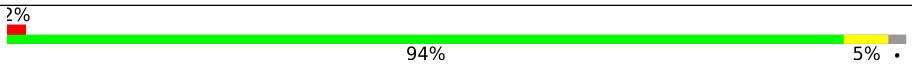
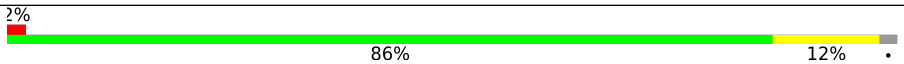
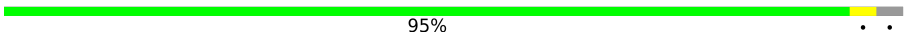
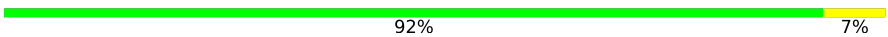
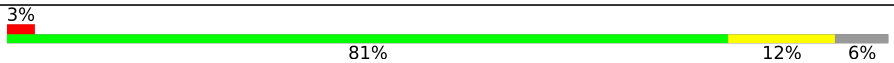
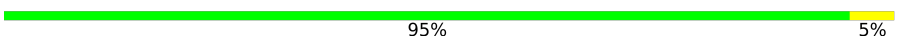
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	88% 9% .
2	B	505	92% 7%
2	b	505	90% 9% .
3	C	455	92% 7% .
3	c	455	91% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	137	91% 9%
17	X	40	90% 5% 5%
17	x	40	90% 5% 5%
18	Y	30	3% 87% 10%
18	y	30	60% 37%
19	Z	62	90% 8%
19	z	62	77% 21%
20	R	34	6% 74% 26%

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
27	GOL	D	412	-	X	-	-
27	GOL	a	418	-	-	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 62674 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	220	0
			4318	2821	715	757	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	22	0
			4166	2735	694	724	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	99	0
			4272	2796	715	743	18			
3	c	455	Total	C	N	O	S	0	101	0
			4316	2827	720	751	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	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	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	5	0
			815	519	135	161			

- 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 289	C 194	N 46	O 49	0	1	0
17	x	38	Total 281	C 188	N 45	O 48	0	0	0

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

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

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

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

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	34	Total 273	C 186	N 47	O 40	0	0	0

- 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 2	Fe 2	0	1
21	a	1	Total 2	Fe 2	0	1

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

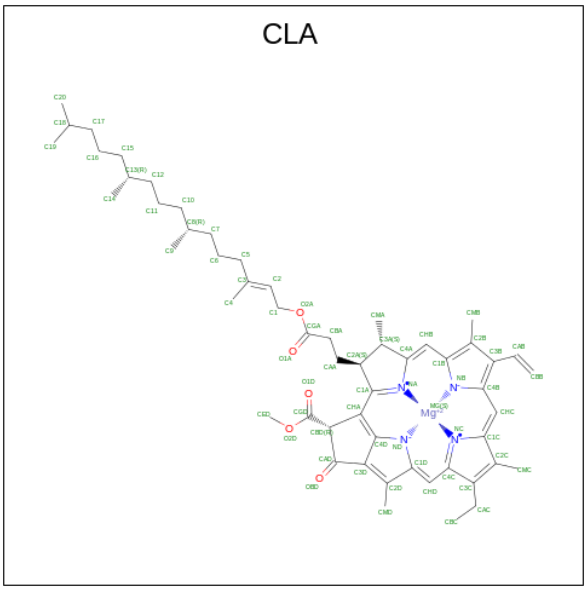
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 4	Cl 4	0	2

Continued on next page...

Continued from previous page...

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

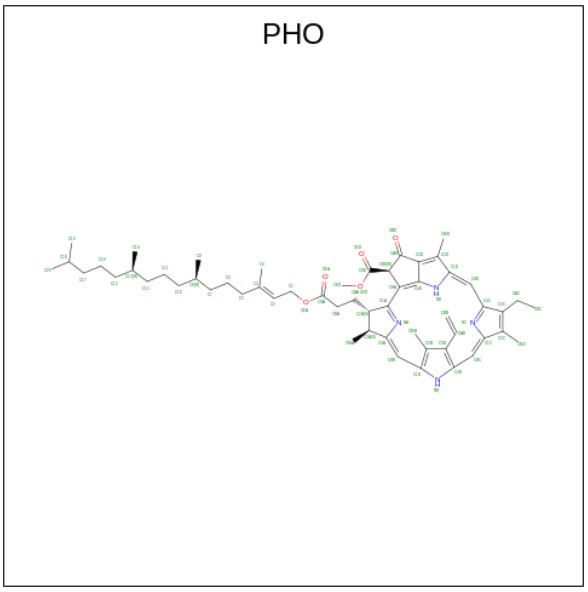
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110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

Continued on next page...

Continued from previous page...

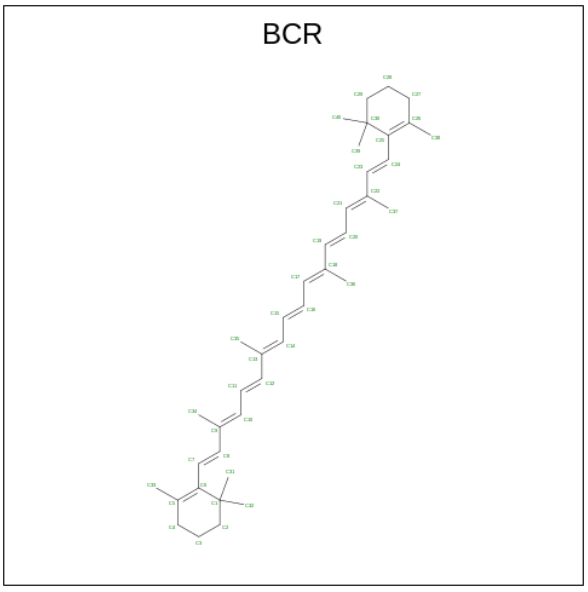
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



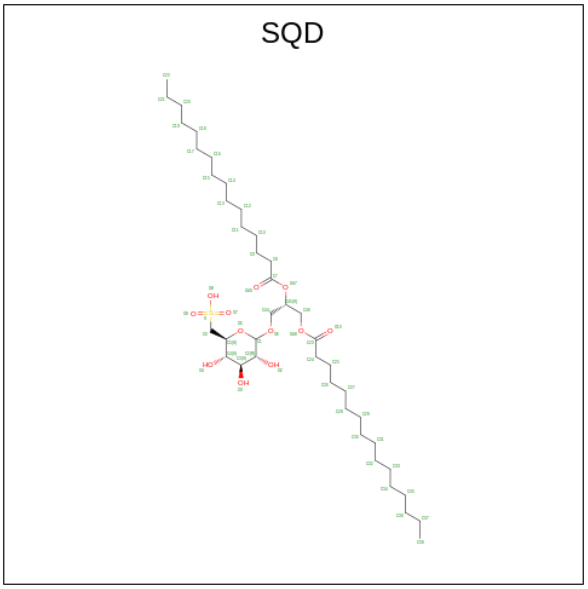
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



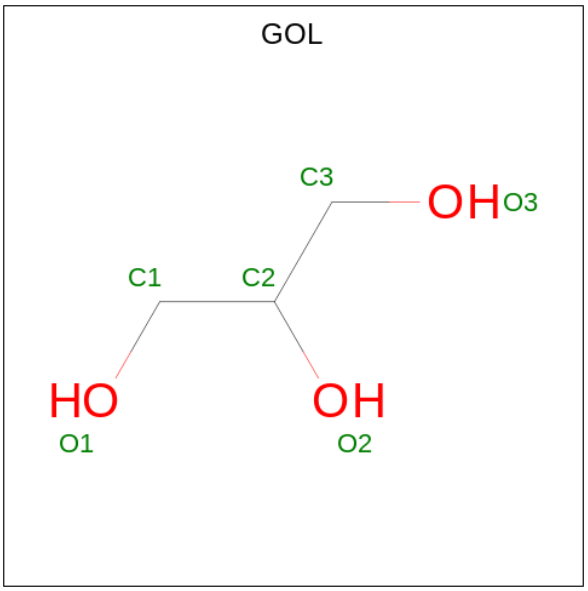
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



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

- Molecule 27 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



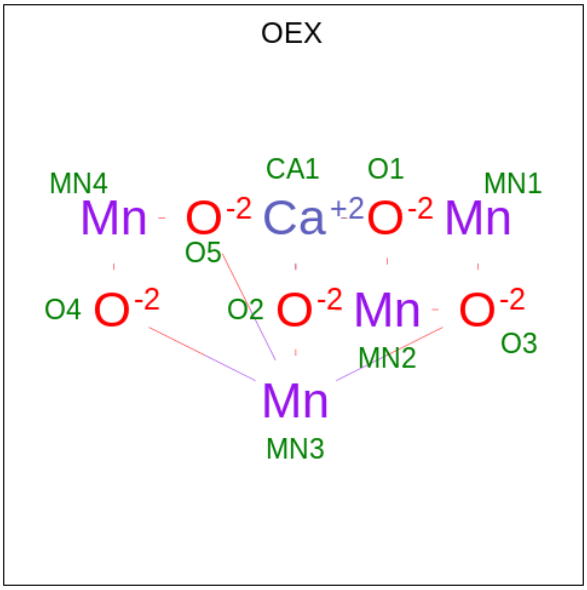
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

Continued on next page...

Continued from previous page...

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

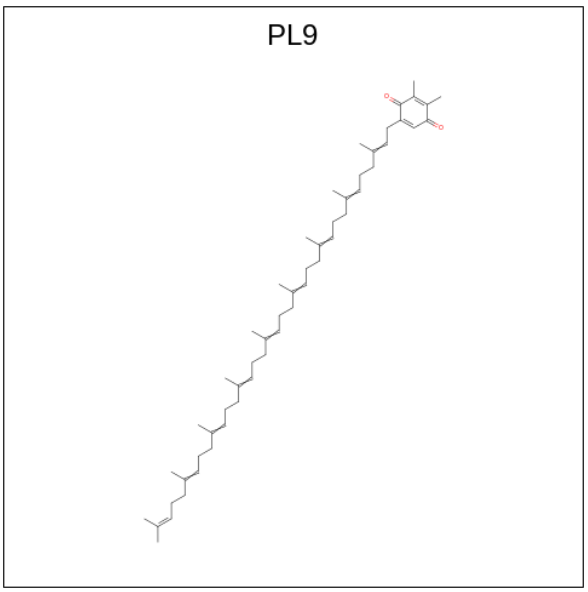
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total Ca Mn O 20 2 8 10	0	1
28	a	1	Total Ca Mn O 20 2 8 10	0	1

- Molecule 29 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$)

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



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

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

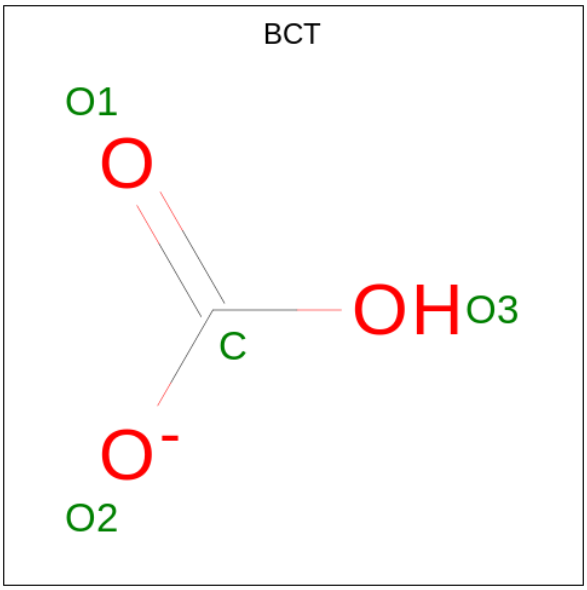
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 68 58 10	0	1
30	X	1	Total C O 18 16 2	0	0

Continued on next page...

Continued from previous page...

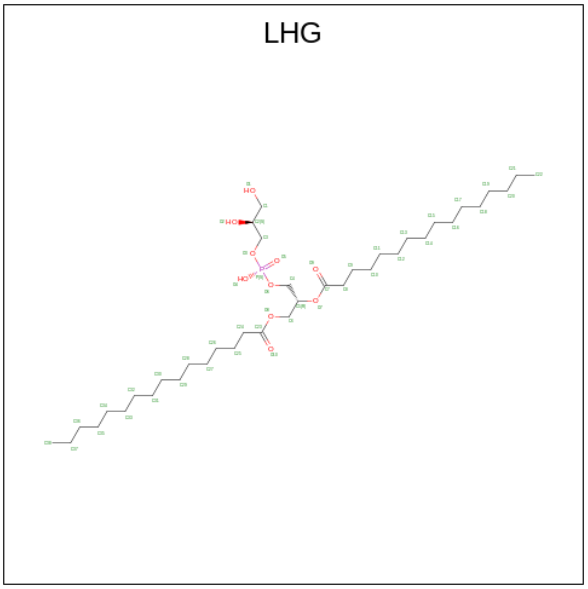
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	2	Total C O 69 59 10	0	0
30	c	1	Total C O 64 54 10	0	1
30	d	1	Total C O 17 16 1	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



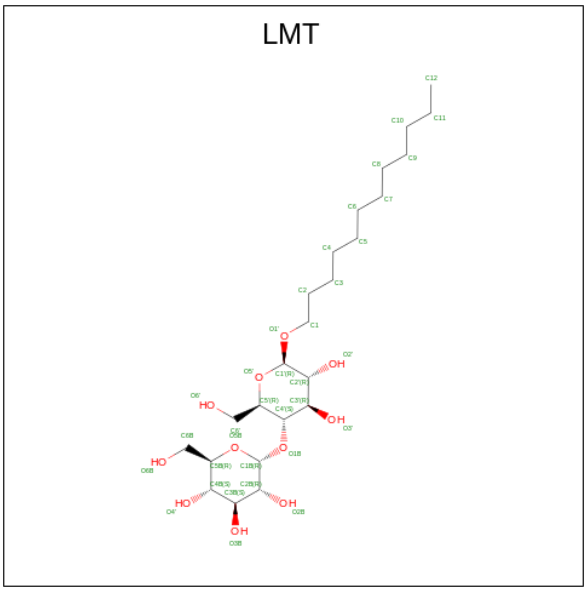
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 8 2 6	0	1
31	d	1	Total C O 8 2 6	0	1

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



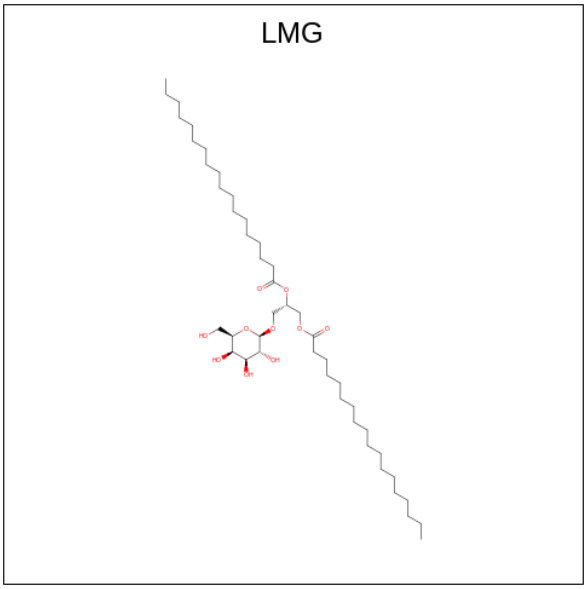
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	b	1	Total	C	O	P	0	1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

- Molecule 33 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



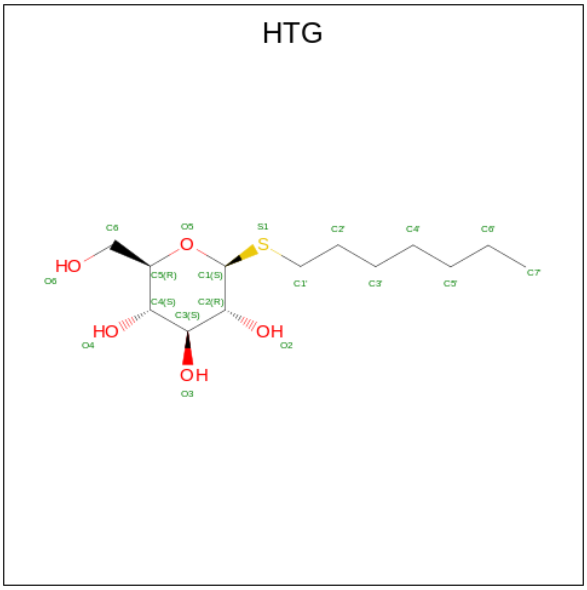
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	A	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			35	24	11		
33	B	1	Total	C	O	0	0
			25	19	6		
33	D	1	Total	C	O	0	0
			35	24	11		
33	F	1	Total	C	O	0	0
			35	24	11		
33	M	1	Total	C	O	0	0
			35	24	11		
33	T	1	Total	C	O	0	0
			35	24	11		
33	a	1	Total	C	O	0	0
			35	24	11		
33	b	1	Total	C	O	0	0
			25	19	6		
33	b	1	Total	C	O	0	0
			25	19	6		
33	e	1	Total	C	O	0	0
			35	24	11		
33	m	1	Total	C	O	0	0
			35	24	11		
33	t	1	Total	C	O	0	0
			26	19	7		

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



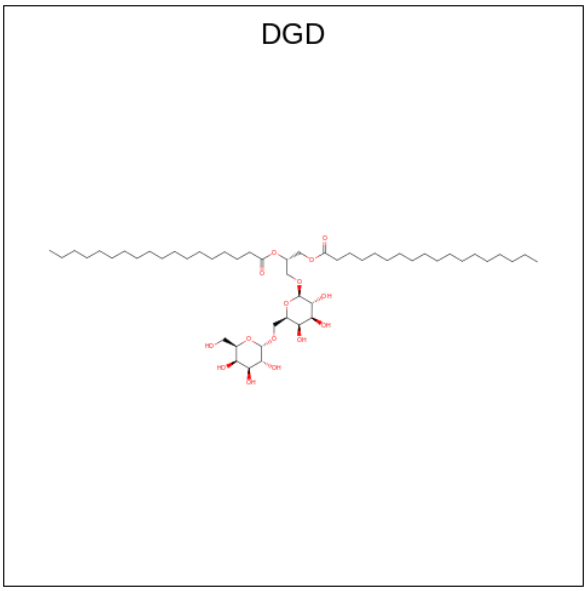
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	C	1	Total C O 51 41 10	0	0
34	D	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	c	1	Total C O 51 41 10	0	0
34	d	1	Total C O 51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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



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

- 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 124 94 30	0	1
36	C	1	Total C O 124 94 30	0	1
36	C	1	Total C O 62 47 15	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 124 94 30	0	1
36	c	1	Total C O 124 94 30	0	1
36	c	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

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

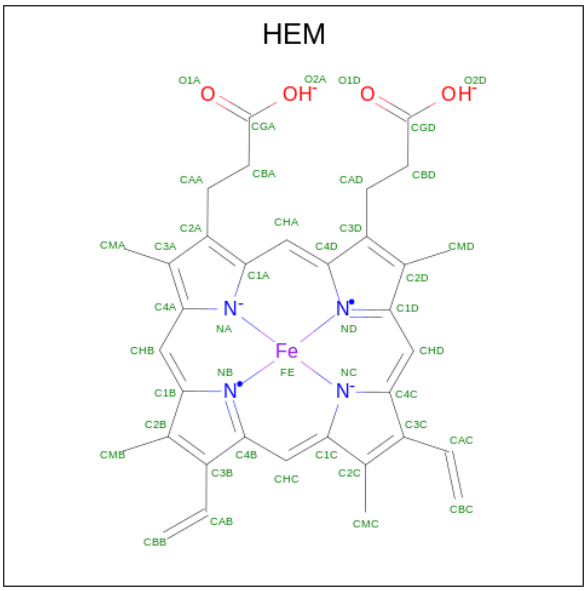
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Ca 1 1	0	0
37	F	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	c	2	Total Ca 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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: $C_{34}H_{32}FeN_4O_4$).

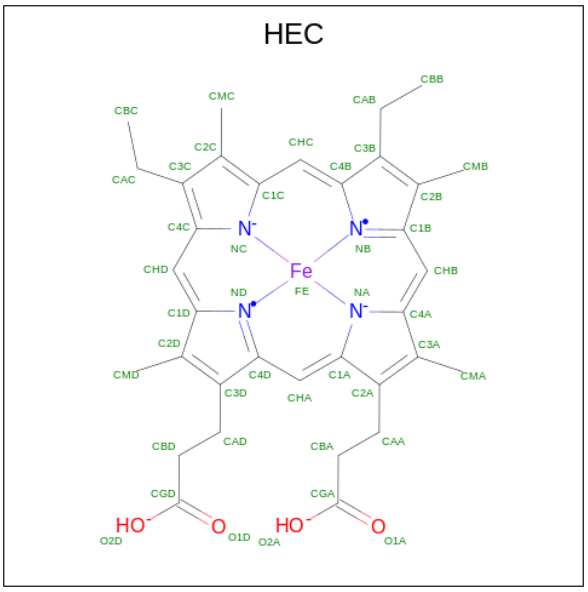


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	F	1	Total C Fe N O 43 34 1 4 4	0	0
38	f	1	Total C Fe N O 43 34 1 4 4	0	0

- 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: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	136	Total	O	0	85
			220	220		
41	B	187	Total	O	0	2
			189	189		
41	C	169	Total	O	0	38
			206	206		
41	D	122	Total	O	0	34
			156	156		
41	E	17	Total	O	0	0
			17	17		
41	F	5	Total	O	0	0
			5	5		
41	H	22	Total	O	0	0
			22	22		
41	I	5	Total	O	0	0
			5	5		
41	J	7	Total	O	0	0
			7	7		
41	K	5	Total	O	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	9	Total O 10 10	0	1
41	M	6	Total O 6 6	0	0
41	O	104	Total O 109 109	0	5
41	T	10	Total O 13 13	0	3
41	U	46	Total O 49 49	0	3
41	V	82	Total O 83 83	0	1
41	X	8	Total O 8 8	0	0
41	a	130	Total O 211 211	0	82
41	b	200	Total O 203 203	0	3
41	c	160	Total O 193 193	0	34
41	d	115	Total O 146 146	0	31
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	12	Total O 12 12	0	0
41	o	100	Total O 104 104	0	4
41	t	7	Total O 10 10	0	3

Continued on next page...

Continued from previous page...

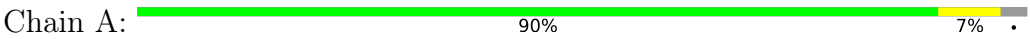
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	u	50	Total O 51 51	0	1
41	v	58	Total O 60 60	0	2
41	x	8	Total O 8 8	0	0
41	y	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

Chain A:



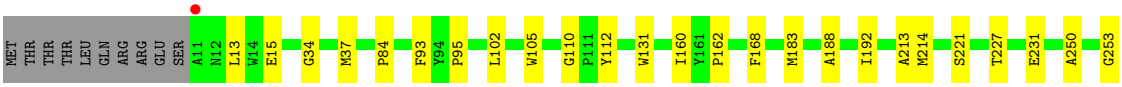




• Molecule 1: Photosystem II protein D1

Chain a:

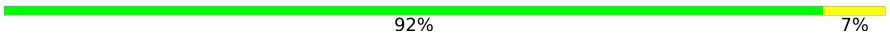


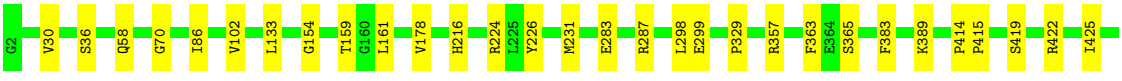


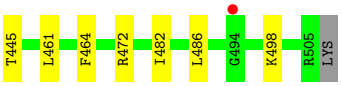


• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



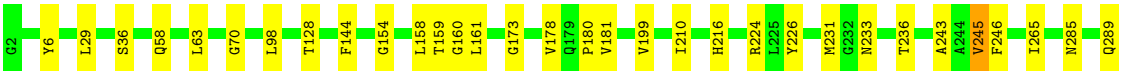


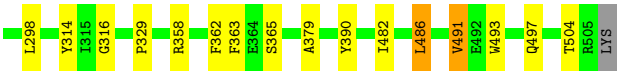


• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



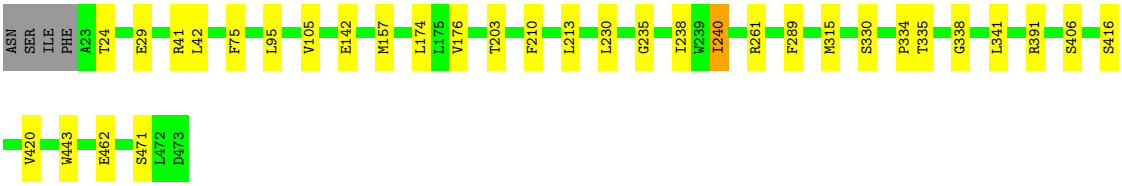




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

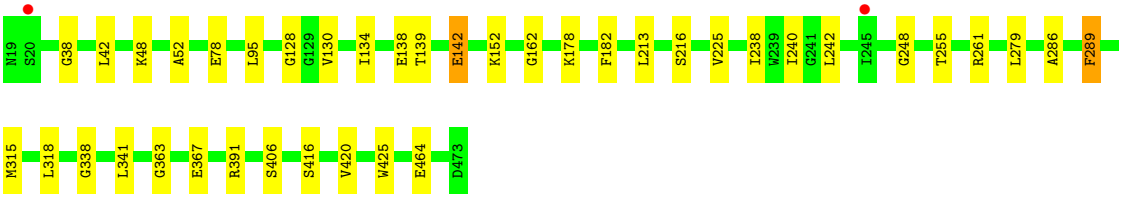




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

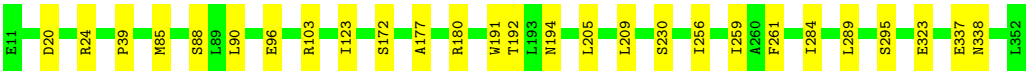




• Molecule 4: Photosystem II D2 protein

Chain D:

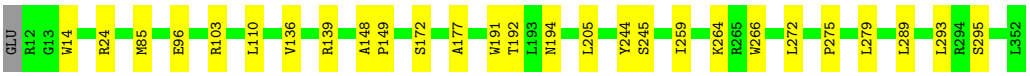




• Molecule 4: Photosystem II D2 protein

Chain d:

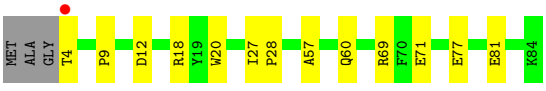




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

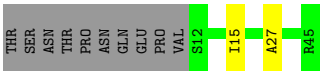




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

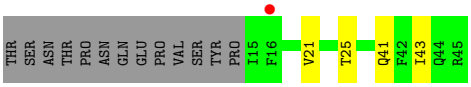




• Molecule 6: Cytochrome b559 subunit beta

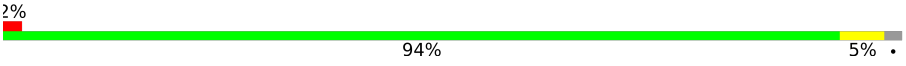
Chain f:

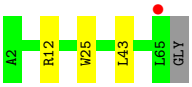




• Molecule 7: Photosystem II reaction center protein H

Chain H:

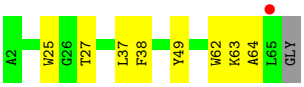




• Molecule 7: Photosystem II reaction center protein H

Chain h:





• Molecule 8: Photosystem II reaction center protein I

Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

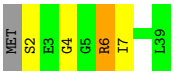




• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:

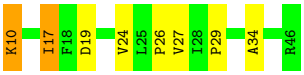




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

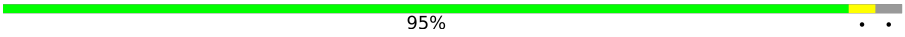
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:

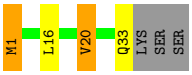




• Molecule 12: Photosystem II reaction center protein M

Chain M:

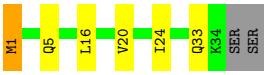




• Molecule 12: Photosystem II reaction center protein M

Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

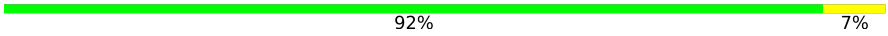






• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

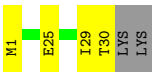




• Molecule 14: Photosystem II reaction center protein T

Chain T:

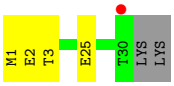




• Molecule 14: Photosystem II reaction center protein T

Chain t:

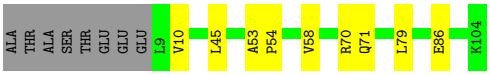




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

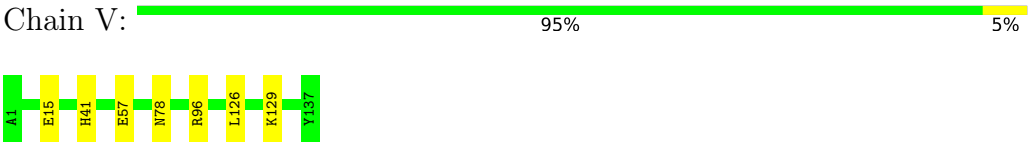
Chain u:





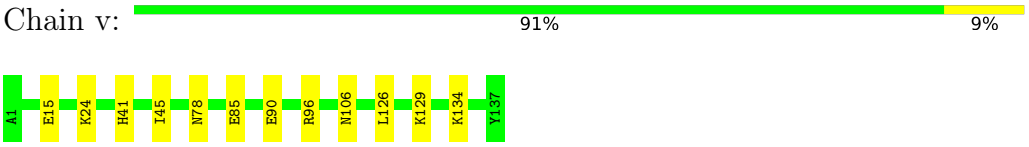
• Molecule 16: Cytochrome c-550

Chain V:



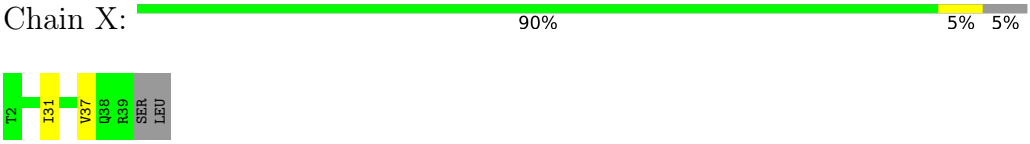
• Molecule 16: Cytochrome c-550

Chain v:



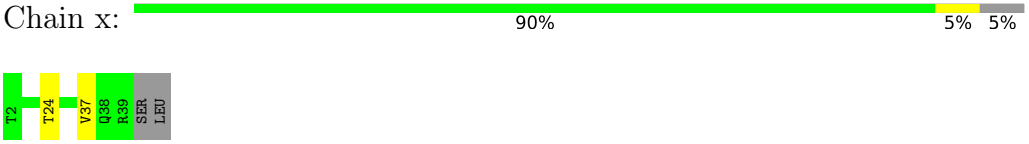
• Molecule 17: Photosystem II reaction center protein X

Chain X:



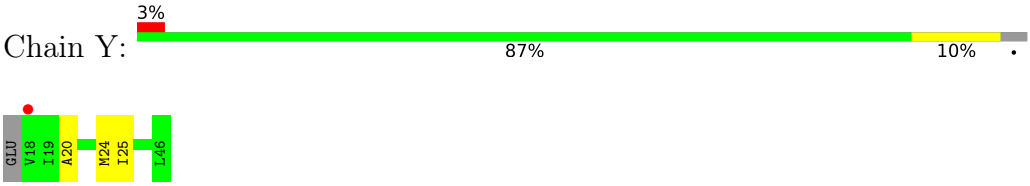
• Molecule 17: Photosystem II reaction center protein X

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



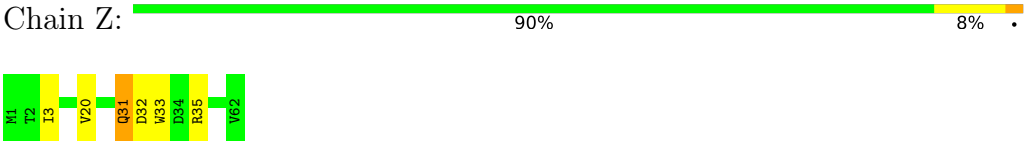
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



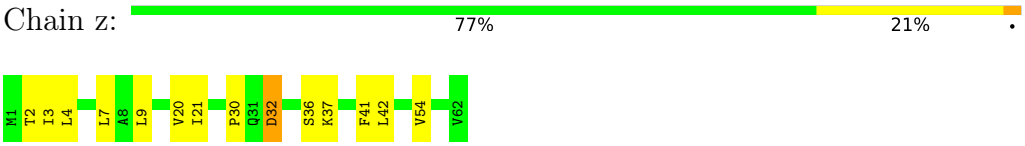
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



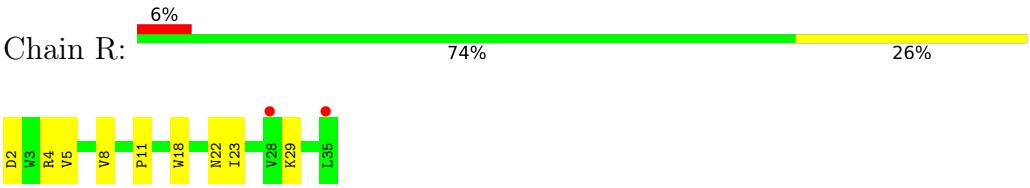
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.20) 99.7 (19.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.140 , 0.176 0.153 , 0.183	Depositor DCC
R_{free} test set	21187 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CLA, BCT, MG, PL9, GOL, LMT, HTG, DGD, CA, FE2, SQD, CL, FME, HEM, LMG, HEC, LHG, UNL, OEX, PHO, BCR

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	0.45	0/6098
1	a	0.25	0/4457	0.41	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.31	0/4285	0.48	0/5841
3	C	0.27	0/4416	0.42	0/6013
3	c	0.27	0/4467	0.42	0/6082
4	D	0.32	0/3746	0.46	0/5102
4	d	0.29	0/3780	0.45	0/5147
5	E	0.31	0/681	0.48	0/928
5	e	0.28	0/690	0.46	0/939
6	F	0.31	0/284	0.43	0/387
6	f	0.26	0/269	0.41	0/365
7	H	0.30	0/519	0.47	0/708
7	h	0.28	0/530	0.46	0/722
8	I	0.27	0/311	0.41	0/419
8	i	0.31	0/311	0.45	0/419
9	J	0.29	0/278	0.36	0/376
9	j	0.27	0/283	0.38	0/383
10	K	0.33	0/303	0.50	0/416
10	k	0.30	0/303	0.45	0/416
11	L	0.35	0/318	0.46	0/433
11	l	0.36	0/318	0.50	0/433
12	M	0.37	0/261	0.52	0/357
12	m	0.31	0/279	0.46	0/380
13	O	0.33	0/1991	0.50	0/2698
13	o	0.31	0/1966	0.49	0/2665
14	T	0.33	0/310	0.41	0/419
14	t	0.33	0/301	0.41	0/406
15	U	0.35	0/811	0.54	0/1095
15	u	0.34	0/826	0.52	0/1116
16	V	0.34	0/1142	0.48	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.29	0/1139	0.46	0/1542
17	X	0.23	0/292	0.34	0/395
17	x	0.23	0/284	0.36	0/384
18	Y	0.24	0/216	0.42	0/289
18	y	0.22	0/216	0.36	0/289
19	Z	0.21	0/490	0.34	0/669
19	z	0.21	0/490	0.39	0/669
20	R	0.24	0/279	0.34	0/383
All	All	0.30	0/50634	0.45	0/68876

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	21	0
1	a	4318	0	4124	36	0
2	B	4166	0	3999	26	0
2	b	4134	0	3976	38	0
3	C	4272	0	4138	22	0
3	c	4316	0	4184	32	0
4	D	3625	0	3489	28	0
4	d	3658	0	3522	26	0
5	E	662	0	648	10	0
5	e	670	0	655	6	0
6	F	275	0	282	2	0
6	f	261	0	269	5	0
7	H	506	0	529	2	0
7	h	517	0	541	6	0
8	I	314	0	328	4	0
8	i	314	0	328	3	0
9	J	272	0	279	5	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	3	0
10	K	293	0	305	6	0
10	k	293	0	305	5	0
11	L	311	0	320	2	0
11	l	311	0	320	4	0
12	M	268	0	285	4	0
12	m	286	0	305	8	0
13	O	1958	0	1920	24	0
13	o	1933	0	1900	8	0
14	T	311	0	318	2	0
14	t	302	0	311	4	0
15	U	800	0	796	5	0
15	u	815	0	817	4	0
16	V	1120	0	1122	4	0
16	v	1117	0	1131	7	0
17	X	289	0	322	2	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	5	0
19	Z	479	0	516	2	0
19	z	479	0	516	3	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	19	0
23	B	1040	0	1152	27	0
23	C	845	0	936	33	0
23	D	195	0	216	7	0
23	a	455	0	504	20	0
23	b	1040	0	1152	21	0
23	c	845	0	936	38	0
23	d	195	0	216	5	0
24	A	256	0	296	5	0
24	a	256	0	296	5	0
25	A	40	0	56	1	0
25	B	120	0	168	5	0
25	C	80	0	112	1	0
25	D	40	0	56	0	0
25	H	40	0	56	2	0
25	K	40	0	56	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	5	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	8	0
25	c	80	0	112	1	0
25	d	40	0	56	3	0
25	h	40	0	56	6	0
25	k	40	0	56	2	0
25	t	40	0	56	4	0
25	y	40	0	56	1	0
26	A	162	0	232	4	0
26	F	43	0	53	3	0
26	L	54	0	78	1	0
26	a	162	0	232	11	0
26	b	54	0	78	4	0
26	f	43	0	53	1	0
27	A	12	0	15	4	0
27	B	18	0	24	2	0
27	C	12	0	16	0	0
27	D	6	0	8	2	0
27	O	12	0	16	4	0
27	V	12	0	16	0	0
27	a	12	0	16	5	0
27	b	12	0	16	3	0
27	c	18	0	24	0	0
27	d	6	0	8	0	0
27	l	12	0	16	2	0
27	o	12	0	16	0	0
27	v	12	0	16	3	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	17	0
29	D	110	0	160	0	0
29	a	110	0	160	10	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	X	18	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	69	0	0	0	0
30	c	64	0	0	0	0
30	d	17	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	8	0	0	0	0
31	d	8	0	0	0	0
32	A	98	0	148	3	0
32	D	196	0	296	13	0
32	E	84	0	114	6	0
32	L	98	0	148	0	0
32	a	84	0	114	8	0
32	b	98	0	148	1	0
32	d	294	0	444	25	0
33	A	35	0	46	2	0
33	B	95	0	127	3	0
33	D	35	0	46	1	0
33	F	35	0	46	0	0
33	M	35	0	46	2	0
33	T	35	0	46	0	0
33	a	35	0	46	2	0
33	b	50	0	70	1	0
33	e	35	0	46	1	0
33	m	35	0	46	0	0
33	t	26	0	35	2	0
34	B	51	0	72	0	0
34	C	153	0	216	2	0
34	D	51	0	72	0	0
34	Z	37	0	44	2	0
34	c	153	0	216	3	0
34	d	51	0	72	4	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	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	c	19	0	26	1	0
35	d	16	0	17	1	0
35	o	19	0	26	1	0
36	C	310	0	410	7	0
36	H	62	0	82	1	0
36	c	310	0	410	8	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	1	0
40	v	43	0	30	0	0
41	A	220	0	0	1	0
41	B	189	0	0	2	0
41	C	206	0	0	2	0
41	D	156	0	0	2	0
41	E	17	0	0	2	0
41	F	5	0	0	0	0
41	H	22	0	0	0	0
41	I	5	0	0	0	0
41	J	7	0	0	0	0
41	K	5	0	0	1	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	109	0	0	1	0
41	T	13	0	0	0	0
41	U	49	0	0	0	0
41	V	83	0	0	0	0
41	X	8	0	0	0	0
41	a	211	0	0	2	0
41	b	203	0	0	0	0
41	c	193	0	0	3	0
41	d	146	0	0	0	0
41	e	9	0	0	0	0
41	f	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	h	17	0	0	0	0
41	i	2	0	0	0	0
41	j	1	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	12	0	0	0	0
41	o	104	0	0	0	0
41	t	10	0	0	0	0
41	u	51	0	0	1	0
41	v	60	0	0	0	0
41	x	8	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61528	582	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 (582) 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	1.47	0.94
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.51	0.92
27:A:418:GOL:H11	12:M:1:FME:HG2	1.52	0.91
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.55	0.87
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.62	0.81
4:d:192[A]:THR:HG23	23:d:402[A]:CLA:HBC2	1.64	0.80
23:B:601:CLA:H12	23:B:601:CLA:H71	1.65	0.77
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
4:d:192[B]:THR:HG23	23:d:402[B]:CLA:HBC2	1.69	0.75
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.70	0.74
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.70	0.73
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.71	0.73
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.72	0.71
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.73	0.70
23:A:408:CLA:H193	23:C:507:CLA:H101	1.73	0.70
32:D:407[A]:LHG:H112	32:D:407[A]:LHG:H382	1.74	0.70
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.73	0.70
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.74	0.69
23:C:514:CLA:H202	34:C:521:LMG:H402	1.74	0.69
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:408:CLA:H192	23:c:506:CLA:H142	1.73	0.69
27:b:628:GOL:HO1	27:b:628:GOL:HO3	1.40	0.69
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.74	0.69
27:a:418:GOL:O2	41:a:501:HOH:O	2.10	0.68
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.76	0.67
23:C:507:CLA:H142	36:C:517[B]:DGD:HAF2	1.77	0.66
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.78	0.66
32:d:406[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.76	0.66
23:a:408:CLA:H152	23:c:507:CLA:H142	1.77	0.65
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.30	0.65
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.78	0.65
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.80	0.64
29:A:414[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.64
33:B:628:LMT:H52	35:o:301:HTG:H4'1	1.78	0.64
27:O:303:GOL:O1	41:O:401:HOH:O	2.15	0.64
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.31	0.64
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.81	0.63
27:b:628:GOL:O3	27:b:628:GOL:O1	2.13	0.63
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.29	0.63
23:a:405[B]:CLA:HHC	23:a:405[B]:CLA:HBB1	1.80	0.62
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H112	1.81	0.62
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.82	0.62
23:C:507:CLA:H142	36:C:517[A]:DGD:HAF2	1.80	0.62
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	1.99	0.62
29:A:414[B]:PL9:H262	32:E:101[B]:LHG:H223	1.80	0.62
20:R:18:TRP:O	20:R:22:ASN:ND2	2.32	0.62
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.82	0.62
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.29	0.61
36:C:517[B]:DGD:O1A	41:C:601[B]:HOH:O	2.16	0.61
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.33	0.61
25:C:515:BCR:H352	34:C:521:LMG:H352	1.83	0.61
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.82	0.61
2:b:285:ASN:O	2:b:289:GLN:HG2	2.00	0.61
10:K:17:ILE:H	10:K:17:ILE:HD13	1.65	0.60
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.83	0.60
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.31	0.60
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.83	0.60
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.84	0.60
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.83	0.60
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	1.83	0.60
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:601:CLA:H72	23:b:601:CLA:H2	1.85	0.59
1:A:102:LEU:HD12	35:b:625:HTG:H61	1.84	0.59
23:a:405[A]:CLA:HHC	23:a:405[A]:CLA:HBB1	1.85	0.58
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.84	0.58
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.85	0.58
26:a:410[A]:SQD:H152	32:d:407[A]:LHG:H172	1.86	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.69	0.58
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.67	0.58
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.03	0.58
2:b:98:LEU:HB2	35:b:622:HTG:H7'1	1.86	0.58
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.36	0.58
27:a:418:GOL:O3	14:t:2:GLU:OE1	2.21	0.57
2:B:226:TYR:HA	2:B:231:MET:HG3	1.85	0.57
29:A:414[B]:PL9:H253	23:D:402[B]:CLA:H141	1.86	0.57
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.35	0.57
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.87	0.56
25:T:102:BCR:H19C	25:b:618:BCR:H363	1.87	0.56
26:a:410[A]:SQD:H321	23:c:509:CLA:H102	1.87	0.56
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.40	0.56
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.05	0.56
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.87	0.56
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.06	0.56
26:a:410[A]:SQD:H141	32:d:407[A]:LHG:H152	1.86	0.56
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.87	0.56
25:b:619:BCR:H331	25:b:619:BCR:C8	2.36	0.56
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.86	0.56
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.41	0.56
23:c:503:CLA:H61	23:c:513:CLA:H42	1.89	0.55
27:a:417:GOL:H32	12:m:1:FME:HG3	1.88	0.55
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.07	0.55
34:z:101:LMG:H302	34:z:101:LMG:H141	1.89	0.55
29:A:414[A]:PL9:H503	26:F:103:SQD:H341	1.89	0.54
24:A:417[B]:PHO:H3A	23:D:402[B]:CLA:H142	1.90	0.54
23:a:406[A]:CLA:H191	32:a:419[A]:LHG:H111	1.88	0.54
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.06	0.54
24:a:415[B]:PHO:HBC3	4:d:279:LEU:HD22	1.90	0.54
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.54
23:a:406[B]:CLA:H191	32:a:419[B]:LHG:H111	1.88	0.54
4:D:261[B]:PHE:CZ	32:D:406[B]:LHG:HC81	2.43	0.54
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.13	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:ILE:HD11	36:H:102:DGD:HAH2	1.89	0.54
25:T:102:BCR:H321	25:T:102:BCR:HC8	1.90	0.54
34:c:520:LMG:H181	10:k:27:VAL:HG11	1.88	0.54
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.31	0.54
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.08	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.43	0.53
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.88	0.53
4:D:192[A]:THR:HG23	23:D:402[A]:CLA:HBC2	1.90	0.53
26:a:410[B]:SQD:H141	32:d:407[B]:LHG:H152	1.89	0.53
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.90	0.53
1:a:214[B]:MET:HB3	29:a:413[B]:PL9:H103	1.91	0.53
26:a:410[B]:SQD:H321	23:c:509:CLA:H102	1.90	0.53
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.91	0.53
19:Z:33:TRP:HZ2	34:Z:101:LMG:HC61	1.74	0.53
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.40	0.52
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.92	0.52
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.10	0.52
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.92	0.52
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.91	0.52
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.39	0.52
36:C:518[B]:DGD:HAT1	36:C:519:DGD:HBE1	1.92	0.52
13:O:42:ARG:O	13:O:241:ALA:HA	2.10	0.52
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.92	0.52
32:a:419[B]:LHG:HC31	5:e:9:PRO:HA	1.91	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.45	0.52
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.92	0.51
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.10	0.51
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.92	0.51
4:D:323[A]:GLU:O	27:D:412:GOL:O2	2.28	0.51
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.90	0.51
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.45	0.51
3:C:210:PHE:HA	3:C:213:LEU:HD13	1.92	0.51
24:a:415[A]:PHO:HBC3	4:d:279:LEU:HD22	1.91	0.51
4:D:85:MET:CE	4:D:96:GLU:HG2	2.40	0.51
2:b:497:GLN:HB2	2:b:504:THR:HB	1.92	0.51
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.92	0.51
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	1.91	0.51
35:B:623:HTG:H61	1:a:102:LEU:HD12	1.92	0.51
4:d:85:MET:CE	4:d:96:GLU:HG2	2.39	0.51
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.46	0.51
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:413[A]:PL9:H28	32:a:419[A]:LHG:H222	1.92	0.51
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.24	0.50
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.92	0.50
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.46	0.50
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.93	0.50
29:A:414[A]:PL9:H253	23:D:402[A]:CLA:H141	1.92	0.50
4:D:192[B]:THR:HG23	23:D:402[B]:CLA:HBC2	1.92	0.50
26:a:410[B]:SQD:H152	32:d:407[B]:LHG:H172	1.93	0.50
32:d:406[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.94	0.50
5:E:77:GLU:O	5:E:81:GLU:HG2	2.12	0.50
1:a:160[B]:ILE:HD11	36:c:517[B]:DGD:HBT1	1.93	0.50
32:a:419[A]:LHG:HC31	5:e:9:PRO:HA	1.93	0.50
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.94	0.50
2:b:226:TYR:HA	2:b:231:MET:HG3	1.93	0.50
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.92	0.50
33:B:629:LMT:H6E	33:t:101:LMT:H6D	1.94	0.49
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.42	0.49
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	1.94	0.49
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.94	0.49
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.93	0.49
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.45	0.49
19:z:32:ASP:O	19:z:36:SER:OG	2.17	0.49
3:C:203:THR:O	3:C:235:GLY:HA3	2.11	0.49
23:c:512:CLA:H191	34:z:101:LMG:H241	1.94	0.49
27:l:102[A]:GOL:H32	14:t:25:GLU:HB2	1.93	0.49
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.47	0.49
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	1.93	0.49
23:a:404[A]:CLA:H201	32:d:406[A]:LHG:H161	1.95	0.49
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.94	0.49
3:C:41:ARG:NH1	23:C:512:CLA:HMD1	2.28	0.49
29:a:413[B]:PL9:H28	32:a:419[B]:LHG:H222	1.95	0.49
3:C:157:MET:HE2	3:C:157:MET:HA	1.95	0.48
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.19	0.48
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.94	0.48
23:A:408:CLA:H41	23:A:408:CLA:H61	1.54	0.48
2:B:383[A]:PHE:CZ	13:O:167:GLY:HA2	2.48	0.48
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.43	0.48
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.94	0.48
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.79	0.48
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.47	0.48
27:a:418:GOL:H11	12:m:1:FME:HE3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:407[A]:LHG:H331	32:d:407[A]:LHG:H361	1.55	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.95	0.48
27:A:411:GOL:O3	27:A:411:GOL:O1	2.27	0.48
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.44	0.48
27:A:418:GOL:O2	41:A:501:HOH:O	2.20	0.48
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.96	0.48
4:D:323[B]:GLU:O	27:D:412:GOL:O2	2.32	0.48
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.94	0.48
3:c:464[B]:GLU:OE2	4:d:245[B]:SER:OG	2.31	0.48
34:c:521:LMG:H232	34:c:521:LMG:H391	1.96	0.48
25:h:101:BCR:H331	25:h:101:BCR:C8	2.43	0.48
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:H132	1.96	0.48
23:a:406[B]:CLA:H203	34:d:410:LMG:H412	1.96	0.48
23:b:601:CLA:H92	25:h:101:BCR:H403	1.96	0.48
36:C:518[A]:DGD:HAT1	36:C:519:DGD:HBE1	1.96	0.48
36:c:517[B]:DGD:HG11	41:c:604[B]:HOH:O	2.14	0.48
32:d:407[A]:LHG:H122	32:d:407[A]:LHG:C38	2.44	0.48
32:A:419[B]:LHG:H252	2:B:464:PHE:CZ	2.49	0.48
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.48
26:F:103:SQD:H102	17:X:31:ILE:HD11	1.95	0.48
26:L:101:SQD:H462	26:L:101:SQD:H1	1.96	0.47
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.74	0.47
29:a:413[B]:PL9:H171	29:a:413[B]:PL9:H151	1.52	0.47
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.95	0.47
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.96	0.47
23:A:408:CLA:H18	23:C:506:CLA:H142	1.97	0.47
23:B:606:CLA:H202	26:a:411:SQD:H302	1.97	0.47
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.96	0.47
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.96	0.47
1:a:15:GLU:HB2	33:a:416:LMT:H6'2	1.97	0.47
25:d:404:BCR:H331	25:d:404:BCR:C8	2.45	0.47
1:A:240[A]:GLY:HA3	14:T:29[A]:ILE:HG23	1.96	0.47
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.96	0.47
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.96	0.47
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.29	0.47
2:B:133:LEU:HB2	27:B:625:GOL:H31	1.97	0.47
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.95	0.47
8:I:35:LYS:O	8:I:37:LEU:N	2.47	0.47
1:a:160[A]:ILE:HD11	36:c:517[A]:DGD:HBT1	1.96	0.47
23:b:604:CLA:H42	23:b:605:CLA:H2	1.96	0.47
29:a:413[A]:PL9:H351	6:f:25:THR:OG1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:410[A]:SQD:H152	26:A:410[A]:SQD:H122	1.54	0.47
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.97	0.47
5:E:57:ALA:H	5:E:60:GLN:HE21	1.61	0.47
13:O:25:THR:O	13:O:27:ARG:N	2.47	0.47
2:b:233:ASN:O	2:b:236:THR:HG22	2.15	0.47
23:d:403:CLA:H162	7:h:37:LEU:HD21	1.97	0.47
32:d:407[B]:LHG:H332	32:d:407[B]:LHG:H302	1.75	0.47
1:A:214[A]:MET:HE2	1:A:255[A]:PHE:CE1	2.49	0.47
4:D:261[B]:PHE:CE1	32:D:406[B]:LHG:HC81	2.50	0.47
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	1.97	0.47
32:d:407[A]:LHG:H332	32:d:407[A]:LHG:H302	1.77	0.47
1:A:183[B]:MET:HA	23:A:404[B]:CLA:HMD1	1.96	0.46
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.45	0.46
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H132	1.97	0.46
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.97	0.46
3:c:48:LYS:HG3	3:c:138:GLU:HG3	1.98	0.46
23:C:505:CLA:H62	23:C:505:CLA:H41	1.70	0.46
23:c:513:CLA:HMB2	23:c:513:CLA:H192	1.97	0.46
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.98	0.46
29:a:413[A]:PL9:H171	29:a:413[A]:PL9:H151	1.57	0.46
2:b:98:LEU:HB2	35:b:622:HTG:C7'	2.45	0.46
3:c:95:LEU:HD21	23:c:502:CLA:OBD	2.16	0.46
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.18	0.46
4:D:180:ARG:HD3	4:D:180:ARG:C	2.41	0.46
23:b:605:CLA:H62	23:b:605:CLA:H41	1.59	0.46
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.97	0.46
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.98	0.46
4:D:103:ARG:HH21	5:E:77:GLU:HG2	1.81	0.46
3:c:216:SER:HB2	34:c:501:LMG:HC71	1.97	0.46
3:c:238:ILE:O	3:c:242:LEU:HG	2.15	0.46
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.97	0.46
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	1.98	0.46
23:B:614:CLA:H71	23:B:614:CLA:H112	1.52	0.46
23:B:614:CLA:H8	25:B:617:BCR:H362	1.98	0.46
23:C:511:CLA:H152	23:C:511:CLA:H112	1.44	0.46
41:E:201:HOH:O	9:J:6:ARG:HG3	2.15	0.46
11:l:20:GLY:O	11:l:24:ILE:HG12	2.16	0.46
15:u:10[A]:VAL:HG12	41:u:242:HOH:O	2.15	0.46
23:B:610:CLA:H122	23:B:615:CLA:HAA1	1.97	0.46
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.16	0.46
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:405[B]:CLA:HBA1	23:a:405[B]:CLA:C4A	2.46	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.98	0.46
33:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.97	0.46
2:B:363:PHE:HB3	2:B:365:SER:O	2.15	0.45
3:C:443[B]:TRP:CE2	23:C:509:CLA:HMD2	2.52	0.45
23:a:405[A]:CLA:HBA1	23:a:405[A]:CLA:C4A	2.45	0.45
2:b:58:GLN:C	2:b:329:PRO:HB3	2.41	0.45
36:c:519:DGD:HBH2	32:d:407[B]:LHG:H211	1.99	0.45
34:d:410:LMG:H221	34:d:410:LMG:H191	1.62	0.45
23:C:504:CLA:CBB	23:C:513:CLA:H41	2.43	0.45
32:D:406[B]:LHG:HC62	11:L:15[B]:THR:HG23	1.99	0.45
23:a:408:CLA:H203	23:c:507:CLA:H101	1.98	0.45
24:A:417[B]:PHO:HBC2	24:A:417[B]:PHO:HHD	1.97	0.45
3:C:334[A]:PRO:HA	13:O:153:THR:OG1	2.16	0.45
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	1.97	0.45
10:k:24:VAL:HG21	18:y:25:ILE:HB	1.97	0.45
3:C:174:LEU:HB3	23:C:503:CLA:H152	1.98	0.45
6:F:27:ALA:HB1	38:F:102:HEM:HAC	1.99	0.45
13:o:58:ASN:C	13:o:60:ARG:H	2.24	0.45
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.82	0.45
32:E:101[B]:LHG:H241	32:E:101[B]:LHG:HC61	1.83	0.45
23:a:404[B]:CLA:H203	23:a:404[B]:CLA:H162	1.79	0.45
25:a:409:BCR:H24C	25:a:409:BCR:H371	1.70	0.45
2:b:224:ARG:HH21	33:b:621:LMT:H1'	1.81	0.45
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.97	0.45
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.98	0.45
23:c:506:CLA:HMD2	23:c:508:CLA:HAB	1.99	0.45
23:c:509:CLA:H18	36:c:518[B]:DGD:HAT2	1.99	0.45
16:v:45[B]:ILE:HD13	27:v:202[B]:GOL:H11	1.99	0.45
26:A:410[B]:SQD:H361	10:K:34:ALA:HA	1.99	0.45
2:B:445:THR:HA	41:B:704:HOH:O	2.17	0.45
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.77	0.45
4:D:230[A]:SER:HB2	41:D:578:HOH:O	2.16	0.45
26:a:410[A]:SQD:H271	32:d:407[A]:LHG:H141	1.98	0.45
32:d:407[A]:LHG:H342	32:d:407[A]:LHG:H151	1.99	0.45
26:A:410[B]:SQD:H122	26:A:410[B]:SQD:H152	1.61	0.45
3:c:182:PHE:HA	35:c:522:HTG:H61	1.99	0.45
23:C:507:CLA:H18	23:C:507:CLA:H152	1.49	0.45
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.99	0.45
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.52	0.45
29:a:413[B]:PL9:H351	6:f:25:THR:OG1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.73	0.45
23:c:513:CLA:H121	23:c:514:CLA:H142	1.99	0.45
23:c:510:CLA:H91	23:c:510:CLA:H111	1.78	0.44
23:A:408:CLA:H171	23:C:507:CLA:H121	1.98	0.44
25:H:101:BCR:H331	25:H:101:BCR:C8	2.47	0.44
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.51	0.44
18:y:20:ALA:O	18:y:24:MET:HG2	2.17	0.44
23:C:513:CLA:H143	23:C:514:CLA:H142	1.99	0.44
25:T:102:BCR:HC7	25:T:102:BCR:H331	1.63	0.44
23:a:404[A]:CLA:H203	23:a:404[A]:CLA:H162	1.80	0.44
25:b:618:BCR:H24C	25:b:618:BCR:H371	1.82	0.44
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.99	0.44
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.86	0.44
23:C:503:CLA:H151	23:C:504:CLA:HMB2	1.99	0.44
4:D:261[A]:PHE:CZ	32:D:406[A]:LHG:HC81	2.52	0.44
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.52	0.44
4:d:266[A]:TRP:CD1	32:d:406[A]:LHG:HC31	2.52	0.44
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.17	0.44
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.83	0.44
29:A:414[B]:PL9:H171	29:A:414[B]:PL9:H151	1.52	0.44
2:B:58:GLN:C	2:B:329:PRO:HB3	2.43	0.44
13:O:54:GLU:HG2	13:O:64:GLU:O	2.17	0.44
13:O:130:GLN:H	13:O:130:GLN:CD	2.24	0.44
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.98	0.44
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.17	0.44
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.85	0.44
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.44
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	2.00	0.44
25:d:404:BCR:H383	34:d:410:LMG:H171	1.99	0.44
15:u:92:VAL:HG12	15:u:97:ARG:HD2	1.99	0.44
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.77	0.44
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.99	0.44
1:A:63[B]:ILE:HB	3:C:335[B]:THR:HG21	2.00	0.44
29:A:414[A]:PL9:H322	29:A:414[A]:PL9:H301	1.77	0.44
23:B:602:CLA:H162	23:B:602:CLA:H203	1.66	0.44
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.99	0.44
13:O:79:ASP:OD1	13:O:80:GLN:N	2.45	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.44
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.87	0.44
23:d:402[A]:CLA:HAA2	23:d:402[A]:CLA:HBD	2.00	0.44
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:GLU:O	2:B:287:ARG:HG3	2.18	0.43
13:O:51:LEU:HD12	13:O:234:LYS:HG2	1.99	0.43
23:b:603:CLA:H62	23:b:603:CLA:H41	1.80	0.43
36:c:517[A]:DGD:HG11	41:c:604[A]:HOH:O	2.18	0.43
32:d:407[B]:LHG:H361	32:d:407[B]:LHG:H331	1.57	0.43
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.67	0.43
23:C:506:CLA:H93	23:C:506:CLA:H111	1.73	0.43
36:h:102:DGD:HB61	36:h:102:DGD:HB91	1.90	0.43
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.99	0.43
23:C:509:CLA:H142	23:C:509:CLA:H111	1.81	0.43
1:a:213[B]:ALA:HB2	4:d:275[B]:PRO:HG2	2.00	0.43
13:o:58:ASN:HB2	13:o:61:GLN:HG2	2.00	0.43
29:A:414[B]:PL9:H301	29:A:414[B]:PL9:H322	1.80	0.43
23:B:613:CLA:H162	23:B:613:CLA:H121	1.63	0.43
8:I:36:ASP:OD1	8:I:36:ASP:N	2.52	0.43
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	2.00	0.43
32:d:407[B]:LHG:H342	32:d:407[B]:LHG:H151	2.01	0.43
7:h:49:TYR:CG	36:h:102:DGD:HB22	2.53	0.43
25:k:101:BCR:H24C	25:k:101:BCR:H371	1.70	0.43
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.82	0.43
23:A:404[A]:CLA:H143	24:A:407[A]:PHO:H61	2.01	0.43
29:A:414[B]:PL9:H503	26:F:103:SQD:H341	2.00	0.43
2:b:29:LEU:HD23	26:b:620:SQD:H201	2.00	0.43
26:b:620:SQD:H462	26:b:620:SQD:H1	1.99	0.43
32:d:407[A]:LHG:H242	32:d:407[A]:LHG:H272	1.86	0.43
15:u:45:LEU:HD21	15:u:71:GLN:HB3	1.99	0.43
32:D:406[A]:LHG:HC62	11:L:15[A]:THR:HG23	2.00	0.43
33:M:101:LMT:H72	12:m:24:ILE:HD13	2.01	0.43
1:a:259[B]:ILE:HG22	1:a:260[B]:PHE:CD1	2.53	0.43
23:a:406[A]:CLA:H203	34:d:410:LMG:H412	2.01	0.43
23:a:408:CLA:H61	23:a:408:CLA:H102	1.83	0.43
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.01	0.43
32:A:419[A]:LHG:H361	23:B:613:CLA:H51	2.01	0.43
25:B:618:BCR:H331	25:B:618:BCR:C8	2.48	0.43
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.01	0.43
36:C:517[A]:DGD:HG11	41:C:601[A]:HOH:O	2.18	0.43
23:b:609:CLA:NC	25:h:101:BCR:H332	2.34	0.43
23:b:614:CLA:H112	23:b:614:CLA:H72	1.61	0.43
23:b:615:CLA:H92	23:b:615:CLA:H61	1.74	0.43
32:d:407[B]:LHG:C38	32:d:407[B]:LHG:H122	2.48	0.43
25:h:101:BCR:H24C	25:h:101:BCR:H371	1.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:t:102:BCR:H382	25:t:102:BCR:H23C	2.00	0.43
33:D:401:LMT:H21	35:b:622:HTG:H1	2.01	0.43
10:K:10:LYS:N	41:K:204:HOH:O	2.52	0.43
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.49	0.43
23:A:405[A]:CLA:HHC	23:A:405[A]:CLA:HBB1	2.01	0.43
24:A:417[A]:PHO:H3A	23:D:402[A]:CLA:H142	1.99	0.43
23:B:613:CLA:H143	23:B:613:CLA:H111	1.81	0.43
25:T:102:BCR:H24C	25:T:102:BCR:H371	1.83	0.43
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	2.01	0.43
3:C:338[B]:GLY:HA3	3:C:341[B]:LEU:O	2.19	0.43
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.01	0.43
23:c:505:CLA:H151	23:c:509:CLA:H143	2.01	0.43
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.19	0.43
14:t:2:GLU:HG2	14:t:3:THR:N	2.34	0.43
32:A:419[A]:LHG:H252	2:B:464:PHE:CZ	2.54	0.42
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.42
41:E:201:HOH:O	9:J:2:SER:N	2.52	0.42
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.19	0.42
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.01	0.42
23:d:402[B]:CLA:HAA2	23:d:402[B]:CLA:HBD	2.01	0.42
25:d:404:BCR:H15C	25:d:404:BCR:H351	1.81	0.42
13:o:92:SER:HB3	13:o:131:PRO:HA	2.00	0.42
33:A:420:LMT:O3'	33:A:420:LMT:H6'2	2.20	0.42
26:a:411:SQD:H1	41:a:621:HOH:O	2.20	0.42
2:b:491[A]:VAL:HG13	4:d:136[A]:VAL:HG13	2.02	0.42
26:b:620:SQD:H311	26:b:620:SQD:H341	1.69	0.42
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.02	0.42
13:O:169:ASP:H	27:O:303:GOL:H12	1.83	0.42
23:a:404[B]:CLA:H152	24:a:407[B]:PHO:H52	2.00	0.42
32:a:419[A]:LHG:H241	32:a:419[A]:LHG:HC61	1.89	0.42
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.02	0.42
27:l:102[B]:GOL:H32	14:t:25:GLU:HB2	2.01	0.42
26:A:410[A]:SQD:H361	10:K:34:ALA:HA	2.02	0.42
23:C:502:CLA:H42	23:C:503:CLA:HMD3	2.01	0.42
23:C:503:CLA:H61	23:C:513:CLA:H42	2.02	0.42
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.02	0.42
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.00	0.42
23:a:404[B]:CLA:H161	23:a:404[B]:CLA:H122	1.86	0.42
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.54	0.42
2:b:358:ARG:HB2	27:b:628:GOL:H31	2.00	0.42
4:d:14:TRP:CD1	35:d:409:HTG:H61	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:f:102:SQD:O7	26:f:102:SQD:H462	2.20	0.42
25:h:101:BCR:H11C	25:h:101:BCR:H341	1.95	0.42
13:o:42:ARG:O	13:o:241:ALA:HA	2.20	0.42
1:A:202:VAL:HG11	23:A:406[B]:CLA:C3D	2.49	0.42
29:A:414[A]:PL9:H171	29:A:414[A]:PL9:H151	1.53	0.42
5:E:9:PRO:HA	32:E:101[B]:LHG:HC31	2.01	0.42
10:K:26:PRO:O	10:K:29:PRO:HD2	2.20	0.42
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.68	0.42
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.54	0.42
26:a:410[B]:SQD:H271	32:d:407[B]:LHG:H141	2.00	0.42
2:b:158:LEU:HB3	2:b:199:VAL:HG22	2.01	0.42
36:c:519:DGD:HBH2	32:d:407[A]:LHG:H211	2.02	0.42
23:B:614:CLA:H92	23:B:614:CLA:H61	1.78	0.42
3:C:338[A]:GLY:HA3	3:C:341[A]:LEU:O	2.20	0.42
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.18	0.42
16:V:41:HIS:CD2	40:V:201:HEC:NB	2.88	0.42
2:b:6[B]:TYR:OH	32:b:630[B]:LHG:O5	2.30	0.42
2:b:36:SER:OG	25:b:618:BCR:H362	2.19	0.42
32:D:407[A]:LHG:H332	32:D:407[A]:LHG:H302	1.85	0.42
25:T:102:BCR:H351	26:b:620:SQD:H211	2.00	0.42
23:c:506:CLA:H93	23:c:506:CLA:H111	1.83	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
23:c:509:CLA:HBC3	23:c:511:CLA:H71	2.01	0.42
20:R:8:VAL:O	20:R:11:PRO:HD2	2.20	0.42
2:B:154:GLY:O	2:B:159:THR:HG23	2.20	0.42
2:B:383[B]:PHE:CZ	13:O:167:GLY:HA2	2.55	0.42
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.02	0.42
1:a:105:TRP:CE2	1:a:110[B]:GLY:HA3	2.55	0.42
32:a:419[B]:LHG:H241	32:a:419[B]:LHG:HC61	1.89	0.42
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.55	0.42
23:c:509:CLA:H18	36:c:518[A]:DGD:HAT2	2.01	0.42
23:A:405[A]:CLA:HBA1	23:A:405[A]:CLA:C4A	2.50	0.42
23:B:615:CLA:H172	23:B:615:CLA:H13	1.87	0.42
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:C11	2.45	0.42
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.02	0.42
2:b:159:THR:HA	2:b:181:VAL:O	2.20	0.42
2:b:363:PHE:HB3	2:b:365:SER:O	2.20	0.42
23:c:513:CLA:HBA2	23:c:513:CLA:H3A	1.79	0.42
33:B:626:LMT:H62	33:B:626:LMT:H91	1.51	0.41
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.20	0.41
23:D:402[B]:CLA:HAA2	23:D:402[B]:CLA:HBD	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.83	0.41
27:a:418:GOL:H31	12:m:1:FME:HG2	2.02	0.41
18:y:34:MET:O	18:y:38:LEU:HG	2.20	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.97	0.41
23:A:404[A]:CLA:H192	23:A:404[A]:CLA:H161	1.80	0.41
27:A:418:GOL:H11	12:M:1:FME:CG	2.36	0.41
23:C:507:CLA:H3A	23:C:507:CLA:HBA1	1.83	0.41
32:D:407[A]:LHG:H362	32:D:407[A]:LHG:H331	1.86	0.41
3:c:391[B]:ARG:NH2	41:c:613:HOH:O	2.53	0.41
23:c:510:CLA:H142	23:c:510:CLA:H112	1.81	0.41
32:d:407[B]:LHG:H142	32:d:407[B]:LHG:H372	2.02	0.41
5:e:20:TRP:HZ2	9:j:12:VAL:HG13	1.84	0.41
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.50	0.41
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.01	0.41
4:D:230[B]:SER:HB2	41:D:578:HOH:O	2.21	0.41
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.20	0.41
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.56	0.41
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.19	0.41
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.02	0.41
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.76	0.41
2:B:102:VAL:HA	25:B:618:BCR:C40	2.50	0.41
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.20	0.41
1:a:214[A]:MET:HB3	29:a:413[A]:PL9:H103	2.01	0.41
24:a:415[A]:PHO:H42	24:a:415[A]:PHO:H11	1.92	0.41
32:d:407[B]:LHG:H242	32:d:407[B]:LHG:H272	1.91	0.41
34:Z:101:LMG:H141	34:Z:101:LMG:H111	1.87	0.41
2:B:482[B]:ILE:HD12	2:B:486[B]:LEU:HD22	2.02	0.41
23:B:603:CLA:H61	23:B:603:CLA:H102	1.83	0.41
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	2.02	0.41
33:M:101:LMT:H6D	11:l:9:PRO:HA	2.03	0.41
15:U:45:LEU:HD23	15:U:45:LEU:HA	1.94	0.41
24:a:407[B]:PHO:HAB	4:d:205[B]:LEU:HD13	2.01	0.41
23:b:615:CLA:H112	23:b:615:CLA:H91	1.79	0.41
3:c:363:GLY:O	3:c:367:GLU:HG2	2.20	0.41
4:d:148[A]:ALA:HB3	4:d:149[A]:PRO:HD3	2.03	0.41
32:d:407[A]:LHG:H372	32:d:407[A]:LHG:H142	2.03	0.41
2:B:357[A]:ARG:HH12	27:B:622:GOL:C3	2.33	0.41
23:B:615:CLA:H71	23:B:616:CLA:H172	2.02	0.41
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	2.03	0.41
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	2.03	0.41
1:A:85[A]:SER:HA	1:A:109[A]:GLY:HA3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B:621:HTG:H7'3	35:B:621:HTG:H4'2	1.90	0.41
1:a:15:GLU:HG3	33:a:416:LMT:O4'	2.21	0.41
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.81	0.41
6:f:21:VAL:O	6:f:25:THR:HG23	2.21	0.41
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.50	0.41
3:C:330:SER:HB3	13:O:100:GLY:O	2.20	0.41
5:E:18:ARG:H	9:J:2:SER:N	2.18	0.41
32:E:101[A]:LHG:H291	32:E:101[A]:LHG:H261	1.75	0.41
13:O:93:LEU:O	13:O:128:SER:HA	2.20	0.41
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.56	0.41
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.03	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.92	0.41
1:A:15:GLU:HG2	33:A:420:LMT:O3B	2.21	0.41
1:A:231:GLU:HB3	41:B:874:HOH:O	2.21	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.89	0.41
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.46	0.41
4:D:209[B]:LEU:HD23	4:D:209[B]:LEU:C	2.46	0.41
16:V:57:GLU:H	16:V:57:GLU:CD	2.28	0.41
1:a:307:ILE:HG22	1:a:313:VAL:HA	2.01	0.41
26:a:410[B]:SQD:H162	26:a:410[B]:SQD:H132	1.91	0.41
23:b:601:CLA:H91	23:b:601:CLA:H111	1.90	0.41
23:b:607:CLA:H91	23:b:607:CLA:H112	1.67	0.41
23:b:614:CLA:H162	23:b:614:CLA:H122	1.83	0.41
3:c:128:GLY:HA3	23:c:514:CLA:C3C	2.51	0.41
3:c:338[A]:GLY:HA2	13:o:103:PHE:HZ	1.86	0.41
3:c:425[A]:TRP:CD1	23:c:505:CLA:HMA3	2.55	0.41
7:h:62:TRP:C	7:h:64:ALA:H	2.29	0.41
8:i:32:PRO:C	8:i:33:LYS:HD2	2.45	0.41
33:t:101:LMT:H112	33:t:101:LMT:H81	1.83	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.78	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.48	0.41
4:d:110:LEU:HD23	4:d:110:LEU:HA	1.93	0.41
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.40
23:A:404[A]:CLA:CBD	23:A:405[A]:CLA:HAC2	2.51	0.40
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.03	0.40
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.36	0.40
8:i:2:GLU:O	8:i:6:ILE:HG12	2.21	0.40
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.56	0.40
29:A:414[A]:PL9:H121	29:A:414[A]:PL9:HC8	1.78	0.40
3:C:176:VAL:HG21	3:C:238:ILE:HG13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:39[A]:ARG:HB2	13:O:246:ALA:HB2	2.02	0.40
13:O:137:THR:C	13:O:139:SER:H	2.29	0.40
1:a:34:GLY:HA2	1:a:37:MET:HB3	2.03	0.40
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CH2	2.57	0.40
29:a:413[B]:PL9:H301	29:a:413[B]:PL9:H321	1.73	0.40
23:c:509:CLA:H162	23:c:509:CLA:H122	1.73	0.40
23:c:513:CLA:H142	23:c:513:CLA:H111	1.94	0.40
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.99	0.40
23:A:404[B]:CLA:CAD	23:A:405[B]:CLA:HAC2	2.51	0.40
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	2.03	0.40
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.02	0.40
23:a:408:CLA:H61	23:a:408:CLA:H41	1.85	0.40
29:a:413[B]:PL9:H503	17:x:24:THR:OG1	2.21	0.40
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.56	0.40
3:c:318:LEU:C	3:c:318:LEU:HD23	2.47	0.40
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:HC2	1.71	0.40
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.03	0.40
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.03	0.40
4:d:148[B]:ALA:HB3	4:d:149[B]:PRO:HD3	2.03	0.40
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.03	0.40
4:d:266[B]:TRP:CD1	32:d:406[B]:LHG:HC31	2.57	0.40
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.86	0.40
23:B:615:CLA:H92	23:B:615:CLA:H61	1.89	0.40
36:C:518[A]:DGD:HAE2	36:C:518[A]:DGD:HA81	1.86	0.40
32:D:407[B]:LHG:H332	32:D:407[B]:LHG:H302	1.91	0.40
5:E:27:ILE:HB	5:E:28:PRO:HD3	2.03	0.40
2:b:154:GLY:O	2:b:159:THR:HG23	2.22	0.40
5:e:60:GLN:HE21	5:e:60:GLN:HB2	1.71	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	34
1	a	551/344 (160%)	541 (98%)	8 (2%)	2 (0%)	30	34
2	B	524/505 (104%)	518 (99%)	6 (1%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	43	51
3	c	554/455 (122%)	544 (98%)	9 (2%)	1 (0%)	43	51
4	D	454/342 (133%)	438 (96%)	16 (4%)	0	100	100
4	d	457/342 (134%)	445 (97%)	12 (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%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	6
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%)	36 (100%)	0	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%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	34
13	o	249/244 (102%)	244 (98%)	5 (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	99/104 (95%)	95 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	25 (93%)	2 (7%)	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 5
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 5
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	6180/5384 (115%)	6047 (98%)	122 (2%)	11 (0%)	43 51

All (11) 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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	444/279 (159%)	441 (99%)	3 (1%)	76 87
1	a	442/279 (158%)	441 (100%)	1 (0%)	87 94
2	B	423/403 (105%)	417 (99%)	6 (1%)	59 75
2	b	420/403 (104%)	410 (98%)	10 (2%)	43 58

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	C	431/356 (121%)	422 (98%)	9 (2%)	47 63
3	c	437/356 (123%)	431 (99%)	6 (1%)	59 75
4	D	368/277 (133%)	365 (99%)	3 (1%)	73 85
4	d	372/277 (134%)	368 (99%)	4 (1%)	65 79
5	E	72/73 (99%)	70 (97%)	2 (3%)	38 52
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 75
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 41
7	h	55/54 (102%)	55 (100%)	0	100 100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18 22
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 51
9	J	26/27 (96%)	25 (96%)	1 (4%)	29 40
9	j	26/27 (96%)	25 (96%)	1 (4%)	29 40
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 3
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 7
11	L	36/35 (103%)	36 (100%)	0	100 100
11	l	36/35 (103%)	36 (100%)	0	100 100
12	M	30/32 (94%)	27 (90%)	3 (10%)	7 7
12	m	32/32 (100%)	30 (94%)	2 (6%)	16 19
13	O	216/207 (104%)	207 (96%)	9 (4%)	26 36
13	o	213/207 (103%)	206 (97%)	7 (3%)	33 45
14	T	32/28 (114%)	28 (88%)	4 (12%)	4 4
14	t	31/28 (111%)	31 (100%)	0	100 100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44 59
15	u	88/89 (99%)	86 (98%)	2 (2%)	44 59
16	V	123/117 (105%)	122 (99%)	1 (1%)	73 85
16	v	123/117 (105%)	119 (97%)	4 (3%)	33 45
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	y	22/23 (96%)	18 (82%)	4 (18%)	2 1
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 22
19	z	52/52 (100%)	44 (85%)	8 (15%)	2 2
20	R	29/29 (100%)	27 (93%)	2 (7%)	14 16
All	All	5110/4403 (116%)	5000 (98%)	110 (2%)	45 61

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	243[A]	GLU
1	A	243[B]	GLU
2	B	161	LEU
2	B	298	LEU
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	142	GLU
3	C	240	ILE
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	462	GLU
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	4	THR
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	16[A]	LEU
12	M	16[B]	LEU
12	M	20	VAL
13	O	4	THR
13	O	49	THR
13	O	55	GLU
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
13	O	180	GLU
13	O	194	LYS
13	O	234	LYS
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
1	a	13	LEU
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	245	VAL
2	b	298	LEU
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	142	GLU
3	c	152	LYS
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	71	GLU
8	i	33	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	90	GLU
18	y	18	VAL
18	y	19	ILE
18	y	30	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	20	VAL
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	21	ILE
19	z	32	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
3	C	415	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	301	GLN
5	E	60	GLN
13	O	231	HIS
15	U	78	ASN
17	X	38	GLN
2	b	14	ASN
2	b	331	ASN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN
19	Z	31	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	$\#\|Z\| > 2$
8	FME	i	1	8	8,9,10	0.70	0	7,9,11	1.20	1 (14%)
12	FME	m	1	12	8,9,10	0.52	0	7,9,11	1.52	2 (28%)
14	FME	T	1	14	8,9,10	0.63	0	7,9,11	1.62	2 (28%)
12	FME	M	1	12	8,9,10	0.57	0	7,9,11	1.33	1 (14%)
8	FME	I	1	8	8,9,10	0.58	0	7,9,11	1.20	1 (14%)
14	FME	t	1	14	8,9,10	0.65	0	7,9,11	1.47	2 (28%)

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
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	1	FME	CA-N-CN	-2.62	118.80	122.82
14	T	1	FME	CA-N-CN	2.49	126.66	122.82
14	t	1	FME	O-C-CA	-2.39	118.50	124.78
14	T	1	FME	CG-CB-CA	2.39	119.59	112.95
14	t	1	FME	CA-N-CN	-2.38	119.17	122.82
12	m	1	FME	O1-CN-N	-2.30	119.20	125.27
12	M	1	FME	O-C-CA	-2.25	118.89	124.78
8	I	1	FME	O-C-CA	-2.20	119.00	124.78
8	i	1	FME	O-C-CA	-2.08	119.33	124.78

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O1-CN-N-CA
12	m	1	FME	O1-CN-N-CA
12	m	1	FME	O-C-CA-CB

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	$\#\|Z\| > 2$
35	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.43	1 (4%)
24	PHO	A	417[B]	-	58,69,69	2.70	14 (24%)	56,99,99	2.97	18 (32%)
26	SQD	A	412	-	53,54,54	1.02	3 (5%)	62,65,65	1.24	6 (9%)
36	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.11	7 (9%)
35	HTG	o	301	-	19,19,19	1.06	2 (10%)	23,24,24	1.49	4 (17%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.32	7 (12%)
27	GOL	c	526[B]	-	5,5,5	1.02	0	5,5,5	0.91	0
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
34	LMG	d	410	39	51,51,55	0.87	2 (3%)	59,59,63	1.14	5 (8%)
23	CLA	B	610	41	69,73,73	2.07	19 (27%)	83,113,113	2.87	32 (38%)
27	GOL	o	304	-	5,5,5	0.97	0	5,5,5	1.10	0
32	LHG	d	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
38	HEM	F	102	6,5	50,50,50	1.54	7 (14%)	66,82,82	1.94	15 (22%)
23	CLA	C	511	3	69,73,73	2.04	21 (30%)	83,113,113	2.96	32 (38%)
23	CLA	C	505	41	69,73,73	1.99	20 (28%)	83,113,113	2.85	29 (34%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
23	CLA	b	602	2	69,73,73	2.09	18 (26%)	83,113,113	2.95	35 (42%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.31	9 (16%)
25	BCR	A	409	-	41,41,41	0.98	1 (2%)	56,56,56	1.43	9 (16%)
35	HTG	b	625	-	19,19,19	1.10	2 (10%)	23,24,24	1.46	4 (17%)
23	CLA	b	614	2	69,73,73	1.97	20 (28%)	83,113,113	2.97	31 (37%)
23	CLA	a	404[B]	1	69,73,73	1.99	20 (28%)	83,113,113	2.89	32 (38%)
23	CLA	a	408	1	69,73,73	1.98	19 (27%)	83,113,113	2.94	31 (37%)
32	LHG	d	406[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.07	4 (7%)
35	HTG	b	623	-	19,19,19	1.06	1 (5%)	23,24,24	1.88	2 (8%)
25	BCR	d	404	-	41,41,41	1.11	2 (4%)	56,56,56	1.96	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	D	404	-	41,41,41	1.13	2 (4%)	56,56,56	1.83	17 (30%)
23	CLA	d	402[B]	4	69,73,73	1.99	20 (28%)	83,113,113	2.84	30 (36%)
36	DGD	c	519	-	63,63,67	0.88	4 (6%)	77,77,81	1.02	5 (6%)
34	LMG	c	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.23	6 (10%)
23	CLA	b	611	2	69,73,73	1.95	21 (30%)	83,113,113	2.90	28 (33%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
27	GOL	c	527	-	5,5,5	1.13	0	5,5,5	0.92	0
36	DGD	C	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	0.97	4 (5%)
29	PL9	d	405[B]	-	55,55,55	0.66	1 (1%)	68,69,69	1.63	17 (25%)
24	PHO	A	407[B]	-	58,69,69	2.65	12 (20%)	56,99,99	2.87	17 (30%)
36	DGD	c	518[B]	-	63,63,67	0.86	3 (4%)	77,77,81	0.96	5 (6%)
40	HEC	v	201	16	50,50,50	1.71	7 (14%)	68,82,82	1.39	8 (11%)
27	GOL	O	302	-	5,5,5	0.87	0	5,5,5	0.90	0
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	11 (19%)
38	HEM	f	101	6,5	50,50,50	1.49	6 (12%)	66,82,82	1.74	11 (16%)
36	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
23	CLA	c	513	3	69,73,73	2.08	19 (27%)	83,113,113	2.89	32 (38%)
33	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.17	2 (6%)
24	PHO	A	417[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
25	BCR	b	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.35	9 (16%)
23	CLA	C	507	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	32 (38%)
29	PL9	a	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
23	CLA	c	509	3	69,73,73	2.11	20 (28%)	83,113,113	2.77	30 (36%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
36	DGD	C	519	-	63,63,67	0.89	3 (4%)	77,77,81	1.00	4 (5%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	11 (21%)
23	CLA	b	616	2	69,73,73	2.01	18 (26%)	83,113,113	2.92	30 (36%)
40	HEC	V	201	16	50,50,50	1.71	6 (12%)	68,82,82	1.53	13 (19%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.29	4 (7%)
27	GOL	D	412	-	5,5,5	1.42	2 (40%)	5,5,5	0.89	0
35	HTG	B	623	-	19,19,19	0.99	2 (10%)	23,24,24	1.13	3 (13%)
25	BCR	k	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.50	11 (19%)
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	603	2	69,73,73	2.01	19 (27%)	83,113,113	2.90	31 (37%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LHG	d	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
29	PL9	A	414[B]	-	55,55,55	0.65	1 (1%)	68,69,69	2.01	25 (36%)
33	LMT	t	101	-	26,26,36	0.90	2 (7%)	31,31,47	1.32	3 (9%)
23	CLA	B	606	2	69,73,73	1.98	20 (28%)	83,113,113	2.88	32 (38%)
32	LHG	L	102[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	2 (3%)
23	CLA	d	402[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
23	CLA	C	503	3	69,73,73	2.03	20 (28%)	83,113,113	2.72	28 (33%)
23	CLA	C	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.84	33 (39%)
23	CLA	c	511	3	69,73,73	2.00	20 (28%)	83,113,113	2.84	32 (38%)
27	GOL	a	418	-	5,5,5	1.31	1 (20%)	5,5,5	0.85	0
23	CLA	C	513	3	69,73,73	2.06	19 (27%)	83,113,113	2.84	35 (42%)
32	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.19	5 (9%)
26	SQD	a	410[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	11 (17%)
23	CLA	b	609	2	69,73,73	2.02	18 (26%)	83,113,113	2.79	31 (37%)
31	BCT	A	416[B]	21	2,3,3	0.63	0	2,3,3	1.15	0
34	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.15	5 (8%)
36	DGD	C	517[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.09	7 (9%)
36	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	D	402[B]	4	69,73,73	2.04	20 (28%)	83,113,113	2.88	30 (36%)
29	PL9	d	405[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
34	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.48	6 (13%)
23	CLA	b	601	41	69,73,73	2.09	19 (27%)	83,113,113	2.79	28 (33%)
23	CLA	a	405[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
36	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
27	GOL	B	622	-	5,5,5	0.97	0	5,5,5	1.14	1 (20%)
23	CLA	c	508	41	69,73,73	2.03	19 (27%)	83,113,113	2.88	29 (34%)
23	CLA	B	613	2	69,73,73	2.02	20 (28%)	83,113,113	2.73	31 (37%)
33	LMT	e	101	-	36,36,36	1.02	2 (5%)	47,47,47	0.99	1 (2%)
33	LMT	B	628	-	36,36,36	1.02	3 (8%)	47,47,47	1.15	5 (10%)
27	GOL	o	303	-	5,5,5	0.97	0	5,5,5	0.97	0
32	LHG	b	630[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.02	3 (5%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
29	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.67	17 (25%)
25	BCR	H	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.44	7 (12%)
32	LHG	D	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.00	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LHG	d	412[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	5 (9%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.73	12 (21%)
34	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.12	4 (6%)
23	CLA	c	504	3	69,73,73	2.08	19 (27%)	83,113,113	2.85	28 (33%)
35	HTG	b	622	-	19,19,19	1.15	2 (10%)	23,24,24	1.94	7 (30%)
23	CLA	c	507	3	69,73,73	2.03	20 (28%)	83,113,113	2.78	30 (36%)
35	HTG	V	202	-	11,11,19	0.31	0	15,15,24	1.01	1 (6%)
27	GOL	a	417	-	5,5,5	1.14	0	5,5,5	1.06	1 (20%)
23	CLA	B	607	41	69,73,73	1.97	21 (30%)	83,113,113	2.84	31 (37%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
23	CLA	C	506	3	69,73,73	2.00	19 (27%)	83,113,113	2.81	30 (36%)
27	GOL	A	418	-	5,5,5	1.42	1 (20%)	5,5,5	0.96	1 (20%)
23	CLA	b	603	2	69,73,73	2.01	20 (28%)	83,113,113	2.90	34 (40%)
27	GOL	d	411	-	5,5,5	0.98	0	5,5,5	1.10	0
27	GOL	l	102[B]	-	5,5,5	0.91	0	5,5,5	0.96	0
23	CLA	a	406[B]	41	69,73,73	2.01	19 (27%)	83,113,113	2.89	30 (36%)
28	OEX	a	412[B]	1,3,41	0,14,14	-	-	-		
33	LMT	T	101	-	36,36,36	1.06	3 (8%)	47,47,47	1.06	3 (6%)
23	CLA	b	610	41	69,73,73	2.02	20 (28%)	83,113,113	2.82	33 (39%)
35	HTG	c	522	-	19,19,19	0.94	1 (5%)	23,24,24	1.64	3 (13%)
23	CLA	b	606	2	69,73,73	1.97	19 (27%)	83,113,113	2.92	31 (37%)
23	CLA	c	514	3	69,73,73	2.10	21 (30%)	83,113,113	2.86	32 (38%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.37	9 (16%)
32	LHG	L	102[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
23	CLA	C	510	3	69,73,73	2.06	19 (27%)	83,113,113	2.83	31 (37%)
23	CLA	b	608	2	69,73,73	1.98	19 (27%)	83,113,113	2.76	32 (38%)
24	PHO	a	415[B]	-	58,69,69	2.79	14 (24%)	56,99,99	2.90	16 (28%)
28	OEX	A	413[B]	1,3,41	0,14,14	-	-	-		
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
26	SQD	F	103	-	42,43,54	1.19	4 (9%)	51,54,65	2.14	14 (27%)
25	BCR	T	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.57	12 (21%)
26	SQD	a	410[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
25	BCR	C	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.29	6 (10%)
36	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
27	GOL	A	411	-	5,5,5	1.11	0	5,5,5	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HTG	D	410	-	16,16,19	1.04	1 (6%)	20,21,24	1.59	1 (5%)
23	CLA	B	611	2	69,73,73	2.55	19 (27%)	83,113,113	4.09	31 (37%)
23	CLA	D	402[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	A	406[B]	41	69,73,73	2.05	19 (27%)	83,113,113	2.84	32 (38%)
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.44	7 (11%)
23	CLA	B	614	2	69,73,73	2.02	20 (28%)	83,113,113	3.01	30 (36%)
23	CLA	c	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.83	30 (36%)
33	LMT	B	629	-	25,25,36	0.89	2 (8%)	30,30,47	1.14	3 (10%)
27	GOL	B	625	-	5,5,5	1.01	0	5,5,5	0.95	0
34	LMG	c	521	-	51,51,55	1.00	2 (3%)	59,59,63	1.37	7 (11%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.68	13 (23%)
23	CLA	D	403	4	69,73,73	2.10	19 (27%)	83,113,113	2.86	34 (40%)
23	CLA	B	604	2	69,73,73	2.00	21 (30%)	83,113,113	2.68	30 (36%)
32	LHG	b	630[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
25	BCR	a	409	-	41,41,41	1.02	1 (2%)	56,56,56	1.35	7 (12%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
23	CLA	d	403	4	69,73,73	2.03	20 (28%)	83,113,113	2.89	31 (37%)
23	CLA	B	615	2	69,73,73	1.99	18 (26%)	83,113,113	2.90	28 (33%)
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.10	4 (9%)
34	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.05	2 (4%)
33	LMT	a	416	-	36,36,36	1.00	1 (2%)	47,47,47	1.01	1 (2%)
23	CLA	A	408	1	69,73,73	1.97	19 (27%)	83,113,113	2.99	35 (42%)
26	SQD	L	101	-	53,54,54	1.06	4 (7%)	62,65,65	1.75	10 (16%)
23	CLA	b	607	41	69,73,73	1.99	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	c	503	3	69,73,73	1.97	18 (26%)	83,113,113	2.71	29 (34%)
31	BCT	d	401[B]	21	2,3,3	0.60	0	2,3,3	1.27	0
33	LMT	b	627	-	25,25,36	0.87	0	30,30,47	1.12	3 (10%)
28	OEX	a	412[A]	1,3,41	0,14,14	-	-	-		
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	a	406[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
33	LMT	F	101	-	36,36,36	1.08	1 (2%)	47,47,47	1.06	3 (6%)
35	HTG	d	409	-	16,16,19	1.01	1 (6%)	20,21,24	1.60	2 (10%)
33	LMT	m	103	-	36,36,36	1.03	2 (5%)	47,47,47	1.08	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	O	303	-	5,5,5	1.00	0	5,5,5	1.07	1 (20%)
23	CLA	C	508	41	69,73,73	1.95	19 (27%)	83,113,113	2.84	29 (34%)
26	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.69	12 (19%)
23	CLA	B	608	2	69,73,73	1.92	19 (27%)	83,113,113	2.86	34 (40%)
24	PHO	a	415[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
28	OEX	A	413[A]	1,3,41	0,14,14	-	-	-		
25	BCR	c	515	-	41,41,41	0.98	1 (2%)	56,56,56	1.64	11 (19%)
34	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.34	6 (10%)
26	SQD	a	411	-	53,54,54	1.07	3 (5%)	62,65,65	1.19	8 (12%)
27	GOL	V	203[B]	-	5,5,5	1.01	0	5,5,5	0.94	0
23	CLA	B	605	2	69,73,73	2.01	19 (27%)	83,113,113	2.95	30 (36%)
23	CLA	B	609	2	69,73,73	2.01	18 (26%)	83,113,113	2.80	29 (34%)
24	PHO	a	407[B]	-	58,69,69	2.77	12 (20%)	56,99,99	2.71	15 (26%)
25	BCR	t	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.67	13 (23%)
29	PL9	a	413[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.90	22 (32%)
23	CLA	A	404[B]	1	69,73,73	2.05	20 (28%)	83,113,113	2.85	31 (37%)
23	CLA	B	602	2	69,73,73	2.02	20 (28%)	83,113,113	2.83	31 (37%)
25	BCR	b	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	5 (8%)
34	LMG	D	411	39	51,51,55	0.82	3 (5%)	59,59,63	1.04	3 (5%)
35	HTG	B	621	-	19,19,19	0.77	1 (5%)	23,24,24	1.49	1 (4%)
33	LMT	A	420	-	36,36,36	1.03	2 (5%)	47,47,47	1.14	4 (8%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
32	LHG	D	406[B]	-	48,48,48	0.85	2 (4%)	51,54,54	0.99	3 (5%)
27	GOL	C	523[B]	-	5,5,5	1.31	0	5,5,5	0.75	0
23	CLA	C	512	3	69,73,73	2.01	20 (28%)	83,113,113	2.77	28 (33%)
31	BCT	A	416[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
32	LHG	d	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	31 (37%)
23	CLA	c	506	3	69,73,73	2.03	18 (26%)	83,113,113	2.75	28 (33%)
25	BCR	K	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.43	10 (17%)
26	SQD	A	410[B]	-	53,54,54	0.93	3 (5%)	62,65,65	1.77	11 (17%)
34	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.29	7 (11%)
23	CLA	b	613	2	69,73,73	1.95	18 (26%)	83,113,113	2.80	31 (37%)
23	CLA	C	509	3	69,73,73	2.05	21 (30%)	83,113,113	2.79	27 (32%)
25	BCR	h	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	b	628	-	5,5,5	0.31	0	5,5,5	1.43	1 (20%)
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
34	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.34	5 (8%)
33	LMT	M	101	-	36,36,36	1.10	3 (8%)	47,47,47	1.17	4 (8%)
27	GOL	b	624	-	5,5,5	1.12	1 (20%)	5,5,5	0.79	0
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.42	8 (14%)
33	LMT	D	401	-	36,36,36	0.93	2 (5%)	47,47,47	1.07	2 (4%)
23	CLA	c	510	3	69,73,73	2.04	18 (26%)	83,113,113	2.84	31 (37%)
23	CLA	a	405[B]	41	69,73,73	2.07	18 (26%)	83,113,113	2.81	32 (38%)
31	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
32	LHG	d	412[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	601	41	69,73,73	2.08	20 (28%)	83,113,113	2.90	30 (36%)
32	LHG	a	419[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	b	615	2	69,73,73	1.97	18 (26%)	83,113,113	2.86	31 (37%)
33	LMT	B	626	-	36,36,36	1.18	4 (11%)	47,47,47	1.38	5 (10%)
36	DGD	H	102	-	63,63,67	0.86	4 (6%)	77,77,81	1.03	6 (7%)
23	CLA	c	512	3	69,73,73	2.06	21 (30%)	83,113,113	2.86	33 (39%)
23	CLA	c	505	41	69,73,73	2.06	21 (30%)	83,113,113	2.84	30 (36%)
27	GOL	v	202[B]	-	5,5,5	1.07	0	5,5,5	0.84	0
23	CLA	B	616	2	69,73,73	1.99	20 (28%)	83,113,113	2.91	28 (33%)
23	CLA	b	604	2	69,73,73	2.03	21 (30%)	83,113,113	2.74	28 (33%)
23	CLA	B	612	2	69,73,73	2.03	21 (30%)	83,113,113	2.82	30 (36%)
23	CLA	C	504	3	69,73,73	2.00	19 (27%)	83,113,113	2.89	29 (34%)
23	CLA	b	605	2	69,73,73	1.95	18 (26%)	83,113,113	2.98	30 (36%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
24	PHO	a	407[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.75	30 (36%)
23	CLA	A	405[B]	41	69,73,73	2.01	19 (27%)	83,113,113	2.78	31 (37%)
36	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.07	5 (6%)
27	GOL	B	627	-	5,5,5	0.97	0	5,5,5	1.01	0

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
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
24	PHO	A	417[B]	-	-	1/37/103/103	0/5/6/6
26	SQD	A	412	-	-	12/49/69/69	0/1/1/1
36	DGD	h	102	-	-	13/51/91/95	0/2/2/2
35	HTG	o	301	-	-	3/10/30/30	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	c	526[B]	-	-	0/4/4/4	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
34	LMG	d	410	39	-	9/46/66/70	0/1/1/1
23	CLA	B	610	41	-	10/39/115/115	-
27	GOL	o	304	-	-	2/4/4/4	-
32	LHG	d	407[A]	-	-	11/53/53/53	-
38	HEM	F	102	6,5	-	6/14/54/54	-
23	CLA	C	511	3	-	14/39/115/115	-
23	CLA	C	505	41	-	7/39/115/115	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	b	602	2	-	4/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
35	HTG	b	625	-	-	4/10/30/30	0/1/1/1
23	CLA	b	614	2	-	14/39/115/115	-
23	CLA	a	404[B]	1	-	4/39/115/115	-
23	CLA	a	408	1	-	9/39/115/115	-
32	LHG	d	406[B]	-	-	15/53/53/53	-
35	HTG	b	623	-	-	3/10/30/30	0/1/1/1
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	d	402[B]	4	-	4/39/115/115	-
36	DGD	c	519	-	-	9/51/91/95	0/2/2/2
34	LMG	c	501	-	-	14/46/66/70	0/1/1/1
23	CLA	b	611	2	-	3/39/115/115	-
32	LHG	a	419[A]	-	-	16/46/46/53	-
27	GOL	c	527	-	-	3/4/4/4	-
36	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
29	PL9	d	405[B]	-	-	9/53/73/73	0/1/1/1
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	c	518[B]	-	-	17/51/91/95	0/2/2/2
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
27	GOL	O	302	-	-	2/4/4/4	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
38	HEM	f	101	6,5	-	6/14/54/54	-
36	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
23	CLA	c	513	3	-	15/39/115/115	-
33	LMT	b	621	-	-	8/17/37/61	0/1/1/2
24	PHO	A	417[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	b	619	-	-	5/29/63/63	0/2/2/2
23	CLA	C	507	3	-	10/39/115/115	-
29	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	c	509	3	-	4/39/115/115	-
27	GOL	c	526[A]	-	-	0/4/4/4	-
36	DGD	C	519	-	-	15/51/91/95	0/2/2/2
26	SQD	f	102	-	-	11/38/58/69	0/1/1/1
23	CLA	b	616	2	-	8/39/115/115	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	GOL	D	412	-	-	4/4/4/4	-
35	HTG	B	623	-	-	5/10/30/30	0/1/1/1
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LHG	D	406[A]	-	-	16/53/53/53	-
23	CLA	B	603	2	-	7/39/115/115	-
23	CLA	a	404[A]	1	-	3/39/115/115	-
32	LHG	d	406[A]	-	-	13/53/53/53	-
29	PL9	A	414[B]	-	-	16/53/73/73	0/1/1/1
33	LMT	t	101	-	-	9/17/38/61	0/1/1/2
23	CLA	B	606	2	-	10/39/115/115	-
32	LHG	L	102[B]	-	-	16/53/53/53	-
23	CLA	d	402[A]	4	-	2/39/115/115	-
23	CLA	C	503	3	-	11/39/115/115	-
23	CLA	C	502	3	-	6/39/115/115	-
23	CLA	c	511	3	-	10/39/115/115	-
27	GOL	a	418	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	513	3	-	12/39/115/115	-
32	LHG	A	419[B]	-	-	12/53/53/53	-
26	SQD	a	410[B]	-	-	10/49/69/69	0/1/1/1
23	CLA	b	609	2	-	3/39/115/115	-
34	LMG	c	520	-	-	12/46/66/70	0/1/1/1
36	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
36	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	D	402[B]	4	-	2/39/115/115	-
29	PL9	d	405[A]	-	-	6/53/73/73	0/1/1/1
34	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
23	CLA	b	601	41	-	17/39/115/115	-
23	CLA	a	405[A]	41	-	8/39/115/115	-
36	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
27	GOL	B	622	-	-	2/4/4/4	-
23	CLA	c	508	41	-	9/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
33	LMT	e	101	-	-	15/21/61/61	0/2/2/2
33	LMT	B	628	-	-	12/21/61/61	0/2/2/2
27	GOL	o	303	-	-	1/4/4/4	-
32	LHG	b	630[B]	-	-	20/53/53/53	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
32	LHG	D	407[B]	-	-	16/53/53/53	-
32	LHG	d	412[B]	-	-	11/53/53/53	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
34	LMG	C	520	-	-	9/46/66/70	0/1/1/1
23	CLA	c	504	3	-	3/39/115/115	-
35	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	c	507	3	-	8/39/115/115	-
35	HTG	V	202	-	-	0/2/19/30	0/1/1/1
27	GOL	a	417	-	-	2/4/4/4	-
23	CLA	B	607	41	-	4/39/115/115	-
23	CLA	A	405[A]	41	-	4/39/115/115	-
23	CLA	C	506	3	-	7/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	A	418	-	-	2/4/4/4	-
23	CLA	b	603	2	-	5/39/115/115	-
27	GOL	d	411	-	-	3/4/4/4	-
27	GOL	l	102[B]	-	-	3/4/4/4	-
23	CLA	a	406[B]	41	-	7/39/115/115	-
33	LMT	T	101	-	-	7/21/61/61	0/2/2/2
35	HTG	c	522	-	-	2/10/30/30	0/1/1/1
23	CLA	b	610	41	-	5/39/115/115	-
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	c	514	3	-	12/39/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LHG	L	102[A]	-	-	19/53/53/53	-
23	CLA	C	510	3	-	5/39/115/115	-
23	CLA	b	608	2	-	4/39/115/115	-
24	PHO	a	415[B]	-	-	1/37/103/103	0/5/6/6
32	LHG	A	419[A]	-	-	10/53/53/53	-
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
25	BCR	T	102	-	-	3/29/63/63	0/2/2/2
26	SQD	a	410[A]	-	-	10/49/69/69	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
35	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	B	611	2	-	2/39/115/115	-
23	CLA	D	402[A]	4	-	0/39/115/115	-
23	CLA	A	406[B]	41	-	6/39/115/115	-
34	LMG	C	501	-	-	11/46/66/70	0/1/1/1
23	CLA	B	614	2	-	13/39/115/115	-
23	CLA	c	502	3	-	4/39/115/115	-
33	LMT	B	629	-	-	11/17/37/61	0/1/1/2
27	GOL	B	625	-	-	1/4/4/4	-
34	LMG	c	521	-	-	13/46/66/70	0/1/1/1
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	D	403	4	-	14/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	604	2	-	2/39/115/115	-
32	LHG	b	630[A]	-	-	20/53/53/53	-
25	BCR	a	409	-	-	0/29/63/63	0/2/2/2
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	d	403	4	-	8/39/115/115	-
23	CLA	B	615	2	-	7/39/115/115	-
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
32	LHG	D	407[A]	-	-	14/53/53/53	-
32	LHG	E	101[B]	-	-	21/46/46/53	-
34	LMG	z	101	-	-	9/34/54/70	0/1/1/1
33	LMT	a	416	-	-	11/21/61/61	0/2/2/2
23	CLA	A	408	1	-	9/39/115/115	-
26	SQD	L	101	-	-	12/49/69/69	0/1/1/1
23	CLA	b	607	41	-	2/39/115/115	-
23	CLA	c	503	3	-	9/39/115/115	-
33	LMT	b	627	-	-	11/17/37/61	0/1/1/2
33	LMT	F	101	-	-	8/21/61/61	0/2/2/2
27	GOL	l	102[A]	-	-	2/4/4/4	-
23	CLA	a	406[A]	41	-	7/39/115/115	-
35	HTG	d	409	-	-	1/7/27/30	0/1/1/1
33	LMT	m	103	-	-	6/21/61/61	0/2/2/2
27	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	508	41	-	9/39/115/115	-
26	SQD	b	620	-	-	17/49/69/69	0/1/1/1
23	CLA	B	608	2	-	4/39/115/115	-
24	PHO	a	415[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
34	LMG	C	521	-	-	13/46/66/70	0/1/1/1
26	SQD	a	411	-	-	14/49/69/69	0/1/1/1
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	B	605	2	-	7/39/115/115	-
23	CLA	B	609	2	-	1/39/115/115	-
24	PHO	a	407[B]	-	-	5/37/103/103	0/5/6/6
25	BCR	t	102	-	-	3/29/63/63	0/2/2/2
29	PL9	a	413[B]	-	-	15/53/73/73	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	404[B]	1	-	6/39/115/115	-
23	CLA	B	602	2	-	9/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
34	LMG	D	411	39	-	10/46/66/70	0/1/1/1
35	HTG	B	621	-	-	4/10/30/30	0/1/1/1
33	LMT	A	420	-	-	15/21/61/61	0/2/2/2
23	CLA	A	406[A]	41	-	7/39/115/115	-
32	LHG	D	406[B]	-	-	19/53/53/53	-
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	C	512	3	-	2/39/115/115	-
32	LHG	d	407[B]	-	-	13/53/53/53	-
23	CLA	C	514	3	-	7/39/115/115	-
23	CLA	c	506	3	-	7/39/115/115	-
25	BCR	K	102	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
34	LMG	m	101	-	-	10/46/66/70	0/1/1/1
23	CLA	b	613	2	-	6/39/115/115	-
23	CLA	C	509	3	-	7/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
27	GOL	b	628	-	-	0/4/4/4	-
32	LHG	E	101[A]	-	-	22/46/46/53	-
34	LMG	B	620	-	-	14/46/66/70	0/1/1/1
33	LMT	M	101	-	-	5/21/61/61	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
33	LMT	D	401	-	-	6/21/61/61	0/2/2/2
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	a	405[B]	41	-	6/39/115/115	-
32	LHG	d	412[A]	-	-	13/53/53/53	-
23	CLA	B	601	41	-	11/39/115/115	-
32	LHG	a	419[B]	-	-	16/46/46/53	-
23	CLA	b	615	2	-	7/39/115/115	-
33	LMT	B	626	-	-	11/21/61/61	0/2/2/2
36	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	c	512	3	-	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	505	41	-	8/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	B	616	2	-	5/39/115/115	-
23	CLA	b	604	2	-	11/39/115/115	-
23	CLA	B	612	2	-	7/39/115/115	-
23	CLA	C	504	3	-	4/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
24	PHO	a	407[A]	-	-	5/37/103/103	0/5/6/6
23	CLA	A	404[A]	1	-	5/39/115/115	-
23	CLA	b	612	2	-	4/39/115/115	-
23	CLA	A	405[B]	41	-	4/39/115/115	-
36	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
27	GOL	B	627	-	-	4/4/4/4	-

All (1860) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407[B]	PHO	C1B-C2B	9.39	1.50	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	415[B]	PHO	C1D-C2D	9.08	1.49	1.39
24	a	407[A]	PHO	C1B-C2B	8.96	1.49	1.39
24	a	415[B]	PHO	C1B-C2B	8.82	1.49	1.39
24	a	415[A]	PHO	C1B-C2B	8.77	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	8.76	1.49	1.39
24	A	417[A]	PHO	C1D-C2D	8.71	1.49	1.39
24	a	415[A]	PHO	C1D-C2D	8.58	1.49	1.39
24	a	407[A]	PHO	C1D-C2D	8.45	1.48	1.39
24	a	407[B]	PHO	C1D-C2D	8.42	1.48	1.39
24	A	407[A]	PHO	C1B-C2B	8.30	1.48	1.39
24	A	417[A]	PHO	C1B-C2B	8.26	1.48	1.39
24	A	407[B]	PHO	C1B-C2B	8.25	1.48	1.39
24	A	417[B]	PHO	C1B-C2B	8.19	1.48	1.39
24	A	417[B]	PHO	C1D-C2D	8.07	1.48	1.39
40	v	201	HEC	C3D-C2D	7.72	1.53	1.36
40	V	201	HEC	C3D-C2D	7.46	1.52	1.36
23	B	611	CLA	CMB-C2B	7.37	1.66	1.50
24	a	415[A]	PHO	C3B-C4B	7.11	1.49	1.41
23	B	611	CLA	C1D-ND	6.98	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C3B-C4B	6.83	1.49	1.41
24	a	415[B]	PHO	C3B-C4B	6.75	1.49	1.41
23	B	611	CLA	C1B-C2B	6.72	1.59	1.43
24	a	407[B]	PHO	C4D-CHA	6.61	1.50	1.39
24	A	417[A]	PHO	C3B-C4B	6.61	1.49	1.41
24	A	417[B]	PHO	C3B-C4B	6.58	1.49	1.41
24	a	407[B]	PHO	C3B-C4B	6.56	1.49	1.41
24	a	407[A]	PHO	C3B-C4B	6.52	1.49	1.41
24	A	407[A]	PHO	C3B-C4B	6.43	1.48	1.41
24	A	417[B]	PHO	C4D-CHA	6.42	1.49	1.39
24	a	407[B]	PHO	C3B-C2B	6.41	1.49	1.40
24	a	407[A]	PHO	C3B-C2B	6.36	1.49	1.40
24	A	417[A]	PHO	C4D-CHA	6.36	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.35	1.49	1.39
24	a	407[A]	PHO	C4D-CHA	6.34	1.49	1.39
24	a	415[B]	PHO	C3B-C2B	6.33	1.49	1.40
24	a	415[B]	PHO	C4D-CHA	6.30	1.49	1.39
24	A	417[B]	PHO	C3B-C2B	6.20	1.49	1.40
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
24	A	417[A]	PHO	C3B-C2B	6.12	1.48	1.40
24	a	415[A]	PHO	C4D-CHA	6.09	1.49	1.39
24	A	417[A]	PHO	C3C-C2C	6.07	1.49	1.36
24	A	407[B]	PHO	C4D-CHA	6.06	1.49	1.39
23	D	403	CLA	C1D-ND	6.05	1.45	1.37
24	A	417[B]	PHO	C3C-C2C	6.03	1.49	1.36
24	a	415[A]	PHO	C3C-C2C	5.98	1.49	1.36
23	a	405[B]	CLA	C1D-ND	5.97	1.45	1.37
24	a	415[A]	PHO	C3B-C2B	5.90	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	5.90	1.48	1.40
24	a	415[B]	PHO	C3C-C2C	5.89	1.49	1.36
23	C	511	CLA	C1D-ND	5.78	1.44	1.37
23	B	611	CLA	CHC-C1C	5.71	1.50	1.38
24	a	407[B]	PHO	C3C-C2C	5.71	1.48	1.36
23	D	403	CLA	C3C-C2C	5.70	1.48	1.36
23	c	509	CLA	C3C-C2C	5.68	1.48	1.36
23	c	513	CLA	C3C-C2C	5.67	1.48	1.36
24	A	407[B]	PHO	C3C-C2C	5.66	1.48	1.36
24	a	407[B]	PHO	C3D-C2D	5.66	1.49	1.39
23	B	611	CLA	C3C-C2C	5.65	1.48	1.36
23	c	510	CLA	C3C-C2C	5.61	1.48	1.36
24	A	407[A]	PHO	C3C-C2C	5.58	1.48	1.36
23	b	601	CLA	C1D-ND	5.57	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C3C-C2C	5.57	1.48	1.36
23	C	503	CLA	C1D-ND	5.56	1.44	1.37
23	b	616	CLA	C1D-ND	5.52	1.44	1.37
23	c	514	CLA	C1D-ND	5.52	1.44	1.37
23	B	610	CLA	C3C-C2C	5.50	1.48	1.36
24	a	407[A]	PHO	C3C-C2C	5.49	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.49	1.48	1.36
23	C	509	CLA	C3C-C2C	5.48	1.48	1.36
23	b	602	CLA	C3C-C2C	5.48	1.48	1.36
23	c	505	CLA	C1D-ND	5.46	1.44	1.37
23	C	513	CLA	C3C-C2C	5.46	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.45	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
23	c	512	CLA	C1D-ND	5.44	1.44	1.37
23	c	504	CLA	C3C-C2C	5.43	1.48	1.36
23	b	615	CLA	C3C-C2C	5.43	1.48	1.36
23	b	609	CLA	O2D-CGD	5.43	1.46	1.33
24	a	407[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	b	614	CLA	C3C-C2C	5.41	1.48	1.36
23	a	408	CLA	C3C-C2C	5.41	1.48	1.36
23	d	403	CLA	C3C-C2C	5.39	1.48	1.36
23	b	605	CLA	C3C-C2C	5.38	1.48	1.36
23	a	404[B]	CLA	C3C-C2C	5.38	1.48	1.36
23	B	605	CLA	C1D-ND	5.37	1.44	1.37
23	a	405[B]	CLA	C3C-C2C	5.37	1.48	1.36
24	a	415[B]	PHO	C3D-C2D	5.36	1.49	1.39
23	d	402[B]	CLA	C3C-C2C	5.35	1.48	1.36
23	A	408	CLA	C3C-C2C	5.35	1.48	1.36
23	a	405[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	B	601	CLA	C3C-C2C	5.35	1.48	1.36
23	C	504	CLA	C3C-C2C	5.35	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.35	1.48	1.36
23	b	607	CLA	C3C-C2C	5.35	1.48	1.36
23	b	606	CLA	C3C-C2C	5.34	1.48	1.36
23	a	406[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	c	514	CLA	C3C-C2C	5.34	1.48	1.36
23	c	506	CLA	C3C-C2C	5.33	1.48	1.36
23	b	603	CLA	C3C-C2C	5.32	1.48	1.36
23	b	601	CLA	C3C-C2C	5.31	1.48	1.36
23	C	514	CLA	C3C-C2C	5.31	1.48	1.36
23	A	404[B]	CLA	C1D-ND	5.30	1.44	1.37
23	C	511	CLA	C3C-C2C	5.29	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C3C-C2C	5.28	1.48	1.36
24	a	415[A]	PHO	C3D-C2D	5.28	1.48	1.39
23	c	509	CLA	O2D-CGD	5.26	1.46	1.33
24	A	417[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	a	405[B]	CLA	O2D-CGD	5.25	1.46	1.33
23	B	601	CLA	C1D-ND	5.24	1.44	1.37
23	c	511	CLA	O2D-CGD	5.24	1.46	1.33
23	B	603	CLA	C3C-C2C	5.24	1.47	1.36
23	C	513	CLA	CHC-C1C	5.24	1.49	1.38
23	d	402[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	C	510	CLA	C3C-C2C	5.23	1.47	1.36
23	b	610	CLA	C3C-C2C	5.23	1.47	1.36
23	c	512	CLA	C3C-C2C	5.22	1.47	1.36
23	D	402[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	c	505	CLA	O2D-CGD	5.22	1.45	1.33
23	D	402[B]	CLA	C3C-C2C	5.21	1.47	1.36
23	b	602	CLA	O2D-CGD	5.21	1.45	1.33
23	B	606	CLA	C3C-C2C	5.21	1.47	1.36
23	d	403	CLA	C1D-ND	5.20	1.44	1.37
23	C	508	CLA	C3C-C2C	5.20	1.47	1.36
23	B	605	CLA	C3C-C2C	5.20	1.47	1.36
23	B	604	CLA	C3C-C2C	5.18	1.47	1.36
23	c	502	CLA	C1D-ND	5.16	1.44	1.37
23	b	616	CLA	C3C-C2C	5.16	1.47	1.36
23	a	405[A]	CLA	C1D-ND	5.16	1.44	1.37
23	C	513	CLA	C1D-ND	5.15	1.44	1.37
23	C	505	CLA	C3C-C2C	5.14	1.47	1.36
23	c	509	CLA	C1D-ND	5.14	1.44	1.37
23	b	611	CLA	C3C-C2C	5.14	1.47	1.36
23	c	510	CLA	O2D-CGD	5.13	1.45	1.33
23	c	502	CLA	C3C-C2C	5.13	1.47	1.36
23	B	614	CLA	C3C-C2C	5.13	1.47	1.36
23	c	503	CLA	C3C-C2C	5.13	1.47	1.36
23	b	605	CLA	C1D-ND	5.13	1.44	1.37
23	c	504	CLA	CHC-C1C	5.12	1.48	1.38
23	B	602	CLA	C1D-ND	5.11	1.44	1.37
24	A	417[B]	PHO	C3D-C2D	5.11	1.48	1.39
23	B	601	CLA	O2D-CGD	5.11	1.45	1.33
23	C	503	CLA	C3C-C2C	5.11	1.47	1.36
23	C	507	CLA	O2D-CGD	5.11	1.45	1.33
23	B	615	CLA	C1D-ND	5.10	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C3C-C2C	5.10	1.47	1.36
25	C	515	BCR	C23-C22	-5.09	1.35	1.45
40	V	201	HEC	FE-ND	5.09	2.10	1.94
23	c	514	CLA	O2D-CGD	5.08	1.45	1.33
23	B	614	CLA	C1D-ND	5.07	1.44	1.37
23	c	504	CLA	C1D-ND	5.07	1.44	1.37
23	C	510	CLA	O2D-CGD	5.06	1.45	1.33
23	B	609	CLA	C3C-C2C	5.06	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
23	c	507	CLA	C3C-C2C	5.05	1.47	1.36
23	B	616	CLA	C3C-C2C	5.04	1.47	1.36
23	C	502	CLA	C3C-C2C	5.04	1.47	1.36
23	b	602	CLA	CHC-C1C	5.03	1.48	1.38
23	A	405[B]	CLA	C3C-C2C	5.03	1.47	1.36
23	b	603	CLA	O2D-CGD	5.03	1.45	1.33
23	B	615	CLA	O2D-CGD	5.03	1.45	1.33
24	a	407[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	c	505	CLA	C3C-C2C	5.03	1.47	1.36
24	a	407[B]	PHO	O2D-CGD	5.02	1.45	1.33
23	D	402[B]	CLA	C1D-ND	5.02	1.44	1.37
23	C	512	CLA	O2D-CGD	5.02	1.45	1.33
23	C	503	CLA	O2D-CGD	5.01	1.45	1.33
23	B	601	CLA	O2A-CGA	5.01	1.48	1.33
23	B	602	CLA	C3C-C2C	5.00	1.47	1.36
23	c	513	CLA	CHC-C1C	4.99	1.48	1.38
23	B	606	CLA	C1D-ND	4.99	1.43	1.37
23	b	613	CLA	C1D-ND	4.99	1.43	1.37
24	a	415[B]	PHO	O2D-CGD	4.99	1.45	1.33
23	C	509	CLA	C1D-ND	4.99	1.43	1.37
23	B	609	CLA	O2D-CGD	4.98	1.45	1.33
23	B	613	CLA	O2D-CGD	4.98	1.45	1.33
23	C	507	CLA	C3C-C2C	4.98	1.47	1.36
23	a	405[A]	CLA	O2D-CGD	4.98	1.45	1.33
23	c	507	CLA	C1D-ND	4.97	1.43	1.37
23	A	406[B]	CLA	O2D-CGD	4.97	1.45	1.33
25	D	404	BCR	C23-C22	-4.97	1.35	1.45
25	K	102	BCR	C23-C22	-4.97	1.35	1.45
23	c	508	CLA	C1D-ND	4.96	1.43	1.37
23	c	513	CLA	C1D-ND	4.96	1.43	1.37
23	A	405[B]	CLA	C1D-ND	4.96	1.43	1.37
23	C	510	CLA	C1D-ND	4.96	1.43	1.37
23	b	610	CLA	O2D-CGD	4.96	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	O2D-CGD	4.96	1.45	1.33
23	D	402[B]	CLA	O2D-CGD	4.96	1.45	1.33
23	C	509	CLA	O2D-CGD	4.95	1.45	1.33
24	a	415[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	B	610	CLA	C1D-ND	4.95	1.43	1.37
23	A	404[B]	CLA	O2D-CGD	4.95	1.45	1.33
23	B	608	CLA	C1D-ND	4.94	1.43	1.37
23	b	601	CLA	O2D-CGD	4.94	1.45	1.33
25	k	101	BCR	C23-C22	-4.93	1.35	1.45
23	b	613	CLA	CHC-C1C	4.93	1.48	1.38
23	c	506	CLA	CHC-C1C	4.93	1.48	1.38
23	C	506	CLA	C3C-C2C	4.93	1.47	1.36
23	d	403	CLA	CHC-C1C	4.92	1.48	1.38
23	c	512	CLA	O2D-CGD	4.92	1.45	1.33
23	b	604	CLA	C1D-ND	4.92	1.43	1.37
23	b	604	CLA	C3C-C2C	4.91	1.47	1.36
24	A	417[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	B	609	CLA	CHC-C1C	4.91	1.48	1.38
23	C	514	CLA	C1D-ND	4.91	1.43	1.37
23	C	512	CLA	C3C-C2C	4.91	1.47	1.36
24	A	417[B]	PHO	O2D-CGD	4.90	1.45	1.33
24	A	407[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	A	406[A]	CLA	O2D-CGD	4.90	1.45	1.33
24	A	407[B]	PHO	O2D-CGD	4.90	1.45	1.33
23	b	603	CLA	C1D-ND	4.89	1.43	1.37
23	A	405[B]	CLA	O2D-CGD	4.89	1.45	1.33
25	b	619	BCR	C23-C22	-4.89	1.35	1.45
23	B	601	CLA	CHC-C1C	4.88	1.48	1.38
25	d	404	BCR	C23-C22	-4.88	1.35	1.45
23	B	613	CLA	C1D-ND	4.88	1.43	1.37
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
38	F	102	HEM	FE-NB	4.88	2.10	1.94
23	B	612	CLA	CHC-C1C	4.88	1.48	1.38
23	B	604	CLA	O2D-CGD	4.88	1.45	1.33
23	c	503	CLA	O2D-CGD	4.87	1.45	1.33
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	B	616	CLA	CHC-C1C	4.87	1.48	1.38
23	b	610	CLA	CHC-C1C	4.86	1.48	1.38
23	b	606	CLA	C1D-ND	4.86	1.43	1.37
23	c	508	CLA	C3C-C2C	4.86	1.47	1.36
23	b	605	CLA	O2D-CGD	4.86	1.45	1.33
23	B	606	CLA	CHC-C1C	4.85	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	CHC-C1C	4.85	1.48	1.38
23	C	514	CLA	O2D-CGD	4.85	1.45	1.33
23	c	507	CLA	O2D-CGD	4.85	1.45	1.33
23	c	513	CLA	O2D-CGD	4.85	1.45	1.33
23	C	504	CLA	CHC-C1C	4.84	1.48	1.38
23	c	508	CLA	O2D-CGD	4.84	1.45	1.33
23	C	502	CLA	C1D-ND	4.84	1.43	1.37
24	a	415[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	a	408	CLA	CHC-C1C	4.84	1.48	1.38
23	B	607	CLA	C3C-C2C	4.84	1.47	1.36
23	B	613	CLA	CHC-C1C	4.84	1.48	1.38
38	f	101	HEM	FE-NB	4.83	2.09	1.94
23	B	615	CLA	C3C-C2C	4.83	1.47	1.36
26	F	103	SQD	O47-C7	4.83	1.47	1.34
23	c	510	CLA	C1D-ND	4.82	1.43	1.37
23	B	610	CLA	O2D-CGD	4.82	1.45	1.33
23	c	511	CLA	C1D-ND	4.82	1.43	1.37
23	b	609	CLA	C3C-C2C	4.82	1.47	1.36
23	D	402[A]	CLA	O2D-CGD	4.80	1.44	1.33
25	C	516	BCR	C23-C22	-4.80	1.35	1.45
23	D	403	CLA	CHC-C1C	4.80	1.48	1.38
23	C	505	CLA	O2D-CGD	4.80	1.44	1.33
25	B	617	BCR	C23-C22	-4.79	1.35	1.45
24	a	415[B]	PHO	OBD-CAD	4.78	1.29	1.22
23	a	406[B]	CLA	C1D-ND	4.77	1.43	1.37
23	a	406[B]	CLA	CHC-C1C	4.77	1.48	1.38
23	C	504	CLA	C1D-ND	4.77	1.43	1.37
23	a	406[B]	CLA	O2D-CGD	4.76	1.44	1.33
23	b	601	CLA	O2A-CGA	4.76	1.47	1.33
23	B	602	CLA	CHC-C1C	4.75	1.48	1.38
23	b	608	CLA	C3C-C2C	4.74	1.46	1.36
23	A	406[B]	CLA	CHC-C1C	4.74	1.48	1.38
23	c	509	CLA	CHC-C1C	4.74	1.48	1.38
23	b	613	CLA	C3C-C2C	4.74	1.46	1.36
23	b	613	CLA	O2D-CGD	4.74	1.44	1.33
25	B	619	BCR	C23-C22	-4.74	1.35	1.45
23	B	613	CLA	C3C-C2C	4.74	1.46	1.36
23	b	614	CLA	O2D-CGD	4.74	1.44	1.33
23	B	608	CLA	C3C-C2C	4.74	1.46	1.36
23	B	604	CLA	CHC-C1C	4.73	1.48	1.38
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	b	616	CLA	CHC-C1C	4.73	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	O2D-CGD	4.73	1.44	1.33
23	a	408	CLA	O2D-CGD	4.73	1.44	1.33
23	C	506	CLA	CHC-C1C	4.73	1.48	1.38
23	B	603	CLA	C1D-ND	4.72	1.43	1.37
23	A	406[A]	CLA	CHC-C1C	4.72	1.48	1.38
23	C	506	CLA	O2D-CGD	4.71	1.44	1.33
23	b	615	CLA	CHC-C1C	4.70	1.48	1.38
23	B	611	CLA	CHC-C4B	4.70	1.50	1.39
23	b	606	CLA	CHC-C1C	4.70	1.48	1.38
23	C	511	CLA	CHC-C1C	4.68	1.48	1.38
23	C	508	CLA	CHC-C1C	4.68	1.48	1.38
23	A	404[B]	CLA	CHC-C1C	4.68	1.48	1.38
23	D	403	CLA	O2D-CGD	4.67	1.44	1.33
23	a	404[B]	CLA	O2D-CGD	4.67	1.44	1.33
23	d	402[A]	CLA	O2D-CGD	4.66	1.44	1.33
23	b	602	CLA	C1D-ND	4.66	1.43	1.37
23	B	603	CLA	O2D-CGD	4.66	1.44	1.33
23	b	611	CLA	O2D-CGD	4.66	1.44	1.33
23	c	512	CLA	CHC-C1C	4.66	1.48	1.38
23	b	616	CLA	O2D-CGD	4.66	1.44	1.33
23	C	513	CLA	O2D-CGD	4.65	1.44	1.33
23	c	514	CLA	CHC-C1C	4.65	1.48	1.38
23	b	609	CLA	C1D-ND	4.64	1.43	1.37
34	c	521	LMG	O7-C10	4.64	1.47	1.34
25	T	102	BCR	C23-C22	-4.63	1.36	1.45
23	c	508	CLA	CHC-C1C	4.63	1.47	1.38
34	C	521	LMG	O7-C10	4.63	1.47	1.34
23	b	604	CLA	CHC-C1C	4.63	1.47	1.38
26	a	411	SQD	O48-C23	4.62	1.46	1.33
23	a	404[B]	CLA	C1D-ND	4.62	1.43	1.37
23	C	511	CLA	O2D-CGD	4.62	1.44	1.33
23	a	404[A]	CLA	C1D-ND	4.62	1.43	1.37
23	b	601	CLA	CHC-C1C	4.61	1.47	1.38
23	b	615	CLA	C1D-ND	4.61	1.43	1.37
25	b	617	BCR	C23-C22	-4.61	1.36	1.45
23	d	402[B]	CLA	O2D-CGD	4.61	1.44	1.33
23	b	606	CLA	O2D-CGD	4.60	1.44	1.33
24	A	417[B]	PHO	OBD-CAD	4.59	1.28	1.22
25	y	101	BCR	C23-C22	-4.59	1.36	1.45
23	A	405[B]	CLA	CHC-C1C	4.58	1.47	1.38
23	c	502	CLA	CHC-C1C	4.58	1.47	1.38
23	d	402[B]	CLA	C1D-ND	4.58	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	O2D-CGD	4.58	1.44	1.33
23	a	406[A]	CLA	CHC-C1C	4.58	1.47	1.38
23	c	506	CLA	O2D-CGD	4.58	1.44	1.33
23	A	408	CLA	O2D-CGD	4.58	1.44	1.33
23	b	602	CLA	CHD-C1D	4.57	1.47	1.38
25	c	516	BCR	C23-C22	-4.56	1.36	1.45
23	B	606	CLA	O2D-CGD	4.55	1.44	1.33
23	b	604	CLA	O2D-CGD	4.55	1.44	1.33
23	A	405[A]	CLA	CHC-C1C	4.55	1.47	1.38
23	C	505	CLA	C1D-ND	4.55	1.43	1.37
23	b	614	CLA	CHC-C1C	4.54	1.47	1.38
23	a	404[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	c	507	CLA	CHC-C1C	4.54	1.47	1.38
23	B	608	CLA	O2D-CGD	4.53	1.44	1.33
23	b	614	CLA	C1D-ND	4.53	1.43	1.37
23	b	604	CLA	CHD-C1D	4.53	1.47	1.38
23	b	605	CLA	CHC-C1C	4.52	1.47	1.38
24	A	407[B]	PHO	C3D-C2D	4.52	1.47	1.39
23	B	616	CLA	O2D-CGD	4.51	1.44	1.33
23	b	609	CLA	CHC-C1C	4.50	1.47	1.38
23	D	402[B]	CLA	CHC-C1C	4.50	1.47	1.38
26	f	102	SQD	O47-C7	4.50	1.47	1.34
26	L	101	SQD	O47-C7	4.50	1.47	1.34
23	B	607	CLA	CHC-C1C	4.50	1.47	1.38
23	a	406[A]	CLA	O2D-CGD	4.50	1.44	1.33
25	c	515	BCR	C23-C22	-4.50	1.36	1.45
23	b	607	CLA	C1D-ND	4.49	1.43	1.37
40	v	201	HEC	FE-ND	4.49	2.08	1.94
23	c	514	CLA	O2A-CGA	4.49	1.46	1.33
23	B	605	CLA	CHC-C1C	4.48	1.47	1.38
23	B	614	CLA	O2D-CGD	4.48	1.44	1.33
23	b	608	CLA	O2D-CGD	4.48	1.44	1.33
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
34	C	521	LMG	O8-C28	4.47	1.46	1.33
25	h	101	BCR	C23-C22	-4.47	1.36	1.45
23	a	405[B]	CLA	CHC-C1C	4.46	1.47	1.38
34	z	101	LMG	O8-C28	4.46	1.46	1.33
32	E	101[B]	LHG	O8-C23	4.46	1.46	1.33
25	A	409	BCR	C23-C22	-4.46	1.36	1.45
23	B	614	CLA	CHB-C1B	4.46	1.49	1.39
23	B	611	CLA	C4B-NB	-4.46	1.32	1.37
23	b	607	CLA	CHC-C1C	4.46	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	CHC-C1C	4.45	1.47	1.38
23	B	604	CLA	C1D-ND	4.45	1.43	1.37
23	C	506	CLA	C1D-ND	4.45	1.43	1.37
23	B	610	CLA	OBD-CAD	4.45	1.30	1.22
23	c	511	CLA	CHC-C1C	4.45	1.47	1.38
23	b	607	CLA	O2D-CGD	4.44	1.44	1.33
25	H	101	BCR	C23-C22	-4.43	1.36	1.45
23	b	607	CLA	CHD-C1D	4.43	1.47	1.38
23	C	507	CLA	C1D-ND	4.43	1.43	1.37
23	b	609	CLA	CHD-C1D	4.43	1.47	1.38
23	c	513	CLA	O2A-CGA	4.43	1.46	1.33
23	C	503	CLA	CHC-C1C	4.43	1.47	1.38
23	A	408	CLA	CHC-C1C	4.43	1.47	1.38
23	B	615	CLA	CHC-C1C	4.42	1.47	1.38
23	B	610	CLA	CHC-C1C	4.42	1.47	1.38
23	a	404[B]	CLA	CHC-C1C	4.42	1.47	1.38
23	b	611	CLA	CHC-C1C	4.42	1.47	1.38
23	c	509	CLA	CHD-C1D	4.42	1.47	1.38
23	b	611	CLA	O2A-CGA	4.41	1.46	1.33
25	a	409	BCR	C23-C22	-4.41	1.36	1.45
23	B	604	CLA	CHD-C1D	4.41	1.46	1.38
23	D	403	CLA	CHD-C1D	4.41	1.46	1.38
25	t	102	BCR	C23-C22	-4.41	1.36	1.45
23	a	405[A]	CLA	CHC-C1C	4.40	1.47	1.38
23	b	612	CLA	O2D-CGD	4.40	1.43	1.33
23	c	506	CLA	CHD-C1D	4.40	1.46	1.38
23	a	405[B]	CLA	C3D-C2D	4.40	1.51	1.39
23	c	504	CLA	CHD-C1D	4.40	1.46	1.38
23	A	406[B]	CLA	CHD-C1D	4.39	1.46	1.38
32	a	419[A]	LHG	O8-C23	4.39	1.46	1.33
23	C	507	CLA	CHD-C1D	4.39	1.46	1.38
23	b	610	CLA	CHD-C1D	4.39	1.46	1.38
23	C	512	CLA	CHC-C1C	4.39	1.47	1.38
34	B	620	LMG	O8-C28	4.39	1.46	1.33
23	a	405[A]	CLA	C3D-C2D	4.38	1.51	1.39
23	c	506	CLA	C1D-ND	4.38	1.43	1.37
23	B	616	CLA	C1D-ND	4.38	1.43	1.37
26	A	412	SQD	O48-C23	4.37	1.46	1.33
23	C	510	CLA	CHC-C1C	4.37	1.47	1.38
32	a	419[B]	LHG	O8-C23	4.37	1.46	1.33
23	C	502	CLA	CHD-C1D	4.37	1.46	1.38
23	c	514	CLA	CHD-C1D	4.37	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	O2D-CGD	4.36	1.43	1.33
26	b	620	SQD	O47-C7	4.36	1.46	1.34
23	B	602	CLA	CHD-C1D	4.36	1.46	1.38
23	C	514	CLA	CHD-C1D	4.36	1.46	1.38
23	a	404[A]	CLA	CHC-C1C	4.36	1.47	1.38
25	Y	101	BCR	C23-C22	-4.36	1.36	1.45
23	B	611	CLA	O2D-CGD	4.36	1.43	1.33
24	a	407[A]	PHO	OBD-CAD	4.36	1.28	1.22
23	b	612	CLA	CHC-C1C	4.35	1.47	1.38
23	d	403	CLA	CHD-C1D	4.35	1.46	1.38
23	b	608	CLA	CHC-C1C	4.35	1.47	1.38
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33
23	b	602	CLA	CHC-C4B	4.34	1.49	1.39
23	C	510	CLA	CHD-C1D	4.34	1.46	1.38
23	C	508	CLA	C1D-ND	4.34	1.43	1.37
23	C	509	CLA	C3D-C2D	4.33	1.51	1.39
23	C	512	CLA	C1D-ND	4.33	1.43	1.37
23	b	601	CLA	CHD-C1D	4.33	1.46	1.38
23	B	612	CLA	C1B-NB	-4.33	1.32	1.37
23	b	608	CLA	C1D-ND	4.32	1.43	1.37
23	C	505	CLA	CHC-C1C	4.32	1.47	1.38
24	A	417[A]	PHO	OBD-CAD	4.31	1.28	1.22
26	b	620	SQD	O48-C23	4.31	1.45	1.33
23	c	513	CLA	CHD-C1D	4.31	1.46	1.38
23	A	404[A]	CLA	CHC-C1C	4.31	1.47	1.38
23	B	609	CLA	C1D-ND	4.31	1.43	1.37
32	d	407[A]	LHG	O8-C23	4.31	1.45	1.33
36	c	519	DGD	O1G-C1A	4.31	1.45	1.33
23	c	503	CLA	O2A-CGA	4.30	1.45	1.33
23	d	403	CLA	O2A-CGA	4.30	1.45	1.33
23	b	602	CLA	CHD-C4C	4.29	1.49	1.39
23	b	609	CLA	OBD-CAD	4.28	1.29	1.22
23	B	614	CLA	CHC-C1C	4.28	1.47	1.38
23	C	514	CLA	CHC-C1C	4.28	1.47	1.38
23	A	406[B]	CLA	C1D-ND	4.28	1.43	1.37
23	c	507	CLA	O2A-CGA	4.27	1.45	1.33
23	c	503	CLA	C1D-ND	4.27	1.43	1.37
23	c	503	CLA	CHC-C1C	4.27	1.47	1.38
23	D	402[A]	CLA	C1D-ND	4.27	1.43	1.37
23	C	504	CLA	O2D-CGD	4.27	1.43	1.33
38	F	102	HEM	FE-NC	4.26	2.09	1.95
23	b	603	CLA	CHC-C1C	4.26	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C1D-ND	4.26	1.43	1.37
23	c	512	CLA	CHB-C1B	4.26	1.49	1.39
23	B	609	CLA	CHD-C1D	4.26	1.46	1.38
23	d	402[B]	CLA	CHC-C1C	4.25	1.47	1.38
23	b	607	CLA	C1B-NB	-4.25	1.32	1.37
23	B	611	CLA	C3B-C2B	4.25	1.55	1.41
23	D	402[A]	CLA	CHC-C1C	4.25	1.47	1.38
23	A	408	CLA	O2A-CGA	4.25	1.45	1.33
23	b	609	CLA	CHB-C1B	4.24	1.48	1.39
23	A	405[B]	CLA	CHD-C1D	4.24	1.46	1.38
23	A	408	CLA	C1D-ND	4.24	1.43	1.37
23	C	511	CLA	CHD-C4C	4.24	1.48	1.39
23	B	603	CLA	C1B-NB	-4.23	1.32	1.37
25	b	618	BCR	C23-C22	-4.23	1.36	1.45
23	b	601	CLA	C3D-C2D	4.23	1.50	1.39
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
23	D	402[A]	CLA	O2A-CGA	4.22	1.45	1.33
34	Z	101	LMG	O7-C10	4.22	1.46	1.34
23	b	610	CLA	C1D-ND	4.22	1.43	1.37
23	c	504	CLA	O2D-CGD	4.22	1.43	1.33
34	m	101	LMG	O8-C28	4.21	1.45	1.33
24	A	407[B]	PHO	OBD-CAD	4.21	1.28	1.22
23	B	612	CLA	CHB-C1B	4.21	1.48	1.39
23	a	408	CLA	O2A-CGA	4.21	1.45	1.33
23	c	504	CLA	CHC-C4B	4.21	1.48	1.39
23	c	505	CLA	CHC-C1C	4.21	1.47	1.38
23	c	505	CLA	CHD-C1D	4.21	1.46	1.38
23	B	613	CLA	C3D-C2D	4.20	1.50	1.39
23	c	510	CLA	CHD-C1D	4.20	1.46	1.38
23	C	514	CLA	O2A-CGA	4.20	1.45	1.33
23	c	503	CLA	CHD-C1D	4.20	1.46	1.38
38	f	101	HEM	FE-NC	4.20	2.09	1.95
34	c	521	LMG	O8-C28	4.20	1.45	1.33
23	B	615	CLA	CHD-C1D	4.20	1.46	1.38
26	f	102	SQD	O48-C23	4.19	1.45	1.33
23	B	603	CLA	CHC-C1C	4.19	1.47	1.38
23	d	403	CLA	O2D-CGD	4.19	1.43	1.33
23	B	613	CLA	C1B-NB	-4.19	1.32	1.37
23	B	611	CLA	C1C-C2C	4.19	1.52	1.44
23	c	512	CLA	O2A-CGA	4.19	1.45	1.33
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	C	512	CLA	CHD-C1D	4.19	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	O2A-CGA	4.19	1.45	1.33
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
23	C	511	CLA	CHB-C1B	4.19	1.48	1.39
26	L	101	SQD	O48-C23	4.19	1.45	1.33
24	a	407[B]	PHO	OBD-CAD	4.19	1.28	1.22
23	C	512	CLA	O2A-CGA	4.19	1.45	1.33
23	d	402[B]	CLA	O2A-CGA	4.18	1.45	1.33
23	C	507	CLA	CHC-C1C	4.18	1.47	1.38
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
23	D	402[B]	CLA	O2A-CGA	4.18	1.45	1.33
23	b	604	CLA	CHC-C4B	4.18	1.48	1.39
23	c	508	CLA	CHD-C1D	4.18	1.46	1.38
34	c	520	LMG	O7-C10	4.18	1.46	1.34
23	c	509	CLA	C3D-C2D	4.17	1.50	1.39
23	c	504	CLA	O2A-CGA	4.17	1.45	1.33
23	C	513	CLA	O2A-CGA	4.17	1.45	1.33
23	c	504	CLA	CHD-C4C	4.17	1.48	1.39
23	C	509	CLA	O2A-CGA	4.16	1.45	1.33
23	c	508	CLA	O2A-CGA	4.16	1.45	1.33
23	B	607	CLA	O2D-CGD	4.15	1.43	1.33
23	a	406[A]	CLA	C1D-ND	4.15	1.42	1.37
23	A	404[B]	CLA	CHD-C1D	4.15	1.46	1.38
32	E	101[B]	LHG	O7-C7	4.15	1.46	1.34
34	C	520	LMG	O8-C28	4.15	1.45	1.33
23	B	609	CLA	C3D-C2D	4.15	1.50	1.39
23	d	403	CLA	C3D-C2D	4.15	1.50	1.39
36	C	517[B]	DGD	O2G-C1B	4.15	1.46	1.34
23	B	614	CLA	CHD-C4C	4.14	1.48	1.39
23	C	514	CLA	CHD-C4C	4.14	1.48	1.39
23	c	508	CLA	OBD-CAD	4.14	1.29	1.22
32	a	419[B]	LHG	O7-C7	4.14	1.46	1.34
24	A	407[A]	PHO	OBD-CAD	4.14	1.28	1.22
23	C	502	CLA	O2A-CGA	4.14	1.45	1.33
23	B	607	CLA	C1B-NB	-4.14	1.32	1.37
23	c	509	CLA	O2A-CGA	4.14	1.45	1.33
23	B	608	CLA	CHD-C1D	4.14	1.46	1.38
23	c	513	CLA	CHD-C4C	4.13	1.48	1.39
32	a	419[A]	LHG	O7-C7	4.13	1.46	1.34
23	B	604	CLA	CHB-C1B	4.13	1.48	1.39
23	d	402[A]	CLA	CHC-C1C	4.13	1.46	1.38
23	C	505	CLA	CHB-C1B	4.13	1.48	1.39
23	a	405[B]	CLA	O2A-CGA	4.13	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	CHD-C1D	4.13	1.46	1.38
23	c	511	CLA	CHB-C1B	4.12	1.48	1.39
23	a	406[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	b	604	CLA	CHB-C1B	4.12	1.48	1.39
23	C	504	CLA	CHD-C1D	4.12	1.46	1.38
23	B	606	CLA	CHD-C1D	4.12	1.46	1.38
23	B	612	CLA	C4B-NB	-4.11	1.32	1.37
23	b	608	CLA	O2A-CGA	4.11	1.45	1.33
36	C	519	DGD	O1G-C1A	4.11	1.45	1.33
23	C	513	CLA	CHD-C1D	4.11	1.46	1.38
23	d	402[A]	CLA	CHB-C1B	4.11	1.48	1.39
23	d	402[B]	CLA	CHB-C1B	4.11	1.48	1.39
36	c	518[B]	DGD	O1G-C1A	4.11	1.45	1.33
23	a	404[B]	CLA	CHD-C4C	4.11	1.48	1.39
26	A	412	SQD	O47-C7	4.11	1.45	1.34
23	A	405[B]	CLA	C3D-C2D	4.10	1.50	1.39
23	c	512	CLA	CHD-C1D	4.10	1.46	1.38
23	c	511	CLA	C3D-C2D	4.10	1.50	1.39
23	a	406[B]	CLA	O2A-CGA	4.10	1.45	1.33
34	c	501	LMG	O7-C10	4.10	1.45	1.34
23	A	405[B]	CLA	O2A-CGA	4.10	1.45	1.33
23	C	502	CLA	O2D-CGD	4.09	1.43	1.33
23	C	513	CLA	CHC-C4B	4.09	1.48	1.39
36	c	517[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	c	506	CLA	CHC-C4B	4.09	1.48	1.39
23	B	610	CLA	CHD-C1D	4.09	1.46	1.38
23	b	615	CLA	CHD-C1D	4.09	1.46	1.38
23	B	603	CLA	CHD-C1D	4.09	1.46	1.38
23	b	613	CLA	C3D-C2D	4.09	1.50	1.39
23	a	405[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	C	508	CLA	CHD-C1D	4.08	1.46	1.38
26	a	410[B]	SQD	O47-C7	4.08	1.45	1.34
32	L	102[B]	LHG	O8-C23	4.08	1.45	1.33
26	a	410[B]	SQD	O48-C23	4.08	1.45	1.33
23	D	402[B]	CLA	CHB-C1B	4.08	1.48	1.39
23	b	611	CLA	C1D-ND	4.08	1.42	1.37
23	b	612	CLA	CHB-C1B	4.07	1.48	1.39
23	B	601	CLA	CHC-C4B	4.07	1.48	1.39
26	a	410[A]	SQD	O47-C7	4.07	1.45	1.34
26	a	411	SQD	O47-C7	4.07	1.45	1.34
23	c	502	CLA	CHD-C1D	4.06	1.46	1.38
23	B	613	CLA	CHD-C1D	4.06	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	520	LMG	O7-C10	4.06	1.45	1.34
23	b	616	CLA	CHD-C1D	4.06	1.46	1.38
23	C	504	CLA	CHC-C4B	4.06	1.48	1.39
36	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
23	D	402[A]	CLA	CHB-C1B	4.06	1.48	1.39
34	z	101	LMG	O7-C10	4.05	1.45	1.34
23	a	404[B]	CLA	CHD-C1D	4.05	1.46	1.38
23	b	608	CLA	CHD-C1D	4.05	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.05	1.50	1.39
23	d	402[A]	CLA	O2A-CGA	4.05	1.45	1.33
23	C	506	CLA	CHD-C1D	4.05	1.46	1.38
23	C	512	CLA	CHD-C4C	4.05	1.48	1.39
23	B	614	CLA	C4B-NB	-4.05	1.32	1.37
23	B	616	CLA	C3D-C2D	4.04	1.50	1.39
25	B	618	BCR	C23-C22	-4.04	1.37	1.45
23	c	507	CLA	CHD-C1D	4.04	1.46	1.38
23	c	505	CLA	C3D-C2D	4.04	1.50	1.39
23	A	404[A]	CLA	CHD-C1D	4.03	1.46	1.38
34	c	501	LMG	O8-C28	4.03	1.45	1.33
23	b	601	CLA	CHD-C4C	4.03	1.48	1.39
23	B	605	CLA	CHC-C4B	4.03	1.48	1.39
23	C	506	CLA	CHC-C4B	4.03	1.48	1.39
23	b	607	CLA	C3D-C2D	4.03	1.50	1.39
23	C	503	CLA	C3D-C2D	4.03	1.50	1.39
23	C	509	CLA	CHD-C1D	4.03	1.46	1.38
36	C	518[B]	DGD	O1G-C1A	4.03	1.45	1.33
23	D	403	CLA	CHD-C4C	4.02	1.48	1.39
34	C	501	LMG	O7-C10	4.02	1.45	1.34
23	b	603	CLA	CHD-C1D	4.02	1.46	1.38
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
34	C	501	LMG	O8-C28	4.02	1.45	1.33
23	b	612	CLA	CHD-C1D	4.02	1.46	1.38
36	c	517[B]	DGD	O2G-C1B	4.02	1.45	1.34
23	B	615	CLA	O2A-CGA	4.02	1.45	1.33
23	A	404[B]	CLA	CHD-C4C	4.02	1.48	1.39
23	c	513	CLA	CHC-C4B	4.02	1.48	1.39
26	F	103	SQD	O48-C23	4.02	1.45	1.33
32	d	406[B]	LHG	O7-C7	4.01	1.45	1.34
23	c	510	CLA	CHC-C1C	4.01	1.46	1.38
23	B	602	CLA	CHD-C4C	4.01	1.48	1.39
23	c	514	CLA	CHD-C4C	4.01	1.48	1.39
23	D	403	CLA	C3D-C2D	4.01	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	CHD-C4C	4.01	1.48	1.39
32	d	412[B]	LHG	O8-C23	4.01	1.45	1.33
23	B	605	CLA	CHB-C1B	4.01	1.48	1.39
23	A	406[B]	CLA	O2A-CGA	4.01	1.45	1.33
23	B	608	CLA	C3D-C2D	4.00	1.50	1.39
23	B	609	CLA	CHC-C4B	4.00	1.48	1.39
32	d	407[B]	LHG	O8-C23	4.00	1.45	1.33
23	b	610	CLA	CHB-C1B	4.00	1.48	1.39
23	B	615	CLA	CHD-C4C	4.00	1.48	1.39
23	a	404[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	c	502	CLA	O2D-CGD	3.99	1.42	1.33
23	b	611	CLA	CHB-C1B	3.99	1.48	1.39
23	A	406[B]	CLA	C3D-C2D	3.99	1.50	1.39
34	c	520	LMG	O8-C28	3.98	1.45	1.33
23	B	601	CLA	CHD-C1D	3.98	1.46	1.38
23	c	512	CLA	CHD-C4C	3.98	1.48	1.39
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
23	B	611	CLA	OBD-CAD	3.98	1.29	1.22
26	a	410[A]	SQD	O48-C23	3.98	1.45	1.33
23	b	615	CLA	CHD-C4C	3.98	1.48	1.39
23	b	614	CLA	CHD-C1D	3.98	1.46	1.38
23	c	510	CLA	CHB-C1B	3.98	1.48	1.39
23	b	615	CLA	O2A-CGA	3.98	1.45	1.33
23	C	513	CLA	C3D-C2D	3.97	1.50	1.39
23	B	603	CLA	C3D-C2D	3.97	1.50	1.39
23	B	612	CLA	C1D-ND	3.97	1.42	1.37
23	c	504	CLA	CHB-C1B	3.97	1.48	1.39
32	D	407[B]	LHG	O7-C7	3.96	1.45	1.34
23	a	406[B]	CLA	C3D-C2D	3.96	1.49	1.39
23	C	505	CLA	CHD-C1D	3.96	1.46	1.38
23	c	509	CLA	OBD-CAD	3.96	1.29	1.22
23	a	404[A]	CLA	CHD-C4C	3.96	1.48	1.39
23	B	612	CLA	O2D-CGD	3.95	1.42	1.33
23	C	504	CLA	CHD-C4C	3.95	1.48	1.39
24	a	415[B]	PHO	O2A-CGA	3.95	1.44	1.33
26	A	410[B]	SQD	O48-C23	3.95	1.44	1.33
23	D	403	CLA	CHC-C4B	3.94	1.48	1.39
23	C	506	CLA	CHB-C1B	3.94	1.48	1.39
23	c	505	CLA	O2A-CGA	3.94	1.44	1.33
23	B	607	CLA	CHB-C1B	3.94	1.48	1.39
23	A	404[B]	CLA	C3D-C2D	3.94	1.49	1.39
23	b	606	CLA	CHD-C1D	3.94	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	O2A-CGA	3.94	1.44	1.33
23	C	514	CLA	C3D-C2D	3.94	1.49	1.39
36	h	102	DGD	O2G-C1B	3.93	1.45	1.34
23	b	616	CLA	O2A-CGA	3.93	1.44	1.33
23	B	610	CLA	C3D-C2D	3.93	1.49	1.39
23	c	508	CLA	C3D-C2D	3.93	1.49	1.39
23	C	510	CLA	CHB-C1B	3.93	1.48	1.39
23	D	402[B]	CLA	CHD-C1D	3.93	1.46	1.38
23	c	509	CLA	CHC-C4B	3.93	1.48	1.39
23	D	402[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	C	507	CLA	O2A-CGA	3.92	1.44	1.33
32	L	102[B]	LHG	O7-C7	3.92	1.45	1.34
23	B	611	CLA	O2A-CGA	3.92	1.44	1.33
36	c	517[B]	DGD	O1G-C1A	3.92	1.44	1.33
23	b	610	CLA	OBD-CAD	3.91	1.29	1.22
23	A	406[B]	CLA	OBD-CAD	3.91	1.29	1.22
23	a	408	CLA	C1D-ND	3.91	1.42	1.37
23	C	506	CLA	CHD-C4C	3.91	1.48	1.39
32	D	407[A]	LHG	O8-C23	3.90	1.44	1.33
23	c	507	CLA	CHD-C4C	3.90	1.48	1.39
23	c	502	CLA	O2A-CGA	3.90	1.44	1.33
23	a	406[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	C	511	CLA	CHD-C1D	3.90	1.46	1.38
23	D	402[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	b	613	CLA	CHC-C4B	3.89	1.48	1.39
23	b	610	CLA	CHC-C4B	3.89	1.48	1.39
23	a	405[B]	CLA	CHD-C4C	3.89	1.48	1.39
23	B	602	CLA	CHC-C4B	3.89	1.48	1.39
23	c	506	CLA	C3D-C2D	3.89	1.49	1.39
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
23	b	603	CLA	CHC-C4B	3.89	1.48	1.39
23	B	611	CLA	CHD-C1D	3.88	1.45	1.38
23	B	611	CLA	CHB-C1B	3.88	1.48	1.39
23	B	607	CLA	CHD-C1D	3.88	1.45	1.38
23	b	608	CLA	C4B-NB	-3.88	1.33	1.37
23	B	613	CLA	CHB-C1B	3.88	1.48	1.39
36	h	102	DGD	O1G-C1A	3.87	1.44	1.33
23	C	509	CLA	OBD-CAD	3.87	1.29	1.22
23	d	402[A]	CLA	C1B-NB	-3.87	1.33	1.37
23	D	402[B]	CLA	CHD-C4C	3.87	1.48	1.39
23	c	510	CLA	O2A-CGA	3.87	1.44	1.33
23	B	615	CLA	OBD-CAD	3.87	1.29	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	CHD-C4C	3.86	1.48	1.39
23	c	507	CLA	CHB-C1B	3.86	1.48	1.39
24	A	407[B]	PHO	O2A-CGA	3.86	1.44	1.33
23	B	607	CLA	CHC-C4B	3.86	1.48	1.39
23	c	508	CLA	CHD-C4C	3.86	1.48	1.39
23	C	512	CLA	CHB-C1B	3.86	1.48	1.39
34	B	620	LMG	O7-C10	3.86	1.45	1.34
23	B	602	CLA	C3D-C2D	3.86	1.49	1.39
23	C	503	CLA	O2A-CGA	3.86	1.44	1.33
23	C	510	CLA	O2A-CGA	3.86	1.44	1.33
23	b	602	CLA	OBD-CAD	3.86	1.29	1.22
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
24	A	417[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	c	503	CLA	CHB-C1B	3.85	1.48	1.39
23	C	510	CLA	C3D-C2D	3.85	1.49	1.39
23	b	616	CLA	C3D-C2D	3.85	1.49	1.39
23	c	507	CLA	C3D-C2D	3.85	1.49	1.39
23	B	615	CLA	C3D-C2D	3.85	1.49	1.39
36	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	C	510	CLA	C4B-NB	-3.85	1.33	1.37
23	b	611	CLA	CHD-C4C	3.85	1.48	1.39
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	C	507	CLA	CHD-C4C	3.84	1.48	1.39
23	b	609	CLA	C3D-C2D	3.84	1.49	1.39
23	B	606	CLA	CHB-C1B	3.84	1.48	1.39
32	d	407[B]	LHG	O7-C7	3.84	1.45	1.34
23	b	612	CLA	C3D-C2D	3.84	1.49	1.39
23	B	606	CLA	O2A-CGA	3.84	1.44	1.33
23	b	611	CLA	CHC-C4B	3.84	1.48	1.39
32	L	102[A]	LHG	O8-C23	3.84	1.44	1.33
23	B	614	CLA	CHC-C4B	3.84	1.48	1.39
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
23	b	612	CLA	OBD-CAD	3.84	1.29	1.22
36	c	518[A]	DGD	O1G-C1A	3.83	1.44	1.33
32	D	407[B]	LHG	O8-C23	3.83	1.44	1.33
23	b	603	CLA	CHD-C4C	3.83	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	B	616	CLA	O2A-CGA	3.83	1.44	1.33
23	C	505	CLA	C3D-C2D	3.83	1.49	1.39
35	b	623	HTG	C1'-S1	-3.83	1.76	1.81
23	a	405[B]	CLA	CHD-C1D	3.83	1.45	1.38
24	a	415[A]	PHO	O2A-CGA	3.83	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C3B-C4B	3.83	1.51	1.42
23	c	502	CLA	CHB-C1B	3.83	1.48	1.39
23	B	607	CLA	CHD-C4C	3.83	1.48	1.39
23	b	605	CLA	CHD-C4C	3.83	1.48	1.39
23	c	513	CLA	CHB-C1B	3.82	1.48	1.39
23	c	508	CLA	CHC-C4B	3.82	1.48	1.39
23	b	606	CLA	CHB-C1B	3.82	1.48	1.39
24	A	417[B]	PHO	O2A-CGA	3.82	1.44	1.33
23	b	610	CLA	CHD-C4C	3.82	1.48	1.39
32	L	102[A]	LHG	O7-C7	3.82	1.45	1.34
23	a	404[B]	CLA	OBD-CAD	3.81	1.29	1.22
23	A	406[B]	CLA	CHD-C4C	3.81	1.47	1.39
32	d	412[B]	LHG	O7-C7	3.81	1.45	1.34
23	d	402[A]	CLA	CHD-C1D	3.81	1.45	1.38
23	C	508	CLA	CHB-C1B	3.81	1.47	1.39
23	b	607	CLA	CHD-C4C	3.80	1.47	1.39
23	b	612	CLA	C1B-NB	-3.80	1.33	1.37
36	C	517[B]	DGD	O1G-C1A	3.80	1.44	1.33
23	c	510	CLA	C1B-NB	-3.80	1.33	1.37
23	c	502	CLA	CHD-C4C	3.80	1.47	1.39
23	b	602	CLA	O2A-CGA	3.80	1.44	1.33
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
23	C	506	CLA	O2A-CGA	3.80	1.44	1.33
23	A	406[A]	CLA	CHC-C4B	3.80	1.47	1.39
23	b	612	CLA	CHC-C4B	3.80	1.47	1.39
23	a	405[A]	CLA	CHD-C1D	3.80	1.45	1.38
34	d	410	LMG	O8-C28	3.79	1.44	1.33
23	C	512	CLA	C3D-C2D	3.79	1.49	1.39
23	C	502	CLA	CHD-C4C	3.79	1.47	1.39
23	c	502	CLA	C3D-C2D	3.79	1.49	1.39
23	c	508	CLA	CHB-C1B	3.79	1.47	1.39
23	a	408	CLA	CHD-C1D	3.79	1.45	1.38
36	H	102	DGD	O1G-C1A	3.79	1.44	1.33
23	B	611	CLA	C3B-C4B	3.78	1.51	1.42
36	C	518[B]	DGD	O2G-C1B	3.78	1.45	1.34
23	b	608	CLA	CHD-C4C	3.78	1.47	1.39
23	B	608	CLA	CHB-C1B	3.78	1.47	1.39
23	A	405[A]	CLA	CHB-C1B	3.78	1.47	1.39
23	C	513	CLA	CHD-C4C	3.78	1.47	1.39
23	c	509	CLA	CHD-C4C	3.78	1.47	1.39
23	b	614	CLA	CHC-C4B	3.78	1.47	1.39
23	c	503	CLA	C3D-C2D	3.78	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C3D-C2D	3.78	1.49	1.39
23	b	615	CLA	C1B-NB	-3.77	1.33	1.37
23	a	405[A]	CLA	OBD-CAD	3.77	1.29	1.22
34	d	410	LMG	O7-C10	3.77	1.44	1.34
23	A	408	CLA	CHD-C1D	3.77	1.45	1.38
23	a	404[B]	CLA	C3D-C2D	3.77	1.49	1.39
23	C	514	CLA	CHB-C1B	3.77	1.47	1.39
36	c	518[B]	DGD	O2G-C1B	3.77	1.44	1.34
23	B	612	CLA	CHD-C1D	3.76	1.45	1.38
23	B	602	CLA	CHB-C1B	3.76	1.47	1.39
23	B	608	CLA	CHC-C1C	3.76	1.46	1.38
23	A	408	CLA	CHD-C4C	3.76	1.47	1.39
23	b	609	CLA	O2A-CGA	3.76	1.44	1.33
23	c	511	CLA	O2A-CGA	3.76	1.44	1.33
23	b	608	CLA	C3D-C2D	3.76	1.49	1.39
23	a	406[A]	CLA	CHB-C1B	3.75	1.47	1.39
23	b	602	CLA	C3D-C2D	3.75	1.49	1.39
32	A	419[B]	LHG	O8-C23	3.75	1.44	1.33
23	B	614	CLA	O2A-CGA	3.75	1.44	1.33
32	b	630[B]	LHG	O7-C7	3.75	1.44	1.34
32	d	412[A]	LHG	O8-C23	3.75	1.44	1.33
23	C	503	CLA	CHB-C1B	3.75	1.47	1.39
23	D	402[B]	CLA	C3D-C2D	3.75	1.49	1.39
23	d	403	CLA	CHC-C4B	3.74	1.47	1.39
23	a	406[B]	CLA	CHD-C4C	3.74	1.47	1.39
23	C	510	CLA	OBD-CAD	3.74	1.28	1.22
23	B	605	CLA	C3D-C2D	3.74	1.49	1.39
24	a	407[B]	PHO	O2A-CGA	3.74	1.44	1.33
23	c	514	CLA	C3D-C2D	3.74	1.49	1.39
23	b	604	CLA	CHD-C4C	3.74	1.47	1.39
23	C	502	CLA	CHC-C4B	3.74	1.47	1.39
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	B	609	CLA	C3B-C4B	3.74	1.51	1.42
23	C	510	CLA	CHD-C4C	3.73	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	B	610	CLA	CHD-C4C	3.73	1.47	1.39
23	b	608	CLA	OBD-CAD	3.73	1.28	1.22
36	C	519	DGD	O2G-C1B	3.73	1.44	1.34
23	b	605	CLA	CHD-C1D	3.73	1.45	1.38
32	D	406[B]	LHG	O7-C7	3.73	1.44	1.34
23	b	611	CLA	C3D-C2D	3.73	1.49	1.39
23	c	506	CLA	CHB-C1B	3.73	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHB-C1B	3.73	1.47	1.39
23	C	513	CLA	OBD-CAD	3.73	1.28	1.22
23	C	503	CLA	CHD-C4C	3.72	1.47	1.39
23	c	514	CLA	CHB-C1B	3.72	1.47	1.39
23	D	402[A]	CLA	C1B-NB	-3.72	1.33	1.37
23	d	402[B]	CLA	CHD-C1D	3.72	1.45	1.38
32	d	406[A]	LHG	O7-C7	3.72	1.44	1.34
23	c	510	CLA	CHD-C4C	3.72	1.47	1.39
23	D	403	CLA	O2A-CGA	3.72	1.44	1.33
23	A	405[A]	CLA	CHD-C1D	3.72	1.45	1.38
23	b	606	CLA	O2A-CGA	3.72	1.44	1.33
23	B	612	CLA	O2A-CGA	3.72	1.44	1.33
36	C	518[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	B	613	CLA	OBD-CAD	3.71	1.28	1.22
23	B	605	CLA	O2A-CGA	3.71	1.44	1.33
23	A	406[B]	CLA	CHC-C4B	3.71	1.47	1.39
23	C	507	CLA	C3D-C2D	3.71	1.49	1.39
23	B	607	CLA	C1D-ND	3.70	1.42	1.37
23	d	402[B]	CLA	CHD-C4C	3.70	1.47	1.39
32	b	630[B]	LHG	O8-C23	3.70	1.44	1.33
26	A	410[B]	SQD	O47-C7	3.70	1.44	1.34
23	b	614	CLA	O2A-CGA	3.70	1.44	1.33
23	C	507	CLA	CHB-C1B	3.70	1.47	1.39
23	C	507	CLA	C4B-NB	-3.70	1.33	1.37
23	b	604	CLA	C3D-C2D	3.70	1.49	1.39
23	C	506	CLA	C3D-C2D	3.69	1.49	1.39
23	a	404[A]	CLA	CHB-C1B	3.69	1.47	1.39
23	C	505	CLA	O2A-CGA	3.69	1.44	1.33
23	b	603	CLA	O2A-CGA	3.69	1.44	1.33
23	b	605	CLA	C3D-C2D	3.68	1.49	1.39
23	b	606	CLA	C3D-C2D	3.68	1.49	1.39
35	b	622	HTG	C1'-S1	-3.68	1.76	1.81
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	B	605	CLA	CHD-C4C	3.68	1.47	1.39
23	a	406[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	B	610	CLA	CHC-C4B	3.68	1.47	1.39
23	A	404[A]	CLA	C4B-NB	-3.68	1.33	1.37
23	B	601	CLA	CHD-C4C	3.68	1.47	1.39
35	o	301	HTG	C1'-S1	-3.68	1.76	1.81
23	D	403	CLA	OBD-CAD	3.67	1.28	1.22
23	C	503	CLA	CHC-C4B	3.67	1.47	1.39
23	b	609	CLA	CHC-C4B	3.67	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	C3D-C2D	3.67	1.49	1.39
23	A	406[A]	CLA	C1B-NB	-3.67	1.33	1.37
23	c	504	CLA	C3D-C2D	3.67	1.49	1.39
23	b	603	CLA	CHB-C1B	3.67	1.47	1.39
23	C	503	CLA	OBD-CAD	3.67	1.28	1.22
23	B	604	CLA	CHC-C4B	3.67	1.47	1.39
23	B	610	CLA	C1B-NB	-3.67	1.33	1.37
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	c	509	CLA	CHB-C1B	3.67	1.47	1.39
23	B	608	CLA	O2A-CGA	3.67	1.44	1.33
23	B	607	CLA	OBD-CAD	3.67	1.28	1.22
23	a	406[B]	CLA	CHD-C1D	3.66	1.45	1.38
23	b	608	CLA	C1B-NB	-3.66	1.33	1.37
23	B	616	CLA	CHC-C4B	3.66	1.47	1.39
23	c	513	CLA	C3D-C2D	3.66	1.49	1.39
23	B	616	CLA	CHB-C1B	3.66	1.47	1.39
23	a	404[A]	CLA	C3D-C2D	3.66	1.49	1.39
23	b	601	CLA	OBD-CAD	3.66	1.28	1.22
32	d	407[A]	LHG	O7-C7	3.66	1.44	1.34
23	A	405[A]	CLA	C1B-NB	-3.66	1.33	1.37
23	c	513	CLA	OBD-CAD	3.65	1.28	1.22
23	B	603	CLA	CHB-C1B	3.65	1.47	1.39
23	b	614	CLA	C3D-C2D	3.65	1.49	1.39
23	B	615	CLA	CHB-C1B	3.65	1.47	1.39
23	a	406[B]	CLA	CHC-C4B	3.65	1.47	1.39
23	C	505	CLA	CHC-C4B	3.65	1.47	1.39
23	D	403	CLA	CHB-C1B	3.65	1.47	1.39
23	B	604	CLA	O2A-CGA	3.65	1.44	1.33
23	d	403	CLA	CHD-C4C	3.65	1.47	1.39
23	C	509	CLA	CHB-C1B	3.64	1.47	1.39
23	b	614	CLA	CHB-C1B	3.64	1.47	1.39
23	c	502	CLA	CHC-C4B	3.64	1.47	1.39
23	b	614	CLA	CHD-C4C	3.64	1.47	1.39
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
23	b	613	CLA	CHD-C4C	3.64	1.47	1.39
23	c	512	CLA	OBD-CAD	3.64	1.28	1.22
23	B	605	CLA	CHD-C1D	3.64	1.45	1.38
23	C	508	CLA	CHC-C4B	3.64	1.47	1.39
23	a	405[B]	CLA	CHB-C1B	3.63	1.47	1.39
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	a	408	CLA	CHC-C4B	3.63	1.47	1.39
23	D	402[B]	CLA	OBD-CAD	3.63	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHD-C4C	3.63	1.47	1.39
23	a	408	CLA	OBD-CAD	3.63	1.28	1.22
23	b	611	CLA	CHD-C1D	3.63	1.45	1.38
23	C	502	CLA	CHB-C1B	3.63	1.47	1.39
23	B	613	CLA	CHC-C4B	3.62	1.47	1.39
23	B	602	CLA	O2A-CGA	3.62	1.43	1.33
23	B	601	CLA	C3D-C2D	3.62	1.49	1.39
23	b	616	CLA	CHC-C4B	3.62	1.47	1.39
36	c	517[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	a	405[A]	CLA	CHD-C4C	3.62	1.47	1.39
23	b	616	CLA	OBD-CAD	3.62	1.28	1.22
23	c	506	CLA	OBD-CAD	3.62	1.28	1.22
23	b	615	CLA	C3D-C2D	3.62	1.49	1.39
32	b	630[A]	LHG	O7-C7	3.62	1.44	1.34
23	a	404[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	608	CLA	CHB-C1B	3.61	1.47	1.39
23	c	503	CLA	CHD-C4C	3.61	1.47	1.39
23	C	504	CLA	CHB-C1B	3.61	1.47	1.39
23	d	402[B]	CLA	C3D-C2D	3.61	1.49	1.39
23	C	505	CLA	CHD-C4C	3.61	1.47	1.39
23	C	509	CLA	CHC-C4B	3.61	1.47	1.39
23	b	615	CLA	CHB-C1B	3.61	1.47	1.39
23	a	404[B]	CLA	O2A-CGA	3.61	1.43	1.33
23	c	514	CLA	CHC-C4B	3.61	1.47	1.39
23	a	405[B]	CLA	CHC-C4B	3.61	1.47	1.39
23	B	603	CLA	CHD-C4C	3.61	1.47	1.39
23	d	402[B]	CLA	OBD-CAD	3.60	1.28	1.22
23	c	511	CLA	CHD-C4C	3.60	1.47	1.39
23	C	511	CLA	O2A-CGA	3.60	1.43	1.33
32	d	406[B]	LHG	O8-C23	3.60	1.43	1.33
23	b	613	CLA	O2A-CGA	3.60	1.43	1.33
23	A	404[B]	CLA	CHB-C1B	3.60	1.47	1.39
23	B	606	CLA	CHD-C4C	3.60	1.47	1.39
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	b	605	CLA	OBD-CAD	3.60	1.28	1.22
34	m	101	LMG	O7-C10	3.60	1.44	1.34
23	b	610	CLA	C3D-C2D	3.59	1.48	1.39
23	D	402[B]	CLA	CHC-C4B	3.59	1.47	1.39
23	b	606	CLA	CHD-C4C	3.59	1.47	1.39
23	c	505	CLA	CHD-C4C	3.59	1.47	1.39
23	c	505	CLA	OBD-CAD	3.59	1.28	1.22
23	B	609	CLA	CHB-C1B	3.58	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	CHD-C4C	3.58	1.47	1.39
23	A	408	CLA	C3D-C2D	3.58	1.48	1.39
23	a	406[B]	CLA	CHB-C1B	3.58	1.47	1.39
23	c	507	CLA	OBD-CAD	3.58	1.28	1.22
23	a	406[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	a	408	CLA	CHB-C1B	3.58	1.47	1.39
23	A	405[B]	CLA	CHC-C4B	3.57	1.47	1.39
23	B	614	CLA	CHD-C1D	3.57	1.45	1.38
23	B	606	CLA	CHC-C4B	3.57	1.47	1.39
23	c	510	CLA	OBD-CAD	3.57	1.28	1.22
23	d	402[A]	CLA	CHD-C4C	3.57	1.47	1.39
23	B	614	CLA	C3D-C2D	3.57	1.48	1.39
23	d	403	CLA	CHB-C1B	3.57	1.47	1.39
23	B	603	CLA	CHC-C4B	3.56	1.47	1.39
23	C	510	CLA	C1B-NB	-3.56	1.33	1.37
23	A	405[A]	CLA	CHD-C4C	3.56	1.47	1.39
23	A	405[A]	CLA	CHC-C4B	3.56	1.47	1.39
23	A	404[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	C	512	CLA	C4B-NB	-3.55	1.33	1.37
23	B	603	CLA	OBD-CAD	3.55	1.28	1.22
23	C	505	CLA	C1B-NB	-3.55	1.33	1.37
36	C	517[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	d	402[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	601	CLA	OBD-CAD	3.55	1.28	1.22
23	c	511	CLA	CHC-C4B	3.55	1.47	1.39
23	a	404[B]	CLA	CHC-C4B	3.54	1.47	1.39
23	a	406[B]	CLA	OBD-CAD	3.54	1.28	1.22
23	a	406[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	c	505	CLA	C1B-NB	-3.54	1.33	1.37
23	B	616	CLA	CHD-C1D	3.54	1.45	1.38
23	c	506	CLA	O2A-CGA	3.54	1.43	1.33
36	c	518[A]	DGD	O2G-C1B	3.53	1.44	1.34
23	b	605	CLA	CHB-C1B	3.53	1.47	1.39
32	d	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	a	408	CLA	CHD-C4C	3.53	1.47	1.39
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	B	606	CLA	C3D-C2D	3.53	1.48	1.39
23	D	403	CLA	C3B-C4B	3.53	1.51	1.42
23	b	616	CLA	CHB-C1B	3.53	1.47	1.39
23	d	402[B]	CLA	CHC-C4B	3.53	1.47	1.39
23	b	607	CLA	CHB-C1B	3.52	1.47	1.39
38	f	101	HEM	C4D-ND	-3.52	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
23	C	502	CLA	C3D-C2D	3.52	1.48	1.39
23	B	609	CLA	CHD-C4C	3.51	1.47	1.39
23	b	601	CLA	CHB-C1B	3.51	1.47	1.39
23	c	511	CLA	CHD-C1D	3.51	1.45	1.38
32	A	419[B]	LHG	O7-C7	3.51	1.44	1.34
23	C	511	CLA	CHC-C4B	3.51	1.47	1.39
23	b	613	CLA	C1B-NB	-3.51	1.33	1.37
23	b	606	CLA	CHC-C4B	3.51	1.47	1.39
32	d	412[A]	LHG	O7-C7	3.50	1.44	1.34
23	c	512	CLA	C3D-C2D	3.50	1.48	1.39
23	C	507	CLA	C1B-NB	-3.50	1.33	1.37
23	b	605	CLA	C1B-NB	-3.50	1.33	1.37
32	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
32	b	630[A]	LHG	O8-C23	3.49	1.43	1.33
23	c	507	CLA	CHC-C4B	3.49	1.47	1.39
23	b	615	CLA	CHC-C4B	3.49	1.47	1.39
23	b	604	CLA	O2A-CGA	3.49	1.43	1.33
23	A	404[B]	CLA	OBD-CAD	3.49	1.28	1.22
23	b	609	CLA	CHD-C4C	3.49	1.47	1.39
23	c	503	CLA	OBD-CAD	3.49	1.28	1.22
23	C	507	CLA	OBD-CAD	3.48	1.28	1.22
23	B	612	CLA	CHC-C4B	3.48	1.47	1.39
23	a	405[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	B	612	CLA	C3D-C2D	3.48	1.48	1.39
23	C	512	CLA	CHC-C4B	3.48	1.47	1.39
23	A	405[B]	CLA	C1B-NB	-3.47	1.33	1.37
23	a	408	CLA	C3D-C2D	3.47	1.48	1.39
23	A	405[B]	CLA	CHB-C1B	3.47	1.47	1.39
23	a	405[A]	CLA	CHC-C4B	3.47	1.47	1.39
23	C	514	CLA	OBD-CAD	3.47	1.28	1.22
23	b	601	CLA	CHC-C4B	3.46	1.47	1.39
23	B	604	CLA	OBD-CAD	3.46	1.28	1.22
34	D	411	LMG	O7-C10	3.46	1.44	1.34
32	D	406[B]	LHG	O8-C23	3.46	1.43	1.33
23	B	611	CLA	CHD-C4C	3.46	1.47	1.39
36	H	102	DGD	O2G-C1B	3.45	1.44	1.34
23	a	405[B]	CLA	C1B-NB	-3.45	1.33	1.37
23	c	507	CLA	C1B-NB	-3.44	1.33	1.37
23	A	405[B]	CLA	OBD-CAD	3.43	1.28	1.22
23	D	402[A]	CLA	C3D-C2D	3.43	1.48	1.39
23	c	510	CLA	C4B-NB	-3.43	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[A]	CLA	CHB-C1B	3.43	1.47	1.39
23	B	601	CLA	CHB-C1B	3.43	1.47	1.39
23	b	613	CLA	CHD-C1D	3.42	1.45	1.38
23	d	402[A]	CLA	CHC-C4B	3.42	1.47	1.39
38	F	102	HEM	C1B-NB	-3.42	1.34	1.40
23	B	603	CLA	C4B-NB	-3.42	1.33	1.37
23	C	511	CLA	C1B-NB	-3.42	1.33	1.37
23	d	402[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	A	408	CLA	OBD-CAD	3.41	1.28	1.22
23	A	404[B]	CLA	O2A-CGA	3.41	1.43	1.33
23	b	604	CLA	OBD-CAD	3.41	1.28	1.22
23	a	405[B]	CLA	OBD-CAD	3.40	1.28	1.22
23	A	408	CLA	CHB-C1B	3.40	1.47	1.39
23	B	613	CLA	O2A-CGA	3.40	1.43	1.33
23	B	610	CLA	O2A-CGA	3.40	1.43	1.33
23	C	509	CLA	CHD-C4C	3.40	1.47	1.39
23	A	406[B]	CLA	C1B-NB	-3.40	1.33	1.37
24	a	407[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	B	608	CLA	CHD-C4C	3.38	1.46	1.39
23	a	404[B]	CLA	CHB-C1B	3.38	1.47	1.39
23	A	404[B]	CLA	CHC-C4B	3.38	1.47	1.39
23	C	513	CLA	CHB-C1B	3.37	1.47	1.39
23	C	504	CLA	C3D-C2D	3.37	1.48	1.39
23	B	612	CLA	CHD-C4C	3.37	1.46	1.39
23	C	512	CLA	OBD-CAD	3.37	1.28	1.22
23	b	613	CLA	CHB-C1B	3.37	1.47	1.39
23	B	612	CLA	OBD-CAD	3.37	1.28	1.22
23	C	511	CLA	C3D-C2D	3.37	1.48	1.39
23	a	404[A]	CLA	CHC-C4B	3.36	1.46	1.39
23	a	405[A]	CLA	C1B-NB	-3.36	1.33	1.37
23	B	604	CLA	C3D-C2D	3.36	1.48	1.39
23	B	601	CLA	C3B-C4B	3.36	1.50	1.42
23	C	508	CLA	CHD-C4C	3.35	1.46	1.39
23	b	614	CLA	OBD-CAD	3.35	1.28	1.22
23	c	512	CLA	CHC-C4B	3.35	1.46	1.39
23	C	502	CLA	C1B-NB	-3.35	1.33	1.37
23	B	616	CLA	C4B-NB	-3.35	1.33	1.37
23	B	616	CLA	C1B-NB	-3.35	1.33	1.37
23	c	514	CLA	OBD-CAD	3.35	1.28	1.22
23	c	505	CLA	CHB-C1B	3.35	1.46	1.39
23	b	615	CLA	OBD-CAD	3.34	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	O2A-CGA	3.34	1.43	1.33
23	D	402[A]	CLA	CHC-C4B	3.33	1.46	1.39
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
34	D	411	LMG	O8-C28	3.33	1.43	1.33
23	b	612	CLA	O2A-CGA	3.33	1.43	1.33
23	D	402[B]	CLA	C1B-NB	-3.33	1.33	1.37
23	d	402[B]	CLA	C4B-NB	-3.33	1.33	1.37
23	C	507	CLA	CHC-C4B	3.33	1.46	1.39
36	c	519	DGD	O2G-C1B	3.32	1.43	1.34
23	C	510	CLA	CHC-C4B	3.32	1.46	1.39
23	c	514	CLA	C1B-NB	-3.32	1.33	1.37
23	A	404[B]	CLA	C4B-NB	-3.32	1.33	1.37
23	b	612	CLA	CHD-C4C	3.31	1.46	1.39
23	b	606	CLA	OBD-CAD	3.31	1.28	1.22
23	B	607	CLA	O2A-CGA	3.31	1.43	1.33
23	A	406[B]	CLA	C3B-C4B	3.30	1.50	1.42
23	B	615	CLA	CHC-C4B	3.30	1.46	1.39
23	d	403	CLA	OBD-CAD	3.30	1.28	1.22
23	a	404[A]	CLA	C1B-NB	-3.30	1.33	1.37
23	c	504	CLA	C3B-C4B	3.30	1.50	1.42
23	C	506	CLA	C1B-NB	-3.30	1.33	1.37
23	b	603	CLA	OBD-CAD	3.29	1.28	1.22
23	b	602	CLA	CHB-C1B	3.29	1.46	1.39
23	b	607	CLA	CHC-C4B	3.29	1.46	1.39
23	B	611	CLA	C3D-C2D	3.29	1.48	1.39
23	A	408	CLA	CHC-C4B	3.28	1.46	1.39
23	B	607	CLA	C3D-C2D	3.28	1.48	1.39
23	A	408	CLA	C4B-NB	-3.28	1.33	1.37
23	b	605	CLA	CHC-C4B	3.28	1.46	1.39
23	d	402[A]	CLA	C1D-ND	3.27	1.41	1.37
23	C	506	CLA	OBD-CAD	3.27	1.28	1.22
23	c	503	CLA	CHC-C4B	3.27	1.46	1.39
23	D	402[A]	CLA	OBD-CAD	3.26	1.28	1.22
23	c	511	CLA	C1B-NB	-3.26	1.33	1.37
35	B	623	HTG	C1'-S1	-3.26	1.77	1.81
23	C	514	CLA	C4B-NB	-3.26	1.33	1.37
23	b	605	CLA	O2A-CGA	3.25	1.42	1.33
35	b	625	HTG	C1'-S1	-3.25	1.77	1.81
23	C	505	CLA	OBD-CAD	3.24	1.28	1.22
23	a	406[A]	CLA	CHC-C4B	3.24	1.46	1.39
23	B	613	CLA	CHD-C4C	3.24	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C3B-C4B	3.24	1.50	1.42
38	f	101	HEM	C1B-NB	-3.24	1.34	1.40
35	d	409	HTG	C1'-S1	-3.23	1.77	1.81
35	b	625	HTG	C1-S1	-3.23	1.75	1.80
23	C	513	CLA	C3B-C4B	3.23	1.50	1.42
23	b	616	CLA	C3B-C4B	3.22	1.50	1.42
38	F	102	HEM	C4D-ND	-3.21	1.34	1.40
23	c	502	CLA	OBD-CAD	3.21	1.28	1.22
23	A	405[A]	CLA	C3B-C4B	3.20	1.50	1.42
23	a	408	CLA	C3B-C4B	3.19	1.50	1.42
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	C	502	CLA	C3B-C4B	3.19	1.50	1.42
23	b	604	CLA	C1B-C2B	3.18	1.50	1.43
35	D	410	HTG	C1'-S1	-3.18	1.77	1.81
23	c	507	CLA	C4B-NB	-3.18	1.33	1.37
23	B	605	CLA	C3B-C4B	3.18	1.50	1.42
23	C	514	CLA	CHC-C4B	3.18	1.46	1.39
23	B	602	CLA	C1C-C2C	3.17	1.50	1.44
23	B	602	CLA	OBD-CAD	3.17	1.27	1.22
23	D	402[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	a	404[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	c	511	CLA	OBD-CAD	3.17	1.27	1.22
23	B	609	CLA	C1B-NB	-3.16	1.33	1.37
23	a	404[B]	CLA	C1B-NB	-3.16	1.33	1.37
23	b	607	CLA	C1B-C2B	3.16	1.50	1.43
23	c	508	CLA	C1B-NB	-3.16	1.33	1.37
23	C	506	CLA	C3B-C4B	3.16	1.50	1.42
23	A	404[A]	CLA	CHC-C4B	3.15	1.46	1.39
23	b	610	CLA	O2A-CGA	3.15	1.42	1.33
23	b	614	CLA	C1B-NB	-3.15	1.33	1.37
23	C	511	CLA	OBD-CAD	3.14	1.27	1.22
23	D	402[B]	CLA	C4B-NB	-3.13	1.33	1.37
23	a	404[B]	CLA	C4B-NB	-3.13	1.33	1.37
35	c	522	HTG	C1'-S1	-3.13	1.77	1.81
23	b	616	CLA	C1B-NB	-3.13	1.33	1.37
23	B	607	CLA	C1C-C2C	3.13	1.50	1.44
23	b	610	CLA	C1B-NB	-3.13	1.33	1.37
23	A	406[A]	CLA	C3B-C4B	3.13	1.50	1.42
23	b	608	CLA	CHC-C4B	3.13	1.46	1.39
23	B	608	CLA	C4B-NB	-3.12	1.33	1.37
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
23	b	601	CLA	C1B-NB	-3.11	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	C3B-C4B	3.11	1.50	1.42
23	d	403	CLA	C3B-C4B	3.11	1.50	1.42
23	b	606	CLA	C1B-NB	-3.10	1.34	1.37
23	a	406[B]	CLA	C3B-C4B	3.10	1.50	1.42
23	B	602	CLA	C1B-NB	-3.10	1.34	1.37
24	A	417[A]	PHO	CHA-CBD	-3.10	1.47	1.51
23	A	404[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	a	406[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	c	506	CLA	C4C-C3C	3.09	1.50	1.45
23	c	514	CLA	C4B-NB	-3.09	1.34	1.37
23	b	601	CLA	C3B-C4B	3.09	1.50	1.42
23	c	514	CLA	C3B-C4B	3.08	1.50	1.42
23	C	511	CLA	C4B-NB	-3.08	1.34	1.37
23	B	604	CLA	C1B-C2B	3.08	1.50	1.43
23	a	404[A]	CLA	O2A-CGA	3.07	1.42	1.33
23	b	612	CLA	C1B-C2B	3.07	1.50	1.43
23	B	606	CLA	C1B-NB	-3.07	1.34	1.37
23	C	503	CLA	C1B-NB	-3.06	1.34	1.37
23	C	504	CLA	C3B-C4B	3.06	1.49	1.42
23	C	509	CLA	C4B-NB	-3.05	1.34	1.37
23	C	506	CLA	C1B-C2B	3.05	1.50	1.43
23	A	404[B]	CLA	C1B-NB	-3.05	1.34	1.37
23	b	602	CLA	C1C-C2C	3.05	1.50	1.44
23	C	514	CLA	C1B-NB	-3.05	1.34	1.37
23	c	512	CLA	C1B-C2B	3.05	1.50	1.43
23	a	406[A]	CLA	C3B-C4B	3.05	1.49	1.42
23	B	616	CLA	CHD-C4C	3.04	1.46	1.39
23	c	505	CLA	C1B-C2B	3.03	1.50	1.43
35	C	522	HTG	C1'-S1	-3.03	1.77	1.81
23	C	504	CLA	OBD-CAD	3.03	1.27	1.22
23	A	408	CLA	C1B-NB	-3.03	1.34	1.37
23	C	513	CLA	C1C-C2C	3.02	1.50	1.44
23	C	505	CLA	C4D-CHA	3.02	1.49	1.38
23	c	504	CLA	C1B-NB	-3.02	1.34	1.37
23	a	406[B]	CLA	C4B-NB	-3.02	1.34	1.37
23	B	608	CLA	CHC-C4B	3.01	1.46	1.39
23	c	513	CLA	C3B-C4B	3.01	1.49	1.42
23	B	606	CLA	OBD-CAD	3.01	1.27	1.22
23	C	508	CLA	OBD-CAD	3.01	1.27	1.22
23	B	614	CLA	OBD-CAD	3.01	1.27	1.22
23	B	610	CLA	C4B-NB	-3.01	1.34	1.37
23	c	504	CLA	OBD-CAD	3.00	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	C4B-NB	-3.00	1.34	1.37
23	B	608	CLA	C1B-NB	-3.00	1.34	1.37
23	c	510	CLA	CHC-C4B	3.00	1.46	1.39
23	b	607	CLA	O2A-CGA	2.99	1.42	1.33
23	b	603	CLA	C4B-NB	-2.99	1.34	1.37
23	c	505	CLA	C4B-NB	-2.99	1.34	1.37
23	d	402[A]	CLA	C4B-NB	-2.99	1.34	1.37
23	B	610	CLA	C3B-C4B	2.99	1.49	1.42
23	a	406[B]	CLA	C1B-NB	-2.99	1.34	1.37
23	c	510	CLA	C1B-C2B	2.98	1.50	1.43
23	B	609	CLA	OBD-CAD	2.97	1.27	1.22
40	v	201	HEC	FE-NC	2.97	2.05	1.95
23	b	611	CLA	OBD-CAD	2.96	1.27	1.22
23	B	615	CLA	C3B-C4B	2.96	1.49	1.42
23	B	606	CLA	C1C-C2C	2.96	1.50	1.44
23	b	609	CLA	C3B-C4B	2.96	1.49	1.42
23	B	611	CLA	MG-NB	2.96	2.11	2.05
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	a	405[A]	CLA	C3B-C4B	2.96	1.49	1.42
23	B	610	CLA	C4C-C3C	2.94	1.50	1.45
23	b	612	CLA	C4B-NB	-2.94	1.34	1.37
23	C	514	CLA	C1B-C2B	2.93	1.50	1.43
23	c	504	CLA	C1C-C2C	2.93	1.50	1.44
23	a	405[B]	CLA	C3B-C4B	2.93	1.49	1.42
23	a	408	CLA	C1B-C2B	2.92	1.50	1.43
23	B	616	CLA	C1B-C2B	2.92	1.50	1.43
23	D	403	CLA	C1B-NB	-2.92	1.34	1.37
23	c	508	CLA	C1B-C2B	2.92	1.50	1.43
23	B	607	CLA	C1B-C2B	2.91	1.50	1.43
23	c	506	CLA	C1B-NB	-2.91	1.34	1.37
23	a	408	CLA	C4B-NB	-2.91	1.34	1.37
23	c	509	CLA	C1B-C2B	2.91	1.50	1.43
23	b	605	CLA	C3B-C4B	2.90	1.49	1.42
23	B	612	CLA	C4D-CHA	2.90	1.48	1.38
23	C	504	CLA	C4B-NB	-2.90	1.34	1.37
23	C	505	CLA	C4B-NB	-2.90	1.34	1.37
23	b	613	CLA	OBD-CAD	2.90	1.27	1.22
23	C	510	CLA	C1B-C2B	2.90	1.50	1.43
23	c	503	CLA	C1B-NB	-2.89	1.34	1.37
23	b	604	CLA	C1B-NB	-2.89	1.34	1.37
23	c	512	CLA	C1B-NB	-2.89	1.34	1.37
23	B	606	CLA	C3B-C4B	2.89	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	C1B-NB	-2.89	1.34	1.37
23	C	508	CLA	C1B-NB	-2.89	1.34	1.37
23	B	615	CLA	C1B-C2B	2.89	1.50	1.43
23	b	603	CLA	C3B-C4B	2.89	1.49	1.42
23	D	403	CLA	C1C-C2C	2.89	1.50	1.44
23	b	601	CLA	C4B-NB	-2.89	1.34	1.37
23	b	613	CLA	C1B-C2B	2.88	1.50	1.43
23	C	512	CLA	C4D-CHA	2.88	1.48	1.38
23	c	511	CLA	C3B-C4B	2.88	1.49	1.42
23	c	511	CLA	C1B-C2B	2.88	1.50	1.43
23	A	406[A]	CLA	C4B-NB	-2.87	1.34	1.37
23	C	513	CLA	C1B-NB	-2.87	1.34	1.37
23	c	513	CLA	C1B-NB	-2.87	1.34	1.37
23	c	509	CLA	C1C-C2C	2.86	1.50	1.44
23	C	508	CLA	C1C-C2C	2.86	1.50	1.44
23	D	402[B]	CLA	C1C-C2C	2.86	1.50	1.44
23	b	602	CLA	C1B-NB	-2.86	1.34	1.37
23	A	408	CLA	C3B-C4B	2.85	1.49	1.42
23	B	616	CLA	C4D-CHA	2.85	1.48	1.38
23	C	504	CLA	C1B-NB	-2.85	1.34	1.37
23	b	607	CLA	OBD-CAD	2.84	1.27	1.22
40	V	201	HEC	FE-NC	2.84	2.04	1.95
23	c	506	CLA	C1C-C2C	2.84	1.50	1.44
23	c	505	CLA	C1C-C2C	2.83	1.50	1.44
23	c	503	CLA	C1B-C2B	2.83	1.49	1.43
23	B	605	CLA	C4B-NB	-2.83	1.34	1.37
23	D	402[A]	CLA	C1B-C2B	2.83	1.49	1.43
24	A	407[A]	PHO	CBD-CGD	-2.83	1.48	1.52
23	B	616	CLA	C3B-C4B	2.83	1.49	1.42
23	b	612	CLA	C1C-C2C	2.82	1.50	1.44
23	B	602	CLA	C3B-C4B	2.82	1.49	1.42
23	B	612	CLA	C1C-C2C	2.82	1.50	1.44
23	C	508	CLA	C4D-CHA	2.82	1.48	1.38
23	b	611	CLA	C1B-C2B	2.82	1.49	1.43
23	B	615	CLA	C1B-NB	-2.81	1.34	1.37
23	c	509	CLA	C3B-C4B	2.81	1.49	1.42
23	B	605	CLA	C1B-NB	-2.81	1.34	1.37
23	c	508	CLA	C1C-C2C	2.81	1.50	1.44
23	C	507	CLA	C4C-C3C	2.80	1.49	1.45
23	B	601	CLA	C1C-C2C	2.79	1.50	1.44
23	b	609	CLA	C1B-NB	-2.79	1.34	1.37
23	c	502	CLA	C1B-C2B	2.79	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C4D-CHA	2.79	1.48	1.38
23	c	502	CLA	C3B-C4B	2.79	1.49	1.42
23	b	606	CLA	C3B-C4B	2.79	1.49	1.42
23	c	506	CLA	C1B-C2B	2.78	1.49	1.43
26	a	410[B]	SQD	C6-S	-2.78	1.67	1.77
23	c	511	CLA	C1C-C2C	2.78	1.50	1.44
23	b	610	CLA	C3B-C4B	2.78	1.49	1.42
23	C	511	CLA	C4C-C3C	2.78	1.49	1.45
23	c	508	CLA	C4B-NB	-2.78	1.34	1.37
34	Z	101	LMG	O8-C28	2.77	1.47	1.33
23	b	614	CLA	C4B-NB	-2.77	1.34	1.37
23	b	606	CLA	C4B-NB	-2.77	1.34	1.37
23	B	604	CLA	C3B-C4B	2.77	1.49	1.42
29	A	414[A]	PL9	C6-C5	2.76	1.49	1.35
23	B	602	CLA	C1B-C2B	2.76	1.49	1.43
23	b	610	CLA	C1C-C2C	2.76	1.49	1.44
23	B	604	CLA	C1B-NB	-2.76	1.34	1.37
23	c	510	CLA	C4C-C3C	2.76	1.49	1.45
29	a	413[A]	PL9	C6-C5	2.75	1.49	1.35
23	A	404[A]	CLA	C1B-C2B	2.75	1.49	1.43
23	B	605	CLA	OBD-CAD	2.75	1.27	1.22
23	C	505	CLA	C1C-C2C	2.75	1.49	1.44
23	b	604	CLA	C4D-CHA	2.75	1.48	1.38
23	B	601	CLA	C1B-NB	-2.75	1.34	1.37
23	c	508	CLA	C4D-CHA	2.75	1.48	1.38
23	D	402[B]	CLA	C1B-C2B	2.75	1.49	1.43
23	c	504	CLA	C4B-NB	-2.74	1.34	1.37
23	C	504	CLA	C4D-CHA	2.74	1.48	1.38
23	B	612	CLA	C1B-C2B	2.74	1.49	1.43
36	H	102	DGD	O5D-C1E	2.74	1.44	1.40
23	B	614	CLA	C1B-C2B	2.74	1.49	1.43
23	b	603	CLA	C1B-C2B	2.73	1.49	1.43
23	B	614	CLA	C1C-C2C	2.73	1.49	1.44
26	a	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	B	613	CLA	C1C-C2C	2.73	1.49	1.44
29	a	413[B]	PL9	C6-C5	2.73	1.49	1.35
23	C	509	CLA	C1B-C2B	2.73	1.49	1.43
23	A	405[A]	CLA	C4B-NB	-2.73	1.34	1.37
23	c	506	CLA	C4D-CHA	2.73	1.48	1.38
26	A	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	C	502	CLA	C4D-CHA	2.73	1.48	1.38
23	A	406[A]	CLA	C4D-CHA	2.72	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406[A]	CLA	C1C-C2C	2.72	1.49	1.44
23	b	607	CLA	C4D-CHA	2.72	1.48	1.38
23	B	608	CLA	OBD-CAD	2.72	1.27	1.22
23	c	509	CLA	C4D-CHA	2.72	1.48	1.38
23	a	405[A]	CLA	C1B-C2B	2.72	1.49	1.43
23	B	613	CLA	C4C-C3C	2.72	1.49	1.45
23	B	609	CLA	C1C-C2C	2.72	1.49	1.44
23	c	507	CLA	C1B-C2B	2.72	1.49	1.43
23	b	616	CLA	C1C-C2C	2.72	1.49	1.44
23	c	514	CLA	C1C-C2C	2.72	1.49	1.44
23	B	614	CLA	C1B-NB	-2.72	1.34	1.37
23	b	608	CLA	C3B-C4B	2.72	1.49	1.42
23	B	606	CLA	C1B-C2B	2.72	1.49	1.43
23	C	511	CLA	C1C-C2C	2.72	1.49	1.44
23	D	402[A]	CLA	C4D-CHA	2.71	1.48	1.38
23	C	507	CLA	C3B-C4B	2.71	1.49	1.42
23	c	505	CLA	C4C-C3C	2.71	1.49	1.45
23	b	613	CLA	C4D-CHA	2.71	1.48	1.38
23	a	406[B]	CLA	C1C-C2C	2.71	1.49	1.44
26	A	410[B]	SQD	C6-S	-2.71	1.67	1.77
23	B	616	CLA	C1C-C2C	2.70	1.49	1.44
23	b	611	CLA	C1B-NB	-2.70	1.34	1.37
23	a	408	CLA	C1C-C2C	2.70	1.49	1.44
24	a	415[B]	PHO	C3A-C2A	-2.70	1.52	1.54
23	c	504	CLA	C1B-C2B	2.70	1.49	1.43
23	B	608	CLA	C4D-CHA	2.70	1.48	1.38
23	C	508	CLA	C1B-C2B	2.70	1.49	1.43
23	d	402[B]	CLA	C1B-C2B	2.70	1.49	1.43
23	C	509	CLA	C4D-CHA	2.70	1.48	1.38
23	b	610	CLA	C4D-CHA	2.69	1.48	1.38
23	D	403	CLA	C4C-C3C	2.69	1.49	1.45
23	A	408	CLA	C1B-C2B	2.69	1.49	1.43
23	B	616	CLA	OBD-CAD	2.69	1.27	1.22
23	B	614	CLA	C4D-CHA	2.69	1.48	1.38
23	d	403	CLA	C4D-CHA	2.69	1.48	1.38
23	b	616	CLA	C1B-C2B	2.69	1.49	1.43
23	D	403	CLA	C1B-C2B	2.69	1.49	1.43
23	C	512	CLA	C1B-C2B	2.68	1.49	1.43
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
29	A	414[B]	PL9	C6-C5	2.68	1.49	1.35
23	c	514	CLA	C1B-C2B	2.68	1.49	1.43
23	b	605	CLA	C4B-NB	-2.68	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C4B-NB	-2.68	1.34	1.37
23	C	502	CLA	OBD-CAD	2.68	1.27	1.22
23	a	406[A]	CLA	C1B-C2B	2.68	1.49	1.43
23	C	508	CLA	C4B-NB	-2.68	1.34	1.37
23	c	511	CLA	C4D-CHA	2.68	1.47	1.38
23	b	609	CLA	C4D-CHA	2.67	1.47	1.38
23	C	503	CLA	C1B-C2B	2.67	1.49	1.43
23	B	610	CLA	C4D-CHA	2.67	1.47	1.38
23	A	405[B]	CLA	C4D-CHA	2.67	1.47	1.38
23	d	403	CLA	C1C-C2C	2.67	1.49	1.44
26	f	102	SQD	C6-S	-2.67	1.67	1.77
23	b	612	CLA	C3B-C4B	2.67	1.49	1.42
23	C	505	CLA	C1B-C2B	2.67	1.49	1.43
23	C	502	CLA	C1B-C2B	2.66	1.49	1.43
23	a	404[A]	CLA	C1B-C2B	2.66	1.49	1.43
23	B	603	CLA	C4C-C3C	2.66	1.49	1.45
23	b	610	CLA	C3D-C4D	-2.66	1.38	1.44
23	B	610	CLA	C1B-C2B	2.66	1.49	1.43
23	B	613	CLA	C1B-C2B	2.65	1.49	1.43
23	d	402[A]	CLA	C1B-C2B	2.65	1.49	1.43
23	b	611	CLA	C4B-NB	-2.65	1.34	1.37
23	B	613	CLA	C4D-CHA	2.65	1.47	1.38
23	C	506	CLA	C4D-CHA	2.65	1.47	1.38
23	C	510	CLA	C3B-C4B	2.65	1.49	1.42
23	B	614	CLA	C3D-C4D	-2.65	1.38	1.44
23	C	506	CLA	C1C-C2C	2.65	1.49	1.44
23	B	613	CLA	C4B-NB	-2.65	1.34	1.37
23	C	509	CLA	C1B-NB	-2.65	1.34	1.37
23	B	610	CLA	C3D-C4D	-2.65	1.38	1.44
23	C	513	CLA	C4D-CHA	2.65	1.47	1.38
23	B	608	CLA	C1B-C2B	2.64	1.49	1.43
23	c	504	CLA	C4D-CHA	2.64	1.47	1.38
23	B	609	CLA	C1B-C2B	2.64	1.49	1.43
23	B	605	CLA	C1B-C2B	2.64	1.49	1.43
26	a	411	SQD	C6-S	-2.63	1.67	1.77
23	a	405[B]	CLA	C1B-C2B	2.63	1.49	1.43
23	b	613	CLA	C4B-NB	-2.63	1.34	1.37
23	C	507	CLA	C4D-CHA	2.63	1.47	1.38
23	c	510	CLA	C4D-CHA	2.63	1.47	1.38
23	C	512	CLA	C1C-C2C	2.63	1.49	1.44
23	a	406[A]	CLA	C4B-NB	-2.63	1.34	1.37
23	A	404[B]	CLA	C1B-C2B	2.62	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C4D-CHA	2.62	1.47	1.38
23	B	616	CLA	C1C-NC	-2.62	1.33	1.37
23	A	404[B]	CLA	C4D-CHA	2.62	1.47	1.38
23	B	607	CLA	C4D-CHA	2.62	1.47	1.38
23	B	605	CLA	C1C-C2C	2.62	1.49	1.44
23	a	406[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	A	405[A]	CLA	C1B-C2B	2.62	1.49	1.43
23	c	512	CLA	C3B-C4B	2.62	1.48	1.42
23	b	615	CLA	C1B-C2B	2.61	1.49	1.43
23	b	614	CLA	C3B-C4B	2.61	1.48	1.42
23	B	615	CLA	C1C-C2C	2.61	1.49	1.44
23	c	502	CLA	C4C-C3C	2.61	1.49	1.45
23	C	507	CLA	C3D-C4D	-2.61	1.38	1.44
23	B	606	CLA	C4D-CHA	2.61	1.47	1.38
36	c	519	DGD	O2G-C2G	-2.60	1.40	1.46
23	b	609	CLA	C4B-NB	-2.60	1.34	1.37
23	A	408	CLA	C3D-C4D	-2.60	1.38	1.44
23	C	503	CLA	C3B-C4B	2.60	1.48	1.42
23	b	614	CLA	C1B-C2B	2.60	1.49	1.43
26	A	412	SQD	C6-S	-2.60	1.67	1.77
23	c	502	CLA	C4D-CHA	2.60	1.47	1.38
23	c	513	CLA	C4B-NB	-2.60	1.34	1.37
23	C	509	CLA	C4C-C3C	2.60	1.49	1.45
23	C	511	CLA	C3B-C4B	2.59	1.48	1.42
23	b	606	CLA	C1C-C2C	2.59	1.49	1.44
23	c	512	CLA	C1C-C2C	2.59	1.49	1.44
23	a	408	CLA	C1B-NB	-2.59	1.34	1.37
23	D	402[B]	CLA	C4C-C3C	2.59	1.49	1.45
23	C	514	CLA	C4D-CHA	2.59	1.47	1.38
23	c	513	CLA	C4D-CHA	2.59	1.47	1.38
23	C	507	CLA	C1B-C2B	2.59	1.49	1.43
23	b	606	CLA	C4D-CHA	2.58	1.47	1.38
33	B	626	LMT	C3'-C2'	2.58	1.58	1.52
36	C	519	DGD	O2G-C2G	-2.58	1.40	1.46
23	A	406[B]	CLA	C1C-C2C	2.58	1.49	1.44
40	V	201	HEC	CAC-C3C	2.58	1.57	1.51
23	d	402[B]	CLA	C4D-CHA	2.58	1.47	1.38
23	d	403	CLA	C4B-NB	-2.57	1.34	1.37
23	b	615	CLA	C3B-C4B	2.57	1.48	1.42
23	C	504	CLA	C1C-C2C	2.57	1.49	1.44
23	C	510	CLA	C1C-C2C	2.57	1.49	1.44
23	a	404[A]	CLA	C3B-C4B	2.57	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C4B-NB	-2.57	1.34	1.37
23	A	405[B]	CLA	C4B-NB	-2.57	1.34	1.37
23	c	512	CLA	C4B-NB	-2.57	1.34	1.37
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	610	CLA	C4C-C3C	2.57	1.49	1.45
23	C	509	CLA	C3B-C2B	2.56	1.49	1.41
23	C	510	CLA	C4C-C3C	2.56	1.49	1.45
23	b	601	CLA	C4D-CHA	2.56	1.47	1.38
23	b	604	CLA	C3B-C4B	2.56	1.48	1.42
23	b	615	CLA	C4D-CHA	2.56	1.47	1.38
23	d	402[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	a	404[B]	CLA	C1B-C2B	2.55	1.49	1.43
23	b	603	CLA	C4D-CHA	2.55	1.47	1.38
23	C	514	CLA	C3B-C4B	2.55	1.48	1.42
35	B	623	HTG	C1-S1	-2.55	1.76	1.80
40	V	201	HEC	FE-NB	2.55	2.02	1.94
23	C	502	CLA	C1C-C2C	2.55	1.49	1.44
23	C	511	CLA	C1B-C2B	2.55	1.49	1.43
38	f	101	HEM	C1D-ND	-2.55	1.33	1.38
23	B	601	CLA	C4B-NB	-2.55	1.34	1.37
23	C	503	CLA	C4B-NB	-2.55	1.34	1.37
27	A	418	GOL	O2-C2	-2.55	1.35	1.43
23	C	503	CLA	C4C-C3C	2.55	1.49	1.45
24	a	415[A]	PHO	C3A-C2A	-2.55	1.52	1.54
23	c	511	CLA	C4B-NB	-2.55	1.34	1.37
23	c	512	CLA	C4D-CHA	2.55	1.47	1.38
23	B	608	CLA	C4C-C3C	2.54	1.49	1.45
33	t	101	LMT	O3'-C3'	-2.54	1.37	1.43
23	b	607	CLA	C1C-C2C	2.54	1.49	1.44
23	a	405[B]	CLA	C4D-CHA	2.54	1.47	1.38
23	A	404[B]	CLA	C3B-C4B	2.54	1.48	1.42
23	c	509	CLA	C1B-NB	-2.54	1.34	1.37
23	b	603	CLA	C1C-C2C	2.54	1.49	1.44
23	c	502	CLA	C1C-C2C	2.53	1.49	1.44
23	C	512	CLA	C3B-C4B	2.53	1.48	1.42
23	B	605	CLA	C4D-CHA	2.53	1.47	1.38
23	d	403	CLA	C1B-C2B	2.53	1.49	1.43
33	A	420	LMT	O3'-C3'	-2.53	1.37	1.43
23	A	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
33	m	103	LMT	O2B-C2B	-2.52	1.37	1.43
23	a	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
23	B	602	CLA	C3D-C4D	-2.52	1.38	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C4D-CHA	2.52	1.47	1.38
35	b	622	HTG	O5-C1	2.51	1.46	1.42
38	F	102	HEM	C1C-C2C	-2.51	1.40	1.45
23	c	502	CLA	C1B-NB	-2.51	1.34	1.37
23	C	514	CLA	C1C-C2C	2.51	1.49	1.44
38	f	101	HEM	C1C-C2C	-2.51	1.40	1.45
23	C	503	CLA	C1C-C2C	2.51	1.49	1.44
23	b	603	CLA	C3B-C2B	2.51	1.49	1.41
23	b	613	CLA	C3B-C4B	2.51	1.48	1.42
23	b	603	CLA	C1B-NB	-2.50	1.34	1.37
23	b	614	CLA	C3D-C4D	-2.50	1.38	1.44
23	b	605	CLA	C1B-C2B	2.50	1.49	1.43
23	B	604	CLA	C4D-CHA	2.50	1.47	1.38
26	b	620	SQD	C6-S	-2.50	1.68	1.77
23	d	402[B]	CLA	C4C-C3C	2.50	1.49	1.45
23	b	616	CLA	C4D-CHA	2.50	1.47	1.38
23	b	608	CLA	C3D-C4D	-2.50	1.38	1.44
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	C	509	CLA	C3B-C4B	2.49	1.48	1.42
23	a	404[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	c	503	CLA	C3B-C2B	2.49	1.49	1.41
34	C	521	LMG	O1-C1	2.49	1.44	1.40
23	C	506	CLA	C4C-C3C	2.49	1.49	1.45
33	B	626	LMT	O3'-C3'	-2.49	1.37	1.43
23	C	511	CLA	C4D-CHA	2.49	1.47	1.38
23	b	606	CLA	C3D-C4D	-2.49	1.38	1.44
23	b	609	CLA	C1B-C2B	2.49	1.49	1.43
24	A	417[B]	PHO	CHA-CBD	-2.48	1.48	1.51
23	B	605	CLA	C3D-C4D	-2.48	1.38	1.44
23	a	404[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	c	513	CLA	C1B-C2B	2.48	1.49	1.43
23	a	405[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.48	1.47	1.38
23	B	603	CLA	C4D-CHA	2.47	1.47	1.38
23	c	507	CLA	C3B-C4B	2.47	1.48	1.42
23	d	403	CLA	C1B-NB	-2.47	1.34	1.37
23	c	504	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	504	CLA	C3D-C4D	-2.46	1.38	1.44
33	B	629	LMT	O3'-C3'	-2.46	1.37	1.43
23	b	607	CLA	C4C-C3C	2.46	1.49	1.45
23	B	612	CLA	C3B-C2B	2.46	1.49	1.41
23	C	507	CLA	C1C-C2C	2.46	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C3B-C2B	2.46	1.49	1.41
23	C	510	CLA	C4D-CHA	2.45	1.47	1.38
23	A	406[B]	CLA	C4D-CHA	2.45	1.47	1.38
33	e	101	LMT	O3'-C3'	-2.45	1.37	1.43
23	c	514	CLA	C4D-CHA	2.45	1.47	1.38
23	C	513	CLA	C4B-NB	-2.45	1.34	1.37
23	B	601	CLA	C1B-C2B	2.44	1.49	1.43
23	b	614	CLA	C4D-CHA	2.44	1.47	1.38
23	c	510	CLA	C3B-C4B	2.44	1.48	1.42
23	D	402[B]	CLA	C4D-CHA	2.44	1.47	1.38
23	a	406[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	A	406[A]	CLA	C1B-C2B	2.44	1.49	1.43
23	c	505	CLA	C4D-CHA	2.44	1.47	1.38
23	c	503	CLA	C3B-C4B	2.43	1.48	1.42
23	A	404[B]	CLA	C3D-C4D	-2.43	1.38	1.44
23	A	405[B]	CLA	C1B-C2B	2.43	1.49	1.43
23	B	610	CLA	C1C-C2C	2.43	1.49	1.44
23	b	601	CLA	C1C-C2C	2.43	1.49	1.44
23	B	616	CLA	C3B-C2B	2.43	1.49	1.41
23	b	611	CLA	C3B-C4B	2.43	1.48	1.42
33	B	628	LMT	O2'-C2'	-2.43	1.37	1.43
23	b	611	CLA	C4D-CHA	2.43	1.47	1.38
23	B	604	CLA	C1C-C2C	2.43	1.49	1.44
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42
23	a	405[B]	CLA	C4B-NB	-2.42	1.34	1.37
23	C	514	CLA	C3D-C4D	-2.42	1.38	1.44
23	A	406[B]	CLA	C1B-C2B	2.42	1.49	1.43
26	L	101	SQD	C6-S	-2.42	1.68	1.77
23	C	511	CLA	C3D-C4D	-2.42	1.38	1.44
29	d	405[B]	PL9	C6-C5	2.42	1.47	1.35
23	B	602	CLA	C4D-CHA	2.41	1.47	1.38
23	c	502	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	602	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	602	CLA	C4C-C3C	2.41	1.49	1.45
23	b	612	CLA	C4D-CHA	2.41	1.47	1.38
23	c	507	CLA	C4C-C3C	2.41	1.49	1.45
23	A	405[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	A	406[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	B	601	CLA	C4D-CHA	2.41	1.47	1.38
23	B	603	CLA	C1B-C2B	2.41	1.48	1.43
23	a	406[B]	CLA	C1B-C2B	2.41	1.48	1.43
23	b	605	CLA	C4D-CHA	2.41	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	C1C-C2C	2.41	1.49	1.44
23	b	611	CLA	C1C-C2C	2.41	1.49	1.44
23	B	612	CLA	C4C-C3C	2.41	1.49	1.45
24	A	417[B]	PHO	C3D-C4D	-2.41	1.37	1.41
23	b	614	CLA	C3B-C2B	2.41	1.49	1.41
23	C	512	CLA	C1B-NB	-2.40	1.34	1.37
24	a	407[B]	PHO	C3A-C2A	-2.40	1.52	1.54
23	b	606	CLA	C1B-C2B	2.40	1.48	1.43
23	a	404[B]	CLA	C4D-CHA	2.40	1.46	1.38
23	b	608	CLA	C4D-CHA	2.40	1.46	1.38
35	B	621	HTG	C1'-S1	-2.40	1.78	1.81
29	D	405[B]	PL9	C6-C5	2.40	1.47	1.35
33	F	101	LMT	O3'-C3'	-2.40	1.37	1.43
33	b	621	LMT	C3'-C2'	2.40	1.58	1.52
23	C	513	CLA	C1B-C2B	2.40	1.48	1.43
36	h	102	DGD	O5D-C1E	2.40	1.44	1.40
23	C	502	CLA	C3D-C4D	-2.40	1.38	1.44
23	D	402[A]	CLA	C3D-C4D	-2.39	1.38	1.44
23	c	509	CLA	C3B-C2B	2.39	1.49	1.41
23	c	512	CLA	C3B-C2B	2.39	1.49	1.41
23	b	615	CLA	C3D-C4D	-2.39	1.38	1.44
23	a	408	CLA	C4D-CHA	2.39	1.46	1.38
24	A	417[B]	PHO	C4B-NB	-2.39	1.34	1.38
23	d	402[B]	CLA	C3D-C4D	-2.38	1.38	1.44
23	c	505	CLA	C3B-C2B	2.38	1.49	1.41
23	b	604	CLA	C4C-C3C	2.38	1.49	1.45
23	A	404[B]	CLA	C3B-C2B	2.38	1.49	1.41
23	a	404[B]	CLA	C3B-C4B	2.38	1.48	1.42
33	M	101	LMT	O3'-C3'	-2.38	1.37	1.43
23	d	402[A]	CLA	C4D-CHA	2.38	1.46	1.38
23	b	603	CLA	C4C-C3C	2.38	1.49	1.45
23	B	615	CLA	C4D-CHA	2.38	1.46	1.38
23	B	608	CLA	C3B-C2B	2.38	1.49	1.41
23	b	613	CLA	C1C-C2C	2.37	1.49	1.44
23	D	403	CLA	C4D-CHA	2.37	1.46	1.38
23	a	404[B]	CLA	C3B-C2B	2.37	1.49	1.41
33	M	101	LMT	O2'-C2'	-2.37	1.37	1.43
23	B	603	CLA	C3B-C4B	2.37	1.48	1.42
23	B	614	CLA	C3B-C4B	2.37	1.48	1.42
23	B	606	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	608	CLA	C3B-C4B	2.36	1.48	1.42
23	B	602	CLA	C4C-C3C	2.36	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C3D-C4D	-2.36	1.38	1.44
23	c	514	CLA	C3D-C4D	-2.36	1.38	1.44
29	d	405[A]	PL9	C6-C5	2.35	1.47	1.35
23	c	507	CLA	C4D-CHA	2.35	1.46	1.38
23	B	602	CLA	C4B-NB	-2.35	1.34	1.37
23	d	402[B]	CLA	C1C-C2C	2.35	1.49	1.44
23	B	603	CLA	C3B-C2B	2.35	1.49	1.41
23	b	604	CLA	C3B-C2B	2.35	1.49	1.41
24	A	417[A]	PHO	C3D-C4D	-2.35	1.37	1.41
33	T	101	LMT	O3'-C3'	-2.34	1.37	1.43
24	A	417[A]	PHO	C3A-C2A	-2.34	1.52	1.54
23	b	610	CLA	C1B-C2B	2.34	1.48	1.43
23	d	402[B]	CLA	C3B-C2B	2.34	1.49	1.41
26	F	103	SQD	C6-S	-2.34	1.68	1.77
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	607	CLA	C3B-C4B	2.34	1.48	1.42
23	b	607	CLA	C3B-C4B	2.34	1.48	1.42
23	b	602	CLA	C4D-CHA	2.34	1.46	1.38
29	D	405[A]	PL9	C6-C5	2.34	1.47	1.35
23	b	612	CLA	C3D-C4D	-2.34	1.38	1.44
33	M	101	LMT	O2B-C2B	-2.34	1.37	1.43
23	C	512	CLA	C4C-C3C	2.34	1.49	1.45
23	B	609	CLA	C3D-C4D	-2.34	1.38	1.44
23	A	405[B]	CLA	C1C-C2C	2.33	1.49	1.44
23	b	608	CLA	C1B-C2B	2.33	1.48	1.43
24	a	407[A]	PHO	CBD-CGD	-2.33	1.49	1.52
23	b	609	CLA	C1C-C2C	2.33	1.49	1.44
23	c	505	CLA	C1C-NC	-2.33	1.34	1.37
23	b	601	CLA	C4C-C3C	2.33	1.49	1.45
23	a	404[A]	CLA	C3B-C2B	2.32	1.49	1.41
23	A	404[A]	CLA	C3B-C2B	2.32	1.49	1.41
23	b	611	CLA	C4C-C3C	2.32	1.49	1.45
23	c	509	CLA	C4C-C3C	2.32	1.49	1.45
23	b	602	CLA	C4B-NB	-2.31	1.34	1.37
26	F	103	SQD	O6-C1	2.31	1.44	1.40
23	c	513	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	612	CLA	C4C-C3C	2.31	1.49	1.45
23	C	506	CLA	C4B-NB	-2.31	1.34	1.37
23	b	604	CLA	MG-NA	2.31	2.11	2.06
23	D	402[B]	CLA	C3D-C4D	-2.31	1.39	1.44
23	C	509	CLA	C1C-C2C	2.31	1.49	1.44
23	d	402[A]	CLA	C1C-C2C	2.30	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	C3D-C4D	-2.30	1.39	1.44
33	a	416	LMT	O3'-C3'	-2.30	1.37	1.43
23	A	404[B]	CLA	C1C-C2C	2.30	1.49	1.44
23	A	408	CLA	C3B-C2B	2.30	1.49	1.41
23	b	608	CLA	C3B-C2B	2.30	1.49	1.41
23	C	512	CLA	C3D-C4D	-2.30	1.39	1.44
23	B	616	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	503	CLA	C4D-CHA	2.30	1.46	1.38
23	c	509	CLA	C4B-NB	-2.30	1.35	1.37
23	b	612	CLA	C3B-C2B	2.29	1.49	1.41
23	C	510	CLA	C3B-C2B	2.29	1.48	1.41
23	B	607	CLA	C4B-NB	-2.29	1.35	1.37
40	v	201	HEC	CAC-C3C	2.29	1.57	1.51
23	A	405[B]	CLA	C3D-C4D	-2.29	1.39	1.44
23	B	604	CLA	MG-NA	2.29	2.11	2.06
23	c	505	CLA	C3B-C4B	2.29	1.48	1.42
23	C	504	CLA	C4C-C3C	2.28	1.49	1.45
23	B	612	CLA	C3B-C4B	2.28	1.48	1.42
23	B	612	CLA	C1C-NC	-2.28	1.34	1.37
40	v	201	HEC	FE-NB	2.28	2.01	1.94
25	d	404	BCR	C30-C25	-2.28	1.50	1.53
23	D	402[B]	CLA	C3B-C2B	2.28	1.48	1.41
23	B	607	CLA	C1C-NC	-2.28	1.34	1.37
23	b	610	CLA	C3B-C2B	2.27	1.48	1.41
33	D	401	LMT	O2'-C2'	-2.27	1.37	1.43
23	b	604	CLA	C4B-NB	-2.27	1.35	1.37
23	c	504	CLA	C4C-C3C	2.27	1.48	1.45
23	B	611	CLA	C4D-CHA	2.27	1.46	1.38
24	A	417[B]	PHO	C3A-C2A	-2.26	1.52	1.54
24	A	417[A]	PHO	C4B-NB	-2.26	1.34	1.38
23	B	605	CLA	C4C-C3C	2.26	1.48	1.45
24	A	407[B]	PHO	CHA-CBD	-2.26	1.48	1.51
27	a	418	GOL	C1-C2	2.26	1.61	1.51
23	C	504	CLA	C1B-C2B	2.25	1.48	1.43
23	a	404[A]	CLA	C1C-C2C	2.25	1.48	1.44
23	a	408	CLA	C4C-C3C	2.25	1.48	1.45
23	b	604	CLA	C1C-C2C	2.25	1.48	1.44
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	607	CLA	C3D-C4D	-2.24	1.39	1.44
23	d	402[A]	CLA	C3B-C4B	2.24	1.48	1.42
23	C	505	CLA	C3B-C4B	2.24	1.48	1.42
23	b	613	CLA	C3B-C2B	2.24	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	C3B-C2B	2.23	1.48	1.41
23	C	503	CLA	C3B-C2B	2.23	1.48	1.41
23	c	513	CLA	C4C-C3C	2.23	1.48	1.45
23	d	403	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	601	CLA	C3B-C2B	2.23	1.48	1.41
27	D	412	GOL	C3-C2	2.23	1.60	1.51
23	B	601	CLA	C3B-C2B	2.23	1.48	1.41
38	F	102	HEM	C3B-C4B	2.22	1.49	1.44
23	c	510	CLA	C3B-C2B	2.22	1.48	1.41
23	B	607	CLA	C3B-C2B	2.22	1.48	1.41
23	B	613	CLA	C3B-C2B	2.21	1.48	1.41
40	V	201	HEC	CMB-C2B	2.21	1.55	1.50
23	a	406[B]	CLA	C3D-C4D	-2.21	1.39	1.44
36	C	518[A]	DGD	O5D-C1E	2.21	1.44	1.40
33	A	420	LMT	O2'-C2'	-2.21	1.37	1.43
23	D	402[A]	CLA	C4C-C3C	2.21	1.48	1.45
29	D	405[B]	PL9	C2-C3	2.21	1.40	1.34
23	c	508	CLA	C3B-C4B	2.20	1.47	1.42
23	c	509	CLA	C3D-C4D	-2.20	1.39	1.44
23	b	616	CLA	C3D-C4D	-2.20	1.39	1.44
33	B	628	LMT	O2B-C2B	-2.20	1.37	1.43
23	B	604	CLA	C1A-CHA	2.20	1.52	1.43
23	a	405[A]	CLA	C4B-NB	-2.20	1.35	1.37
23	B	608	CLA	C3D-C4D	-2.20	1.39	1.44
24	A	417[A]	PHO	C1D-ND	-2.20	1.34	1.38
23	D	402[A]	CLA	C3B-C2B	2.19	1.48	1.41
23	c	511	CLA	C3B-C2B	2.19	1.48	1.41
29	a	413[A]	PL9	C2-C3	2.19	1.40	1.34
23	c	507	CLA	C3B-C2B	2.19	1.48	1.41
33	B	628	LMT	O3'-C3'	-2.19	1.37	1.43
23	c	512	CLA	MG-NA	2.18	2.11	2.06
23	b	615	CLA	C4C-C3C	2.18	1.48	1.45
33	m	103	LMT	C3'-C2'	2.17	1.57	1.52
23	B	604	CLA	C4C-C3C	2.17	1.48	1.45
23	B	602	CLA	C3B-C2B	2.17	1.48	1.41
23	C	505	CLA	C3D-C4D	-2.17	1.39	1.44
29	a	413[B]	PL9	C2-C3	2.17	1.40	1.34
23	C	508	CLA	C3B-C2B	2.17	1.48	1.41
23	b	608	CLA	C1C-C2C	2.17	1.48	1.44
23	C	508	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	507	CLA	C3D-C4D	-2.16	1.39	1.44
23	c	514	CLA	C3B-C2B	2.16	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402[A]	CLA	C3B-C4B	2.16	1.47	1.42
23	A	406[B]	CLA	C3D-C4D	-2.16	1.39	1.44
23	b	601	CLA	C1B-C2B	2.16	1.48	1.43
23	a	404[B]	CLA	C1C-C2C	2.16	1.48	1.44
23	d	403	CLA	C4C-C3C	2.16	1.48	1.45
23	c	511	CLA	C4C-C3C	2.16	1.48	1.45
23	a	405[B]	CLA	C1C-C2C	2.16	1.48	1.44
23	C	506	CLA	C3D-C4D	-2.15	1.39	1.44
23	C	505	CLA	C3B-C2B	2.15	1.48	1.41
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	615	CLA	MG-NA	2.15	2.11	2.06
23	C	503	CLA	C3D-C4D	-2.15	1.39	1.44
23	b	614	CLA	C4C-C3C	2.15	1.48	1.45
23	C	513	CLA	C3D-C4D	-2.14	1.39	1.44
24	a	407[A]	PHO	C4B-NB	-2.14	1.34	1.38
23	A	406[B]	CLA	C4C-C3C	2.14	1.48	1.45
23	b	611	CLA	C3B-C2B	2.14	1.48	1.41
33	T	101	LMT	O3B-C3B	-2.14	1.37	1.43
23	B	604	CLA	C3B-C2B	2.13	1.48	1.41
23	B	607	CLA	C4C-C3C	2.13	1.48	1.45
24	a	415[B]	PHO	C1B-NB	-2.13	1.34	1.38
23	a	404[B]	CLA	C3D-C4D	-2.13	1.39	1.44
24	a	415[A]	PHO	C4B-NB	-2.13	1.34	1.38
23	A	405[B]	CLA	C3B-C2B	2.13	1.48	1.41
23	c	502	CLA	C4B-NB	-2.13	1.35	1.37
24	A	407[A]	PHO	C4B-NB	-2.12	1.34	1.38
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
23	c	503	CLA	C3D-C4D	-2.12	1.39	1.44
23	C	508	CLA	C4C-C3C	2.12	1.48	1.45
23	a	405[A]	CLA	C1C-C2C	2.12	1.48	1.44
27	D	412	GOL	O2-C2	-2.12	1.37	1.43
23	B	614	CLA	C4C-C3C	2.12	1.48	1.45
24	a	415[B]	PHO	CHA-CBD	-2.12	1.49	1.51
23	d	402[B]	CLA	C3B-C4B	2.11	1.47	1.42
23	C	502	CLA	C3B-C2B	2.11	1.48	1.41
36	H	102	DGD	O2G-C2G	-2.11	1.41	1.46
23	b	611	CLA	C3D-C4D	-2.11	1.39	1.44
23	D	403	CLA	C4B-NB	-2.11	1.35	1.37
23	B	613	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	514	CLA	C1D-C2D	2.11	1.49	1.45
35	o	301	HTG	O5-C1	2.10	1.45	1.42
33	D	401	LMT	O3'-C3'	-2.10	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	511	CLA	C3D-C4D	-2.10	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.10	1.39	1.44
23	C	505	CLA	C4C-C3C	2.10	1.48	1.45
24	A	407[B]	PHO	C4B-NB	-2.10	1.34	1.38
24	A	407[A]	PHO	C1B-NB	-2.09	1.34	1.38
23	B	609	CLA	C4C-C3C	2.09	1.48	1.45
23	b	605	CLA	C1D-C2D	2.09	1.49	1.45
23	B	614	CLA	C3B-C2B	2.09	1.48	1.41
23	D	402[B]	CLA	C3B-C4B	2.09	1.47	1.42
23	B	606	CLA	C4C-C3C	2.09	1.48	1.45
23	c	514	CLA	C4C-C3C	2.09	1.48	1.45
33	B	626	LMT	O5'-C5'	-2.09	1.39	1.44
23	c	507	CLA	C1C-C2C	2.09	1.48	1.44
23	a	406[A]	CLA	C4C-C3C	2.08	1.48	1.45
23	c	508	CLA	C3D-C4D	-2.08	1.39	1.44
23	C	511	CLA	C3B-C2B	2.08	1.48	1.41
23	b	606	CLA	C3B-C2B	2.08	1.48	1.41
23	d	402[A]	CLA	C3B-C2B	2.07	1.48	1.41
23	b	611	CLA	C1D-C2D	2.07	1.49	1.45
27	b	624	GOL	C3-C2	2.07	1.60	1.51
23	A	408	CLA	C1C-NC	-2.07	1.34	1.37
36	c	518[B]	DGD	O3G-C1D	2.07	1.43	1.40
33	B	629	LMT	O2'-C2'	-2.07	1.38	1.43
23	C	513	CLA	C3B-C2B	2.07	1.48	1.41
24	A	407[A]	PHO	C1D-ND	-2.07	1.34	1.38
23	b	616	CLA	C3B-C2B	2.06	1.48	1.41
23	C	502	CLA	C4C-C3C	2.06	1.48	1.45
23	C	507	CLA	C1D-C2D	2.06	1.49	1.45
26	L	101	SQD	O6-C1	2.06	1.43	1.40
23	b	603	CLA	C3D-C4D	-2.06	1.39	1.44
40	v	201	HEC	CMD-C2D	2.06	1.55	1.50
23	c	512	CLA	C4C-C3C	2.06	1.48	1.45
23	b	615	CLA	C4B-NB	-2.06	1.35	1.37
23	c	505	CLA	C3D-C4D	-2.06	1.39	1.44
23	B	606	CLA	C3B-C2B	2.05	1.48	1.41
23	B	613	CLA	C3B-C4B	2.05	1.47	1.42
23	B	615	CLA	C4B-NB	-2.05	1.35	1.37
23	C	514	CLA	C1C-NC	-2.05	1.34	1.37
23	b	605	CLA	C1C-C2C	2.05	1.48	1.44
29	D	405[A]	PL9	C2-C3	2.04	1.40	1.34
23	C	509	CLA	C1A-CHA	2.04	1.51	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C1C-C2C	2.04	1.48	1.44
24	a	415[A]	PHO	C1B-NB	-2.03	1.34	1.38
23	b	610	CLA	C4B-NB	-2.03	1.35	1.37
23	B	603	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	612	CLA	C3D-C4D	-2.03	1.39	1.44
23	b	607	CLA	C3B-C2B	2.03	1.48	1.41
33	e	101	LMT	O2B-C2B	-2.03	1.38	1.43
25	D	404	BCR	C5-C6	2.03	1.37	1.34
32	b	630[A]	LHG	O7-C5	-2.02	1.41	1.46
38	F	102	HEM	C3C-C4C	-2.02	1.42	1.46
40	v	201	HEC	CMC-C2C	2.02	1.55	1.50
23	C	509	CLA	C3D-C4D	-2.02	1.39	1.44
24	a	415[B]	PHO	C4B-NB	-2.02	1.34	1.38
23	a	405[B]	CLA	C3B-C2B	2.02	1.48	1.41
23	b	604	CLA	C1A-CHA	2.02	1.51	1.43
24	a	407[B]	PHO	C4B-NB	-2.02	1.34	1.38
23	B	606	CLA	MG-NA	2.02	2.11	2.06
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
23	d	403	CLA	C3B-C2B	2.02	1.48	1.41
33	T	101	LMT	O2'-C2'	-2.01	1.38	1.43
36	c	519	DGD	O5D-C1E	2.01	1.43	1.40
34	D	411	LMG	O7-C8	-2.01	1.41	1.46
23	c	508	CLA	C4C-C3C	2.01	1.48	1.45
23	D	403	CLA	C3D-C4D	-2.01	1.39	1.44
23	c	512	CLA	C1D-C2D	2.01	1.49	1.45
23	a	406[B]	CLA	C3B-C2B	2.01	1.48	1.41
23	B	601	CLA	C4C-C3C	2.01	1.48	1.45
33	B	626	LMT	O4'-C4B	-2.01	1.38	1.43
23	a	408	CLA	C3B-C2B	2.00	1.48	1.41
33	t	101	LMT	O2'-C2'	-2.00	1.38	1.43
24	a	415[A]	PHO	CBD-CGD	-2.00	1.49	1.52
23	c	506	CLA	C4B-NB	-2.00	1.35	1.37
23	C	511	CLA	C1D-C2D	2.00	1.49	1.45

