Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:38 AM UTC

PDB ID	:	8IRG / pdb_00008irg
Title	:	XFEL structure of cyanobacterial photosystem II following two flashes (2F) with a 30-microsecond delay
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

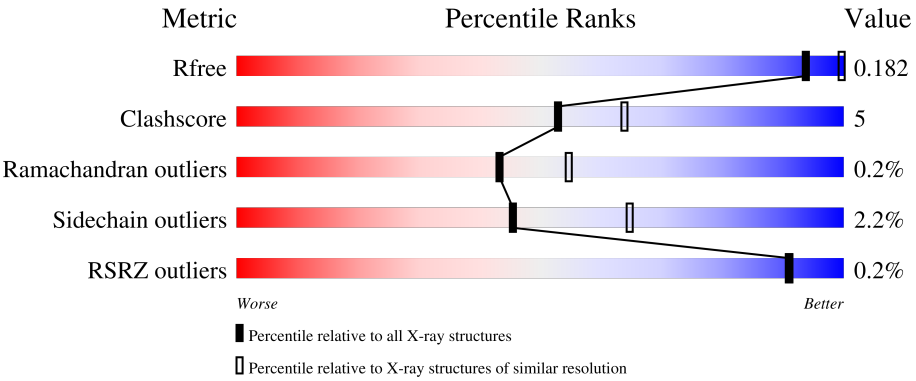
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



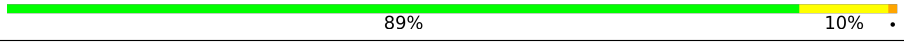
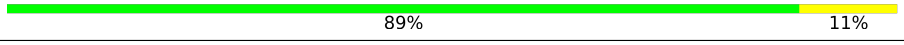
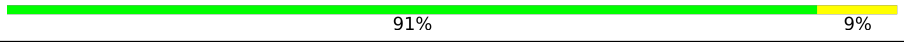
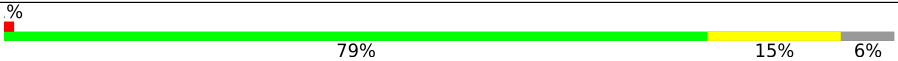
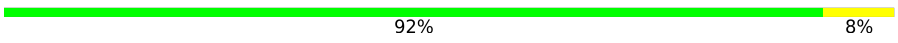
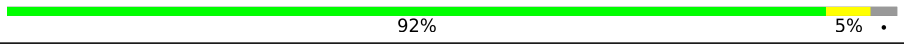
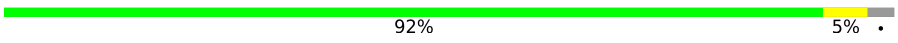
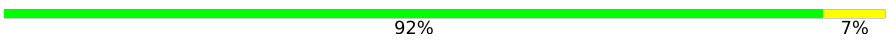
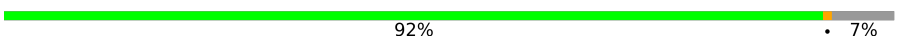
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	88% 9% .
1	a	344	85% 12% .
2	B	505	92% 7%
2	b	505	% 91% 8% .
3	C	455	91% 8% .

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	V	137	96%
16	v	137	91% 9%
17	X	40	82% 12% 5%
17	x	40	88% 8% 5%
18	Y	30	87% 10%
18	y	30	50% 43%
19	Z	62	87% 11%
19	z	62	76% 24%
20	R	34	6% 74% 24%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[A]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	407	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	C	515	X	-	-	-
23	CLA	D	404[A]	X	-	-	-
23	CLA	D	404[B]	X	-	-	-
23	CLA	D	405	X	-	-	-
23	CLA	a	405[A]	X	-	-	-
23	CLA	a	405[B]	X	-	-	-
23	CLA	a	406[A]	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-
23	CLA	c	512	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	513	X	-	-	-
23	CLA	c	514	X	-	-	-
23	CLA	d	401[A]	X	-	-	-
23	CLA	d	401[B]	X	-	-	-
23	CLA	d	402	X	-	-	-
25	GOL	D	403	-	-	X	-
25	GOL	D	414	-	X	-	-
25	GOL	a	419	-	-	X	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 62602 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	221	0
			4330	2830	716	759	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	20	0
			4146	2721	692	720	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	18			

There are 8 discrepancies between the modelled and reference sequences:

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

Continued on next page...

Continued from previous page...

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

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

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

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			662	432	107	123			
5	e	79	Total	C	N	O	0	2	0
			670	439	110	121			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	34	Total	C	N	O	S	0	0	0
			275	187	45	42	1			
6	f	31	Total	C	N	O	S	0	1	0
			261	179	43	38	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	38	Total	C	N	O	S	0	0	0
			272	182	42	47	1			
9	j	39	Total	C	N	O	S	0	0	0
			277	185	43	48	1			

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	33	Total	C	N	O	S	0	1	0
			268	179	39	49	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	2	0
			286	190	43	52	1			

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	6	0
			311	213	48	48	2			
14	t	30	Total	C	N	O	S	0	5	0
			302	208	47	45	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	6	0
			1120	711	185	220	4			
16	v	137	Total	C	N	O	S	0	6	0
			1117	712	185	216	4			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	X	38	Total 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).

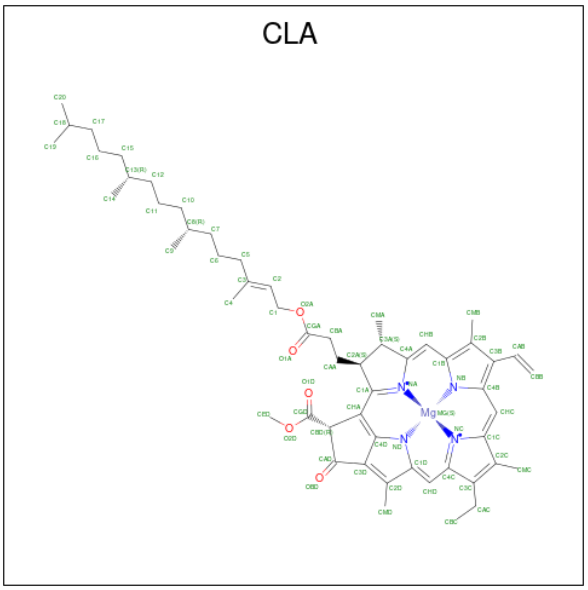
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 4	Cl 4	0	2

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...

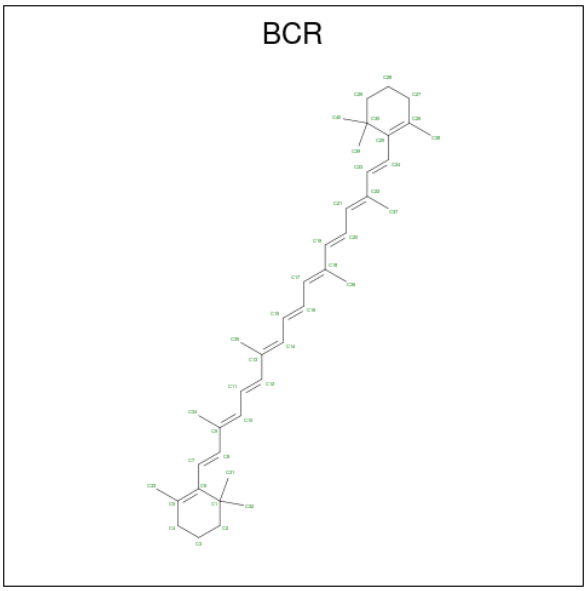
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110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

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



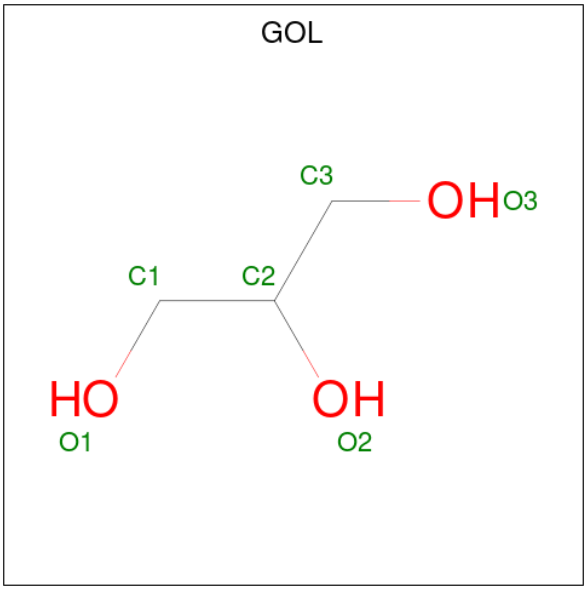
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	K	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	Y	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 25 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



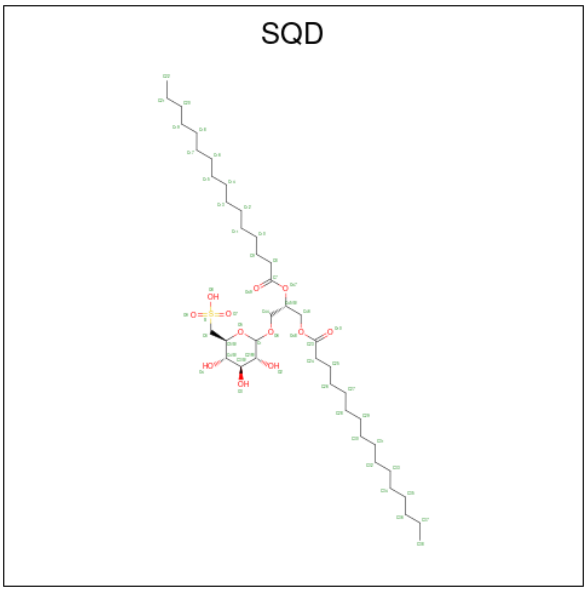
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O 6 3 3	0	0
25	B	1	Total C O 6 3 3	0	0
25	B	1	Total C O 6 3 3	0	0

Continued on next page...

Continued from previous page...

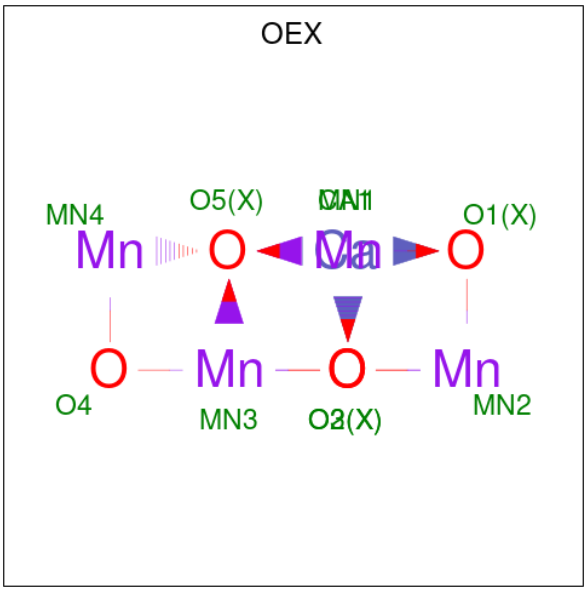
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
25	B	1	Total	C	O	0	0
			6	3	3		
25	C	1	Total	C	O	0	1
			12	6	6		
25	D	1	Total	C	O	0	0
			6	3	3		
25	D	1	Total	C	O	0	0
			6	3	3		
25	O	1	Total	C	O	0	0
			6	3	3		
25	O	1	Total	C	O	0	0
			6	3	3		
25	V	1	Total	C	O	0	1
			12	6	6		
25	a	1	Total	C	O	0	0
			6	3	3		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

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



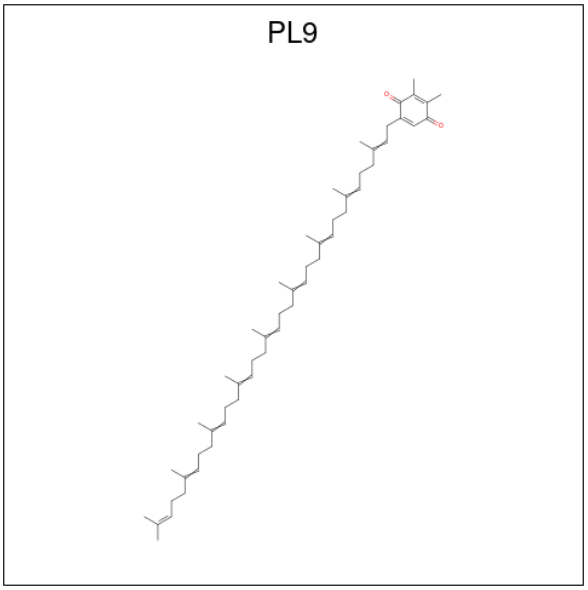
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	B	1	Total	C	O	S	0	0
			54	41	12	1		
26	C	1	Total	C	O	S	0	1
			108	82	24	2		
26	F	1	Total	C	O	S	0	0
			43	30	12	1		
26	a	1	Total	C	O	S	0	1
			108	82	24	2		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	b	1	Total	C	O	S	0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

- Molecule 27 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



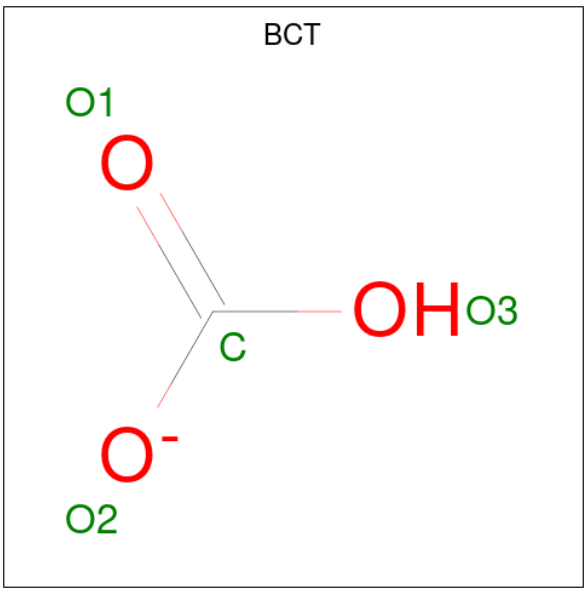
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 110 106 4	0	1
28	D	1	Total C O 110 106 4	0	1
28	a	1	Total C O 110 106 4	0	1
28	d	1	Total C O 110 106 4	0	1

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 28 23 5	0	0
29	B	2	Total C O 73 63 10	0	0
29	D	2	Total C O 57 51 6	0	0
29	I	1	Total C O 40 35 5	0	0
29	J	1	Total C 10 10	0	0
29	K	1	Total C O 68 58 10	0	1
29	M	1	Total C 10 10	0	0
29	X	1	Total C O 18 16 2	0	0
29	a	1	Total C O 30 25 5	0	0
29	b	2	Total C O 69 59 10	0	0
29	c	1	Total C O 64 54 10	0	1
29	d	1	Total C O 17 16 1	0	0
29	j	1	Total C 10 10	0	0
29	m	1	Total C 10 10	0	0
29	x	1	Total C O 18 16 2	0	0

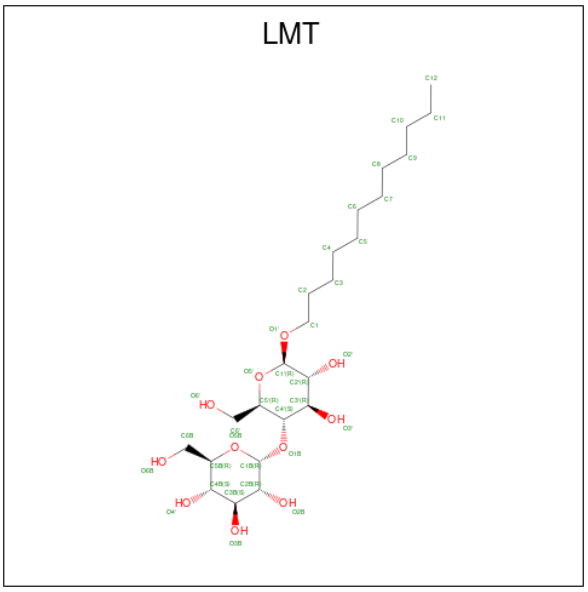
- Molecule 30 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand

of Interest" by depositor).



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

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



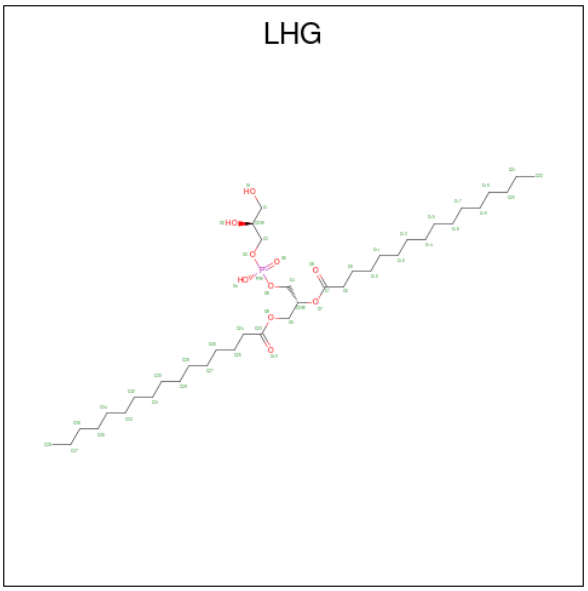
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0

Continued on next page...

Continued from previous page...

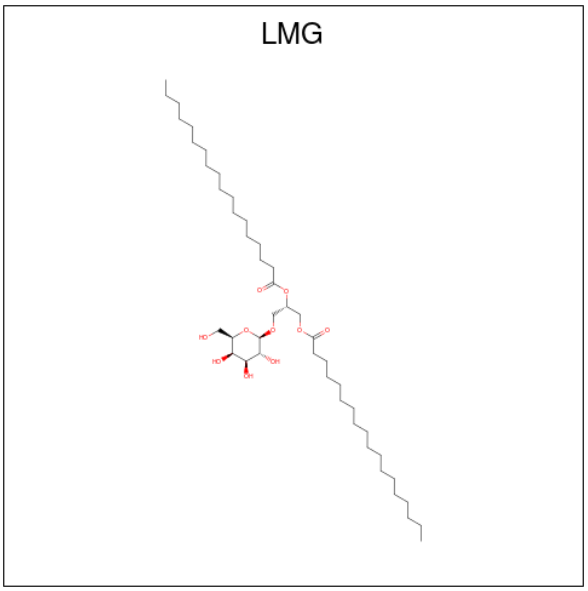
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	T	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 6	0	0
31	c	1	Total C O 35 24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

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



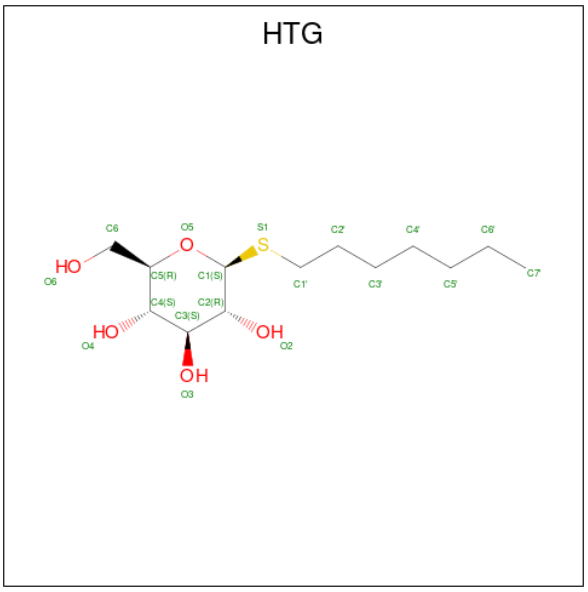
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	D	1	Total	C	O	P	0	1
			98	76	20	2		
32	E	1	Total	C	O	P	0	1
			84	62	20	2		
32	L	1	Total	C	O	P	0	1
			98	76	20	2		
32	a	1	Total	C	O	P	0	1
			84	62	20	2		
32	d	1	Total	C	O	P	0	1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

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



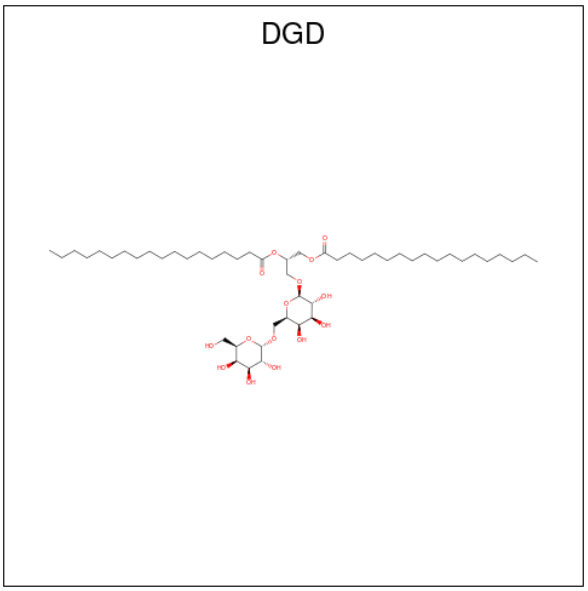
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 37 27 10	0	0
33	D	1	Total C O 51 41 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51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

- Molecule 34 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



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

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



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

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

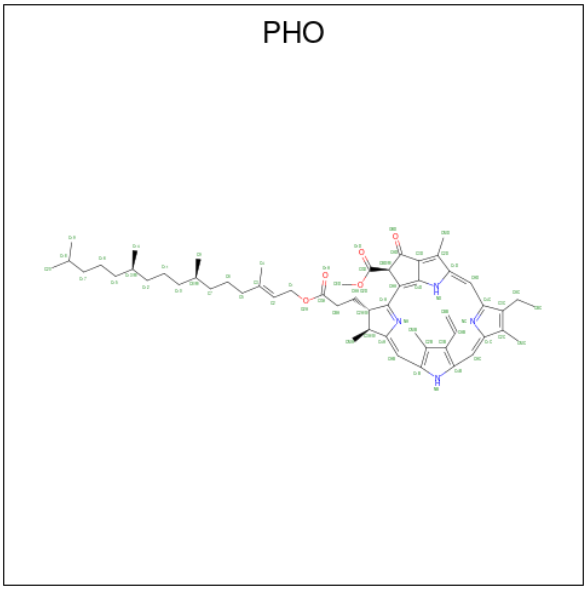
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	V	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0

Continued on next page...

Continued from previous page...

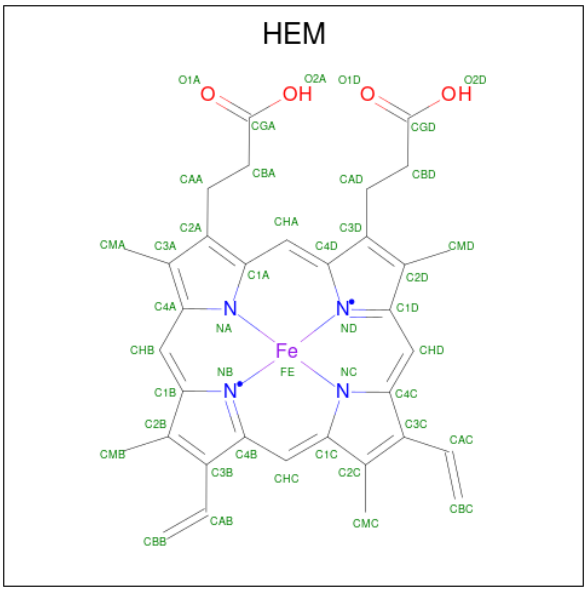
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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

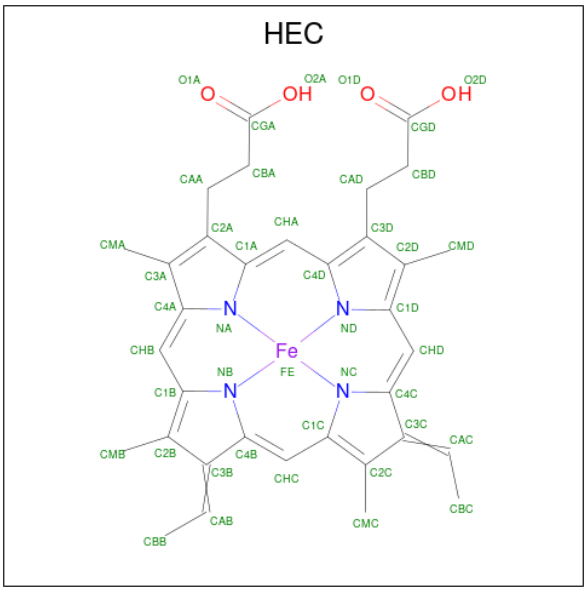


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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	137	Total	O	0	84
			219	219		
41	B	190	Total	O	0	3
			193	193		
41	C	170	Total	O	0	37
			207	207		
41	D	122	Total	O	0	34
			156	156		
41	E	15	Total	O	0	0
			15	15		
41	F	6	Total	O	0	0
			6	6		
41	H	22	Total	O	0	0
			22	22		
41	I	6	Total	O	0	0
			6	6		
41	J	5	Total	O	0	0
			5	5		
41	K	7	Total	O	0	0
			7	7		

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	98	Total O 103 103	0	5
41	T	11	Total O 14 14	0	3
41	U	46	Total O 48 48	0	2
41	V	80	Total O 82 82	0	2
41	X	8	Total O 8 8	0	0
41	a	129	Total O 208 208	0	81
41	b	201	Total O 204 204	0	3
41	c	162	Total O 195 195	0	33
41	d	122	Total O 155 155	0	33
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	17	Total O 17 17	0	0
41	i	3	Total O 3 3	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	7	Total O 8 8	0	1
41	m	13	Total O 13 13	0	0
41	o	95	Total O 99 99	0	4
41	t	6	Total O 9 9	0	3

Continued on next page...

Continued from previous page...