All (3339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	17.25	121.80	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.68	90.65	107.16
23	B	611	CLA	C1D-ND-C4D	-12.02	97.79	106.33
24	a	415[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	A	417[B]	PHO	C2D-C1D-ND	11.65	117.57	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	415[B]	PHO	C2D-C1D-ND	11.54	117.49	109.53
24	A	407[A]	PHO	C2D-C1D-ND	11.43	117.42	109.53
24	a	407[A]	PHO	C2D-C1D-ND	11.21	117.26	109.53
24	A	407[B]	PHO	C2D-C1D-ND	11.06	117.17	109.53
24	a	407[B]	PHO	C2D-C1D-ND	10.83	117.01	109.53
24	A	417[A]	PHO	C2D-C1D-ND	10.73	116.93	109.53
23	B	611	CLA	CHB-C1B-NB	-10.72	112.91	124.26
23	a	408	CLA	C1D-ND-C4D	-10.70	98.73	106.33
23	B	612	CLA	C1D-ND-C4D	-10.65	98.77	106.33
23	B	611	CLA	C2D-C1D-ND	10.27	117.67	110.10
23	A	408	CLA	C1D-ND-C4D	-10.19	99.10	106.33
23	b	605	CLA	C1D-ND-C4D	-10.15	99.13	106.33
23	C	511	CLA	C1D-ND-C4D	-10.11	99.15	106.33
23	a	406[B]	CLA	C1D-ND-C4D	-10.08	99.17	106.33
23	B	615	CLA	C1D-ND-C4D	-10.02	99.22	106.33
23	c	512	CLA	C1D-ND-C4D	-9.96	99.26	106.33
23	C	504	CLA	C1D-ND-C4D	-9.86	99.33	106.33
23	B	601	CLA	C1D-ND-C4D	-9.79	99.38	106.33
23	B	614	CLA	C1D-ND-C4D	-9.73	99.42	106.33
23	a	406[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	d	402[B]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	b	614	CLA	C1D-ND-C4D	-9.67	99.47	106.33
23	b	611	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	B	605	CLA	C1D-ND-C4D	-9.56	99.55	106.33
23	c	504	CLA	C1D-ND-C4D	-9.53	99.56	106.33
23	a	408	CLA	C2D-C1D-ND	9.50	117.10	110.10
23	C	502	CLA	C1D-ND-C4D	-9.49	99.59	106.33
23	c	507	CLA	C1D-ND-C4D	-9.46	99.62	106.33
23	B	615	CLA	C2D-C1D-ND	9.44	117.06	110.10
23	A	406[A]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	c	514	CLA	C1D-ND-C4D	-9.40	99.66	106.33
23	D	402[B]	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	a	404[B]	CLA	C1D-ND-C4D	-9.33	99.71	106.33
23	B	612	CLA	C2D-C1D-ND	9.33	116.98	110.10
23	C	505	CLA	C1D-ND-C4D	-9.29	99.73	106.33
23	C	506	CLA	C1D-ND-C4D	-9.29	99.74	106.33
23	A	408	CLA	C2D-C1D-ND	9.27	116.93	110.10
23	A	406[B]	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	b	615	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	B	607	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	B	606	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	d	403	CLA	C1D-ND-C4D	-9.20	99.80	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C2D-C1D-ND	9.20	116.88	110.10
23	D	402[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	603	CLA	C1D-ND-C4D	-9.14	99.85	106.33
23	c	502	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	b	616	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	b	613	CLA	C2D-C1D-ND	9.11	116.82	110.10
23	b	614	CLA	C2D-C1D-ND	9.10	116.81	110.10
23	b	602	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	c	506	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	b	601	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	A	405[A]	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	A	405[A]	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	c	510	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	c	513	CLA	C1D-ND-C4D	-9.05	99.90	106.33
23	b	609	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	d	402[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	a	406[B]	CLA	C2D-C1D-ND	9.01	116.75	110.10
23	a	404[A]	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	B	614	CLA	C2D-C1D-ND	8.95	116.70	110.10
23	b	606	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	C	514	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	b	611	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	B	609	CLA	C1D-ND-C4D	-8.87	100.03	106.33
23	b	610	CLA	C1D-ND-C4D	-8.84	100.05	106.33
23	b	605	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	B	602	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	D	403	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	C	510	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	a	406[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	C	504	CLA	C2D-C1D-ND	8.81	116.59	110.10
23	c	512	CLA	C2D-C1D-ND	8.80	116.59	110.10
23	B	606	CLA	C2D-C1D-ND	8.77	116.57	110.10
23	c	508	CLA	C1D-ND-C4D	-8.75	100.12	106.33
23	c	505	CLA	C1D-ND-C4D	-8.75	100.12	106.33
23	B	608	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	B	616	CLA	C2D-C1D-ND	8.70	116.52	110.10
23	b	613	CLA	C1D-ND-C4D	-8.70	100.16	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	b	607	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	B	608	CLA	C2D-C1D-ND	8.63	116.47	110.10
23	c	503	CLA	C1D-ND-C4D	-8.62	100.21	106.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	C	503	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	C	512	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	B	605	CLA	C2D-C1D-ND	8.56	116.41	110.10
23	C	508	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	B	601	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	a	405[A]	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	b	608	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-8.49	100.31	106.33
23	D	402[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	513	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	b	612	CLA	C1D-ND-C4D	-8.45	100.33	106.33
23	b	616	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	D	402[B]	CLA	C2D-C1D-ND	8.43	116.31	110.10
23	C	507	CLA	C1D-ND-C4D	-8.40	100.37	106.33
23	C	508	CLA	C2D-C1D-ND	8.39	116.29	110.10
23	c	511	CLA	C1D-ND-C4D	-8.39	100.38	106.33
23	B	613	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	B	610	CLA	C1D-ND-C4D	-8.35	100.40	106.33
23	b	602	CLA	C2B-C1B-NB	8.35	115.83	110.23
23	C	509	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	c	509	CLA	C2D-C1D-ND	8.32	116.24	110.10
23	B	616	CLA	C1D-ND-C4D	-8.32	100.42	106.33
23	d	403	CLA	C2D-C1D-ND	8.31	116.23	110.10
23	A	406[B]	CLA	C2D-C1D-ND	8.30	116.22	110.10
23	B	603	CLA	C1D-ND-C4D	-8.30	100.44	106.33
23	B	613	CLA	C1D-ND-C4D	-8.29	100.44	106.33
23	c	509	CLA	C1D-ND-C4D	-8.24	100.48	106.33
23	B	611	CLA	CHD-C4C-C3C	-8.24	112.73	124.84
23	c	513	CLA	C2B-C1B-NB	8.24	115.75	110.23
23	c	504	CLA	C2D-C1D-ND	8.24	116.17	110.10
23	B	607	CLA	C2D-C1D-ND	8.23	116.17	110.10
23	b	606	CLA	C2D-C1D-ND	8.21	116.15	110.10
23	b	615	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	c	507	CLA	C2D-C1D-ND	8.20	116.14	110.10
23	c	503	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	c	511	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	C	509	CLA	C1D-ND-C4D	-8.18	100.52	106.33
23	c	508	CLA	C2D-C1D-ND	8.18	116.14	110.10
23	C	510	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	d	402[B]	CLA	C2D-C1D-ND	8.15	116.11	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	C2B-C1B-NB	8.14	115.69	110.23
23	b	609	CLA	C2D-C1D-ND	8.14	116.10	110.10
23	D	403	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	a	405[B]	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	502	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	C	502	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	c	505	CLA	C2D-C1D-ND	8.05	116.03	110.10
23	b	601	CLA	C2D-C1D-ND	8.04	116.03	110.10
23	B	609	CLA	C2D-C1D-ND	8.04	116.03	110.10
23	b	604	CLA	C1D-ND-C4D	-8.04	100.63	106.33
23	d	403	CLA	C2B-C1B-NB	8.03	115.62	110.23
23	a	404[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	B	601	CLA	C2B-C1B-NB	8.03	115.61	110.23
23	b	603	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	C	513	CLA	C2B-C1B-NB	7.97	115.58	110.23
23	A	406[B]	CLA	C2B-C1B-NB	7.96	115.57	110.23
23	B	610	CLA	C2D-C1D-ND	7.94	115.95	110.10
23	d	402[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	b	614	CLA	C2B-C1B-NB	7.91	115.53	110.23
24	a	407[B]	PHO	O2D-CGD-CBD	7.90	121.00	111.00
23	C	511	CLA	C2D-C1D-ND	7.86	115.89	110.10
23	A	405[B]	CLA	C2D-C1D-ND	7.86	115.89	110.10
23	c	513	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	C	512	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	b	607	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	C	514	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	a	404[B]	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	c	514	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	c	510	CLA	C2D-C1D-ND	7.79	115.85	110.10
23	B	603	CLA	C2D-C1D-ND	7.79	115.85	110.10
23	C	506	CLA	C2D-C1D-ND	7.76	115.83	110.10
23	B	604	CLA	C1D-ND-C4D	-7.76	100.82	106.33
23	b	602	CLA	C4A-NA-C1A	-7.76	103.22	106.71
23	C	504	CLA	C2B-C1B-NB	7.70	115.40	110.23
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	C	513	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	C	503	CLA	C2D-C1D-ND	7.66	115.75	110.10
24	A	407[B]	PHO	O2D-CGD-CBD	7.66	120.70	111.00
23	B	602	CLA	C2D-C1D-ND	7.64	115.73	110.10
23	b	601	CLA	C2B-C1B-NB	7.64	115.35	110.23
23	c	506	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	B	616	CLA	C2B-C1B-NB	7.59	115.32	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	D	403	CLA	C2B-C1B-NB	7.56	115.30	110.23
23	c	505	CLA	C2B-C1B-NB	7.56	115.30	110.23
23	C	511	CLA	CMD-C2D-C1D	7.55	138.01	124.71
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	b	610	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	a	404[B]	CLA	C2B-C1B-NB	7.52	115.27	110.23
23	c	504	CLA	C4A-NA-C1A	-7.50	103.33	106.71
23	C	512	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	c	514	CLA	C2B-C1B-NB	7.45	115.22	110.23
23	C	511	CLA	C2B-C1B-NB	7.44	115.22	110.23
23	b	604	CLA	C2D-C1D-ND	7.44	115.58	110.10
23	a	406[B]	CLA	C2B-C1B-NB	7.43	115.22	110.23
23	A	404[B]	CLA	C2B-C1B-NB	7.40	115.19	110.23
23	b	605	CLA	C2B-C1B-NB	7.39	115.19	110.23
23	C	514	CLA	C2B-C1B-NB	7.39	115.19	110.23
35	b	623	HTG	C1'-S1-C1	7.38	113.89	100.09
24	A	417[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	b	616	CLA	C2B-C1B-NB	7.36	115.17	110.23
23	b	615	CLA	C4A-NA-C1A	-7.34	103.41	106.71
23	b	603	CLA	C2B-C1B-NB	7.33	115.14	110.23
23	B	611	CLA	CMB-C2B-C1B	7.29	136.47	125.37
23	b	606	CLA	C2B-C1B-NB	7.29	115.12	110.23
23	b	602	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	B	616	CLA	CHD-C4C-C3C	-7.24	114.20	124.84
23	b	612	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	C	504	CLA	C4A-NA-C1A	-7.22	103.46	106.71
23	a	405[B]	CLA	C2B-C1B-NB	7.22	115.07	110.23
24	a	415[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
23	b	608	CLA	C2B-C1B-NB	7.20	115.06	110.23
24	a	415[B]	PHO	O2D-CGD-CBD	7.20	120.12	111.00
23	A	404[A]	CLA	C2B-C1B-NB	7.20	115.06	110.23
23	B	609	CLA	C4A-NA-C1A	-7.20	103.47	106.71
26	F	103	SQD	O6-C1-C2	7.19	119.53	108.30
23	C	509	CLA	C2B-C1B-NB	7.19	115.05	110.23
23	c	508	CLA	O2D-CGD-CBD	7.19	124.04	111.27
23	c	504	CLA	C2B-C1B-NB	7.17	115.04	110.23
23	C	503	CLA	C2B-C1B-NB	7.16	115.03	110.23
24	a	407[A]	PHO	O2D-CGD-CBD	7.16	120.07	111.00
23	A	404[B]	CLA	C2D-C1D-ND	7.16	115.38	110.10
23	B	603	CLA	C2B-C1B-NB	7.15	115.03	110.23
24	a	407[A]	PHO	C1C-C2C-C3C	-7.15	102.67	108.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C2B-C1B-NB	7.14	115.02	110.23
24	A	417[B]	PHO	C2B-C1B-NB	7.13	114.45	109.53
24	A	417[A]	PHO	C2B-C1B-NB	7.12	114.44	109.53
23	B	606	CLA	CMD-C2D-C1D	7.12	137.25	124.71
24	a	415[A]	PHO	C2B-C1B-NB	7.11	114.44	109.53
23	A	406[A]	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	B	605	CLA	CHD-C4C-C3C	-7.09	114.41	124.84
24	A	407[B]	PHO	C4D-ND-C1D	-7.09	101.61	108.83
24	a	415[A]	PHO	C4D-ND-C1D	-7.08	101.62	108.83
24	A	417[B]	PHO	C1C-C2C-C3C	-7.07	102.73	108.61
23	B	614	CLA	CMD-C2D-C1D	7.07	137.18	124.71
23	C	510	CLA	C2B-C1B-NB	7.05	114.96	110.23
23	b	613	CLA	C2B-C1B-NB	7.05	114.95	110.23
24	A	417[B]	PHO	O2D-CGD-CBD	7.04	119.92	111.00
23	C	507	CLA	C2D-C1D-ND	7.04	115.29	110.10
23	b	615	CLA	C2B-C1B-NB	7.04	114.95	110.23
23	A	405[B]	CLA	C2B-C1B-NB	7.01	114.93	110.23
23	a	404[A]	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	B	616	CLA	O2D-CGD-CBD	6.98	123.68	111.27
23	a	408	CLA	C2B-C1B-NB	6.98	114.91	110.23
24	A	417[B]	PHO	C4D-ND-C1D	-6.98	101.73	108.83
23	C	506	CLA	C2B-C1B-NB	6.97	114.91	110.23
24	A	407[B]	PHO	C2B-C1B-NB	6.91	114.30	109.53
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	b	605	CLA	C4A-NA-C1A	-6.91	103.60	106.71
23	b	606	CLA	CHD-C4C-C3C	-6.91	114.69	124.84
24	a	415[A]	PHO	C1C-C2C-C3C	-6.90	102.87	108.61
23	c	508	CLA	CMD-C2D-C1D	6.89	136.86	124.71
23	B	604	CLA	C2D-C1D-ND	6.87	115.17	110.10
23	B	609	CLA	C2B-C1B-NB	6.87	114.84	110.23
23	a	406[A]	CLA	C2B-C1B-NB	6.86	114.83	110.23
24	A	407[A]	PHO	C4D-ND-C1D	-6.85	101.86	108.83
23	B	602	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	B	603	CLA	O2D-CGD-CBD	6.81	123.36	111.27
24	a	415[B]	PHO	C4D-ND-C1D	-6.80	101.91	108.83
23	c	511	CLA	C2B-C1B-NB	6.80	114.79	110.23
23	c	514	CLA	CMD-C2D-C1D	6.79	136.69	124.71
23	c	510	CLA	C2B-C1B-NB	6.79	114.78	110.23
23	c	502	CLA	CMD-C2D-C1D	6.78	136.66	124.71
23	c	506	CLA	C2B-C1B-NB	6.77	114.77	110.23
23	B	603	CLA	C4A-NA-C1A	-6.75	103.67	106.71
23	c	502	CLA	C2B-C1B-NB	6.74	114.75	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404[B]	CLA	C4A-NA-C1A	-6.74	103.68	106.71
23	a	406[B]	CLA	CHD-C4C-C3C	-6.74	114.93	124.84
23	B	610	CLA	O2D-CGD-CBD	6.73	123.23	111.27
24	a	415[B]	PHO	C1C-C2C-C3C	-6.72	103.02	108.61
23	B	606	CLA	CHD-C1D-ND	-6.71	118.28	124.45
24	A	407[B]	PHO	C1C-C2C-C3C	-6.71	103.03	108.61
23	A	405[A]	CLA	C2B-C1B-NB	6.70	114.72	110.23
35	D	410	HTG	C1'-S1-C1	6.69	112.61	100.09
24	a	415[B]	PHO	C2B-C1B-NB	6.69	114.15	109.53
23	C	502	CLA	C2B-C1B-NB	6.69	114.72	110.23
23	C	508	CLA	O2D-CGD-CBD	6.68	123.14	111.27
23	B	610	CLA	C2B-C1B-NB	6.68	114.71	110.23
23	a	405[A]	CLA	C2B-C1B-NB	6.67	114.71	110.23
23	B	608	CLA	C2B-C1B-NB	6.67	114.70	110.23
23	b	605	CLA	CHD-C1D-ND	-6.66	118.33	124.45
23	b	611	CLA	C2B-C1B-NB	6.66	114.70	110.23
23	C	508	CLA	CMD-C2D-C1D	6.66	136.45	124.71
23	b	607	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	b	616	CLA	C4A-NA-C1A	-6.65	103.72	106.71
23	d	402[B]	CLA	C2C-C1C-NC	6.63	116.18	109.97
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	612	CLA	C2B-C1B-NB	6.62	114.67	110.23
23	B	611	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	606	CLA	CMD-C2D-C1D	6.61	136.37	124.71
23	b	604	CLA	C2C-C1C-NC	6.61	116.16	109.97
23	C	513	CLA	C4A-NA-C1A	-6.60	103.74	106.71
23	B	615	CLA	C4A-NA-C1A	-6.59	103.74	106.71
23	c	509	CLA	C2B-C1B-NB	6.59	114.65	110.23
23	b	616	CLA	CHD-C4C-C3C	-6.58	115.17	124.84
23	B	601	CLA	CMD-C2D-C1D	6.58	136.31	124.71
24	A	417[A]	PHO	C1C-C2C-C3C	-6.58	103.14	108.61
23	A	404[B]	CLA	CMD-C2D-C1D	6.57	136.30	124.71
23	C	508	CLA	CHD-C4C-C3C	-6.56	115.20	124.84
23	B	601	CLA	CHD-C4C-C3C	-6.55	115.22	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.55	115.22	124.84
23	C	509	CLA	C2C-C1C-NC	6.54	116.10	109.97
23	C	513	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
23	D	402[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	b	605	CLA	CHD-C4C-C3C	-6.52	115.25	124.84
23	b	606	CLA	C4A-NA-C1A	-6.52	103.78	106.71
23	d	402[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	A	408	CLA	CMD-C2D-C1D	6.51	136.19	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	CMD-C2D-C1D	6.50	136.17	124.71
23	c	502	CLA	CHD-C1D-ND	-6.50	118.48	124.45
23	b	609	CLA	C2B-C1B-NB	6.49	114.58	110.23
23	a	406[B]	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	c	508	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	D	402[B]	CLA	CMD-C2D-C1D	6.47	136.11	124.71
23	D	402[B]	CLA	CHD-C1D-ND	-6.47	118.51	124.45
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
35	c	522	HTG	C1'-S1-C1	6.46	112.17	100.09
23	b	613	CLA	CHD-C4C-C3C	-6.46	115.35	124.84
23	b	615	CLA	CMD-C2D-C1D	6.45	136.09	124.71
23	C	507	CLA	C2C-C1C-NC	6.45	116.01	109.97
23	B	605	CLA	C2B-C1B-NB	6.45	114.55	110.23
23	C	505	CLA	C2C-C1C-NC	6.44	116.00	109.97
23	B	605	CLA	CMD-C2D-C1D	6.43	136.05	124.71
24	a	407[B]	PHO	C1C-C2C-C3C	-6.43	103.26	108.61
24	A	417[A]	PHO	C4D-ND-C1D	-6.42	102.30	108.83
24	a	407[A]	PHO	C2B-C1B-NB	6.41	113.95	109.53
23	d	403	CLA	CHD-C1D-ND	-6.41	118.57	124.45
23	c	505	CLA	CHD-C1D-ND	-6.41	118.57	124.45
23	b	611	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	c	512	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	c	504	CLA	CHD-C4C-C3C	-6.38	115.47	124.84
23	D	403	CLA	CMD-C2D-C1D	6.38	135.95	124.71
23	B	613	CLA	C2B-C1B-NB	6.37	114.50	110.23
23	C	507	CLA	CMD-C2D-C1D	6.35	135.91	124.71
23	B	615	CLA	CHD-C1D-ND	-6.35	118.62	124.45
23	c	513	CLA	CMD-C2D-C1D	6.35	135.90	124.71
23	a	408	CLA	CHD-C4C-C3C	-6.35	115.51	124.84
23	b	607	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	a	407[A]	PHO	C4D-ND-C1D	-6.34	102.38	108.83
26	F	103	SQD	O47-C7-C8	6.34	125.17	111.50
23	a	406[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	c	504	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	C	504	CLA	CHD-C4C-C3C	-6.33	115.54	124.84
23	d	402[B]	CLA	CMD-C2D-C1D	6.33	135.86	124.71
23	c	513	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	B	614	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	a	406[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	B	605	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	C	502	CLA	C4A-NA-C1A	-6.28	103.88	106.71
40	V	201	HEC	C1D-ND-C4D	6.28	111.56	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
23	d	403	CLA	CMD-C2D-C1D	6.26	135.75	124.71
23	b	610	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	D	402[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	c	503	CLA	C2B-C1B-NB	6.26	114.43	110.23
23	B	614	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	a	404[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	B	615	CLA	C2B-C1B-NB	6.25	114.42	110.23
24	A	407[A]	PHO	C2B-C1B-NB	6.25	113.84	109.53
23	b	616	CLA	O2D-CGD-CBD	6.24	122.36	111.27
23	c	514	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	B	608	CLA	C2C-C1C-NC	6.23	115.81	109.97
23	B	614	CLA	C2B-C1B-NB	6.22	114.40	110.23
23	D	402[B]	CLA	C2C-C1C-NC	6.22	115.80	109.97
23	a	405[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	b	605	CLA	CMD-C2D-C1D	6.21	135.67	124.71
23	b	603	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	a	405[B]	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
23	c	503	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	a	404[B]	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	C	511	CLA	CHD-C1D-ND	-6.19	118.76	124.45
23	c	505	CLA	CMD-C2D-C1D	6.19	135.63	124.71
23	a	404[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	b	610	CLA	C2B-C1B-NB	6.19	114.38	110.23
23	b	601	CLA	O2D-CGD-CBD	6.18	122.26	111.27
23	B	606	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	C	505	CLA	C2B-C1B-NB	6.18	114.38	110.23
23	b	611	CLA	CMD-C2D-C1D	6.17	135.59	124.71
23	C	514	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	A	408	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	D	402[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	C	505	CLA	CHD-C1D-ND	-6.16	118.79	124.45
24	A	407[A]	PHO	C1C-C2C-C3C	-6.15	103.49	108.61
23	a	404[B]	CLA	CMD-C2D-C1D	6.15	135.56	124.71
23	B	614	CLA	C2C-C1C-NC	6.15	115.73	109.97
23	b	614	CLA	CMD-C2D-C1D	6.15	135.55	124.71
23	B	610	CLA	CMD-C2D-C1D	6.14	135.54	124.71
23	B	602	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
23	c	512	CLA	CMD-C2D-C1D	6.13	135.51	124.71
23	c	503	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	C	506	CLA	CHD-C4C-C3C	-6.12	115.84	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402[B]	CLA	C2B-C1B-NB	6.12	114.33	110.23
23	a	404[B]	CLA	C2C-C1C-NC	6.12	115.70	109.97
23	c	508	CLA	CHD-C4C-C3C	-6.11	115.85	124.84
23	B	604	CLA	C2B-C1B-NB	6.11	114.33	110.23
23	c	507	CLA	C2B-C1B-NB	6.11	114.33	110.23
23	c	507	CLA	CHD-C1D-ND	-6.10	118.84	124.45
23	b	609	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
23	B	610	CLA	C2C-C1C-NC	6.09	115.68	109.97
23	b	601	CLA	C4A-NA-C1A	-6.08	103.97	106.71
23	B	612	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	D	403	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	A	406[B]	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	B	603	CLA	C2C-C1C-NC	6.07	115.66	109.97
23	d	403	CLA	O2D-CGD-CBD	6.06	122.04	111.27
23	b	614	CLA	O2D-CGD-CBD	6.06	122.03	111.27
23	A	408	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	c	512	CLA	CHD-C1D-ND	-6.04	118.91	124.45
23	b	612	CLA	CHD-C4C-C3C	-6.04	115.97	124.84
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	d	402[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	c	512	CLA	C2B-C1B-NB	6.03	114.27	110.23
23	B	601	CLA	CHD-C1D-ND	-6.02	118.92	124.45
24	a	407[B]	PHO	C4D-ND-C1D	-6.01	102.72	108.83
23	C	503	CLA	C2C-C1C-NC	5.99	115.59	109.97
23	b	602	CLA	CHD-C1D-ND	-5.99	118.95	124.45
23	C	502	CLA	O2D-CGD-CBD	5.99	121.91	111.27
23	c	509	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	B	602	CLA	CMD-C2D-C1D	5.98	135.26	124.71
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	C	509	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	b	611	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	b	615	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	a	404[B]	CLA	C4A-NA-C1A	-5.97	104.02	106.71
23	c	514	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	C	507	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	b	602	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	C	502	CLA	CMD-C2D-C1D	5.95	135.21	124.71
23	B	604	CLA	C2C-C1C-NC	5.95	115.55	109.97
23	C	511	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	B	616	CLA	C3C-C4C-NC	5.94	117.24	110.57
23	c	513	CLA	CHD-C1D-ND	-5.94	118.99	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	C2C-C1C-NC	5.94	115.53	109.97
23	b	616	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	c	507	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	b	602	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	B	607	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
23	B	607	CLA	CHD-C1D-ND	-5.92	119.01	124.45
23	d	402[B]	CLA	C2B-C1B-NB	5.92	114.20	110.23
23	a	405[B]	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	c	506	CLA	CHD-C4C-C3C	-5.92	116.14	124.84
23	A	406[B]	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	B	602	CLA	C4A-NA-C1A	-5.91	104.05	106.71
26	L	101	SQD	O6-C1-C2	5.91	117.53	108.30
23	b	610	CLA	CMD-C2D-C1D	5.91	135.13	124.71
23	B	601	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	B	615	CLA	CMD-C2D-C1D	5.91	135.12	124.71
23	b	603	CLA	CMD-C2D-C1D	5.91	135.12	124.71
23	b	602	CLA	O2D-CGD-CBD	5.91	121.76	111.27
23	C	502	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	b	603	CLA	CHD-C4C-C3C	-5.90	116.17	124.84
23	B	606	CLA	C4A-NA-C1A	-5.90	104.06	106.71
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414[A]	PL9	C7-C8-C9	-5.89	116.99	126.79
23	b	606	CLA	CHD-C1D-ND	-5.89	119.04	124.45
23	A	404[A]	CLA	C4A-NA-C1A	-5.89	104.06	106.71
24	a	407[B]	PHO	C2B-C1B-NB	5.88	113.59	109.53
23	d	402[B]	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	A	406[A]	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	C	504	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	d	403	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	b	601	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
23	D	402[A]	CLA	C2B-C1B-NB	5.87	114.17	110.23
23	C	508	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	b	610	CLA	O2D-CGD-CBD	5.86	121.69	111.27
23	A	405[B]	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	B	612	CLA	O2D-CGD-CBD	5.86	121.68	111.27
23	b	601	CLA	CMD-C2D-C1D	5.86	135.03	124.71
23	C	514	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	A	404[A]	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	C	510	CLA	C2C-C1C-NC	5.81	115.41	109.97
23	B	610	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
23	B	607	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	c	511	CLA	CMD-C2D-C1D	5.80	134.93	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	CMD-C2D-C1D	5.79	134.92	124.71
23	C	512	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	B	606	CLA	O2D-CGD-CBD	5.79	121.56	111.27
23	B	611	CLA	C3D-C2D-C1D	-5.79	97.94	105.83
23	b	614	CLA	CHD-C4C-C3C	-5.78	116.34	124.84
23	a	405[B]	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	B	609	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	c	507	CLA	C2C-C1C-NC	5.78	115.38	109.97
23	b	601	CLA	CHD-C1D-ND	-5.78	119.15	124.45
23	B	602	CLA	O2D-CGD-CBD	5.77	121.53	111.27
23	A	404[B]	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	c	504	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	c	508	CLA	C2B-C1B-NB	5.76	114.09	110.23
23	B	613	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	a	404[A]	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	a	405[A]	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	C	512	CLA	CMD-C2D-C1D	5.74	134.84	124.71
23	D	403	CLA	C4A-NA-C1A	-5.74	104.12	106.71
23	A	405[B]	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	c	513	CLA	O2D-CGD-CBD	5.74	121.46	111.27
23	c	510	CLA	C1-C2-C3	-5.73	116.13	126.04
23	C	510	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
23	d	402[B]	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
23	c	506	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	A	404[B]	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	c	506	CLA	O2D-CGD-CBD	5.72	121.42	111.27
23	C	503	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	c	509	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	a	405[B]	CLA	CHD-C1D-ND	-5.71	119.20	124.45
35	d	409	HTG	C1'-S1-C1	5.71	110.78	100.09
23	B	608	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	c	510	CLA	CMD-C2D-C1D	5.71	134.78	124.71
23	b	614	CLA	CHD-C1D-ND	-5.71	119.21	124.45
23	C	503	CLA	CMD-C2D-C1D	5.70	134.76	124.71
38	F	102	HEM	CAD-CBD-CGD	5.70	125.86	113.60
23	D	402[B]	CLA	C4A-NA-C1A	-5.69	104.15	106.71
23	C	502	CLA	CHD-C1D-ND	-5.69	119.23	124.45
23	B	607	CLA	C2B-C1B-NB	5.68	114.04	110.23
23	A	404[B]	CLA	C2C-C1C-NC	5.68	115.30	109.97
23	b	608	CLA	CMD-C2D-C1D	5.68	134.73	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	c	509	CLA	C4A-NA-C1A	-5.68	104.15	106.71
23	b	603	CLA	C2C-C1C-NC	5.67	115.29	109.97
23	d	402[A]	CLA	C2B-C1B-NB	5.67	114.03	110.23
23	C	505	CLA	CMD-C2D-C1D	5.66	134.69	124.71
23	B	604	CLA	CHD-C4C-C3C	-5.66	116.52	124.84
35	B	621	HTG	C1'-S1-C1	5.66	110.67	100.09
23	C	511	CLA	O2D-CGD-CBD	5.65	121.31	111.27
23	b	615	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	b	615	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	C	514	CLA	C2C-C1C-NC	5.64	115.26	109.97
23	d	402[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	A	406[B]	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	B	603	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
23	b	604	CLA	O2D-CGD-CBD	5.63	121.27	111.27
23	b	608	CLA	C2C-C1C-NC	5.62	115.24	109.97
23	B	603	CLA	CMD-C2D-C1D	5.62	134.62	124.71
23	B	609	CLA	CMD-C2D-C1D	5.62	134.62	124.71
23	c	507	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	B	616	CLA	C4A-NA-C1A	-5.61	104.18	106.71
23	b	611	CLA	O2D-CGD-CBD	5.61	121.24	111.27
23	b	607	CLA	CHD-C1D-ND	-5.61	119.30	124.45
23	C	506	CLA	C2C-C1C-NC	5.61	115.23	109.97
35	C	522	HTG	C1'-S1-C1	5.61	110.58	100.09
23	a	405[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	A	405[B]	CLA	CHD-C1D-ND	-5.60	119.30	124.45
23	D	402[B]	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	B	605	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	A	408	CLA	C2C-C1C-NC	5.60	115.22	109.97
23	a	406[B]	CLA	CMD-C2D-C1D	5.60	134.58	124.71
23	c	514	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	B	606	CLA	C2B-C1B-NB	5.58	113.97	110.23
26	a	410[A]	SQD	O6-C1-C2	5.58	117.02	108.30
23	A	405[A]	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	b	603	CLA	CHD-C1D-ND	-5.57	119.33	124.45
23	b	612	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	a	408	CLA	O2D-CGD-CBD	5.56	121.16	111.27
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	b	607	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
23	b	604	CLA	C2B-C1B-NB	5.56	113.96	110.23
26	A	410[B]	SQD	O6-C1-C2	5.56	116.98	108.30
23	d	402[A]	CLA	CHD-C1D-ND	-5.56	119.35	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[A]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	c	505	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	C	513	CLA	CMD-C2D-C1D	5.55	134.50	124.71
23	C	506	CLA	O2D-CGD-CBD	5.55	121.13	111.27
23	A	406[B]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
40	v	201	HEC	C1D-ND-C4D	5.55	110.81	105.07
23	d	402[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.54	116.69	124.84
23	C	510	CLA	CHD-C1D-ND	-5.54	119.37	124.45
23	C	514	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	b	611	CLA	C2C-C1C-NC	5.53	115.16	109.97
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	C	508	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	C	511	CLA	C2C-C1C-NC	5.53	115.15	109.97
25	Y	101	BCR	C33-C5-C6	-5.52	118.33	124.53
23	B	603	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	B	614	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	B	612	CLA	CHD-C1D-ND	-5.50	119.39	124.45
23	c	505	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	c	511	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	b	613	CLA	C2C-C1C-NC	5.48	115.11	109.97
23	B	611	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	b	607	CLA	CMD-C2D-C1D	5.48	134.37	124.71
23	a	406[B]	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	b	609	CLA	CMD-C2D-C1D	5.47	134.35	124.71
23	b	613	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	b	606	CLA	O2D-CGD-CBD	5.46	120.97	111.27
23	D	403	CLA	CHD-C1D-ND	-5.46	119.43	124.45
23	b	604	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
23	b	609	CLA	CHD-C1D-ND	-5.44	119.45	124.45
23	B	606	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	A	408	CLA	C3D-C2D-C1D	-5.44	98.41	105.83
23	B	614	CLA	O2D-CGD-CBD	5.44	120.94	111.27
23	a	405[A]	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	C	512	CLA	C2C-C1C-NC	5.44	115.06	109.97
23	B	607	CLA	O2D-CGD-CBD	5.43	120.92	111.27
26	b	620	SQD	O6-C1-C2	5.42	116.76	108.30
23	B	606	CLA	C3D-C2D-C1D	-5.41	98.44	105.83
23	B	608	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	B	604	CLA	CMD-C2D-C1D	5.41	134.24	124.71
23	C	505	CLA	CHD-C4C-C3C	-5.40	116.90	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CMD-C2D-C1D	5.39	134.21	124.71
23	a	404[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	c	508	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	C	505	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
23	B	611	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	B	614	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
24	a	415[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	b	610	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	b	604	CLA	CMD-C2D-C1D	5.35	134.15	124.71
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	b	613	CLA	CMD-C2D-C1D	5.35	134.14	124.71
23	c	511	CLA	CHD-C1D-ND	-5.35	119.54	124.45
23	A	405[B]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	c	502	CLA	CHD-C4C-C3C	-5.34	116.99	124.84
23	a	406[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
29	A	414[B]	PL9	C7-C8-C9	-5.34	117.91	126.79
23	C	512	CLA	C3B-C2B-C1B	-5.34	100.72	107.16
23	b	611	CLA	C4A-NA-C1A	-5.34	104.31	106.71
23	B	604	CLA	O2D-CGD-CBD	5.33	120.74	111.27
23	A	406[A]	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	a	404[B]	CLA	CHD-C4C-C3C	-5.33	117.01	124.84
23	b	604	CLA	CHD-C1D-ND	-5.33	119.56	124.45
23	B	605	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
23	a	408	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	D	403	CLA	O2D-CGD-CBD	5.31	120.71	111.27
23	B	604	CLA	C3C-C4C-NC	5.30	116.52	110.57
25	D	404	BCR	C7-C8-C9	-5.30	118.23	126.23
23	B	615	CLA	C3D-C2D-C1D	-5.29	98.61	105.83
23	c	510	CLA	CHD-C4C-C3C	-5.29	117.06	124.84
23	a	404[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	B	616	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
23	B	608	CLA	CMD-C2D-C1D	5.28	134.02	124.71
23	C	508	CLA	C2B-C1B-NB	5.27	113.77	110.23
23	b	614	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	b	609	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	A	405[B]	CLA	C4A-NA-C1A	-5.25	104.34	106.71
23	c	511	CLA	C2C-C1C-NC	5.25	114.89	109.97
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	b	608	CLA	CHD-C1D-ND	-5.24	119.64	124.45
23	b	614	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	B	613	CLA	CMD-C2D-C1D	5.24	133.94	124.71
23	B	612	CLA	C2B-C1B-NB	5.24	113.74	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[B]	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.22	117.16	124.84
23	b	609	CLA	C4A-NA-C1A	-5.22	104.36	106.71
23	B	609	CLA	C2C-C1C-NC	5.21	114.86	109.97
26	a	410[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	C	506	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	B	605	CLA	C2C-C1C-NC	5.21	114.85	109.97
23	b	613	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
23	C	509	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	B	605	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	c	502	CLA	C2C-C1C-NC	5.20	114.84	109.97
23	c	505	CLA	C3B-C2B-C1B	-5.19	100.89	107.16
26	L	101	SQD	O47-C7-C8	5.19	122.69	111.50
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	a	405[A]	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	b	616	CLA	CHD-C1D-ND	-5.18	119.69	124.45
24	A	407[A]	PHO	C3D-C4D-ND	5.17	114.77	107.72
23	C	512	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	B	616	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	C	508	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	B	602	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	B	611	CLA	CMC-C2C-C1C	5.16	132.90	125.04
23	C	506	CLA	C3C-C4C-NC	5.15	116.35	110.57
23	B	613	CLA	C1-C2-C3	-5.14	117.15	126.04
23	B	608	CLA	C3D-C2D-C1D	-5.14	98.82	105.83
23	c	513	CLA	C3B-C2B-C1B	-5.14	100.96	107.16
26	b	620	SQD	O47-C7-C8	5.14	122.57	111.50
23	B	608	CLA	O2D-CGD-CBD	5.13	120.39	111.27
23	C	506	CLA	CMD-C2D-C1D	5.13	133.76	124.71
25	t	102	BCR	C33-C5-C6	-5.13	118.77	124.53
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	B	610	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	c	512	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	a	415[B]	PHO	C3D-C4D-ND	5.11	114.69	107.72
23	C	504	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	c	509	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	b	616	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	C	512	CLA	O2D-CGD-CBD	5.10	120.32	111.27
23	B	602	CLA	CHD-C1D-ND	-5.09	119.78	124.45
23	b	608	CLA	C4A-NA-C1A	-5.09	104.42	106.71
24	a	415[A]	PHO	C3D-C4D-ND	5.09	114.66	107.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	O2D-CGD-CBD	5.08	120.29	111.27
23	b	613	CLA	C3C-C4C-NC	5.08	116.26	110.57
23	c	509	CLA	O2D-CGD-CBD	5.07	120.28	111.27
38	f	101	HEM	CHC-C4B-NB	5.06	129.92	124.42
23	C	503	CLA	CHD-C1D-ND	-5.06	119.80	124.45
24	A	407[B]	PHO	C3D-C4D-ND	5.05	114.61	107.72
23	c	509	CLA	CMD-C2D-C1D	5.05	133.62	124.71
23	b	605	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	b	603	CLA	O2D-CGD-CBD	5.05	120.24	111.27
23	b	606	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	C	505	CLA	O2D-CGD-CBD	5.04	120.23	111.27
23	a	408	CLA	CHD-C1D-ND	-5.04	119.82	124.45
23	c	506	CLA	CMD-C2D-C1D	5.04	133.59	124.71
23	b	614	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
23	c	508	CLA	C4A-NA-C1A	-5.04	104.44	106.71
26	F	103	SQD	C1-O5-C5	-5.03	103.81	113.69
23	C	508	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
23	c	514	CLA	C2C-C1C-NC	5.02	114.68	109.97
23	B	604	CLA	C4A-NA-C1A	-5.02	104.45	106.71
23	C	513	CLA	CHD-C1D-ND	-5.02	119.84	124.45
23	B	608	CLA	C4A-NA-C1A	-5.01	104.45	106.71
23	b	605	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	C	513	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	c	502	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	c	510	CLA	CHD-C1D-ND	-5.00	119.86	124.45
23	B	616	CLA	C3B-C2B-C1B	-4.99	101.14	107.16
23	b	611	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	B	613	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	c	506	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	A	408	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
23	C	509	CLA	C3C-C4C-NC	4.98	116.15	110.57
23	C	509	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	D	403	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
23	C	506	CLA	CHD-C1D-ND	-4.97	119.88	124.45
23	c	512	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
23	b	612	CLA	C3C-C4C-NC	4.97	116.15	110.57
23	C	504	CLA	C3B-C2B-C1B	-4.97	101.16	107.16
23	d	403	CLA	C2C-C1C-NC	4.97	114.62	109.97
23	c	502	CLA	O2D-CGD-CBD	4.96	120.08	111.27
26	f	102	SQD	O47-C7-C8	4.95	122.17	111.50
23	B	615	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	a	406[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402[B]	CLA	C3D-C2D-C1D	-4.93	99.10	105.83
23	b	610	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	b	601	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	C	510	CLA	C3B-C2B-C1B	-4.93	101.22	107.16
23	a	406[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
24	A	417[A]	PHO	C3D-C4D-ND	4.91	114.42	107.72
23	B	604	CLA	C1-C2-C3	-4.91	117.56	126.04
23	b	610	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	B	610	CLA	CHD-C1D-ND	-4.91	119.95	124.45
23	d	403	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
23	c	506	CLA	CHD-C1D-ND	-4.90	119.95	124.45
23	a	405[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	A	404[A]	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
26	a	410[B]	SQD	O6-C1-C2	4.88	115.93	108.30
23	C	502	CLA	C2C-C1C-NC	4.88	114.55	109.97
23	A	405[B]	CLA	C1C-C2C-C3C	-4.87	101.84	106.96
23	c	508	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	a	404[B]	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
23	b	612	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	C	513	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
24	A	417[B]	PHO	C3D-C4D-ND	4.85	114.33	107.72
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	a	405[B]	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
23	d	403	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
23	B	614	CLA	C3B-C2B-C1B	-4.85	101.31	107.16
23	A	404[B]	CLA	C3B-C2B-C1B	-4.84	101.31	107.16
25	d	404	BCR	C7-C8-C9	-4.84	118.92	126.23
23	c	504	CLA	C2C-C1C-NC	4.84	114.51	109.97
23	b	610	CLA	C1-C2-C3	-4.84	117.67	126.04
23	c	507	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	c	505	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	C	507	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	b	606	CLA	C2C-C1C-NC	4.84	114.50	109.97
23	B	601	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	c	510	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	B	612	CLA	C3C-C4C-NC	4.83	115.99	110.57
23	a	406[B]	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	C	514	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
23	C	509	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
23	c	504	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	c	506	CLA	C4A-NA-C1A	-4.80	104.55	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	b	607	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	b	612	CLA	CMD-C2D-C1D	4.79	133.16	124.71
23	C	509	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	B	609	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	B	611	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	c	502	CLA	O2D-CGD-O1D	-4.79	114.47	123.84
23	c	511	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	B	613	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	a	405[B]	CLA	O2D-CGD-CBD	4.78	119.77	111.27
23	b	614	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	c	502	CLA	CMB-C2B-C1B	4.78	132.65	125.37
23	b	604	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	B	612	CLA	O2D-CGD-O1D	-4.77	114.51	123.84
23	c	514	CLA	C3D-C2D-C1D	-4.77	99.33	105.83
23	b	604	CLA	C1-C2-C3	-4.76	117.81	126.04
23	C	511	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	b	605	CLA	C2C-C1C-NC	4.76	114.43	109.97
23	b	611	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	c	502	CLA	C4A-NA-C1A	-4.75	104.57	106.71
23	c	505	CLA	O2D-CGD-CBD	4.75	119.71	111.27
23	B	606	CLA	C3C-C4C-NC	4.75	115.90	110.57
23	C	502	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	a	405[B]	CLA	C4A-NA-C1A	-4.74	104.58	106.71
23	b	605	CLA	C3D-C4D-ND	4.74	117.91	110.24
24	a	415[B]	PHO	C1-C2-C3	-4.73	117.86	126.04
23	C	514	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	c	511	CLA	O2D-CGD-CBD	4.73	119.67	111.27
23	a	408	CLA	C3D-C4D-ND	4.72	117.88	110.24
23	b	615	CLA	C3D-C2D-C1D	-4.72	99.38	105.83
23	c	505	CLA	C4A-NA-C1A	-4.72	104.58	106.71
23	B	612	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	A	405[B]	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
26	a	410[B]	SQD	O47-C7-C8	4.72	121.66	111.50
23	b	603	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	C	504	CLA	C2C-C1C-NC	4.71	114.39	109.97
23	A	405[A]	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
23	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	C	505	CLA	C1C-C2C-C3C	-4.71	102.01	106.96
23	B	601	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
23	c	507	CLA	C3D-C2D-C1D	-4.70	99.41	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[B]	CLA	C3D-C4D-ND	4.70	117.84	110.24
23	c	503	CLA	C1C-C2C-C3C	-4.70	102.02	106.96
23	B	603	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	C	508	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	B	607	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	c	504	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	b	607	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	c	504	CLA	O2D-CGD-CBD	4.69	119.59	111.27
23	b	609	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	a	406[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.68	115.96	126.06
23	B	616	CLA	CMD-C2D-C1D	4.68	132.96	124.71
23	c	512	CLA	O2D-CGD-CBD	4.68	119.58	111.27
23	c	508	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
23	C	510	CLA	O2D-CGD-CBD	4.67	119.57	111.27
23	C	505	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	b	604	CLA	C3C-C4C-NC	4.67	115.81	110.57
24	a	407[A]	PHO	C3D-C4D-ND	4.67	114.08	107.72
23	b	602	CLA	C3D-C4D-ND	4.67	117.79	110.24
23	d	402[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	a	408	CLA	C3C-C4C-NC	4.67	115.80	110.57
34	C	501	LMG	C7-O1-C1	-4.67	104.62	113.74
23	c	512	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	B	601	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	c	510	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
23	B	612	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
23	c	511	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	c	503	CLA	C3B-C2B-C1B	-4.65	101.54	107.16
23	B	605	CLA	C3C-C4C-NC	4.65	115.79	110.57
35	b	622	HTG	C1-O5-C5	4.65	121.16	112.58
25	b	617	BCR	C7-C8-C9	-4.65	119.21	126.23
23	C	510	CLA	C1-C2-C3	-4.65	118.00	126.04
23	a	408	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	A	406[B]	CLA	C3D-C4D-ND	4.64	117.75	110.24
23	C	509	CLA	CMD-C2D-C1D	4.64	132.89	124.71
25	H	101	BCR	C38-C26-C25	-4.64	119.32	124.53
23	C	511	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	C	503	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
38	F	102	HEM	CHC-C4B-NB	4.62	129.44	124.42
23	C	507	CLA	O2D-CGD-CBD	4.62	119.48	111.27
23	c	514	CLA	O2D-CGD-CBD	4.62	119.48	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	417[B]	PHO	C1-C2-C3	-4.62	118.06	126.04
23	a	406[B]	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
23	b	606	CLA	C3C-C4C-NC	4.61	115.74	110.57
23	c	509	CLA	CHD-C1D-ND	-4.61	120.22	124.45
23	b	613	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
29	a	413[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	B	610	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	C	507	CLA	C3B-C2B-C1B	-4.60	101.60	107.16
23	A	406[B]	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	C	510	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	c	509	CLA	C3C-C4C-NC	4.60	115.72	110.57
23	C	509	CLA	CHD-C1D-ND	-4.59	120.23	124.45
23	C	514	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	a	404[B]	CLA	C3D-C4D-ND	4.59	117.66	110.24
23	C	511	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	b	601	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	c	513	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	B	615	CLA	CMB-C2B-C1B	4.58	132.34	125.37
23	a	405[B]	CLA	C1C-C2C-C3C	-4.58	102.14	106.96
23	a	406[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	A	404[B]	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
23	B	602	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
23	D	402[B]	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	c	507	CLA	C3D-C4D-ND	4.56	117.62	110.24
23	b	606	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
23	D	402[A]	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	A	406[A]	CLA	C3D-C4D-ND	4.55	117.61	110.24
26	f	102	SQD	C1-O5-C5	4.55	122.62	113.69
23	C	510	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	C	503	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
23	b	611	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	B	612	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	d	402[B]	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	B	612	CLA	CMD-C2D-C1D	4.55	132.72	124.71
23	B	603	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
23	d	402[B]	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	B	613	CLA	CHD-C1D-ND	-4.54	120.28	124.45
23	B	602	CLA	C3C-C4C-NC	4.54	115.67	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	c	506	CLA	C3D-C4D-ND	4.54	117.58	110.24
23	a	408	CLA	CMD-C2D-C1D	4.54	132.71	124.71
23	C	507	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
23	c	507	CLA	O2D-CGD-CBD	4.53	119.32	111.27
23	A	408	CLA	C3D-C4D-ND	4.53	117.57	110.24
23	A	405[B]	CLA	O2D-CGD-CBD	4.53	119.31	111.27
23	B	607	CLA	C4A-NA-C1A	-4.53	104.67	106.71
24	A	417[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
23	b	607	CLA	C3B-C4B-NB	4.53	114.71	110.52
23	b	605	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
26	A	410[B]	SQD	C1-O5-C5	-4.52	104.81	113.69
23	C	503	CLA	O2D-CGD-CBD	4.52	119.31	111.27
23	C	512	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	B	603	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	d	402[B]	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	B	611	CLA	CHD-C4C-NC	4.52	131.32	124.20
23	C	513	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	B	608	CLA	C3B-C2B-C1B	-4.52	101.71	107.16
23	A	406[B]	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
23	b	608	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	C	506	CLA	C3D-C4D-ND	4.51	117.53	110.24
23	b	601	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	b	603	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
34	B	620	LMG	O7-C10-C11	4.50	121.19	111.50
23	b	613	CLA	C4A-NA-C1A	-4.50	104.69	106.71
23	D	403	CLA	C2C-C1C-NC	4.49	114.18	109.97
23	D	402[B]	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
23	A	406[B]	CLA	O2D-CGD-CBD	4.49	119.25	111.27
23	C	507	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	B	611	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	a	405[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	c	514	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
23	b	603	CLA	C3C-C4C-NC	4.49	115.60	110.57
23	b	608	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
23	a	404[A]	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	b	610	CLA	CHD-C1D-ND	-4.48	120.34	124.45
23	a	408	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
23	B	610	CLA	O2A-CGA-CBA	4.48	125.96	111.91
23	a	408	CLA	C4A-NA-C1A	-4.47	104.70	106.71
23	c	513	CLA	C2C-C1C-NC	4.47	114.16	109.97
23	b	612	CLA	CHD-C1D-ND	-4.47	120.35	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	101	BCR	C33-C5-C6	-4.47	119.51	124.53
23	d	402[B]	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
24	a	407[B]	PHO	C3D-C4D-ND	4.46	113.80	107.72
23	b	612	CLA	O2D-CGD-CBD	4.46	119.20	111.27
23	b	602	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	B	610	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
25	d	404	BCR	C15-C14-C13	-4.45	120.96	127.31
23	d	402[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	d	402[B]	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	c	504	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	B	613	CLA	O2D-CGD-CBD	4.44	119.16	111.27
23	b	608	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
23	d	402[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	d	402[B]	CLA	C1C-C2C-C3C	-4.44	102.29	106.96
23	b	608	CLA	C3B-C2B-C1B	-4.44	101.81	107.16
23	B	609	CLA	C3D-C4D-ND	4.44	117.41	110.24
23	b	610	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	c	510	CLA	C4A-NA-C1A	-4.43	104.71	106.71
23	B	614	CLA	C1C-C2C-C3C	-4.43	102.30	106.96
23	C	513	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
33	t	101	LMT	C3'-C4'-C5'	-4.42	100.78	110.93
23	a	406[B]	CLA	C2C-C1C-NC	4.42	114.11	109.97
23	c	509	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
23	C	505	CLA	C4A-NA-C1A	-4.42	104.72	106.71
23	C	506	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
23	c	508	CLA	CMC-C2C-C1C	4.41	131.75	125.04
23	C	510	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	B	608	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	C	503	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	b	609	CLA	C3C-C4C-NC	4.40	115.51	110.57
23	b	614	CLA	O2D-CGD-O1D	-4.40	115.24	123.84
23	b	607	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	b	604	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	D	402[A]	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
23	a	405[A]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	b	611	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	b	602	CLA	C2C-C1C-NC	4.39	114.08	109.97
23	c	512	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
26	A	410[B]	SQD	O9-S-C6	4.39	112.15	106.94
23	b	612	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
23	b	601	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	B	605	CLA	C3B-C2B-C1B	-4.38	101.87	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404[B]	CLA	C1D-CHD-C4C	-4.38	116.61	126.06
29	a	413[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	B	602	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
23	a	406[B]	CLA	O2D-CGD-CBD	4.38	119.04	111.27
23	C	513	CLA	C2C-C1C-NC	4.38	114.07	109.97
23	b	612	CLA	C1-C2-C3	-4.37	118.48	126.04
23	b	603	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	b	616	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
23	A	408	CLA	C4A-NA-C1A	-4.36	104.75	106.71
23	B	615	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	B	614	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	502	CLA	O2D-CGD-O1D	-4.35	115.34	123.84
23	B	607	CLA	C1C-C2C-C3C	-4.35	102.39	106.96
23	C	502	CLA	C3D-C4D-ND	4.34	117.26	110.24
23	C	512	CLA	C4A-NA-C1A	-4.34	104.75	106.71
23	B	616	CLA	O2D-CGD-O1D	-4.34	115.35	123.84
23	c	503	CLA	CMD-C2D-C1D	4.34	132.36	124.71
23	B	612	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
38	F	102	HEM	C1B-NB-C4B	4.34	109.55	105.07
23	c	508	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	c	511	CLA	C1-C2-C3	-4.33	118.56	126.04
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
34	c	521	LMG	O6-C5-C4	4.32	117.55	109.69
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	d	403	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
23	c	510	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	c	514	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	B	601	CLA	C2C-C1C-NC	4.32	114.02	109.97
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.52	110.52
23	C	514	CLA	C3B-C4B-NB	4.31	114.52	110.52
23	D	402[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	a	404[B]	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
23	B	613	CLA	C3B-C2B-C1B	-4.31	101.95	107.16
34	Z	101	LMG	O7-C10-C11	4.31	120.79	111.50
23	B	605	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	b	609	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	B	601	CLA	C3D-C4D-ND	4.30	117.20	110.24
34	c	501	LMG	O7-C10-C11	4.30	120.77	111.50
23	A	404[B]	CLA	C3D-C4D-ND	4.30	117.19	110.24
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	C	504	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	c	503	CLA	C4A-NA-C1A	-4.30	104.78	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
23	d	403	CLA	C3D-C4D-ND	4.29	117.18	110.24
25	d	404	BCR	C40-C30-C25	-4.29	103.34	110.30
23	b	604	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
23	c	507	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
23	B	603	CLA	O2D-CGD-O1D	-4.29	115.46	123.84
23	a	404[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	B	601	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	b	610	CLA	C3D-C4D-ND	4.27	117.15	110.24
23	D	402[B]	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	a	405[B]	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
23	c	514	CLA	C1D-CHD-C4C	-4.26	116.86	126.06
23	C	514	CLA	C3D-C4D-ND	4.26	117.13	110.24
26	b	620	SQD	C1-O5-C5	-4.26	105.33	113.69
23	d	403	CLA	C4A-NA-C1A	-4.26	104.79	106.71
29	D	405[B]	PL9	C42-C43-C44	-4.26	117.41	127.66
23	b	607	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
23	D	402[B]	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	a	406[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
25	b	617	BCR	C33-C5-C6	-4.25	119.75	124.53
23	A	405[B]	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	c	514	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	c	504	CLA	C1D-CHD-C4C	-4.25	116.90	126.06
23	C	514	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	b	607	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	b	616	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	c	512	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	A	406[B]	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	c	504	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	c	502	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
23	b	607	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
23	C	511	CLA	C1-C2-C3	-4.23	118.72	126.04
23	C	512	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	C	504	CLA	O2D-CGD-CBD	4.23	118.79	111.27
23	C	507	CLA	C3D-C4D-ND	4.23	117.07	110.24
26	A	410[B]	SQD	C1-C2-C3	-4.22	101.20	110.00
23	D	403	CLA	O2D-CGD-O1D	-4.22	115.58	123.84
23	b	606	CLA	O2D-CGD-O1D	-4.22	115.59	123.84
23	a	404[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	C	504	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	406[A]	CLA	C3B-C2B-C1B	-4.21	102.07	107.16
23	B	602	CLA	C3D-C4D-ND	4.21	117.05	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	c	502	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	a	404[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	B	615	CLA	C3C-C4C-NC	4.20	115.29	110.57
32	E	101[B]	LHG	O7-C7-C8	4.20	120.56	111.50
23	C	503	CLA	C3D-C4D-ND	4.20	117.03	110.24
29	A	414[B]	PL9	C32-C33-C34	-4.20	117.56	127.66
29	a	413[B]	PL9	C7-C8-C9	-4.20	119.81	126.79
23	b	603	CLA	C1D-CHD-C4C	-4.20	117.01	126.06
23	b	602	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	c	510	CLA	C3B-C4B-NB	4.19	114.40	110.52
26	a	410[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	a	404[B]	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	c	505	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	b	615	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	d	402[B]	CLA	O2D-CGD-CBD	4.18	118.70	111.27
23	B	613	CLA	CAC-C3C-C4C	4.18	130.24	124.81
23	B	607	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	C	506	CLA	CMB-C2B-C1B	4.18	131.73	125.37
23	b	614	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	a	404[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	C	503	CLA	C4A-NA-C1A	-4.17	104.83	106.71
23	C	514	CLA	C1C-C2C-C3C	-4.17	102.58	106.96
23	c	510	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
23	B	616	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	a	406[B]	CLA	C3C-C4C-NC	4.16	115.24	110.57
23	b	616	CLA	C2C-C1C-NC	4.16	113.87	109.97
23	b	609	CLA	O2D-CGD-CBD	4.16	118.66	111.27
23	C	505	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
34	d	410	LMG	O7-C10-C11	4.16	120.46	111.50
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	D	403	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
34	C	501	LMG	O1-C1-C2	4.14	114.77	108.30
23	B	616	CLA	C4C-C3C-C2C	-4.14	100.86	106.90
23	A	404[B]	CLA	C3C-C4C-NC	4.14	115.22	110.57
23	D	402[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	c	512	CLA	C3D-C4D-ND	4.14	116.94	110.24
34	C	501	LMG	O7-C10-C11	4.14	120.42	111.50
23	C	511	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
23	b	615	CLA	C3B-C2B-C1B	-4.14	102.17	107.16
23	B	610	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
23	b	612	CLA	C3D-C4D-ND	4.13	116.92	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	C1D-CHD-C4C	-4.12	117.17	126.06
23	a	405[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	b	607	CLA	O2D-CGD-CBD	4.12	118.58	111.27
23	D	403	CLA	C1D-CHD-C4C	-4.12	117.18	126.06
29	A	414[A]	PL9	C7-C3-C2	-4.12	117.89	123.30
23	c	503	CLA	C3D-C4D-ND	4.12	116.89	110.24
23	d	402[A]	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	d	402[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	c	508	CLA	CMB-C2B-C1B	4.11	131.63	125.37
23	c	508	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
23	a	408	CLA	CMC-C2C-C1C	4.11	131.30	125.04
23	c	505	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	A	404[B]	CLA	CAA-C2A-C3A	-4.11	101.54	112.78
26	L	101	SQD	C3-C4-C5	4.10	117.56	110.24
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
38	F	102	HEM	C4C-NC-C1C	4.10	109.36	105.35
23	C	504	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
23	a	404[A]	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	c	513	CLA	C3D-C4D-ND	4.09	116.86	110.24
23	b	605	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	503	CLA	C3C-C4C-NC	4.08	115.15	110.57
23	c	503	CLA	C1D-CHD-C4C	-4.08	117.25	126.06
34	c	521	LMG	O7-C10-C11	4.08	120.30	111.50
23	b	609	CLA	C1-C2-C3	-4.08	118.98	126.04
23	c	503	CLA	CHD-C1D-ND	-4.08	120.70	124.45
23	B	609	CLA	O2D-CGD-CBD	4.08	118.52	111.27
23	C	513	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
23	A	404[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
23	A	405[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
36	C	517[A]	DGD	O2G-C1B-C2B	4.08	120.29	111.50
25	A	409	BCR	C24-C23-C22	-4.08	120.08	126.23
23	D	402[B]	CLA	O2D-CGD-CBD	4.07	118.51	111.27
26	a	410[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
23	D	402[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	B	604	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
25	d	404	BCR	C29-C30-C25	4.06	116.74	110.48
23	c	506	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	c	507	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	b	604	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	A	408	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	b	612	CLA	C3B-C4B-NB	4.06	114.28	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
26	A	410[B]	SQD	C44-O6-C1	-4.06	105.82	113.74
23	C	505	CLA	C3D-C4D-ND	4.05	116.80	110.24
23	a	404[B]	CLA	C1D-CHD-C4C	-4.05	117.31	126.06
26	L	101	SQD	O7-S-C6	4.05	111.76	106.94
23	B	606	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	b	616	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	C	509	CLA	C3B-C4B-NB	4.05	114.27	110.52
34	C	521	LMG	O7-C10-C11	4.04	120.22	111.50
23	c	509	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	C	503	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	B	614	CLA	CMC-C2C-C1C	4.04	131.19	125.04
38	f	101	HEM	C4C-NC-C1C	4.04	109.30	105.35
23	C	510	CLA	C3D-C4D-ND	4.04	116.77	110.24
26	a	410[B]	SQD	C1-O5-C5	-4.04	105.76	113.69
23	d	403	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	C	511	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
23	b	610	CLA	C3B-C2B-C1B	-4.03	102.29	107.16
23	A	405[B]	CLA	C3B-C2B-C1B	-4.03	102.30	107.16
23	C	509	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	B	603	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	b	608	CLA	C3D-C4D-ND	4.02	116.75	110.24
34	m	101	LMG	O7-C10-C11	4.02	120.17	111.50
23	C	502	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
23	D	403	CLA	CMB-C2B-C1B	4.02	131.49	125.37
34	c	520	LMG	O7-C10-C11	4.02	120.16	111.50
23	c	513	CLA	C1-C2-C3	-4.02	119.09	126.04
23	C	510	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
34	C	521	LMG	O6-C5-C4	4.01	116.98	109.69
23	c	502	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	a	405[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	b	602	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
23	b	601	CLA	C3C-C4C-NC	4.01	115.07	110.57
38	f	101	HEM	CAD-CBD-CGD	4.01	122.23	113.60
23	c	512	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
23	b	609	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
23	C	514	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	C	513	CLA	C1-C2-C3	-4.00	119.12	126.04
23	c	510	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	C	508	CLA	O2D-CGD-O1D	-4.00	116.01	123.84
23	B	605	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
23	d	402[A]	CLA	C3B-C2B-C1B	-4.00	102.34	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	C3D-C4D-ND	3.99	116.70	110.24
23	c	505	CLA	C3B-C4B-NB	3.99	114.22	110.52
23	a	405[A]	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
23	B	601	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	C	506	CLA	C3D-C2D-C1D	-3.99	100.39	105.83
23	a	408	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
34	c	521	LMG	C3-C4-C5	3.98	117.34	110.24
23	b	610	CLA	C1D-CHD-C4C	-3.98	117.47	126.06
23	B	607	CLA	C3B-C2B-C1B	-3.98	102.36	107.16
23	c	510	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	b	608	CLA	C3B-C4B-NB	3.98	114.20	110.52
23	B	610	CLA	C3C-C4C-NC	3.97	115.03	110.57
33	B	626	LMT	C1'-O5'-C5'	-3.97	105.89	113.69
23	D	403	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	A	405[B]	CLA	CBC-CAC-C3C	-3.97	101.49	112.43
23	c	508	CLA	C3D-C4D-ND	3.97	116.66	110.24
23	a	404[B]	CLA	CAA-C2A-C3A	-3.97	101.92	112.78
23	a	405[B]	CLA	C3D-C4D-ND	3.97	116.65	110.24
23	A	408	CLA	C3B-C4B-NB	3.96	114.19	110.52
23	B	608	CLA	C3B-C4B-NB	3.96	114.19	110.52
23	A	405[B]	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
23	C	505	CLA	C3B-C4B-NB	3.96	114.19	110.52
23	b	616	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
25	y	101	BCR	C15-C14-C13	-3.95	121.67	127.31
23	a	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	606	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	D	403	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	b	615	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	A	406[A]	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
23	A	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	615	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
23	b	614	CLA	C3C-C4C-NC	3.94	114.99	110.57
23	a	408	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	B	602	CLA	C1D-CHD-C4C	-3.94	117.57	126.06
29	d	405[A]	PL9	C42-C43-C44	-3.93	118.19	127.66
23	C	508	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	a	404[B]	CLA	C3B-C4B-NB	3.93	114.16	110.52
23	c	505	CLA	C1-O2A-CGA	3.93	126.76	116.44
26	F	103	SQD	O8-S-C6	3.93	112.00	105.74
23	a	406[B]	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
23	D	402[A]	CLA	C1-C2-C3	-3.93	119.25	126.04
23	b	615	CLA	C3C-C4C-NC	3.93	114.98	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[A]	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	B	604	CLA	CHD-C1D-ND	-3.93	120.84	124.45
23	B	608	CLA	C3D-C4D-ND	3.93	116.59	110.24
26	A	410[B]	SQD	O47-C7-C8	3.93	119.96	111.50
23	a	405[B]	CLA	C1D-CHD-C4C	-3.92	117.59	126.06
23	b	606	CLA	C4-C3-C5	3.92	121.87	115.27
23	C	513	CLA	C3D-C4D-ND	3.92	116.58	110.24
23	b	601	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
23	B	614	CLA	C1-C2-C3	-3.92	119.26	126.04
36	c	518[B]	DGD	O2G-C1B-C2B	3.92	119.94	111.50
26	a	410[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
23	A	404[B]	CLA	C3B-C4B-NB	3.91	114.14	110.52
23	A	405[A]	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
23	a	404[B]	CLA	C3C-C4C-NC	3.91	114.95	110.57
29	A	414[A]	PL9	C7-C3-C4	3.91	120.05	116.88
29	a	413[A]	PL9	C32-C33-C34	-3.89	118.28	127.66
23	B	608	CLA	CAC-C3C-C4C	3.89	129.86	124.81
34	C	520	LMG	O7-C10-C11	3.89	119.88	111.50
23	b	608	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	A	406[B]	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
23	C	502	CLA	C3B-C2B-C1B	-3.88	102.47	107.16
32	A	419[A]	LHG	O8-C23-O10	-3.88	113.79	123.59
36	c	517[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	C	506	CLA	CAC-C3C-C4C	3.88	129.85	124.81
23	A	405[A]	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	b	610	CLA	O2A-CGA-CBA	3.88	124.09	111.91
23	B	614	CLA	C3D-C4D-ND	3.88	116.51	110.24
23	a	405[A]	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
29	a	413[B]	PL9	C32-C33-C34	-3.86	118.36	127.66
23	B	603	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
26	A	412	SQD	O8-S-C6	3.86	111.90	105.74
23	C	509	CLA	C3D-C4D-ND	3.86	116.48	110.24
23	C	511	CLA	C4A-NA-C1A	-3.86	104.97	106.71
23	B	602	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
23	C	512	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
23	B	604	CLA	C3D-C2D-C1D	-3.86	100.57	105.83
23	c	509	CLA	C1-C2-C3	-3.86	119.38	126.04
23	B	610	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	B	615	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	d	402[B]	CLA	C3B-C4B-NB	3.85	114.09	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C3D-C4D-ND	3.85	116.47	110.24
23	C	508	CLA	C1D-CHD-C4C	-3.85	117.76	126.06
23	a	408	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
23	b	612	CLA	CAC-C3C-C4C	3.84	129.80	124.81
23	b	612	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
36	C	517[B]	DGD	O2G-C1B-C2B	3.84	119.78	111.50
29	a	413[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
23	a	405[B]	CLA	C3C-C4C-NC	3.84	114.87	110.57
23	b	616	CLA	O2A-CGA-CBA	3.83	123.94	111.91
23	c	507	CLA	C1-C2-C3	-3.83	119.42	126.04
23	B	613	CLA	C3D-C4D-ND	3.83	116.43	110.24
23	B	615	CLA	C1D-CHD-C4C	-3.82	117.81	126.06
23	b	611	CLA	C1-C2-C3	-3.82	119.43	126.04
23	B	606	CLA	C3D-C4D-ND	3.82	116.42	110.24
23	b	616	CLA	CMB-C2B-C1B	3.82	131.18	125.37
23	B	616	CLA	C3D-C4D-ND	3.82	116.41	110.24
23	C	502	CLA	C3C-C4C-NC	3.82	114.85	110.57
23	c	511	CLA	CMC-C2C-C1C	3.81	130.84	125.04
23	B	603	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
23	B	616	CLA	C3B-C4B-NB	3.81	114.05	110.52
29	A	414[B]	PL9	C7-C3-C2	-3.80	118.30	123.30
23	C	510	CLA	C3B-C4B-NB	3.80	114.04	110.52
23	D	402[B]	CLA	C3B-C4B-NB	3.80	114.04	110.52
23	B	614	CLA	C1D-CHD-C4C	-3.80	117.85	126.06
29	a	413[B]	PL9	C7-C3-C4	3.80	119.97	116.88
23	b	615	CLA	C1C-C2C-C3C	-3.80	102.96	106.96
23	a	405[A]	CLA	CMB-C2B-C1B	3.80	131.16	125.37
32	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	417[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
23	A	404[B]	CLA	C1C-C2C-C3C	-3.80	102.97	106.96
23	b	610	CLA	C4C-C3C-C2C	-3.80	101.36	106.90
23	b	608	CLA	CMC-C2C-C1C	3.79	130.82	125.04
23	c	506	CLA	C3D-C2D-C1D	-3.79	100.66	105.83
29	A	414[B]	PL9	C37-C38-C39	-3.79	118.54	127.66
34	Z	101	LMG	C1-C2-C3	3.79	117.89	110.00
25	C	516	BCR	C7-C8-C9	-3.79	120.51	126.23
23	B	610	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	C	509	CLA	C1-C2-C3	-3.78	119.50	126.04
38	F	102	HEM	CHD-C4C-NC	3.78	128.53	124.44
23	A	408	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
32	L	102[B]	LHG	O7-C7-C8	3.78	119.65	111.50
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C3B-C4B-NB	3.78	114.02	110.52
23	B	612	CLA	C4C-C3C-C2C	-3.78	101.39	106.90
23	A	408	CLA	C1C-C2C-C3C	-3.78	102.99	106.96
38	F	102	HEM	CBD-CAD-C3D	-3.78	102.14	112.63
23	B	615	CLA	CMC-C2C-C1C	3.78	130.79	125.04
23	b	603	CLA	C3B-C4B-NB	3.77	114.02	110.52
25	Y	101	BCR	C15-C14-C13	-3.77	121.92	127.31
25	Y	101	BCR	C16-C17-C18	-3.77	121.93	127.31
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	b	604	CLA	C3B-C4B-NB	3.77	114.01	110.52
23	b	605	CLA	O2D-CGD-O1D	-3.76	116.48	123.84
32	d	412[B]	LHG	O7-C7-C8	3.76	119.61	111.50
23	b	614	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
23	b	616	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
24	a	415[A]	PHO	C4-C3-C5	3.76	121.59	115.27
23	c	513	CLA	C1D-CHD-C4C	-3.76	117.95	126.06
23	C	509	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
23	a	404[B]	CLA	O2D-CGD-CBD	3.76	117.94	111.27
25	t	102	BCR	C11-C10-C9	-3.75	121.95	127.31
23	c	511	CLA	C3D-C4D-ND	3.75	116.31	110.24
23	c	503	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	c	513	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	c	506	CLA	CAC-C3C-C4C	3.75	129.67	124.81
34	B	620	LMG	O8-C28-C29	3.74	123.65	111.91
25	K	102	BCR	C7-C8-C9	-3.74	120.58	126.23
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
23	d	403	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
29	a	413[A]	PL9	C15-C14-C16	3.74	121.56	115.27
23	b	613	CLA	C3B-C4B-NB	3.74	113.98	110.52
23	B	613	CLA	C3B-C4B-NB	3.73	113.98	110.52
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	b	612	CLA	C4-C3-C5	3.73	121.55	115.27
23	B	609	CLA	C3B-C2B-C1B	-3.73	102.66	107.16
23	C	507	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	c	507	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	b	613	CLA	C3D-C4D-ND	3.72	116.26	110.24
26	a	411	SQD	O47-C7-C8	3.72	119.52	111.50
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	B	608	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
23	B	607	CLA	C4-C3-C5	3.72	121.52	115.27
25	H	101	BCR	C16-C17-C18	-3.72	122.01	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[B]	CLA	CAA-C2A-C3A	-3.72	102.60	112.78
32	d	407[B]	LHG	O7-C7-C8	3.71	119.51	111.50
23	B	616	CLA	CHD-C1D-ND	-3.71	121.04	124.45
23	C	507	CLA	C1-C2-C3	-3.71	119.63	126.04
26	A	412	SQD	O47-C7-C8	3.71	119.50	111.50
23	B	606	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
23	b	604	CLA	C3D-C4D-ND	3.70	116.23	110.24
23	C	503	CLA	CMB-C2B-C1B	3.70	131.01	125.37
25	B	618	BCR	C29-C30-C25	3.70	116.18	110.48
23	c	505	CLA	C1C-C2C-C3C	-3.70	103.07	106.96
23	c	506	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
23	b	613	CLA	C1-C2-C3	-3.70	119.65	126.04
36	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	b	608	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	C	514	CLA	C1D-CHD-C4C	-3.69	118.09	126.06
23	b	603	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	c	511	CLA	C1C-C2C-C3C	-3.69	103.08	106.96
23	B	604	CLA	C1C-C2C-C3C	-3.68	103.08	106.96
23	c	506	CLA	CMB-C2B-C1B	3.68	130.98	125.37
26	F	103	SQD	C44-O6-C1	-3.68	106.54	113.74
23	C	508	CLA	C3D-C4D-ND	3.68	116.19	110.24
32	L	102[A]	LHG	O7-C7-C8	3.68	119.43	111.50
23	A	406[A]	CLA	CMB-C2B-C1B	3.68	130.97	125.37
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
23	c	512	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
36	c	517[B]	DGD	O2G-C1B-C2B	3.67	119.40	111.50
23	a	404[A]	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	d	402[B]	CLA	C1-C2-C3	-3.66	119.71	126.04
23	c	509	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
25	a	409	BCR	C38-C26-C25	-3.66	120.42	124.53
23	A	405[B]	CLA	CMC-C2C-C1C	3.66	130.61	125.04
23	C	506	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
29	d	405[B]	PL9	C42-C43-C44	-3.66	118.86	127.66
38	f	101	HEM	C1B-NB-C4B	3.66	108.85	105.07
23	B	607	CLA	CMC-C2C-C1C	3.65	130.60	125.04
23	C	507	CLA	C3B-C4B-NB	3.65	113.90	110.52
23	b	613	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
23	B	605	CLA	C4-C3-C5	3.65	121.41	115.27
23	B	607	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
26	a	410[B]	SQD	C44-O6-C1	-3.64	106.63	113.74
23	b	609	CLA	CBC-CAC-C3C	-3.64	102.39	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402[A]	CLA	C3B-C4B-NB	3.64	113.89	110.52
26	a	410[A]	SQD	O9-S-C6	3.63	111.25	106.94
23	B	605	CLA	CMB-C2B-C1B	3.62	130.89	125.37
23	d	403	CLA	CMB-C2B-C1B	3.62	130.88	125.37
35	b	622	HTG	C1'-S1-C1	3.62	106.86	100.09
23	C	512	CLA	C4-C3-C5	3.62	121.36	115.27
23	b	602	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	B	610	CLA	CAA-C2A-C3A	-3.62	102.88	112.78
23	B	610	CLA	CMB-C2B-C1B	3.62	130.88	125.37
23	C	512	CLA	C1C-C2C-C3C	-3.62	103.16	106.96
23	B	613	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	b	611	CLA	C3B-C4B-NB	3.61	113.87	110.52
23	B	603	CLA	CAA-C2A-C3A	-3.61	102.89	112.78
25	C	515	BCR	C33-C5-C6	-3.61	120.48	124.53
23	B	602	CLA	CMC-C2C-C1C	3.61	130.53	125.04
23	B	615	CLA	O2D-CGD-CBD	3.61	117.68	111.27
29	A	414[B]	PL9	C7-C3-C4	3.60	119.81	116.88
23	A	408	CLA	C1-C2-C3	-3.60	119.81	126.04
40	V	201	HEC	CBD-CAD-C3D	-3.60	102.62	112.63
23	A	408	CLA	O2D-CGD-CBD	3.60	117.67	111.27
23	b	607	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
23	b	606	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	b	604	CLA	CAC-C3C-C4C	3.60	129.48	124.81
23	c	512	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
24	A	417[A]	PHO	C4D-CHA-CBD	3.59	110.14	108.52
23	b	603	CLA	CAA-C2A-C3A	-3.59	102.94	112.78
23	c	510	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	c	502	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	c	508	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
23	B	604	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
23	C	512	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
23	B	608	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	d	402[A]	CLA	C3B-C4B-NB	3.58	113.84	110.52
23	b	614	CLA	C1-C2-C3	-3.58	119.85	126.04
23	c	511	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
25	h	101	BCR	C38-C26-C25	-3.58	120.51	124.53
23	B	604	CLA	C3D-C4D-ND	3.58	116.03	110.24
23	c	507	CLA	C3B-C4B-NB	3.58	113.83	110.52
23	c	510	CLA	CAC-C3C-C4C	3.58	129.45	124.81
24	A	407[B]	PHO	C1A-C2A-C3A	-3.57	99.44	102.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
23	c	511	CLA	C3B-C4B-NB	3.57	113.83	110.52
23	a	406[B]	CLA	CHD-C4C-NC	3.57	129.83	124.20
23	b	612	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	b	611	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	B	614	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	d	402[A]	CLA	C1-C2-C3	-3.56	119.89	126.04
23	B	613	CLA	O2A-CGA-O1A	-3.56	114.62	123.59
23	B	606	CLA	C3B-C2B-C1B	-3.56	102.87	107.16
23	C	508	CLA	CMB-C2B-C1B	3.55	130.78	125.37
23	C	502	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	c	514	CLA	C3B-C4B-NB	3.55	113.81	110.52
23	B	602	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
23	B	611	CLA	CHB-C4A-NA	3.55	129.42	124.51
23	B	605	CLA	CHD-C4C-NC	3.55	129.79	124.20
29	d	405[A]	PL9	C40-C39-C41	3.55	121.23	115.27
23	D	402[B]	CLA	C1-C2-C3	-3.54	119.91	126.04
29	a	413[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
23	b	609	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
25	k	101	BCR	C29-C30-C25	3.54	115.93	110.48
25	T	102	BCR	C11-C10-C9	-3.54	122.26	127.31
23	d	402[B]	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
23	C	503	CLA	C3B-C4B-NB	3.53	113.79	110.52
23	b	615	CLA	CMB-C2B-C1B	3.53	130.75	125.37
26	L	101	SQD	O9-S-C6	3.53	111.14	106.94
23	B	605	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	B	606	CLA	O2D-CGD-O1D	-3.53	116.93	123.84
26	F	103	SQD	C1-C2-C3	-3.53	102.64	110.00
29	d	405[B]	PL9	C7-C8-C9	-3.53	120.92	126.79
23	b	615	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	B	607	CLA	O2A-CGA-O1A	-3.53	114.69	123.59
23	b	611	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	B	608	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	C	513	CLA	C4-C3-C5	3.52	121.19	115.27
23	B	607	CLA	C3B-C4B-NB	3.52	113.78	110.52
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66
23	A	406[B]	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
25	c	515	BCR	C11-C10-C9	-3.51	122.30	127.31
29	A	414[A]	PL9	C15-C14-C16	3.51	121.18	115.27
23	B	610	CLA	CAA-CBA-CGA	-3.51	103.00	113.25
23	A	404[A]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	c	503	CLA	CBC-CAC-C3C	-3.50	102.78	112.43
23	c	509	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
29	D	405[A]	PL9	C53-C6-C1	3.50	122.15	114.99
23	B	609	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
36	C	518[B]	DGD	O2G-C1B-C2B	3.50	119.04	111.50
29	A	414[B]	PL9	C15-C14-C16	3.50	121.15	115.27
23	a	406[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	b	613	CLA	O2D-CGD-CBD	3.49	117.47	111.27
23	b	602	CLA	CAA-C2A-C3A	-3.49	103.23	112.78
23	b	611	CLA	C1D-CHD-C4C	-3.49	118.54	126.06
23	B	603	CLA	C3B-C4B-NB	3.49	113.75	110.52
23	b	612	CLA	CMC-C2C-C1C	3.48	130.34	125.04
29	A	414[B]	PL9	C22-C23-C24	-3.48	119.28	127.66
23	B	604	CLA	C3B-C4B-NB	3.48	113.75	110.52
29	a	413[A]	PL9	C30-C29-C31	3.48	121.13	115.27
23	A	404[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
34	C	521	LMG	C3-C4-C5	3.48	116.45	110.24
23	b	612	CLA	C1D-CHD-C4C	-3.48	118.55	126.06
23	B	605	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
23	b	609	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
38	F	102	HEM	CHD-C1D-ND	3.48	128.20	124.42
23	c	512	CLA	C4-C3-C5	3.48	121.12	115.27
29	D	405[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
23	b	616	CLA	O2A-CGA-O1A	-3.47	114.83	123.59
23	c	514	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	604	CLA	CAC-C3C-C4C	3.47	129.31	124.81
23	a	404[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	C	506	CLA	C4C-C3C-C2C	-3.47	101.84	106.90
25	d	404	BCR	C38-C26-C25	-3.46	120.64	124.53
29	a	413[B]	PL9	C15-C14-C16	3.46	121.10	115.27
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
32	A	419[B]	LHG	O8-C23-O10	-3.46	114.85	123.59
23	d	402[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	c	504	CLA	CMB-C2B-C1B	3.46	130.64	125.37
25	D	404	BCR	C29-C30-C25	3.45	115.80	110.48
29	d	405[B]	PL9	C40-C39-C41	3.45	121.08	115.27
32	b	630[B]	LHG	O7-C7-C8	3.45	118.94	111.50
23	B	614	CLA	C3B-C4B-NB	3.45	113.72	110.52
23	b	602	CLA	C1-C2-C3	-3.45	120.08	126.04
34	c	501	LMG	C7-O1-C1	-3.45	107.00	113.74
23	c	506	CLA	C1C-C2C-C3C	-3.45	103.33	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
35	b	625	HTG	C1-O5-C5	3.45	118.94	112.58
23	c	512	CLA	C3B-C4B-NB	3.45	113.71	110.52
23	C	509	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
25	c	516	BCR	C7-C8-C9	-3.45	121.03	126.23
32	A	419[B]	LHG	O7-C7-C8	3.45	118.93	111.50
23	c	511	CLA	C4-C3-C5	3.44	121.06	115.27
23	b	615	CLA	C3B-C4B-NB	3.44	113.71	110.52
23	c	513	CLA	C4-C3-C5	3.44	121.06	115.27
23	b	610	CLA	CAA-C2A-C3A	-3.44	103.35	112.78
25	c	515	BCR	C15-C14-C13	-3.44	122.40	127.31
23	b	614	CLA	C3B-C4B-NB	3.44	113.70	110.52
23	c	506	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
23	b	610	CLA	CAC-C3C-C4C	3.44	129.27	124.81
23	C	506	CLA	C1-C2-C3	-3.43	120.10	126.04
23	B	602	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	a	406[B]	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	c	505	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
24	a	415[B]	PHO	C4-C3-C5	3.43	121.04	115.27
34	Z	101	LMG	O6-C1-C2	3.43	117.61	110.35
23	b	612	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
23	B	615	CLA	C4-C3-C5	3.43	121.04	115.27
23	C	511	CLA	CHD-C4C-NC	3.43	129.60	124.20
23	b	605	CLA	CHD-C4C-NC	3.42	129.60	124.20
25	T	102	BCR	C15-C16-C17	-3.42	116.46	123.47
23	d	403	CLA	C1D-CHD-C4C	-3.41	118.69	126.06
29	D	405[B]	PL9	C53-C6-C1	3.41	121.97	114.99
23	a	404[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
29	a	413[A]	PL9	C35-C34-C36	3.41	121.01	115.27
32	d	412[B]	LHG	O8-C23-C24	3.41	122.60	111.91
23	b	606	CLA	CHD-C4C-NC	3.41	129.57	124.20
23	C	509	CLA	C4C-C3C-C2C	-3.41	101.93	106.90
23	B	610	CLA	O2A-CGA-O1A	-3.40	115.01	123.59
23	B	614	CLA	O2A-CGA-O1A	-3.39	115.03	123.59
23	B	609	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
25	t	102	BCR	C15-C16-C17	-3.39	116.53	123.47
29	D	405[A]	PL9	C25-C24-C26	3.39	120.97	115.27
23	B	613	CLA	C4A-NA-C1A	-3.39	105.18	106.71
25	D	404	BCR	C28-C27-C26	-3.38	108.03	114.08
23	b	604	CLA	CMC-C2C-C1C	3.38	130.19	125.04
23	b	612	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
38	f	101	HEM	CHA-C4D-ND	3.38	128.54	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	619	BCR	C24-C23-C22	-3.38	121.13	126.23
23	c	509	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	b	604	CLA	CMB-C2B-C1B	3.38	130.51	125.37
23	B	609	CLA	CMC-C2C-C1C	3.37	130.18	125.04
36	c	518[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	c	506	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
23	b	616	CLA	CHD-C4C-NC	3.36	129.50	124.20
23	c	510	CLA	CHC-C1C-C2C	-3.36	117.39	126.73
23	C	512	CLA	C3B-C4B-NB	3.36	113.63	110.52
25	y	101	BCR	C38-C26-C25	-3.36	120.75	124.53
23	B	611	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	C	503	CLA	C1D-CHD-C4C	-3.35	118.82	126.06
35	o	301	HTG	C1'-S1-C1	3.35	106.36	100.09
26	a	410[B]	SQD	C1-C2-C3	-3.35	103.02	110.00
23	C	511	CLA	C4-C3-C5	3.35	120.91	115.27
29	a	413[B]	PL9	C30-C29-C31	3.35	120.91	115.27
23	B	611	CLA	O2D-CGD-O1D	-3.35	117.30	123.84
23	C	507	CLA	CAC-C3C-C4C	3.34	129.15	124.81
23	b	603	CLA	C2A-C1A-CHA	-3.34	118.01	123.86
23	b	616	CLA	C3B-C4B-NB	3.34	113.61	110.52
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
23	b	609	CLA	CAC-C3C-C4C	3.34	129.14	124.81
23	C	510	CLA	C1D-CHD-C4C	-3.34	118.86	126.06
25	d	404	BCR	C10-C11-C12	-3.33	112.81	123.22
23	d	402[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	A	404[B]	CLA	O2A-CGA-CBA	3.33	122.36	111.91
23	C	511	CLA	C3C-C4C-NC	3.33	114.31	110.57
25	C	515	BCR	C15-C14-C13	-3.33	122.56	127.31
23	c	507	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
23	C	507	CLA	O2D-CGD-O1D	-3.33	117.34	123.84
25	k	101	BCR	C7-C8-C9	-3.32	121.21	126.23
23	c	502	CLA	CAC-C3C-C4C	3.32	129.12	124.81
29	a	413[B]	PL9	C27-C28-C29	-3.32	119.66	127.66
23	D	403	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	A	406[A]	CLA	C3B-C4B-NB	3.32	113.59	110.52
23	c	504	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
23	B	613	CLA	O2A-CGA-CBA	3.31	122.31	111.91
23	C	505	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
23	c	510	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
29	a	413[B]	PL9	C7-C3-C2	-3.31	118.95	123.30
23	a	405[B]	CLA	CHD-C4C-NC	3.31	129.42	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	BCR	C15-C14-C13	-3.31	122.59	127.31
23	A	405[B]	CLA	C3C-C4C-NC	3.30	114.28	110.57
23	B	601	CLA	CHD-C4C-NC	3.30	129.41	124.20
34	c	501	LMG	C8-O7-C10	-3.30	109.66	117.79
23	b	608	CLA	C1-C2-C3	-3.30	120.34	126.04
23	C	506	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	b	604	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
23	b	604	CLA	C1D-CHD-C4C	-3.30	118.94	126.06
23	c	507	CLA	CAC-C3C-C4C	3.30	129.09	124.81
32	d	412[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
40	V	201	HEC	CAD-CBD-CGD	-3.30	106.51	113.60
23	a	405[B]	CLA	C3B-C4B-NB	3.30	113.57	110.52
23	A	408	CLA	CAA-C2A-C3A	-3.30	103.75	112.78
23	B	612	CLA	C1D-CHD-C4C	-3.30	118.95	126.06
23	a	408	CLA	C3B-C4B-NB	3.29	113.57	110.52
32	d	407[A]	LHG	O7-C7-C8	3.29	118.59	111.50
33	D	401	LMT	O5B-C5B-C4B	3.29	115.67	109.69
23	b	601	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	D	404	BCR	C16-C17-C18	-3.29	122.62	127.31
23	B	612	CLA	C11-C12-C13	-3.28	105.30	115.92
25	D	404	BCR	C38-C26-C25	-3.28	120.84	124.53
23	C	513	CLA	C1C-C2C-C3C	-3.28	103.50	106.96
23	b	613	CLA	C1D-CHD-C4C	-3.28	118.98	126.06
25	B	617	BCR	C33-C5-C6	-3.28	120.84	124.53
25	b	618	BCR	C15-C14-C13	-3.28	122.63	127.31
23	b	615	CLA	C4-C3-C5	3.28	120.78	115.27
25	c	515	BCR	C16-C17-C18	-3.27	122.64	127.31
23	B	604	CLA	CMB-C2B-C1B	3.27	130.35	125.37
23	C	508	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
23	A	405[B]	CLA	CAA-C2A-C3A	-3.27	103.82	112.78
23	B	610	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	c	508	CLA	C4-C3-C5	3.27	120.77	115.27
23	a	405[B]	CLA	CMB-C2B-C1B	3.27	130.35	125.37
23	B	601	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
23	C	513	CLA	CMC-C2C-C1C	3.27	130.01	125.04
23	c	513	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
23	b	611	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
35	V	202	HTG	C1-O5-C5	3.27	116.62	112.19
34	z	101	LMG	O7-C10-C11	3.26	118.53	111.50
35	b	622	HTG	O2-C2-C1	3.26	116.26	110.27
23	b	613	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	C	510	CLA	CAC-C3C-C4C	3.26	129.04	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414[B]	PL9	C20-C19-C21	3.26	120.75	115.27
23	B	608	CLA	CHC-C1C-C2C	-3.26	117.68	126.73
23	c	508	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
23	c	513	CLA	CMB-C2B-C1B	3.25	130.32	125.37
23	b	602	CLA	CMC-C2C-C1C	3.25	129.99	125.04
23	b	605	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
23	b	607	CLA	CHC-C1C-C2C	-3.25	117.70	126.73
23	a	408	CLA	CAA-C2A-C3A	-3.25	103.88	112.78
23	C	502	CLA	CMC-C2C-C1C	3.25	129.99	125.04
32	d	412[A]	LHG	O7-C7-C8	3.25	118.50	111.50
25	C	515	BCR	C7-C8-C9	-3.25	121.33	126.23
23	A	405[B]	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	b	609	CLA	CMC-C2C-C1C	3.25	129.98	125.04
25	d	404	BCR	C16-C17-C18	-3.25	122.68	127.31
34	c	521	LMG	C9-C8-C7	-3.24	104.11	111.79
23	c	502	CLA	C3B-C4B-NB	3.24	113.52	110.52
29	a	413[B]	PL9	C25-C24-C26	3.24	120.72	115.27
23	b	612	CLA	O2A-CGA-O1A	-3.24	115.42	123.59
23	b	602	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
23	C	506	CLA	CMC-C2C-C1C	3.23	129.96	125.04
33	B	626	LMT	C4B-C3B-C2B	3.23	116.46	110.82
23	c	513	CLA	O2A-CGA-CBA	3.23	122.04	111.91
23	B	611	CLA	C1-C2-C3	-3.23	120.46	126.04
23	A	405[A]	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	C	504	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
32	d	406[B]	LHG	O7-C7-C8	3.22	118.45	111.50
23	C	507	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
24	a	415[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
26	a	411	SQD	O48-C23-C24	3.22	122.01	111.91
23	B	603	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
32	d	412[A]	LHG	O8-C23-C24	3.22	122.00	111.91
23	b	614	CLA	O2A-CGA-O1A	-3.21	115.48	123.59
23	b	607	CLA	C4-C3-C5	3.21	120.68	115.27
23	A	406[B]	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
23	C	509	CLA	CHC-C1C-C2C	-3.21	117.81	126.73
23	a	404[B]	CLA	CHC-C1C-C2C	-3.21	117.82	126.73
23	B	611	CLA	C2A-C1A-CHA	-3.21	118.25	123.86
23	B	603	CLA	CHC-C1C-C2C	-3.21	117.83	126.73
25	T	102	BCR	C12-C13-C14	-3.20	114.02	118.94
29	d	405[B]	PL9	C7-C3-C4	3.20	119.48	116.88
38	F	102	HEM	CHB-C1B-NB	3.20	128.32	124.37
35	o	301	HTG	O5-C1-C2	3.20	114.34	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[B]	CLA	C3B-C4B-NB	3.20	113.48	110.52
25	h	101	BCR	C7-C8-C9	-3.19	121.41	126.23
23	a	404[A]	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
23	B	605	CLA	O2A-CGA-O1A	-3.19	115.53	123.59
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
26	b	620	SQD	O8-S-C6	3.19	110.82	105.74
23	b	601	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	C	505	CLA	C1-O2A-CGA	3.19	124.81	116.44
23	B	608	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	C	512	CLA	CAC-C3C-C4C	3.19	128.94	124.81
29	a	413[A]	PL9	C17-C18-C19	-3.19	119.99	127.66
23	b	601	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
32	D	407[B]	LHG	O7-C7-C8	3.18	118.36	111.50
25	D	404	BCR	C10-C11-C12	-3.18	113.29	123.22
23	A	406[A]	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	b	616	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
29	A	414[A]	PL9	C27-C28-C29	-3.18	120.01	127.66
23	c	512	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	C	511	CLA	CHC-C1C-C2C	-3.17	117.91	126.73
23	B	612	CLA	CAC-C3C-C4C	3.17	128.93	124.81
26	F	103	SQD	O7-S-C6	3.17	110.71	106.94
24	a	407[B]	PHO	CMA-C3A-C4A	-3.17	107.43	114.38
29	a	413[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	D	402[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	C	512	CLA	C1-O2A-CGA	3.17	124.76	116.44
26	b	620	SQD	O7-S-C6	3.17	110.70	106.94
29	D	405[B]	PL9	C17-C18-C19	-3.16	120.04	127.66
23	B	609	CLA	CMB-C2B-C1B	3.16	130.19	125.37
23	A	406[B]	CLA	CAA-C2A-C3A	-3.16	104.11	112.78
38	f	101	HEM	CHD-C1D-ND	3.16	127.85	124.42
23	B	607	CLA	CBC-CAC-C3C	-3.16	103.72	112.43
23	b	613	CLA	O2A-CGA-O1A	-3.16	115.62	123.59
25	a	409	BCR	C40-C30-C25	-3.16	105.18	110.30
23	c	503	CLA	C3B-C4B-NB	3.16	113.44	110.52
23	C	506	CLA	C4-C3-C5	3.16	120.58	115.27
24	A	417[A]	PHO	C4-C3-C5	3.15	120.58	115.27
23	b	603	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	C	514	CLA	C1-C2-C3	-3.15	120.59	126.04
23	a	405[A]	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	A	405[A]	CLA	CMB-C2B-C1B	3.15	130.17	125.37
32	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	O2A-CGA-CBA	3.15	121.79	111.91
32	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
35	b	625	HTG	O5-C5-C4	3.15	115.41	109.69
23	B	614	CLA	O2A-CGA-CBA	3.15	121.78	111.91
23	B	602	CLA	C3B-C4B-NB	3.14	113.43	110.52
38	f	101	HEM	C4D-ND-C1D	3.14	108.32	105.07
23	b	612	CLA	C2A-C1A-CHA	-3.14	118.36	123.86
23	c	505	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
25	c	515	BCR	C37-C22-C21	-3.14	118.52	122.92
23	B	605	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	c	504	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
23	a	408	CLA	C4-C3-C5	3.14	120.55	115.27
26	f	102	SQD	O5-C1-C2	3.14	116.99	110.35
23	B	613	CLA	CMC-C2C-C1C	3.13	129.81	125.04
23	b	616	CLA	CBC-CAC-C3C	-3.13	103.79	112.43
23	b	602	CLA	C4C-C3C-C2C	-3.13	102.33	106.90
23	D	402[B]	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	B	616	CLA	C1-O2A-CGA	3.13	124.66	116.44
34	m	101	LMG	O8-C28-C29	3.13	121.73	111.91
23	a	405[A]	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	a	406[A]	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	B	613	CLA	C4-C3-C5	3.13	120.53	115.27
23	C	513	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	a	406[A]	CLA	C1-C2-C3	-3.13	120.64	126.04
23	c	507	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
23	D	402[B]	CLA	CMC-C2C-C1C	3.13	129.80	125.04
23	d	402[A]	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	C	503	CLA	CHC-C1C-C2C	-3.13	118.05	126.73
24	A	417[B]	PHO	C4D-CHA-CBD	3.12	109.93	108.52
33	b	627	LMT	C3'-C4'-C5'	-3.12	103.77	110.93
23	a	408	CLA	O2A-CGA-CBA	3.12	121.70	111.91
23	A	404[B]	CLA	O2D-CGD-CBD	3.12	116.81	111.27
23	c	505	CLA	CAC-C3C-C4C	3.12	128.86	124.81
32	A	419[B]	LHG	O8-C23-C24	3.12	121.69	111.91
29	D	405[A]	PL9	C51-C49-C50	3.12	121.49	114.60
23	C	503	CLA	CAC-C3C-C4C	3.12	128.85	124.81
23	b	604	CLA	CHC-C1C-C2C	-3.12	118.08	126.73
23	C	505	CLA	C1D-CHD-C4C	-3.11	119.34	126.06
23	B	606	CLA	C3B-C4B-NB	3.11	113.40	110.52
26	f	102	SQD	C4-C3-C2	-3.11	105.39	110.82
23	c	503	CLA	CMC-C2C-C1C	3.11	129.78	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
24	A	417[B]	PHO	C1A-C2A-C3A	-3.11	99.88	102.84
23	B	601	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
36	C	519	DGD	O1G-C1A-C2A	3.11	121.66	111.91
23	B	615	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	b	603	CLA	C4-C3-C5	3.11	120.50	115.27
23	a	404[B]	CLA	O2A-CGA-CBA	3.11	121.66	111.91
29	D	405[A]	PL9	C10-C9-C11	3.11	120.50	115.27
23	D	403	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	C	511	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
23	B	614	CLA	CAC-C3C-C4C	3.10	128.83	124.81
23	C	507	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	b	601	CLA	C4-C3-C5	3.10	120.48	115.27
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
23	c	511	CLA	CAC-C3C-C4C	3.10	128.83	124.81
23	b	607	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
23	C	504	CLA	CHD-C4C-NC	3.09	129.08	124.20
32	b	630[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	C	510	CLA	O2A-CGA-CBA	3.09	121.61	111.91
29	d	405[B]	PL9	C10-C9-C11	3.09	120.47	115.27
25	D	404	BCR	C40-C30-C25	-3.09	105.29	110.30
23	c	507	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	B	613	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	A	408	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	C	503	CLA	O2D-CGD-O1D	-3.09	117.81	123.84
23	B	606	CLA	O2A-CGA-O1A	-3.08	115.81	123.59
23	B	605	CLA	C1-C2-C3	-3.08	120.71	126.04
24	a	415[A]	PHO	CMB-C2B-C3B	3.08	130.44	124.68
29	A	414[B]	PL9	C27-C28-C29	-3.08	120.24	127.66
29	a	413[A]	PL9	C10-C9-C11	3.08	120.45	115.27
23	d	403	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
23	b	614	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
34	C	521	LMG	O8-C28-C29	3.08	121.56	111.91
23	C	503	CLA	C1-C2-C3	-3.08	120.72	126.04
26	A	412	SQD	O48-C23-C24	3.08	121.56	111.91
23	C	510	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
23	c	503	CLA	CMB-C2B-C1B	3.07	130.05	125.37
23	c	510	CLA	C4-C3-C5	3.07	120.44	115.27
23	a	404[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
32	a	419[B]	LHG	O7-C7-C8	3.07	118.12	111.50
23	c	502	CLA	C4C-C3C-C2C	-3.07	102.42	106.90
23	b	615	CLA	C11-C10-C8	-3.07	106.00	115.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	C3B-C4B-NB	3.07	113.36	110.52
23	A	406[B]	CLA	CMB-C2B-C1B	3.06	130.04	125.37
23	d	402[B]	CLA	O2A-CGA-CBA	3.06	121.52	111.91
23	c	514	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
33	B	628	LMT	O1'-C1'-C2'	3.06	113.08	108.30
34	C	520	LMG	O8-C28-C29	3.06	121.51	111.91
23	A	406[B]	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
23	B	609	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	B	603	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	c	509	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
32	A	419[B]	LHG	C5-O7-C7	-3.06	110.27	117.79
23	B	613	CLA	C1D-CHD-C4C	-3.06	119.46	126.06
23	D	403	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
34	Z	101	LMG	C4-C3-C2	3.06	116.16	110.82
23	C	512	CLA	CMC-C2C-C1C	3.06	129.69	125.04
32	D	406[B]	LHG	O7-C7-C8	3.06	118.08	111.50
25	K	102	BCR	C20-C21-C22	-3.05	122.95	127.31
29	d	405[A]	PL9	C10-C9-C11	3.05	120.41	115.27
23	c	503	CLA	CHD-C4C-NC	3.05	129.01	124.20
23	a	404[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	D	402[A]	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	406[A]	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	a	406[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	C	504	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	b	610	CLA	CAA-CBA-CGA	-3.05	104.34	113.25
23	c	511	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	c	509	CLA	C4-C3-C5	3.05	120.40	115.27
23	a	406[B]	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	b	605	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	d	402[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	A	408	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	A	404[B]	CLA	O2A-CGA-O1A	-3.05	115.90	123.59
23	d	402[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	a	404[B]	CLA	CAA-C2A-C1A	-3.04	102.01	111.97
23	B	610	CLA	C3B-C4B-NB	3.04	113.34	110.52
23	D	402[B]	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	c	506	CLA	CMC-C2C-C1C	3.04	129.66	125.04
23	A	404[B]	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	B	614	CLA	C2A-C1A-CHA	-3.04	118.55	123.86
23	C	513	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	B	604	CLA	CMC-C2C-C1C	3.03	129.66	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	L	101	SQD	O48-C23-C24	3.03	121.42	111.91
23	C	502	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	c	513	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	d	402[A]	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	A	406[A]	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
23	c	503	CLA	CHC-C1C-C2C	-3.03	118.33	126.73
23	c	502	CLA	C1-C2-C3	-3.02	120.81	126.04
23	d	402[A]	CLA	C4-C3-C5	3.02	120.36	115.27
40	v	201	HEC	CBD-CAD-C3D	-3.02	104.23	112.63
29	d	405[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
23	b	605	CLA	O2A-CGA-O1A	-3.02	115.97	123.59
23	C	502	CLA	CAC-C3C-C4C	3.02	128.73	124.81
29	A	414[B]	PL9	C17-C18-C19	-3.02	120.39	127.66
23	B	602	CLA	CAC-C3C-C4C	3.02	128.72	124.81
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
23	c	510	CLA	O2A-CGA-CBA	3.01	121.37	111.91
23	c	512	CLA	CMB-C2B-C1B	3.01	129.96	125.37
29	a	413[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
23	b	605	CLA	C2A-C1A-CHA	-3.01	118.59	123.86
29	D	405[B]	PL9	C25-C24-C26	3.01	120.34	115.27
29	d	405[B]	PL9	C37-C38-C39	-3.01	120.41	127.66
23	a	408	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
32	d	406[A]	LHG	O7-C7-C8	3.01	117.99	111.50
23	D	402[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	B	603	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
23	c	510	CLA	O2A-C1-C2	3.01	116.54	108.64
23	b	609	CLA	C3B-C4B-NB	3.01	113.31	110.52
25	b	618	BCR	C37-C22-C21	-3.01	118.71	122.92
23	D	403	CLA	CAA-C2A-C3A	-3.01	104.55	112.78
23	b	614	CLA	CMB-C2B-C1B	3.00	129.94	125.37
33	B	626	LMT	O1'-C1'-C2'	3.00	112.99	108.30
24	a	407[B]	PHO	C1A-C2A-C3A	-3.00	99.98	102.84
23	c	512	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	A	406[B]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	A	405[A]	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	410[A]	SQD	C45-O47-C7	-3.00	110.42	117.79
23	b	608	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	D	402[B]	CLA	O2A-CGA-CBA	2.99	121.31	111.91
23	d	403	CLA	C4-C3-C5	2.99	120.31	115.27
23	A	408	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	A	404[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	b	603	CLA	CAC-C3C-C4C	2.99	128.68	124.81
29	a	413[B]	PL9	C37-C38-C39	-2.98	120.47	127.66
32	D	407[A]	LHG	O8-C23-C24	2.98	121.27	111.91
23	b	608	CLA	CAC-C3C-C4C	2.98	128.68	124.81
23	c	507	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
23	d	402[B]	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
29	a	413[B]	PL9	C22-C23-C24	-2.98	120.49	127.66
23	B	616	CLA	CAC-C3C-C4C	2.98	128.67	124.81
23	B	609	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
32	d	412[B]	LHG	O8-C23-O10	-2.97	116.09	123.59
32	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	b	614	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	b	612	CLA	CHB-C1B-NB	-2.97	121.11	124.26
29	a	413[B]	PL9	C17-C18-C19	-2.97	120.51	127.66
32	D	407[B]	LHG	O8-C23-C24	2.97	121.23	111.91
23	c	502	CLA	C1D-CHD-C4C	-2.97	119.65	126.06
24	A	407[B]	PHO	O1D-CGD-CBD	-2.97	119.79	124.74
23	b	606	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	b	605	CLA	C4-C3-C5	2.97	120.27	115.27
23	B	614	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	A	406[B]	CLA	C3B-C4B-NB	2.97	113.27	110.52
23	b	608	CLA	CBC-CAC-C3C	-2.97	104.25	112.43
23	B	612	CLA	C4A-NA-C1A	-2.97	105.37	106.71
36	h	102	DGD	O2G-C1B-C2B	2.96	117.89	111.50
23	B	602	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	A	405[B]	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
23	b	609	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	c	510	CLA	C1-O2A-CGA	2.96	124.22	116.44
23	b	613	CLA	O2A-CGA-CBA	2.96	121.20	111.91
25	b	619	BCR	C24-C23-C22	-2.96	121.76	126.23
24	A	417[B]	PHO	C4-C3-C5	2.96	120.25	115.27
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	c	502	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
23	B	610	CLA	CHC-C1C-C2C	-2.95	118.52	126.73
23	d	402[B]	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
35	b	622	HTG	O5-C5-C4	2.95	115.06	109.69
23	c	510	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
23	a	405[A]	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
26	A	410[B]	SQD	O48-C23-C24	2.95	121.17	111.91
23	B	604	CLA	C6-C5-C3	-2.95	105.72	113.45
24	a	407[B]	PHO	O1D-CGD-CBD	-2.95	119.83	124.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[B]	CLA	CHC-C1C-C2C	-2.95	118.55	126.73
23	B	601	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
26	L	101	SQD	C1-O5-C5	-2.95	107.91	113.69
29	A	414[B]	PL9	C30-C29-C31	2.95	120.23	115.27
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
23	B	611	CLA	C4A-NA-C1A	-2.94	105.38	106.71
25	B	618	BCR	C7-C8-C9	-2.94	121.79	126.23
23	A	408	CLA	CBC-CAC-C3C	-2.94	104.31	112.43
23	c	511	CLA	CHD-C4C-NC	2.94	128.84	124.20
23	B	605	CLA	CMC-C2C-C1C	2.94	129.52	125.04
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
23	C	510	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
25	C	516	BCR	C33-C5-C6	-2.94	121.23	124.53
32	E	101[B]	LHG	O8-C23-C24	2.94	121.12	111.91
32	a	419[A]	LHG	O7-C7-C8	2.94	117.83	111.50
23	c	506	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
23	C	514	CLA	CBC-CAC-C3C	-2.93	104.34	112.43
23	A	406[A]	CLA	CHD-C4C-NC	2.93	128.83	124.20
29	A	414[A]	PL9	C17-C18-C19	-2.93	120.59	127.66
32	D	406[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
23	B	607	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
23	C	507	CLA	C4-C3-C5	2.93	120.20	115.27
29	d	405[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
24	a	415[B]	PHO	C4A-C3A-C2A	-2.93	100.05	102.84
23	c	512	CLA	O2A-CGA-CBA	2.93	121.10	111.91
23	b	610	CLA	C4-C3-C5	2.93	120.19	115.27
29	d	405[A]	PL9	C27-C28-C29	-2.93	120.61	127.66
23	A	404[A]	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	B	606	CLA	O2A-CGA-CBA	2.93	121.09	111.91
23	D	403	CLA	O2A-CGA-O1A	-2.92	116.21	123.59
23	C	504	CLA	CMB-C2B-C1B	2.92	129.82	125.37
29	a	413[B]	PL9	C35-C34-C36	2.92	120.19	115.27
25	d	404	BCR	C28-C27-C26	-2.92	108.86	114.08
23	b	612	CLA	O2A-CGA-CBA	2.92	121.08	111.91
23	a	405[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	b	613	CLA	CHC-C1C-C2C	-2.92	118.62	126.73
23	A	406[A]	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	C	511	CLA	O2A-CGA-O1A	-2.92	116.22	123.59
23	B	615	CLA	C11-C10-C8	-2.92	106.49	115.92
29	d	405[A]	PL9	C53-C6-C1	2.92	120.95	114.99
23	c	509	CLA	CMB-C2B-C1B	2.92	129.81	125.37
29	a	413[A]	PL9	C22-C23-C24	-2.92	120.64	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[B]	CLA	C4-C3-C5	2.91	120.17	115.27
23	b	608	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
23	b	606	CLA	C3B-C4B-NB	2.91	113.22	110.52
23	D	402[B]	CLA	C1D-CHD-C4C	-2.91	119.78	126.06
23	b	611	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91
25	B	617	BCR	C7-C8-C9	-2.91	121.84	126.23
32	D	407[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
23	C	514	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
23	c	512	CLA	CMC-C2C-C1C	2.91	129.47	125.04
25	b	619	BCR	C38-C26-C25	-2.91	121.26	124.53
23	B	607	CLA	CMB-C2B-C1B	2.91	129.80	125.37
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
23	C	511	CLA	O2A-CGA-CBA	2.91	121.03	111.91
23	A	408	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
23	a	404[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	a	406[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	b	602	CLA	CMA-C3A-C4A	-2.90	103.97	111.77
23	c	513	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	C	510	CLA	O2A-CGA-O1A	-2.90	116.27	123.59
23	C	504	CLA	O2A-CGA-O1A	-2.90	116.28	123.59
23	a	405[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
25	a	409	BCR	C24-C23-C22	-2.90	121.86	126.23
23	C	506	CLA	C3B-C4B-NB	2.90	113.20	110.52
29	a	413[B]	PL9	C42-C43-C44	-2.90	120.69	127.66
23	a	406[A]	CLA	CMB-C2B-C1B	2.89	129.78	125.37
23	B	608	CLA	C1-C2-C3	-2.89	121.04	126.04
26	b	620	SQD	C3-C4-C5	2.89	115.40	110.24
23	b	615	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	B	616	CLA	C1C-C2C-C3C	-2.89	103.92	106.96
38	F	102	HEM	CBA-CAA-C2A	-2.89	104.59	112.63
25	K	102	BCR	C24-C23-C22	-2.89	121.87	126.23
23	b	603	CLA	O2A-CGA-CBA	2.89	120.97	111.91
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	C	502	CLA	C1-O2A-CGA	2.89	124.02	116.44
23	C	510	CLA	CMC-C2C-C1C	2.89	129.43	125.04
24	a	415[B]	PHO	CMB-C2B-C3B	2.89	130.08	124.68
23	C	506	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
25	D	404	BCR	C37-C22-C23	2.88	122.62	118.08
23	C	510	CLA	CHB-C1B-NB	-2.88	121.20	124.26
29	a	413[B]	PL9	C53-C6-C1	2.88	120.89	114.99
23	b	614	CLA	CHB-C1B-NB	-2.88	121.20	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	D	402[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	B	606	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	b	607	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
33	A	420	LMT	O5B-C5B-C4B	2.88	114.92	109.69
25	k	101	BCR	C24-C23-C22	-2.88	121.89	126.23
23	c	513	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	b	606	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	a	407[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
26	a	410[B]	SQD	O9-S-C6	2.87	110.35	106.94
23	D	402[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	C	513	CLA	CMB-C2B-C1B	2.87	129.74	125.37
23	a	406[B]	CLA	CAA-C2A-C3A	-2.87	104.92	112.78
29	D	405[B]	PL9	C51-C49-C50	2.87	120.94	114.60
23	B	607	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
29	A	414[B]	PL9	C10-C9-C11	2.87	120.09	115.27
23	b	610	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	C	503	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
23	b	601	CLA	CHD-C4C-NC	2.86	128.72	124.20
29	a	413[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
23	B	607	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
23	B	605	CLA	C2A-C1A-CHA	-2.86	118.85	123.86
23	C	505	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
23	c	508	CLA	CHD-C4C-NC	2.86	128.71	124.20
40	v	201	HEC	CHA-C4D-ND	2.86	127.53	124.42
40	V	201	HEC	CBC-CAC-C3C	2.86	120.31	112.43
23	A	404[B]	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
25	y	101	BCR	C24-C23-C22	-2.86	121.92	126.23
26	a	410[B]	SQD	O8-S-C6	2.86	110.29	105.74
23	B	604	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
34	D	411	LMG	O8-C28-O10	-2.85	116.39	123.59
23	d	403	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	A	404[B]	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
23	C	513	CLA	CBC-CAC-C3C	-2.85	104.57	112.43
24	a	407[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	c	505	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
23	b	603	CLA	CMA-C3A-C2A	-2.85	102.33	113.83
32	b	630[A]	LHG	O8-C23-C24	2.85	120.84	111.91
25	c	515	BCR	C36-C18-C17	-2.85	118.93	122.92
23	a	408	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	c	508	CLA	CAC-C3C-C4C	2.85	128.50	124.81
23	d	403	CLA	CHD-C4C-NC	2.85	128.69	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	CMC-C2C-C1C	2.85	129.37	125.04
23	B	612	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
23	b	616	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
24	A	407[B]	PHO	CMB-C2B-C3B	2.85	130.00	124.68
23	b	603	CLA	CHC-C1C-C2C	-2.84	118.84	126.73
24	a	407[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
23	b	610	CLA	O2A-CGA-O1A	-2.84	116.42	123.59
23	D	403	CLA	C3B-C4B-NB	2.84	113.15	110.52
23	c	504	CLA	CHD-C4C-NC	2.84	128.68	124.20
25	K	102	BCR	C38-C26-C25	-2.84	121.34	124.53
23	b	610	CLA	CMC-C2C-C1C	2.84	129.36	125.04
25	c	516	BCR	C11-C10-C9	-2.84	123.26	127.31
23	D	402[B]	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	B	609	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
23	C	506	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
23	B	610	CLA	CHD-C4C-NC	2.83	128.67	124.20
23	b	614	CLA	CHD-C4C-NC	2.83	128.67	124.20
23	D	403	CLA	O2A-CGA-CBA	2.83	120.79	111.91
23	C	504	CLA	C1-C2-C3	-2.83	121.15	126.04
23	b	608	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
25	D	404	BCR	C3-C4-C5	-2.83	109.03	114.08
23	D	402[B]	CLA	C4-C3-C5	2.82	120.02	115.27
23	a	405[B]	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
23	C	502	CLA	C3B-C4B-NB	2.82	113.13	110.52
23	b	602	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
23	b	605	CLA	CMB-C2B-C1B	2.82	129.66	125.37
38	f	101	HEM	CHB-C1B-NB	2.82	127.85	124.37
23	D	403	CLA	C4-C3-C5	2.82	120.01	115.27
23	b	602	CLA	CHD-C4C-NC	2.82	128.64	124.20
23	c	513	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	b	611	CLA	CHD-C4C-NC	2.82	128.64	124.20
36	c	517[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	B	606	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	B	613	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	a	406[B]	CLA	C1-C2-C3	-2.81	121.18	126.04
23	B	606	CLA	CMC-C2C-C1C	2.81	129.32	125.04
34	z	101	LMG	O8-C28-C29	2.81	120.72	111.91
23	c	514	CLA	O2A-CGA-CBA	2.80	120.71	111.91
23	c	514	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	B	604	CLA	C6-C7-C8	-2.80	106.86	115.92
34	c	520	LMG	O8-C28-C29	2.80	120.70	111.91
34	c	520	LMG	O1-C7-C8	-2.80	104.14	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
25	d	404	BCR	C21-C20-C19	-2.80	114.48	123.22
23	b	609	CLA	CHD-C4C-NC	2.80	128.61	124.20
23	c	510	CLA	CHB-C1B-NB	-2.80	121.30	124.26
23	d	402[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.73
36	C	517[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
25	c	516	BCR	C32-C1-C6	-2.79	105.77	110.30
23	C	504	CLA	C4-C3-C5	2.79	119.96	115.27
36	c	519	DGD	O3G-C3G-C2G	-2.79	104.17	110.90
35	B	623	HTG	C1'-S1-C1	2.79	105.31	100.09
23	A	406[A]	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
32	D	407[A]	LHG	O7-C7-C8	2.79	117.50	111.50
23	C	510	CLA	C4-C3-C5	2.78	119.95	115.27
23	a	406[B]	CLA	CMB-C2B-C1B	2.78	129.61	125.37
26	a	410[A]	SQD	O47-C7-O49	-2.78	116.98	123.70
34	D	411	LMG	O7-C10-C11	2.78	117.50	111.50
25	t	102	BCR	C35-C13-C12	2.78	122.46	118.08
23	c	506	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
24	A	417[B]	PHO	O2D-CGD-O1D	-2.78	118.41	123.84
23	b	609	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
23	B	612	CLA	C2A-C1A-CHA	-2.78	119.00	123.86
23	c	514	CLA	CHD-C4C-NC	2.77	128.57	124.20
26	b	620	SQD	O9-S-C6	2.77	110.23	106.94
29	a	413[B]	PL9	C10-C9-C11	2.77	119.93	115.27
25	t	102	BCR	C28-C27-C26	-2.77	109.13	114.08
23	B	610	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
26	L	101	SQD	C4-C3-C2	2.77	115.66	110.82
23	b	601	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
23	c	503	CLA	O2A-CGA-CBA	2.77	120.59	111.91
33	B	626	LMT	C2'-C3'-C4'	2.77	116.00	109.68
35	b	622	HTG	O2-C2-C3	-2.76	103.96	110.35
23	B	616	CLA	CHD-C4C-NC	2.76	128.56	124.20
23	A	405[B]	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
23	c	514	CLA	CMC-C2C-C1C	2.76	129.25	125.04
32	b	630[B]	LHG	O8-C23-C24	2.76	120.58	111.91
29	a	413[A]	PL9	C53-C6-C1	2.76	120.64	114.99
24	a	407[B]	PHO	O2A-CGA-CBA	2.76	120.57	111.91
29	D	405[B]	PL9	C27-C28-C29	-2.76	121.02	127.66
23	D	402[B]	CLA	CHC-C1C-C2C	-2.76	119.08	126.73
23	b	604	CLA	C4C-C3C-C2C	-2.76	102.88	106.90
23	C	514	CLA	C2A-C1A-CHA	-2.75	119.05	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[B]	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	C	502	CLA	CBC-CAC-C3C	-2.75	104.85	112.43
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
23	a	408	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	B	616	CLA	O2A-CGA-CBA	2.75	120.53	111.91
23	b	613	CLA	CMA-C3A-C4A	-2.75	104.39	111.77
23	d	402[B]	CLA	C2A-C1A-CHA	-2.75	119.06	123.86
24	A	417[B]	PHO	CED-O2D-CGD	2.75	122.15	115.94
23	C	514	CLA	CMB-C2B-C1B	2.75	129.55	125.37
23	A	406[B]	CLA	CHD-C4C-NC	2.75	128.53	124.20
32	D	406[B]	LHG	O8-C23-O10	-2.74	116.67	123.59
23	B	611	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
23	B	608	CLA	CMA-C3A-C4A	-2.74	104.40	111.77
23	c	509	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
29	A	414[B]	PL9	C53-C6-C1	2.74	120.59	114.99
25	k	101	BCR	C11-C10-C9	-2.74	123.40	127.31
23	c	508	CLA	O2A-CGA-CBA	2.74	120.50	111.91
23	B	602	CLA	CHD-C4C-NC	2.74	128.52	124.20
24	A	407[B]	PHO	CBC-CAC-C3C	-2.74	108.87	112.88
23	D	402[B]	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
33	M	101	LMT	C3'-C4'-C5'	-2.74	104.65	110.93
29	A	414[A]	PL9	C10-C9-C8	-2.74	116.66	123.68
36	H	102	DGD	O1G-C1A-C2A	2.73	120.49	111.91
23	a	405[B]	CLA	O2A-CGA-O1A	-2.73	116.69	123.59
23	A	404[A]	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	B	601	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	C	509	CLA	CAC-C3C-C4C	2.73	128.35	124.81
23	C	505	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	C	514	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	D	405[B]	PL9	C10-C9-C11	2.73	119.86	115.27
23	C	507	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
36	C	517[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
23	c	514	CLA	C2A-C1A-CHA	-2.73	119.09	123.86
25	y	101	BCR	C11-C10-C9	-2.73	123.42	127.31
23	b	610	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
32	d	407[A]	LHG	O8-C23-C24	2.73	120.46	111.91
23	B	601	CLA	CMB-C2B-C1B	2.72	129.52	125.37
32	D	407[B]	LHG	O8-C23-O10	-2.72	116.72	123.59
23	c	509	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
25	A	409	BCR	C16-C17-C18	-2.72	123.42	127.31
23	D	403	CLA	CHC-C1C-C2C	-2.72	119.17	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMB-C2B-C1B	2.72	129.52	125.37
23	B	614	CLA	CHC-C1C-C2C	-2.72	119.17	126.73
23	a	405[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
26	a	410[B]	SQD	C45-O47-C7	-2.72	111.09	117.79
23	b	609	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
29	D	405[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	402[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	b	615	CLA	CHD-C4C-NC	2.72	128.49	124.20
25	T	102	BCR	C21-C20-C19	-2.72	114.73	123.22
26	f	102	SQD	O8-S-C6	2.72	110.07	105.74
23	A	406[B]	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
25	k	101	BCR	C20-C21-C22	-2.72	123.43	127.31
32	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
26	A	412	SQD	C4-C3-C2	-2.72	106.08	110.82
25	h	101	BCR	C24-C23-C22	-2.72	122.13	126.23
23	b	606	CLA	CHC-C1C-C2C	-2.72	119.19	126.73
25	c	515	BCR	C36-C18-C19	2.71	122.35	118.08
29	d	405[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
23	A	404[B]	CLA	C1-C2-C3	-2.71	121.35	126.04
23	a	406[B]	CLA	C4-C3-C5	2.71	119.83	115.27
23	C	502	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
23	B	602	CLA	C11-C12-C13	-2.71	107.16	115.92
25	H	101	BCR	C24-C23-C22	-2.71	122.14	126.23
23	a	406[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	b	612	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
24	a	407[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	D	402[B]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	c	504	CLA	CMC-C2C-C1C	2.71	129.16	125.04
38	F	102	HEM	CHA-C4D-ND	2.71	127.71	124.37
23	A	406[A]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	c	514	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
23	A	404[A]	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
34	m	101	LMG	C8-O7-C10	-2.70	111.14	117.79
32	d	406[B]	LHG	O8-C23-O10	-2.70	116.77	123.59
23	C	505	CLA	CMB-C2B-C1B	2.70	129.48	125.37
23	b	609	CLA	CMB-C2B-C1B	2.70	129.48	125.37
36	h	102	DGD	O1G-C1A-C2A	2.70	120.39	111.91
23	c	506	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	C	512	CLA	CHC-C1C-C2C	-2.70	119.23	126.73
23	A	406[B]	CLA	O2A-CGA-CBA	2.70	120.38	111.91
34	c	521	LMG	O8-C28-C29	2.70	120.38	111.91
23	b	616	CLA	CHC-C1C-C2C	-2.70	119.23	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
23	B	601	CLA	C1-O2A-CGA	2.70	123.52	116.44
36	C	518[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	D	402[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	d	403	CLA	C3B-C4B-NB	2.70	113.02	110.52
27	b	628	GOL	C3-C2-C1	-2.70	101.22	111.70
23	a	404[B]	CLA	C4-C3-C5	2.70	119.81	115.27
23	B	613	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	C	514	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
36	c	519	DGD	O1G-C1A-C2A	2.69	120.36	111.91
23	c	510	CLA	CMB-C2B-C1B	2.69	129.47	125.37
26	a	411	SQD	O7-S-C6	2.69	110.14	106.94
23	B	608	CLA	C11-C12-C13	-2.69	107.23	115.92
23	b	602	CLA	CMB-C2B-C1B	2.69	129.46	125.37
23	B	603	CLA	O2A-CGA-CBA	2.69	120.34	111.91
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
25	h	101	BCR	C16-C17-C18	-2.69	123.48	127.31
23	D	403	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
25	T	102	BCR	C3-C4-C5	-2.68	109.28	114.08
25	t	102	BCR	C36-C18-C19	2.68	122.31	118.08
36	h	102	DGD	O1G-C1A-O1A	-2.68	116.82	123.59
23	B	612	CLA	C3B-C4B-NB	2.68	113.00	110.52
35	b	622	HTG	O5-C1-C2	2.68	113.69	110.31
33	a	416	LMT	C3'-C4'-C5'	-2.68	104.78	110.93
36	h	102	DGD	O3G-C1D-C2D	2.68	112.49	108.30
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
34	C	501	LMG	C6-C5-C4	2.68	119.28	113.00
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
25	T	102	BCR	C35-C13-C12	2.68	122.30	118.08
23	a	405[B]	CLA	O2A-CGA-CBA	2.68	120.32	111.91
23	a	404[B]	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
23	B	609	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	C	508	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	b	605	CLA	C3B-C4B-NB	2.68	113.00	110.52
26	f	102	SQD	O5-C5-C4	2.68	114.56	109.69
23	a	406[A]	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
23	C	503	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
32	a	419[A]	LHG	O8-C23-C24	2.68	120.30	111.91
24	a	415[A]	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
36	c	517[A]	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	405[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
24	a	415[B]	PHO	O2D-CGD-O1D	-2.67	118.61	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
23	b	607	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
23	B	606	CLA	CBC-CAC-C3C	-2.67	105.06	112.43
25	Y	101	BCR	C15-C16-C17	-2.67	118.00	123.47
23	C	502	CLA	CMB-C2B-C1B	2.67	129.44	125.37
23	A	408	CLA	O2A-CGA-CBA	2.67	120.29	111.91
23	a	404[B]	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
23	b	614	CLA	O2A-CGA-CBA	2.67	120.28	111.91
29	a	413[B]	PL9	C20-C19-C21	2.67	119.76	115.27
23	C	510	CLA	C16-C15-C13	-2.67	107.30	115.92
25	c	515	BCR	C28-C27-C26	-2.67	109.32	114.08
23	c	506	CLA	C3B-C4B-NB	2.67	112.99	110.52
23	B	601	CLA	O2A-CGA-CBA	2.67	120.27	111.91
23	a	404[B]	CLA	C1-C2-C3	-2.66	121.44	126.04
25	Y	101	BCR	C10-C11-C12	-2.66	114.91	123.22
23	a	405[B]	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
23	a	406[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	B	601	CLA	C3B-C4B-NB	2.66	112.98	110.52
23	C	502	CLA	C4C-C3C-C2C	-2.66	103.03	106.90
23	C	511	CLA	CMC-C2C-C1C	2.65	129.08	125.04
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59
23	b	613	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	a	404[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	A	404[B]	CLA	CMA-C3A-C2A	-2.65	103.13	113.83
23	b	611	CLA	C2A-C1A-CHA	-2.65	119.22	123.86
25	C	515	BCR	C16-C17-C18	-2.65	123.53	127.31
23	B	608	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	c	511	CLA	CHC-C1C-C2C	-2.65	119.37	126.73
25	H	101	BCR	C7-C8-C9	-2.65	122.23	126.23
29	D	405[B]	PL9	C20-C19-C21	2.65	119.73	115.27
23	C	505	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
29	D	405[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	B	610	CLA	CMC-C2C-C1C	2.65	129.07	125.04
38	F	102	HEM	O2A-CGA-CBA	2.64	122.53	114.03
24	A	417[B]	PHO	CMB-C2B-C3B	2.64	129.62	124.68
26	a	411	SQD	C3-C4-C5	2.64	114.95	110.24
25	b	617	BCR	C29-C30-C25	2.64	114.55	110.48
23	c	512	CLA	CHC-C1C-C2C	-2.64	119.39	126.73
23	B	615	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
26	F	103	SQD	O5-C1-O6	2.64	116.22	109.97
23	b	613	CLA	CED-O2D-CGD	2.64	121.91	115.94
23	a	408	CLA	O2A-CGA-O1A	-2.64	116.94	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	d	403	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
23	b	606	CLA	CMB-C2B-C1B	2.64	129.38	125.37
23	D	402[B]	CLA	O2A-CGA-O1A	-2.63	116.94	123.59
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
23	C	512	CLA	CHD-C4C-NC	2.63	128.35	124.20
36	c	519	DGD	O2G-C1B-C2B	2.63	117.18	111.50
24	A	417[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
23	B	609	CLA	O2A-CGA-CBA	2.63	120.17	111.91
23	B	608	CLA	C11-C10-C8	-2.63	107.42	115.92
25	b	619	BCR	C11-C10-C9	-2.63	123.56	127.31
23	A	404[B]	CLA	CHD-C4C-NC	2.63	128.35	124.20
23	B	606	CLA	CHD-C4C-NC	2.63	128.35	124.20
35	b	625	HTG	C1'-S1-C1	2.63	105.01	100.09
23	B	609	CLA	CAC-C3C-C4C	2.63	128.22	124.81
25	a	409	BCR	C7-C8-C9	-2.63	122.27	126.23
23	c	508	CLA	C3B-C4B-NB	2.63	112.95	110.52
23	B	616	CLA	CHC-C1C-C2C	-2.62	119.44	126.73
23	C	505	CLA	CHB-C1B-NB	-2.62	121.48	124.26
23	c	508	CLA	O1D-CGD-CBD	-2.62	119.12	124.48
29	a	413[B]	PL9	C40-C39-C41	2.62	119.68	115.27
32	a	419[B]	LHG	O8-C23-C24	2.62	120.13	111.91
23	a	406[B]	CLA	C3B-C4B-NB	2.62	112.94	110.52
23	d	402[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
34	D	411	LMG	O8-C28-C29	2.62	120.13	111.91
29	D	405[B]	PL9	C42-C41-C39	-2.62	104.37	112.98
29	A	414[B]	PL9	C40-C39-C41	2.62	119.67	115.27
23	b	609	CLA	C16-C15-C13	-2.62	107.46	115.92
32	d	406[B]	LHG	O8-C23-C24	2.62	120.12	111.91
23	C	507	CLA	CMB-C2B-C1B	2.62	129.35	125.37
25	c	515	BCR	C20-C21-C22	-2.61	123.58	127.31
26	f	102	SQD	O48-C23-C24	2.61	120.11	111.91
29	D	405[B]	PL9	C37-C38-C39	-2.61	121.37	127.66
23	C	511	CLA	CAC-C3C-C4C	2.61	128.20	124.81
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
23	C	508	CLA	C4-C3-C5	2.61	119.66	115.27
29	d	405[B]	PL9	C36-C37-C38	-2.61	103.30	111.88
23	a	408	CLA	CMB-C2B-C1B	2.61	129.34	125.37
33	b	621	LMT	C1'-O5'-C5'	-2.61	108.57	113.69
23	c	508	CLA	C4C-C3C-C2C	-2.61	103.09	106.90
32	D	406[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	b	614	CLA	CBC-CAC-C3C	-2.61	105.24	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.50
23	B	615	CLA	C6-C7-C8	-2.61	107.50	115.92
23	B	606	CLA	CMB-C2B-C1B	2.61	129.34	125.37
24	A	407[B]	PHO	CMA-C3A-C4A	-2.61	108.67	114.38
23	c	505	CLA	CMB-C2B-C1B	2.61	129.34	125.37
23	B	609	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
23	c	505	CLA	CHB-C1B-NB	-2.60	121.50	124.26
25	B	619	BCR	C21-C20-C19	-2.60	115.10	123.22
23	C	505	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
23	c	509	CLA	O2A-CGA-CBA	2.60	120.07	111.91
32	L	102[A]	LHG	O8-C23-C24	2.60	120.06	111.91
23	b	605	CLA	C1-C2-C3	-2.60	121.55	126.04
25	H	101	BCR	C16-C15-C14	-2.60	118.16	123.47
25	B	618	BCR	C37-C22-C21	-2.60	119.29	122.92
23	C	514	CLA	O2A-CGA-CBA	2.60	120.05	111.91
23	d	402[B]	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
23	c	504	CLA	C4-C3-C5	2.59	119.64	115.27
23	a	406[B]	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
23	a	405[A]	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	A	405[A]	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	c	507	CLA	CHD-C4C-NC	2.59	128.29	124.20
23	B	607	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
23	c	504	CLA	C3B-C4B-NB	2.59	112.92	110.52
23	b	609	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
32	D	406[B]	LHG	O8-C23-C24	2.59	120.03	111.91
23	C	504	CLA	CMC-C2C-C1C	2.59	128.98	125.04
23	b	610	CLA	CMB-C2B-C1B	2.59	129.31	125.37
23	a	404[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
25	B	618	BCR	C2-C1-C6	2.59	114.46	110.48
23	b	602	CLA	C11-C12-C13	-2.59	107.56	115.92
23	B	614	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
23	a	404[B]	CLA	CMA-C3A-C4A	-2.58	104.83	111.77
23	B	611	CLA	CMB-C2B-C3B	2.58	132.84	126.59
38	f	101	HEM	CBD-CAD-C3D	-2.58	105.45	112.63
23	b	601	CLA	C1-O2A-CGA	2.58	123.22	116.44
29	d	405[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
23	b	610	CLA	CHD-C4C-NC	2.58	128.27	124.20
23	a	406[B]	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
25	T	102	BCR	C15-C14-C13	2.58	130.99	127.31
23	C	504	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
25	Y	101	BCR	C34-C9-C8	2.58	122.14	118.08
23	B	604	CLA	O2A-CGA-O1A	-2.58	117.09	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	CHC-C1C-C2C	-2.58	119.58	126.73
23	b	602	CLA	CHB-C1B-C2B	-2.57	119.97	127.24
23	b	606	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
25	B	618	BCR	C37-C22-C23	2.57	122.13	118.08
25	d	404	BCR	C39-C30-C25	-2.57	106.13	110.30
25	h	101	BCR	C36-C18-C17	-2.57	119.32	122.92
23	B	603	CLA	C4-C3-C5	2.57	119.60	115.27
23	B	603	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	C	507	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
23	d	403	CLA	CBC-CAC-C3C	-2.57	105.34	112.43
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	A	404[B]	CLA	CAA-C2A-C1A	-2.57	103.56	111.97
23	B	612	CLA	CMC-C2C-C1C	2.57	128.95	125.04
23	C	504	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
23	C	502	CLA	C4-C3-C5	2.56	119.58	115.27
33	T	101	LMT	C3'-C4'-C5'	-2.56	105.05	110.93
23	D	402[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	D	402[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	C	508	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
23	B	608	CLA	CMA-C3A-C2A	-2.56	103.50	113.83
23	b	615	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
36	c	517[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
34	c	501	LMG	O6-C5-C4	2.56	114.34	109.69
25	B	618	BCR	C38-C26-C25	-2.56	121.66	124.53
23	C	514	CLA	CHD-C4C-NC	2.56	128.23	124.20
23	A	408	CLA	C4-C3-C5	2.56	119.57	115.27
23	c	509	CLA	CHD-C4C-NC	2.56	128.23	124.20
26	F	103	SQD	O48-C23-C24	2.56	119.93	111.91
29	D	405[B]	PL9	C7-C8-C9	-2.56	122.54	126.79
23	B	604	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	t	102	BCR	C37-C22-C23	2.56	122.10	118.08
23	c	507	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
23	b	614	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	B	607	CLA	CED-O2D-CGD	2.55	121.71	115.94
35	c	522	HTG	O5-C1-C2	2.55	113.52	110.31
25	T	102	BCR	C2-C1-C6	2.55	114.41	110.48
23	b	603	CLA	CHD-C4C-NC	2.55	128.22	124.20
25	y	101	BCR	C10-C11-C12	-2.55	115.26	123.22
23	b	616	CLA	CAC-C3C-C4C	2.55	128.12	124.81
25	A	409	BCR	C38-C26-C25	-2.55	121.67	124.53
23	c	514	CLA	CHC-C1C-C2C	-2.55	119.66	126.73
26	F	103	SQD	O47-C7-O49	-2.54	117.56	123.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	b	610	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
23	C	505	CLA	C4-C3-C5	2.54	119.54	115.27
24	a	415[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	B	601	CLA	CMC-C2C-C1C	2.54	128.90	125.04
23	B	609	CLA	C1-C2-C3	-2.54	121.66	126.04
23	C	507	CLA	O2A-CGA-CBA	2.54	119.86	111.91
23	b	601	CLA	C3B-C4B-NB	2.54	112.87	110.52
23	b	607	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
23	b	607	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
25	y	101	BCR	C21-C20-C19	-2.53	115.31	123.22
23	B	612	CLA	C1-C2-C3	-2.53	121.66	126.04
36	H	102	DGD	O1G-C1A-O1A	-2.53	117.20	123.59
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
23	b	604	CLA	O2A-CGA-CBA	2.53	119.85	111.91
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	609	CLA	CMA-C3A-C4A	-2.53	104.97	111.77
23	b	611	CLA	CMB-C2B-C1B	2.53	129.22	125.37
23	C	512	CLA	C1-C2-C3	-2.53	121.67	126.04
34	B	620	LMG	O8-C28-O10	-2.53	117.22	123.59
23	B	610	CLA	O1D-CGD-CBD	-2.53	119.32	124.48
36	C	519	DGD	O3G-C3G-C2G	-2.52	104.81	110.90
23	B	609	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
33	e	101	LMT	O1'-C1'-C2'	2.52	112.24	108.30
23	a	406[A]	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	A	406[A]	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
24	A	417[B]	PHO	C4A-C3A-C2A	-2.52	100.44	102.84
23	b	611	CLA	O2A-CGA-O1A	-2.52	117.23	123.59
23	C	508	CLA	C1-C2-C3	-2.52	121.69	126.04
26	a	411	SQD	O8-S-C6	2.52	109.75	105.74
25	b	618	BCR	C29-C30-C25	2.52	114.36	110.48
26	a	410[B]	SQD	O48-C23-C24	2.52	119.81	111.91
32	d	407[B]	LHG	O8-C23-C24	2.52	119.81	111.91
23	D	403	CLA	CMA-C3A-C2A	-2.52	103.68	113.83
23	A	405[B]	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	B	608	CLA	O2A-CGA-O1A	-2.52	117.24	123.59
23	c	512	CLA	CBC-CAC-C3C	-2.52	105.50	112.43
23	b	616	CLA	CMC-C2C-C1C	2.51	128.87	125.04
23	B	609	CLA	C16-C15-C13	-2.51	107.79	115.92
24	A	407[B]	PHO	C1-C2-C3	-2.51	121.69	126.04
23	A	405[B]	CLA	C2A-C1A-CHA	-2.51	119.46	123.86
34	C	501	LMG	C8-O7-C10	-2.51	111.60	117.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	413[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	c	511	CLA	O2A-CGA-CBA	2.51	119.79	111.91
23	B	609	CLA	C3B-C4B-NB	2.51	112.85	110.52
29	A	414[B]	PL9	C35-C34-C36	2.51	119.50	115.27
23	a	405[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	A	407[A]	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407[A]	PHO	CMB-C2B-C3B	2.51	129.37	124.68
23	A	405[B]	CLA	C4-C3-C5	2.51	119.49	115.27
23	b	602	CLA	C4-C3-C5	2.51	119.49	115.27
23	C	511	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	a	406[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	b	614	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
25	Y	101	BCR	C36-C18-C17	-2.51	119.41	122.92
26	f	102	SQD	O47-C7-O49	-2.50	117.65	123.70
33	A	420	LMT	O5'-C5'-C6'	2.50	112.66	106.44
25	c	516	BCR	C33-C5-C6	-2.50	121.72	124.53
26	a	411	SQD	C1-O5-C5	2.50	118.60	113.69
33	B	629	LMT	C3'-C4'-C5'	-2.50	105.19	110.93
24	A	417[B]	PHO	OBD-CAD-C3D	-2.50	123.83	127.98
23	c	507	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
25	Y	101	BCR	C37-C22-C23	2.50	122.02	118.08
23	d	402[B]	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
23	B	611	CLA	C3B-C4B-NB	2.50	112.83	110.52
26	b	620	SQD	C1-C2-C3	-2.50	104.79	110.00
40	V	201	HEC	C1D-C2D-C3D	-2.50	104.33	106.96
23	c	507	CLA	C4-C3-C5	2.50	119.47	115.27
23	a	404[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	b	607	CLA	CAC-C3C-C4C	2.50	128.05	124.81
23	B	614	CLA	OBD-CAD-C3D	-2.49	122.52	128.52
23	C	503	CLA	C4-C3-C5	2.49	119.46	115.27
23	c	502	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	d	403	CLA	O2A-CGA-CBA	2.49	119.72	111.91
33	B	629	LMT	O1'-C1'-C2'	2.49	112.19	108.30
23	d	402[B]	CLA	CAA-C2A-C3A	-2.49	105.96	112.78
25	T	102	BCR	C16-C17-C18	-2.49	123.76	127.31
23	a	406[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
36	C	518[B]	DGD	O1G-C1A-C2A	2.49	119.71	111.91
25	k	101	BCR	C2-C1-C6	2.49	114.31	110.48
24	a	407[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
23	C	508	CLA	CMC-C2C-C1C	2.48	128.82	125.04
23	b	603	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
35	b	623	HTG	O5-C1-C2	2.48	113.43	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	O2A-CGA-CBA	2.48	119.69	111.91
36	c	517[B]	DGD	O3G-C3G-C2G	-2.48	104.91	110.90
29	A	414[B]	PL9	C12-C13-C14	-2.48	121.69	127.66
36	C	517[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	405[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
23	b	606	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
23	C	510	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
23	b	616	CLA	C4-C3-C5	2.48	119.44	115.27
23	c	514	CLA	C1-C2-C3	-2.48	121.76	126.04
23	B	615	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
25	D	404	BCR	C24-C23-C22	-2.48	122.49	126.23
36	C	517[B]	DGD	O5D-C6D-C5D	-2.48	104.47	109.05
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
33	F	101	LMT	C1'-O5'-C5'	-2.47	108.83	113.69
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	b	606	CLA	C1-C2-C3	-2.47	121.77	126.04
25	h	101	BCR	C11-C10-C9	-2.47	123.78	127.31
36	c	518[B]	DGD	O1G-C1A-C2A	2.47	119.67	111.91
23	C	514	CLA	CMC-C2C-C1C	2.47	128.80	125.04
25	A	409	BCR	C31-C1-C6	-2.47	106.29	110.30
23	B	612	CLA	CHD-C4C-NC	2.47	128.09	124.20
25	t	102	BCR	C21-C20-C19	-2.47	115.52	123.22
29	a	413[B]	PL9	C47-C48-C49	-2.47	119.32	127.75
25	c	516	BCR	C37-C22-C21	-2.47	119.47	122.92
23	C	507	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	B	602	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
23	c	510	CLA	C2A-C1A-CHA	-2.47	119.55	123.86
38	f	101	HEM	CHD-C4C-NC	2.47	127.11	124.44
23	B	614	CLA	CMB-C2B-C1B	2.46	129.12	125.37
23	b	601	CLA	C2A-C1A-CHA	-2.46	119.55	123.86
23	a	405[B]	CLA	CMC-C2C-C1C	2.46	128.79	125.04
32	d	406[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
23	a	405[B]	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
26	a	410[A]	SQD	O7-S-C6	2.46	109.86	106.94
23	C	513	CLA	O2A-CGA-O1A	-2.46	117.39	123.59
23	C	510	CLA	CHD-C4C-NC	2.46	128.07	124.20
33	B	628	LMT	O5'-C5'-C6'	2.45	112.54	106.44
23	B	611	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
33	m	103	LMT	C3'-C4'-C5'	-2.45	105.30	110.93
25	t	102	BCR	C12-C13-C14	-2.45	115.18	118.94
23	B	602	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
23	a	405[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[B]	CLA	O2A-CGA-CBA	2.45	119.60	111.91
24	A	407[B]	PHO	O2A-CGA-CBA	2.45	119.60	111.91
23	C	513	CLA	CMA-C3A-C4A	-2.45	105.18	111.77
25	c	515	BCR	C7-C8-C9	-2.45	122.53	126.23
23	B	605	CLA	OBD-CAD-C3D	-2.45	122.62	128.52
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
32	b	630[B]	LHG	O8-C23-O10	-2.45	117.41	123.59
23	C	507	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
23	C	507	CLA	C4C-C3C-C2C	-2.45	103.33	106.90
29	a	413[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	B	610	CLA	CBC-CAC-C3C	-2.45	105.69	112.43
25	c	516	BCR	C29-C30-C25	2.45	114.25	110.48
23	C	513	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	B	606	CLA	C4-C3-C5	2.45	119.39	115.27
24	a	407[B]	PHO	C1-C2-C3	-2.45	121.81	126.04
23	a	405[B]	CLA	CAA-CBA-CGA	2.45	120.40	113.25
23	c	509	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
29	D	405[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
23	c	505	CLA	CHD-C4C-NC	2.44	128.06	124.20
29	a	413[A]	PL9	C20-C19-C21	2.44	119.38	115.27
23	C	503	CLA	CHD-C4C-NC	2.44	128.06	124.20
23	A	405[B]	CLA	CAA-CBA-CGA	2.44	120.39	113.25
23	b	604	CLA	C4-C3-C5	2.44	119.38	115.27
23	b	607	CLA	C1-O2A-CGA	2.44	122.85	116.44
23	b	602	CLA	CAC-C3C-C4C	2.44	127.98	124.81
26	L	101	SQD	O48-C23-O10	-2.44	117.43	123.59
23	B	601	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
24	a	415[B]	PHO	C1A-C2A-C3A	-2.44	100.52	102.84
23	A	405[A]	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	A	406[B]	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
23	a	404[A]	CLA	CHD-C4C-NC	2.44	128.05	124.20
29	d	405[B]	PL9	C47-C48-C49	-2.44	119.42	127.75
26	A	410[B]	SQD	O48-C23-O10	-2.44	117.44	123.59
23	c	503	CLA	C4C-C3C-C2C	-2.44	103.34	106.90
23	a	404[B]	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
23	c	505	CLA	C1-C2-C3	-2.44	121.83	126.04
23	C	507	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	B	619	BCR	C38-C26-C25	-2.43	121.79	124.53
23	B	608	CLA	CHD-C4C-NC	2.43	128.04	124.20
34	c	520	LMG	C8-O7-C10	-2.43	111.80	117.79
25	D	404	BCR	C21-C20-C19	-2.43	115.62	123.22
23	a	404[B]	CLA	CHD-C4C-NC	2.43	128.04	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
29	D	405[B]	PL9	C45-C44-C46	2.43	119.36	115.27
29	D	405[B]	PL9	C12-C13-C14	-2.43	121.81	127.66
23	C	503	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	B	607	CLA	CHD-C4C-NC	2.43	128.03	124.20
23	A	406[B]	CLA	C1-C2-C3	-2.43	121.84	126.04
24	a	407[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
26	A	410[B]	SQD	O8-S-C6	2.43	109.61	105.74
23	c	505	CLA	CMC-C2C-C1C	2.43	128.74	125.04
23	B	612	CLA	CHC-C1C-C2C	-2.43	119.98	126.73
25	T	102	BCR	C33-C5-C6	-2.43	121.80	124.53
23	c	508	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
23	a	408	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
23	A	408	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
29	d	405[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
23	C	511	CLA	C4C-C3C-C2C	-2.42	103.36	106.90
23	B	615	CLA	CHC-C1C-C2C	-2.42	120.01	126.73
23	B	601	CLA	CHB-C4A-NA	2.42	127.85	124.51
29	A	414[B]	PL9	C42-C43-C44	-2.42	121.84	127.66
23	d	402[B]	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
26	a	410[A]	SQD	O8-S-C6	2.41	109.59	105.74
23	c	508	CLA	CHC-C1C-C2C	-2.41	120.02	126.73
24	a	407[B]	PHO	O2A-CGA-O1A	-2.41	117.50	123.59
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68
33	M	101	LMT	C1'-O5'-C5'	-2.41	108.95	113.69
38	F	102	HEM	O2D-CGD-CBD	2.41	121.78	114.03
25	b	619	BCR	C39-C30-C25	-2.41	106.39	110.30
23	a	406[B]	CLA	CMC-C2C-C1C	2.41	128.71	125.04
23	c	512	CLA	C1-O2A-CGA	2.41	122.77	116.44
23	C	508	CLA	O2A-CGA-CBA	2.41	119.47	111.91
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
23	B	612	CLA	C4-C3-C5	2.40	119.32	115.27
23	C	511	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
23	C	504	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
33	B	628	LMT	O5'-C5'-C4'	2.40	114.82	109.75
36	c	518[B]	DGD	C2G-O2G-C1B	-2.40	111.88	117.79
23	b	601	CLA	CAC-C3C-C4C	2.40	127.92	124.81
33	A	420	LMT	O1'-C1'-C2'	2.40	112.05	108.30
23	b	609	CLA	O2A-CGA-CBA	2.40	119.44	111.91
23	C	504	CLA	O2A-CGA-CBA	2.40	119.43	111.91
25	K	102	BCR	C3-C4-C5	-2.40	109.80	114.08
23	b	605	CLA	CMC-C2C-C1C	2.40	128.69	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	101	BCR	C10-C11-C12	-2.40	115.74	123.22
23	C	506	CLA	O2A-CGA-CBA	2.40	119.43	111.91
35	b	625	HTG	C1-C2-C3	-2.40	105.86	110.59
23	c	505	CLA	CBC-CAC-C3C	-2.40	105.83	112.43
23	A	408	CLA	CHB-C4A-NA	2.40	127.82	124.51
23	B	613	CLA	CHB-C4A-NA	2.40	127.82	124.51
38	F	102	HEM	C4D-ND-C1D	2.39	107.55	105.07
23	B	612	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
23	a	405[B]	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
33	B	626	LMT	C1B-C2B-C3B	2.39	114.98	110.00
25	k	101	BCR	C15-C14-C13	-2.39	123.89	127.31
23	c	504	CLA	O2A-CGA-CBA	2.39	119.42	111.91
29	D	405[B]	PL9	C40-C39-C41	2.39	119.29	115.27
23	d	403	CLA	CHB-C4A-NA	2.39	127.82	124.51
24	a	407[B]	PHO	O2D-CGD-O1D	-2.39	119.16	123.84
23	D	402[B]	CLA	CMB-C2B-C1B	2.39	129.01	125.37
23	C	502	CLA	C2A-C1A-CHA	-2.39	119.68	123.86
29	A	414[B]	PL9	C47-C48-C49	-2.39	119.59	127.75
23	C	503	CLA	O2A-CGA-CBA	2.39	119.40	111.91
32	A	419[B]	LHG	O7-C7-O9	-2.39	117.94	123.70
23	C	514	CLA	CHB-C1B-NB	-2.39	121.73	124.26
25	H	101	BCR	C10-C11-C12	-2.38	115.78	123.22
23	c	504	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
23	B	610	CLA	CMA-C3A-C4A	-2.38	105.37	111.77
23	c	504	CLA	C1-C2-C3	-2.38	121.92	126.04
23	c	502	CLA	C4-C3-C5	2.38	119.28	115.27
29	A	414[B]	PL9	C45-C44-C46	2.38	119.28	115.27
26	A	412	SQD	O48-C23-O10	-2.38	117.58	123.59
32	L	102[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
25	d	404	BCR	C36-C18-C17	-2.38	119.59	122.92
23	a	404[B]	CLA	CAC-C3C-C4C	2.38	127.90	124.81
23	B	607	CLA	C11-C10-C8	-2.38	108.23	115.92
23	A	406[B]	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
29	a	413[A]	PL9	C10-C9-C8	-2.38	117.58	123.68
23	d	402[B]	CLA	CHD-C4C-NC	2.38	127.95	124.20
29	d	405[A]	PL9	C7-C8-C9	-2.38	122.84	126.79
33	B	629	LMT	O5'-C5'-C4'	2.38	114.76	109.75
29	D	405[A]	PL9	C45-C44-C46	2.38	119.27	115.27
23	c	512	CLA	CAC-C3C-C4C	2.38	127.89	124.81
25	A	409	BCR	C37-C22-C21	-2.38	119.60	122.92
38	F	102	HEM	C4A-NA-C1A	2.37	107.67	105.35
23	c	512	CLA	CMA-C3A-C4A	2.37	118.15	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	C4-C3-C5	2.37	119.26	115.27
23	A	404[B]	CLA	C4-C3-C5	2.37	119.26	115.27
23	b	608	CLA	CMA-C3A-C4A	-2.37	105.40	111.77
36	C	517[B]	DGD	C2G-O2G-C1B	-2.37	111.95	117.79
34	C	521	LMG	C9-C8-C7	-2.37	106.18	111.79
23	C	514	CLA	C4-C3-C5	2.37	119.26	115.27
23	C	507	CLA	CGD-CBD-CAD	-2.37	103.06	110.73
23	A	404[B]	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
23	c	502	CLA	CHD-C4C-NC	2.37	127.93	124.20
23	c	505	CLA	O2A-CGA-CBA	2.37	119.34	111.91
32	d	406[B]	LHG	C6-C5-C4	-2.37	106.19	111.79
36	h	102	DGD	C6D-C5D-C4D	2.37	117.03	112.09
25	B	619	BCR	C7-C8-C9	-2.37	122.66	126.23
23	C	510	CLA	C11-C12-C13	-2.37	108.27	115.92
23	c	512	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
29	d	405[B]	PL9	C17-C18-C19	-2.36	121.97	127.66
23	C	503	CLA	O2A-CGA-O1A	-2.36	117.62	123.59
23	A	408	CLA	CMC-C2C-C1C	2.36	128.64	125.04
34	m	101	LMG	C7-O1-C1	-2.36	109.12	113.74
23	a	406[B]	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
23	b	606	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	B	602	CLA	CMB-C2B-C1B	2.36	128.96	125.37
23	c	509	CLA	CMC-C2C-C1C	2.36	128.63	125.04
23	B	615	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
40	V	201	HEC	CBA-CAA-C2A	-2.36	106.07	112.63
29	D	405[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
25	a	409	BCR	C33-C5-C6	-2.36	121.88	124.53
25	b	617	BCR	C24-C23-C22	-2.36	122.67	126.23
34	C	520	LMG	O8-C28-O10	-2.36	117.64	123.59
23	c	513	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	a	408	CLA	CHC-C1C-C2C	-2.36	120.18	126.73
23	a	405[B]	CLA	C4-C3-C5	2.36	119.23	115.27
25	A	409	BCR	C33-C5-C6	-2.36	121.88	124.53
23	A	404[B]	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	b	608	CLA	C11-C10-C8	-2.36	108.31	115.92
23	C	505	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
23	c	503	CLA	CAC-C3C-C4C	2.35	127.86	124.81
24	A	417[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
23	b	615	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
23	A	404[B]	CLA	CMC-C2C-C1C	2.35	128.62	125.04
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
36	C	518[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	413[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	a	405[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	B	601	CLA	CAC-C3C-C4C	2.35	127.85	124.81
23	b	604	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
25	K	102	BCR	C29-C30-C25	2.35	114.09	110.48
23	C	508	CLA	CBC-CAC-C3C	-2.35	105.97	112.43
23	A	406[B]	CLA	CMC-C2C-C1C	2.34	128.61	125.04
23	C	509	CLA	O2A-CGA-CBA	2.34	119.26	111.91
36	C	518[B]	DGD	O1G-C1A-O1A	-2.34	117.68	123.59
25	h	101	BCR	C36-C18-C19	2.34	121.77	118.08
25	Y	101	BCR	C38-C26-C25	-2.34	121.90	124.53
23	A	408	CLA	CMB-C2B-C1B	2.34	128.93	125.37
23	C	505	CLA	CAC-C3C-C4C	2.34	127.85	124.81
23	c	513	CLA	CBA-CAA-C2A	-2.34	106.95	113.86
26	A	410[B]	SQD	O9-S-O7	-2.34	105.85	113.95
23	C	506	CLA	CHB-C1B-NB	-2.34	121.78	124.26
23	b	606	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	d	405[B]	PL9	C53-C6-C1	2.34	119.77	114.99
36	H	102	DGD	C3B-C2B-C1B	-2.34	105.12	113.62
23	d	402[B]	CLA	CAC-C3C-C4C	2.34	127.84	124.81
23	c	505	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
25	H	101	BCR	C31-C1-C6	-2.34	106.51	110.30
23	c	504	CLA	CAC-C3C-C4C	2.34	127.84	124.81
23	b	612	CLA	CHD-C4C-NC	2.34	127.88	124.20
23	c	510	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	b	608	CLA	O2A-CGA-CBA	2.33	119.23	111.91
23	C	513	CLA	CHC-C1C-C2C	-2.33	120.25	126.73
33	A	420	LMT	O5'-C5'-C4'	2.33	114.67	109.75
23	D	402[A]	CLA	CHD-C4C-NC	2.33	127.88	124.20
38	f	101	HEM	CMD-C2D-C1D	2.33	128.59	125.04
23	a	405[A]	CLA	C1-O2A-CGA	2.33	122.56	116.44
29	A	414[B]	PL9	C37-C36-C34	-2.33	105.32	112.98
23	B	608	CLA	CBC-CAC-C3C	-2.33	106.01	112.43
29	a	413[A]	PL9	C35-C34-C33	-2.33	117.70	123.68
36	C	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
35	o	301	HTG	C2'-C1'-S1	-2.33	104.88	112.40
23	B	607	CLA	O2A-CGA-CBA	2.33	119.21	111.91
36	c	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
40	v	201	HEC	CBA-CAA-C2A	-2.33	106.16	112.63
23	B	610	CLA	CMA-C3A-C2A	-2.33	104.45	113.83
32	d	406[A]	LHG	O8-C23-C24	2.33	119.21	111.91
23	b	603	CLA	CMC-C2C-C1C	2.33	128.58	125.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	410[B]	SQD	O47-C7-O49	-2.32	118.09	123.70
36	c	517[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
23	a	406[A]	CLA	C4-C3-C5	2.32	119.17	115.27
23	b	613	CLA	C4-C3-C5	2.32	119.17	115.27
23	A	405[B]	CLA	CED-O2D-CGD	2.32	121.18	115.94
23	b	607	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
26	a	410[A]	SQD	O48-C23-C24	2.32	119.17	111.91
25	B	619	BCR	C2-C1-C6	2.32	114.05	110.48
23	c	511	CLA	C4-C3-C2	-2.31	117.74	123.68
23	c	511	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
23	C	514	CLA	CAA-C2A-C3A	-2.31	106.44	112.78
23	C	505	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
23	c	507	CLA	CMB-C2B-C1B	2.31	128.89	125.37
25	B	618	BCR	C28-C27-C26	-2.31	109.95	114.08
23	B	607	CLA	CHC-C1C-C2C	-2.31	120.31	126.73
34	m	101	LMG	O8-C28-O10	-2.31	117.76	123.59
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
23	b	610	CLA	C3B-C4B-NB	2.31	112.66	110.52
34	d	410	LMG	O7-C10-O9	-2.31	118.12	123.70
23	c	514	CLA	CHB-C1B-NB	-2.31	121.81	124.26
23	b	603	CLA	C7-C6-C5	-2.31	107.09	113.36
25	D	404	BCR	C15-C14-C13	-2.31	124.02	127.31
23	c	505	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	c	511	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
26	b	620	SQD	O48-C23-C24	2.30	119.14	111.91
23	d	402[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	b	615	CLA	C6-C7-C8	-2.30	108.47	115.92
23	c	513	CLA	C3B-C4B-NB	2.30	112.65	110.52
23	A	406[B]	CLA	C4-C3-C5	2.30	119.14	115.27
36	C	517[B]	DGD	O3G-C3G-C2G	-2.30	105.34	110.90
26	a	411	SQD	O48-C23-O10	-2.30	117.78	123.59
33	T	101	LMT	C1'-O5'-C5'	-2.30	109.17	113.69
23	c	505	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
23	D	403	CLA	CAC-C3C-C4C	2.30	127.80	124.81
23	C	514	CLA	CAC-C3C-C4C	2.30	127.80	124.81
34	c	521	LMG	O8-C28-O10	-2.30	117.79	123.59
25	B	619	BCR	C3-C4-C5	-2.30	109.97	114.08
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
29	D	405[B]	PL9	C30-C29-C31	2.30	119.14	115.27
23	d	402[B]	CLA	CMB-C2B-C1B	2.30	128.87	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	618	BCR	C8-C7-C6	-2.30	120.75	127.20
23	b	603	CLA	CMB-C2B-C1B	2.29	128.86	125.37
23	c	514	CLA	CMB-C2B-C1B	2.29	128.86	125.37
23	C	508	CLA	C6-C7-C8	-2.29	108.50	115.92
29	A	414[B]	PL9	C51-C49-C50	2.29	119.67	114.60
25	C	516	BCR	C32-C1-C6	-2.29	106.58	110.30
23	c	507	CLA	CMC-C2C-C1C	2.29	128.53	125.04
23	A	405[B]	CLA	CMB-C2B-C1B	2.29	128.86	125.37
24	A	407[B]	PHO	C4A-C3A-C2A	-2.29	100.66	102.84
23	C	513	CLA	CAC-C3C-C4C	2.29	127.78	124.81
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	415[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
23	a	404[B]	CLA	C7-C6-C5	-2.29	107.14	113.36
32	d	407[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
25	d	404	BCR	C40-C30-C39	2.29	115.55	108.53
23	a	406[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	B	612	CLA	CMA-C3A-C2A	-2.29	104.60	113.83
23	C	506	CLA	CHD-C4C-NC	2.29	127.81	124.20
23	C	510	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	b	601	CLA	O2A-CGA-CBA	2.29	119.08	111.91
23	b	608	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
23	b	608	CLA	C4C-C3C-C2C	-2.28	103.57	106.90
23	b	611	CLA	O2A-CGA-CBA	2.28	119.07	111.91
25	b	618	BCR	C37-C22-C23	2.28	121.67	118.08
23	C	509	CLA	CHD-C4C-NC	2.28	127.80	124.20
23	c	513	CLA	CHB-C4A-NA	2.28	127.67	124.51
23	a	405[B]	CLA	CMA-C3A-C2A	-2.28	104.63	113.83
23	B	602	CLA	CMA-C3A-C4A	-2.28	105.65	111.77
25	d	404	BCR	C11-C10-C9	-2.28	124.06	127.31
23	B	603	CLA	CHD-C4C-NC	2.28	127.79	124.20
33	m	103	LMT	C1'-O5'-C5'	-2.27	109.22	113.69
23	b	608	CLA	C11-C12-C13	-2.27	108.57	115.92
23	a	404[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	C	511	CLA	CMB-C2B-C1B	2.27	128.83	125.37
29	d	405[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
25	c	516	BCR	C21-C20-C19	-2.27	116.13	123.22
29	a	413[B]	PL9	C45-C44-C46	2.27	119.09	115.27
25	C	516	BCR	C29-C30-C25	2.27	113.97	110.48
40	V	201	HEC	CHA-C4D-ND	2.27	126.88	124.42
23	B	605	CLA	CED-O2D-CGD	2.27	121.07	115.94
24	A	417[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
23	A	408	CLA	OBD-CAD-C3D	-2.27	123.07	128.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	508	CLA	CBC-CAC-C3C	-2.27	106.18	112.43
23	a	406[B]	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
25	c	515	BCR	C38-C26-C25	-2.27	121.98	124.53
23	c	513	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
34	d	410	LMG	C7-O1-C1	-2.26	109.32	113.74
40	v	201	HEC	C4B-NB-C1B	2.26	107.41	105.07
23	B	605	CLA	CBC-CAC-C3C	-2.26	106.19	112.43
25	t	102	BCR	C20-C21-C22	-2.26	124.08	127.31
36	c	517[B]	DGD	C3G-C2G-C1G	-2.26	106.44	111.79
35	b	622	HTG	C6-C5-C4	-2.26	107.71	113.00
32	d	412[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
35	B	623	HTG	O5-C5-C4	2.26	113.80	109.69
25	b	617	BCR	C11-C10-C9	-2.26	124.08	127.31
23	c	503	CLA	C1-O2A-CGA	2.26	122.37	116.44
25	b	618	BCR	C33-C5-C6	-2.26	121.99	124.53
23	D	402[A]	CLA	C4-C3-C5	2.26	119.07	115.27
23	C	511	CLA	C4-C3-C2	-2.26	117.88	123.68
29	d	405[B]	PL9	C51-C49-C50	2.26	119.59	114.60
32	d	406[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
25	B	617	BCR	C31-C1-C6	-2.26	106.63	110.30
23	A	408	CLA	CMA-C3A-C2A	-2.26	104.72	113.83
35	o	301	HTG	O2-C2-C3	-2.26	105.13	110.35
23	b	602	CLA	C11-C10-C8	-2.26	108.62	115.92
23	c	512	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
32	b	630[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
23	c	507	CLA	O2A-CGA-CBA	2.26	118.99	111.91
24	a	415[A]	PHO	C4-C3-C2	-2.26	117.89	123.68
23	B	603	CLA	CMC-C2C-C1C	2.25	128.47	125.04
23	B	603	CLA	CMA-C3A-C2A	-2.25	104.73	113.83
23	b	615	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
23	B	603	CLA	CHB-C1B-C2B	-2.25	120.88	127.24
26	f	102	SQD	O7-S-C6	2.25	109.61	106.94
23	c	502	CLA	CMC-C2C-C1C	2.25	128.47	125.04
29	D	405[A]	PL9	C20-C19-C21	2.25	119.05	115.27
32	d	412[B]	LHG	O7-C7-O9	-2.25	118.27	123.70
24	A	417[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68
34	C	520	LMG	C8-O7-C10	-2.25	112.26	117.79
25	B	617	BCR	C15-C14-C13	-2.25	124.10	127.31
23	a	408	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
23	C	513	CLA	C4-C3-C2	-2.25	117.91	123.68
23	A	405[B]	CLA	CAC-C3C-C4C	2.25	127.72	124.81
23	D	403	CLA	C2A-C1A-CHA	-2.25	119.93	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	CHB-C1B-C2B	-2.24	120.90	127.24
40	V	201	HEC	C4A-NA-C1A	2.24	107.55	105.35
35	B	623	HTG	C3-C4-C5	2.24	114.24	110.24
23	a	406[B]	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	c	503	CLA	C1-C2-C3	-2.24	122.17	126.04
24	a	415[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
23	d	403	CLA	CAC-C3C-C4C	2.24	127.72	124.81
23	c	514	CLA	C4-C3-C5	2.24	119.04	115.27
23	C	506	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
23	b	602	CLA	CHC-C1C-C2C	-2.24	120.51	126.73
25	y	101	BCR	C35-C13-C14	-2.24	119.79	122.92
23	d	403	CLA	C2A-C1A-CHA	-2.24	119.95	123.86
23	A	405[B]	CLA	CMA-C3A-C2A	-2.24	104.81	113.83
34	m	101	LMG	O7-C10-O9	-2.24	118.30	123.70
23	c	514	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
25	c	516	BCR	C15-C14-C13	-2.23	124.12	127.31
26	F	103	SQD	O48-C23-O10	-2.23	117.95	123.59
29	D	405[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
23	b	615	CLA	CHA-C1A-NA	-2.23	121.29	126.40
23	a	405[B]	CLA	C1-C2-C3	-2.23	122.18	126.04
29	A	414[B]	PL9	C25-C24-C26	2.23	119.02	115.27
23	c	504	CLA	CHC-C1C-C2C	-2.23	120.53	126.73
25	t	102	BCR	C1-C6-C7	2.23	122.08	115.78
23	c	510	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
34	d	410	LMG	O8-C28-O10	-2.23	117.97	123.59
36	C	517[B]	DGD	O6D-C1D-O3G	-2.23	104.70	109.97
23	a	408	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
23	b	615	CLA	O2A-CGA-CBA	2.23	118.89	111.91
36	c	518[B]	DGD	O2G-C1B-O1B	-2.22	118.33	123.70
23	B	602	CLA	O2A-CGA-CBA	2.22	118.89	111.91
29	d	405[B]	PL9	C12-C13-C14	-2.22	122.31	127.66
26	F	103	SQD	C46-C45-C44	-2.22	106.53	111.79
23	a	404[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
23	b	605	CLA	O2A-C1-C2	-2.22	102.79	108.64
23	D	402[B]	CLA	CHD-C4C-NC	2.22	127.71	124.20
26	A	410[A]	SQD	O8-S-C6	2.22	109.28	105.74
23	d	403	CLA	C1-O2A-CGA	2.22	122.27	116.44
23	c	506	CLA	CHD-C4C-NC	2.22	127.70	124.20
25	Y	101	BCR	C1-C6-C7	2.22	122.06	115.78
23	A	408	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
29	A	414[B]	PL9	C2-C3-C4	2.22	121.86	118.80
23	B	601	CLA	C2A-C1A-CHA	-2.22	119.98	123.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C1-O2A-CGA	2.22	122.27	116.44
36	h	102	DGD	O4D-C4D-C3D	-2.22	105.22	110.35
26	a	410[B]	SQD	C3-C4-C5	2.22	114.20	110.24
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	c	507	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
24	A	407[B]	PHO	O2D-CGD-O1D	-2.22	119.50	123.84
23	C	502	CLA	C1-C2-C3	-2.22	122.21	126.04
23	c	512	CLA	C1-C2-C3	-2.22	122.21	126.04
36	C	517[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
34	d	410	LMG	O8-C28-C29	2.22	118.86	111.91
36	c	518[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
25	Y	101	BCR	C36-C18-C19	2.22	121.57	118.08
25	T	102	BCR	C1-C6-C7	2.21	122.04	115.78
26	F	103	SQD	O5-C1-C2	-2.21	105.66	110.35
25	C	516	BCR	C11-C10-C9	-2.21	124.15	127.31
23	b	614	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	d	405[B]	PL9	C20-C19-C21	2.21	118.99	115.27
23	b	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	B	611	CLA	OBD-CAD-C3D	-2.21	123.20	128.52
36	H	102	DGD	O6E-C5E-C6E	2.21	111.94	106.44
23	B	606	CLA	C7-C6-C5	-2.21	107.35	113.36
23	C	513	CLA	CBA-CAA-C2A	-2.21	107.34	113.86
23	C	513	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
23	C	506	CLA	CHA-C1A-NA	-2.21	121.34	126.40
23	B	611	CLA	O2A-CGA-CBA	2.21	118.84	111.91
23	B	616	CLA	C2A-C1A-CHA	-2.21	120.00	123.86
25	c	515	BCR	C33-C5-C6	-2.21	122.05	124.53
23	c	502	CLA	O2A-CGA-CBA	2.21	118.84	111.91
23	C	504	CLA	CAC-C3C-C4C	2.21	127.67	124.81
23	b	615	CLA	C11-C12-C13	-2.21	108.78	115.92
40	v	201	HEC	C4A-NA-C1A	2.21	107.51	105.35
23	b	608	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
32	L	102[B]	LHG	O8-C23-C24	2.21	118.83	111.91
40	V	201	HEC	C2A-C1A-NA	-2.21	108.18	110.32
23	B	613	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
23	c	502	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
34	c	521	LMG	C1-C2-C3	-2.20	105.41	110.00
24	A	417[B]	PHO	C6-C5-C3	-2.20	107.68	113.45
23	B	608	CLA	O2A-CGA-CBA	2.20	118.81	111.91
23	A	408	CLA	CHB-C1B-NB	-2.20	121.93	124.26
24	A	407[A]	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	406[A]	CLA	CAC-C3C-C4C	2.20	127.67	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	404	BCR	C37-C22-C23	2.20	121.54	118.08
25	C	515	BCR	C40-C30-C25	-2.20	106.73	110.30
23	C	511	CLA	CHB-C1B-NB	-2.20	121.93	124.26
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
23	C	512	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
25	K	102	BCR	C36-C18-C19	2.20	121.54	118.08
23	c	511	CLA	C11-C10-C8	-2.20	108.82	115.92
24	A	417[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
25	b	618	BCR	C7-C8-C9	-2.20	122.92	126.23
23	B	608	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
23	a	404[B]	CLA	CMA-C3A-C2A	-2.19	104.97	113.83
25	b	619	BCR	C16-C15-C14	-2.19	118.98	123.47
25	K	102	BCR	C32-C1-C6	-2.19	106.74	110.30
23	b	608	CLA	CMB-C2B-C3B	2.19	131.90	126.59
23	b	605	CLA	C1-O2A-CGA	2.19	122.19	116.44
23	B	604	CLA	C11-C12-C13	-2.19	108.84	115.92
23	b	614	CLA	CMC-C2C-C1C	2.19	128.37	125.04
23	c	503	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	A	407[B]	PHO	CBA-CAA-C2A	-2.19	107.42	113.81
36	H	102	DGD	O2G-C1B-C2B	2.19	116.21	111.50
23	C	502	CLA	O2A-CGA-CBA	2.19	118.77	111.91
24	a	415[B]	PHO	CBA-CAA-C2A	-2.19	107.42	113.81
29	d	405[B]	PL9	C7-C3-C2	-2.19	120.42	123.30
25	B	618	BCR	C15-C14-C13	-2.19	124.19	127.31
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
25	C	515	BCR	C24-C23-C22	-2.18	122.94	126.23
26	a	410[A]	SQD	O9-S-O7	-2.18	106.39	113.95
23	b	615	CLA	C1-C2-C3	-2.18	122.27	126.04
24	a	407[B]	PHO	CMB-C2B-C3B	2.18	128.76	124.68
23	B	610	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	b	604	CLA	C6-C5-C3	-2.18	107.74	113.45
29	A	414[B]	PL9	C10-C9-C8	-2.18	118.09	123.68
26	L	101	SQD	C44-O6-C1	-2.18	109.48	113.74
29	d	405[A]	PL9	C51-C49-C50	2.18	119.42	114.60
38	F	102	HEM	C4B-C3B-C2B	-2.18	105.39	107.11
32	d	407[B]	LHG	O8-C23-O10	-2.18	118.09	123.59
35	c	522	HTG	C1-O5-C5	2.18	116.60	112.58
23	d	402[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
36	c	518[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
23	b	616	CLA	C1-C2-C3	-2.18	122.28	126.04
23	C	510	CLA	CMB-C2B-C1B	2.18	128.68	125.37
33	t	101	LMT	C1-O1'-C1'	2.17	117.45	113.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	Z	101	LMG	C1-O6-C5	2.17	117.95	113.69
25	D	404	BCR	C15-C16-C17	-2.17	119.03	123.47
23	B	604	CLA	O2A-CGA-CBA	2.17	118.72	111.91
23	b	611	CLA	CMC-C2C-C1C	2.17	128.34	125.04
34	C	501	LMG	O6-C1-O1	-2.17	104.83	109.97
23	b	602	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
24	a	407[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
32	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24
23	D	403	CLA	CHC-C4B-NB	-2.17	121.96	124.26
23	C	502	CLA	C11-C12-C13	-2.17	108.92	115.92
23	c	511	CLA	C7-C6-C5	-2.17	107.48	113.36
23	D	402[B]	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
23	B	609	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
25	y	101	BCR	C40-C30-C25	-2.16	106.79	110.30
29	d	405[B]	PL9	C15-C14-C16	2.16	118.91	115.27
27	B	622	GOL	C3-C2-C1	-2.16	103.29	111.70
23	A	408	CLA	CAC-C3C-C4C	2.16	127.62	124.81
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
26	b	620	SQD	C44-O6-C1	-2.16	109.52	113.74
23	C	513	CLA	C3B-C4B-NB	2.16	112.52	110.52
40	v	201	HEC	CMC-C2C-C1C	-2.16	122.08	125.37
25	b	618	BCR	C38-C26-C25	-2.16	122.10	124.53
29	d	405[B]	PL9	C45-C44-C46	2.16	118.90	115.27
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	C	509	CLA	CAA-C2A-C3A	-2.16	106.87	112.78
23	C	511	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
23	B	603	CLA	CMB-C2B-C3B	2.16	131.81	126.59
25	h	101	BCR	C16-C15-C14	-2.16	119.06	123.47
23	d	402[B]	CLA	CMC-C2C-C1C	2.16	128.32	125.04
23	D	403	CLA	CHB-C1B-NB	-2.16	121.97	124.26
40	V	201	HEC	C4B-NB-C1B	2.16	107.30	105.07
23	b	603	CLA	CBC-CAC-C3C	-2.15	106.49	112.43
34	C	521	LMG	O1-C1-C2	2.15	111.67	108.30
23	A	406[B]	CLA	CAC-C3C-C4C	2.15	127.60	124.81
23	b	610	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
23	B	605	CLA	O2A-CGA-CBA	2.15	118.66	111.91
25	t	102	BCR	C29-C28-C27	-2.15	106.57	111.38
25	C	515	BCR	C38-C26-C25	-2.15	122.11	124.53
36	C	518[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	b	610	CLA	C4-C3-C2	-2.15	118.16	123.68
23	B	615	CLA	CED-O2D-CGD	2.15	120.80	115.94
25	b	619	BCR	C29-C30-C25	2.15	113.79	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	410[B]	SQD	O6-C44-C45	-2.15	105.71	110.90
23	c	514	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
36	c	517[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
29	d	405[A]	PL9	C35-C34-C36	2.15	118.88	115.27
25	C	516	BCR	C37-C22-C23	2.15	121.46	118.08
36	c	517[B]	DGD	C2G-O2G-C1B	-2.14	112.51	117.79
25	d	404	BCR	C38-C26-C27	2.14	117.73	113.62
23	C	508	CLA	C3B-C4B-NB	2.14	112.50	110.52
26	A	412	SQD	O6-C44-C45	-2.14	105.73	110.90
36	c	519	DGD	O3G-C1D-C2D	-2.14	104.96	108.30
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27
23	B	606	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
23	b	605	CLA	C6-C7-C8	-2.14	109.00	115.92
40	V	201	HEC	C3D-C4D-ND	-2.14	108.28	110.36
23	C	509	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
23	B	606	CLA	CAC-C3C-C4C	2.14	127.58	124.81
23	b	613	CLA	CAC-C3C-C4C	2.14	127.58	124.81
25	y	101	BCR	C35-C13-C12	2.14	121.44	118.08
40	V	201	HEC	CAA-CBA-CGA	-2.14	109.01	113.60
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
34	c	520	LMG	O8-C28-O10	-2.13	118.20	123.59
23	b	606	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
29	a	413[B]	PL9	C51-C49-C50	2.13	119.32	114.60
23	c	509	CLA	CAC-C3C-C4C	2.13	127.58	124.81
25	h	101	BCR	C10-C11-C12	-2.13	116.57	123.22
25	b	618	BCR	C35-C13-C14	-2.13	119.94	122.92
23	B	616	CLA	CMB-C2B-C3B	2.13	131.75	126.59
24	A	417[B]	PHO	O2A-CGA-CBA	2.13	118.59	111.91
23	c	510	CLA	C4-C3-C2	-2.13	118.22	123.68
33	m	103	LMT	C3B-C4B-C5B	-2.13	106.44	110.24
25	a	409	BCR	C8-C7-C6	-2.13	121.22	127.20
36	C	517[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
23	b	612	CLA	CMB-C2B-C1B	2.13	128.61	125.37
24	a	415[B]	PHO	O2A-CGA-CBA	2.13	118.58	111.91
36	c	518[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
23	B	602	CLA	CHB-C4A-NA	2.13	127.45	124.51
23	a	405[B]	CLA	CHB-C4A-NA	2.13	127.45	124.51
32	E	101[B]	LHG	O7-C7-O9	-2.13	118.57	123.70
23	b	603	CLA	CGD-CBD-CAD	-2.12	103.85	110.73
25	d	404	BCR	C33-C5-C6	-2.12	122.14	124.53
26	b	620	SQD	O5-C1-C2	-2.12	105.85	110.35
24	a	415[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	621	LMT	C2'-C3'-C4'	2.12	114.53	109.68
33	M	101	LMT	O5B-C5B-C6B	2.12	111.72	106.44
23	c	506	CLA	CHB-C1B-NB	-2.12	122.01	124.26
23	C	502	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
23	B	611	CLA	C11-C12-C13	-2.12	109.06	115.92
23	C	513	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
36	C	517[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
29	D	405[B]	PL9	C36-C37-C38	-2.12	104.92	111.88
25	d	404	BCR	C29-C28-C27	-2.12	106.64	111.38
25	A	409	BCR	C8-C7-C6	-2.12	121.25	127.20
36	C	517[B]	DGD	C3G-C2G-C1G	-2.12	106.78	111.79
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
23	D	403	CLA	OBD-CAD-C3D	-2.12	123.43	128.52
33	t	101	LMT	O5'-C1'-O1'	-2.12	104.96	109.97
25	c	516	BCR	C2-C1-C6	2.12	113.74	110.48
23	B	601	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
23	D	403	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	B	605	CLA	C3B-C4B-NB	2.11	112.47	110.52
36	C	517[B]	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
23	b	604	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
25	B	618	BCR	C40-C30-C25	-2.11	106.88	110.30
23	B	616	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
23	c	502	CLA	CBC-CAC-C3C	-2.11	106.63	112.43
23	B	610	CLA	C1-C2-C3	-2.11	122.40	126.04
23	C	502	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
24	A	417[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
23	B	606	CLA	C11-C10-C8	-2.10	109.11	115.92
36	h	102	DGD	C3B-C2B-C1B	-2.10	105.97	113.62
23	c	514	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
29	d	405[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
23	b	611	CLA	CAC-C3C-C4C	2.10	127.54	124.81
25	C	515	BCR	C37-C22-C23	2.10	121.39	118.08
23	B	606	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
32	b	630[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
36	H	102	DGD	O3G-C3G-C2G	-2.10	105.83	110.90
23	d	403	CLA	C6-C7-C8	-2.10	109.13	115.92
25	B	619	BCR	C16-C15-C14	-2.10	119.18	123.47
40	V	201	HEC	CMD-C2D-C1D	2.10	128.23	125.04
33	F	101	LMT	C2'-C3'-C4'	2.10	114.47	109.68
26	b	620	SQD	O47-C7-O49	-2.10	118.64	123.70
23	b	610	CLA	CMA-C3A-C4A	-2.10	106.14	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	CHA-C1A-NA	-2.10	121.60	126.40
23	b	601	CLA	CHB-C1B-C2B	-2.09	121.32	127.24
25	y	101	BCR	C16-C15-C14	-2.09	119.18	123.47
32	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
23	D	402[A]	CLA	CMB-C2B-C1B	2.09	128.56	125.37
25	b	619	BCR	C7-C6-C5	2.09	126.53	121.46
23	c	512	CLA	C11-C10-C8	-2.09	109.16	115.92
23	b	607	CLA	C1-C2-C3	-2.09	122.43	126.04
25	k	101	BCR	C36-C18-C19	2.09	121.37	118.08
23	A	406[B]	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36
33	F	101	LMT	C3B-C4B-C5B	-2.09	106.52	110.24
33	M	101	LMT	C3B-C4B-C5B	-2.09	106.52	110.24
29	a	413[B]	PL9	C10-C9-C8	-2.09	118.33	123.68
23	B	611	CLA	C2C-C1C-NC	2.08	111.92	109.97
23	c	504	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
23	d	402[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
24	a	415[B]	PHO	O1D-CGD-CBD	-2.08	121.27	124.74
23	b	607	CLA	CMB-C2B-C1B	2.08	128.54	125.37
26	f	102	SQD	O48-C23-O10	-2.08	118.33	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
33	D	401	LMT	C4B-C3B-C2B	-2.08	107.19	110.82
23	A	408	CLA	C11-C12-C13	-2.08	109.19	115.92
23	a	404[B]	CLA	CHB-C4A-NA	2.08	127.39	124.51
23	B	602	CLA	C1-O2A-CGA	2.08	121.90	116.44
25	D	404	BCR	C29-C28-C27	-2.08	106.73	111.38
29	A	414[B]	PL9	C35-C34-C33	-2.08	118.34	123.68
34	B	620	LMG	C8-O7-C10	-2.08	112.67	117.79
23	c	507	CLA	CAA-CBA-CGA	2.08	119.33	113.25
25	K	102	BCR	C37-C22-C21	-2.08	120.01	122.92
36	C	519	DGD	O1G-C1A-O1A	-2.08	118.34	123.59
23	b	610	CLA	C11-C12-C13	-2.08	109.20	115.92
23	b	614	CLA	C4-C3-C5	2.08	118.77	115.27
23	B	616	CLA	C4-C3-C2	-2.08	118.35	123.68
25	K	102	BCR	C2-C1-C6	2.08	113.68	110.48
23	B	616	CLA	CMC-C2C-C1C	2.08	128.20	125.04
23	b	603	CLA	C1-O2A-CGA	2.08	121.89	116.44
33	B	628	LMT	O5B-C5B-C6B	2.07	111.59	106.44
23	c	506	CLA	C1-C2-C3	-2.07	122.46	126.04
23	B	607	CLA	CMA-C3A-C2A	-2.07	105.47	113.83
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405[A]	PL9	C12-C13-C14	-2.07	122.68	127.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	627	LMT	O1'-C1'-C2'	2.07	111.53	108.30
23	B	614	CLA	CBC-CAC-C3C	-2.07	106.73	112.43
40	v	201	HEC	C2A-C1A-NA	-2.07	108.31	110.32
29	D	405[B]	PL9	C22-C23-C24	-2.07	122.68	127.66
23	B	613	CLA	CHB-C1B-NB	-2.07	122.07	124.26
23	C	512	CLA	O2A-CGA-CBA	2.07	118.39	111.91
23	B	613	CLA	C2A-C1A-CHA	-2.07	120.25	123.86
23	c	512	CLA	CHB-C1B-NB	-2.07	122.07	124.26
34	Z	101	LMG	C9-C8-C7	-2.07	106.90	111.79
29	D	405[A]	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	413[A]	PL9	C51-C49-C50	2.07	119.17	114.60
25	c	516	BCR	C37-C22-C23	2.07	121.33	118.08
25	A	409	BCR	C11-C10-C9	-2.07	124.36	127.31
23	B	601	CLA	C4-C3-C5	2.06	118.74	115.27
29	D	405[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
25	k	101	BCR	C34-C9-C8	2.06	121.33	118.08
32	E	101[B]	LHG	C5-O7-C7	-2.06	112.72	117.79
23	B	611	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	d	404	BCR	C24-C23-C22	-2.06	123.12	126.23
25	D	404	BCR	C30-C25-C24	2.06	121.60	115.78
25	b	619	BCR	C15-C14-C13	-2.06	124.37	127.31
23	c	514	CLA	C1-O2A-CGA	2.06	121.84	116.44
23	b	611	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
24	a	407[B]	PHO	CBA-CAA-C2A	-2.06	107.80	113.81
23	b	606	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
35	d	409	HTG	C4-C3-C2	-2.06	107.23	110.82
36	c	517[B]	DGD	O6D-C1D-O3G	-2.05	105.11	109.97
23	B	612	CLA	C7-C6-C5	-2.05	107.78	113.36
36	C	517[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	C	508	CLA	CHA-C1A-NA	-2.05	121.70	126.40
23	C	505	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
34	B	620	LMG	C4-C3-C2	-2.05	107.24	110.82
25	h	101	BCR	C20-C21-C22	-2.05	124.38	127.31
23	b	609	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	c	509	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
32	d	412[B]	LHG	C5-O7-C7	-2.05	112.75	117.79
23	A	404[A]	CLA	CHB-C4A-NA	2.05	127.34	124.51
34	C	501	LMG	C9-C8-C7	-2.05	106.94	111.79
23	c	513	CLA	CHB-C1B-C2B	-2.05	121.45	127.24
36	C	518[B]	DGD	C6D-C5D-C4D	2.05	116.37	112.09
23	c	509	CLA	CHA-C1A-NA	-2.05	121.71	126.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	h	101	BCR	C34-C9-C8	2.05	121.30	118.08
23	b	613	CLA	CMB-C2B-C1B	2.05	128.49	125.37
26	F	103	SQD	O8-S-O7	-2.05	106.28	111.27
23	a	406[B]	CLA	CHB-C1B-C2B	-2.04	121.46	127.24
23	C	514	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
29	a	413[B]	PL9	C35-C34-C33	-2.04	118.44	123.68
32	D	407[A]	LHG	O4-P-O5	2.04	122.34	112.24
23	c	503	CLA	C2A-C1A-CHA	-2.04	120.29	123.86
25	D	404	BCR	C37-C22-C21	-2.04	120.06	122.92
33	b	627	LMT	C1'-O5'-C5'	-2.04	109.68	113.69
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27
27	O	303	GOL	C3-C2-C1	-2.04	103.77	111.70
23	b	612	CLA	C4D-CHA-C1A	-2.04	118.77	121.25
23	C	513	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
25	T	102	BCR	C39-C30-C25	-2.04	106.99	110.30
23	B	604	CLA	CHB-C1B-NB	-2.04	122.10	124.26
23	c	502	CLA	CHB-C1B-NB	-2.04	122.10	124.26
29	d	405[B]	PL9	C32-C33-C34	-2.04	122.75	127.66
23	c	511	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
23	B	613	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
24	A	407[B]	PHO	O2A-CGA-O1A	-2.04	118.45	123.59
26	a	411	SQD	O5-C5-C4	2.04	113.39	109.69
33	B	628	LMT	C3B-C4B-C5B	-2.04	106.61	110.24
23	b	602	CLA	CMA-C3A-C2A	-2.04	105.62	113.83
26	f	102	SQD	C44-O6-C1	-2.04	109.76	113.74
23	C	502	CLA	O2A-CGA-O1A	-2.04	118.46	123.59
23	C	513	CLA	C2A-C1A-CHA	-2.03	120.30	123.86
34	c	501	LMG	O8-C28-C29	2.03	118.29	111.91
25	t	102	BCR	C37-C22-C21	-2.03	120.07	122.92
33	T	101	LMT	O5B-C5B-C6B	2.03	111.49	106.44
23	C	508	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
36	C	519	DGD	O2G-C1B-C2B	2.03	115.88	111.50
25	y	101	BCR	C1-C6-C7	2.03	121.53	115.78
23	a	404[A]	CLA	CMB-C2B-C3B	2.03	131.51	126.59
23	a	408	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	b	601	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
23	B	604	CLA	C4-C3-C5	2.03	118.69	115.27
23	a	405[A]	CLA	CAC-C3C-C2C	2.03	131.00	127.53
26	a	410[A]	SQD	O48-C23-O10	-2.03	118.47	123.59
24	a	407[A]	PHO	CBC-CAC-C3C	-2.03	109.91	112.88
25	a	409	BCR	C2-C3-C4	-2.03	106.85	111.38
23	c	511	CLA	CED-O2D-CGD	2.03	120.52	115.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	BCR	C38-C26-C27	2.03	117.51	113.62
29	d	405[A]	PL9	C45-C44-C46	2.03	118.68	115.27
23	b	615	CLA	C2A-C1A-CHA	-2.03	120.32	123.86
23	B	606	CLA	CHB-C1B-C2B	-2.03	121.52	127.24
24	a	415[B]	PHO	CBC-CAC-C3C	-2.02	109.92	112.88
23	c	508	CLA	C1-C2-C3	-2.02	122.54	126.04
23	B	603	CLA	C2A-C3A-C4A	-2.02	98.60	101.87
23	b	613	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
23	c	511	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
23	b	603	CLA	C5-C3-C2	-2.02	117.02	121.12
34	c	501	LMG	O7-C10-O9	-2.02	118.82	123.70
24	a	415[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91
25	Y	101	BCR	C3-C4-C5	-2.02	110.47	114.08
23	B	614	CLA	CMA-C3A-C2A	-2.02	105.68	113.83
23	b	605	CLA	CHB-C1B-C2B	-2.02	121.53	127.24
23	c	513	CLA	CMC-C2C-C1C	2.02	128.12	125.04
23	b	613	CLA	CHB-C1B-NB	-2.02	122.12	124.26
23	b	609	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
23	c	513	CLA	C2A-C1A-CHA	-2.02	120.33	123.86
25	k	101	BCR	C39-C30-C25	-2.02	107.03	110.30
23	B	602	CLA	C4-C3-C5	2.02	118.67	115.27
23	c	506	CLA	C4-C3-C5	2.02	118.66	115.27
23	b	607	CLA	CHD-C4C-NC	2.02	127.38	124.20
24	A	417[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	d	402[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
23	A	405[B]	CLA	O2A-CGA-CBA	2.01	118.23	111.91
24	a	407[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
25	y	101	BCR	C37-C22-C23	2.01	121.25	118.08
23	A	406[B]	CLA	CHB-C4A-NA	2.01	127.30	124.51
23	b	613	CLA	CHB-C4A-NA	2.01	127.30	124.51
23	C	506	CLA	C11-C10-C8	-2.01	109.42	115.92
24	A	417[B]	PHO	CBA-CAA-C2A	-2.01	107.93	113.81
31	A	416[A]	BCT	O2-C-O1	2.01	124.76	119.55
27	A	418	GOL	C3-C2-C1	-2.01	103.89	111.70
23	D	402[A]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
31	d	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
23	D	403	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	B	608	CLA	OBD-CAD-C3D	-2.01	123.68	128.52
23	b	613	CLA	CHA-C1A-NA	-2.01	121.80	126.40
36	c	519	DGD	O2G-C1B-O1B	-2.01	118.85	123.70
23	B	613	CLA	CHD-C4C-NC	2.01	127.37	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	405[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
23	b	602	CLA	O2A-CGA-CBA	2.01	118.21	111.91
23	C	507	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	b	606	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
25	b	619	BCR	C31-C1-C6	-2.01	107.05	110.30
23	b	616	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
23	b	601	CLA	CAA-C2A-C3A	-2.01	107.29	112.78
27	a	417	GOL	C3-C2-C1	-2.01	103.91	111.70
23	C	509	CLA	CMB-C2B-C1B	2.00	128.42	125.37
23	c	513	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
23	b	616	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
36	c	518[B]	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
23	A	404[B]	CLA	CHB-C1B-C2B	-2.00	121.58	127.24
25	c	516	BCR	C16-C17-C18	-2.00	124.45	127.31
34	m	101	LMG	C3-C4-C5	2.00	113.81	110.24
23	B	615	CLA	O2A-CGA-O1A	-2.00	118.54	123.59