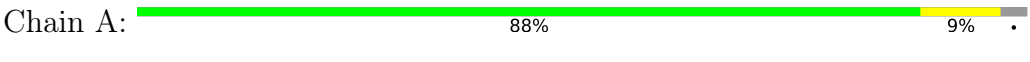
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	u	50	Total O 51 51	0	1
41	v	57	Total O 60 60	0	3
41	x	8	Total O 8 8	0	0
41	y	2	Total O 2 2	0	0

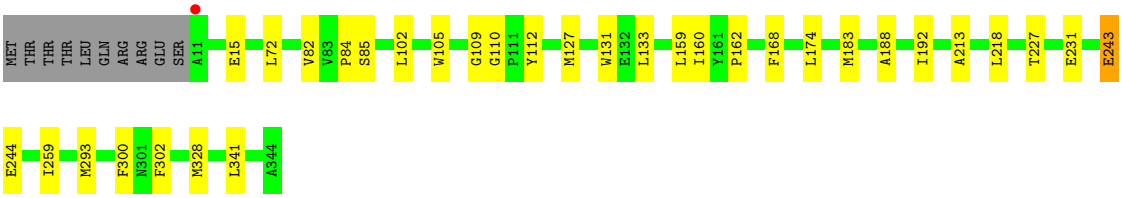
3 Residue-property plots (i)

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:

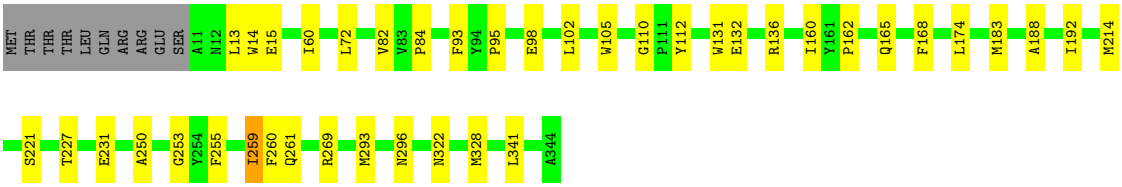




• Molecule 1: Photosystem II protein D1

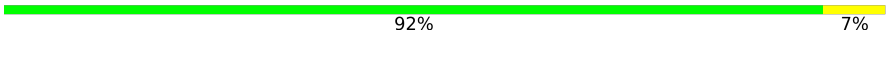
Chain a:

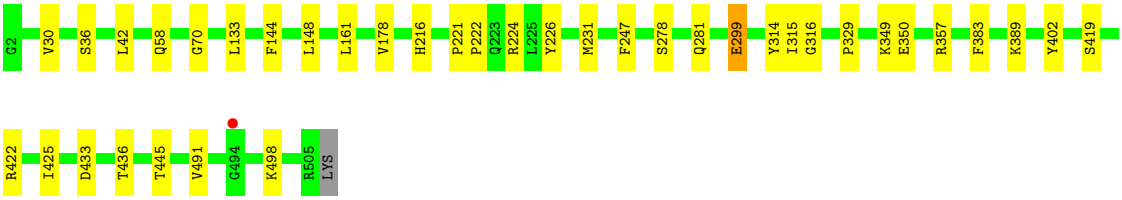




• Molecule 2: Photosystem II CP47 reaction center protein

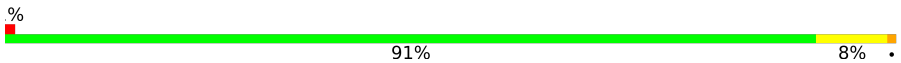
Chain B:

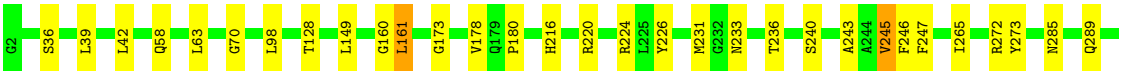




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



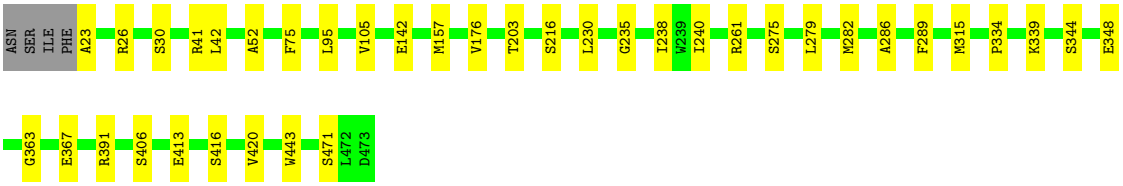




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

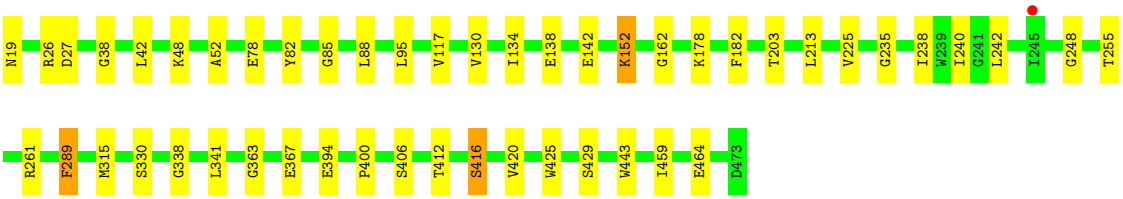




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:





• Molecule 4: Photosystem II D2 protein

Chain D:

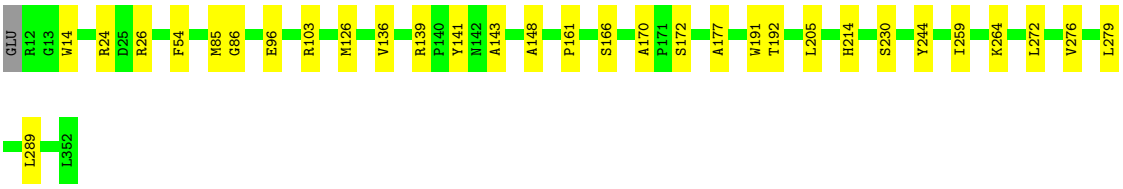




• Molecule 4: Photosystem II D2 protein

Chain d:

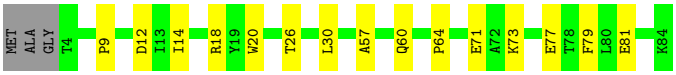




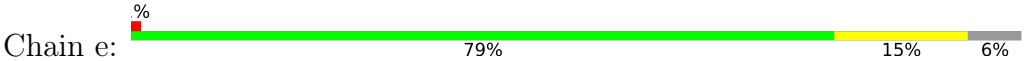
• Molecule 5: Cytochrome b559 subunit alpha

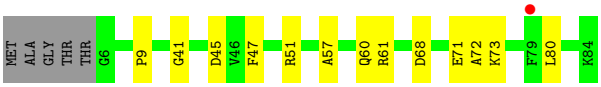
Chain E:





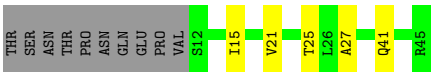
• Molecule 5: Cytochrome b559 subunit alpha





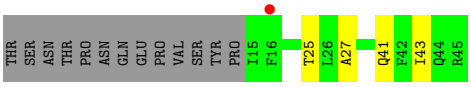
• Molecule 6: Cytochrome b559 subunit beta



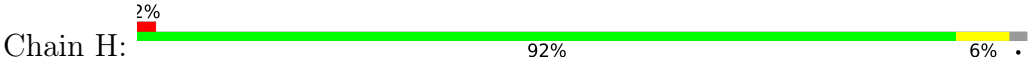


• Molecule 6: Cytochrome b559 subunit beta



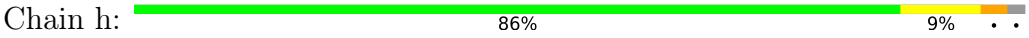


• Molecule 7: Photosystem II reaction center protein H



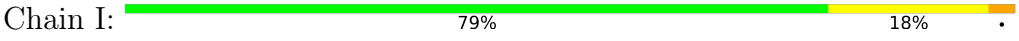


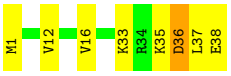
• Molecule 7: Photosystem II reaction center protein H



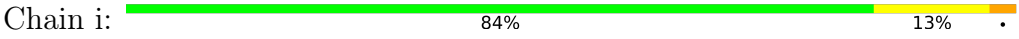


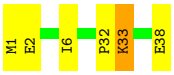
• Molecule 8: Photosystem II reaction center protein I





• Molecule 8: Photosystem II reaction center protein I

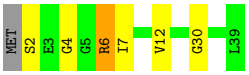




• Molecule 9: Photosystem II reaction center protein J

Chain J:

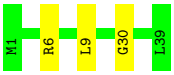




• Molecule 9: Photosystem II reaction center protein J

Chain j:

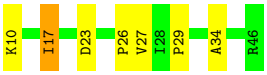




• Molecule 10: Photosystem II reaction center protein K

Chain K:

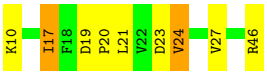




• Molecule 10: Photosystem II reaction center protein K

Chain k:

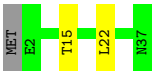




• Molecule 11: Photosystem II reaction center protein L

Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:

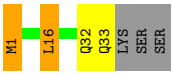




• Molecule 12: Photosystem II reaction center protein M

Chain M:

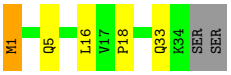




• Molecule 12: Photosystem II reaction center protein M

Chain m:

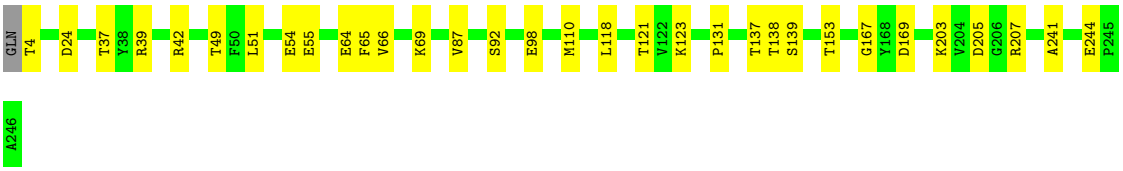




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

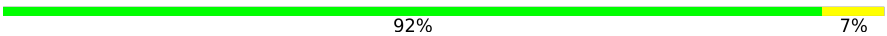
Chain O:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

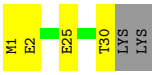




• Molecule 14: Photosystem II reaction center protein T

Chain T:

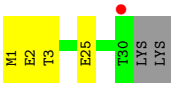




• Molecule 14: Photosystem II reaction center protein T

Chain t:

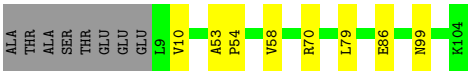




• Molecule 15: Photosystem II 12 kDa extrinsic protein

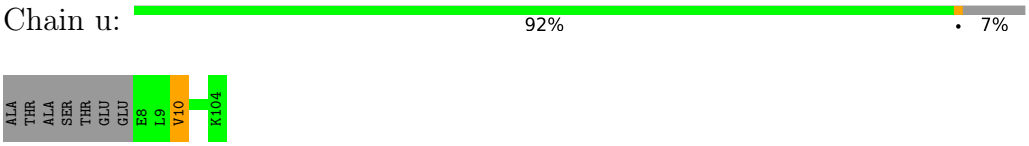
Chain U:





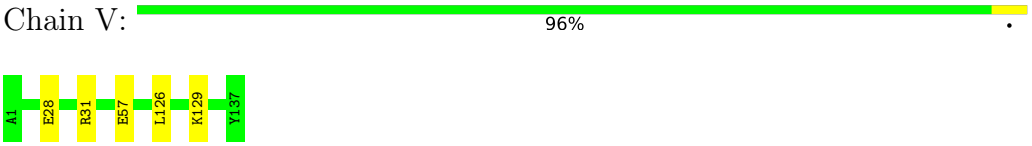
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



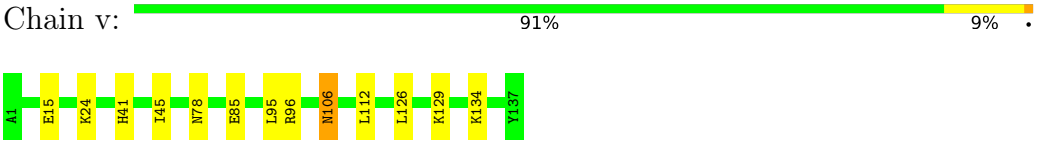
• Molecule 16: Cytochrome c-550

Chain V:



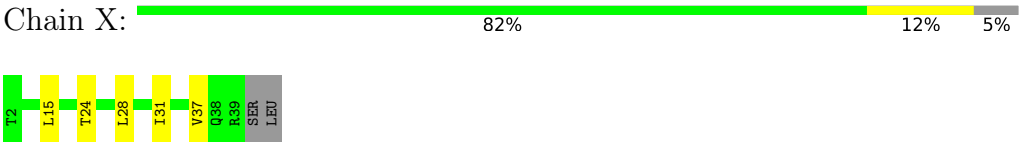
• Molecule 16: Cytochrome c-550

Chain v:



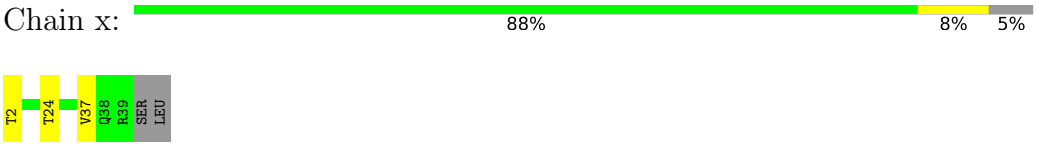
• Molecule 17: Photosystem II reaction center protein X

Chain X:



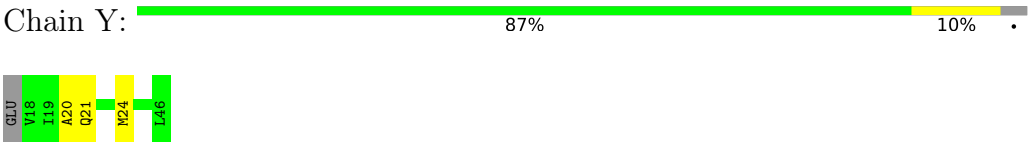
• Molecule 17: Photosystem II reaction center protein X

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:

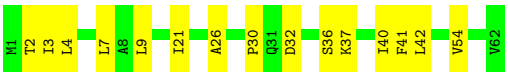




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

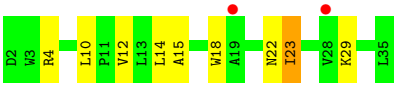




• Molecule 20: Photosystem II protein Y

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	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.30 19.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.30) 99.7 (19.99-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.90 (at 2.30Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.141 , 0.180 0.142 , 0.182	Depositor DCC
R_{free} test set	28224 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 76.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	62602	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 1.68% 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: CL, LMG, DGD, CLA, PL9, CA, HEC, BCT, OEX, HEM, SQD, GOL, LMT, FE2, UNL, FME, MG, BCR, LHG, PHO, HTG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/4478	0.43	0/6098
1	a	0.25	0/4470	0.40	0/6087
2	B	0.38	0/4293	0.50	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.30	0/4404	0.44	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.34	0/3741	0.47	0/5095
4	d	0.31	0/3749	0.45	0/5106
5	E	0.35	0/681	0.52	0/928
5	e	0.30	0/690	0.48	0/939
6	F	0.35	0/284	0.45	0/387
6	f	0.29	0/269	0.47	0/365
7	H	0.35	0/519	0.53	0/708
7	h	0.31	0/530	0.46	0/722
8	I	0.30	0/311	0.46	0/419
8	i	0.35	0/311	0.45	0/419
9	J	0.32	0/278	0.40	0/376
9	j	0.28	0/283	0.40	0/383
10	K	0.34	0/303	0.48	0/416
10	k	0.33	0/303	0.47	0/416
11	L	0.37	0/318	0.47	0/433
11	l	0.37	0/318	0.45	0/433
12	M	0.38	0/261	0.54	0/357
12	m	0.39	0/279	0.47	0/380
13	O	0.36	0/1991	0.52	0/2698
13	o	0.34	0/1966	0.51	0/2665
14	T	0.34	0/310	0.43	0/419
14	t	0.32	0/301	0.42	0/406
15	U	0.38	0/811	0.54	0/1095
15	u	0.36	0/818	0.54	0/1105
16	V	0.36	0/1142	0.51	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.31	0/1139	0.48	0/1542
17	X	0.25	0/292	0.37	0/395
17	x	0.25	0/284	0.37	0/384
18	Y	0.25	0/216	0.47	0/289
18	y	0.24	0/216	0.39	0/289
19	Z	0.23	0/490	0.37	0/669
19	z	0.24	0/490	0.36	0/669
20	R	0.23	0/279	0.35	0/383
All	All	0.32	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	28	0
1	a	4330	0	4132	40	0
2	B	4146	0	3983	25	0
2	b	4134	0	3976	40	0
3	C	4260	0	4123	27	0
3	c	4308	0	4172	36	0
4	D	3620	0	3484	37	0
4	d	3628	0	3490	22	0
5	E	662	0	648	12	0
5	e	670	0	655	9	0
6	F	275	0	282	5	0
6	f	261	0	269	5	0
7	H	506	0	529	3	0
7	h	517	0	541	8	0
8	I	314	0	328	5	0
8	i	314	0	328	3	0
9	J	272	0	279	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	4	0
10	k	293	0	305	7	0
11	L	311	0	320	3	0
11	l	311	0	320	2	0
12	M	268	0	285	6	0
12	m	286	0	305	7	0
13	O	1958	0	1920	15	0
13	o	1933	0	1900	9	0
14	T	311	0	318	1	0
14	t	302	0	311	3	0
15	U	800	0	796	5	0
15	u	807	0	805	1	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	8	0
17	X	289	0	322	4	0
17	x	281	0	312	3	0
18	Y	215	0	246	2	0
18	y	215	0	246	8	0
19	Z	479	0	516	3	0
19	z	479	0	516	5	0
20	R	273	0	305	5	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	14	0
23	B	1040	0	1152	26	0
23	C	845	0	936	37	0
23	D	195	0	216	7	0
23	a	455	0	504	15	0
23	b	1040	0	1152	30	0
23	c	845	0	936	32	0
23	d	195	0	216	7	0
24	A	40	0	56	1	0
24	B	120	0	168	4	0
24	C	80	0	112	0	0
24	D	40	0	56	2	0
24	H	40	0	56	2	0
24	K	40	0	56	1	0
24	T	40	0	56	6	0
24	Y	40	0	56	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	40	0	56	1	0
24	b	120	0	168	10	0
24	c	80	0	112	4	0
24	d	40	0	56	2	0
24	h	40	0	56	5	0
24	k	40	0	56	2	0
24	t	40	0	56	3	0
24	y	40	0	56	2	0
25	A	6	0	8	1	0
25	B	18	0	24	3	0
25	C	12	0	16	1	0
25	D	12	0	14	8	0
25	O	12	0	16	2	0
25	V	12	0	16	1	0
25	a	12	0	16	7	0
25	b	12	0	16	2	0
25	c	24	0	32	1	0
25	d	6	0	8	0	0
25	l	12	0	16	1	0
25	o	6	0	8	0	0
25	v	12	0	16	2	0
26	A	54	0	78	1	0
26	B	54	0	78	3	0
26	C	108	0	155	2	0
26	F	43	0	53	2	0
26	a	162	0	233	9	0
26	b	54	0	78	2	0
26	f	43	0	53	1	0
27	A	20	0	0	0	0
27	a	20	0	0	0	0
28	A	110	0	160	19	0
28	D	110	0	160	1	0
28	a	110	0	160	10	0
28	d	110	0	160	1	0
29	A	28	0	0	0	0
29	B	73	0	0	0	0
29	D	57	0	0	0	0
29	I	40	0	0	0	0
29	J	10	0	0	0	0
29	K	68	0	0	0	0
29	M	10	0	0	0	0
29	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
29	a	30	0	0	0	0
29	b	69	0	0	0	0
29	c	64	0	0	0	0
29	d	17	0	0	0	0
29	j	10	0	0	0	0
29	m	10	0	0	0	0
29	x	18	0	0	0	0
30	A	8	0	0	0	0
30	a	8	0	0	0	0
31	A	70	0	92	3	0
31	B	70	0	92	3	0
31	F	35	0	46	0	0
31	M	35	0	46	0	0
31	T	35	0	45	0	0
31	b	50	0	70	1	0
31	c	35	0	46	2	0
31	e	35	0	46	1	0
31	m	35	0	46	2	0
31	t	51	0	67	2	0
32	A	98	0	148	1	0
32	D	196	0	296	13	0
32	E	84	0	114	6	0
32	L	98	0	148	1	0
32	a	84	0	114	8	0
32	d	294	0	444	24	0
32	l	98	0	148	0	0
33	B	51	0	72	1	0
33	C	190	0	260	4	0
33	D	51	0	72	0	0
33	a	51	0	72	1	0
33	c	102	0	144	2	0
33	d	51	0	72	1	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	3	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	2	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	310	0	410	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	62	0	82	1	0
35	c	310	0	410	12	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	O	1	0	0	0	0
36	V	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	256	0	296	5	0
37	a	256	0	296	4	0
38	F	43	0	30	1	0
38	f	43	0	30	1	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	219	0	0	0	0
41	B	193	0	0	2	0
41	C	207	0	0	3	0
41	D	156	0	0	6	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	22	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	7	0	0	0	0
41	L	10	0	0	0	0
41	M	6	0	0	0	0
41	O	103	0	0	0	0
41	T	14	0	0	0	0
41	U	48	0	0	0	0
41	V	82	0	0	1	0
41	X	8	0	0	0	0
41	a	208	0	0	2	0
41	b	204	0	0	0	0
41	c	195	0	0	3	0
41	d	155	0	0	1	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	17	0	0	0	0
41	i	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	j	1	0	0	0	0
41	k	3	0	0	0	0
41	l	8	0	0	0	0
41	m	13	0	0	0	0
41	o	99	0	0	0	0
41	t	9	0	0	1	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	62602	0	61441	609	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 (609) 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)
25:D:403:GOL:H11	12:M:1:FME:HG2	1.43	0.99
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.50	0.94
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.56	0.88
24:b:619:BCR:H331	24:b:619:BCR:HC8	1.60	0.84
23:B:601:CLA:H12	23:B:601:CLA:H71	1.65	0.78
4:d:192[B]:THR:HG23	23:d:401[B]:CLA:HBC2	1.66	0.78
4:d:192[A]:THR:HG23	23:d:401[A]:CLA:HBC2	1.66	0.77
23:A:406[A]:CLA:H152	28:A:412[A]:PL9:H252	1.67	0.76
23:B:604:CLA:H42	23:B:605:CLA:H2	1.67	0.75
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.68	0.74
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.69	0.74
23:A:407:CLA:H193	23:C:508:CLA:H101	1.70	0.73
23:C:507:CLA:HHC	23:C:507:CLA:HBB1	1.70	0.73
23:A:406[B]:CLA:H152	28:A:412[B]:PL9:H252	1.71	0.73
23:c:503:CLA:H61	23:c:513:CLA:H42	1.71	0.71
32:D:409[B]:LHG:H382	32:D:409[B]:LHG:H112	1.73	0.71
23:a:409:CLA:H192	23:c:506:CLA:H142	1.71	0.71
25:D:403:GOL:O2	41:D:501:HOH:O	2.08	0.71
1:a:15:GLU:HB2	31:c:501:LMT:H6'2	1.73	0.70
23:a:409:CLA:H152	23:c:507:CLA:H142	1.73	0.70
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.74	0.69
13:O:42:ARG:HH12	25:O:302:GOL:H12	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.75	0.69
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.75	0.69
23:C:508:CLA:H142	35:C:518[B]:DGD:HAF2	1.75	0.68
31:t:101:LMT:H6E	31:t:102:LMT:H6D	1.75	0.68
32:D:409[A]:LHG:H112	32:D:409[A]:LHG:H382	1.76	0.68
23:C:505:CLA:HBB1	23:C:514:CLA:H41	1.77	0.67
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.75	0.67
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.28	0.67
23:C:515:CLA:H202	33:C:522:LMG:H402	1.78	0.66
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.76	0.66
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.78	0.66
25:a:418:GOL:H32	12:m:1:FME:HG3	1.77	0.66
25:a:419:GOL:H11	12:m:1:FME:HE3	1.78	0.66
25:a:419:GOL:H31	12:m:1:FME:HG2	1.78	0.66
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	1.78	0.66
3:C:286:ALA:HB2	23:C:504:CLA:HMD1	1.77	0.66
24:y:101:BCR:H321	24:y:101:BCR:HC8	1.78	0.66
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.78	0.65
23:C:503:CLA:H193	23:C:509:CLA:HBB1	1.79	0.65
23:C:507:CLA:CMD	23:C:509:CLA:HAB	2.27	0.65
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.77	0.65
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.78	0.64
23:c:512:CLA:H191	33:z:101:LMG:H241	1.79	0.64
4:D:192[B]:THR:HG23	23:D:404[B]:CLA:HBC2	1.79	0.64
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:HBB1	1.80	0.64
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.80	0.64
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.80	0.64
26:a:411[A]:SQD:H321	23:c:509:CLA:H102	1.78	0.64
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.80	0.64
28:A:412[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.63
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.29	0.63
23:C:512:CLA:HBC3	23:C:512:CLA:H192	1.81	0.63
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.30	0.63
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.81	0.63
10:K:17:ILE:H	10:K:17:ILE:HD13	1.64	0.62
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.80	0.62
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.32	0.62
26:a:411[A]:SQD:H152	32:d:406[A]:LHG:H172	1.82	0.62
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.32	0.62
13:O:169:ASP:OD1	25:O:303:GOL:H12	2.00	0.62
34:B:622:HTG:H4'1	31:B:630:LMT:H52	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:514:CLA:HBB1	24:c:515:BCR:H24C	1.80	0.62
23:C:508:CLA:H142	35:C:518[A]:DGD:HAF2	1.81	0.61
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.30	0.61
35:c:518[B]:DGD:HAF1	35:c:518[B]:DGD:HA81	1.83	0.61
4:D:205[B]:LEU:HD13	37:D:401[B]:PHO:HAB	1.83	0.60
2:B:226:TYR:HA	2:B:231:MET:HG3	1.82	0.60
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.35	0.60
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.36	0.59
32:d:405[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.85	0.59
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.84	0.59
24:t:103:BCR:H321	24:t:103:BCR:HC8	1.83	0.59
26:a:411[B]:SQD:H321	23:c:509:CLA:H102	1.82	0.59
26:a:411[A]:SQD:H141	32:d:406[A]:LHG:H152	1.84	0.59
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.33	0.59
28:A:412[B]:PL9:H262	32:E:101[B]:LHG:H223	1.84	0.58
23:C:510:CLA:HBC3	23:C:512:CLA:H71	1.84	0.58
1:a:214[B]:MET:HB3	28:a:414[B]:PL9:H103	1.86	0.58
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.33	0.58
2:b:285:ASN:O	2:b:289:GLN:HG2	2.03	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.69	0.58
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.67	0.58
23:b:601:CLA:H72	23:b:601:CLA:H2	1.86	0.57
25:D:403:GOL:H31	12:M:1:FME:HE3	1.85	0.57
4:D:192[A]:THR:HG23	23:D:404[A]:CLA:HBC2	1.87	0.57
23:A:407:CLA:H18	23:C:507:CLA:H142	1.87	0.57
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.87	0.57
23:a:407[A]:CLA:H191	32:a:420[A]:LHG:H111	1.85	0.57
37:a:416[A]:PHO:HBC3	4:d:279:LEU:HD22	1.86	0.56
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.06	0.56
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.85	0.56
4:D:323[A]:GLU:O	25:D:414:GOL:O2	2.23	0.56
26:a:411[B]:SQD:H141	32:d:406[B]:LHG:H152	1.86	0.56
35:c:517[A]:DGD:HG11	41:c:606[A]:HOH:O	2.06	0.56
5:E:57:ALA:H	5:E:60:GLN:HE21	1.51	0.56
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.87	0.56
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.19	0.55
32:D:408[B]:LHG:HC62	11:L:15[B]:THR:HG23	1.89	0.55
3:c:27:ASP:HB3	10:k:46:ARG:HG3	1.89	0.55
25:a:419:GOL:O2	41:a:501:HOH:O	2.09	0.55
10:k:24:VAL:HG22	18:y:25:ILE:HD13	1.89	0.55
4:D:327:ALA:HB2	25:D:414:GOL:H2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.12	0.55
8:I:35:LYS:O	8:I:37:LEU:N	2.40	0.54
1:a:183[A]:MET:HA	23:a:405[A]:CLA:HMD1	1.89	0.54
16:v:134[A]:LYS:HE2	25:v:202[A]:GOL:H32	1.88	0.54
26:F:103:SQD:H102	17:X:31:ILE:HD11	1.90	0.54
32:D:409[A]:LHG:H382	32:D:409[A]:LHG:H132	1.89	0.54
25:b:628:GOL:O3	25:b:628:GOL:O1	2.21	0.54
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.88	0.54
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.88	0.54
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.90	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.42	0.54
3:c:182:PHE:HA	34:c:522:HTG:H61	1.90	0.54
23:a:407[B]:CLA:H191	32:a:420[B]:LHG:H111	1.89	0.54
23:d:402:CLA:H162	7:h:37:LEU:HD21	1.90	0.54
28:A:412[A]:PL9:H253	23:D:404[A]:CLA:H141	1.89	0.54
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.90	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.42	0.53
5:E:77:GLU:O	5:E:81:GLU:HG2	2.08	0.53
23:a:406[B]:CLA:HBB1	23:a:406[B]:CLA:HHC	1.90	0.53
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.21	0.53
4:D:317[B]:LYS:NZ	41:D:513[B]:HOH:O	2.38	0.53
23:a:405[B]:CLA:H152	37:a:408[B]:PHO:H52	1.89	0.53
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.89	0.53
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.08	0.53
24:Y:101:BCR:H321	24:Y:101:BCR:HC8	1.91	0.53
1:a:160[B]:ILE:HD11	35:c:517[B]:DGD:HBT1	1.89	0.53
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.90	0.53
23:C:503:CLA:C3D	23:C:505:CLA:H2	2.39	0.53
25:l:801[A]:GOL:H32	14:t:25:GLU:HB2	1.89	0.53
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.89	0.53
1:A:341[B]:LEU:HD13	25:C:524[B]:GOL:H31	1.90	0.53
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.90	0.52
23:B:607:CLA:HMB1	23:B:607:CLA:HBB1	1.91	0.52
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.91	0.52
3:C:95:LEU:HD21	23:C:503:CLA:OBD	2.09	0.52
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.90	0.52
32:D:409[B]:LHG:H382	32:D:409[B]:LHG:H132	1.91	0.52
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.44	0.52
26:B:620:SQD:H381	31:m:103:LMT:H121	1.92	0.52
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.10	0.52
33:z:101:LMG:H302	33:z:101:LMG:H141	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.44	0.52
2:B:36[B]:SER:OG	24:B:618:BCR:H362	2.09	0.52
35:c:519:DGD:HBH2	32:d:406[A]:LHG:H211	1.92	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.91	0.51
23:A:404[B]:CLA:HBB1	23:D:404[B]:CLA:C4B	2.17	0.51
23:A:406[B]:CLA:HHC	23:A:406[B]:CLA:HBB1	1.91	0.51
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.93	0.51
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.91	0.51
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.93	0.51
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.45	0.51
2:b:226:TYR:HA	2:b:231:MET:HG3	1.91	0.51
24:b:619:BCR:H331	24:b:619:BCR:C8	2.34	0.51
28:A:412[A]:PL9:H472	4:D:39:PRO:HD3	1.92	0.51
15:u:10[A]:VAL:HG12	41:u:246:HOH:O	2.09	0.51
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.92	0.51
24:T:102:BCR:H321	24:T:102:BCR:HC8	1.93	0.51
32:a:420[A]:LHG:HC31	5:e:9:PRO:HA	1.92	0.51
23:c:509:CLA:H18	35:c:518[A]:DGD:HAT2	1.93	0.51
23:C:514:CLA:H143	23:C:515:CLA:H142	1.91	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.51
16:v:134[B]:LYS:HE2	25:v:202[B]:GOL:H32	1.92	0.51
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.93	0.51
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.41	0.51
24:h:101:BCR:H331	24:h:101:BCR:C8	2.40	0.51
25:D:403:GOL:H11	12:M:1:FME:CG	2.30	0.51
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.11	0.51
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.41	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.46	0.50
28:A:412[B]:PL9:H472	4:D:39:PRO:HD3	1.93	0.50
23:C:512:CLA:H52	32:D:409[A]:LHG:H371	1.92	0.50
28:A:412[B]:PL9:H253	23:D:404[B]:CLA:H141	1.91	0.50
3:C:176:VAL:HG21	3:C:238:ILE:HG13	1.93	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	2.42	0.50
3:c:363:GLY:O	3:c:367:GLU:HG2	2.12	0.50
6:f:27:ALA:HB1	38:f:101:HEM:HAC	1.92	0.50
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.93	0.50
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.92	0.50
23:A:406[B]:CLA:HED1	35:C:520:DGD:HAE2	1.93	0.50
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.50
4:d:85:MET:CE	4:d:96:GLU:HG2	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:606:CLA:H202	26:a:412:SQD:H302	1.94	0.50
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.12	0.50
26:a:411[B]:SQD:H271	32:d:406[B]:LHG:H141	1.92	0.50
3:c:117:VAL:HG12	33:c:521:LMG:H221	1.94	0.49
28:a:414[A]:PL9:H351	6:f:25:THR:OG1	2.12	0.49
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.12	0.49
3:C:279:LEU:HD22	23:C:511:CLA:HED2	1.94	0.49
1:a:165[B]:GLN:OE1	41:a:518[B]:HOH:O	2.20	0.49
2:B:247:PHE:CE2	23:B:602:CLA:H102	2.47	0.49
13:O:137:THR:C	13:O:139:SER:H	2.19	0.49
23:a:405[A]:CLA:H201	32:d:405[A]:LHG:H161	1.95	0.49
18:y:20:ALA:O	18:y:24:MET:HG2	2.12	0.49
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	1.95	0.49
3:C:443[B]:TRP:CE2	23:C:510:CLA:HMD2	2.48	0.49
28:a:414[B]:PL9:H351	6:f:25:THR:OG1	2.13	0.49
4:d:14:TRP:CD1	34:d:408:HTG:H61	2.47	0.49
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.12	0.49
32:d:405[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.95	0.49
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.10	0.49
23:C:512:CLA:H52	32:D:409[B]:LHG:H371	1.95	0.49
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.12	0.49
23:C:513:CLA:HBB1	23:C:513:CLA:HMB3	1.94	0.48
25:D:403:GOL:H12	14:T:2:GLU:OE1	2.13	0.48
3:C:42:LEU:HD21	23:C:513:CLA:H2A	1.95	0.48
37:D:402[A]:PHO:H3A	23:D:404[A]:CLA:H142	1.94	0.48
3:c:425[A]:TRP:CD1	23:c:505:CLA:HMA2	2.48	0.48
32:d:406[A]:LHG:H122	32:d:406[A]:LHG:C38	2.44	0.48
2:b:36:SER:OG	24:b:618:BCR:H362	2.13	0.48
3:c:152:LYS:HD2	41:c:756:HOH:O	2.12	0.48
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.96	0.48
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	1.94	0.48
31:t:102:LMT:H112	31:t:102:LMT:H81	1.46	0.48
3:C:157:MET:HE2	3:C:157:MET:HA	1.96	0.48
4:D:261[B]:PHE:CZ	32:D:408[B]:LHG:HC81	2.49	0.48
9:J:2:SER:N	41:J:201:HOH:O	2.46	0.48
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.95	0.48
34:B:622:HTG:O5	25:B:629:GOL:H12	2.14	0.48
32:a:420[B]:LHG:HC31	5:e:9:PRO:HA	1.94	0.48
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.96	0.48
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.95	0.48
37:a:408[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B:621:LMG:H112	33:B:621:LMG:H141	1.71	0.48
32:D:408[A]:LHG:HC62	11:L:15[A]:THR:HG23	1.96	0.48
25:V:204[B]:GOL:H12	41:V:324[B]:HOH:O	2.12	0.48
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.49	0.48
1:A:218[B]:LEU:HD12	28:A:412[B]:PL9:C3	2.44	0.47
4:D:264[B]:LYS:NZ	41:D:505[B]:HOH:O	2.46	0.47
26:b:620:SQD:H462	26:b:620:SQD:H1	1.95	0.47
24:t:103:BCR:H331	24:t:103:BCR:HC7	1.56	0.47
1:A:105:TRP:CE2	1:A:110[A]:GLY:HA3	2.50	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.47
4:D:230[A]:SER:HB2	41:D:529:HOH:O	2.14	0.47
25:a:419:GOL:O3	14:t:2:GLU:OE1	2.28	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.40	0.47
23:B:604:CLA:HMD1	23:B:612:CLA:H203	1.96	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HG3	1.97	0.47
35:c:517[B]:DGD:HG11	41:c:606[B]:HOH:O	2.15	0.47
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.96	0.47
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.97	0.47
23:C:512:CLA:H152	23:C:512:CLA:H112	1.51	0.47
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.49	0.47
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.50	0.47
2:b:220:ARG:HG3	7:h:20:LYS:HG2	1.96	0.47
23:b:601:CLA:H92	24:h:101:BCR:H403	1.96	0.47
32:d:406[A]:LHG:H342	32:d:406[A]:LHG:H151	1.97	0.47
5:E:9:PRO:HA	32:E:101[A]:LHG:HC31	1.95	0.47
28:A:412[B]:PL9:H151	28:A:412[B]:PL9:H171	1.54	0.47
32:A:416[A]:LHG:H361	23:B:613:CLA:H51	1.97	0.47
26:C:501[B]:SQD:H361	10:K:34:ALA:HA	1.97	0.47
10:K:23:ASP:OD2	18:Y:21:GLN:NE2	2.48	0.47
35:c:519:DGD:HBH2	32:d:406[B]:LHG:H211	1.97	0.47
7:h:56:ASP:OD2	17:x:2:THR:OG1	2.32	0.47
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.29	0.47
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.97	0.47
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.80	0.47
4:D:241[B]:GLU:CD	4:D:241[B]:GLU:H	2.23	0.47
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.97	0.47
32:d:406[A]:LHG:H302	32:d:406[A]:LHG:H332	1.67	0.47
2:B:58:GLN:C	2:B:329:PRO:HB3	2.40	0.47
15:U:53:ALA:HB1	15:U:54:PRO:HA	1.96	0.47
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.79	0.47
23:a:407[B]:CLA:HMB2	23:d:401[B]:CLA:H122	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:414[A]:PL9:H171	28:a:414[A]:PL9:H151	1.58	0.47
32:d:406[B]:LHG:H122	32:d:406[B]:LHG:C38	2.45	0.47
13:o:142:PHE:HB2	13:o:199:LEU:HB2	1.97	0.47
19:z:32:ASP:O	19:z:36:SER:OG	2.21	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.96	0.46
1:A:192[A]:ILE:HG13	1:A:293[A]:MET:HE1	1.97	0.46
3:C:443[B]:TRP:CD2	23:C:510:CLA:HMD2	2.50	0.46
23:a:405[B]:CLA:HBB1	23:d:401[B]:CLA:C4B	2.15	0.46
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.97	0.46
8:I:36:ASP:OD1	8:I:36:ASP:N	2.48	0.46
23:a:406[A]:CLA:HBA1	23:a:406[A]:CLA:C4A	2.45	0.46
25:A:409:GOL:O3	25:A:409:GOL:O1	2.32	0.46
1:a:14:TRP:HD1	31:c:501:LMT:H6'1	1.81	0.46
26:a:411[A]:SQD:H271	32:d:406[A]:LHG:H141	1.97	0.46
2:b:149[B]:LEU:HD11	23:b:604:CLA:H152	1.97	0.46
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.80	0.46
26:a:411[B]:SQD:H152	32:d:406[B]:LHG:H172	1.98	0.46
3:c:85:GLY:O	23:c:505:CLA:HED2	2.16	0.46
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.97	0.46
2:B:133:LEU:HB2	25:B:627:GOL:H31	1.98	0.46
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.97	0.46
32:d:406[A]:LHG:H331	32:d:406[A]:LHG:H361	1.46	0.46
18:y:34:MET:O	18:y:38:LEU:HG	2.15	0.46
23:B:612:CLA:H162	23:B:612:CLA:H122	1.79	0.46
13:O:92:SER:HB3	13:O:131:PRO:HA	1.97	0.46
24:T:102:BCR:HC7	24:T:102:BCR:H331	1.59	0.46
1:a:82[B]:VAL:HB	1:a:174[B]:LEU:HB2	1.97	0.46
28:a:414[B]:PL9:H171	28:a:414[B]:PL9:H151	1.53	0.46
24:d:403:BCR:C8	24:d:403:BCR:H331	2.45	0.46
24:t:103:BCR:H23C	24:t:103:BCR:H382	1.98	0.46
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.45	0.46
24:B:619:BCR:H371	24:B:619:BCR:H24C	1.73	0.46
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.46
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.16	0.46
24:b:619:BCR:HC7	24:b:619:BCR:H311	1.60	0.46
23:d:402:CLA:H41	23:d:402:CLA:H61	1.64	0.46
26:A:410:SQD:H301	23:b:606:CLA:H202	1.98	0.45
3:C:41:ARG:NH1	23:C:513:CLA:HMD1	2.31	0.45
23:C:507:CLA:H111	23:C:507:CLA:H93	1.68	0.45
23:b:605:CLA:H41	23:b:605:CLA:H62	1.56	0.45
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:6:ARG:HG3	41:J:201:HOH:O	2.16	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.98	0.45
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	1.98	0.45
33:c:520:LMG:H181	10:k:27:VAL:HG11	1.99	0.45
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.96	0.45
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.80	0.45
28:a:414[B]:PL9:H28	32:a:420[B]:LHG:H222	1.97	0.45
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	1.98	0.45
23:B:614:CLA:H71	23:B:614:CLA:H112	1.48	0.45
23:C:508:CLA:H18	23:C:508:CLA:H152	1.43	0.45
23:b:614:CLA:H72	23:b:614:CLA:H112	1.58	0.45
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.98	0.45
4:D:261[A]:PHE:CZ	32:D:408[A]:LHG:HC81	2.52	0.45
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.52	0.45
12:M:32:GLN:HG2	31:m:103:LMT:H6'2	1.99	0.45
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.97	0.45
35:c:518[A]:DGD:HAT1	35:c:519:DGD:HBF2	1.99	0.45
13:o:43:LEU:HB3	13:o:81:ILE:HB	1.99	0.45
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.52	0.45
32:d:406[A]:LHG:H142	32:d:406[A]:LHG:H372	1.97	0.45
1:a:341[B]:LEU:HD22	25:c:526[B]:GOL:H12	1.98	0.45
24:b:617:BCR:H24C	24:b:617:BCR:H371	1.77	0.45
2:B:445:THR:HA	41:B:712:HOH:O	2.16	0.45
24:T:102:BCR:H351	26:b:620:SQD:H211	1.99	0.45
2:b:233:ASN:O	2:b:236:THR:HG22	2.17	0.45
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.45
19:z:26:ALA:HB3	19:z:40:ILE:HD11	1.99	0.45
23:C:510:CLA:HBC2	32:D:409[A]:LHG:H351	2.00	0.45
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.83	0.45
20:R:18:TRP:O	20:R:22:ASN:ND2	2.40	0.45
23:C:507:CLA:H101	23:C:507:CLA:H61	1.79	0.44
5:E:14:ILE:HD12	9:J:12:VAL:HG11	1.98	0.44
5:E:64:PRO:HB2	5:E:79:PHE:CD2	2.52	0.44
7:h:43:LEU:O	7:h:47:GLU:HG3	2.17	0.44
3:c:238:ILE:O	3:c:242:LEU:HG	2.17	0.44
35:c:518[B]:DGD:HAT1	35:c:519:DGD:HBF2	1.99	0.44
28:A:412[A]:PL9:H151	28:A:412[A]:PL9:H171	1.55	0.44
28:A:412[A]:PL9:H301	28:A:412[A]:PL9:H322	1.76	0.44
3:C:23:ALA:HB1	3:C:26:ARG:HB2	1.98	0.44
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.17	0.44
37:D:402[B]:PHO:HHD	37:D:402[B]:PHO:HBC2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.18	0.44
23:A:407:CLA:H61	23:A:407:CLA:H41	1.60	0.44
31:A:417:LMT:H6'2	31:A:417:LMT:O3'	2.18	0.44
5:E:30:LEU:HD23	20:R:12:VAL:HG22	2.00	0.44
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.99	0.44
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.53	0.44
28:a:414[A]:PL9:H503	17:x:24:THR:OG1	2.18	0.44
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.52	0.44
4:d:214[B]:HIS:HA	28:d:404[B]:PL9:O2	2.17	0.44
5:e:68:ASP:O	5:e:72:ALA:HB2	2.17	0.44
28:A:412[B]:PL9:H351	6:F:25:THR:OG1	2.17	0.44
2:B:357[A]:ARG:HH12	25:B:624:GOL:C3	2.30	0.44
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.78	0.44
23:C:503:CLA:C4D	23:C:505:CLA:H2	2.47	0.44
1:a:105:TRP:CE2	1:a:110[B]:GLY:HA3	2.52	0.44
23:b:615:CLA:H61	23:b:615:CLA:H92	1.65	0.44
4:D:230[B]:SER:HB2	41:D:529:HOH:O	2.18	0.44
1:a:214[A]:MET:HB3	28:a:414[A]:PL9:H103	1.98	0.44
16:V:28:GLU:CD	16:V:31:ARG:HH21	2.26	0.44
23:b:606:CLA:H142	23:b:606:CLA:H111	1.89	0.44
3:c:95:LEU:HD21	23:c:502:CLA:OBD	2.18	0.44
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.18	0.44
3:c:330:SER:HB3	13:o:100:GLY:O	2.17	0.44
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	1.99	0.44
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.89	0.44
23:b:614:CLA:H8	24:b:617:BCR:H362	2.00	0.44
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.32	0.44
23:C:505:CLA:H101	23:C:505:CLA:H62	1.63	0.44
35:C:520:DGD:HBE2	35:C:520:DGD:HB81	1.75	0.44
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.44
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.32	0.44
23:b:607:CLA:H112	23:b:607:CLA:H91	1.62	0.44
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.00	0.43
37:D:402[B]:PHO:H3A	23:D:404[B]:CLA:H142	2.00	0.43
28:a:414[A]:PL9:H28	32:a:420[A]:LHG:H222	1.99	0.43
20:R:10:LEU:O	20:R:14:LEU:HG	2.18	0.43
31:B:628:LMT:H91	31:B:628:LMT:H62	1.59	0.43
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.43
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.00	0.43
1:a:259[A]:ILE:HG22	1:a:260[A]:PHE:CD1	2.53	0.43
18:y:31:ALA:O	18:y:35:ILE:HG13	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:408:BCR:H24C	24:A:408:BCR:H371	1.76	0.43
3:C:275:SER:HB3	23:C:511:CLA:HED3	2.00	0.43
35:C:518[B]:DGD:HG11	41:C:601[B]:HOH:O	2.18	0.43
24:T:102:BCR:H19C	24:b:618:BCR:H363	1.99	0.43
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.54	0.43
33:a:417:LMG:H172	33:a:417:LMG:H201	1.74	0.43
23:c:505:CLA:H151	23:c:509:CLA:H143	1.98	0.43
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.99	0.43
28:A:412[A]:PL9:HC2	28:A:412[A]:PL9:HC8	1.71	0.43
28:A:412[A]:PL9:H221	28:A:412[A]:PL9:H201	1.88	0.43
28:D:407[A]:PL9:H401	28:D:407[A]:PL9:H422	1.75	0.43
13:O:54:GLU:HG2	13:O:64:GLU:O	2.19	0.43
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	2.00	0.43
2:B:422:ARG:O	2:B:425:ILE:HG12	2.17	0.43
35:C:518[B]:DGD:O1A	41:C:601[B]:HOH:O	2.21	0.43
24:T:102:BCR:H382	24:T:102:BCR:H23C	1.99	0.43
25:a:418:GOL:H12	41:t:201:HOH:O	2.18	0.43
1:A:131:TRP:CD2	1:A:131:TRP:C	2.95	0.43
14:t:2:GLU:HG2	14:t:3:THR:N	2.34	0.43
26:C:501[A]:SQD:H122	26:C:501[A]:SQD:H152	1.52	0.43
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.85	0.43
35:c:518[B]:DGD:HBF2	35:c:518[B]:DGD:HBE1	1.87	0.43
4:d:126:MET:HE3	4:d:143[A]:ALA:O	2.18	0.43
2:B:278:SER:HB3	2:B:281:GLN:HB3	2.00	0.43
4:D:49:LEU:HD13	24:D:406:BCR:C15	2.48	0.43
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	2.01	0.43
24:c:516:BCR:H24C	24:c:516:BCR:H371	1.85	0.43
4:d:148[B]:ALA:HB2	4:d:276[B]:VAL:HG13	2.00	0.43
5:E:26:THR:HG22	20:R:15:ALA:HB1	2.00	0.43
3:c:26:ARG:NH2	18:y:46:LEU:OXT	2.43	0.43
3:c:48:LYS:HG3	3:c:138:GLU:HG3	2.01	0.43
23:c:506:CLA:HAA1	23:c:506:CLA:HBD	2.01	0.43
23:B:602:CLA:H162	23:B:602:CLA:H203	1.64	0.42
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.84	0.42
3:C:344[A]:SER:OG	3:C:348:GLU:OE1	2.36	0.42
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.44	0.42
32:E:101[B]:LHG:H261	32:E:101[B]:LHG:H291	1.79	0.42
1:a:60[B]:ILE:HD12	1:a:84[B]:PRO:HD2	2.02	0.42
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.54	0.42
23:b:616:CLA:H92	23:b:616:CLA:H62	1.75	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:406[B]:LHG:H331	32:d:406[B]:LHG:H361	1.57	0.42
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.53	0.42
4:D:205[A]:LEU:HD13	37:D:401[A]:PHO:HAB	2.00	0.42
6:F:27:ALA:HB1	38:F:102:HEM:HAC	2.00	0.42
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.00	0.42
28:a:414[B]:PL9:H471	26:f:102:SQD:H292	2.01	0.42
2:b:247:PHE:CE2	23:b:602:CLA:H121	2.55	0.42
3:c:88:LEU:HD13	23:c:504:CLA:HED3	2.01	0.42
2:B:42:LEU:HD23	2:B:42:LEU:HA	1.91	0.42
23:B:616:CLA:H41	23:B:616:CLA:H61	1.69	0.42
26:B:620:SQD:H1	26:B:620:SQD:H462	2.01	0.42
1:a:296[B]:ASN:HB2	3:c:400[B]:PRO:O	2.19	0.42
23:b:607:CLA:H201	32:d:411[B]:LHG:H131	2.01	0.42
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.01	0.42
23:d:401[B]:CLA:HAA2	23:d:401[B]:CLA:HBD	2.01	0.42
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.76	0.42
35:C:519[B]:DGD:HBF2	35:C:519[B]:DGD:HBE2	1.79	0.42
24:D:406:BCR:H11C	24:D:406:BCR:H341	1.88	0.42
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.02	0.42
1:A:127:MET:HE3	23:C:507:CLA:HMB2	2.01	0.42
34:D:412:HTG:H1'2	7:H:25:TRP:CE3	2.55	0.42
11:L:22:LEU:HD23	32:L:101[B]:LHG:H172	2.00	0.42
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.01	0.42
1:A:82[A]:VAL:HB	1:A:174[A]:LEU:HB2	2.01	0.42
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.02	0.42
23:B:613:CLA:H162	23:B:613:CLA:H121	1.78	0.42
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.86	0.42
33:C:526:LMG:H141	33:C:526:LMG:H111	1.87	0.42
24:Y:101:BCR:H15C	24:Y:101:BCR:H351	1.84	0.42
1:a:269[B]:ARG:HB3	41:d:544[B]:HOH:O	2.20	0.42
24:y:101:BCR:H15C	24:y:101:BCR:H351	1.84	0.42
1:A:231:GLU:HB3	41:B:873:HOH:O	2.20	0.42
3:C:413[B]:GLU:OE2	41:C:612[B]:HOH:O	2.21	0.42
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.55	0.42
23:b:612:CLA:H122	23:b:612:CLA:H162	1.88	0.42
7:h:38:PHE:HB2	24:h:101:BCR:C10	2.49	0.42
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.02	0.42
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.54	0.42
24:b:618:BCR:H24C	24:b:618:BCR:H371	1.83	0.42
8:i:32:PRO:C	8:i:33:LYS:HD2	2.44	0.42
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.88	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
1:A:300[B]:PHE:HB3	1:A:302:PHE:CE2	2.55	0.42
23:B:601:CLA:H62	23:B:601:CLA:H92	1.84	0.42
23:B:602:CLA:H141	23:B:602:CLA:H161	1.91	0.42
32:D:409[A]:LHG:H302	32:D:409[A]:LHG:H332	1.81	0.42
24:T:102:BCR:H24C	24:T:102:BCR:H371	1.85	0.42
24:a:410:BCR:H24C	24:a:410:BCR:H371	1.81	0.42
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	2.02	0.42
24:B:618:BCR:H15C	24:B:618:BCR:H351	1.88	0.42
32:E:101[B]:LHG:H241	32:E:101[B]:LHG:HC61	1.80	0.42
8:I:12:VAL:O	8:I:16:VAL:HG23	2.19	0.42
24:K:102:BCR:H15C	24:K:102:BCR:H351	1.89	0.42
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.41
3:C:279:LEU:HD12	3:C:282:MET:HE3	2.02	0.41
37:a:416[B]:PHO:HBC2	37:a:416[B]:PHO:HHD	2.02	0.41
23:b:616:CLA:H102	23:b:616:CLA:H13	1.72	0.41
23:c:502:CLA:H42	23:c:503:CLA:HMD3	2.02	0.41
24:k:101:BCR:H15C	24:k:101:BCR:H351	1.90	0.41
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.50	0.41
23:C:504:CLA:HAA1	23:C:504:CLA:HBD	2.03	0.41
23:C:511:CLA:HMB1	23:C:511:CLA:HBB1	2.02	0.41
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.20	0.41
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.41
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.02	0.41
23:b:609:CLA:NC	24:h:101:BCR:H332	2.35	0.41
1:A:213[B]:ALA:HB2	4:D:275[B]:PRO:HG2	2.02	0.41
3:C:363:GLY:O	3:C:367:GLU:HG2	2.20	0.41
32:a:420[A]:LHG:H241	32:a:420[A]:LHG:HC61	1.90	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.86	0.41
8:i:2:GLU:O	8:i:6:ILE:HG12	2.20	0.41
16:v:106:ASN:OD1	16:v:106:ASN:N	2.52	0.41
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.01	0.41
1:A:160[B]:ILE:HD11	35:C:518[B]:DGD:HBT2	2.02	0.41
23:B:606:CLA:H122	23:B:606:CLA:H161	1.90	0.41
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	2.01	0.41
3:C:52:ALA:HB2	23:C:513:CLA:HMA2	2.01	0.41
3:C:339[B]:LYS:NZ	15:U:99:ASN:O	2.51	0.41
4:D:264[B]:LYS:NZ	41:D:526[B]:HOH:O	2.53	0.41
24:H:101:BCR:H11C	24:H:101:BCR:H341	1.98	0.41
24:Y:101:BCR:HC7	24:Y:101:BCR:H331	1.84	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:322[B]:ASN:OD1	3:c:412[B]:THR:HA	2.20	0.41
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:CBB	2.48	0.41
25:a:419:GOL:C3	12:m:1:FME:HG2	2.47	0.41
3:c:443[B]:TRP:CZ2	23:c:509:CLA:HMD1	2.55	0.41
23:c:510:CLA:H43	23:c:510:CLA:H12	1.91	0.41
24:c:515:BCR:H11C	24:c:515:BCR:H341	1.78	0.41
32:d:411[B]:LHG:H211	12:m:18:PRO:HG3	2.03	0.41
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.03	0.41
28:A:412[A]:PL9:H43	28:A:412[A]:PL9:H471	1.69	0.41
31:A:415:LMT:H71	2:b:39:LEU:HD13	2.02	0.41
23:C:504:CLA:H141	23:C:504:CLA:H161	1.86	0.41
23:a:406[B]:CLA:HBA1	23:a:406[B]:CLA:C4A	2.49	0.41
2:b:226:TYR:CD2	2:b:231:MET:HB2	2.55	0.41
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.50	0.41
32:d:406[A]:LHG:H131	32:d:406[A]:LHG:H102	1.91	0.41
23:B:603:CLA:HAB	23:B:605:CLA:H171	2.02	0.41
33:C:502:LMG:H201	33:C:502:LMG:H231	1.76	0.41
24:H:101:BCR:H331	24:H:101:BCR:C8	2.50	0.41
17:X:15[B]:LEU:HD23	17:X:15[B]:LEU:HA	1.92	0.41
3:c:459[B]:ILE:HG21	3:c:464[B]:GLU:HG3	2.03	0.41
23:c:507:CLA:HBA1	23:c:507:CLA:H3A	1.80	0.41
5:e:41:GLY:HA3	5:e:51[B]:ARG:HH22	1.86	0.41
5:e:80:LEU:HD23	5:e:80:LEU:HA	1.92	0.41
19:Z:7:LEU:HD23	19:Z:7:LEU:HA	1.88	0.41
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	2.01	0.41
26:B:620:SQD:H332	26:B:620:SQD:H301	1.92	0.41
4:D:210[B]:LEU:HA	4:D:213[B]:ILE:HG22	2.03	0.41
28:A:412[A]:PL9:H503	26:F:103:SQD:H341	2.02	0.41
2:B:349:LYS:HG3	2:B:350:GLU:OE1	2.21	0.41
2:B:491[A]:VAL:HG12	4:D:136[A]:VAL:HG13	2.03	0.41
24:B:618:BCR:C8	24:B:618:BCR:H331	2.50	0.41
35:C:519[A]:DGD:HAE2	35:C:519[A]:DGD:HA81	1.91	0.41
32:D:409[B]:LHG:H332	32:D:409[B]:LHG:H302	1.92	0.41
6:F:21:VAL:O	6:F:25:THR:HG23	2.20	0.41
12:M:16[B]:LEU:HD22	12:M:16[B]:LEU:HA	1.95	0.41
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.03	0.41
2:b:272:ARG:HG3	2:b:273:TYR:N	2.36	0.41
23:b:606:CLA:H72	24:b:619:BCR:HC7	2.03	0.41
23:b:613:CLA:H72	23:b:613:CLA:H111	1.89	0.41
24:b:619:BCR:H15C	24:b:619:BCR:H351	1.88	0.41
3:c:429:SER:HA	35:c:518[B]:DGD:HBW1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:505:CLA:H92	23:c:505:CLA:H61	1.77	0.41
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.55	0.41
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.01	0.41
4:d:161:PRO:HG3	4:d:170:ALA:HB2	2.03	0.41
28:A:412[A]:PL9:HC8	28:A:412[A]:PL9:H121	1.79	0.41
34:B:625:HTG:H61	1:a:102:LEU:HD12	2.03	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.95	0.41
4:D:203[B]:GLY:HA3	4:D:278[B]:GLY:HA3	2.03	0.41
17:X:24:THR:O	17:X:28:LEU:HG	2.21	0.41
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.03	0.41
33:d:409:LMG:H221	33:d:409:LMG:H191	1.67	0.41
5:e:45:ASP:CG	5:e:51[A]:ARG:HH22	2.29	0.41
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.41
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.21	0.41
3:C:216:SER:HB2	33:C:502:LMG:HC71	2.02	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.56	0.40
13:O:137:THR:C	13:O:139:SER:N	2.79	0.40
32:a:420[A]:LHG:H142	32:a:420[A]:LHG:H172	1.83	0.40
2:b:42:LEU:HD23	2:b:42:LEU:HA	1.92	0.40
24:k:101:BCR:H24C	24:k:101:BCR:H371	1.77	0.40
28:A:412[B]:PL9:H322	28:A:412[B]:PL9:H301	1.72	0.40
10:K:26:PRO:O	10:K:29:PRO:HD2	2.21	0.40
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.88	0.40
23:b:616:CLA:H3A	23:b:616:CLA:HBA1	1.91	0.40
4:d:86:GLY:O	4:d:166:SER:HB2	2.20	0.40
32:d:406[A]:LHG:H242	32:d:406[A]:LHG:H272	1.92	0.40
13:o:58:ASN:ND2	13:o:61:GLN:HG3	2.33	0.40
1:A:159[B]:LEU:C	1:A:162[B]:PRO:HD2	2.46	0.40
2:B:221:PRO:HA	2:B:222:PRO:HD3	2.01	0.40
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.34	0.40
23:C:506:CLA:H62	23:C:506:CLA:H41	1.74	0.40
13:O:121:THR:OG1	13:O:123:LYS:HG3	2.21	0.40
1:a:95:PRO:HD2	1:a:98:GLU:HG3	2.03	0.40
23:a:405[B]:CLA:H122	23:a:405[B]:CLA:H161	1.89	0.40
23:b:601:CLA:HAC1	24:h:101:BCR:H383	2.04	0.40
23:c:509:CLA:H162	23:c:509:CLA:H122	1.78	0.40
24:c:515:BCR:H351	24:c:515:BCR:H15C	1.82	0.40
4:d:141[B]:TYR:OH	32:d:411[B]:LHG:O4	2.29	0.40
32:d:406[B]:LHG:H372	32:d:406[B]:LHG:H142	2.03	0.40
1:A:15:GLU:HG2	31:A:417:LMT:O3B	2.22	0.40
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:323[B]:GLU:O	25:D:414:GOL:O2	2.39	0.40
15:U:86[B]:GLU:OE1	15:U:86[B]:GLU:N	2.25	0.40
16:V:57:GLU:H	16:V:57:GLU:CD	2.29	0.40
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CZ3	2.55	0.40
2:b:358:ARG:HB2	25:b:628:GOL:H31	2.02	0.40
2:b:497:GLN:HB2	2:b:504:THR:HB	2.03	0.40
23:c:506:CLA:HMD2	23:c:508:CLA:HAB	2.04	0.40
35:c:518[A]:DGD:HBF2	35:c:518[A]:DGD:HBE1	1.91	0.40
31:B:630:LMT:H11	1:a:72:LEU:HD13	2.03	0.40
5:E:18:ARG:H	9:J:2:SER:N	2.20	0.40
3:c:82:TYR:OH	3:c:394[A]:GLU:OE2	2.31	0.40
24:d:403:BCR:H15C	24:d:403:BCR:H351	1.83	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%)	548 (99%)	3 (0%)	2 (0%)	30	38
1	a	552/344 (160%)	545 (99%)	5 (1%)	2 (0%)	30	38
2	B	522/505 (103%)	515 (99%)	7 (1%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	546/455 (120%)	540 (99%)	5 (1%)	1 (0%)	43	55
3	c	553/455 (122%)	540 (98%)	12 (2%)	1 (0%)	43	55
4	D	453/342 (132%)	437 (96%)	16 (4%)	0	100	100
4	d	454/342 (133%)	443 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	77 (98%)	2 (2%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	58 (92%)	5 (8%)	0	100	100
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	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%)	240 (96%)	10 (4%)	1 (0%)	30	38
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	98/104 (94%)	95 (97%)	3 (3%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	133 (95%)	7 (5%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	0	100	100
18	y	27/30 (90%)	27 (100%)	0	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	7
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	7
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6171/5384 (115%)	6035 (98%)	126 (2%)	10 (0%)	43	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
3	c	416	SER
19	Z	31	GLN
13	O	138	THR
19	z	30	PRO
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%)	440 (99%)	4 (1%)	70	84
1	a	443/279 (159%)	442 (100%)	1 (0%)	87	94
2	B	421/403 (104%)	416 (99%)	5 (1%)	63	79
2	b	420/403 (104%)	410 (98%)	10 (2%)	43	62
3	C	430/356 (121%)	424 (99%)	6 (1%)	59	76
3	c	436/356 (122%)	428 (98%)	8 (2%)	51	70
4	D	368/277 (133%)	365 (99%)	3 (1%)	73	86
4	d	369/277 (133%)	362 (98%)	7 (2%)	50	69
5	E	72/73 (99%)	71 (99%)	1 (1%)	59	76
5	e	72/73 (99%)	70 (97%)	2 (3%)	38	56
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%)	51 (94%)	3 (6%)	19	28
7	h	55/54 (102%)	53 (96%)	2 (4%)	31	47
8	I	34/34 (100%)	33 (97%)	1 (3%)	37	55
8	i	34/34 (100%)	33 (97%)	1 (3%)	37	55
9	J	26/27 (96%)	25 (96%)	1 (4%)	29	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	j	26/27 (96%)	25 (96%)	1 (4%)	29 44
10	K	30/30 (100%)	27 (90%)	3 (10%)	7 9
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 9
11	L	36/35 (103%)	36 (100%)	0	100 100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 56
12	M	30/32 (94%)	28 (93%)	2 (7%)	15 21
12	m	32/32 (100%)	30 (94%)	2 (6%)	16 23
13	O	216/207 (104%)	207 (96%)	9 (4%)	26 40
13	o	213/207 (103%)	206 (97%)	7 (3%)	33 50
14	T	32/28 (114%)	28 (88%)	4 (12%)	4 5
14	t	31/28 (111%)	31 (100%)	0	100 100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44 63
15	u	87/89 (98%)	85 (98%)	2 (2%)	44 63
16	V	123/117 (105%)	123 (100%)	0	100 100
16	v	123/117 (105%)	119 (97%)	4 (3%)	33 50
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100
18	y	22/23 (96%)	17 (77%)	5 (23%)	1 1
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 26
19	z	52/52 (100%)	46 (88%)	6 (12%)	5 6
20	R	29/29 (100%)	26 (90%)	3 (10%)	7 8
All	All	5103/4403 (116%)	4991 (98%)	112 (2%)	45 65