All (2) chirality outliers are listed below:

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

All (1668) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	606	CLA	CHA-CBD-CGD-O1D
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	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	CHA-CBD-CGD-O1D
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	508	CLA	C2-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C4-C3-C5-C6
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	403	CLA	C4-C3-C5-C6
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	C8-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	F	103	SQD	C2-C1-O6-C44
26	F	103	SQD	O49-C7-O47-C45
26	F	103	SQD	C8-C7-O47-C45
26	L	101	SQD	O5-C1-O6-C44
26	L	101	SQD	O49-C7-O47-C45
26	a	411	SQD	O6-C44-C45-O47
26	a	411	SQD	C5-C6-S-O7
26	a	411	SQD	C5-C6-S-O8
26	a	411	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	B	622	GOL	C1-C2-C3-O3
27	B	622	GOL	O2-C2-C3-O3
27	B	627	GOL	O1-C1-C2-C3
27	D	412	GOL	C1-C2-C3-O3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	O2-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
27	o	304	GOL	C1-C2-C3-O3
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C15-C14-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	A	414[B]	PL9	C14-C16-C17-C18
29	a	413[A]	PL9	C9-C11-C12-C13
29	a	413[A]	PL9	C14-C16-C17-C18
29	a	413[A]	PL9	C25-C24-C26-C27
29	a	413[B]	PL9	C9-C11-C12-C13
29	a	413[B]	PL9	C14-C16-C17-C18
29	a	413[B]	PL9	C23-C24-C26-C27
29	a	413[B]	PL9	C25-C24-C26-C27
32	D	406[A]	LHG	O2-C2-C3-O3
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5
32	D	406[A]	LHG	C3-O3-P-O6
32	D	406[A]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	O2-C2-C3-O3
32	D	406[B]	LHG	C3-O3-P-O4
32	D	406[B]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C4-O6-P-O5
32	D	407[B]	LHG	C4-O6-P-O4
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	102[A]	LHG	C4-O6-P-O4
32	L	102[A]	LHG	C4-O6-P-O5
32	L	102[B]	LHG	C4-O6-P-O4
32	a	419[A]	LHG	C3-O3-P-O4
32	a	419[A]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	O10-C23-O8-C6
32	a	419[A]	LHG	C24-C23-O8-C6
32	a	419[B]	LHG	C3-O3-P-O4
32	a	419[B]	LHG	C4-O6-P-O5
32	a	419[B]	LHG	O10-C23-O8-C6
32	a	419[B]	LHG	C24-C23-O8-C6
32	b	630[A]	LHG	C4-O6-P-O3
32	b	630[A]	LHG	C4-O6-P-O4
32	b	630[A]	LHG	C4-O6-P-O5
32	b	630[B]	LHG	C4-O6-P-O4
32	b	630[B]	LHG	C4-O6-P-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	d	406[A]	LHG	C3-O3-P-O5
32	d	406[A]	LHG	C4-O6-P-O4
32	d	406[B]	LHG	C3-O3-P-O4
32	d	406[B]	LHG	C3-O3-P-O5
32	d	406[B]	LHG	C3-O3-P-O6
32	d	406[B]	LHG	C4-O6-P-O4
32	d	412[A]	LHG	C3-O3-P-O5
33	A	420	LMT	O5'-C1'-O1'-C1
33	B	628	LMT	C2'-C1'-O1'-C1
33	B	629	LMT	O5'-C1'-O1'-C1
33	B	629	LMT	C2-C1-O1'-C1'
33	D	401	LMT	C2'-C1'-O1'-C1
33	D	401	LMT	O5'-C1'-O1'-C1
33	F	101	LMT	C2'-C1'-O1'-C1
33	F	101	LMT	O5'-C1'-O1'-C1
33	T	101	LMT	C2-C1-O1'-C1'
33	b	627	LMT	C2'-C1'-O1'-C1
33	b	627	LMT	O5'-C1'-O1'-C1
33	t	101	LMT	O5'-C1'-O1'-C1
33	t	101	LMT	C2-C1-O1'-C1'
34	C	521	LMG	C11-C10-O7-C8
34	c	521	LMG	O9-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
35	c	522	HTG	C2'-C1'-S1-C1
35	o	301	HTG	C2'-C1'-S1-C1
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
33	B	628	LMT	C4'-C5'-C6'-O6'
33	A	420	LMT	O5B-C1B-O1B-C4'
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
34	z	101	LMG	O9-C10-O7-C8
23	b	616	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
33	a	416	LMT	O5B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	L	101	SQD	C8-C7-O47-C45
34	c	521	LMG	C11-C10-O7-C8
34	z	101	LMG	C11-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	T	101	LMT	O5'-C5'-C6'-O6'
23	C	505	CLA	C4-C3-C5-C6
23	a	408	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
33	B	626	LMT	C4'-C5'-C6'-O6'
33	T	101	LMT	C4B-C5B-C6B-O6B
23	A	408	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	d	403	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C18-C19-C21-C22
23	B	614	CLA	C3-C5-C6-C7
23	D	403	CLA	C3-C5-C6-C7
33	B	626	LMT	O5'-C5'-C6'-O6'
33	F	101	LMT	O5'-C5'-C6'-O6'
35	D	410	HTG	O5-C5-C6-O6
33	m	103	LMT	C4B-C5B-C6B-O6B
33	B	626	LMT	C6-C7-C8-C9
35	D	410	HTG	S1-C1'-C2'-C3'
35	b	625	HTG	S1-C1'-C2'-C3'
33	m	103	LMT	O5B-C5B-C6B-O6B
34	C	521	LMG	O9-C10-O7-C8
33	B	628	LMT	O5B-C5B-C6B-O6B
33	b	621	LMT	O5'-C5'-C6'-O6'
23	C	514	CLA	CBD-CGD-O2D-CED
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	406[A]	LHG	O2-C2-C3-O3
32	d	406[B]	LHG	O2-C2-C3-O3
23	B	616	CLA	C3-C5-C6-C7
34	c	521	LMG	C4-C5-C6-O5
23	C	504	CLA	CBD-CGD-O2D-CED
23	c	514	CLA	CBD-CGD-O2D-CED
34	C	521	LMG	O6-C5-C6-O5
35	b	625	HTG	O5-C5-C6-O6
33	a	416	LMT	C4B-C5B-C6B-O6B
40	V	201	HEC	C2C-C3C-CAC-CBC
35	D	410	HTG	C4-C5-C6-O6
33	A	420	LMT	O5B-C5B-C6B-O6B
33	A	420	LMT	O5'-C5'-C6'-O6'
33	B	629	LMT	O5'-C5'-C6'-O6'
33	b	627	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	T	101	LMT	C4'-C5'-C6'-O6'
33	e	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	413[A]	PL9	C15-C14-C16-C17
29	a	413[A]	PL9	C30-C29-C31-C32
29	a	413[B]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C30-C29-C31-C32
33	F	101	LMT	C4'-C5'-C6'-O6'
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	614	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C28-C29-C31-C32
29	a	413[B]	PL9	C13-C14-C16-C17
29	a	413[B]	PL9	C28-C29-C31-C32
23	b	606	CLA	C2A-CAA-CBA-CGA
36	h	102	DGD	C6B-C7B-C8B-C9B
33	B	626	LMT	O5B-C5B-C6B-O6B
33	B	628	LMT	O5'-C5'-C6'-O6'
33	T	101	LMT	O5B-C5B-C6B-O6B
33	e	101	LMT	O5'-C1'-O1'-C1
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[A]	PL9	C39-C41-C42-C43
36	C	519	DGD	C6B-C7B-C8B-C9B
23	B	605	CLA	CBD-CGD-O2D-CED
33	t	101	LMT	O5'-C5'-C6'-O6'
33	B	628	LMT	C4B-C5B-C6B-O6B
33	A	420	LMT	C4B-C5B-C6B-O6B
34	B	620	LMG	C39-C40-C41-C42
34	B	620	LMG	C15-C16-C17-C18
32	d	406[A]	LHG	C1-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
23	a	408	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	b	623	HTG	C1'-C2'-C3'-C4'
32	D	407[A]	LHG	C33-C34-C35-C36
33	B	629	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
32	E	101[B]	LHG	O2-C2-C3-O3
33	A	420	LMT	C2'-C1'-O1'-C1
33	B	629	LMT	C2'-C1'-O1'-C1
33	t	101	LMT	C2'-C1'-O1'-C1
40	V	201	HEC	C4C-C3C-CAC-CBC
40	v	201	HEC	C2C-C3C-CAC-CBC
34	c	521	LMG	O6-C5-C6-O5
33	b	621	LMT	C4'-C5'-C6'-O6'
23	a	408	CLA	C2-C3-C5-C6
29	a	413[A]	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
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
23	c	505	CLA	C11-C12-C13-C14
23	c	514	CLA	C6-C7-C8-C9
26	L	101	SQD	C30-C31-C32-C33
23	B	606	CLA	C2A-CAA-CBA-CGA
33	b	627	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C10-C11-C12-C13
23	B	606	CLA	C10-C11-C12-C13
40	V	201	HEC	C2B-C3B-CAB-CBB
23	b	611	CLA	C15-C16-C17-C18
23	c	513	CLA	C15-C16-C17-C18
35	B	623	HTG	O5-C5-C6-O6
36	c	518[B]	DGD	C1B-C2B-C3B-C4B
33	B	626	LMT	C4B-C5B-C6B-O6B
33	A	420	LMT	C5'-C4'-O1B-C1B
33	B	626	LMT	C5'-C4'-O1B-C1B
33	e	101	LMT	O5'-C5'-C6'-O6'
23	A	408	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
23	C	508	CLA	C5-C6-C7-C8
23	b	611	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C8-C10-C11-C12
26	b	620	SQD	C18-C19-C20-C21
27	B	627	GOL	O1-C1-C2-O2
27	O	302	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
26	A	410[B]	SQD	C7-C8-C9-C10
26	F	103	SQD	C23-C24-C25-C26
26	L	101	SQD	C7-C8-C9-C10
23	B	603	CLA	C13-C15-C16-C17
23	c	510	CLA	CBA-CGA-O2A-C1
35	b	622	HTG	S1-C1'-C2'-C3'
35	d	409	HTG	S1-C1'-C2'-C3'
23	B	616	CLA	C2-C1-O2A-CGA
33	A	420	LMT	O1'-C1-C2-C3
32	E	101[A]	LHG	C23-C24-C25-C26
34	Z	101	LMG	C10-C11-C12-C13
36	c	518[A]	DGD	C1B-C2B-C3B-C4B
23	C	502	CLA	CBD-CGD-O2D-CED
23	c	513	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	c	510	CLA	C3-C5-C6-C7
23	a	408	CLA	O1A-CGA-O2A-C1
23	c	510	CLA	O1A-CGA-O2A-C1
33	a	416	LMT	O1'-C1-C2-C3
23	B	614	CLA	C8-C10-C11-C12
23	C	511	CLA	C10-C11-C12-C13
33	A	420	LMT	C4'-C5'-C6'-O6'
26	F	103	SQD	O5-C1-O6-C44
33	B	628	LMT	O5'-C1'-O1'-C1
33	b	621	LMT	O5'-C1'-O1'-C1
29	A	414[A]	PL9	C44-C46-C47-C48
29	D	405[B]	PL9	C39-C41-C42-C43
29	d	405[A]	PL9	C39-C41-C42-C43
29	d	405[B]	PL9	C39-C41-C42-C43
32	E	101[B]	LHG	C23-C24-C25-C26
35	B	623	HTG	S1-C1'-C2'-C3'
36	c	517[B]	DGD	O6D-C5D-C6D-O5D
32	D	407[B]	LHG	C33-C34-C35-C36
33	e	101	LMT	O5B-C5B-C6B-O6B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C3-C5-C6-C7
23	c	514	CLA	C10-C11-C12-C13
36	C	519	DGD	CAB-CBB-CCB-CDB
23	a	404[B]	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13
23	c	507	CLA	C15-C16-C17-C18
23	B	614	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
23	a	404[A]	CLA	C15-C16-C17-C18
23	b	606	CLA	C13-C15-C16-C17
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	L	102[A]	LHG	C4-O6-P-O3
32	L	102[B]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C4-O6-P-O3
32	a	419[B]	LHG	C3-O3-P-O6
32	a	419[B]	LHG	C4-O6-P-O3
32	b	630[B]	LHG	C4-O6-P-O3
32	d	406[A]	LHG	C3-O3-P-O6
35	o	301	HTG	C1'-C2'-C3'-C4'
26	A	410[A]	SQD	C7-C8-C9-C10
32	D	406[A]	LHG	C1-C2-C3-O3
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	406[B]	LHG	C1-C2-C3-O3
34	Z	101	LMG	O6-C5-C6-O5
34	B	620	LMG	O9-C10-O7-C8
23	b	604	CLA	C5-C6-C7-C8
23	b	610	CLA	C2A-CAA-CBA-CGA
36	C	519	DGD	C2B-C3B-C4B-C5B
25	T	102	BCR	C13-C14-C15-C16
26	A	410[A]	SQD	C15-C16-C17-C18
32	L	102[A]	LHG	C12-C13-C14-C15
32	L	102[B]	LHG	C12-C13-C14-C15
23	D	403	CLA	CBD-CGD-O2D-CED
34	B	620	LMG	C11-C10-O7-C8
26	F	103	SQD	C30-C31-C32-C33
26	f	102	SQD	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	D	406[B]	LHG	C16-C17-C18-C19
32	L	102[A]	LHG	C17-C18-C19-C20
32	d	412[A]	LHG	C16-C17-C18-C19
33	b	627	LMT	C7-C8-C9-C10
34	B	620	LMG	C34-C35-C36-C37
36	C	517[B]	DGD	C5B-C6B-C7B-C8B
36	c	517[B]	DGD	C2B-C3B-C4B-C5B
36	c	518[A]	DGD	CAA-CBA-CCA-CDA
36	c	518[B]	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	C7B-C8B-C9B-CAB
23	a	408	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
32	L	102[B]	LHG	C13-C14-C15-C16
33	A	420	LMT	C3-C4-C5-C6
34	D	411	LMG	C35-C36-C37-C38
35	b	622	HTG	C2'-C3'-C4'-C5'
36	c	518[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[B]	DGD	CAA-CBA-CCA-CDA
36	c	518[B]	DGD	CBA-CCA-CDA-CEA
26	A	410[B]	SQD	C15-C16-C17-C18
32	L	102[B]	LHG	C17-C18-C19-C20
34	C	521	LMG	C18-C19-C20-C21
36	C	518[A]	DGD	CCB-CDB-CEB-CFB
33	M	101	LMT	O5'-C5'-C6'-O6'
34	D	411	LMG	C30-C31-C32-C33
35	B	621	HTG	C3'-C4'-C5'-C6'
36	c	517[A]	DGD	C2B-C3B-C4B-C5B
36	c	517[B]	DGD	C9A-CAA-CBA-CCA
23	D	403	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
26	F	103	SQD	C24-C25-C26-C27
32	L	102[B]	LHG	C25-C26-C27-C28
33	D	401	LMT	O1'-C1-C2-C3
36	C	517[A]	DGD	C4B-C5B-C6B-C7B
26	A	412	SQD	C2-C1-O6-C44
33	b	621	LMT	C2'-C1'-O1'-C1
33	e	101	LMT	C2'-C1'-O1'-C1
36	C	518[A]	DGD	C2E-C1E-O5D-C6D
32	D	407[B]	LHG	C32-C33-C34-C35
34	C	501	LMG	C17-C18-C19-C20
34	D	411	LMG	C19-C20-C21-C22
36	C	517[A]	DGD	C5B-C6B-C7B-C8B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	c	517[A]	DGD	C9A-CAA-CBA-CCA
23	b	614	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C45-C44-C46-C47
32	A	419[B]	LHG	C34-C35-C36-C37
32	D	406[A]	LHG	C16-C17-C18-C19
32	a	419[A]	LHG	C26-C27-C28-C29
32	b	630[A]	LHG	C14-C15-C16-C17
32	b	630[B]	LHG	C14-C15-C16-C17
32	d	412[B]	LHG	C16-C17-C18-C19
33	e	101	LMT	C4-C5-C6-C7
33	t	101	LMT	C4-C5-C6-C7
34	C	501	LMG	C12-C13-C14-C15
36	H	102	DGD	C5B-C6B-C7B-C8B
29	d	405[A]	PL9	C13-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C14
23	a	406[A]	CLA	C11-C12-C13-C14
23	a	406[B]	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
32	D	407[A]	LHG	C32-C33-C34-C35
32	L	102[A]	LHG	C15-C16-C17-C18
34	C	521	LMG	C17-C18-C19-C20
34	c	520	LMG	C34-C35-C36-C37
36	c	519	DGD	CBB-CCB-CDB-CEB
23	B	610	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
36	c	517[B]	DGD	C4D-C5D-C6D-O5D
25	b	619	BCR	C7-C8-C9-C34
32	a	419[B]	LHG	C26-C27-C28-C29
32	d	412[A]	LHG	C32-C33-C34-C35
33	B	628	LMT	C2-C3-C4-C5
33	e	101	LMT	C5-C6-C7-C8
36	C	518[B]	DGD	CCB-CDB-CEB-CFB
36	c	518[A]	DGD	CBA-CCA-CDA-CEA
27	A	411	GOL	O1-C1-C2-C3
27	B	627	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	417	GOL	O1-C1-C2-C3
27	d	411	GOL	O1-C1-C2-C3
27	l	102[B]	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
27	v	202[B]	GOL	O1-C1-C2-C3
25	b	619	BCR	C7-C8-C9-C10
23	C	510	CLA	C3-C5-C6-C7
36	c	517[B]	DGD	O6E-C5E-C6E-O5E
32	A	419[B]	LHG	C12-C13-C14-C15
32	L	102[A]	LHG	C25-C26-C27-C28
33	t	101	LMT	C4'-C5'-C6'-O6'
34	c	520	LMG	C10-C11-C12-C13
26	A	412	SQD	C17-C18-C19-C20
32	A	419[A]	LHG	C34-C35-C36-C37
32	d	406[A]	LHG	C11-C10-C9-C8
33	B	628	LMT	C5-C6-C7-C8
34	c	501	LMG	C30-C31-C32-C33
34	c	501	LMG	C34-C35-C36-C37
34	m	101	LMG	C39-C40-C41-C42
36	C	517[B]	DGD	C4B-C5B-C6B-C7B
36	H	102	DGD	CCB-CDB-CEB-CFB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	a	408	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C19
23	d	403	CLA	C16-C17-C18-C20
26	A	412	SQD	O5-C1-O6-C44
23	b	606	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C12-C13-C14-C15
32	d	407[B]	LHG	C27-C28-C29-C30
33	B	626	LMT	C5-C6-C7-C8
32	L	102[A]	LHG	C13-C14-C15-C16
32	d	406[A]	LHG	C34-C35-C36-C37
34	m	101	LMG	C35-C36-C37-C38
36	H	102	DGD	C7A-C8A-C9A-CAA
26	a	411	SQD	C25-C26-C27-C28
32	d	407[A]	LHG	C27-C28-C29-C30
33	B	629	LMT	C3-C4-C5-C6
33	B	629	LMT	C4-C5-C6-C7
34	d	410	LMG	C29-C30-C31-C32
33	A	420	LMT	C1-C2-C3-C4
23	C	513	CLA	CBA-CGA-O2A-C1
36	C	517[B]	DGD	O6D-C5D-C6D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	E	101[B]	LHG	C24-C25-C26-C27
34	C	501	LMG	C19-C20-C21-C22
34	C	520	LMG	C16-C17-C18-C19
34	C	520	LMG	C17-C18-C19-C20
23	C	507	CLA	C5-C6-C7-C8
33	a	416	LMT	C1-C2-C3-C4
33	A	420	LMT	C2-C1-O1'-C1'
33	F	101	LMT	C2-C1-O1'-C1'
33	b	627	LMT	C2-C1-O1'-C1'
34	c	520	LMG	C33-C34-C35-C36
23	C	514	CLA	O1D-CGD-O2D-CED
23	B	603	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
26	a	411	SQD	C31-C32-C33-C34
32	A	419[A]	LHG	C12-C13-C14-C15
32	b	630[A]	LHG	C16-C17-C18-C19
33	M	101	LMT	C3-C4-C5-C6
33	T	101	LMT	C7-C8-C9-C10
32	E	101[A]	LHG	C24-C25-C26-C27
32	d	406[B]	LHG	C34-C35-C36-C37
33	m	103	LMT	C7-C8-C9-C10
34	B	620	LMG	C17-C18-C19-C20
36	h	102	DGD	C9A-CAA-CBA-CCA
36	h	102	DGD	CAA-CBA-CCA-CDA
36	c	517[A]	DGD	O6D-C5D-C6D-O5D
34	C	501	LMG	C10-C11-C12-C13
26	F	103	SQD	C29-C30-C31-C32
29	D	405[B]	PL9	C15-C14-C16-C17
29	d	405[A]	PL9	C15-C14-C16-C17
36	c	517[A]	DGD	C2A-C1A-O1G-C1G
24	a	407[B]	PHO	C2-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[A]	PL9	C43-C44-C46-C47
29	D	405[A]	PL9	C13-C14-C16-C17
29	d	405[B]	PL9	C13-C14-C16-C17
36	c	519	DGD	C2B-C3B-C4B-C5B
27	D	412	GOL	O1-C1-C2-O2
27	b	624	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
32	d	412[B]	LHG	C32-C33-C34-C35
34	m	101	LMG	C38-C39-C40-C41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	c	518[A]	DGD	CBB-CCB-CDB-CEB
23	b	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
23	C	508	CLA	C2B-C3B-CAB-CBB
23	a	406[A]	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
23	A	406[B]	CLA	C13-C15-C16-C17
32	D	407[A]	LHG	C15-C16-C17-C18
34	C	521	LMG	C19-C20-C21-C22
36	H	102	DGD	C9B-CAB-CBB-CCB
36	c	517[A]	DGD	C5A-C6A-C7A-C8A
36	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	C	510	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C13-C14-C15-C16
32	d	412[A]	LHG	C29-C30-C31-C32
34	D	411	LMG	C36-C37-C38-C39
23	A	404[B]	CLA	C13-C15-C16-C17
23	C	513	CLA	C10-C11-C12-C13
33	B	629	LMT	O1'-C1-C2-C3
33	B	629	LMT	C11-C10-C9-C8
36	c	517[A]	DGD	C7A-C8A-C9A-CAA
34	c	501	LMG	C10-C11-C12-C13
33	b	621	LMT	C3'-C4'-O1B-C1B
25	D	404	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
36	c	518[B]	DGD	CBB-CCB-CDB-CEB
36	h	102	DGD	C2B-C3B-C4B-C5B
23	C	503	CLA	C15-C16-C17-C18
34	m	101	LMG	C11-C10-O7-C8
36	c	518[A]	DGD	C6A-C7A-C8A-C9A
23	C	513	CLA	O1A-CGA-O2A-C1
35	b	622	HTG	C3'-C4'-C5'-C6'
36	c	519	DGD	CBA-CCA-CDA-CEA
23	B	608	CLA	C13-C15-C16-C17
23	b	614	CLA	C10-C11-C12-C13
33	B	626	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	C	501	LMG	C36-C37-C38-C39
23	D	403	CLA	C4-C3-C5-C6
24	a	407[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C15-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C10-C8-C7
23	a	406[A]	CLA	C11-C12-C13-C15
23	a	406[B]	CLA	C11-C12-C13-C15
23	c	505	CLA	C12-C13-C15-C16
29	A	414[B]	PL9	C12-C11-C9-C8
29	D	405[B]	PL9	C13-C14-C16-C17
33	A	420	LMT	C3'-C4'-O1B-C1B
34	c	520	LMG	C31-C32-C33-C34
26	A	412	SQD	C26-C27-C28-C29
26	L	101	SQD	C11-C10-C9-C8
32	D	407[A]	LHG	C29-C30-C31-C32
32	D	407[B]	LHG	C15-C16-C17-C18
33	e	101	LMT	C1-C2-C3-C4
23	C	512	CLA	C8-C10-C11-C12
26	b	620	SQD	C27-C28-C29-C30
32	D	406[A]	LHG	C13-C14-C15-C16
32	b	630[B]	LHG	C12-C13-C14-C15
33	B	628	LMT	C6-C7-C8-C9
33	b	627	LMT	C5-C6-C7-C8
32	b	630[B]	LHG	C27-C28-C29-C30
32	d	407[B]	LHG	C25-C26-C27-C28
32	d	412[B]	LHG	C24-C25-C26-C27
36	C	517[A]	DGD	C8A-C9A-CAA-CBA
36	c	517[A]	DGD	O1A-C1A-O1G-C1G
23	B	610	CLA	C16-C17-C18-C19
36	C	518[A]	DGD	O6E-C1E-O5D-C6D
36	c	517[B]	DGD	O6E-C1E-O5D-C6D
36	c	518[B]	DGD	O6E-C1E-O5D-C6D
23	b	604	CLA	C15-C16-C17-C18
26	a	410[A]	SQD	C9-C10-C11-C12
26	a	410[B]	SQD	C9-C10-C11-C12
26	a	410[B]	SQD	C12-C13-C14-C15
32	b	630[B]	LHG	C16-C17-C18-C19
33	b	621	LMT	C11-C10-C9-C8
34	C	521	LMG	C13-C14-C15-C16
36	C	517[B]	DGD	C8A-C9A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	L	101	SQD	C34-C35-C36-C37
32	d	407[B]	LHG	C29-C30-C31-C32
33	b	627	LMT	C3-C4-C5-C6
26	f	102	SQD	C25-C26-C27-C28
36	c	517[B]	DGD	CAA-CBA-CCA-CDA
34	m	101	LMG	O9-C10-O7-C8
36	C	517[B]	DGD	C4D-C5D-C6D-O5D
26	A	412	SQD	C27-C28-C29-C30
32	L	102[B]	LHG	C15-C16-C17-C18
36	c	518[B]	DGD	C2B-C3B-C4B-C5B
23	C	504	CLA	O1D-CGD-O2D-CED
36	c	517[B]	DGD	C2E-C1E-O5D-C6D
36	c	518[B]	DGD	C2E-C1E-O5D-C6D
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
34	C	520	LMG	C31-C32-C33-C34
36	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	B	610	CLA	C16-C17-C18-C20
26	b	620	SQD	C14-C15-C16-C17
36	C	517[A]	DGD	C9A-CAA-CBA-CCA
36	c	518[A]	DGD	C2B-C3B-C4B-C5B
29	A	414[B]	PL9	C45-C44-C46-C47
23	D	403	CLA	C2-C3-C5-C6
23	b	609	CLA	C2-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
23	D	403	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
36	C	517[A]	DGD	O6E-C5E-C6E-O5E
26	b	620	SQD	C26-C27-C28-C29
32	b	630[A]	LHG	C13-C14-C15-C16
36	c	518[B]	DGD	C6A-C7A-C8A-C9A
23	b	607	CLA	C3-C5-C6-C7
23	B	601	CLA	C2A-CAA-CBA-CGA
33	B	626	LMT	C1-C2-C3-C4
32	d	412[B]	LHG	C25-C26-C27-C28
34	c	501	LMG	C35-C36-C37-C38
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	b	614	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
32	D	407[A]	LHG	C17-C18-C19-C20
35	o	301	HTG	C2'-C3'-C4'-C5'
23	A	406[A]	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	t	101	LMT	O1'-C1-C2-C3
34	m	101	LMG	C37-C38-C39-C40
23	c	514	CLA	O1D-CGD-O2D-CED
34	c	520	LMG	C4-C5-C6-O5
32	d	406[B]	LHG	C24-C23-O8-C6
36	c	517[B]	DGD	C2A-C1A-O1G-C1G
36	h	102	DGD	CAB-CBB-CCB-CDB
36	C	517[B]	DGD	O6E-C5E-C6E-O5E
23	A	404[A]	CLA	C13-C15-C16-C17
23	C	511	CLA	C13-C15-C16-C17
23	d	402[A]	CLA	C16-C17-C18-C20
32	d	407[A]	LHG	C25-C26-C27-C28
32	d	412[B]	LHG	C29-C30-C31-C32
36	c	517[B]	DGD	C5A-C6A-C7A-C8A
23	B	605	CLA	O1D-CGD-O2D-CED
23	c	513	CLA	CBA-CGA-O2A-C1
23	d	403	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C31-C32-C33-C34
34	c	501	LMG	C29-C30-C31-C32
34	C	520	LMG	C36-C37-C38-C39
36	c	518[A]	DGD	C4A-C5A-C6A-C7A
36	c	518[B]	DGD	C4A-C5A-C6A-C7A
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	L	101	SQD	C44-C45-C46-O48
26	a	410[A]	SQD	O6-C44-C45-C46
26	a	410[B]	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	D	407[B]	LHG	C29-C30-C31-C32
32	E	101[B]	LHG	C4-C5-C6-O8
34	c	501	LMG	C7-C8-C9-O8
23	B	614	CLA	C5-C6-C7-C8
23	b	601	CLA	C8-C10-C11-C12
32	E	101[A]	LHG	C25-C26-C27-C28
36	C	518[A]	DGD	C2G-C3G-O3G-C1D
36	C	518[A]	DGD	C5D-C6D-O5D-C1E
36	C	518[B]	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	D	411	LMG	C12-C13-C14-C15
35	c	522	HTG	C4'-C5'-C6'-C7'
36	C	518[A]	DGD	CDA-CEA-CFA-CGA
23	C	503	CLA	C13-C15-C16-C17
32	L	102[B]	LHG	C27-C28-C29-C30
33	a	416	LMT	C2-C3-C4-C5
36	C	518[B]	DGD	CDA-CEA-CFA-CGA
36	c	517[A]	DGD	C4D-C5D-C6D-O5D
34	D	411	LMG	O6-C5-C6-O5
35	b	623	HTG	O5-C5-C6-O6
23	d	403	CLA	O1A-CGA-O2A-C1
36	C	517[A]	DGD	C3B-C4B-C5B-C6B
23	B	615	CLA	C10-C11-C12-C13
29	a	413[B]	PL9	C24-C26-C27-C28
27	A	411	GOL	O1-C1-C2-O2
27	B	627	GOL	O2-C2-C3-O3
27	D	412	GOL	O2-C2-C3-O3
27	o	304	GOL	O2-C2-C3-O3
23	b	610	CLA	C15-C16-C17-C18
33	a	416	LMT	O5'-C5'-C6'-O6'
32	d	412[B]	LHG	C33-C34-C35-C36
23	A	405[A]	CLA	C15-C16-C17-C18
23	B	615	CLA	C5-C6-C7-C8
34	d	410	LMG	O6-C5-C6-O5
36	c	517[A]	DGD	O6E-C5E-C6E-O5E
23	C	511	CLA	C4-C3-C5-C6
23	b	609	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
29	a	413[A]	PL9	C12-C11-C9-C10
29	a	413[B]	PL9	C12-C11-C9-C10
32	d	407[B]	LHG	C28-C29-C30-C31
36	h	102	DGD	CDB-CEB-CFB-CGB
34	c	520	LMG	C28-C29-C30-C31
33	A	420	LMT	C4-C5-C6-C7
34	C	521	LMG	C35-C36-C37-C38
40	v	201	HEC	C2B-C3B-CAB-CBB
23	B	602	CLA	C15-C16-C17-C18
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
32	d	412[A]	LHG	C33-C34-C35-C36
26	b	620	SQD	C46-C45-O47-C7
33	m	103	LMT	O5'-C5'-C6'-O6'
23	b	608	CLA	C2-C1-O2A-CGA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C11-C10-C9-C8
32	d	407[A]	LHG	C34-C35-C36-C37
34	z	101	LMG	C14-C15-C16-C17
26	a	410[A]	SQD	C12-C13-C14-C15
32	D	406[A]	LHG	C12-C13-C14-C15
33	a	416	LMT	C9-C10-C11-C12
33	e	101	LMT	C3-C4-C5-C6
26	b	620	SQD	C24-C23-O48-C46
34	c	521	LMG	C29-C28-O8-C9
36	c	519	DGD	C2A-C1A-O1G-C1G
23	d	402[B]	CLA	C16-C17-C18-C20
36	H	102	DGD	CAB-CBB-CCB-CDB
32	d	406[B]	LHG	O10-C23-O8-C6
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
34	C	501	LMG	C13-C14-C15-C16
35	b	622	HTG	C1'-C2'-C3'-C4'
23	B	601	CLA	C13-C15-C16-C17
23	B	601	CLA	C15-C16-C17-C18
36	C	518[B]	DGD	C2E-C1E-O5D-C6D
34	B	620	LMG	O8-C28-C29-C30
26	a	410[B]	SQD	O6-C44-C45-O47
32	D	406[B]	LHG	C13-C14-C15-C16
36	C	517[A]	DGD	O6D-C5D-C6D-O5D
36	c	517[B]	DGD	O1A-C1A-O1G-C1G
23	d	402[A]	CLA	C16-C17-C18-C19
32	D	407[B]	LHG	C13-C14-C15-C16
32	D	407[B]	LHG	C17-C18-C19-C20
32	d	407[A]	LHG	C29-C30-C31-C32
34	C	520	LMG	C30-C31-C32-C33
32	d	407[B]	LHG	C34-C35-C36-C37
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	C	503	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	511	CLA	C2-C3-C5-C6
23	D	403	CLA	C12-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C2-C3-C5-C6
23	c	507	CLA	C11-C10-C8-C7
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	514	CLA	C11-C10-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
32	d	407[A]	LHG	C28-C29-C30-C31
33	b	621	LMT	C7-C8-C9-C10
34	C	501	LMG	C39-C40-C41-C42
32	D	407[B]	LHG	C24-C23-O8-C6
32	A	419[B]	LHG	C18-C19-C20-C21
23	b	606	CLA	C16-C17-C18-C20
36	c	517[B]	DGD	C7A-C8A-C9A-CAA
27	B	625	GOL	C1-C2-C3-O3
32	b	630[A]	LHG	C27-C28-C29-C30
33	A	420	LMT	C5-C6-C7-C8
23	b	601	CLA	CBA-CGA-O2A-C1
26	a	411	SQD	C16-C17-C18-C19
35	B	623	HTG	C4'-C5'-C6'-C7'
36	C	518[A]	DGD	C5B-C6B-C7B-C8B
23	A	406[A]	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C4B-C3B-CAB-CBB
23	D	402[B]	CLA	C4B-C3B-CAB-CBB
23	a	406[A]	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
23	B	613	CLA	C13-C15-C16-C17
32	E	101[A]	LHG	O6-C4-C5-C6
32	b	630[A]	LHG	O6-C4-C5-C6
23	C	509	CLA	O1D-CGD-O2D-CED
32	D	406[A]	LHG	C10-C11-C12-C13
32	D	407[A]	LHG	C13-C14-C15-C16
32	d	407[A]	LHG	C9-C10-C11-C12
23	B	610	CLA	C13-C15-C16-C17
23	c	513	CLA	C10-C11-C12-C13
33	b	621	LMT	C3-C4-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	d	405[A]	PL9	C45-C44-C46-C47
32	A	419[A]	LHG	C26-C27-C28-C29
32	d	406[A]	LHG	C13-C14-C15-C16
32	d	406[B]	LHG	C11-C10-C9-C8
23	B	608	CLA	C16-C17-C18-C20
33	a	416	LMT	C3-C4-C5-C6
33	e	101	LMT	C9-C10-C11-C12
23	c	512	CLA	CBA-CGA-O2A-C1
34	C	520	LMG	C37-C38-C39-C40
36	C	517[A]	DGD	C7A-C8A-C9A-CAA
36	C	517[B]	DGD	C3B-C4B-C5B-C6B
23	c	513	CLA	O1D-CGD-O2D-CED
32	D	406[B]	LHG	C12-C13-C14-C15
33	B	626	LMT	C2-C1-O1'-C1'
33	e	101	LMT	C2-C1-O1'-C1'
32	d	407[B]	LHG	C9-C10-C11-C12
36	h	102	DGD	C9B-CAB-CBB-CCB
32	E	101[B]	LHG	C25-C26-C27-C28
34	Z	101	LMG	C19-C20-C21-C22
36	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	c	510	CLA	C15-C16-C17-C18
26	A	410[B]	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
32	a	419[A]	LHG	C4-C5-C6-O8
32	a	419[B]	LHG	C4-C5-C6-O8
32	L	102[A]	LHG	C24-C25-C26-C27
32	a	419[A]	LHG	C10-C11-C12-C13
33	t	101	LMT	C7-C8-C9-C10
34	C	520	LMG	C34-C35-C36-C37
36	C	517[B]	DGD	C7A-C8A-C9A-CAA
32	b	630[A]	LHG	C12-C13-C14-C15
24	a	407[A]	PHO	O2A-C1-C2-C3
32	D	407[B]	LHG	C10-C11-C12-C13
40	v	201	HEC	C4C-C3C-CAC-CBC
23	C	502	CLA	O1D-CGD-O2D-CED
36	c	518[A]	DGD	C5A-C6A-C7A-C8A
36	h	102	DGD	CBA-CCA-CDA-CEA
36	c	519	DGD	O1A-C1A-O1G-C1G
24	a	407[A]	PHO	C4-C3-C5-C6
29	A	414[B]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C43-C44-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	F	103	SQD	C34-C35-C36-C37
32	L	102[A]	LHG	C11-C12-C13-C14
24	A	417[B]	PHO	C2C-C3C-CAC-CBC
32	b	630[B]	LHG	C17-C18-C19-C20
40	V	201	HEC	C4B-C3B-CAB-CBB
32	d	406[B]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C7-C8-C9-C10
32	D	407[B]	LHG	O10-C23-O8-C6
35	b	622	HTG	O5-C5-C6-O6
27	a	417	GOL	O1-C1-C2-O2
27	c	527	GOL	O1-C1-C2-O2
27	o	303	GOL	O2-C2-C3-O3
32	E	101[B]	LHG	C17-C18-C19-C20
34	m	101	LMG	C11-C12-C13-C14
32	E	101[A]	LHG	O6-C4-C5-O7
26	A	410[B]	SQD	C12-C13-C14-C15
32	D	406[B]	LHG	C10-C11-C12-C13
33	a	416	LMT	C4'-C5'-C6'-O6'
23	c	513	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	O10-C23-O48-C46
34	c	521	LMG	O10-C28-O8-C9
23	A	406[A]	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
23	d	402[B]	CLA	C16-C17-C18-C19
32	b	630[A]	LHG	C31-C32-C33-C34
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	402[B]	CLA	C2B-C3B-CAB-CBB
23	c	512	CLA	O1A-CGA-O2A-C1
26	a	410[A]	SQD	C34-C35-C36-C37
26	a	410[A]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
34	c	501	LMG	O7-C8-C9-O8
32	d	407[B]	LHG	C24-C23-O8-C6
23	B	615	CLA	C13-C15-C16-C17
32	b	630[B]	LHG	C13-C14-C15-C16
36	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	C	502	CLA	C16-C17-C18-C20
32	E	101[A]	LHG	C17-C18-C19-C20
29	a	413[A]	PL9	C24-C26-C27-C28
26	b	620	SQD	C28-C29-C30-C31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	D	407[A]	LHG	C10-C11-C12-C13
32	a	419[B]	LHG	C10-C11-C12-C13
32	b	630[B]	LHG	C25-C26-C27-C28
32	b	630[B]	LHG	C34-C35-C36-C37
36	C	519	DGD	CDB-CEB-CFB-CGB
23	B	610	CLA	C14-C13-C15-C16
23	B	613	CLA	C11-C12-C13-C14
23	a	406[B]	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	d	403	CLA	C11-C12-C13-C14
23	C	511	CLA	CBA-CGA-O2A-C1
33	M	101	LMT	C2-C3-C4-C5
33	F	101	LMT	C2-C3-C4-C5
36	C	518[B]	DGD	C5B-C6B-C7B-C8B
32	D	407[B]	LHG	C2-C3-O3-P
32	d	407[B]	LHG	C2-C3-O3-P
34	B	620	LMG	C36-C37-C38-C39
34	C	501	LMG	C11-C12-C13-C14
36	C	518[A]	DGD	C8A-C9A-CAA-CBA
23	C	503	CLA	C16-C17-C18-C19
25	B	617	BCR	C5-C6-C7-C8
25	D	404	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	b	619	BCR	C1-C6-C7-C8
32	d	412[A]	LHG	C25-C26-C27-C28
34	Z	101	LMG	C11-C12-C13-C14
25	D	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C21-C22-C23-C24
23	B	612	CLA	C10-C11-C12-C13
23	b	602	CLA	C10-C11-C12-C13
32	D	406[B]	LHG	C26-C27-C28-C29
34	C	501	LMG	C18-C19-C20-C21
23	B	605	CLA	C5-C6-C7-C8
32	D	406[B]	LHG	O6-C4-C5-C6
32	b	630[B]	LHG	O6-C4-C5-C6
26	F	103	SQD	C32-C33-C34-C35
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	601	CLA	C6-C7-C8-C10
23	b	616	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
24	a	407[A]	PHO	C2-C3-C5-C6
29	A	414[B]	PL9	C43-C44-C46-C47
32	E	101[B]	LHG	C13-C14-C15-C16
23	c	510	CLA	C8-C10-C11-C12
23	c	512	CLA	C8-C10-C11-C12
25	t	102	BCR	C13-C14-C15-C16
32	L	102[A]	LHG	C11-C10-C9-C8
32	d	412[A]	LHG	C24-C25-C26-C27
34	d	410	LMG	C10-C11-C12-C13
32	b	630[A]	LHG	C34-C35-C36-C37
36	C	519	DGD	C8A-C9A-CAA-CBA
36	c	518[B]	DGD	C5A-C6A-C7A-C8A
23	C	508	CLA	C13-C15-C16-C17
23	b	601	CLA	C13-C15-C16-C17
36	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	b	630[A]	LHG	C9-C10-C11-C12
32	D	407[B]	LHG	C27-C28-C29-C30
32	d	406[B]	LHG	C13-C14-C15-C16
34	B	620	LMG	C20-C21-C22-C23
23	c	513	CLA	C13-C15-C16-C17
26	a	410[B]	SQD	C34-C35-C36-C37
36	C	519	DGD	CAA-CBA-CCA-CDA
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	407[B]	PHO	CAD-CBD-CGD-O2D
26	L	101	SQD	C46-C45-O47-C7
38	f	101	HEM	C2B-C3B-CAB-CBB
32	E	101[A]	LHG	C13-C14-C15-C16
35	b	625	HTG	C4-C5-C6-O6
26	a	410[A]	SQD	C27-C28-C29-C30
34	C	501	LMG	C20-C21-C22-C23
34	z	101	LMG	C19-C20-C21-C22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	608	CLA	C16-C17-C18-C19
32	D	406[A]	LHG	C34-C35-C36-C37
36	C	518[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[A]	LHG	C4-C5-C6-O8
32	b	630[A]	LHG	O6-C4-C5-O7
32	b	630[B]	LHG	O6-C4-C5-O7
36	C	518[A]	DGD	C7A-C8A-C9A-CAA
23	A	406[B]	CLA	C16-C17-C18-C20
32	A	419[B]	LHG	C1-C2-C3-O3
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	503	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	O1A-CGA-O2A-C1
26	F	103	SQD	O47-C45-C46-O48
32	a	419[A]	LHG	O7-C5-C6-O8
23	c	511	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C45-C44-C46-C47
29	d	405[B]	PL9	C45-C44-C46-C47
32	d	407[B]	LHG	O10-C23-O8-C6
36	c	518[A]	DGD	C1A-C2A-C3A-C4A
29	a	413[B]	PL9	C4-C3-C7-C8
23	B	614	CLA	C14-C13-C15-C16
36	C	517[A]	DGD	C4D-C5D-C6D-O5D
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	C13-C15-C16-C17
23	B	601	CLA	CAA-CBA-CGA-O2A
23	b	601	CLA	CAA-CBA-CGA-O2A
25	d	404	BCR	C37-C22-C23-C24
23	b	613	CLA	CBD-CGD-O2D-CED
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
34	c	501	LMG	C4-C5-C6-O5
23	B	604	CLA	C1A-C2A-CAA-CBA
23	a	405[A]	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
36	C	518[B]	DGD	C1A-C2A-C3A-C4A
23	B	601	CLA	CBA-CGA-O2A-C1
26	F	103	SQD	C24-C23-O48-C46
32	d	407[A]	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	419[A]	LHG	C32-C33-C34-C35
32	D	406[A]	LHG	C4-O6-P-O3
32	D	407[B]	LHG	C4-O6-P-O3
32	d	412[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C23-C24-C25-C26
26	a	410[A]	SQD	C35-C36-C37-C38
34	c	501	LMG	C21-C22-C23-C24
29	D	405[B]	PL9	C45-C44-C46-C47
36	H	102	DGD	O2G-C1B-C2B-C3B
32	D	407[A]	LHG	C2-C3-O3-P
32	d	407[A]	LHG	C2-C3-O3-P
23	C	513	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
32	D	406[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	L	102[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C4-O6-P-O4
32	a	419[B]	LHG	C4-O6-P-O4
32	d	406[A]	LHG	C3-O3-P-O4
32	d	406[B]	LHG	C4-O6-P-O5
23	c	503	CLA	C16-C17-C18-C19
26	F	103	SQD	C7-C8-C9-C10
34	z	101	LMG	C10-C11-C12-C13
32	L	102[B]	LHG	C24-C25-C26-C27
36	C	517[B]	DGD	CCA-CDA-CEA-CFA
36	c	517[A]	DGD	O6E-C1E-O5D-C6D
32	L	102[A]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
36	C	518[B]	DGD	C8B-C9B-CAB-CBB
26	A	412	SQD	C30-C31-C32-C33
33	F	101	LMT	C4-C5-C6-C7
34	C	520	LMG	C11-C12-C13-C14
32	d	412[A]	LHG	C27-C28-C29-C30
36	c	517[A]	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
33	B	628	LMT	C1-C2-C3-C4
23	c	508	CLA	C5-C6-C7-C8
34	Z	101	LMG	C29-C28-O8-C9
32	a	419[B]	LHG	C23-C24-C25-C26
32	D	407[A]	LHG	C24-C23-O8-C6
33	b	627	LMT	C1-C2-C3-C4
23	D	403	CLA	O1D-CGD-O2D-CED
32	E	101[A]	LHG	C1-C2-C3-O3
23	B	616	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
23	d	402[B]	CLA	C11-C12-C13-C15
29	d	405[B]	PL9	C28-C29-C31-C32
23	A	405[B]	CLA	C15-C16-C17-C18
32	d	407[A]	LHG	O10-C23-O8-C6
34	c	501	LMG	C33-C34-C35-C36
33	b	627	LMT	O1'-C1-C2-C3
36	C	518[A]	DGD	C1A-C2A-C3A-C4A
36	C	519	DGD	CBA-CCA-CDA-CEA
32	D	407[A]	LHG	O10-C23-O8-C6
36	c	517[A]	DGD	C8B-C9B-CAB-CBB
23	C	503	CLA	C16-C17-C18-C20
26	A	410[A]	SQD	C34-C35-C36-C37
33	B	628	LMT	C3-C4-C5-C6
26	L	101	SQD	O47-C45-C46-O48
32	E	101[A]	LHG	O7-C5-C6-O8
32	a	419[B]	LHG	O7-C5-C6-O8
34	C	501	LMG	C29-C30-C31-C32
34	C	521	LMG	C38-C39-C40-C41
34	c	520	LMG	C29-C30-C31-C32
26	a	410[A]	SQD	C11-C12-C13-C14
36	c	518[B]	DGD	C2G-C3G-O3G-C1D
33	M	101	LMT	O1'-C1-C2-C3
32	D	406[B]	LHG	C11-C10-C9-C8
23	b	616	CLA	C5-C6-C7-C8
29	d	405[B]	PL9	C15-C14-C16-C17
23	c	507	CLA	C13-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	406[A]	CLA	C14-C13-C15-C16
23	B	610	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	C	511	CLA	C14-C13-C15-C16
23	a	408	CLA	C11-C10-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	c	510	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	B	607	CLA	C3-C5-C6-C7
34	B	620	LMG	C37-C38-C39-C40
24	a	407[A]	PHO	C8-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
26	F	103	SQD	O10-C23-O48-C46
23	A	406[A]	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C3-C5-C6-C7
26	a	410[B]	SQD	C35-C36-C37-C38
32	d	406[B]	LHG	C16-C17-C18-C19
34	C	521	LMG	C12-C13-C14-C15
23	c	511	CLA	C2-C3-C5-C6
29	a	413[A]	PL9	C12-C11-C9-C8
29	a	413[B]	PL9	C43-C44-C46-C47
32	d	412[A]	LHG	C34-C35-C36-C37
23	B	613	CLA	C15-C16-C17-C18
32	d	407[A]	LHG	C32-C33-C34-C35
34	m	101	LMG	C14-C15-C16-C17
32	a	419[B]	LHG	C7-C8-C9-C10
23	C	502	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	C	514	CLA	C2-C1-O2A-CGA
23	a	404[B]	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
26	A	410[A]	SQD	C16-C17-C18-C19
33	b	627	LMT	C6-C7-C8-C9
34	z	101	LMG	C13-C14-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
36	c	518[B]	DGD	C7B-C8B-C9B-CAB
32	d	406[A]	LHG	O10-C23-O8-C6
32	D	406[B]	LHG	O6-C4-C5-O7
32	L	102[A]	LHG	O6-C4-C5-O7
34	d	410	LMG	C16-C17-C18-C19
25	B	617	BCR	C1-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	d	404	BCR	C23-C24-C25-C30
29	A	414[A]	PL9	C28-C29-C31-C32
29	a	413[B]	PL9	C12-C11-C9-C8
33	D	401	LMT	O5B-C5B-C6B-O6B
32	d	406[A]	LHG	C24-C23-O8-C6
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
33	B	629	LMT	C1-C2-C3-C4
36	H	102	DGD	CCA-CDA-CEA-CFA
36	c	518[A]	DGD	O6E-C1E-O5D-C6D
34	m	101	LMG	C32-C33-C34-C35
36	C	517[A]	DGD	C6A-C7A-C8A-C9A
34	Z	101	LMG	C2-C1-O1-C7
36	c	517[A]	DGD	C2E-C1E-O5D-C6D
36	c	518[A]	DGD	C2E-C1E-O5D-C6D
32	L	102[A]	LHG	C26-C27-C28-C29
36	c	519	DGD	CDA-CEA-CFA-CGA
32	E	101[B]	LHG	O7-C5-C6-O8
23	C	507	CLA	C15-C16-C17-C18
32	D	406[B]	LHG	C34-C35-C36-C37
32	d	412[B]	LHG	C3-O3-P-O6
32	d	407[B]	LHG	C33-C34-C35-C36
32	L	102[A]	LHG	C27-C28-C29-C30
32	D	406[B]	LHG	C28-C29-C30-C31
23	C	514	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C15
33	T	101	LMT	C9-C10-C11-C12
34	c	501	LMG	C31-C32-C33-C34
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
34	d	410	LMG	C35-C36-C37-C38
36	c	519	DGD	O6D-C5D-C6D-O5D
26	A	410[B]	SQD	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	629	LMT	C6-C7-C8-C9
23	b	615	CLA	C10-C11-C12-C13
23	c	507	CLA	C10-C11-C12-C13
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
26	A	410[B]	SQD	C16-C17-C18-C19
32	L	102[B]	LHG	C26-C27-C28-C29
32	a	419[B]	LHG	C24-C25-C26-C27
36	C	518[B]	DGD	C7A-C8A-C9A-CAA
26	a	410[B]	SQD	C11-C12-C13-C14
32	D	407[A]	LHG	C27-C28-C29-C30
36	C	518[B]	DGD	C3B-C4B-C5B-C6B
25	D	404	BCR	C37-C22-C23-C24
25	T	102	BCR	C11-C12-C13-C35
23	c	503	CLA	C16-C17-C18-C20
36	h	102	DGD	C3B-C4B-C5B-C6B
23	b	612	CLA	C10-C11-C12-C13
33	B	626	LMT	C9-C10-C11-C12
36	c	517[A]	DGD	C4B-C5B-C6B-C7B
32	A	419[B]	LHG	C17-C18-C19-C20
32	d	412[A]	LHG	C1-C2-C3-O3
27	l	102[B]	GOL	O1-C1-C2-O2
23	b	616	CLA	CBA-CGA-O2A-C1
32	d	407[A]	LHG	C33-C34-C35-C36
23	b	616	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	B	606	CLA	C16-C17-C18-C19
36	C	517[B]	DGD	O6E-C1E-O5D-C6D
36	c	517[B]	DGD	CCB-CDB-CEB-CFB
23	c	510	CLA	C10-C11-C12-C13
34	d	410	LMG	C11-C12-C13-C14
26	L	101	SQD	C29-C30-C31-C32
23	b	601	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C25-C24-C26-C27
33	e	101	LMT	C2-C3-C4-C5
36	C	519	DGD	CDA-CEA-CFA-CGA
23	C	506	CLA	C2-C3-C5-C6
26	A	410[A]	SQD	C11-C10-C9-C8
23	C	509	CLA	C5-C6-C7-C8
23	b	612	CLA	C8-C10-C11-C12
32	b	630[A]	LHG	C25-C26-C27-C28
34	c	501	LMG	O8-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	502	CLA	C16-C17-C18-C19
32	D	406[A]	LHG	C11-C10-C9-C8
33	F	101	LMT	C6-C7-C8-C9
32	A	419[B]	LHG	C26-C27-C28-C29
23	C	508	CLA	C2A-CAA-CBA-CGA
26	a	410[B]	SQD	C27-C28-C29-C30
32	a	419[A]	LHG	C24-C25-C26-C27
23	c	507	CLA	C3A-C2A-CAA-CBA
38	F	102	HEM	CAD-CBD-CGD-O1D
23	C	507	CLA	C16-C17-C18-C20
34	C	520	LMG	C29-C30-C31-C32
23	a	405[B]	CLA	C4C-C3C-CAC-CBC
29	A	414[B]	PL9	C4-C3-C7-C8
29	a	413[A]	PL9	C4-C3-C7-C8
23	B	611	CLA	C11-C12-C13-C14
23	B	615	CLA	C14-C13-C15-C16
23	a	406[A]	CLA	C6-C7-C8-C9
23	d	402[B]	CLA	C11-C12-C13-C14
34	d	410	LMG	C18-C19-C20-C21
36	C	517[B]	DGD	CDB-CEB-CFB-CGB
36	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	b	608	CLA	C13-C15-C16-C17
36	H	102	DGD	O1G-C1G-C2G-C3G
32	L	102[A]	LHG	C23-C24-C25-C26
32	d	412[B]	LHG	C34-C35-C36-C37
24	A	407[B]	PHO	O2A-C1-C2-C3
34	C	521	LMG	C4-C5-C6-O5
33	a	416	LMT	O5'-C1'-O1'-C1
36	h	102	DGD	C6A-C7A-C8A-C9A
32	d	407[B]	LHG	C32-C33-C34-C35
23	a	405[A]	CLA	C15-C16-C17-C18
26	a	410[B]	SQD	C10-C11-C12-C13
26	A	410[A]	SQD	C13-C14-C15-C16
23	b	616	CLA	C4-C3-C5-C6
29	a	413[B]	PL9	C45-C44-C46-C47
23	C	502	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16
23	a	406[B]	CLA	C6-C7-C8-C10
23	b	608	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
35	b	625	HTG	C1'-C2'-C3'-C4'
32	A	419[A]	LHG	C18-C19-C20-C21
32	b	630[A]	LHG	C17-C18-C19-C20
32	L	102[B]	LHG	C11-C10-C9-C8
26	a	411	SQD	C26-C27-C28-C29
23	b	605	CLA	C3-C5-C6-C7
23	a	405[B]	CLA	C15-C16-C17-C18
36	C	519	DGD	C2A-C1A-O1G-C1G
32	D	406[A]	LHG	C26-C27-C28-C29
38	F	102	HEM	CAD-CBD-CGD-O2D
40	V	201	HEC	CAD-CBD-CGD-O1D
40	V	201	HEC	CAD-CBD-CGD-O2D
26	A	412	SQD	C31-C32-C33-C34
32	d	406[A]	LHG	C16-C17-C18-C19
34	D	411	LMG	C34-C35-C36-C37
23	b	601	CLA	C2-C3-C5-C6
29	d	405[A]	PL9	C43-C44-C46-C47
23	C	503	CLA	C2B-C3B-CAB-CBB
23	a	406[B]	CLA	C2B-C3B-CAB-CBB
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
34	d	410	LMG	C19-C20-C21-C22
36	C	519	DGD	O1A-C1A-O1G-C1G
23	c	512	CLA	C3-C5-C6-C7
32	L	102[B]	LHG	C11-C12-C13-C14
36	H	102	DGD	O1G-C1G-C2G-O2G
36	C	518[B]	DGD	C8A-C9A-CAA-CBA
23	A	406[A]	CLA	C16-C17-C18-C19
36	c	517[B]	DGD	C8B-C9B-CAB-CBB
23	C	511	CLA	C15-C16-C17-C18
34	D	411	LMG	C18-C19-C20-C21
23	D	403	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1D-CGD-O2D-CED
29	A	414[A]	PL9	C39-C41-C42-C43
29	A	414[B]	PL9	C39-C41-C42-C43
29	D	405[B]	PL9	C35-C34-C36-C37
29	a	413[A]	PL9	C45-C44-C46-C47
32	d	412[B]	LHG	C17-C18-C19-C20
23	A	404[B]	CLA	C2-C1-O2A-CGA
40	v	201	HEC	C4B-C3B-CAB-CBB
23	D	403	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C6-C7-C8-C9
23	a	406[B]	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
34	d	410	LMG	C38-C39-C40-C41
36	C	519	DGD	C7A-C8A-C9A-CAA
23	b	601	CLA	C3-C5-C6-C7
36	h	102	DGD	O2G-C1B-C2B-C3B
32	A	419[A]	LHG	C29-C30-C31-C32
36	c	517[A]	DGD	CAB-CBB-CCB-CDB
23	B	612	CLA	O1A-CGA-O2A-C1
25	c	515	BCR	C23-C24-C25-C30
25	d	404	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
23	a	408	CLA	C15-C16-C17-C18
23	b	615	CLA	C5-C6-C7-C8
36	C	517[B]	DGD	C6A-C7A-C8A-C9A
27	l	102[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
32	d	412[B]	LHG	C13-C14-C15-C16
29	D	405[A]	PL9	C35-C34-C36-C37
36	c	519	DGD	O6E-C5E-C6E-O5E
23	c	504	CLA	C8-C10-C11-C12
29	D	405[B]	PL9	C43-C44-C46-C47
29	a	413[A]	PL9	C43-C44-C46-C47
29	d	405[B]	PL9	C43-C44-C46-C47
34	B	620	LMG	O10-C28-C29-C30
32	D	406[B]	LHG	C32-C33-C34-C35
33	e	101	LMT	C2B-C1B-O1B-C4'
36	c	517[B]	DGD	C5D-C6D-O5D-C1E
36	c	518[B]	DGD	CDA-CEA-CFA-CGA
26	a	410[B]	SQD	C18-C19-C20-C21
23	C	511	CLA	C8-C10-C11-C12
34	z	101	LMG	O7-C10-C11-C12
23	A	404[A]	CLA	C16-C17-C18-C19
32	E	101[B]	LHG	O6-C4-C5-O7
26	f	102	SQD	C23-C24-C25-C26
32	A	419[A]	LHG	C35-C36-C37-C38
23	C	510	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	C4B-C3B-CAB-CBB
23	A	408	CLA	C16-C17-C18-C19
32	b	630[A]	LHG	C10-C11-C12-C13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
23	B	613	CLA	C11-C12-C13-C15
23	a	406[A]	CLA	C6-C7-C8-C10
23	b	615	CLA	C11-C12-C13-C15
23	b	616	CLA	C2-C3-C5-C6
32	L	102[A]	LHG	C16-C17-C18-C19
32	b	630[B]	LHG	C28-C29-C30-C31
33	B	628	LMT	C7-C8-C9-C10
35	b	623	HTG	S1-C1'-C2'-C3'
34	m	101	LMG	C2-C1-O1-C7
36	C	517[B]	DGD	C2E-C1E-O5D-C6D
23	a	404[B]	CLA	C2C-C3C-CAC-CBC
32	E	101[B]	LHG	C1-C2-C3-O3
34	c	521	LMG	O1-C7-C8-O7
34	C	521	LMG	C20-C21-C22-C23
33	t	101	LMT	C2-C3-C4-C5
36	c	517[B]	DGD	CBA-CCA-CDA-CEA
36	c	517[B]	DGD	CAB-CBB-CCB-CDB
23	b	604	CLA	C10-C11-C12-C13
23	D	403	CLA	C15-C16-C17-C18
23	B	606	CLA	C16-C17-C18-C20
23	C	513	CLA	CAA-CBA-CGA-O2A
32	A	419[A]	LHG	O8-C23-C24-C25
23	c	508	CLA	C8-C10-C11-C12
34	z	101	LMG	C20-C21-C22-C23
29	D	405[B]	PL9	C18-C19-C21-C22
35	B	621	HTG	C4'-C5'-C6'-C7'
36	c	518[A]	DGD	C9B-CAB-CBB-CCB
32	A	419[B]	LHG	C11-C12-C13-C14
23	A	408	CLA	C11-C12-C13-C14
23	A	408	CLA	C14-C13-C15-C16
23	B	616	CLA	C14-C13-C15-C16
23	C	514	CLA	C6-C7-C8-C9
23	a	406[A]	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C6-C7-C8-C9
34	c	521	LMG	C28-C29-C30-C31
34	c	521	LMG	C32-C33-C34-C35
36	c	519	DGD	C7B-C8B-C9B-CAB
34	c	521	LMG	C31-C32-C33-C34
23	B	603	CLA	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	415[A]	PHO	CAD-CBD-CGD-O2D
32	D	407[A]	LHG	C28-C29-C30-C31
23	c	502	CLA	C2A-CAA-CBA-CGA
32	b	630[A]	LHG	C30-C31-C32-C33
23	B	612	CLA	C8-C10-C11-C12
23	B	608	CLA	C2-C1-O2A-CGA
23	a	404[B]	CLA	C4C-C3C-CAC-CBC
32	L	102[A]	LHG	O7-C7-C8-C9
32	a	419[A]	LHG	O8-C23-C24-C25
34	c	520	LMG	O7-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
23	C	507	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C25-C24-C26-C27
32	b	630[B]	LHG	C31-C32-C33-C34
25	T	102	BCR	C11-C12-C13-C14
25	b	619	BCR	C21-C22-C23-C24
25	y	101	BCR	C21-C22-C23-C24
32	A	419[B]	LHG	C32-C33-C34-C35
34	c	520	LMG	C30-C31-C32-C33
34	C	521	LMG	C10-C11-C12-C13
26	F	103	SQD	C44-C45-C46-O48
34	B	620	LMG	O1-C7-C8-C9
32	b	630[A]	LHG	O7-C7-C8-C9
32	b	630[B]	LHG	O7-C7-C8-C9
34	Z	101	LMG	O7-C10-C11-C12
35	B	623	HTG	C4-C5-C6-O6
36	c	517[B]	DGD	C7B-C8B-C9B-CAB
36	c	518[B]	DGD	C1A-C2A-C3A-C4A
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	606	CLA	C8-C10-C11-C12
23	B	602	CLA	O2A-C1-C2-C3
24	A	407[A]	PHO	O2A-C1-C2-C3
24	a	407[B]	PHO	O2A-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
36	C	519	DGD	C6A-C7A-C8A-C9A
38	f	101	HEM	C4B-C3B-CAB-CBB
23	B	612	CLA	CBA-CGA-O2A-C1
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
40	v	201	HEC	CAD-CBD-CGD-O2D
23	A	404[B]	CLA	C16-C17-C18-C19
32	L	102[B]	LHG	C23-C24-C25-C26
32	A	419[B]	LHG	O2-C2-C3-O3
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-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
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-O2D
23	b	612	CLA	CHA-CBD-CGD-O2D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
38	f	101	HEM	CAD-CBD-CGD-O1D
40	v	201	HEC	CAD-CBD-CGD-O1D
32	L	102[B]	LHG	O7-C7-C8-C9
26	f	102	SQD	C26-C27-C28-C29
23	c	513	CLA	CAA-CBA-CGA-O2A
32	E	101[B]	LHG	O7-C7-C8-C9
32	A	419[A]	LHG	C17-C18-C19-C20
32	d	412[A]	LHG	C13-C14-C15-C16
32	d	406[B]	LHG	O7-C5-C6-O8
36	C	518[A]	DGD	CAB-CBB-CCB-CDB
23	C	504	CLA	C8-C10-C11-C12
24	a	415[B]	PHO	C2C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
27	O	303	GOL	O1-C1-C2-O2
27	d	411	GOL	O1-C1-C2-O2
26	A	410[B]	SQD	C34-C35-C36-C37
34	c	501	LMG	C13-C14-C15-C16
33	D	401	LMT	C2B-C1B-O1B-C4'
26	b	620	SQD	C10-C11-C12-C13
23	C	511	CLA	CAA-CBA-CGA-O2A
38	f	101	HEM	CAD-CBD-CGD-O2D
35	B	623	HTG	C2'-C3'-C4'-C5'
36	h	102	DGD	CDA-CEA-CFA-CGA
23	a	405[A]	CLA	C11-C12-C13-C15
29	A	414[A]	PL9	C4-C3-C7-C8
23	b	613	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
23	C	506	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	b	606	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	c	514	CLA	C14-C13-C15-C16
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
26	A	412	SQD	C24-C23-O48-C46
23	B	613	CLA	CAA-CBA-CGA-O2A
34	D	411	LMG	O7-C10-C11-C12
32	d	412[A]	LHG	C18-C19-C20-C21
23	B	614	CLA	C2A-CAA-CBA-CGA
29	D	405[B]	PL9	C11-C12-C13-C14
29	d	405[B]	PL9	C11-C12-C13-C14
32	b	630[A]	LHG	C24-C25-C26-C27
23	B	612	CLA	CAA-CBA-CGA-O2A
32	a	419[B]	LHG	O8-C23-C24-C25
26	L	101	SQD	C24-C25-C26-C27
23	b	604	CLA	C4-C3-C5-C6
34	c	521	LMG	C39-C40-C41-C42
27	A	418	GOL	O1-C1-C2-C3
27	A	418	GOL	C1-C2-C3-O3
27	a	418	GOL	C1-C2-C3-O3
27	d	411	GOL	C1-C2-C3-O3
27	l	102[A]	GOL	C1-C2-C3-O3
27	l	102[B]	GOL	C1-C2-C3-O3
35	B	621	HTG	C1'-C2'-C3'-C4'
23	c	511	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	D	405[A]	PL9	C28-C29-C31-C32
33	D	401	LMT	C1-C2-C3-C4
23	C	513	CLA	CAA-CBA-CGA-O1A
23	D	403	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	C15-C16-C17-C18
32	D	407[B]	LHG	C28-C29-C30-C31
32	A	419[A]	LHG	O10-C23-C24-C25
33	e	101	LMT	C4B-C5B-C6B-O6B
34	Z	101	LMG	O10-C28-O8-C9
32	a	419[A]	LHG	O10-C23-C24-C25
32	b	630[A]	LHG	O9-C7-C8-C9
36	c	517[A]	DGD	O2G-C1B-C2B-C3B
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
24	a	407[B]	PHO	C8-C10-C11-C12
32	A	419[B]	LHG	C30-C31-C32-C33
36	H	102	DGD	C6A-C7A-C8A-C9A
32	E	101[A]	LHG	O7-C7-C8-C9
34	c	501	LMG	O9-C10-O7-C8
23	c	513	CLA	CAA-CBA-CGA-O1A
34	c	520	LMG	O9-C10-C11-C12
29	A	414[B]	PL9	C23-C24-C26-C27
26	a	411	SQD	O10-C23-O48-C46
33	a	416	LMT	C2'-C1'-O1'-C1
23	b	603	CLA	C5-C6-C7-C8
23	b	611	CLA	C13-C15-C16-C17
33	e	101	LMT	O1'-C1-C2-C3
23	A	406[B]	CLA	C4B-C3B-CAB-CBB
23	a	406[B]	CLA	C4B-C3B-CAB-CBB
32	D	406[B]	LHG	C3-O3-P-O5
32	D	407[B]	LHG	C4-O6-P-O5
32	d	406[A]	LHG	C4-O6-P-O5
32	d	412[B]	LHG	C3-O3-P-O5
33	m	103	LMT	C9-C10-C11-C12
23	B	613	CLA	CAA-CBA-CGA-O1A
32	E	101[B]	LHG	O9-C7-C8-C9
32	a	419[B]	LHG	O10-C23-C24-C25
36	c	517[B]	DGD	O2G-C1B-C2B-C3B
34	B	620	LMG	O6-C1-O1-C7
38	f	101	HEM	CAA-CBA-CGA-O2A
23	c	514	CLA	C3-C5-C6-C7
25	h	101	BCR	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	t	102	BCR	C1-C6-C7-C8
25	t	102	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C26
32	L	102[A]	LHG	O9-C7-C8-C9
32	L	102[B]	LHG	O9-C7-C8-C9
32	b	630[B]	LHG	O9-C7-C8-C9
34	Z	101	LMG	O9-C10-C11-C12
24	A	417[A]	PHO	C2C-C3C-CAC-CBC
36	c	517[A]	DGD	C1A-C2A-C3A-C4A
38	F	102	HEM	CAA-CBA-CGA-O2A
36	C	518[B]	DGD	O2G-C1B-C2B-C3B
23	A	404[B]	CLA	C15-C16-C17-C18
34	c	520	LMG	C14-C15-C16-C17
23	b	613	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
29	d	405[B]	PL9	C35-C34-C36-C37
29	d	405[A]	PL9	C11-C12-C13-C14
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	a	405[B]	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
26	a	410[A]	SQD	C10-C11-C12-C13
32	b	630[B]	LHG	C10-C11-C12-C13
34	c	520	LMG	C32-C33-C34-C35
23	B	607	CLA	C14-C13-C15-C16
23	a	405[A]	CLA	C11-C12-C13-C14
23	b	601	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16
23	c	511	CLA	CBD-CGD-O2D-CED
23	b	613	CLA	C5-C6-C7-C8
26	A	412	SQD	O10-C23-O48-C46
23	C	506	CLA	CAA-CBA-CGA-O2A
26	a	411	SQD	O48-C23-C24-C25
32	A	419[B]	LHG	O8-C23-C24-C25
32	D	407[A]	LHG	O8-C23-C24-C25
23	c	505	CLA	O1A-CGA-O2A-C1
32	b	630[B]	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C2A-CAA-CBA-CGA
32	D	407[B]	LHG	O8-C23-C24-C25
36	C	519	DGD	O1G-C1A-C2A-C3A
23	C	509	CLA	C13-C15-C16-C17
36	c	518[B]	DGD	C9B-CAB-CBB-CCB
26	a	410[A]	SQD	C19-C20-C21-C22
32	A	419[B]	LHG	C25-C26-C27-C28
29	A	414[B]	PL9	C12-C11-C9-C10
29	D	405[A]	PL9	C40-C39-C41-C42
29	a	413[B]	PL9	C35-C34-C36-C37
29	d	405[B]	PL9	C30-C29-C31-C32
23	A	405[B]	CLA	C13-C15-C16-C17
36	c	517[A]	DGD	CBA-CCA-CDA-CEA
23	A	406[B]	CLA	C11-C10-C8-C7
23	B	602	CLA	C6-C7-C8-C10
23	B	613	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	b	601	CLA	C11-C12-C13-C15
23	b	614	CLA	C11-C10-C8-C7
38	f	101	HEM	CAA-CBA-CGA-O1A
36	C	519	DGD	C8B-C9B-CAB-CBB
32	E	101[A]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
32	d	407[B]	LHG	O8-C23-C24-C25
34	c	521	LMG	O7-C10-C11-C12
36	C	518[A]	DGD	O2G-C1B-C2B-C3B
26	a	411	SQD	C15-C16-C17-C18
32	D	406[A]	LHG	C28-C29-C30-C31
35	B	621	HTG	C2'-C3'-C4'-C5'
32	D	407[A]	LHG	O10-C23-C24-C25
32	d	407[B]	LHG	O10-C23-C24-C25
36	c	517[A]	DGD	O1B-C1B-C2B-C3B
38	F	102	HEM	CAA-CBA-CGA-O1A
36	C	518[A]	DGD	C3A-C4A-C5A-C6A
33	m	103	LMT	C2-C1-O1'-C1'
34	B	620	LMG	O7-C10-C11-C12
33	M	101	LMT	O5'-C1'-O1'-C1
34	D	411	LMG	O9-C10-C11-C12
26	a	411	SQD	C24-C23-O48-C46
23	b	610	CLA	C5-C6-C7-C8
23	B	612	CLA	CAA-CBA-CGA-O1A
23	C	511	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[A]	LHG	O10-C23-C24-C25
34	c	521	LMG	O9-C10-C11-C12
23	C	504	CLA	C2A-CAA-CBA-CGA
23	c	504	CLA	C2A-CAA-CBA-CGA
23	B	605	CLA	C8-C10-C11-C12
23	b	605	CLA	C5-C6-C7-C8
26	a	411	SQD	O10-C23-C24-C25
32	E	101[B]	LHG	O10-C23-C24-C25
36	C	518[A]	DGD	O1B-C1B-C2B-C3B
26	b	620	SQD	C16-C17-C18-C19
32	b	630[B]	LHG	C11-C12-C13-C14
36	C	519	DGD	C9A-CAA-CBA-CCA
26	A	412	SQD	O48-C23-C24-C25

There are no ring outliers.

173 monomers are involved in 354 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	417[B]	PHO	2	0
36	h	102	DGD	2	0
35	o	301	HTG	1	0
34	d	410	LMG	4	0
23	B	610	CLA	1	0
32	d	407[A]	LHG	10	0
38	F	102	HEM	1	0
23	C	511	CLA	3	0
23	C	505	CLA	1	0
26	A	410[A]	SQD	2	0
25	b	618	BCR	4	0
25	A	409	BCR	1	0
35	b	625	HTG	1	0
23	b	614	CLA	2	0
23	a	404[B]	CLA	4	0
23	a	408	CLA	5	0
32	d	406[B]	LHG	2	0
25	d	404	BCR	3	0
23	d	402[B]	CLA	2	0
36	c	519	DGD	2	0
34	c	501	LMG	1	0
32	a	419[A]	LHG	4	0
36	C	518[B]	DGD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	c	518[B]	DGD	1	0
27	O	302	GOL	1	0
36	c	517[A]	DGD	2	0
23	c	513	CLA	6	0
33	b	621	LMT	1	0
24	A	417[A]	PHO	1	0
25	b	619	BCR	3	0
23	C	507	CLA	6	0
29	a	413[A]	PL9	4	0
23	c	509	CLA	7	0
36	C	519	DGD	2	0
26	f	102	SQD	1	0
23	b	616	CLA	1	0
40	V	201	HEC	1	0
25	B	617	BCR	1	0
27	D	412	GOL	2	0
35	B	623	HTG	1	0
25	k	101	BCR	2	0
32	D	406[A]	LHG	2	0
23	B	603	CLA	1	0
23	a	404[A]	CLA	3	0
32	d	406[A]	LHG	3	0
29	A	414[B]	PL9	7	0
33	t	101	LMT	2	0
23	B	606	CLA	1	0
23	d	402[A]	CLA	2	0
23	C	503	CLA	4	0
23	C	502	CLA	6	0
23	c	511	CLA	1	0
27	a	418	GOL	4	0
23	C	513	CLA	4	0
32	A	419[B]	LHG	1	0
26	a	410[B]	SQD	5	0
23	b	609	CLA	5	0
34	c	520	LMG	1	0
36	C	517[B]	DGD	2	0
36	C	518[A]	DGD	2	0
23	D	402[B]	CLA	4	0
34	Z	101	LMG	2	0
23	b	601	CLA	3	0
23	a	405[A]	CLA	2	0
36	c	518[A]	DGD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	B	622	GOL	1	0
23	c	508	CLA	2	0
23	B	613	CLA	4	0
33	e	101	LMT	1	0
33	B	628	LMT	1	0
32	b	630[B]	LHG	1	0
27	v	202[A]	GOL	1	0
25	H	101	BCR	2	0
32	D	407[B]	LHG	3	0
25	Y	101	BCR	1	0
23	c	504	CLA	3	0
35	b	622	HTG	3	0
23	c	507	CLA	3	0
27	a	417	GOL	1	0
23	A	405[A]	CLA	4	0
23	C	506	CLA	5	0
27	A	418	GOL	3	0
23	b	603	CLA	1	0
27	l	102[B]	GOL	1	0
23	a	406[B]	CLA	2	0
35	c	522	HTG	1	0
23	b	606	CLA	1	0
23	c	514	CLA	3	0
29	A	414[A]	PL9	10	0
25	B	618	BCR	4	0
23	C	510	CLA	1	0
24	a	415[B]	PHO	1	0
32	A	419[A]	LHG	2	0
26	F	103	SQD	3	0
25	T	102	BCR	5	0
26	a	410[A]	SQD	4	0
36	C	517[A]	DGD	2	0
27	A	411	GOL	1	0
23	D	402[A]	CLA	3	0
23	A	406[B]	CLA	2	0
23	B	614	CLA	4	0
23	c	502	CLA	3	0
33	B	629	LMT	1	0
27	B	625	GOL	1	0
34	c	521	LMG	1	0
25	y	101	BCR	1	0
23	B	604	CLA	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	409	BCR	1	0
24	A	407[A]	PHO	2	0
23	d	403	CLA	1	0
23	B	615	CLA	7	0
32	D	407[A]	LHG	5	0
32	E	101[B]	LHG	3	0
34	z	101	LMG	2	0
33	a	416	LMT	2	0
23	A	408	CLA	4	0
26	L	101	SQD	1	0
23	b	607	CLA	1	0
23	c	503	CLA	2	0
27	l	102[A]	GOL	1	0
23	a	406[A]	CLA	2	0
35	d	409	HTG	1	0
27	O	303	GOL	3	0
23	C	508	CLA	2	0
26	b	620	SQD	4	0
24	a	415[A]	PHO	2	0
25	c	515	BCR	1	0
34	C	521	LMG	2	0
26	a	411	SQD	2	0
23	B	605	CLA	4	0
23	B	609	CLA	2	0
24	a	407[B]	PHO	2	0
25	t	102	BCR	4	0
29	a	413[B]	PL9	6	0
23	A	404[B]	CLA	3	0
23	B	602	CLA	1	0
25	b	617	BCR	1	0
35	B	621	HTG	1	0
33	A	420	LMT	2	0
23	A	406[A]	CLA	1	0
32	D	406[B]	LHG	3	0
23	C	512	CLA	2	0
32	d	407[B]	LHG	10	0
23	C	514	CLA	2	0
23	c	506	CLA	6	0
25	K	102	BCR	1	0
26	A	410[B]	SQD	2	0
23	b	613	CLA	1	0
23	C	509	CLA	3	0

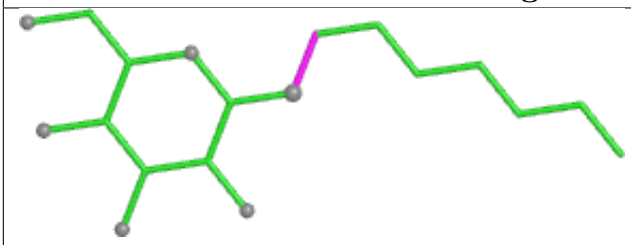
Continued on next page...

Continued from previous page...

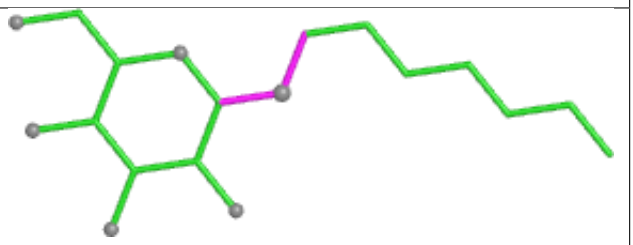
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	h	101	BCR	6	0
27	b	628	GOL	3	0
32	E	101[A]	LHG	3	0
33	M	101	LMT	2	0
25	C	515	BCR	1	0
33	D	401	LMT	1	0
23	c	510	CLA	3	0
23	a	405[B]	CLA	2	0
23	B	601	CLA	2	0
32	a	419[B]	LHG	4	0
23	b	615	CLA	2	0
33	B	626	LMT	1	0
36	H	102	DGD	1	0
23	c	512	CLA	6	0
23	c	505	CLA	2	0
27	v	202[B]	GOL	2	0
23	B	616	CLA	4	0
23	b	604	CLA	1	0
23	C	504	CLA	5	0
23	b	605	CLA	3	0
23	A	404[A]	CLA	5	0
23	b	612	CLA	1	0
23	A	405[B]	CLA	3	0
36	c	517[B]	DGD	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 then 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.

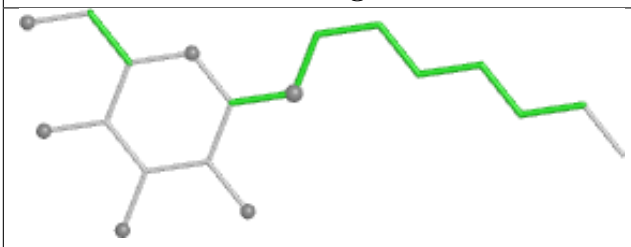
Ligand HTG C 522



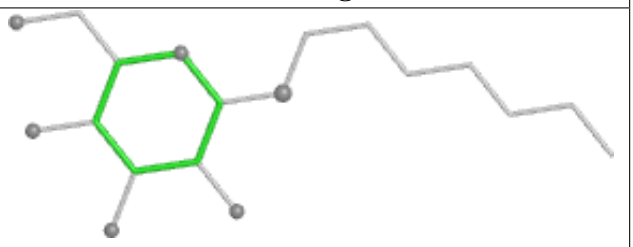
Bond lengths



Bond angles



Torsions

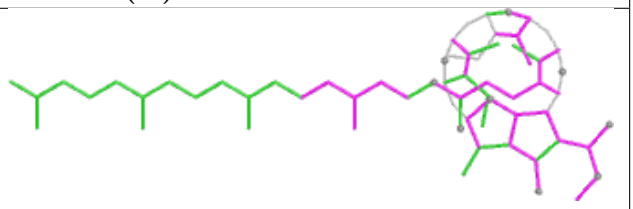


Rings

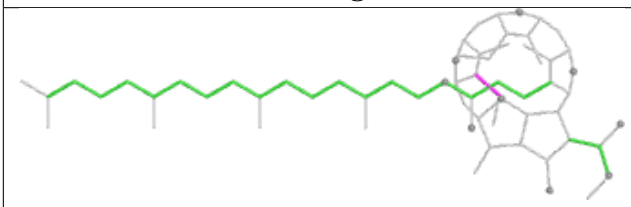
Ligand PHO A 417 (B)



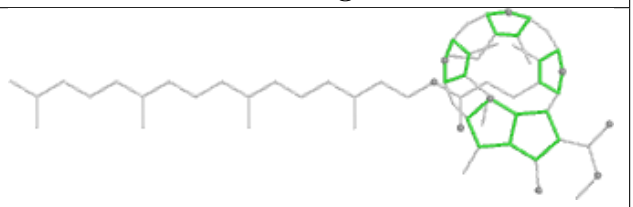
Bond lengths



Bond angles

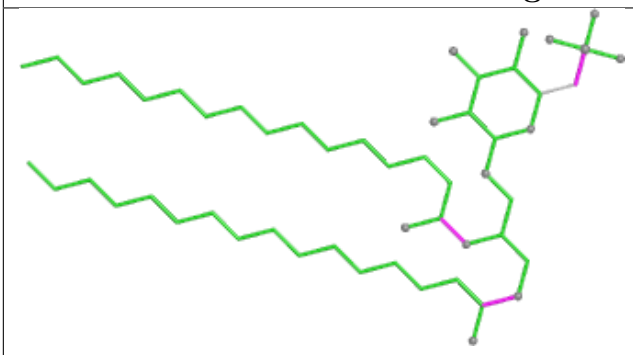


Torsions

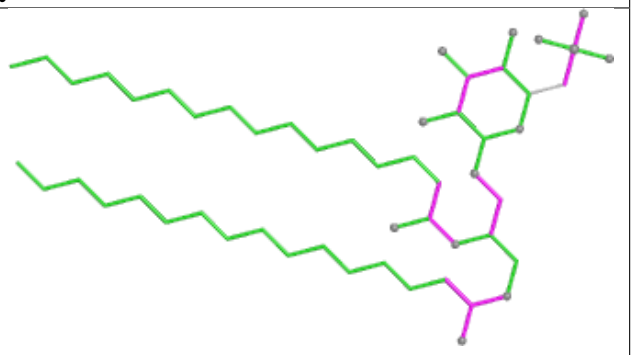


Rings

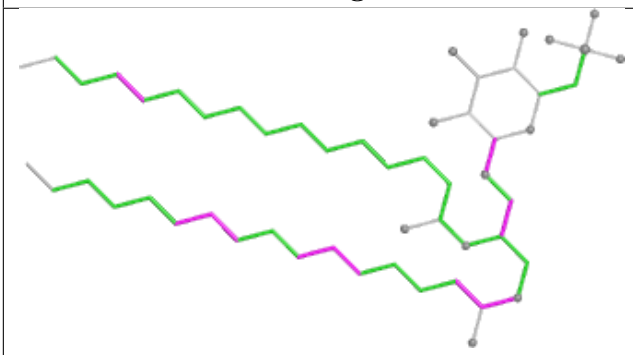
Ligand SQD A 412



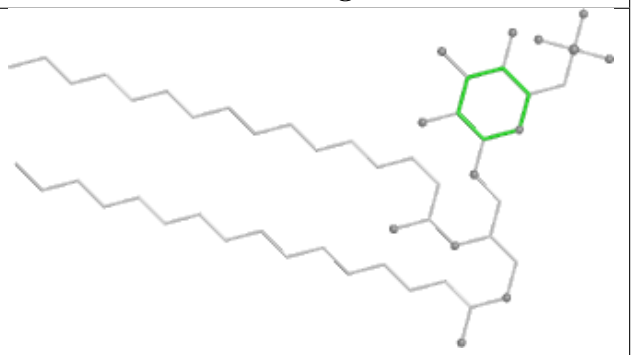
Bond lengths



Bond angles

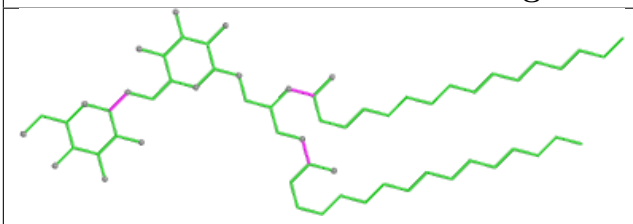


Torsions

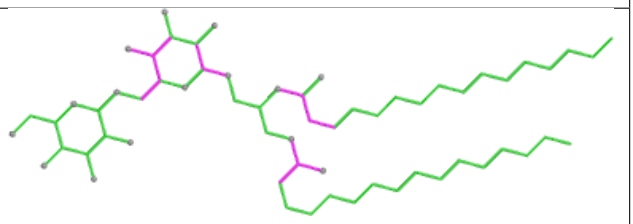


Rings

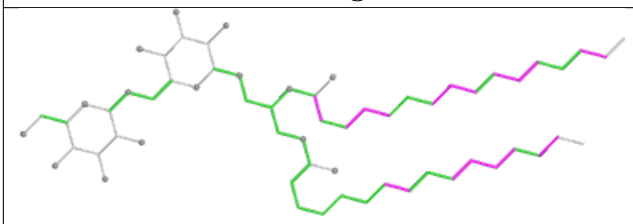
Ligand DGD h 102



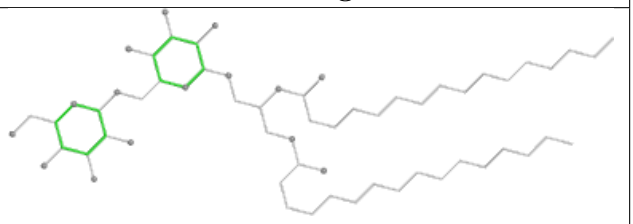
Bond lengths



Bond angles

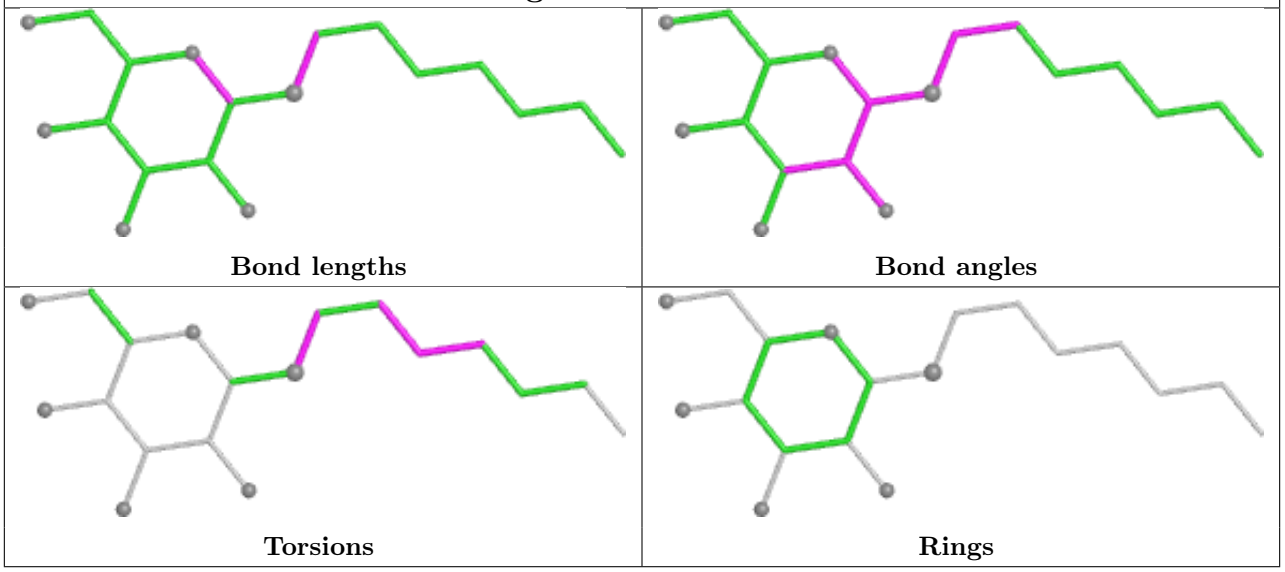


Torsions

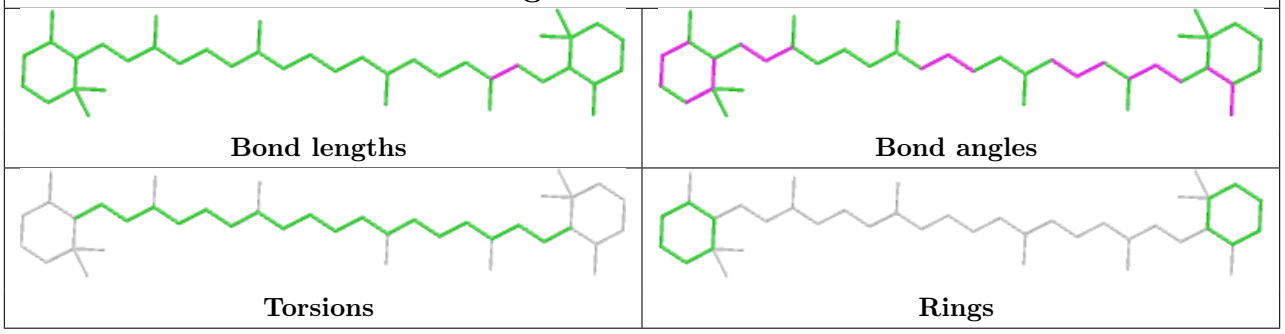


Rings

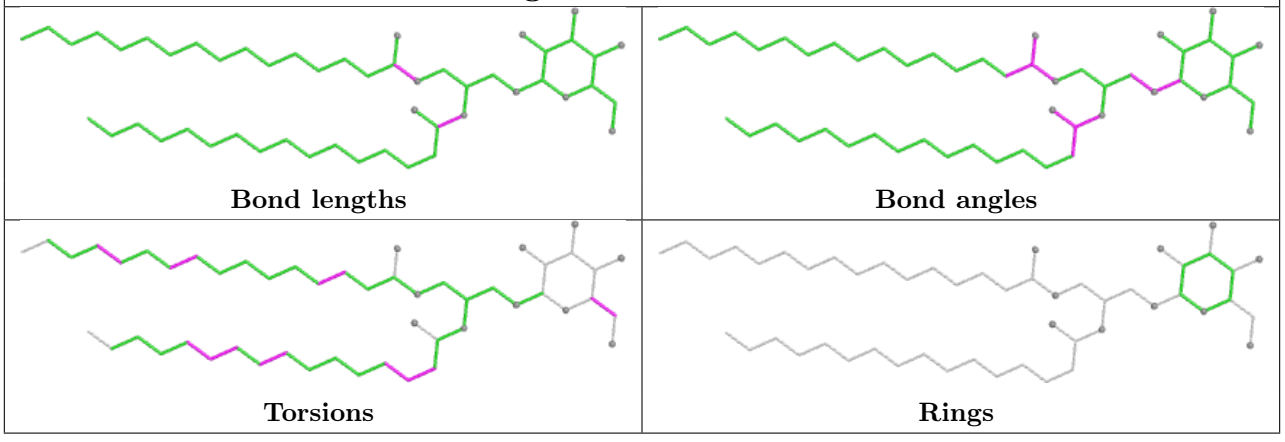
Ligand HTG o 301



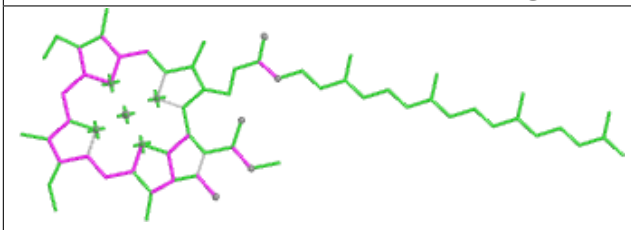
Ligand BCR B 619



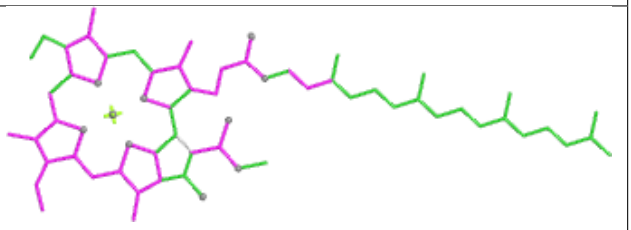
Ligand LMG d 410



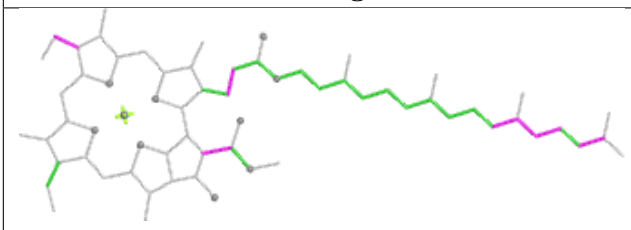
Ligand CLA B 610



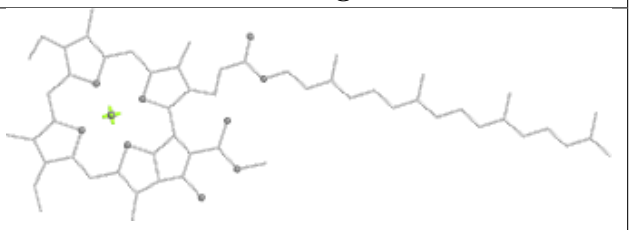
Bond lengths



Bond angles

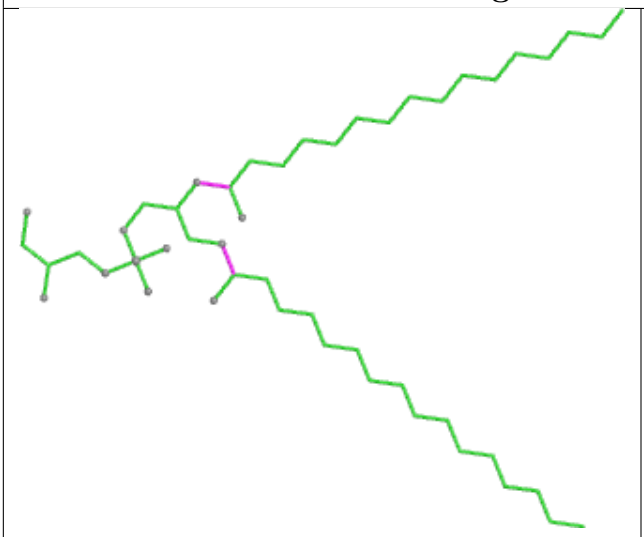


Torsions

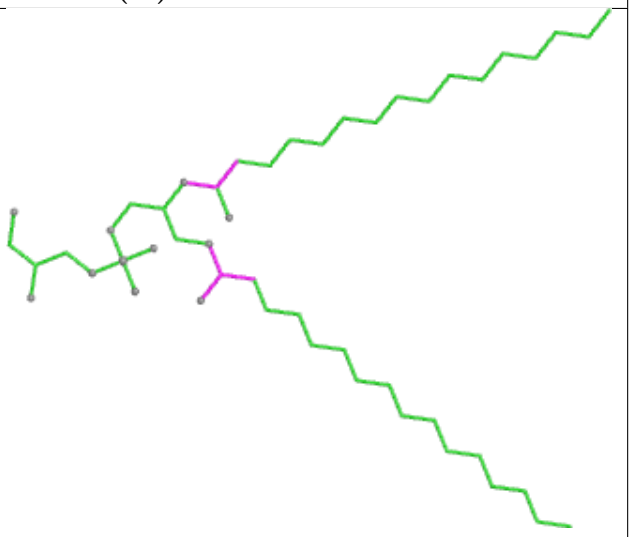


Rings

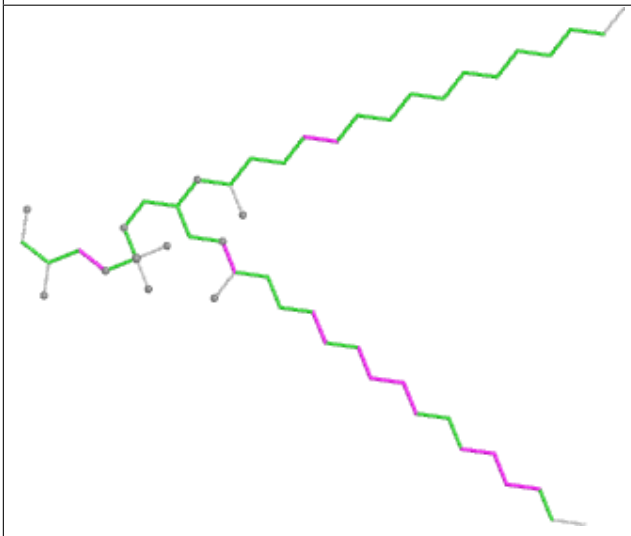
Ligand LHG d 407 (A)



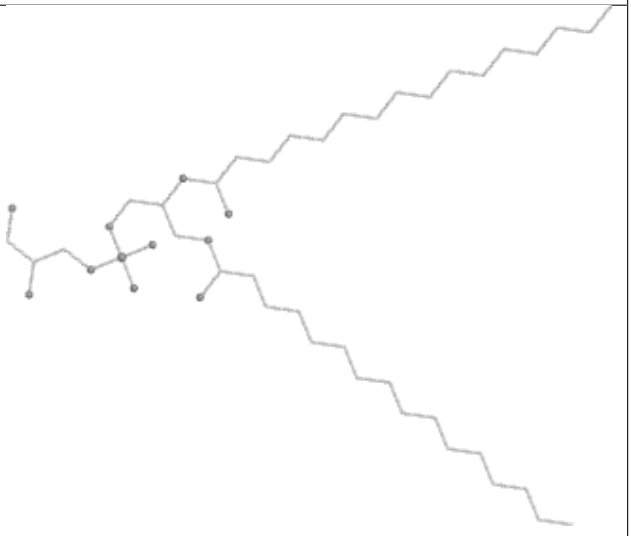
Bond lengths



Bond angles

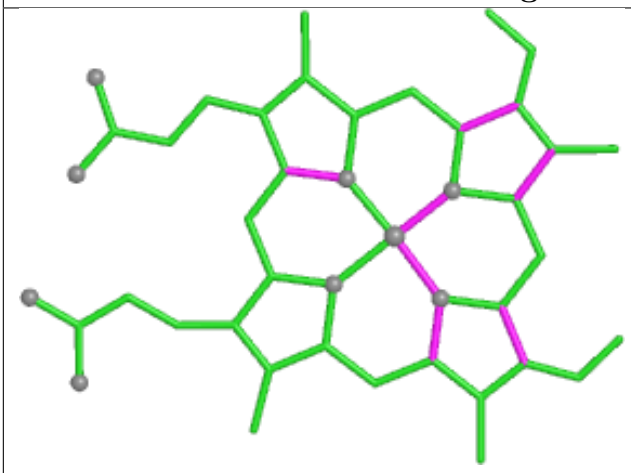


Torsions

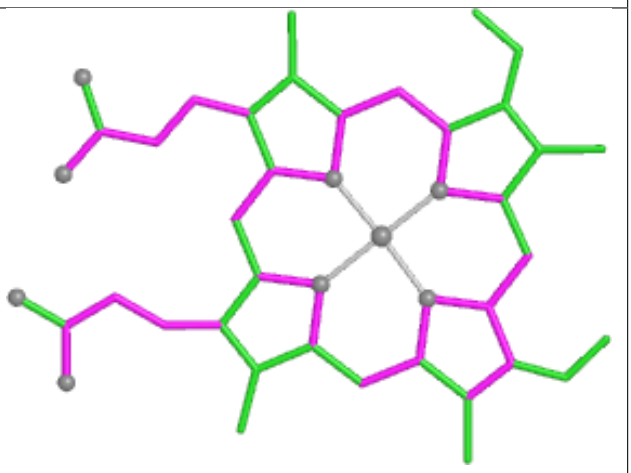


Rings

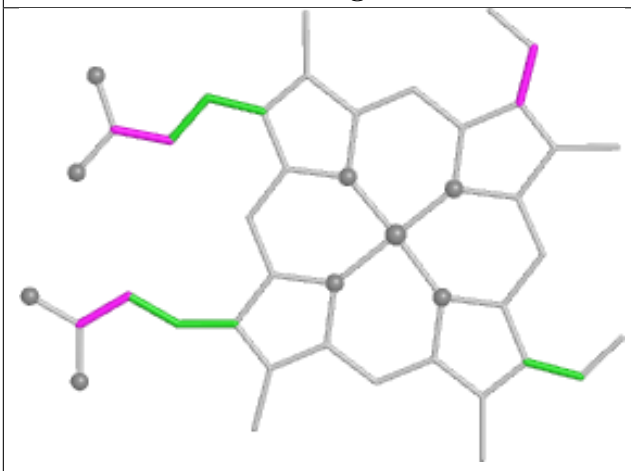
Ligand HEM F 102



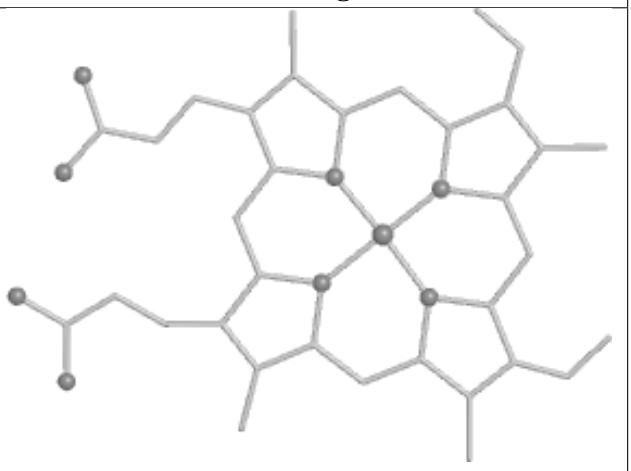
Bond lengths



Bond angles

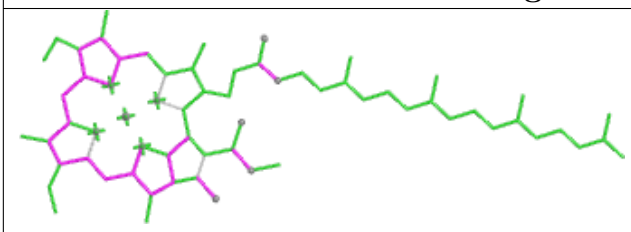


Torsions

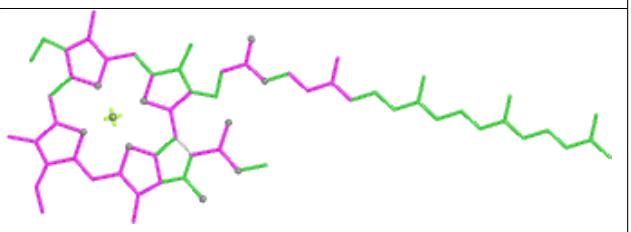


Rings

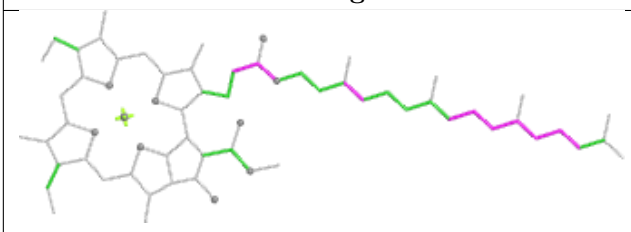
Ligand CLA C 511



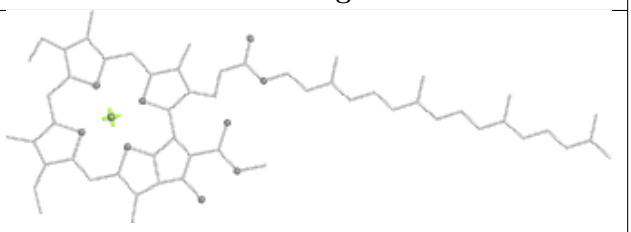
Bond lengths



Bond angles

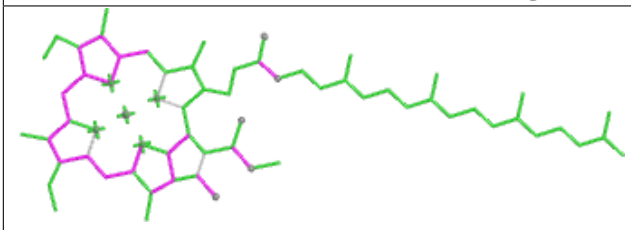


Torsions

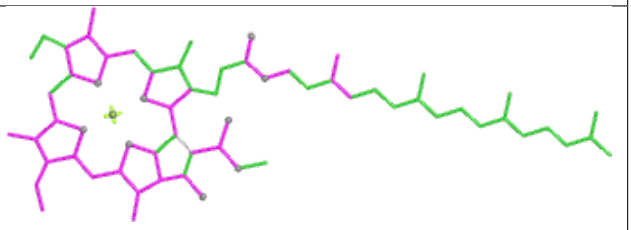


Rings

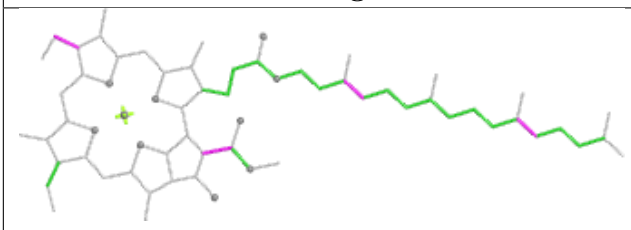
Ligand CLA C 505



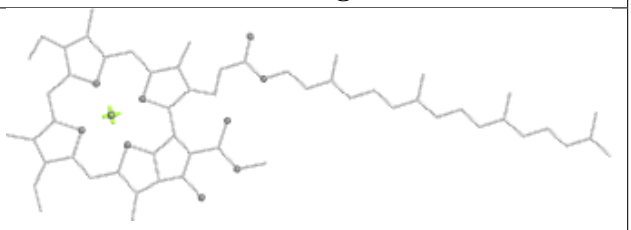
Bond lengths



Bond angles

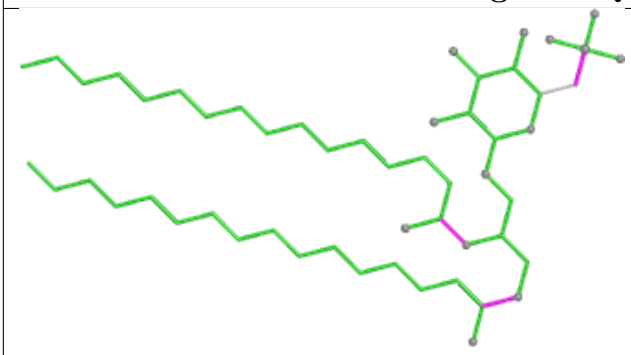


Torsions

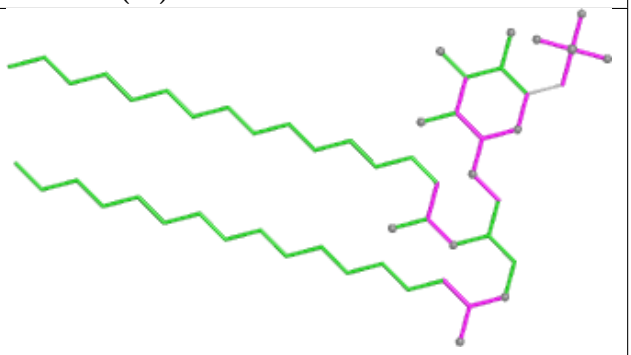


Rings

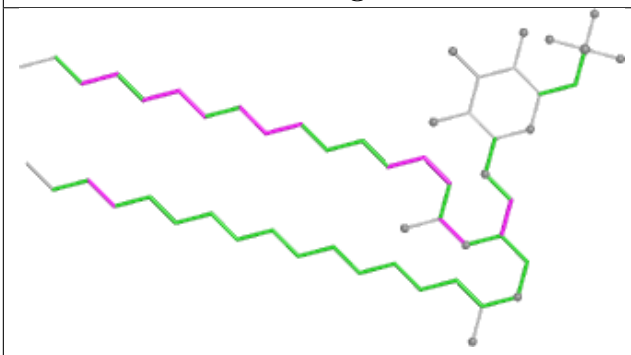
Ligand SQD A 410 (A)