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
1	A	244[A]	GLU
1	A	244[B]	GLU
2	B	161	LEU
2	B	299	GLU
2	B	315	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	389	LYS
2	B	419	SER
3	C	30	SER
3	C	142	GLU
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
7	H	52	THR
8	I	33	LYS
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
13	O	4	THR
13	O	37	THR
13	O	49	THR
13	O	55	GLU
13	O	69	LYS
13	O	87	VAL
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
1	a	13	LEU
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	240	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	b	245	VAL
2	b	362	PHE
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	491[A]	VAL
2	b	491[B]	VAL
3	c	19	ASN
3	c	142	GLU
3	c	152	LYS
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
3	c	416	SER
4	d	26	ARG
4	d	230[A]	SER
4	d	230[B]	SER
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	61	ARG
5	e	71	GLU
7	h	27	THR
7	h	43	LEU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	106	ASN
18	y	18	VAL
18	y	19	ILE
18	y	22	LEU
18	y	30	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	31	GLN
19	Z	62	VAL
20	R	4	ARG
20	R	23	ILE
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	21	ILE
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	374	ASN
2	B	394	GLN
5	E	60	GLN
15	U	78	ASN
17	X	38	GLN
1	a	12	ASN
1	a	75	ASN
2	b	14	ASN
2	b	331	ASN
3	c	19	ASN
3	c	201	ASN
11	l	8	GLN
13	o	58	ASN
13	o	132	ASN
15	u	78	ASN
16	v	86	GLN
19	Z	31	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	8,9,11	1.26	1 (12%)
12	FME	m	1	12	8,9,10	0.51	0	8,9,11	1.35	2 (25%)
14	FME	T	1	14	8,9,10	0.62	0	8,9,11	1.50	1 (12%)
8	FME	I	1	8	8,9,10	0.69	0	8,9,11	1.05	1 (12%)
14	FME	t	1	14	8,9,10	0.82	0	8,9,11	1.37	1 (12%)
12	FME	M	1	12	8,9,10	0.74	0	8,9,11	1.31	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	i	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	1/7/9/11	-
14	FME	t	1	14	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O-C-CA	-2.81	117.54	124.77
12	m	1	FME	O-C-CA	-2.40	118.59	124.77
12	m	1	FME	O1-CN-N	-2.26	119.49	125.32
14	T	1	FME	CB-CA-N	-2.25	106.42	110.52
8	i	1	FME	O-C-CA	-2.21	119.08	124.77
12	M	1	FME	O-C-CA	-2.20	119.11	124.77
12	M	1	FME	CA-N-CN	-2.17	119.48	122.82
8	I	1	FME	O-C-CA	-2.09	119.41	124.77

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	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	$\#\|Z\|>2$
23	CLA	a	407[B]	41	69,73,73	2.02	19 (27%)	82,113,113	2.73	32 (39%)
25	GOL	l	801[A]	-	5,5,5	0.98	0	5,5,5	1.05	1 (20%)
40	HEC	V	202	16	46,50,50	1.87	5 (10%)	58,82,82	1.81	7 (12%)
23	CLA	c	510	-	69,73,73	2.01	19 (27%)	82,113,113	2.81	32 (39%)
25	GOL	O	302	-	5,5,5	1.04	0	5,5,5	0.94	0
23	CLA	b	604	-	69,73,73	1.96	20 (28%)	82,113,113	2.63	30 (36%)
30	BCT	A	414[B]	21	3,3,3	0.51	0	2,3,3	0.87	0
31	LMT	t	101	-	25,25,36	0.88	1 (4%)	30,30,47	1.21	3 (10%)
32	LHG	D	409[B]	-	48,48,48	0.94	2 (4%)	51,54,54	1.03	3 (5%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.98	4 (5%)
26	SQD	C	501[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.85	10 (16%)
24	BCR	c	515	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	12 (21%)
32	LHG	d	405[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	C	505	-	69,73,73	1.93	19 (27%)	82,113,113	2.67	30 (36%)
28	PL9	A	412[A]	-	55,55,55	0.71	3 (5%)	68,69,69	2.05	25 (36%)
23	CLA	C	506	41	69,73,73	1.90	19 (27%)	82,113,113	2.66	31 (37%)
23	CLA	C	508	-	69,73,73	2.00	21 (30%)	82,113,113	2.71	33 (40%)
25	GOL	V	204[B]	-	5,5,5	1.00	0	5,5,5	1.09	0
37	PHO	D	401[B]	-	58,69,69	2.72	15 (25%)	55,99,99	3.00	16 (29%)
23	CLA	B	602	-	69,73,73	2.06	20 (28%)	82,113,113	2.72	33 (40%)
25	GOL	B	629	-	5,5,5	0.90	0	5,5,5	1.12	0
23	CLA	C	511	-	69,73,73	2.03	20 (28%)	82,113,113	2.68	30 (36%)
26	SQD	F	103	-	41,43,54	1.17	3 (7%)	51,54,65	2.03	14 (27%)
23	CLA	a	405[B]	-	69,73,73	2.02	19 (27%)	82,113,113	2.74	36 (43%)
37	PHO	a	416[A]	-	58,69,69	2.79	14 (24%)	55,99,99	3.05	17 (30%)
23	CLA	b	616	-	69,73,73	1.96	19 (27%)	82,113,113	2.81	32 (39%)
23	CLA	B	608	-	69,73,73	1.90	21 (30%)	82,113,113	2.70	35 (42%)
23	CLA	B	606	-	69,73,73	1.97	20 (28%)	82,113,113	2.77	33 (40%)
23	CLA	b	608	-	69,73,73	2.00	21 (30%)	82,113,113	2.67	31 (37%)
23	CLA	B	613	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	31 (37%)
23	CLA	c	502	-	69,73,73	2.00	21 (30%)	82,113,113	2.61	29 (35%)
23	CLA	D	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	34 (41%)
24	BCR	d	403	-	41,41,41	1.10	2 (4%)	56,56,56	1.95	15 (26%)
28	PL9	d	404[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.69	18 (26%)
26	SQD	a	411[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.80	11 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	512	3	69,73,73	2.05	20 (28%)	82,113,113	2.70	32 (39%)
23	CLA	c	508	41	69,73,73	1.97	17 (24%)	82,113,113	2.75	32 (39%)
25	GOL	c	526[B]	-	5,5,5	0.98	0	5,5,5	1.03	0
23	CLA	a	406[A]	41	69,73,73	2.01	17 (24%)	82,113,113	2.72	31 (37%)
32	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.12	3 (6%)
27	OEX	A	411[B]	41,1,3	0,15,15	-	-	-		
25	GOL	b	628	-	5,5,5	0.55	0	5,5,5	1.43	1 (20%)
35	DGD	C	518[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	7 (9%)
31	LMT	t	102	-	26,26,36	0.93	2 (7%)	31,31,47	1.24	2 (6%)
31	LMT	T	101	-	36,36,36	1.05	1 (2%)	47,47,47	1.12	3 (6%)
23	CLA	B	612	-	69,73,73	1.96	19 (27%)	82,113,113	2.70	33 (40%)
23	CLA	b	612	-	69,73,73	2.03	20 (28%)	82,113,113	2.66	32 (39%)
25	GOL	c	527	-	5,5,5	1.28	1 (20%)	5,5,5	0.98	0
35	DGD	C	520	-	63,63,67	0.88	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	A	404[B]	-	69,73,73	2.04	19 (27%)	82,113,113	2.75	33 (40%)
33	LMG	C	521	-	51,51,55	0.97	2 (3%)	59,59,63	1.18	4 (6%)
28	PL9	D	407[B]	-	55,55,55	0.62	2 (3%)	68,69,69	1.69	17 (25%)
23	CLA	B	609	-	69,73,73	2.02	17 (24%)	82,113,113	2.68	31 (37%)
23	CLA	A	407	-	69,73,73	1.94	20 (28%)	82,113,113	2.80	36 (43%)
25	GOL	B	624	-	5,5,5	0.80	0	5,5,5	1.17	1 (20%)
25	GOL	D	403	-	5,5,5	1.57	2 (40%)	5,5,5	0.89	0
38	HEM	F	102	5,6	50,50,50	1.53	8 (16%)	67,82,82	1.80	15 (22%)
24	BCR	A	408	-	41,41,41	1.08	2 (4%)	56,56,56	1.47	8 (14%)
24	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.57	11 (19%)
25	GOL	o	302	-	5,5,5	1.32	1 (20%)	5,5,5	1.13	0
23	CLA	B	603	-	69,73,73	1.96	18 (26%)	82,113,113	2.83	31 (37%)
32	LHG	d	411[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.13	4 (7%)
24	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	11 (19%)
34	HTG	b	623	-	19,19,19	0.98	1 (5%)	23,24,24	1.76	4 (17%)
28	PL9	a	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.03	23 (33%)
24	BCR	b	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	10 (17%)
23	CLA	b	611	-	69,73,73	1.93	20 (28%)	82,113,113	2.78	30 (36%)
25	GOL	B	627	-	5,5,5	1.04	0	5,5,5	1.03	0
30	BCT	a	404[A]	21	3,3,3	0.49	0	2,3,3	1.49	0
35	DGD	H	102	-	63,63,67	0.82	3 (4%)	77,77,81	1.11	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	509	41	69,73,73	1.96	18 (26%)	82,113,113	2.79	31 (37%)
23	CLA	b	614	-	69,73,73	2.01	20 (28%)	82,113,113	2.78	32 (39%)
33	LMG	m	101	-	51,51,55	0.86	2 (3%)	59,59,63	1.41	8 (13%)
32	LHG	L	101[A]	-	48,48,48	0.89	3 (6%)	51,54,54	1.16	4 (7%)
24	BCR	t	103	-	41,41,41	1.07	1 (2%)	56,56,56	1.58	12 (21%)
23	CLA	b	613	-	69,73,73	1.94	18 (26%)	82,113,113	2.70	31 (37%)
26	SQD	f	102	-	41,43,54	1.15	2 (4%)	51,54,65	1.55	12 (23%)
23	CLA	a	407[A]	41	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
33	LMG	c	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.17	6 (10%)
23	CLA	C	503	-	69,73,73	1.99	19 (27%)	82,113,113	2.70	31 (37%)
31	LMT	F	101	-	36,36,36	1.02	1 (2%)	47,47,47	1.05	3 (6%)
23	CLA	A	405[A]	41	69,73,73	2.00	18 (26%)	82,113,113	2.70	35 (42%)
30	BCT	A	414[A]	21	3,3,3	0.55	0	2,3,3	1.29	0
37	PHO	a	408[B]	-	58,69,69	2.75	14 (24%)	55,99,99	2.86	16 (29%)
32	LHG	A	416[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.20	5 (9%)
25	GOL	a	419	-	5,5,5	1.47	1 (20%)	5,5,5	1.08	1 (20%)
32	LHG	a	420[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
32	LHG	l	802[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	4 (7%)
38	HEM	f	101	5,6	50,50,50	1.51	6 (12%)	67,82,82	1.68	12 (17%)
33	LMG	C	526	-	37,37,55	1.01	2 (5%)	45,45,63	1.48	8 (17%)
34	HTG	b	622	-	19,19,19	1.16	3 (15%)	23,24,24	2.15	8 (34%)
23	CLA	b	610	41	69,73,73	1.99	19 (27%)	82,113,113	2.80	32 (39%)
23	CLA	A	406[B]	41	69,73,73	2.08	20 (28%)	82,113,113	2.73	33 (40%)
25	GOL	V	204[A]	-	5,5,5	1.41	1 (20%)	5,5,5	0.86	0
33	LMG	C	502	-	51,51,55	0.91	2 (3%)	59,59,63	1.58	10 (16%)
23	CLA	d	402	-	69,73,73	2.01	20 (28%)	82,113,113	2.67	30 (36%)
37	PHO	D	401[A]	-	58,69,69	2.66	12 (20%)	55,99,99	2.93	14 (25%)
23	CLA	b	609	-	69,73,73	2.01	18 (26%)	82,113,113	2.72	32 (39%)
23	CLA	c	504	-	69,73,73	2.08	20 (28%)	82,113,113	2.78	30 (36%)
23	CLA	a	405[A]	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	34 (41%)
26	SQD	B	620	-	52,54,54	1.02	3 (5%)	62,65,65	1.70	11 (17%)
34	HTG	C	523	-	19,19,19	0.82	1 (5%)	23,24,24	1.24	2 (8%)
23	CLA	b	602	-	69,73,73	2.05	20 (28%)	82,113,113	2.89	33 (40%)
34	HTG	V	203	-	11,11,19	0.35	0	15,15,24	1.32	1 (6%)
35	DGD	C	519[A]	-	63,63,67	0.91	3 (4%)	77,77,81	1.04	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	GOL	l	801[B]	-	5,5,5	0.93	0	5,5,5	1.08	0
32	LHG	d	406[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.02	4 (7%)
23	CLA	B	611	-	69,73,73	2.49	20 (28%)	82,113,113	3.53	31 (37%)
23	CLA	C	514	-	69,73,73	2.01	19 (27%)	82,113,113	2.66	32 (39%)
24	BCR	y	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.76	12 (21%)
32	LHG	D	408[A]	-	48,48,48	0.88	3 (6%)	51,54,54	1.02	3 (5%)
34	HTG	D	412	-	16,16,19	0.94	1 (6%)	20,21,24	1.29	1 (5%)
35	DGD	c	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	0.96	5 (6%)
25	GOL	v	202[A]	-	5,5,5	1.26	0	5,5,5	0.88	0
26	SQD	A	410	-	52,54,54	1.01	2 (3%)	62,65,65	1.19	4 (6%)
26	SQD	C	501[B]	-	52,54,54	0.88	2 (3%)	62,65,65	1.61	11 (17%)
31	LMT	A	415	-	36,36,36	0.86	0	47,47,47	1.11	2 (4%)
32	LHG	d	405[B]	-	48,48,48	0.91	3 (6%)	51,54,54	1.06	4 (7%)
25	GOL	O	303	-	5,5,5	0.88	0	5,5,5	1.16	1 (20%)
23	CLA	C	512	-	69,73,73	2.00	20 (28%)	82,113,113	2.81	34 (41%)
25	GOL	D	414	-	5,5,5	1.90	2 (40%)	5,5,5	0.60	0
25	GOL	c	526[A]	-	5,5,5	1.04	0	5,5,5	1.05	0
28	PL9	A	412[B]	-	55,55,55	0.65	2 (3%)	68,69,69	2.04	25 (36%)
35	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.12	6 (7%)
23	CLA	B	604	-	69,73,73	2.04	21 (30%)	82,113,113	2.62	31 (37%)
24	BCR	D	406	-	41,41,41	1.09	1 (2%)	56,56,56	1.83	18 (32%)
27	OEX	A	411[A]	41,1,3	0,15,15	-	-	-		
35	DGD	C	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	1.20	6 (7%)
33	LMG	z	101	-	39,39,55	1.11	2 (5%)	47,47,63	1.12	5 (10%)
40	HEC	v	201	16	46,50,50	1.94	6 (13%)	58,82,82	1.75	5 (8%)
31	LMT	B	630	-	36,36,36	0.98	2 (5%)	47,47,47	1.20	4 (8%)
31	LMT	b	621	-	25,25,36	0.94	1 (4%)	30,30,47	1.16	2 (6%)
23	CLA	d	401[B]	-	69,73,73	1.98	19 (27%)	82,113,113	2.71	31 (37%)
25	GOL	c	528	-	5,5,5	1.23	1 (20%)	5,5,5	0.92	0
24	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	11 (19%)
28	PL9	D	407[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.61	17 (25%)
26	SQD	b	620	-	52,54,54	1.01	2 (3%)	62,65,65	1.67	11 (17%)
25	GOL	C	524[B]	-	5,5,5	1.27	0	5,5,5	0.88	0
24	BCR	c	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.45	12 (21%)
31	LMT	c	501	-	36,36,36	0.97	2 (5%)	47,47,47	1.03	1 (2%)
24	BCR	B	619	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.50	7 (12%)
23	CLA	B	615	-	69,73,73	2.02	18 (26%)	82,113,113	2.73	32 (39%)
31	LMT	M	101	-	36,36,36	1.08	3 (8%)	47,47,47	1.26	5 (10%)
34	HTG	b	625	-	19,19,19	0.94	2 (10%)	23,24,24	1.44	3 (13%)
23	CLA	c	513	-	69,73,73	2.05	20 (28%)	82,113,113	2.66	32 (39%)
23	CLA	a	406[B]	41	69,73,73	2.02	19 (27%)	82,113,113	2.67	32 (39%)
32	LHG	D	409[A]	-	48,48,48	0.94	2 (4%)	51,54,54	1.04	4 (7%)
24	BCR	C	517	-	41,41,41	1.07	2 (4%)	56,56,56	1.50	11 (19%)
23	CLA	C	513	3	69,73,73	2.01	20 (28%)	82,113,113	2.53	28 (34%)
23	CLA	C	507	-	69,73,73	1.99	19 (27%)	82,113,113	2.72	30 (36%)
37	PHO	D	402[B]	-	58,69,69	2.84	14 (24%)	55,99,99	2.92	16 (29%)
24	BCR	B	617	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	8 (14%)
23	CLA	c	509	-	69,73,73	2.08	20 (28%)	82,113,113	2.63	31 (37%)
35	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	1.03	5 (6%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.12	5 (6%)
23	CLA	C	510	-	69,73,73	2.04	19 (27%)	82,113,113	2.70	30 (36%)
27	OEX	a	413[B]	41,1,3	0,15,15	-	-	-		
31	LMT	e	101	-	36,36,36	0.98	1 (2%)	47,47,47	1.04	1 (2%)
23	CLA	C	504	-	69,73,73	2.01	19 (27%)	82,113,113	2.54	29 (35%)
23	CLA	A	406[A]	41	69,73,73	2.01	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	b	603	-	69,73,73	1.96	20 (28%)	82,113,113	2.74	32 (39%)
24	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	11 (19%)
28	PL9	a	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.95	22 (32%)
23	CLA	b	606	-	69,73,73	1.96	19 (27%)	82,113,113	2.81	33 (40%)
31	LMT	B	628	-	36,36,36	1.13	3 (8%)	47,47,47	1.34	5 (10%)
33	LMG	B	621	-	51,51,55	0.89	2 (3%)	59,59,63	1.32	5 (8%)
23	CLA	c	511	-	69,73,73	1.99	20 (28%)	82,113,113	2.75	35 (42%)
23	CLA	b	601	41	69,73,73	2.04	18 (26%)	82,113,113	2.72	29 (35%)
23	CLA	B	605	-	69,73,73	2.01	18 (26%)	82,113,113	2.82	29 (35%)
23	CLA	b	605	-	69,73,73	1.93	19 (27%)	82,113,113	2.97	30 (36%)
23	CLA	b	607	41	69,73,73	1.95	20 (28%)	82,113,113	2.62	28 (34%)
24	BCR	K	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.45	11 (19%)
28	PL9	d	404[A]	-	55,55,55	0.72	1 (1%)	68,69,69	1.61	17 (25%)
32	LHG	L	101[B]	-	48,48,48	0.91	3 (6%)	51,54,54	1.06	5 (9%)
33	LMG	D	413	39	51,51,55	0.83	2 (3%)	59,59,63	1.07	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.82	15 (26%)
23	CLA	c	507	-	69,73,73	2.02	19 (27%)	82,113,113	2.61	31 (37%)
23	CLA	c	505	41	69,73,73	2.02	20 (28%)	82,113,113	2.62	32 (39%)
23	CLA	b	615	-	69,73,73	1.99	17 (24%)	82,113,113	2.66	35 (42%)
24	BCR	b	617	-	41,41,41	1.07	2 (4%)	56,56,56	1.36	6 (10%)
32	LHG	d	406[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.02	3 (5%)
23	CLA	c	503	-	69,73,73	1.95	19 (27%)	82,113,113	2.62	28 (34%)
24	BCR	a	410	-	41,41,41	1.04	2 (4%)	56,56,56	1.36	9 (16%)
23	CLA	A	405[B]	41	69,73,73	1.97	21 (30%)	82,113,113	2.71	34 (41%)
23	CLA	c	506	-	69,73,73	2.01	18 (26%)	82,113,113	2.64	28 (34%)
34	HTG	c	522	-	19,19,19	0.85	1 (5%)	23,24,24	1.39	3 (13%)
23	CLA	B	601	41	69,73,73	2.07	21 (30%)	82,113,113	2.70	31 (37%)
23	CLA	A	404[A]	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	31 (37%)
33	LMG	a	417	-	51,51,55	0.93	2 (3%)	59,59,63	1.19	6 (10%)
23	CLA	B	607	41	69,73,73	1.91	21 (30%)	82,113,113	2.69	33 (40%)
25	GOL	d	410	-	5,5,5	1.09	0	5,5,5	1.02	0
37	PHO	a	416[B]	-	58,69,69	2.80	14 (24%)	55,99,99	3.03	16 (29%)
34	HTG	B	623	-	19,19,19	0.73	1 (5%)	23,24,24	1.39	2 (8%)
23	CLA	B	610	41	69,73,73	2.01	19 (27%)	82,113,113	2.84	32 (39%)
23	CLA	D	404[B]	-	69,73,73	1.98	19 (27%)	82,113,113	2.80	30 (36%)
23	CLA	d	401[A]	-	69,73,73	1.94	19 (27%)	82,113,113	2.64	33 (40%)
34	HTG	d	408	-	16,16,19	0.88	1 (6%)	20,21,24	1.39	2 (10%)
25	GOL	a	418	-	5,5,5	1.40	2 (40%)	5,5,5	0.97	0
31	LMT	b	627	-	25,25,36	0.88	1 (4%)	30,30,47	1.13	2 (6%)
25	GOL	C	524[A]	-	5,5,5	1.16	0	5,5,5	0.94	0
23	CLA	B	616	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	31 (37%)
26	SQD	a	411[B]	-	52,54,54	0.92	2 (3%)	62,65,65	1.53	10 (16%)
35	DGD	C	519[B]	-	63,63,67	0.88	3 (4%)	77,77,81	1.04	6 (7%)
23	CLA	B	614	-	69,73,73	2.01	20 (28%)	82,113,113	2.87	32 (39%)
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.13	4 (9%)
32	LHG	D	408[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.03	5 (9%)
33	LMG	C	522	-	51,51,55	1.08	3 (5%)	59,59,63	1.35	6 (10%)
25	GOL	v	202[B]	-	5,5,5	1.07	0	5,5,5	0.98	0
26	SQD	a	412	-	52,54,54	1.04	2 (3%)	62,65,65	1.15	7 (11%)
25	GOL	A	409	-	5,5,5	1.17	0	5,5,5	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	PHO	a	408[A]	-	58,69,69	2.77	13 (22%)	55,99,99	2.94	14 (25%)
33	LMG	c	521	-	51,51,55	1.02	2 (3%)	59,59,63	1.33	6 (10%)
32	LHG	A	416[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.29	6 (11%)
23	CLA	c	514	-	69,73,73	2.08	21 (30%)	82,113,113	2.71	32 (39%)
31	LMT	A	417	-	36,36,36	1.01	2 (5%)	47,47,47	1.15	4 (8%)
32	LHG	a	420[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.93	2 (4%)
32	LHG	l	802[A]	-	48,48,48	0.84	3 (6%)	51,54,54	1.05	4 (7%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.19	4 (17%)
34	HTG	B	622	-	19,19,19	1.11	2 (10%)	23,24,24	1.58	6 (26%)
23	CLA	a	409	-	69,73,73	1.97	19 (27%)	82,113,113	2.82	31 (37%)
37	PHO	D	402[A]	-	58,69,69	2.81	14 (24%)	55,99,99	2.93	16 (29%)
23	CLA	C	515	-	69,73,73	2.01	19 (27%)	82,113,113	2.74	31 (37%)
31	LMT	m	103	-	36,36,36	1.04	2 (5%)	47,47,47	1.17	4 (8%)
32	LHG	d	411[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
35	DGD	c	517[A]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	8 (10%)
25	GOL	b	624	-	5,5,5	1.24	1 (20%)	5,5,5	0.86	0
33	LMG	d	409	39	51,51,55	0.92	2 (3%)	59,59,63	1.12	5 (8%)
24	BCR	B	618	-	41,41,41	1.02	2 (4%)	56,56,56	1.33	5 (8%)
24	BCR	b	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.26	9 (16%)
30	BCT	a	404[B]	21	3,3,3	0.51	0	2,3,3	0.90	0
27	OEX	a	413[A]	41,1,3	0,15,15	-	-	-		
23	CLA	D	405	-	69,73,73	2.12	18 (26%)	82,113,113	2.64	31 (37%)

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
23	CLA	a	407[B]	41	-	5/39/115/115	-
25	GOL	l	801[A]	-	-	2/4/4/4	-
40	HEC	V	202	16	-	6/14/54/54	-
23	CLA	c	510	-	1/1/15/20	15/39/115/115	-
25	GOL	O	302	-	-	2/4/4/4	-
23	CLA	b	604	-	1/1/15/20	11/39/115/115	-
31	LMT	t	101	-	-	11/17/37/61	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	D	409[B]	-	-	12/53/53/53	-
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
26	SQD	C	501[A]	-	-	12/49/69/69	0/1/1/1
24	BCR	c	515	-	-	0/29/63/63	0/2/2/2
32	LHG	d	405[A]	-	-	12/53/53/53	-
23	CLA	C	505	-	-	4/39/115/115	-
28	PL9	A	412[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	C	506	41	1/1/15/20	7/39/115/115	-
23	CLA	C	508	-	1/1/15/20	11/39/115/115	-
25	GOL	V	204[B]	-	-	2/4/4/4	-
37	PHO	D	401[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	B	602	-	1/1/15/20	12/39/115/115	-
25	GOL	B	629	-	-	4/4/4/4	-
23	CLA	C	511	-	1/1/15/20	4/39/115/115	-
26	SQD	F	103	-	-	13/38/58/69	0/1/1/1
23	CLA	a	405[B]	-	1/1/15/20	9/39/115/115	-
37	PHO	a	416[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	b	616	-	1/1/15/20	9/39/115/115	-
23	CLA	B	608	-	-	3/39/115/115	-
23	CLA	B	606	-	1/1/15/20	4/39/115/115	-
23	CLA	b	608	-	-	6/39/115/115	-
23	CLA	B	613	-	1/1/15/20	7/39/115/115	-
23	CLA	c	502	-	1/1/15/20	7/39/115/115	-
23	CLA	D	404[A]	-	1/1/15/20	2/39/115/115	-
24	BCR	d	403	-	-	4/29/63/63	0/2/2/2
28	PL9	d	404[B]	-	-	8/53/73/73	0/1/1/1
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
23	CLA	c	512	3	1/1/15/20	6/39/115/115	-
23	CLA	c	508	41	1/1/15/20	8/39/115/115	-
25	GOL	c	526[B]	-	-	0/4/4/4	-
23	CLA	a	406[A]	41	1/1/15/20	4/39/115/115	-
32	LHG	E	101[A]	-	-	21/46/46/53	-
25	GOL	b	628	-	-	0/4/4/4	-
35	DGD	C	518[B]	-	-	15/51/91/95	0/2/2/2
31	LMT	t	102	-	-	9/17/38/61	0/1/1/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	T	101	-	-	9/21/61/61	0/2/2/2
23	CLA	B	612	-	1/1/15/20	3/39/115/115	-
23	CLA	b	612	-	1/1/15/20	5/39/115/115	-
25	GOL	c	527	-	-	3/4/4/4	-
35	DGD	C	520	-	-	23/51/91/95	0/2/2/2
23	CLA	A	404[B]	-	1/1/15/20	5/39/115/115	-
33	LMG	C	521	-	-	10/46/66/70	0/1/1/1
28	PL9	D	407[B]	-	-	7/53/73/73	0/1/1/1
23	CLA	B	609	-	1/1/15/20	2/39/115/115	-
23	CLA	A	407	-	1/1/15/20	8/39/115/115	-
25	GOL	B	624	-	-	2/4/4/4	-
25	GOL	D	403	-	-	2/4/4/4	-
38	HEM	F	102	5,6	-	6/14/54/54	-
24	BCR	A	408	-	-	0/29/63/63	0/2/2/2
24	BCR	T	102	-	-	1/29/63/63	0/2/2/2
25	GOL	o	302	-	-	2/4/4/4	-
23	CLA	B	603	-	1/1/15/20	2/39/115/115	-
32	LHG	d	411[A]	-	-	15/53/53/53	-
24	BCR	k	101	-	-	0/29/63/63	0/2/2/2
34	HTG	b	623	-	-	3/10/30/30	0/1/1/1
28	PL9	a	414[A]	-	-	14/53/73/73	0/1/1/1
24	BCR	b	619	-	-	4/29/63/63	0/2/2/2
23	CLA	b	611	-	1/1/15/20	2/39/115/115	-
25	GOL	B	627	-	-	4/4/4/4	-
35	DGD	H	102	-	-	10/51/91/95	0/2/2/2
23	CLA	C	509	41	1/1/15/20	11/39/115/115	-
23	CLA	b	614	-	1/1/15/20	10/39/115/115	-
33	LMG	m	101	-	-	14/46/66/70	0/1/1/1
32	LHG	L	101[A]	-	-	20/53/53/53	-
24	BCR	t	103	-	-	1/29/63/63	0/2/2/2
23	CLA	b	613	-	1/1/15/20	3/39/115/115	-
26	SQD	f	102	-	-	15/38/58/69	0/1/1/1
23	CLA	a	407[A]	41	-	6/39/115/115	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
23	CLA	C	503	-	1/1/15/20	4/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
23	CLA	A	405[A]	41	1/1/15/20	1/39/115/115	-
37	PHO	a	408[B]	-	-	4/37/103/103	0/5/6/6
32	LHG	A	416[B]	-	-	11/53/53/53	-
25	GOL	a	419	-	-	0/4/4/4	-
32	LHG	a	420[B]	-	-	15/46/46/53	-
32	LHG	l	802[B]	-	-	15/53/53/53	-
38	HEM	f	101	5,6	-	8/14/54/54	-
33	LMG	C	526	-	-	10/31/51/70	0/1/1/1
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	b	610	41	1/1/15/20	6/39/115/115	-
23	CLA	A	406[B]	41	-	4/39/115/115	-
25	GOL	V	204[A]	-	-	2/4/4/4	-
33	LMG	C	502	-	-	16/46/66/70	0/1/1/1
23	CLA	d	402	-	1/1/15/20	8/39/115/115	-
37	PHO	D	401[A]	-	-	0/37/103/103	0/5/6/6
23	CLA	b	609	-	1/1/15/20	1/39/115/115	-
23	CLA	c	504	-	1/1/15/20	3/39/115/115	-
23	CLA	a	405[A]	-	1/1/15/20	4/39/115/115	-
26	SQD	B	620	-	-	16/49/69/69	0/1/1/1
34	HTG	C	523	-	-	0/10/30/30	0/1/1/1
23	CLA	b	602	-	1/1/15/20	5/39/115/115	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1
35	DGD	C	519[A]	-	-	12/51/91/95	0/2/2/2
25	GOL	l	801[B]	-	-	0/4/4/4	-
32	LHG	d	406[B]	-	-	13/53/53/53	-
23	CLA	B	611	-	1/1/15/20	3/39/115/115	-
23	CLA	C	514	-	1/1/15/20	8/39/115/115	-
24	BCR	y	101	-	-	5/29/63/63	0/2/2/2
32	LHG	D	408[A]	-	-	17/53/53/53	-
34	HTG	D	412	-	-	3/7/27/30	0/1/1/1
35	DGD	c	518[B]	-	-	14/51/91/95	0/2/2/2
25	GOL	v	202[A]	-	-	2/4/4/4	-
26	SQD	A	410	-	-	14/49/69/69	0/1/1/1
26	SQD	C	501[B]	-	-	9/49/69/69	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	A	415	-	-	8/21/61/61	0/2/2/2
32	LHG	d	405[B]	-	-	13/53/53/53	-
25	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	512	-	1/1/15/20	13/39/115/115	-
25	GOL	D	414	-	-	4/4/4/4	-
25	GOL	c	526[A]	-	-	0/4/4/4	-
28	PL9	A	412[B]	-	-	14/53/73/73	0/1/1/1
35	DGD	c	519	-	-	10/51/91/95	0/2/2/2
23	CLA	B	604	-	1/1/15/20	4/39/115/115	-
24	BCR	D	406	-	-	4/29/63/63	0/2/2/2
35	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
33	LMG	z	101	-	-	10/34/54/70	0/1/1/1
40	HEC	v	201	16	-	6/14/54/54	-
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
31	LMT	b	621	-	-	9/17/37/61	0/1/1/2
23	CLA	d	401[B]	-	1/1/15/20	4/39/115/115	-
25	GOL	c	528	-	-	2/4/4/4	-
24	BCR	H	101	-	-	2/29/63/63	0/2/2/2
28	PL9	D	407[A]	-	-	6/53/73/73	0/1/1/1
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
25	GOL	C	524[B]	-	-	0/4/4/4	-
24	BCR	c	516	-	-	2/29/63/63	0/2/2/2
31	LMT	c	501	-	-	10/21/61/61	0/2/2/2
24	BCR	B	619	-	-	0/29/63/63	0/2/2/2
24	BCR	C	516	-	-	1/29/63/63	0/2/2/2
23	CLA	B	615	-	1/1/15/20	6/39/115/115	-
31	LMT	M	101	-	-	5/21/61/61	0/2/2/2
34	HTG	b	625	-	-	4/10/30/30	0/1/1/1
23	CLA	c	513	-	1/1/15/20	13/39/115/115	-
23	CLA	a	406[B]	41	-	4/39/115/115	-
32	LHG	D	409[A]	-	-	13/53/53/53	-
24	BCR	C	517	-	-	0/29/63/63	0/2/2/2
23	CLA	C	513	3	1/1/15/20	4/39/115/115	-
23	CLA	C	507	-	1/1/15/20	4/39/115/115	-
37	PHO	D	402[B]	-	-	1/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	617	-	-	2/29/63/63	0/2/2/2
23	CLA	c	509	-	1/1/15/20	3/39/115/115	-
35	DGD	c	517[B]	-	-	18/51/91/95	0/2/2/2
35	DGD	h	102	-	-	13/51/91/95	0/2/2/2
23	CLA	C	510	-	1/1/15/20	6/39/115/115	-
31	LMT	e	101	-	-	12/21/61/61	0/2/2/2
23	CLA	C	504	-	1/1/15/20	9/39/115/115	-
23	CLA	A	406[A]	41	-	5/39/115/115	-
23	CLA	b	603	-	1/1/15/20	6/39/115/115	-
24	BCR	h	101	-	-	2/29/63/63	0/2/2/2
28	PL9	a	414[B]	-	-	17/53/73/73	0/1/1/1
23	CLA	b	606	-	1/1/15/20	12/39/115/115	-
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
33	LMG	B	621	-	-	21/46/66/70	0/1/1/1
23	CLA	c	511	-	1/1/15/20	11/39/115/115	-
23	CLA	b	601	41	1/1/15/20	18/39/115/115	-
23	CLA	B	605	-	1/1/15/20	5/39/115/115	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
24	BCR	K	102	-	-	2/29/63/63	0/2/2/2
28	PL9	d	404[A]	-	-	6/53/73/73	0/1/1/1
32	LHG	L	101[B]	-	-	18/53/53/53	-
33	LMG	D	413	39	-	10/46/66/70	0/1/1/1
24	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
23	CLA	c	507	-	1/1/15/20	7/39/115/115	-
23	CLA	c	505	41	1/1/15/20	11/39/115/115	-
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-
24	BCR	b	617	-	-	2/29/63/63	0/2/2/2
32	LHG	d	406[A]	-	-	12/53/53/53	-
23	CLA	c	503	-	1/1/15/20	2/39/115/115	-
24	BCR	a	410	-	-	3/29/63/63	0/2/2/2
23	CLA	A	405[B]	41	1/1/15/20	4/39/115/115	-
23	CLA	c	506	-	1/1/15/20	6/39/115/115	-
34	HTG	c	522	-	-	1/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	601	41	1/1/15/20	12/39/115/115	-
23	CLA	A	404[A]	-	1/1/15/20	3/39/115/115	-
33	LMG	a	417	-	-	14/46/66/70	0/1/1/1
23	CLA	B	607	41	1/1/15/20	3/39/115/115	-
25	GOL	d	410	-	-	1/4/4/4	-
37	PHO	a	416[B]	-	-	2/37/103/103	0/5/6/6
34	HTG	B	623	-	-	3/10/30/30	0/1/1/1
23	CLA	B	610	41	1/1/15/20	9/39/115/115	-
23	CLA	D	404[B]	-	1/1/15/20	3/39/115/115	-
23	CLA	d	401[A]	-	1/1/15/20	4/39/115/115	-
34	HTG	d	408	-	-	1/7/27/30	0/1/1/1
25	GOL	a	418	-	-	2/4/4/4	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
25	GOL	C	524[A]	-	-	0/4/4/4	-
23	CLA	B	616	-	1/1/15/20	8/39/115/115	-
26	SQD	a	411[B]	-	-	9/49/69/69	0/1/1/1
35	DGD	C	519[B]	-	-	10/51/91/95	0/2/2/2
23	CLA	B	614	-	1/1/15/20	12/39/115/115	-
32	LHG	E	101[B]	-	-	20/46/46/53	-
32	LHG	D	408[B]	-	-	19/53/53/53	-
33	LMG	C	522	-	-	14/46/66/70	0/1/1/1
25	GOL	v	202[B]	-	-	2/4/4/4	-
26	SQD	a	412	-	-	14/49/69/69	0/1/1/1
25	GOL	A	409	-	-	2/4/4/4	-
37	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
33	LMG	c	521	-	-	9/46/66/70	0/1/1/1
32	LHG	A	416[A]	-	-	14/53/53/53	-
23	CLA	c	514	-	1/1/15/20	11/39/115/115	-
31	LMT	A	417	-	-	16/21/61/61	0/2/2/2
32	LHG	a	420[A]	-	-	16/46/46/53	-
32	LHG	l	802[A]	-	-	15/53/53/53	-
34	HTG	B	625	-	-	3/10/30/30	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	a	409	-	-	9/39/115/115	-
37	PHO	D	402[A]	-	-	1/37/103/103	0/5/6/6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	515	-	1/1/15/20	6/39/115/115	-
31	LMT	m	103	-	-	6/21/61/61	0/2/2/2
32	LHG	d	411[B]	-	-	14/53/53/53	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
25	GOL	b	624	-	-	2/4/4/4	-
33	LMG	d	409	39	-	8/46/66/70	0/1/1/1
24	BCR	B	618	-	-	0/29/63/63	0/2/2/2
24	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	D	405	-	1/1/15/20	13/39/115/115	-