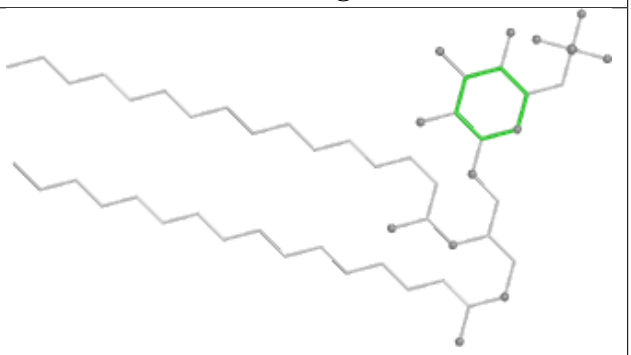
Bond lengths



Bond angles

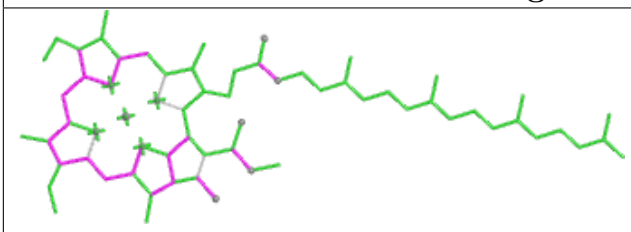


Torsions

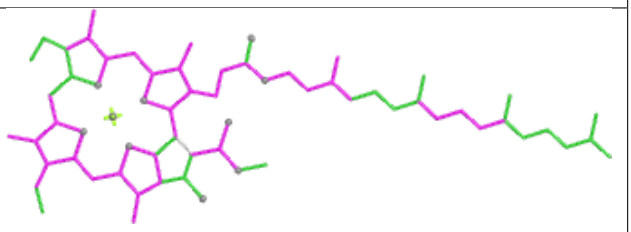


Rings

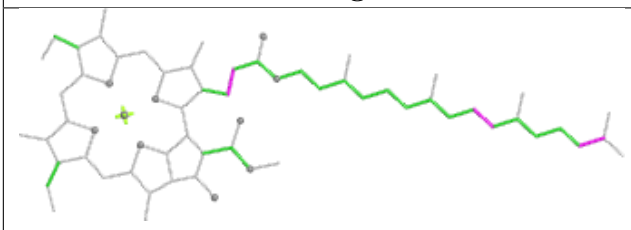
Ligand CLA b 602



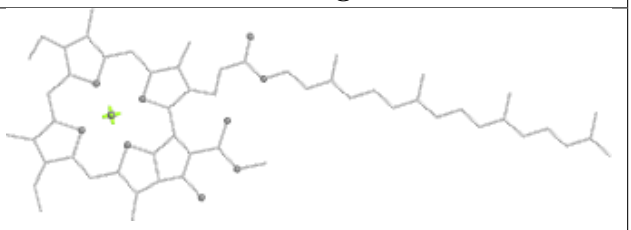
Bond lengths



Bond angles



Torsions

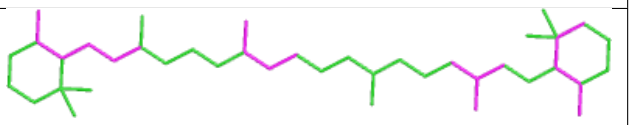


Rings

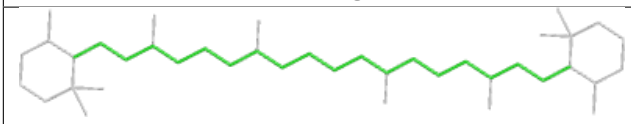
Ligand BCR b 618



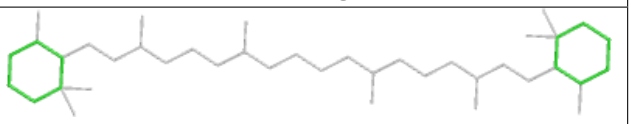
Bond lengths



Bond angles

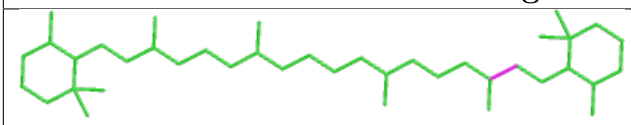


Torsions

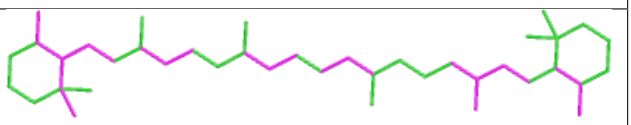


Rings

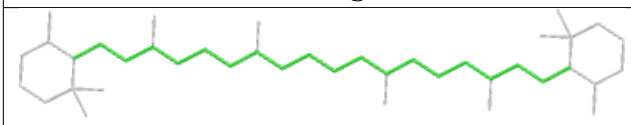
Ligand BCR A 409



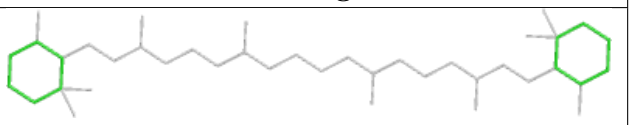
Bond lengths



Bond angles

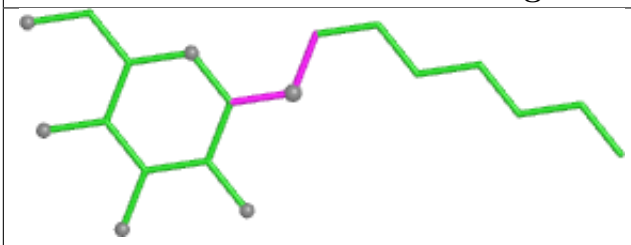


Torsions

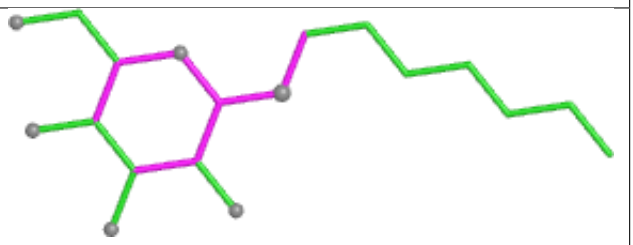


Rings

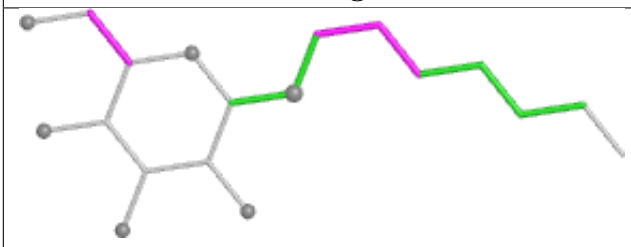
Ligand HTG b 625



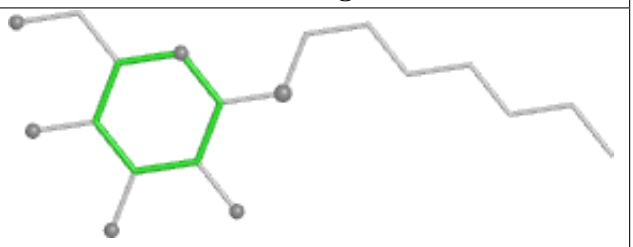
Bond lengths



Bond angles

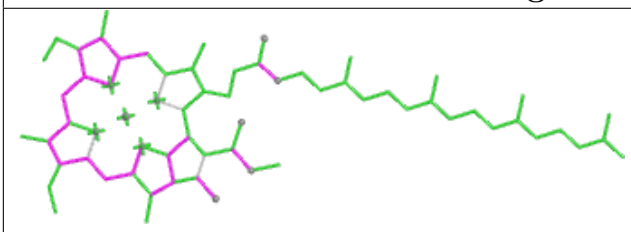


Torsions

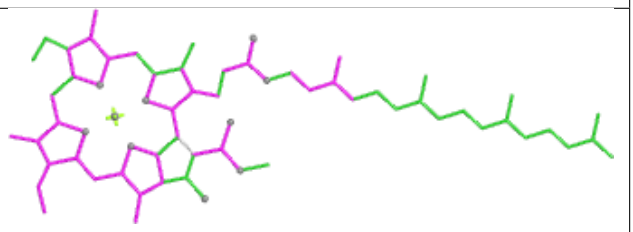


Rings

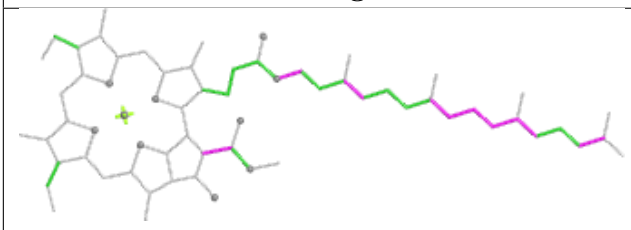
Ligand CLA b 614



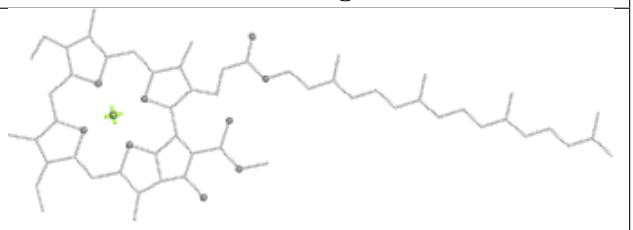
Bond lengths



Bond angles

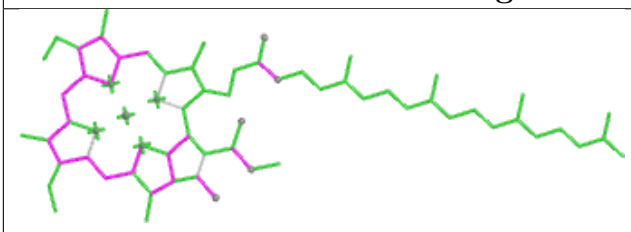


Torsions

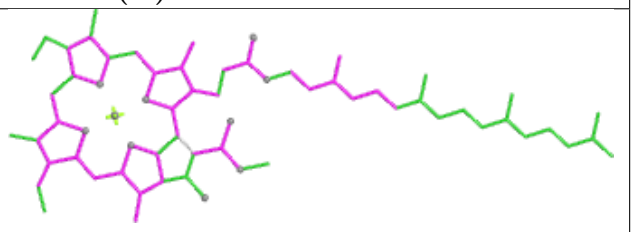


Rings

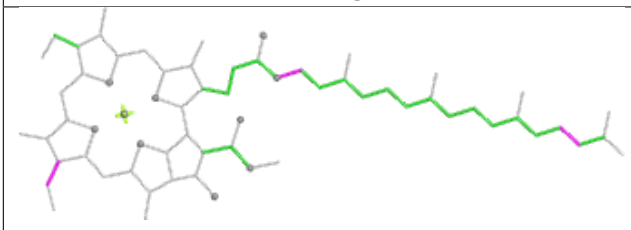
Ligand CLA a 404 (B)



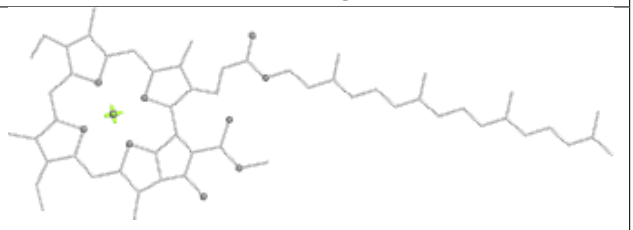
Bond lengths



Bond angles

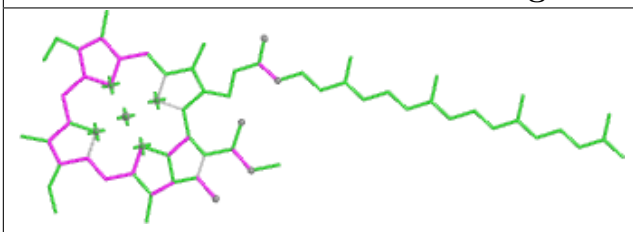


Torsions

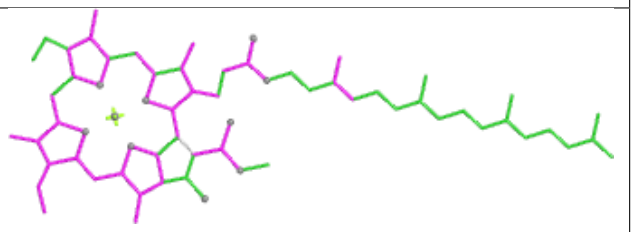


Rings

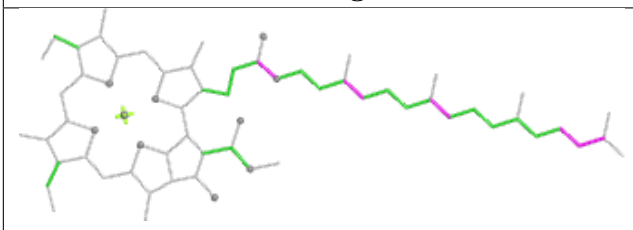
Ligand CLA a 408



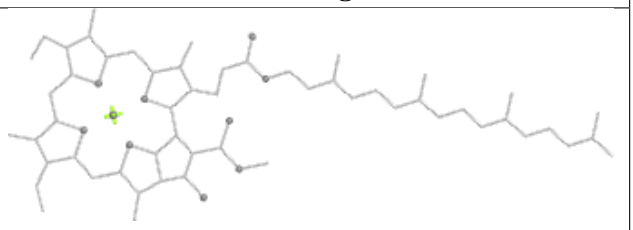
Bond lengths



Bond angles

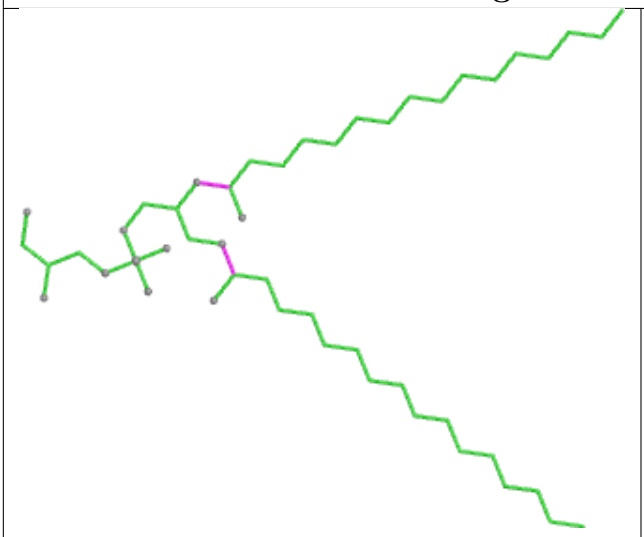


Torsions

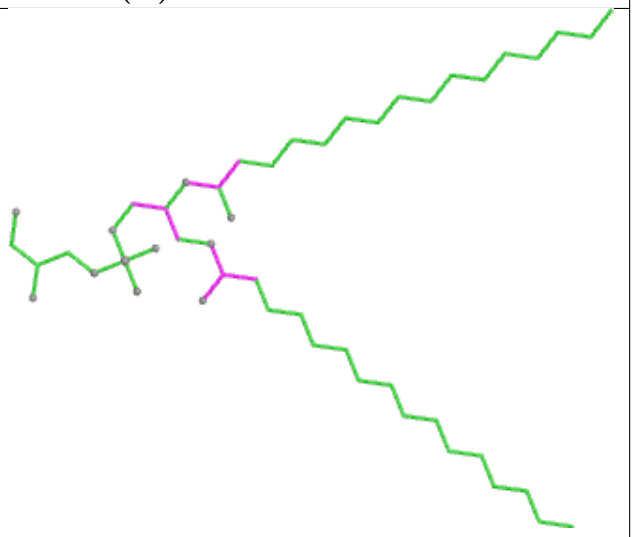


Rings

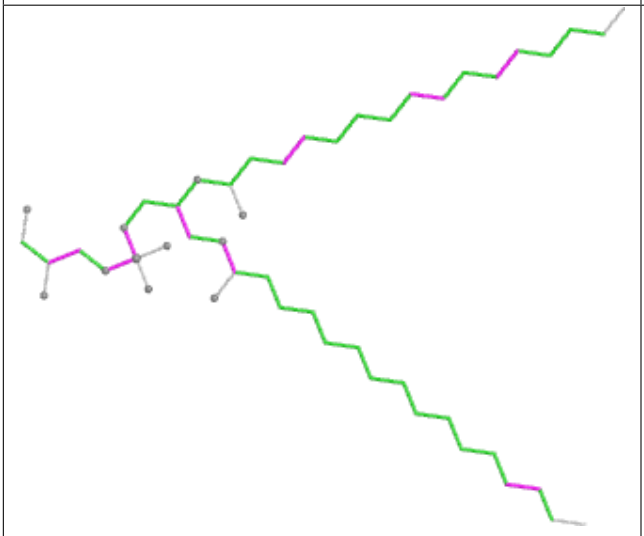
Ligand LHG d 406 (B)



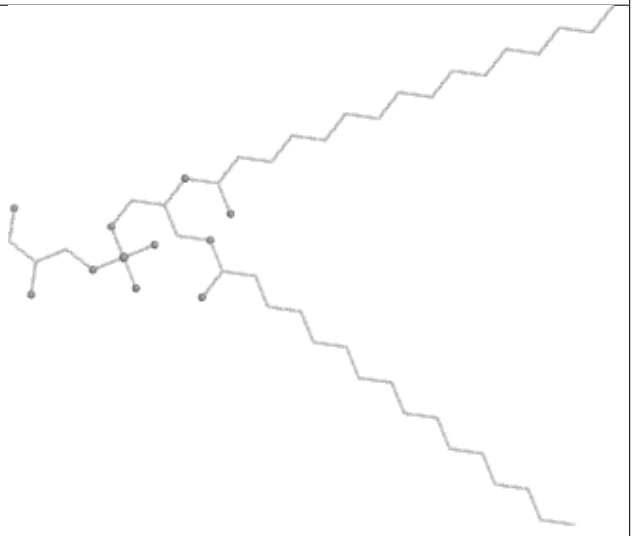
Bond lengths



Bond angles

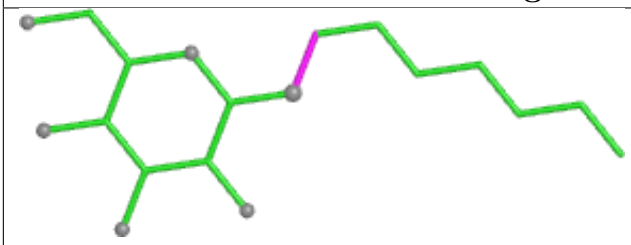


Torsions

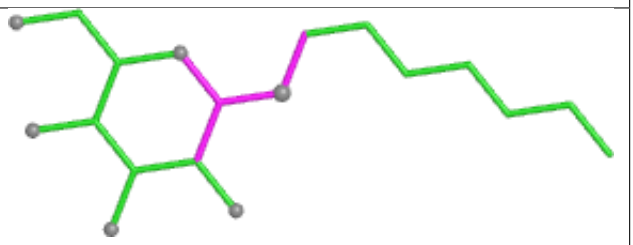


Rings

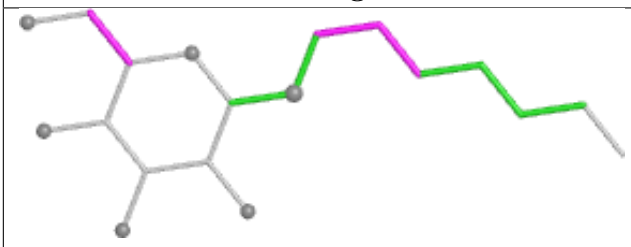
Ligand HTG b 623



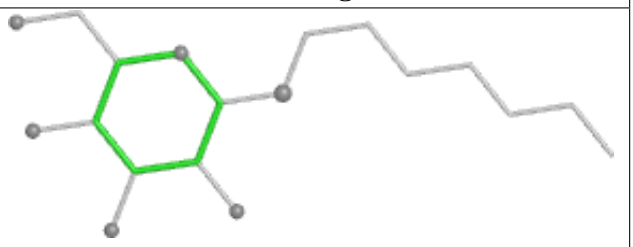
Bond lengths



Bond angles



Torsions

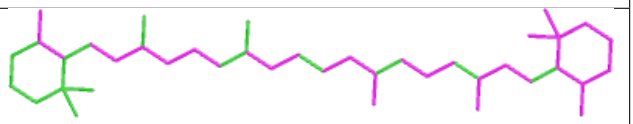


Rings

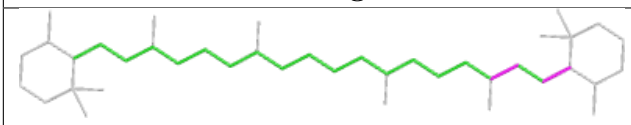
Ligand BCR d 404



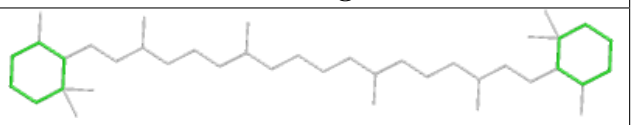
Bond lengths



Bond angles

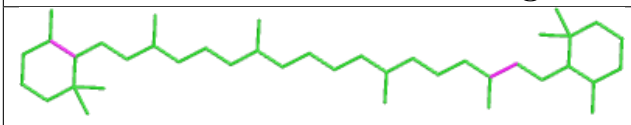


Torsions

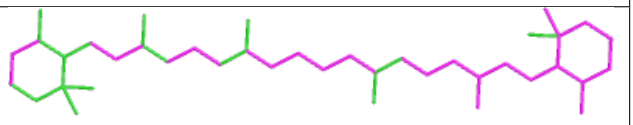


Rings

Ligand BCR D 404



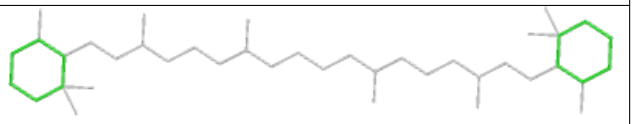
Bond lengths



Bond angles

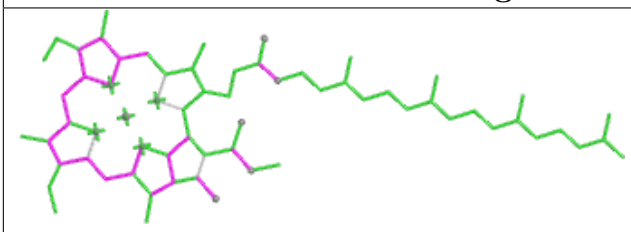


Torsions

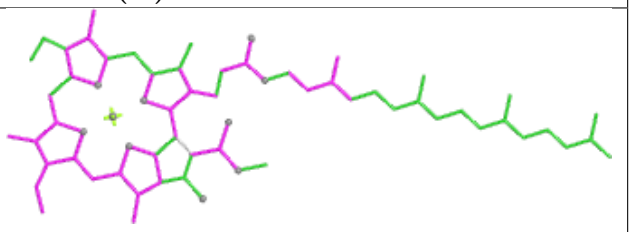


Rings

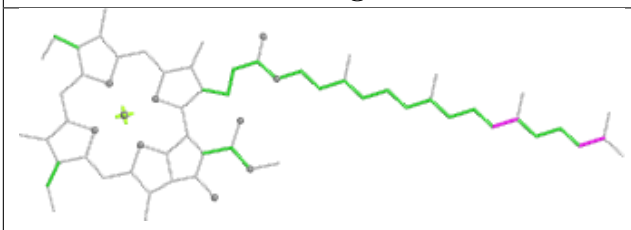
Ligand CLA d 402 (B)



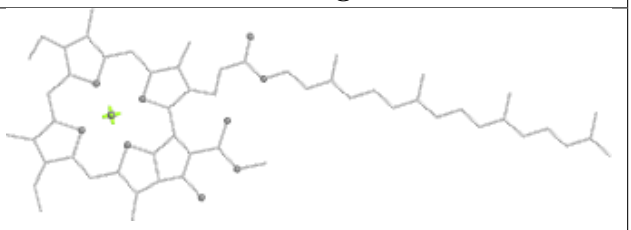
Bond lengths



Bond angles

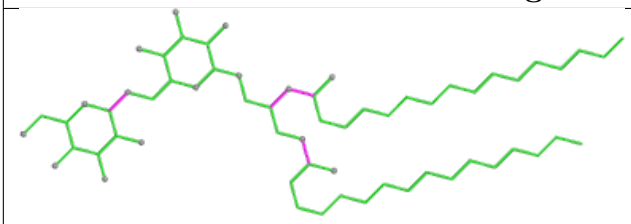


Torsions

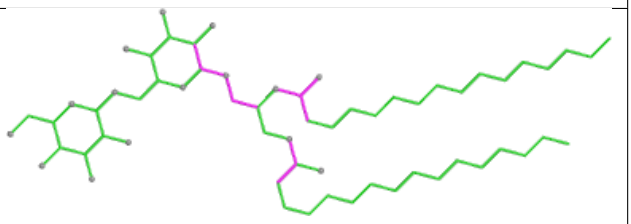


Rings

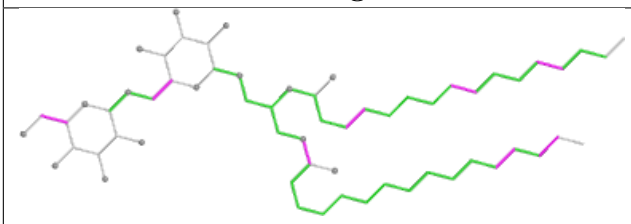
Ligand DGD c 519



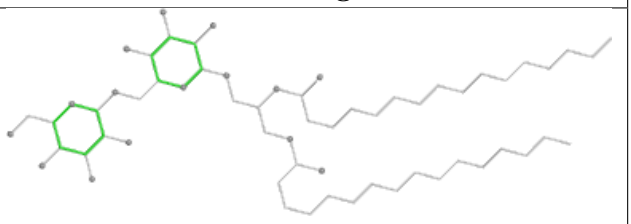
Bond lengths



Bond angles

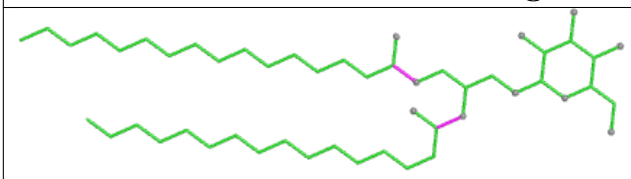


Torsions

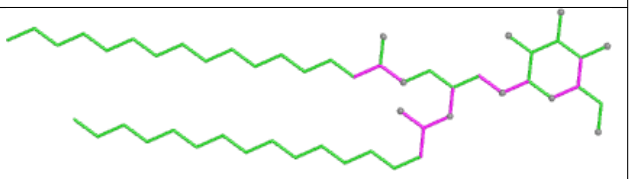


Rings

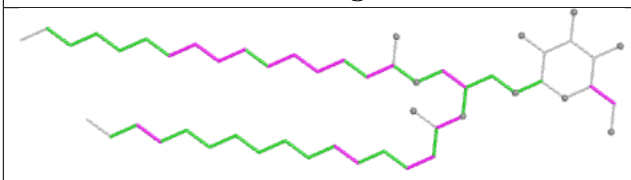
Ligand LMG c 501



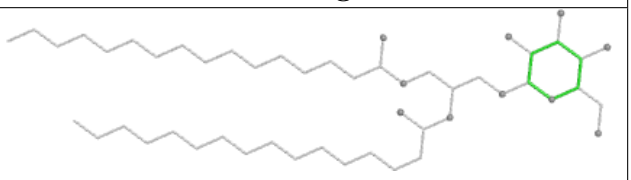
Bond lengths



Bond angles

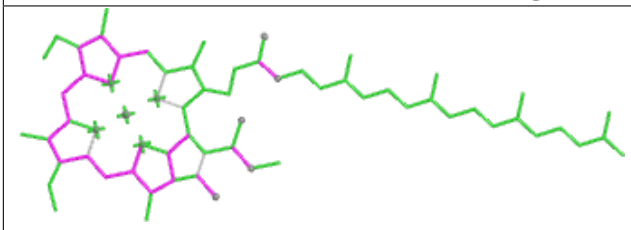


Torsions

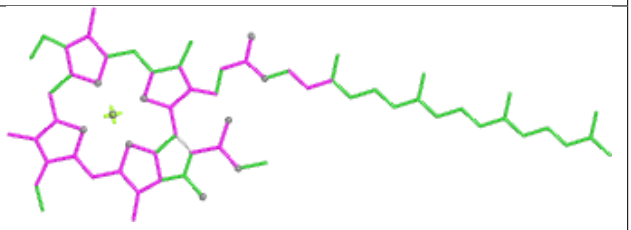


Rings

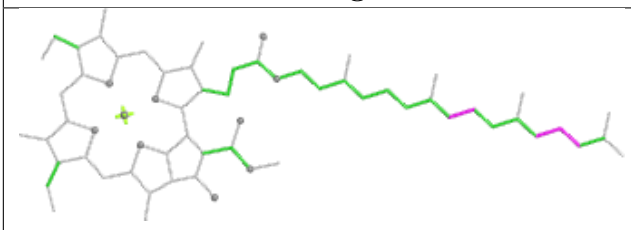
Ligand CLA b 611



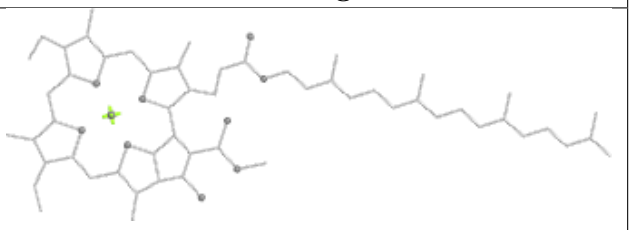
Bond lengths



Bond angles

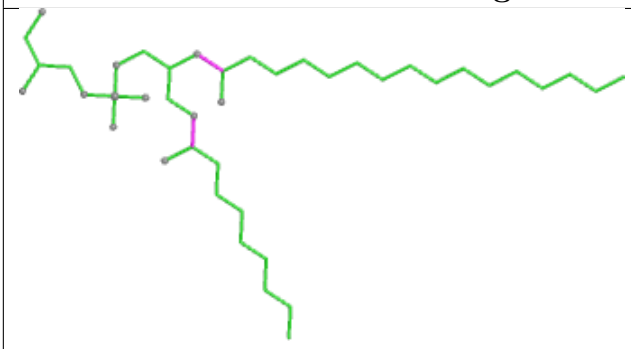


Torsions

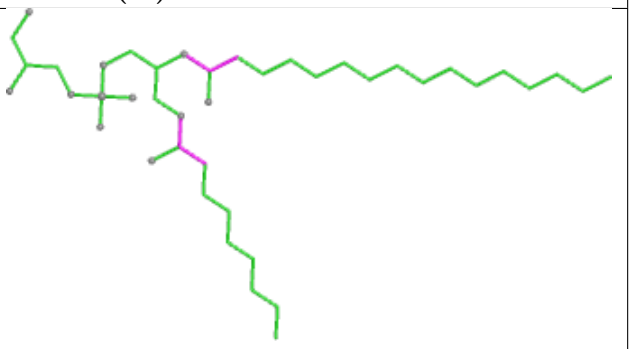


Rings

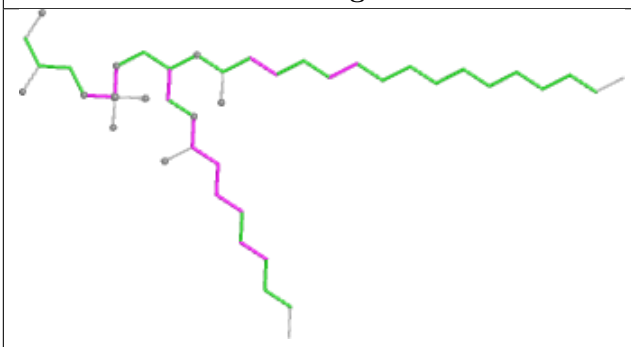
Ligand LHG a 419 (A)



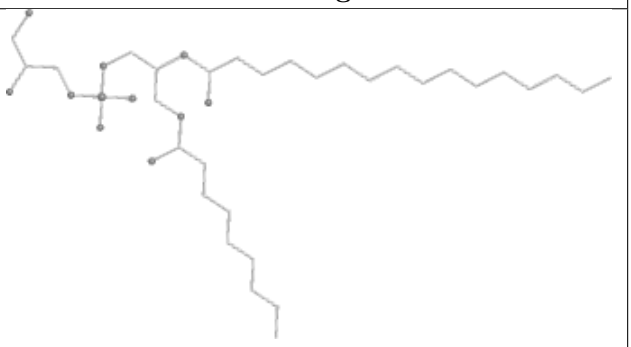
Bond lengths



Bond angles

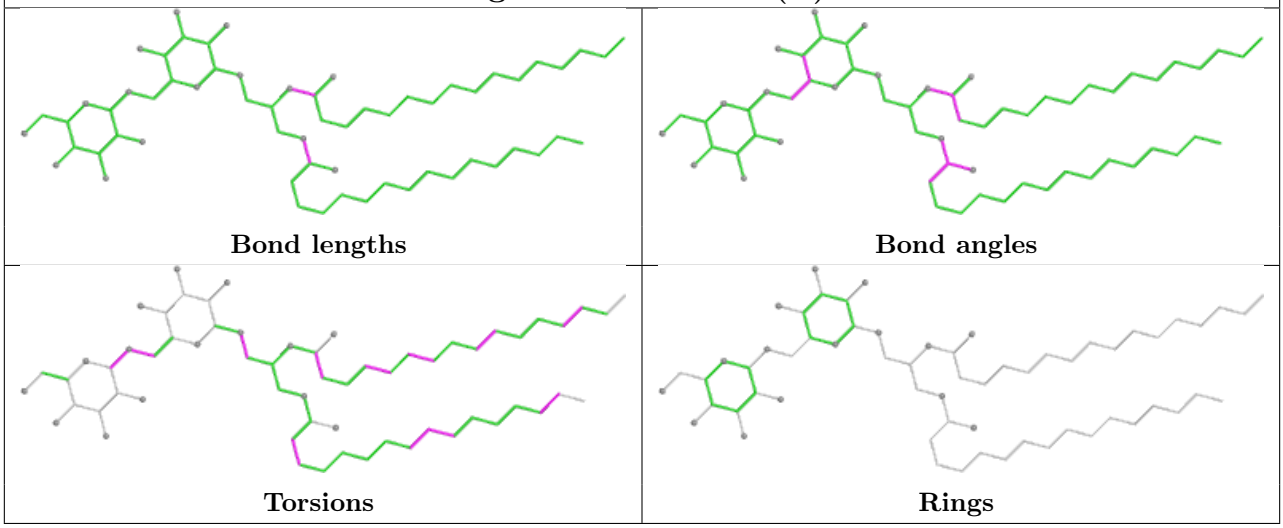


Torsions

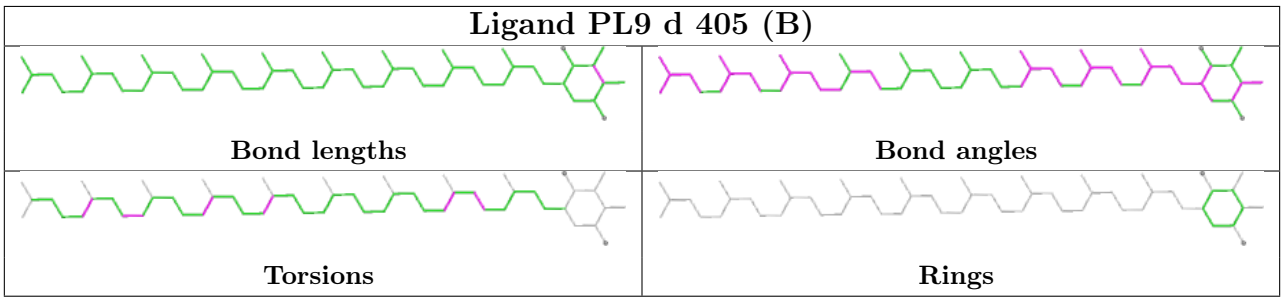


Rings

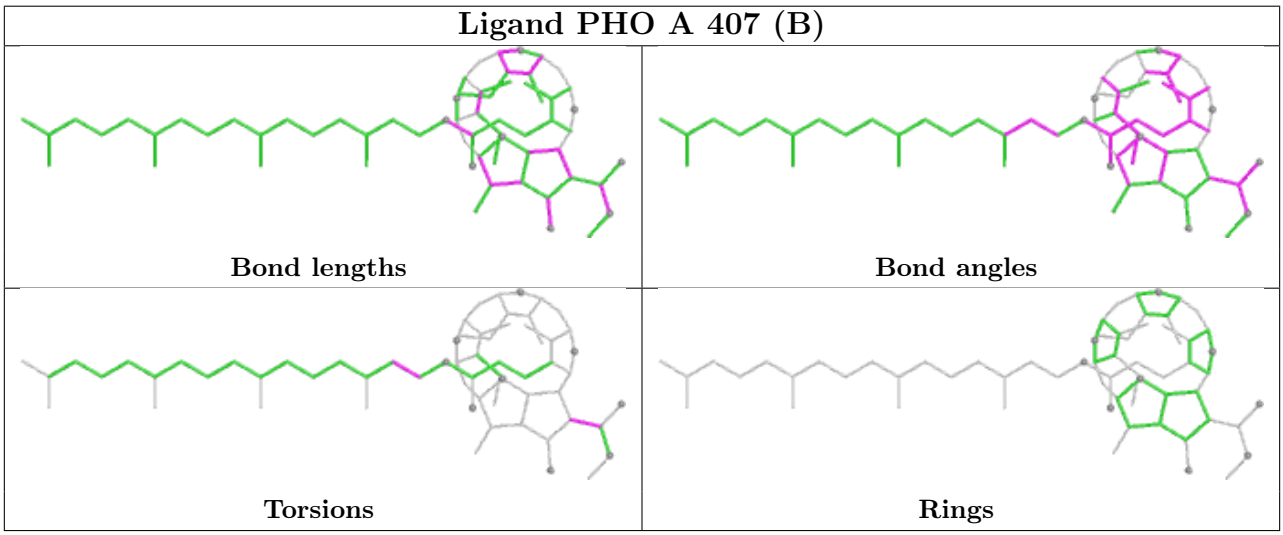
Ligand DGD C 518 (B)



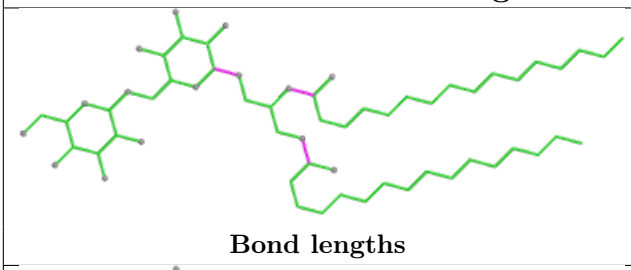
Ligand PL9 d 405 (B)



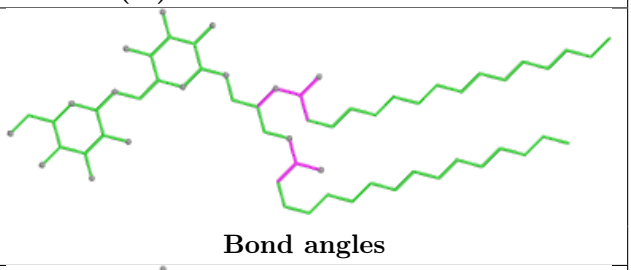
Ligand PHO A 407 (B)



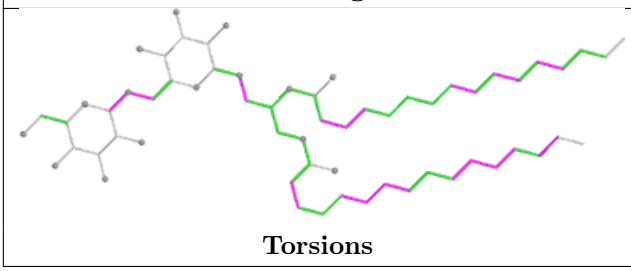
Ligand DGD c 518 (B)



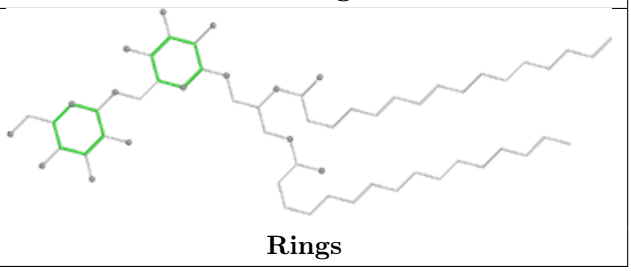
Bond lengths



Bond angles

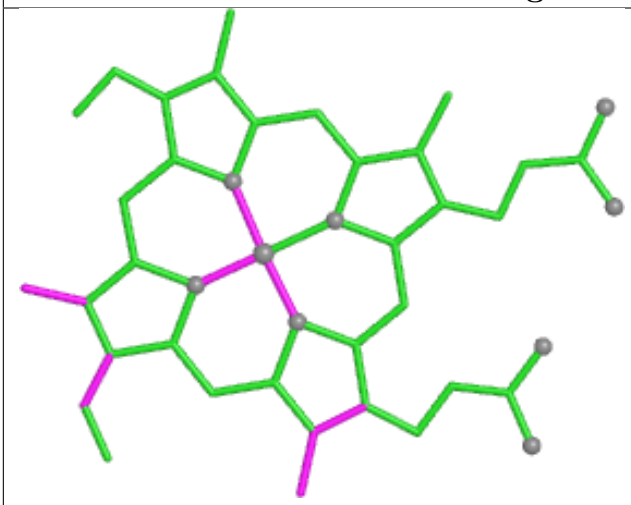


Torsions

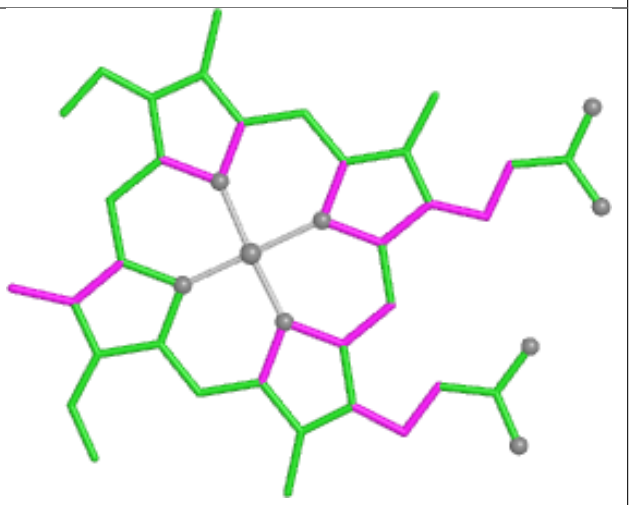


Rings

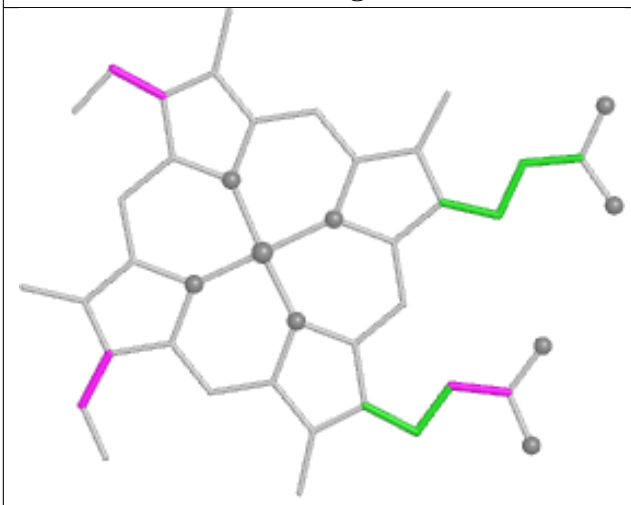
Ligand HEC v 201



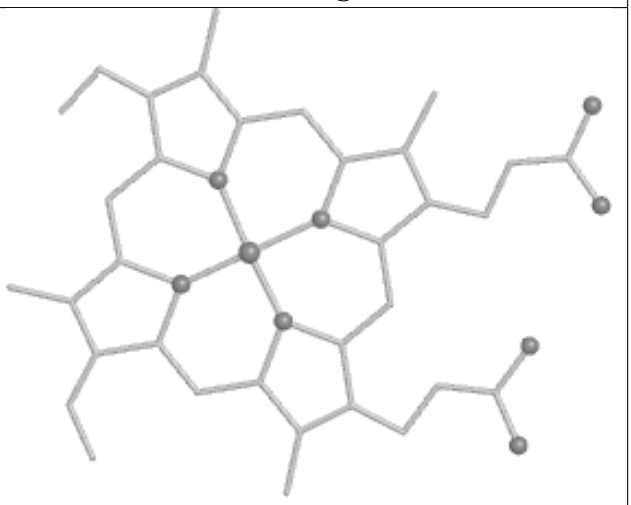
Bond lengths



Bond angles

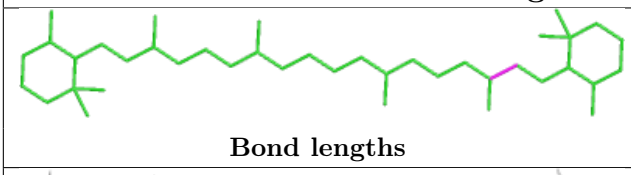


Torsions

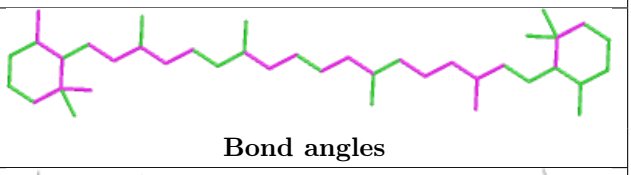


Rings

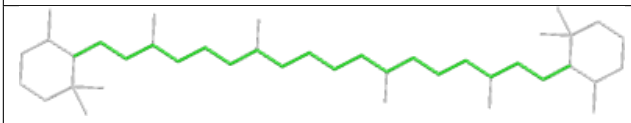
Ligand BCR c 516



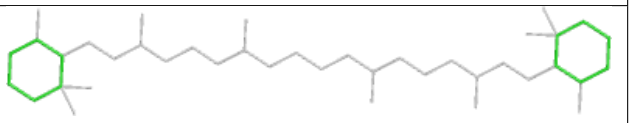
Bond lengths



Bond angles

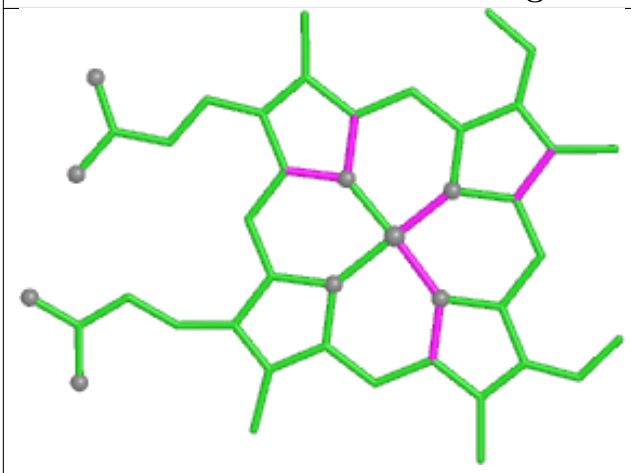


Torsions

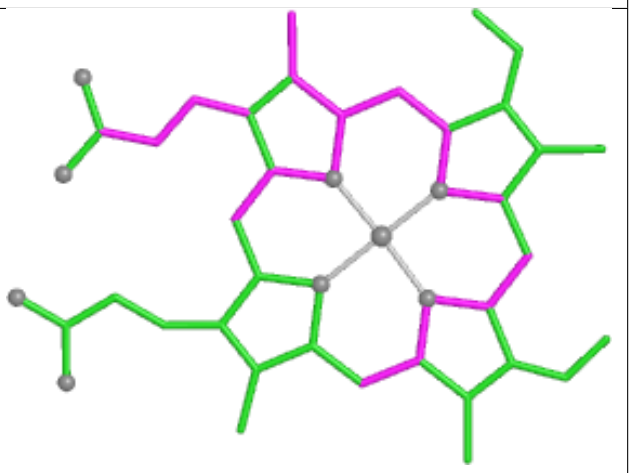


Rings

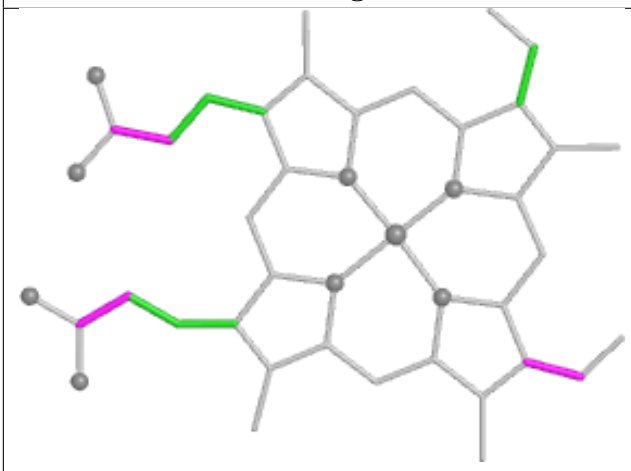
Ligand HEM f 101



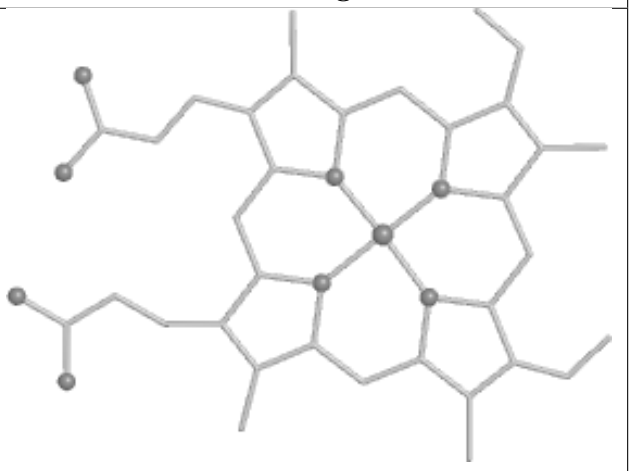
Bond lengths



Bond angles

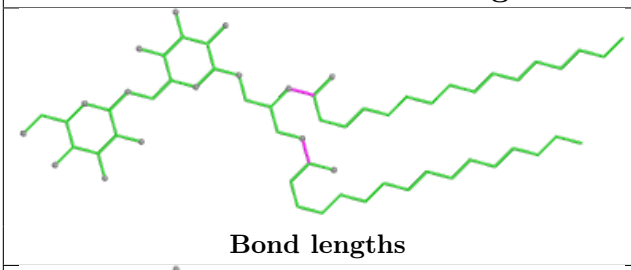


Torsions

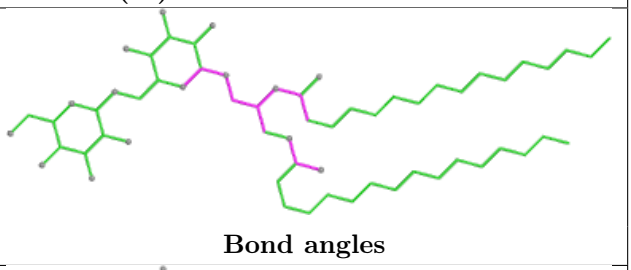


Rings

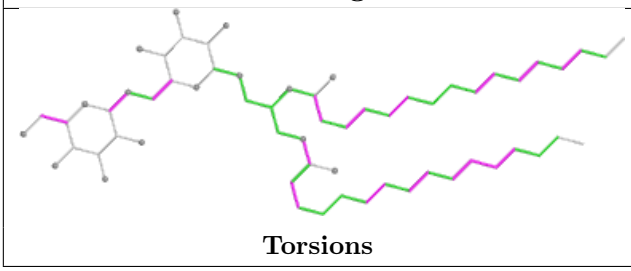
Ligand DGD c 517 (A)



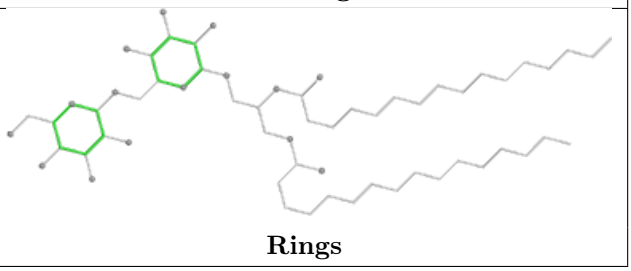
Bond lengths



Bond angles

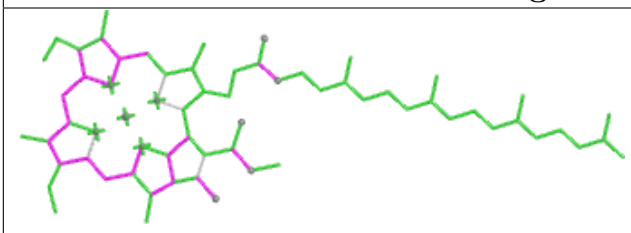


Torsions

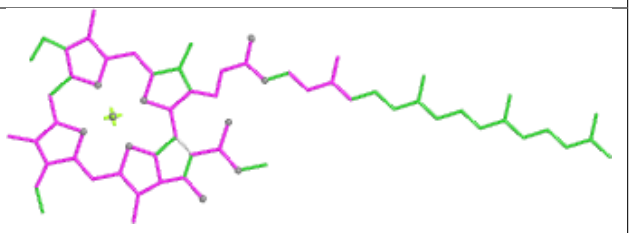


Rings

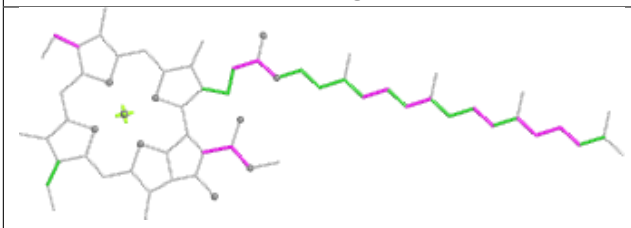
Ligand CLA c 513



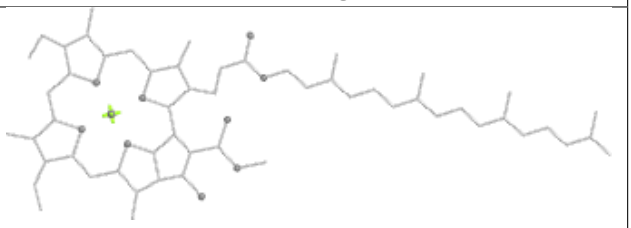
Bond lengths



Bond angles

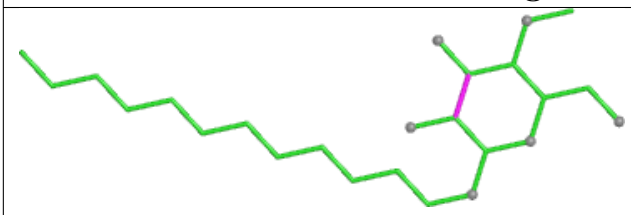


Torsions

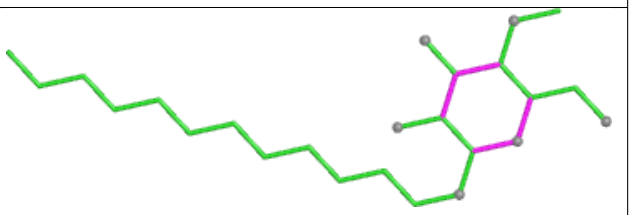


Rings

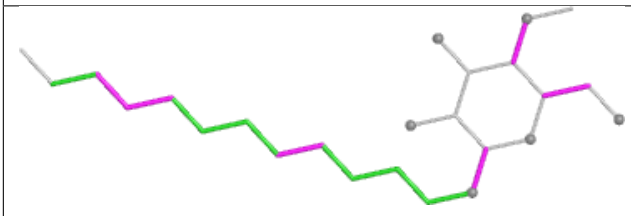
Ligand LMT b 621



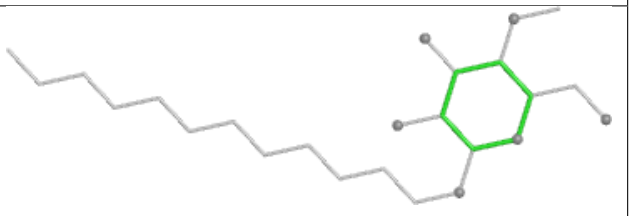
Bond lengths



Bond angles

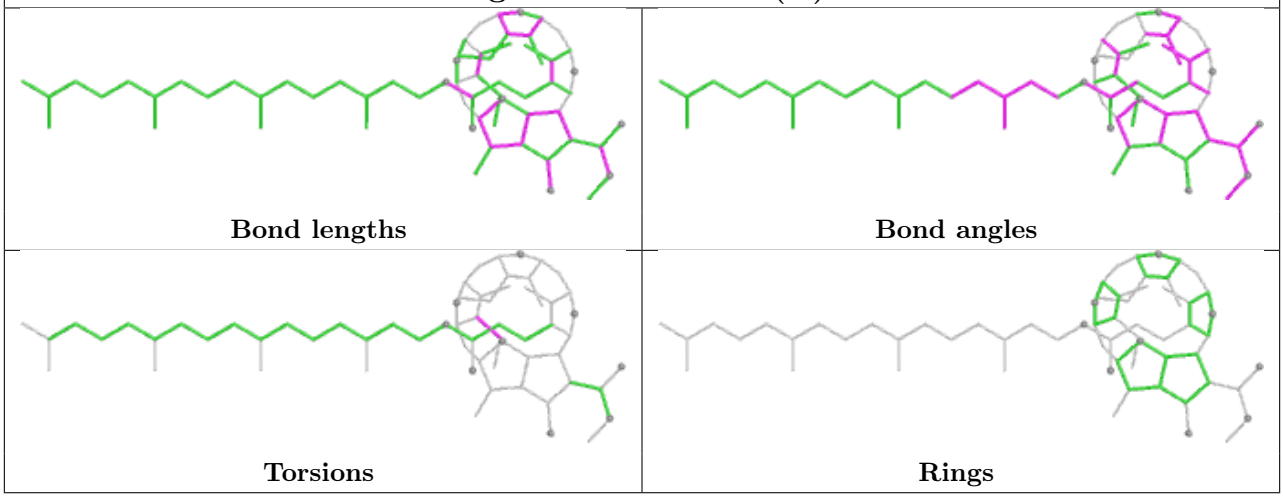


Torsions

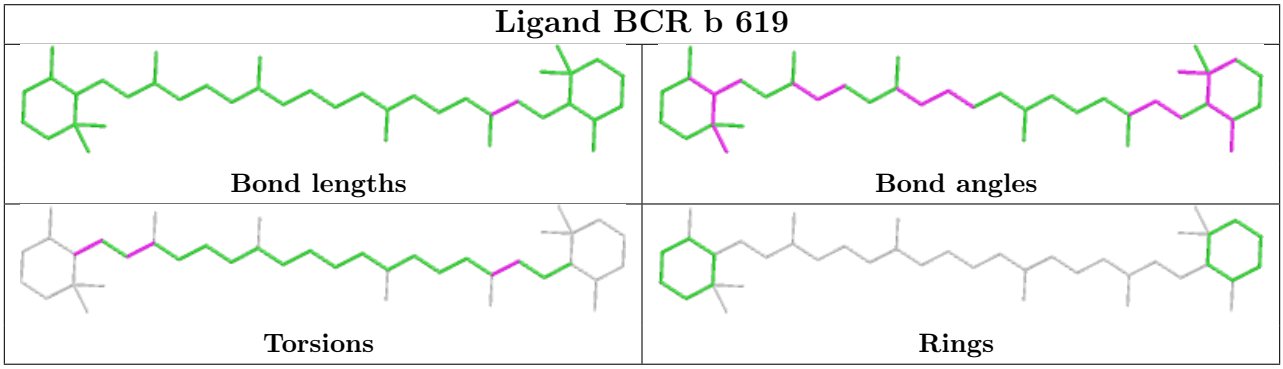


Rings

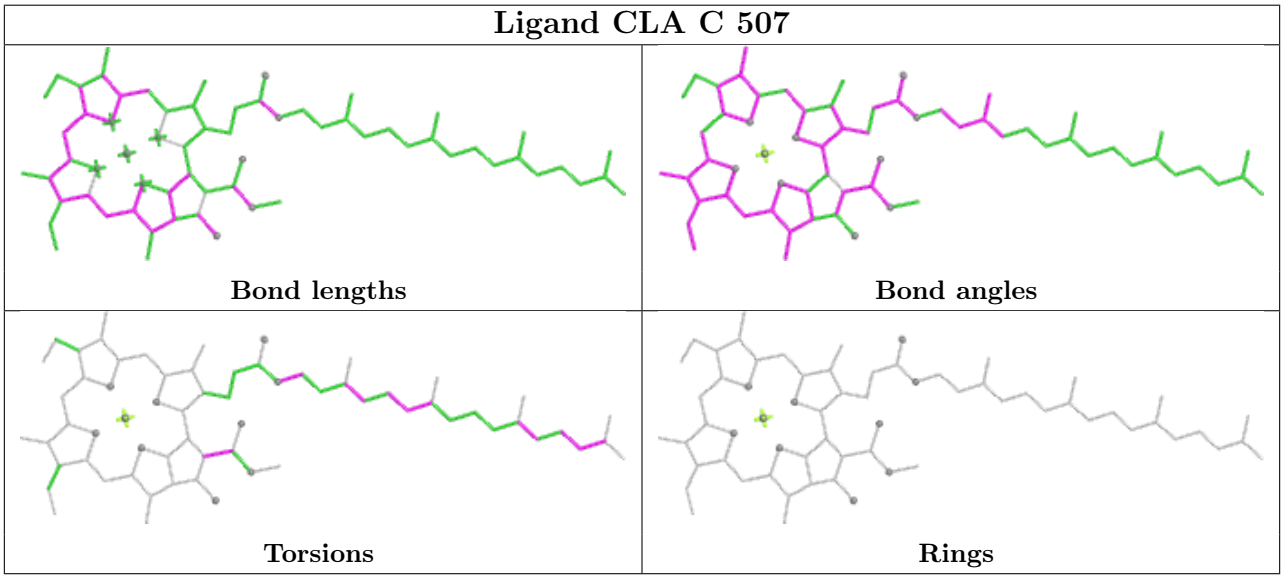
Ligand PHO A 417 (A)



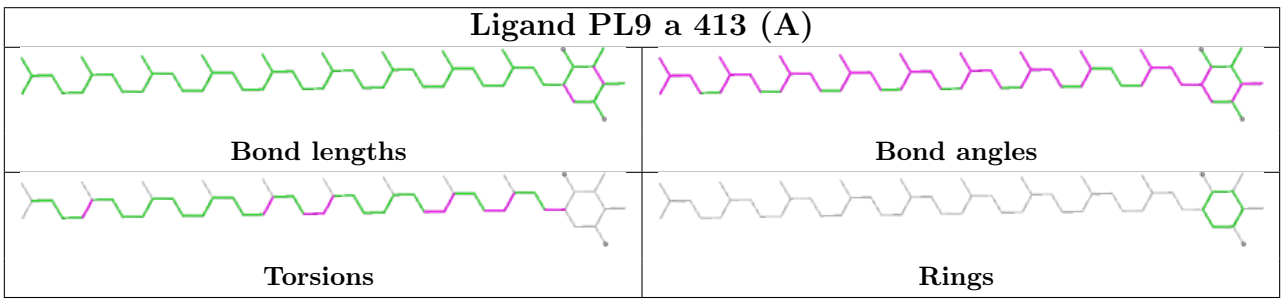
Ligand BCR b 619



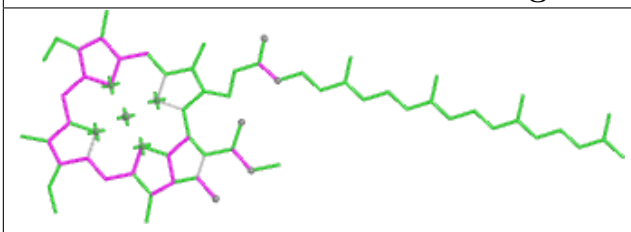
Ligand CLA C 507



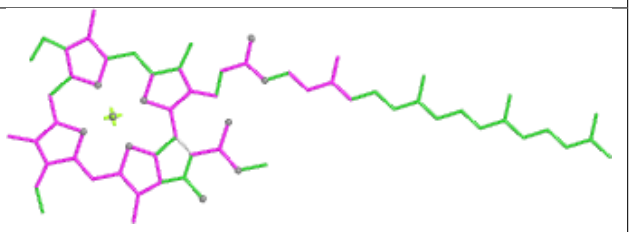
Ligand PL9 a 413 (A)



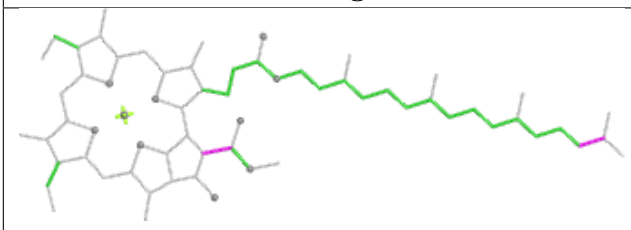
Ligand CLA c 509



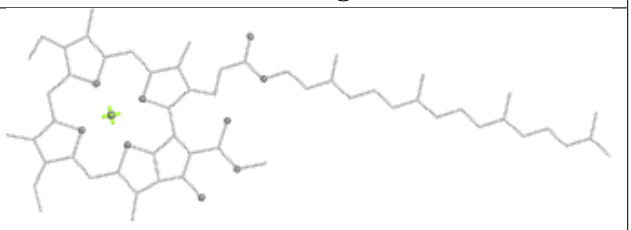
Bond lengths



Bond angles

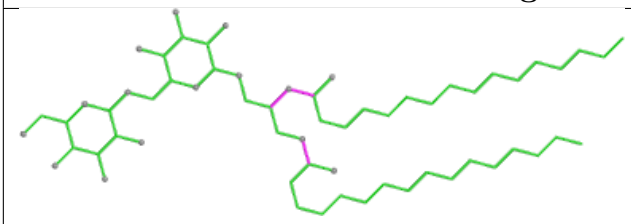


Torsions

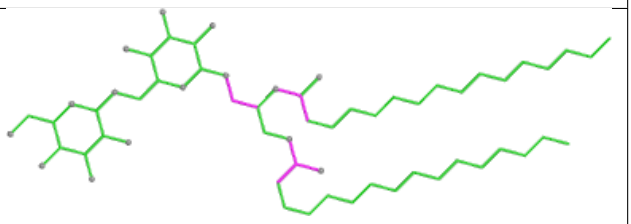


Rings

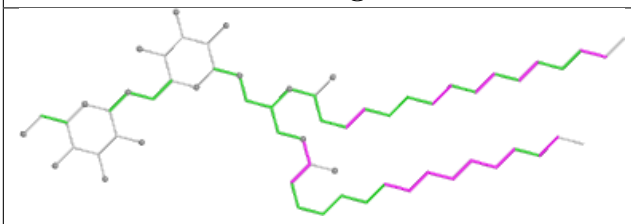
Ligand DGD C 519



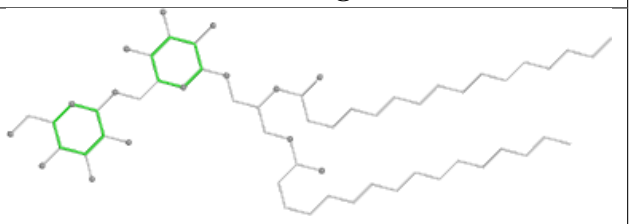
Bond lengths



Bond angles

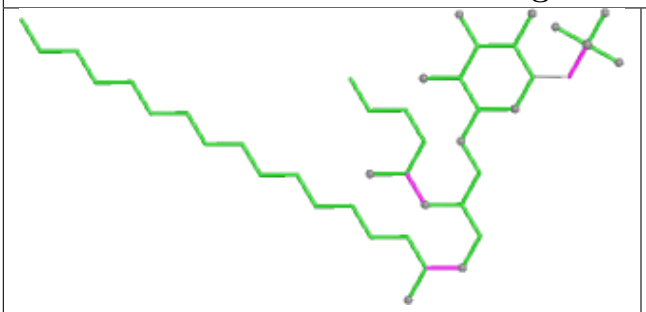


Torsions

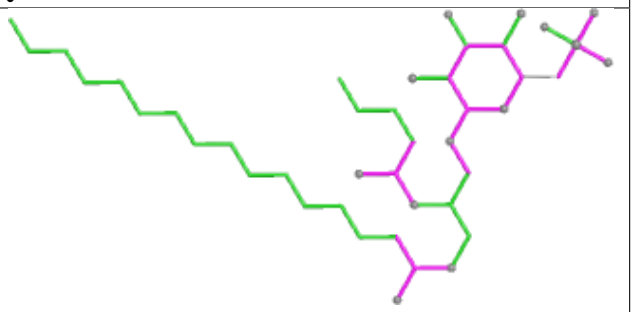


Rings

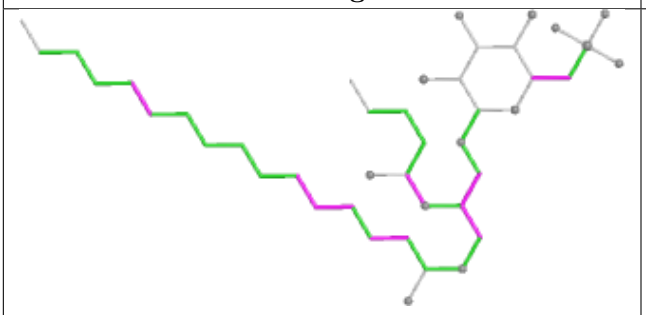
Ligand SQD f 102



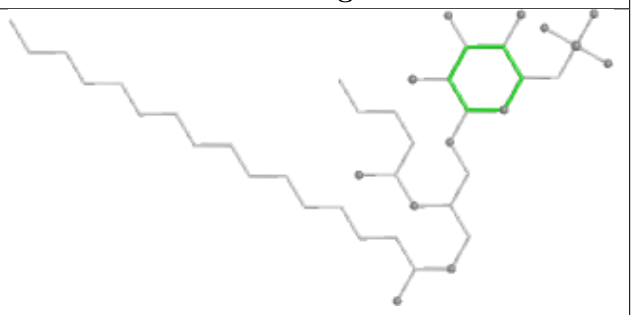
Bond lengths



Bond angles

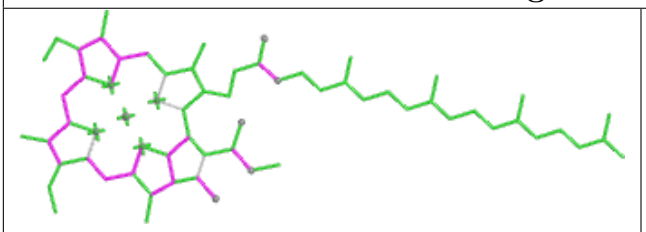


Torsions

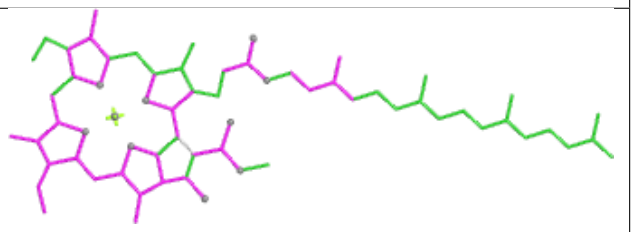


Rings

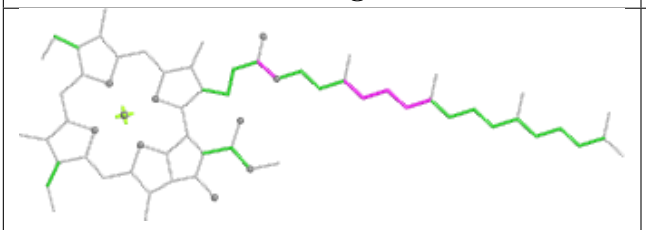
Ligand CLA b 616



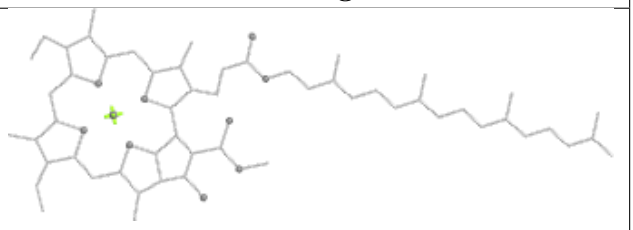
Bond lengths



Bond angles

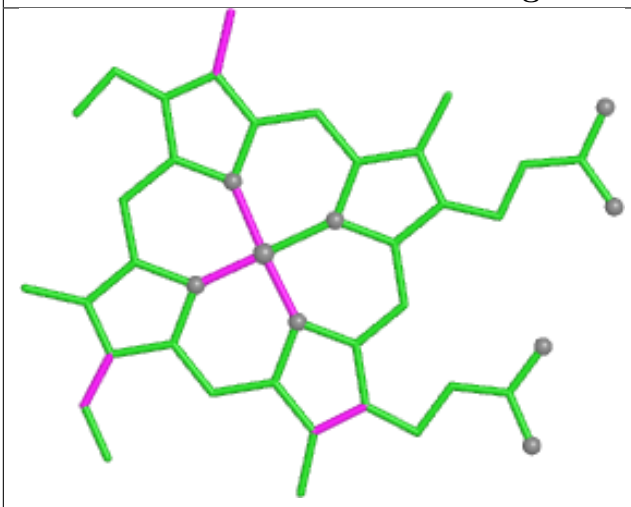


Torsions

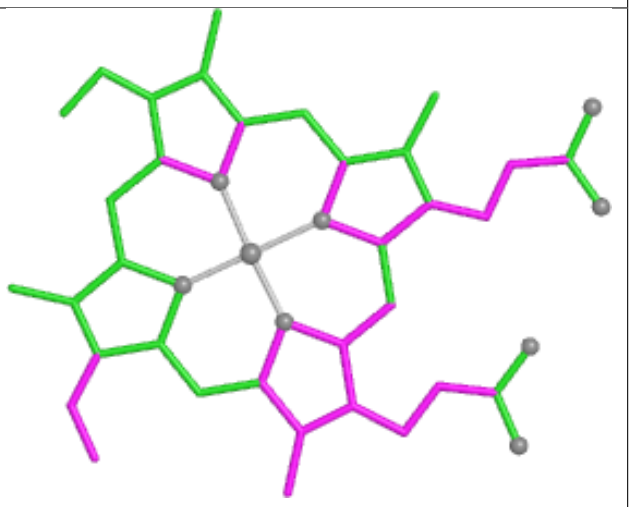


Rings

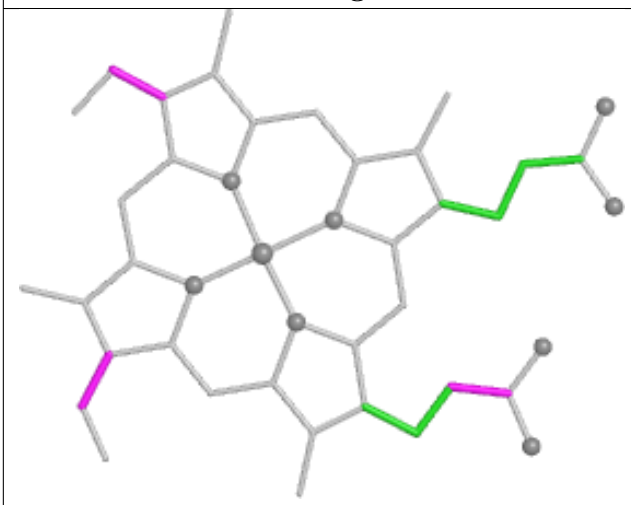
Ligand HEC V 201



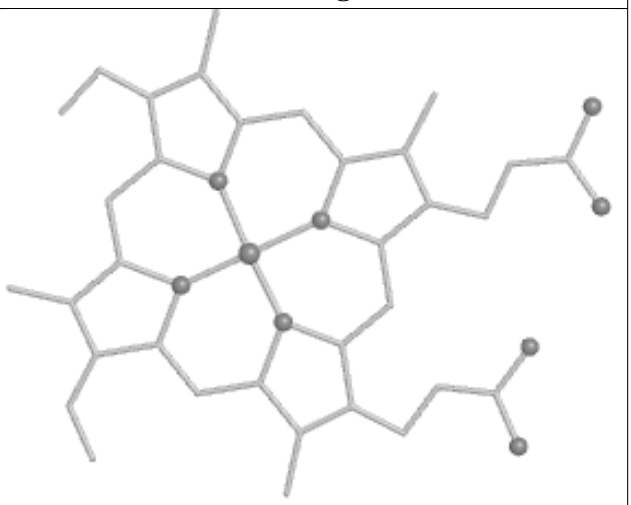
Bond lengths



Bond angles



Torsions

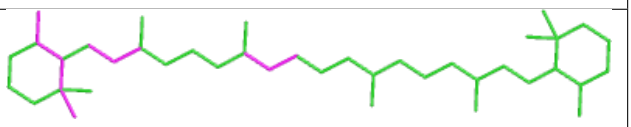


Rings

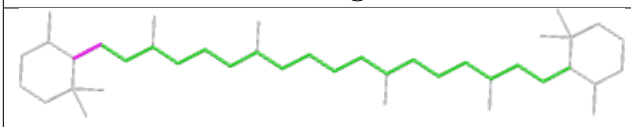
Ligand BCR B 617



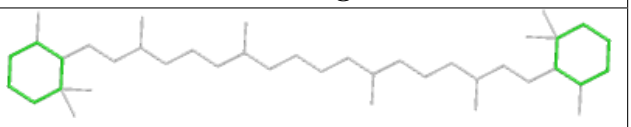
Bond lengths



Bond angles

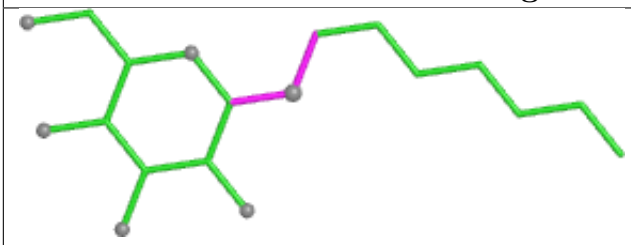


Torsions

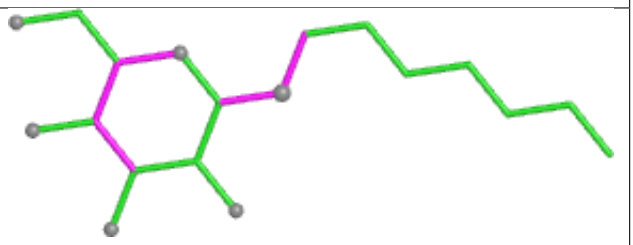


Rings

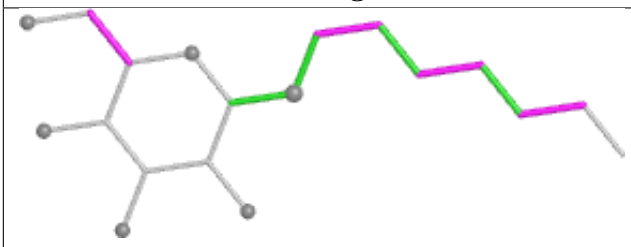
Ligand HTG B 623



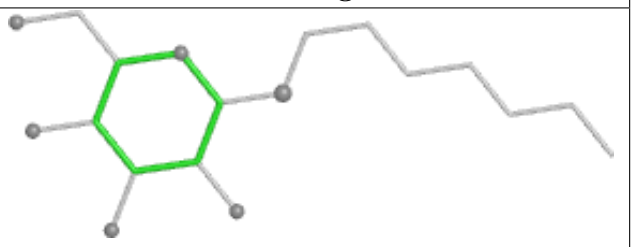
Bond lengths



Bond angles



Torsions

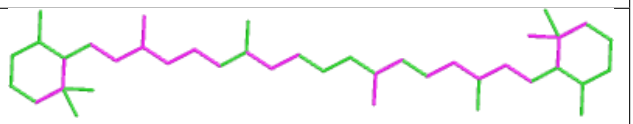


Rings

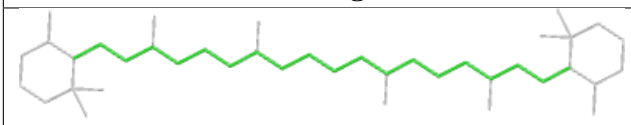
Ligand BCR k 101



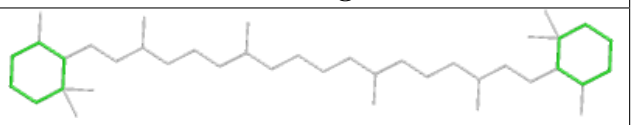
Bond lengths



Bond angles

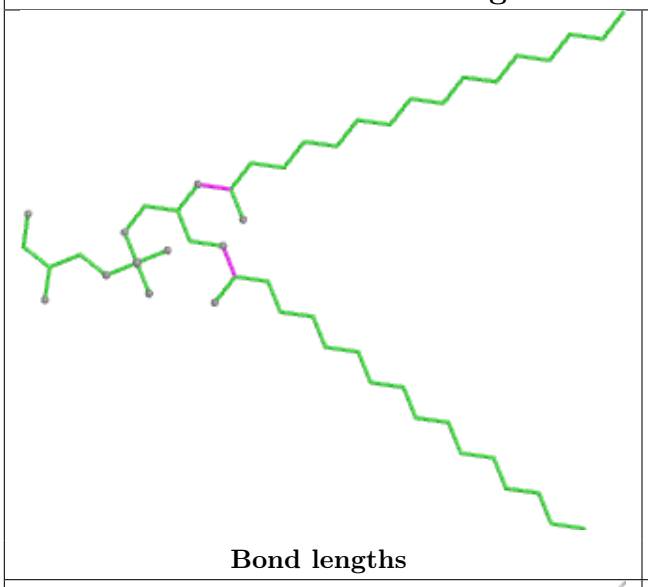


Torsions

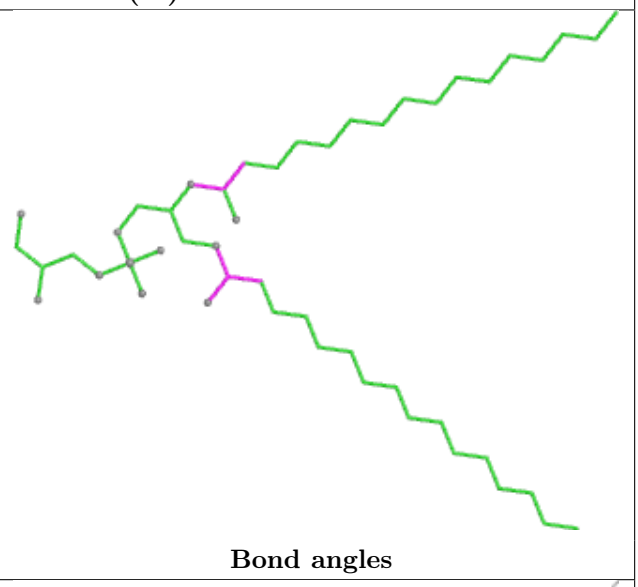


Rings

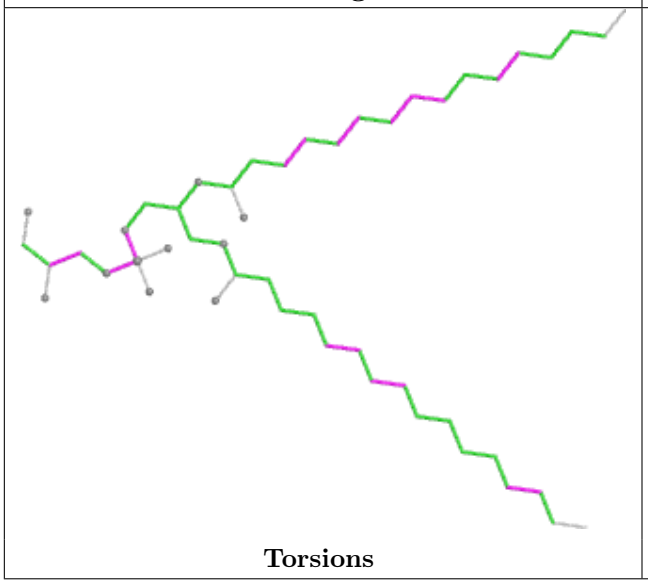
Ligand LHG D 406 (A)



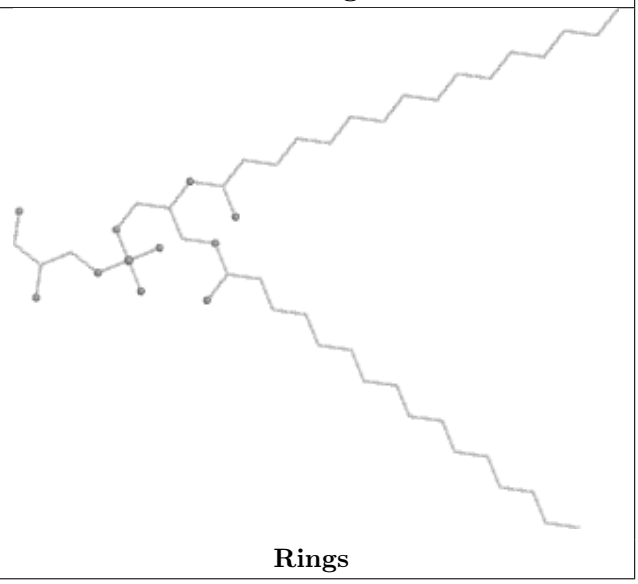
Bond lengths



Bond angles

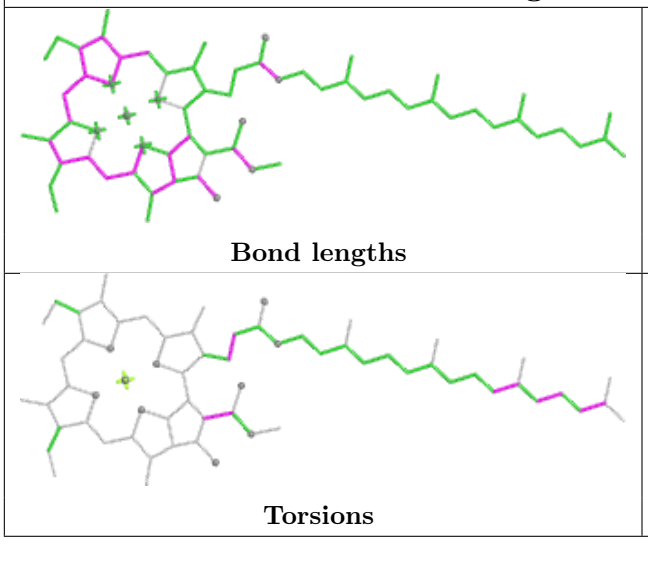


Torsions

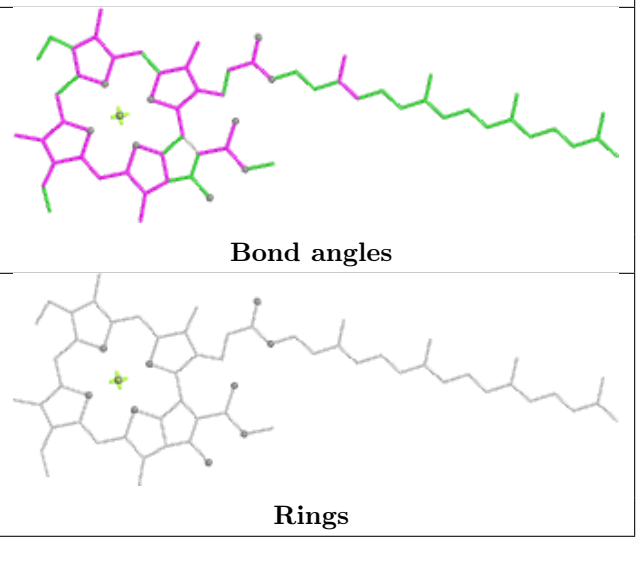


Rings

Ligand CLA B 603



Bond lengths

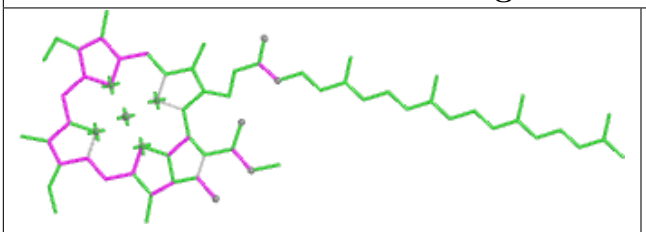


Bond angles

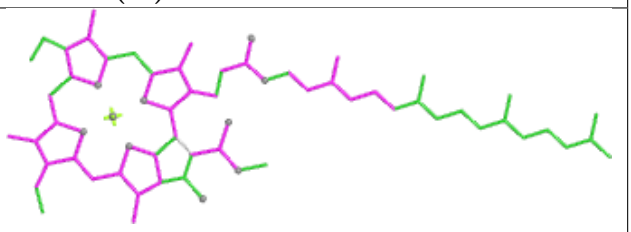
Torsions

Rings

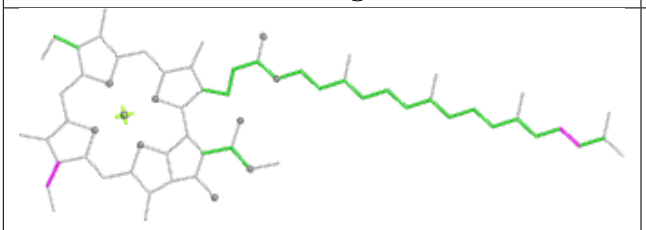
Ligand CLA a 404 (A)



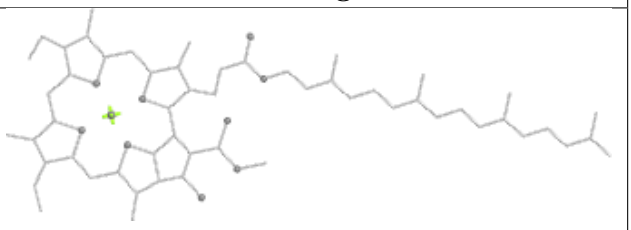
Bond lengths



Bond angles

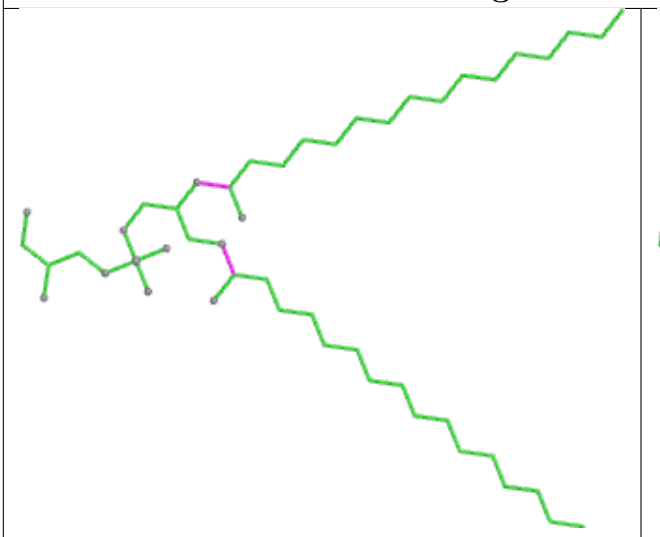


Torsions

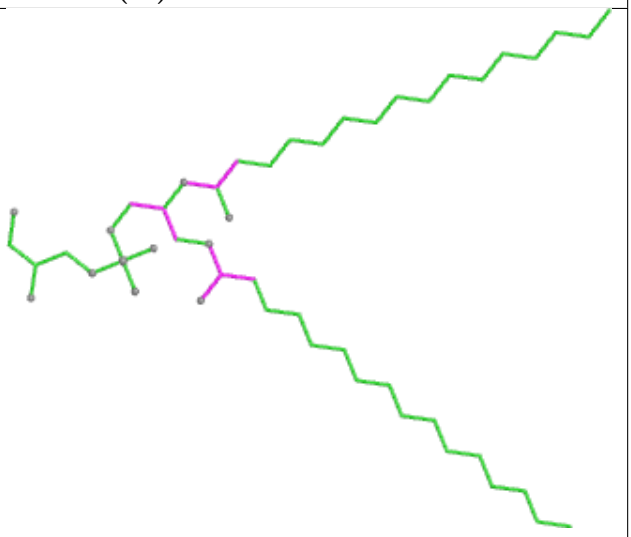


Rings

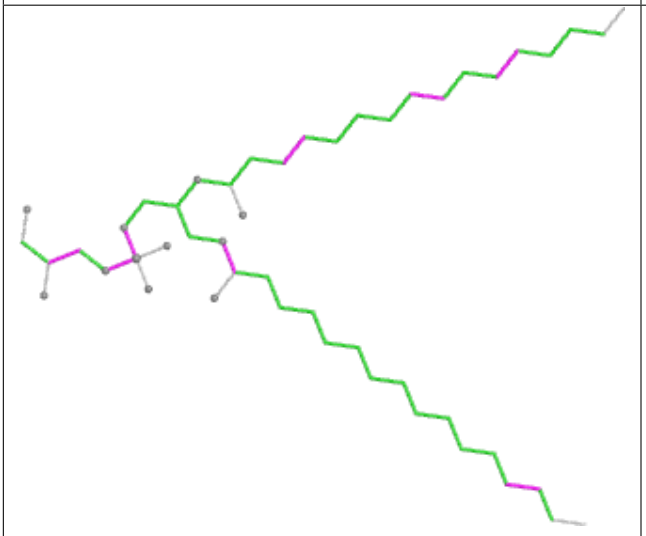
Ligand LHG d 406 (A)



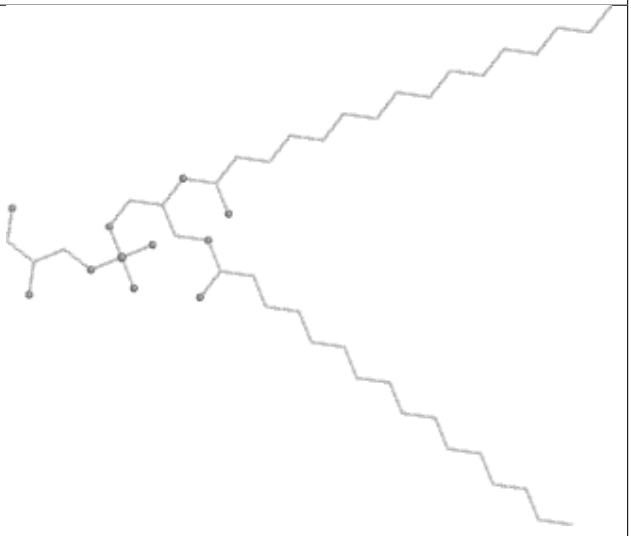
Bond lengths



Bond angles

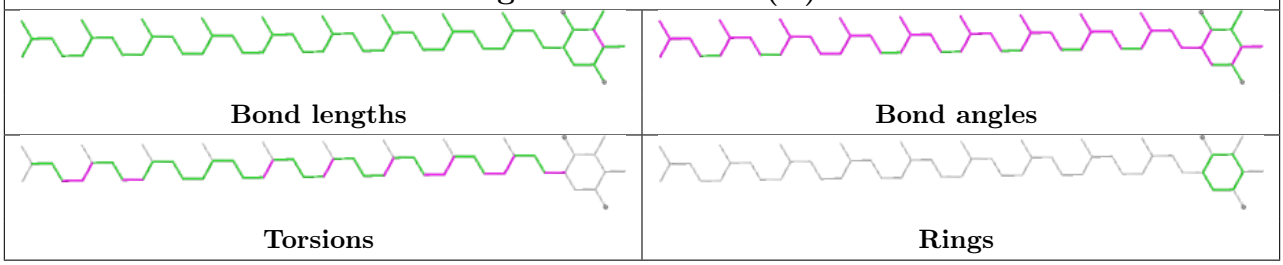


Torsions

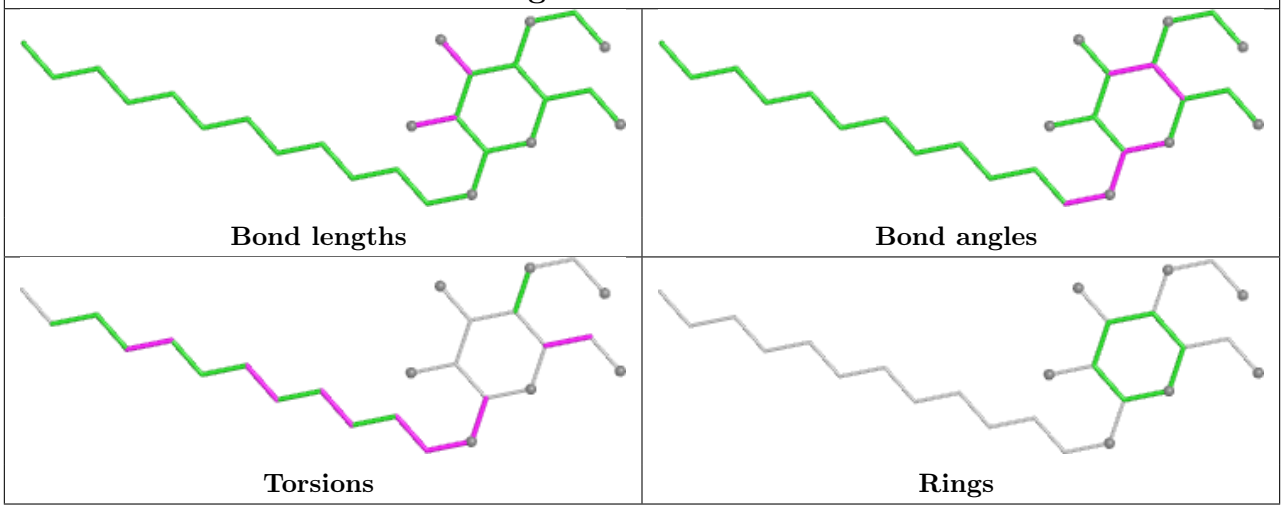


Rings

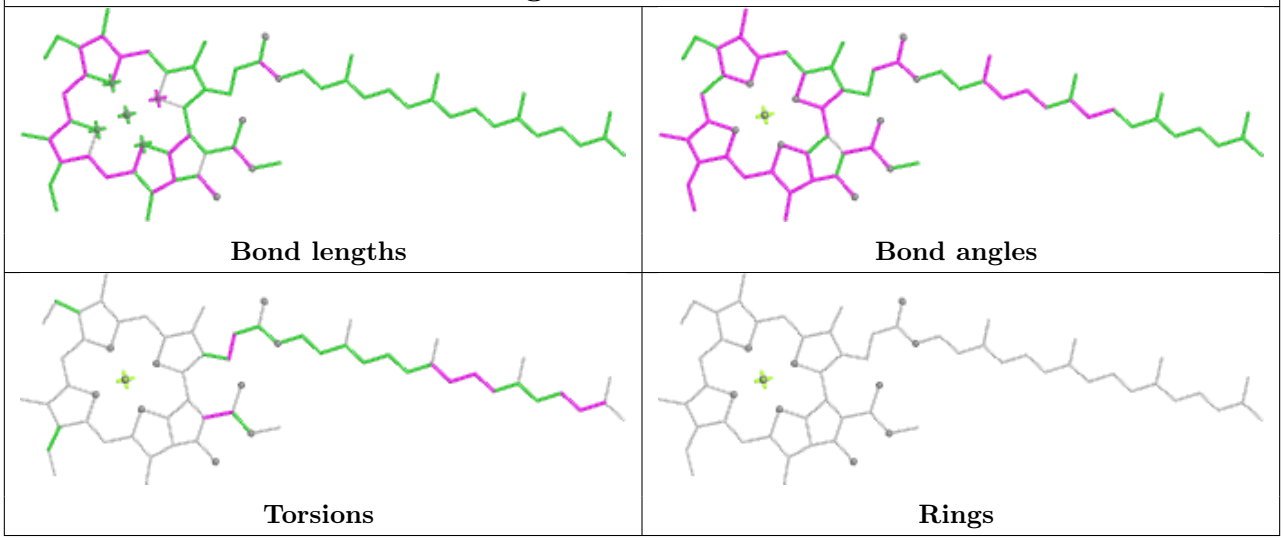
Ligand PL9 A 414 (B)



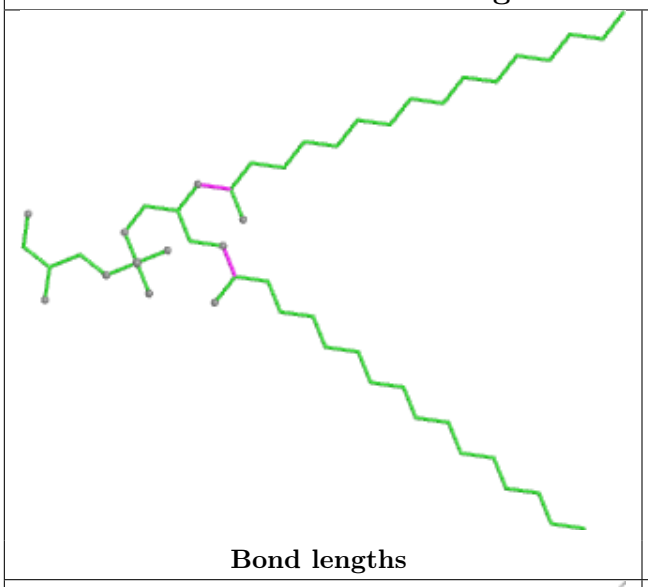
Ligand LMT t 101



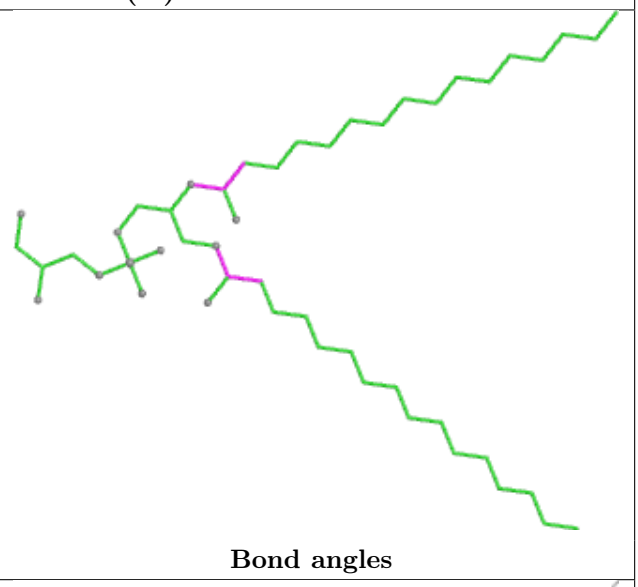
Ligand CLA B 606



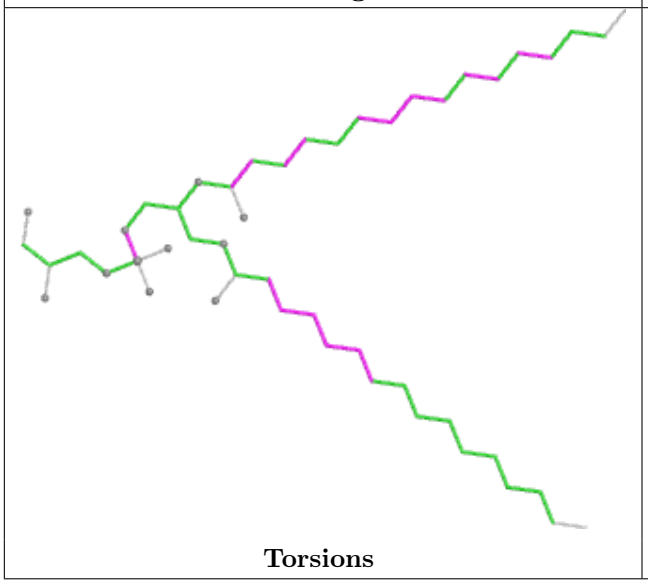
Ligand LHG L 102 (B)



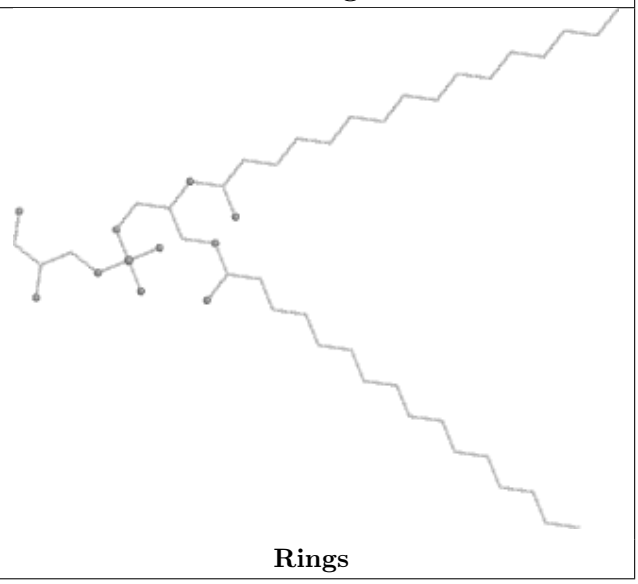
Bond lengths



Bond angles

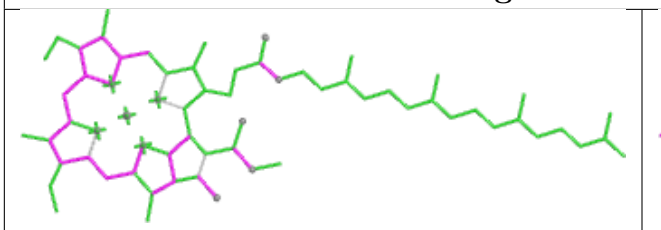


Torsions

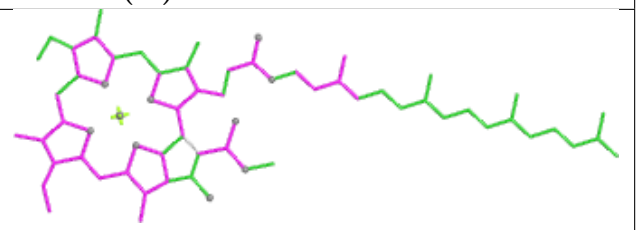


Rings

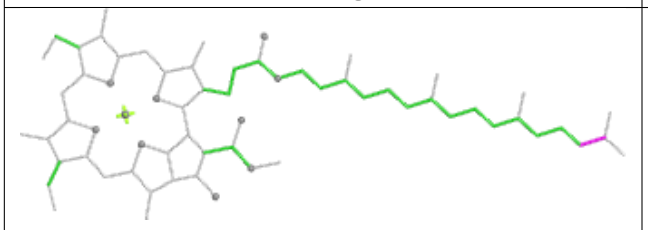
Ligand CLA d 402 (A)



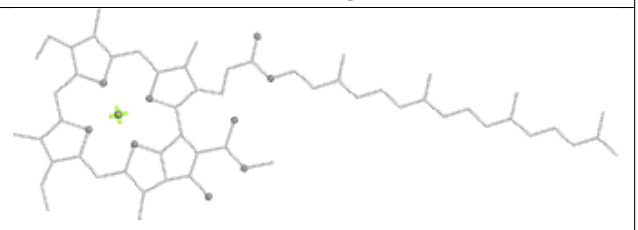
Bond lengths



Bond angles

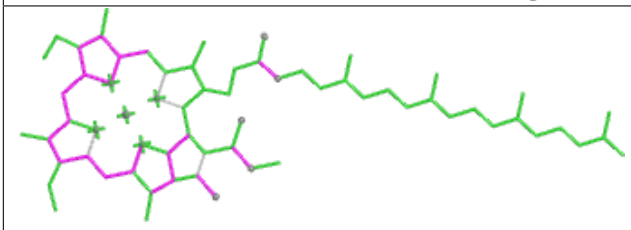


Torsions

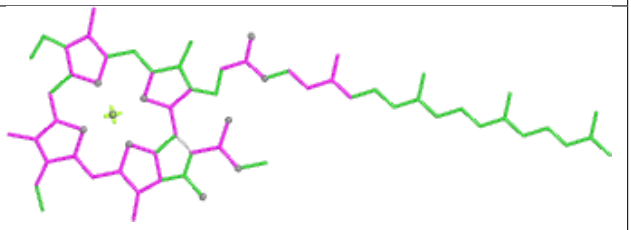


Rings

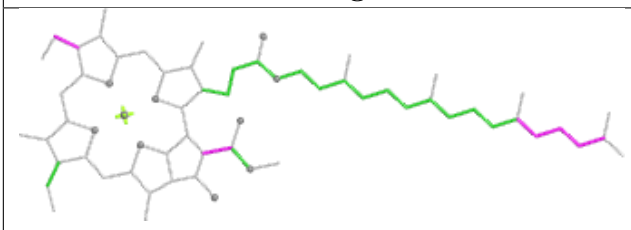
Ligand CLA C 503



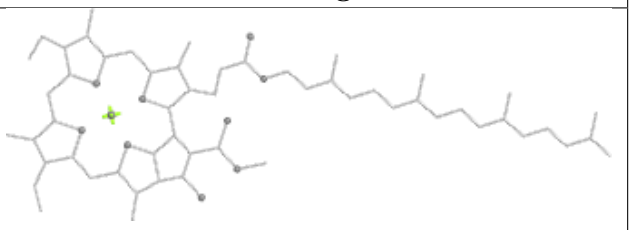
Bond lengths



Bond angles

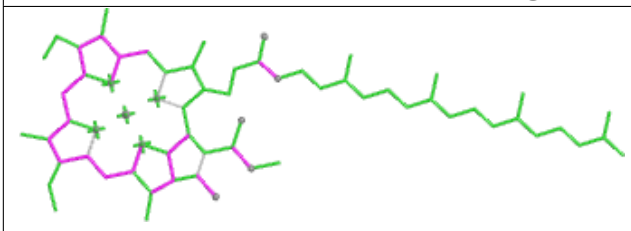


Torsions

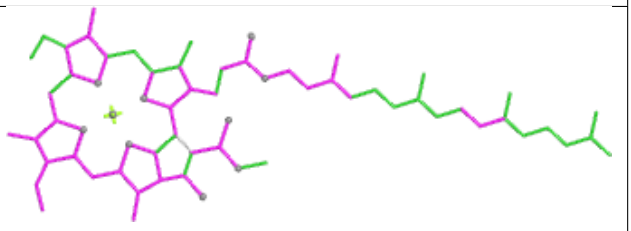


Rings

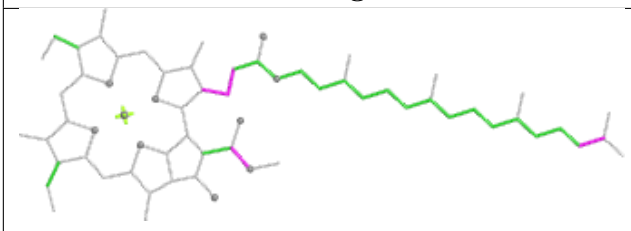
Ligand CLA C 502



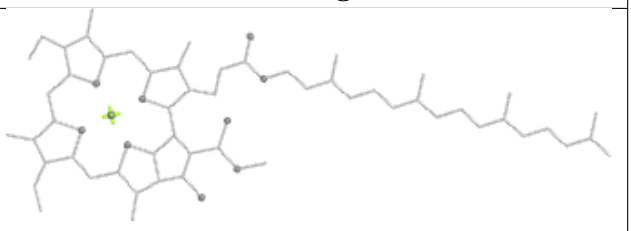
Bond lengths



Bond angles

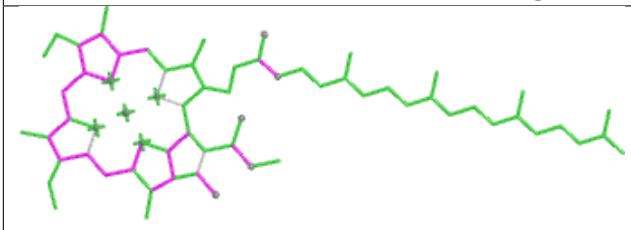


Torsions

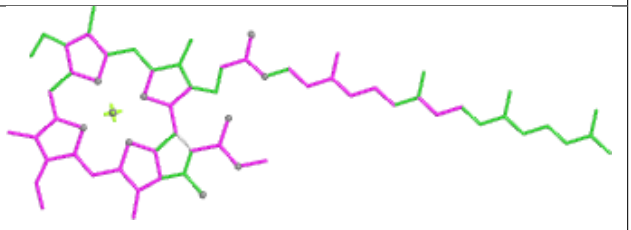


Rings

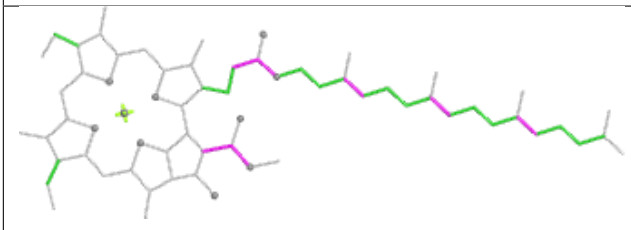
Ligand CLA c 511



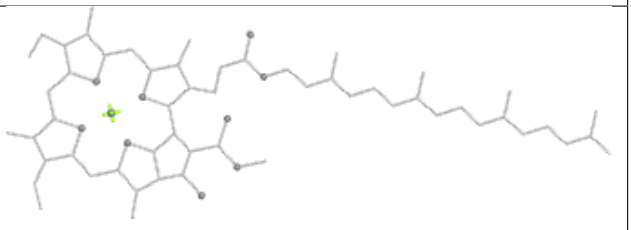
Bond lengths



Bond angles

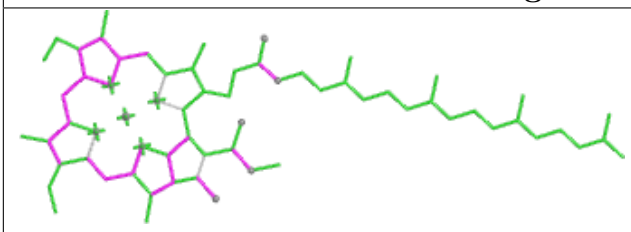


Torsions

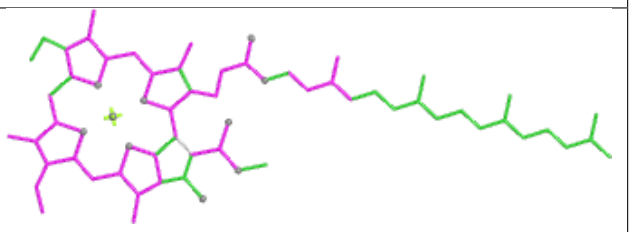


Rings

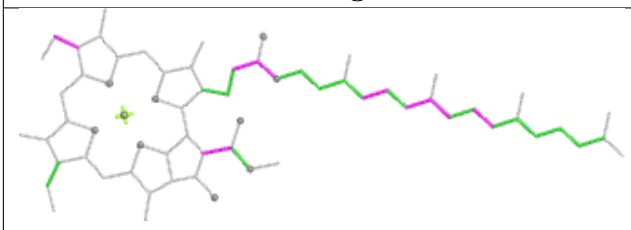
Ligand CLA C 513



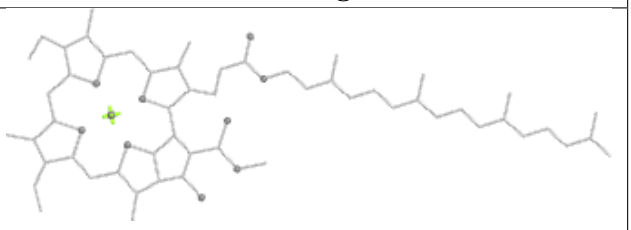
Bond lengths



Bond angles

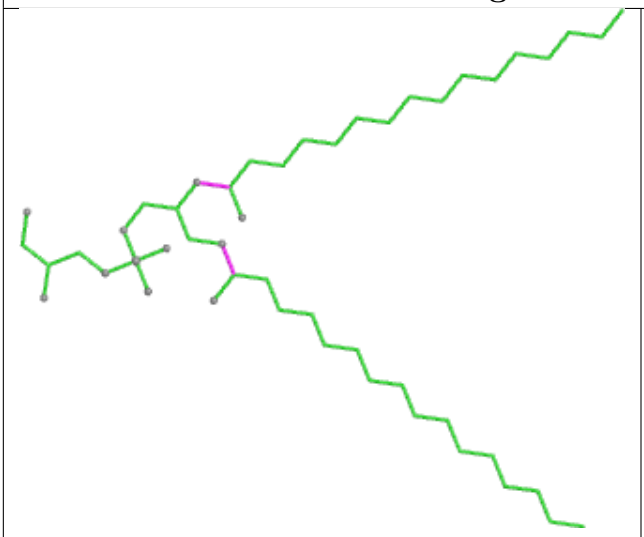


Torsions

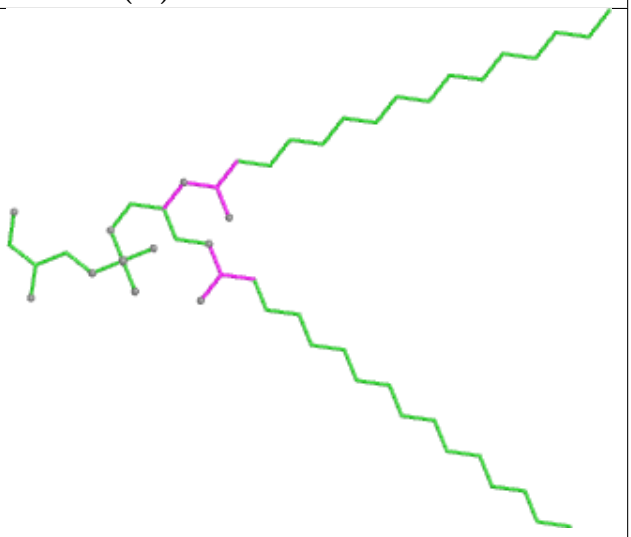


Rings

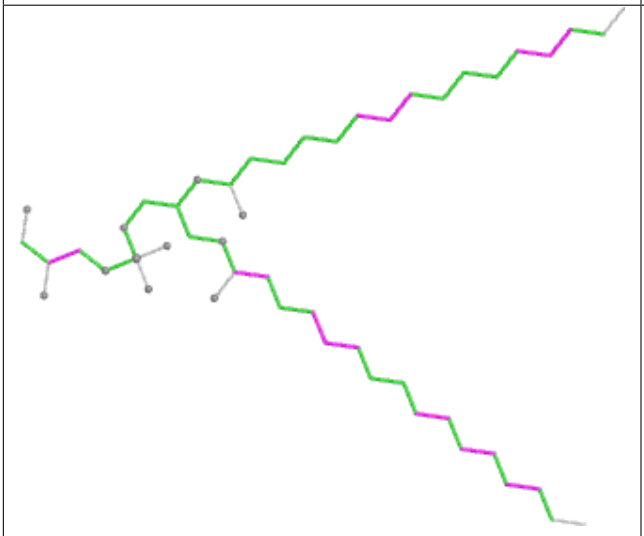
Ligand LHG A 419 (B)



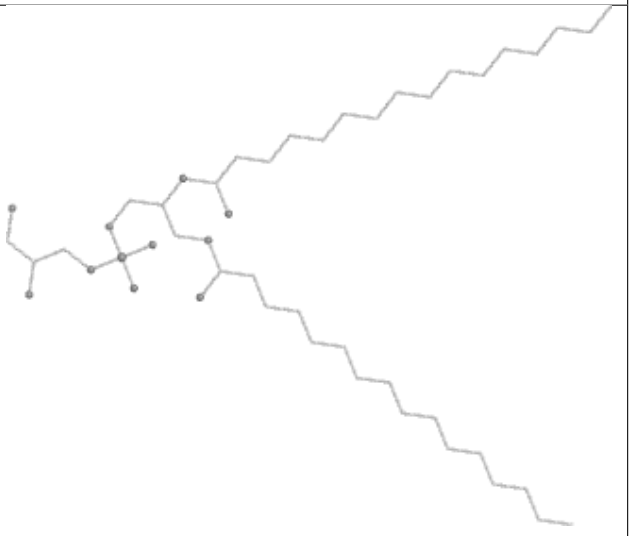
Bond lengths



Bond angles

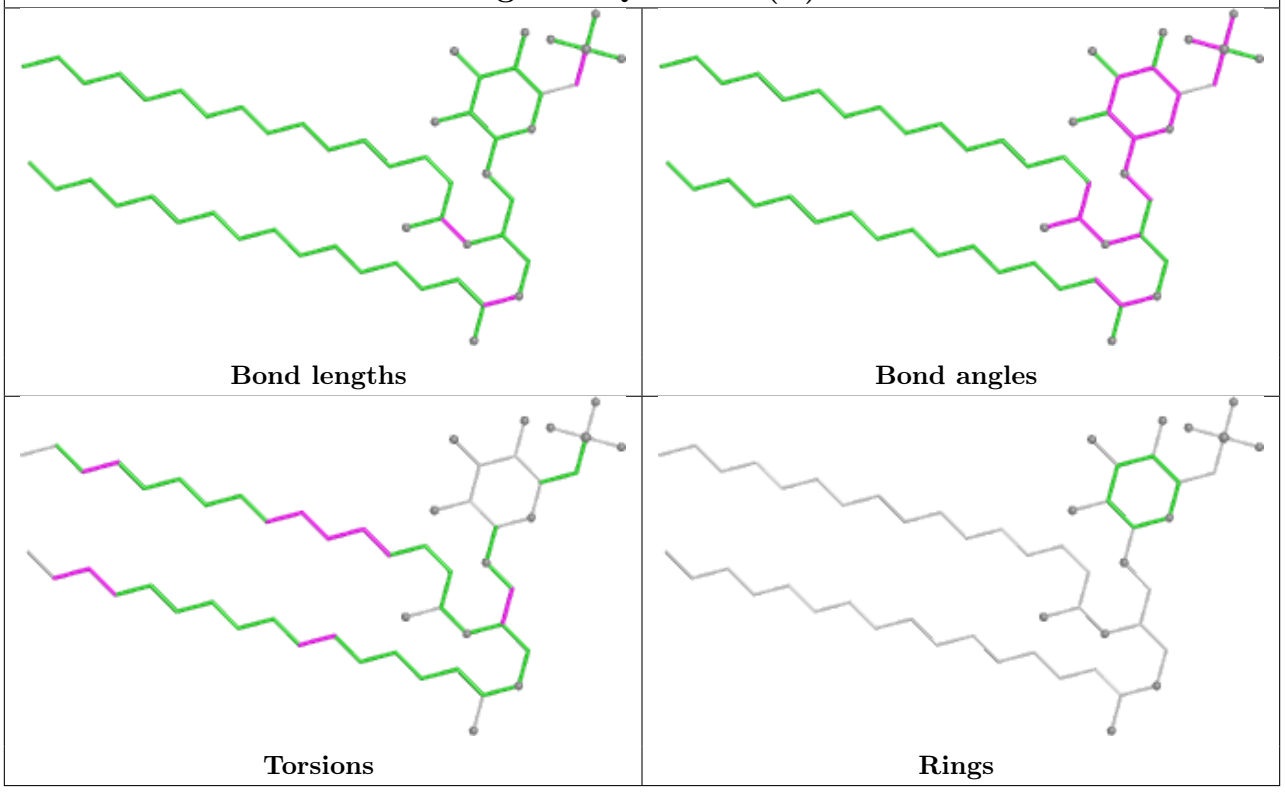


Torsions

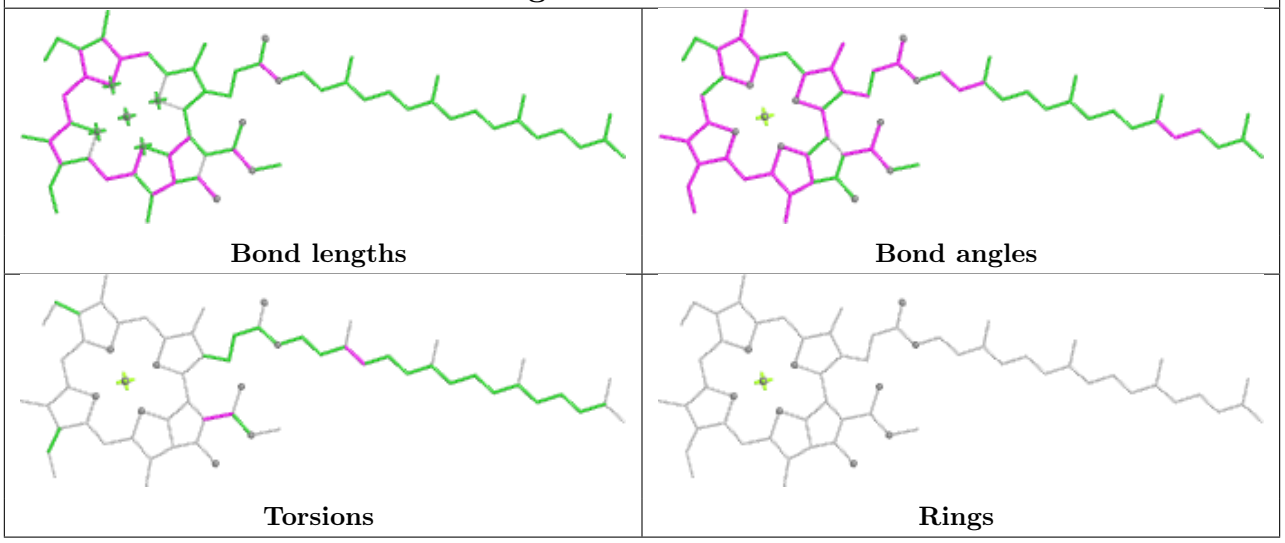


Rings

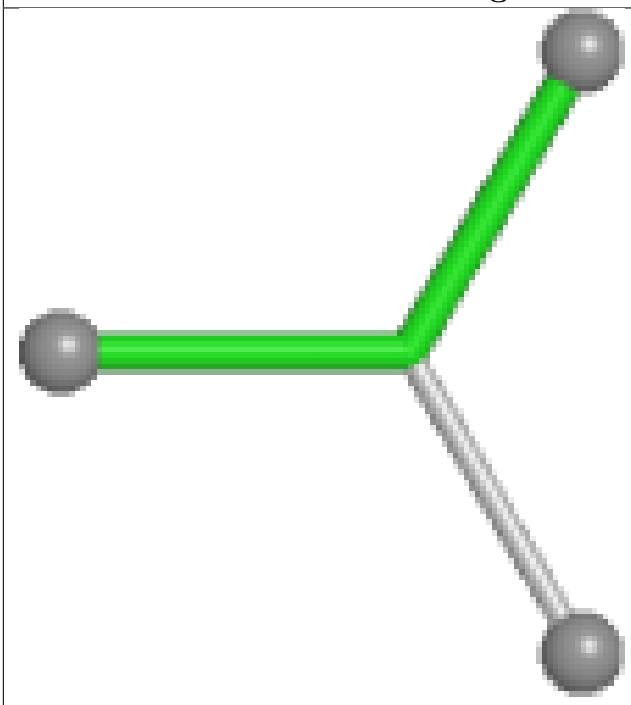
Ligand SQD a 410 (B)



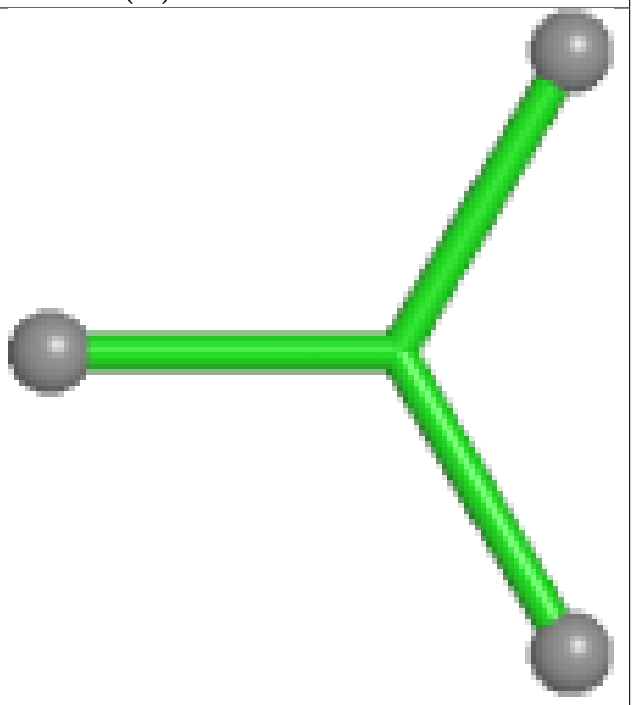
Ligand CLA b 609



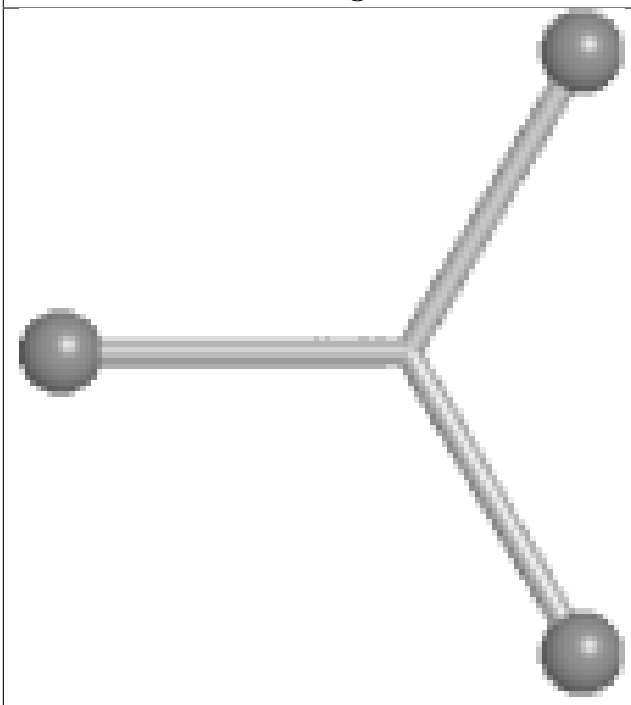
Ligand BCT A 416 (B)



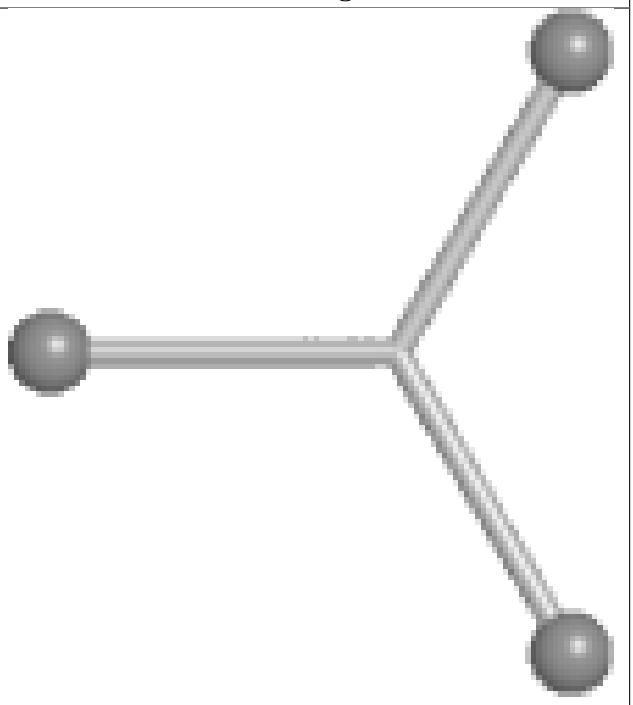
Bond lengths



Bond angles

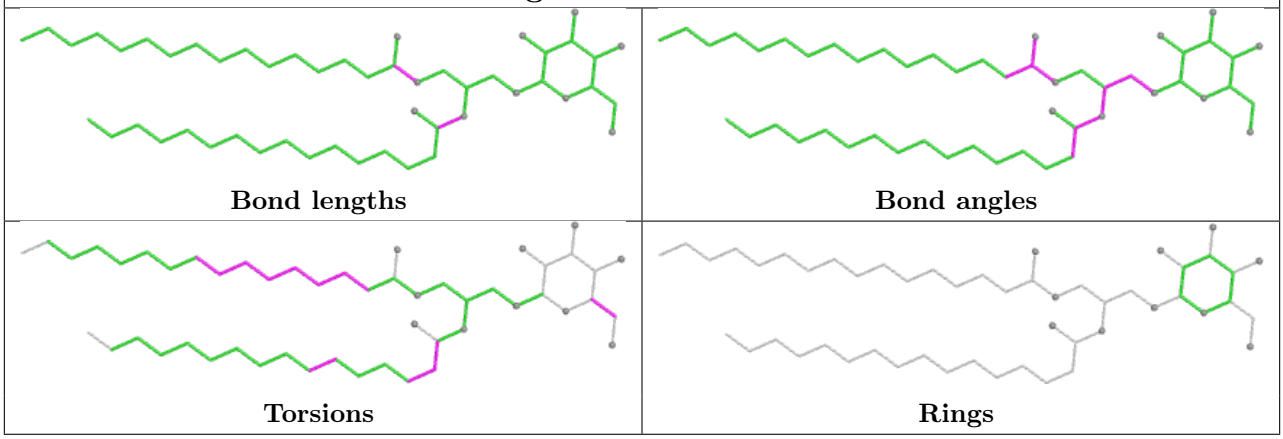


Torsions

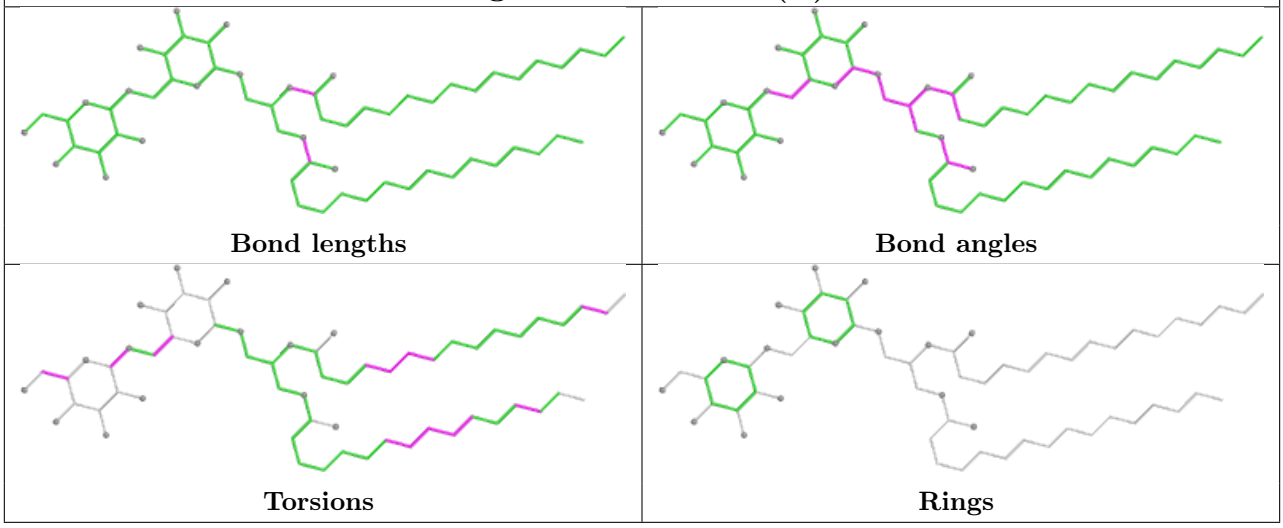


Rings

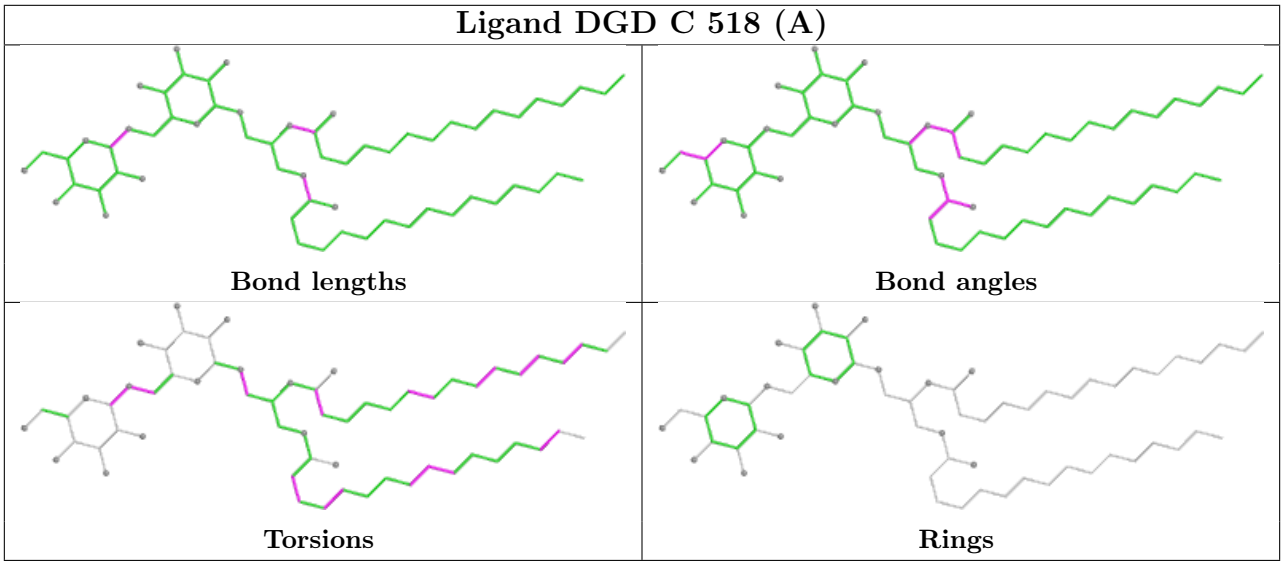
Ligand LMG c 520



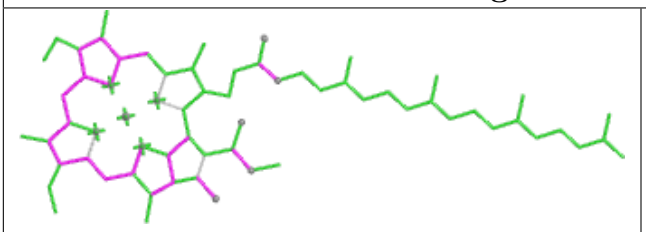
Ligand DGD C 517 (B)

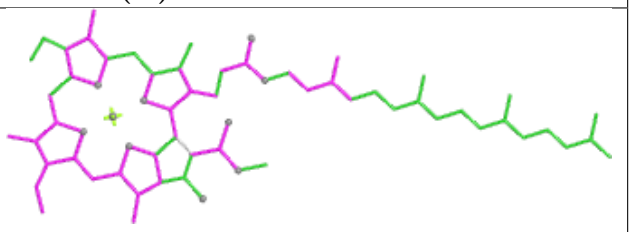


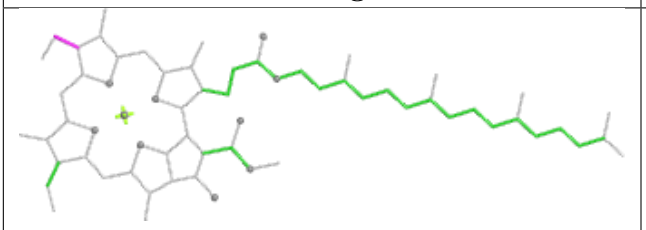
Ligand DGD C 518 (A)

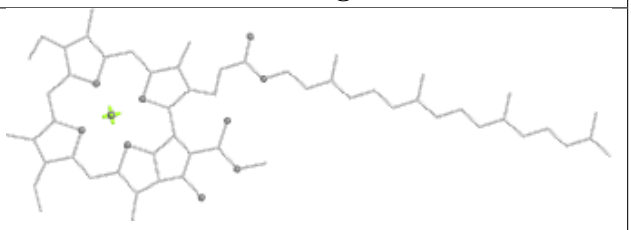


Ligand CLA D 402 (B)


Bond lengths


Bond angles


Torsions

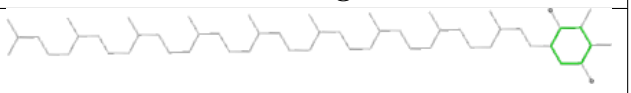

Rings

Ligand PL9 d 405 (A)

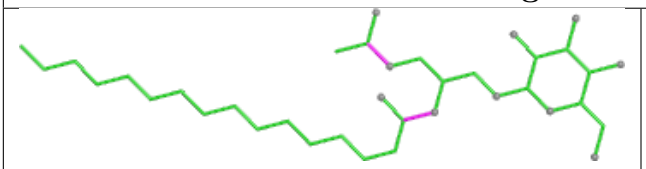

Bond lengths

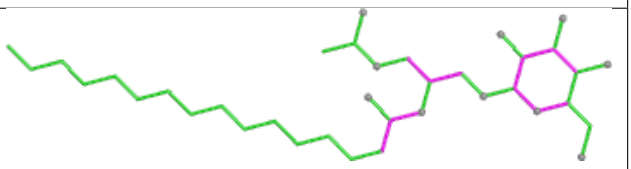

Bond angles

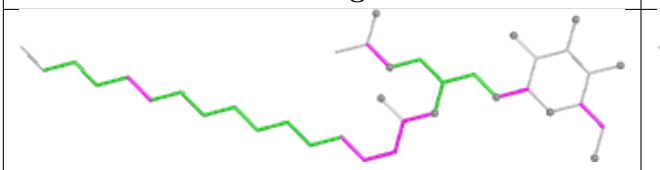

Torsions

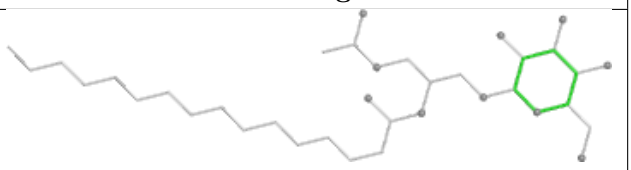

Rings

Ligand LMG Z 101

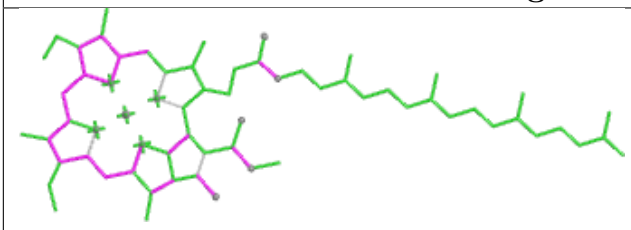

Bond lengths


Bond angles

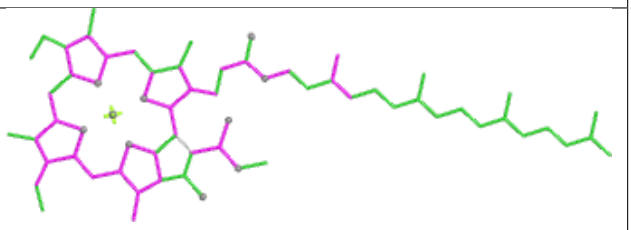

Torsions


Rings

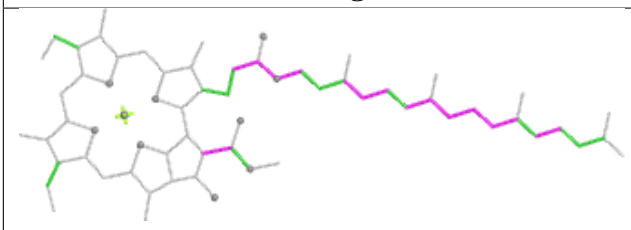
Ligand CLA b 601



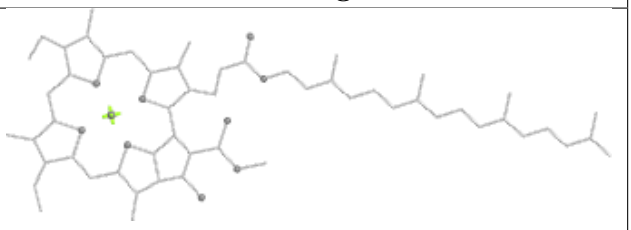
Bond lengths



Bond angles

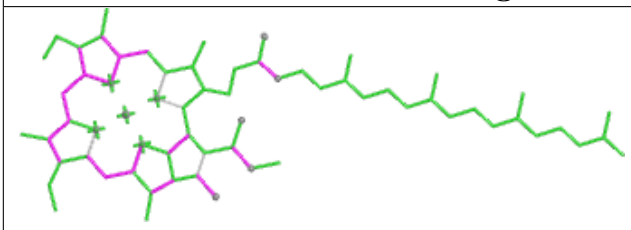


Torsions

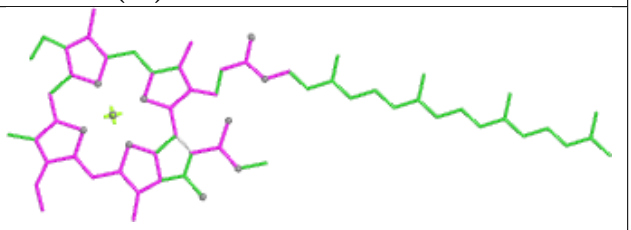


Rings

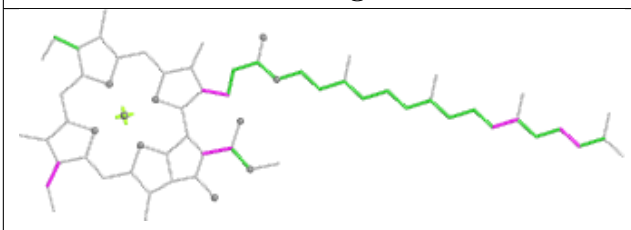
Ligand CLA a 405 (A)



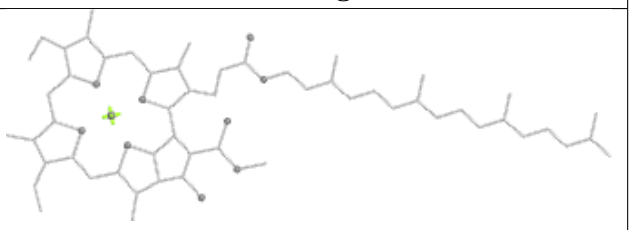
Bond lengths



Bond angles

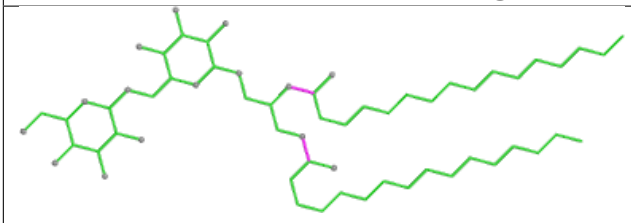


Torsions

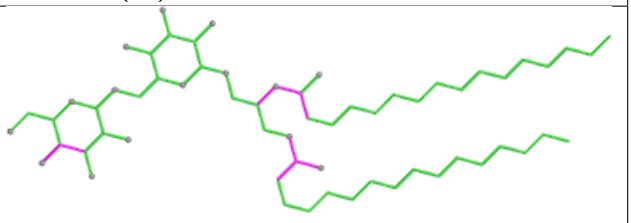


Rings

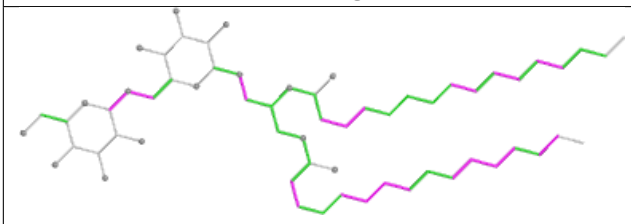
Ligand DGD c 518 (A)



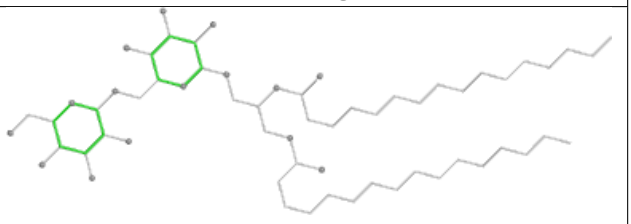
Bond lengths



Bond angles

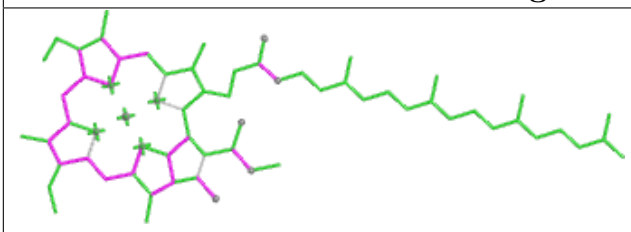


Torsions

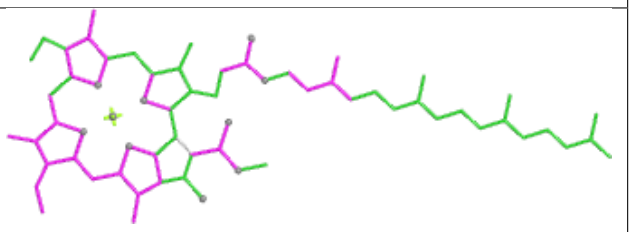


Rings

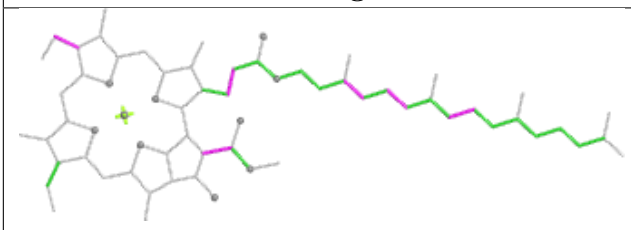
Ligand CLA c 508



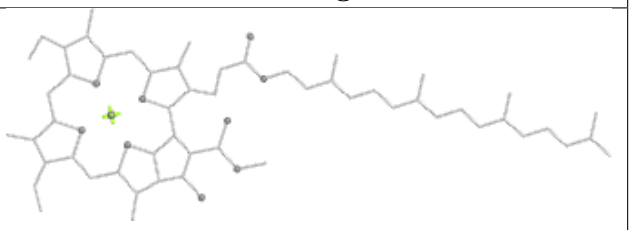
Bond lengths



Bond angles

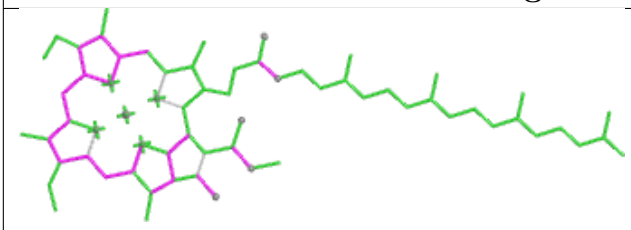


Torsions

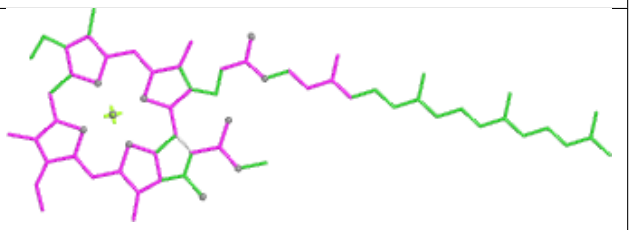


Rings

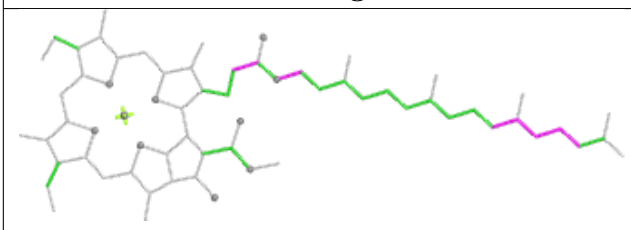
Ligand CLA B 613



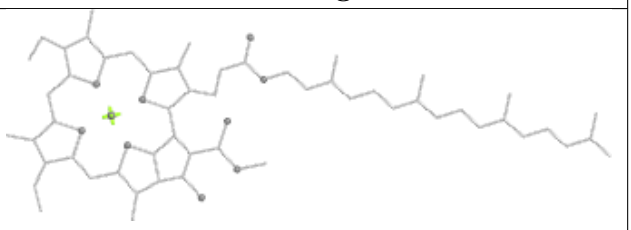
Bond lengths



Bond angles

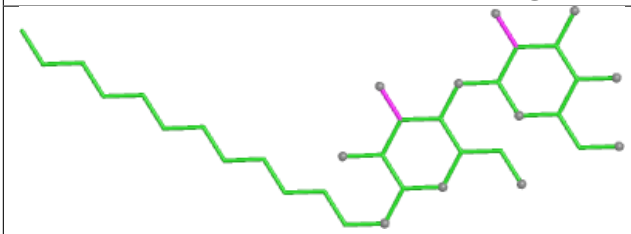


Torsions

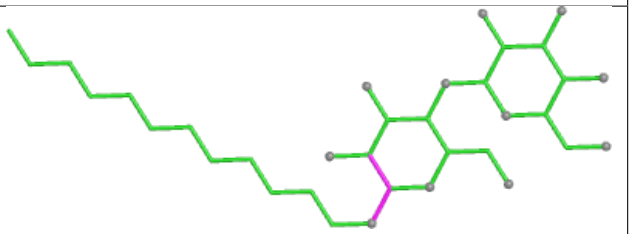


Rings

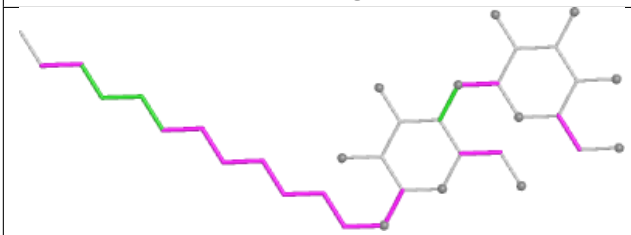
Ligand LMT e 101



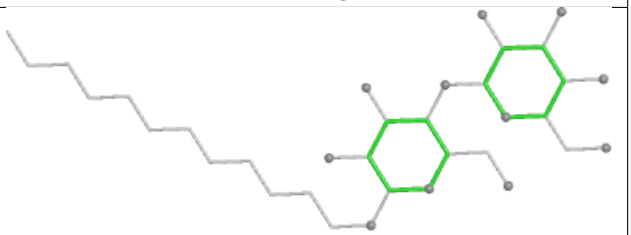
Bond lengths



Bond angles

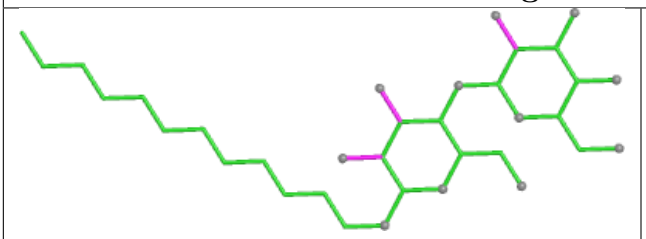


Torsions

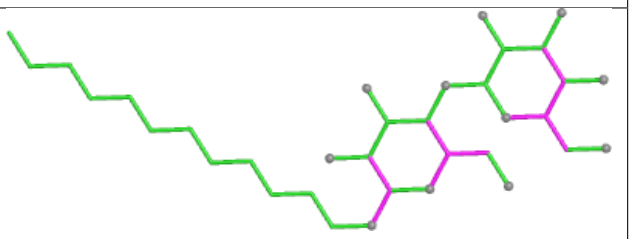


Rings

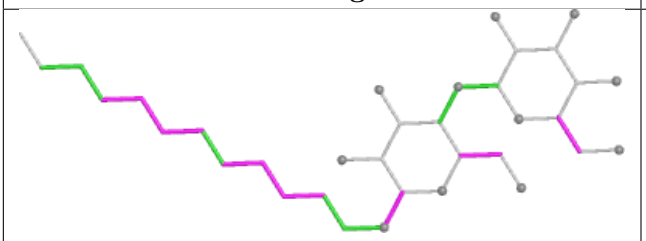
Ligand LMT B 628



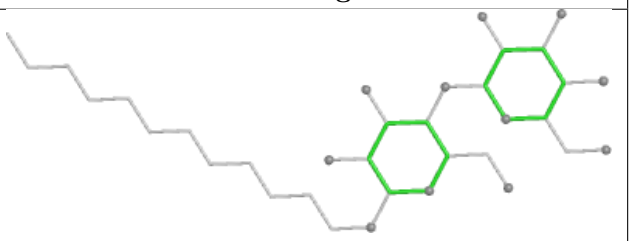
Bond lengths



Bond angles

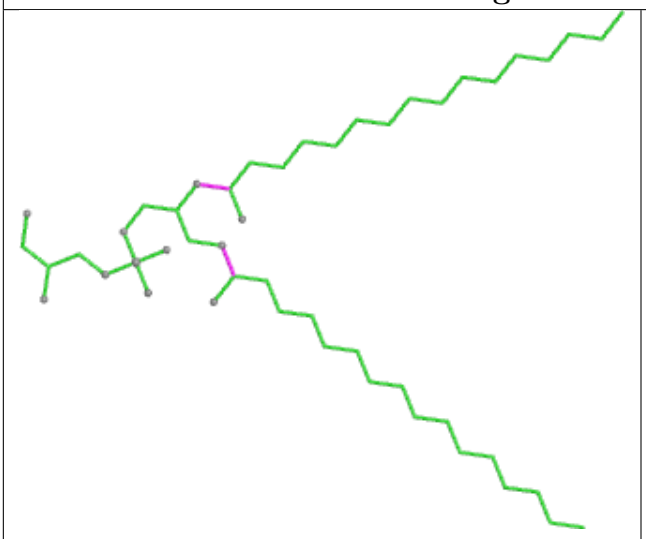


Torsions

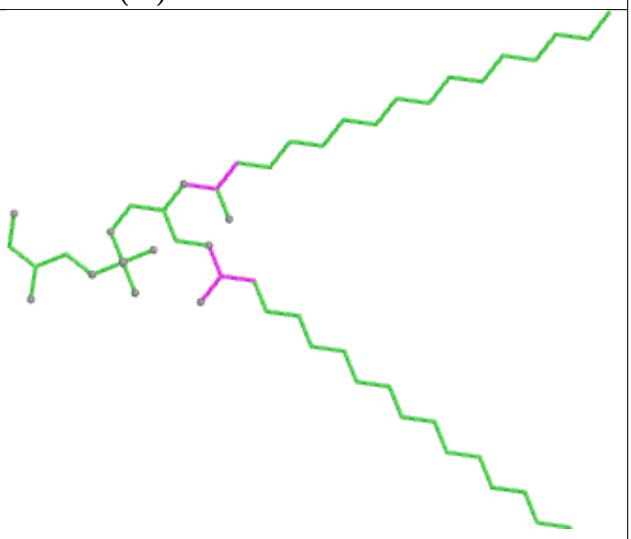


Rings

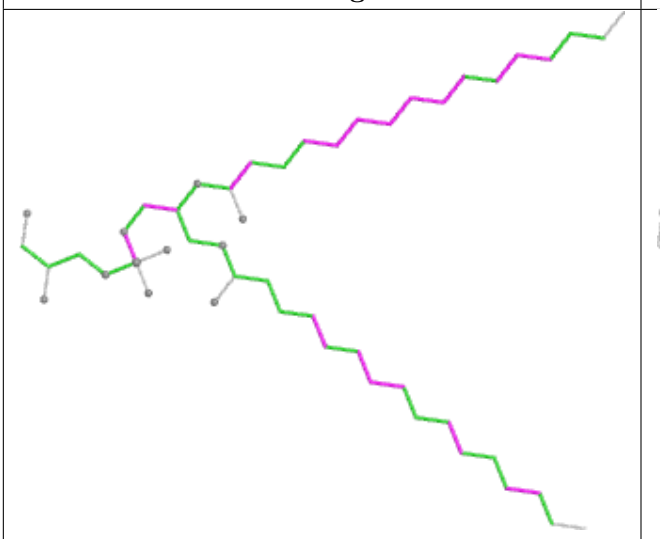
Ligand LHG b 630 (B)



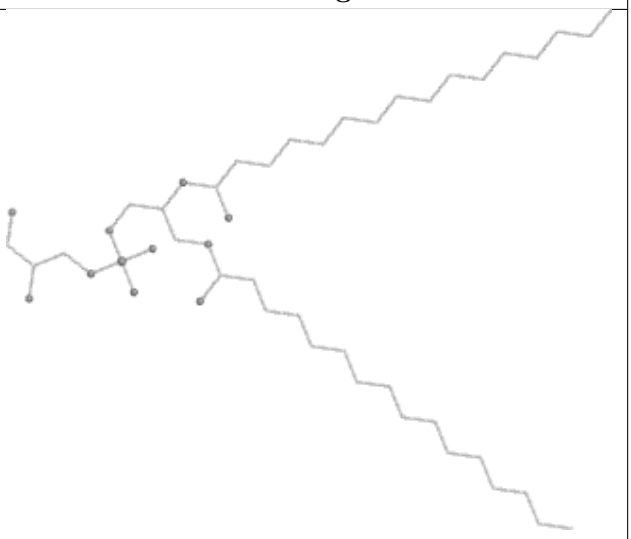
Bond lengths



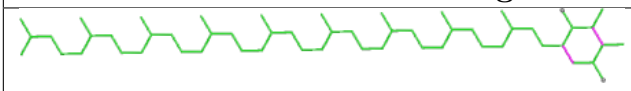
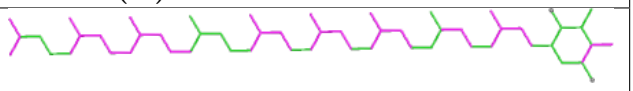
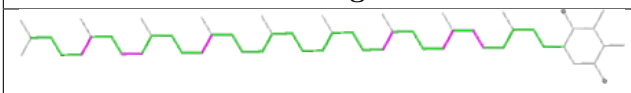
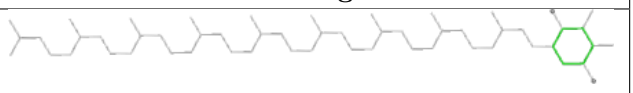
Bond angles

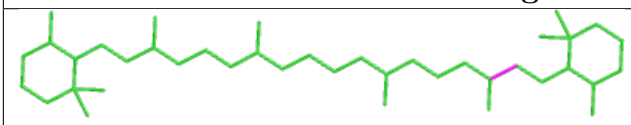
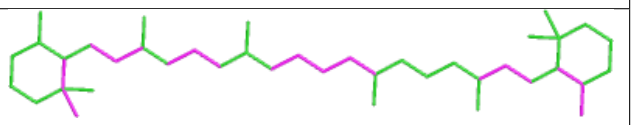
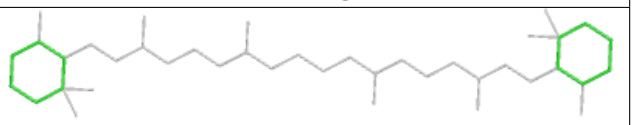


Torsions

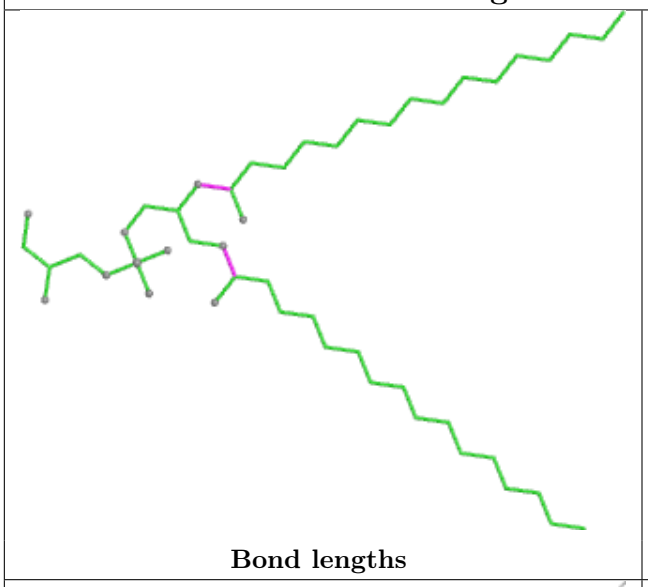


Rings

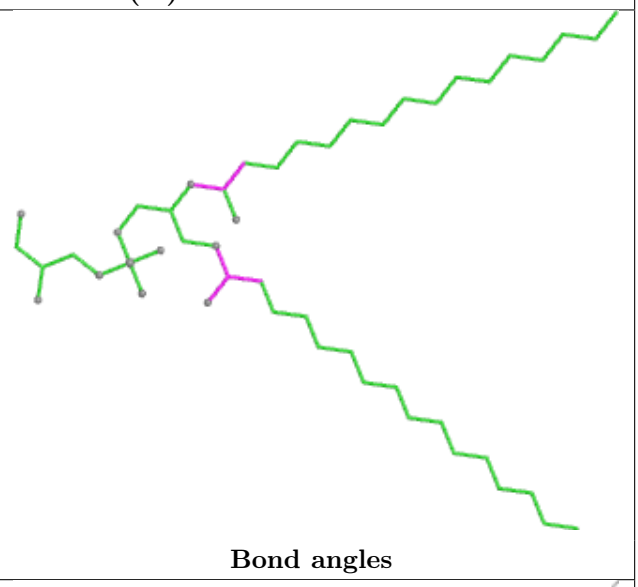
Ligand PL9 D 405 (B)	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR H 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

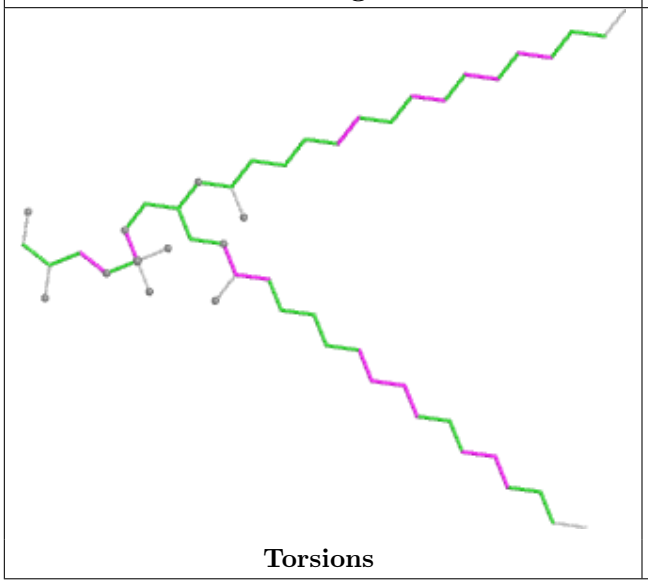
Ligand LHG D 407 (B)



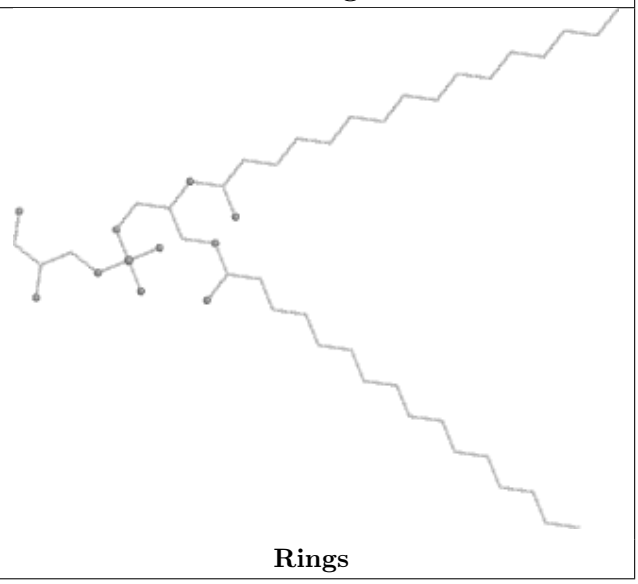
Bond lengths



Bond angles

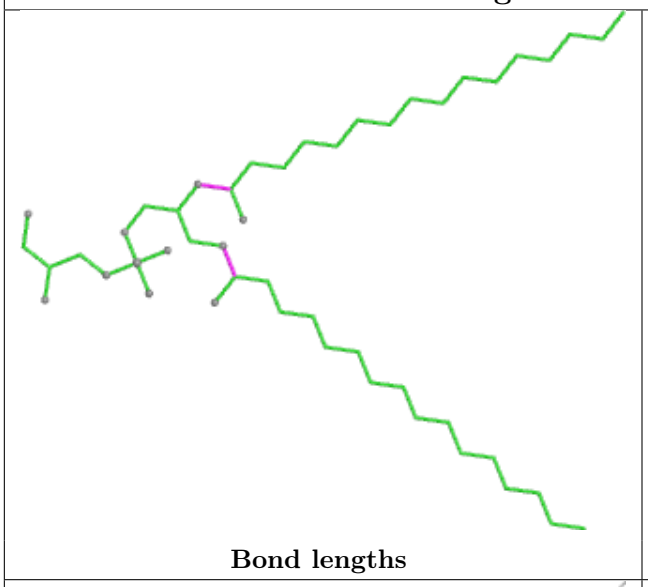


Torsions

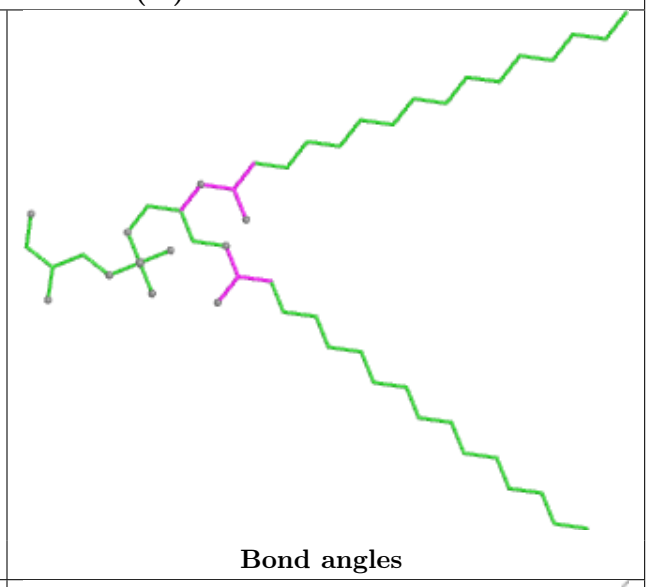


Rings

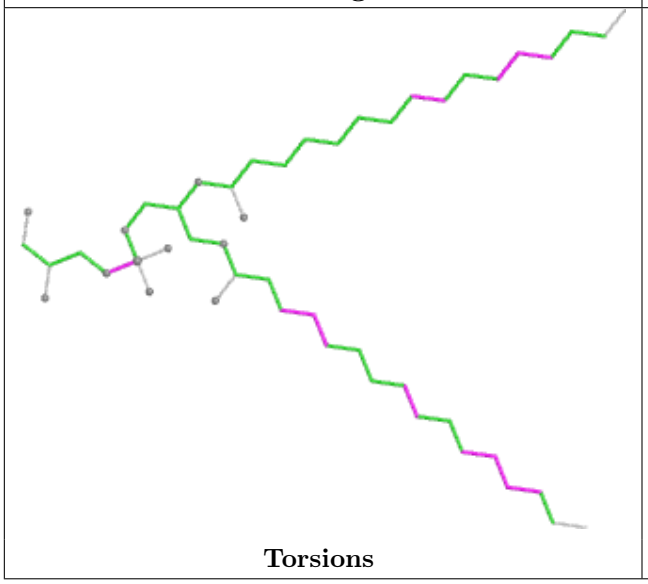
Ligand LHG d 412 (B)



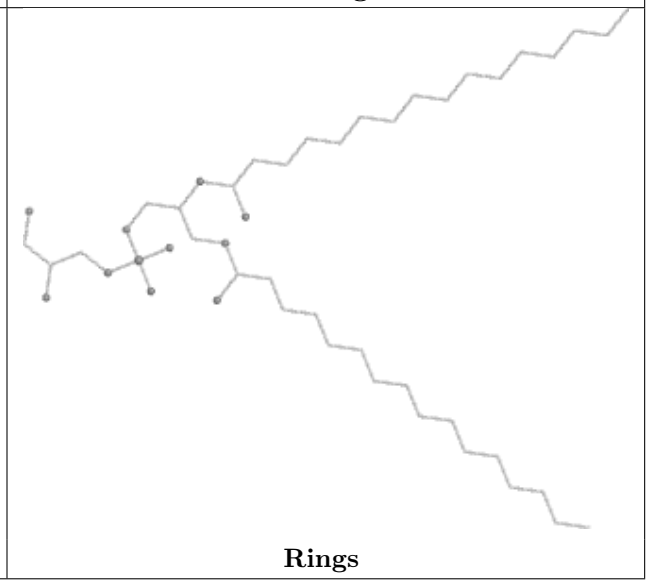
Bond lengths



Bond angles



Torsions

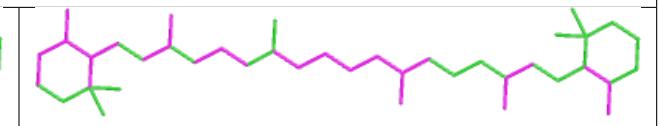


Rings

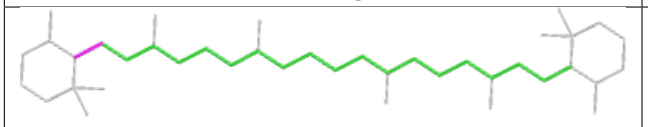
Ligand BCR Y 101



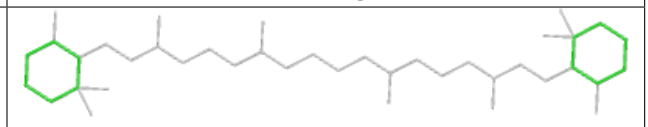
Bond lengths



Bond angles

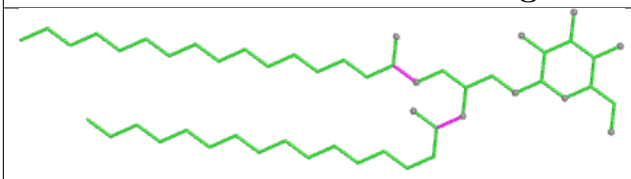


Torsions

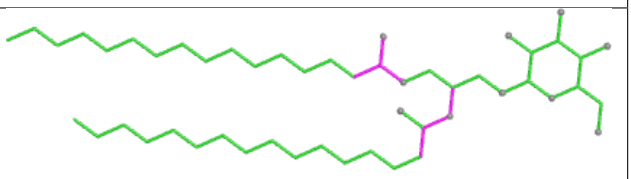


Rings

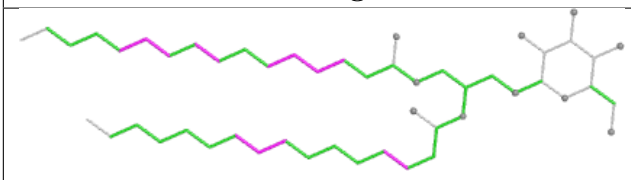
Ligand LMG C 520



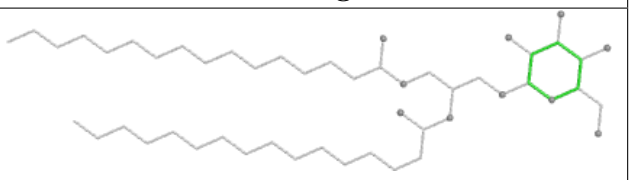
Bond lengths



Bond angles

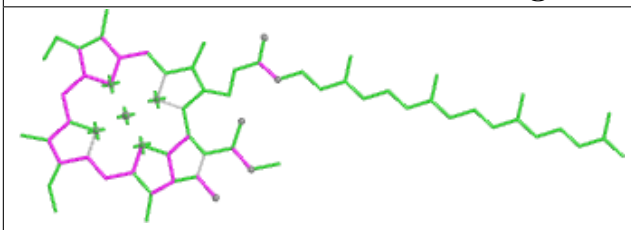


Torsions

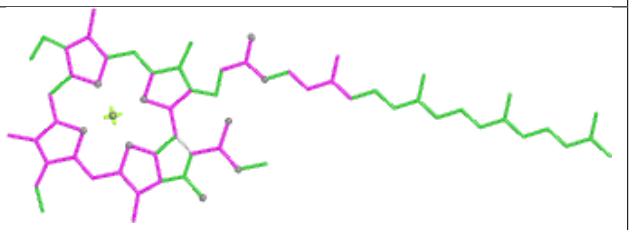


Rings

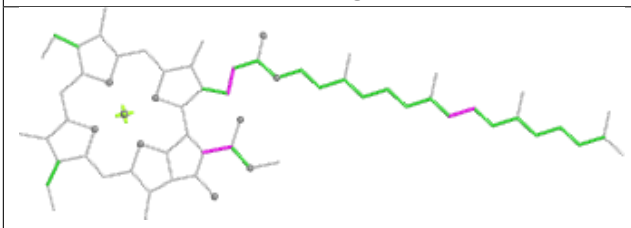
Ligand CLA c 504



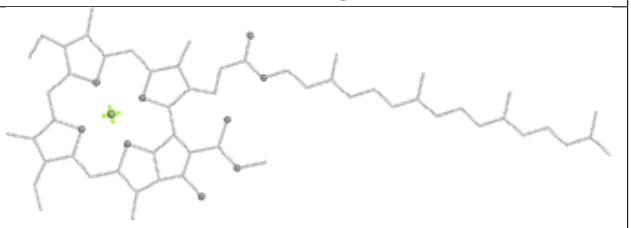
Bond lengths



Bond angles

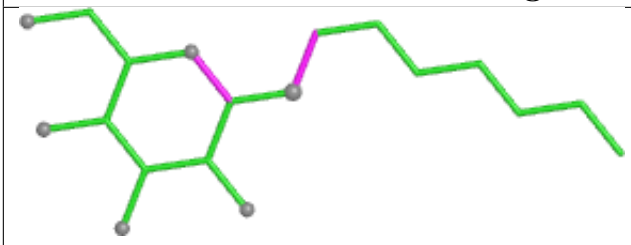


Torsions

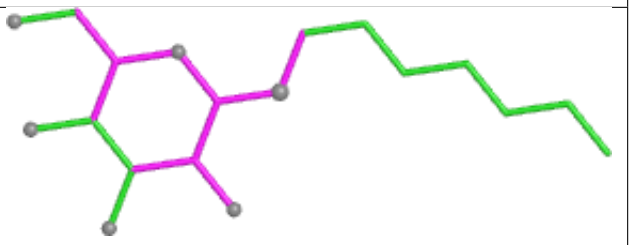


Rings

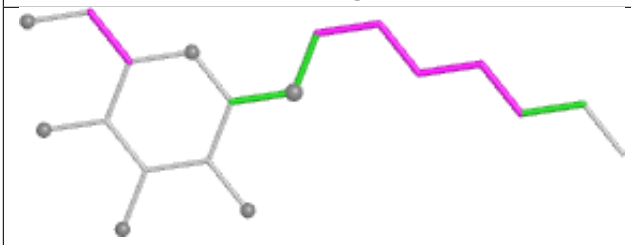
Ligand HTG b 622



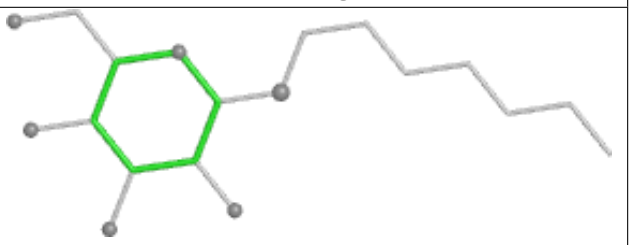
Bond lengths



Bond angles

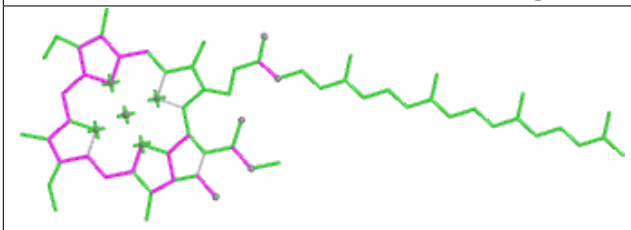


Torsions

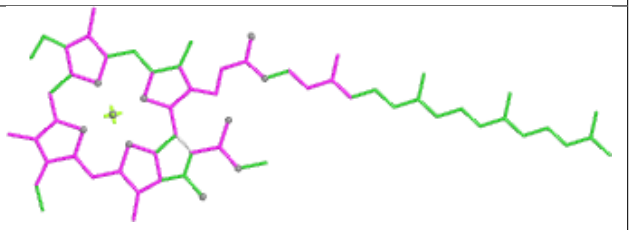


Rings

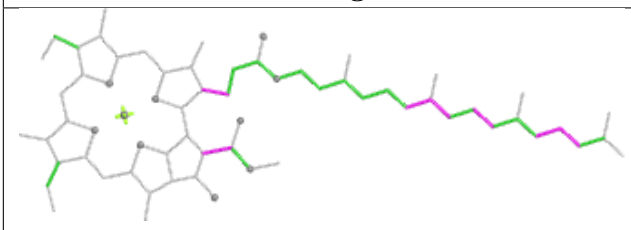
Ligand CLA c 507



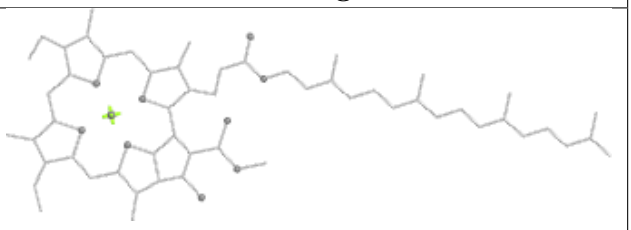
Bond lengths



Bond angles

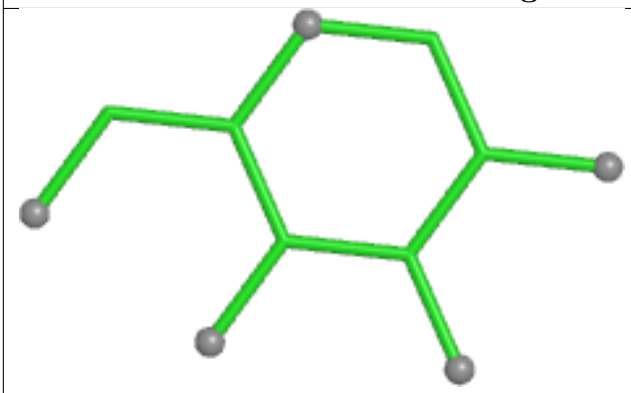


Torsions

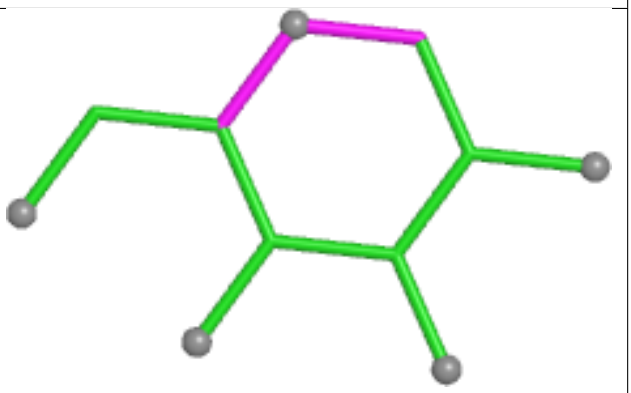


Rings

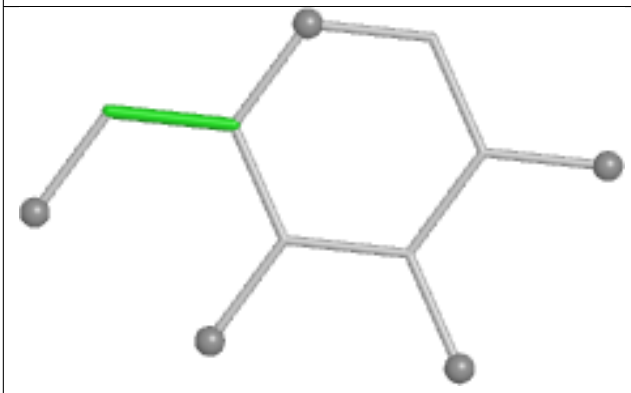
Ligand HTG V 202



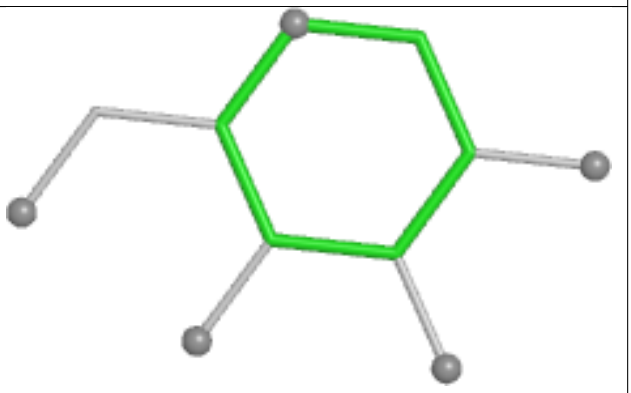
Bond lengths



Bond angles

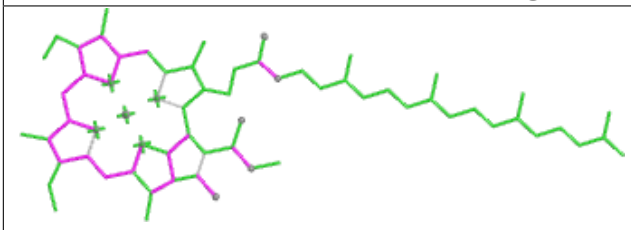


Torsions

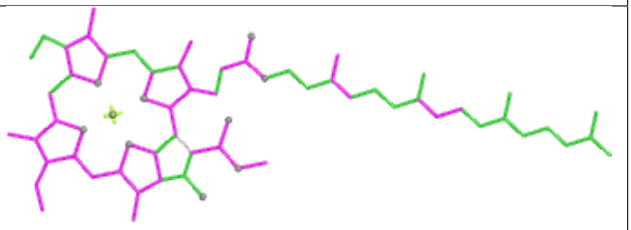


Rings

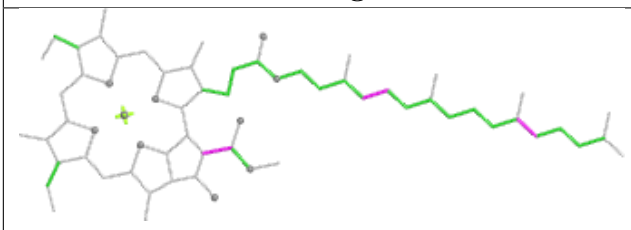
Ligand CLA B 607



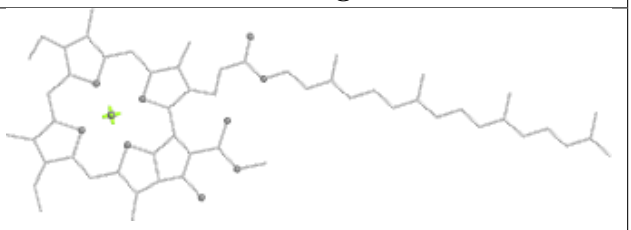
Bond lengths



Bond angles

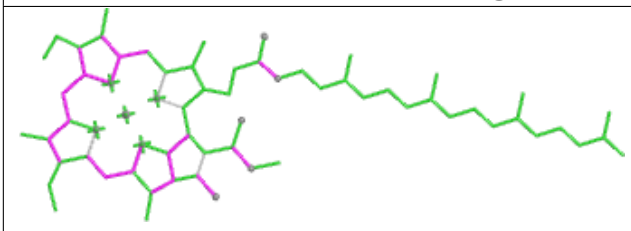


Torsions

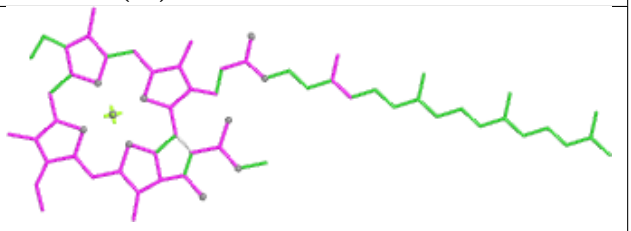


Rings

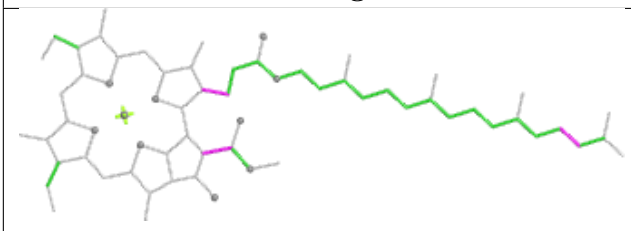
Ligand CLA A 405 (A)