All (1859) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	408[A]	PHO	C1B-C2B	9.37	1.49	1.39
37	a	416[B]	PHO	C1B-C2B	9.27	1.49	1.39
37	D	401[B]	PHO	C1D-C2D	9.25	1.49	1.39
37	D	402[B]	PHO	C1B-C2B	9.11	1.49	1.39
37	D	401[A]	PHO	C1D-C2D	9.05	1.49	1.39
37	a	408[B]	PHO	C1D-C2D	9.00	1.49	1.39
37	D	401[B]	PHO	C1B-C2B	8.92	1.49	1.39
37	a	408[B]	PHO	C1B-C2B	8.90	1.49	1.39
37	a	416[A]	PHO	C1B-C2B	8.84	1.49	1.39
37	a	416[B]	PHO	C1D-C2D	8.83	1.49	1.39
37	D	402[A]	PHO	C1B-C2B	8.80	1.49	1.39
37	a	416[A]	PHO	C1D-C2D	8.76	1.49	1.39
37	D	402[B]	PHO	C3B-C4B	8.75	1.50	1.41
37	D	402[A]	PHO	C1D-C2D	8.67	1.49	1.39
37	D	401[A]	PHO	C1B-C2B	8.59	1.48	1.39
37	a	408[A]	PHO	C1D-C2D	8.55	1.48	1.39
37	D	402[B]	PHO	C1D-C2D	8.36	1.48	1.39
37	a	416[A]	PHO	C3B-C4B	8.28	1.49	1.41
37	D	402[A]	PHO	C3B-C4B	8.05	1.49	1.41
37	a	408[A]	PHO	C3B-C4B	7.53	1.49	1.41
37	a	408[B]	PHO	C3B-C4B	7.50	1.49	1.41
37	a	416[B]	PHO	C3B-C4B	7.43	1.49	1.41
37	D	401[B]	PHO	C3B-C4B	7.16	1.48	1.41
40	V	202	HEC	CAC-C3C	7.04	1.57	1.35
37	a	408[A]	PHO	C4D-CHA	7.01	1.50	1.39
23	B	611	CLA	CMB-C2B	6.98	1.65	1.50
37	D	401[A]	PHO	C3B-C4B	6.95	1.48	1.41
37	D	402[B]	PHO	C4D-CHA	6.88	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	416[B]	PHO	C4D-CHA	6.86	1.49	1.39
23	B	611	CLA	C1B-C2B	6.79	1.59	1.43
40	v	201	HEC	CAC-C3C	6.76	1.57	1.35
37	D	402[A]	PHO	C4D-CHA	6.72	1.49	1.39
37	D	401[B]	PHO	C4D-CHA	6.69	1.49	1.39
37	a	408[B]	PHO	C4D-CHA	6.66	1.49	1.39
40	v	201	HEC	CAB-C3B	6.62	1.56	1.35
37	D	401[A]	PHO	C4D-CHA	6.57	1.49	1.39
37	a	408[A]	PHO	C3B-C2B	6.55	1.49	1.40
37	a	416[A]	PHO	C4D-CHA	6.48	1.49	1.39
37	D	402[B]	PHO	C3B-C2B	6.39	1.49	1.40
37	a	416[B]	PHO	C3B-C2B	6.32	1.48	1.40
37	D	401[A]	PHO	C3B-C2B	6.28	1.48	1.40
37	a	408[B]	PHO	C3B-C2B	6.23	1.48	1.40
37	D	401[B]	PHO	C3B-C2B	6.11	1.48	1.40
37	D	402[A]	PHO	C3B-C2B	6.09	1.48	1.40
40	V	202	HEC	CAB-C3B	6.07	1.54	1.35
23	B	611	CLA	C1D-ND	6.02	1.45	1.37
37	a	416[A]	PHO	C3B-C2B	6.02	1.48	1.40
37	a	416[B]	PHO	C3D-C2D	5.99	1.49	1.39
37	D	402[B]	PHO	C3D-C2D	5.75	1.49	1.39
23	B	611	CLA	C3C-C2C	5.71	1.49	1.36
23	B	605	CLA	C3C-C2C	5.70	1.49	1.36
37	a	416[A]	PHO	OBD-CAD	5.65	1.29	1.22
40	v	201	HEC	C3D-C2D	5.64	1.53	1.38
37	D	402[A]	PHO	OBD-CAD	5.63	1.29	1.22
37	a	416[A]	PHO	C3D-C2D	5.62	1.49	1.39
37	a	408[A]	PHO	C3D-C2D	5.61	1.49	1.39
23	b	605	CLA	C3C-C2C	5.57	1.48	1.36
23	c	513	CLA	C3C-C2C	5.55	1.48	1.36
23	c	509	CLA	O2D-CGD	5.54	1.46	1.33
23	C	514	CLA	C3C-C2C	5.50	1.48	1.36
23	B	610	CLA	C3C-C2C	5.50	1.48	1.36
23	a	406[A]	CLA	C3C-C2C	5.48	1.48	1.36
37	D	402[A]	PHO	C3D-C2D	5.48	1.49	1.39
23	b	601	CLA	C3C-C2C	5.47	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.47	1.48	1.36
23	B	604	CLA	C3C-C2C	5.45	1.48	1.36
23	c	509	CLA	C3C-C2C	5.45	1.48	1.36
37	a	408[B]	PHO	C3D-C2D	5.42	1.48	1.39
23	C	510	CLA	C3C-C2C	5.40	1.48	1.36
23	d	402	CLA	C3C-C2C	5.40	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C3C-C2C	5.40	1.48	1.36
23	a	407[B]	CLA	C3C-C2C	5.39	1.48	1.36
23	c	504	CLA	C3C-C2C	5.39	1.48	1.36
23	d	401[B]	CLA	C3C-C2C	5.38	1.48	1.36
23	C	511	CLA	C3C-C2C	5.37	1.48	1.36
23	a	405[B]	CLA	C3C-C2C	5.37	1.48	1.36
23	D	404[B]	CLA	C3C-C2C	5.37	1.48	1.36
23	b	614	CLA	C3C-C2C	5.36	1.48	1.36
23	B	609	CLA	CHC-C1C	5.35	1.49	1.38
23	D	405	CLA	C3C-C2C	5.34	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.33	1.48	1.36
23	C	509	CLA	CHC-C1C	5.33	1.49	1.38
23	c	511	CLA	O2D-CGD	5.33	1.46	1.33
23	b	607	CLA	C3C-C2C	5.32	1.48	1.36
23	b	615	CLA	C3C-C2C	5.31	1.48	1.36
23	b	609	CLA	O2D-CGD	5.30	1.46	1.33
37	D	402[B]	PHO	OBD-CAD	5.30	1.29	1.22
23	A	406[B]	CLA	C3C-C2C	5.29	1.48	1.36
23	b	612	CLA	C3C-C2C	5.28	1.48	1.36
23	C	505	CLA	C3C-C2C	5.27	1.48	1.36
23	B	602	CLA	C3C-C2C	5.27	1.48	1.36
23	B	601	CLA	C3C-C2C	5.26	1.48	1.36
23	B	614	CLA	C3C-C2C	5.24	1.48	1.36
23	B	605	CLA	O2D-CGD	5.24	1.46	1.33
37	a	416[B]	PHO	OBD-CAD	5.23	1.29	1.22
23	a	409	CLA	CHC-C1C	5.23	1.49	1.38
23	a	409	CLA	C3C-C2C	5.22	1.48	1.36
23	c	514	CLA	C3C-C2C	5.22	1.48	1.36
23	A	404[B]	CLA	C1D-ND	5.22	1.44	1.37
23	a	407[A]	CLA	C3C-C2C	5.21	1.48	1.36
23	b	610	CLA	CHC-C1C	5.21	1.48	1.38
23	b	602	CLA	CHC-C1C	5.21	1.48	1.38
23	D	404[A]	CLA	C3C-C2C	5.21	1.48	1.36
37	a	408[A]	PHO	O2D-CGD	5.19	1.46	1.33
23	B	610	CLA	C1D-ND	5.18	1.44	1.37
23	C	512	CLA	C1D-ND	5.16	1.44	1.37
23	b	603	CLA	C3C-C2C	5.16	1.47	1.36
23	b	606	CLA	C3C-C2C	5.15	1.47	1.36
23	B	606	CLA	CHC-C1C	5.14	1.48	1.38
23	A	404[B]	CLA	C3C-C2C	5.12	1.47	1.36
23	B	611	CLA	CHC-C1C	5.12	1.48	1.38
23	C	504	CLA	C1D-ND	5.12	1.44	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	O2D-CGD	5.11	1.45	1.33
23	B	616	CLA	C3C-C2C	5.11	1.47	1.36
23	b	602	CLA	C3C-C2C	5.10	1.47	1.36
23	b	610	CLA	C3C-C2C	5.10	1.47	1.36
23	B	601	CLA	O2A-CGA	5.10	1.48	1.33
23	A	404[B]	CLA	CHC-C1C	5.09	1.48	1.38
23	c	510	CLA	C3C-C2C	5.09	1.47	1.36
23	A	405[A]	CLA	O2D-CGD	5.09	1.45	1.33
23	b	603	CLA	O2D-CGD	5.08	1.45	1.33
23	d	402	CLA	C1D-ND	5.07	1.44	1.37
38	f	101	HEM	FE-NB	5.07	2.10	1.94
23	c	506	CLA	CHC-C1C	5.07	1.48	1.38
24	C	516	BCR	C23-C22	-5.07	1.35	1.46
23	B	603	CLA	C3C-C2C	5.07	1.47	1.36
23	A	405[B]	CLA	C3C-C2C	5.07	1.47	1.36
23	c	512	CLA	C3C-C2C	5.06	1.47	1.36
23	C	514	CLA	CHC-C1C	5.06	1.48	1.38
23	b	601	CLA	C1D-ND	5.06	1.44	1.37
23	b	609	CLA	CHC-C1C	5.04	1.48	1.38
23	a	407[B]	CLA	CHC-C1C	5.04	1.48	1.38
23	A	406[A]	CLA	C3C-C2C	5.04	1.47	1.36
23	D	404[B]	CLA	O2D-CGD	5.04	1.45	1.33
23	A	406[A]	CLA	CHC-C1C	5.03	1.48	1.38
23	c	511	CLA	C3C-C2C	5.03	1.47	1.36
23	c	510	CLA	O2D-CGD	5.03	1.45	1.33
23	C	515	CLA	C3C-C2C	5.03	1.47	1.36
23	B	613	CLA	O2D-CGD	5.03	1.45	1.33
38	F	102	HEM	FE-NB	5.02	2.10	1.94
23	c	513	CLA	CHC-C1C	5.02	1.48	1.38
23	b	609	CLA	C3C-C2C	5.02	1.47	1.36
23	c	514	CLA	O2D-CGD	5.02	1.45	1.33
37	D	401[B]	PHO	OBD-CAD	5.02	1.28	1.22
23	a	406[A]	CLA	C1D-ND	5.01	1.44	1.37
23	B	606	CLA	C3C-C2C	5.01	1.47	1.36
23	a	406[B]	CLA	C1D-ND	5.01	1.44	1.37
23	D	405	CLA	CHC-C1C	5.00	1.48	1.38
23	C	512	CLA	C3C-C2C	5.00	1.47	1.36
23	d	401[A]	CLA	C3C-C2C	5.00	1.47	1.36
23	a	405[B]	CLA	CHC-C1C	4.99	1.48	1.38
23	c	505	CLA	C1D-ND	4.98	1.44	1.37
23	C	508	CLA	O2D-CGD	4.98	1.45	1.33
23	C	510	CLA	O2D-CGD	4.98	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C3C-C2C	4.97	1.47	1.36
23	C	504	CLA	O2D-CGD	4.97	1.45	1.33
23	A	406[B]	CLA	O2D-CGD	4.97	1.45	1.33
23	c	514	CLA	C1D-ND	4.97	1.44	1.37
23	b	605	CLA	O2D-CGD	4.97	1.45	1.33
23	A	406[B]	CLA	CHC-C1C	4.96	1.48	1.38
23	c	512	CLA	C1D-ND	4.96	1.44	1.37
23	C	508	CLA	C3C-C2C	4.96	1.47	1.36
37	D	402[B]	PHO	O2D-CGD	4.96	1.45	1.33
23	b	616	CLA	C3C-C2C	4.96	1.47	1.36
23	c	503	CLA	C3C-C2C	4.95	1.47	1.36
23	B	601	CLA	O2D-CGD	4.95	1.45	1.33
23	C	513	CLA	O2D-CGD	4.95	1.45	1.33
23	D	405	CLA	C1D-ND	4.95	1.44	1.37
24	y	101	BCR	C23-C22	-4.95	1.35	1.46
23	B	613	CLA	CHC-C1C	4.94	1.48	1.38
24	k	101	BCR	C23-C22	-4.94	1.35	1.46
23	b	616	CLA	C1D-ND	4.94	1.44	1.37
24	d	403	BCR	C23-C22	-4.94	1.35	1.46
23	C	503	CLA	CHC-C1C	4.94	1.48	1.38
23	A	407	CLA	C3C-C2C	4.94	1.47	1.36
23	c	509	CLA	CHC-C1C	4.94	1.48	1.38
23	b	613	CLA	C3C-C2C	4.93	1.47	1.36
23	a	405[A]	CLA	C3C-C2C	4.93	1.47	1.36
24	c	516	BCR	C23-C22	-4.93	1.35	1.46
23	c	504	CLA	CHC-C1C	4.93	1.48	1.38
23	C	507	CLA	CHC-C1C	4.92	1.48	1.38
23	C	507	CLA	C3C-C2C	4.91	1.47	1.36
37	a	408[B]	PHO	O2D-CGD	4.91	1.45	1.33
37	D	401[A]	PHO	C3D-C2D	4.91	1.48	1.39
23	D	405	CLA	CHD-C1D	4.91	1.48	1.38
37	D	401[B]	PHO	C3D-C2D	4.91	1.48	1.39
23	a	406[A]	CLA	O2D-CGD	4.90	1.45	1.33
37	D	402[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	C	509	CLA	C3C-C2C	4.90	1.47	1.36
23	C	503	CLA	C3C-C2C	4.90	1.47	1.36
40	V	202	HEC	C3D-C2D	4.90	1.51	1.38
23	B	609	CLA	C3C-C2C	4.89	1.47	1.36
23	c	512	CLA	O2D-CGD	4.89	1.45	1.33
37	a	416[B]	PHO	O2D-CGD	4.88	1.45	1.33
23	b	602	CLA	O2D-CGD	4.88	1.45	1.33
23	B	610	CLA	CHC-C1C	4.88	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C1D-ND	4.88	1.44	1.37
23	b	613	CLA	CHC-C1C	4.87	1.48	1.38
23	b	601	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	4.86	1.48	1.38
37	a	408[B]	PHO	OBD-CAD	4.86	1.28	1.22
23	a	405[B]	CLA	C1D-ND	4.86	1.44	1.37
23	c	502	CLA	C3C-C2C	4.86	1.47	1.36
23	C	511	CLA	O2D-CGD	4.86	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	4.86	1.45	1.33
37	D	401[A]	PHO	O2D-CGD	4.86	1.45	1.33
24	A	408	BCR	C23-C22	-4.86	1.35	1.46
23	B	601	CLA	CHC-C1C	4.85	1.48	1.38
23	b	604	CLA	C3C-C2C	4.85	1.47	1.36
23	a	406[B]	CLA	O2D-CGD	4.85	1.45	1.33
24	K	102	BCR	C23-C22	-4.84	1.35	1.46
23	c	513	CLA	C1D-ND	4.84	1.44	1.37
24	C	517	BCR	C23-C22	-4.84	1.35	1.46
23	B	615	CLA	CHC-C1C	4.84	1.48	1.38
23	b	615	CLA	CHC-C1C	4.84	1.48	1.38
23	B	602	CLA	CHC-C1C	4.83	1.48	1.38
23	B	612	CLA	CHC-C1C	4.83	1.48	1.38
23	D	404[A]	CLA	O2D-CGD	4.83	1.45	1.33
23	B	612	CLA	C3C-C2C	4.83	1.47	1.36
23	B	615	CLA	C3C-C2C	4.83	1.47	1.36
23	c	507	CLA	O2D-CGD	4.82	1.45	1.33
23	D	405	CLA	O2D-CGD	4.82	1.45	1.33
23	C	512	CLA	CHC-C1C	4.82	1.48	1.38
23	A	406[B]	CLA	C1D-ND	4.82	1.44	1.37
23	B	606	CLA	C1D-ND	4.81	1.44	1.37
23	c	508	CLA	CHC-C1C	4.81	1.48	1.38
23	c	505	CLA	O2D-CGD	4.80	1.45	1.33
33	c	521	LMG	O7-C10	4.80	1.47	1.34
23	c	504	CLA	CHD-C1D	4.80	1.47	1.38
23	b	615	CLA	O2D-CGD	4.80	1.45	1.33
37	a	416[A]	PHO	O2D-CGD	4.79	1.45	1.33
26	F	103	SQD	O47-C7	4.79	1.47	1.34
23	A	405[B]	CLA	C1D-ND	4.79	1.44	1.37
23	b	601	CLA	O2A-CGA	4.79	1.47	1.33
23	a	407[B]	CLA	O2D-CGD	4.78	1.45	1.33
23	C	515	CLA	C1D-ND	4.78	1.44	1.37
23	c	505	CLA	C3C-C2C	4.78	1.47	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	CHC-C1C	4.77	1.48	1.38
24	c	515	BCR	C23-C22	-4.77	1.35	1.46
23	b	614	CLA	CHC-C1C	4.75	1.48	1.38
23	C	504	CLA	C3C-C2C	4.75	1.47	1.36
23	b	611	CLA	CHC-C1C	4.75	1.48	1.38
24	B	619	BCR	C23-C22	-4.74	1.35	1.46
23	a	405[A]	CLA	C1D-ND	4.74	1.44	1.37
23	b	616	CLA	O2D-CGD	4.74	1.44	1.33
23	A	404[A]	CLA	C1D-ND	4.74	1.44	1.37
23	a	405[B]	CLA	O2D-CGD	4.74	1.44	1.33
23	C	515	CLA	O2D-CGD	4.74	1.44	1.33
23	A	407	CLA	O2D-CGD	4.73	1.44	1.33
23	a	405[A]	CLA	CHC-C1C	4.72	1.47	1.38
23	A	404[A]	CLA	O2D-CGD	4.72	1.44	1.33
23	c	511	CLA	C1D-ND	4.72	1.44	1.37
23	B	611	CLA	C4B-NB	-4.72	1.31	1.37
23	c	514	CLA	CHC-C1C	4.72	1.47	1.38
23	b	608	CLA	O2D-CGD	4.72	1.44	1.33
37	D	401[B]	PHO	O2D-CGD	4.71	1.44	1.33
23	d	402	CLA	CHC-C1C	4.71	1.47	1.38
23	b	610	CLA	O2D-CGD	4.71	1.44	1.33
23	B	610	CLA	O2D-CGD	4.71	1.44	1.33
23	c	508	CLA	C3C-C2C	4.70	1.46	1.36
23	B	613	CLA	C3C-C2C	4.70	1.46	1.36
23	A	405[A]	CLA	CHC-C1C	4.69	1.47	1.38
23	C	505	CLA	CHC-C1C	4.69	1.47	1.38
23	a	407[A]	CLA	CHC-C1C	4.69	1.47	1.38
23	b	612	CLA	CHC-C1C	4.68	1.47	1.38
23	b	606	CLA	C1D-ND	4.68	1.44	1.37
23	b	611	CLA	C3C-C2C	4.68	1.46	1.36
23	B	605	CLA	CHC-C1C	4.68	1.47	1.38
23	A	406[A]	CLA	O2D-CGD	4.68	1.44	1.33
24	T	102	BCR	C23-C22	-4.67	1.36	1.46
23	c	507	CLA	C3C-C2C	4.67	1.46	1.36
26	a	412	SQD	O48-C23	4.66	1.46	1.33
23	b	601	CLA	CHC-C1C	4.66	1.47	1.38
23	d	401[B]	CLA	O2D-CGD	4.65	1.44	1.33
33	C	522	LMG	O7-C10	4.65	1.47	1.34
23	C	512	CLA	O2D-CGD	4.65	1.44	1.33
24	b	619	BCR	C23-C22	-4.65	1.36	1.46
23	B	609	CLA	O2D-CGD	4.65	1.44	1.33
23	c	508	CLA	O2D-CGD	4.64	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	O2D-CGD	4.64	1.44	1.33
23	b	613	CLA	C1D-ND	4.64	1.44	1.37
23	b	602	CLA	CHD-C1D	4.63	1.47	1.38
23	c	503	CLA	C1D-ND	4.63	1.43	1.37
23	C	510	CLA	C1D-ND	4.62	1.43	1.37
23	D	404[A]	CLA	CHC-C1C	4.62	1.47	1.38
23	C	513	CLA	CHC-C1C	4.62	1.47	1.38
23	a	407[A]	CLA	O2D-CGD	4.60	1.44	1.33
23	c	507	CLA	C1D-ND	4.60	1.43	1.37
23	B	616	CLA	CHC-C1C	4.60	1.47	1.38
24	t	103	BCR	C23-C22	-4.60	1.36	1.46
23	C	504	CLA	CHC-C1C	4.59	1.47	1.38
23	b	606	CLA	O2D-CGD	4.59	1.44	1.33
23	B	602	CLA	C1D-ND	4.59	1.43	1.37
23	A	405[B]	CLA	O2D-CGD	4.59	1.44	1.33
23	c	503	CLA	O2D-CGD	4.58	1.44	1.33
32	E	101[A]	LHG	O8-C23	4.58	1.46	1.33
23	B	604	CLA	O2D-CGD	4.58	1.44	1.33
33	z	101	LMG	O8-C28	4.58	1.46	1.33
23	c	502	CLA	CHC-C1C	4.58	1.47	1.38
23	b	608	CLA	C3C-C2C	4.57	1.46	1.36
23	b	614	CLA	CHD-C1D	4.57	1.47	1.38
23	C	506	CLA	C3C-C2C	4.57	1.46	1.36
23	b	607	CLA	CHC-C1C	4.57	1.47	1.38
23	c	502	CLA	C1D-ND	4.56	1.43	1.37
23	b	606	CLA	CHC-C1C	4.56	1.47	1.38
23	b	605	CLA	CHC-C1C	4.56	1.47	1.38
23	A	404[A]	CLA	CHC-C1C	4.56	1.47	1.38
24	h	101	BCR	C23-C22	-4.55	1.36	1.46
23	b	614	CLA	C1D-ND	4.55	1.43	1.37
23	B	602	CLA	O2D-CGD	4.54	1.44	1.33
23	B	602	CLA	CHD-C1D	4.54	1.47	1.38
23	C	514	CLA	O2D-CGD	4.54	1.44	1.33
23	d	401[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	B	604	CLA	CHC-C1C	4.54	1.47	1.38
23	B	601	CLA	C1D-ND	4.54	1.43	1.37
23	C	510	CLA	CHC-C1C	4.53	1.47	1.38
23	B	603	CLA	O2D-CGD	4.53	1.44	1.33
23	d	401[B]	CLA	CHC-C1C	4.53	1.47	1.38
23	c	514	CLA	CHD-C1D	4.52	1.47	1.38
23	a	406[A]	CLA	CHC-C1C	4.52	1.47	1.38
26	A	410	SQD	O48-C23	4.52	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	CHC-C1C	4.52	1.47	1.38
23	B	613	CLA	C1D-ND	4.52	1.43	1.37
32	a	420[A]	LHG	O8-C23	4.51	1.46	1.33
23	B	607	CLA	C3C-C2C	4.51	1.46	1.36
24	B	617	BCR	C23-C22	-4.51	1.36	1.46
33	C	522	LMG	O8-C28	4.50	1.46	1.33
23	D	404[B]	CLA	CHC-C1C	4.50	1.47	1.38
23	c	512	CLA	CHD-C1D	4.50	1.47	1.38
23	b	615	CLA	C1D-ND	4.50	1.43	1.37
24	b	618	BCR	C23-C22	-4.50	1.36	1.46
23	C	513	CLA	C3C-C2C	4.50	1.46	1.36
23	C	514	CLA	C1D-ND	4.50	1.43	1.37
23	C	507	CLA	O2D-CGD	4.49	1.44	1.33
26	f	102	SQD	O47-C7	4.49	1.47	1.34
23	c	507	CLA	CHD-C1D	4.49	1.47	1.38
23	a	406[B]	CLA	C3D-C2D	4.48	1.51	1.39
23	B	603	CLA	C1D-ND	4.48	1.43	1.37
23	B	612	CLA	C1B-NB	-4.48	1.32	1.37
23	c	512	CLA	CHC-C1C	4.47	1.47	1.38
23	b	612	CLA	C1D-ND	4.47	1.43	1.37
23	B	604	CLA	CHD-C1D	4.47	1.47	1.38
23	B	615	CLA	CHD-C1D	4.47	1.47	1.38
23	b	608	CLA	CHD-C1D	4.46	1.47	1.38
26	B	620	SQD	O47-C7	4.46	1.46	1.34
23	C	508	CLA	CHD-C1D	4.46	1.47	1.38
23	b	614	CLA	O2D-CGD	4.45	1.44	1.33
23	B	609	CLA	CHD-C1D	4.45	1.47	1.38
23	C	515	CLA	CHC-C1C	4.45	1.47	1.38
23	B	606	CLA	O2D-CGD	4.45	1.44	1.33
26	b	620	SQD	O48-C23	4.44	1.46	1.33
23	c	506	CLA	O2D-CGD	4.44	1.44	1.33
24	D	406	BCR	C23-C22	-4.44	1.36	1.46
23	B	615	CLA	C1D-ND	4.44	1.43	1.37
23	c	514	CLA	O2A-CGA	4.44	1.46	1.33
23	c	513	CLA	O2D-CGD	4.44	1.44	1.33
23	C	509	CLA	O2D-CGD	4.43	1.44	1.33
23	c	510	CLA	C1D-ND	4.43	1.43	1.37
32	E	101[B]	LHG	O8-C23	4.43	1.46	1.33
23	B	607	CLA	CHC-C1C	4.43	1.47	1.38
23	A	407	CLA	CHD-C1D	4.43	1.47	1.38
24	b	617	BCR	C23-C22	-4.43	1.36	1.46
23	a	406[B]	CLA	CHC-C1C	4.42	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	CHC-C1C	4.42	1.47	1.38
23	B	605	CLA	C1D-ND	4.42	1.43	1.37
23	c	512	CLA	CHB-C1B	4.42	1.49	1.39
23	b	603	CLA	CHC-C1C	4.42	1.47	1.38
26	b	620	SQD	O47-C7	4.41	1.46	1.34
23	c	509	CLA	C1D-ND	4.41	1.43	1.37
37	D	401[A]	PHO	OBD-CAD	4.41	1.28	1.22
23	C	506	CLA	O2D-CGD	4.40	1.44	1.33
23	b	612	CLA	O2D-CGD	4.40	1.44	1.33
23	B	604	CLA	CHB-C1B	4.40	1.49	1.39
23	B	611	CLA	OBD-CAD	4.40	1.30	1.22
23	b	607	CLA	O2D-CGD	4.40	1.44	1.33
23	c	502	CLA	CHD-C1D	4.40	1.47	1.38
23	d	402	CLA	O2A-CGA	4.40	1.46	1.33
23	b	604	CLA	CHC-C1C	4.40	1.47	1.38
26	f	102	SQD	O48-C23	4.40	1.46	1.33
23	B	614	CLA	CHC-C1C	4.39	1.47	1.38
23	b	612	CLA	CHB-C1B	4.39	1.49	1.39
26	A	410	SQD	O47-C7	4.38	1.46	1.34
23	c	505	CLA	CHC-C1C	4.38	1.47	1.38
23	C	508	CLA	CHC-C1C	4.38	1.47	1.38
23	A	407	CLA	O2A-CGA	4.38	1.46	1.33
23	b	602	CLA	CHC-C4B	4.37	1.49	1.39
32	a	420[B]	LHG	O8-C23	4.37	1.46	1.33
23	C	511	CLA	CHD-C1D	4.37	1.46	1.38
24	a	410	BCR	C23-C22	-4.36	1.36	1.46
23	a	406[A]	CLA	C3D-C2D	4.36	1.50	1.39
23	c	507	CLA	CHC-C1C	4.35	1.47	1.38
23	B	607	CLA	O2D-CGD	4.34	1.43	1.33
23	A	407	CLA	CHC-C1C	4.34	1.47	1.38
23	c	513	CLA	O2A-CGA	4.34	1.46	1.33
24	H	101	BCR	C23-C22	-4.34	1.36	1.46
33	C	521	LMG	O8-C28	4.34	1.46	1.33
23	a	405[A]	CLA	O2D-CGD	4.34	1.43	1.33
23	a	409	CLA	O2A-CGA	4.33	1.46	1.33
23	B	616	CLA	O2D-CGD	4.33	1.43	1.33
23	C	503	CLA	CHD-C1D	4.33	1.46	1.38
23	C	505	CLA	O2D-CGD	4.32	1.43	1.33
23	b	609	CLA	OBD-CAD	4.32	1.29	1.22
23	C	507	CLA	C1D-ND	4.31	1.43	1.37
23	C	504	CLA	C3D-C2D	4.31	1.50	1.39
23	C	510	CLA	C3D-C2D	4.30	1.50	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	CHC-C4B	4.30	1.49	1.39
23	d	402	CLA	CHD-C1D	4.29	1.46	1.38
23	c	510	CLA	CHD-C1D	4.29	1.46	1.38
23	b	613	CLA	O2D-CGD	4.29	1.43	1.33
23	c	508	CLA	C1D-ND	4.29	1.43	1.37
23	b	612	CLA	CHD-C1D	4.29	1.46	1.38
23	A	405[B]	CLA	O2A-CGA	4.29	1.45	1.33
32	a	420[A]	LHG	O7-C7	4.28	1.46	1.34
23	d	401[A]	CLA	CHC-C1C	4.28	1.47	1.38
23	D	404[B]	CLA	O2A-CGA	4.28	1.45	1.33
33	c	521	LMG	O8-C28	4.28	1.45	1.33
23	a	407[B]	CLA	C1D-ND	4.27	1.43	1.37
23	C	514	CLA	CHD-C1D	4.27	1.46	1.38
23	C	513	CLA	O2A-CGA	4.26	1.45	1.33
23	b	607	CLA	C1B-NB	-4.25	1.32	1.37
23	b	611	CLA	O2A-CGA	4.25	1.45	1.33
23	B	611	CLA	CHD-C1D	4.25	1.46	1.38
23	A	406[B]	CLA	CHD-C1D	4.25	1.46	1.38
23	d	401[B]	CLA	O2A-CGA	4.25	1.45	1.33
23	c	505	CLA	C3D-C2D	4.24	1.50	1.39
23	c	511	CLA	CHC-C1C	4.24	1.47	1.38
23	B	615	CLA	O2A-CGA	4.24	1.45	1.33
23	B	611	CLA	O2D-CGD	4.24	1.43	1.33
23	C	511	CLA	C1D-ND	4.24	1.43	1.37
33	c	520	LMG	O7-C10	4.23	1.46	1.34
23	B	608	CLA	C1D-ND	4.23	1.43	1.37
23	b	607	CLA	CHD-C1D	4.23	1.46	1.38
23	c	513	CLA	CHD-C1D	4.23	1.46	1.38
23	c	509	CLA	C3D-C2D	4.22	1.50	1.39
23	c	508	CLA	CHD-C1D	4.22	1.46	1.38
23	C	512	CLA	CHD-C4C	4.22	1.48	1.39
23	c	506	CLA	CHD-C4C	4.22	1.48	1.39
26	a	412	SQD	O47-C7	4.22	1.46	1.34
32	E	101[A]	LHG	O7-C7	4.22	1.46	1.34
23	b	611	CLA	O2D-CGD	4.22	1.43	1.33
23	b	605	CLA	C1D-ND	4.21	1.43	1.37
38	F	102	HEM	FE-NC	4.21	2.09	1.95
23	c	514	CLA	CHD-C4C	4.21	1.48	1.39
38	f	101	HEM	FE-NC	4.21	2.09	1.95
32	d	406[A]	LHG	O8-C23	4.20	1.45	1.33
23	c	503	CLA	O2A-CGA	4.20	1.45	1.33
23	a	406[B]	CLA	O2A-CGA	4.20	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[A]	CLA	C1D-ND	4.20	1.43	1.37
23	B	606	CLA	CHB-C1B	4.20	1.48	1.39
23	b	611	CLA	C1D-ND	4.19	1.43	1.37
33	m	101	LMG	O8-C28	4.19	1.45	1.33
24	Y	101	BCR	C23-C22	-4.19	1.37	1.46
23	B	608	CLA	CHC-C1C	4.19	1.46	1.38
23	c	502	CLA	O2D-CGD	4.19	1.43	1.33
26	B	620	SQD	O48-C23	4.19	1.45	1.33
23	D	404[A]	CLA	O2A-CGA	4.19	1.45	1.33
23	b	602	CLA	CHD-C4C	4.19	1.48	1.39
23	b	604	CLA	O2D-CGD	4.19	1.43	1.33
35	C	520	DGD	O1G-C1A	4.18	1.45	1.33
32	d	406[B]	LHG	O8-C23	4.18	1.45	1.33
23	B	614	CLA	C1D-ND	4.18	1.43	1.37
35	c	518[B]	DGD	O1G-C1A	4.17	1.45	1.33
23	C	515	CLA	O2A-CGA	4.17	1.45	1.33
33	C	521	LMG	O7-C10	4.17	1.46	1.34
23	b	610	CLA	CHC-C4B	4.17	1.48	1.39
23	b	602	CLA	C1D-ND	4.17	1.43	1.37
23	C	504	CLA	CHD-C1D	4.17	1.46	1.38
23	C	508	CLA	C1D-ND	4.16	1.43	1.37
23	B	601	CLA	CHC-C4B	4.16	1.48	1.39
26	a	411[B]	SQD	O47-C7	4.16	1.46	1.34
23	C	507	CLA	CHD-C1D	4.16	1.46	1.38
23	D	404[A]	CLA	CHD-C1D	4.16	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.15	1.50	1.39
23	d	401[B]	CLA	CHD-C1D	4.15	1.46	1.38
23	b	611	CLA	CHB-C1B	4.15	1.48	1.39
23	b	609	CLA	CHD-C1D	4.15	1.46	1.38
23	c	510	CLA	O2A-CGA	4.15	1.45	1.33
33	B	621	LMG	O8-C28	4.15	1.45	1.33
35	c	519	DGD	O1G-C1A	4.15	1.45	1.33
23	c	504	CLA	CHD-C4C	4.14	1.48	1.39
23	C	515	CLA	CHD-C1D	4.14	1.46	1.38
23	c	506	CLA	CHD-C1D	4.14	1.46	1.38
32	a	420[B]	LHG	O7-C7	4.14	1.46	1.34
23	A	406[B]	CLA	CHD-C4C	4.14	1.48	1.39
23	A	405[B]	CLA	C3D-C2D	4.14	1.50	1.39
32	L	101[B]	LHG	O8-C23	4.14	1.45	1.33
23	B	612	CLA	CHD-C1D	4.13	1.46	1.38
23	a	407[A]	CLA	C1D-ND	4.13	1.43	1.37
23	b	601	CLA	CHD-C1D	4.13	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	518[A]	DGD	O2G-C1B	4.13	1.46	1.34
37	a	408[A]	PHO	OBD-CAD	4.13	1.27	1.22
23	c	509	CLA	O2A-CGA	4.13	1.45	1.33
23	B	609	CLA	C1D-ND	4.13	1.43	1.37
23	b	614	CLA	C3D-C2D	4.13	1.50	1.39
23	B	614	CLA	O2A-CGA	4.13	1.45	1.33
26	F	103	SQD	O48-C23	4.13	1.45	1.33
23	b	601	CLA	C3D-C2D	4.13	1.50	1.39
26	a	411[B]	SQD	O48-C23	4.13	1.45	1.33
23	B	614	CLA	CHC-C4B	4.13	1.48	1.39
23	a	406[A]	CLA	O2A-CGA	4.13	1.45	1.33
23	A	406[B]	CLA	O2A-CGA	4.13	1.45	1.33
23	a	405[A]	CLA	CHD-C4C	4.12	1.48	1.39
33	C	526	LMG	O7-C10	4.12	1.45	1.34
23	C	513	CLA	CHB-C1B	4.12	1.48	1.39
23	b	603	CLA	OBD-CAD	4.12	1.29	1.22
23	a	407[B]	CLA	O2A-CGA	4.12	1.45	1.33
23	C	513	CLA	C3D-C2D	4.12	1.50	1.39
33	d	409	LMG	O8-C28	4.12	1.45	1.33
23	b	608	CLA	CHB-C1B	4.12	1.48	1.39
23	c	504	CLA	O2A-CGA	4.12	1.45	1.33
23	c	512	CLA	O2A-CGA	4.12	1.45	1.33
23	A	406[A]	CLA	C1B-NB	-4.11	1.32	1.37
23	C	509	CLA	CHD-C1D	4.11	1.46	1.38
23	D	405	CLA	C3D-C2D	4.11	1.50	1.39
23	C	514	CLA	O2A-CGA	4.11	1.45	1.33
23	c	508	CLA	O2A-CGA	4.11	1.45	1.33
23	B	602	CLA	CHB-C1B	4.11	1.48	1.39
35	c	517[B]	DGD	O2G-C1B	4.11	1.45	1.34
32	D	409[B]	LHG	O7-C7	4.10	1.45	1.34
23	C	503	CLA	C1D-ND	4.10	1.43	1.37
33	c	520	LMG	O8-C28	4.10	1.45	1.33
23	a	405[B]	CLA	CHD-C4C	4.10	1.48	1.39
23	b	615	CLA	CHD-C1D	4.10	1.46	1.38
23	a	405[B]	CLA	CHD-C1D	4.10	1.46	1.38
23	a	406[B]	CLA	CHD-C1D	4.09	1.46	1.38
23	b	608	CLA	CHC-C1C	4.09	1.46	1.38
23	D	405	CLA	CHB-C1B	4.09	1.48	1.39
23	B	610	CLA	C3D-C2D	4.09	1.50	1.39
23	B	616	CLA	C3D-C2D	4.09	1.50	1.39
23	B	609	CLA	O2A-CGA	4.09	1.45	1.33
23	C	503	CLA	O2D-CGD	4.09	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	O2D-CGD	4.08	1.43	1.33
23	C	512	CLA	CHB-C1B	4.08	1.48	1.39
23	c	513	CLA	CHB-C1B	4.08	1.48	1.39
23	a	405[A]	CLA	CHD-C1D	4.08	1.46	1.38
23	A	405[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	c	502	CLA	C3D-C2D	4.08	1.50	1.39
23	C	509	CLA	O2A-CGA	4.08	1.45	1.33
35	c	517[B]	DGD	O1G-C1A	4.08	1.45	1.33
33	a	417	LMG	O7-C10	4.08	1.45	1.34
32	d	411[B]	LHG	O8-C23	4.07	1.45	1.33
23	C	515	CLA	C3D-C2D	4.07	1.50	1.39
23	A	406[A]	CLA	CHD-C1D	4.07	1.46	1.38
32	E	101[B]	LHG	O7-C7	4.07	1.45	1.34
23	B	611	CLA	C3B-C2B	4.06	1.54	1.41
23	c	507	CLA	CHD-C4C	4.06	1.48	1.39
23	C	508	CLA	O2A-CGA	4.06	1.45	1.33
23	C	510	CLA	O2A-CGA	4.06	1.45	1.33
23	D	405	CLA	CHC-C4B	4.06	1.48	1.39
23	C	507	CLA	CHB-C1B	4.05	1.48	1.39
23	C	513	CLA	CHD-C1D	4.05	1.46	1.38
23	C	507	CLA	CHC-C4B	4.05	1.48	1.39
23	c	504	CLA	O2D-CGD	4.05	1.43	1.33
23	c	513	CLA	CHC-C4B	4.05	1.48	1.39
26	a	411[A]	SQD	O47-C7	4.05	1.45	1.34
23	B	611	CLA	C1C-C2C	4.05	1.52	1.44
23	b	616	CLA	O2A-CGA	4.05	1.45	1.33
23	c	509	CLA	CHD-C4C	4.05	1.48	1.39
23	c	511	CLA	CHD-C4C	4.04	1.48	1.39
23	c	507	CLA	C3D-C2D	4.04	1.50	1.39
33	a	417	LMG	O8-C28	4.04	1.45	1.33
23	B	609	CLA	C3D-C2D	4.04	1.50	1.39
23	B	610	CLA	OBD-CAD	4.04	1.29	1.22
23	B	604	CLA	C1D-ND	4.04	1.43	1.37
23	c	509	CLA	CHD-C1D	4.04	1.46	1.38
23	B	609	CLA	CHC-C4B	4.04	1.48	1.39
23	B	604	CLA	OBD-CAD	4.03	1.29	1.22
23	a	409	CLA	CHD-C1D	4.03	1.46	1.38
23	b	615	CLA	C3D-C2D	4.03	1.50	1.39
23	A	406[B]	CLA	OBD-CAD	4.03	1.29	1.22
23	b	604	CLA	C1D-ND	4.03	1.43	1.37
23	C	506	CLA	C3D-C2D	4.03	1.50	1.39
23	b	615	CLA	O2A-CGA	4.03	1.45	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	402[A]	PHO	O2A-CGA	4.03	1.45	1.33
23	B	611	CLA	O2A-CGA	4.02	1.45	1.33
23	C	505	CLA	CHD-C4C	4.02	1.48	1.39
32	d	405[B]	LHG	O7-C7	4.02	1.45	1.34
23	b	601	CLA	CHD-C4C	4.02	1.48	1.39
23	c	510	CLA	CHD-C4C	4.02	1.48	1.39
23	b	608	CLA	C3D-C2D	4.02	1.50	1.39
23	C	513	CLA	CHD-C4C	4.02	1.48	1.39
35	h	102	DGD	O2G-C1B	4.02	1.45	1.34
23	D	404[A]	CLA	CHB-C1B	4.02	1.48	1.39
23	C	505	CLA	C1D-ND	4.02	1.43	1.37
23	B	612	CLA	CHB-C1B	4.02	1.48	1.39
23	C	504	CLA	O2A-CGA	4.02	1.45	1.33
23	a	407[B]	CLA	CHD-C1D	4.01	1.46	1.38
23	a	407[A]	CLA	C3D-C2D	4.01	1.49	1.39
35	C	518[B]	DGD	O2G-C1B	4.01	1.45	1.34
23	a	405[A]	CLA	CHB-C1B	4.01	1.48	1.39
35	c	518[A]	DGD	O1G-C1A	4.01	1.45	1.33
23	b	614	CLA	CHC-C4B	4.01	1.48	1.39
32	D	409[B]	LHG	O8-C23	4.00	1.45	1.33
23	b	606	CLA	CHD-C1D	4.00	1.46	1.38
23	b	609	CLA	O2A-CGA	4.00	1.45	1.33
23	B	603	CLA	CHC-C1C	4.00	1.46	1.38
23	A	406[A]	CLA	C3D-C2D	4.00	1.49	1.39
23	B	603	CLA	C3D-C2D	4.00	1.49	1.39
23	b	604	CLA	CHD-C1D	4.00	1.46	1.38
23	C	513	CLA	C1D-ND	4.00	1.43	1.37
23	c	502	CLA	CHD-C4C	3.99	1.48	1.39
23	c	511	CLA	CHB-C1B	3.99	1.48	1.39
23	c	503	CLA	C3D-C2D	3.99	1.49	1.39
23	b	608	CLA	O2A-CGA	3.99	1.45	1.33
23	b	610	CLA	CHB-C1B	3.99	1.48	1.39
23	d	401[A]	CLA	CHB-C1B	3.99	1.48	1.39
23	B	615	CLA	CHB-C1B	3.99	1.48	1.39
23	b	612	CLA	CHC-C4B	3.99	1.48	1.39
23	c	513	CLA	C3D-C2D	3.99	1.49	1.39
23	C	503	CLA	CHD-C4C	3.99	1.48	1.39
23	B	611	CLA	CHB-C1B	3.99	1.48	1.39
23	B	605	CLA	CHC-C4B	3.98	1.48	1.39
23	b	609	CLA	C1D-ND	3.98	1.43	1.37
23	A	404[B]	CLA	CHD-C4C	3.98	1.48	1.39
23	b	612	CLA	C3D-C2D	3.98	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402	CLA	C3D-C2D	3.98	1.49	1.39
26	a	411[A]	SQD	O48-C23	3.98	1.44	1.33
23	B	613	CLA	CHB-C1B	3.98	1.48	1.39
23	C	503	CLA	O2A-CGA	3.97	1.44	1.33
23	B	603	CLA	C1B-NB	-3.97	1.32	1.37
23	A	404[B]	CLA	CHD-C1D	3.97	1.46	1.38
23	a	407[A]	CLA	O2A-CGA	3.97	1.44	1.33
26	C	501[B]	SQD	O48-C23	3.97	1.44	1.33
37	D	401[B]	PHO	O2A-CGA	3.96	1.44	1.33
23	d	401[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	b	605	CLA	C1B-NB	-3.96	1.32	1.37
23	b	616	CLA	C3D-C2D	3.96	1.49	1.39
23	A	406[B]	CLA	C3D-C2D	3.96	1.49	1.39
23	b	604	CLA	CHC-C4B	3.96	1.48	1.39
23	c	506	CLA	C1D-ND	3.96	1.43	1.37
23	c	507	CLA	CHB-C1B	3.95	1.48	1.39
35	c	518[B]	DGD	O2G-C1B	3.95	1.45	1.34
23	A	405[B]	CLA	CHD-C1D	3.95	1.46	1.38
23	C	514	CLA	CHC-C4B	3.95	1.48	1.39
23	B	616	CLA	C1D-ND	3.95	1.43	1.37
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	B	601	CLA	CHD-C1D	3.95	1.46	1.38
23	c	506	CLA	CHB-C1B	3.95	1.48	1.39
23	C	509	CLA	C1D-ND	3.95	1.43	1.37
23	B	602	CLA	CHD-C4C	3.95	1.48	1.39
23	B	602	CLA	CHC-C4B	3.94	1.48	1.39
23	b	613	CLA	C3D-C2D	3.94	1.49	1.39
23	c	513	CLA	CHD-C4C	3.94	1.48	1.39
23	A	405[A]	CLA	CHD-C1D	3.94	1.46	1.38
23	c	504	CLA	CHB-C1B	3.94	1.48	1.39
37	D	402[B]	PHO	O2A-CGA	3.94	1.44	1.33
23	c	504	CLA	CHC-C4B	3.94	1.48	1.39
23	b	608	CLA	OBD-CAD	3.94	1.29	1.22
23	B	605	CLA	C3D-C2D	3.93	1.49	1.39
23	c	503	CLA	CHC-C1C	3.93	1.46	1.38
23	B	607	CLA	OBD-CAD	3.93	1.29	1.22
23	d	402	CLA	O2D-CGD	3.93	1.42	1.33
23	C	503	CLA	CHC-C4B	3.93	1.48	1.39
23	C	511	CLA	C4B-NB	-3.92	1.32	1.37
32	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
33	C	502	LMG	O7-C10	3.92	1.45	1.34
35	C	519[B]	DGD	O1G-C1A	3.92	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404[A]	CLA	C1D-ND	3.92	1.43	1.37
23	d	401[B]	CLA	C1D-ND	3.92	1.43	1.37
24	B	618	BCR	C23-C22	-3.92	1.37	1.46
23	b	614	CLA	CHD-C4C	3.91	1.48	1.39
23	a	407[B]	CLA	OBD-CAD	3.91	1.29	1.22
32	D	409[A]	LHG	O8-C23	3.91	1.44	1.33
23	d	401[B]	CLA	CHD-C4C	3.91	1.48	1.39
23	c	507	CLA	O2A-CGA	3.91	1.44	1.33
23	c	509	CLA	CHB-C1B	3.91	1.48	1.39
23	B	608	CLA	C3D-C2D	3.91	1.49	1.39
33	z	101	LMG	O7-C10	3.91	1.45	1.34
23	A	406[B]	CLA	CHC-C4B	3.91	1.48	1.39
23	c	506	CLA	CHC-C4B	3.91	1.48	1.39
23	a	406[A]	CLA	C1B-NB	-3.90	1.32	1.37
23	D	404[B]	CLA	C1D-ND	3.90	1.43	1.37
32	d	405[A]	LHG	O7-C7	3.90	1.45	1.34
23	c	502	CLA	O2A-CGA	3.90	1.44	1.33
23	A	404[B]	CLA	CHC-C4B	3.90	1.48	1.39
23	C	514	CLA	C3D-C2D	3.90	1.49	1.39
23	d	401[A]	CLA	CHD-C1D	3.89	1.46	1.38
23	B	609	CLA	CHD-C4C	3.89	1.48	1.39
32	D	409[A]	LHG	O7-C7	3.89	1.45	1.34
23	B	606	CLA	CHD-C1D	3.89	1.46	1.38
23	b	608	CLA	CHD-C4C	3.89	1.48	1.39
23	b	606	CLA	O2A-CGA	3.89	1.44	1.33
23	B	603	CLA	CHB-C1B	3.89	1.48	1.39
23	b	609	CLA	CHC-C4B	3.88	1.48	1.39
23	B	608	CLA	O2D-CGD	3.88	1.42	1.33
23	B	605	CLA	O2A-CGA	3.88	1.44	1.33
23	c	505	CLA	CHB-C1B	3.88	1.48	1.39
33	C	502	LMG	O8-C28	3.88	1.44	1.33
32	l	802[B]	LHG	O7-C7	3.88	1.45	1.34
23	b	609	CLA	CHB-C1B	3.87	1.48	1.39
23	D	404[B]	CLA	CHD-C4C	3.87	1.48	1.39
32	d	411[B]	LHG	O7-C7	3.87	1.45	1.34
23	B	614	CLA	C4B-NB	-3.87	1.32	1.37
23	a	405[B]	CLA	C3D-C2D	3.87	1.49	1.39
23	b	608	CLA	C1D-ND	3.87	1.42	1.37
32	D	408[B]	LHG	O7-C7	3.87	1.45	1.34
23	D	405	CLA	OBD-CAD	3.87	1.29	1.22
23	C	511	CLA	C3D-C2D	3.87	1.49	1.39
23	c	508	CLA	C3D-C2D	3.86	1.49	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C3D-C2D	3.86	1.49	1.39
23	B	614	CLA	CHB-C1B	3.86	1.48	1.39
23	B	607	CLA	O2A-CGA	3.86	1.44	1.33
23	A	404[A]	CLA	C3D-C2D	3.86	1.49	1.39
23	C	510	CLA	CHD-C1D	3.86	1.45	1.38
23	B	615	CLA	C3D-C2D	3.86	1.49	1.39
23	b	610	CLA	C1D-ND	3.86	1.42	1.37
23	D	404[B]	CLA	CHD-C1D	3.85	1.45	1.38
23	B	603	CLA	CHC-C4B	3.85	1.48	1.39
32	A	416[B]	LHG	O8-C23	3.85	1.44	1.33
37	a	416[A]	PHO	O2A-CGA	3.85	1.44	1.33
23	c	514	CLA	CHB-C1B	3.85	1.48	1.39
23	b	610	CLA	C3D-C2D	3.85	1.49	1.39
23	a	407[B]	CLA	CHC-C4B	3.85	1.48	1.39
23	C	512	CLA	O2A-CGA	3.85	1.44	1.33
35	C	519[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	b	610	CLA	CHD-C4C	3.85	1.48	1.39
23	C	510	CLA	OBD-CAD	3.85	1.29	1.22
23	c	503	CLA	CHD-C1D	3.84	1.45	1.38
23	a	406[A]	CLA	OBD-CAD	3.84	1.29	1.22
23	B	606	CLA	O2A-CGA	3.84	1.44	1.33
33	d	409	LMG	O7-C10	3.84	1.45	1.34
23	B	606	CLA	CHC-C4B	3.84	1.48	1.39
23	C	507	CLA	O2A-CGA	3.84	1.44	1.33
23	c	503	CLA	CHD-C4C	3.84	1.47	1.39
35	C	519[B]	DGD	O2G-C1B	3.84	1.45	1.34
23	b	604	CLA	C3D-C2D	3.84	1.49	1.39
23	C	505	CLA	CHD-C1D	3.84	1.45	1.38
23	B	613	CLA	C1B-NB	-3.84	1.32	1.37
32	D	408[B]	LHG	O8-C23	3.83	1.44	1.33
23	C	509	CLA	CHC-C4B	3.83	1.48	1.39
32	d	406[B]	LHG	O7-C7	3.83	1.45	1.34
23	a	407[B]	CLA	CHD-C4C	3.83	1.47	1.39
23	C	504	CLA	CHB-C1B	3.83	1.48	1.39
23	b	603	CLA	CHD-C1D	3.82	1.45	1.38
37	a	416[B]	PHO	O2A-CGA	3.82	1.44	1.33
23	a	407[B]	CLA	C3D-C2D	3.82	1.49	1.39
37	a	408[B]	PHO	O2A-CGA	3.81	1.44	1.33
23	A	405[A]	CLA	CHD-C4C	3.81	1.47	1.39
23	b	605	CLA	CHD-C4C	3.81	1.47	1.39
23	B	609	CLA	CHB-C1B	3.81	1.48	1.39
35	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407[A]	CLA	CHD-C4C	3.81	1.47	1.39
23	B	613	CLA	OBD-CAD	3.81	1.29	1.22
23	B	615	CLA	OBD-CAD	3.81	1.29	1.22
23	C	503	CLA	C1B-NB	-3.81	1.32	1.37
35	h	102	DGD	O1G-C1A	3.80	1.44	1.33
23	C	508	CLA	CHD-C4C	3.80	1.47	1.39
23	c	506	CLA	O2A-CGA	3.80	1.44	1.33
23	c	512	CLA	C3D-C2D	3.80	1.49	1.39
23	b	610	CLA	CHD-C1D	3.80	1.45	1.38
23	B	613	CLA	C3D-C2D	3.80	1.49	1.39
23	C	504	CLA	CHC-C4B	3.80	1.47	1.39
23	c	505	CLA	O2A-CGA	3.80	1.44	1.33
35	C	519[A]	DGD	O1G-C1A	3.80	1.44	1.33
23	B	614	CLA	CHD-C4C	3.79	1.47	1.39
23	A	404[A]	CLA	CHB-C1B	3.79	1.47	1.39
23	D	404[B]	CLA	OBD-CAD	3.79	1.29	1.22
32	l	802[B]	LHG	O8-C23	3.79	1.44	1.33
23	b	615	CLA	CHD-C4C	3.79	1.47	1.39
23	c	514	CLA	C3D-C2D	3.79	1.49	1.39
23	c	511	CLA	C3D-C2D	3.79	1.49	1.39
23	b	615	CLA	CHB-C1B	3.79	1.47	1.39
35	c	517[A]	DGD	O1G-C1A	3.79	1.44	1.33
23	b	606	CLA	C3D-C2D	3.78	1.49	1.39
23	B	610	CLA	CHD-C4C	3.78	1.47	1.39
23	C	506	CLA	CHB-C1B	3.78	1.47	1.39
23	A	407	CLA	C1D-ND	3.78	1.42	1.37
23	B	612	CLA	O2A-CGA	3.78	1.44	1.33
23	C	507	CLA	CHD-C4C	3.78	1.47	1.39
23	B	601	CLA	C3D-C2D	3.78	1.49	1.39
23	B	610	CLA	CHB-C1B	3.78	1.47	1.39
23	a	409	CLA	OBD-CAD	3.78	1.29	1.22
37	D	401[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	C	510	CLA	CHB-C1B	3.77	1.47	1.39
23	c	502	CLA	CHC-C4B	3.77	1.47	1.39
23	a	406[B]	CLA	CHD-C4C	3.77	1.47	1.39
23	B	613	CLA	CHD-C1D	3.77	1.45	1.38
23	a	405[B]	CLA	OBD-CAD	3.77	1.29	1.22
23	A	406[A]	CLA	C1D-ND	3.77	1.42	1.37
23	B	614	CLA	CHD-C1D	3.77	1.45	1.38
23	C	515	CLA	CHD-C4C	3.77	1.47	1.39
23	b	602	CLA	OBD-CAD	3.77	1.29	1.22
32	L	101[B]	LHG	O7-C7	3.77	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	501[A]	SQD	O48-C23	3.76	1.44	1.33
23	B	616	CLA	CHC-C4B	3.76	1.47	1.39
23	c	511	CLA	CHD-C1D	3.76	1.45	1.38
23	A	405[A]	CLA	CHC-C4B	3.76	1.47	1.39
37	D	402[A]	PHO	CHA-CBD	-3.76	1.47	1.51
23	b	616	CLA	CHC-C4B	3.76	1.47	1.39
23	C	503	CLA	C3D-C2D	3.76	1.49	1.39
23	b	609	CLA	C3D-C2D	3.76	1.49	1.39
23	b	613	CLA	CHB-C1B	3.76	1.47	1.39
23	d	401[B]	CLA	CHB-C1B	3.75	1.47	1.39
23	a	409	CLA	CHC-C4B	3.75	1.47	1.39
23	b	615	CLA	CHC-C4B	3.75	1.47	1.39
23	c	505	CLA	CHD-C1D	3.75	1.45	1.38
23	B	604	CLA	CHD-C4C	3.75	1.47	1.39
23	C	506	CLA	CHD-C4C	3.75	1.47	1.39
35	C	518[B]	DGD	O1G-C1A	3.75	1.44	1.33
26	C	501[B]	SQD	O47-C7	3.75	1.44	1.34
23	c	508	CLA	CHD-C4C	3.74	1.47	1.39
23	B	615	CLA	CHD-C4C	3.74	1.47	1.39
23	C	514	CLA	CHD-C4C	3.74	1.47	1.39
23	B	616	CLA	O2A-CGA	3.74	1.44	1.33
23	c	510	CLA	CHC-C1C	3.74	1.46	1.38
23	b	612	CLA	O2A-CGA	3.74	1.44	1.33
23	c	508	CLA	CHC-C4B	3.74	1.47	1.39
23	c	512	CLA	CHD-C4C	3.74	1.47	1.39
33	B	621	LMG	O7-C10	3.74	1.44	1.34
23	c	502	CLA	CHB-C1B	3.74	1.47	1.39
23	a	405[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	c	503	CLA	OBD-CAD	3.74	1.28	1.22
23	C	511	CLA	CHD-C4C	3.74	1.47	1.39
23	A	406[A]	CLA	O2A-CGA	3.74	1.44	1.33
23	C	508	CLA	C3D-C2D	3.74	1.49	1.39
23	C	503	CLA	CHB-C1B	3.73	1.47	1.39
23	d	402	CLA	CHD-C4C	3.73	1.47	1.39
23	c	505	CLA	CHD-C4C	3.73	1.47	1.39
23	b	613	CLA	CHC-C4B	3.73	1.47	1.39
23	A	406[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	C	513	CLA	C4B-NB	-3.73	1.33	1.37
23	B	602	CLA	O2A-CGA	3.73	1.44	1.33
23	b	612	CLA	CHD-C4C	3.72	1.47	1.39
23	a	405[A]	CLA	C3D-C2D	3.72	1.49	1.39
23	C	505	CLA	CHB-C1B	3.72	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	OBD-CAD	3.72	1.28	1.22
23	C	511	CLA	O2A-CGA	3.72	1.44	1.33
23	B	603	CLA	O2A-CGA	3.72	1.44	1.33
23	B	607	CLA	C3D-C2D	3.72	1.49	1.39
23	B	603	CLA	CHD-C1D	3.71	1.45	1.38
23	b	603	CLA	O2A-CGA	3.71	1.44	1.33
23	b	613	CLA	CHD-C1D	3.71	1.45	1.38
23	c	508	CLA	OBD-CAD	3.71	1.28	1.22
23	c	509	CLA	CHC-C4B	3.71	1.47	1.39
23	d	402	CLA	CHB-C1B	3.70	1.47	1.39
23	C	515	CLA	OBD-CAD	3.70	1.28	1.22
23	A	404[A]	CLA	CHD-C4C	3.69	1.47	1.39
23	d	402	CLA	CHC-C4B	3.69	1.47	1.39
23	a	409	CLA	C1D-ND	3.69	1.42	1.37
32	L	101[A]	LHG	O7-C7	3.69	1.44	1.34
26	C	501[A]	SQD	O47-C7	3.68	1.44	1.34
23	b	607	CLA	C3D-C2D	3.68	1.49	1.39
23	C	509	CLA	CHD-C4C	3.68	1.47	1.39