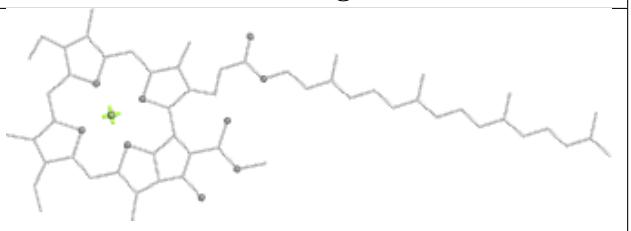
Bond lengths



Bond angles

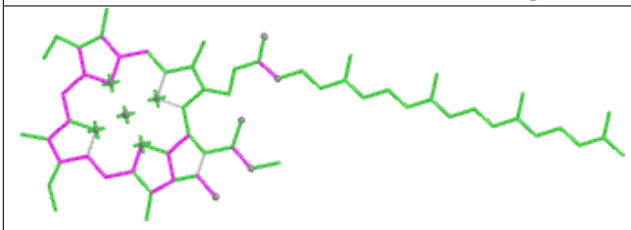


Torsions

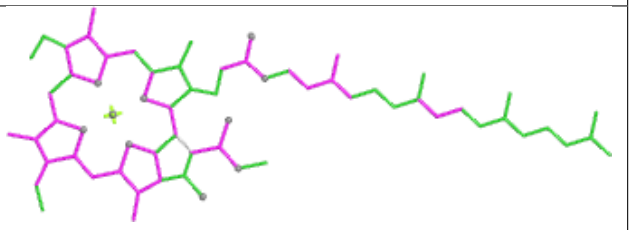


Rings

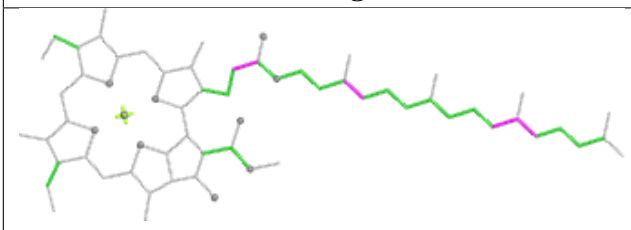
Ligand CLA C 506



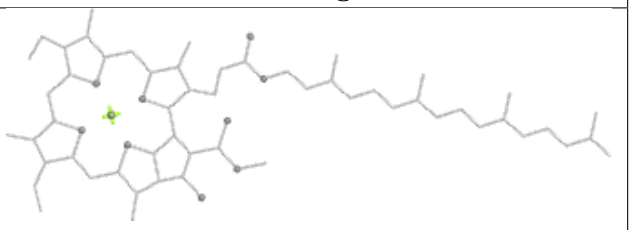
Bond lengths



Bond angles

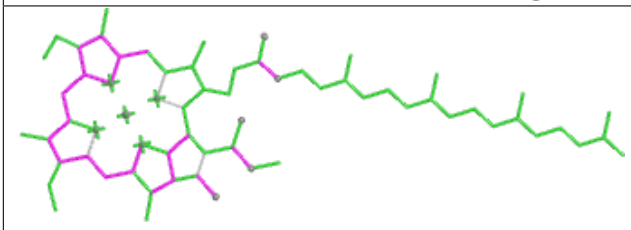


Torsions

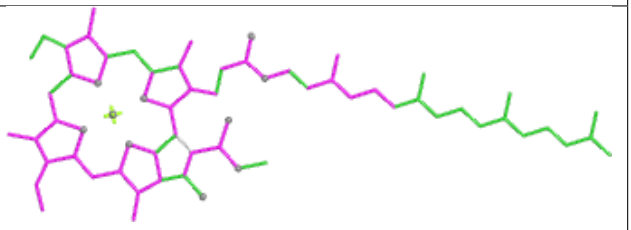


Rings

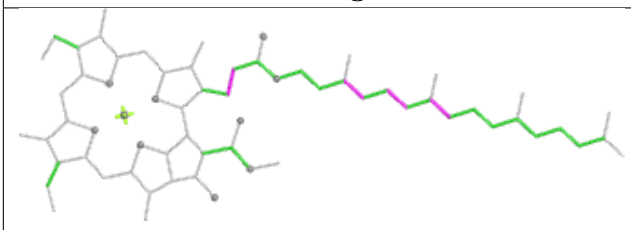
Ligand CLA b 603



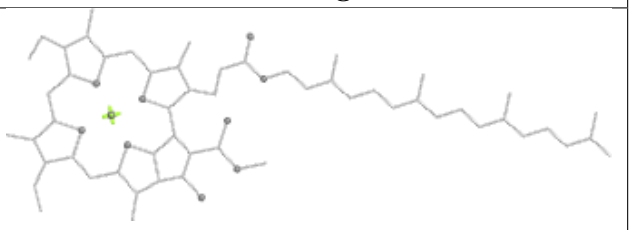
Bond lengths



Bond angles

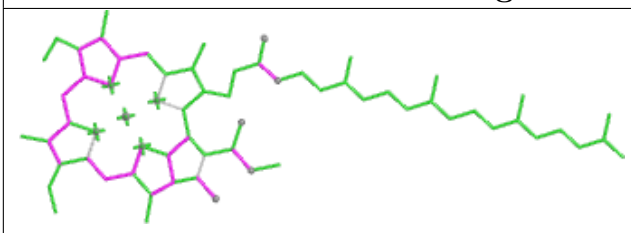


Torsions

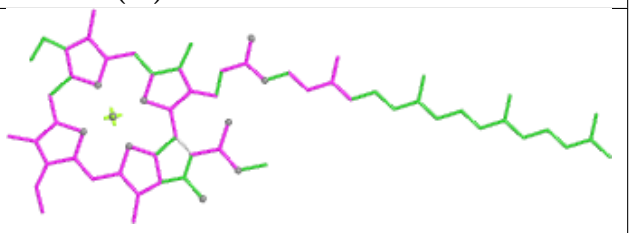


Rings

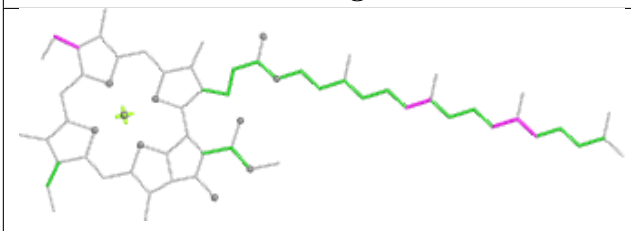
Ligand CLA a 406 (B)



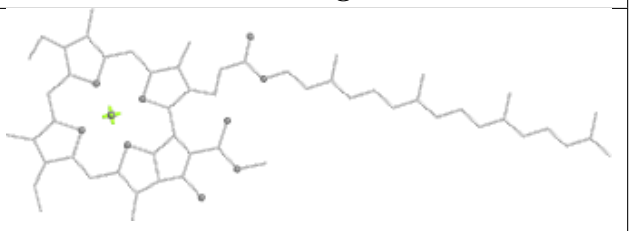
Bond lengths



Bond angles

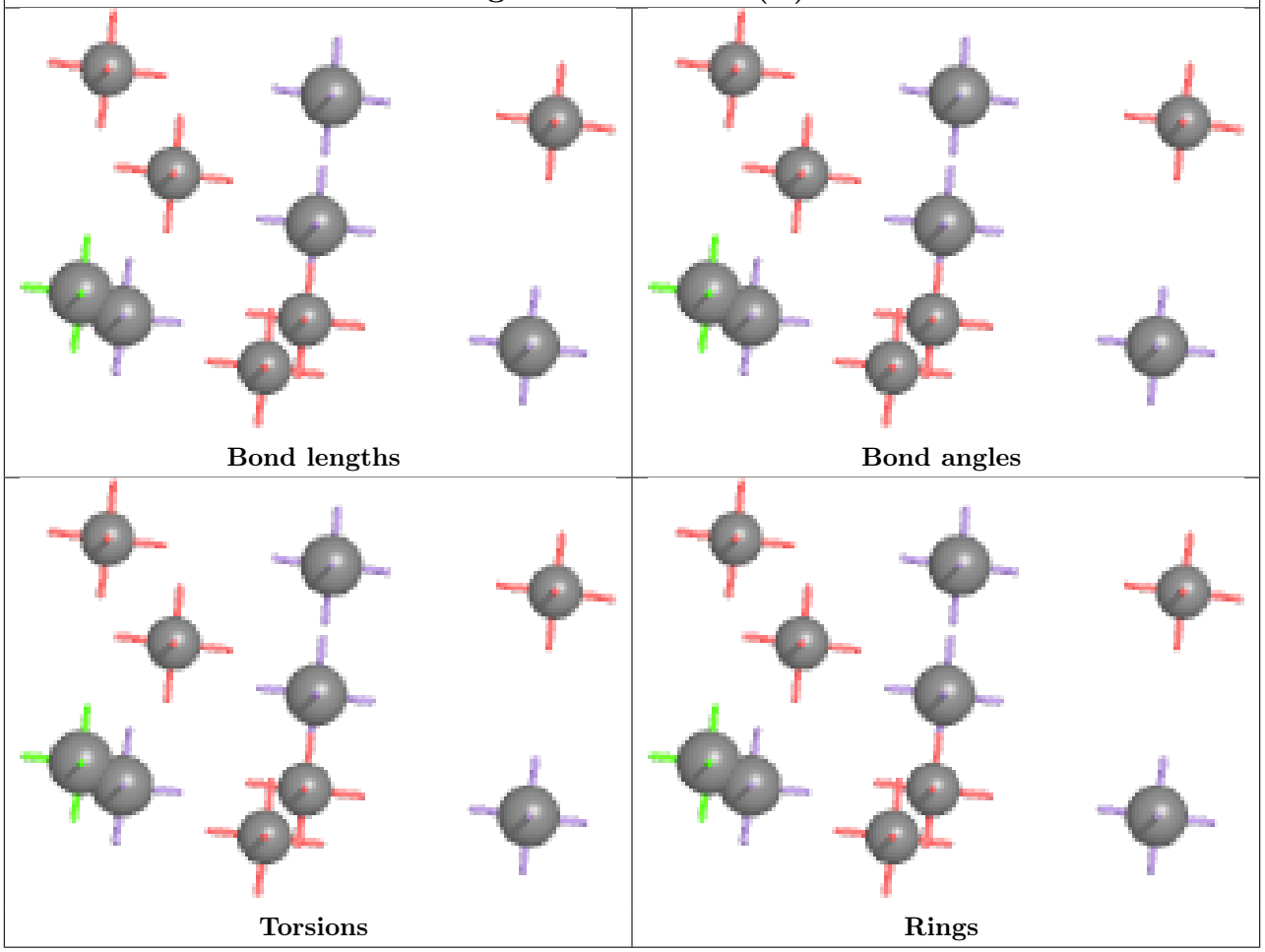


Torsions

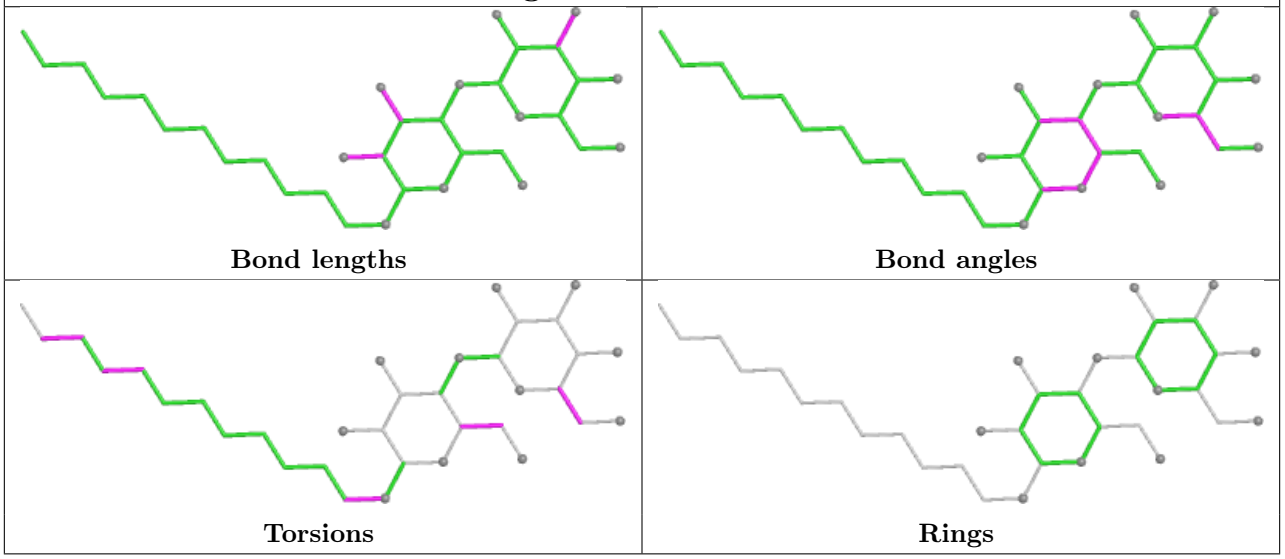


Rings

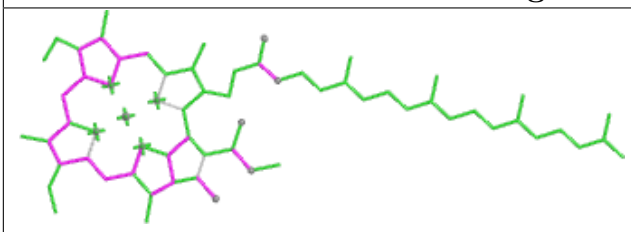
Ligand OEX a 412 (B)

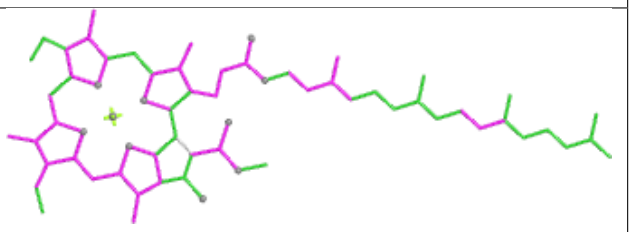


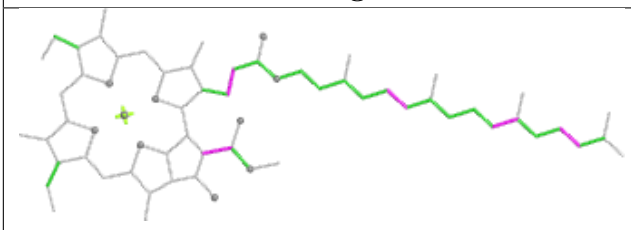
Ligand LMT T 101

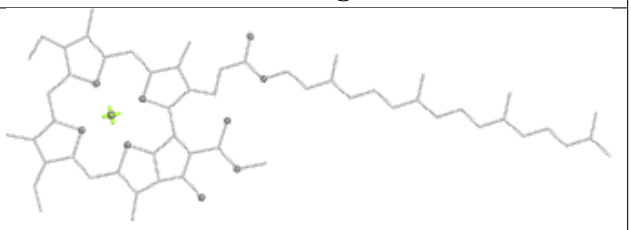


Ligand CLA b 610

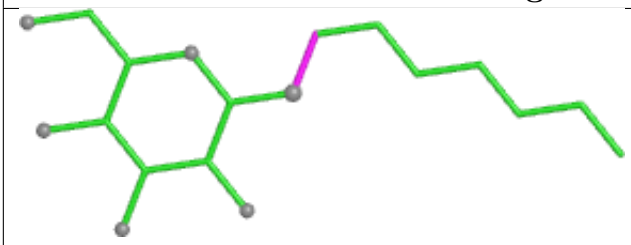

Bond lengths

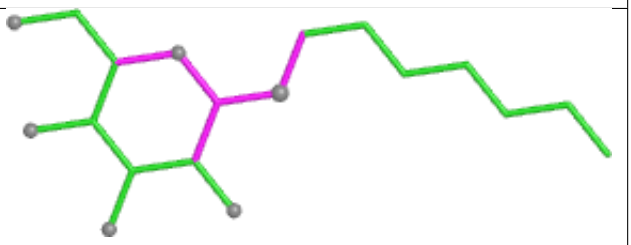

Bond angles

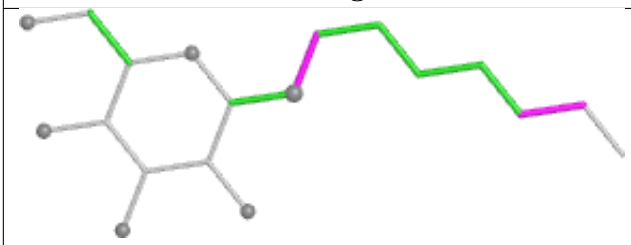

Torsions

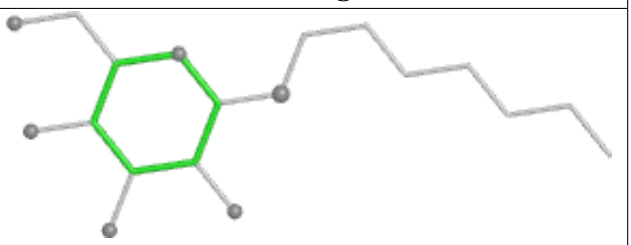

Rings

Ligand HTG c 522

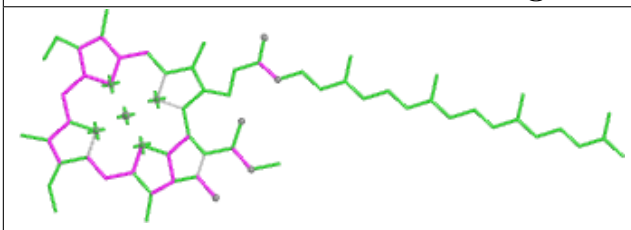

Bond lengths

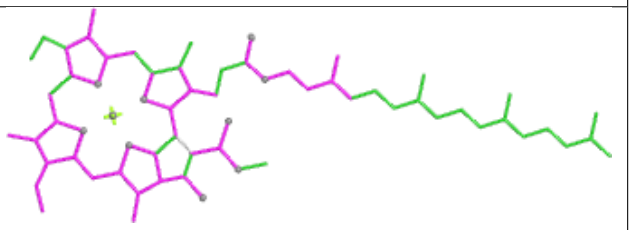

Bond angles

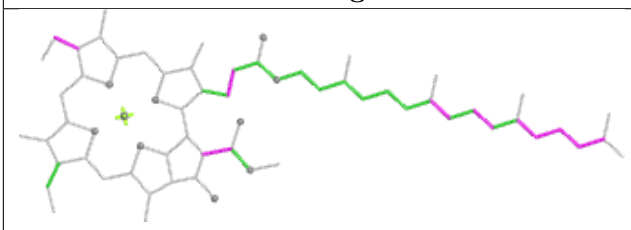

Torsions

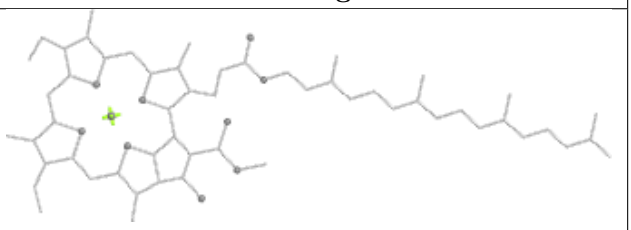

Rings

Ligand CLA b 606

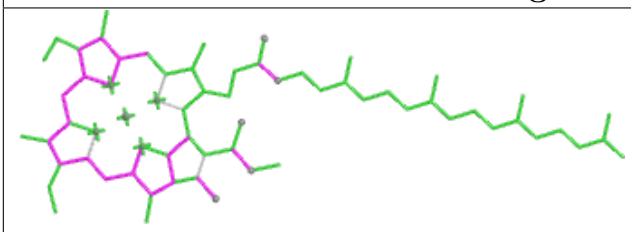

Bond lengths


Bond angles

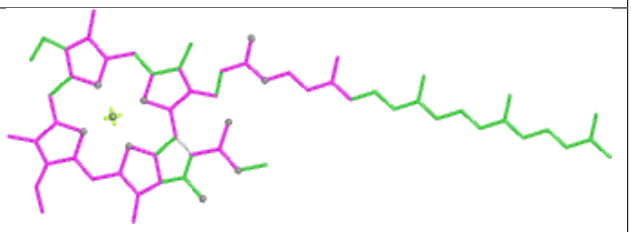

Torsions


Rings

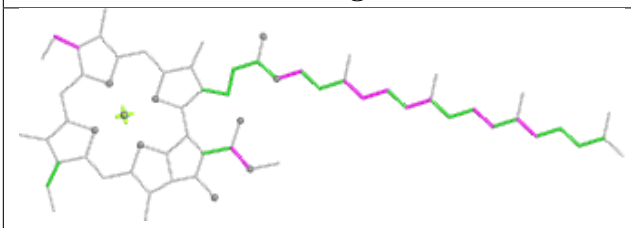
Ligand CLA c 514



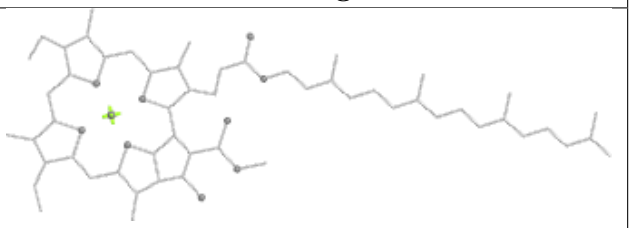
Bond lengths



Bond angles



Torsions

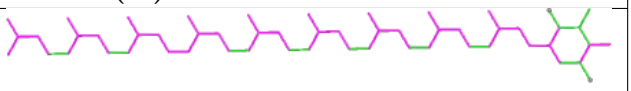


Rings

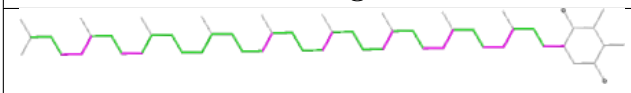
Ligand PL9 A 414 (A)



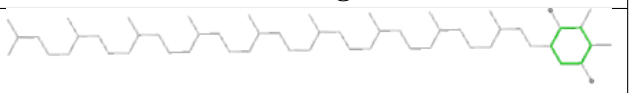
Bond lengths



Bond angles



Torsions

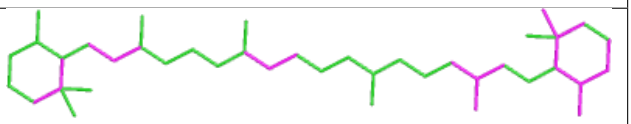


Rings

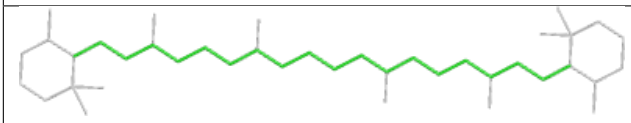
Ligand BCR B 618



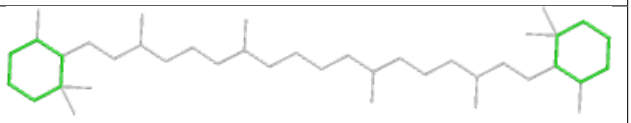
Bond lengths



Bond angles

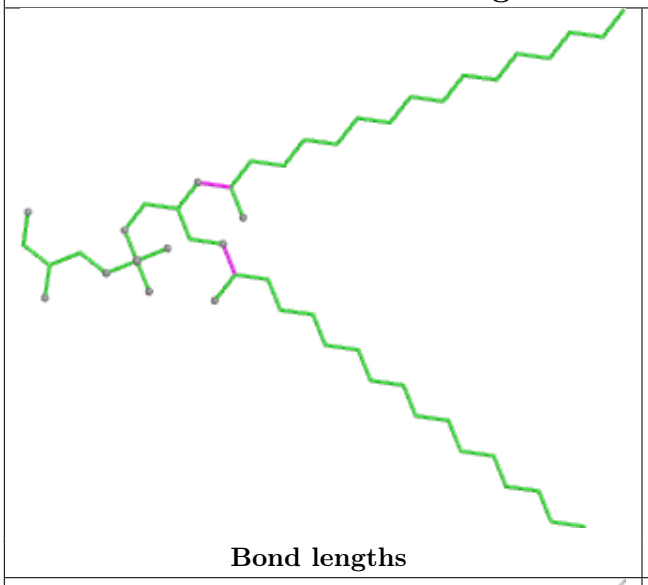


Torsions

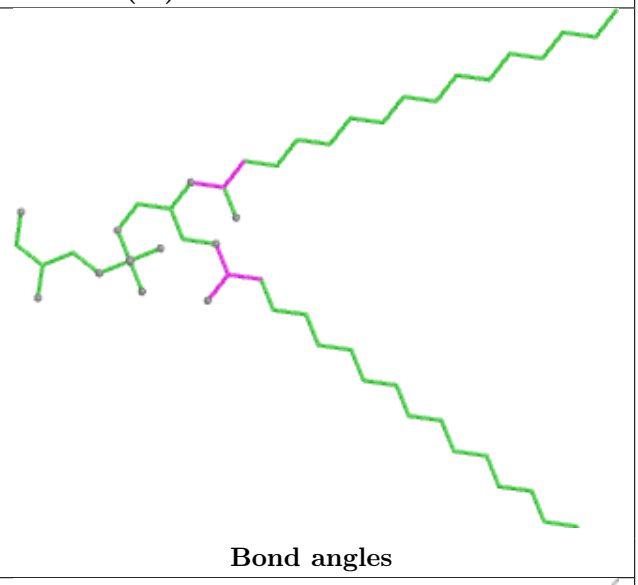


Rings

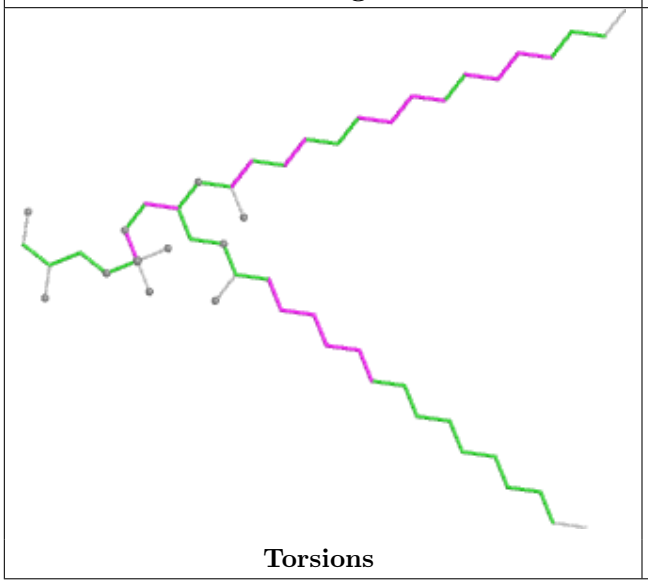
Ligand LHG L 102 (A)



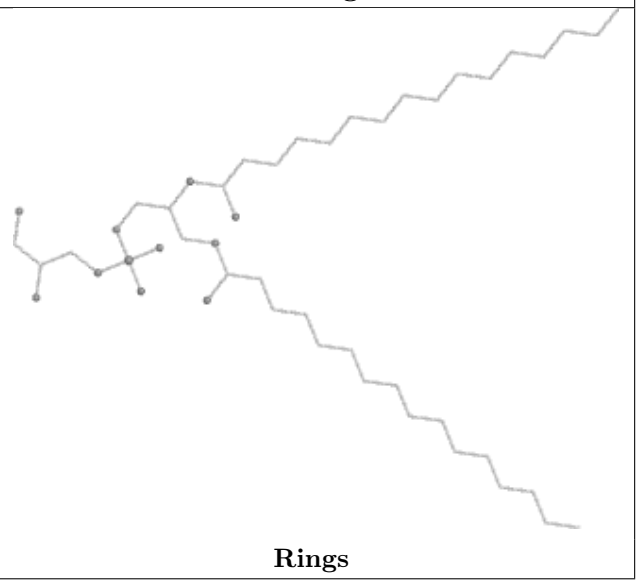
Bond lengths



Bond angles

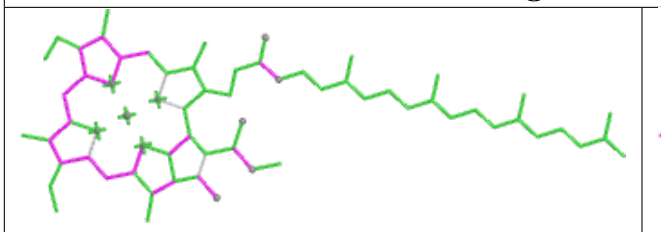


Torsions

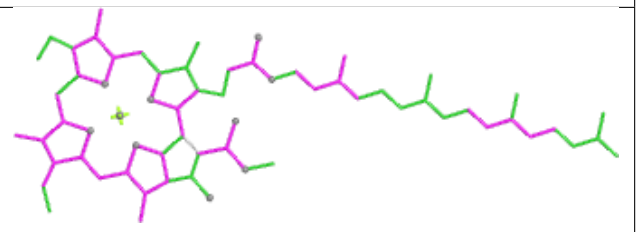


Rings

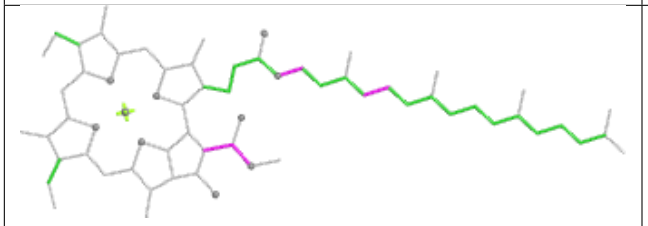
Ligand CLA C 510



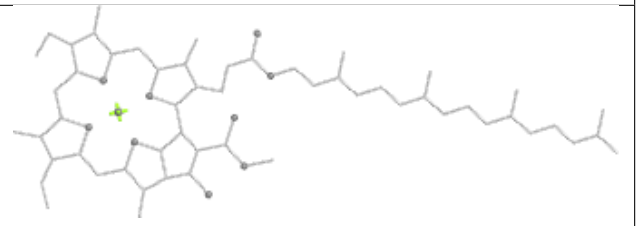
Bond lengths



Bond angles

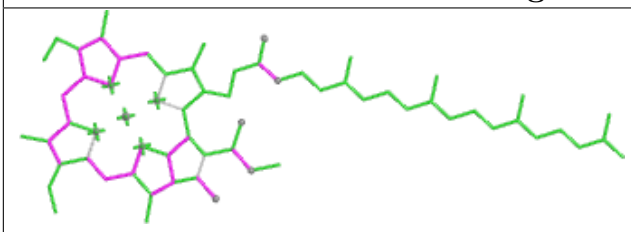


Torsions

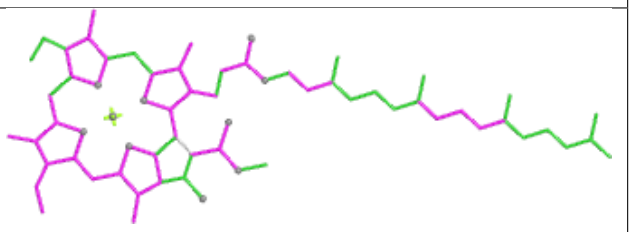


Rings

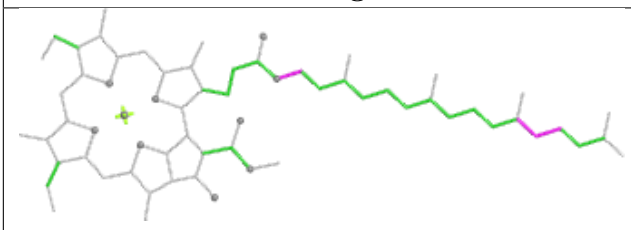
Ligand CLA b 608



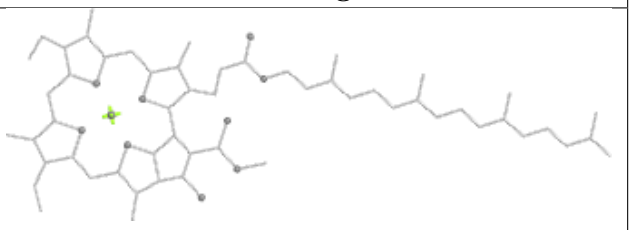
Bond lengths



Bond angles



Torsions

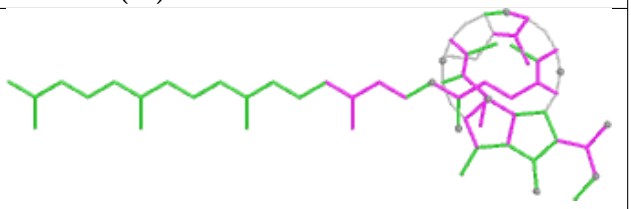


Rings

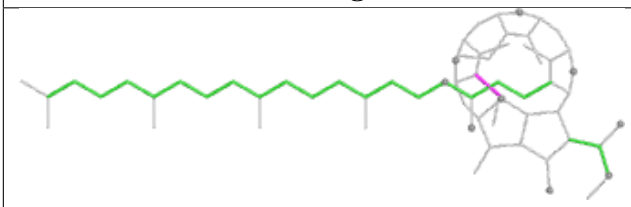
Ligand PHO a 415 (B)



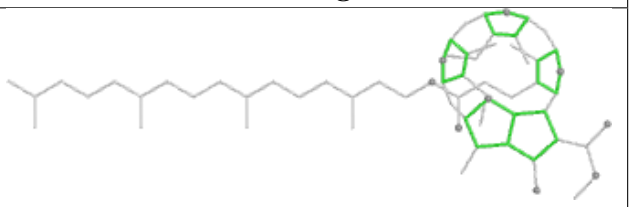
Bond lengths



Bond angles

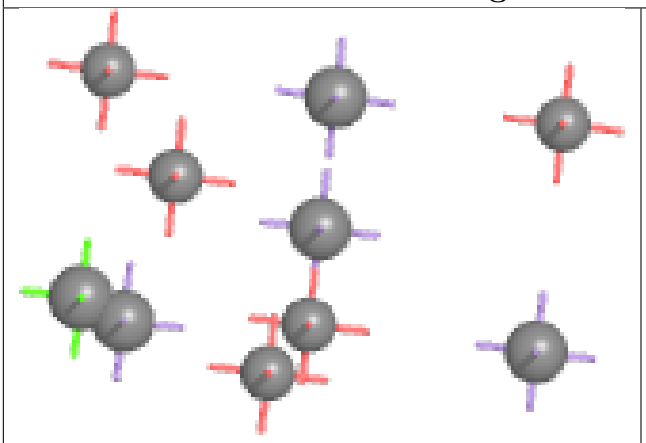


Torsions

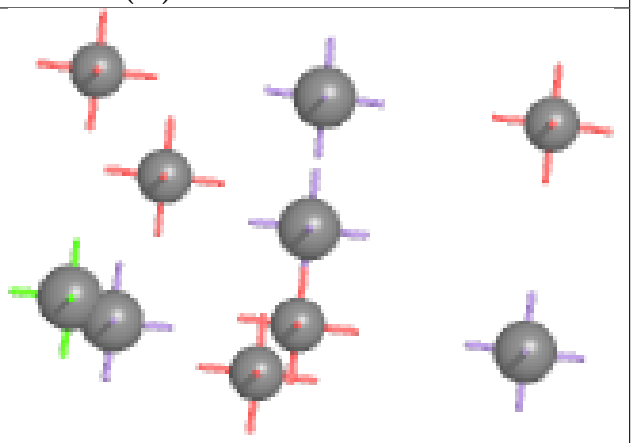


Rings

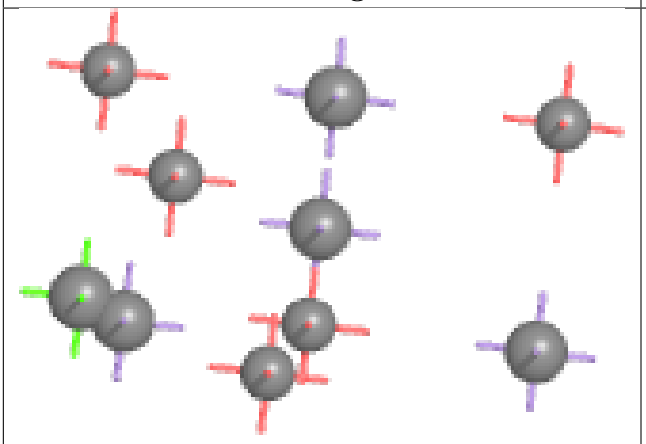
Ligand OEX A 413 (B)



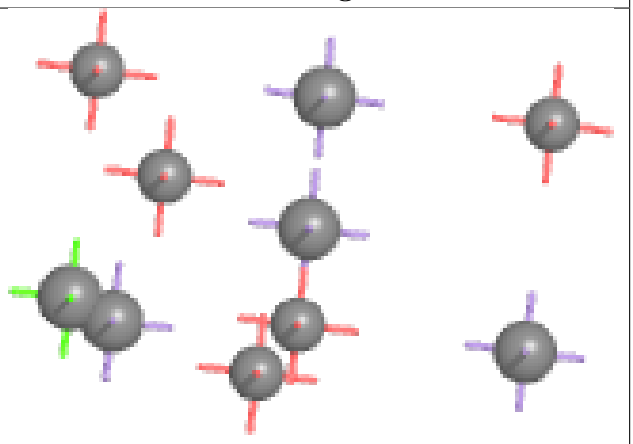
Bond lengths



Bond angles

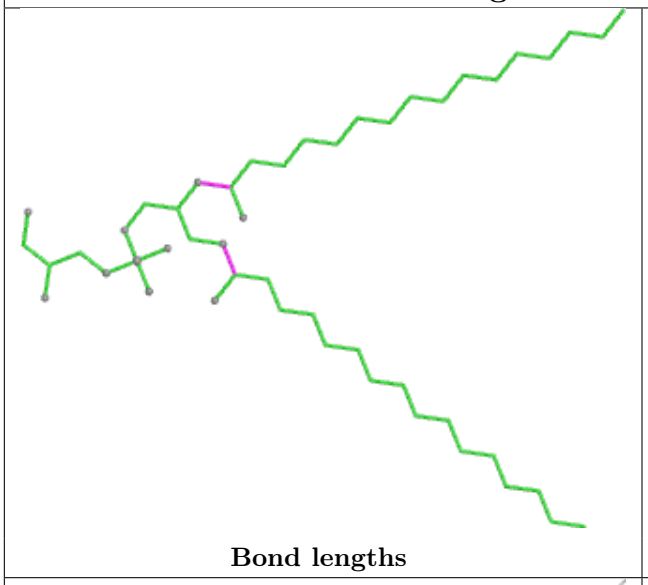


Torsions

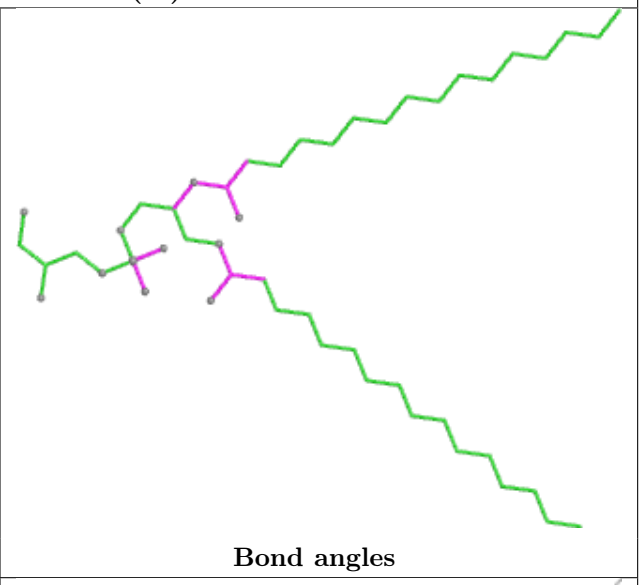


Rings

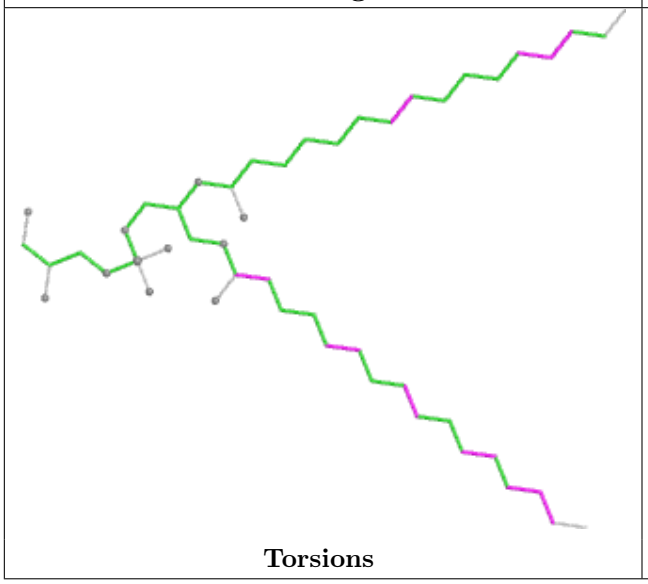
Ligand LHG A 419 (A)



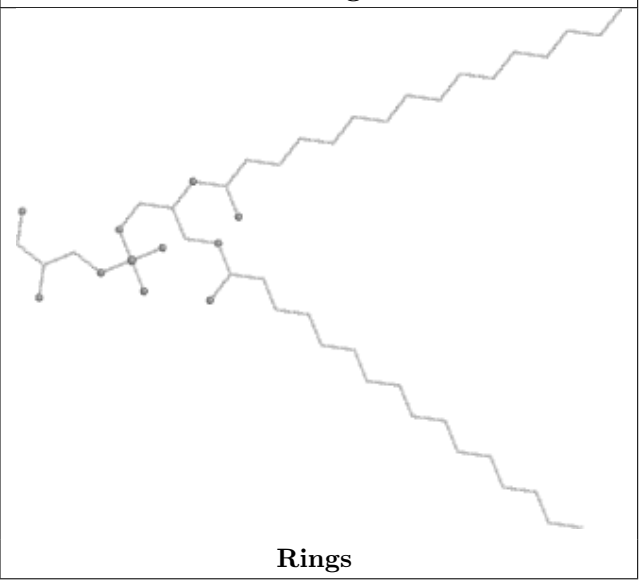
Bond lengths



Bond angles

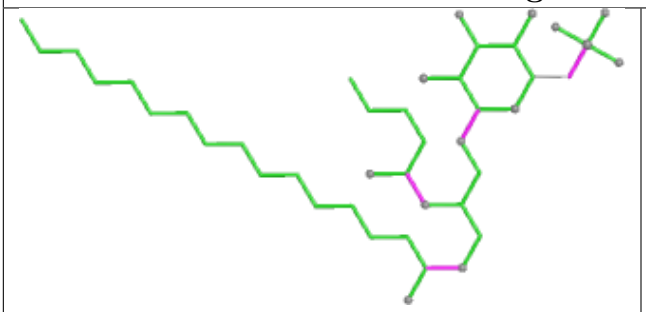


Torsions

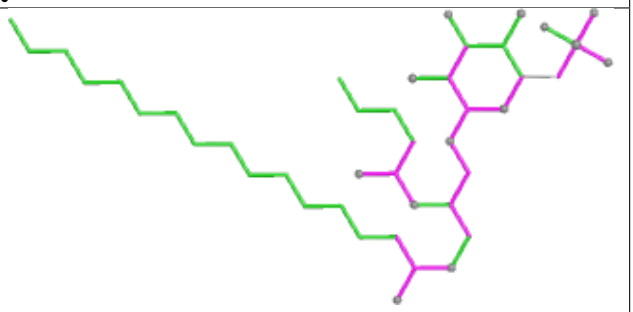


Rings

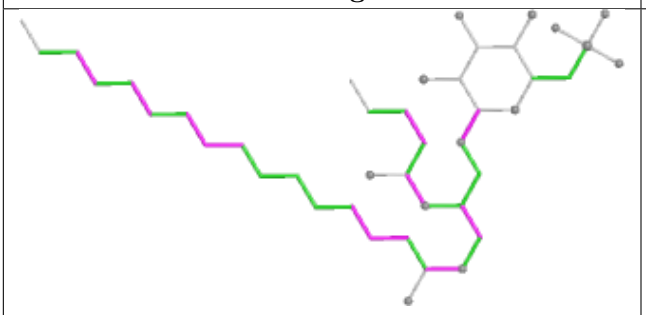
Ligand SQD F 103



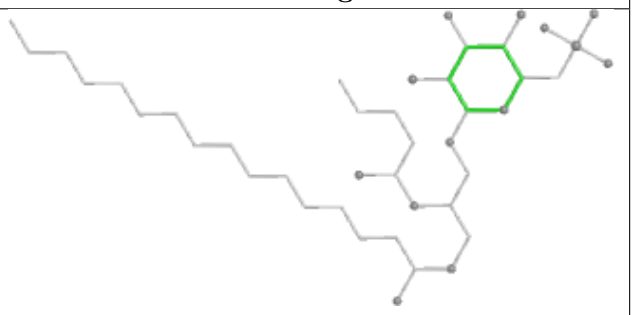
Bond lengths



Bond angles



Torsions

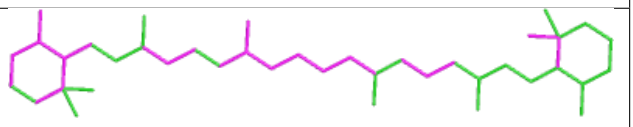


Rings

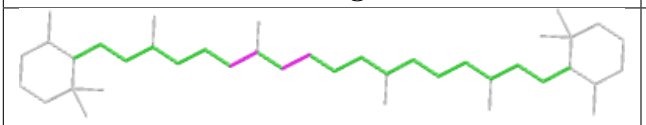
Ligand BCR T 102



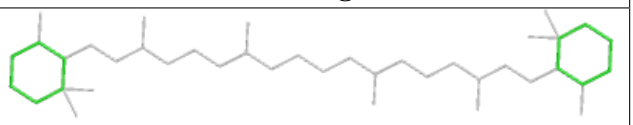
Bond lengths



Bond angles

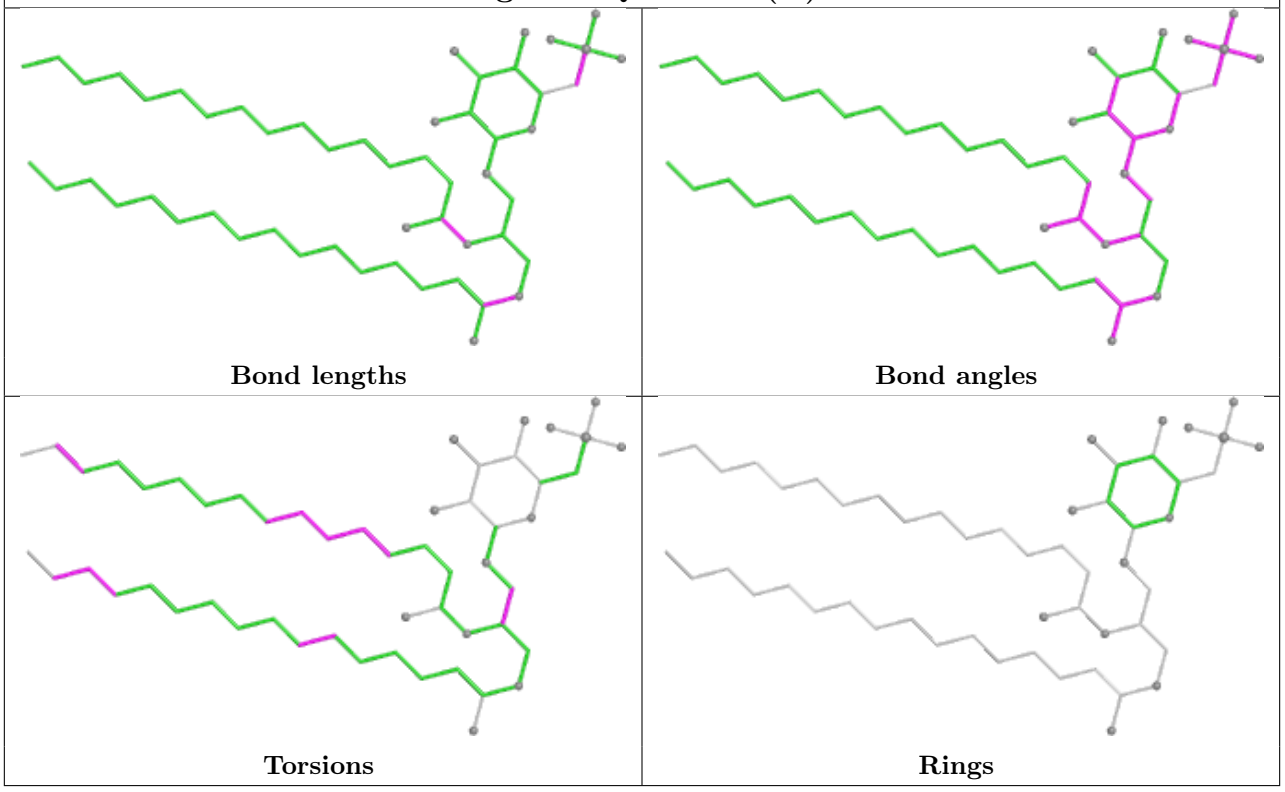


Torsions

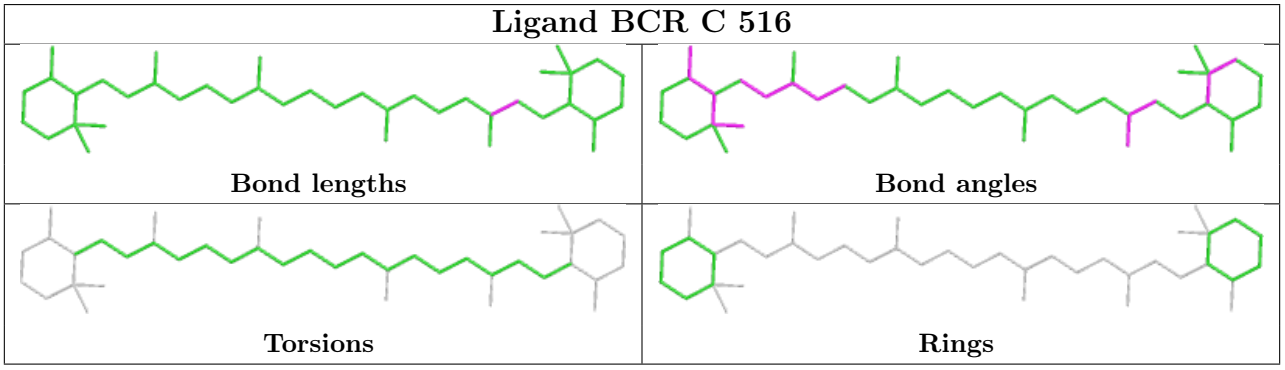


Rings

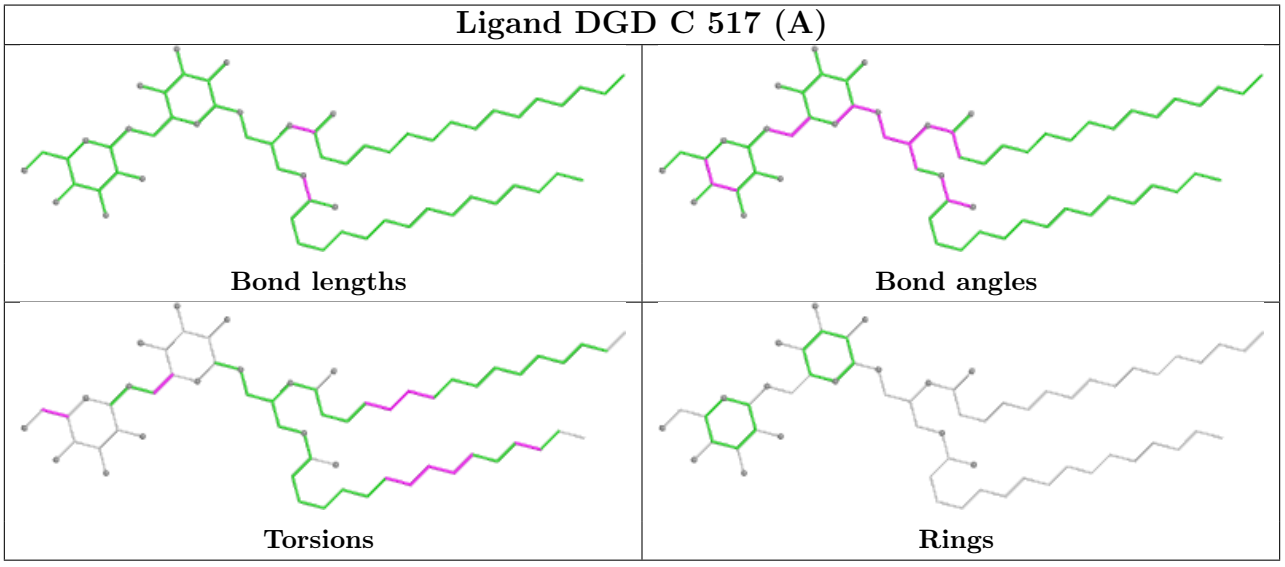
Ligand SQD a 410 (A)

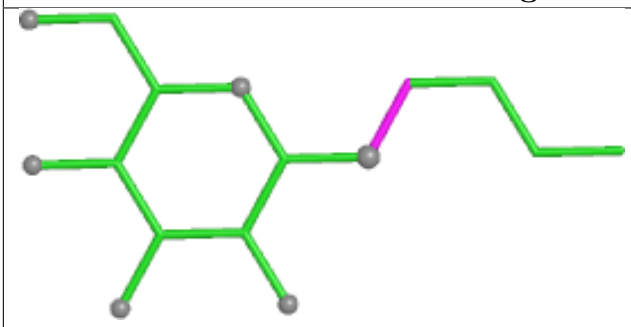
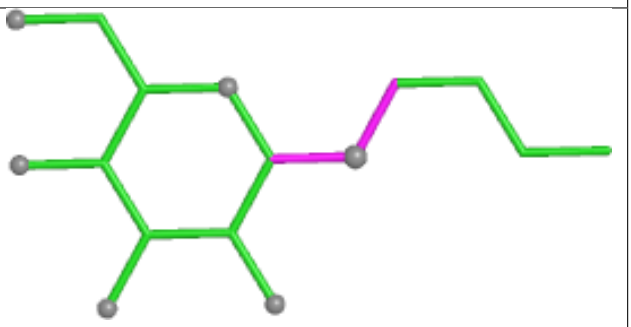
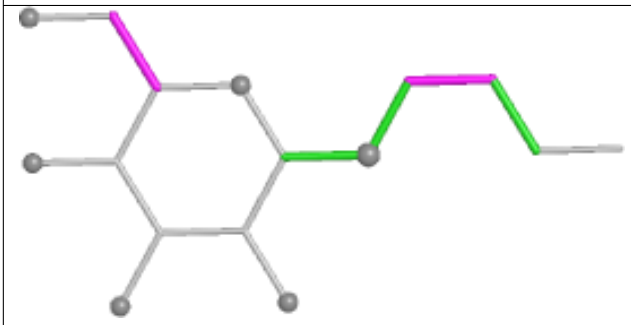
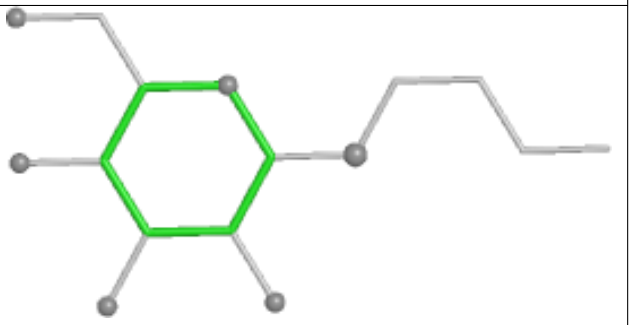


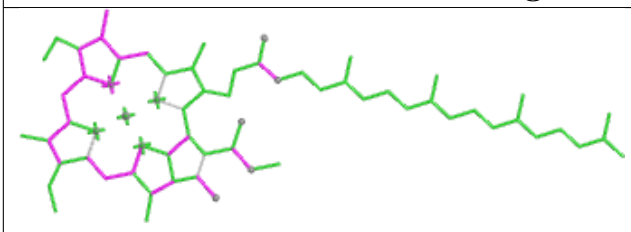
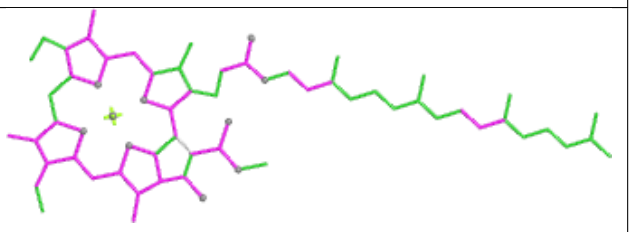
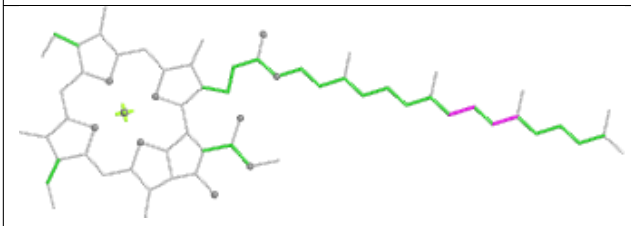
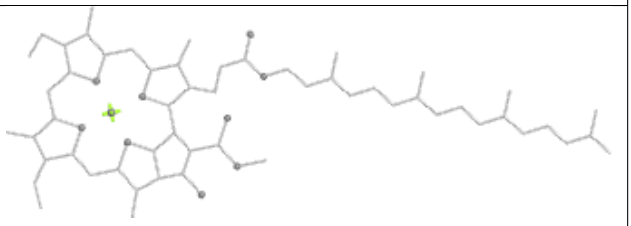
Ligand BCR C 516



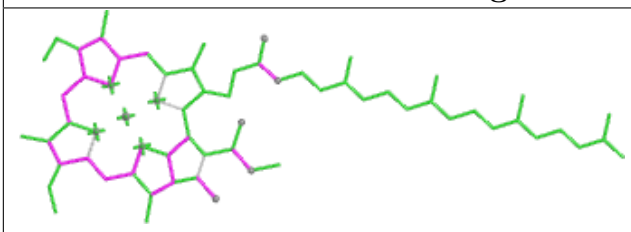
Ligand DGD C 517 (A)



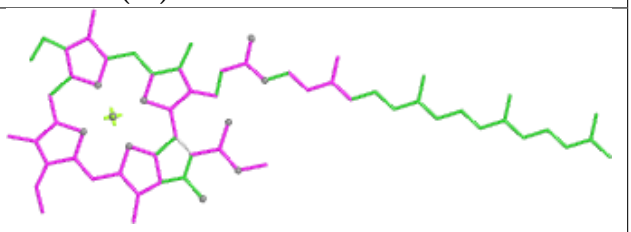
Ligand HTG D 410	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

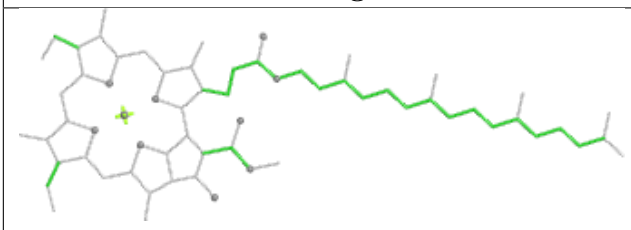
Ligand CLA D 402 (A)



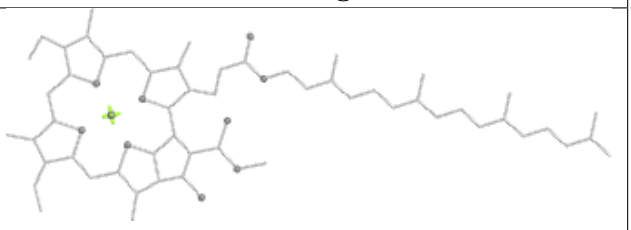
Bond lengths



Bond angles

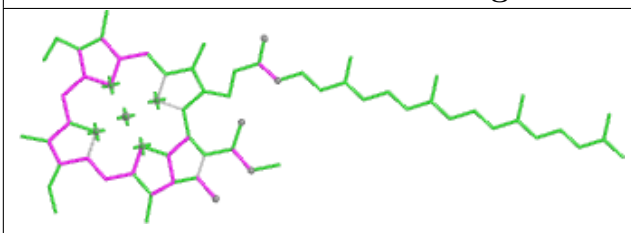


Torsions

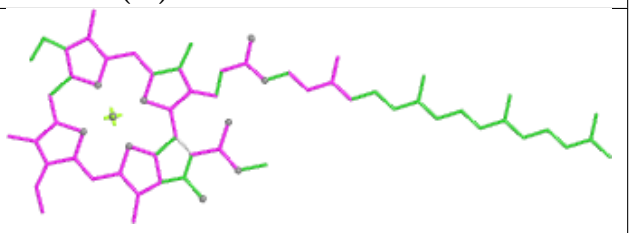


Rings

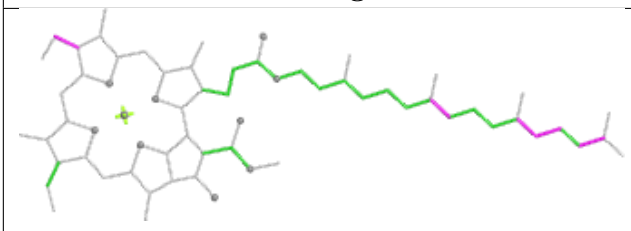
Ligand CLA A 406 (B)



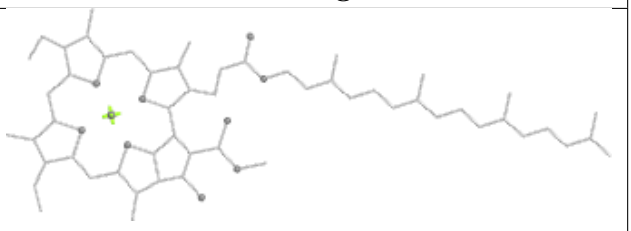
Bond lengths



Bond angles

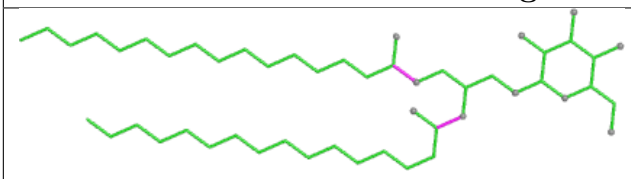


Torsions

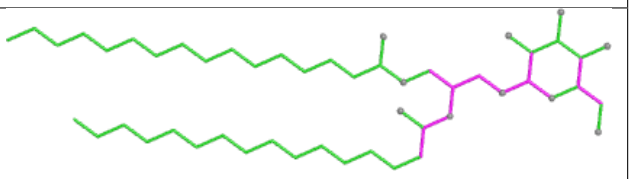


Rings

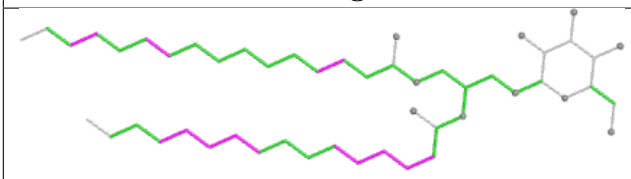
Ligand LMG C 501



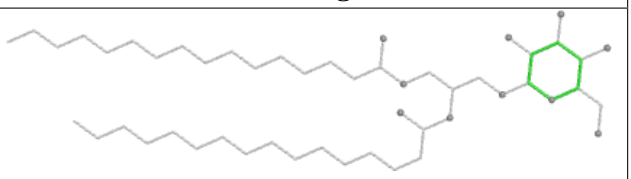
Bond lengths



Bond angles

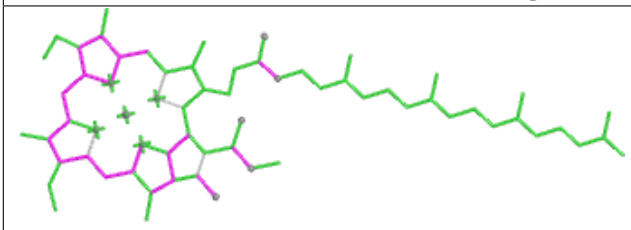


Torsions

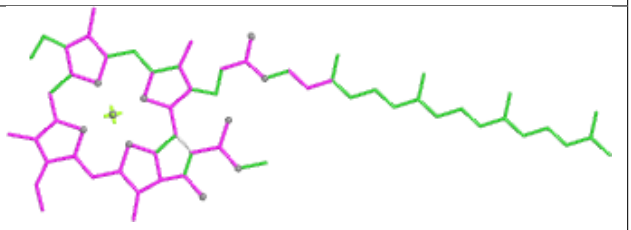


Rings

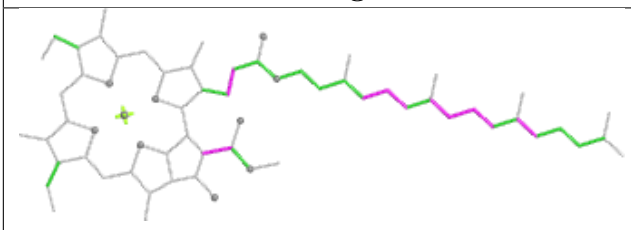
Ligand CLA B 614



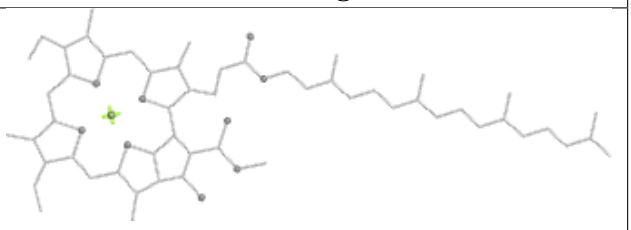
Bond lengths



Bond angles

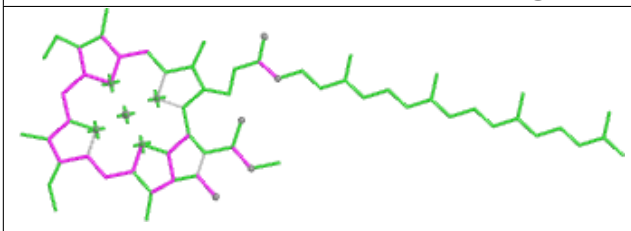


Torsions

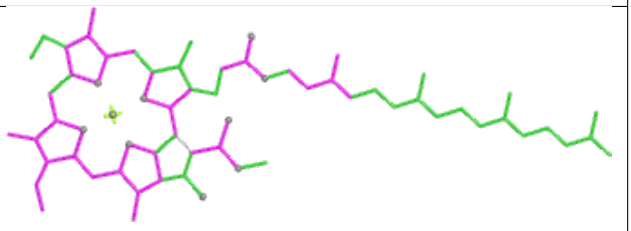


Rings

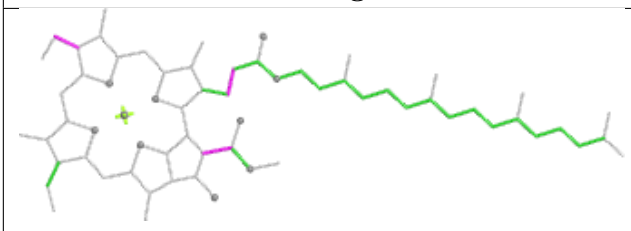
Ligand CLA c 502



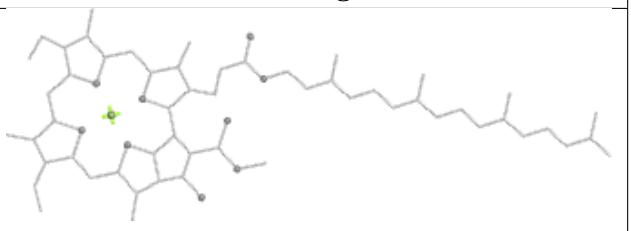
Bond lengths



Bond angles

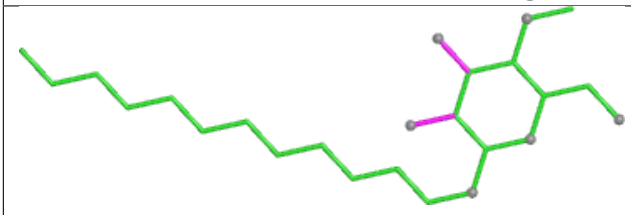


Torsions

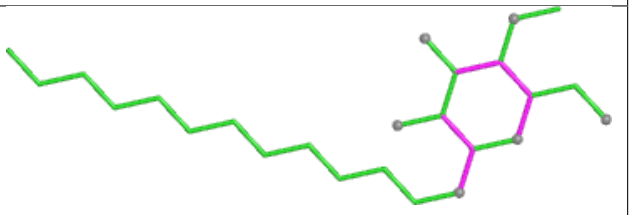


Rings

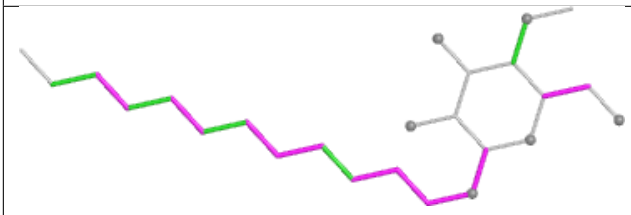
Ligand LMT B 629



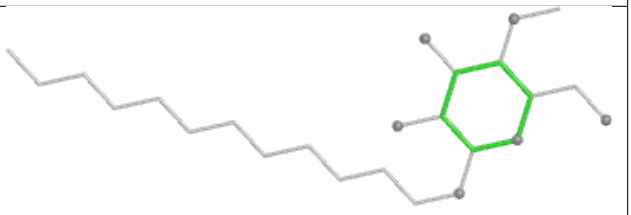
Bond lengths



Bond angles

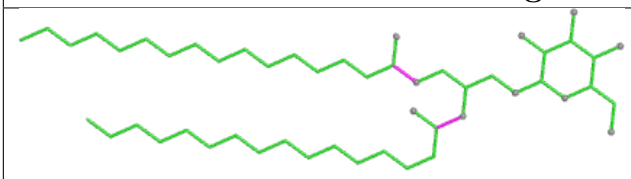


Torsions

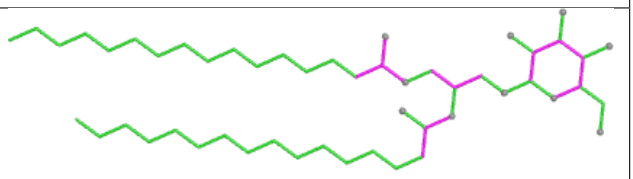


Rings

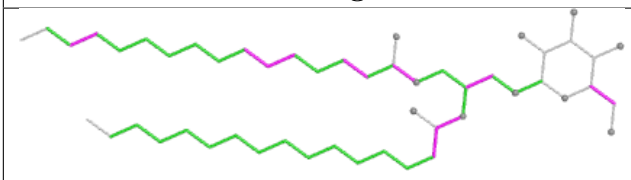
Ligand LMG c 521



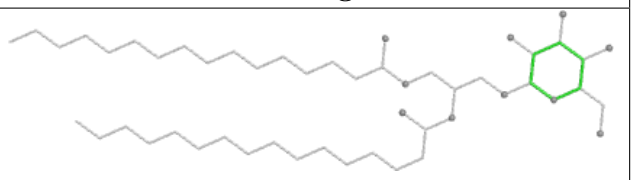
Bond lengths



Bond angles

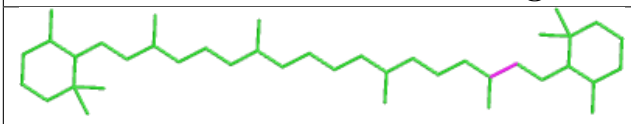


Torsions

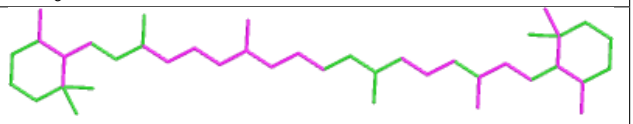


Rings

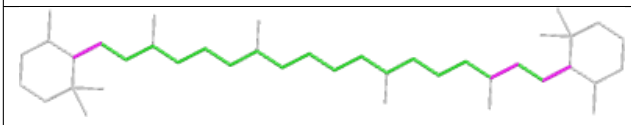
Ligand BCR y 101



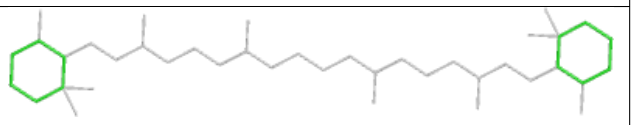
Bond lengths



Bond angles

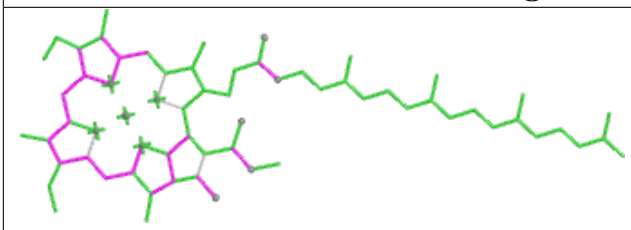


Torsions

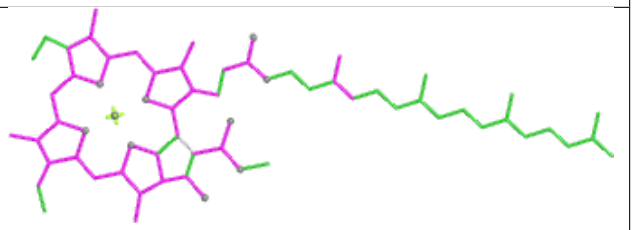


Rings

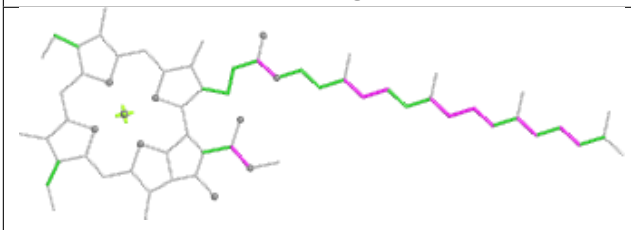
Ligand CLA D 403



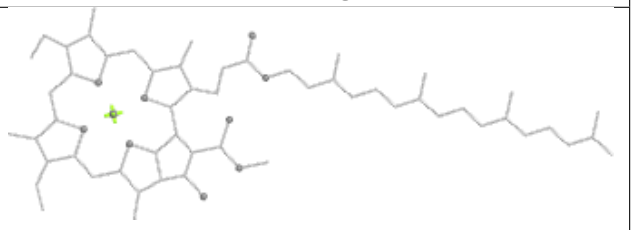
Bond lengths



Bond angles

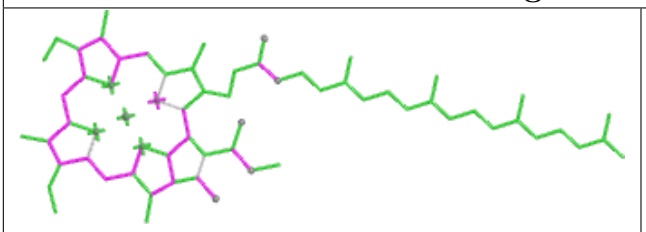


Torsions

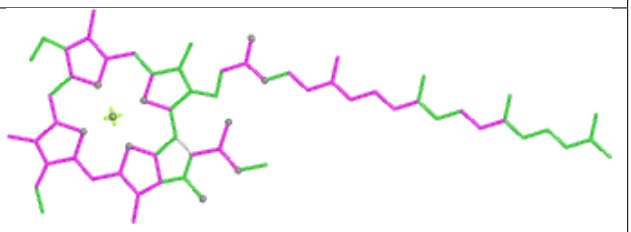


Rings

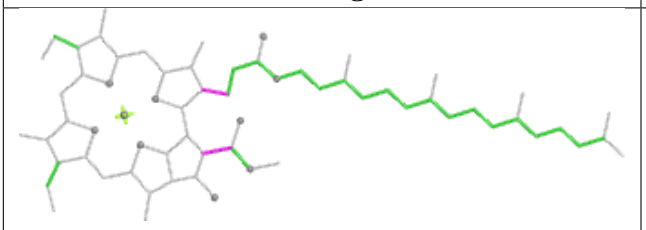
Ligand CLA B 604



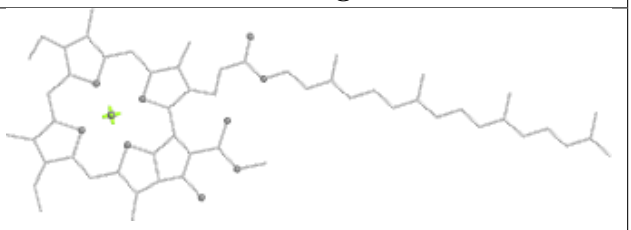
Bond lengths



Bond angles

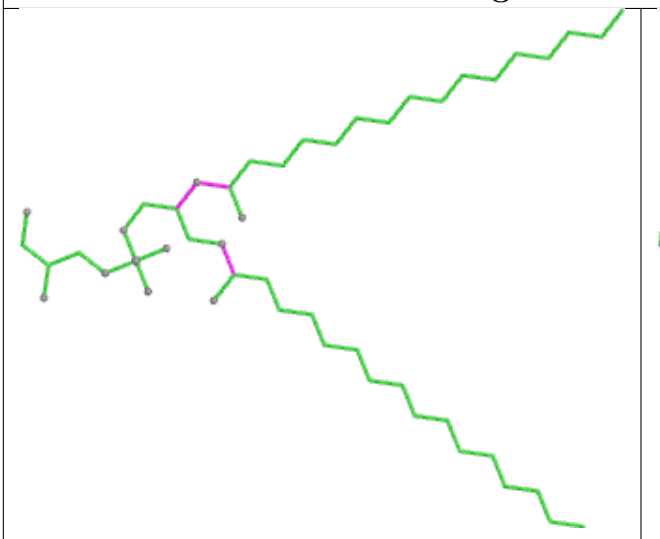


Torsions

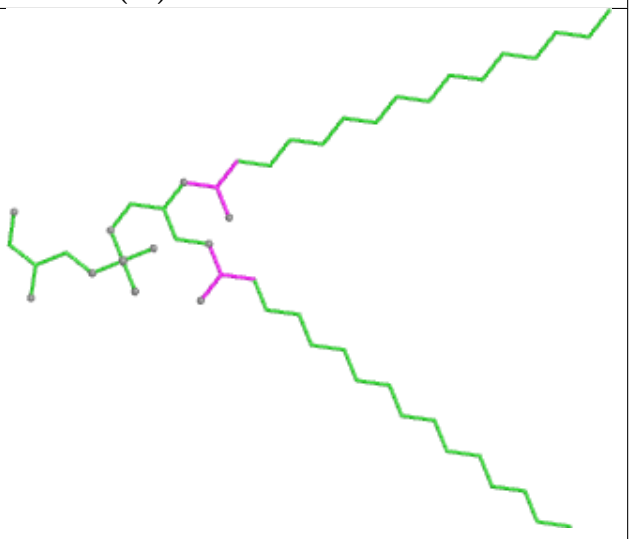


Rings

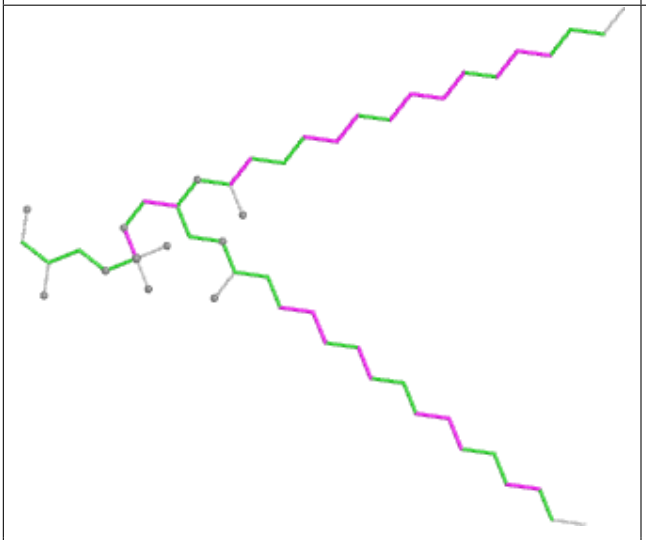
Ligand LHG b 630 (A)



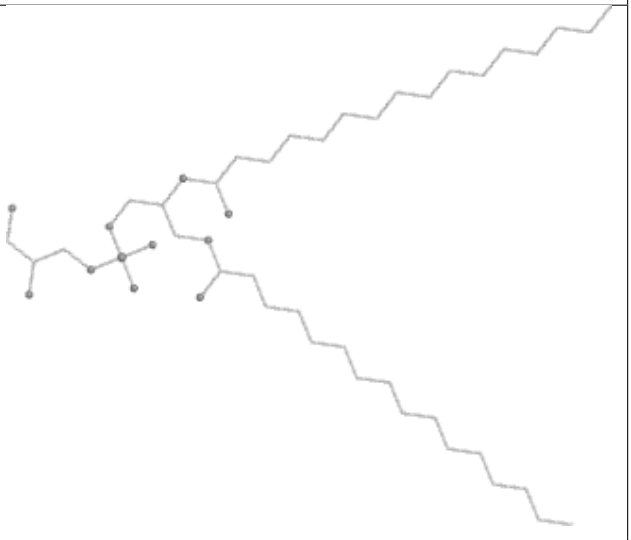
Bond lengths



Bond angles

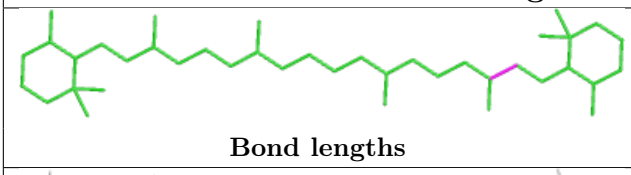


Torsions

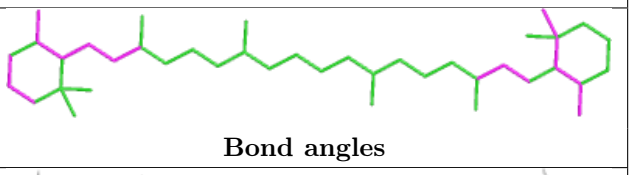


Rings

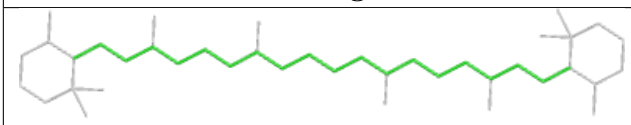
Ligand BCR a 409



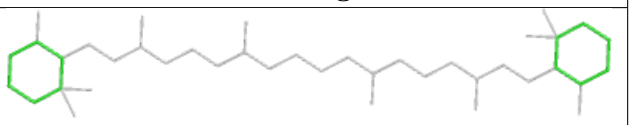
Bond lengths



Bond angles



Torsions

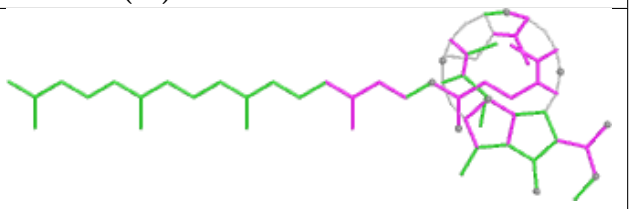


Rings

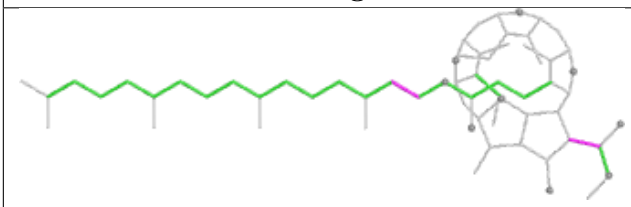
Ligand PHO A 407 (A)



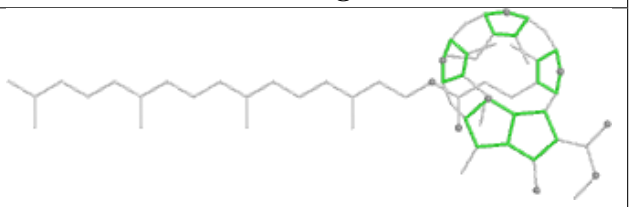
Bond lengths



Bond angles

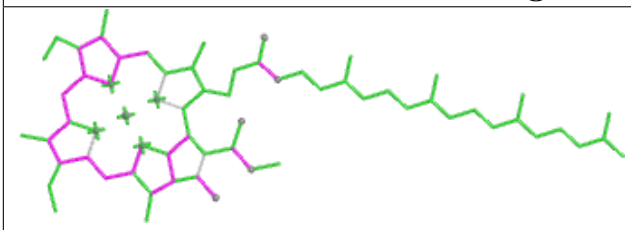


Torsions

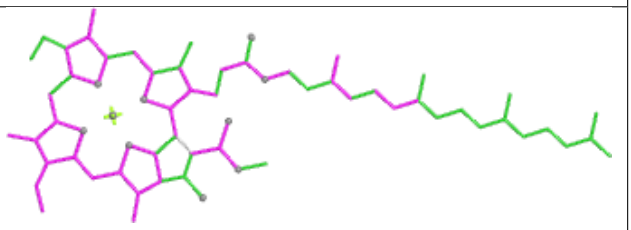


Rings

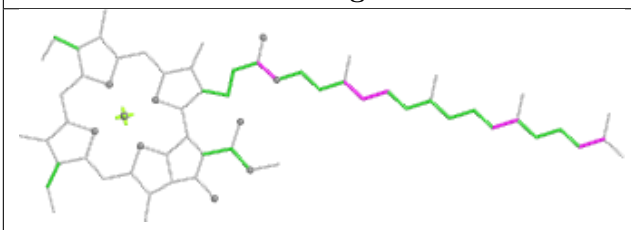
Ligand CLA d 403



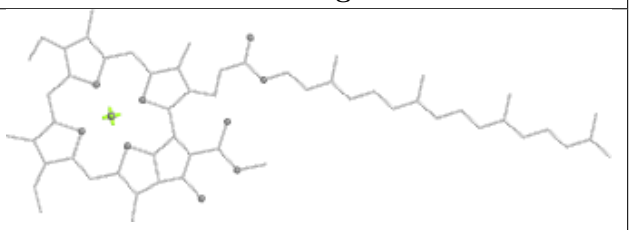
Bond lengths



Bond angles

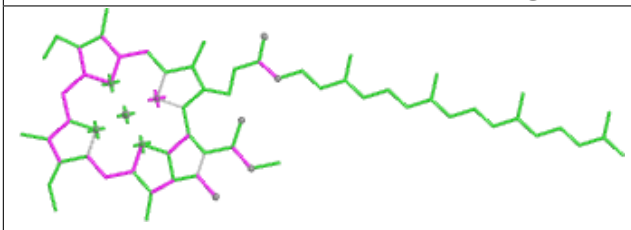


Torsions

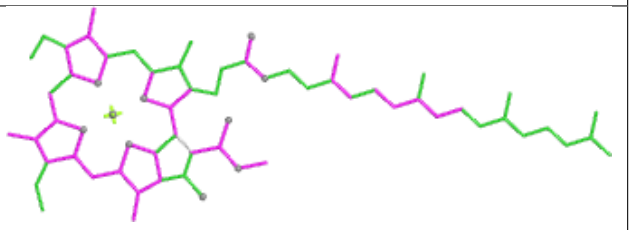


Rings

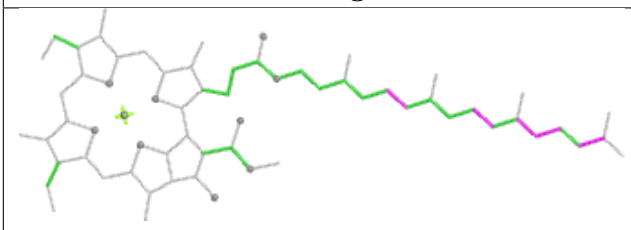
Ligand CLA B 615



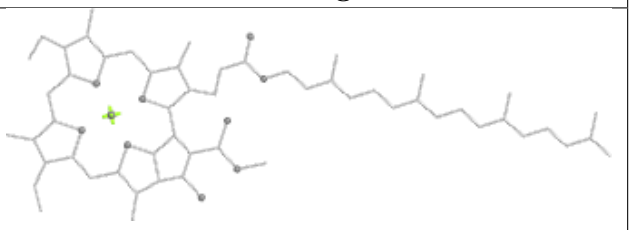
Bond lengths



Bond angles



Torsions

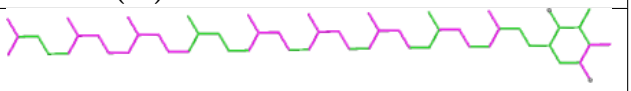


Rings

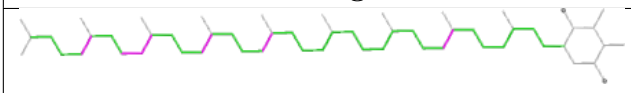
Ligand PL9 D 405 (A)



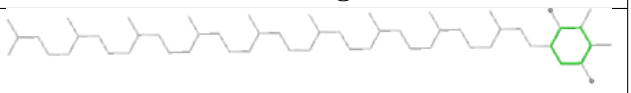
Bond lengths



Bond angles

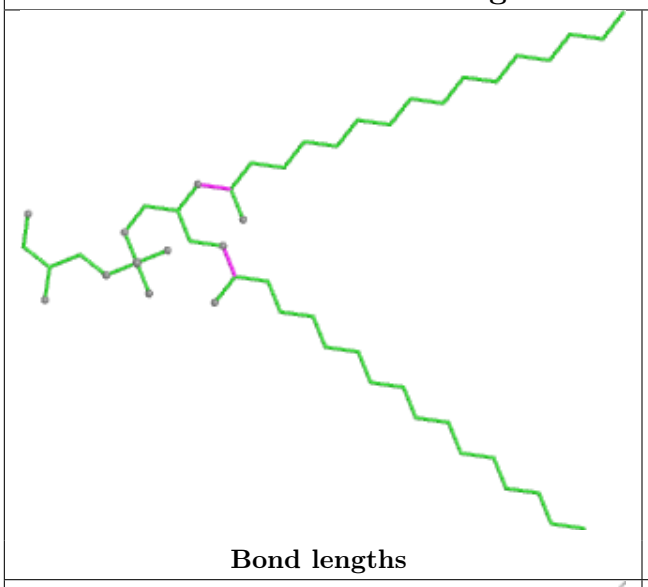


Torsions

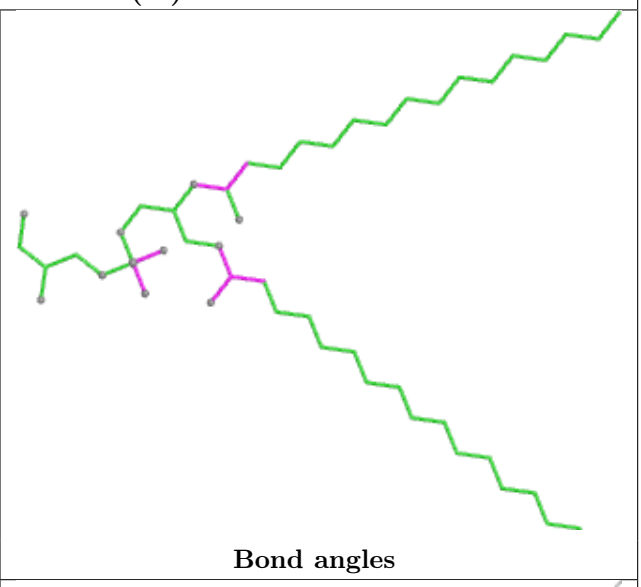


Rings

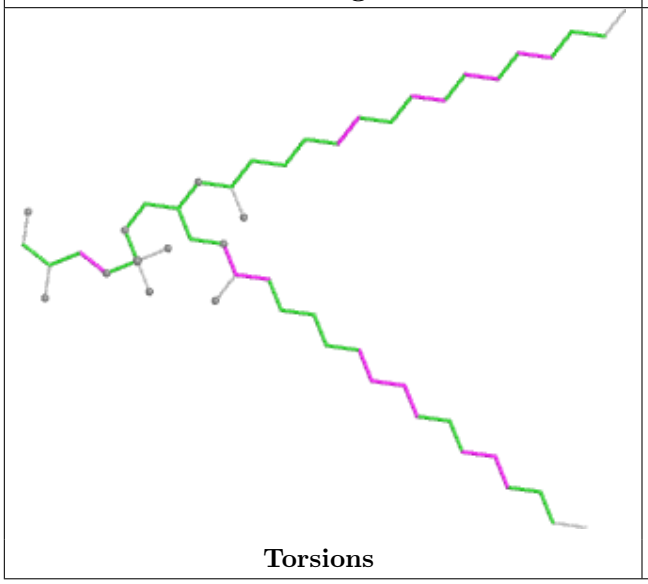
Ligand LHG D 407 (A)



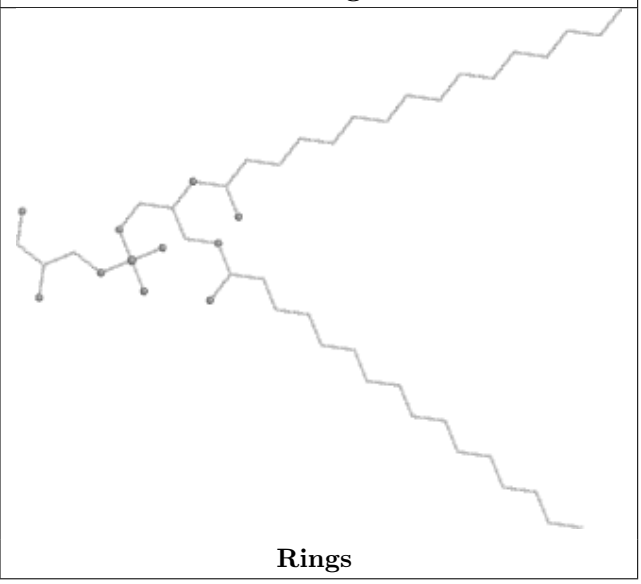
Bond lengths



Bond angles

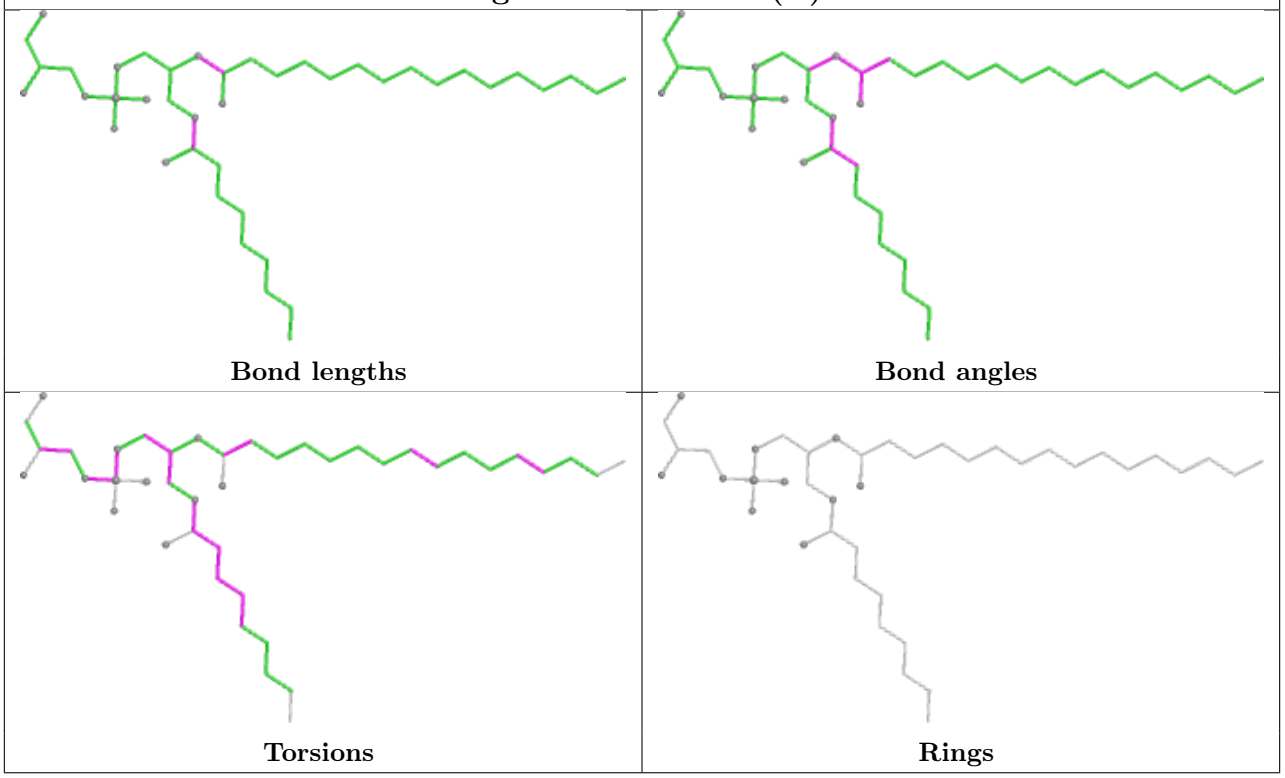


Torsions

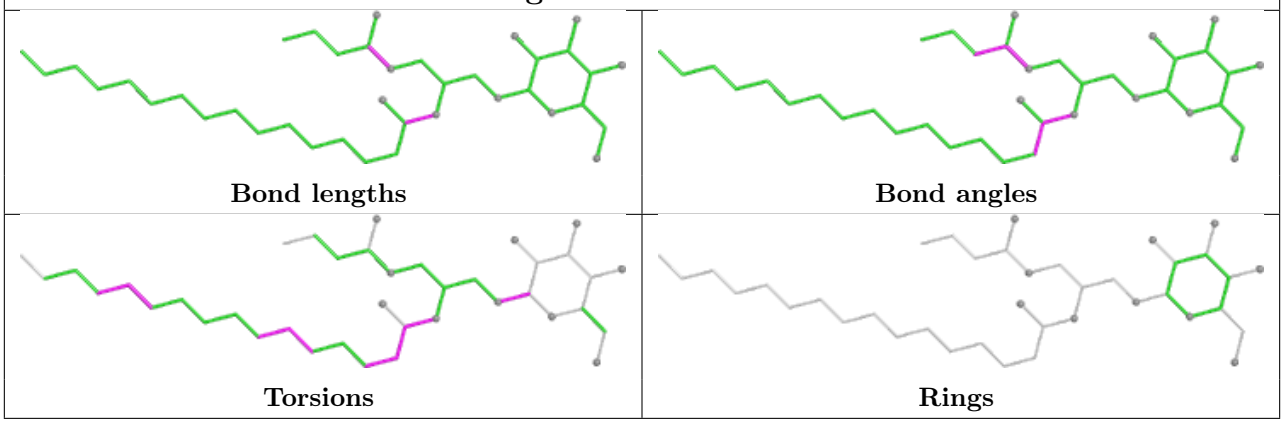


Rings

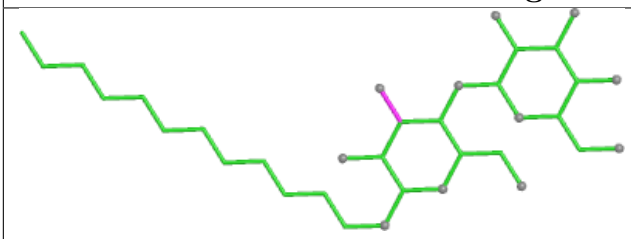
Ligand LHG E 101 (B)



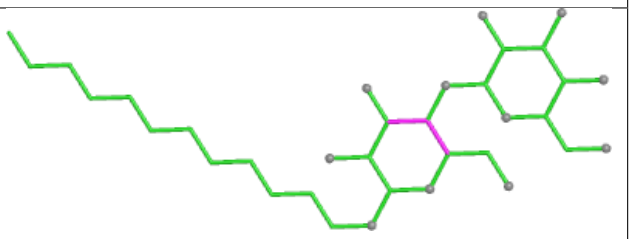
Ligand LMG z 101



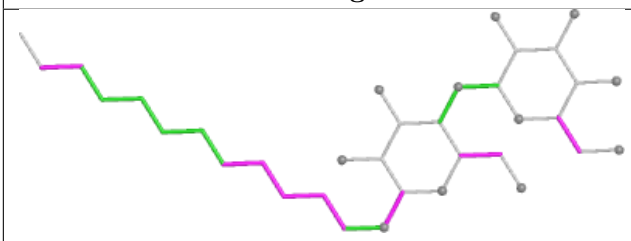
Ligand LMT a 416



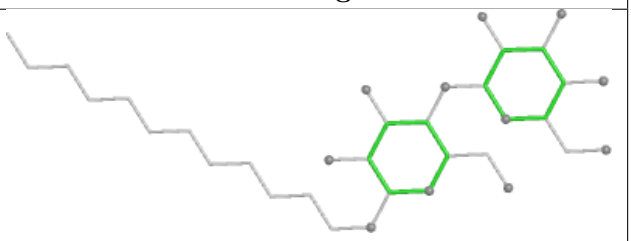
Bond lengths



Bond angles

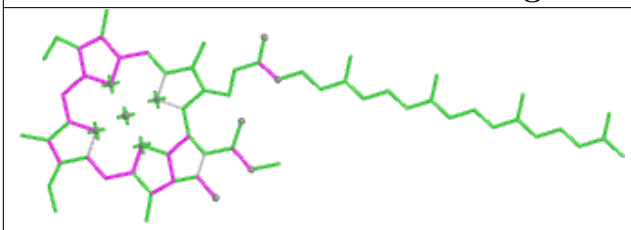


Torsions

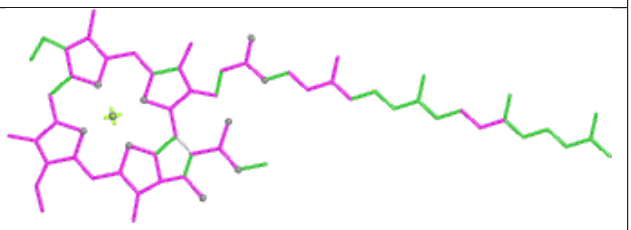


Rings

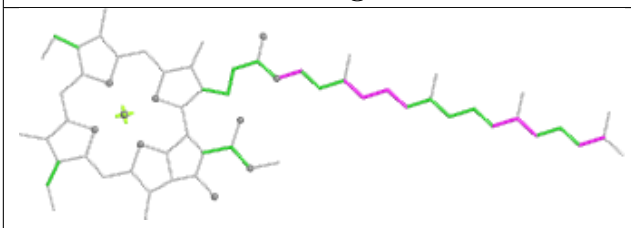
Ligand CLA A 408



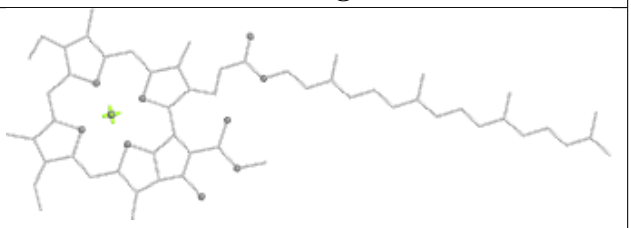
Bond lengths



Bond angles

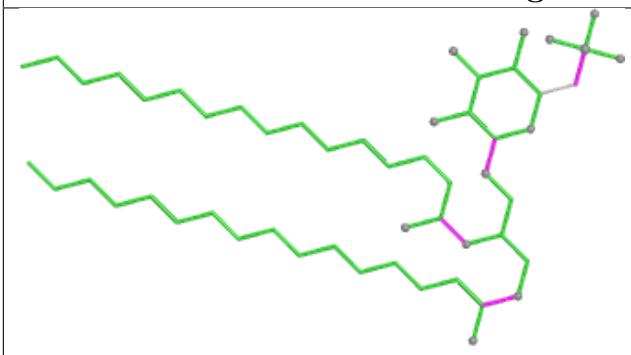


Torsions

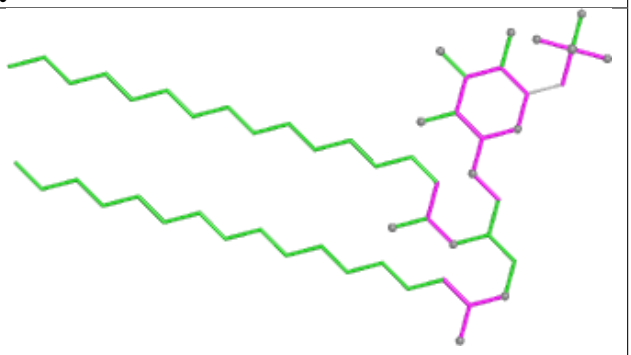


Rings

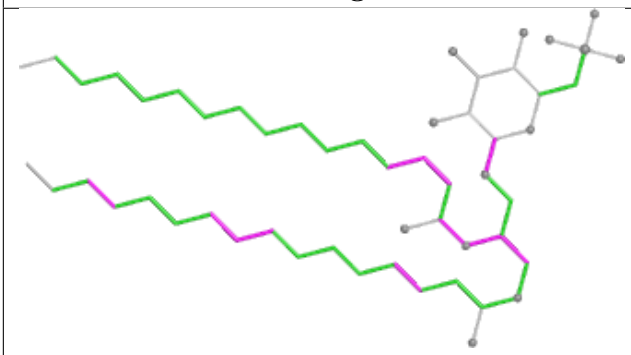
Ligand SQD L 101



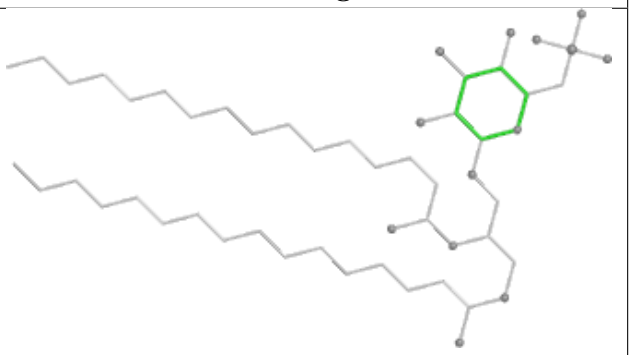
Bond lengths



Bond angles

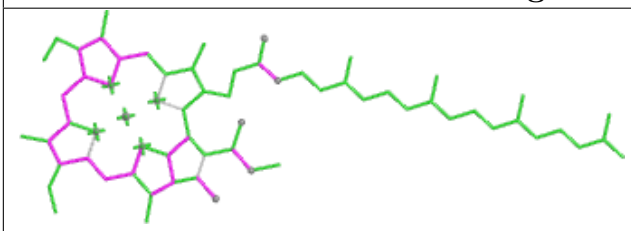


Torsions

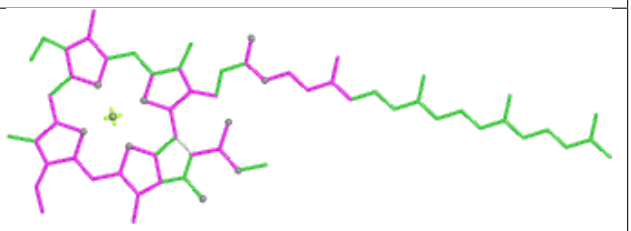


Rings

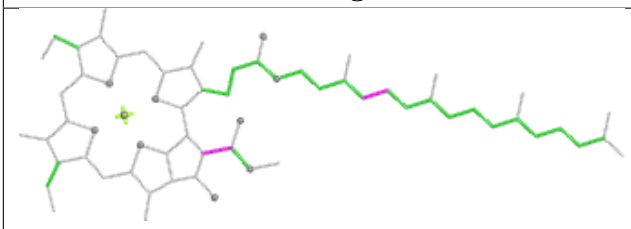
Ligand CLA b 607



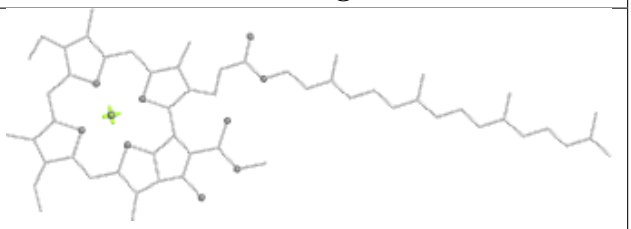
Bond lengths



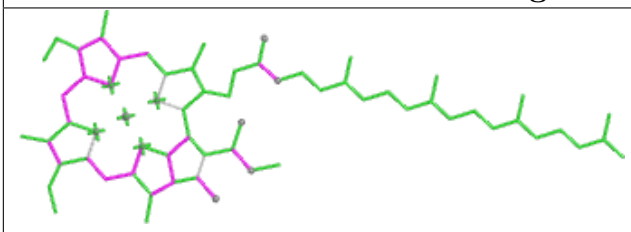
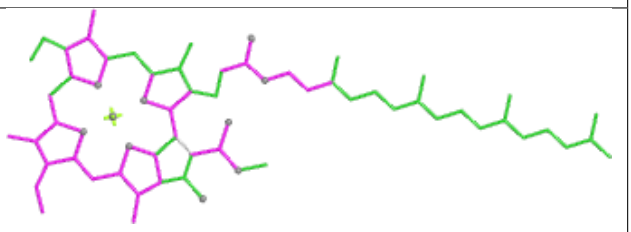
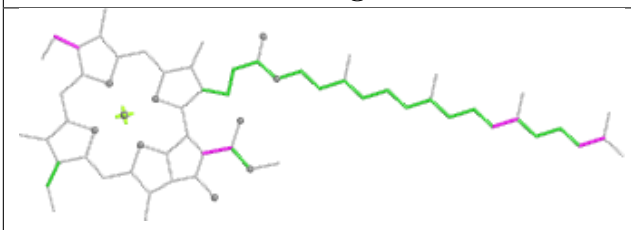
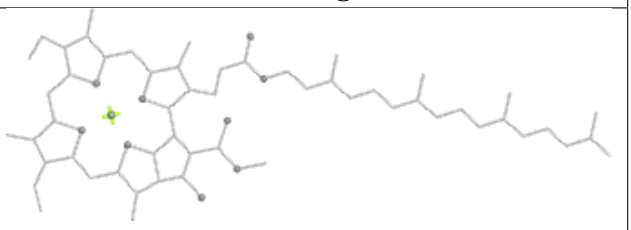
Bond angles



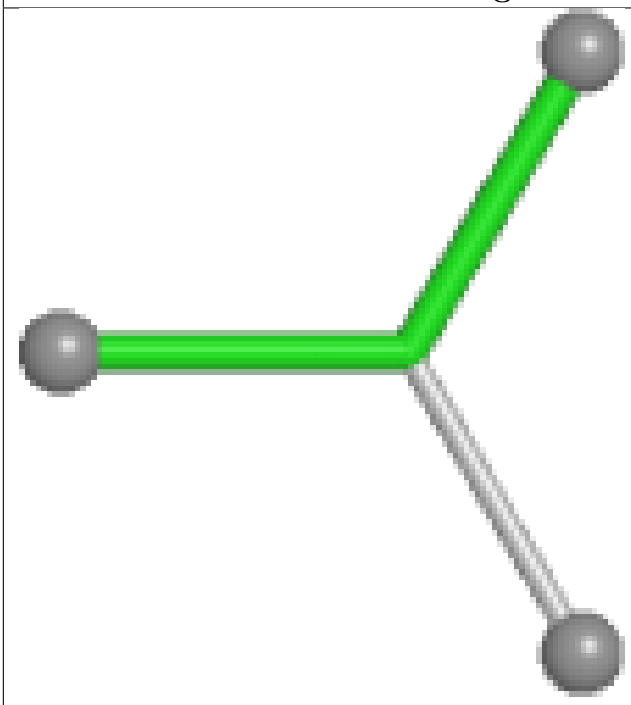
Torsions



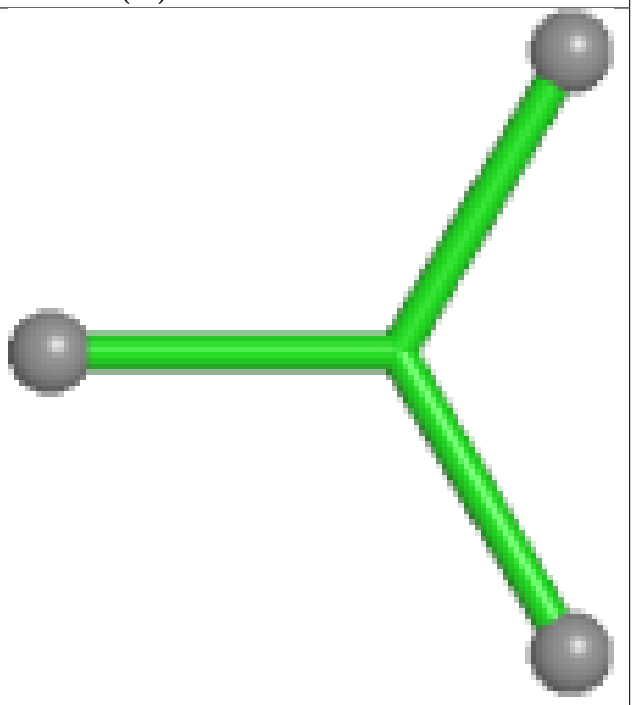
Rings

Ligand CLA c 503	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

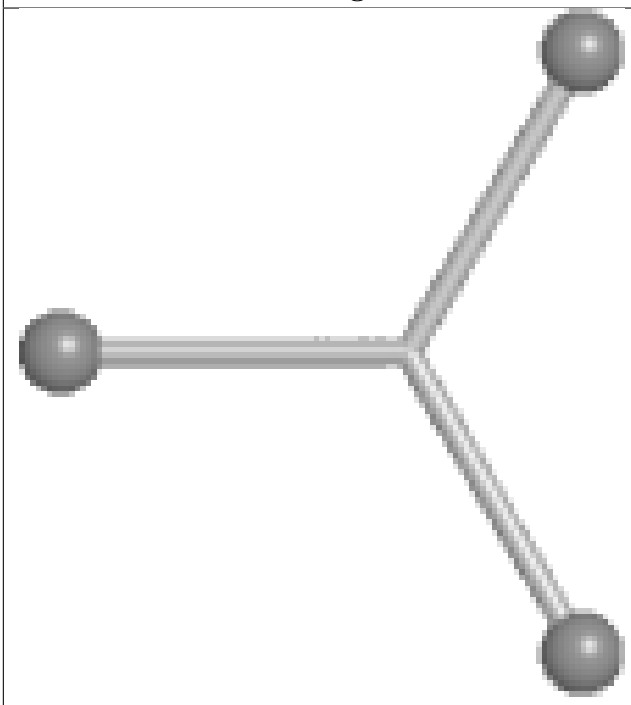
Ligand BCT d 401 (B)



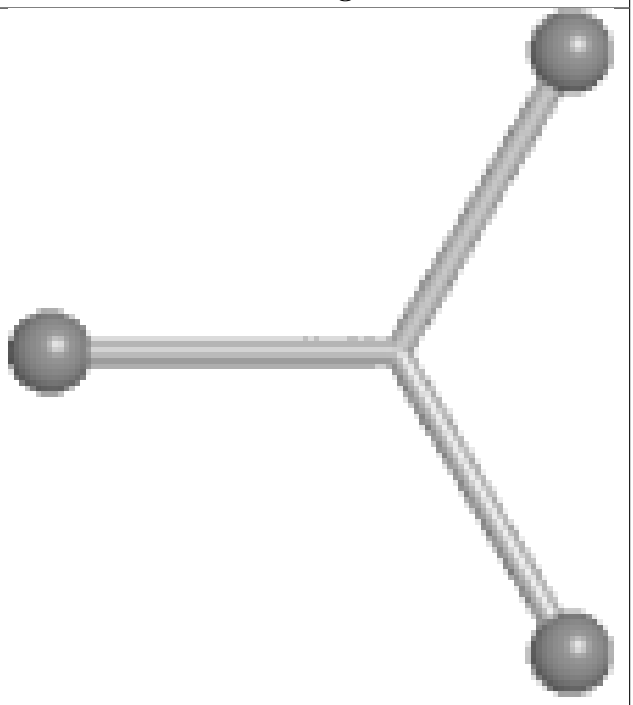
Bond lengths



Bond angles

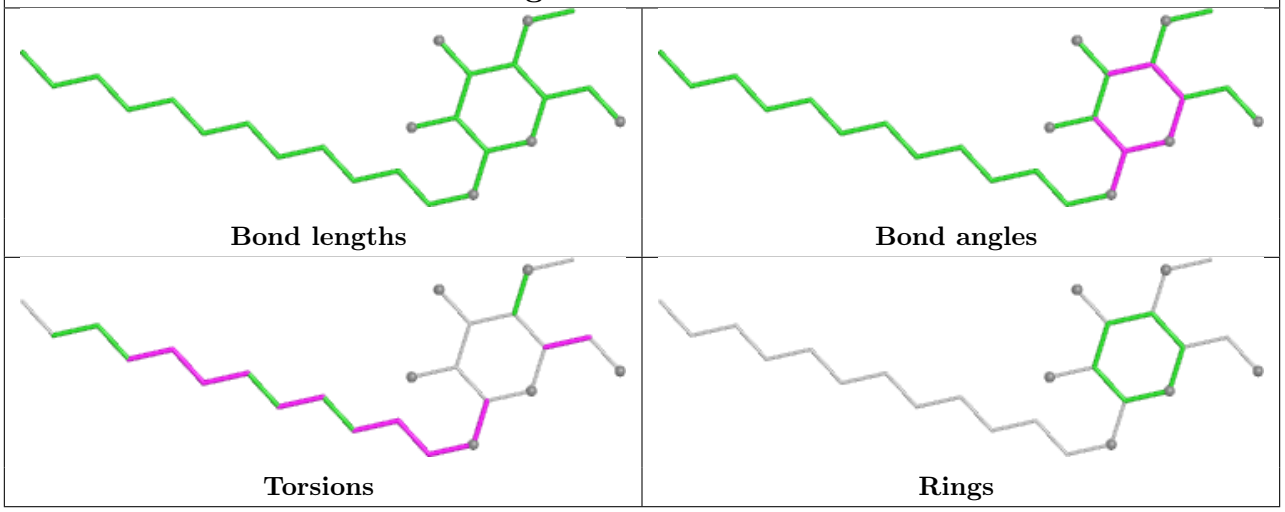


Torsions

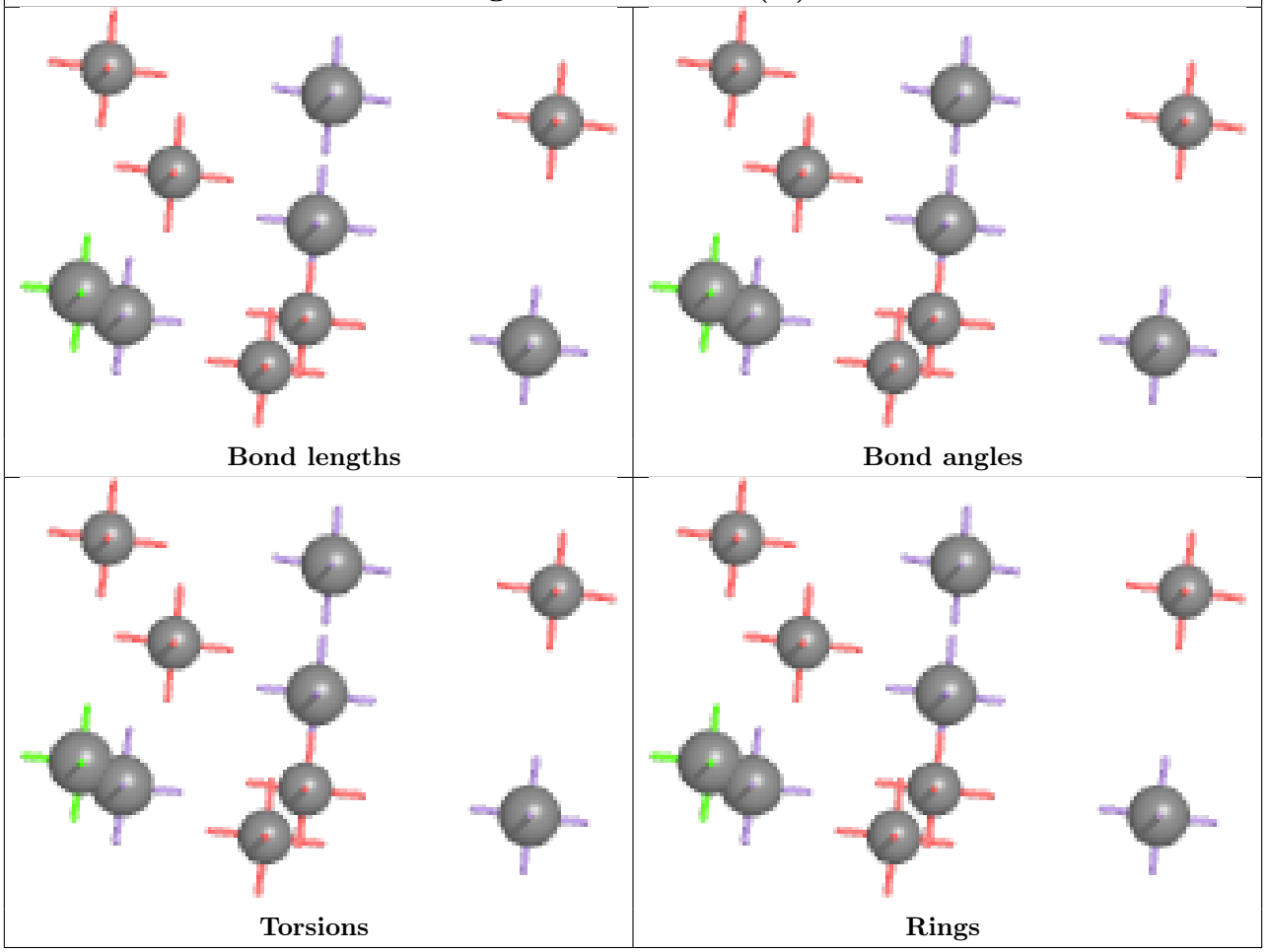


Rings

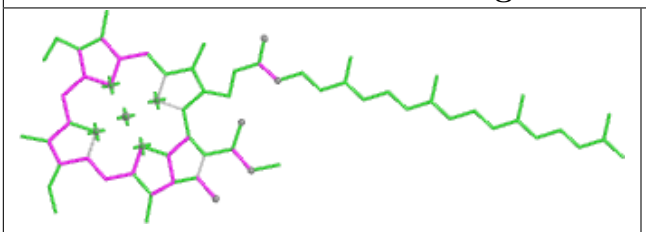
Ligand LMT b 627



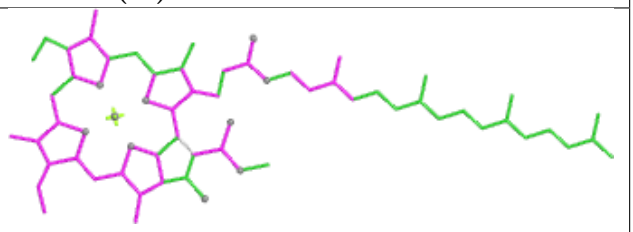
Ligand OEX a 412 (A)



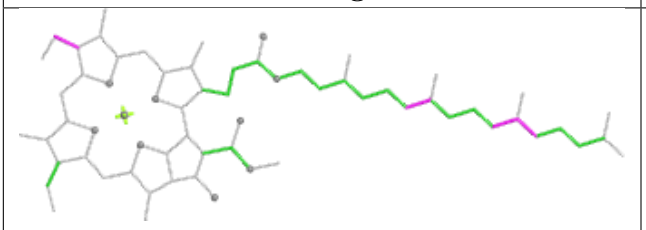
Ligand CLA a 406 (A)



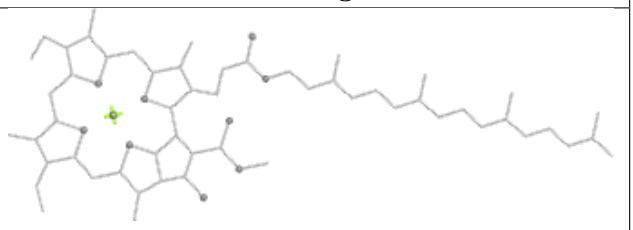
Bond lengths



Bond angles

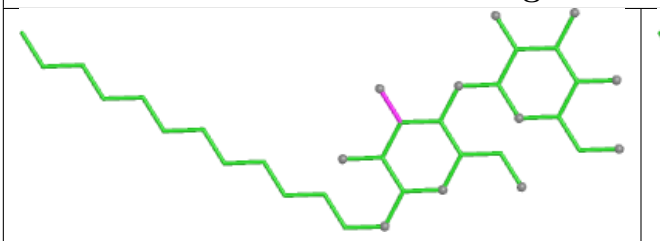


Torsions

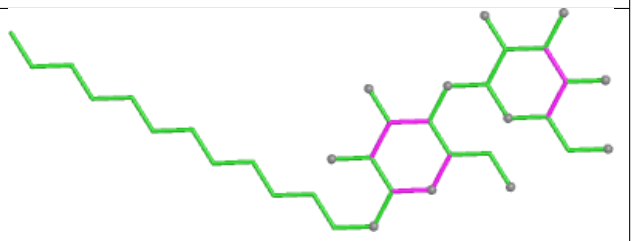


Rings

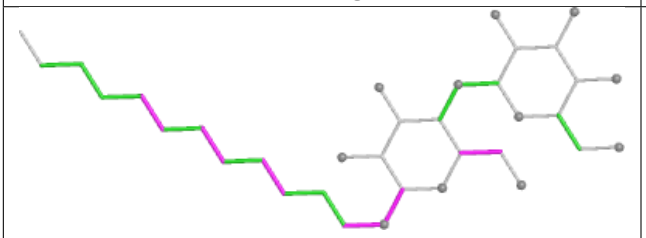
Ligand LMT F 101



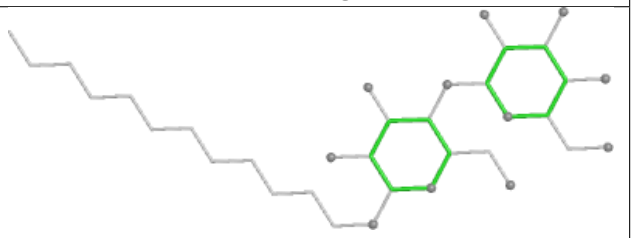
Bond lengths



Bond angles

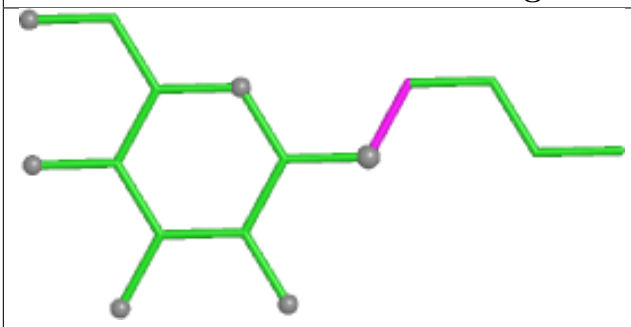


Torsions

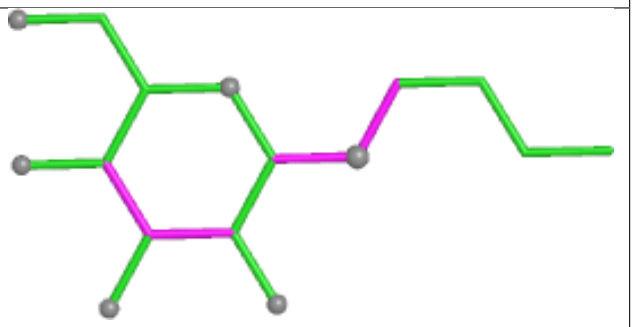


Rings

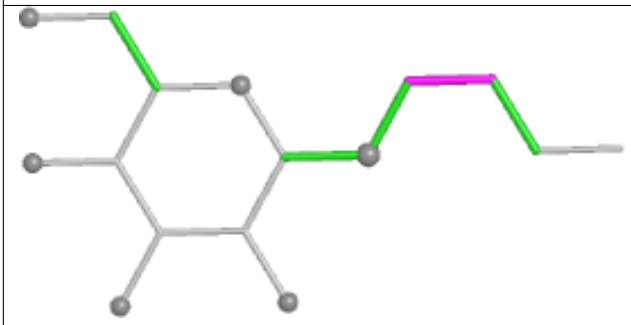
Ligand HTG d 409



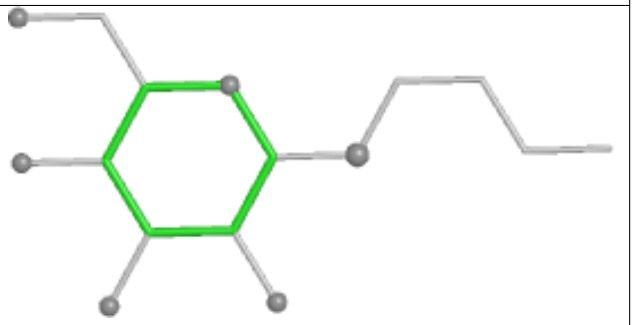
Bond lengths



Bond angles

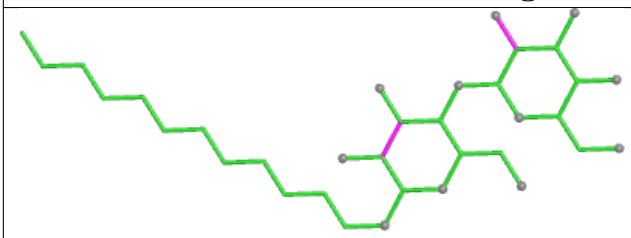


Torsions

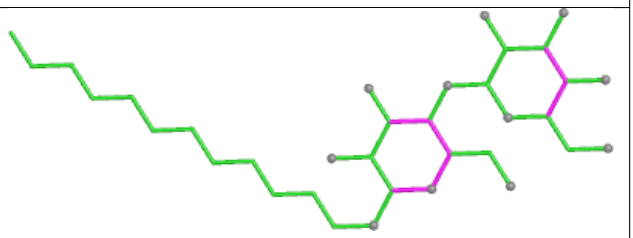


Rings

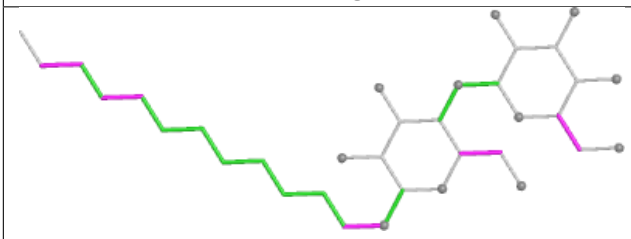
Ligand LMT m 103



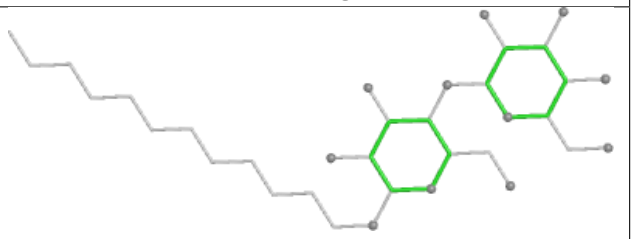
Bond lengths



Bond angles

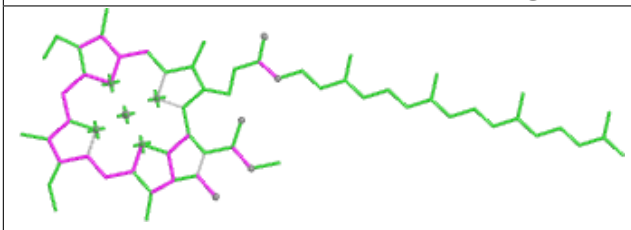


Torsions

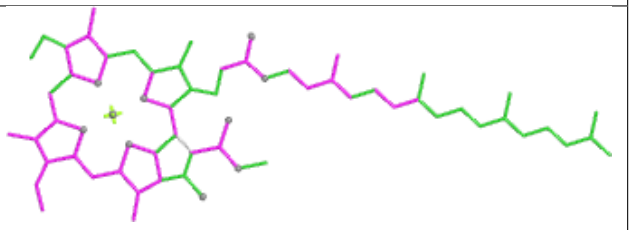


Rings

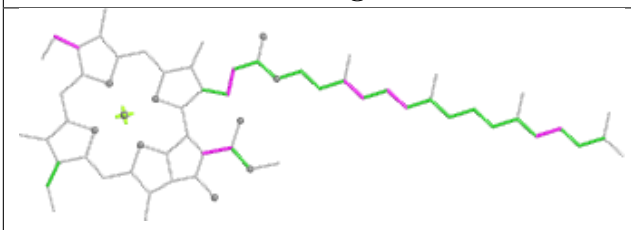
Ligand CLA C 508



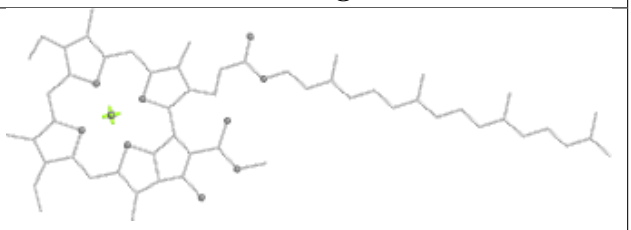
Bond lengths



Bond angles

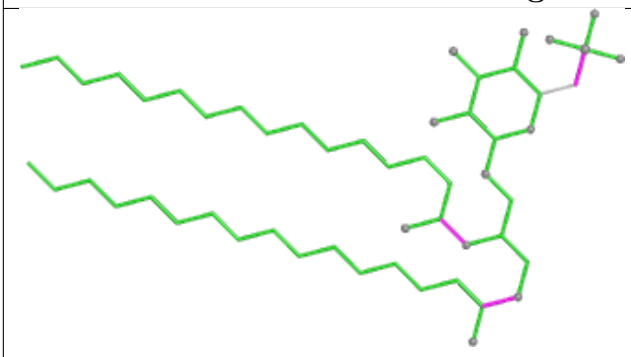


Torsions

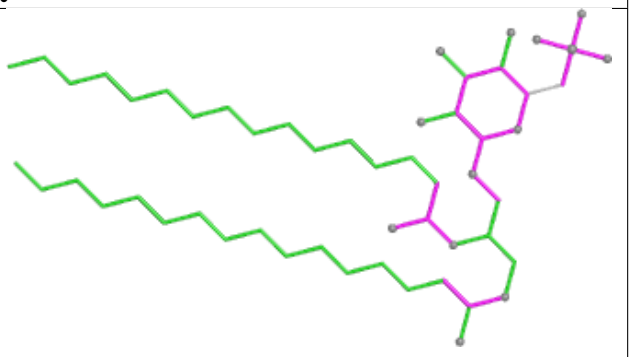


Rings

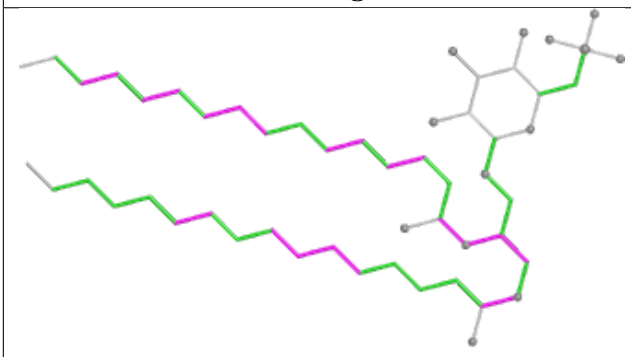
Ligand SQD b 620



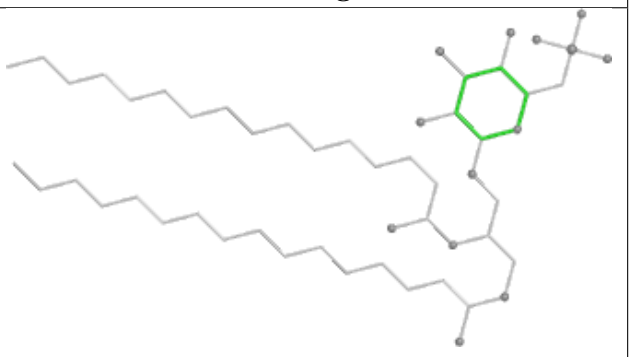
Bond lengths



Bond angles

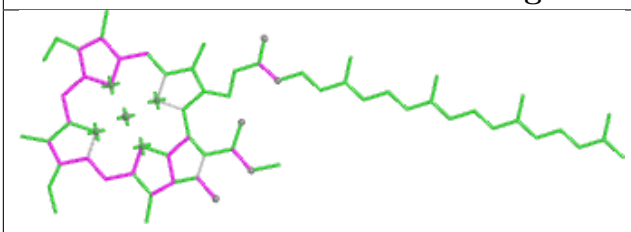


Torsions

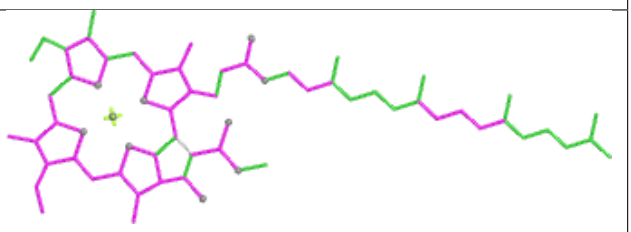


Rings

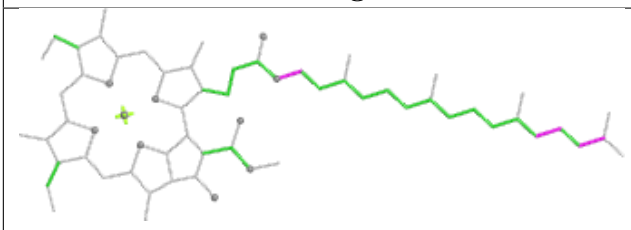
Ligand CLA B 608



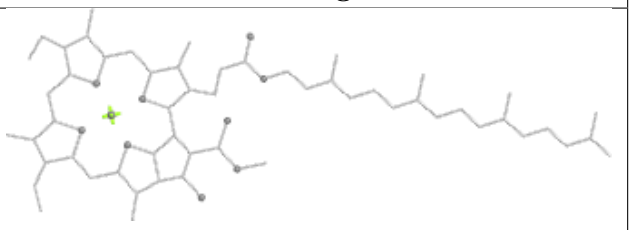
Bond lengths



Bond angles

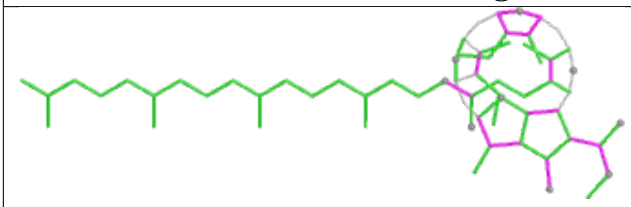


Torsions

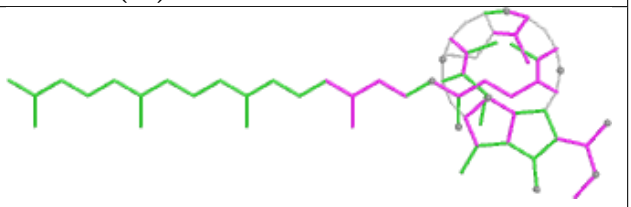


Rings

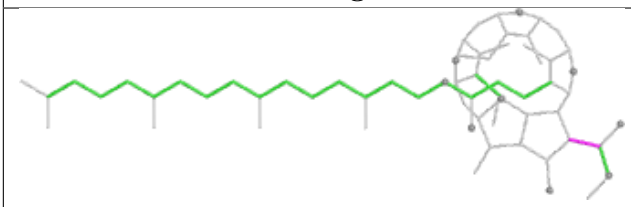
Ligand PHO a 415 (A)



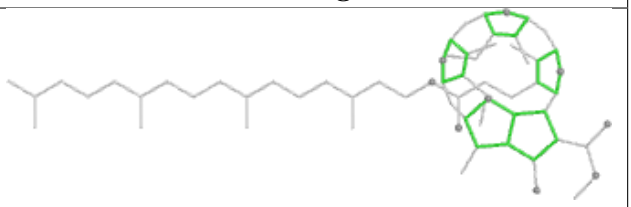
Bond lengths



Bond angles

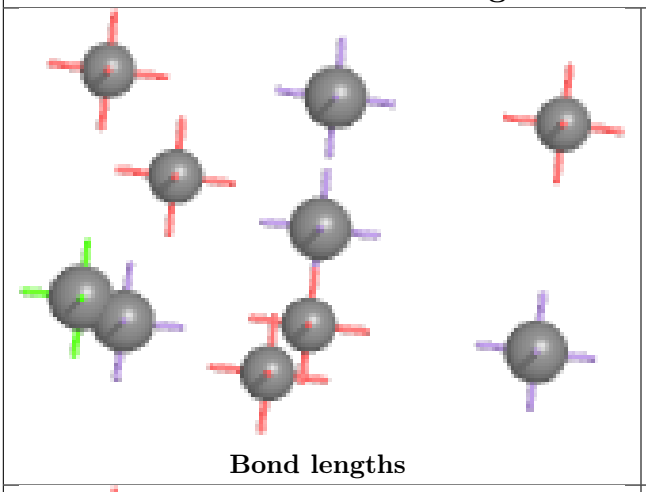


Torsions

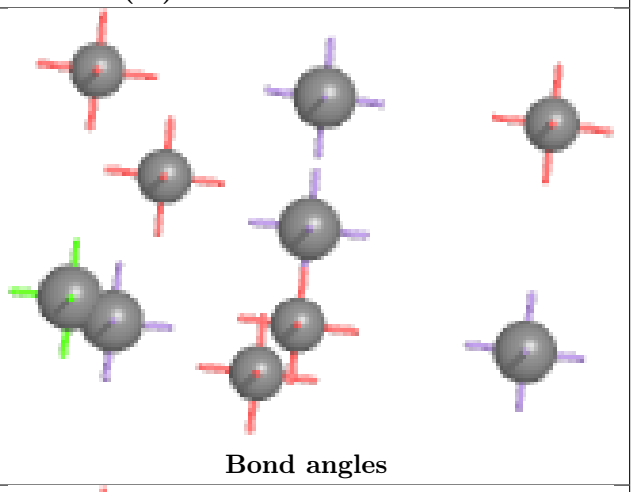


Rings

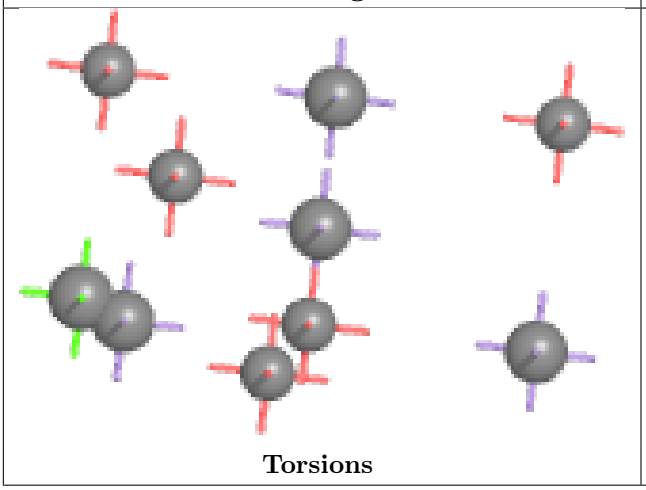
Ligand OEX A 413 (A)



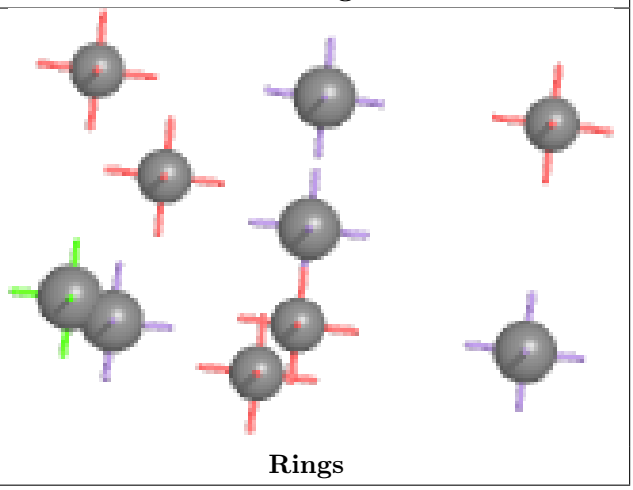
Bond lengths



Bond angles

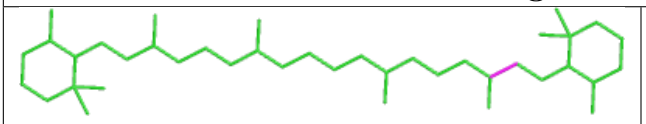


Torsions

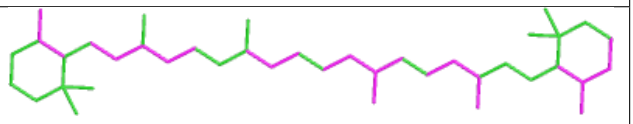


Rings

Ligand BCR c 515



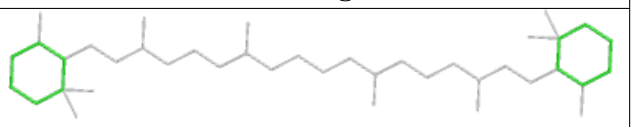
Bond lengths



Bond angles

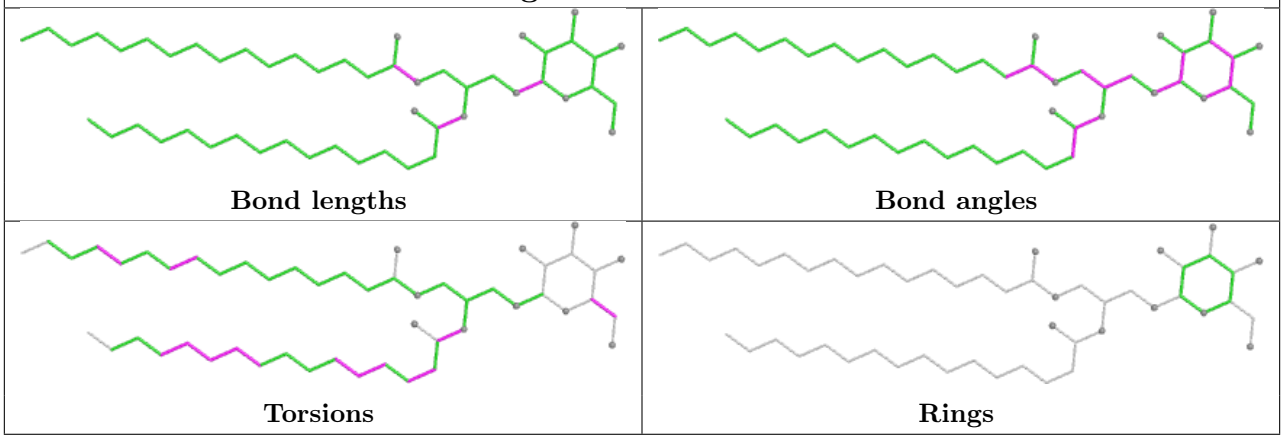


Torsions

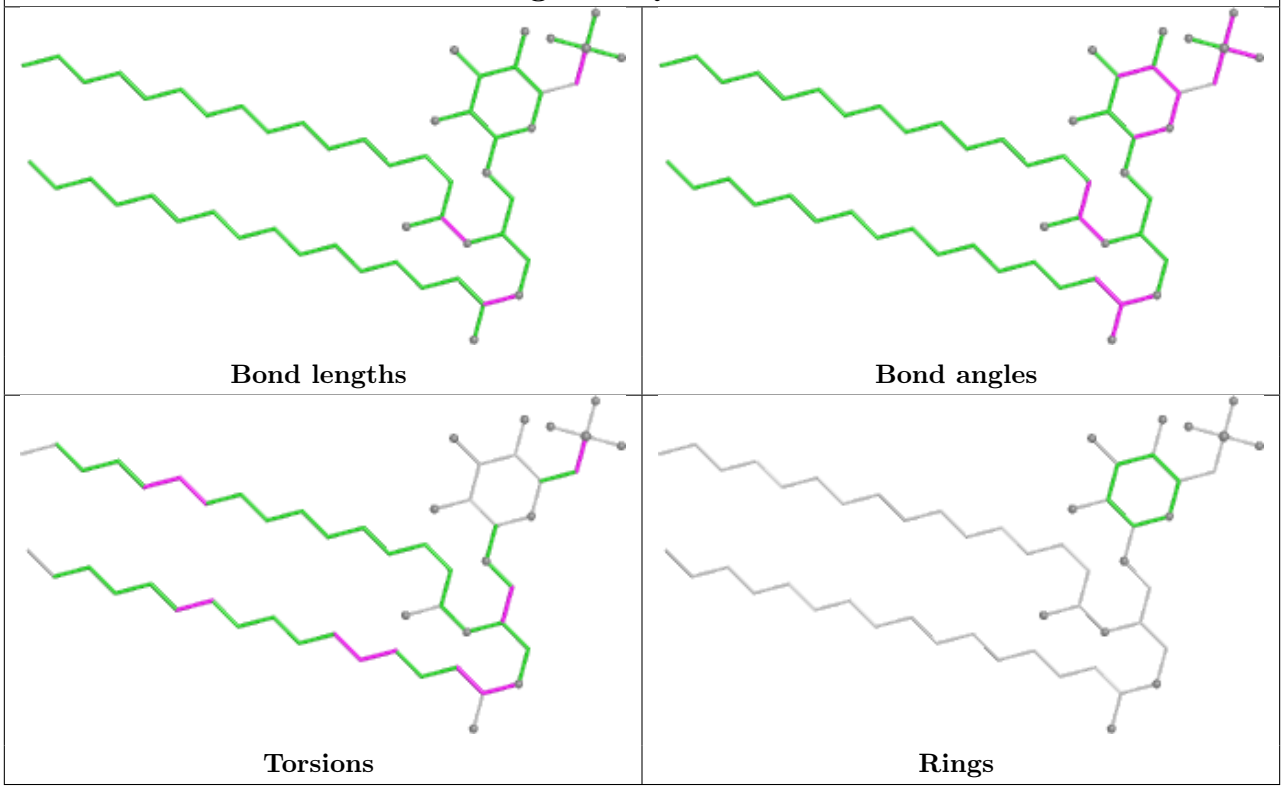


Rings

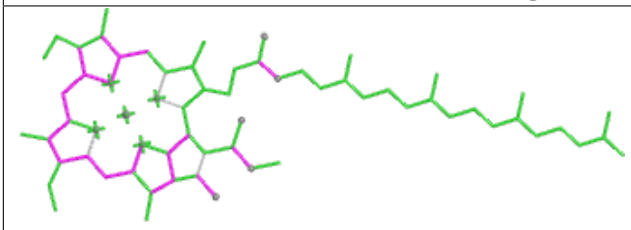
Ligand LMG C 521



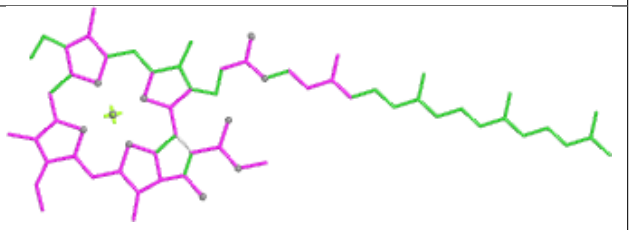
Ligand SQD a 411



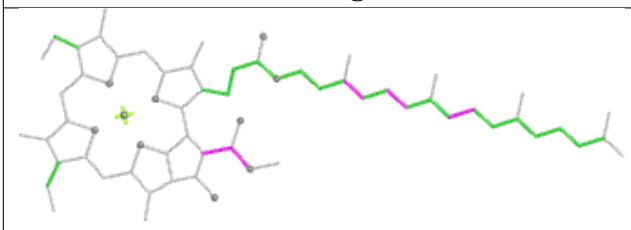
Ligand CLA B 605



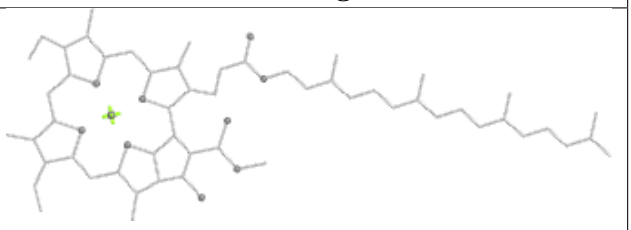
Bond lengths



Bond angles

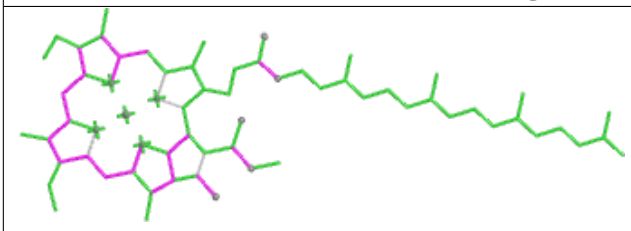


Torsions

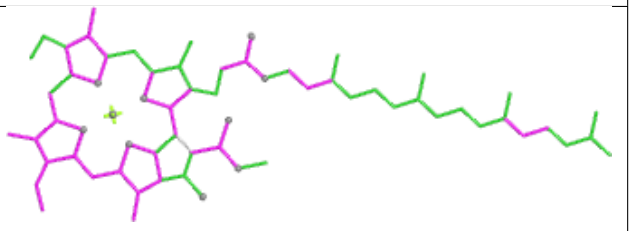


Rings

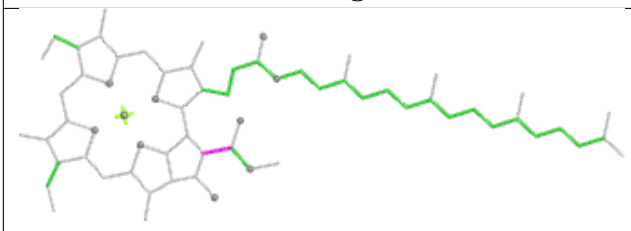
Ligand CLA B 609



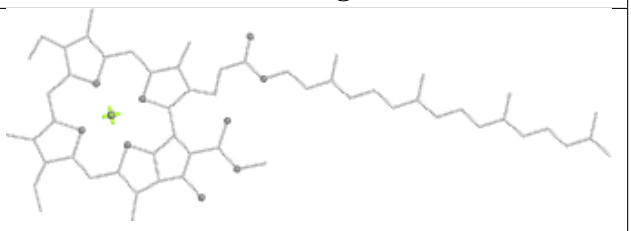
Bond lengths



Bond angles

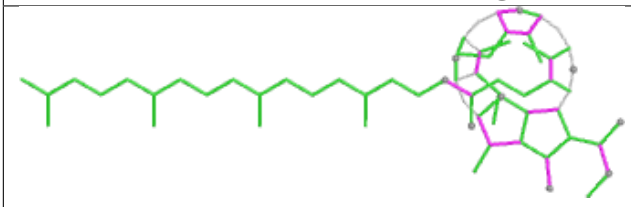


Torsions

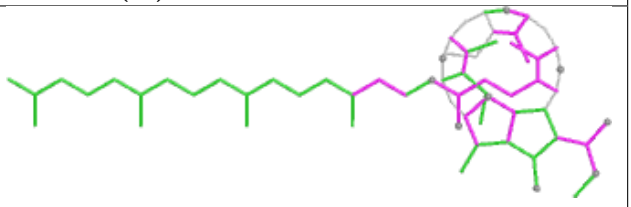


Rings

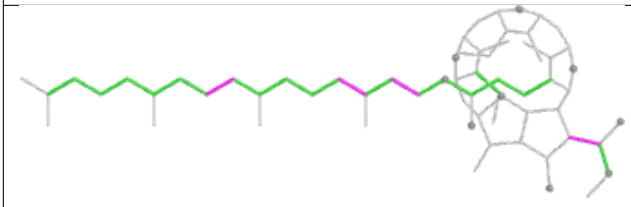
Ligand PHO a 407 (B)



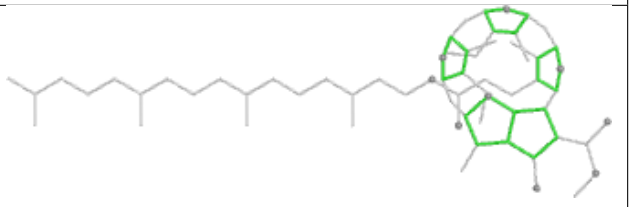
Bond lengths



Bond angles

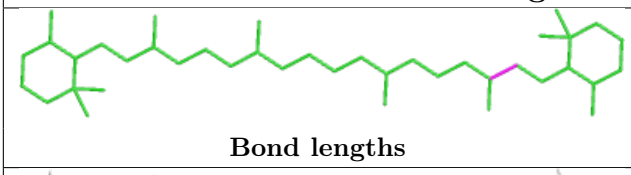


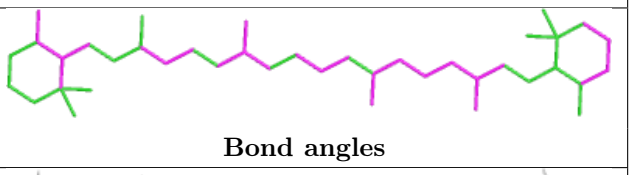
Torsions

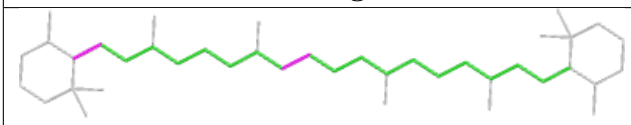


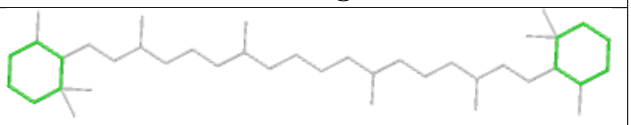
Rings

Ligand BCR t 102


Bond lengths


Bond angles

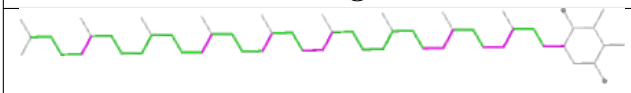

Torsions

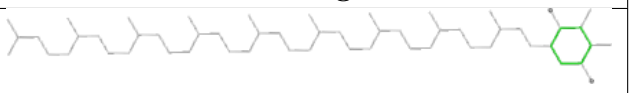

Rings

Ligand PL9 a 413 (B)

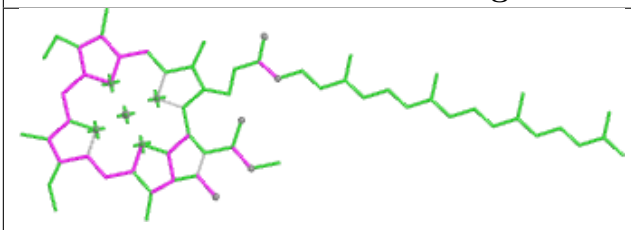

Bond lengths

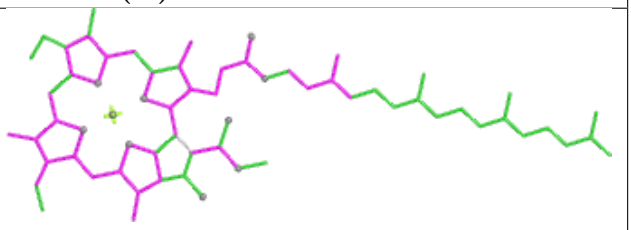

Bond angles

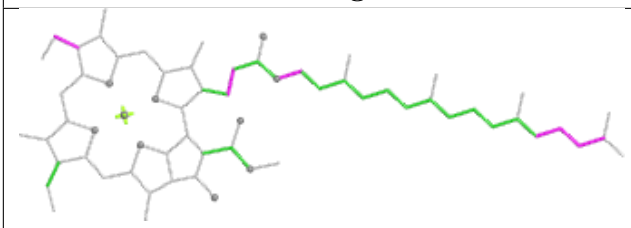

Torsions

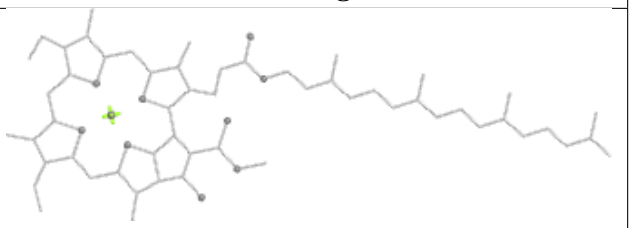

Rings

Ligand CLA A 404 (B)

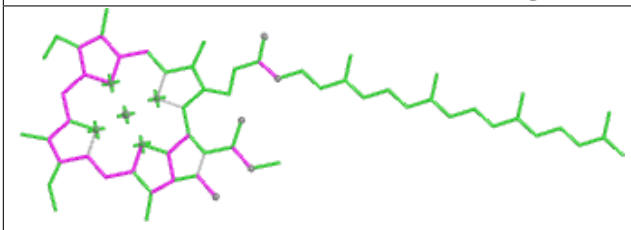

Bond lengths


Bond angles

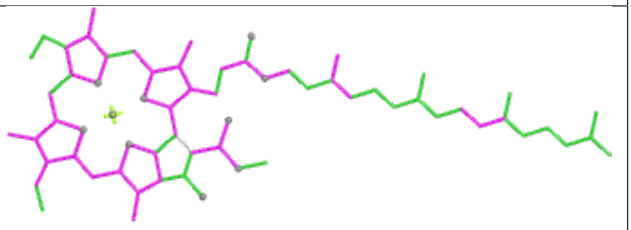

Torsions


Rings

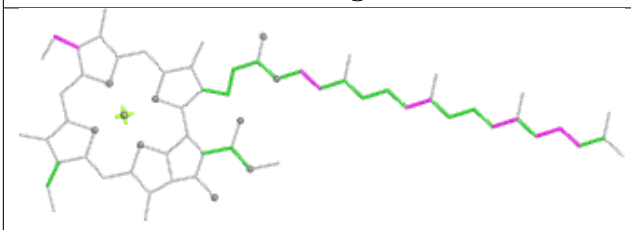
Ligand CLA B 602



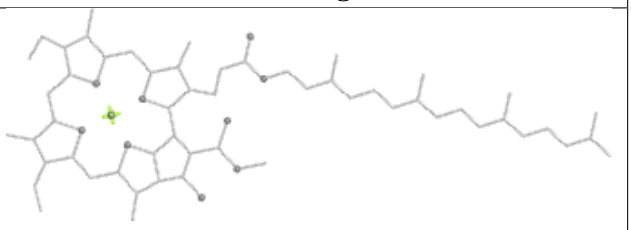
Bond lengths



Bond angles



Torsions

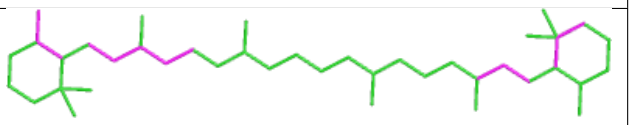


Rings

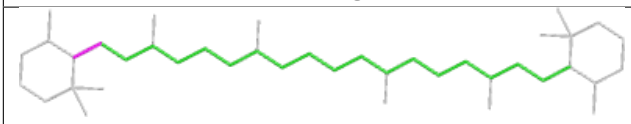
Ligand BCR b 617



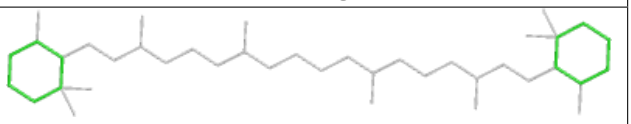
Bond lengths



Bond angles

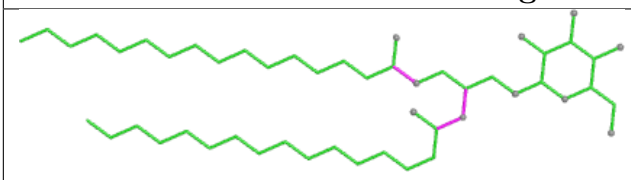


Torsions

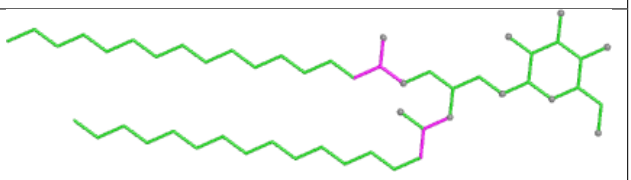


Rings

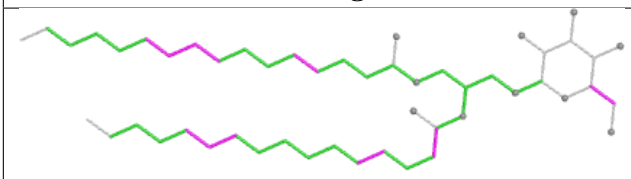
Ligand LMG D 411



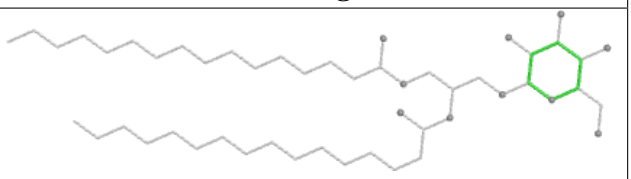
Bond lengths



Bond angles

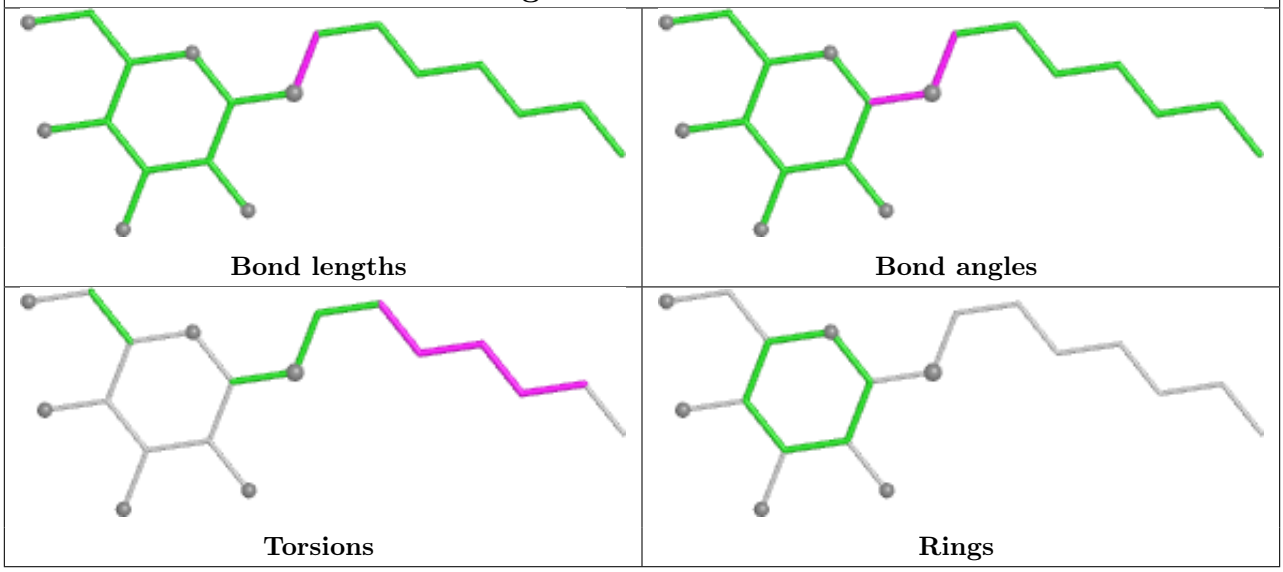


Torsions

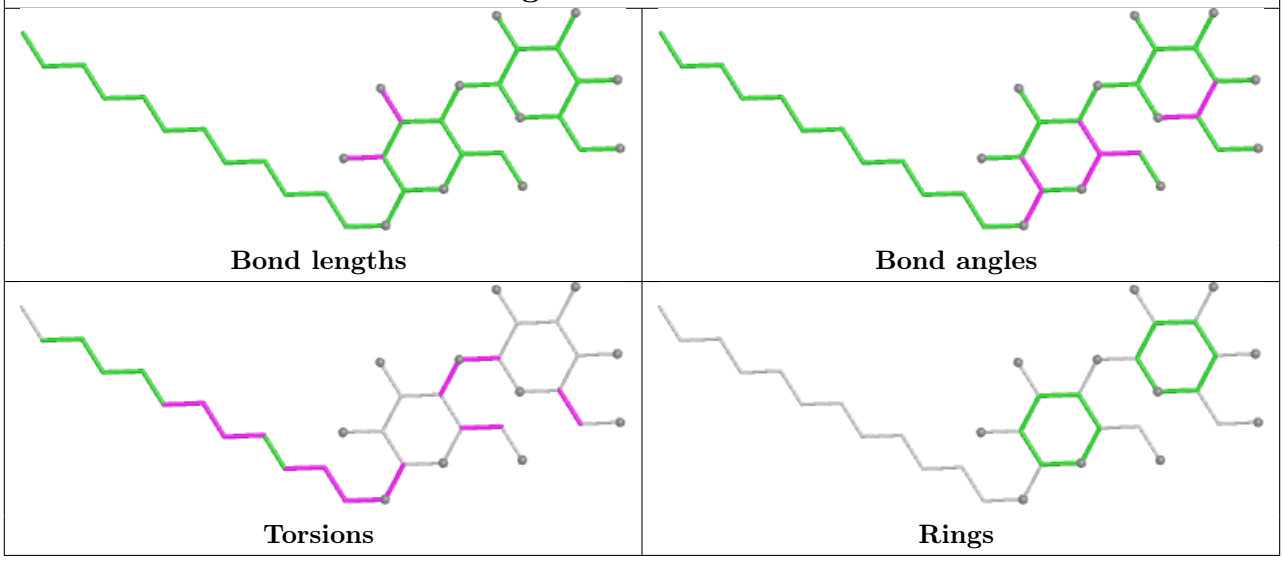


Rings

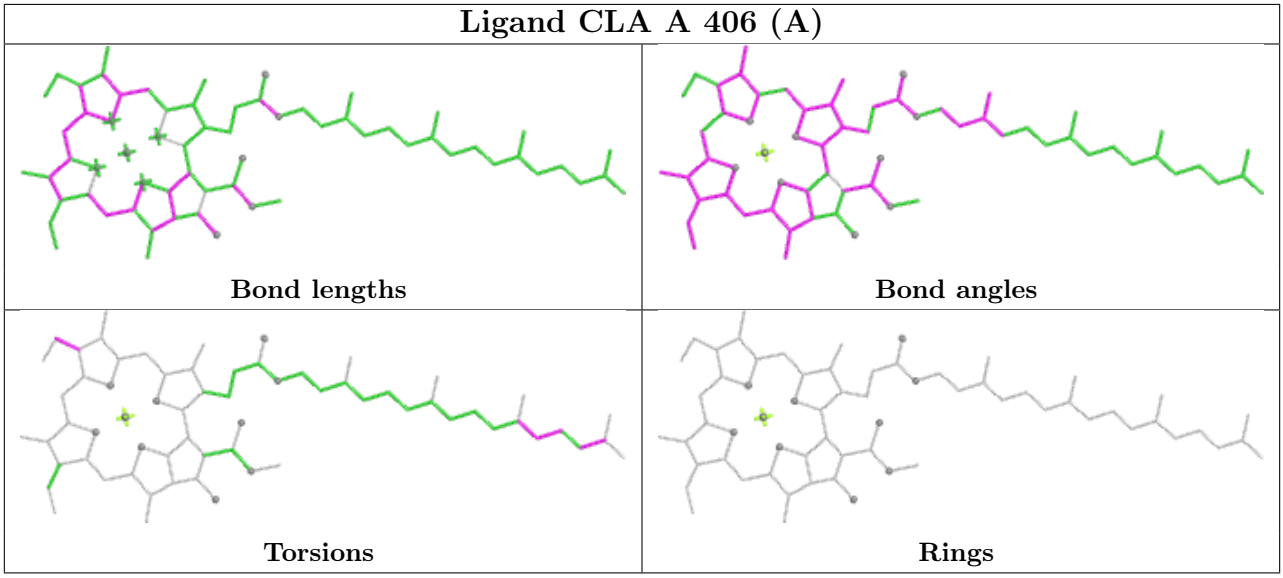
Ligand HTG B 621



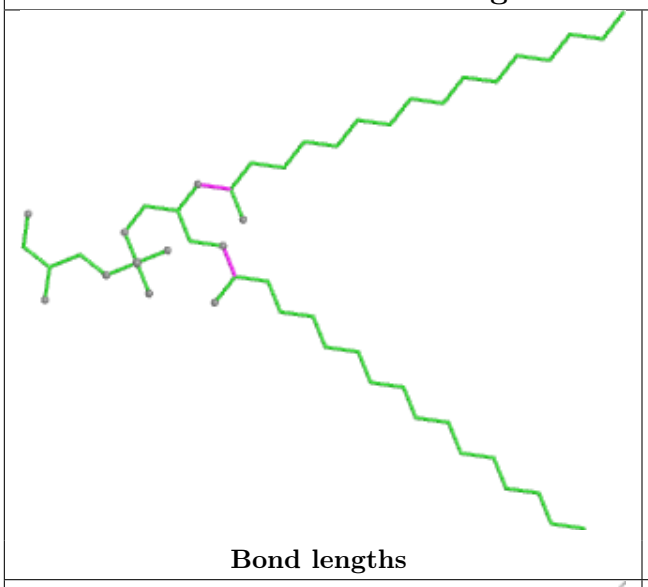
Ligand LMT A 420



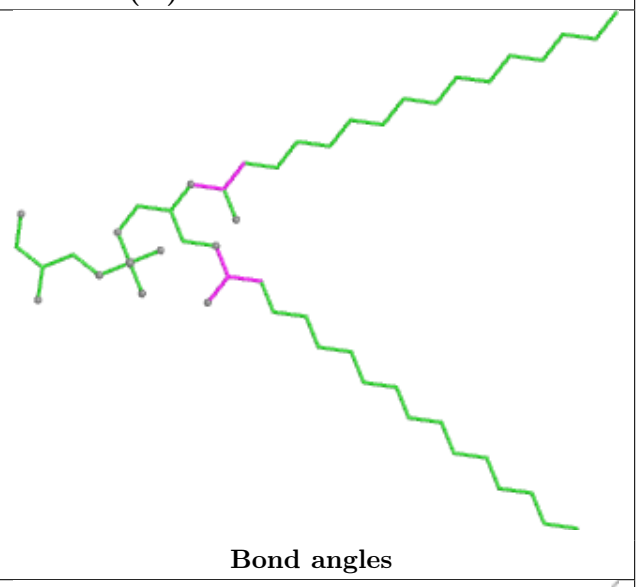
Ligand CLA A 406 (A)



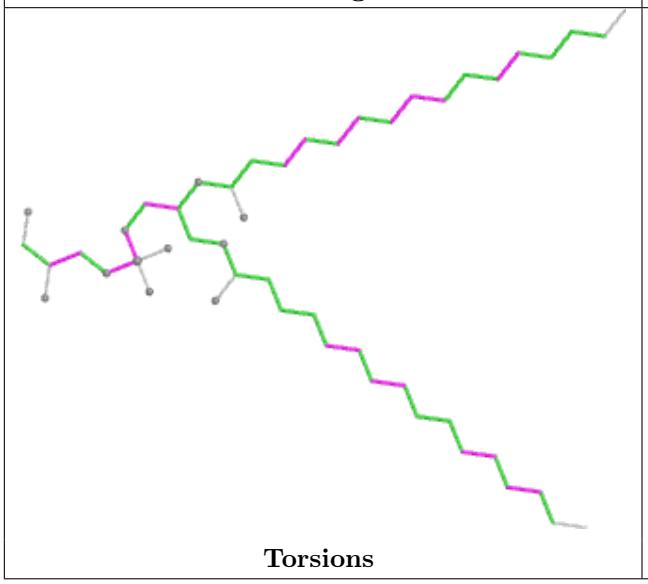
Ligand LHG D 406 (B)



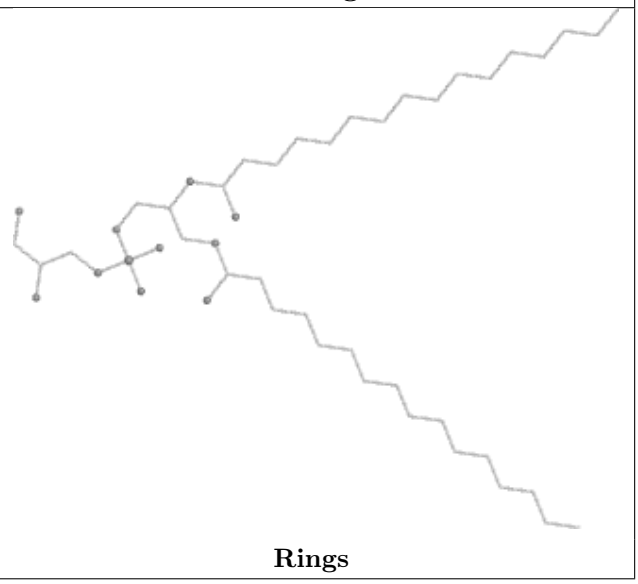
Bond lengths



Bond angles

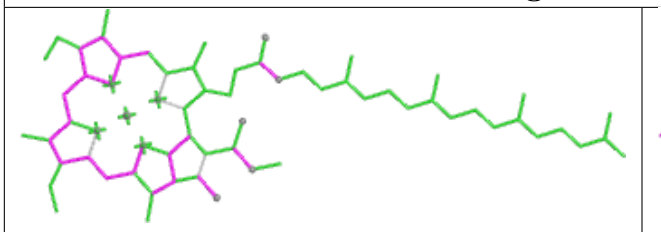


Torsions

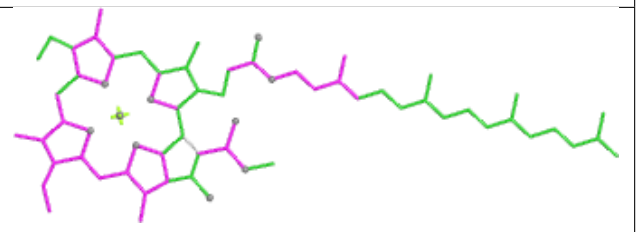


Rings

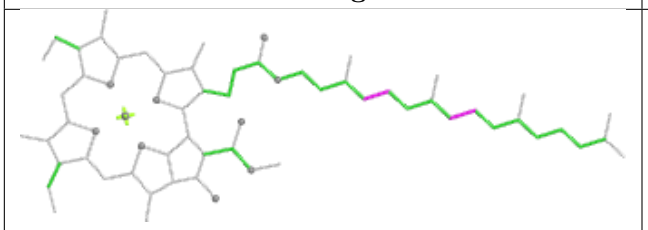
Ligand CLA C 512



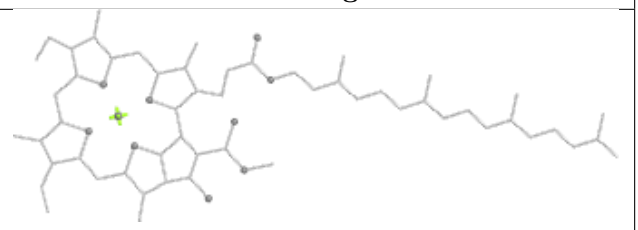
Bond lengths



Bond angles

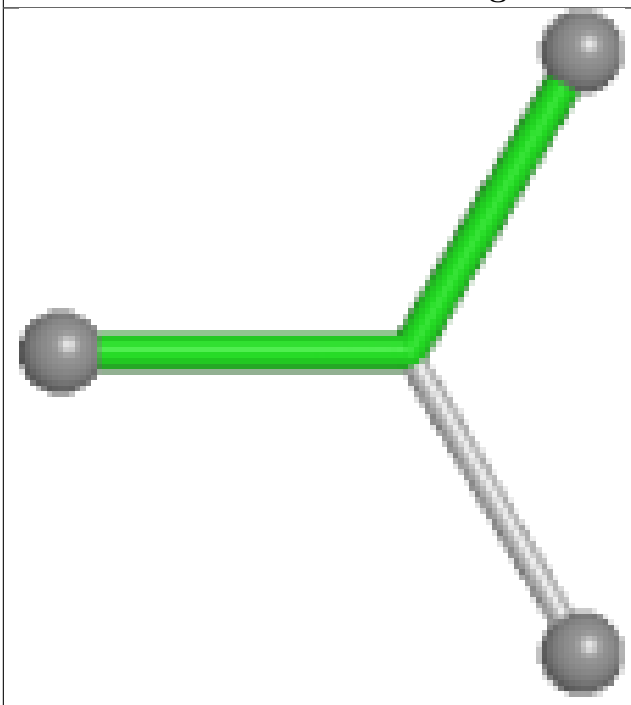


Torsions

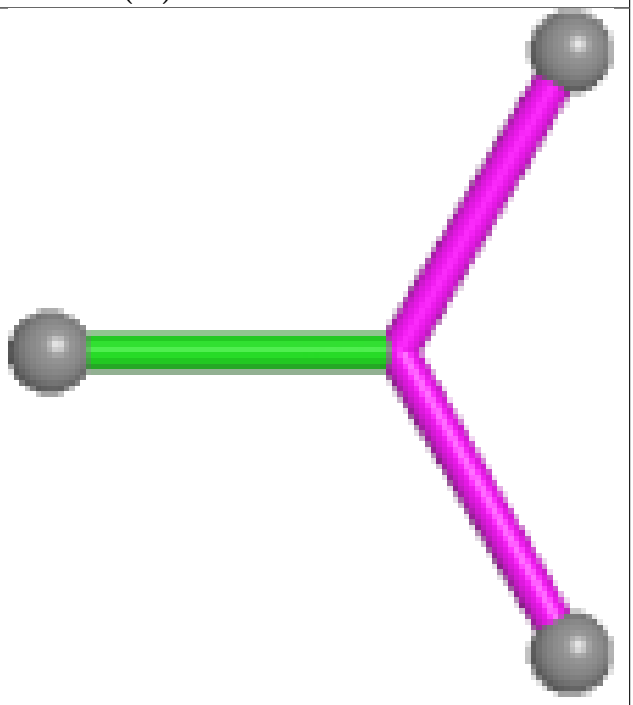


Rings

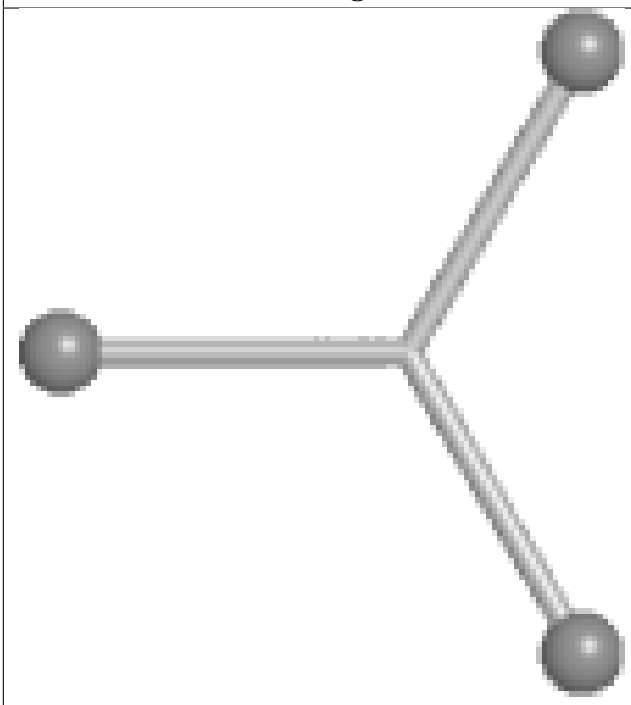
Ligand BCT A 416 (A)



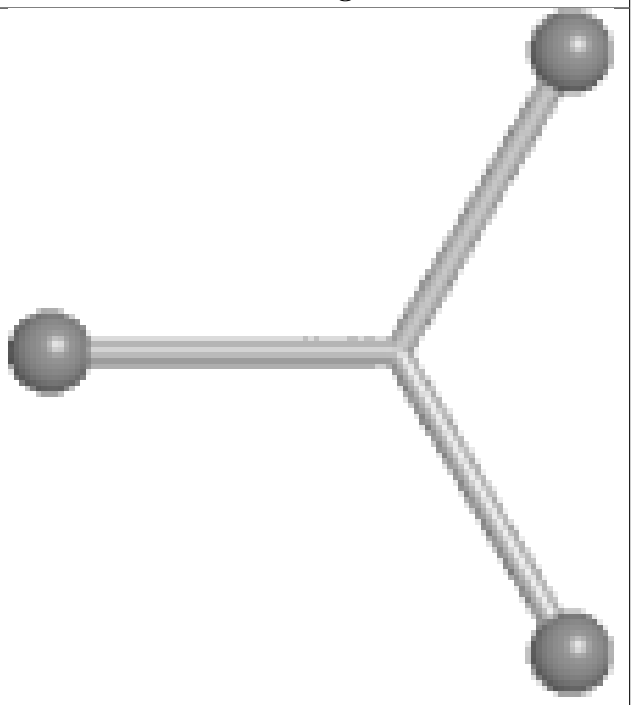
Bond lengths



Bond angles

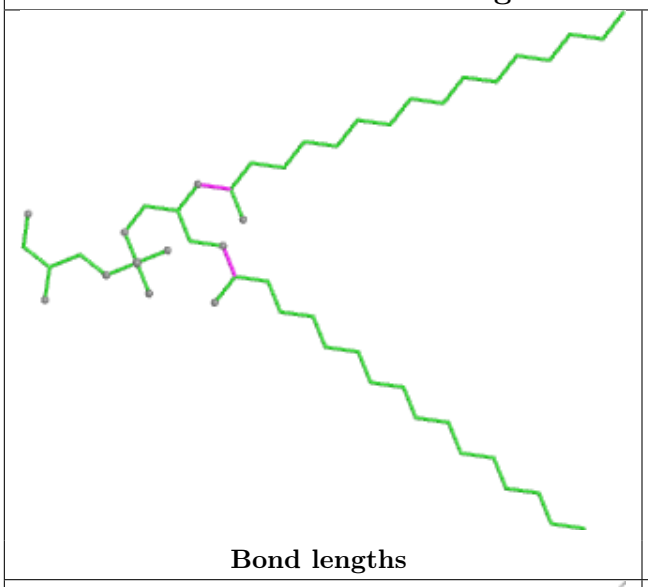


Torsions

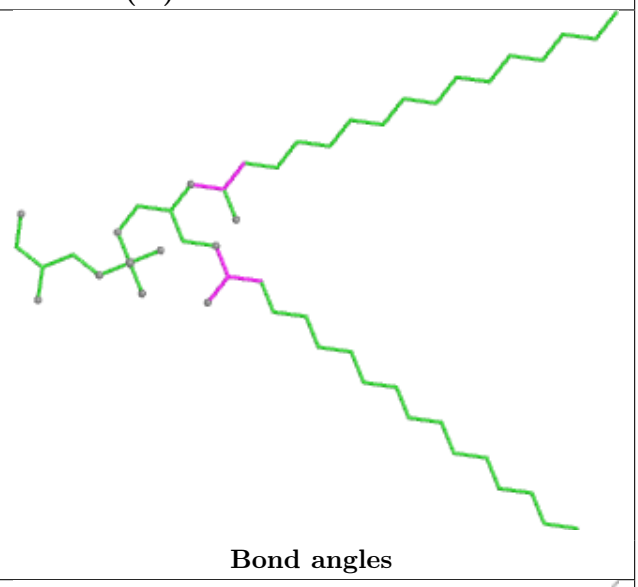


Rings

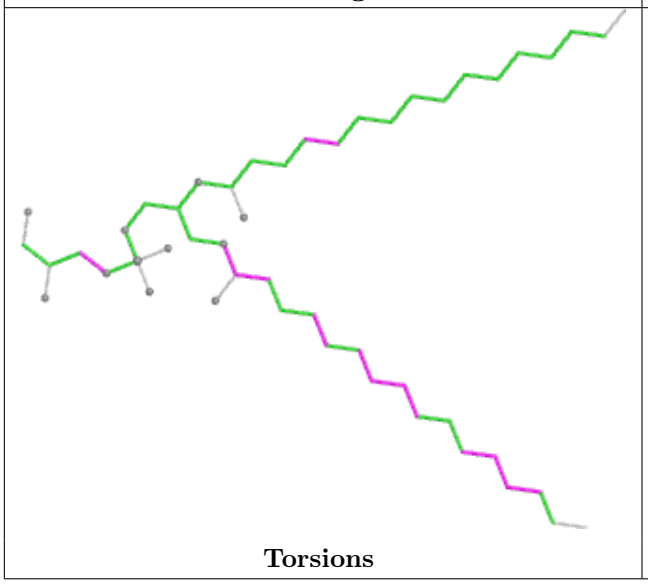
Ligand LHG d 407 (B)



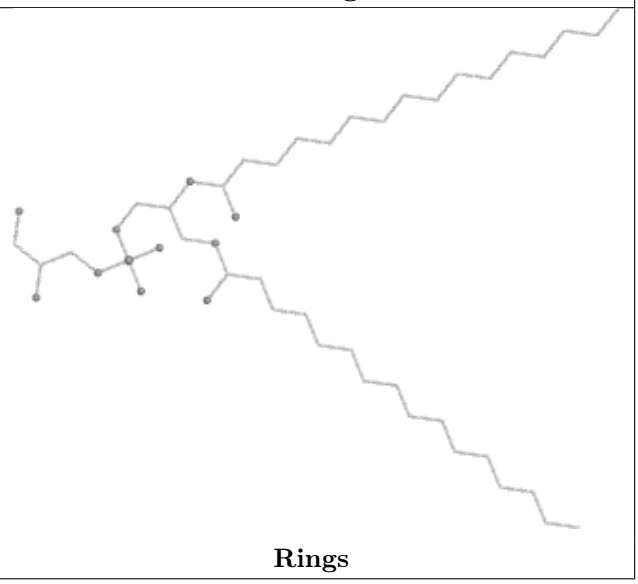
Bond lengths



Bond angles

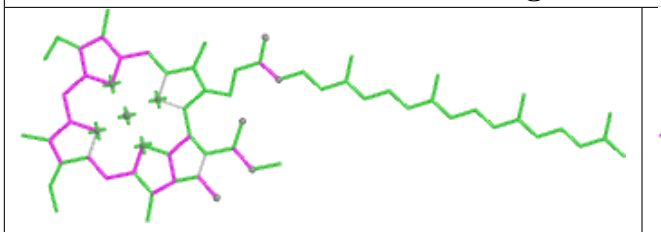


Torsions

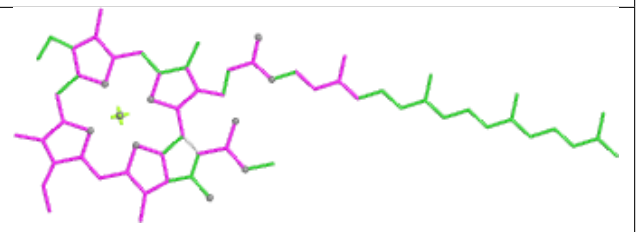


Rings

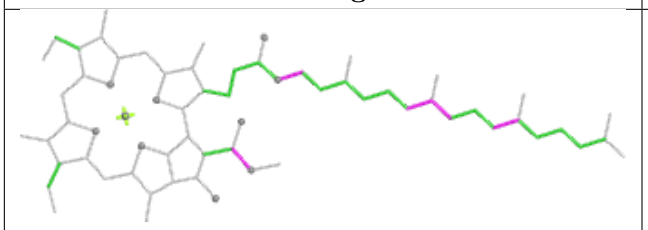
Ligand CLA C 514



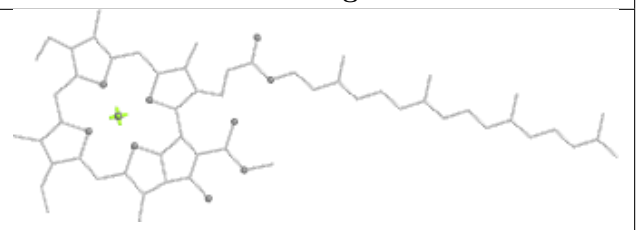
Bond lengths



Bond angles

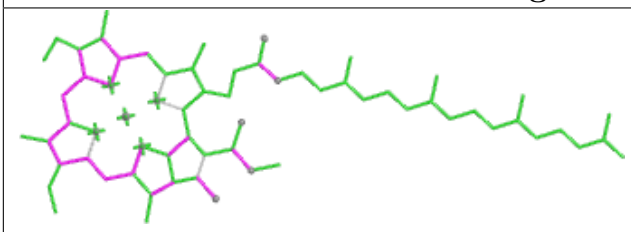


Torsions

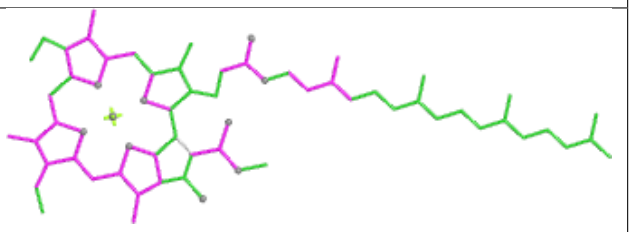


Rings

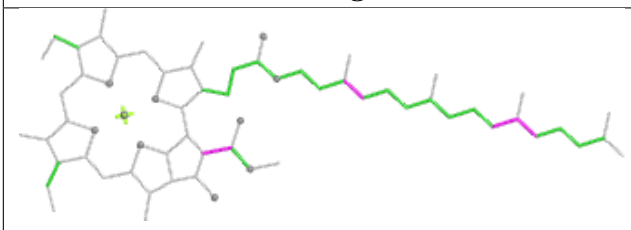
Ligand CLA c 506



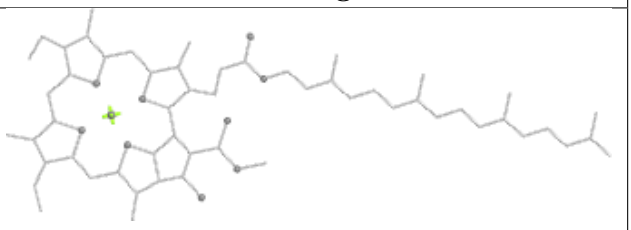
Bond lengths



Bond angles



Torsions



Rings

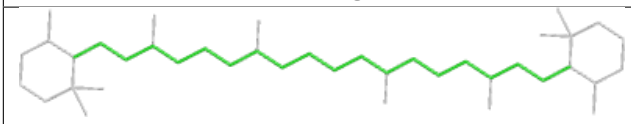
Ligand BCR K 102



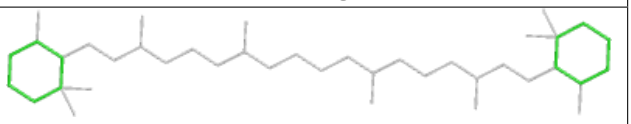
Bond lengths



Bond angles

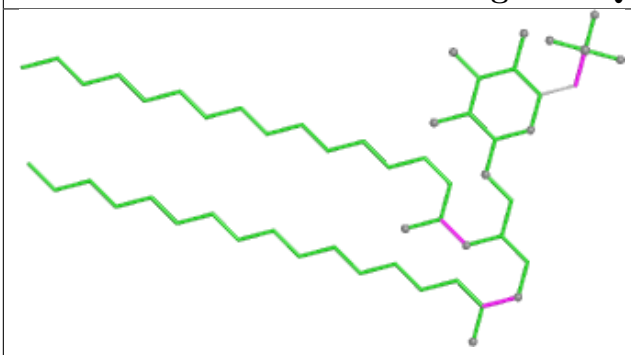


Torsions

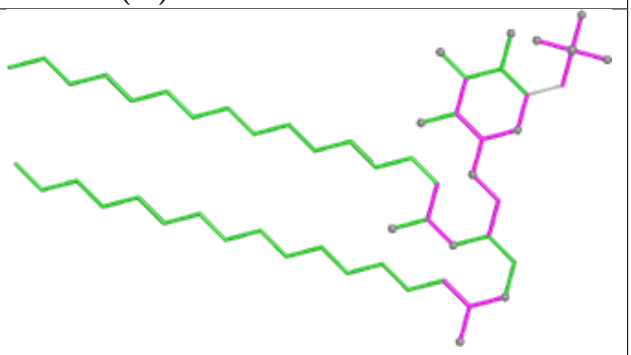


Rings

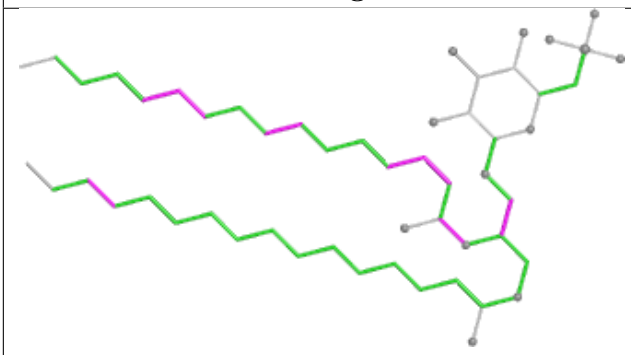
Ligand SQD A 410 (B)



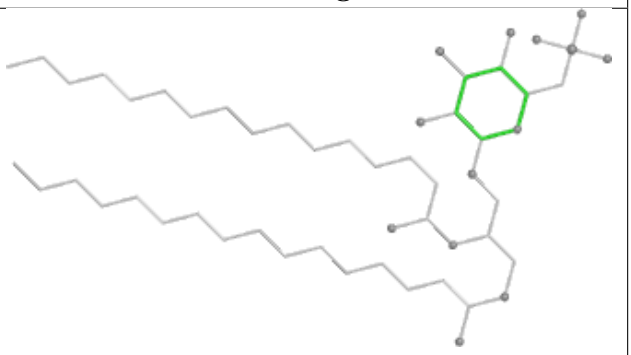
Bond lengths



Bond angles

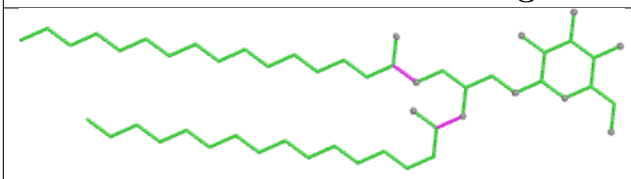


Torsions

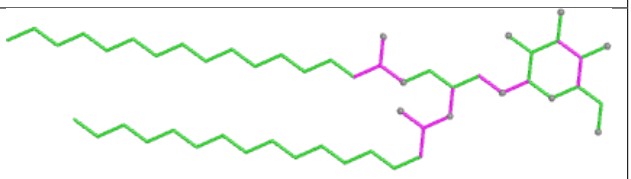


Rings

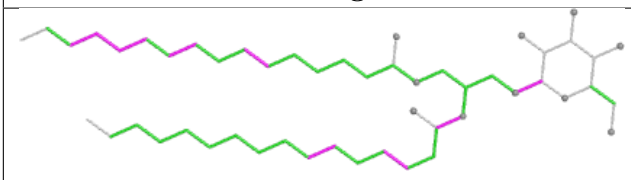
Ligand LMG m 101



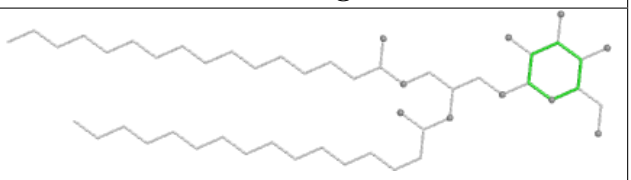
Bond lengths



Bond angles

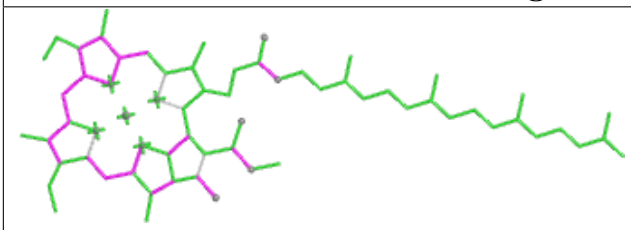


Torsions

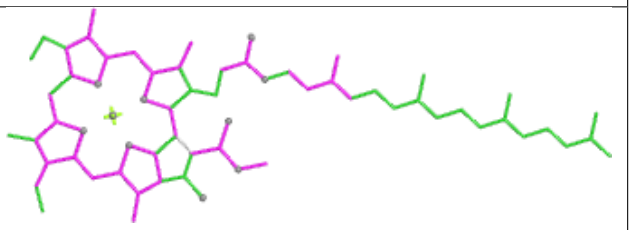


Rings

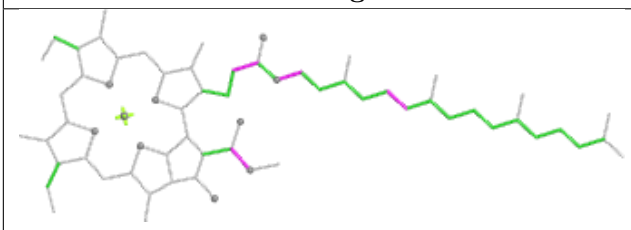
Ligand CLA b 613



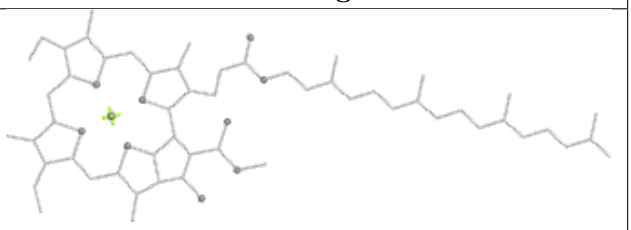
Bond lengths



Bond angles

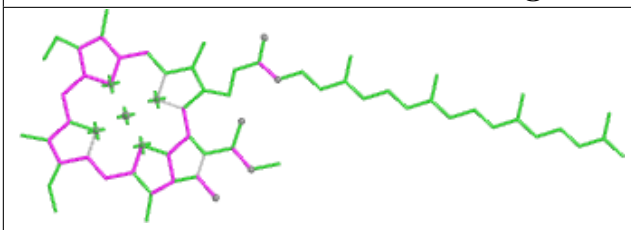


Torsions

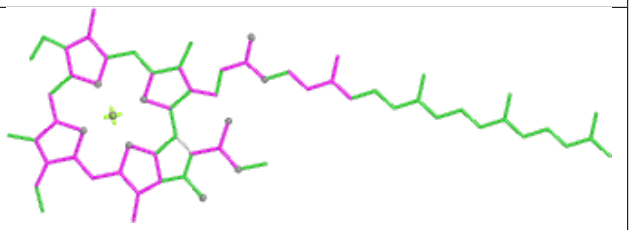


Rings

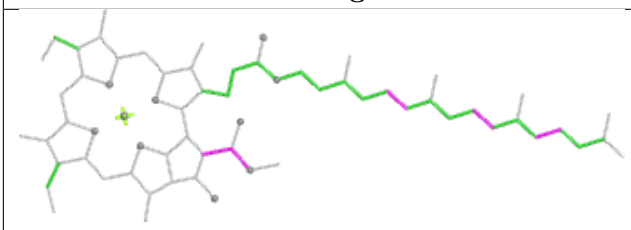
Ligand CLA C 509



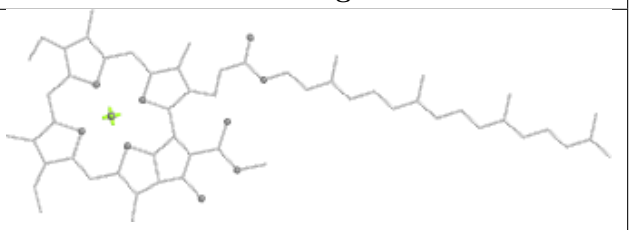
Bond lengths



Bond angles

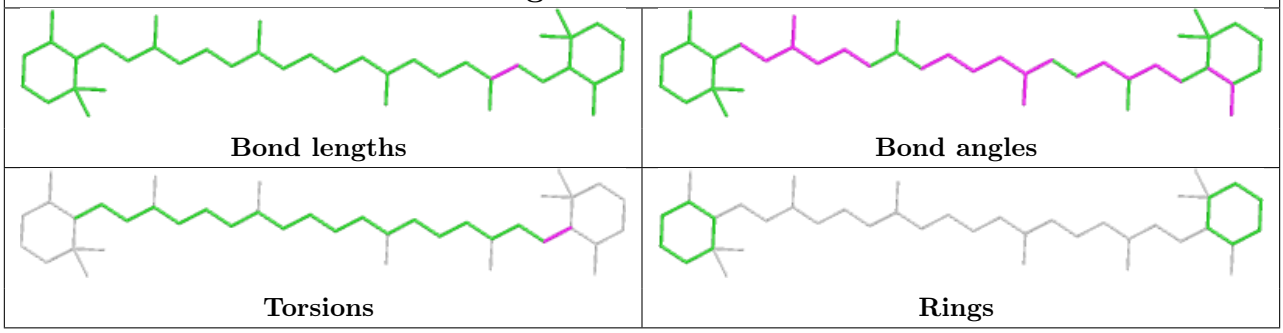


Torsions

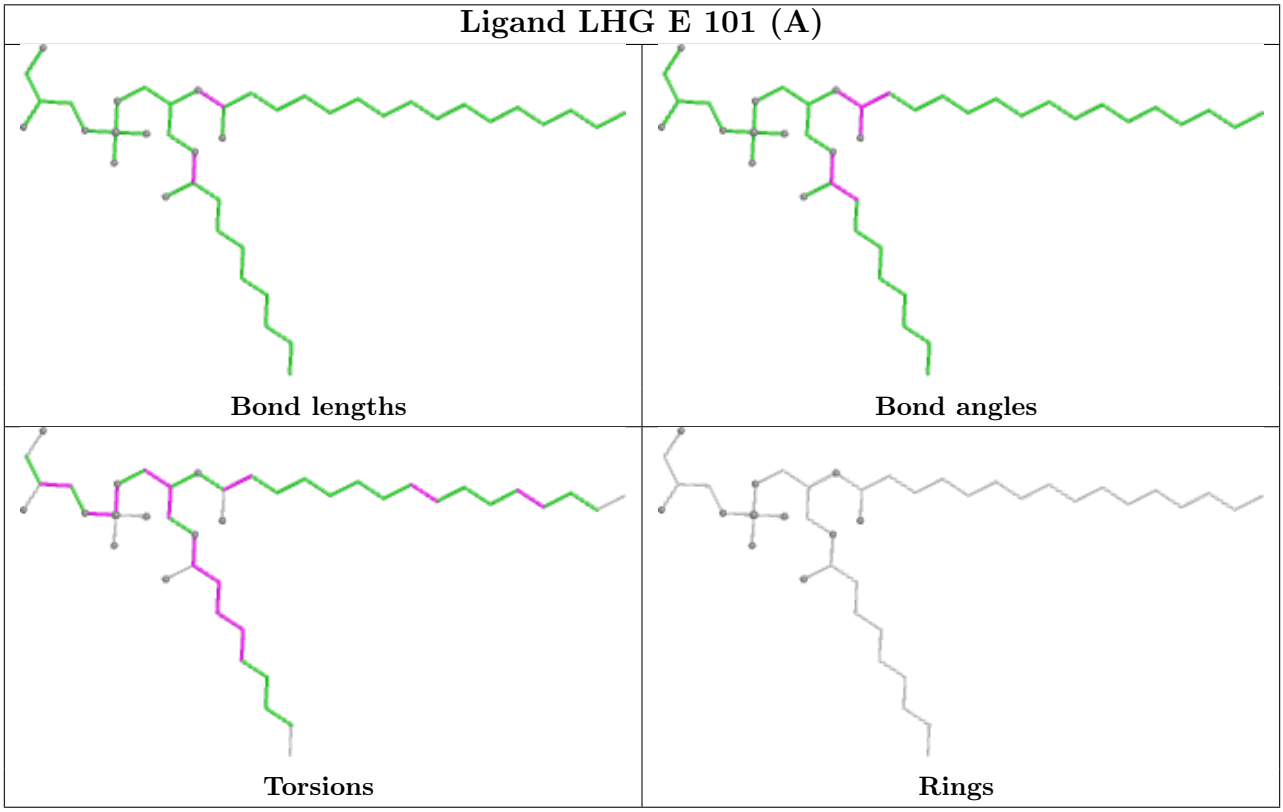


Rings

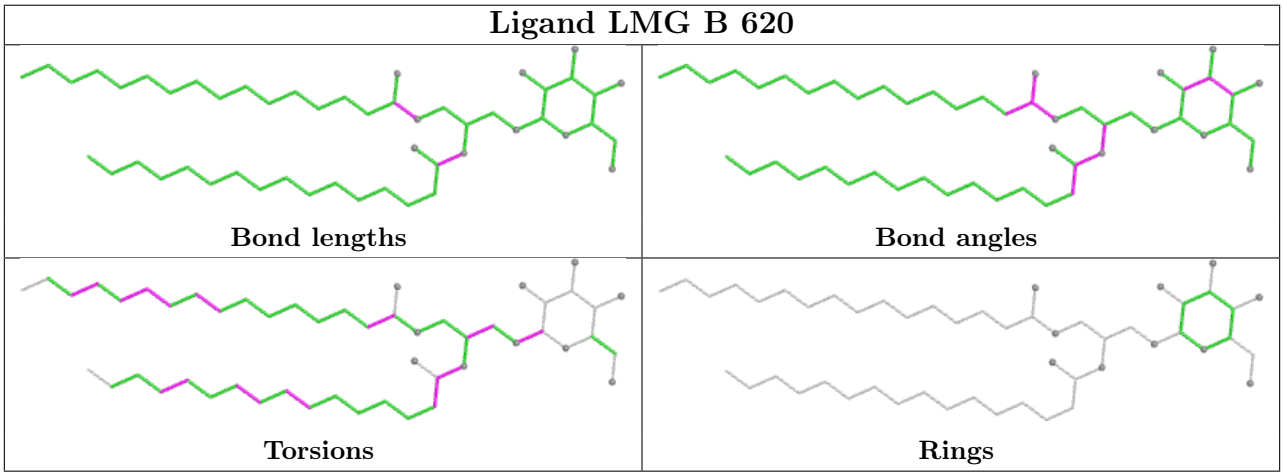
Ligand BCR h 101



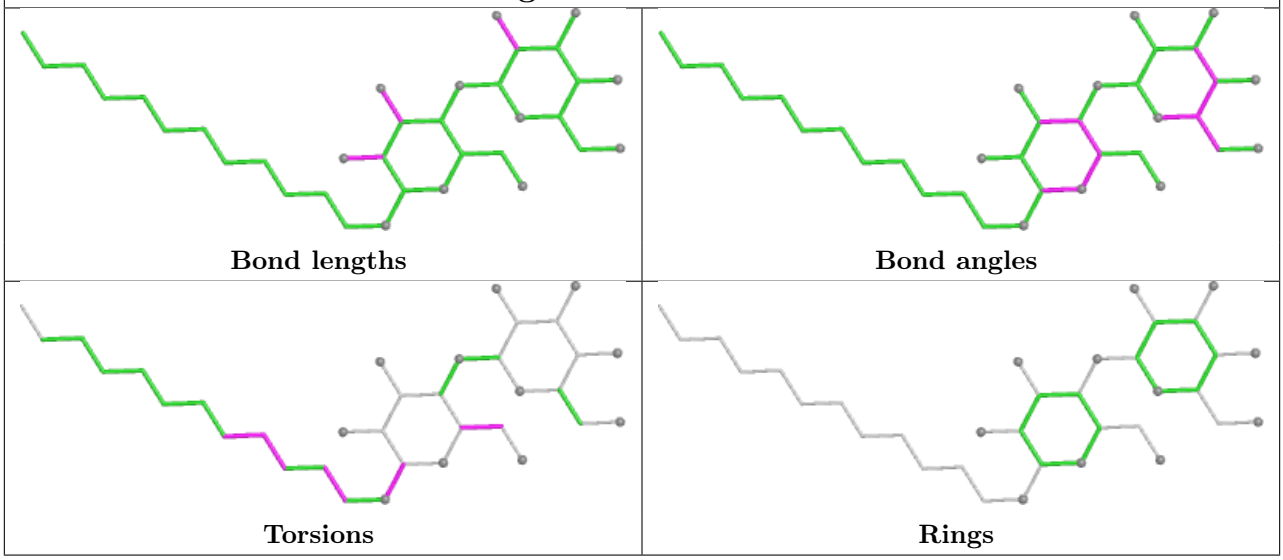
Ligand LHG E 101 (A)



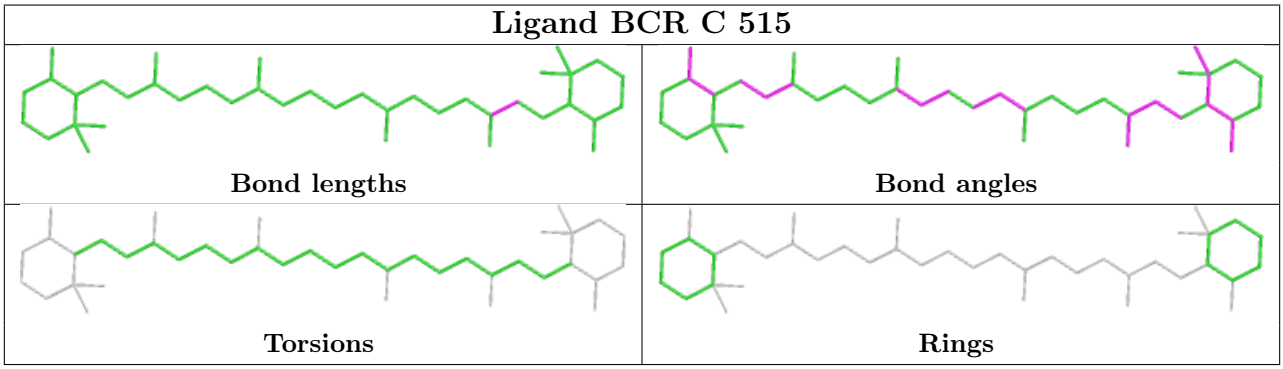
Ligand LMG B 620



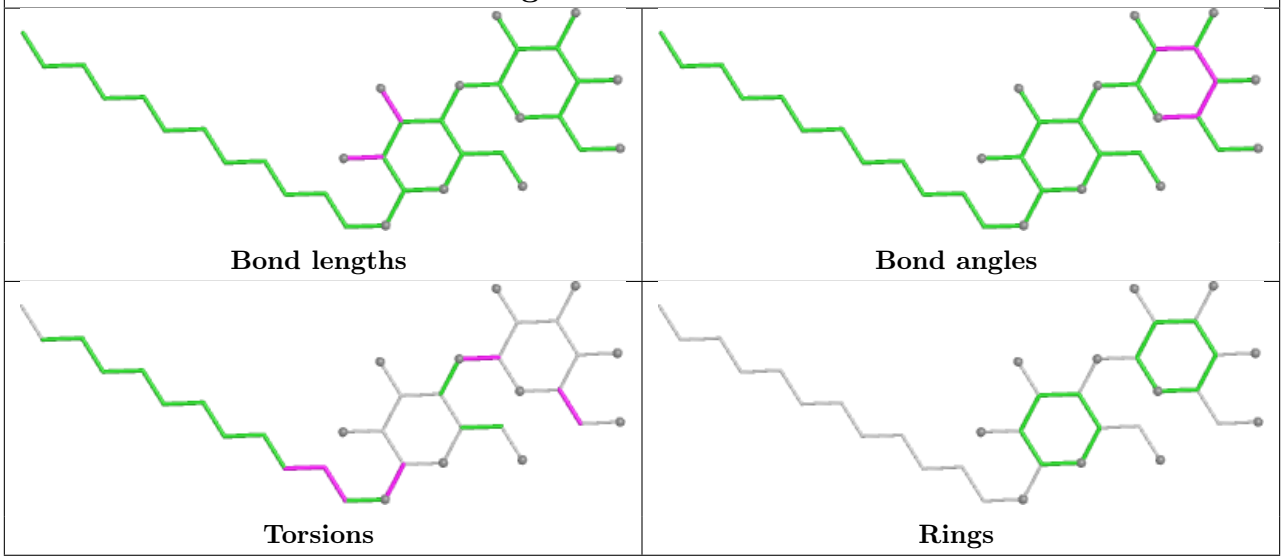
Ligand LMT M 101



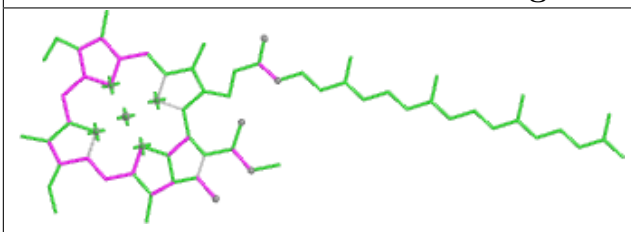
Ligand BCR C 515



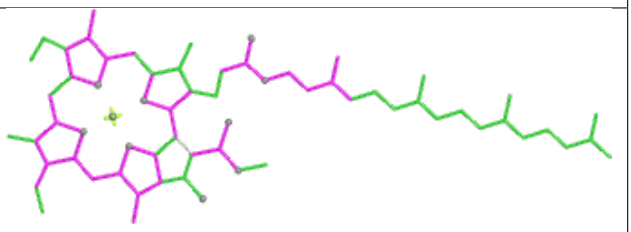
Ligand LMT D 401



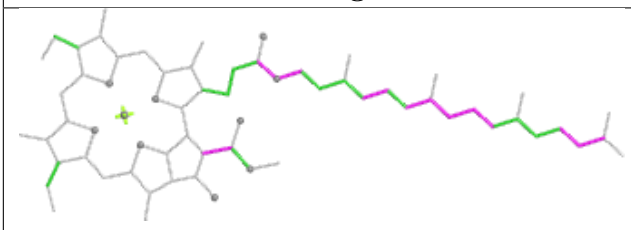
Ligand CLA c 510



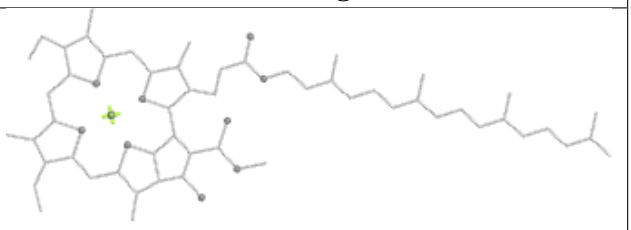
Bond lengths



Bond angles

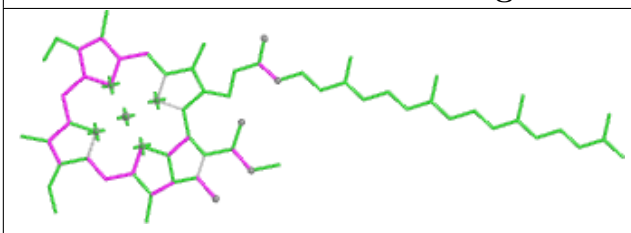


Torsions

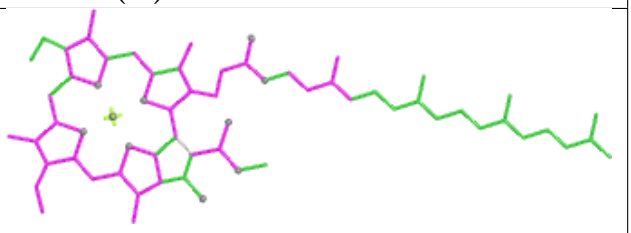


Rings

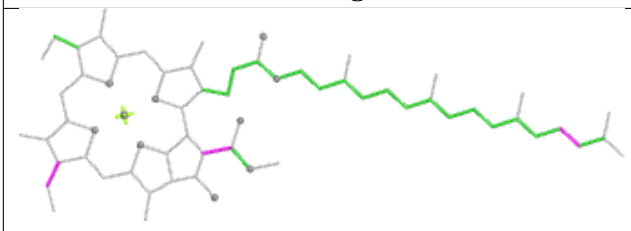
Ligand CLA a 405 (B)



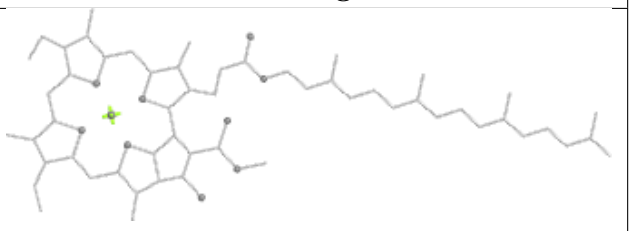
Bond lengths



Bond angles

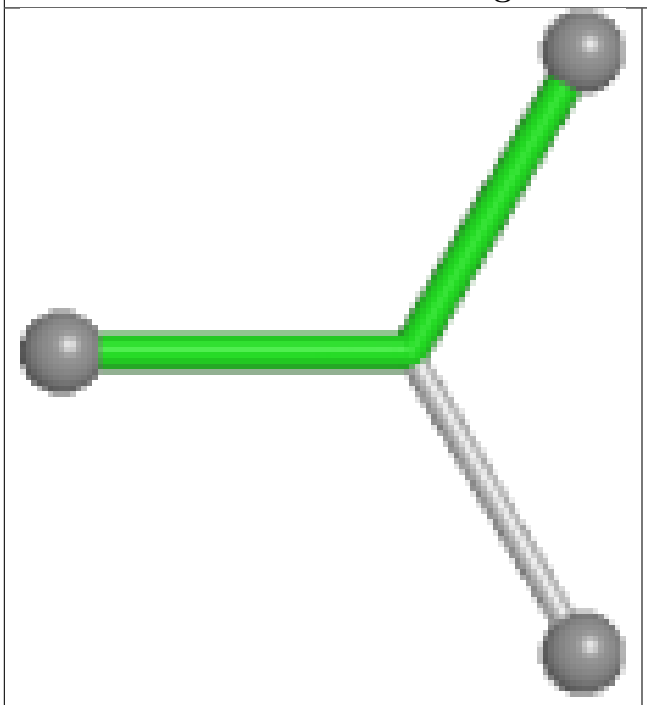


Torsions

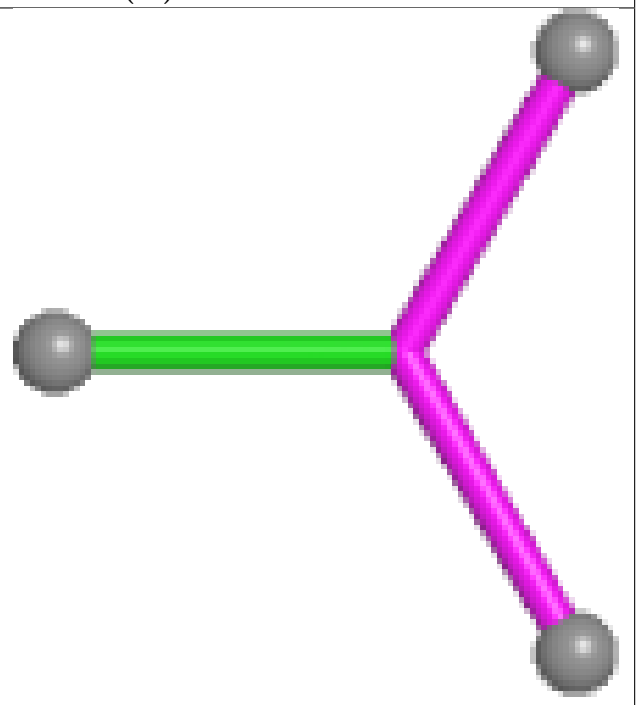


Rings

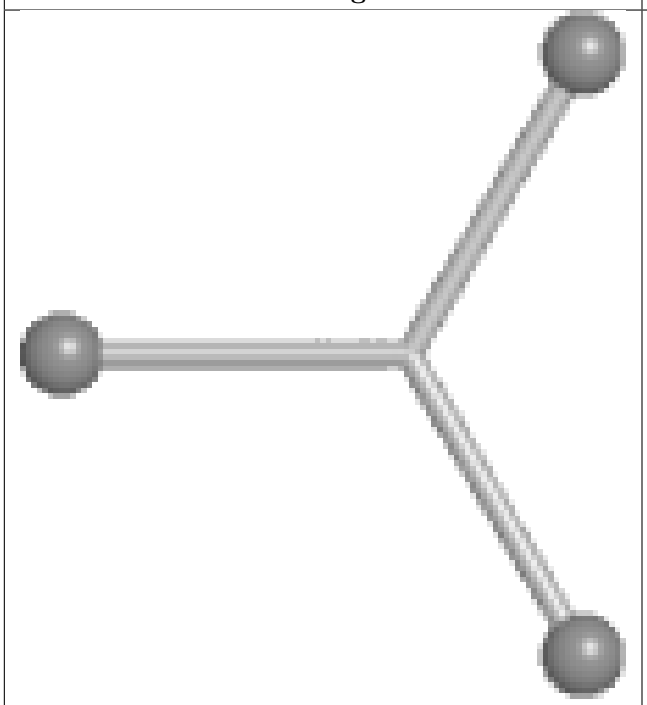
Ligand BCT d 401 (A)



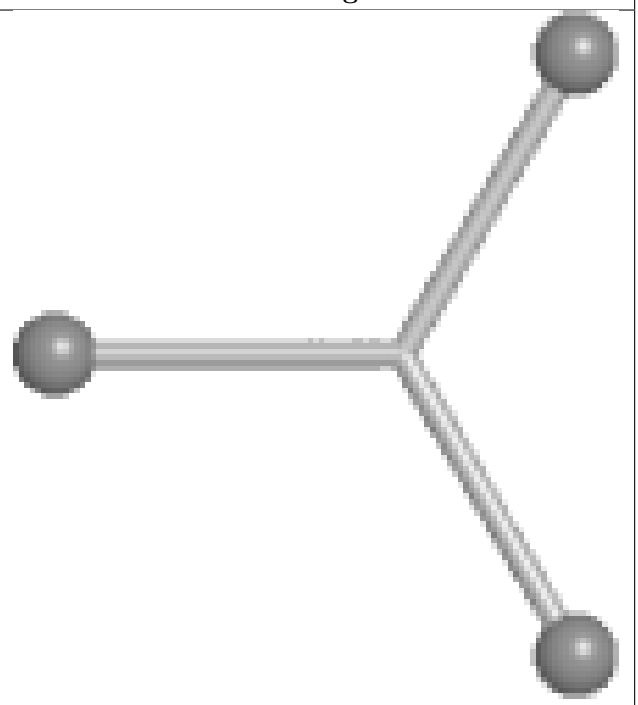
Bond lengths



Bond angles

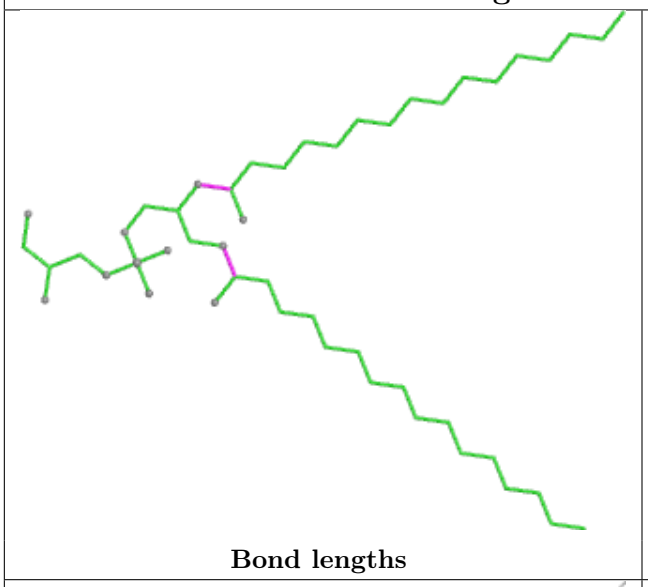


Torsions

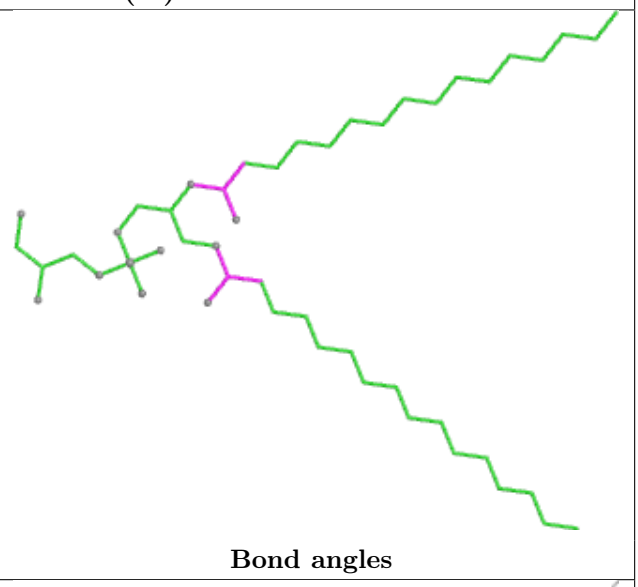


Rings

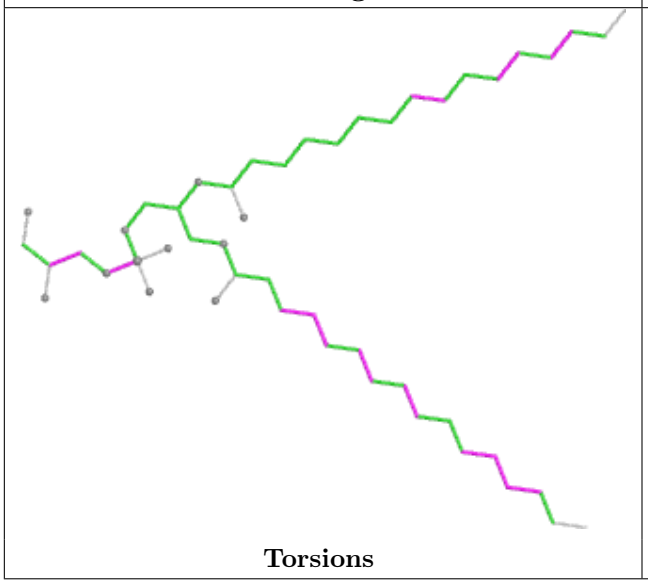
Ligand LHG d 412 (A)



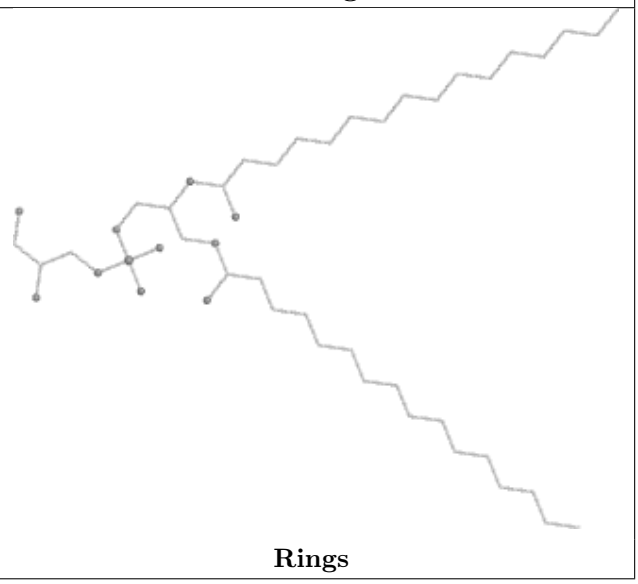
Bond lengths



Bond angles

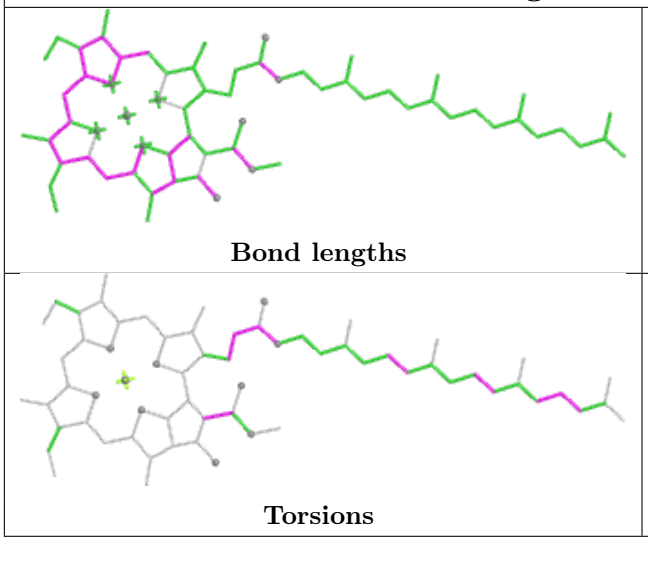


Torsions

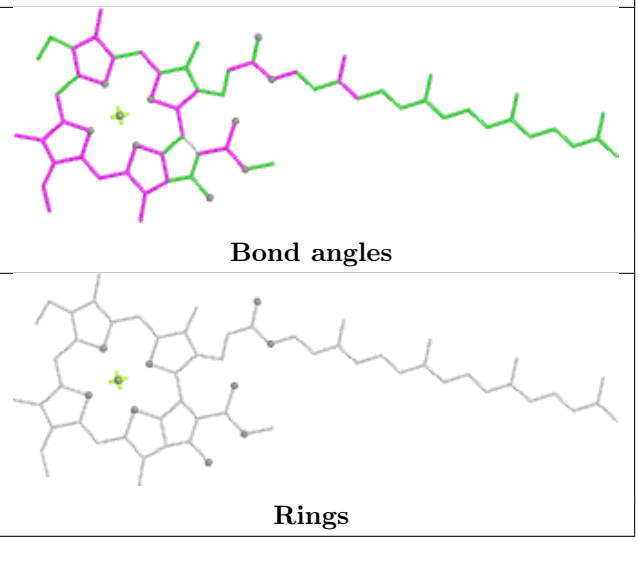


Rings

Ligand CLA B 601



Bond lengths

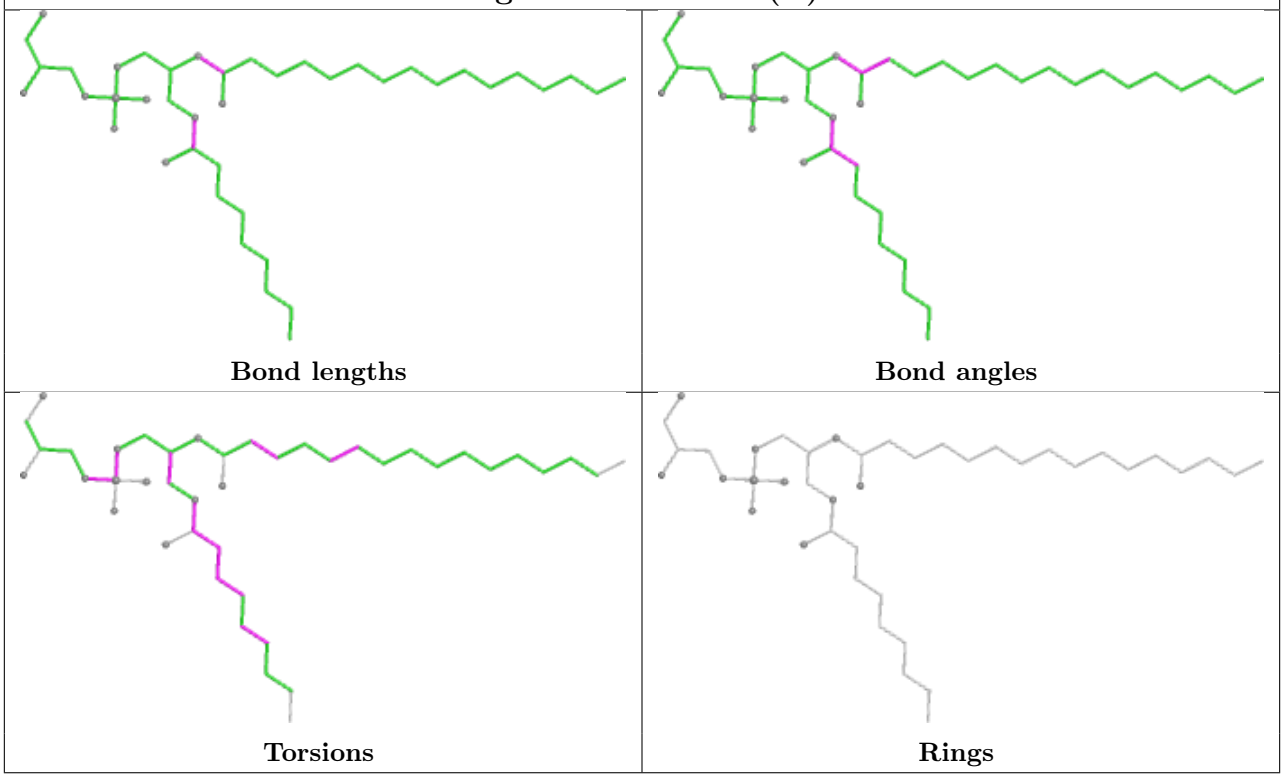


Bond angles

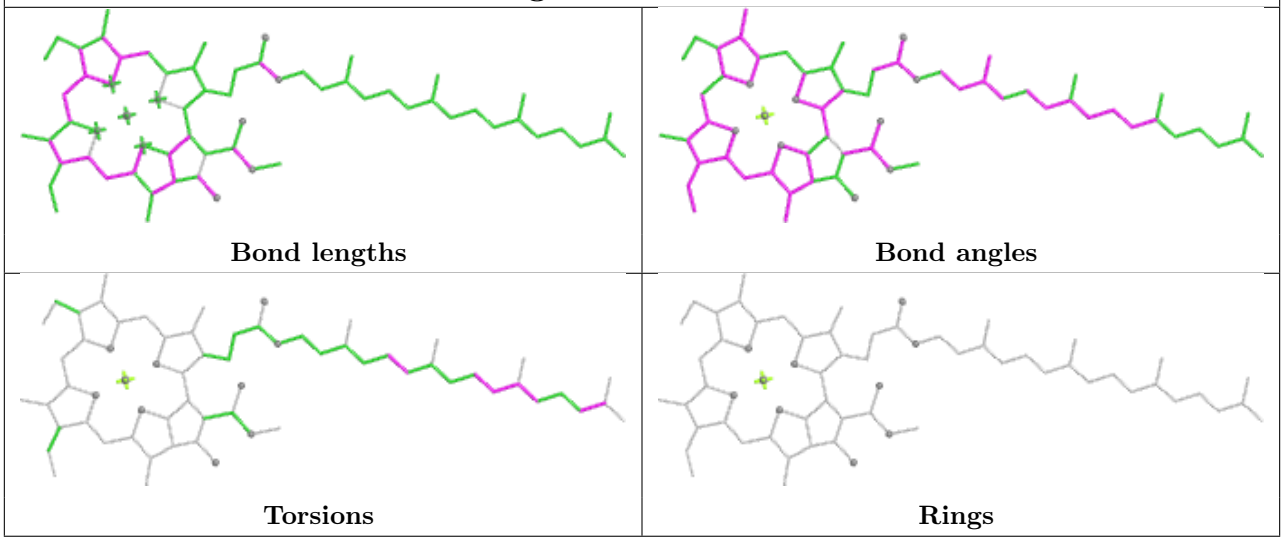
Torsions

Rings

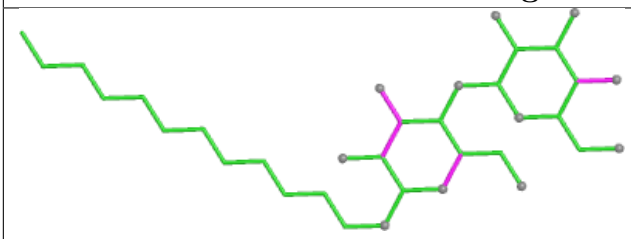
Ligand LHG a 419 (B)



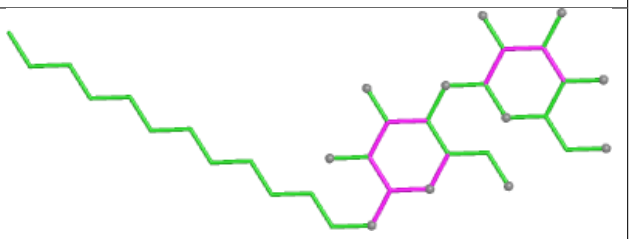
Ligand CLA b 615



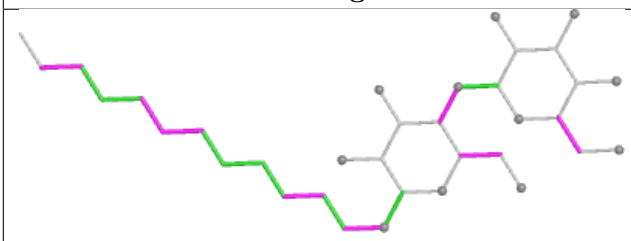
Ligand LMT B 626



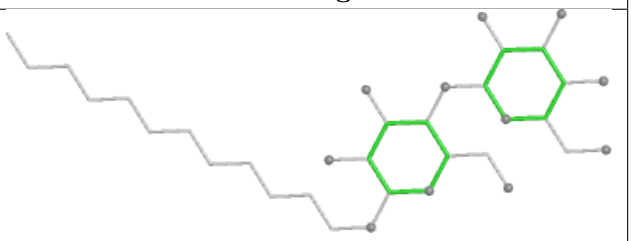
Bond lengths



Bond angles

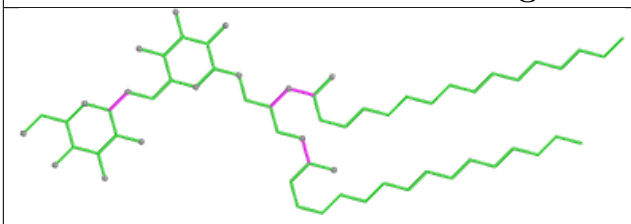


Torsions

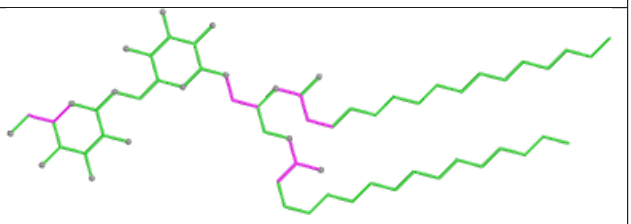


Rings

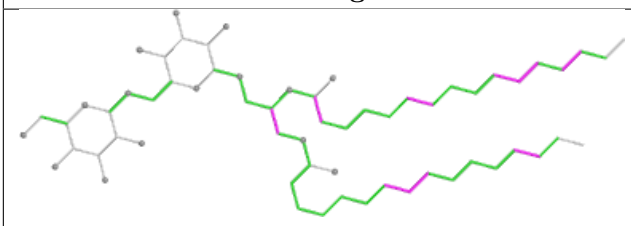
Ligand DGD H 102



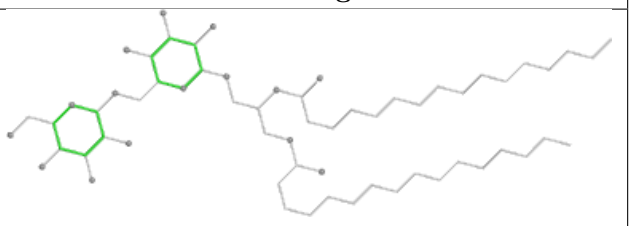
Bond lengths



Bond angles

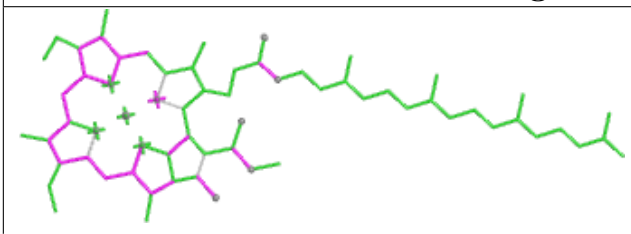


Torsions

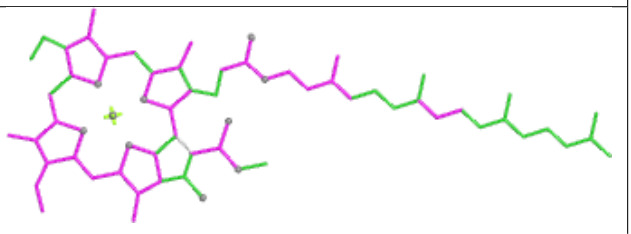


Rings

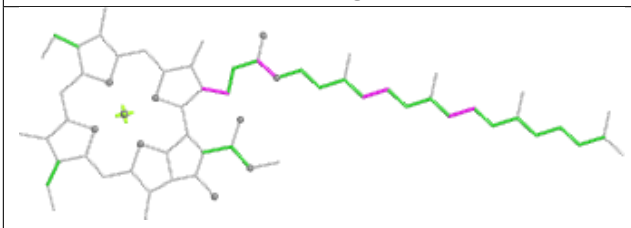
Ligand CLA c 512



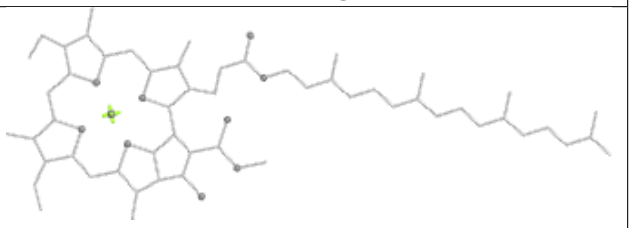
Bond lengths



Bond angles

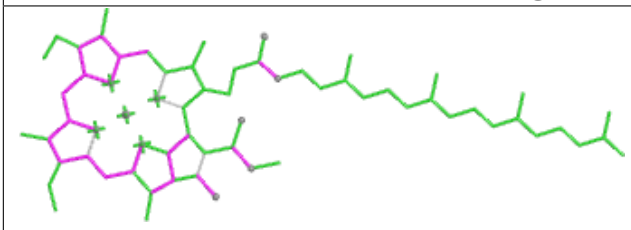


Torsions

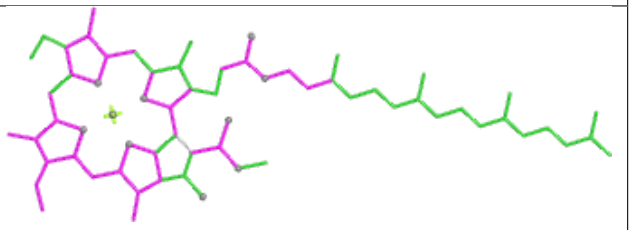


Rings

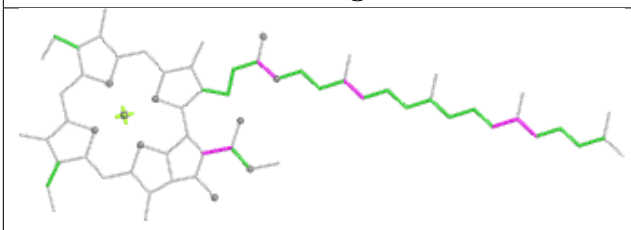
Ligand CLA c 505



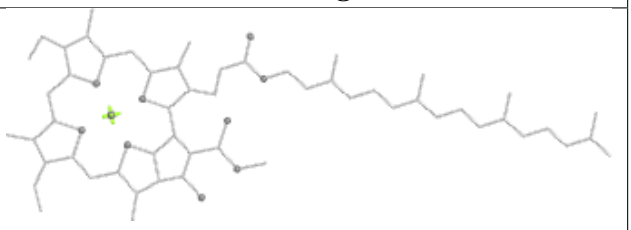
Bond lengths



Bond angles

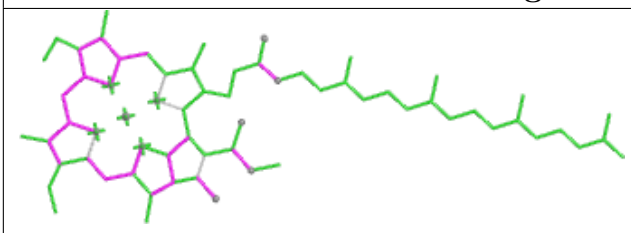


Torsions

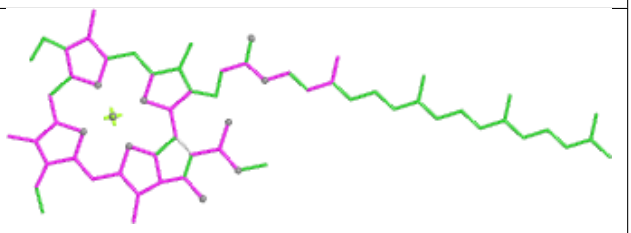


Rings

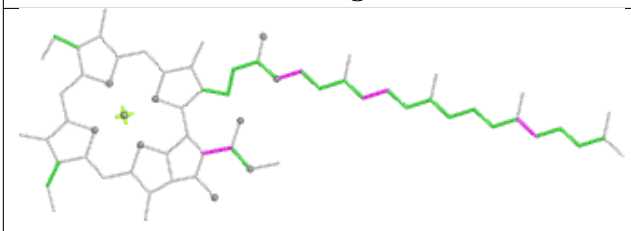
Ligand CLA B 616



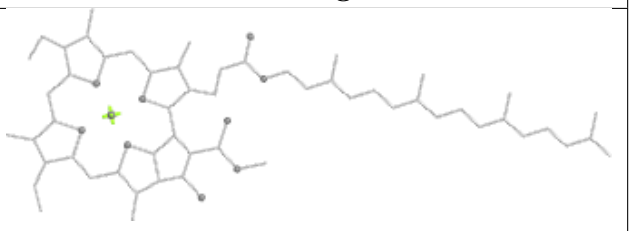
Bond lengths



Bond angles

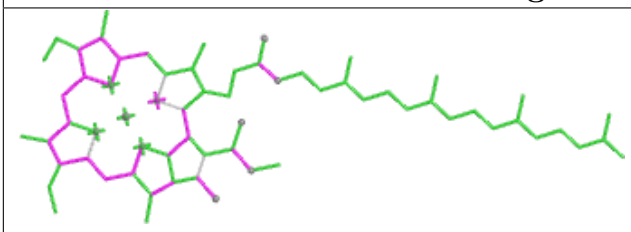


Torsions

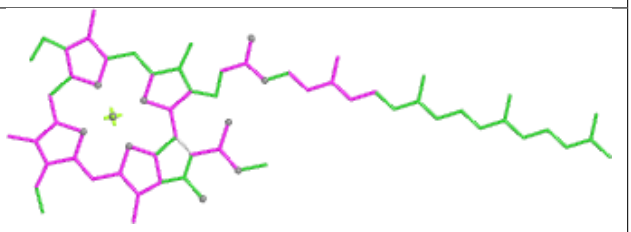


Rings

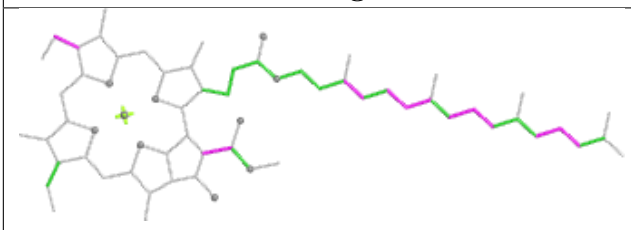
Ligand CLA b 604



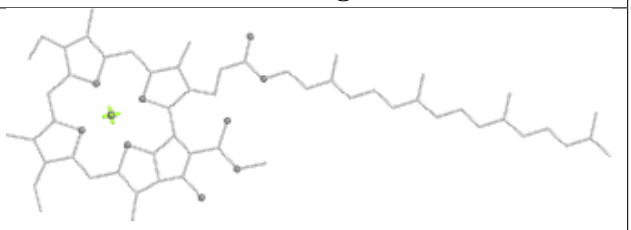
Bond lengths



Bond angles

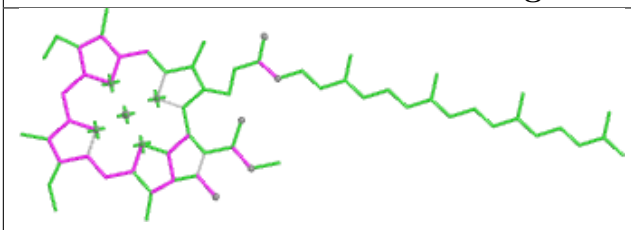


Torsions

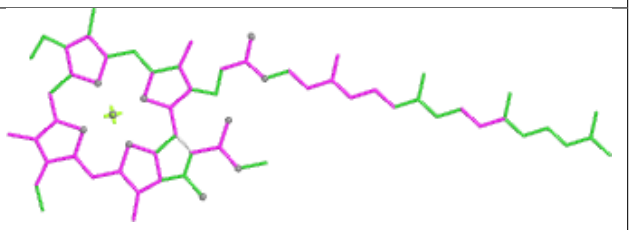


Rings

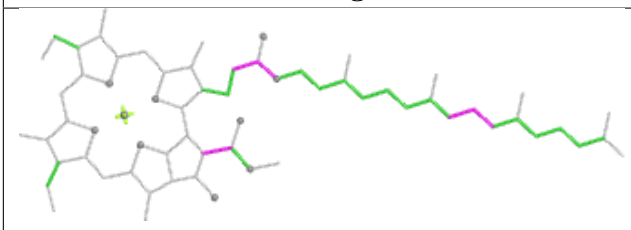
Ligand CLA B 612



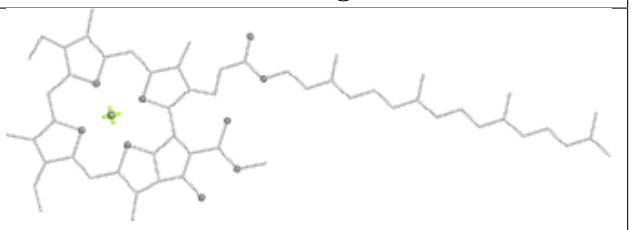
Bond lengths



Bond angles

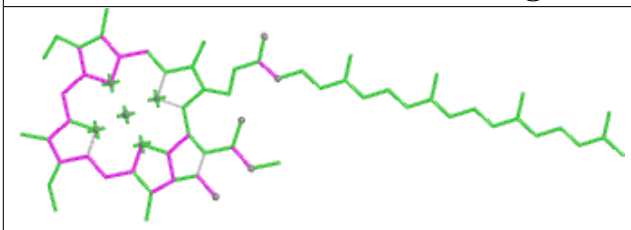


Torsions

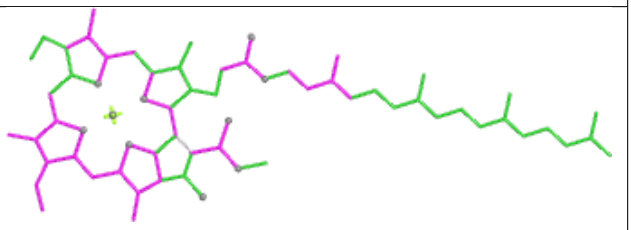


Rings

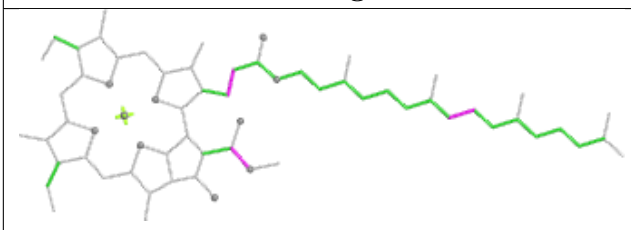
Ligand CLA C 504



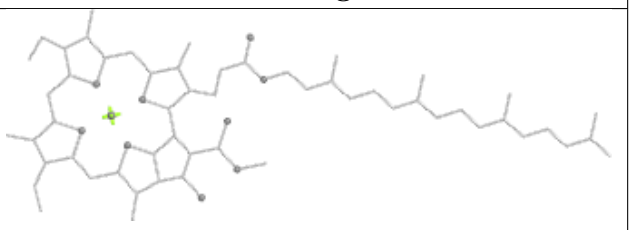
Bond lengths



Bond angles

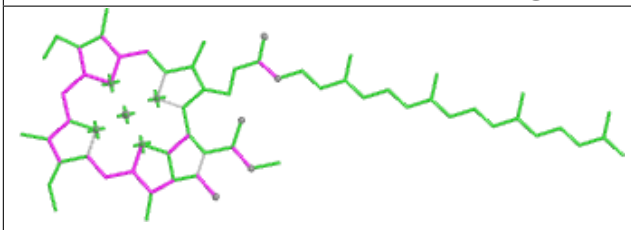


Torsions

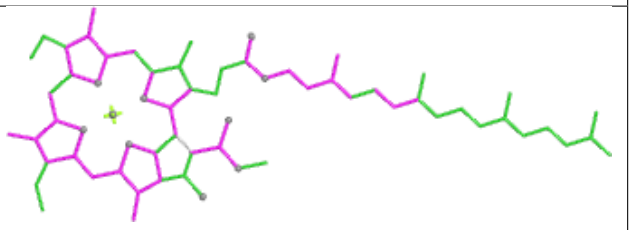


Rings

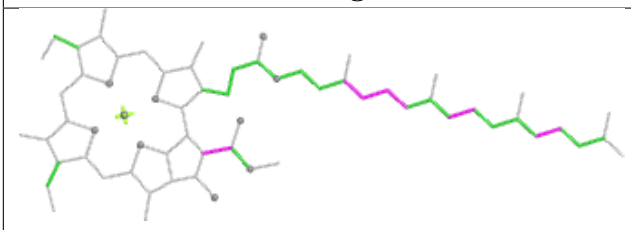
Ligand CLA b 605



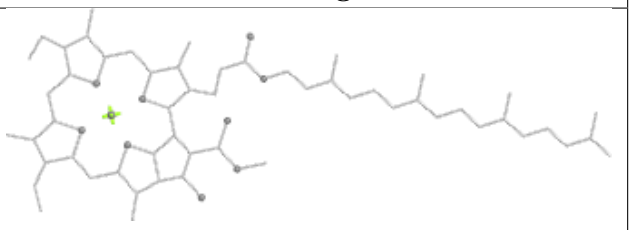
Bond lengths



Bond angles

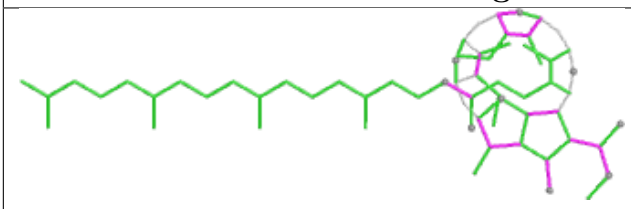


Torsions

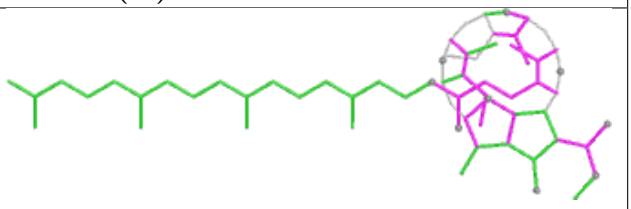


Rings

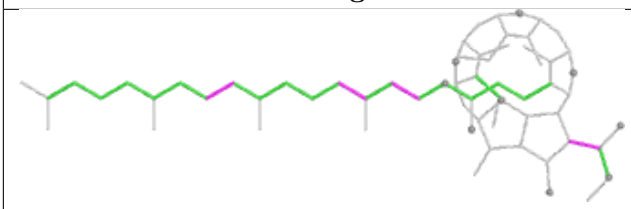
Ligand PHO a 407 (A)



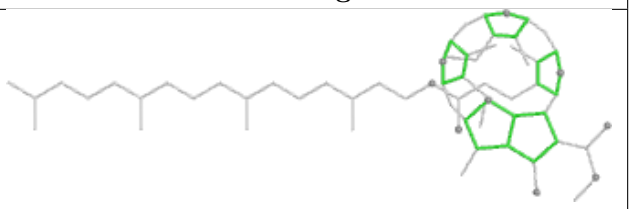
Bond lengths



Bond angles

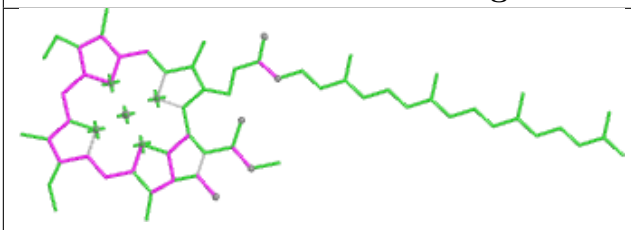


Torsions

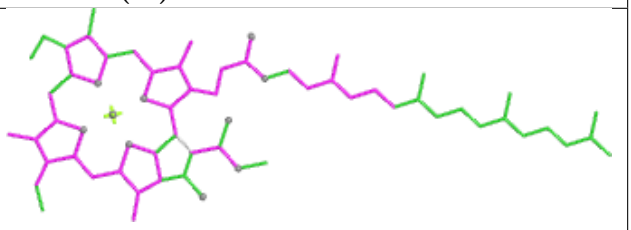


Rings

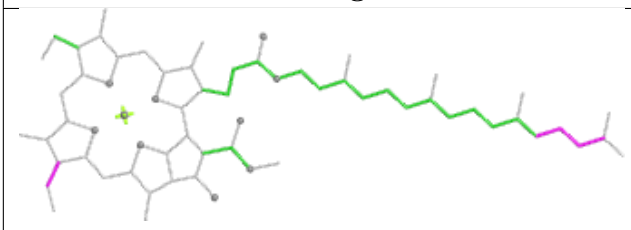
Ligand CLA A 404 (A)



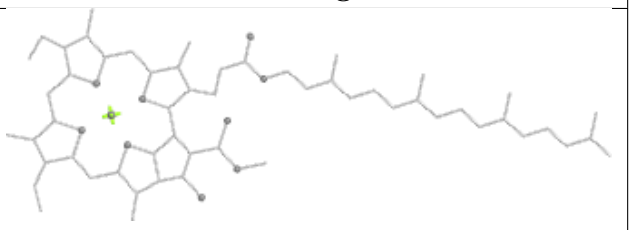
Bond lengths



Bond angles

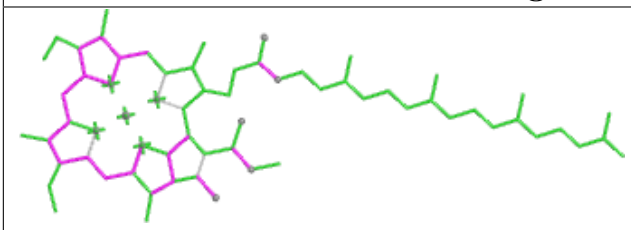


Torsions

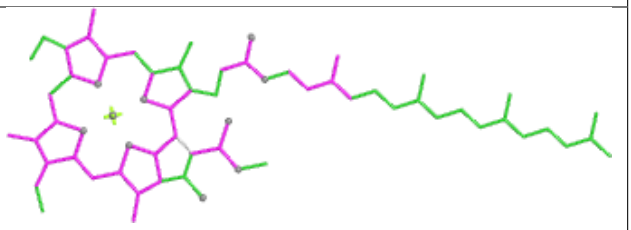


Rings

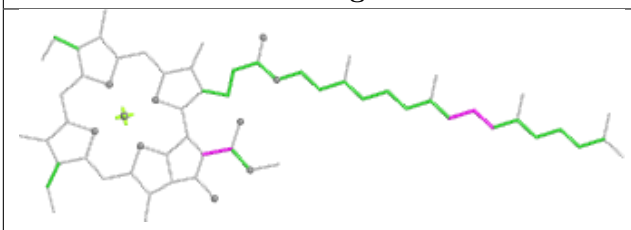
Ligand CLA b 612



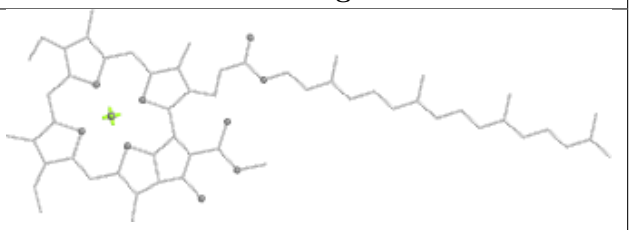
Bond lengths



Bond angles

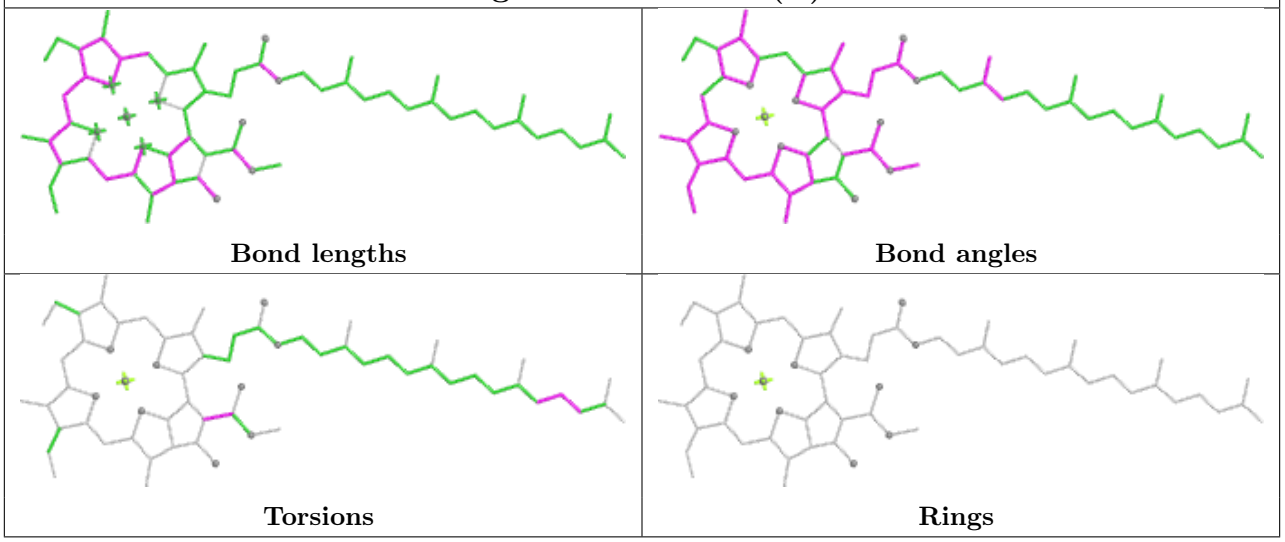


Torsions

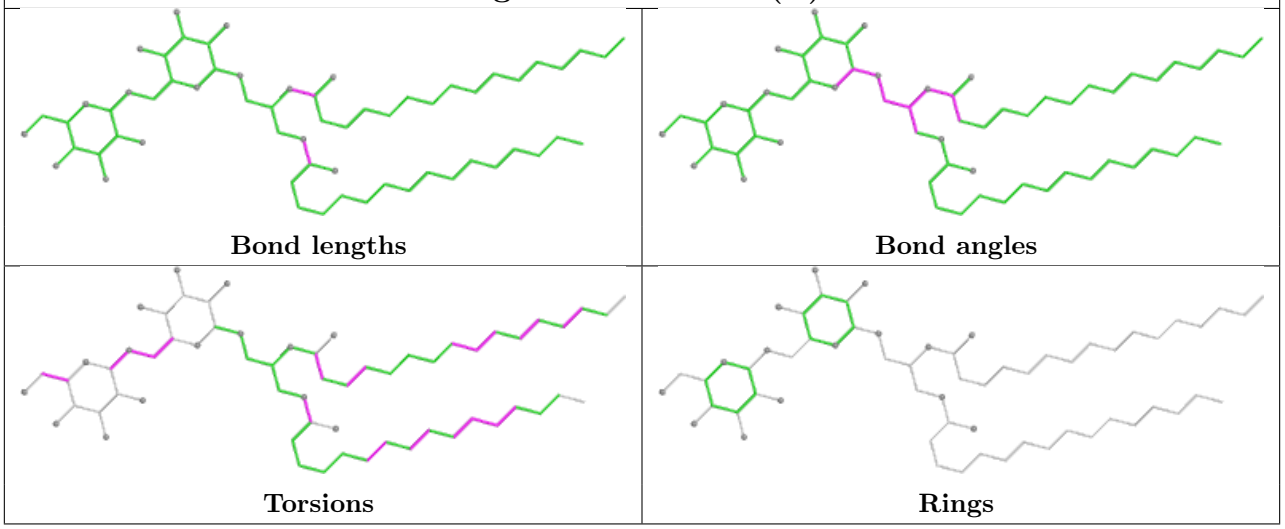


Rings

Ligand CLA A 405 (B)



Ligand DGD c 517 (B)



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%)	-0.57	1 (0%) 90 88	20, 26, 60, 128	222 (66%)
1	a	334/344 (97%)	-0.53	1 (0%) 90 88	22, 29, 66, 141	220 (65%)
2	B	504/505 (99%)	-0.47	1 (0%) 91 90	23, 54, 81, 119	22 (4%)
2	b	504/505 (99%)	-0.40	0 100 100	24, 57, 96, 162	19 (3%)
3	C	451/455 (99%)	-0.52	0 100 100	23, 59, 81, 162	99 (21%)
3	c	455/455 (100%)	-0.43	2 (0%) 88 87	25, 66, 86, 126	101 (22%)
4	D	342/342 (100%)	-0.58	0 100 100	21, 47, 65, 137	115 (33%)
4	d	341/342 (99%)	-0.57	0 100 100	22, 51, 73, 132	119 (34%)
5	E	81/84 (96%)	-0.30	1 (1%) 76 74	52, 69, 101, 170	0
5	e	79/84 (94%)	-0.27	1 (1%) 75 73	32, 77, 117, 152	2 (2%)
6	F	34/44 (77%)	-0.60	0 100 100	55, 61, 86, 108	0
6	f	31/44 (70%)	-0.40	1 (3%) 50 47	53, 66, 94, 148	1 (3%)
7	H	64/65 (98%)	-0.27	1 (1%) 70 67	52, 63, 84, 109	0
7	h	64/65 (98%)	-0.35	1 (1%) 70 67	39, 69, 93, 108	1 (1%)
8	I	37/38 (97%)	-0.18	0 100 100	57, 63, 124, 165	0
8	i	37/38 (97%)	-0.21	0 100 100	55, 64, 121, 139	0
9	J	38/39 (97%)	-0.31	0 100 100	51, 70, 118, 182	0
9	j	39/39 (100%)	-0.27	0 100 100	60, 76, 127, 174	0
10	K	37/37 (100%)	-0.59	0 100 100	59, 68, 86, 108	0
10	k	37/37 (100%)	-0.49	0 100 100	67, 74, 95, 113	0
11	L	36/37 (97%)	-0.55	0 100 100	24, 47, 104, 147	2 (5%)
11	l	36/37 (97%)	-0.54	0 100 100	25, 48, 104, 121	2 (5%)
12	M	32/36 (88%)	-0.50	0 100 100	27, 50, 79, 143	1 (3%)
12	m	33/36 (91%)	-0.44	0 100 100	24, 50, 74, 151	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%)	-0.47	0 100 100	22, 65, 121, 186	10 (4%)
13	o	243/244 (99%)	-0.42	0 100 100	22, 66, 125, 171	8 (3%)
14	T	29/32 (90%)	-0.58	0 100 100	27, 48, 57, 68	6 (20%)
14	t	29/32 (90%)	-0.57	1 (3%) 48 45	28, 49, 67, 75	5 (17%)
15	U	96/104 (92%)	-0.57	0 100 100	26, 60, 93, 101	4 (4%)
15	u	97/104 (93%)	-0.58	0 100 100	28, 62, 84, 139	5 (5%)
16	V	137/137 (100%)	-0.64	0 100 100	24, 58, 83, 107	6 (4%)
16	v	137/137 (100%)	-0.53	0 100 100	28, 71, 102, 136	6 (4%)
17	X	38/40 (95%)	-0.27	0 100 100	35, 71, 93, 113	1 (2%)
17	x	38/40 (95%)	0.01	0 100 100	63, 77, 123, 169	0
18	Y	29/30 (96%)	0.08	1 (3%) 48 45	68, 86, 120, 126	0
18	y	29/30 (96%)	-0.22	0 100 100	73, 90, 111, 118	0
19	Z	62/62 (100%)	-0.29	0 100 100	66, 81, 133, 169	0
19	z	62/62 (100%)	0.13	0 100 100	79, 95, 146, 202	0
20	R	34/34 (100%)	0.47	2 (5%) 28 25	75, 100, 130, 139	0
All	All	5283/5384 (98%)	-0.46	14 (0%) 90 88	20, 58, 99, 202	979 (18%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	e	79[A]	PHE	4.0
7	H	65	LEU	3.6
6	f	16[A]	PHE	2.9
14	t	30[A]	THR	2.7
1	a	11	ALA	2.5
2	B	494	GLY	2.4
20	R	28	VAL	2.4
3	c	20	SER	2.4
20	R	35	LEU	2.3
7	h	65	LEU	2.2
18	Y	18	VAL	2.2
5	E	4	THR	2.2
1	A	11	ALA	2.1
3	c	245[A]	ILE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.93	0.09	46,60,72,76	0
8	FME	I	1	10/11	0.95	0.07	60,70,80,86	0
8	FME	i	1	10/11	0.96	0.07	57,69,76,89	0
14	FME	t	1	10/11	0.96	0.07	43,51,58,76	0
12	FME	m	1	10/11	0.97	0.07	55,64,93,112	0
12	FME	M	1	10/11	0.97	0.06	49,63,97,109	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	a	417	6/6	0.64	0.15	81,102,107,110	0
33	LMT	B	628	35/35	0.67	0.15	64,119,146,159	0
30	UNL	j	101	10/-	0.69	0.19	78,94,106,108	0
30	UNL	A	415	28/-	0.70	0.15	91,115,134,158	0
33	LMT	D	401	35/35	0.70	0.14	67,118,139,144	0
33	LMT	F	101	35/35	0.70	0.15	106,136,178,183	0
30	UNL	J	101	10/-	0.71	0.25	72,83,90,96	0
35	HTG	B	621	19/19	0.71	0.17	65,93,115,117	0
30	UNL	I	101	40/-	0.72	0.16	80,106,158,169	0
30	UNL	m	102	10/-	0.72	0.21	74,79,100,101	0
30	UNL	a	414	30/-	0.72	0.12	95,123,145,159	0
33	LMT	A	420	35/35	0.73	0.13	97,135,158,172	0
26	SQD	f	102	43/54	0.74	0.13	96,131,177,190	0
30	UNL	K	101[B]	34/-	0.75	0.14	89,113,127,128	34
27	GOL	o	303	6/6	0.75	0.18	80,102,112,119	0
33	LMT	a	416	35/35	0.75	0.13	108,138,156,164	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LMT	e	101	35/35	0.75	0.13	113,151,189,195	0
30	UNL	K	101[A]	34/-	0.75	0.14	90,113,127,128	34
30	UNL	l	101	10/-	0.76	0.17	68,79,90,99	0
35	HTG	C	522	19/19	0.76	0.12	110,129,143,150	0
27	GOL	l	102[A]	6/6	0.77	0.20	67,100,107,110	6
27	GOL	l	102[B]	6/6	0.77	0.20	66,101,108,110	6
30	UNL	i	101	40/-	0.78	0.14	78,110,152,169	0
34	LMG	C	521	51/55	0.78	0.11	58,118,157,172	0
37	CA	F	104	1/1	0.78	0.23	131,131,131,131	0
27	GOL	O	303	6/6	0.79	0.15	84,101,109,113	0
30	UNL	b	626	33/-	0.80	0.12	67,100,154,165	0
30	UNL	b	629	36/-	0.80	0.12	71,98,130,143	0
33	LMT	b	621	25/35	0.80	0.13	83,115,157,170	0
35	HTG	D	410	16/19	0.80	0.12	90,106,132,143	0
30	UNL	D	409	40/-	0.80	0.13	67,96,135,148	0
30	UNL	c	525[A]	32/-	0.81	0.15	102,115,127,138	32
30	UNL	c	525[B]	32/-	0.81	0.15	102,115,127,139	32
27	GOL	o	304	6/6	0.82	0.15	82,93,102,108	0
27	GOL	B	625	6/6	0.82	0.13	69,87,98,117	0
27	GOL	b	624	6/6	0.82	0.15	91,98,104,106	0
27	GOL	d	411	6/6	0.82	0.14	53,74,81,90	0
32	LHG	a	419[A]	42/49	0.82	0.11	95,143,157,167	42
35	HTG	b	623	19/19	0.82	0.11	80,130,155,167	0
35	HTG	c	522	19/19	0.82	0.09	111,128,145,148	0
32	LHG	a	419[B]	42/49	0.82	0.11	95,143,157,168	42
27	GOL	O	302	6/6	0.83	0.10	79,86,105,110	0
26	SQD	a	411	54/54	0.83	0.10	69,97,137,153	0
33	LMT	B	626	35/35	0.83	0.11	70,98,140,150	0
30	UNL	B	624	33/-	0.83	0.14	57,106,145,153	0
35	HTG	V	202	11/19	0.84	0.09	82,114,126,133	0
27	GOL	a	418	6/6	0.84	0.14	58,83,85,95	0
27	GOL	A	411	6/6	0.84	0.13	69,78,88,94	0
33	LMT	B	629	25/35	0.84	0.12	65,91,149,165	0
40	HEC	V	201	43/43	0.84	0.10	38,52,72,137	0
29	PL9	A	414[A]	55/55	0.85	0.15	73,100,112,119	55
29	PL9	A	414[B]	55/55	0.85	0.15	73,100,112,120	55
33	LMT	T	101	35/35	0.85	0.11	75,127,183,186	0
27	GOL	A	418	6/6	0.85	0.16	54,76,86,91	0
26	SQD	A	412	54/54	0.85	0.11	70,92,134,155	0
27	GOL	v	202[A]	6/6	0.85	0.12	66,81,84,86	6
35	HTG	d	409	16/19	0.85	0.11	96,124,142,151	0
27	GOL	v	202[B]	6/6	0.85	0.12	66,81,85,86	6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	LMG	Z	101	37/55	0.85	0.13	70,119,155,173	0
35	HTG	b	622	19/19	0.86	0.12	59,87,116,126	0
34	LMG	z	101	39/55	0.86	0.12	75,129,151,168	0
33	LMT	t	101	26/35	0.86	0.12	75,106,147,156	0
29	PL9	a	413[A]	55/55	0.86	0.15	90,109,123,132	55
34	LMG	c	521	51/55	0.86	0.10	75,136,166,190	0
29	PL9	a	413[B]	55/55	0.86	0.15	90,109,123,133	55
32	LHG	E	101[A]	42/49	0.87	0.12	79,104,116,124	42
32	LHG	E	101[B]	42/49	0.87	0.12	79,104,117,125	42
27	GOL	D	412	6/6	0.87	0.13	47,69,75,95	0
33	LMT	b	627	25/35	0.87	0.12	57,100,147,164	0
27	GOL	V	203[A]	6/6	0.87	0.14	60,72,77,80	6
35	HTG	o	301	19/19	0.87	0.12	61,88,118,123	0
33	LMT	m	103	35/35	0.87	0.10	60,91,109,119	0
27	GOL	V	203[B]	6/6	0.87	0.14	60,72,77,80	6
26	SQD	F	103	43/54	0.88	0.11	68,103,125,140	0
33	LMT	M	101	35/35	0.88	0.10	61,101,124,129	0
37	CA	f	103	1/1	0.88	0.11	125,125,125,125	0
27	GOL	c	527	6/6	0.88	0.17	104,117,125,127	0
26	SQD	b	620	54/54	0.89	0.10	66,97,127,132	0
26	SQD	L	101	54/54	0.89	0.10	66,95,137,148	0
23	CLA	b	601	65/65	0.89	0.10	59,90,127,159	0
37	CA	o	302	1/1	0.89	0.07	105,105,105,105	0
30	UNL	D	408	17/-	0.89	0.11	60,77,101,120	0
23	CLA	B	601	65/65	0.90	0.09	56,77,109,160	0
27	GOL	B	627	6/6	0.90	0.12	78,80,94,94	0
23	CLA	c	514	65/65	0.91	0.09	70,90,125,145	0
35	HTG	B	623	19/19	0.91	0.08	70,82,99,105	0
34	LMG	c	501	51/55	0.91	0.09	67,96,114,125	0
30	UNL	d	408	17/-	0.91	0.10	68,83,114,123	0
34	LMG	m	101	51/55	0.91	0.09	61,77,101,115	0
34	LMG	C	501	51/55	0.91	0.09	72,92,119,131	0
34	LMG	C	520	51/55	0.91	0.10	53,86,115,129	0
32	LHG	A	419[B]	49/49	0.92	0.10	52,66,87,90	49
34	LMG	B	620	51/55	0.92	0.09	58,73,95,116	0
34	LMG	c	520	51/55	0.92	0.09	60,94,129,159	0
25	BCR	T	102	40/40	0.92	0.07	46,58,74,84	0
35	HTG	b	625	19/19	0.92	0.08	66,81,97,116	0
32	LHG	A	419[A]	49/49	0.92	0.10	52,66,87,90	49
23	CLA	C	514	65/65	0.93	0.08	58,87,113,121	0
23	CLA	d	403	65/65	0.93	0.09	46,66,124,153	0
26	SQD	a	410[A]	54/54	0.93	0.09	62,83,118,122	54

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LHG	D	407[A]	49/49	0.93	0.10	50,61,110,111	49
32	LHG	D	407[B]	49/49	0.93	0.10	50,61,110,112	49
26	SQD	a	410[B]	54/54	0.93	0.09	62,83,118,123	54
25	BCR	D	404	40/40	0.93	0.09	49,59,106,108	0
25	BCR	K	102	40/40	0.93	0.10	57,65,80,81	0
23	CLA	b	616	65/65	0.93	0.09	50,64,127,139	0
32	LHG	d	412[A]	49/49	0.93	0.09	55,69,84,93	49
32	LHG	d	412[B]	49/49	0.93	0.09	55,69,84,94	49
25	BCR	d	404	40/40	0.93	0.08	53,68,104,112	0
25	BCR	t	102	40/40	0.93	0.07	45,60,80,86	0
34	LMG	D	411	51/55	0.93	0.09	49,70,124,136	0
36	DGD	C	518[A]	62/66	0.93	0.08	51,64,111,116	62
36	DGD	C	518[B]	62/66	0.93	0.08	51,64,111,117	62
36	DGD	c	517[A]	62/66	0.93	0.08	48,65,100,106	62
36	DGD	c	517[B]	62/66	0.93	0.08	47,65,100,106	62
36	DGD	c	518[A]	62/66	0.93	0.08	56,69,117,131	62
36	DGD	c	518[B]	62/66	0.93	0.08	56,69,117,131	62
26	SQD	A	410[A]	54/54	0.93	0.09	56,80,114,116	54
37	CA	c	523	1/1	0.93	0.10	74,74,74,74	0
26	SQD	A	410[B]	54/54	0.93	0.09	56,81,114,117	54
23	CLA	c	513	65/65	0.93	0.09	62,81,130,136	0
34	LMG	d	410	51/55	0.93	0.08	54,71,117,148	0
23	CLA	c	508	65/65	0.94	0.09	50,68,85,90	0
23	CLA	C	505	65/65	0.94	0.08	40,58,106,138	0
23	CLA	C	507	65/65	0.94	0.08	51,70,120,142	0
23	CLA	C	513	65/65	0.94	0.08	56,73,115,137	0
25	BCR	A	409	40/40	0.94	0.07	42,52,68,69	0
25	BCR	B	619	40/40	0.94	0.08	48,60,96,97	0
25	BCR	C	515	40/40	0.94	0.08	53,75,88,91	0
23	CLA	A	408	65/65	0.94	0.09	45,53,130,148	0
25	BCR	H	101	40/40	0.94	0.08	51,67,85,88	0
31	BCT	d	401[A]	4/4	0.94	0.08	58,59,70,78	4
31	BCT	d	401[B]	4/4	0.94	0.08	58,60,70,80	4
27	GOL	B	622	6/6	0.94	0.08	72,82,89,91	0
23	CLA	a	408	65/65	0.94	0.10	43,56,141,159	0
23	CLA	B	606	65/65	0.94	0.08	39,56,110,130	0
36	DGD	C	519	62/66	0.94	0.08	45,63,102,116	0
36	DGD	H	102	62/66	0.94	0.09	47,63,75,84	0
25	BCR	b	618	40/40	0.94	0.07	46,58,82,94	0
25	BCR	c	515	40/40	0.94	0.08	68,84,93,98	0
23	CLA	b	606	65/65	0.94	0.08	44,60,114,128	0
25	BCR	h	101	40/40	0.94	0.09	53,69,93,101	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	c	519	62/66	0.94	0.08	51,68,108,132	0
36	DGD	h	102	62/66	0.94	0.09	53,66,79,85	0
23	CLA	b	614	65/65	0.94	0.07	42,53,103,117	0
23	CLA	B	614	65/65	0.94	0.08	39,50,105,124	0
23	CLA	c	505	65/65	0.94	0.08	52,66,110,134	0
23	CLA	c	507	65/65	0.94	0.09	50,70,121,138	0
27	GOL	b	628	6/6	0.94	0.07	83,90,91,96	0
31	BCT	A	416[A]	4/4	0.95	0.08	55,57,61,66	4
31	BCT	A	416[B]	4/4	0.95	0.08	54,56,62,72	4
23	CLA	C	509	65/65	0.95	0.07	45,57,119,142	0
23	CLA	c	502	65/65	0.95	0.08	55,68,80,95	0
23	CLA	B	603	65/65	0.95	0.08	40,54,72,91	0
25	BCR	Y	101	40/40	0.95	0.08	52,67,83,91	0
29	PL9	D	405[A]	55/55	0.95	0.07	38,50,61,70	55
29	PL9	D	405[B]	55/55	0.95	0.07	38,50,61,70	55
25	BCR	a	409	40/40	0.95	0.07	45,55,69,71	0
25	BCR	b	617	40/40	0.95	0.06	44,55,65,72	0
23	CLA	B	616	65/65	0.95	0.09	48,60,131,143	0
27	GOL	C	523[A]	6/6	0.95	0.09	59,64,68,70	6
32	LHG	b	630[A]	49/49	0.95	0.08	54,61,73,98	49
32	LHG	b	630[B]	49/49	0.95	0.08	53,61,73,98	49
32	LHG	d	406[A]	49/49	0.95	0.08	49,59,74,80	49
32	LHG	d	406[B]	49/49	0.95	0.08	48,59,74,80	49
32	LHG	d	407[A]	49/49	0.95	0.09	53,64,111,128	49
32	LHG	d	407[B]	49/49	0.95	0.09	53,65,111,129	49
27	GOL	C	523[B]	6/6	0.95	0.09	63,64,69,70	6
25	BCR	b	619	40/40	0.95	0.08	46,62,87,92	0
23	CLA	D	403	65/65	0.95	0.08	48,58,126,139	0
36	DGD	C	517[A]	62/66	0.95	0.07	47,58,101,106	62
36	DGD	C	517[B]	62/66	0.95	0.07	46,59,101,106	62
23	CLA	c	509	65/65	0.95	0.07	43,63,126,150	0
23	CLA	a	406[A]	65/65	0.95	0.07	42,54,123,132	65
25	BCR	k	101	40/40	0.95	0.09	57,73,84,88	0
30	UNL	X	101	18/-	0.95	0.10	61,78,111,113	0
23	CLA	a	406[B]	65/65	0.95	0.07	41,54,123,132	65
25	BCR	y	101	40/40	0.95	0.08	59,71,88,101	0
23	CLA	C	502	65/65	0.95	0.07	50,62,74,80	0
24	PHO	a	415[A]	64/64	0.95	0.07	44,56,62,69	64
24	PHO	a	415[B]	64/64	0.95	0.07	44,56,62,69	64
23	CLA	B	610	65/65	0.95	0.08	43,55,67,89	0
25	BCR	B	618	40/40	0.95	0.06	44,57,73,84	0
23	CLA	B	611	65/65	0.95	0.07	37,48,68,78	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	612	65/65	0.95	0.08	43,53,65,73	0
23	CLA	C	508	65/65	0.95	0.08	48,63,87,92	0
30	UNL	x	101	18/-	0.95	0.10	72,83,135,137	0
23	CLA	A	405[A]	65/65	0.96	0.06	37,44,58,69	65
23	CLA	b	607	65/65	0.96	0.07	39,50,84,97	0
23	CLA	b	609	65/65	0.96	0.07	46,65,79,89	0
23	CLA	b	611	65/65	0.96	0.07	40,51,73,84	0
23	CLA	C	506	65/65	0.96	0.07	48,61,96,107	0
23	CLA	b	613	65/65	0.96	0.06	41,50,86,107	0
27	GOL	c	526[A]	6/6	0.96	0.07	67,71,76,79	6
27	GOL	c	526[B]	6/6	0.96	0.07	67,73,77,80	6
23	CLA	A	405[B]	65/65	0.96	0.06	37,44,58,70	65
23	CLA	B	607	65/65	0.96	0.06	38,48,81,86	0
25	BCR	c	516	40/40	0.96	0.06	56,66,83,85	0
23	CLA	B	609	65/65	0.96	0.07	46,60,71,85	0
32	LHG	D	406[A]	49/49	0.96	0.08	49,56,70,78	49
32	LHG	D	406[B]	49/49	0.96	0.08	49,56,70,79	49
23	CLA	c	504	65/65	0.96	0.07	50,69,80,97	0
23	CLA	C	510	65/65	0.96	0.08	48,58,85,100	0
23	CLA	c	506	65/65	0.96	0.07	50,65,98,100	0
23	CLA	C	512	65/65	0.96	0.07	50,64,79,88	0
32	LHG	L	102[A]	49/49	0.96	0.07	50,59,69,95	49
32	LHG	L	102[B]	49/49	0.96	0.07	50,59,68,95	49
23	CLA	A	406[A]	65/65	0.96	0.06	41,49,115,126	65
23	CLA	A	406[B]	65/65	0.96	0.06	41,49,115,126	65
23	CLA	c	512	65/65	0.96	0.08	55,68,86,100	0
23	CLA	D	402[A]	65/65	0.96	0.07	33,44,69,79	65
23	CLA	D	402[B]	65/65	0.96	0.07	33,44,69,81	65
23	CLA	B	613	65/65	0.96	0.06	40,48,94,111	0
29	PL9	d	405[A]	55/55	0.96	0.07	41,52,63,72	55
29	PL9	d	405[B]	55/55	0.96	0.07	41,53,63,72	55
24	PHO	A	417[A]	64/64	0.96	0.06	40,51,58,65	64
24	PHO	A	417[B]	64/64	0.96	0.06	39,51,58,65	64
24	PHO	a	407[A]	64/64	0.96	0.06	44,50,56,61	64
24	PHO	a	407[B]	64/64	0.96	0.06	44,50,56,61	64
23	CLA	A	404[A]	65/65	0.96	0.07	37,44,64,71	65
23	CLA	A	404[B]	65/65	0.96	0.07	37,44,66,71	65
23	CLA	B	602	65/65	0.96	0.07	46,56,71,88	0
25	BCR	B	617	40/40	0.96	0.06	42,54,65,65	0
23	CLA	C	504	65/65	0.96	0.06	48,61,73,83	0
37	CA	C	524	1/1	0.96	0.05	74,74,74,74	0
23	CLA	b	602	65/65	0.96	0.07	48,60,82,91	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	603	65/65	0.96	0.07	46,57,82,94	0
25	BCR	C	516	40/40	0.96	0.06	51,64,76,88	0
23	CLA	b	604	65/65	0.96	0.07	39,51,100,123	0
23	CLA	b	605	65/65	0.96	0.07	39,52,73,84	0
23	CLA	d	402[B]	65/65	0.97	0.07	40,46,81,96	65
23	CLA	B	604	65/65	0.97	0.06	39,48,115,134	0
24	PHO	A	407[A]	64/64	0.97	0.05	39,47,55,58	64
24	PHO	A	407[B]	64/64	0.97	0.05	38,47,55,58	64
23	CLA	b	610	65/65	0.97	0.07	46,57,68,77	0
23	CLA	a	404[A]	65/65	0.97	0.06	41,47,67,78	65
23	CLA	a	404[B]	65/65	0.97	0.06	41,47,68,78	65
23	CLA	a	405[A]	65/65	0.97	0.05	40,46,68,74	65
23	CLA	a	405[B]	65/65	0.97	0.05	40,46,68,74	65
23	CLA	b	615	65/65	0.97	0.06	47,62,87,96	0
23	CLA	B	612	65/65	0.97	0.06	37,50,64,68	0
23	CLA	B	605	65/65	0.97	0.06	41,49,68,84	0
23	CLA	c	503	65/65	0.97	0.07	46,59,95,113	0
22	CL	a	402[A]	1/1	0.97	0.06	49,49,49,49	1
23	CLA	B	615	65/65	0.97	0.06	44,54,82,92	0
23	CLA	C	511	65/65	0.97	0.06	48,59,82,90	0
22	CL	a	402[B]	1/1	0.97	0.06	49,49,49,49	1
23	CLA	B	608	65/65	0.97	0.05	42,52,72,79	0
23	CLA	C	503	65/65	0.97	0.06	46,54,84,94	0
23	CLA	c	510	65/65	0.97	0.08	46,63,92,102	0
23	CLA	c	511	65/65	0.97	0.06	49,64,81,98	0
37	CA	O	301	1/1	0.97	0.04	105,105,105,105	0
22	CL	A	403[A]	1/1	0.97	0.04	47,47,47,47	1
22	CL	A	403[B]	1/1	0.97	0.04	47,47,47,47	1
23	CLA	b	608	65/65	0.97	0.06	43,58,85,97	0
23	CLA	d	402[A]	65/65	0.97	0.07	40,46,81,95	65
22	CL	A	402[A]	1/1	0.98	0.05	44,44,44,44	1
22	CL	A	402[B]	1/1	0.98	0.05	44,44,44,44	1
22	CL	a	403[A]	1/1	0.98	0.07	52,52,52,52	1
38	HEM	F	102	43/43	0.98	0.06	52,68,80,88	0
38	HEM	f	101	43/43	0.98	0.08	56,82,118,130	0
39	MG	J	102	1/1	0.98	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.98	0.07	64,64,64,64	0
22	CL	a	403[B]	1/1	0.98	0.07	52,52,52,52	1
40	HEC	v	201	43/43	0.98	0.07	47,61,69,71	0
37	CA	c	524	1/1	0.99	0.03	77,77,77,77	0
21	FE2	A	401[B]	1/1	0.99	0.02	52,52,52,52	1
21	FE2	a	401[A]	1/1	0.99	0.03	54,54,54,54	1

Continued on next page...

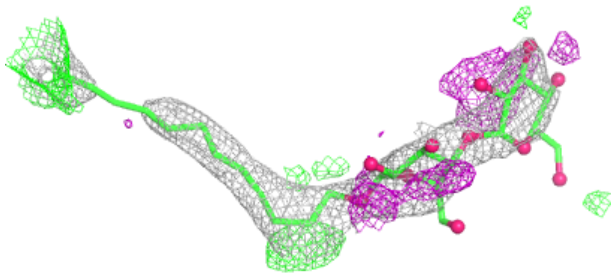
Continued from previous page...

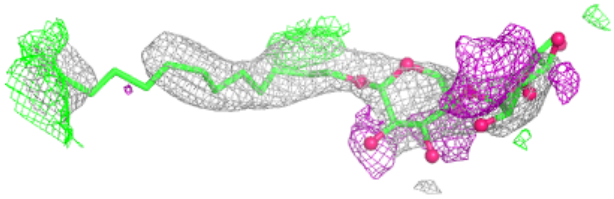
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	a	401[B]	1/1	0.99	0.03	55,55,55,55	1
28	OEX	A	413[A]	10/10	0.99	0.03	40,45,49,49	10
28	OEX	A	413[B]	10/10	0.99	0.03	39,44,49,50	10
28	OEX	a	412[A]	10/10	0.99	0.03	46,49,51,55	10
28	OEX	a	412[B]	10/10	0.99	0.03	45,50,51,55	10
21	FE2	A	401[A]	1/1	0.99	0.02	51,51,51,51	1

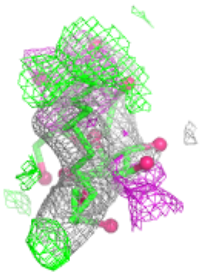
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LMT B 628:

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

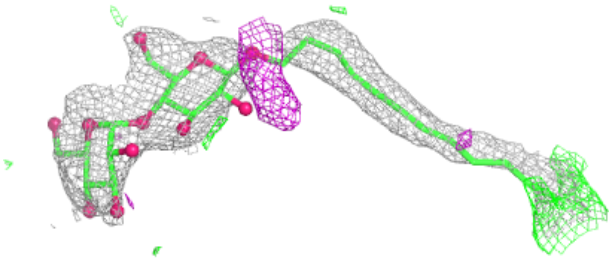


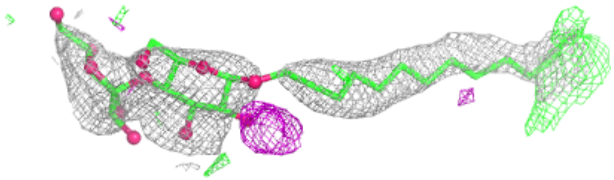


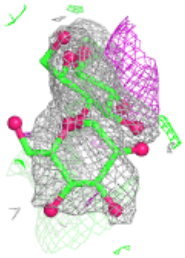


Electron density around LMT D 401:

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

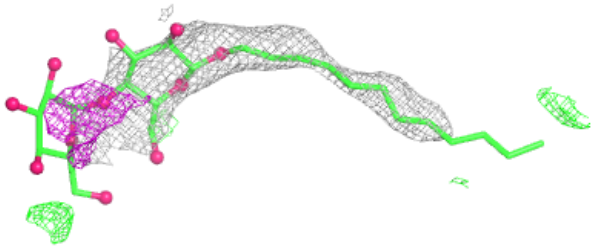


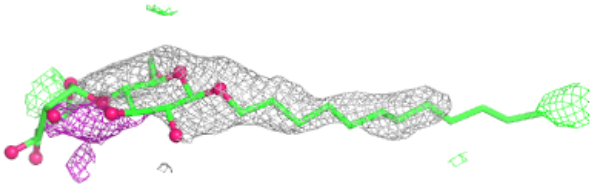


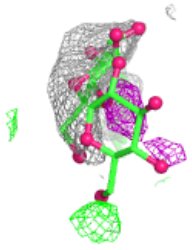


Electron density around LMT F 101:

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

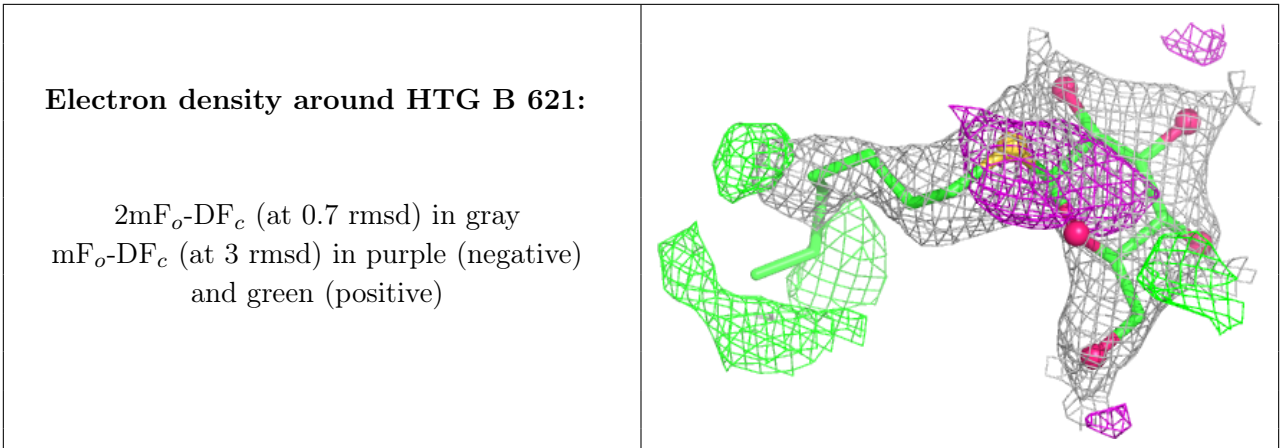






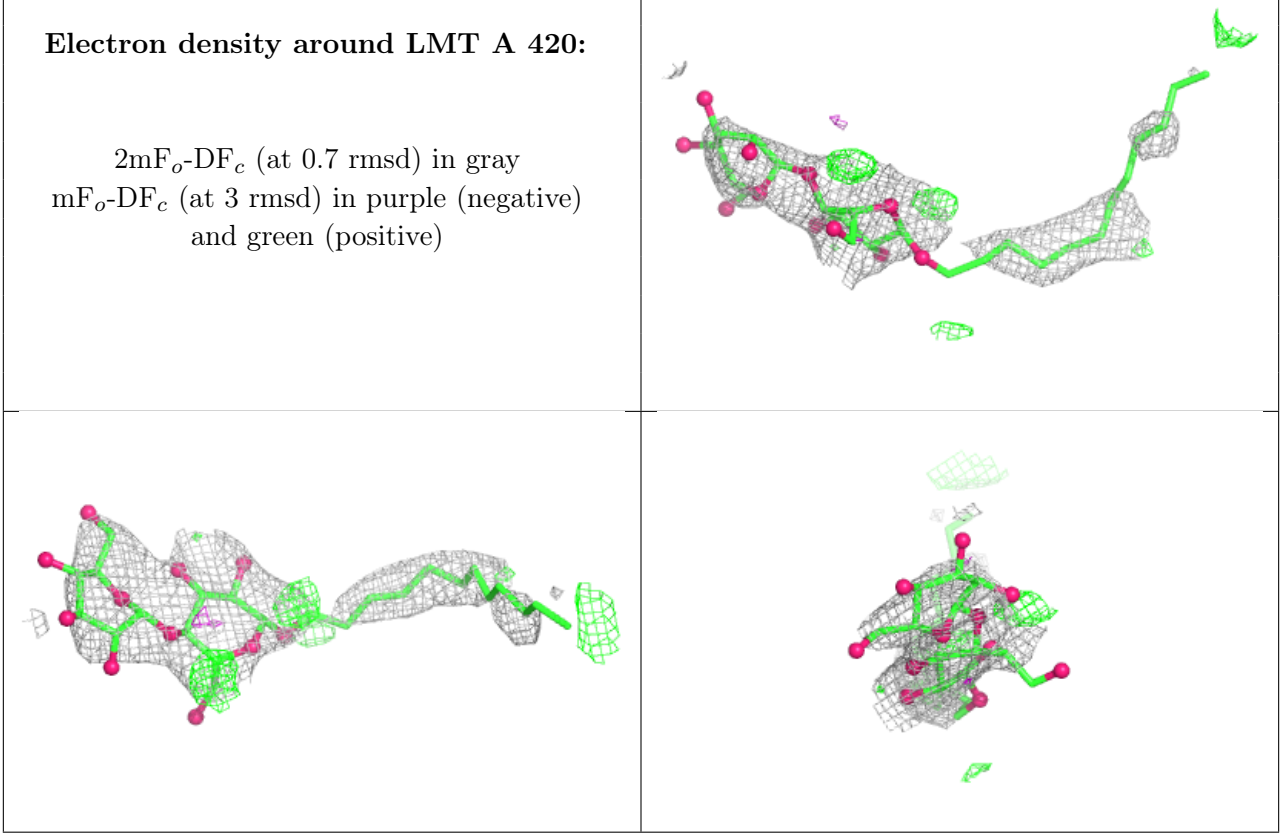
Electron density around HTG B 621:

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



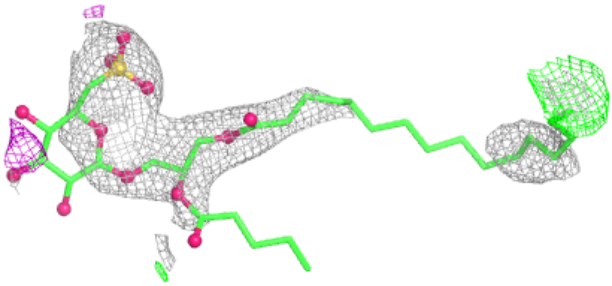
Electron density around LMT A 420:

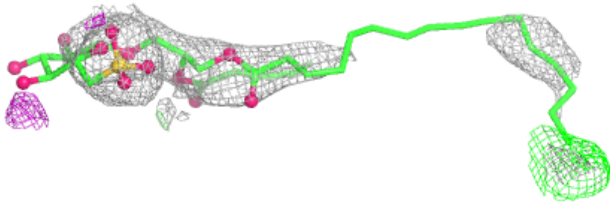
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

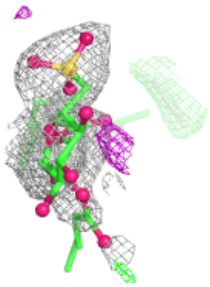


Electron density around SQD f 102:

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

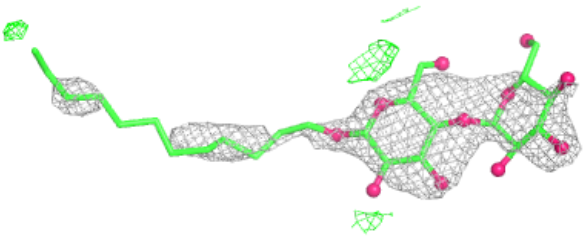


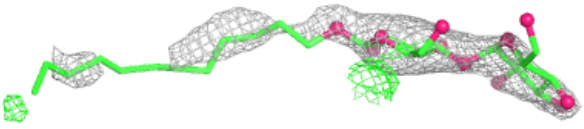


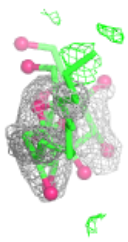


Electron density around LMT a 416:

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

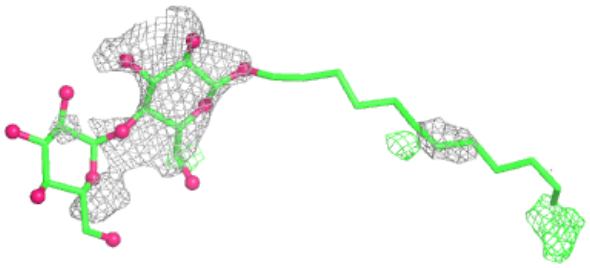


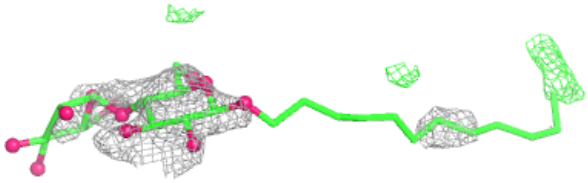


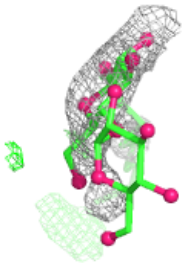


Electron density around LMT e 101:

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

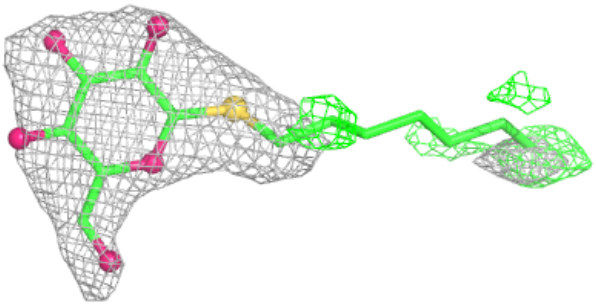


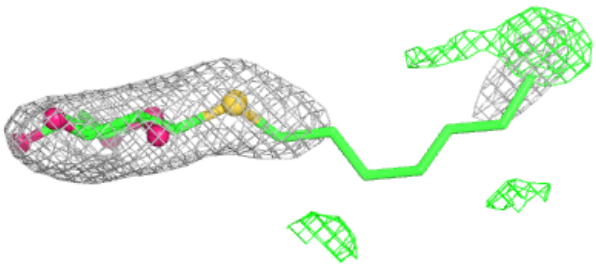


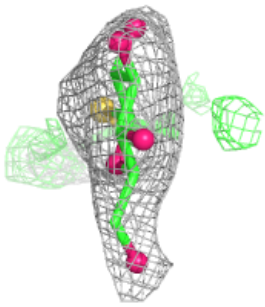


Electron density around HTG C 522:

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

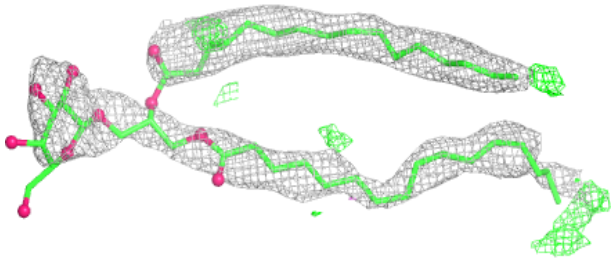


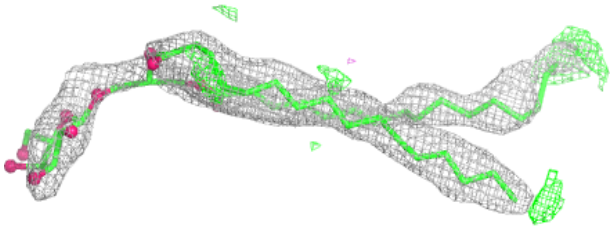


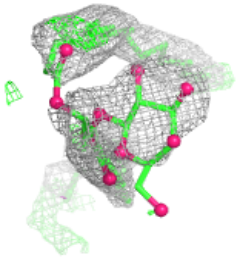


Electron density around LMG C 521:

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

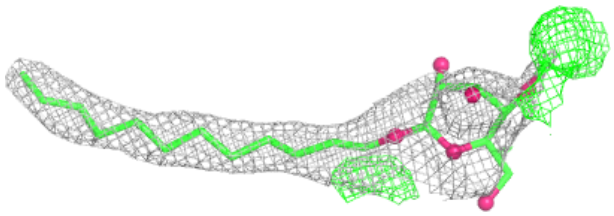


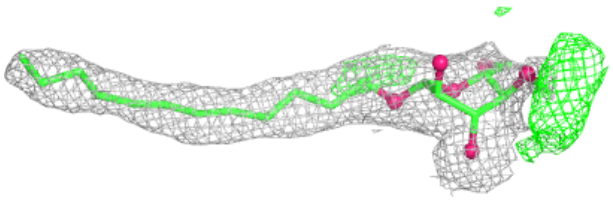


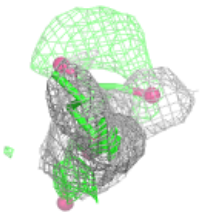


Electron density around LMT b 621:

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

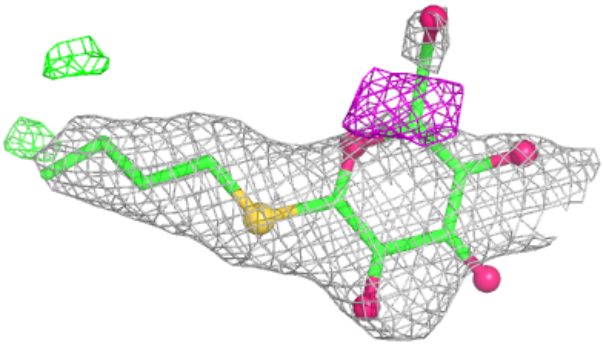


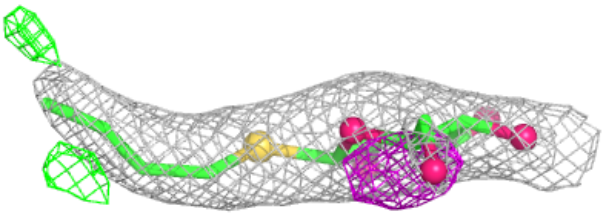


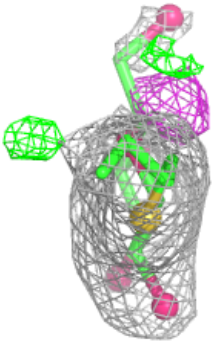


Electron density around HTG D 410:

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

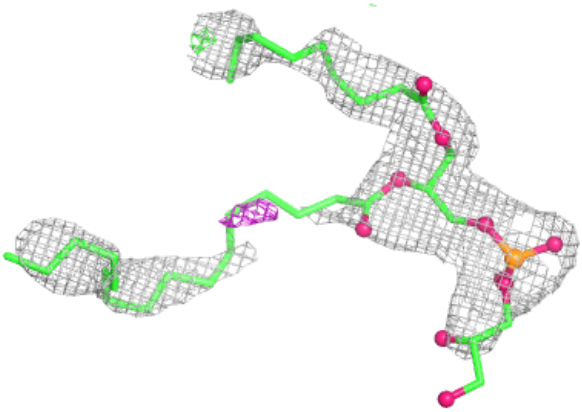


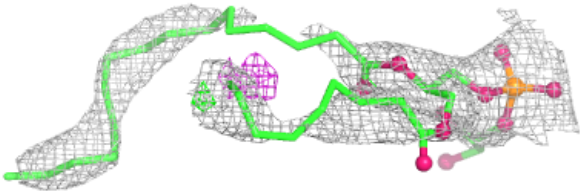


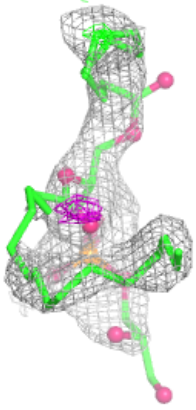


Electron density around LHG a 419 (A):

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

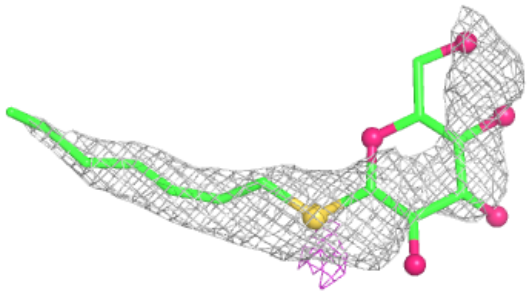


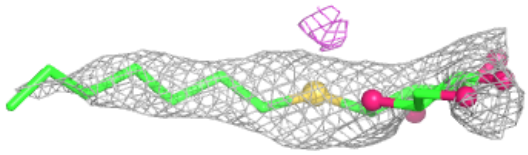


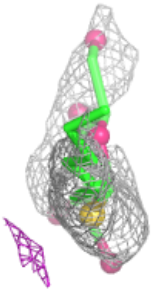


Electron density around HTG b 623:

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

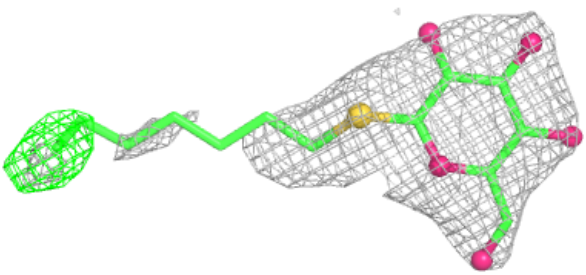


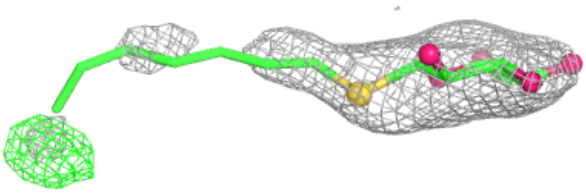


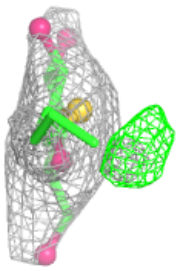


Electron density around HTG c 522:

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

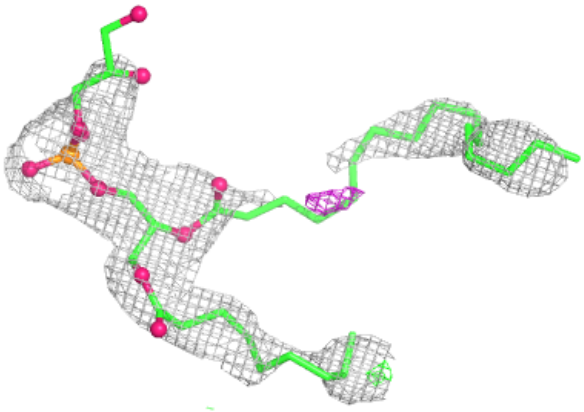


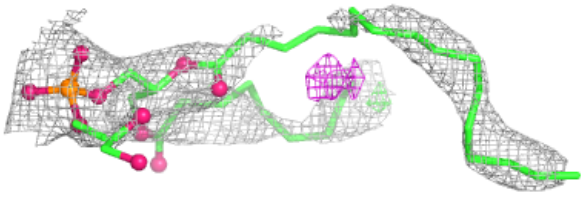


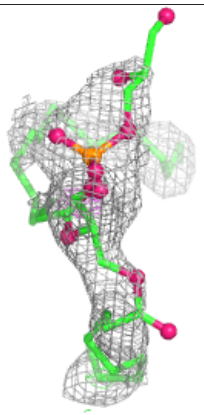


Electron density around LHG a 419 (B):

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

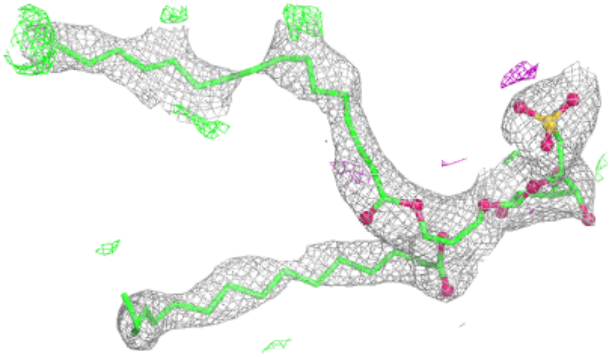


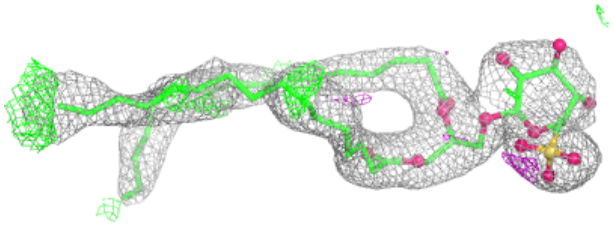


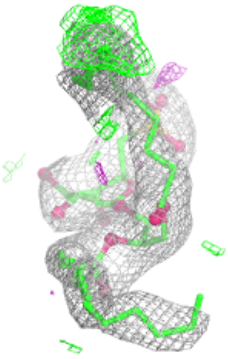


Electron density around SQD a 411:

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

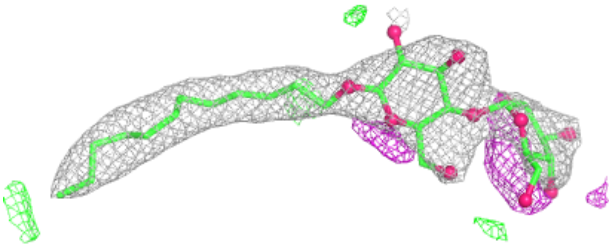


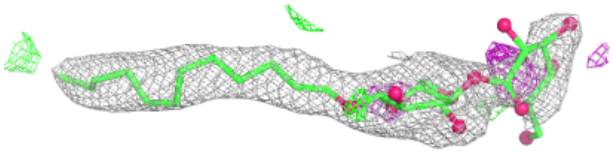


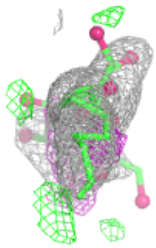


Electron density around LMT B 626:

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

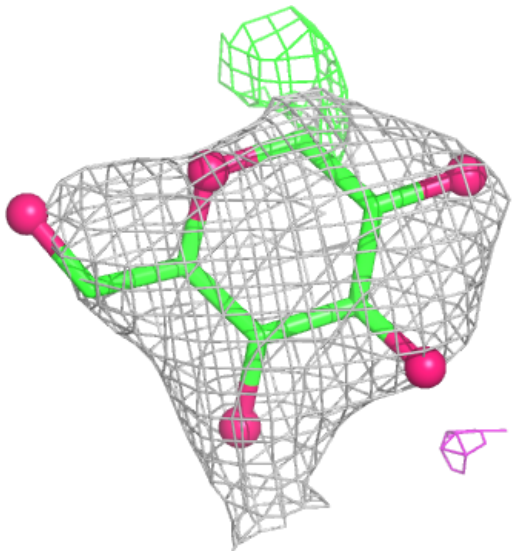


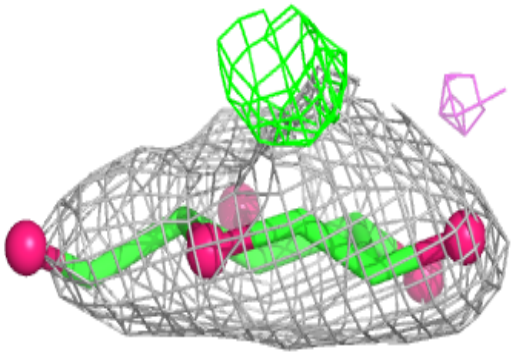


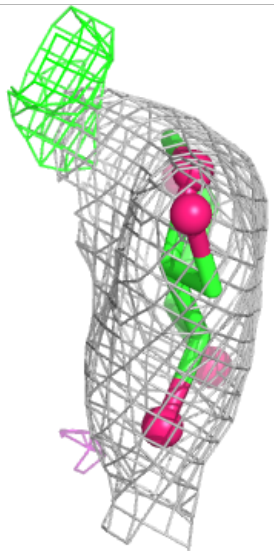


Electron density around HTG V 202:

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

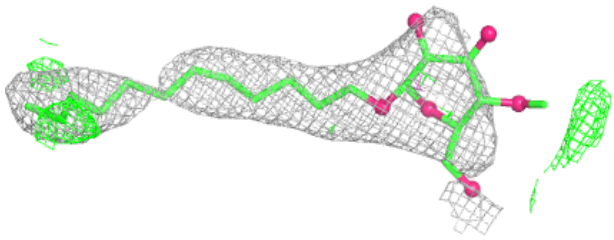


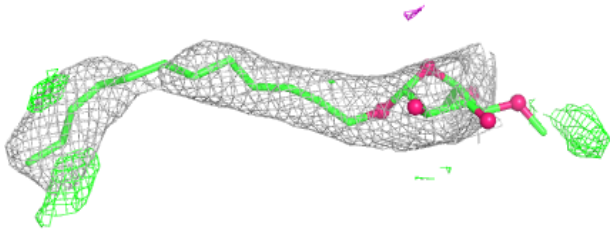


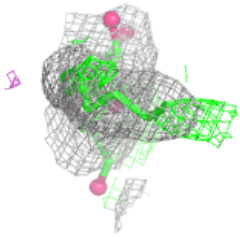


Electron density around LMT B 629:

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

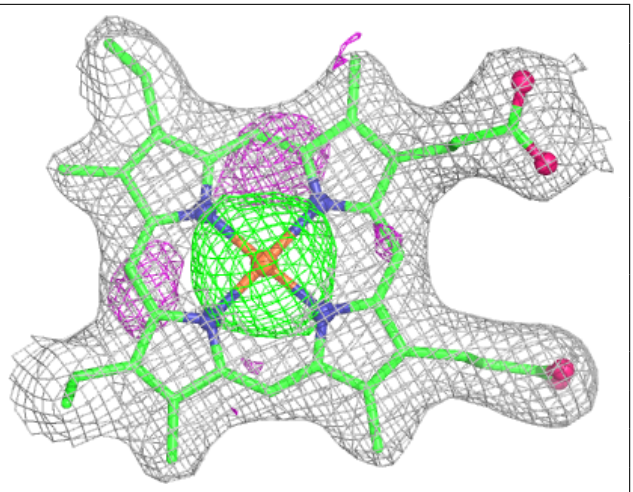


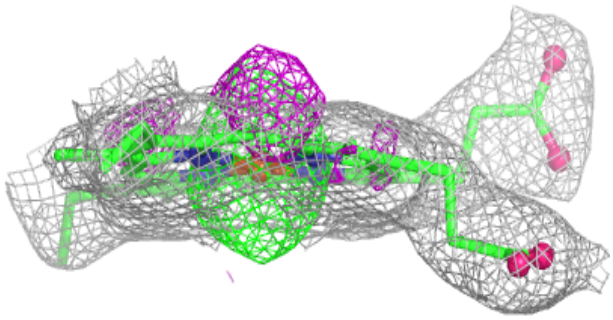


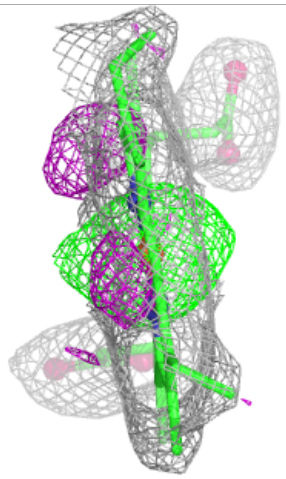


Electron density around HEC V 201:

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

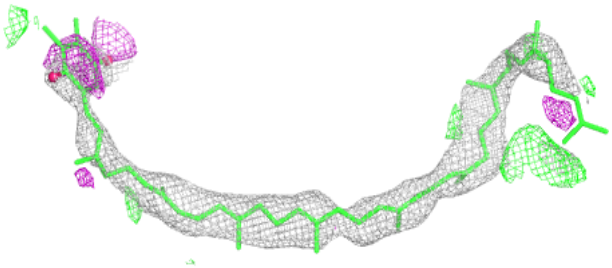


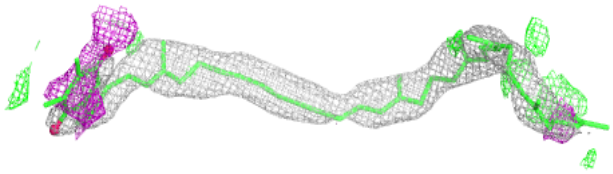


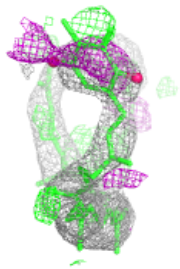


Electron density around PL9 A 414 (A):

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

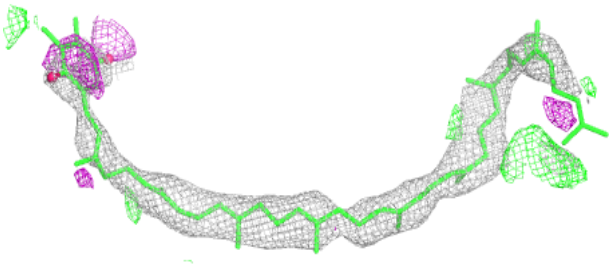


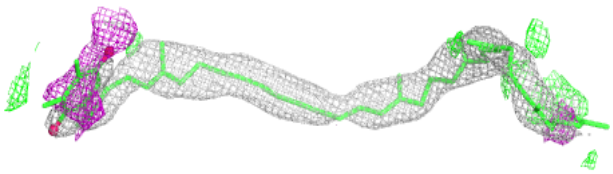


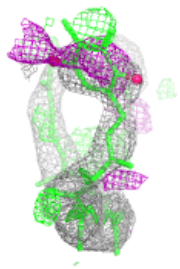


Electron density around PL9 A 414 (B):

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

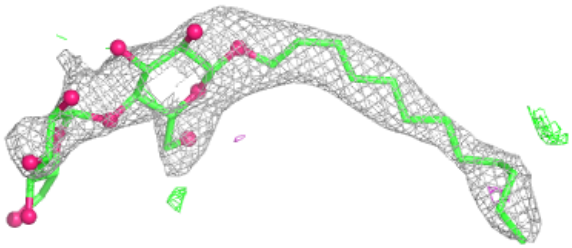


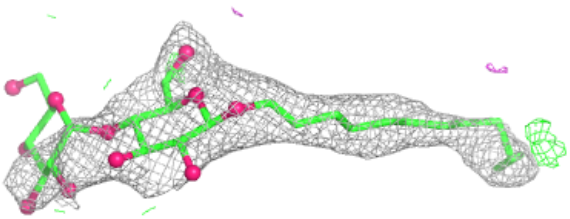




Electron density around LMT T 101:

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

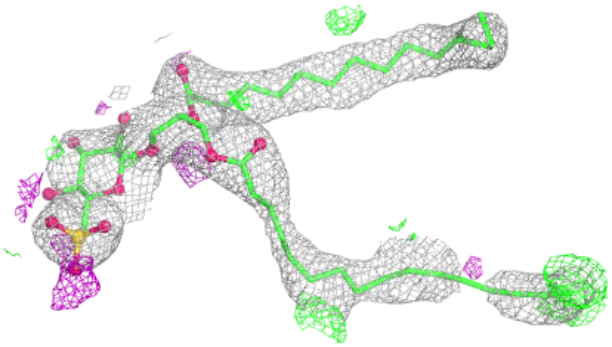


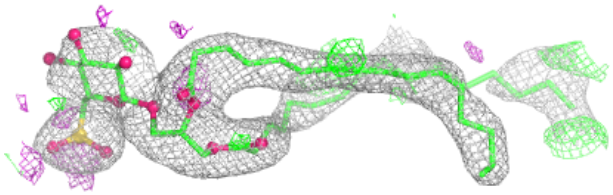


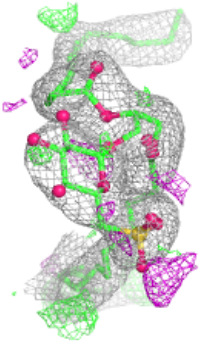


Electron density around SQD A 412:

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

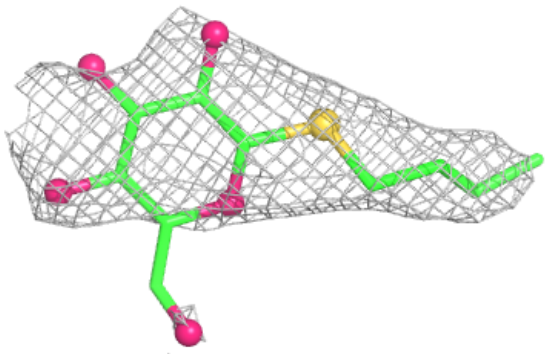


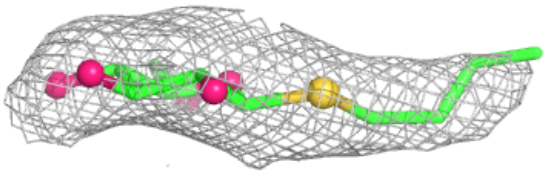


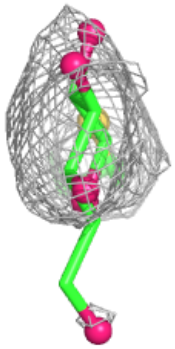


Electron density around HTG d 409:

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

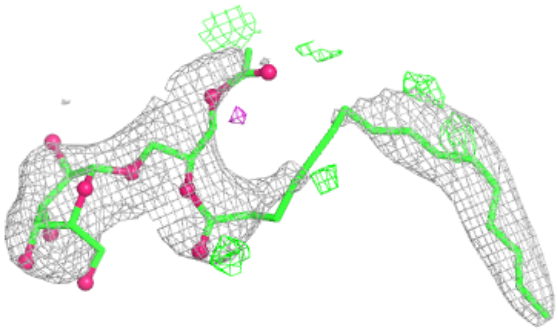


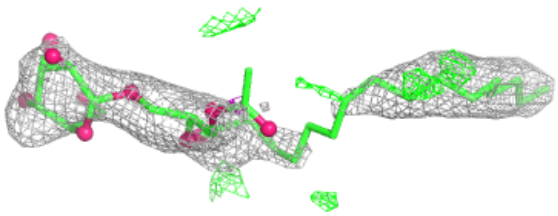


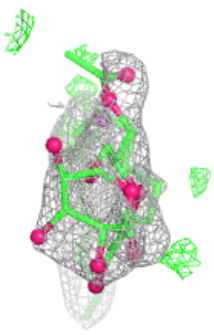


Electron density around LMG Z 101:

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

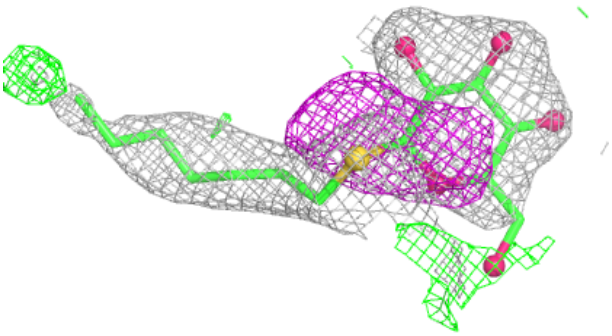


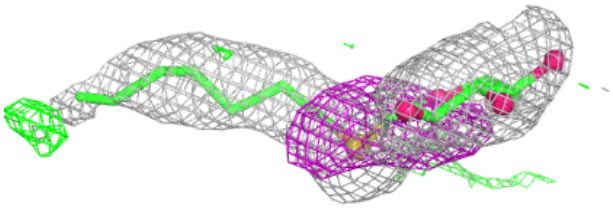


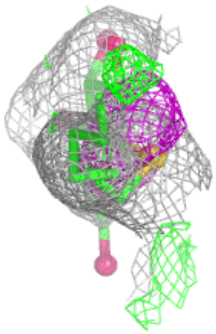


Electron density around HTG b 622:

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

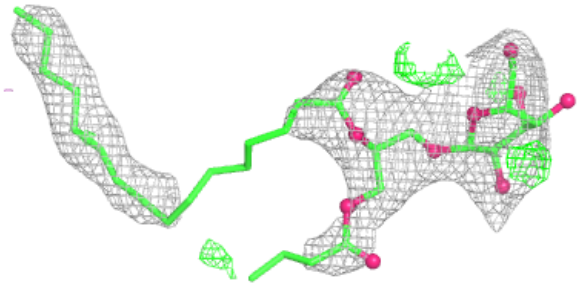


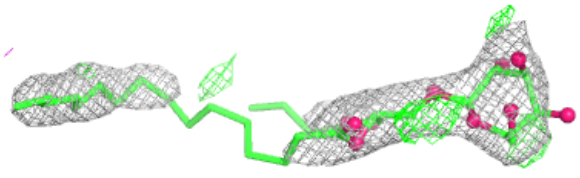


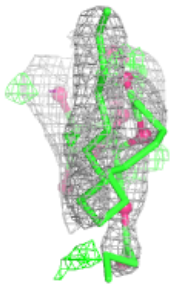


Electron density around LMG z 101:

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

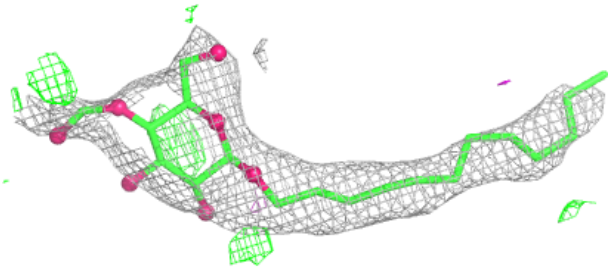


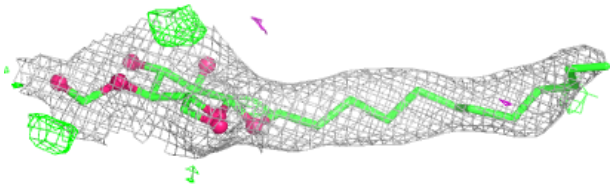


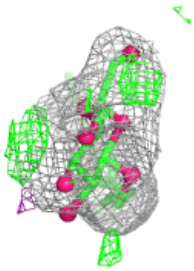


Electron density around LMT t 101:

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

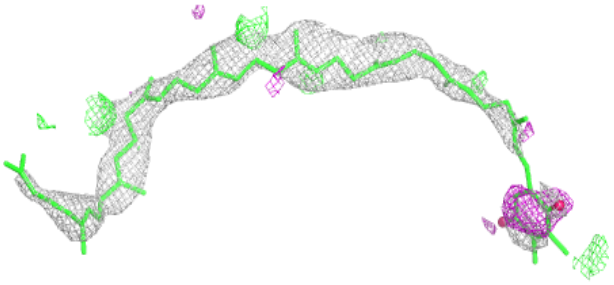


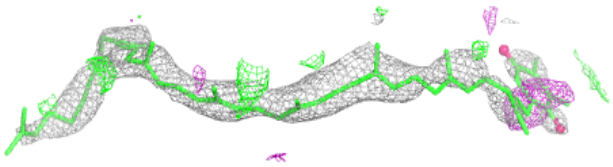


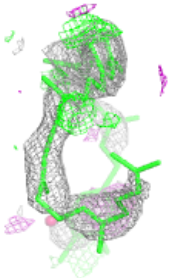


Electron density around PL9 a 413 (A):

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

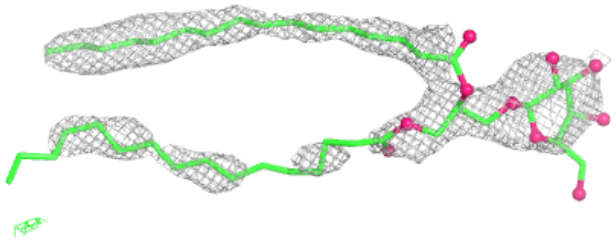


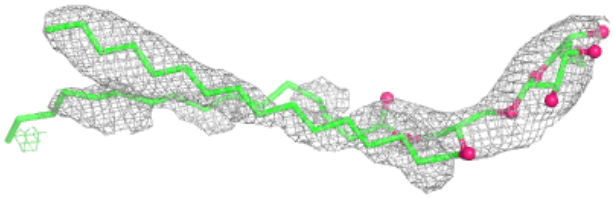


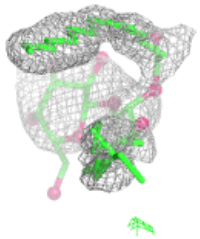


Electron density around LMG c 521:

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

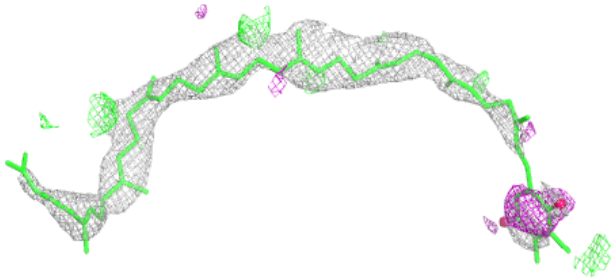


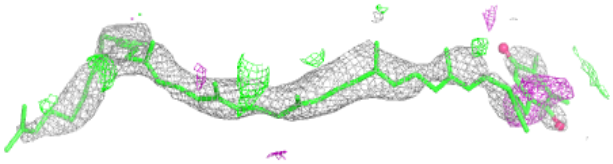


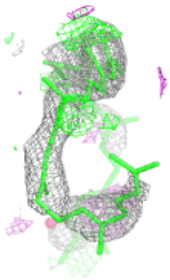


Electron density around PL9 a 413 (B):

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

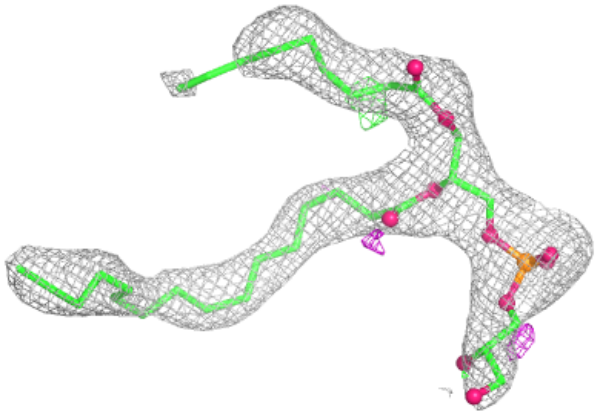


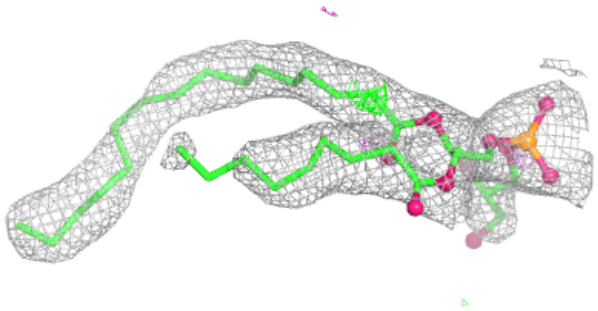


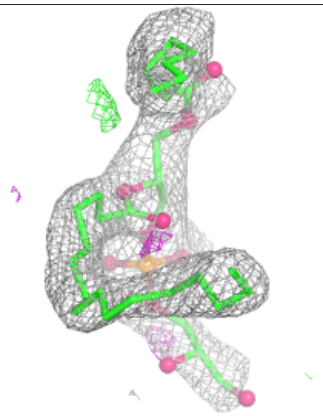


Electron density around LHG E 101 (A):

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

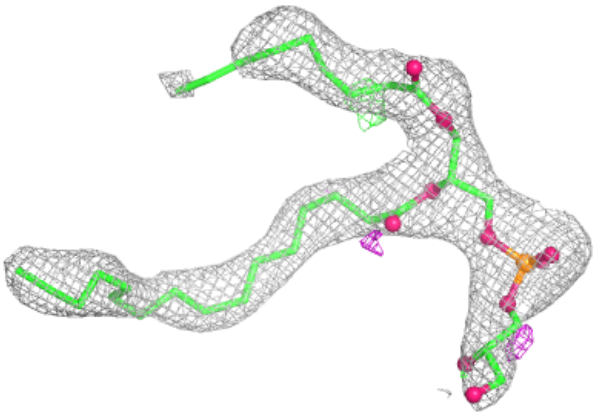


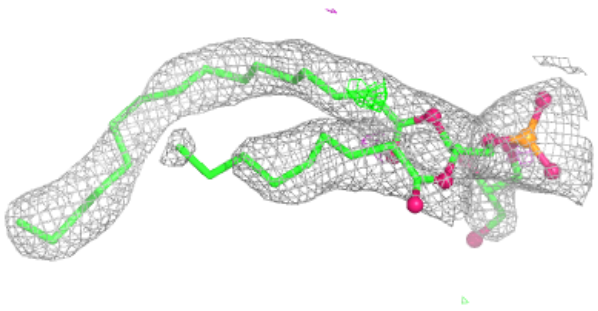


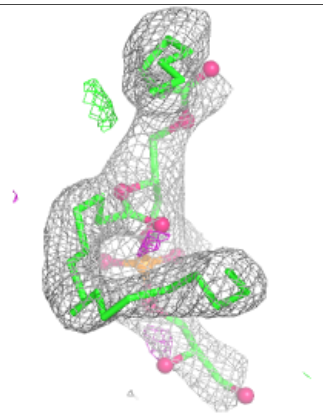


Electron density around LHG E 101 (B):

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

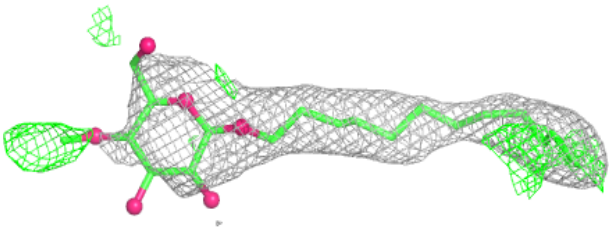


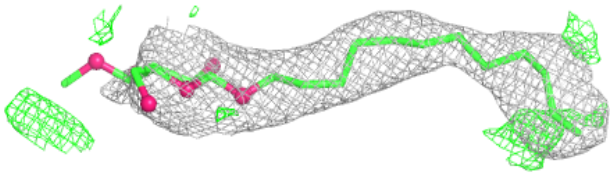


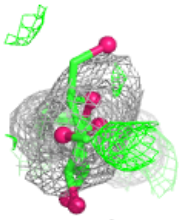


Electron density around LMT b 627:

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

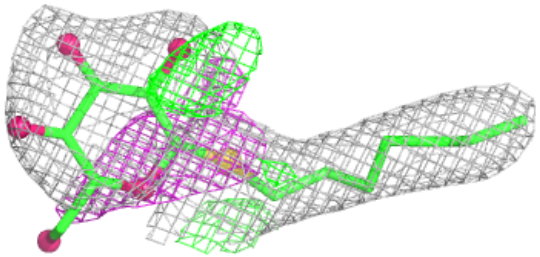


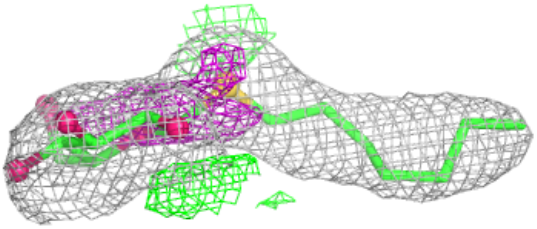


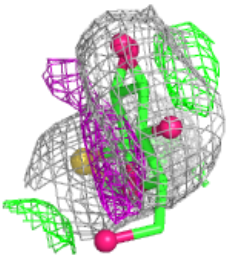


Electron density around HTG o 301:

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

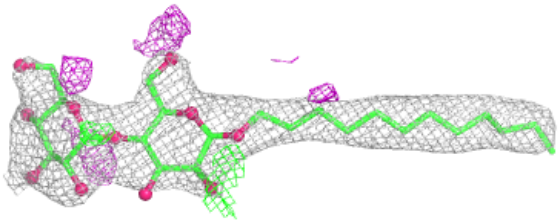


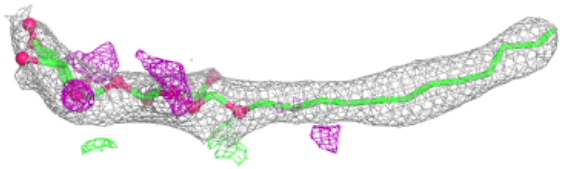


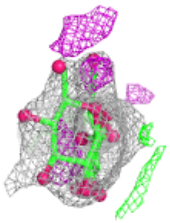


Electron density around LMT m 103:

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

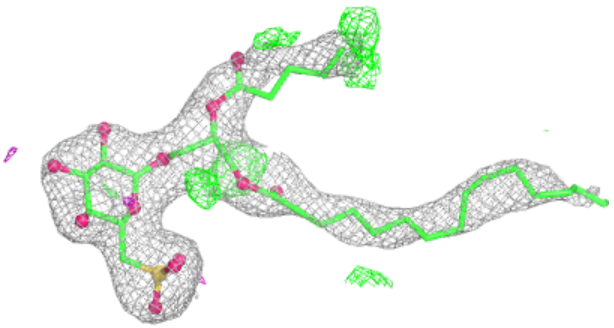


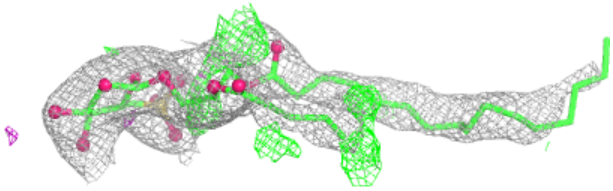


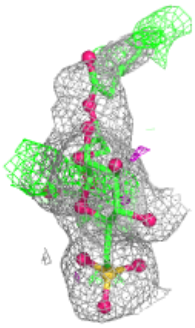


Electron density around SQD F 103:

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

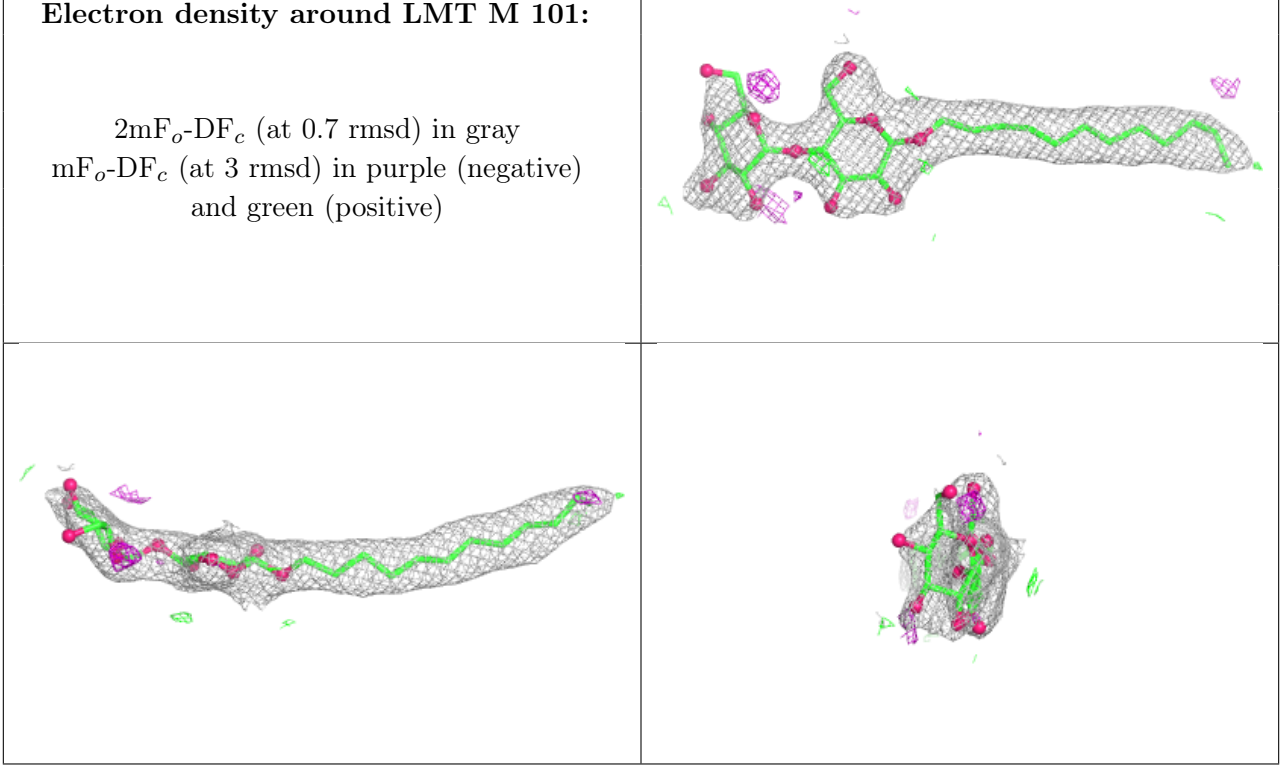






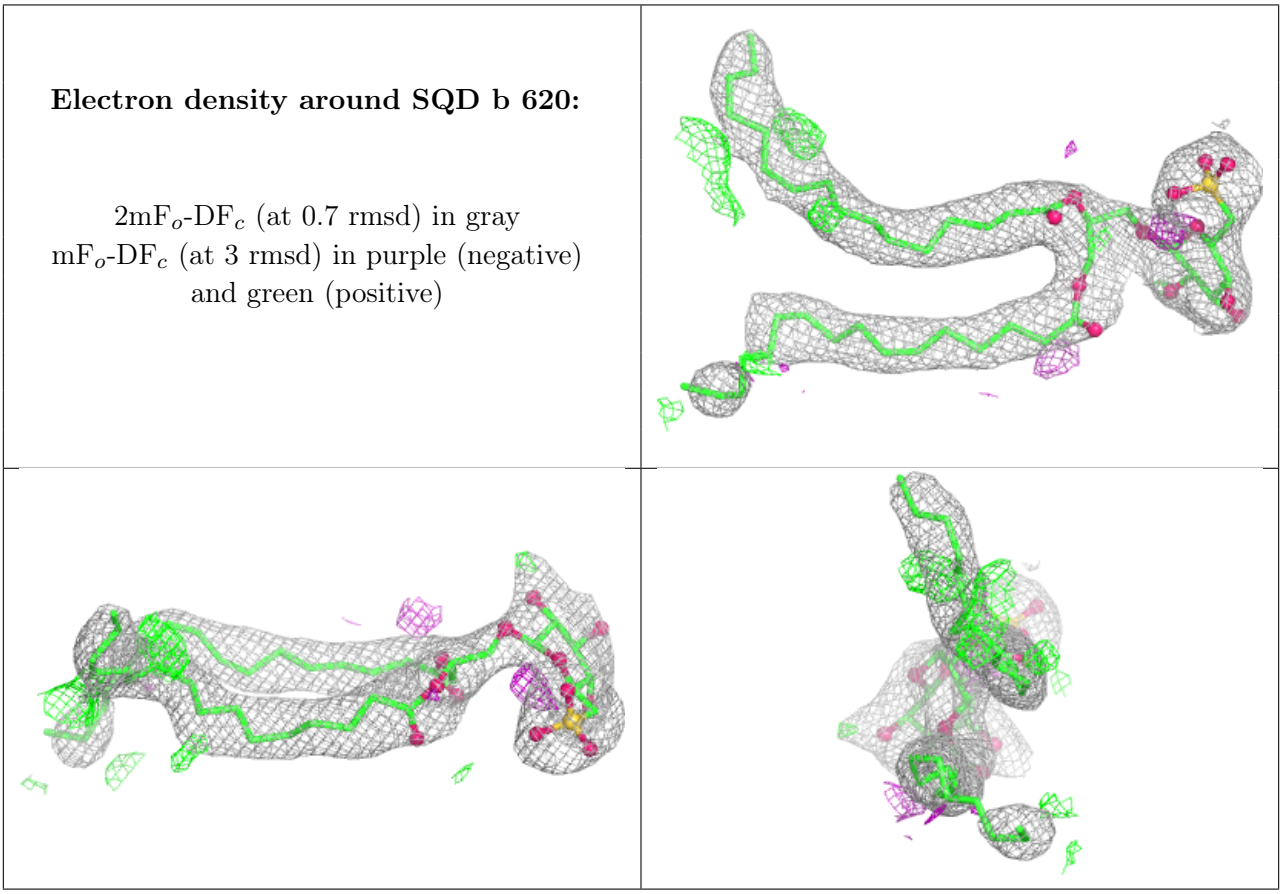
Electron density around LMT M 101:

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



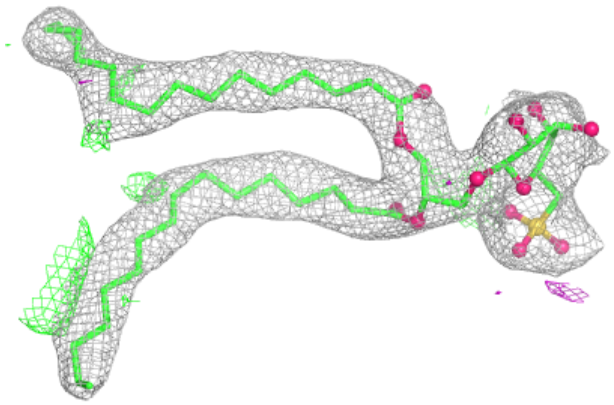
Electron density around SQD b 620:

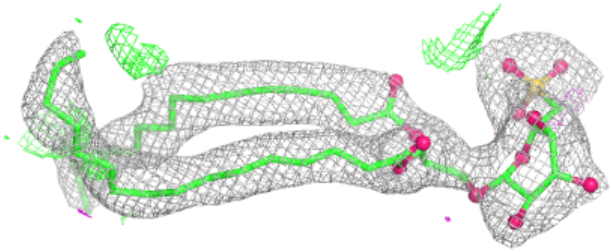
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

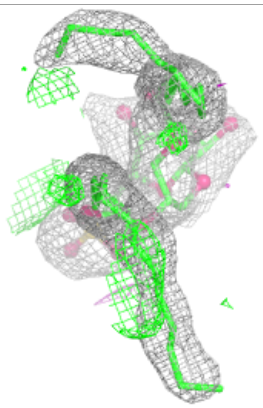


Electron density around SQD L 101:

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

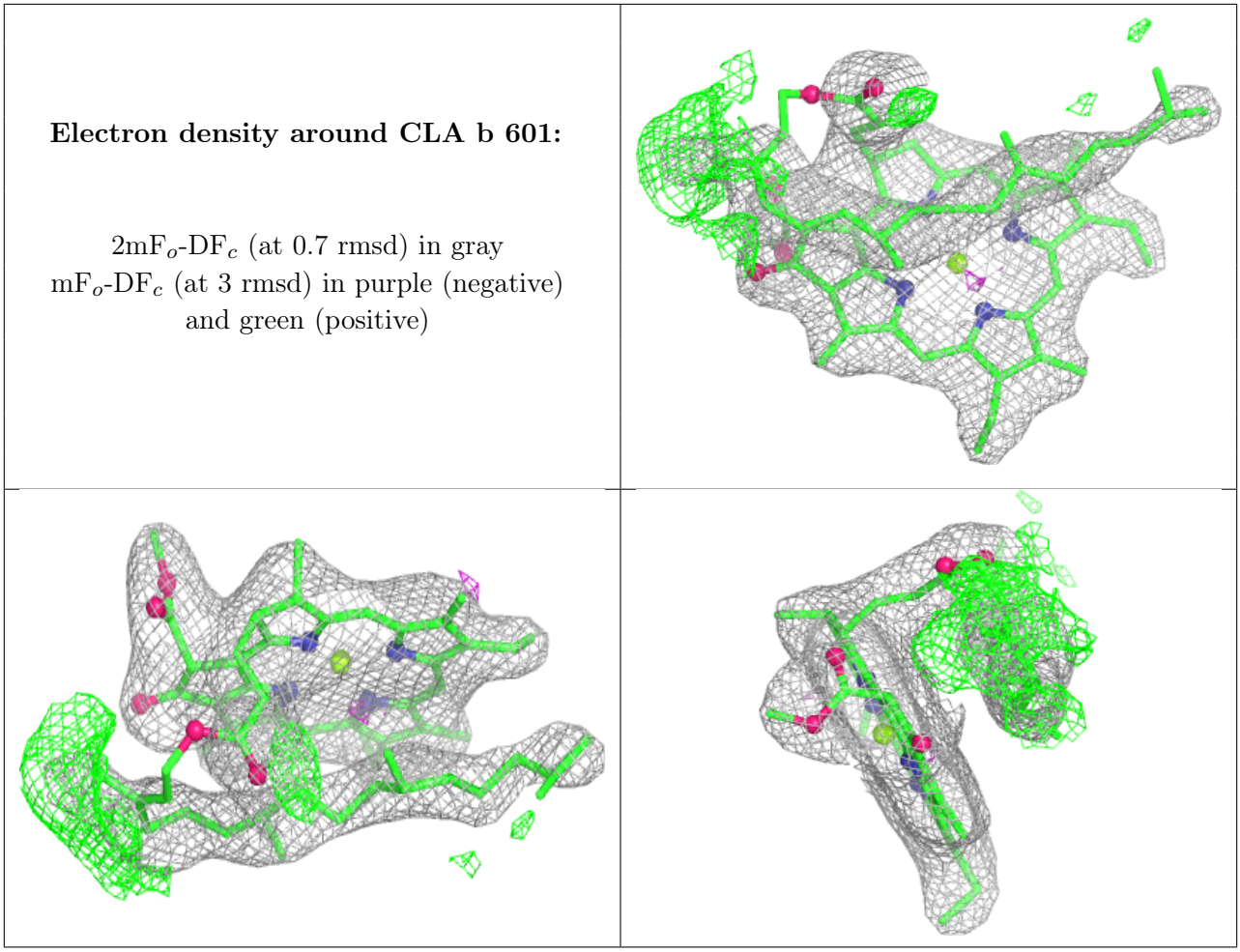






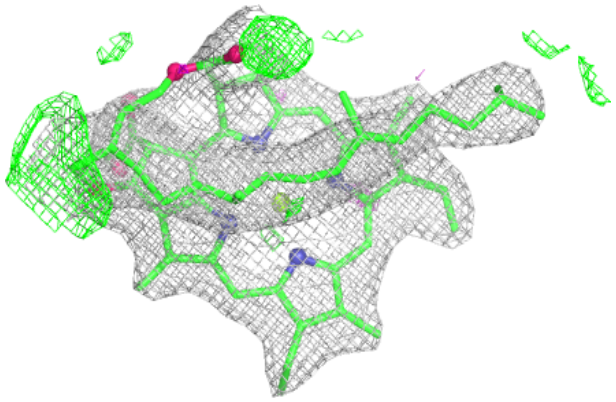
Electron density around CLA b 601:

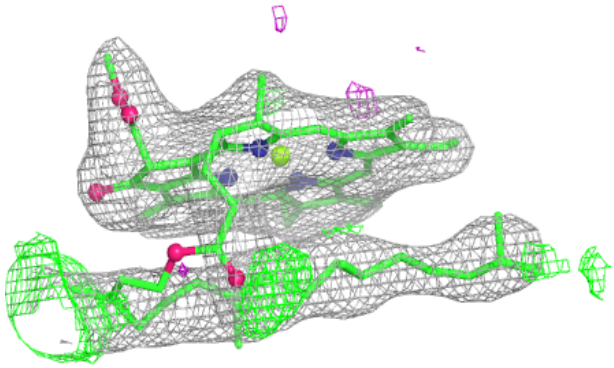
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

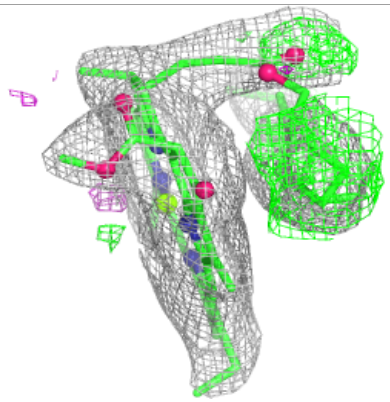


Electron density around CLA B 601:

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

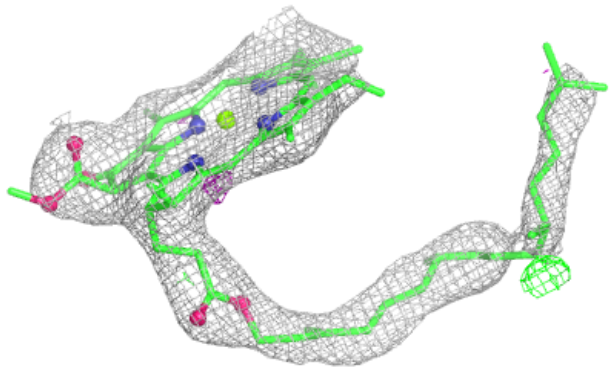


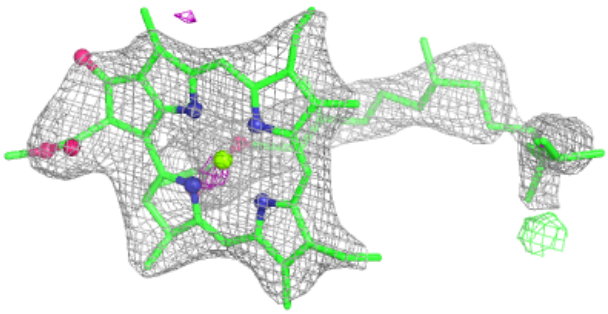


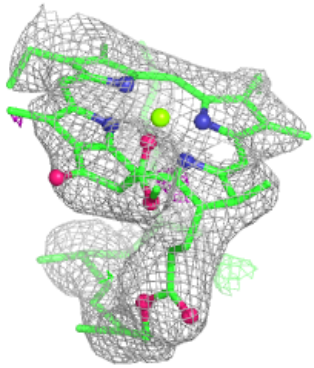


Electron density around CLA c 514:

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

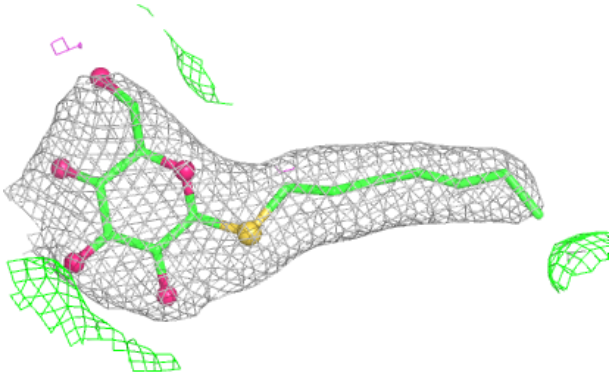


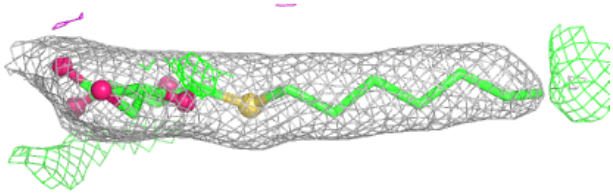


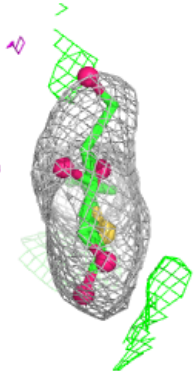


Electron density around HTG B 623:

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

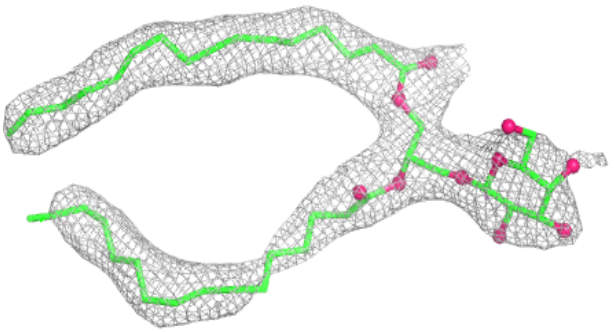


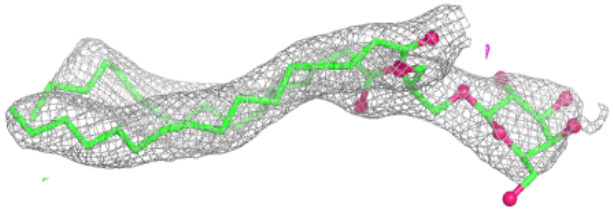


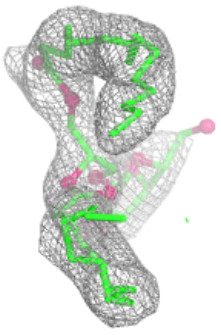


Electron density around LMG c 501:

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

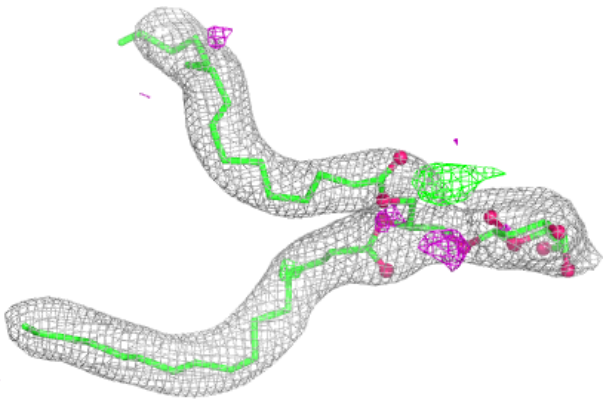


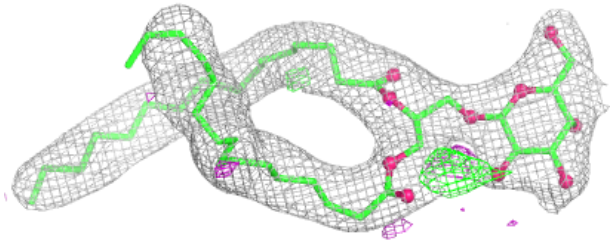


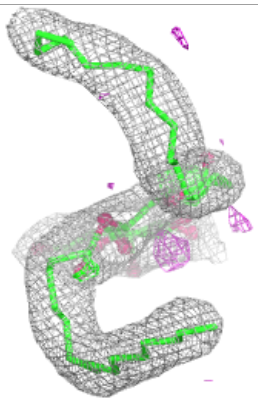


Electron density around LMG m 101:

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

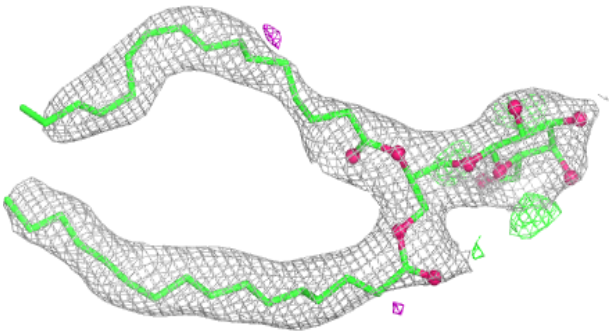


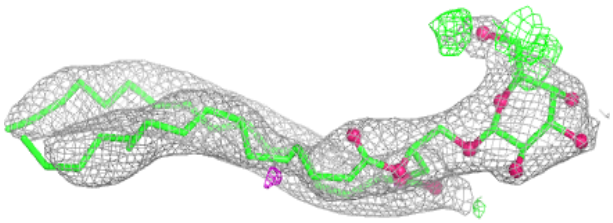


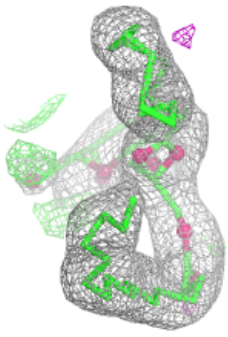


Electron density around LMG C 501:

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

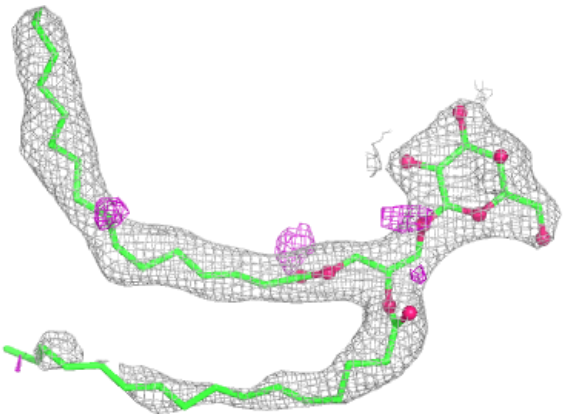


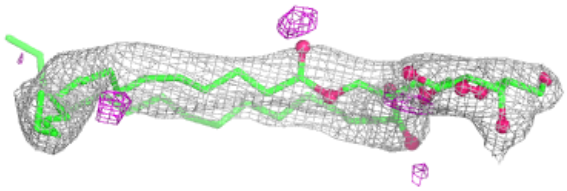


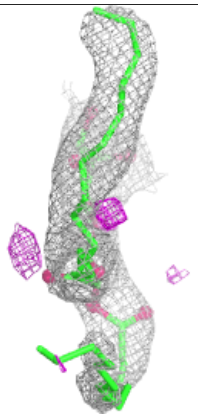


Electron density around LMG C 520:

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

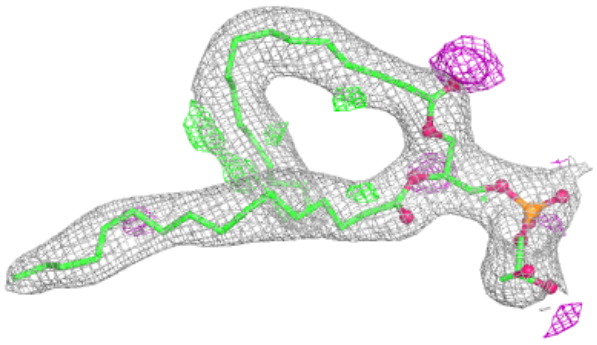


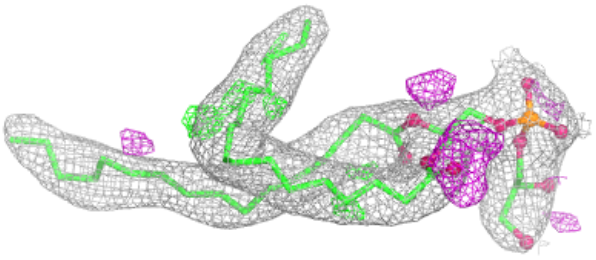


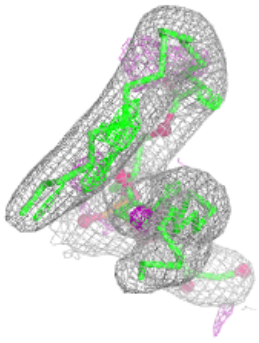


Electron density around LHG A 419 (B):

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

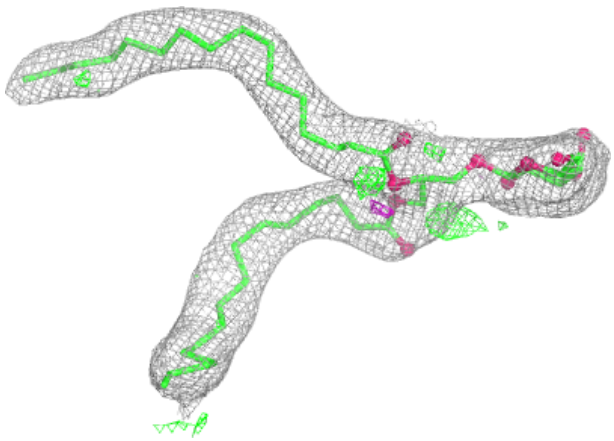


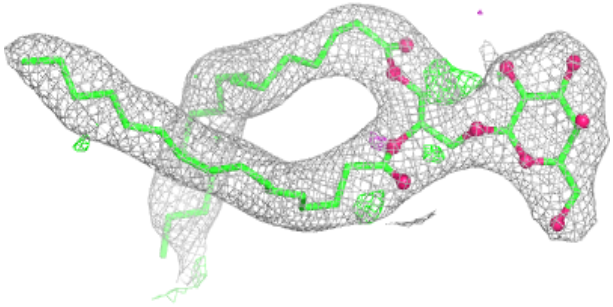


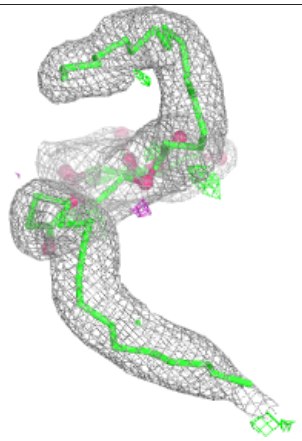


Electron density around LMG B 620:

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

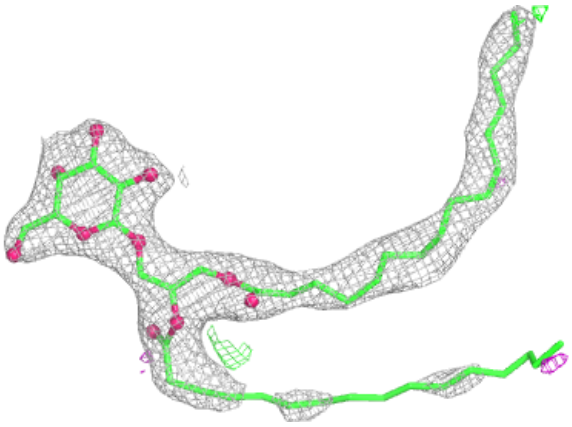


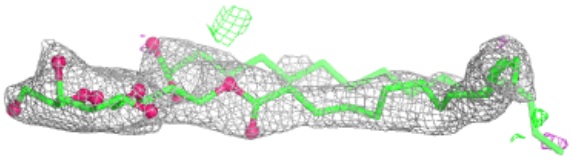


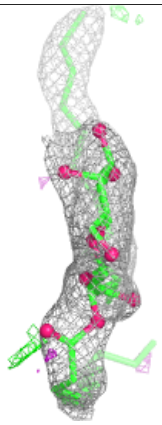


Electron density around LMG c 520:

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

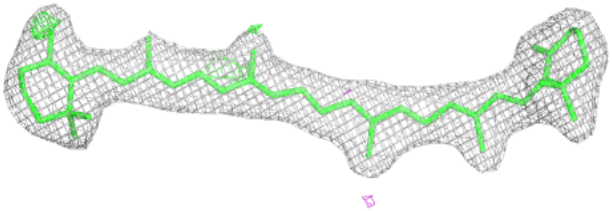


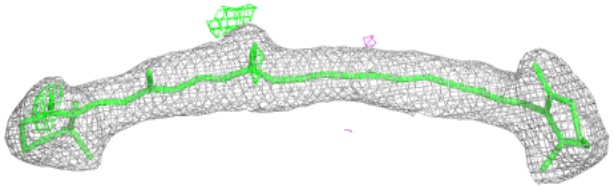


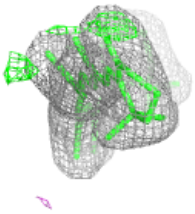


Electron density around BCR T 102:

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

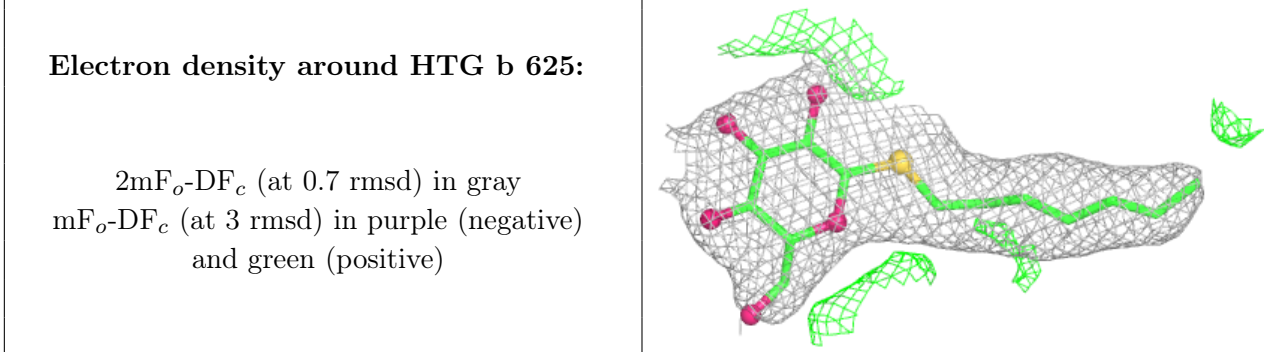


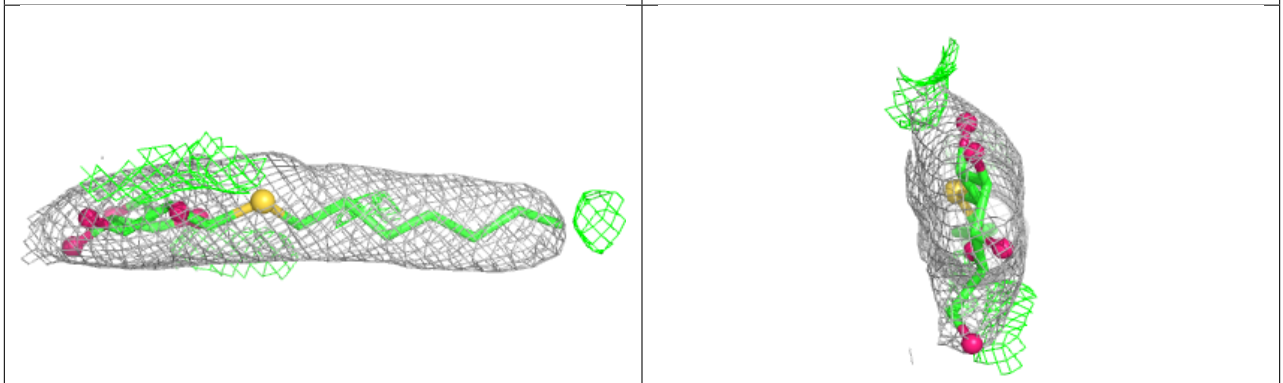




Electron density around HTG b 625:

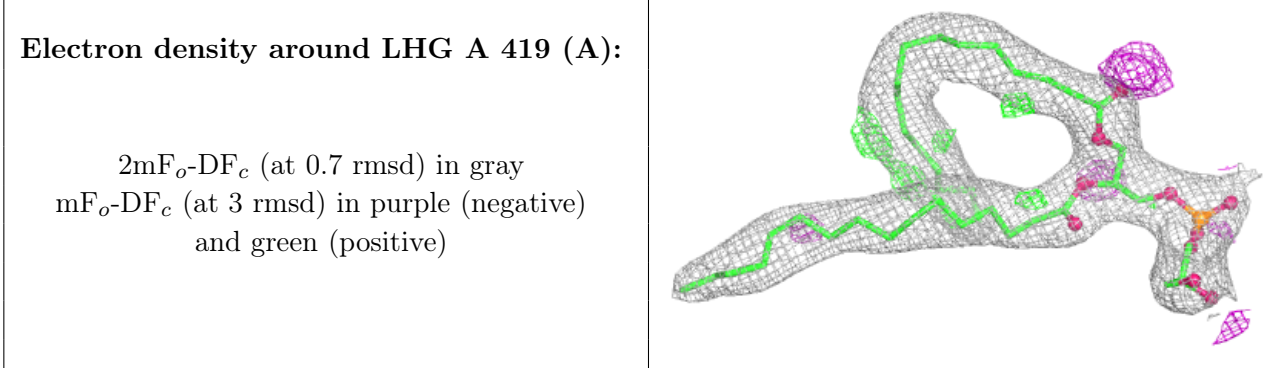
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

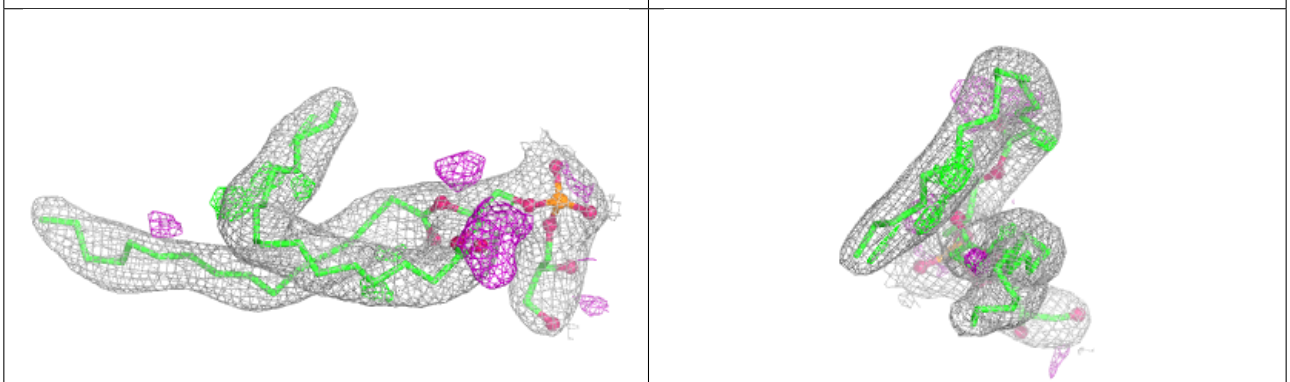




Electron density around LHG A 419 (A):

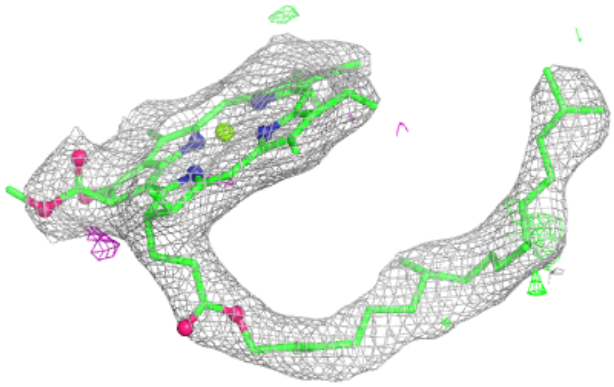
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

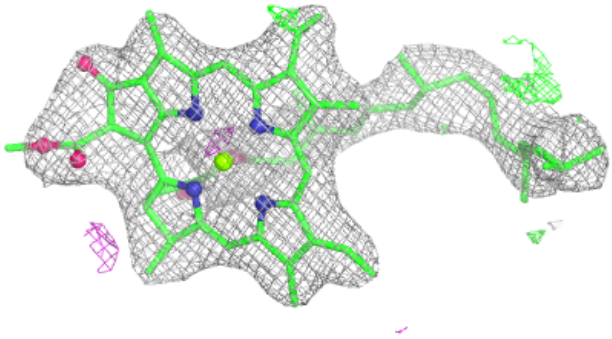


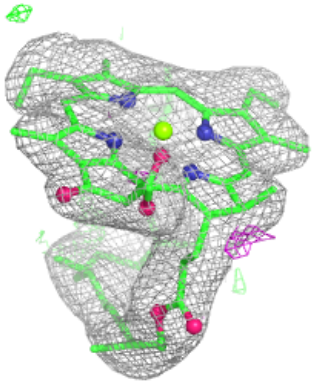


Electron density around CLA C 514:

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

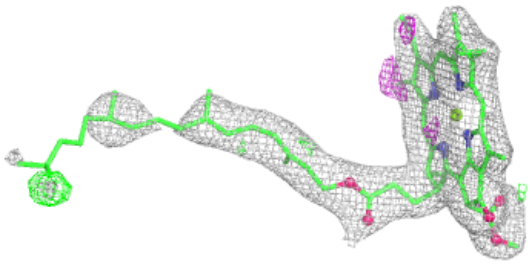


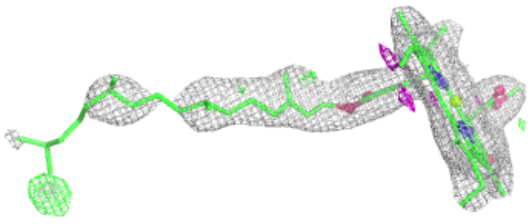


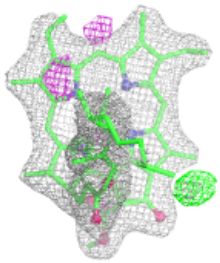


Electron density around CLA d 403:

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

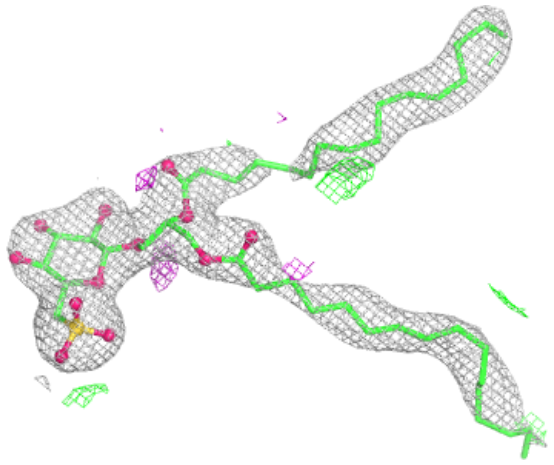


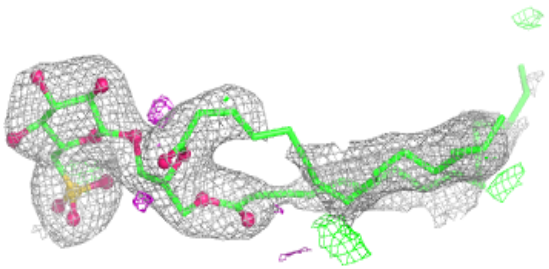


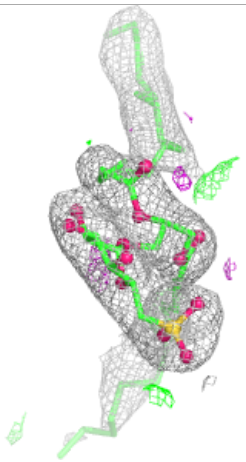


Electron density around SQD a 410 (A):

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

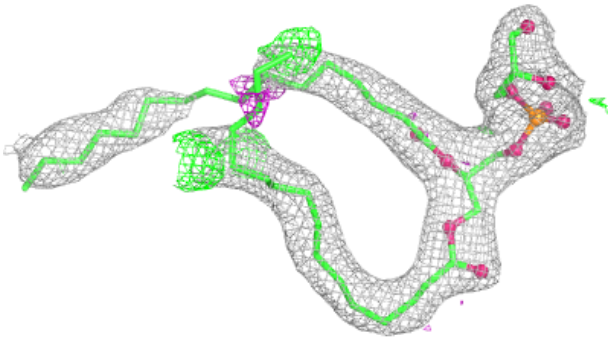


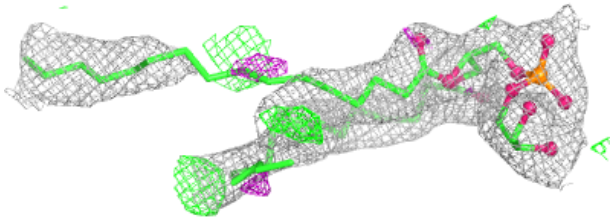


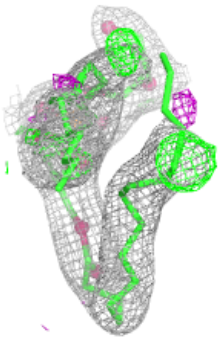


Electron density around LHG D 407 (A):

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

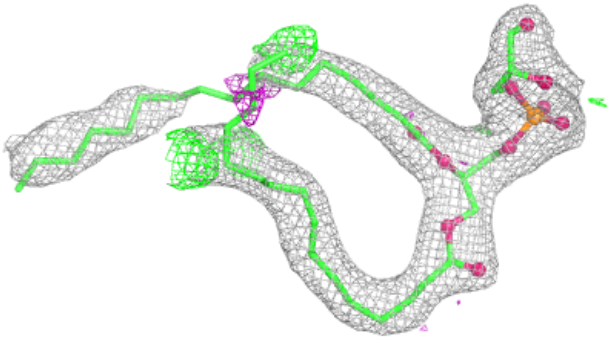


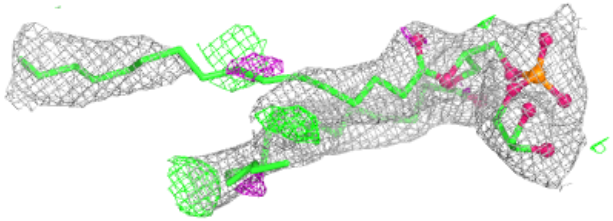


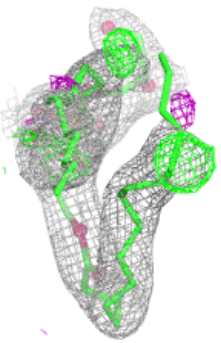


Electron density around LHG D 407 (B):

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

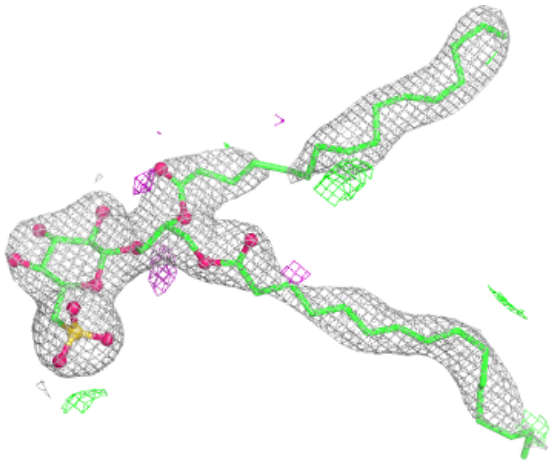


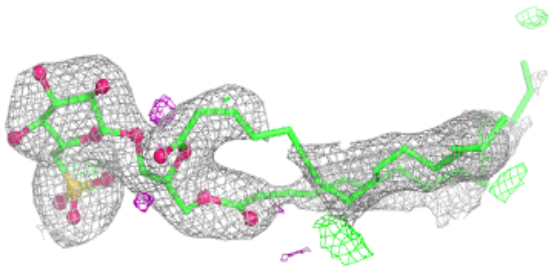


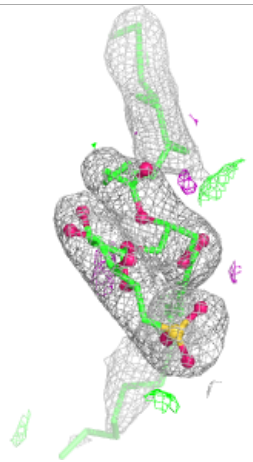


Electron density around SQD a 410 (B):

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

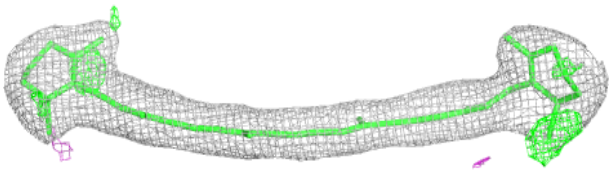


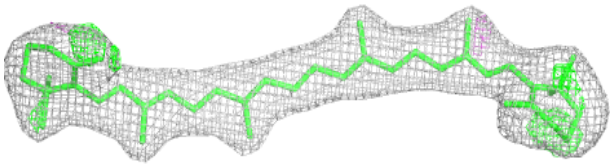


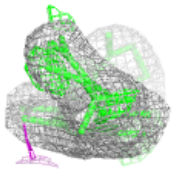


Electron density around BCR D 404:

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

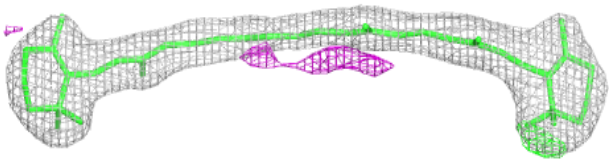


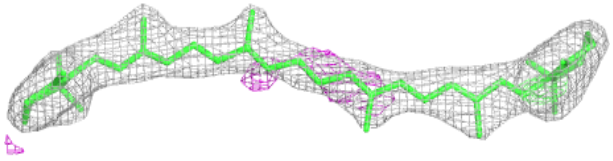


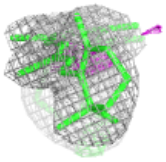


Electron density around BCR K 102:

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

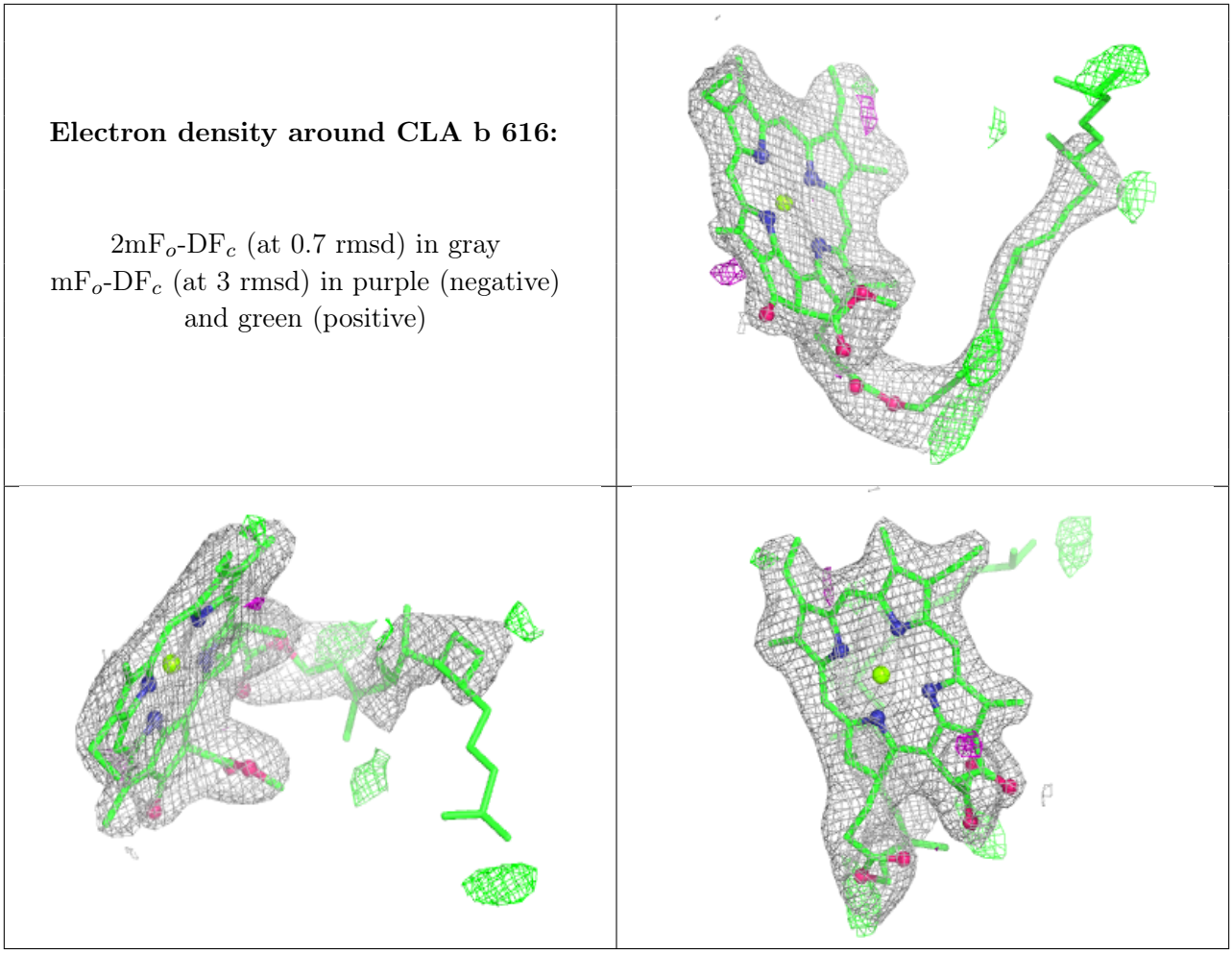






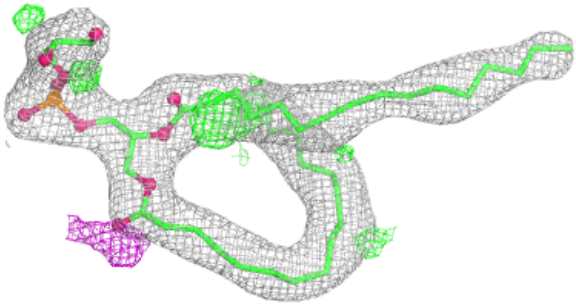
Electron density around CLA b 616:

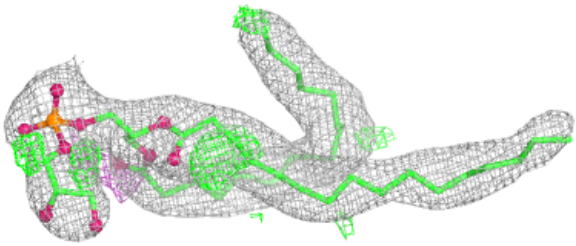
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

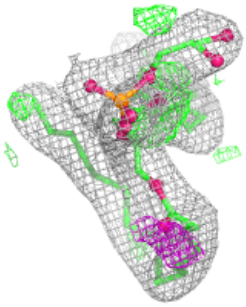


Electron density around LHG d 412 (A):

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

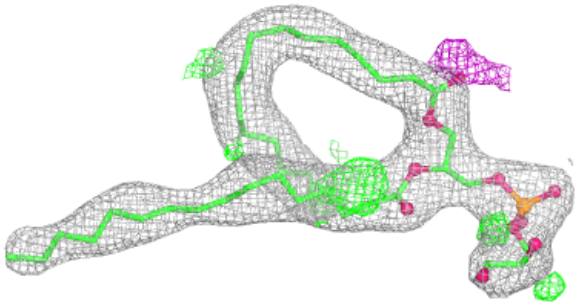


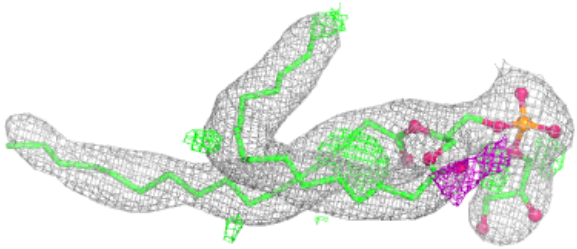


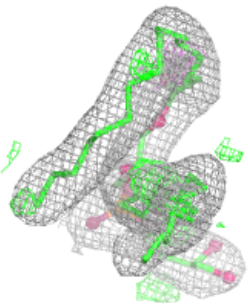


Electron density around LHG d 412 (B):

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

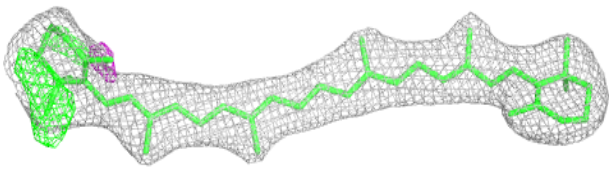


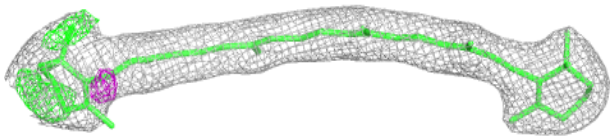


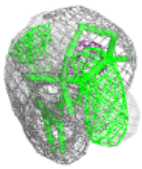


Electron density around BCR d 404:

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

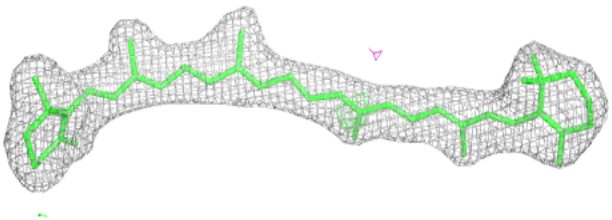


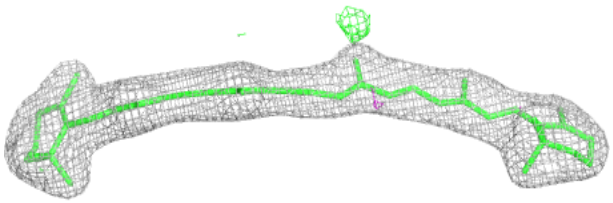


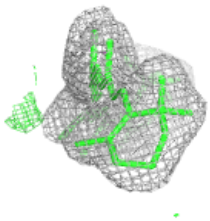


Electron density around BCR t 102:

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

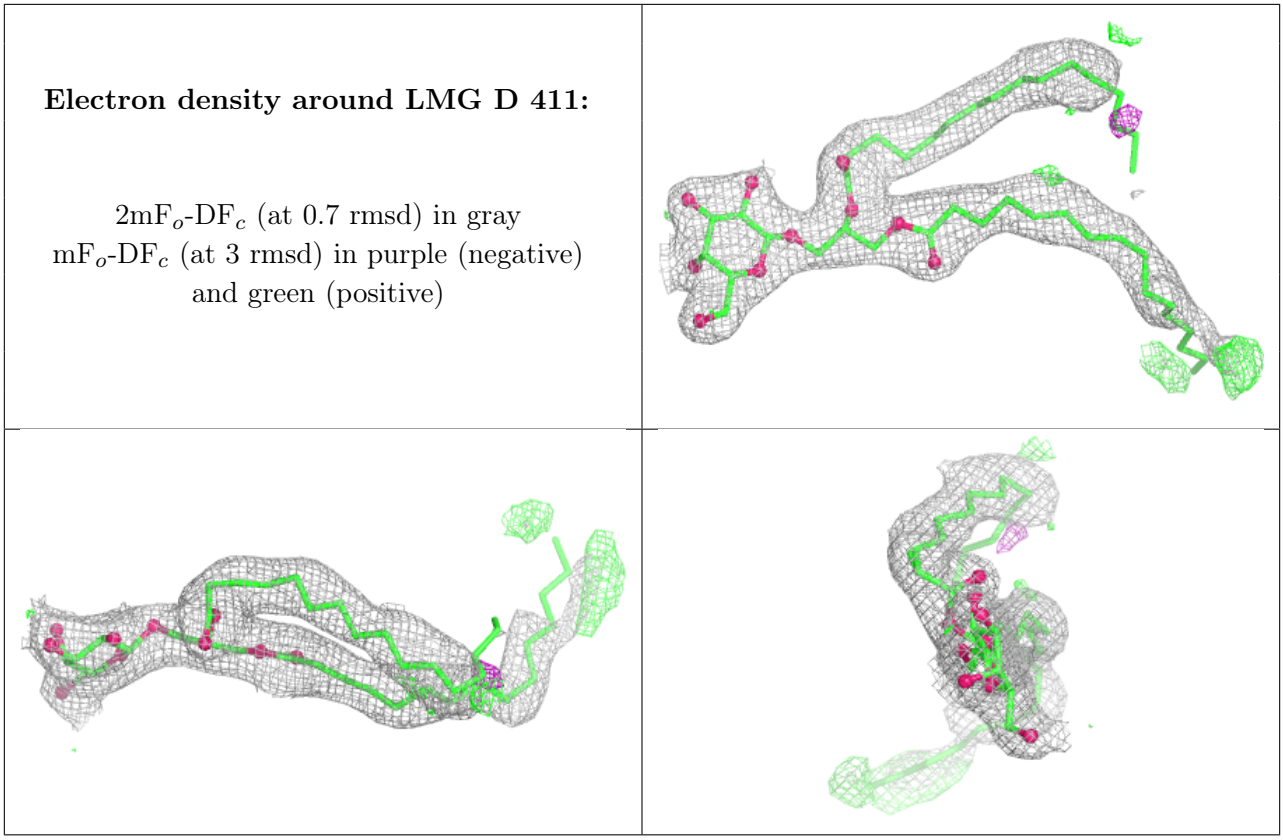






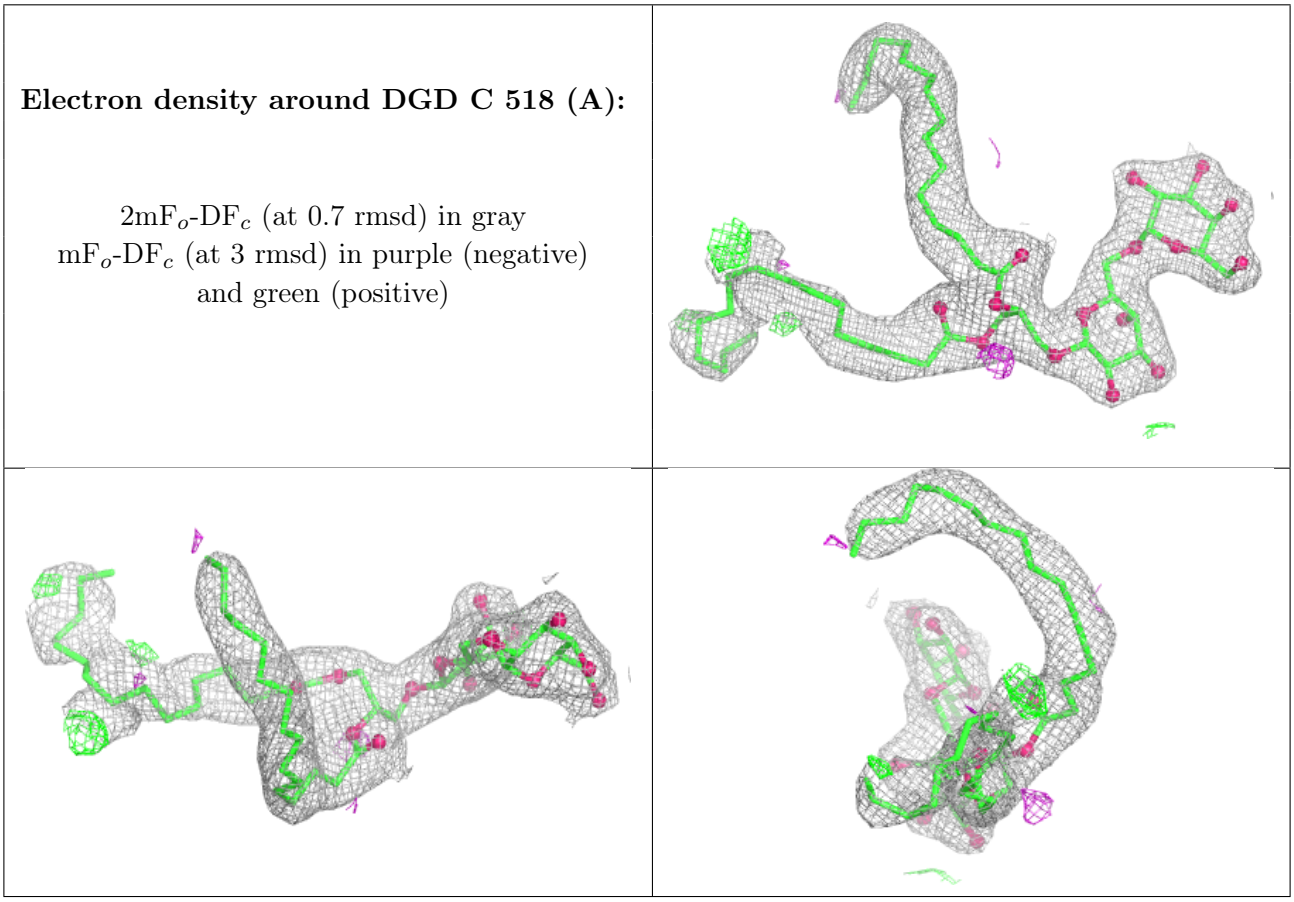
Electron density around LMG D 411:

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



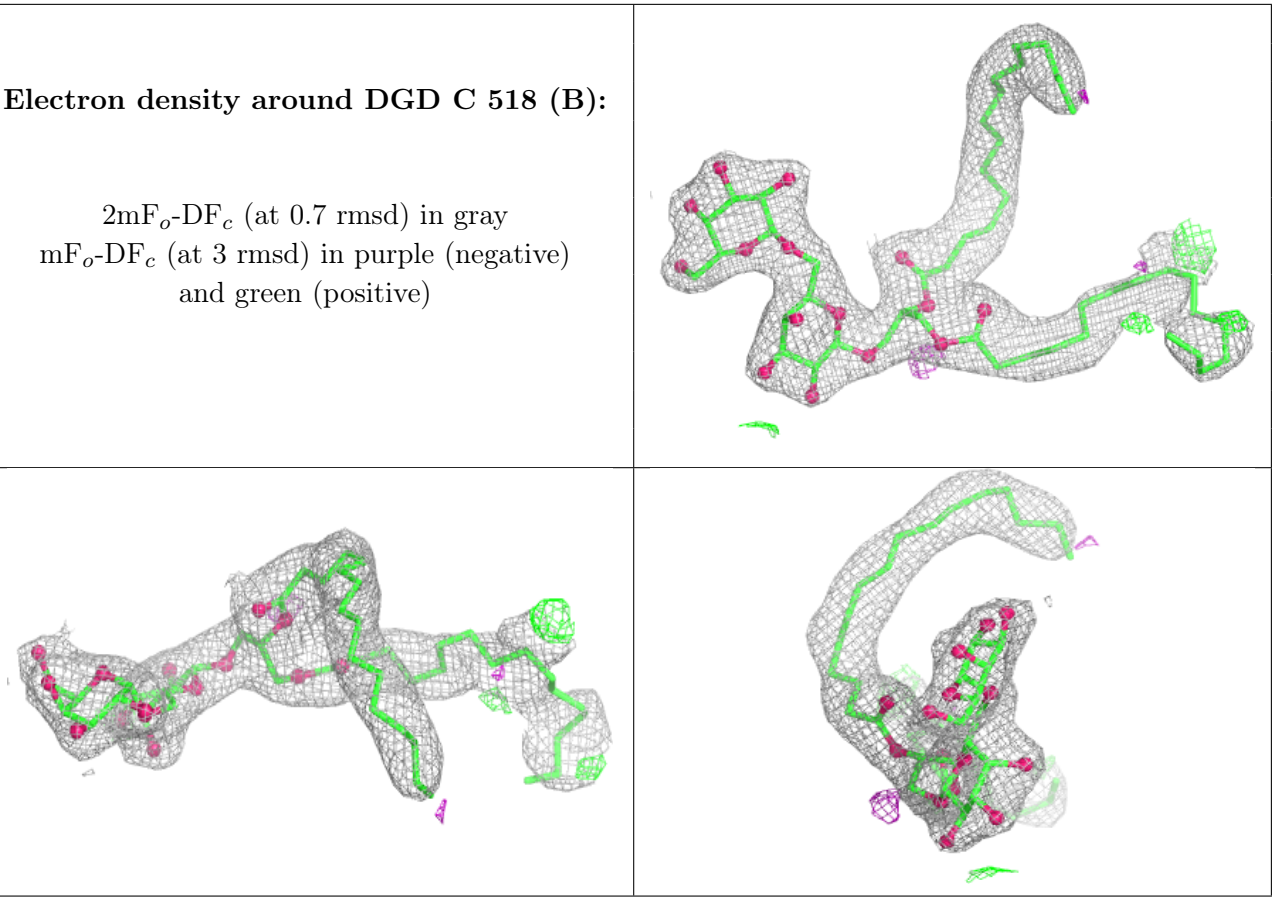
Electron density around DGD C 518 (A):

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



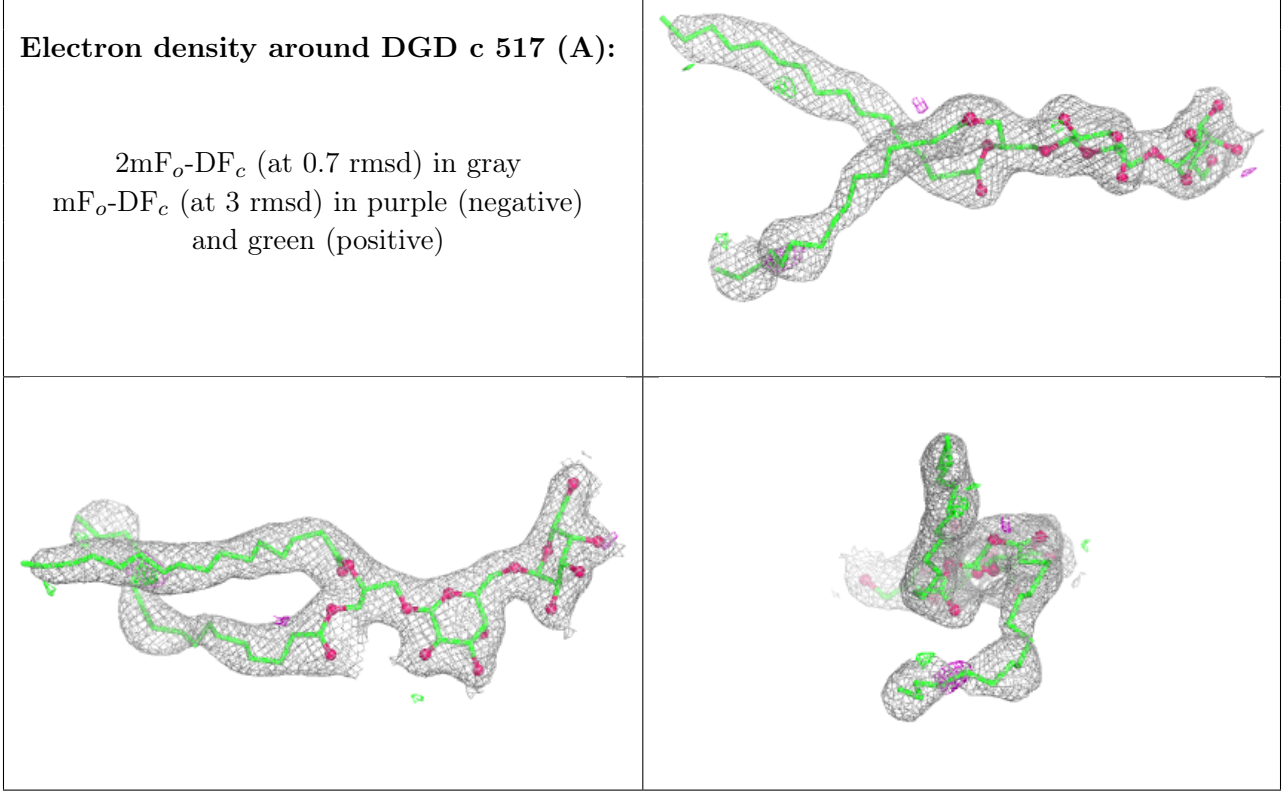
Electron density around DGD C 518 (B):

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



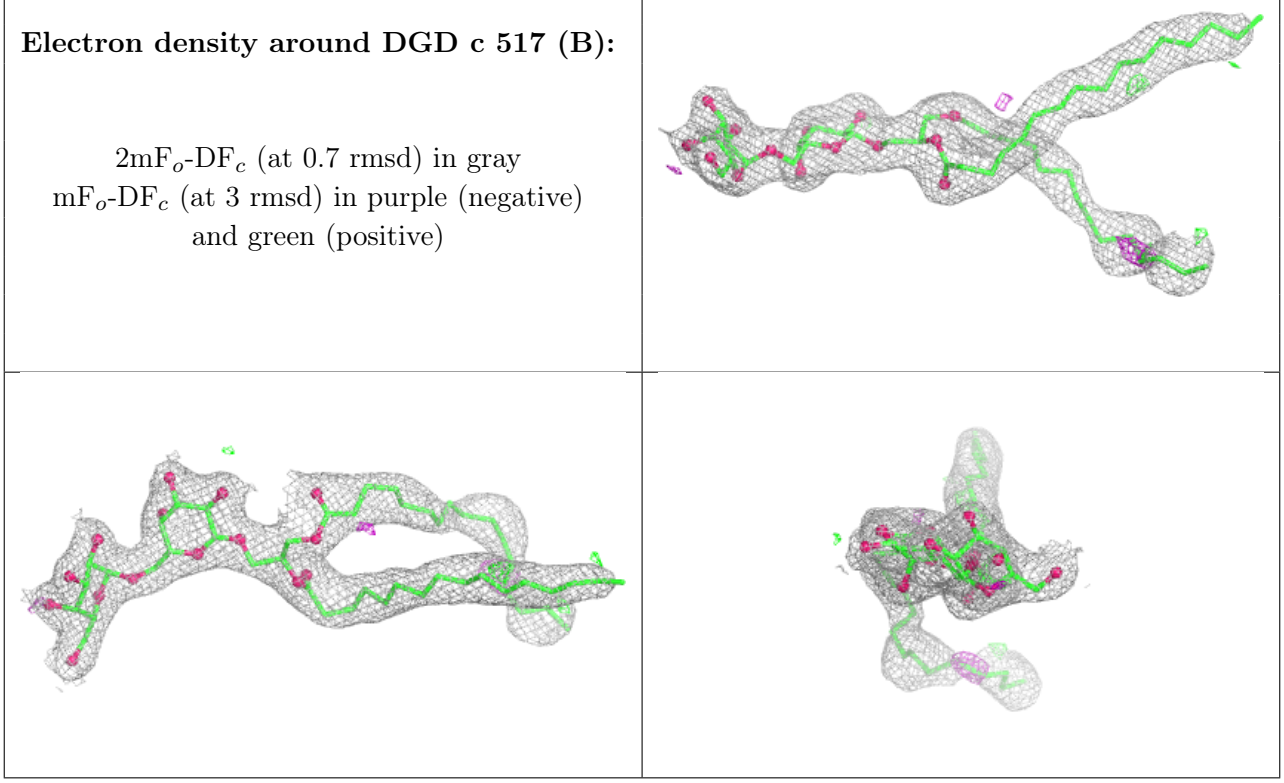
Electron density around DGD c 517 (A):

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



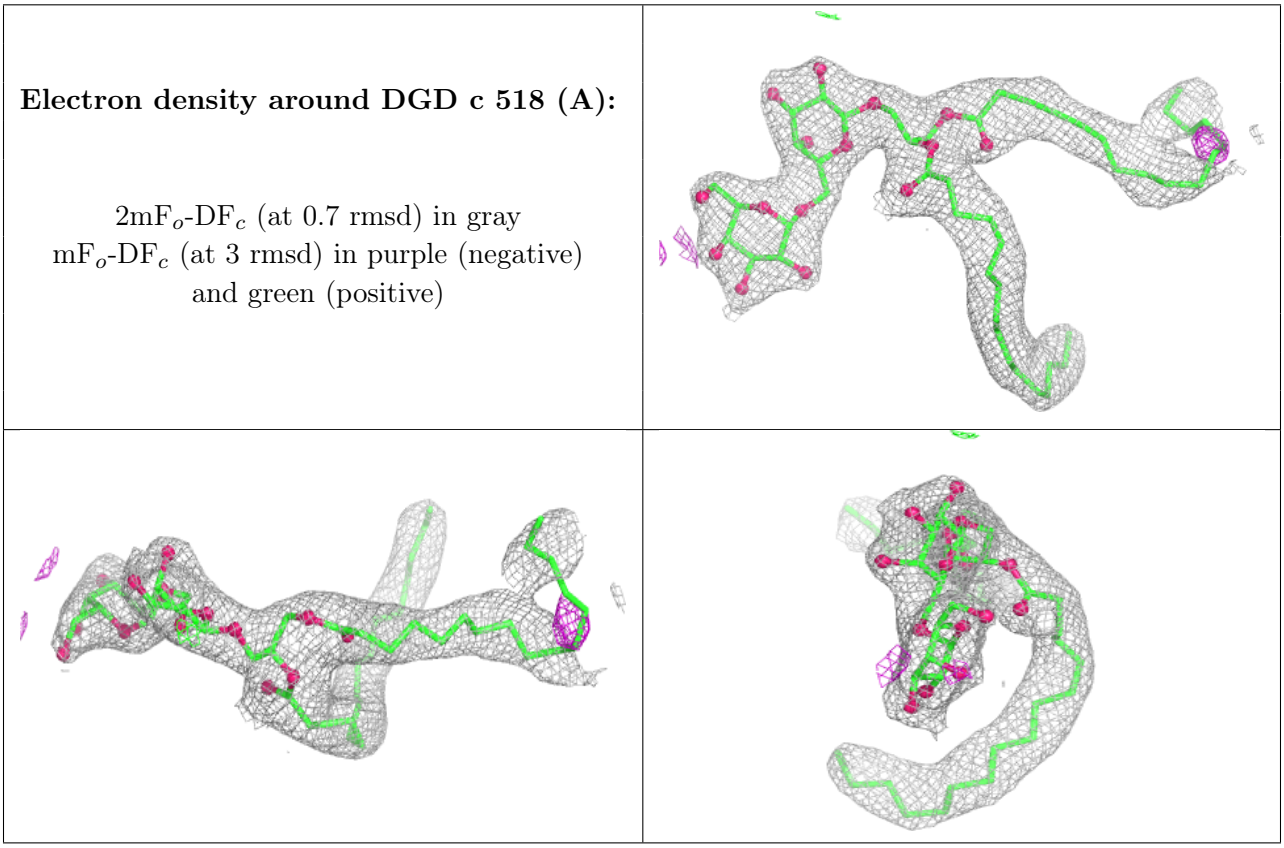
Electron density around DGD c 517 (B):

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



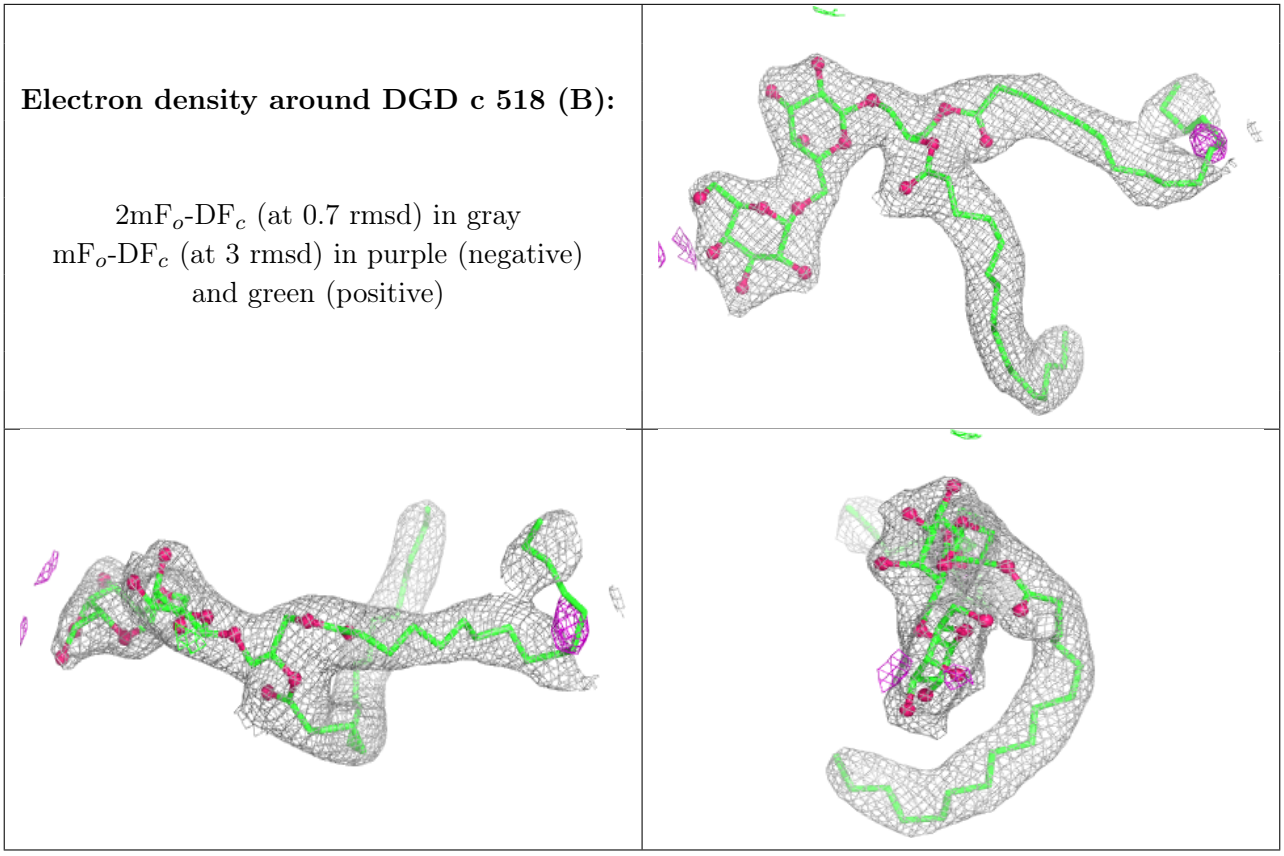
Electron density around DGD c 518 (A):

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



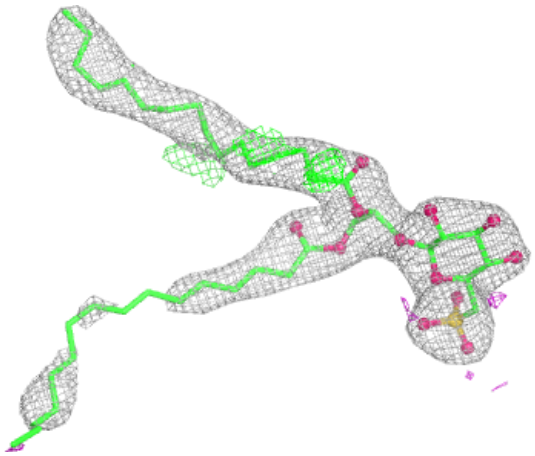
Electron density around DGD c 518 (B):

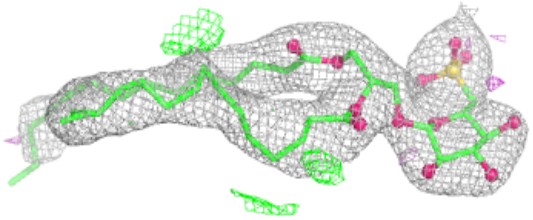
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

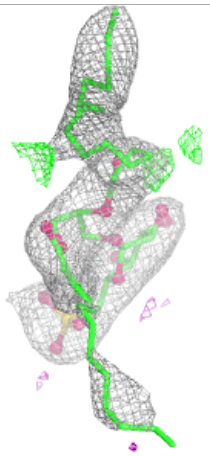


Electron density around SQD A 410 (A):

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

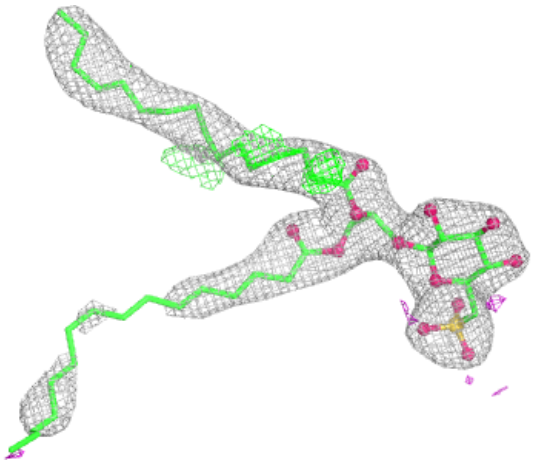


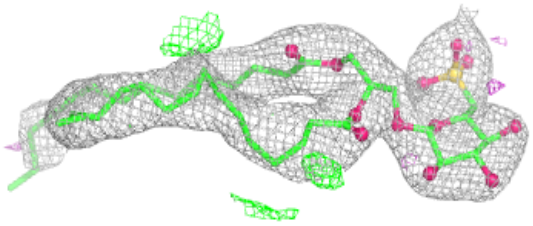


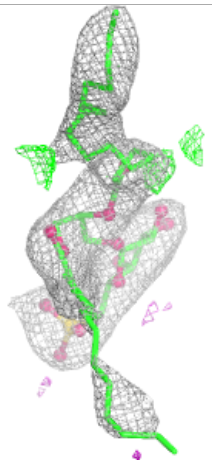


Electron density around SQD A 410 (B):

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

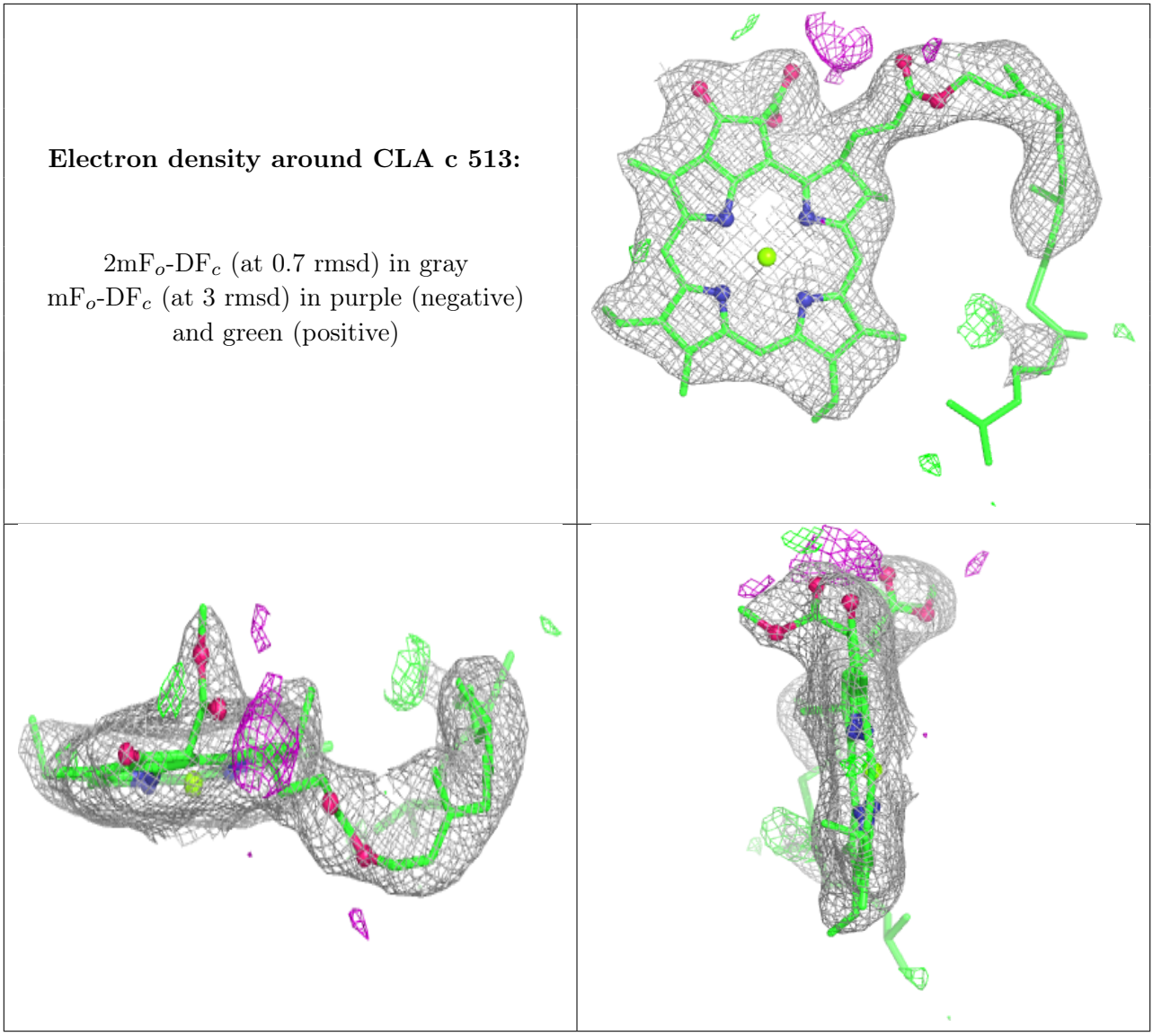






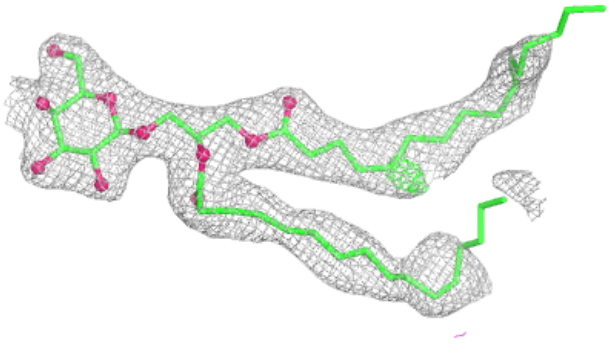
Electron density around CLA c 513:

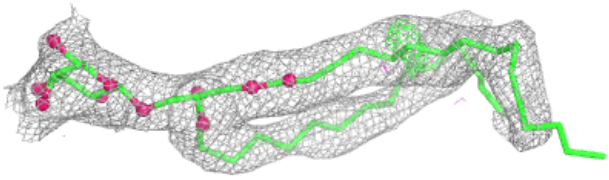
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

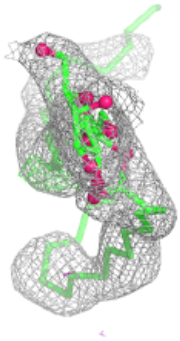


Electron density around LMG d 410:

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

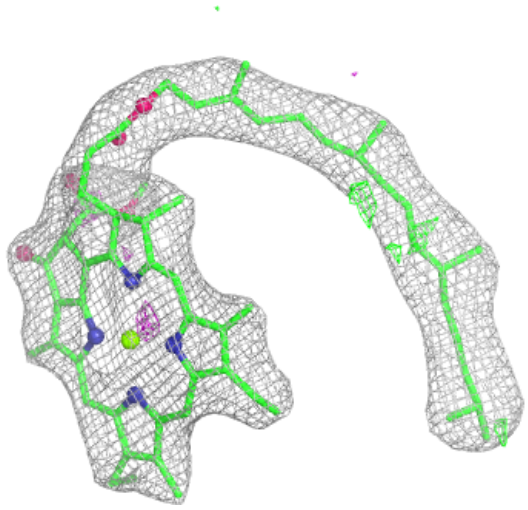


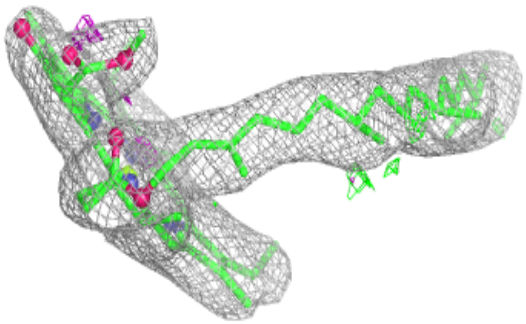


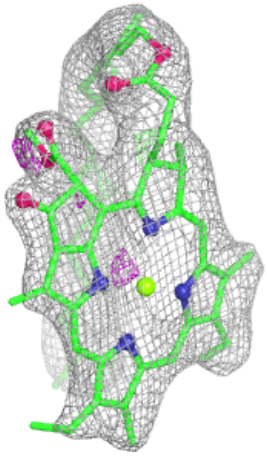


Electron density around CLA c 508:

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

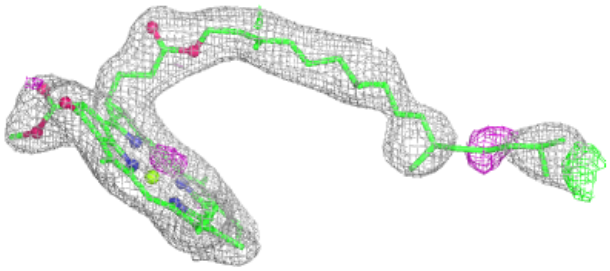


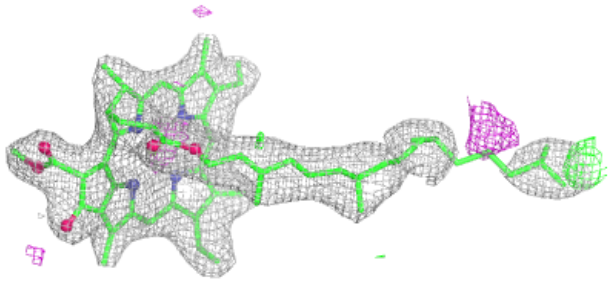


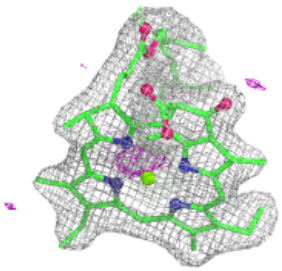


Electron density around CLA C 505:

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

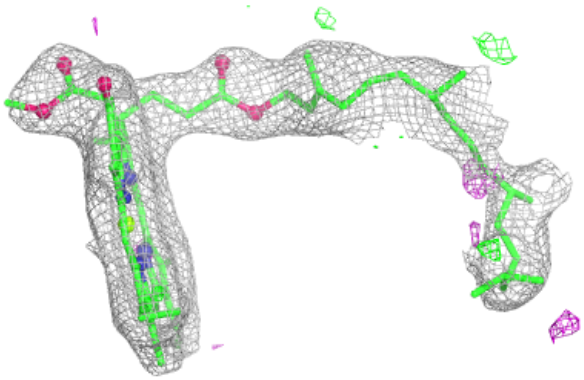


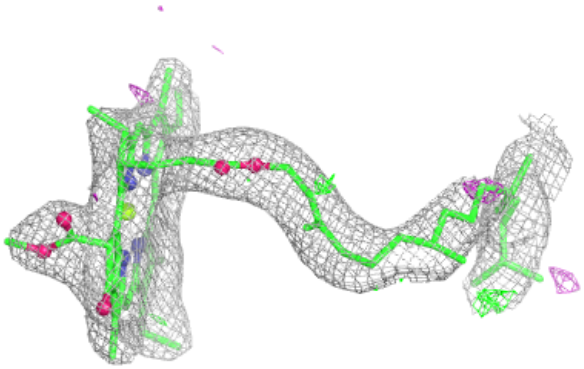


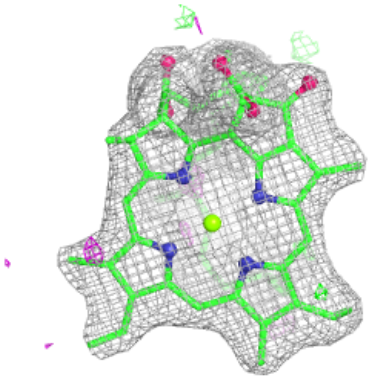


Electron density around CLA C 507:

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

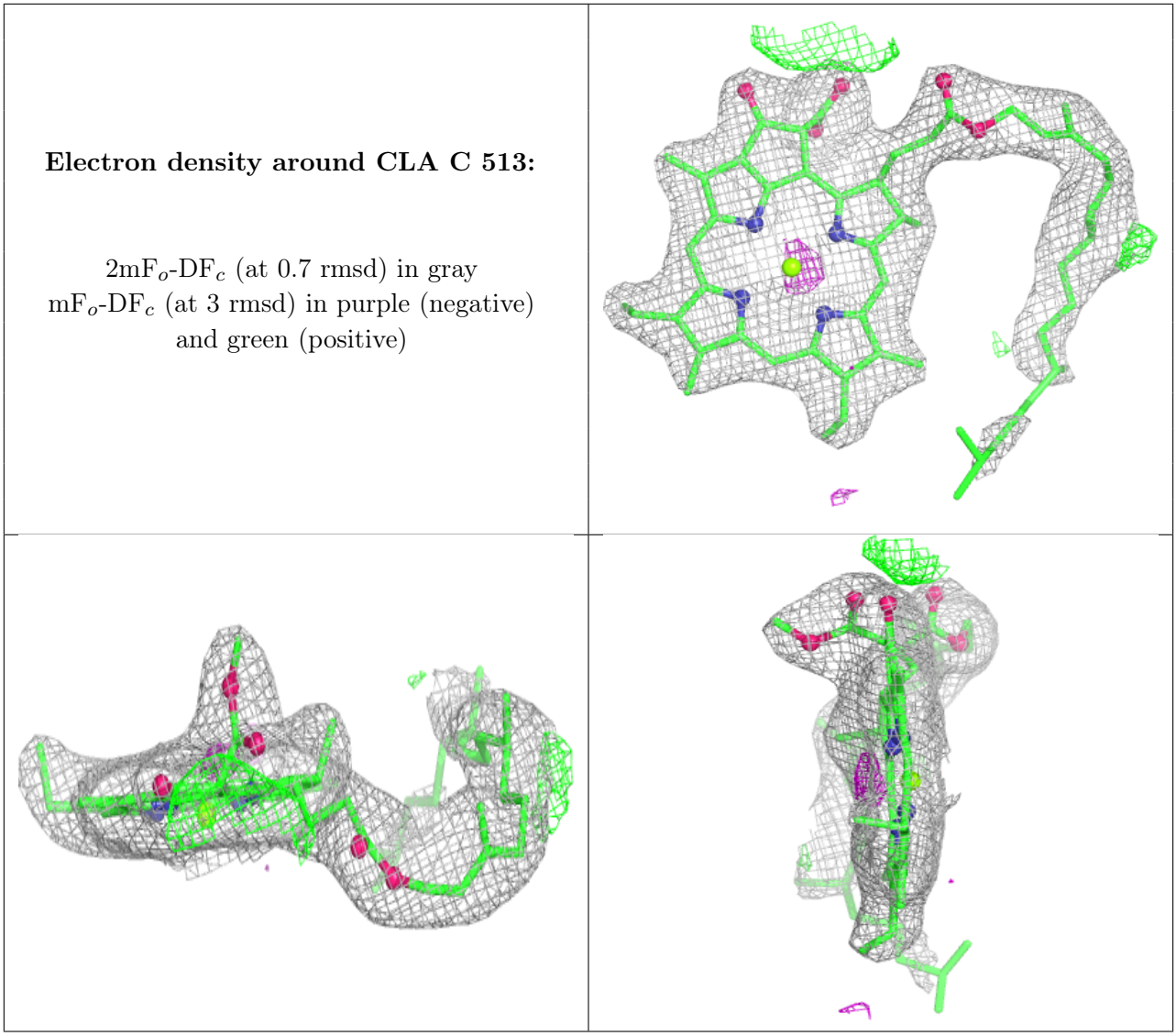






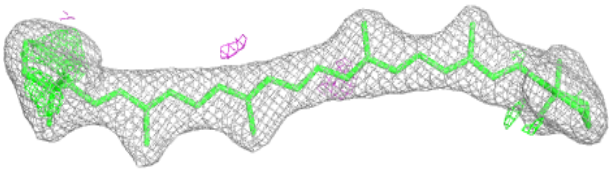
Electron density around CLA C 513:

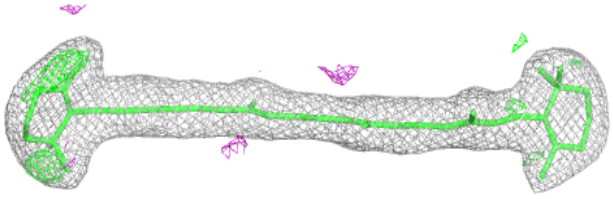
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

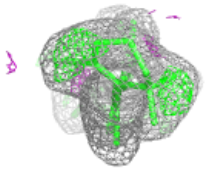


Electron density around BCR A 409:

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

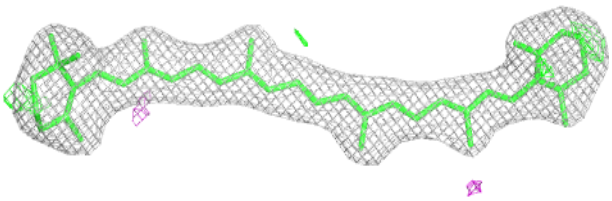


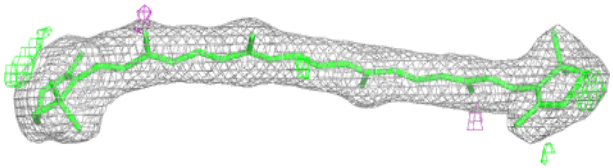


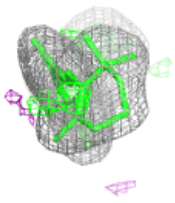


Electron density around BCR B 619:

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



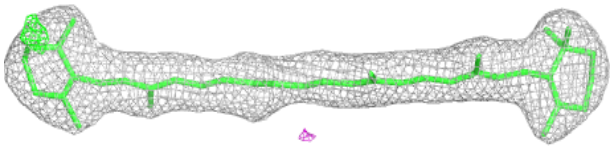


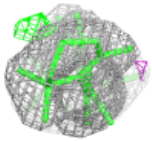


Electron density around BCR C 515:

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

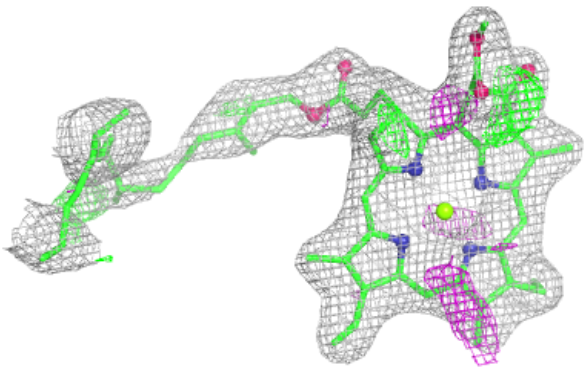


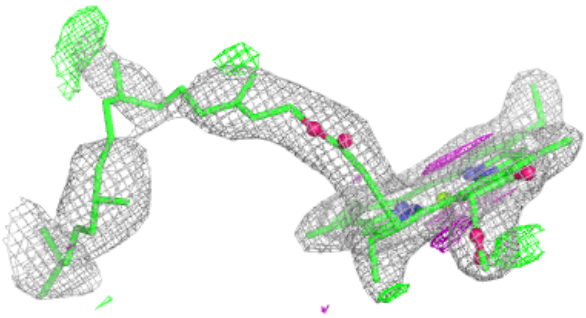


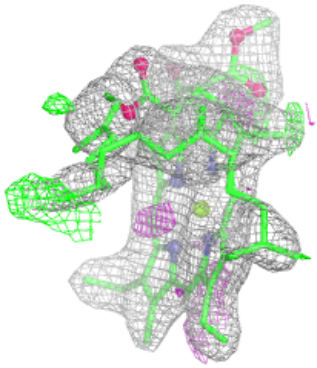


Electron density around CLA A 408:

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

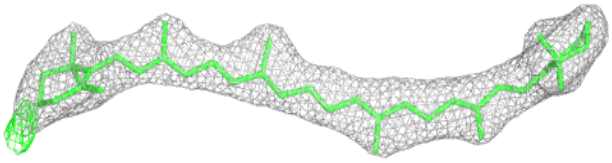


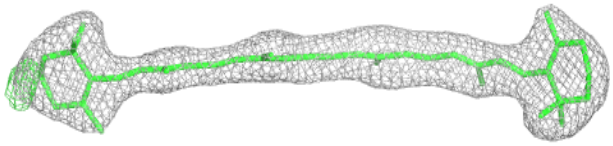


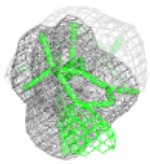


Electron density around BCR H 101:

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

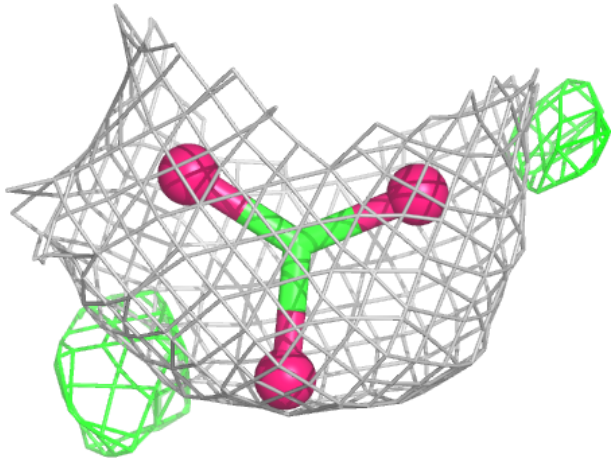


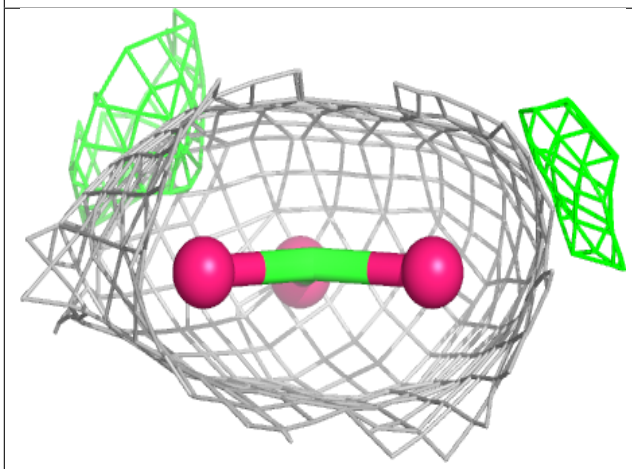


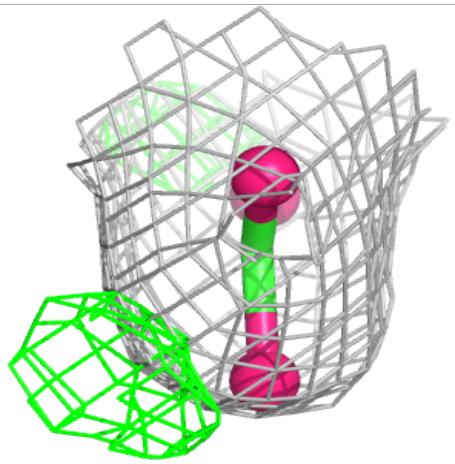


Electron density around BCT d 401 (A):

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

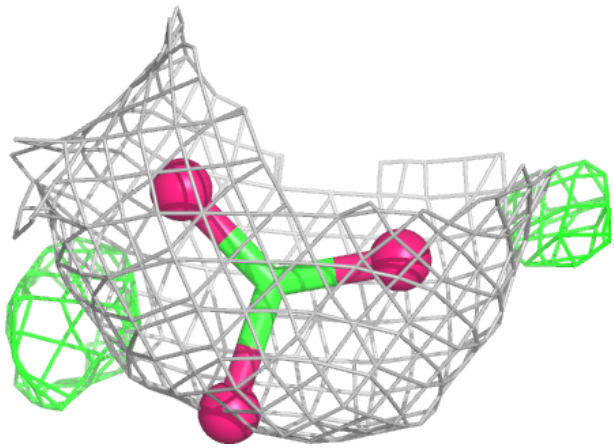


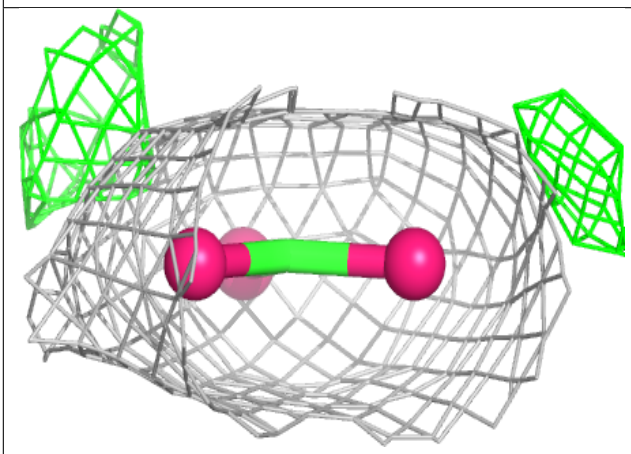


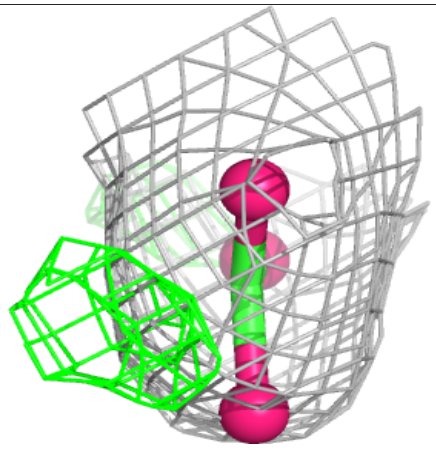


Electron density around BCT d 401 (B):

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

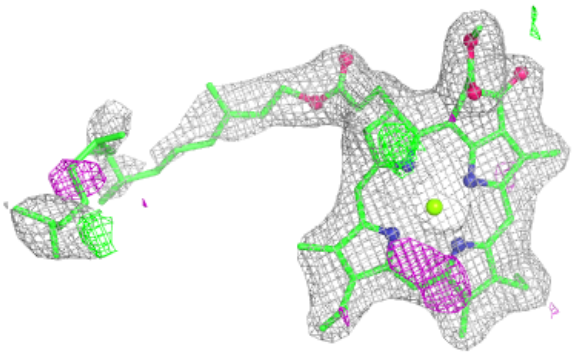


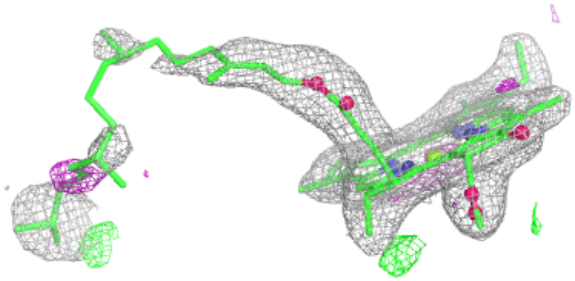


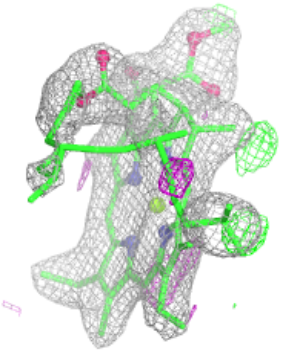


Electron density around CLA a 408:

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

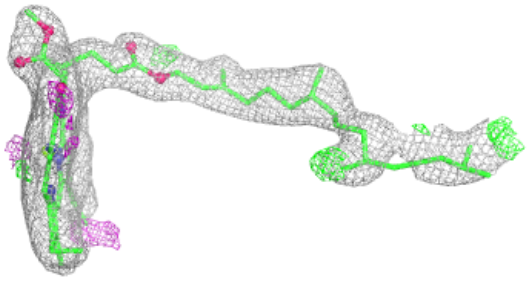


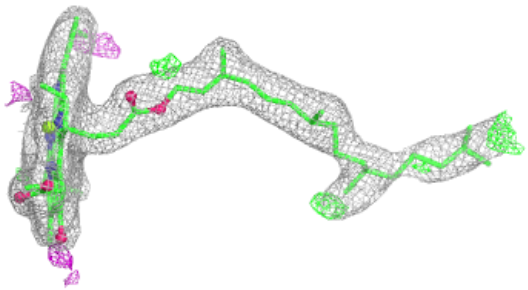


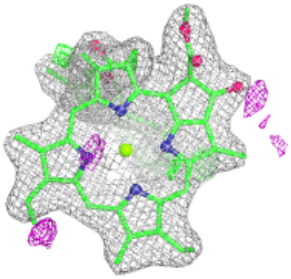


Electron density around CLA B 606:

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

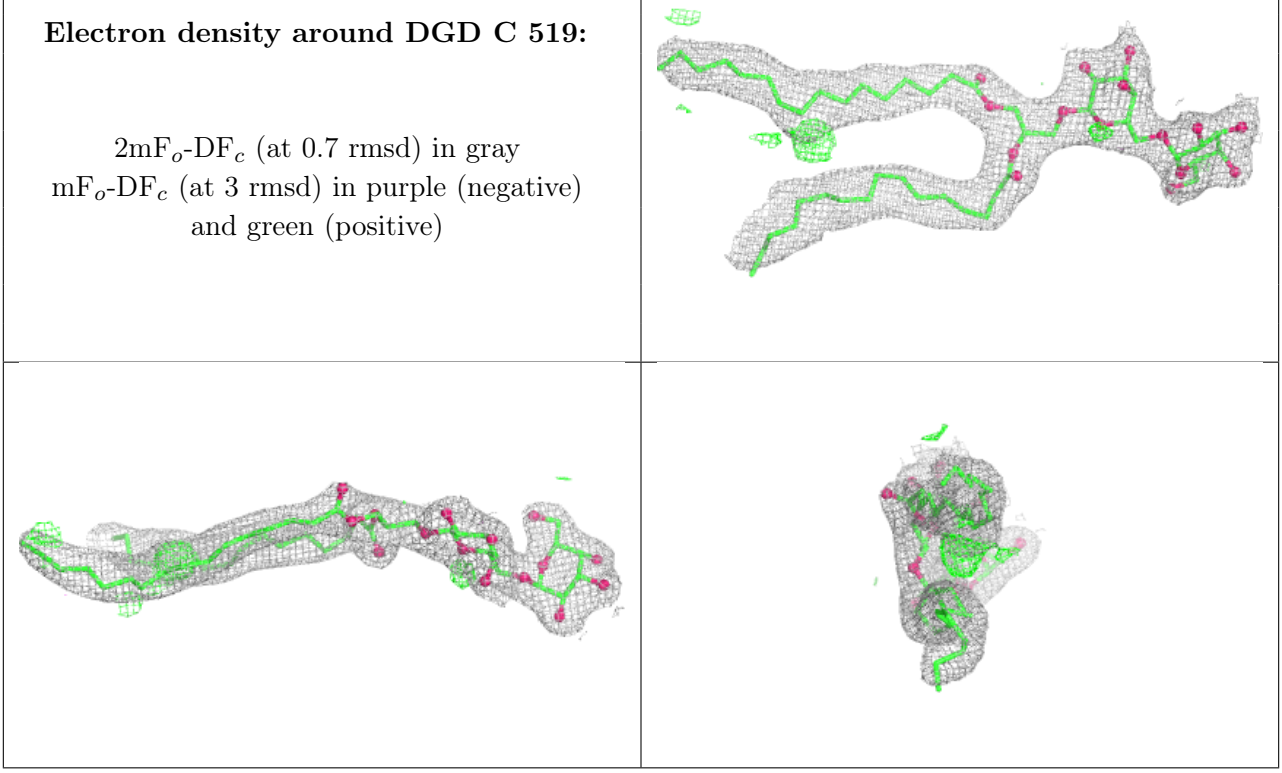






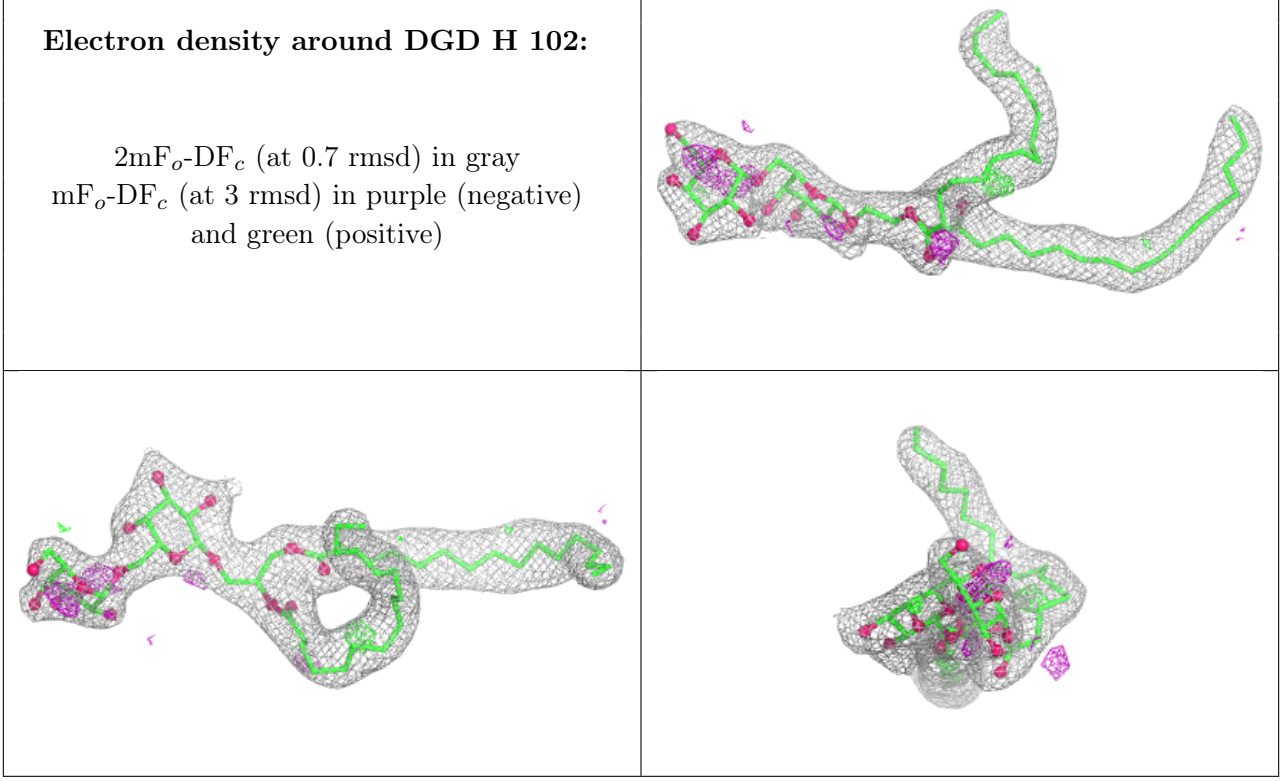
Electron density around DGD C 519:

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



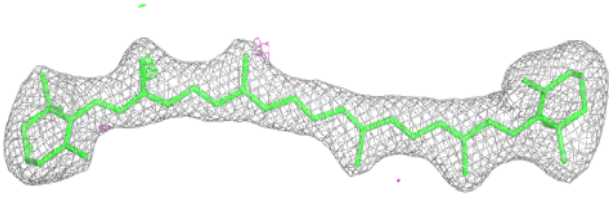
Electron density around DGD H 102:

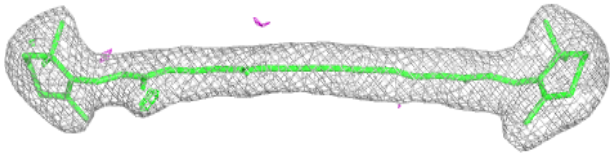
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

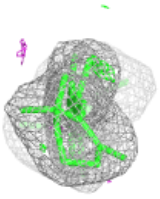


Electron density around BCR b 618:

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

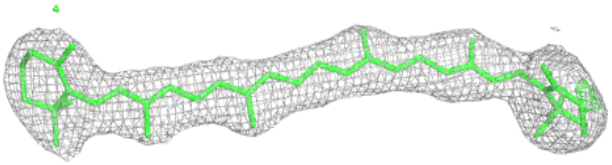


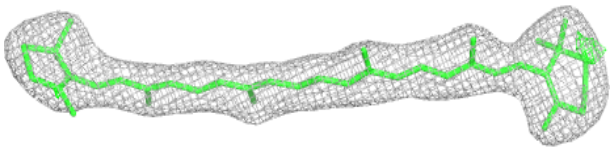


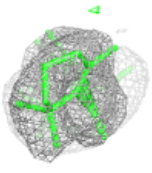


Electron density around BCR c 515:

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

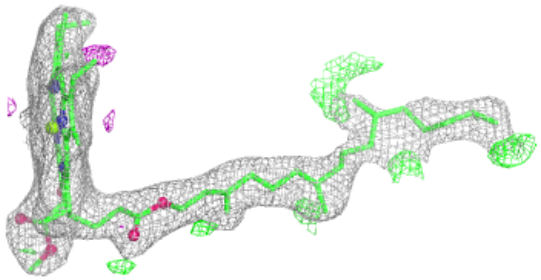


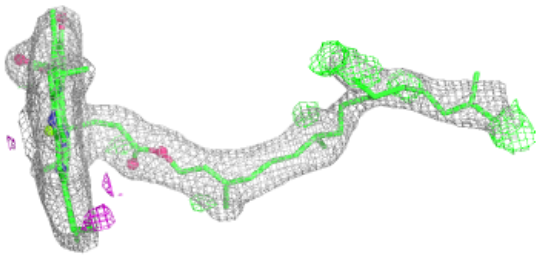


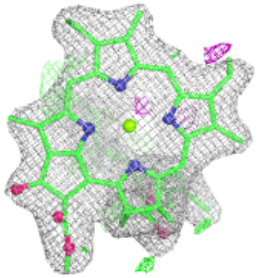


Electron density around CLA b 606:

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

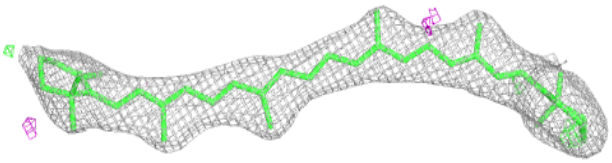


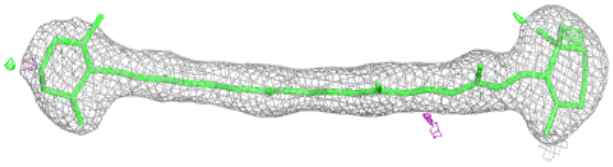


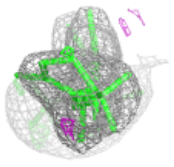


Electron density around BCR h 101:

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

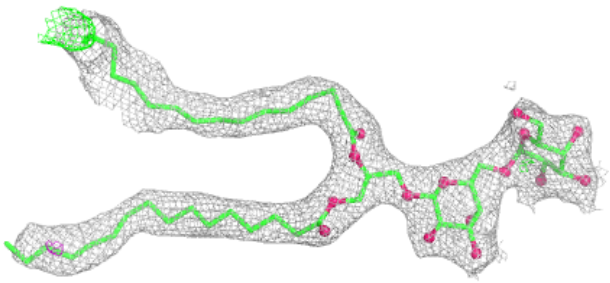


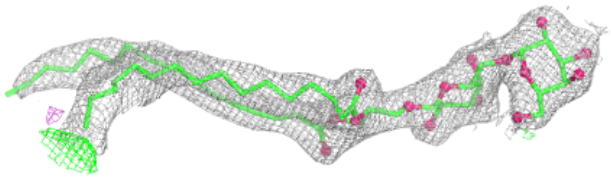


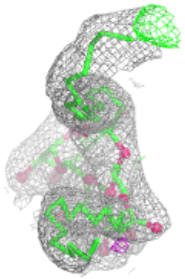


Electron density around DGD c 519:

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

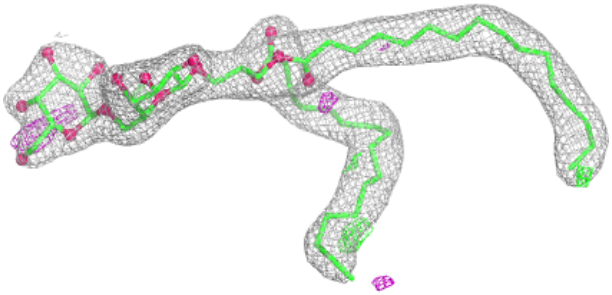


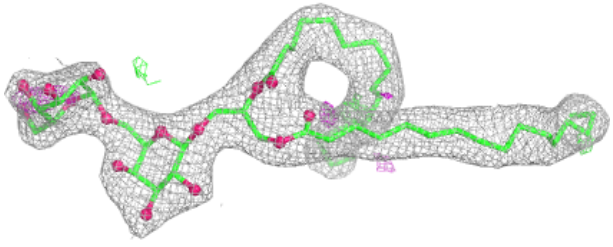


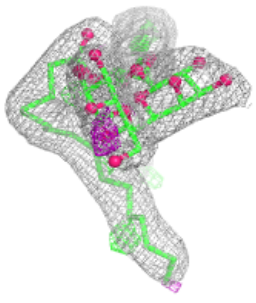


Electron density around DGD h 102:

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

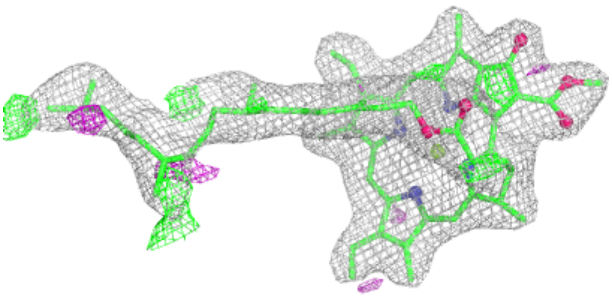


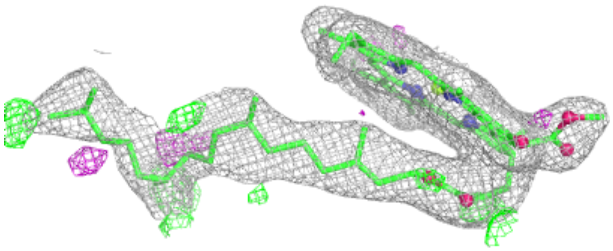


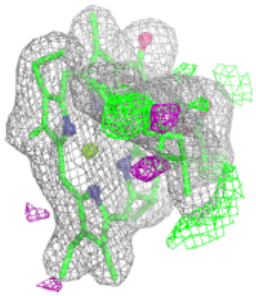


Electron density around CLA b 614:

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

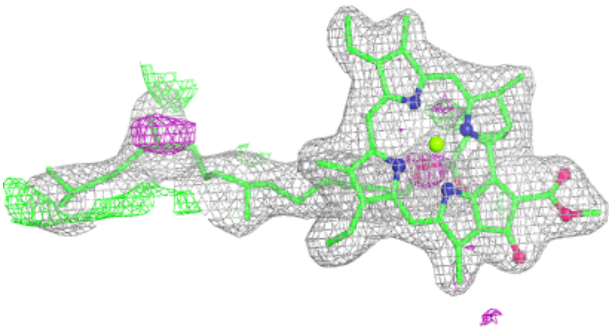


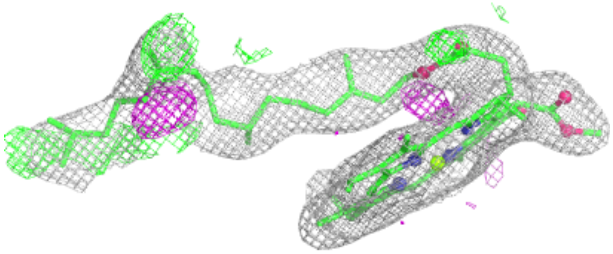


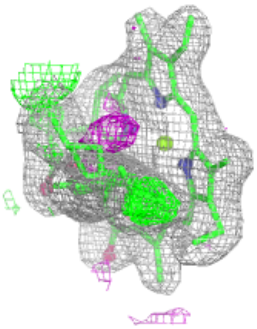


Electron density around CLA B 614:

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

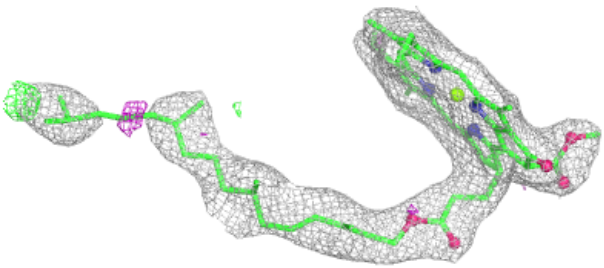


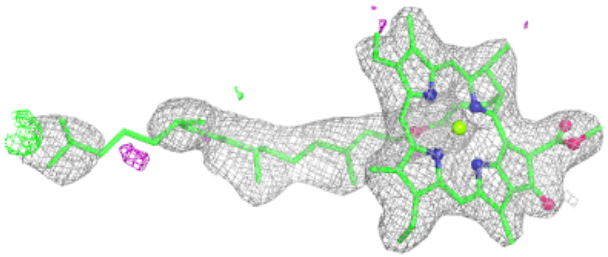


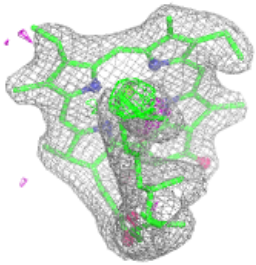


Electron density around CLA c 505:

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

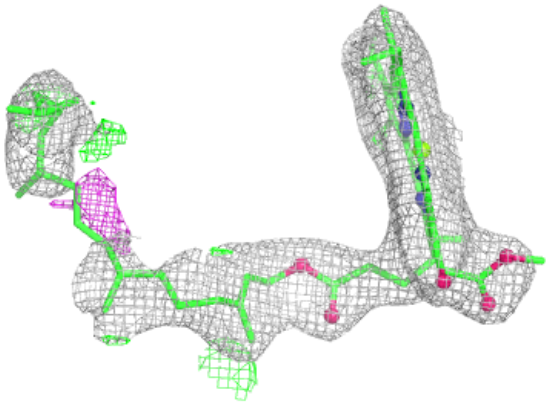


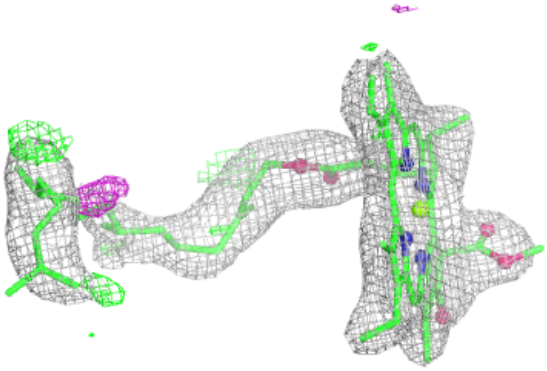


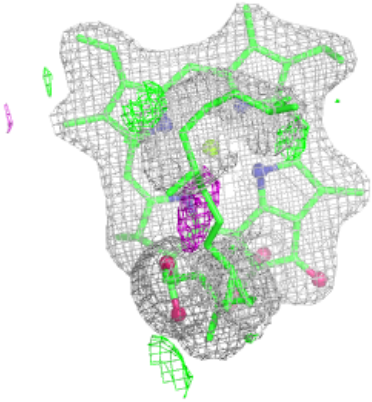


Electron density around CLA c 507:

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

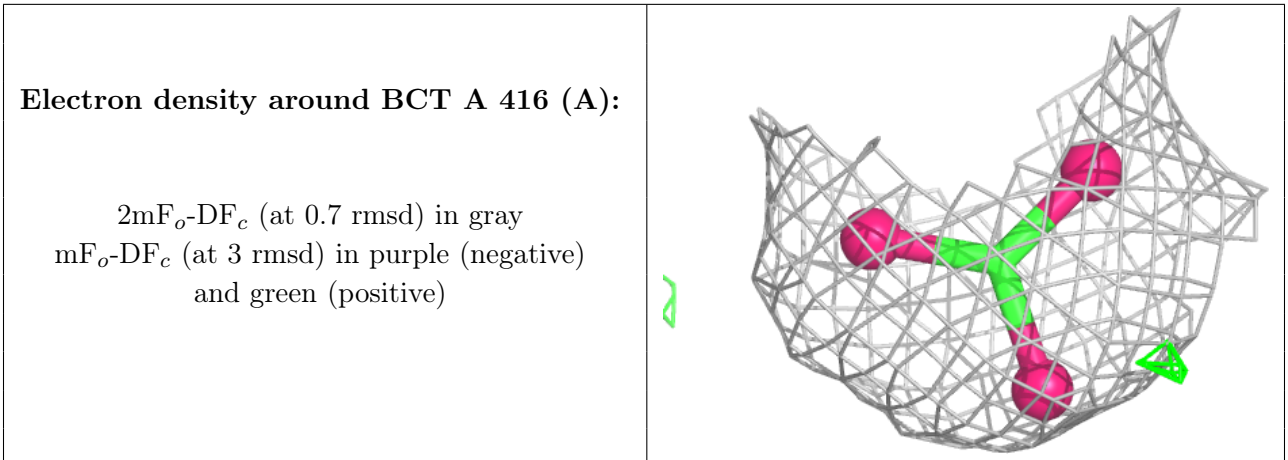


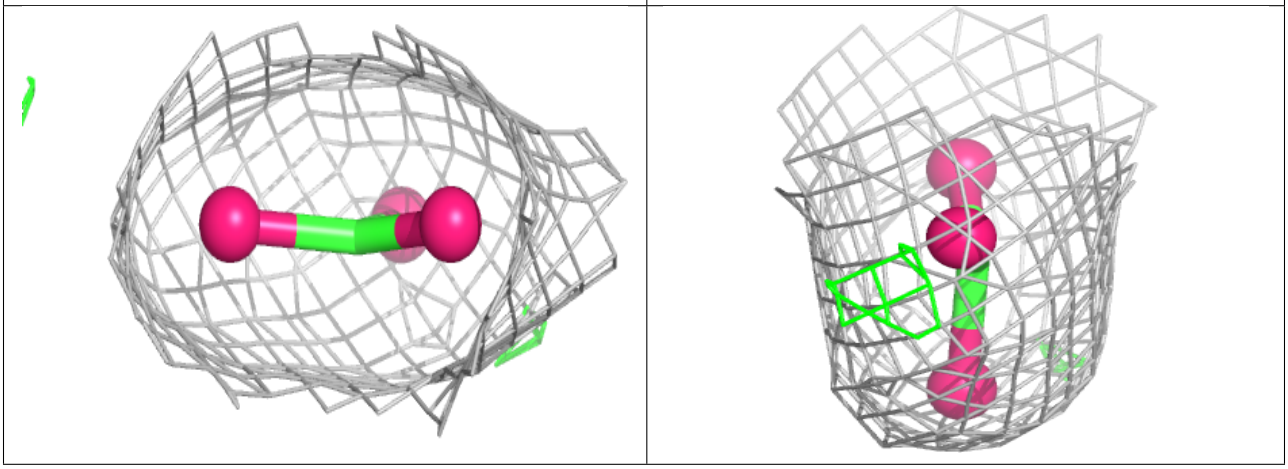




Electron density around BCT A 416 (A):

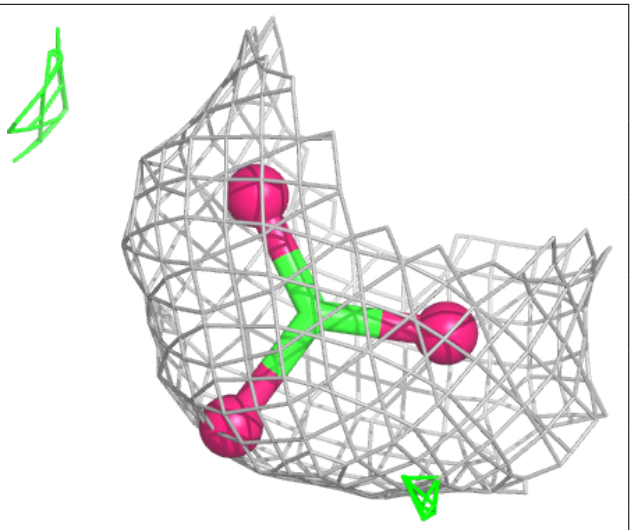
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

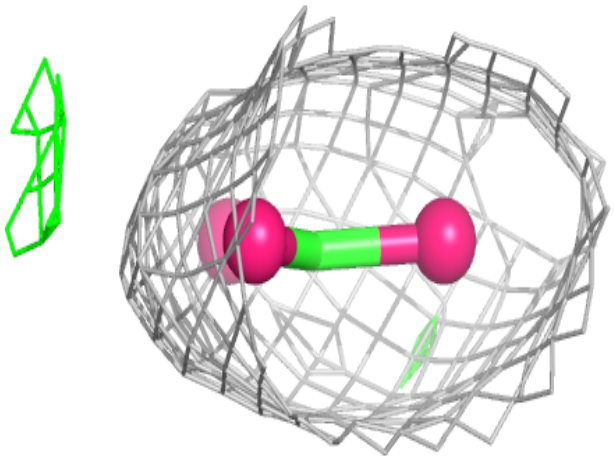


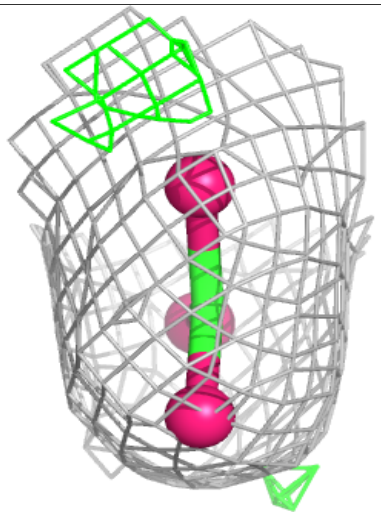


Electron density around BCT A 416 (B):

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

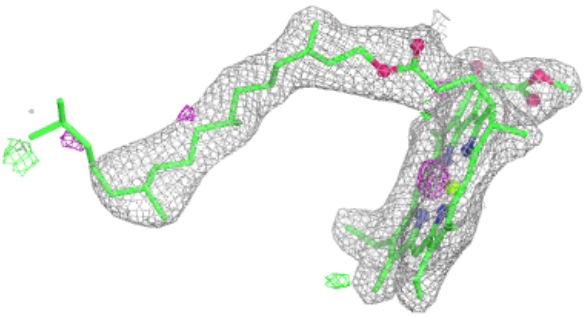


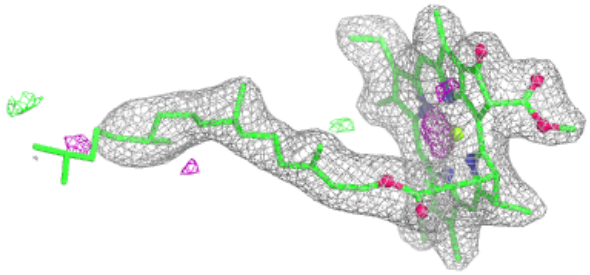


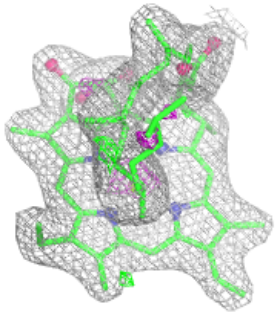


Electron density around CLA C 509:

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

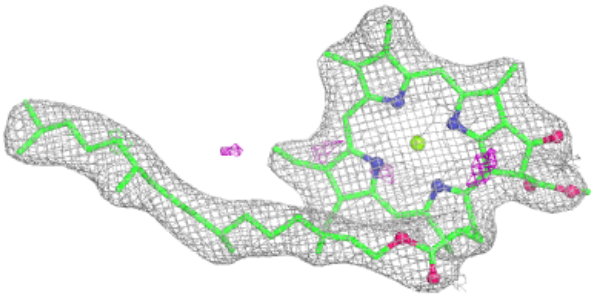


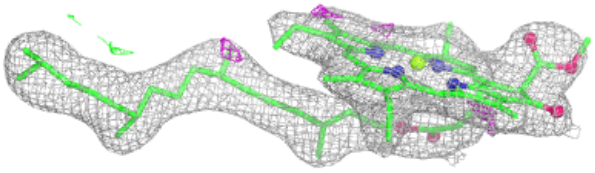


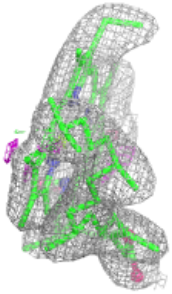


Electron density around CLA c 502:

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

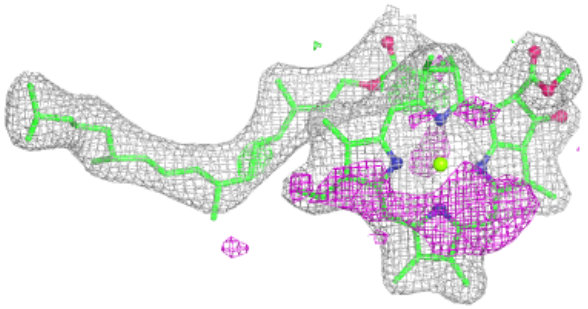


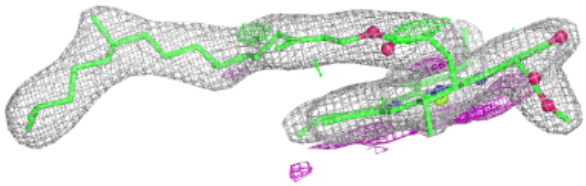


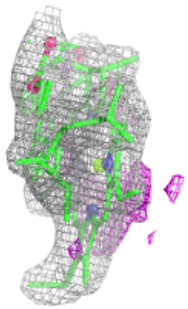


Electron density around CLA B 603:

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

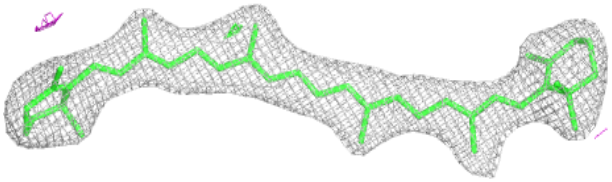


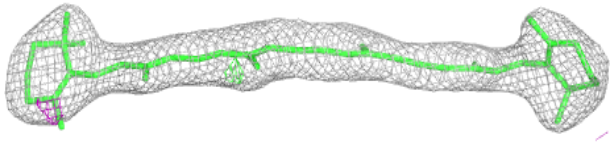


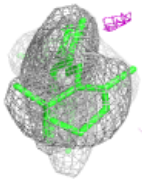


Electron density around BCR Y 101:

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

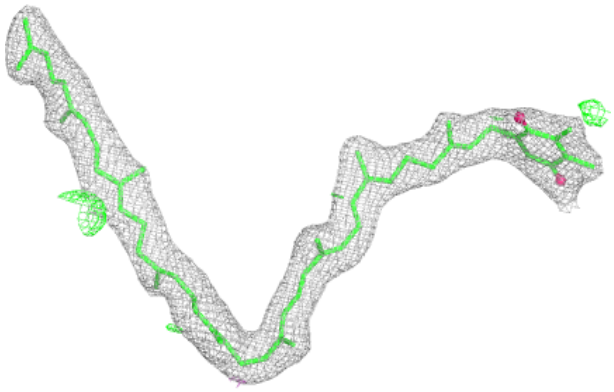


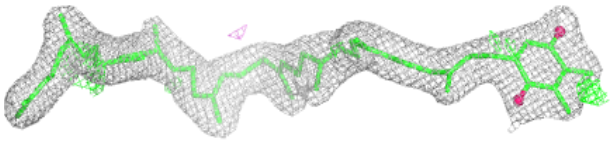


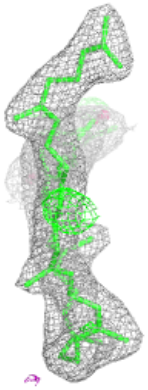


Electron density around PL9 D 405 (A):

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

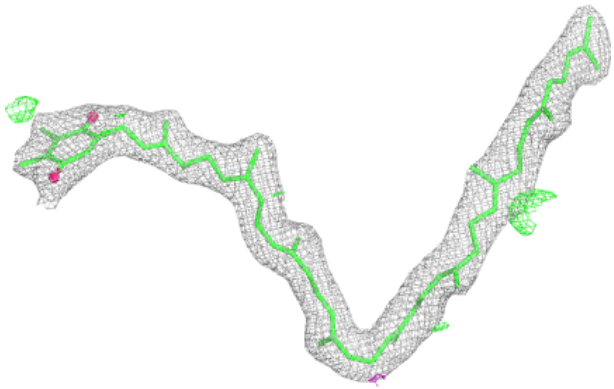


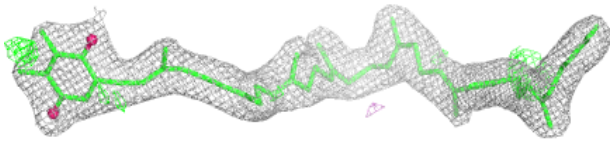




Electron density around PL9 D 405 (B):

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

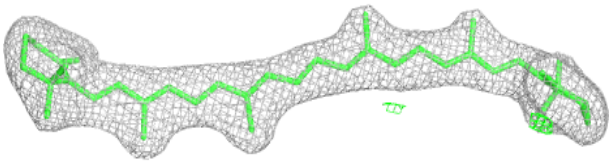


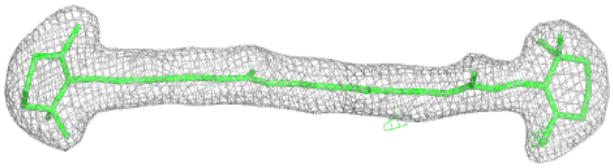


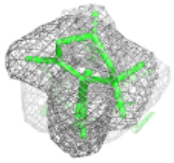


Electron density around BCR a 409:

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

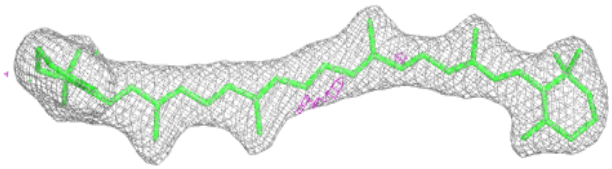


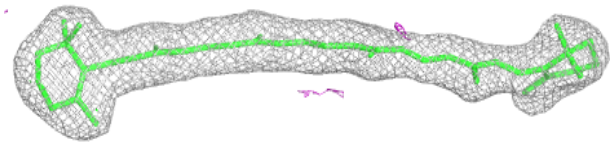


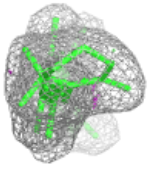


Electron density around BCR b 617:

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

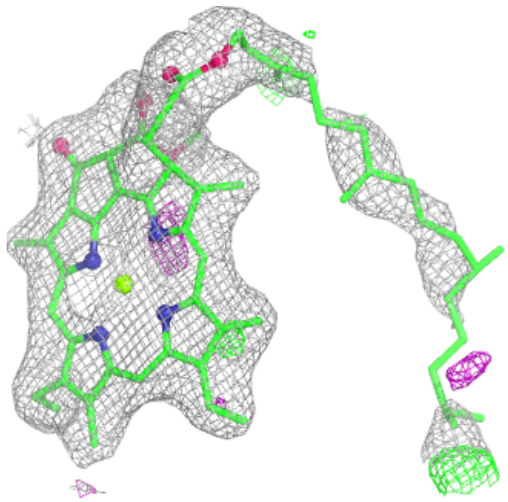


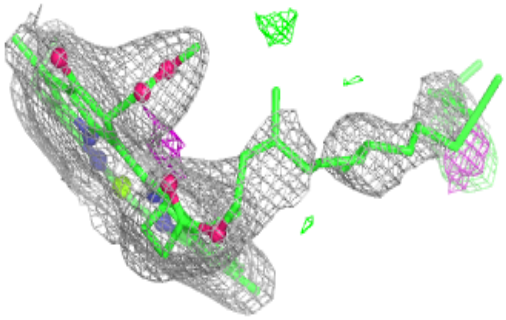


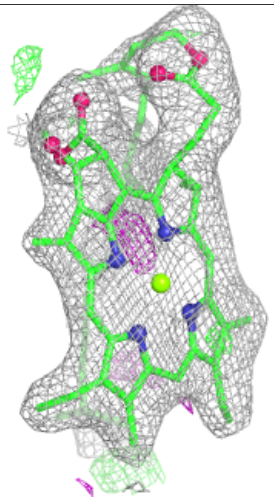


Electron density around CLA B 616:

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

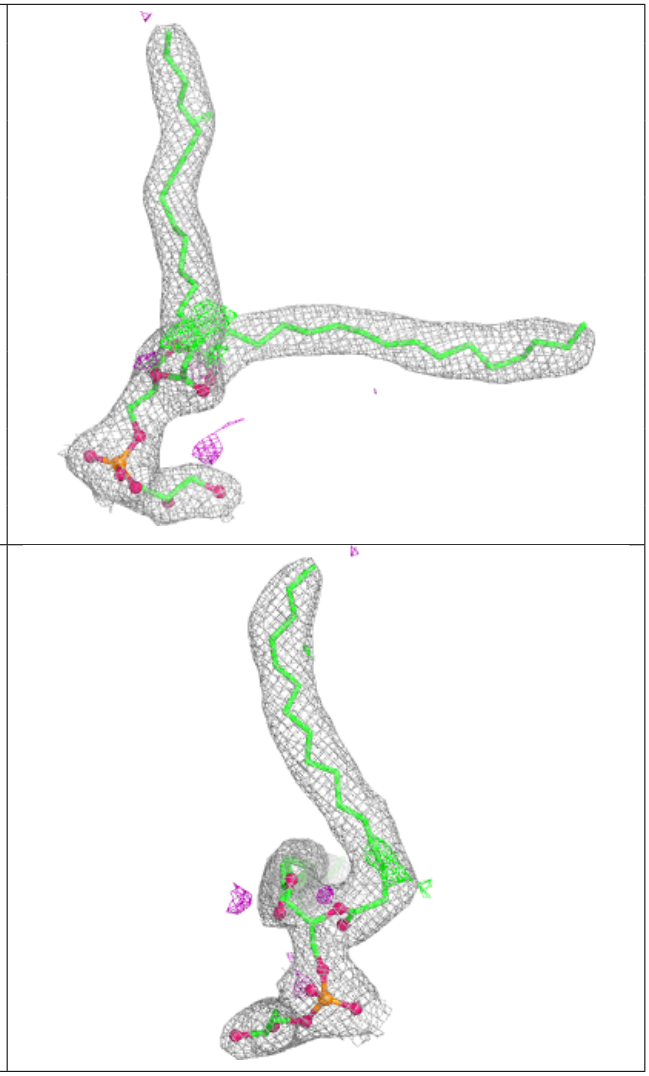


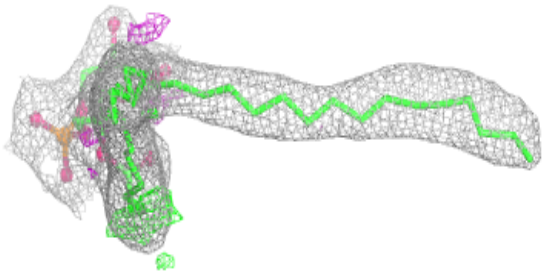




Electron density around LHG b 630 (A):

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

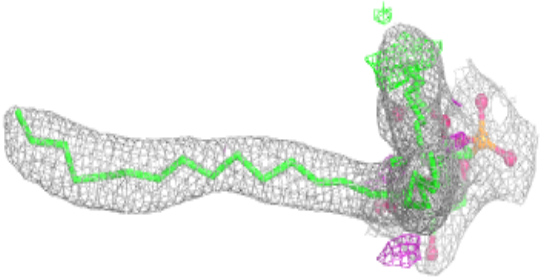


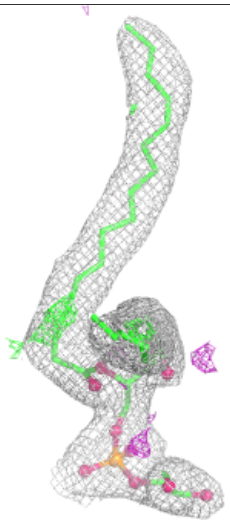


Electron density around LHG b 630 (B):

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

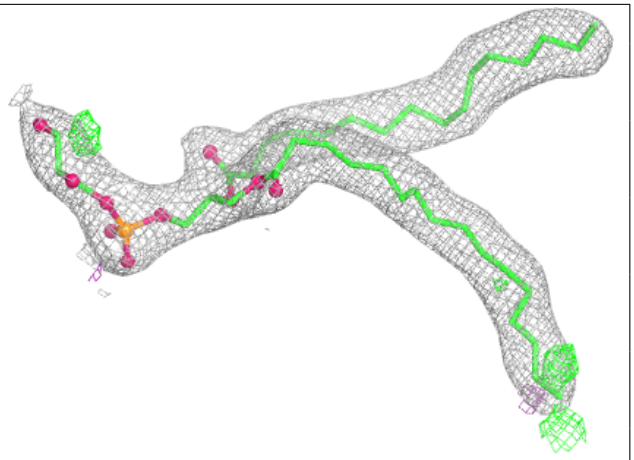


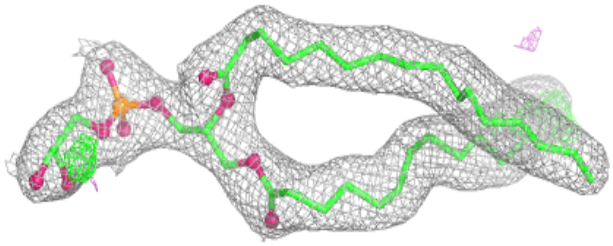


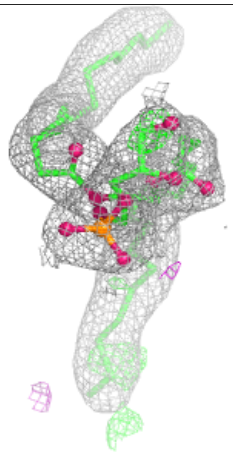


Electron density around LHG d 406 (A):

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

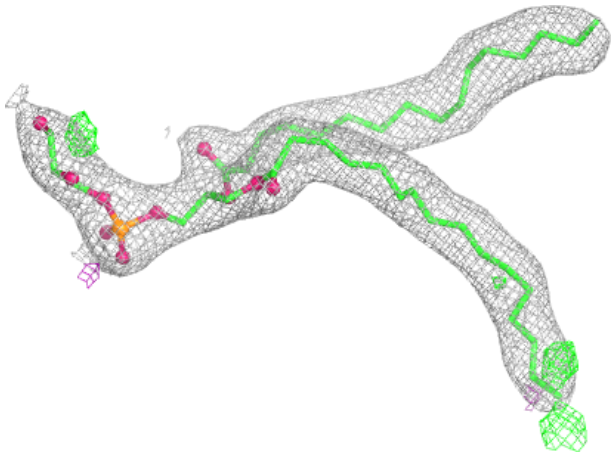


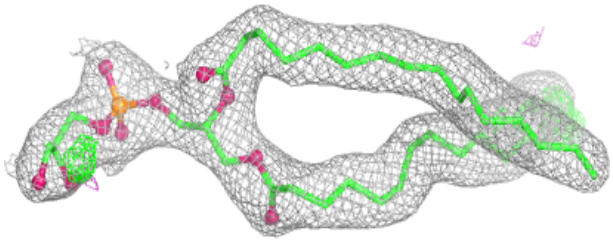


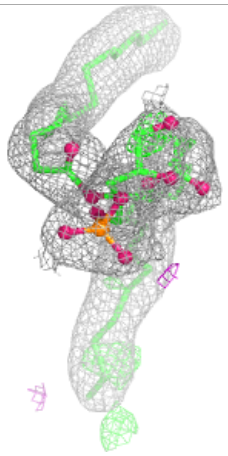


Electron density around LHG d 406 (B):

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

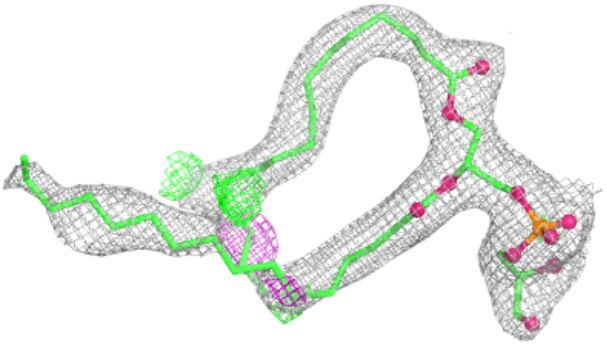


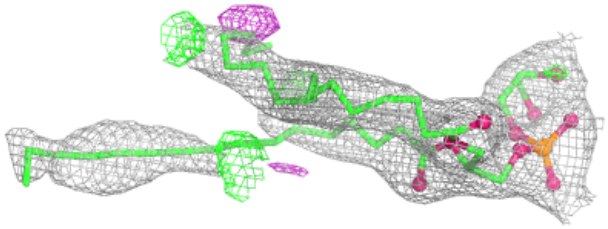


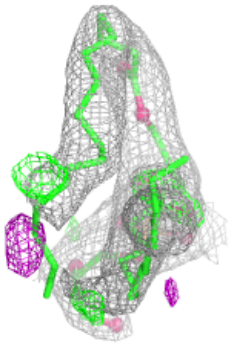


Electron density around LHG d 407 (A):

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

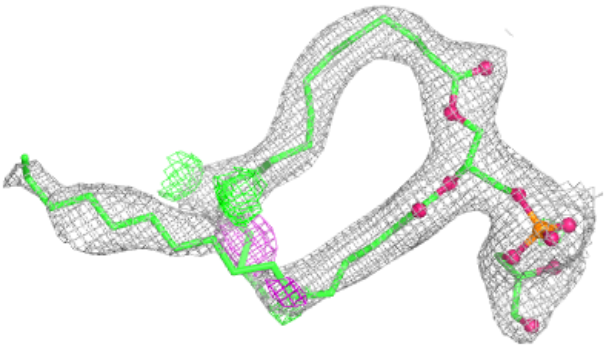


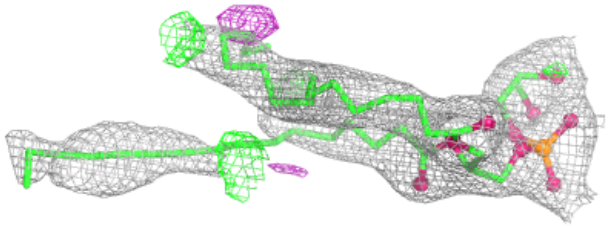


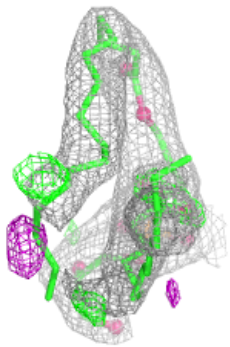


Electron density around LHG d 407 (B):

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

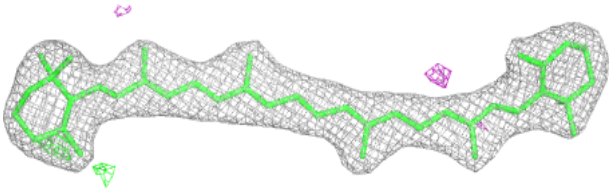


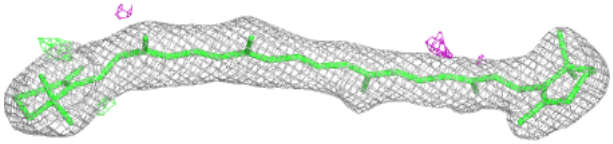


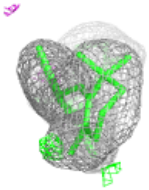


Electron density around BCR b 619:

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

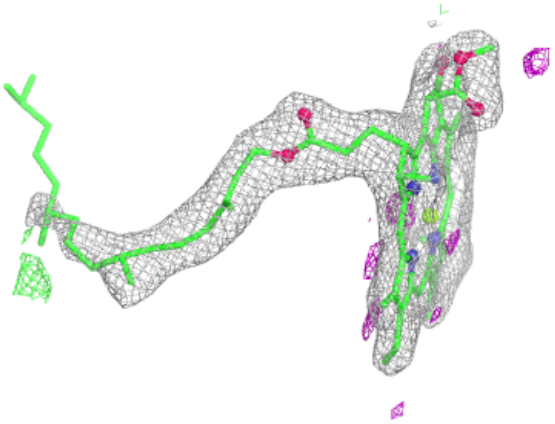


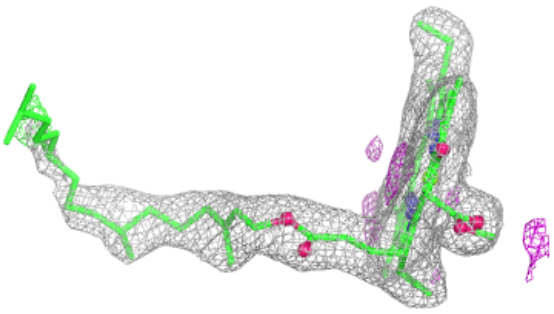


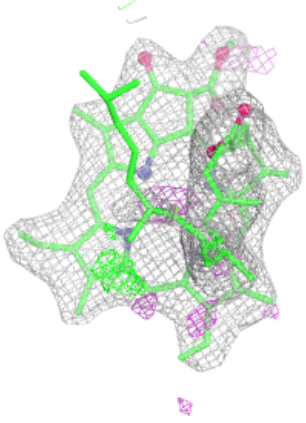


Electron density around CLA D 403:

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

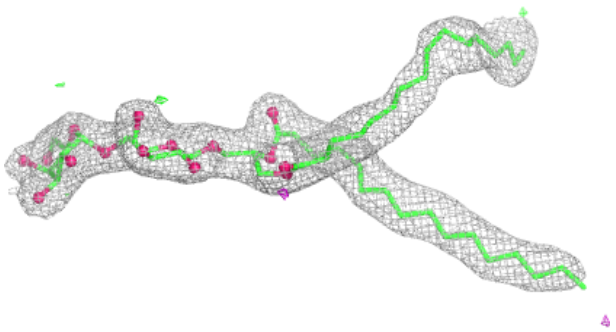


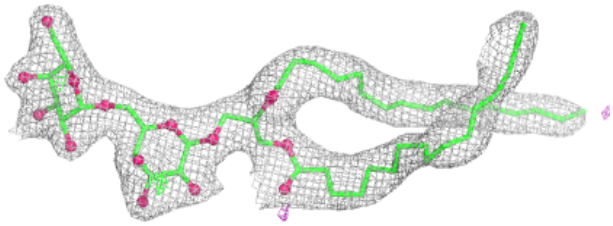


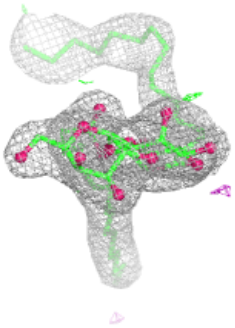


Electron density around DGD C 517 (A):

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

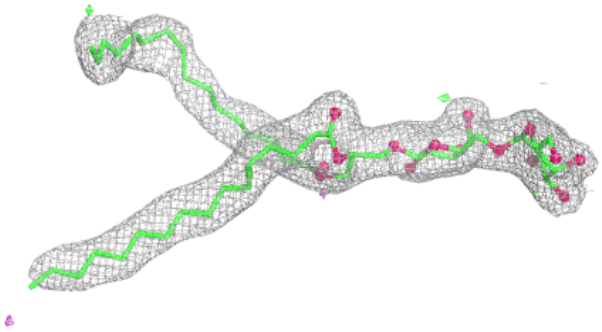


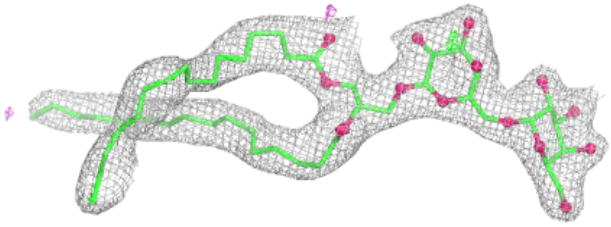


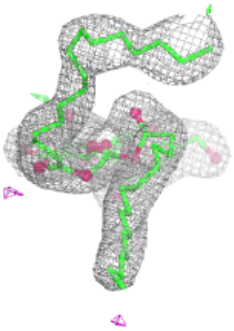


Electron density around DGD C 517 (B):

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

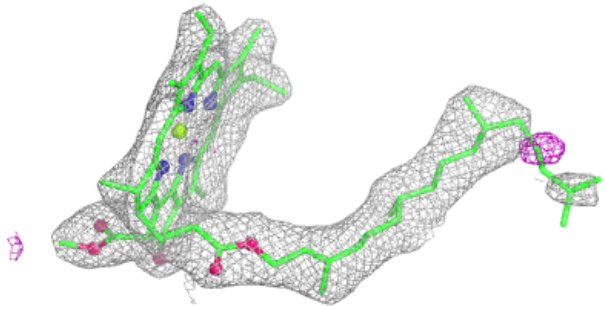


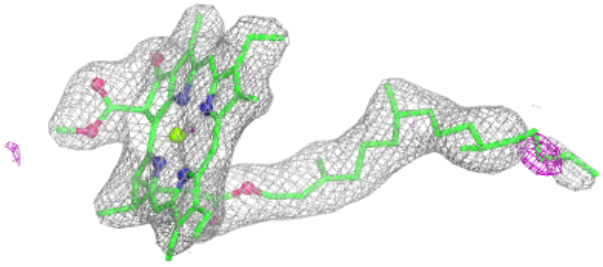


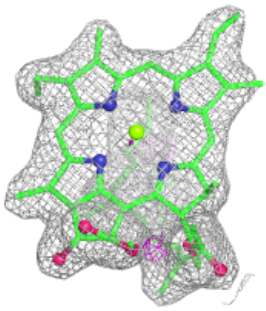


Electron density around CLA c 509:

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

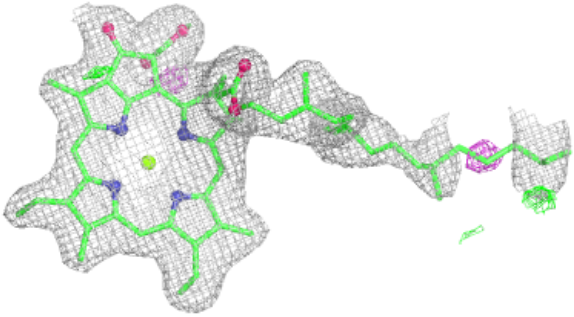


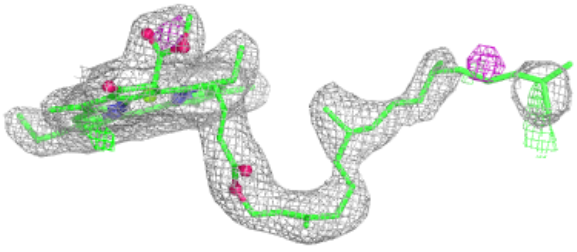




Electron density around CLA a 406 (A):

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

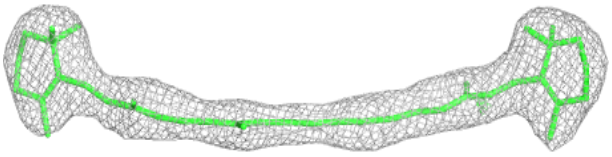


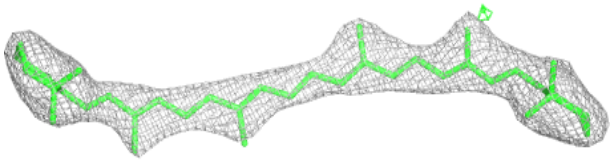


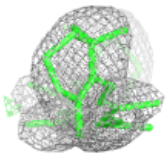


Electron density around BCR k 101:

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

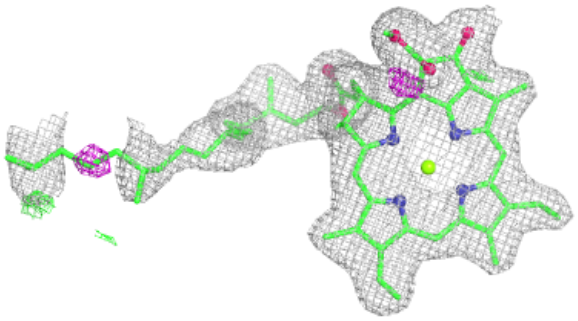


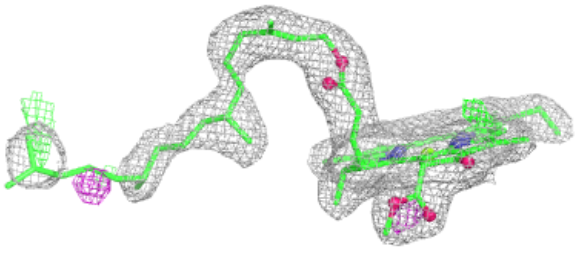


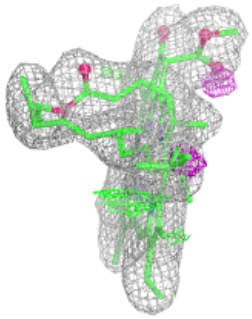


Electron density around CLA a 406 (B):

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

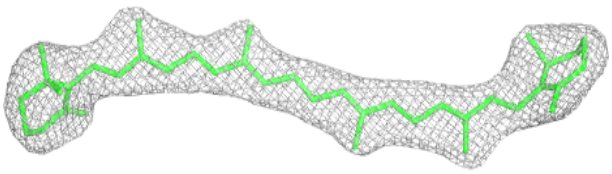


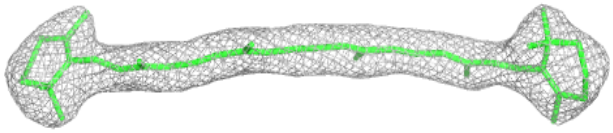


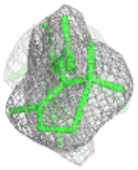


Electron density around BCR y 101:

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

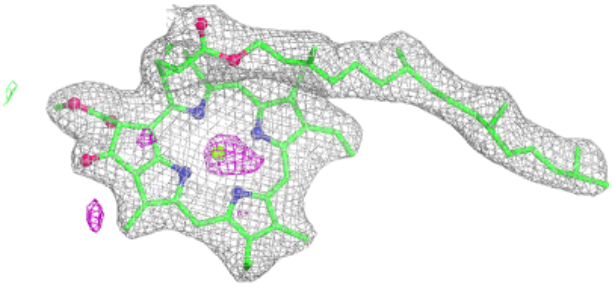


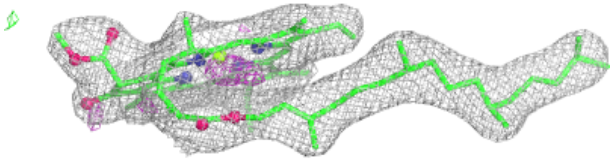


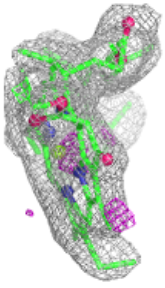


Electron density around CLA C 502:

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

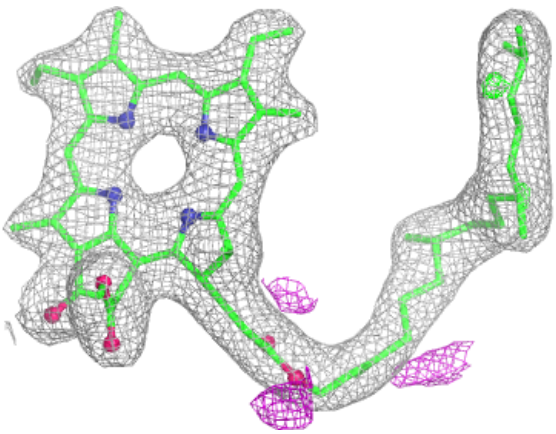


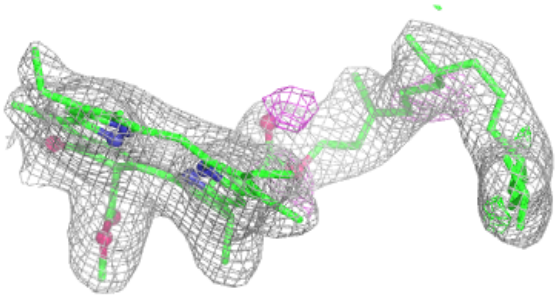


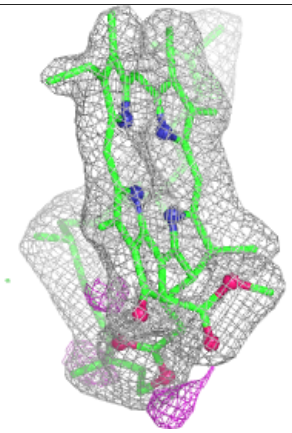


Electron density around PHO a 415 (A):

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

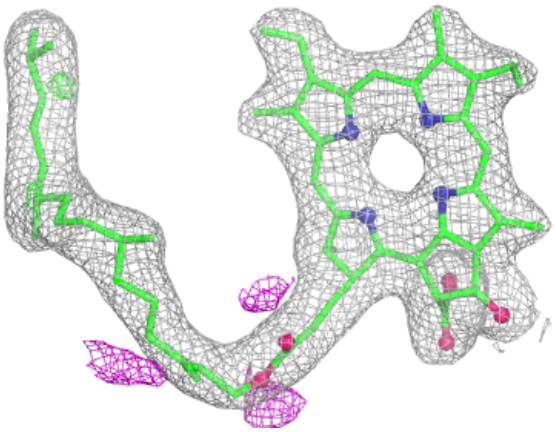


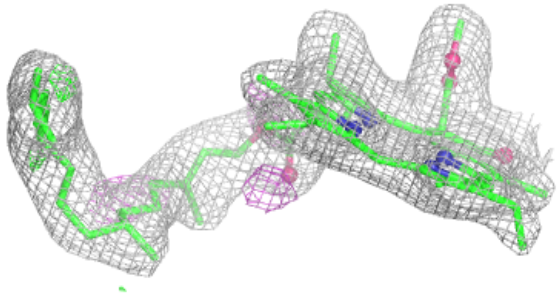


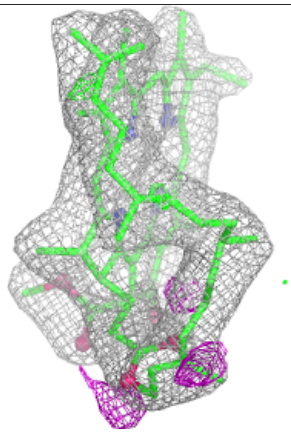


Electron density around PHO a 415 (B):

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

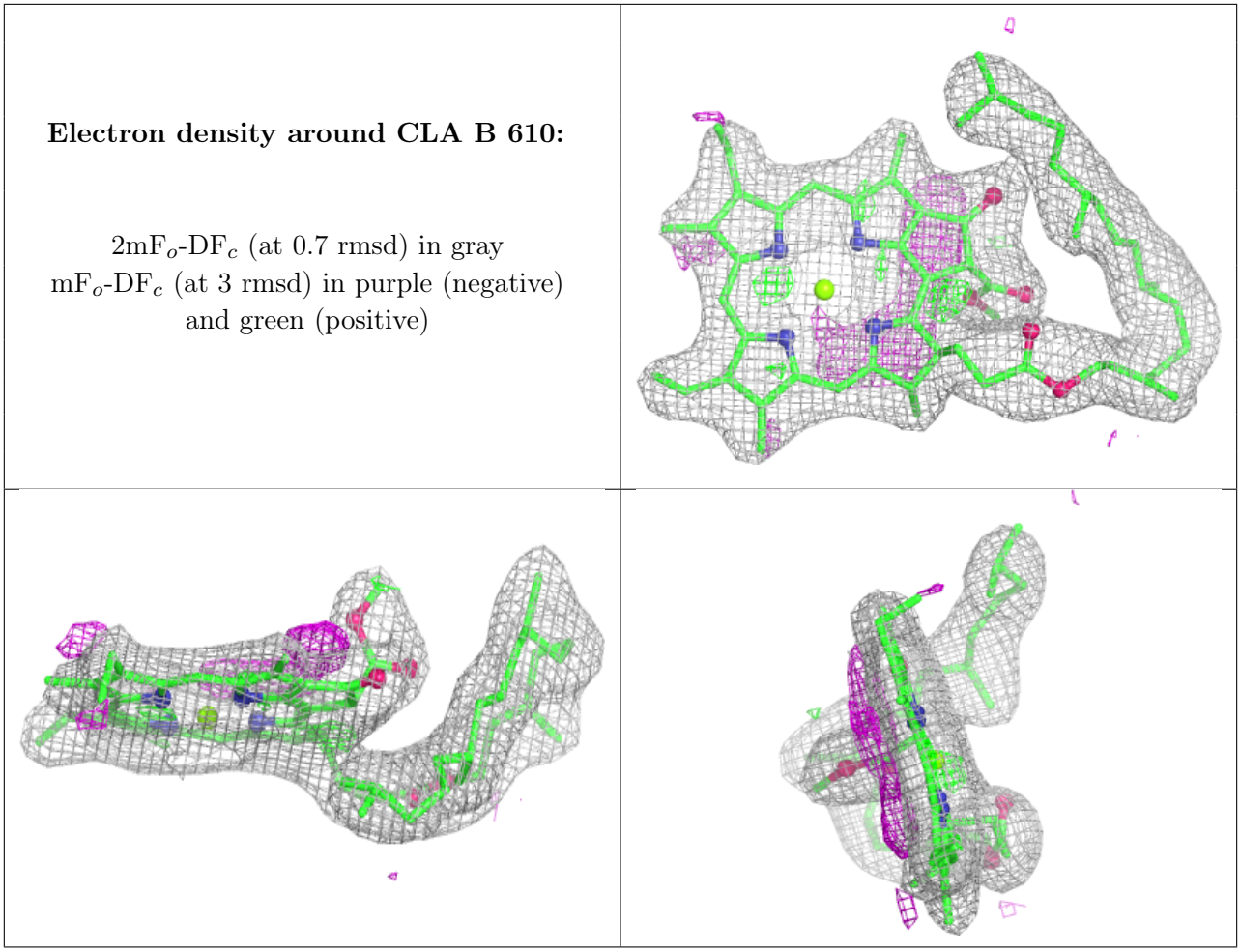






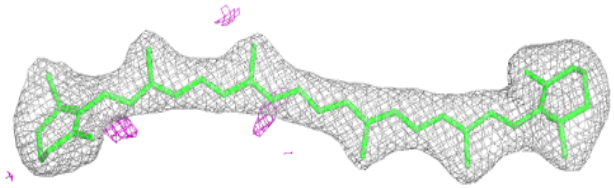
Electron density around CLA B 610:

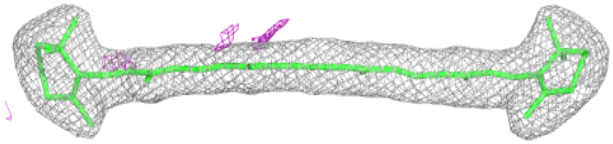
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

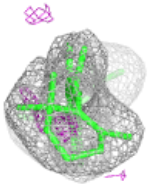


Electron density around BCR B 618:

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

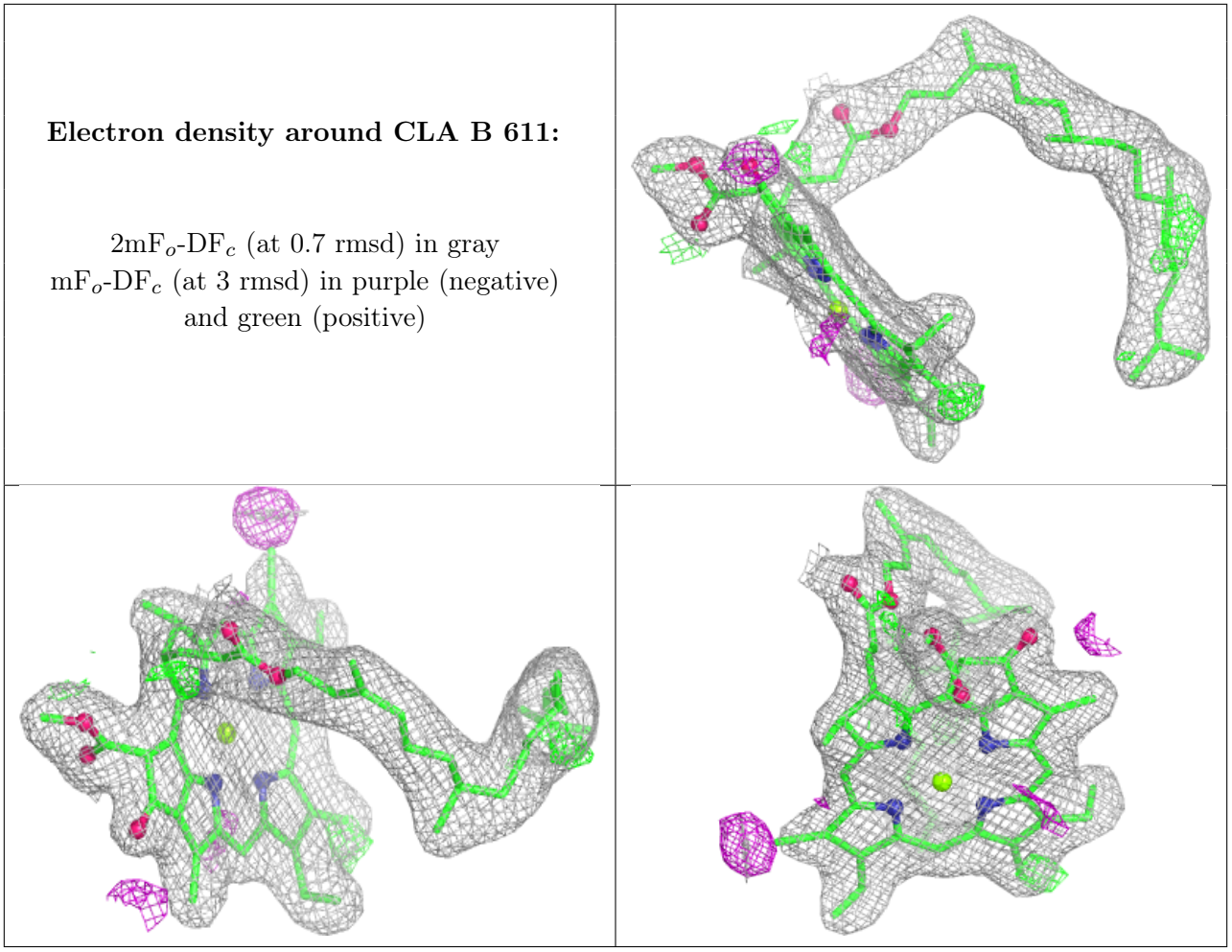






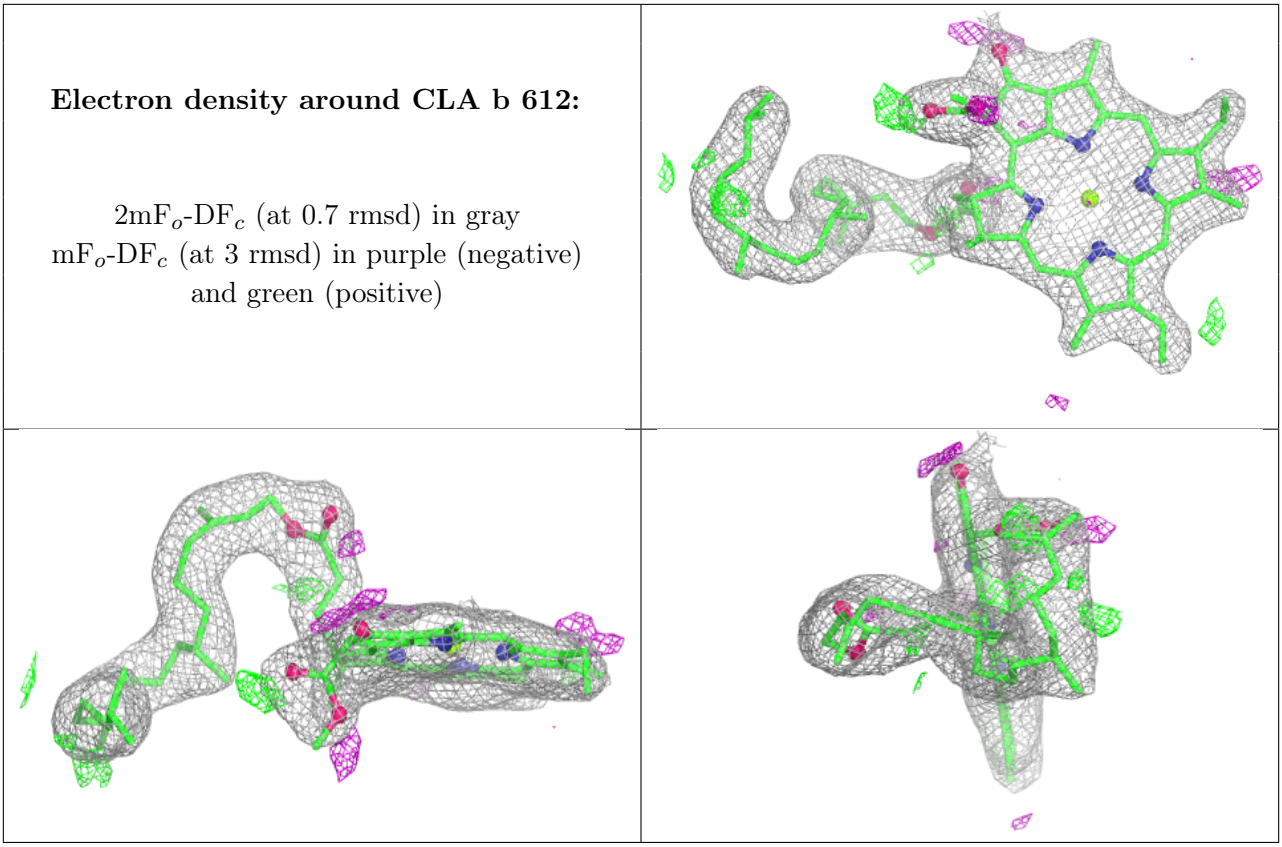
Electron density around CLA B 611:

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



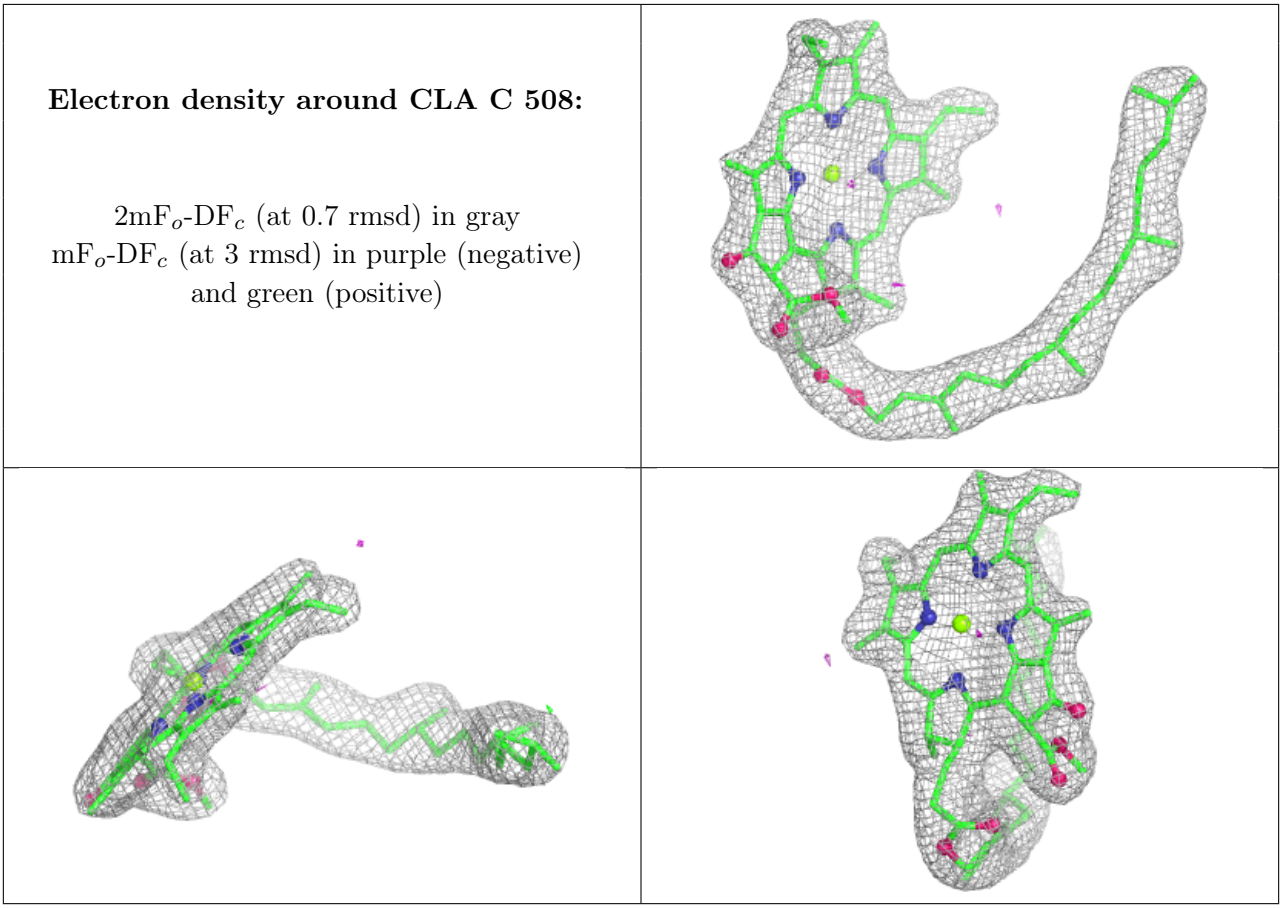
Electron density around CLA b 612:

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



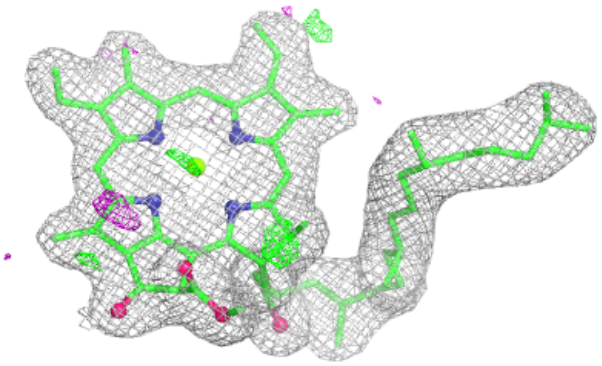
Electron density around CLA C 508:

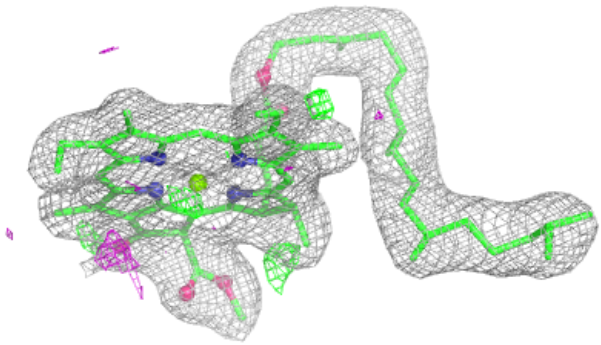
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

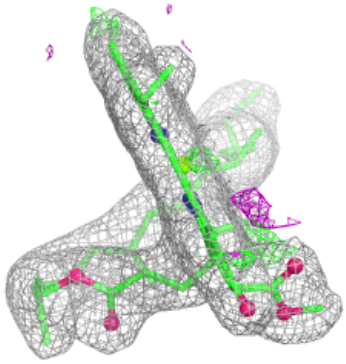


Electron density around CLA A 405 (A):

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

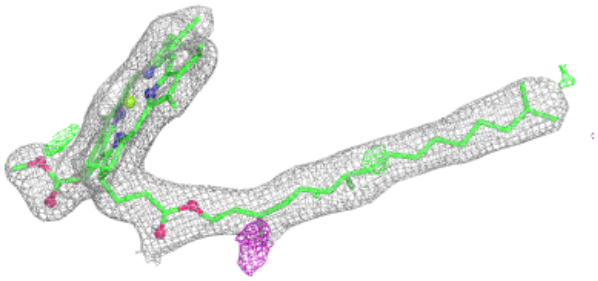


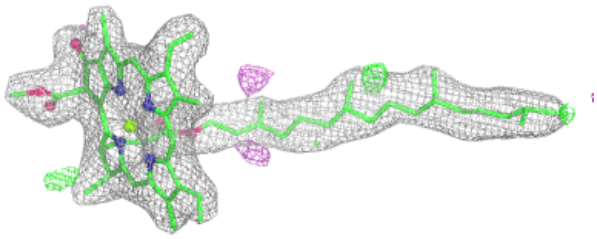


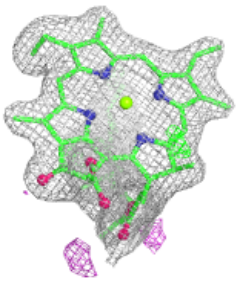


Electron density around CLA b 607:

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

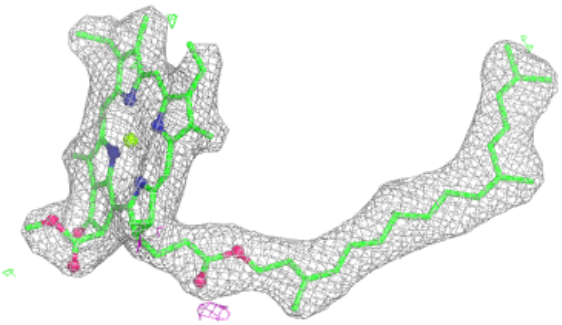


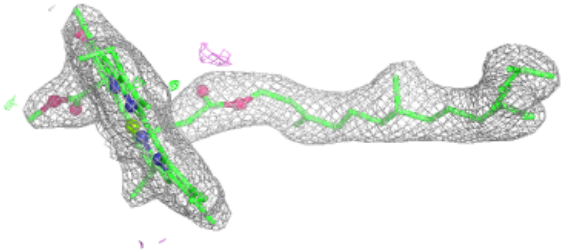


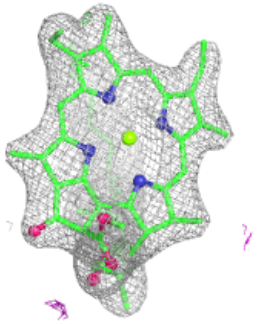


Electron density around CLA b 609:

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

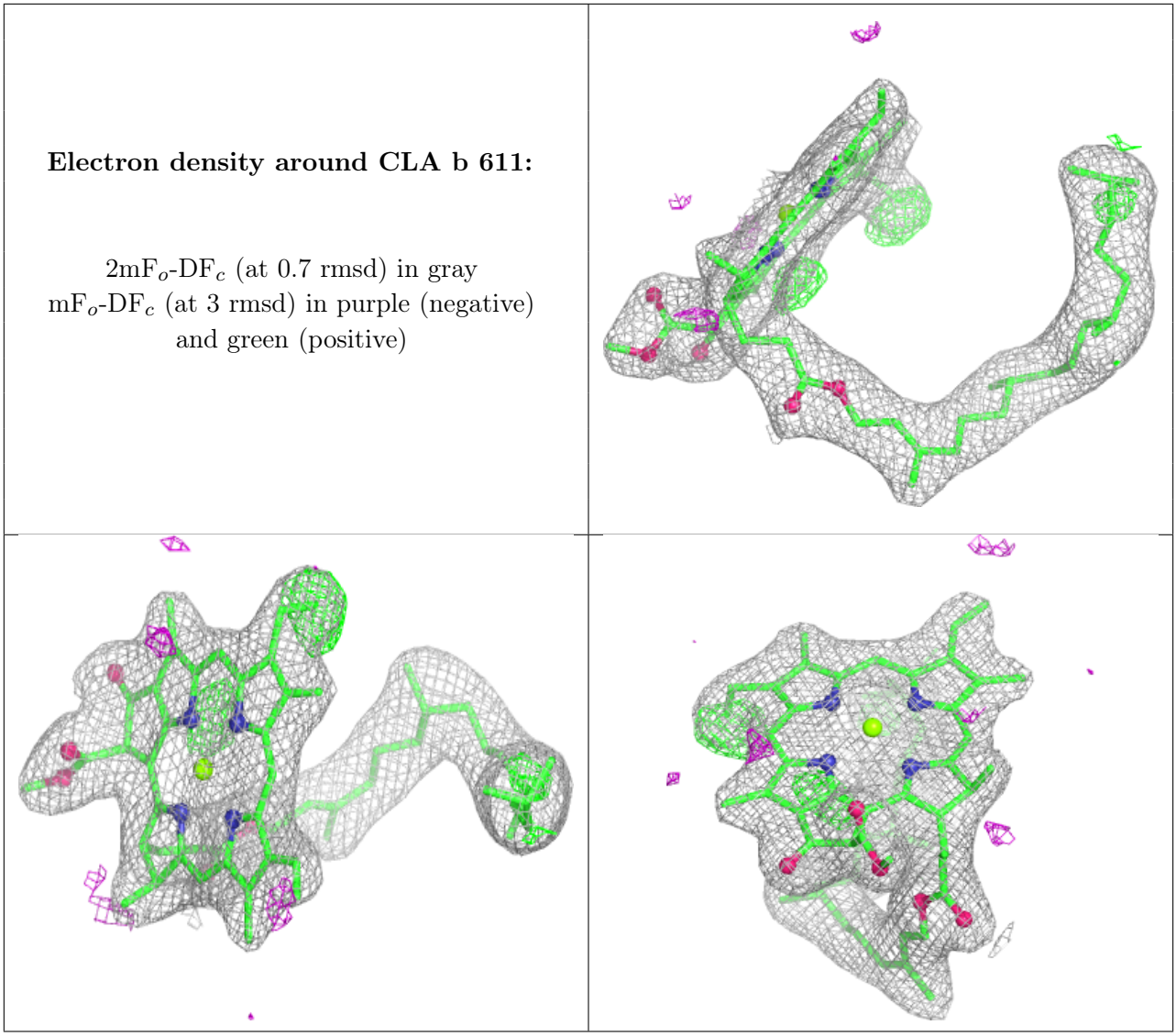






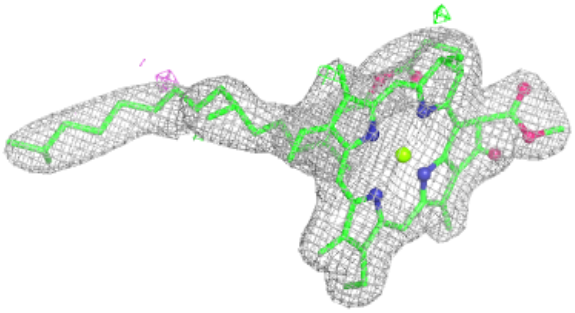
Electron density around CLA b 611:

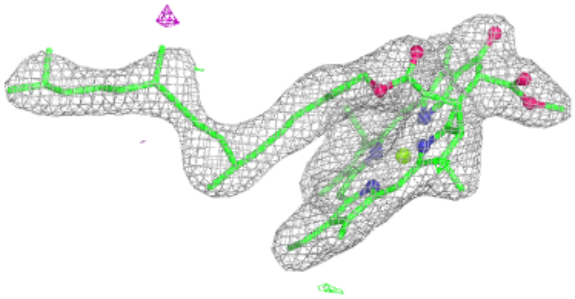
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

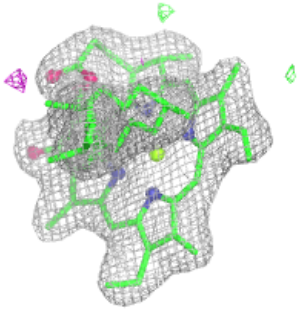


Electron density around CLA C 506:

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

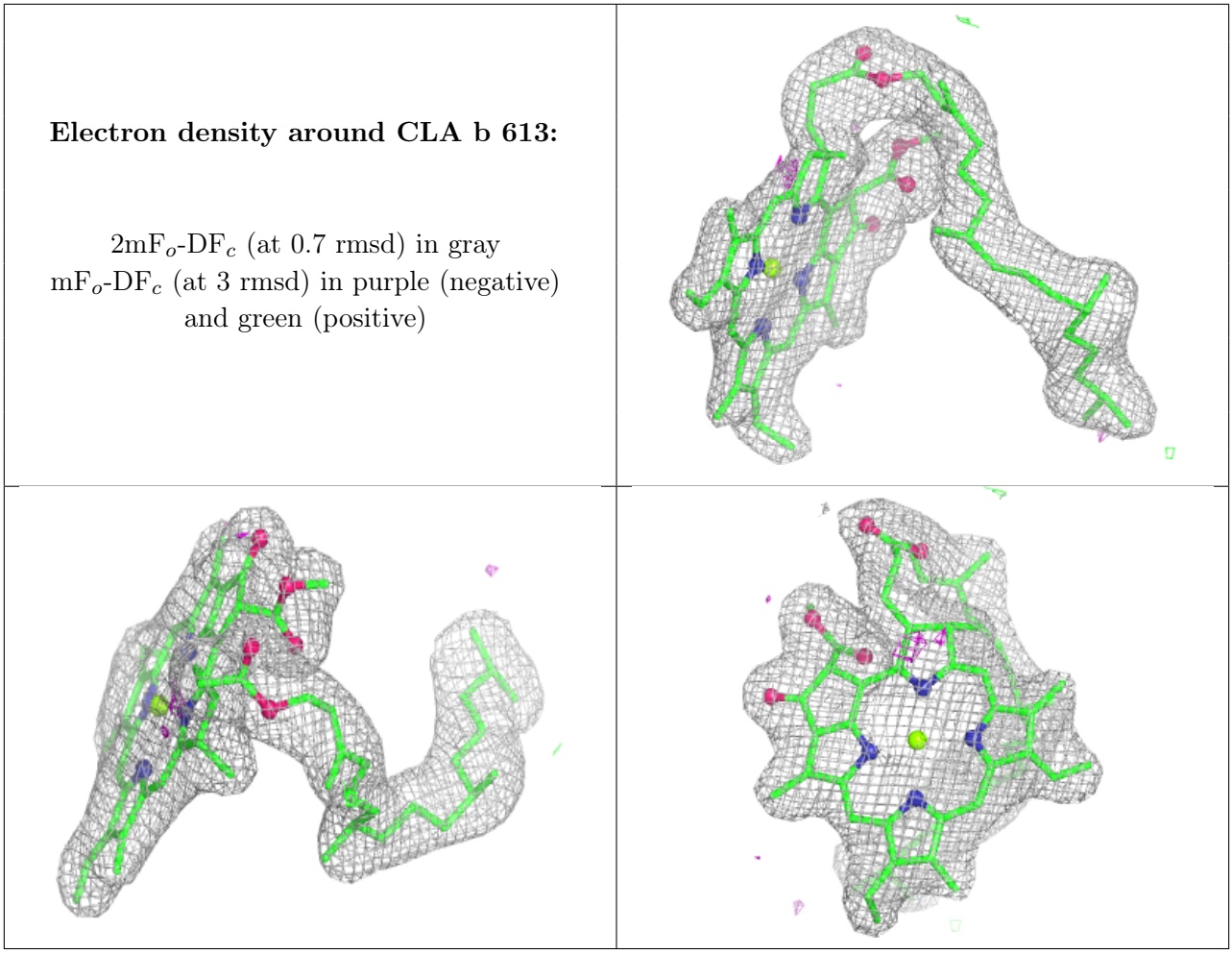






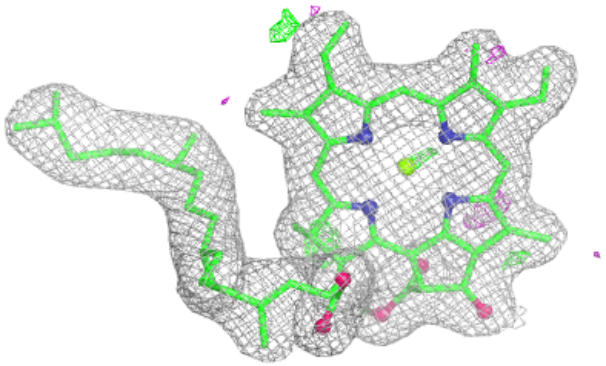
Electron density around CLA b 613:

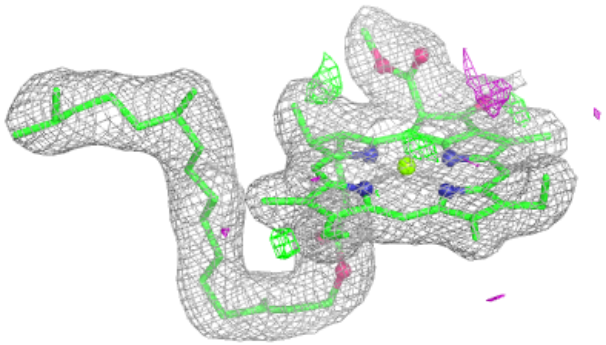
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

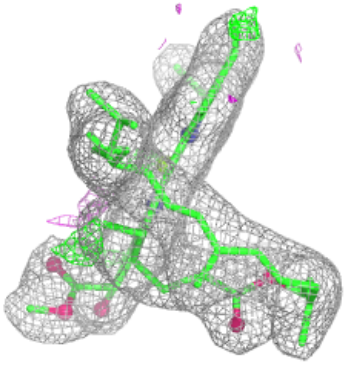


Electron density around CLA A 405 (B):

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

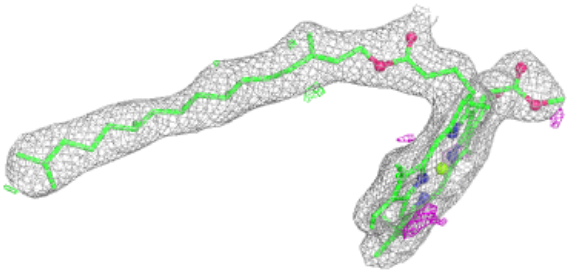


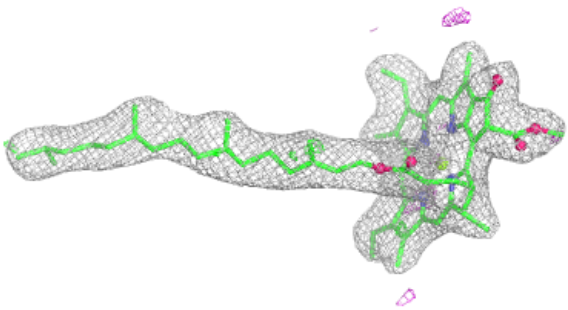


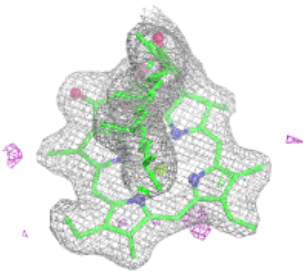


Electron density around CLA B 607:

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

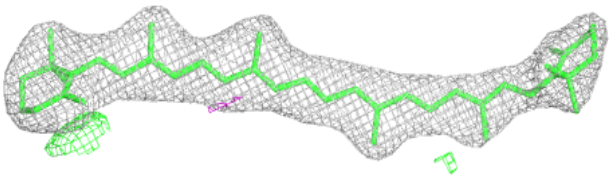


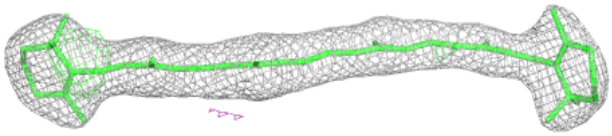


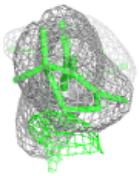


Electron density around BCR c 516:

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

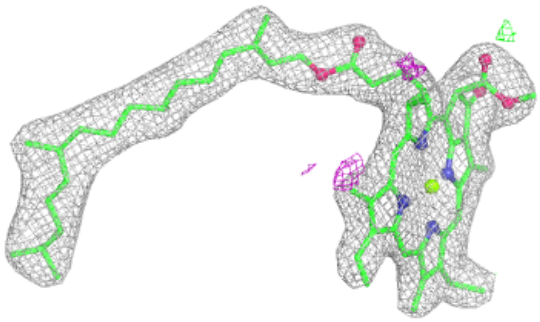


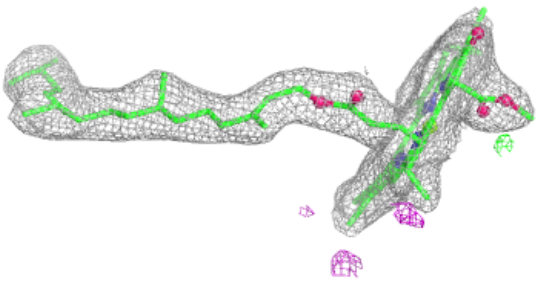


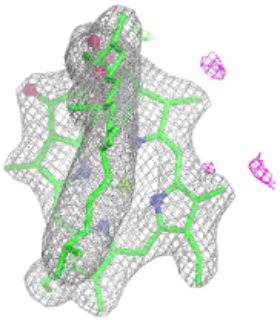


Electron density around CLA B 609:

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

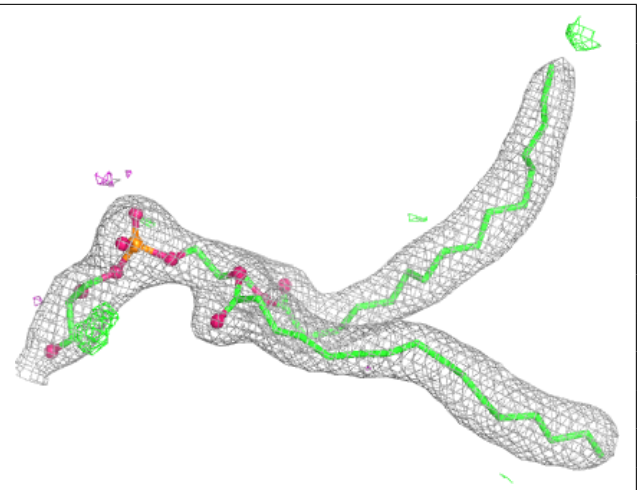


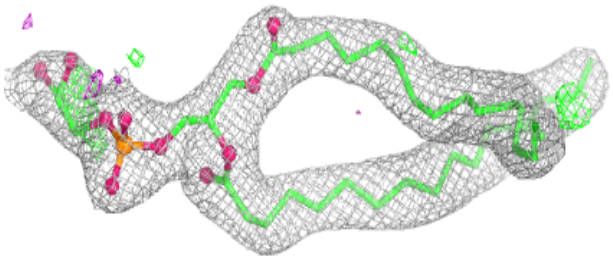


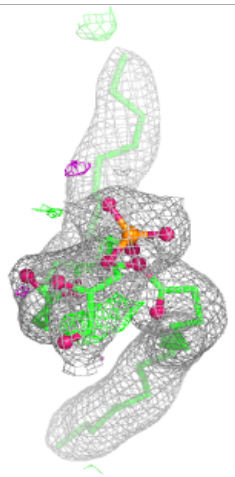


Electron density around LHG D 406 (A):

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

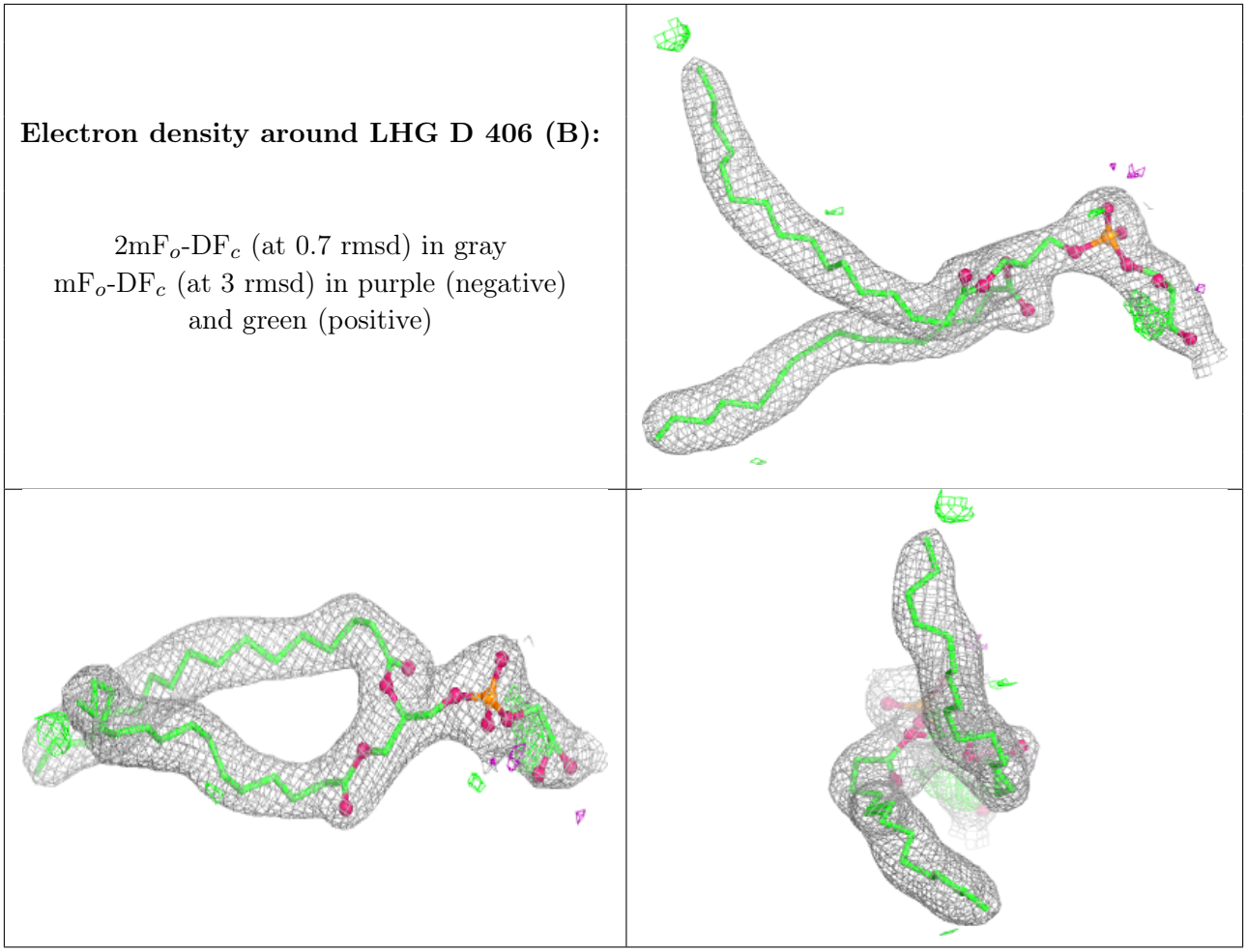






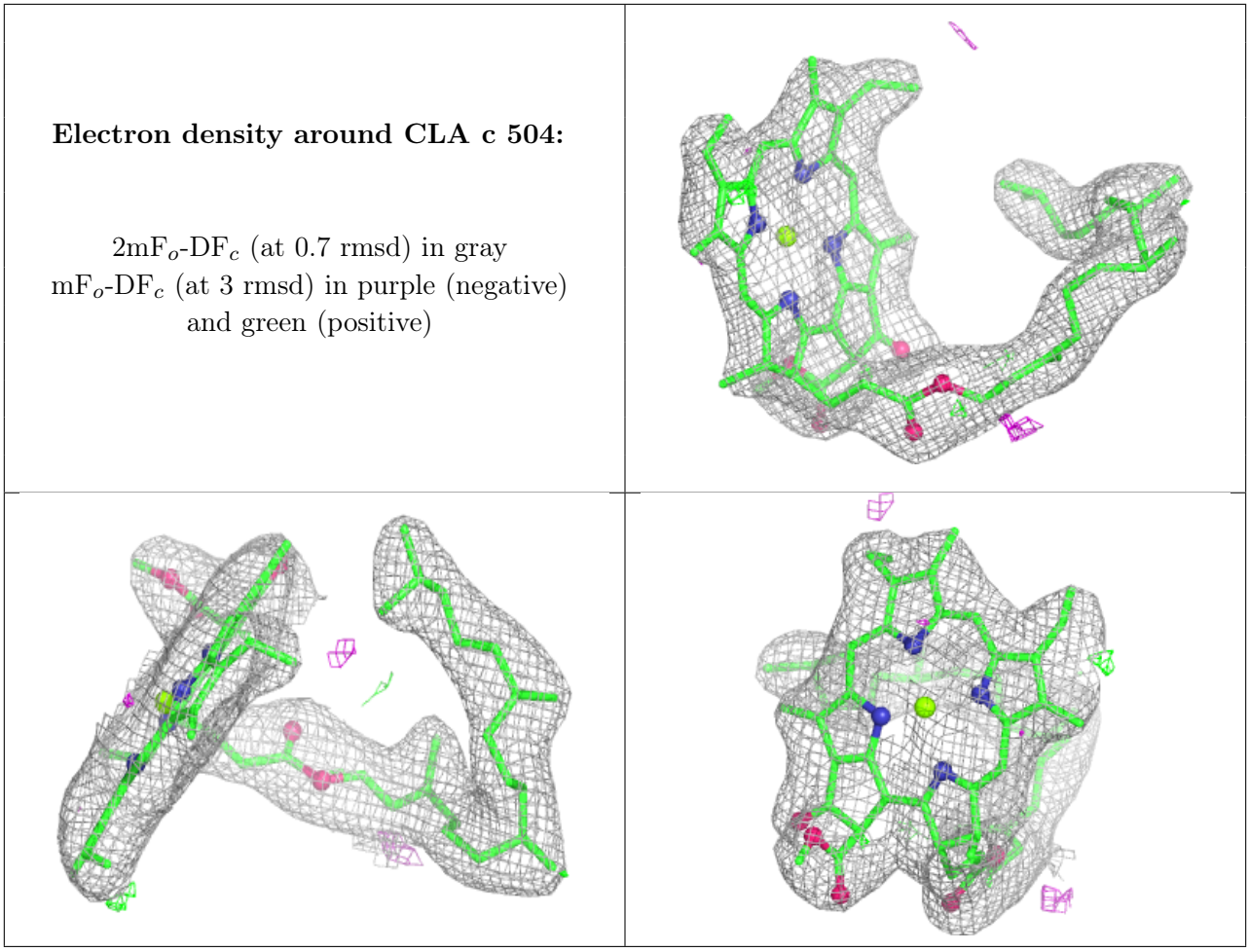
Electron density around LHG D 406 (B):

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



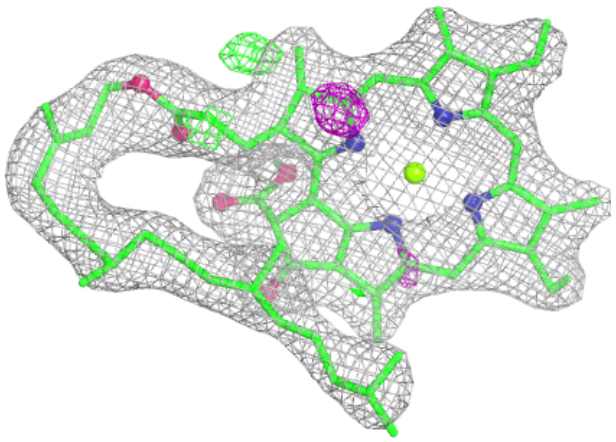
Electron density around CLA c 504:

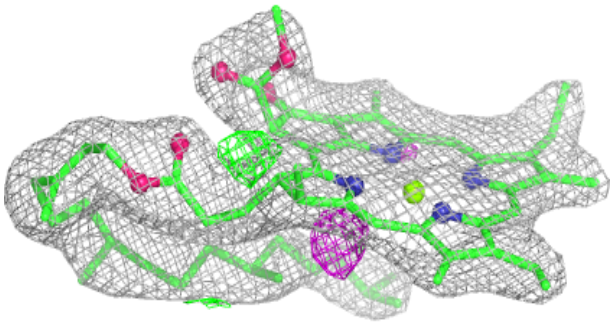
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA 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)

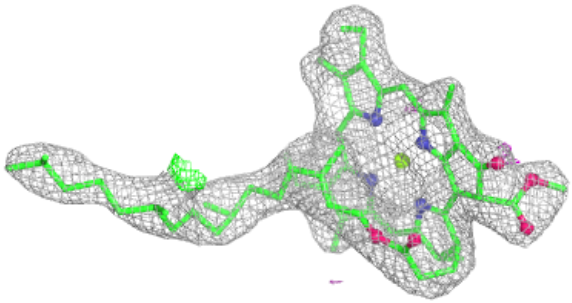


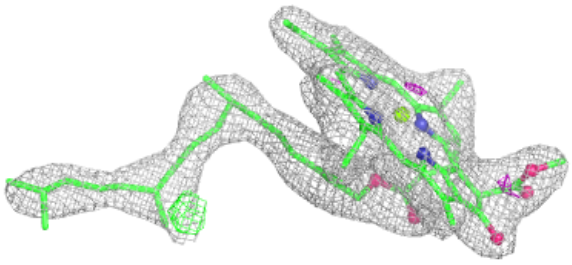


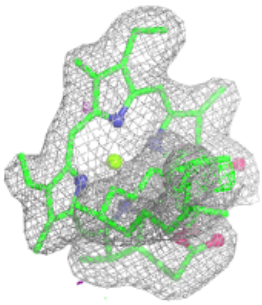


Electron density around CLA c 506:

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

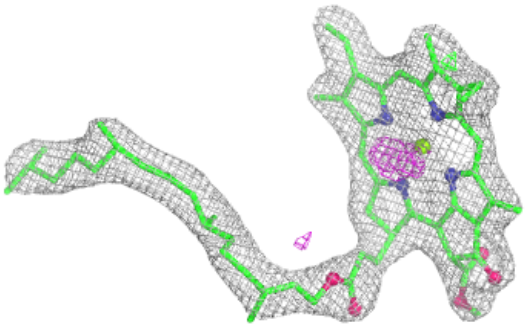


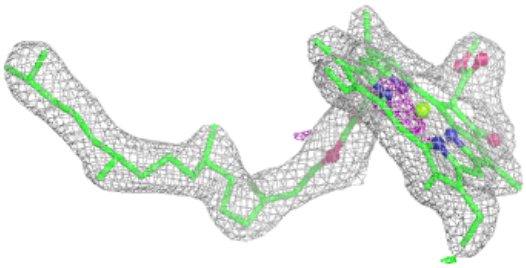


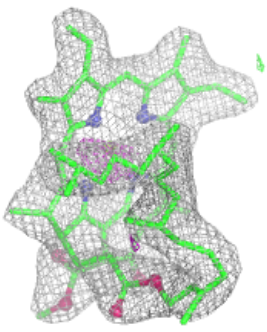


Electron density around CLA C 512:

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

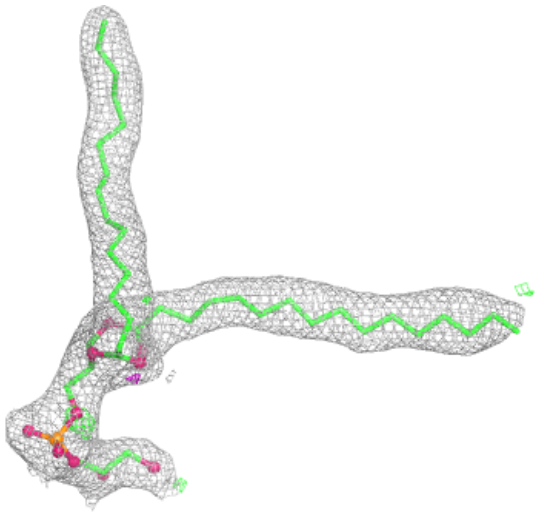


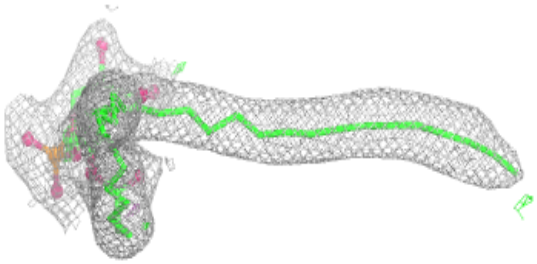


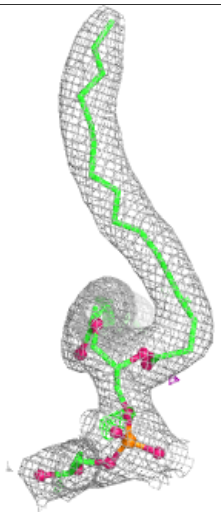


Electron density around LHG L 102 (A):

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

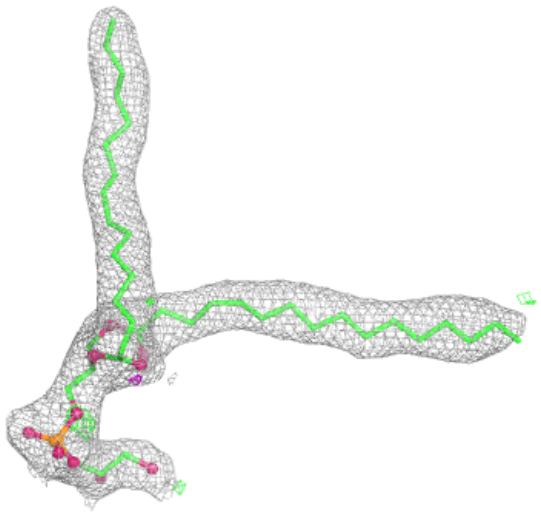


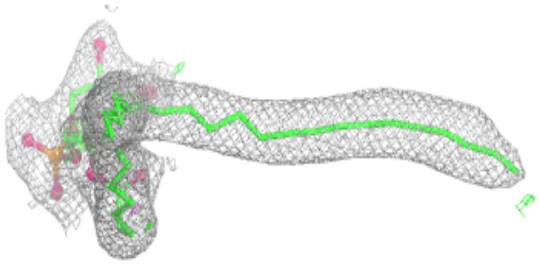


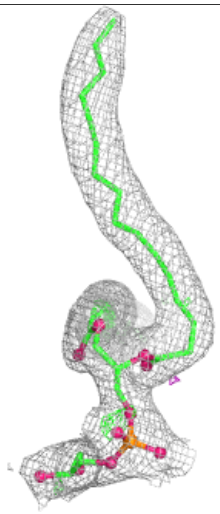


Electron density around LHG L 102 (B):

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

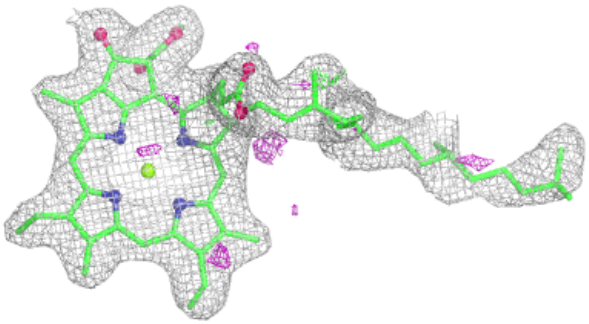


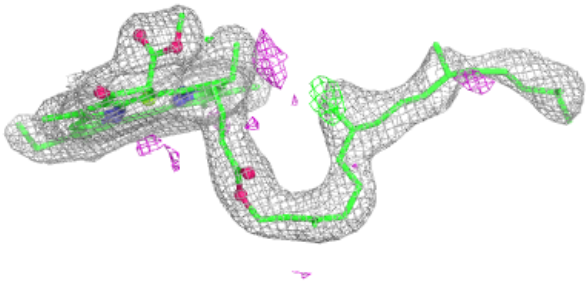


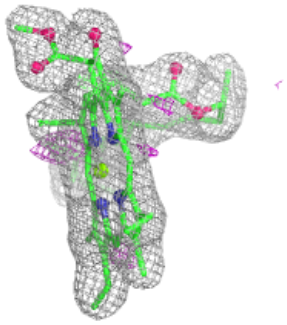


Electron density around CLA A 406 (A):

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

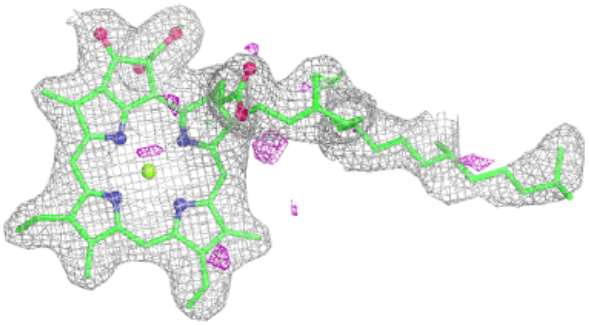


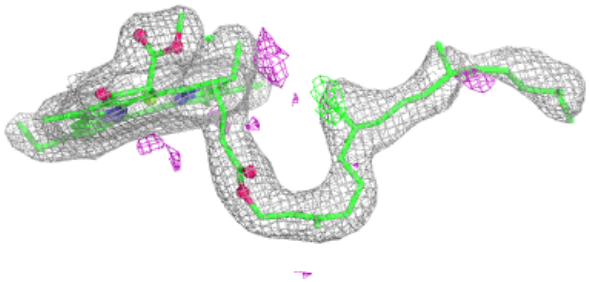


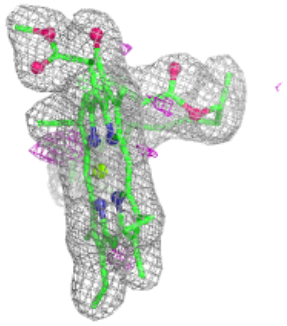


Electron density around CLA A 406 (B):

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

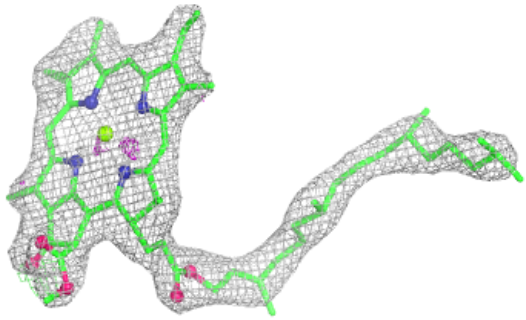


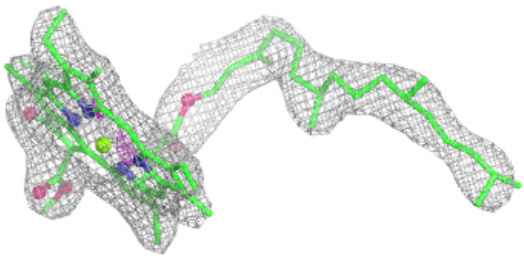


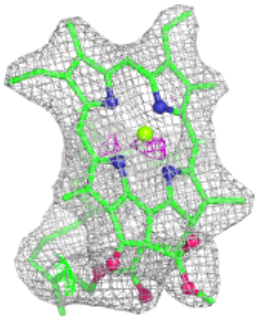


Electron density around CLA c 512:

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

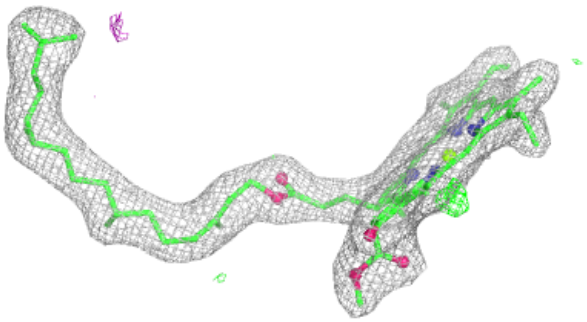


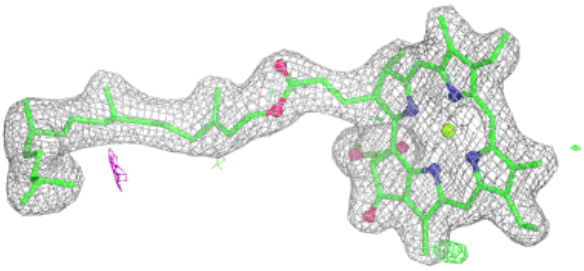


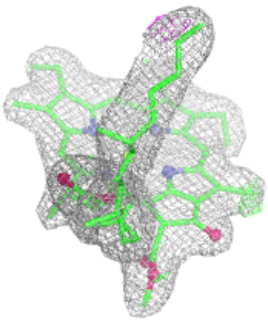


Electron density around CLA D 402 (A):

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

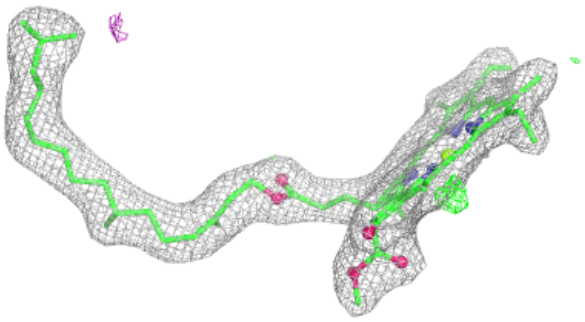


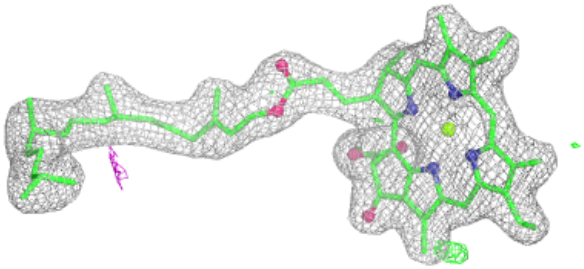


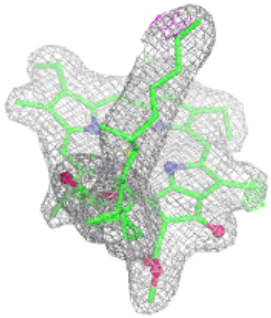


Electron density around CLA D 402 (B):

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

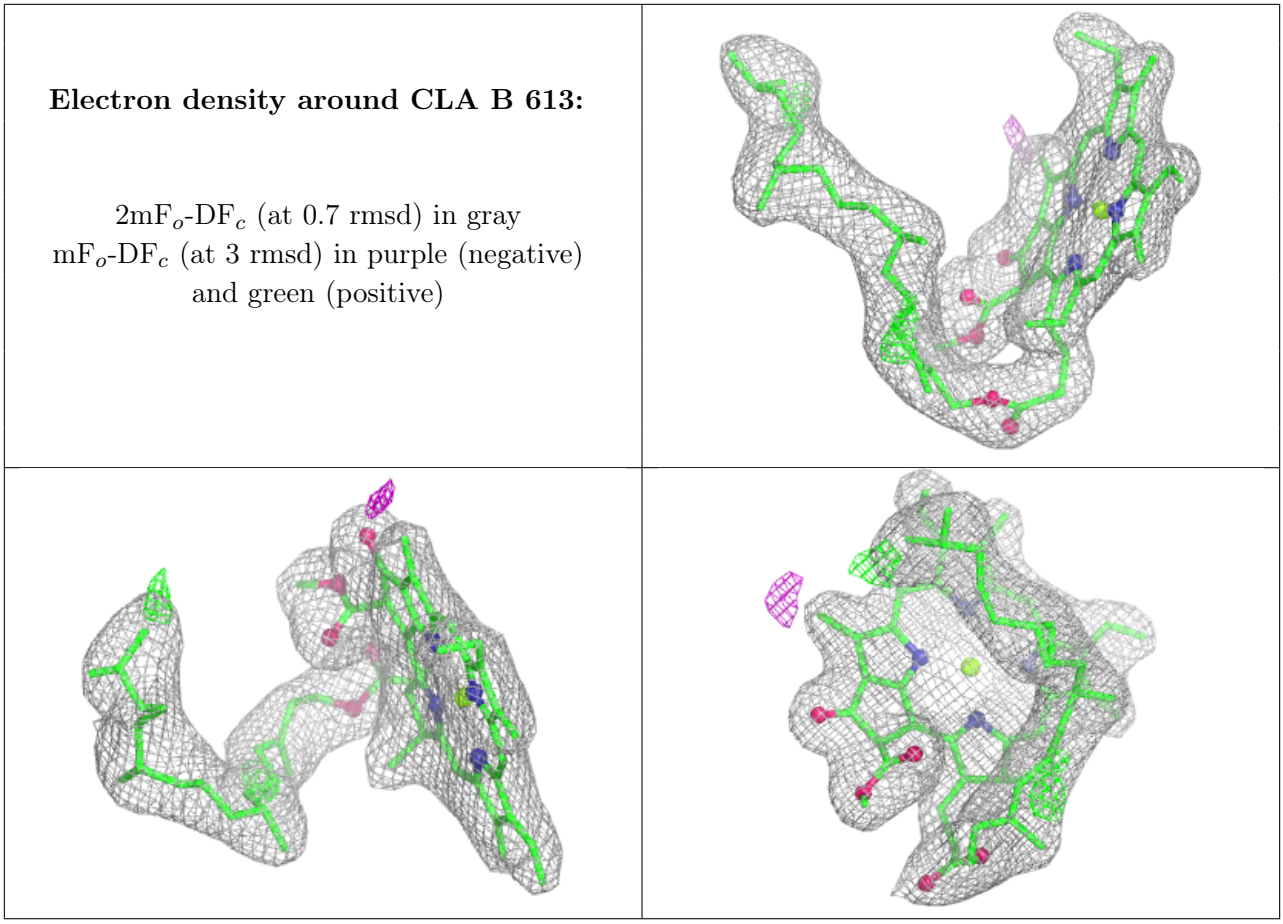






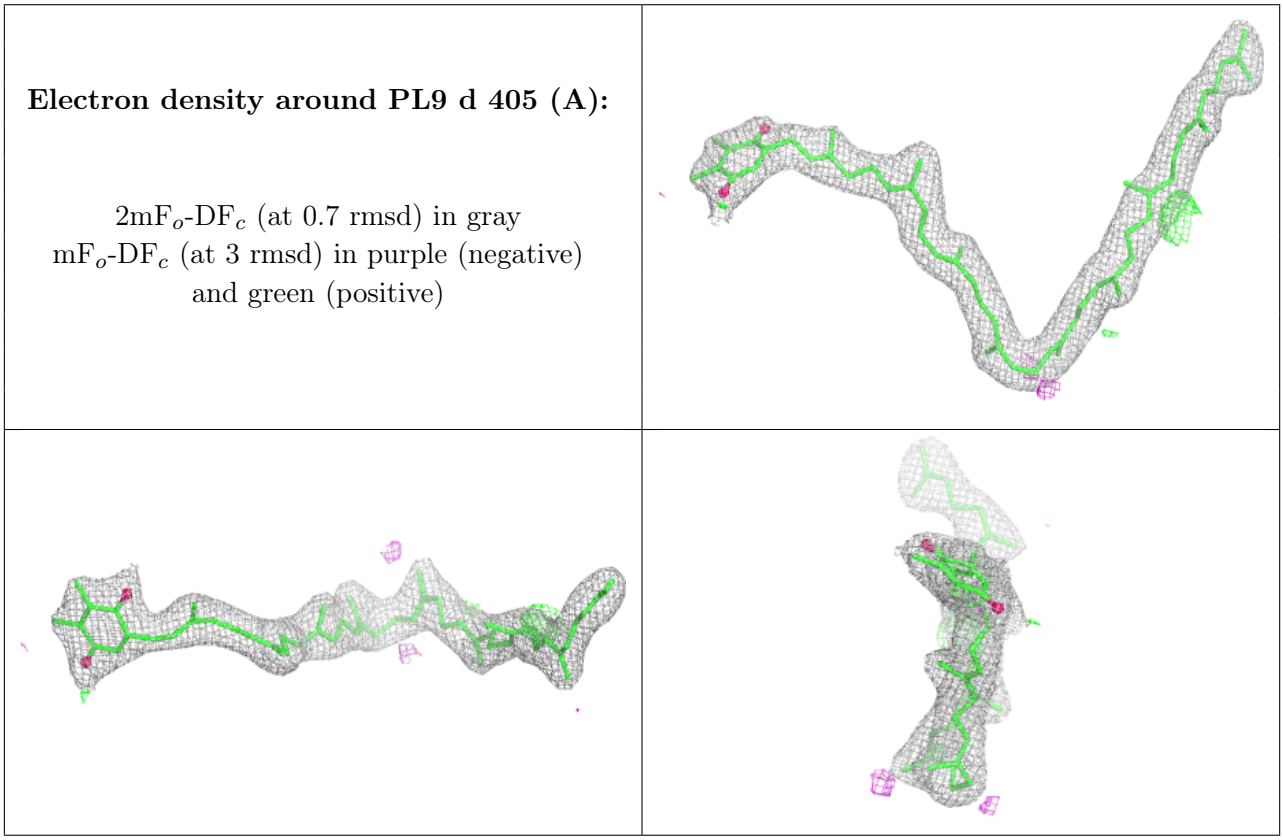
Electron density around CLA B 613:

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



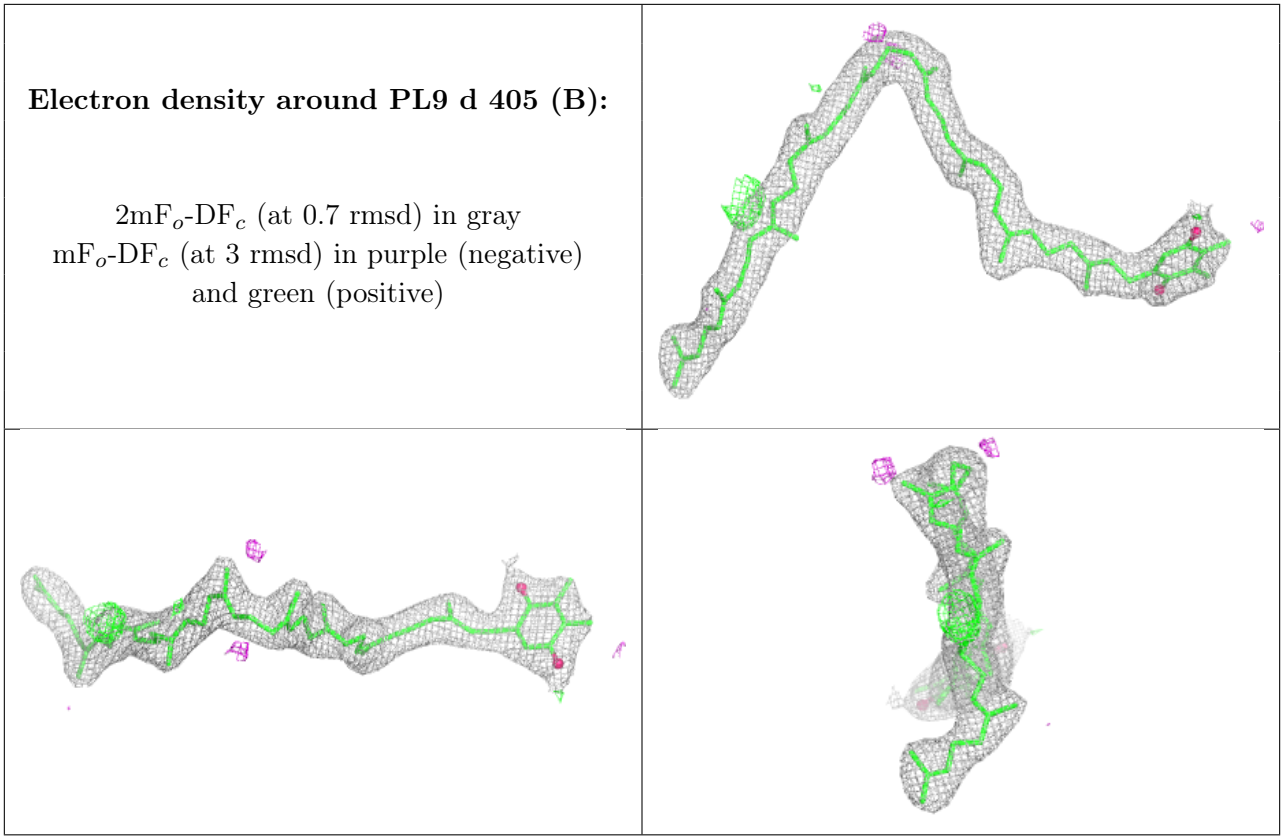
Electron density around PL9 d 405 (A):

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



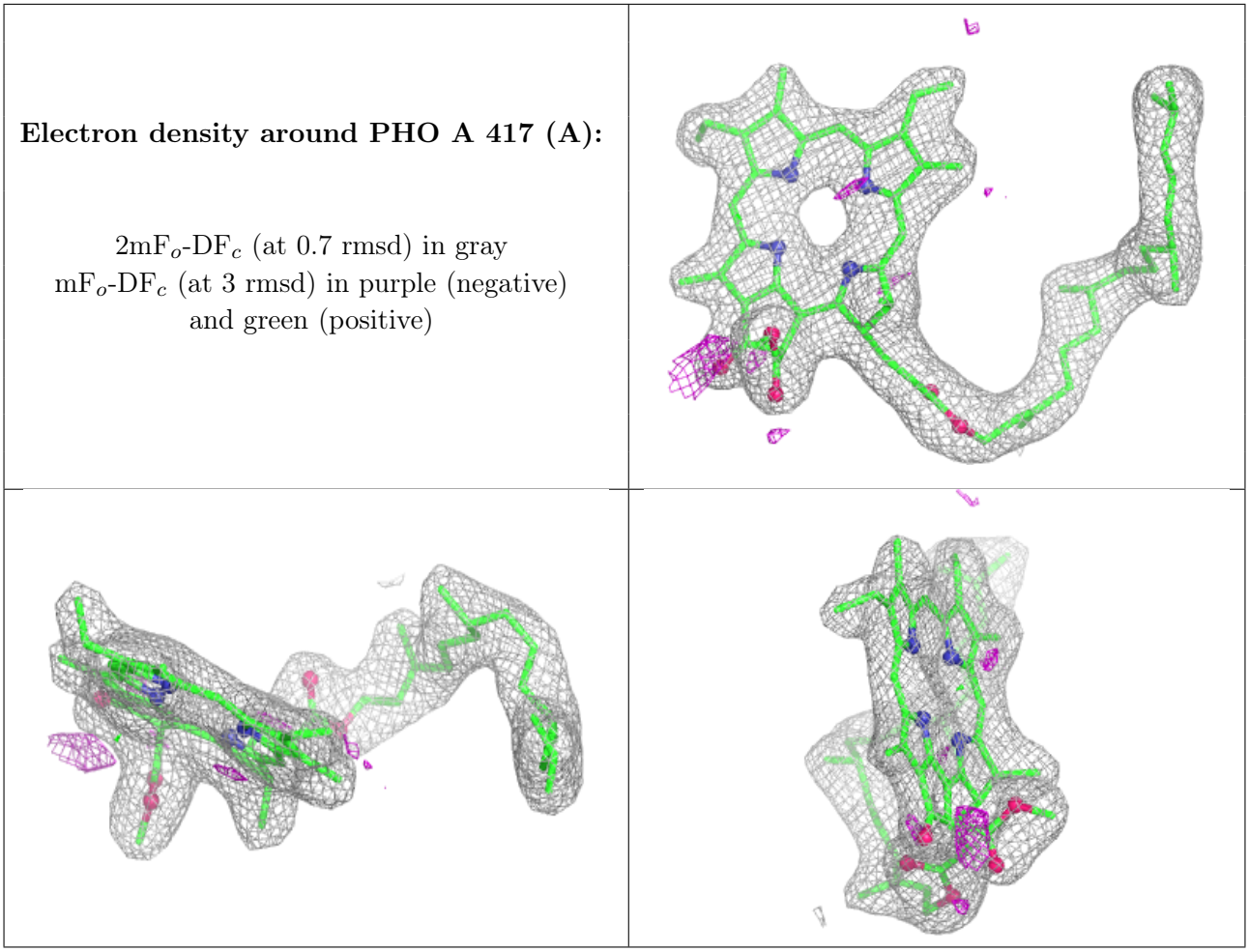
Electron density around PL9 d 405 (B):

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



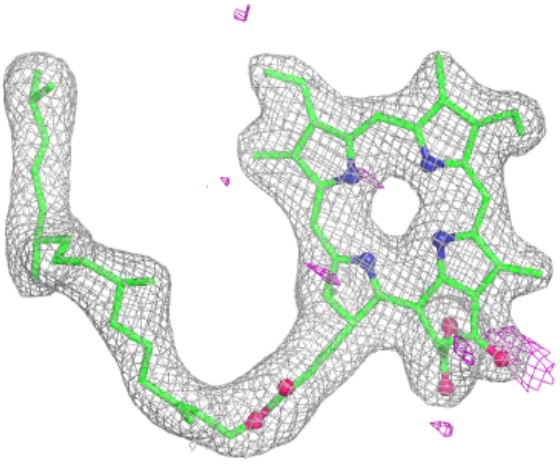
Electron density around PHO A 417 (A):

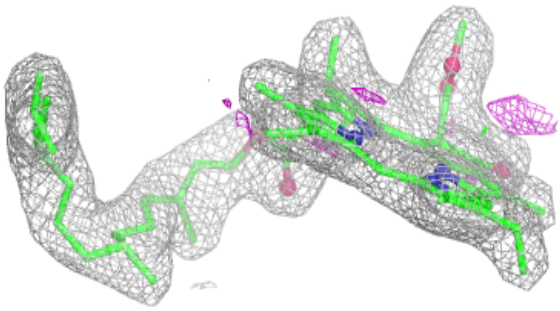
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

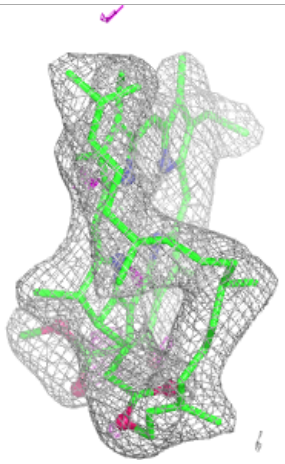


Electron density around PHO A 417 (B):

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

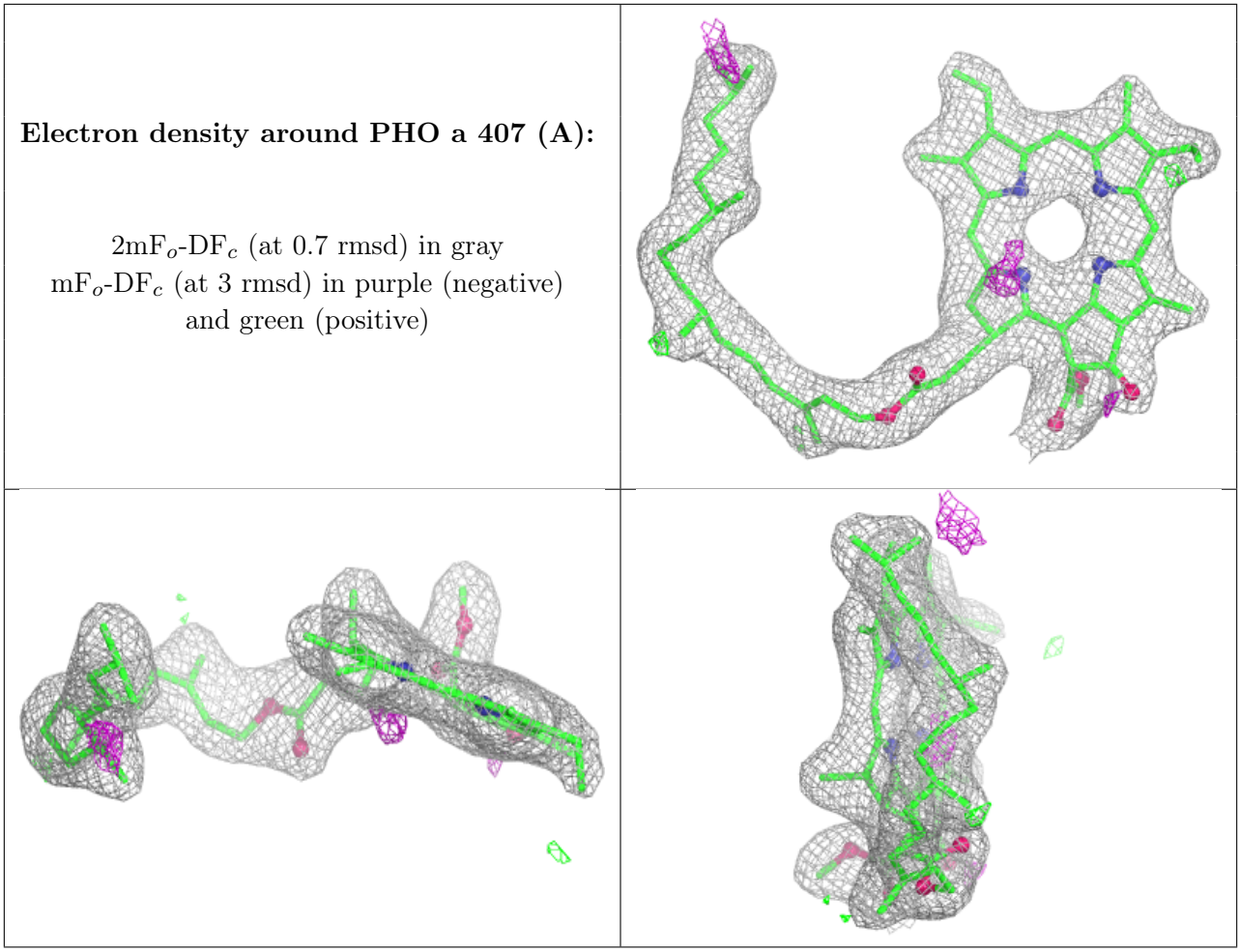






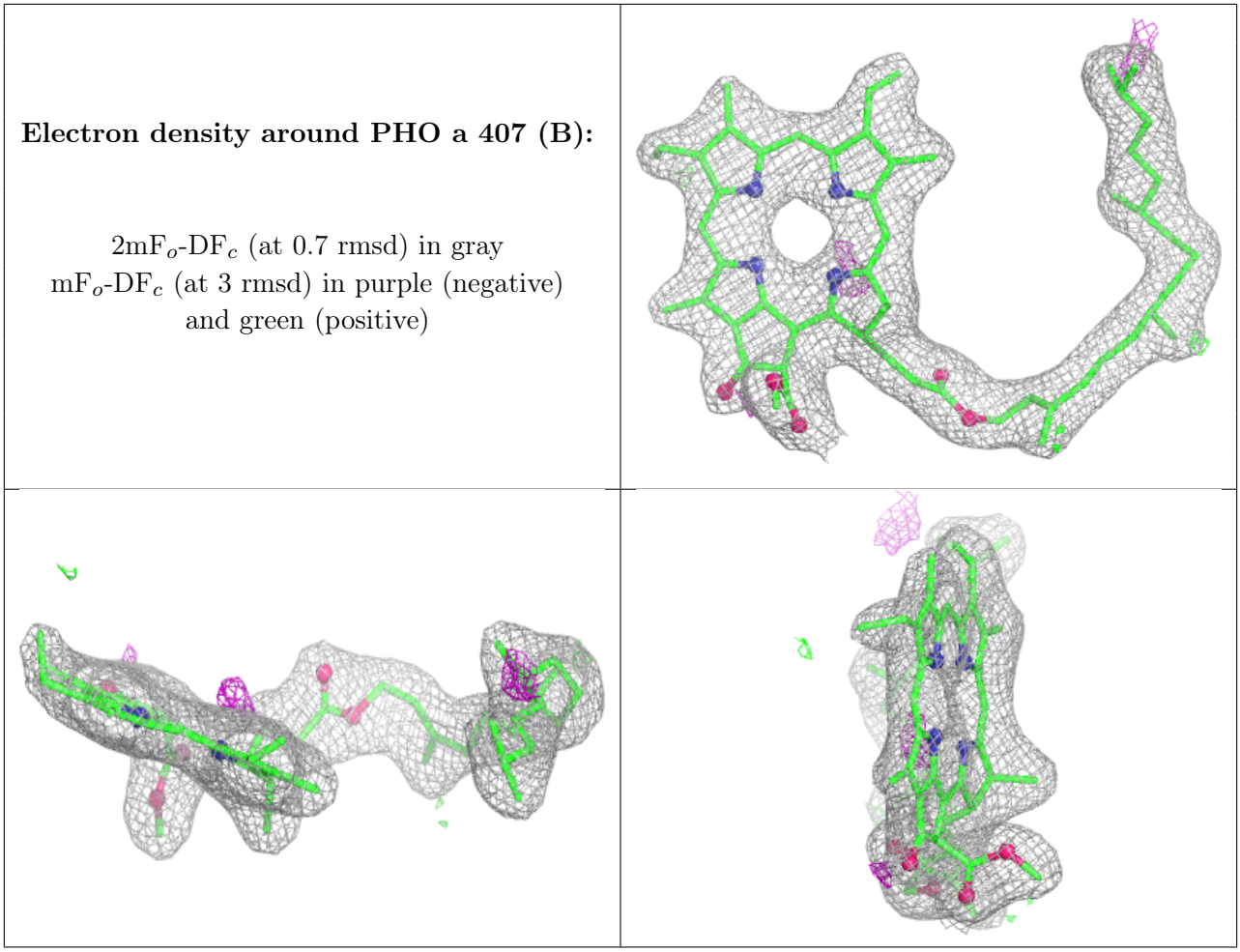
Electron density around PHO a 407 (A):

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



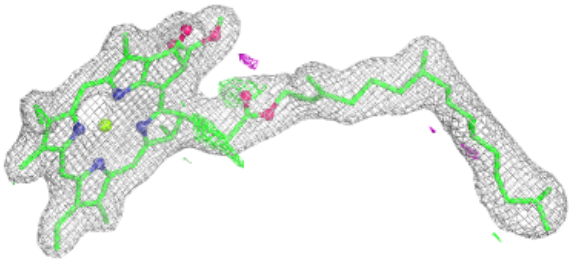
Electron density around PHO a 407 (B):

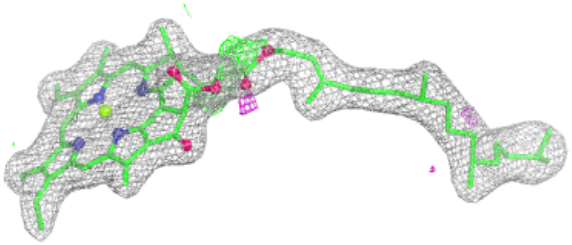
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

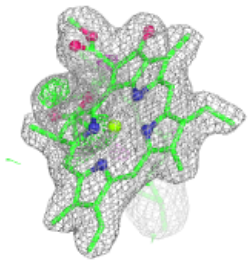


Electron density around CLA A 404 (A):

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

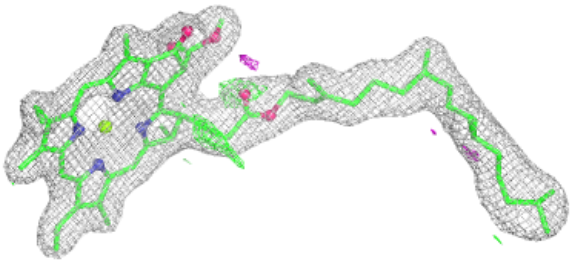


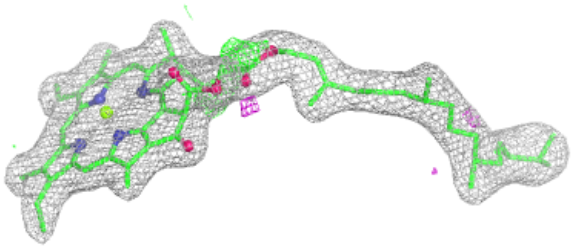


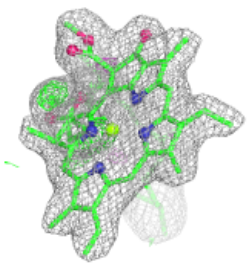


Electron density around CLA A 404 (B):

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

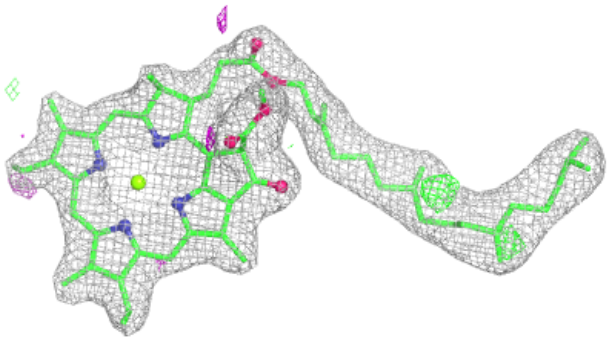


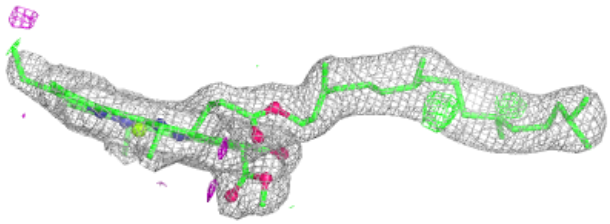


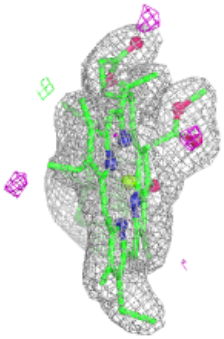


Electron density around CLA B 602:

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

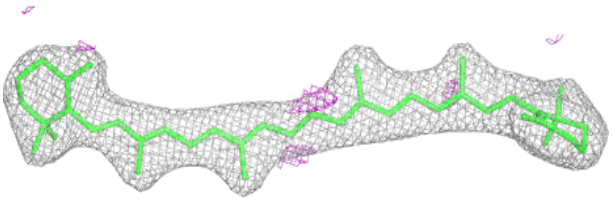


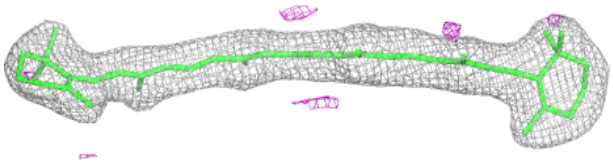


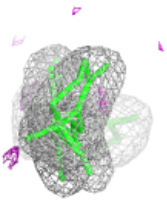


Electron density around BCR B 617:

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

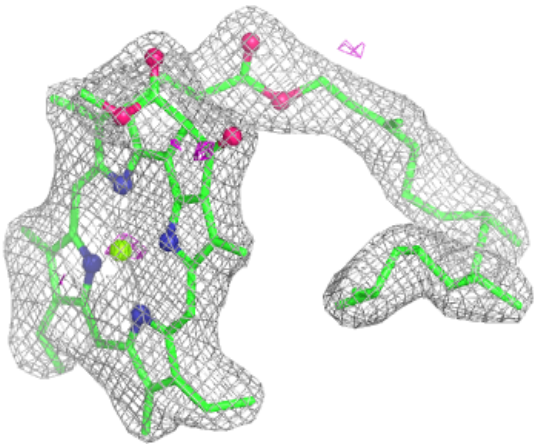


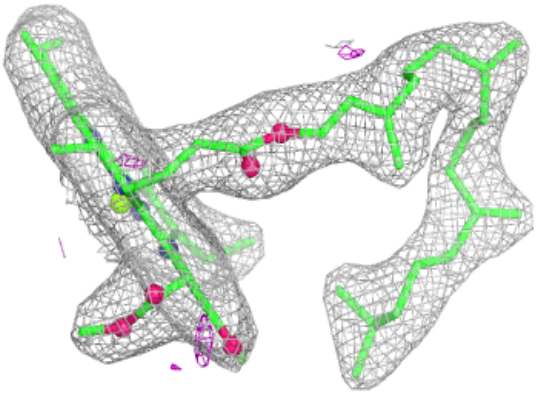


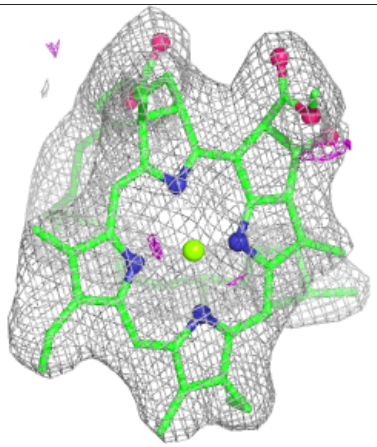


Electron density around CLA C 504:

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

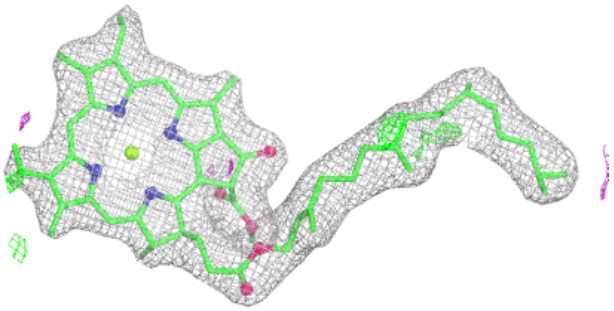


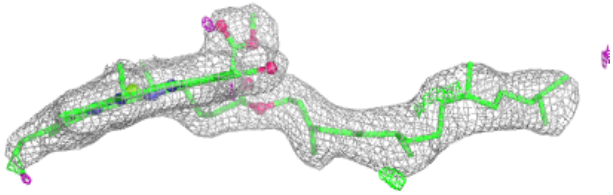


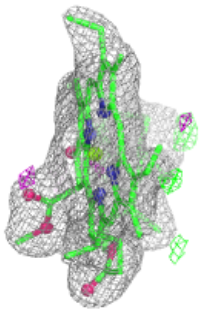


Electron density around CLA b 602:

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

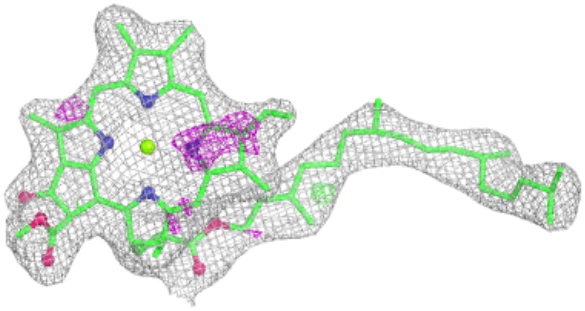


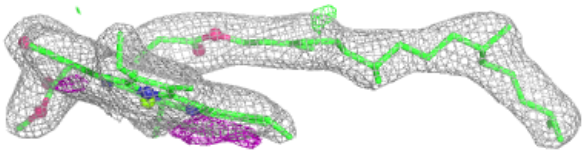


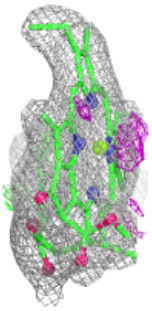


Electron density around CLA b 603:

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

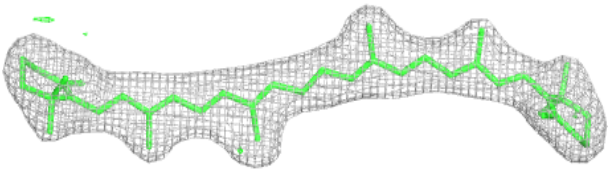


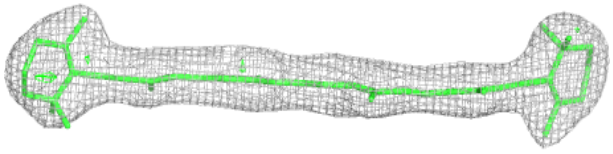


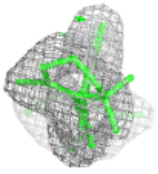


Electron density around BCR C 516:

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

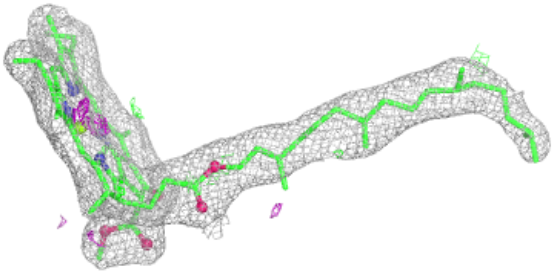


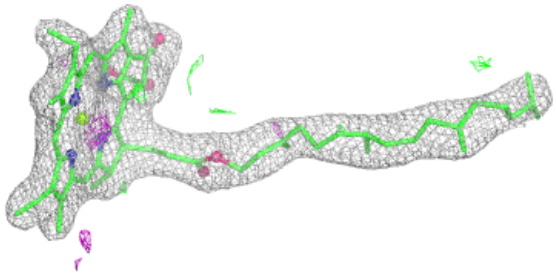


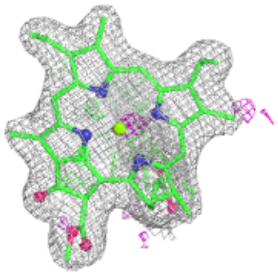


Electron density around CLA b 604:

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

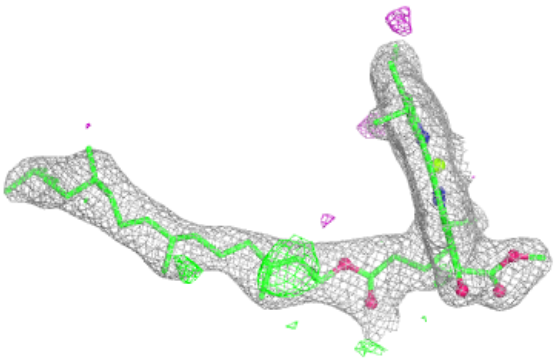


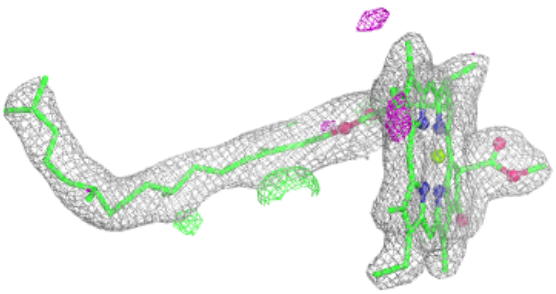


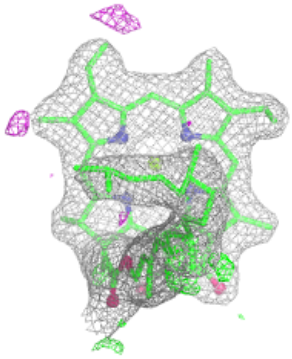


Electron density around CLA b 605:

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

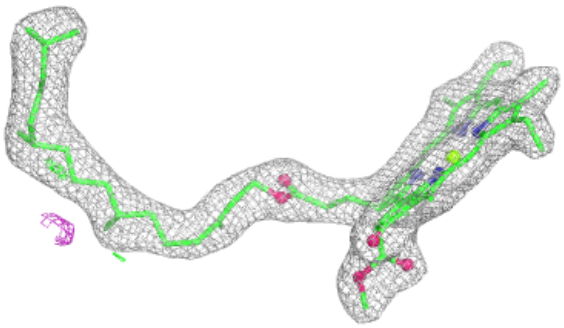


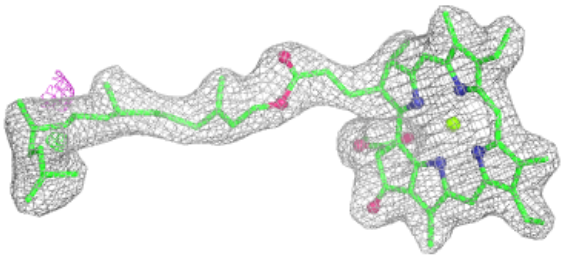


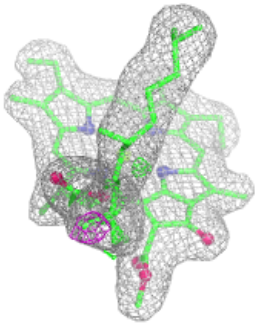


Electron density around CLA d 402 (B):

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

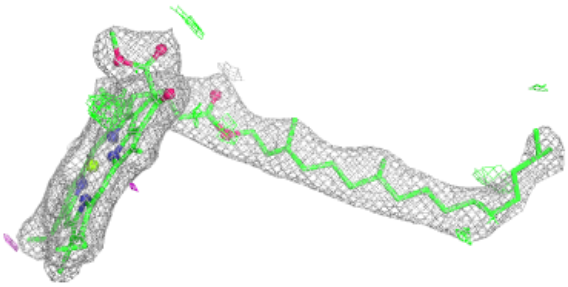


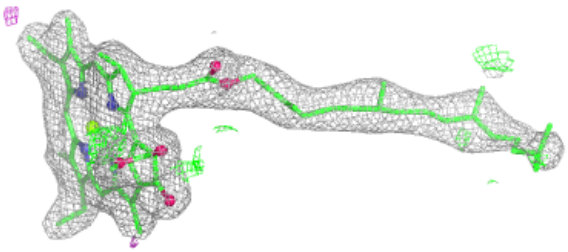


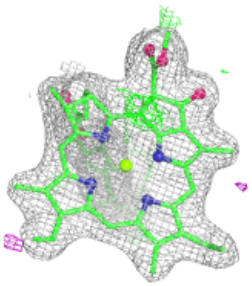


Electron density around CLA B 604:

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

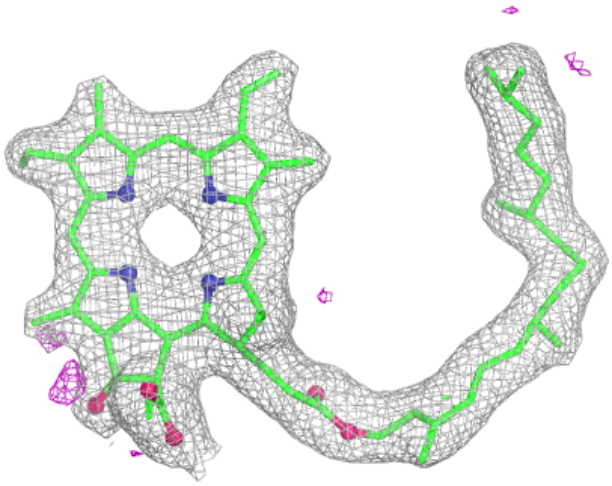


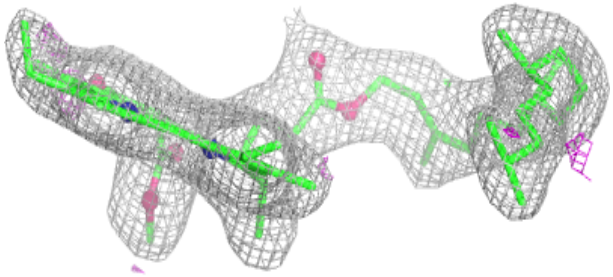


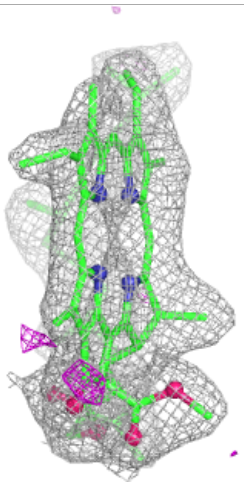


Electron density around PHO A 407 (A):

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

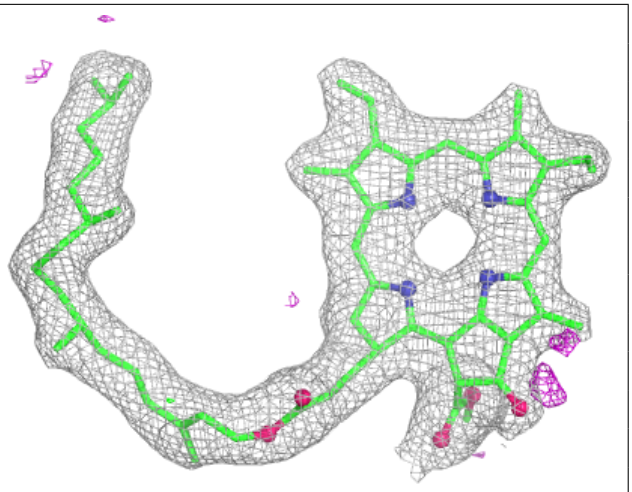


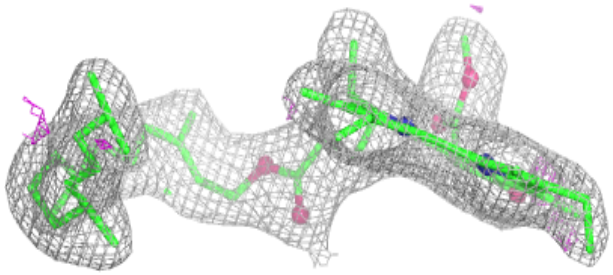


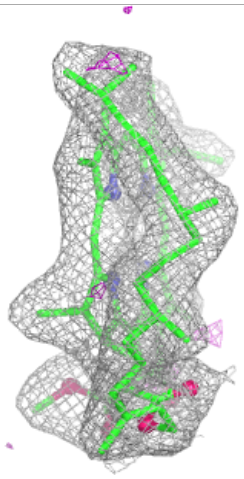


Electron density around PHO A 407 (B):

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

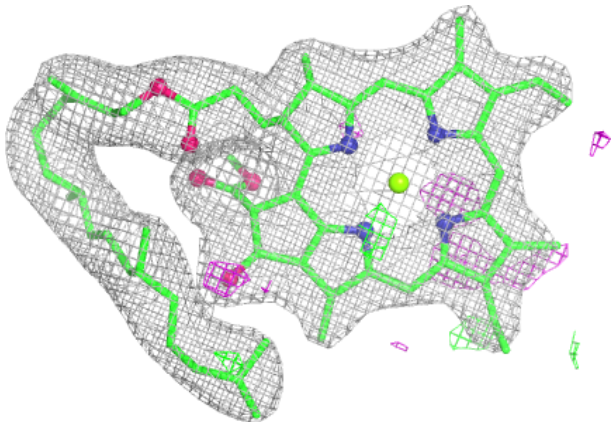


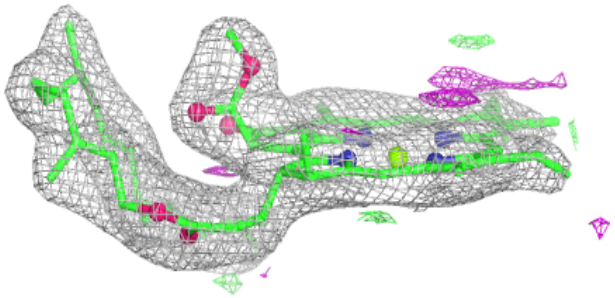


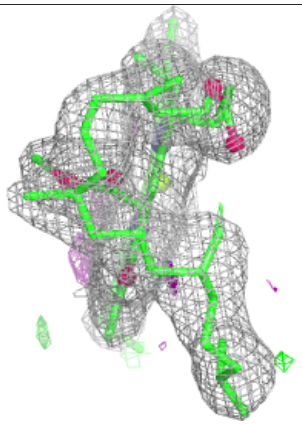


Electron density around CLA b 610:

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

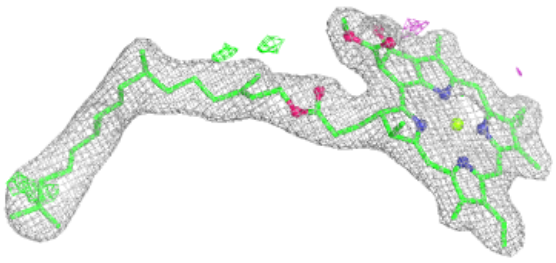


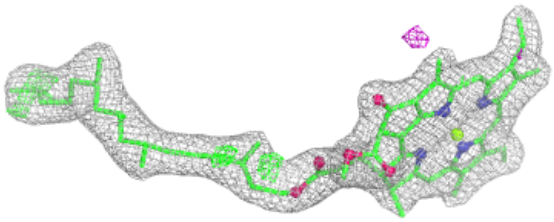


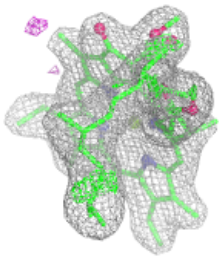


Electron density around CLA a 404 (A):

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

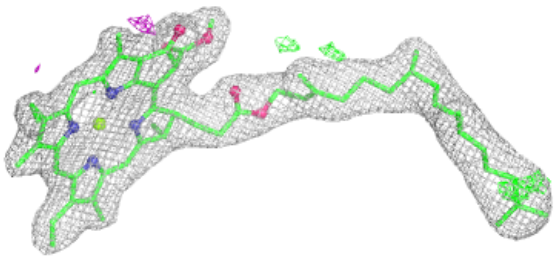


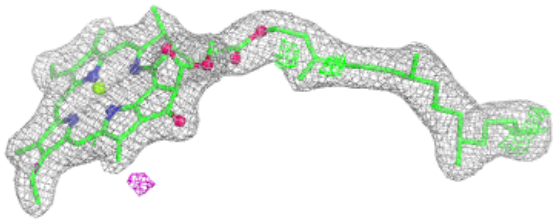


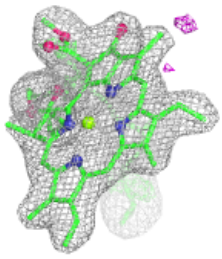


Electron density around CLA a 404 (B):

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

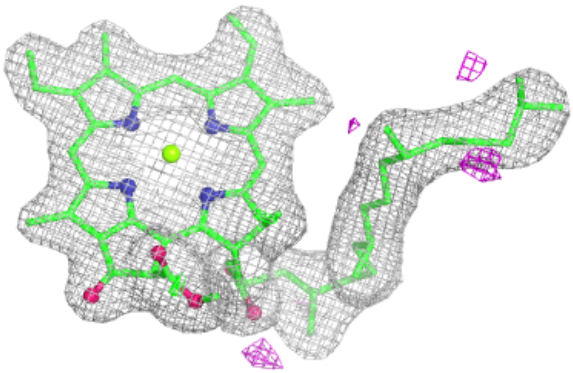


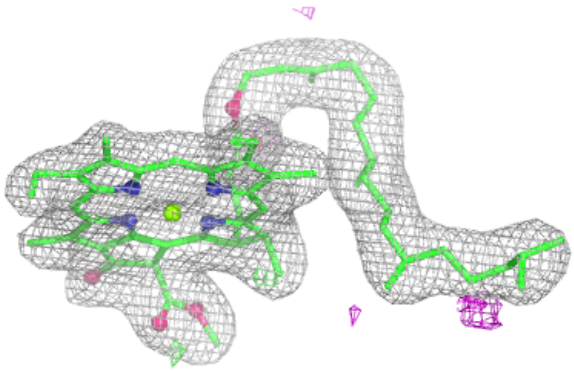


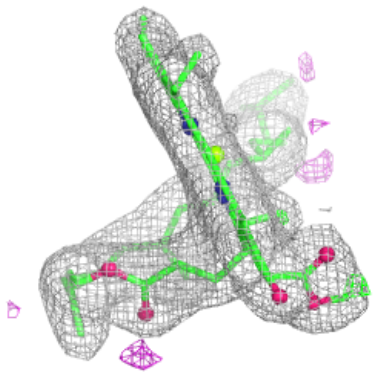


Electron density around CLA a 405 (A):

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

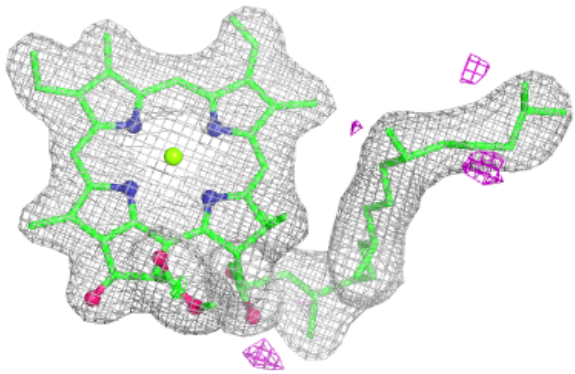


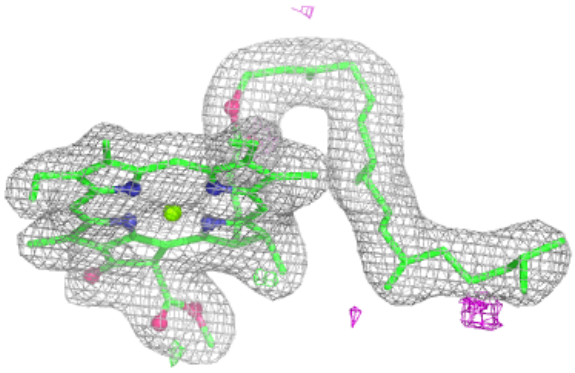


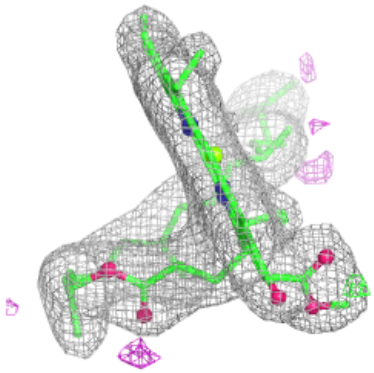


Electron density around CLA a 405 (B):

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

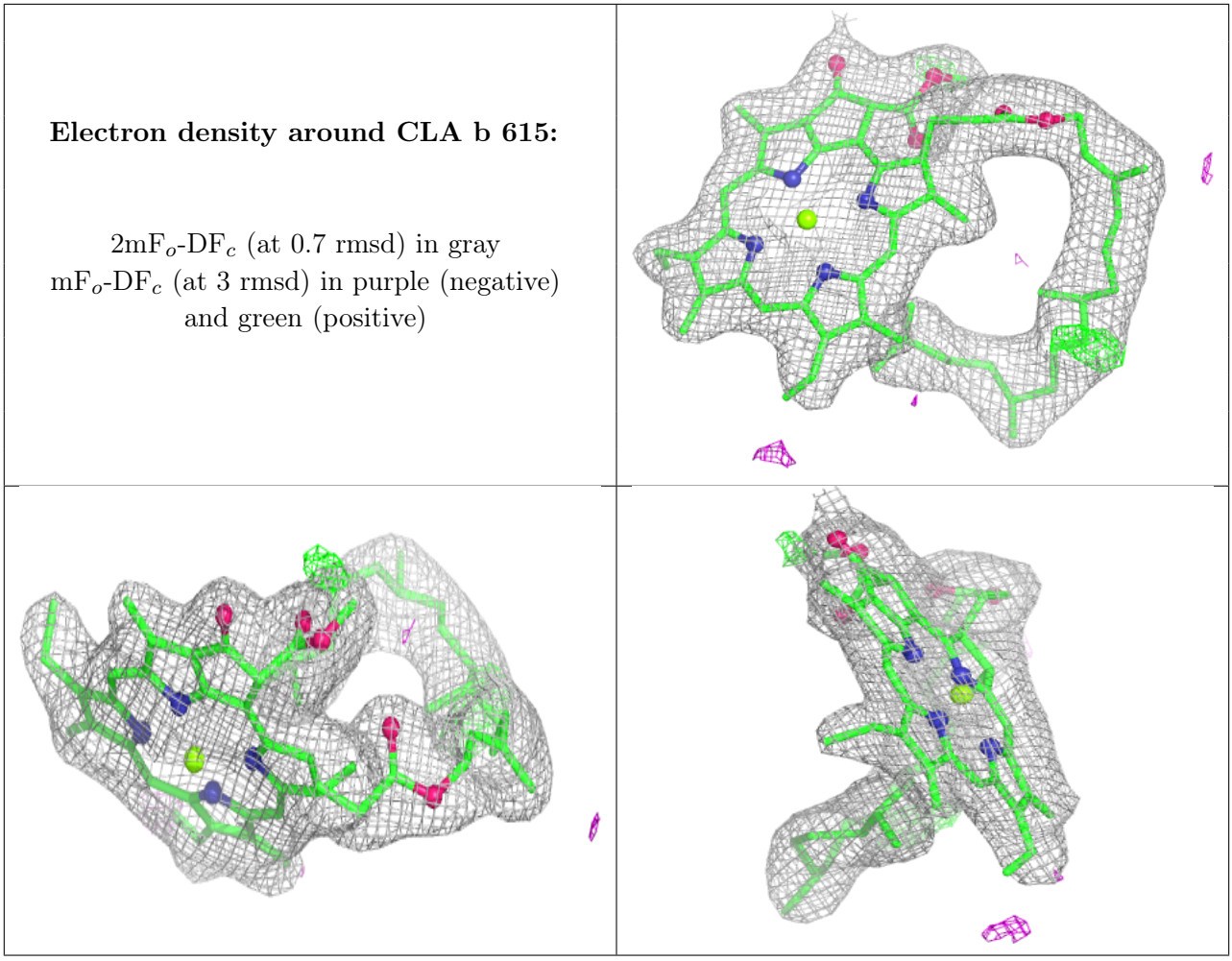






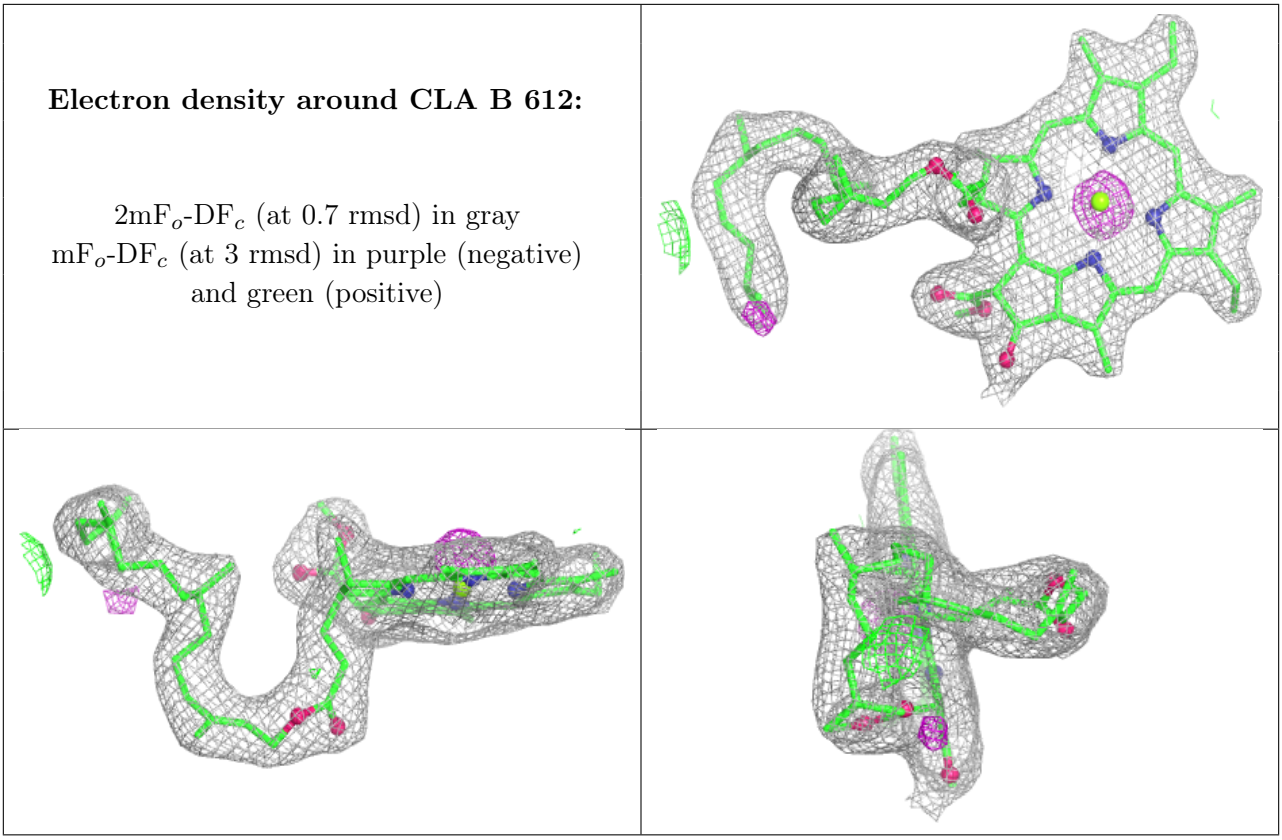
Electron density around CLA b 615:

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



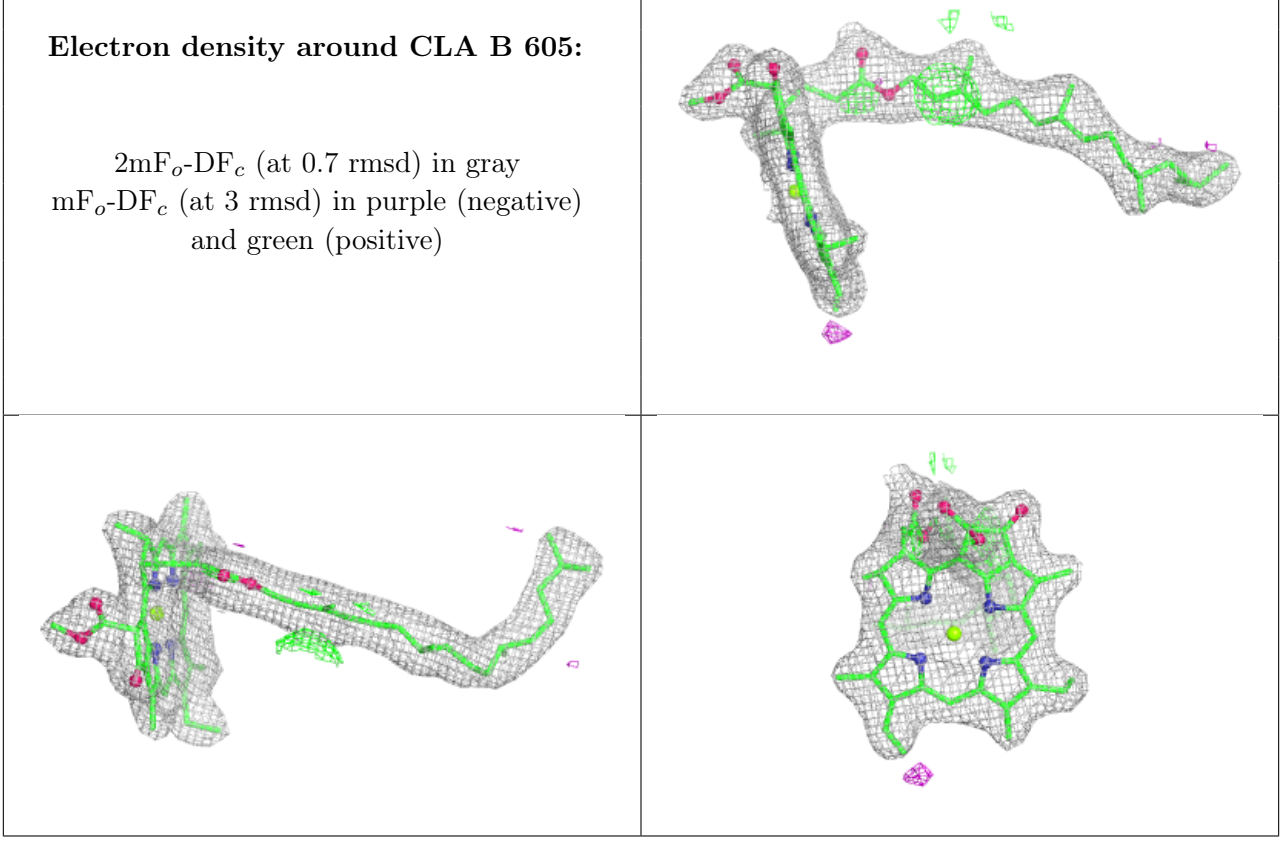
Electron density around CLA B 612:

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



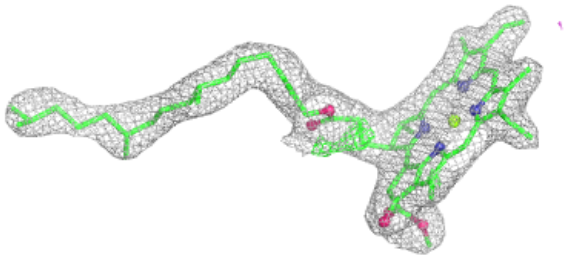
Electron density around CLA B 605:

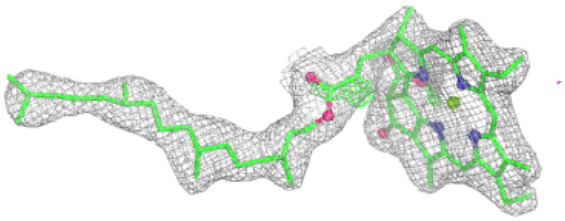
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

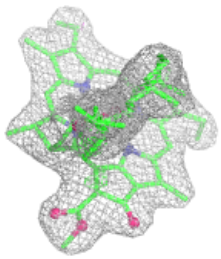


Electron density around CLA c 503:

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

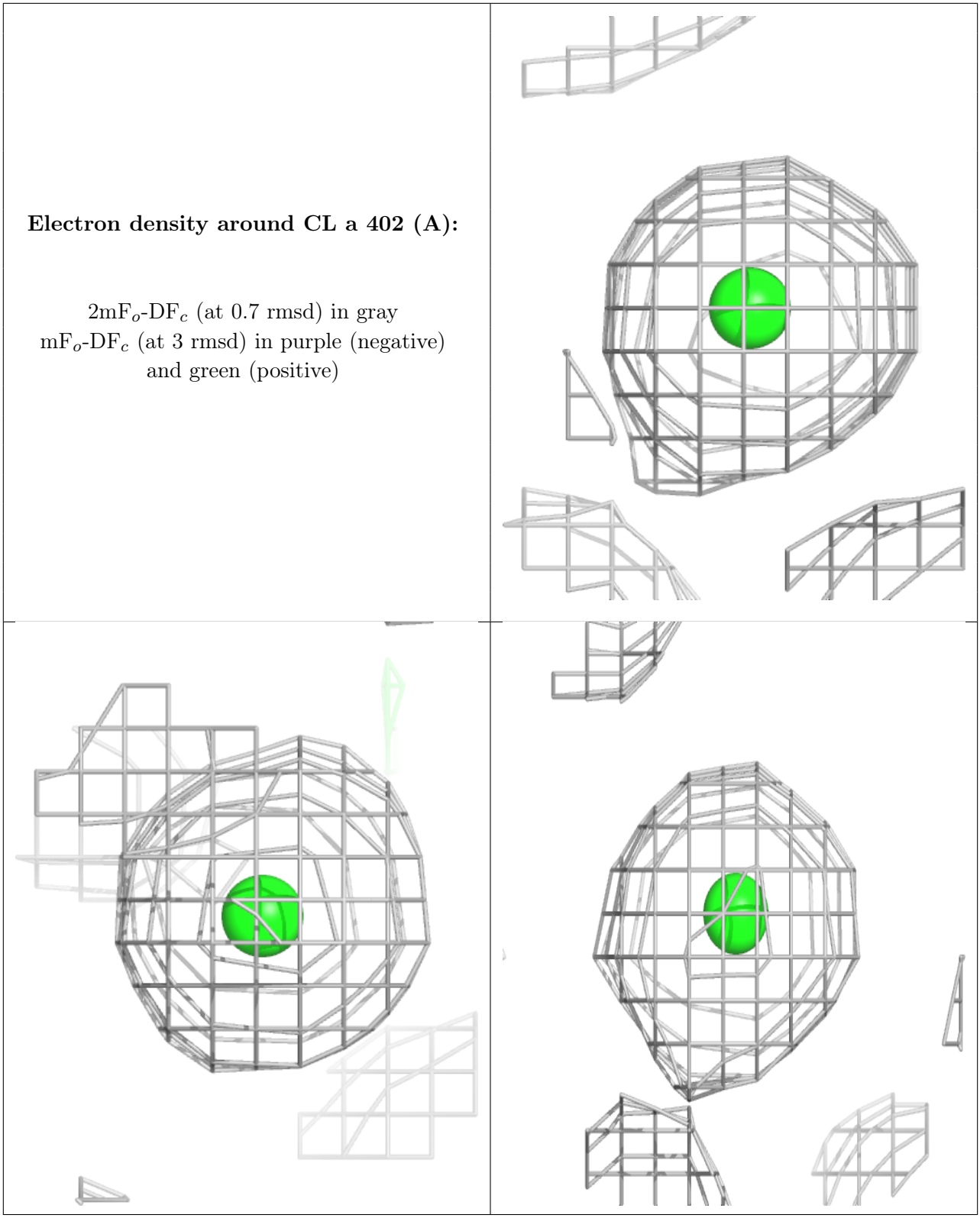






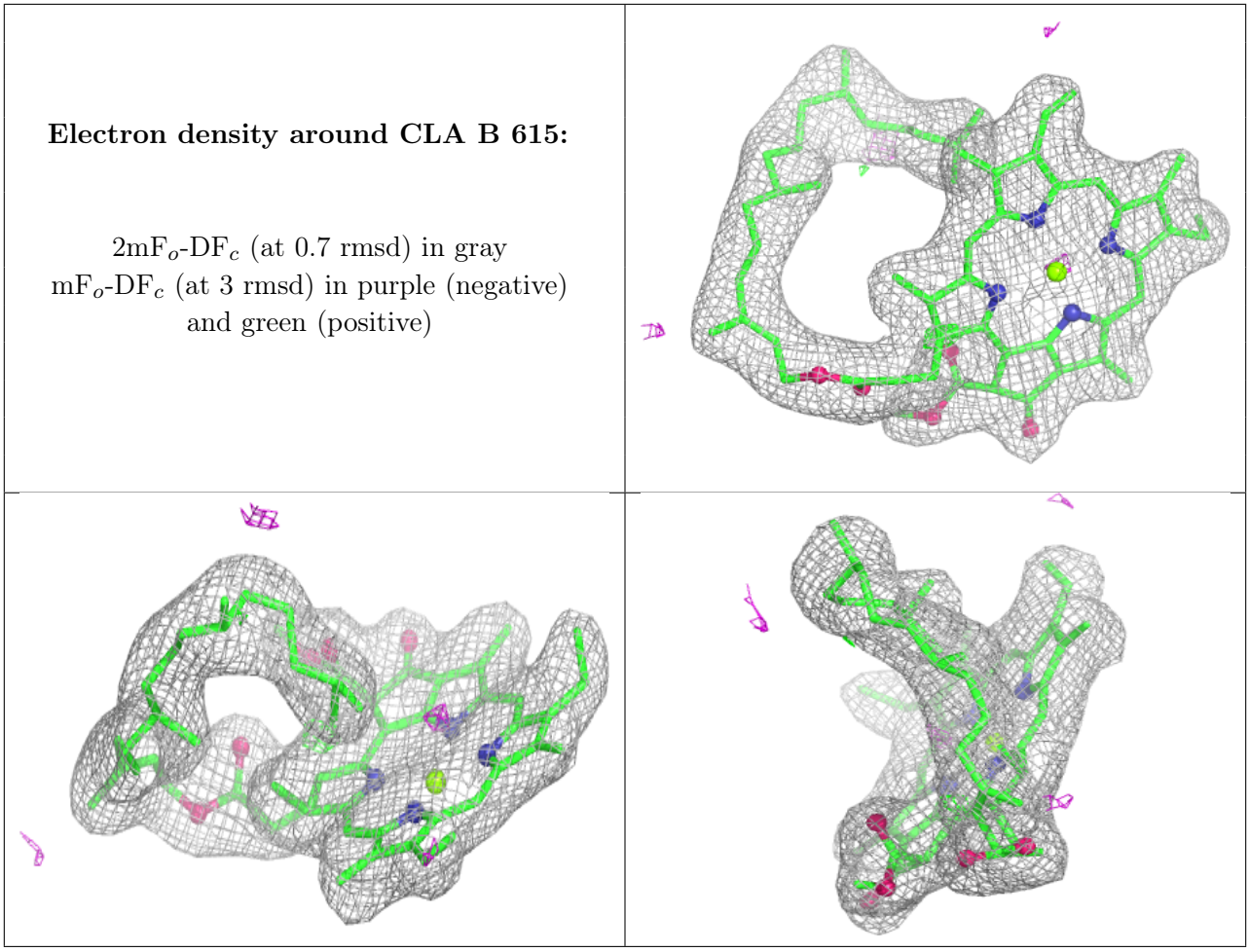
Electron density around CL a 402 (A):

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



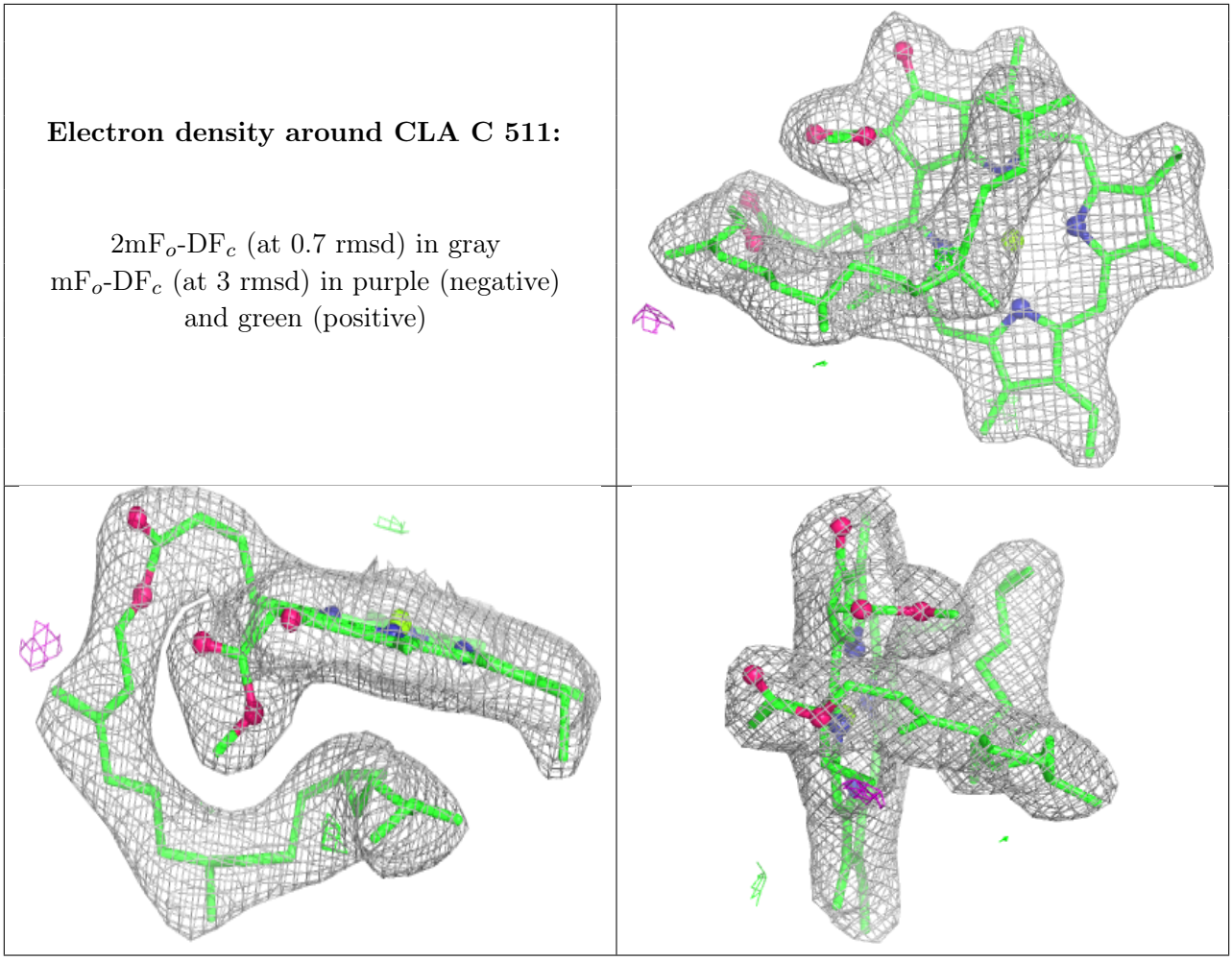
Electron density around CLA B 615:

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



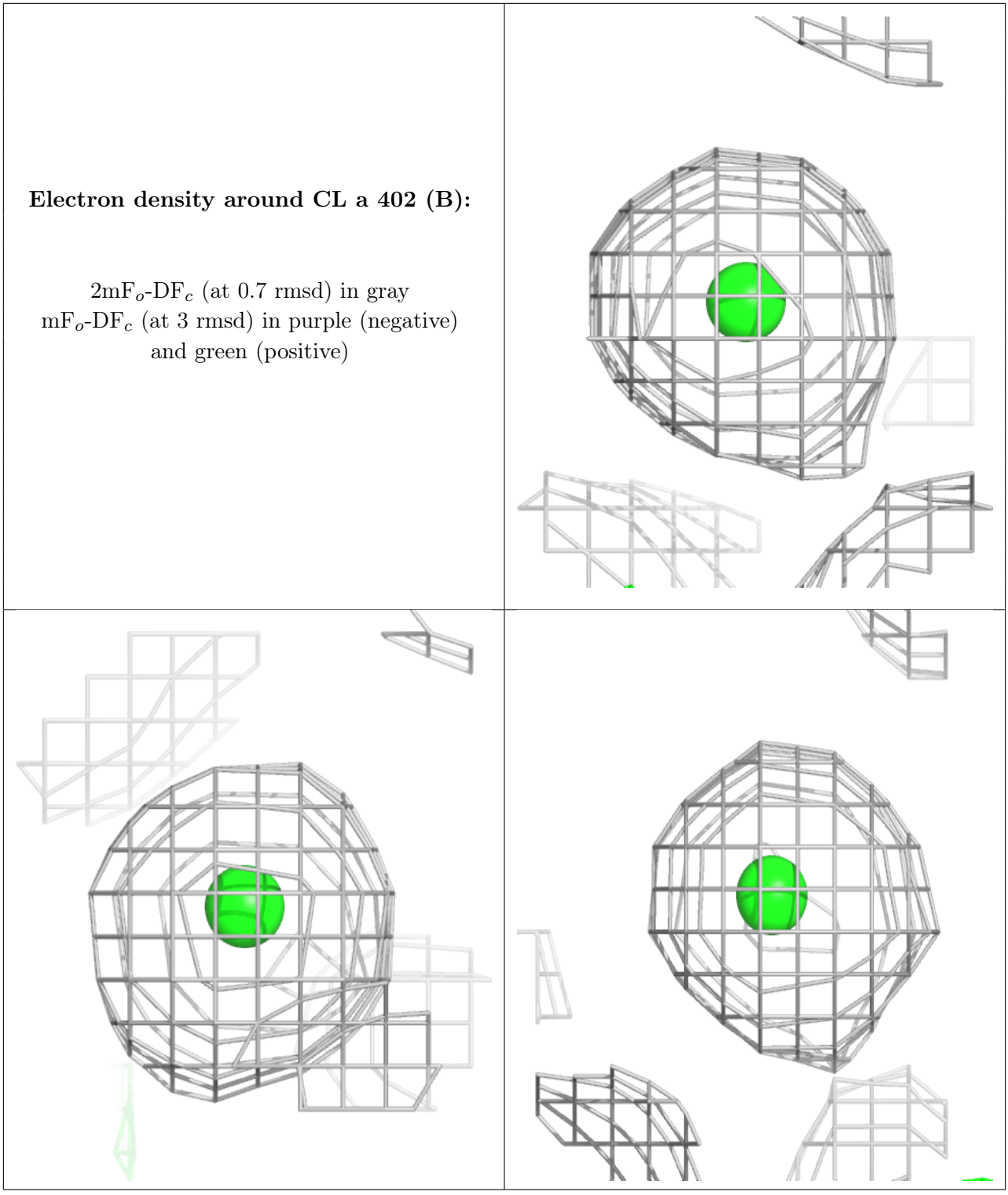
Electron density around CLA C 511:

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



Electron density around CL a 402 (B):

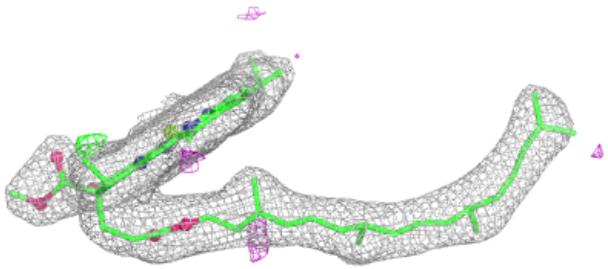
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

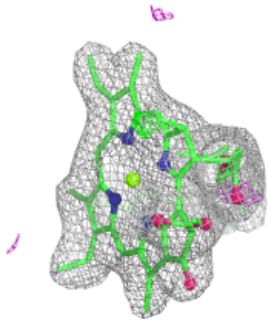


Electron density around CLA B 608:

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

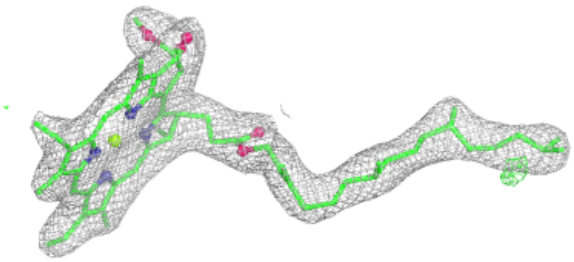


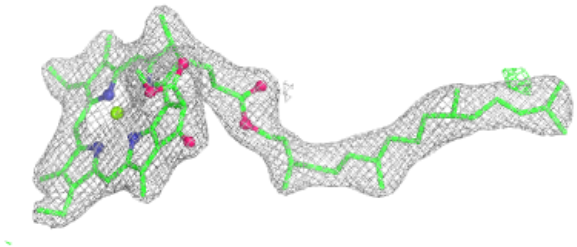


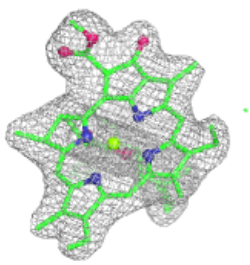


Electron density around CLA C 503:

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

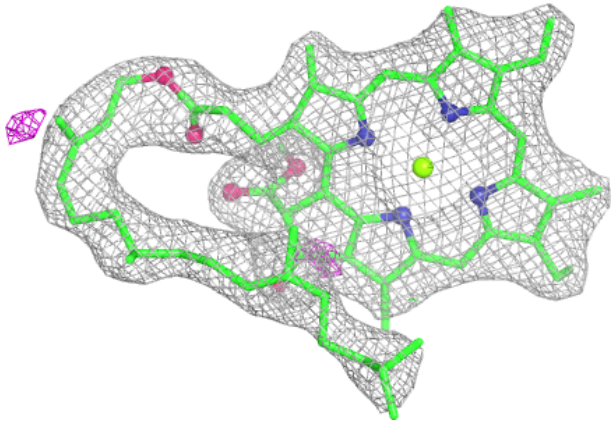


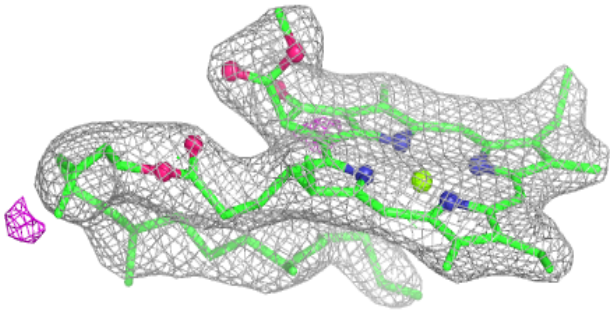


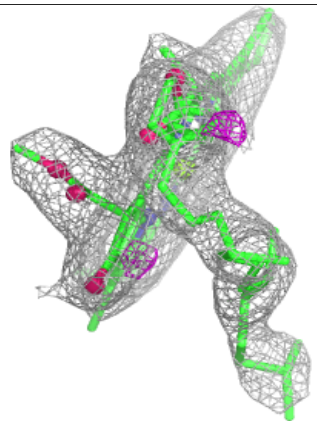


Electron density around CLA c 510:

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

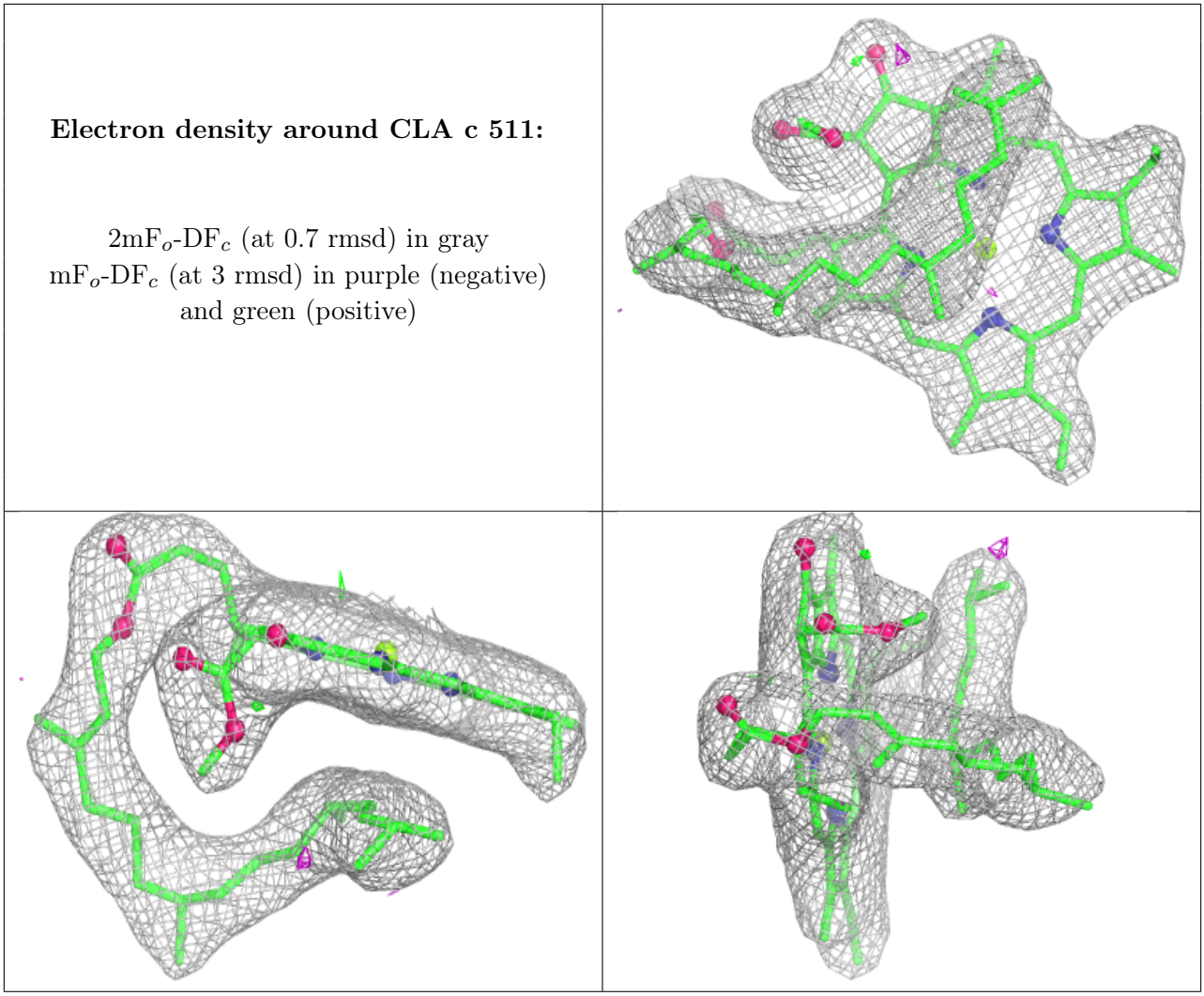






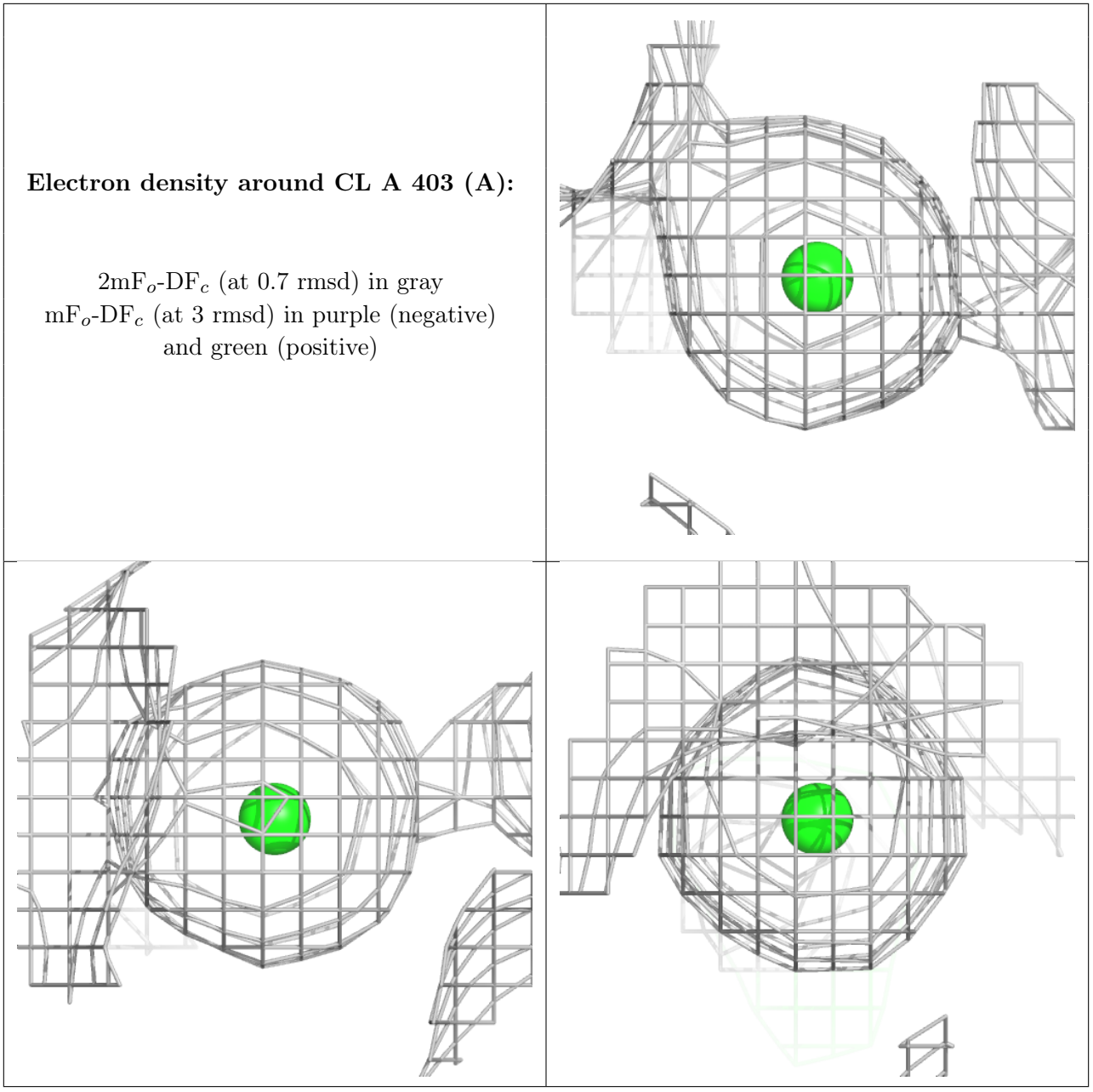
Electron density around CLA c 511:

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



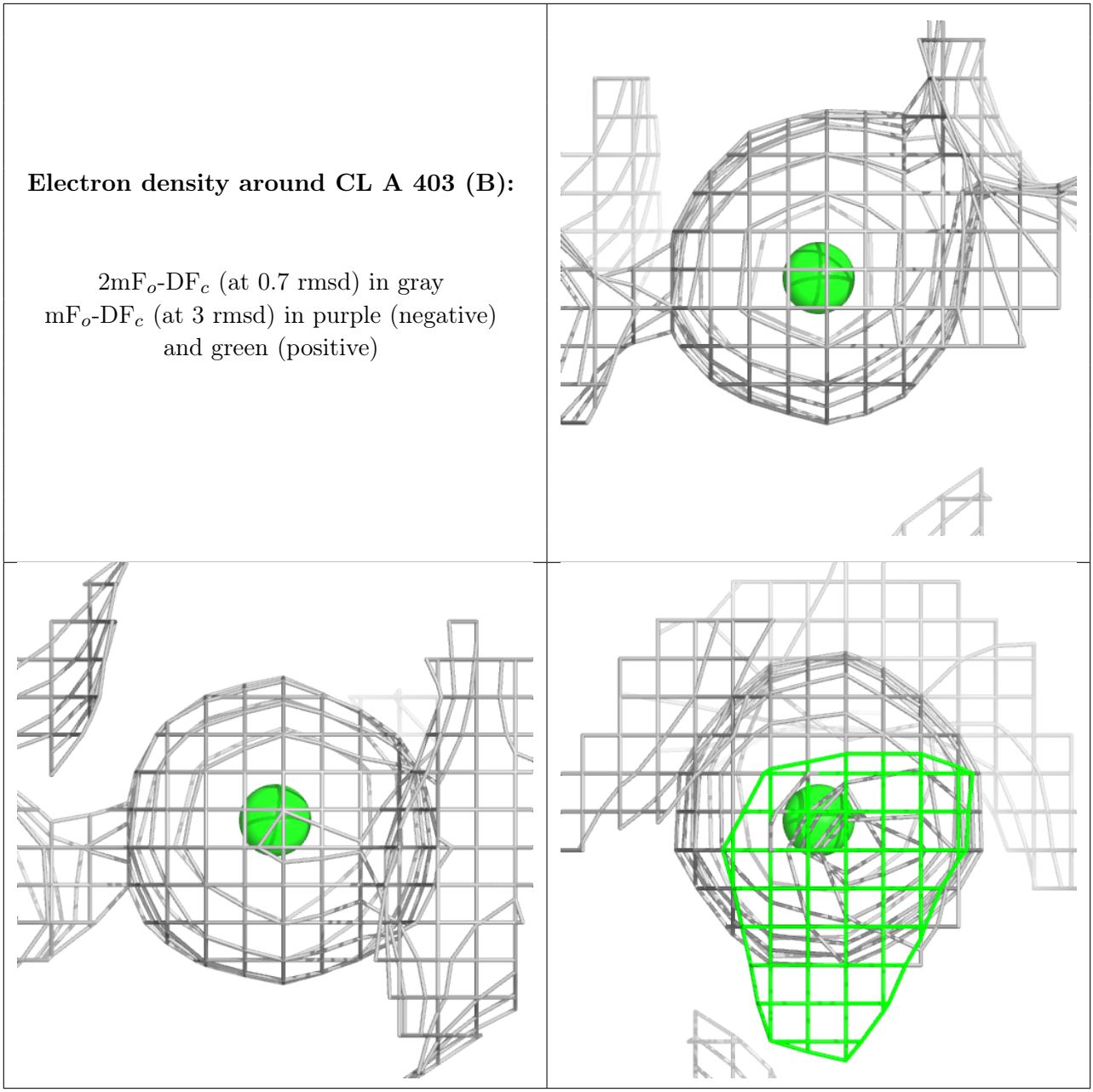
Electron density around CL A 403 (A):

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



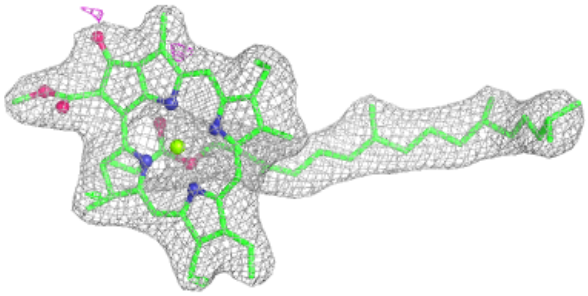
Electron density around CL A 403 (B):

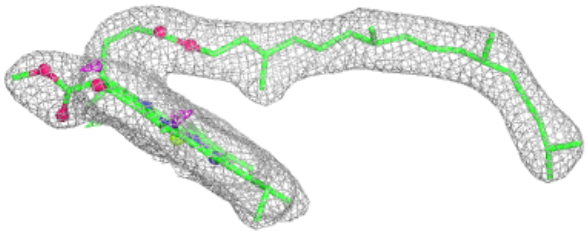
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

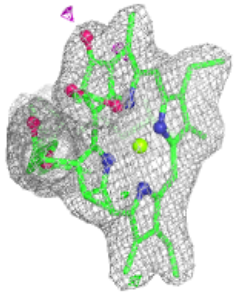


Electron density around CLA b 608:

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

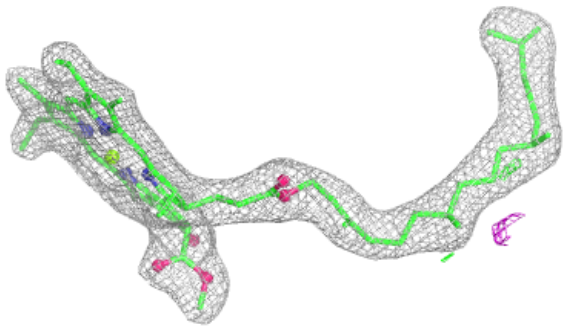


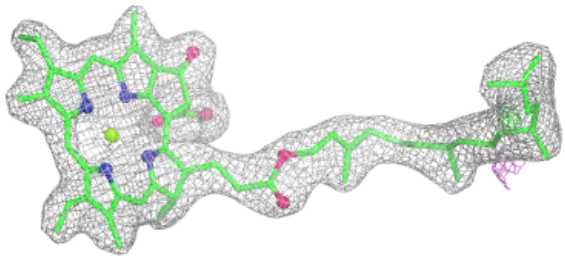


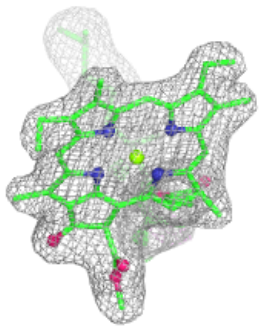


Electron density around CLA d 402 (A):

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

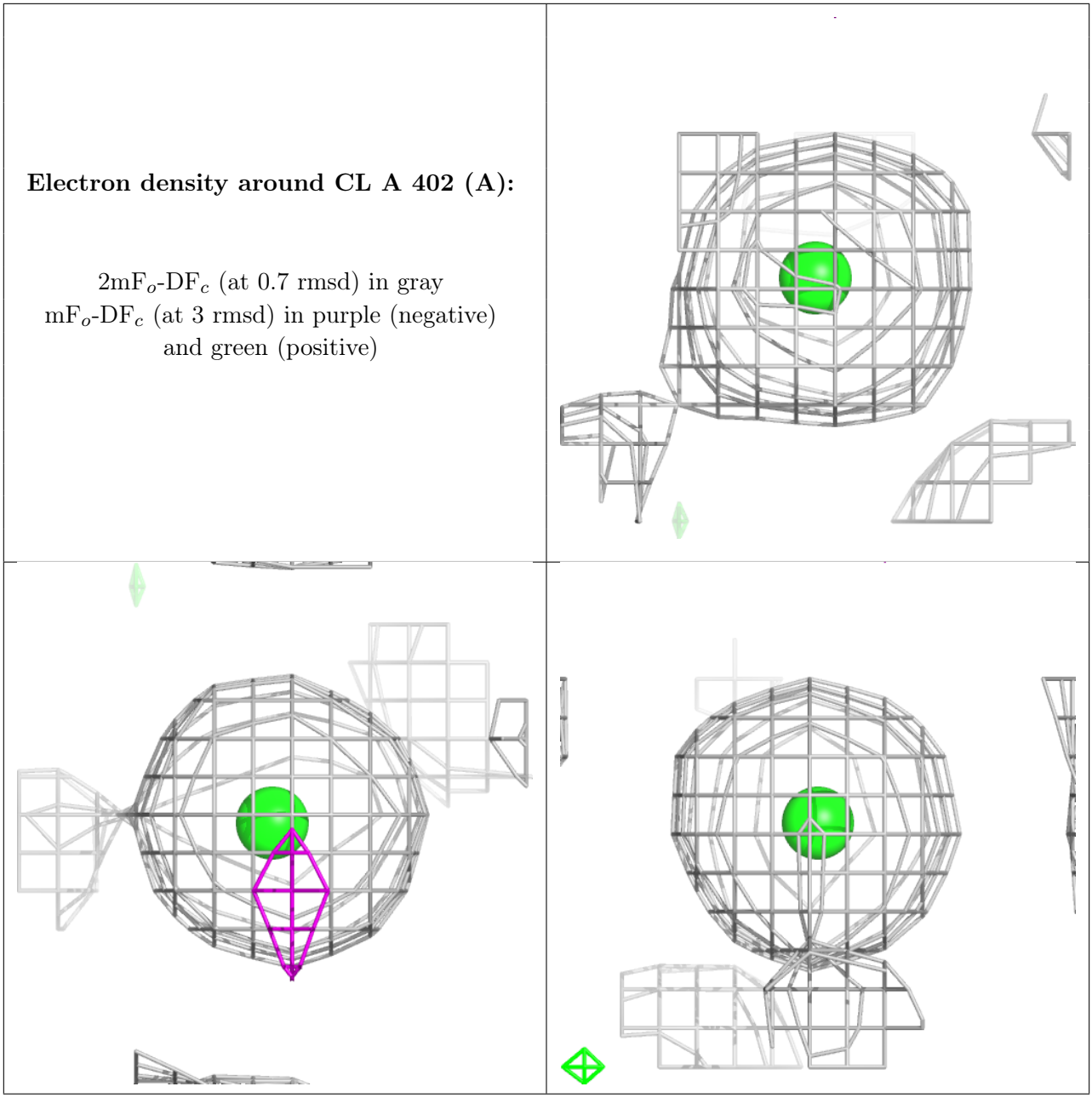






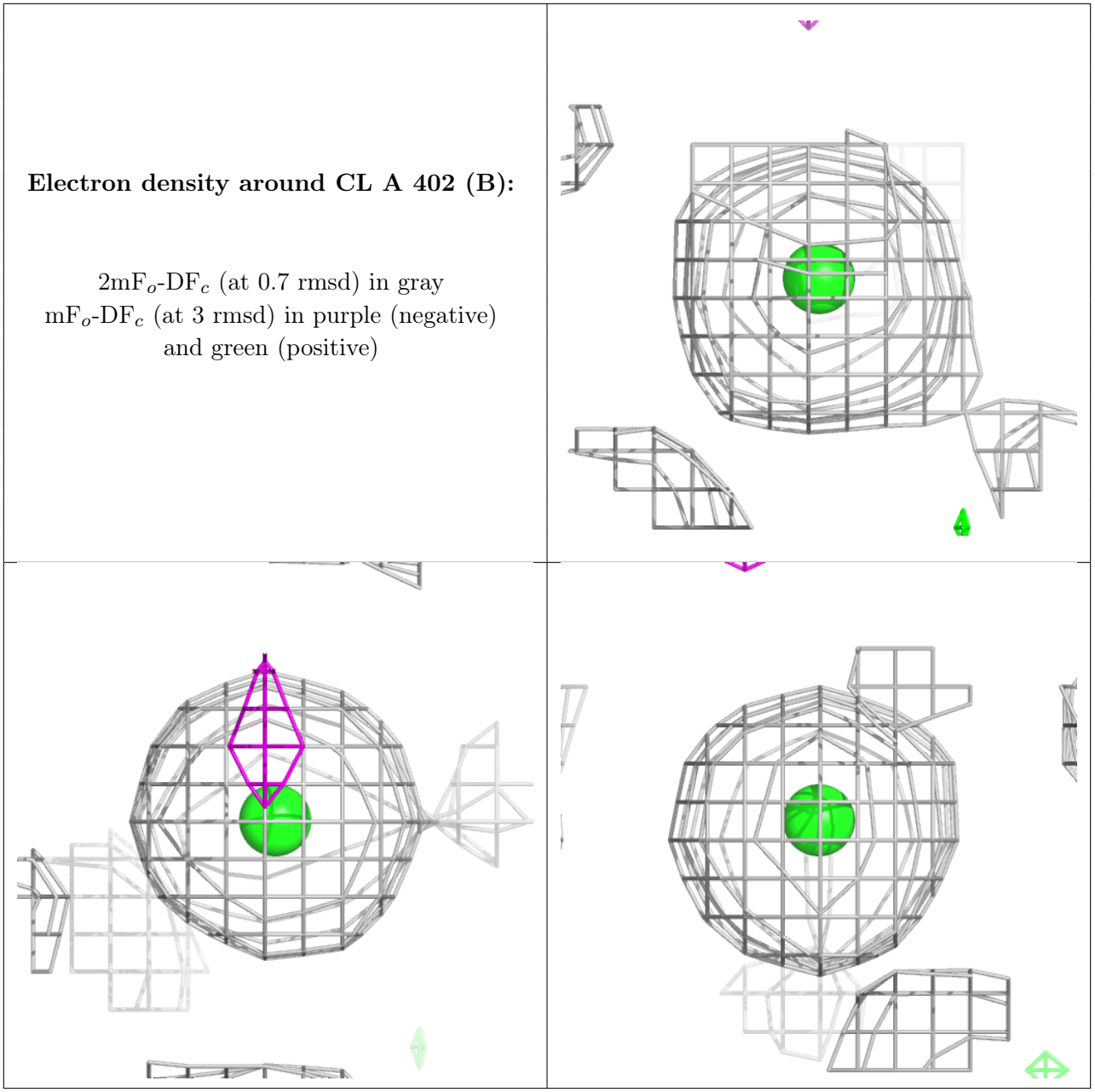
Electron density around CL A 402 (A):

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



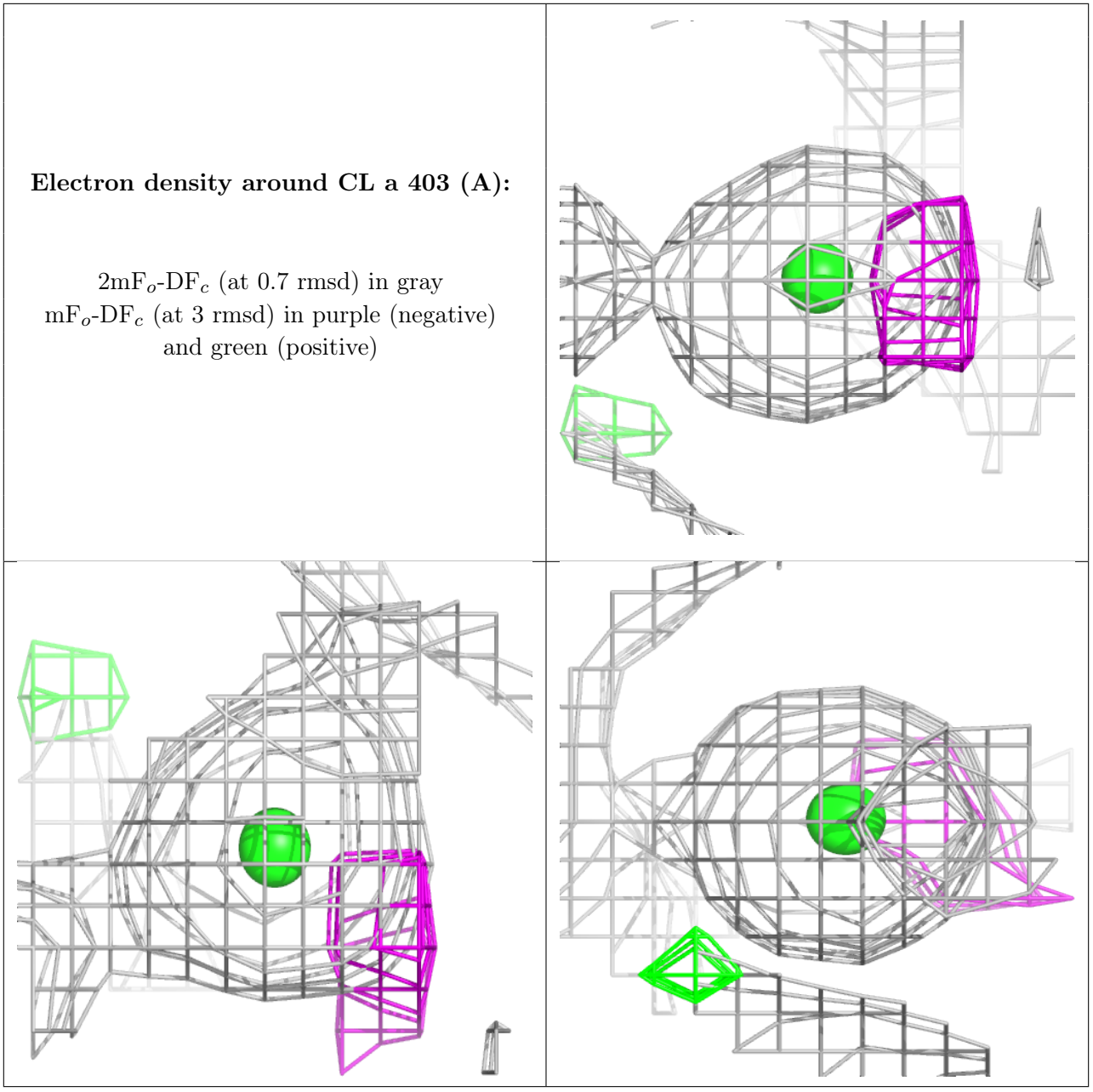
Electron density around CL A 402 (B):

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



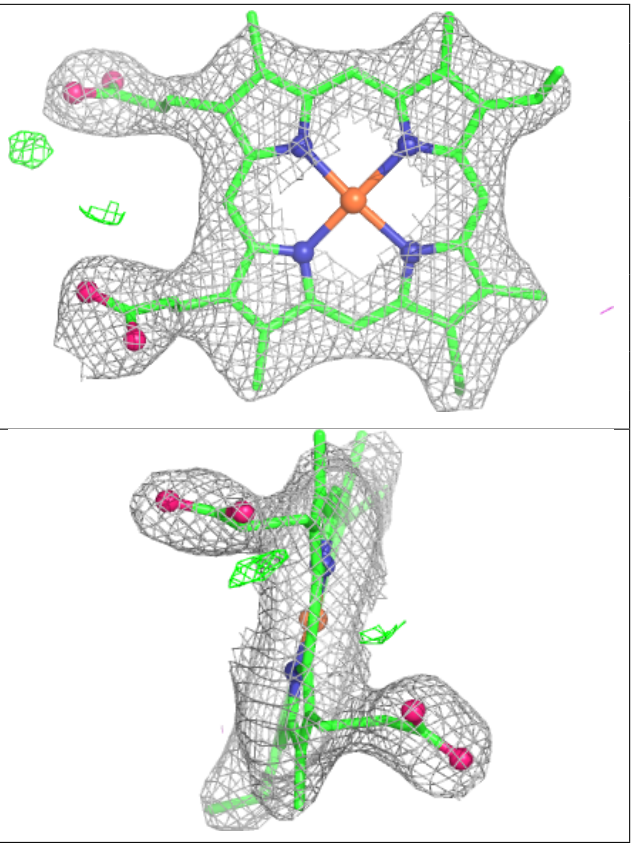
Electron density around CL a 403 (A):

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



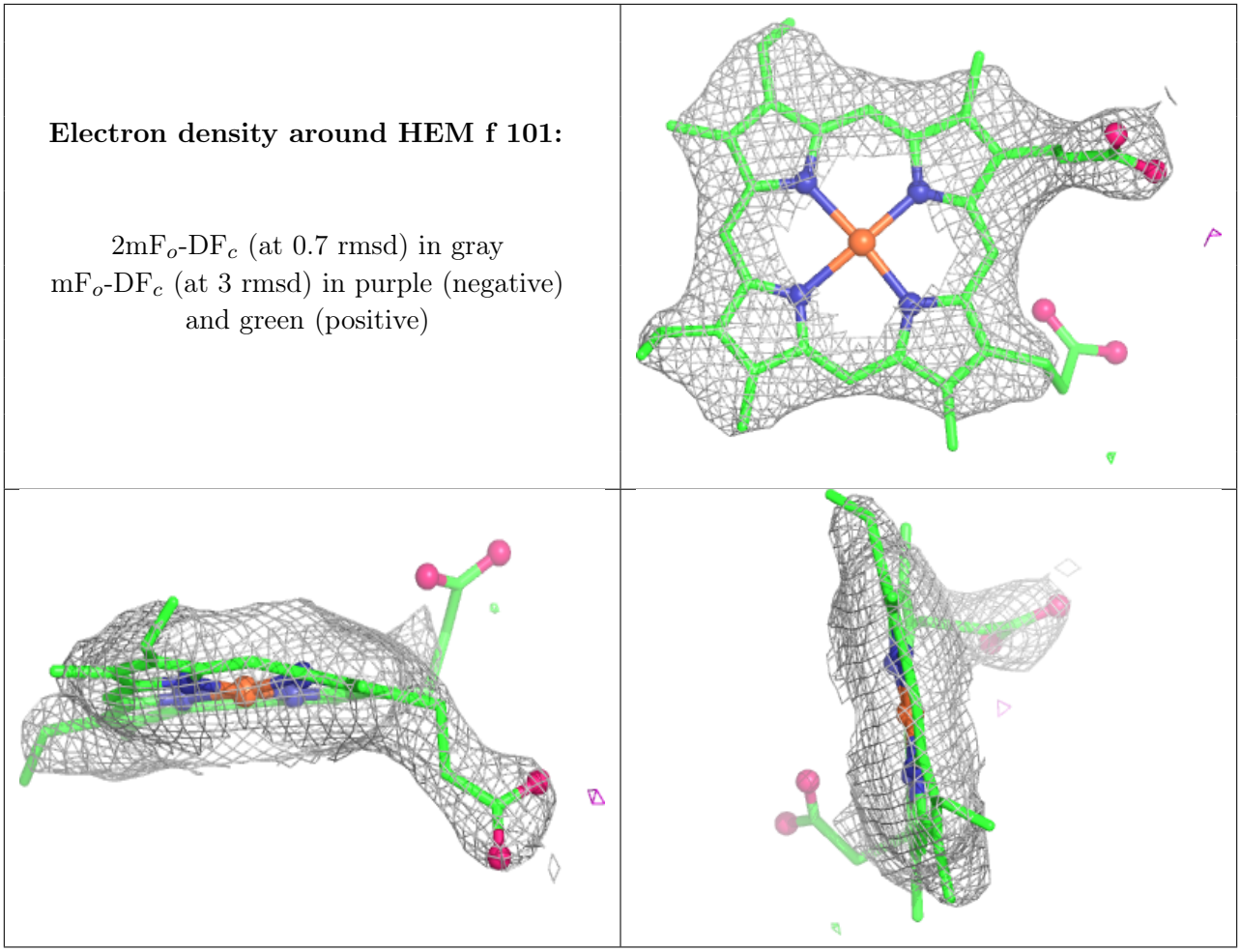
Electron density around HEM F 102:

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



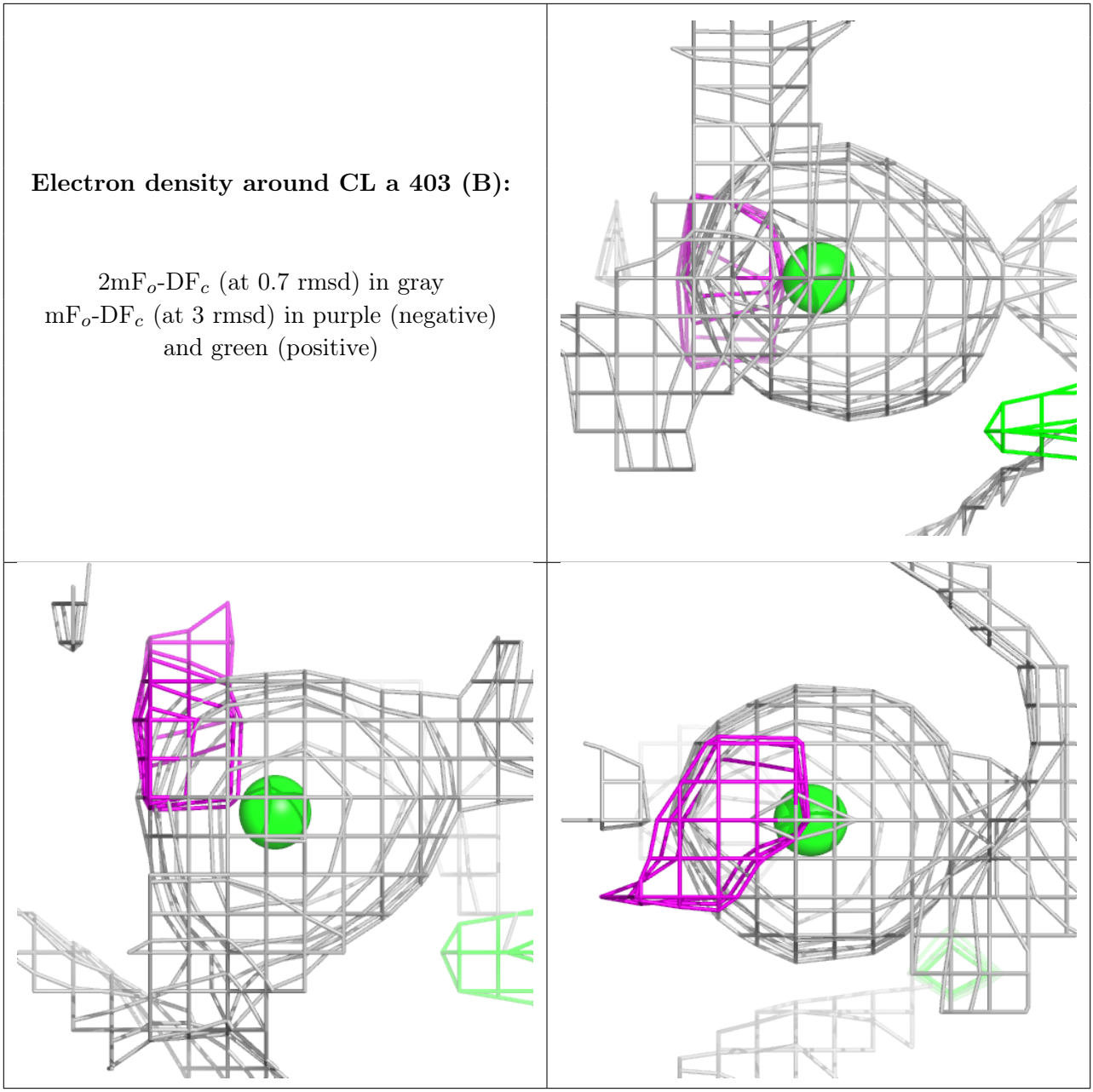
Electron density around HEM f 101:

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



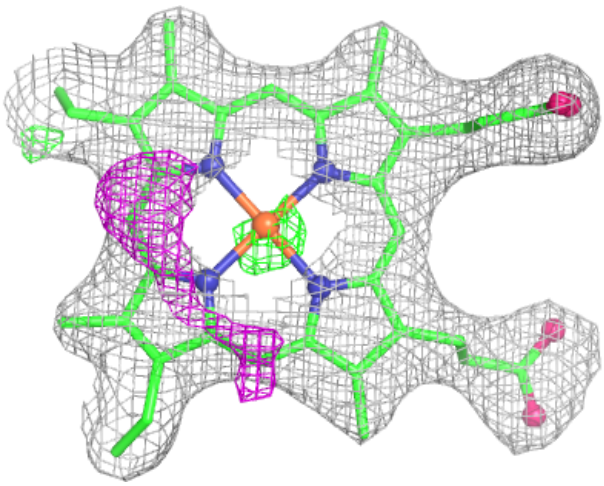
Electron density around CL a 403 (B):

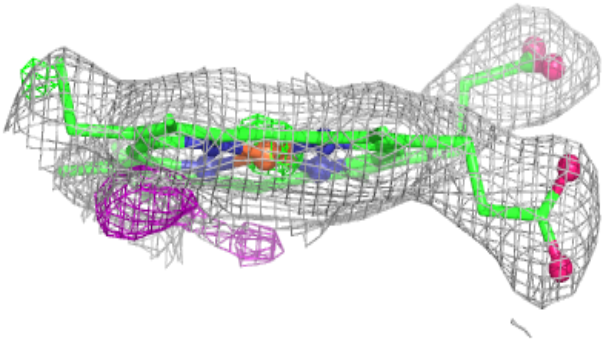
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

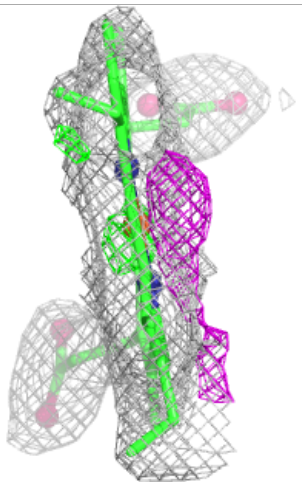


Electron density around HEC v 201:

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

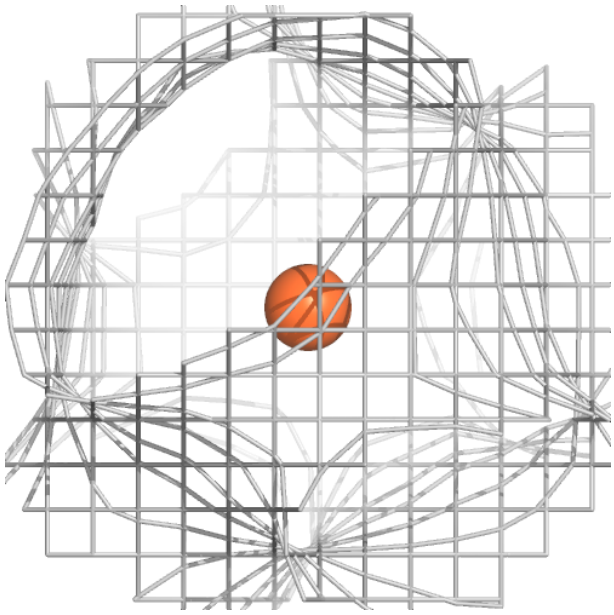


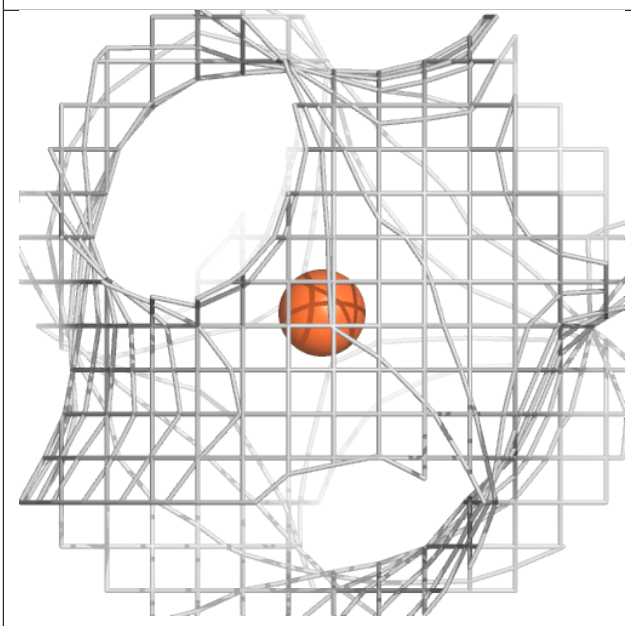


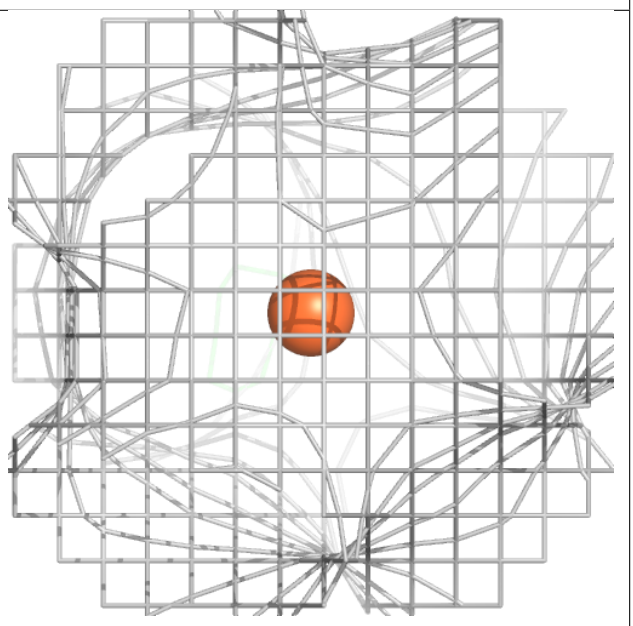


Electron density around FE2 A 401 (B):

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

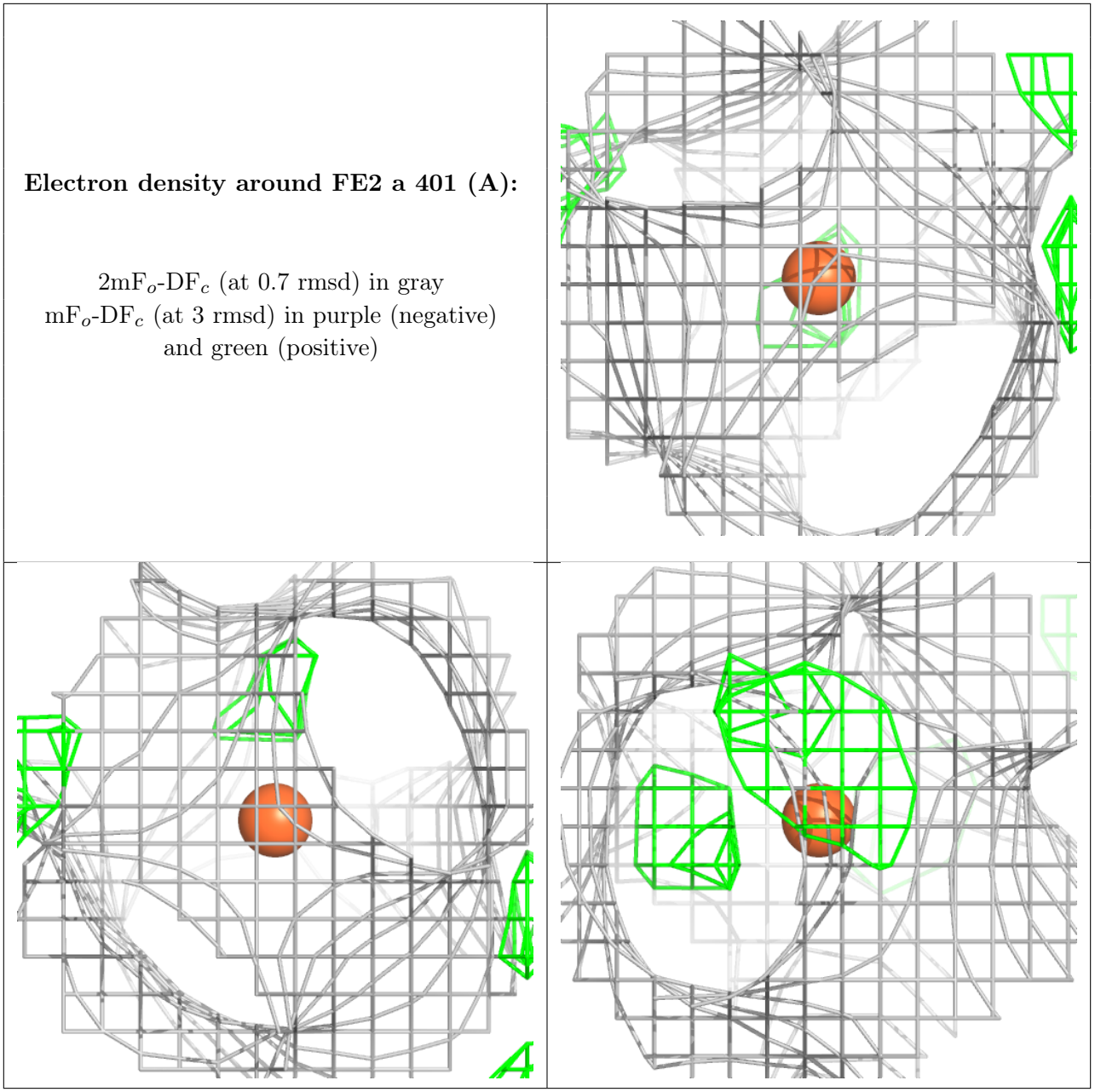






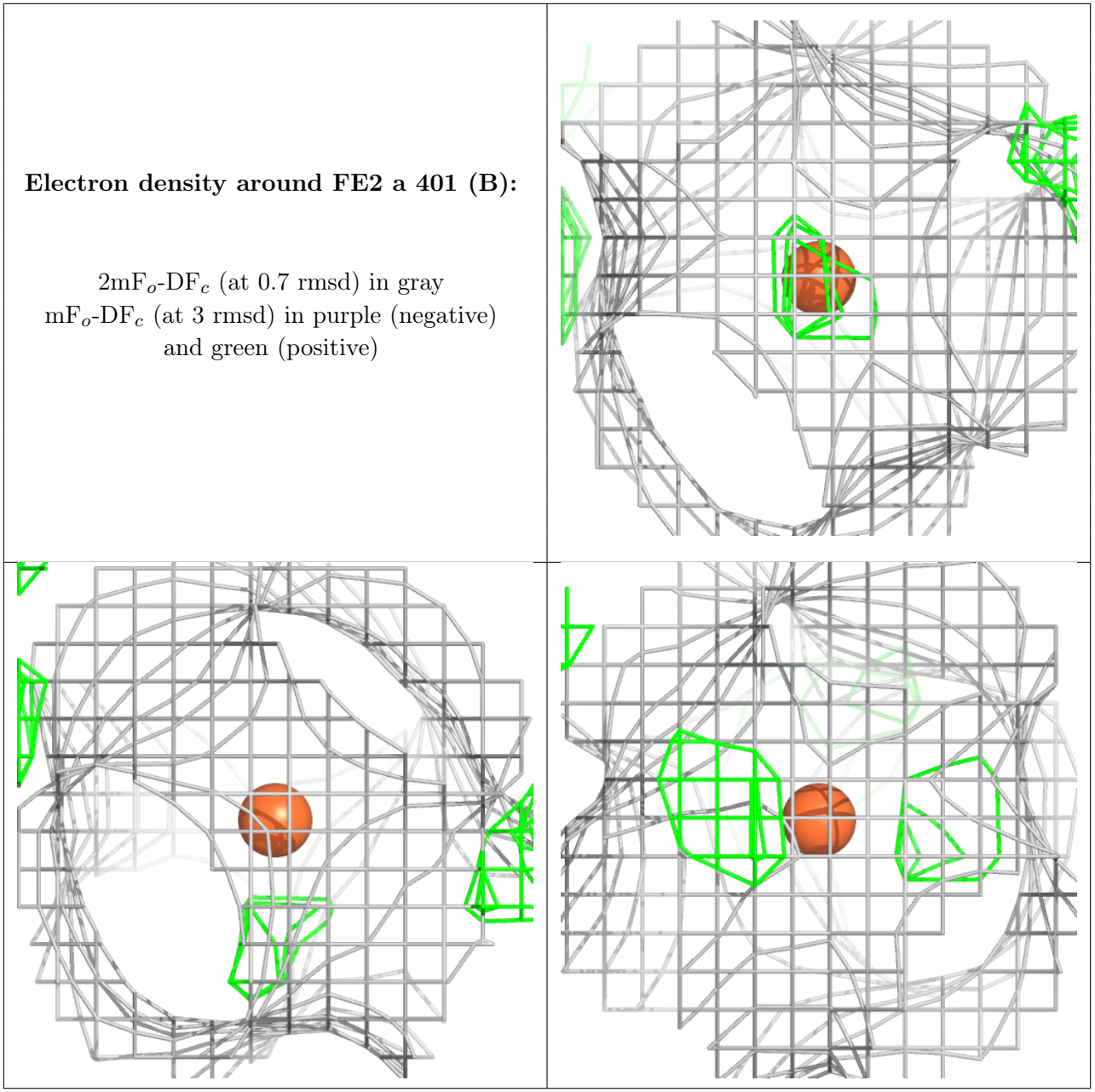
Electron density around FE2 a 401 (A):

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



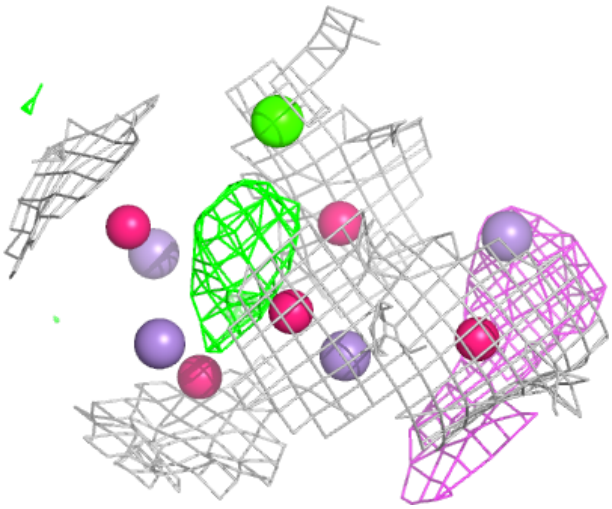
Electron density around FE2 a 401 (B):

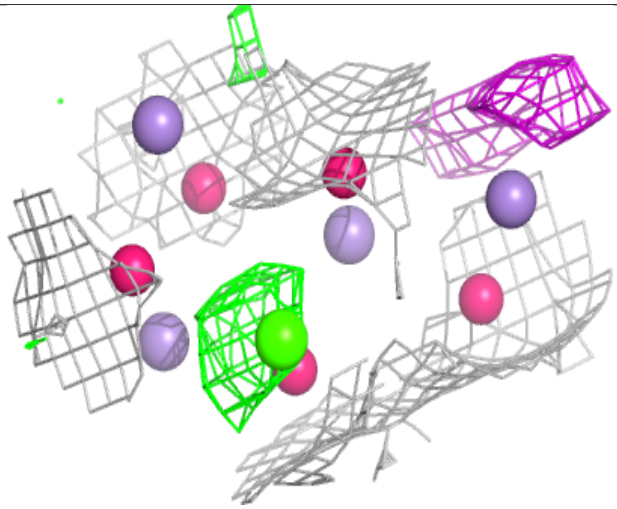
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

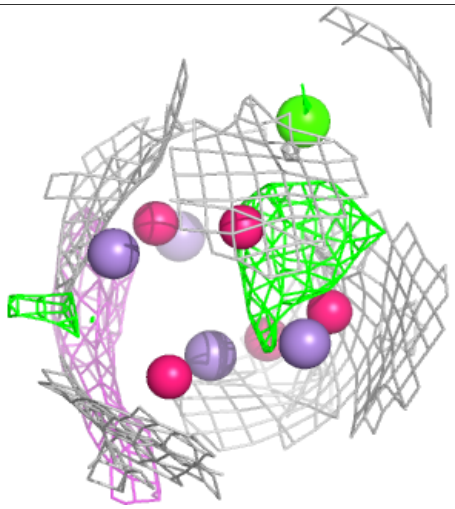


Electron density around OEX A 413 (A):

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

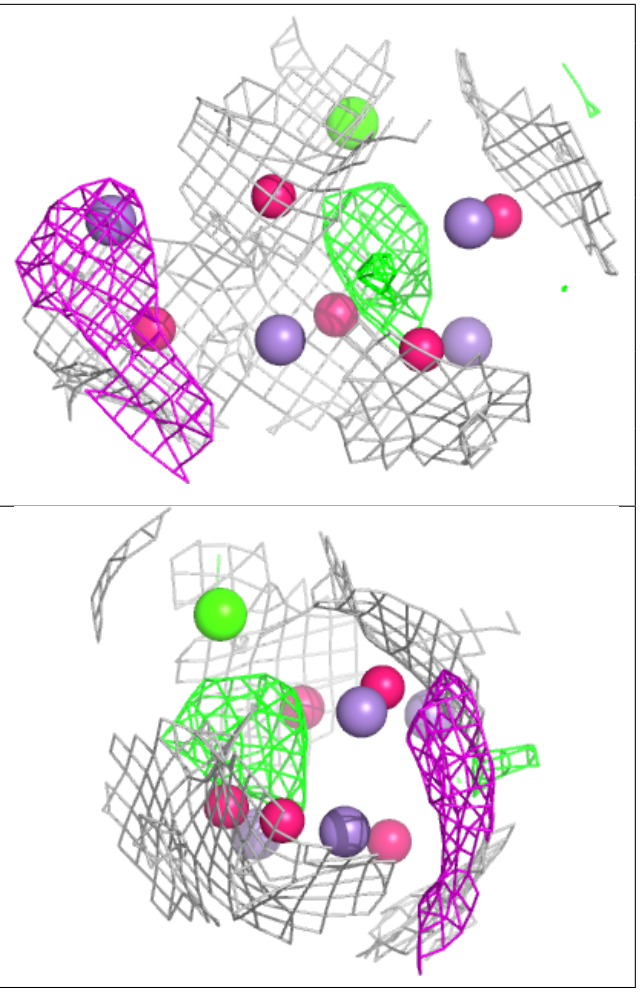






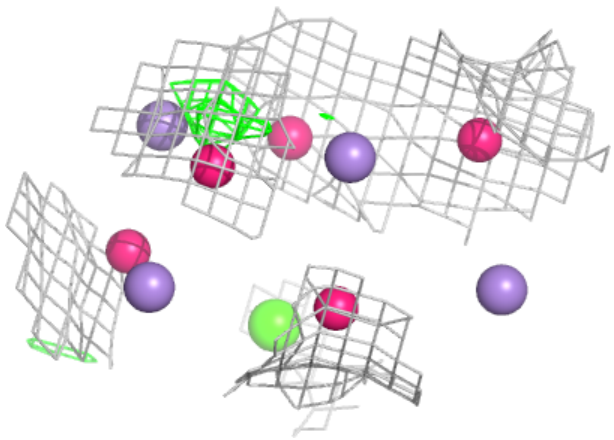
Electron density around OEX A 413 (B):

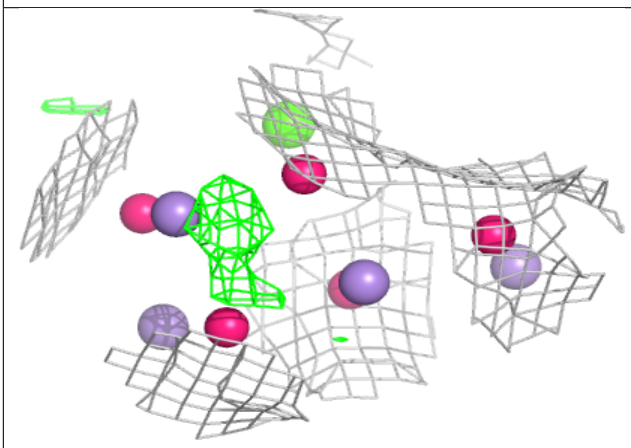
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

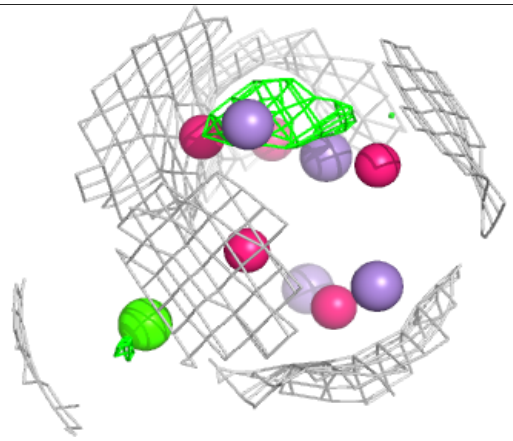


Electron density around OEX a 412 (A):

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

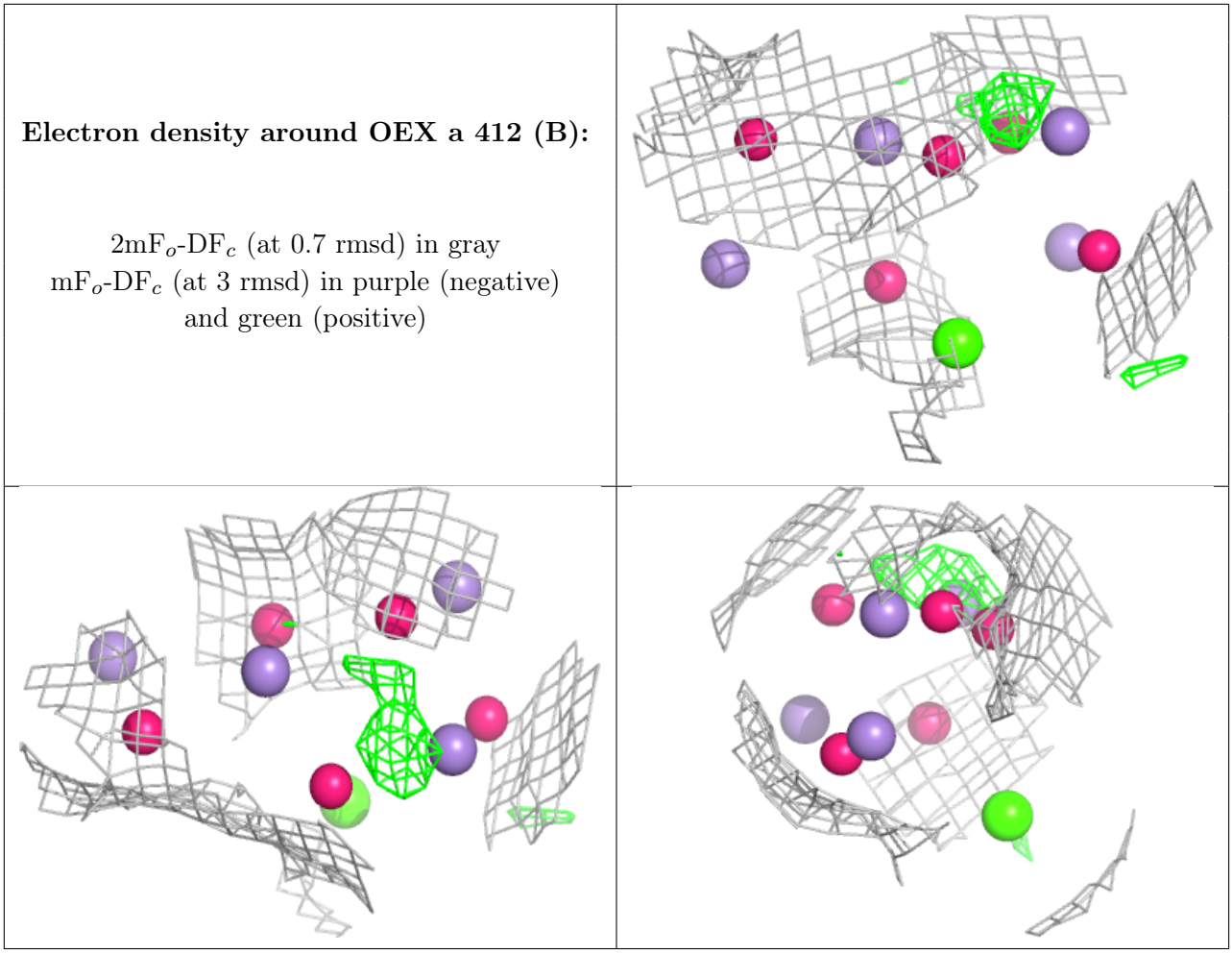






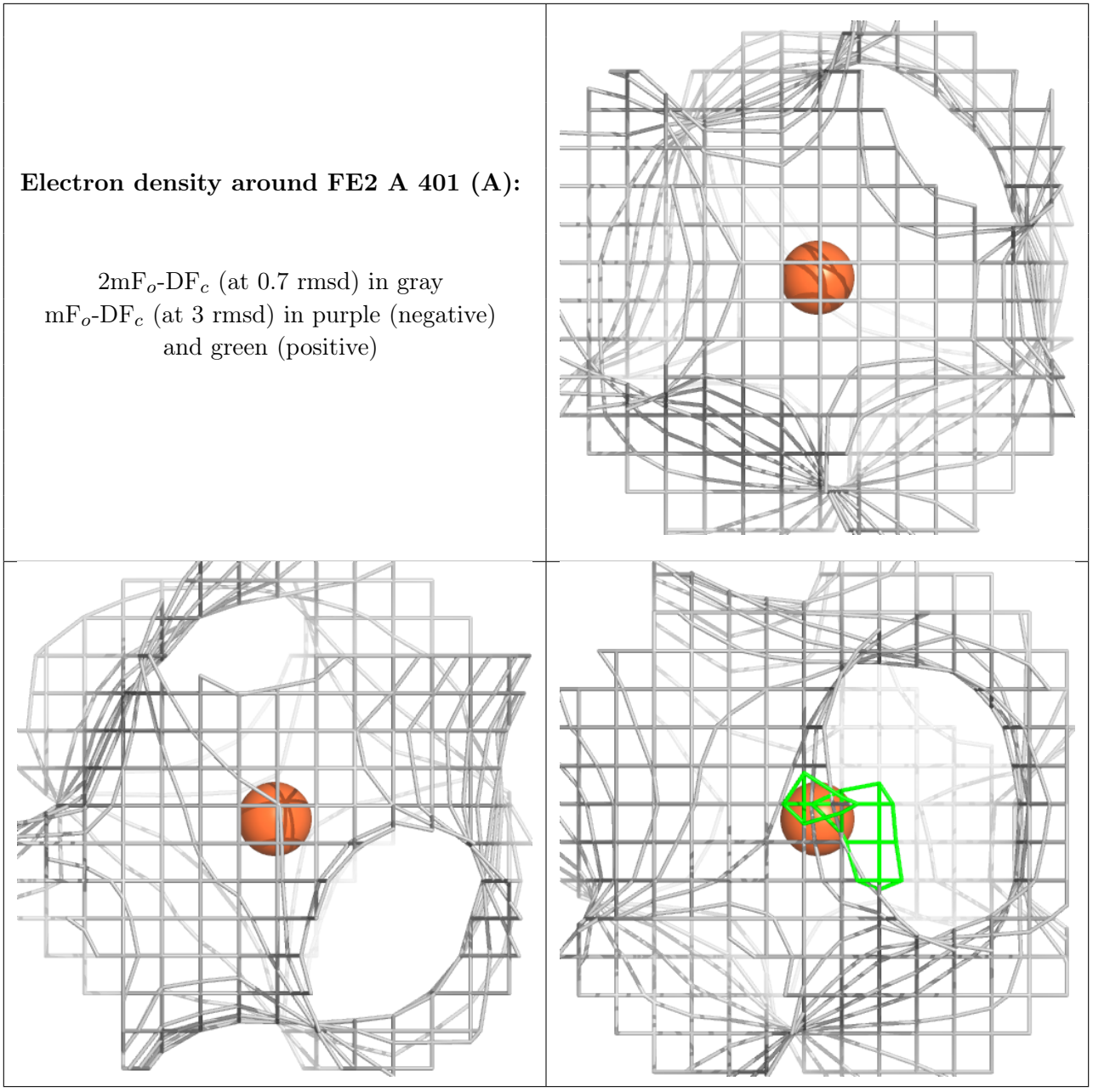
Electron density around OEX a 412 (B):

$2mF_o$-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)



6.5 Other polymers

There are no such residues in this entry.