23	D	404[B]	CLA	CHB-C1B	3.68	1.47	1.39
23	c	513	CLA	OBD-CAD	3.68	1.28	1.22
23	C	504	CLA	OBD-CAD	3.68	1.28	1.22
23	b	609	CLA	CHD-C4C	3.68	1.47	1.39
32	d	406[A]	LHG	O7-C7	3.68	1.44	1.34
23	d	401[B]	CLA	CHC-C4B	3.68	1.47	1.39
23	b	607	CLA	CHB-C1B	3.68	1.47	1.39
23	c	510	CLA	C1B-NB	-3.68	1.33	1.37
23	b	614	CLA	O2A-CGA	3.68	1.44	1.33
23	B	616	CLA	CHD-C1D	3.67	1.45	1.38
23	B	605	CLA	CHD-C1D	3.67	1.45	1.38
23	b	614	CLA	CHB-C1B	3.67	1.47	1.39
23	C	512	CLA	CHD-C1D	3.67	1.45	1.38
23	D	404[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	A	404[A]	CLA	CHD-C1D	3.67	1.45	1.38
32	D	408[A]	LHG	O7-C7	3.67	1.44	1.34
23	B	610	CLA	CHC-C4B	3.66	1.47	1.39
23	B	606	CLA	CHD-C4C	3.66	1.47	1.39
23	B	607	CLA	CHD-C4C	3.66	1.47	1.39
23	A	407	CLA	C3D-C2D	3.66	1.49	1.39
35	C	518[A]	DGD	O1G-C1A	3.66	1.44	1.33
23	b	602	CLA	C3D-C2D	3.65	1.49	1.39
23	b	616	CLA	CHD-C1D	3.65	1.45	1.38
32	d	411[A]	LHG	O8-C23	3.65	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	CHD-C4C	3.65	1.47	1.39
23	b	606	CLA	CHB-C1B	3.65	1.47	1.39
23	b	601	CLA	CHB-C1B	3.65	1.47	1.39
33	m	101	LMG	O7-C10	3.65	1.44	1.34
23	A	405[A]	CLA	CHB-C1B	3.65	1.47	1.39
23	D	405	CLA	O2A-CGA	3.64	1.44	1.33
23	b	603	CLA	C3D-C2D	3.64	1.48	1.39
23	B	616	CLA	CHB-C1B	3.64	1.47	1.39
23	C	515	CLA	CHB-C1B	3.64	1.47	1.39
23	B	608	CLA	CHB-C1B	3.64	1.47	1.39
23	c	510	CLA	CHB-C1B	3.64	1.47	1.39
23	b	608	CLA	C1B-NB	-3.64	1.33	1.37
23	A	406[A]	CLA	CHC-C4B	3.64	1.47	1.39
23	B	612	CLA	CHD-C4C	3.64	1.47	1.39
23	B	612	CLA	C1D-ND	3.63	1.42	1.37
23	B	602	CLA	C3D-C2D	3.63	1.48	1.39
23	c	512	CLA	OBD-CAD	3.63	1.28	1.22
23	a	406[B]	CLA	CHC-C4B	3.63	1.47	1.39
23	b	616	CLA	CHD-C4C	3.63	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.63	1.48	1.39
23	c	511	CLA	CHC-C4B	3.63	1.47	1.39
23	d	401[A]	CLA	CHD-C4C	3.62	1.47	1.39
23	C	508	CLA	C1B-NB	-3.62	1.33	1.37
23	b	602	CLA	O2A-CGA	3.62	1.43	1.33
32	d	405[B]	LHG	O8-C23	3.62	1.43	1.33
23	a	406[A]	CLA	CHD-C1D	3.62	1.45	1.38
23	D	405	CLA	CHD-C4C	3.62	1.47	1.39
23	C	505	CLA	CHC-C4B	3.62	1.47	1.39
23	B	612	CLA	C4B-NB	-3.61	1.33	1.37
23	A	405[B]	CLA	CHD-C4C	3.61	1.47	1.39
23	A	406[B]	CLA	C1B-NB	-3.61	1.33	1.37
23	d	401[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	D	404[B]	CLA	C3D-C2D	3.61	1.48	1.39
32	l	802[A]	LHG	O7-C7	3.61	1.44	1.34
32	D	408[A]	LHG	O8-C23	3.61	1.43	1.33
23	B	601	CLA	CHD-C4C	3.61	1.47	1.39
23	B	605	CLA	CHB-C1B	3.61	1.47	1.39
35	H	102	DGD	O1G-C1A	3.60	1.43	1.33
23	A	406[A]	CLA	CHB-C1B	3.60	1.47	1.39
23	D	404[B]	CLA	CHC-C4B	3.60	1.47	1.39
32	A	416[A]	LHG	O7-C7	3.60	1.44	1.34
23	b	606	CLA	CHD-C4C	3.60	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404[A]	CLA	C3D-C2D	3.60	1.48	1.39
23	b	604	CLA	CHD-C4C	3.59	1.47	1.39
23	a	407[B]	CLA	CHB-C1B	3.59	1.47	1.39
23	b	603	CLA	C1D-ND	3.59	1.42	1.37
23	B	608	CLA	O2A-CGA	3.59	1.43	1.33
23	c	509	CLA	OBD-CAD	3.59	1.28	1.22
23	C	506	CLA	CHD-C1D	3.59	1.45	1.38
23	a	409	CLA	CHD-C4C	3.59	1.47	1.39
23	a	405[B]	CLA	O2A-CGA	3.59	1.43	1.33
32	d	405[A]	LHG	O8-C23	3.58	1.43	1.33
23	a	407[A]	CLA	CHD-C1D	3.58	1.45	1.38
23	d	401[A]	CLA	C3D-C2D	3.58	1.48	1.39
34	B	625	HTG	C1'-S1	-3.58	1.76	1.81
23	B	611	CLA	CHD-C4C	3.58	1.47	1.39
23	c	510	CLA	C4B-NB	-3.58	1.33	1.37
23	b	603	CLA	CHD-C4C	3.58	1.47	1.39
23	c	507	CLA	OBD-CAD	3.58	1.28	1.22
23	B	612	CLA	O2D-CGD	3.57	1.42	1.33
23	C	507	CLA	OBD-CAD	3.57	1.28	1.22
23	C	511	CLA	CHB-C1B	3.57	1.47	1.39
23	B	607	CLA	CHB-C1B	3.57	1.47	1.39
23	b	604	CLA	C1B-NB	-3.57	1.33	1.37
23	C	505	CLA	C3D-C2D	3.57	1.48	1.39
23	B	605	CLA	CHD-C4C	3.57	1.47	1.39
23	C	511	CLA	OBD-CAD	3.56	1.28	1.22
23	c	508	CLA	CHB-C1B	3.56	1.47	1.39
23	C	509	CLA	C3D-C2D	3.56	1.48	1.39
23	B	612	CLA	C3D-C2D	3.56	1.48	1.39
23	C	506	CLA	C1D-ND	3.56	1.42	1.37
23	C	508	CLA	OBD-CAD	3.55	1.28	1.22
23	a	405[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	C	511	CLA	CHC-C4B	3.55	1.47	1.39
23	a	407[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	a	406[A]	CLA	CHD-C4C	3.55	1.47	1.39
23	b	611	CLA	CHD-C4C	3.54	1.47	1.39
35	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	c	506	CLA	C3D-C2D	3.54	1.48	1.39
23	B	606	CLA	C3D-C2D	3.54	1.48	1.39
23	B	601	CLA	OBD-CAD	3.54	1.28	1.22
23	b	605	CLA	CHD-C1D	3.53	1.45	1.38
23	A	404[B]	CLA	O2A-CGA	3.53	1.43	1.33
23	A	407	CLA	CHD-C4C	3.53	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	CHB-C1B	3.53	1.47	1.39
23	b	605	CLA	C3D-C2D	3.52	1.48	1.39
23	A	405[B]	CLA	CHC-C4B	3.52	1.47	1.39
23	B	608	CLA	CHD-C1D	3.52	1.45	1.38
23	B	616	CLA	C4B-NB	-3.52	1.33	1.37
23	d	401[B]	CLA	OBD-CAD	3.52	1.28	1.22
23	C	512	CLA	C3D-C2D	3.51	1.48	1.39
32	d	411[A]	LHG	O7-C7	3.51	1.44	1.34
23	b	602	CLA	CHB-C1B	3.51	1.47	1.39
23	b	612	CLA	OBD-CAD	3.50	1.28	1.22
23	a	406[B]	CLA	CHB-C1B	3.50	1.47	1.39
32	A	416[A]	LHG	O8-C23	3.50	1.43	1.33
23	c	505	CLA	OBD-CAD	3.50	1.28	1.22
23	a	407[A]	CLA	OBD-CAD	3.50	1.28	1.22
23	A	404[B]	CLA	CHB-C1B	3.50	1.47	1.39
23	B	613	CLA	CHD-C4C	3.49	1.47	1.39
23	D	404[A]	CLA	CHC-C4B	3.49	1.47	1.39
23	A	404[B]	CLA	C1B-NB	-3.49	1.33	1.37
23	b	613	CLA	O2A-CGA	3.49	1.43	1.33
23	C	515	CLA	CHC-C4B	3.49	1.47	1.39
23	C	506	CLA	O2A-CGA	3.49	1.43	1.33
23	C	507	CLA	C3D-C2D	3.48	1.48	1.39
23	a	409	CLA	CHB-C1B	3.48	1.47	1.39
23	C	512	CLA	OBD-CAD	3.48	1.28	1.22
23	A	404[B]	CLA	OBD-CAD	3.48	1.28	1.22
23	b	608	CLA	C4B-NB	-3.48	1.33	1.37
23	b	606	CLA	CHC-C4B	3.48	1.47	1.39
23	a	406[A]	CLA	CHB-C1B	3.47	1.47	1.39
23	c	505	CLA	C1B-NB	-3.47	1.33	1.37
23	c	511	CLA	O2A-CGA	3.47	1.43	1.33
23	b	604	CLA	OBD-CAD	3.47	1.28	1.22
23	B	616	CLA	C1B-NB	-3.47	1.33	1.37
23	B	615	CLA	CHC-C4B	3.47	1.47	1.39
23	b	605	CLA	CHB-C1B	3.46	1.47	1.39
23	a	406[B]	CLA	OBD-CAD	3.46	1.28	1.22
32	A	416[B]	LHG	O7-C7	3.46	1.44	1.34
23	b	613	CLA	C1B-NB	-3.45	1.33	1.37
23	b	611	CLA	CHD-C1D	3.45	1.45	1.38
23	C	514	CLA	CHB-C1B	3.45	1.47	1.39
38	f	101	HEM	C4D-ND	-3.44	1.34	1.40
23	c	502	CLA	OBD-CAD	3.44	1.28	1.22
23	B	608	CLA	CHD-C4C	3.44	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CHB-C1B	3.44	1.47	1.39
23	b	611	CLA	C3D-C2D	3.44	1.48	1.39
23	c	514	CLA	CHC-C4B	3.44	1.47	1.39
23	c	504	CLA	OBD-CAD	3.44	1.28	1.22
23	C	504	CLA	CHD-C4C	3.44	1.47	1.39
23	b	604	CLA	CHB-C1B	3.43	1.47	1.39
23	C	509	CLA	CHB-C1B	3.42	1.47	1.39
23	a	406[B]	CLA	C1B-NB	-3.42	1.33	1.37
23	B	608	CLA	CHC-C4B	3.42	1.47	1.39
23	c	512	CLA	C1B-C2B	3.41	1.51	1.43
23	a	405[B]	CLA	CHC-C4B	3.41	1.47	1.39
23	c	506	CLA	C1B-NB	-3.41	1.33	1.37
23	c	503	CLA	CHC-C4B	3.41	1.47	1.39
23	B	613	CLA	O2A-CGA	3.40	1.43	1.33
23	c	506	CLA	OBD-CAD	3.40	1.28	1.22
23	c	514	CLA	OBD-CAD	3.40	1.28	1.22
23	B	604	CLA	C3D-C2D	3.40	1.48	1.39
23	B	614	CLA	C3D-C2D	3.40	1.48	1.39
23	C	514	CLA	OBD-CAD	3.40	1.28	1.22
23	b	606	CLA	C1B-NB	-3.40	1.33	1.37
23	b	605	CLA	CHC-C4B	3.40	1.47	1.39
23	b	610	CLA	OBD-CAD	3.40	1.28	1.22
23	B	603	CLA	CHD-C4C	3.40	1.46	1.39
23	A	406[B]	CLA	CHB-C1B	3.40	1.47	1.39
32	l	802[A]	LHG	O8-C23	3.40	1.43	1.33
23	c	505	CLA	C4B-NB	-3.39	1.33	1.37
33	D	413	LMG	O7-C10	3.39	1.43	1.34
23	B	604	CLA	CHC-C4B	3.39	1.47	1.39
23	A	404[A]	CLA	C4B-NB	-3.39	1.33	1.37
23	b	616	CLA	CHB-C1B	3.39	1.47	1.39
23	c	507	CLA	C1B-NB	-3.38	1.33	1.37
23	b	611	CLA	CHC-C4B	3.38	1.47	1.39
23	A	405[B]	CLA	OBD-CAD	3.37	1.28	1.22
23	C	513	CLA	CHC-C4B	3.37	1.47	1.39
23	d	401[A]	CLA	CHC-C4B	3.37	1.47	1.39
34	b	623	HTG	C1'-S1	-3.37	1.76	1.81
23	b	601	CLA	OBD-CAD	3.37	1.28	1.22
23	B	607	CLA	CHC-C4B	3.37	1.47	1.39
23	C	510	CLA	CHC-C4B	3.36	1.47	1.39
23	b	603	CLA	C4B-NB	-3.36	1.33	1.37
23	b	611	CLA	OBD-CAD	3.36	1.28	1.22
34	B	622	HTG	C1'-S1	-3.36	1.76	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22
23	B	604	CLA	O2A-CGA	3.36	1.43	1.33
37	a	408[A]	PHO	O2A-CGA	3.36	1.43	1.33
23	b	607	CLA	O2A-CGA	3.35	1.43	1.33
23	C	508	CLA	CHB-C1B	3.35	1.46	1.39
23	B	609	CLA	C1B-NB	-3.35	1.33	1.37
23	b	603	CLA	CHB-C1B	3.35	1.46	1.39
23	B	607	CLA	C1B-NB	-3.35	1.33	1.37
23	b	606	CLA	OBD-CAD	3.35	1.28	1.22
23	C	506	CLA	CHC-C4B	3.34	1.46	1.39
23	b	603	CLA	CHC-C4B	3.34	1.46	1.39
35	H	102	DGD	O2G-C1B	3.34	1.43	1.34
33	D	413	LMG	O8-C28	3.34	1.43	1.33
23	b	601	CLA	CHC-C4B	3.34	1.46	1.39
23	A	407	CLA	OBD-CAD	3.33	1.28	1.22
35	c	519	DGD	O2G-C1B	3.33	1.43	1.34
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
23	d	401[A]	CLA	C1D-ND	3.32	1.42	1.37
23	A	405[A]	CLA	C1B-NB	-3.32	1.33	1.37
23	b	611	CLA	C1B-NB	-3.31	1.33	1.37
23	B	612	CLA	CHC-C4B	3.31	1.46	1.39
23	b	615	CLA	OBD-CAD	3.30	1.28	1.22
23	c	504	CLA	C3D-C2D	3.30	1.48	1.39
23	A	407	CLA	C4B-NB	-3.30	1.33	1.37
23	b	613	CLA	CHD-C4C	3.30	1.46	1.39
23	D	404[B]	CLA	C4B-NB	-3.29	1.33	1.37
23	a	405[B]	CLA	C1B-NB	-3.29	1.33	1.37
23	b	604	CLA	O2A-CGA	3.29	1.43	1.33
23	B	602	CLA	C1C-C2C	3.29	1.51	1.44
23	A	407	CLA	CHC-C4B	3.29	1.46	1.39
23	C	508	CLA	CHC-C4B	3.29	1.46	1.39
23	c	505	CLA	CHC-C4B	3.29	1.46	1.39
23	B	611	CLA	C3D-C2D	3.29	1.48	1.39
23	A	405[B]	CLA	CHB-C1B	3.29	1.46	1.39
23	B	616	CLA	C1B-C2B	3.28	1.50	1.43
23	d	401[B]	CLA	C3D-C2D	3.28	1.47	1.39
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	C	511	CLA	C1B-NB	-3.28	1.33	1.37
23	C	505	CLA	OBD-CAD	3.27	1.28	1.22
23	b	605	CLA	O2A-CGA	3.27	1.42	1.33
23	b	607	CLA	CHD-C4C	3.27	1.46	1.39
23	a	407[A]	CLA	CHC-C4B	3.26	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405	CLA	C1C-C2C	3.26	1.51	1.44
23	C	507	CLA	C1B-C2B	3.25	1.50	1.43
23	D	405	CLA	C4C-C3C	3.25	1.50	1.45
23	d	401[A]	CLA	C1B-NB	-3.25	1.33	1.37
23	b	607	CLA	CHC-C4B	3.25	1.46	1.39
23	C	505	CLA	O2A-CGA	3.25	1.42	1.33
23	D	405	CLA	C1B-NB	-3.24	1.33	1.37
38	f	101	HEM	C1B-NB	-3.24	1.34	1.40
23	b	616	CLA	OBD-CAD	3.24	1.28	1.22
23	B	609	CLA	OBD-CAD	3.24	1.28	1.22
23	D	404[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	C	503	CLA	C1B-C2B	3.23	1.50	1.43
23	a	406[A]	CLA	CHC-C4B	3.23	1.46	1.39
23	c	510	CLA	C4C-C3C	3.23	1.50	1.45
23	c	507	CLA	CHC-C4B	3.23	1.46	1.39
23	d	401[B]	CLA	C1B-NB	-3.22	1.33	1.37
23	c	512	CLA	CHC-C4B	3.22	1.46	1.39
23	B	607	CLA	CHD-C1D	3.22	1.44	1.38
23	c	507	CLA	C4B-NB	-3.22	1.33	1.37
23	B	604	CLA	C1B-C2B	3.22	1.50	1.43
23	c	511	CLA	OBD-CAD	3.21	1.28	1.22
23	a	409	CLA	C3D-C2D	3.21	1.47	1.39
23	B	605	CLA	C1B-C2B	3.21	1.50	1.43
23	B	607	CLA	C1D-ND	3.20	1.42	1.37
23	B	602	CLA	OBD-CAD	3.20	1.28	1.22
23	a	405[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	C	509	CLA	OBD-CAD	3.18	1.28	1.22
38	F	102	HEM	C4D-ND	-3.18	1.34	1.40
23	B	606	CLA	OBD-CAD	3.17	1.27	1.22
23	B	610	CLA	O2A-CGA	3.17	1.42	1.33
23	A	407	CLA	CHB-C1B	3.17	1.46	1.39
23	d	401[B]	CLA	C4B-NB	-3.16	1.33	1.37
23	B	602	CLA	C1B-NB	-3.16	1.33	1.37
23	C	506	CLA	OBD-CAD	3.16	1.27	1.22
23	C	508	CLA	C4B-NB	-3.16	1.33	1.37
23	B	610	CLA	CHD-C1D	3.16	1.44	1.38
38	F	102	HEM	C1B-NB	-3.14	1.34	1.40
23	C	515	CLA	C1B-NB	-3.14	1.33	1.37
23	d	402	CLA	OBD-CAD	3.14	1.27	1.22
23	b	610	CLA	C1B-NB	-3.13	1.33	1.37
23	B	603	CLA	OBD-CAD	3.13	1.27	1.22
23	b	615	CLA	C1B-NB	-3.13	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	520	DGD	O2G-C1B	3.13	1.43	1.34
23	c	511	CLA	C1B-C2B	3.13	1.50	1.43
34	b	622	HTG	C1'-S1	-3.12	1.77	1.81
23	C	509	CLA	C1B-NB	-3.12	1.33	1.37
23	C	509	CLA	C1B-C2B	3.12	1.50	1.43
23	c	503	CLA	C1B-C2B	3.12	1.50	1.43
23	C	513	CLA	C4D-CHA	3.11	1.49	1.38
23	B	607	CLA	C4B-NB	-3.11	1.33	1.37
23	B	612	CLA	C1B-C2B	3.10	1.50	1.43
23	b	614	CLA	C1B-NB	-3.10	1.33	1.37
23	b	612	CLA	C1B-C2B	3.10	1.50	1.43
23	a	405[B]	CLA	CHB-C1B	3.10	1.46	1.39
23	b	603	CLA	C1B-NB	-3.09	1.33	1.37
23	b	614	CLA	C1B-C2B	3.09	1.50	1.43
23	B	613	CLA	CHC-C4B	3.09	1.46	1.39
23	C	512	CLA	CHC-C4B	3.08	1.46	1.39
23	c	514	CLA	C4B-NB	-3.08	1.33	1.37
23	B	612	CLA	OBD-CAD	3.08	1.27	1.22
23	C	515	CLA	C1B-C2B	3.07	1.50	1.43
23	c	510	CLA	OBD-CAD	3.07	1.27	1.22
23	b	610	CLA	O2A-CGA	3.07	1.42	1.33
23	c	504	CLA	C4B-NB	-3.06	1.33	1.37
23	b	602	CLA	C1C-C2C	3.06	1.50	1.44
23	b	608	CLA	CHC-C4B	3.06	1.46	1.39
23	b	604	CLA	C4D-CHA	3.05	1.48	1.38
23	D	404[A]	CLA	C1B-NB	-3.05	1.33	1.37
23	c	503	CLA	C4B-NB	-3.05	1.33	1.37
23	c	510	CLA	C4D-CHA	3.05	1.48	1.38
23	B	608	CLA	C1B-C2B	3.05	1.50	1.43
23	b	613	CLA	C4B-NB	-3.03	1.33	1.37
23	b	607	CLA	C1D-ND	3.03	1.41	1.37
23	C	509	CLA	C1C-C2C	3.03	1.50	1.44
23	A	406[A]	CLA	C1B-C2B	3.03	1.50	1.43
23	b	604	CLA	C1B-C2B	3.03	1.50	1.43
23	B	615	CLA	C1B-C2B	3.02	1.50	1.43
23	a	409	CLA	C1B-C2B	3.02	1.50	1.43
23	B	601	CLA	C1C-C2C	3.02	1.50	1.44
23	c	504	CLA	C1B-NB	-3.02	1.33	1.37
23	A	404[A]	CLA	CHC-C4B	3.01	1.46	1.39
23	B	615	CLA	C1B-NB	-2.99	1.33	1.37
23	c	505	CLA	C1B-C2B	2.99	1.50	1.43
28	A	412[A]	PL9	C6-C5	2.99	1.49	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C1B-NB	-2.99	1.33	1.37
37	D	401[A]	PHO	CBD-CGD	-2.99	1.48	1.52
23	B	614	CLA	C4D-CHA	2.99	1.48	1.38
23	b	605	CLA	OBD-CAD	2.98	1.27	1.22
23	C	503	CLA	OBD-CAD	2.98	1.27	1.22
23	b	612	CLA	C4B-NB	-2.98	1.33	1.37
23	C	510	CLA	C4B-NB	-2.98	1.33	1.37
23	B	610	CLA	C1B-NB	-2.98	1.33	1.37
23	C	508	CLA	C4C-C3C	2.98	1.50	1.45
23	B	611	CLA	C3B-C4B	2.98	1.51	1.42
23	B	612	CLA	C1C-C2C	2.98	1.50	1.44
23	B	604	CLA	C4D-CHA	2.98	1.48	1.38
23	C	506	CLA	C1B-NB	-2.97	1.34	1.37
23	B	616	CLA	OBD-CAD	2.97	1.27	1.22
34	D	412	HTG	C1'-S1	-2.97	1.77	1.81
35	C	520	DGD	O2G-C2G	-2.96	1.39	1.46
23	B	604	CLA	C1C-C2C	2.96	1.50	1.44
25	a	419	GOL	C1-C2	2.96	1.63	1.51
23	A	404[A]	CLA	C1B-NB	-2.95	1.34	1.37
23	c	509	CLA	C4D-CHA	2.95	1.48	1.38
23	b	613	CLA	OBD-CAD	2.95	1.27	1.22
23	A	405[B]	CLA	C1B-NB	-2.95	1.34	1.37
23	d	401[A]	CLA	C4B-NB	-2.95	1.34	1.37
23	B	608	CLA	C4B-NB	-2.95	1.34	1.37
23	C	506	CLA	C1B-C2B	2.94	1.50	1.43
23	B	601	CLA	C1B-NB	-2.94	1.34	1.37
23	c	514	CLA	C1B-NB	-2.93	1.34	1.37
23	b	607	CLA	C1B-C2B	2.93	1.50	1.43
23	C	510	CLA	C1B-C2B	2.92	1.50	1.43
28	a	414[A]	PL9	C6-C5	2.92	1.49	1.35
23	a	405[A]	CLA	C1B-NB	-2.92	1.34	1.37
23	a	405[A]	CLA	C4B-NB	-2.91	1.34	1.37
23	B	614	CLA	C1B-C2B	2.91	1.50	1.43
23	a	409	CLA	C1C-C2C	2.91	1.50	1.44
23	C	515	CLA	C4B-NB	-2.91	1.34	1.37
23	a	407[A]	CLA	C1B-NB	-2.91	1.34	1.37
23	c	508	CLA	C4D-CHA	2.91	1.48	1.38
23	D	404[B]	CLA	C1B-NB	-2.90	1.34	1.37
23	c	508	CLA	C1B-NB	-2.90	1.34	1.37
23	c	508	CLA	C4B-NB	-2.90	1.34	1.37
23	C	512	CLA	C1B-C2B	2.90	1.49	1.43
23	c	511	CLA	C4D-CHA	2.90	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4D-CHA	2.90	1.48	1.38
23	A	404[A]	CLA	C4C-C3C	2.88	1.49	1.45
23	b	615	CLA	C4D-CHA	2.88	1.48	1.38
23	B	613	CLA	C1C-C2C	2.88	1.50	1.44
23	c	505	CLA	C4D-CHA	2.88	1.48	1.38
23	c	510	CLA	CHC-C4B	2.88	1.45	1.39
23	B	614	CLA	OBD-CAD	2.88	1.27	1.22
23	C	511	CLA	C4D-CHA	2.87	1.48	1.38
28	a	414[B]	PL9	C6-C5	2.87	1.49	1.35
23	b	610	CLA	C3D-C4D	-2.87	1.37	1.44
23	b	602	CLA	C3B-C4B	2.87	1.51	1.42
23	B	610	CLA	C1B-C2B	2.87	1.49	1.43
23	c	504	CLA	C1B-C2B	2.87	1.49	1.43
23	c	510	CLA	C1B-C2B	2.87	1.49	1.43
23	B	605	CLA	C1C-C2C	2.87	1.50	1.44
23	b	607	CLA	C4B-NB	-2.87	1.34	1.37
23	D	404[A]	CLA	C1B-C2B	2.86	1.49	1.43
23	a	407[B]	CLA	C4B-NB	-2.86	1.34	1.37
23	C	506	CLA	C4D-CHA	2.86	1.48	1.38
23	B	604	CLA	C1B-NB	-2.86	1.34	1.37
23	B	615	CLA	C1C-C2C	2.86	1.50	1.44
23	B	601	CLA	C4B-NB	-2.85	1.34	1.37
23	C	513	CLA	C1C-C2C	2.85	1.50	1.44
23	c	502	CLA	C1B-NB	-2.85	1.34	1.37
23	B	616	CLA	CHD-C4C	2.85	1.45	1.39
23	B	613	CLA	C1B-C2B	2.84	1.49	1.43
23	B	612	CLA	C4D-CHA	2.84	1.48	1.38
23	c	514	CLA	C1B-C2B	2.84	1.49	1.43
23	c	512	CLA	C4D-CHA	2.84	1.48	1.38
23	d	401[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	b	611	CLA	C1B-C2B	2.83	1.49	1.43
23	c	512	CLA	C4B-NB	-2.83	1.34	1.37
23	b	616	CLA	C1B-NB	-2.83	1.34	1.37
23	b	605	CLA	C4D-CHA	2.83	1.48	1.38
23	A	404[A]	CLA	C1B-C2B	2.83	1.49	1.43
23	a	409	CLA	C1B-NB	-2.82	1.34	1.37
23	B	602	CLA	C1B-C2B	2.82	1.49	1.43
23	D	405	CLA	C3B-C4B	2.82	1.50	1.42
34	d	408	HTG	C1'-S1	-2.82	1.77	1.81
34	b	622	HTG	O5-C1	2.82	1.46	1.42
23	b	612	CLA	C1C-C2C	2.81	1.50	1.44
23	c	508	CLA	C1B-C2B	2.81	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	506	CLA	C1B-C2B	2.81	1.49	1.43
23	C	507	CLA	C1C-C2C	2.81	1.50	1.44
23	C	514	CLA	C1C-C2C	2.81	1.50	1.44
33	C	526	LMG	O8-C28	2.80	1.46	1.33
23	B	609	CLA	C3B-C4B	2.80	1.50	1.42
23	c	513	CLA	C4D-CHA	2.80	1.48	1.38
23	B	605	CLA	C1B-NB	-2.80	1.34	1.37
23	a	407[A]	CLA	C1C-C2C	2.79	1.50	1.44
23	C	506	CLA	C1C-C2C	2.79	1.50	1.44
25	D	414	GOL	O2-C2	-2.79	1.35	1.43
23	A	405[A]	CLA	C4D-CHA	2.79	1.48	1.38
37	a	408[A]	PHO	CBD-CGD	-2.79	1.49	1.52
23	B	603	CLA	C4D-CHA	2.79	1.47	1.38
23	B	613	CLA	C4D-CHA	2.79	1.47	1.38
23	C	509	CLA	C4D-CHA	2.79	1.47	1.38
28	A	412[B]	PL9	C6-C5	2.78	1.48	1.35
23	B	602	CLA	C4D-CHA	2.78	1.47	1.38
23	c	513	CLA	C1B-NB	-2.78	1.34	1.37
23	c	502	CLA	C1B-C2B	2.77	1.49	1.43
23	a	407[A]	CLA	C4D-CHA	2.77	1.47	1.38
23	B	603	CLA	C4B-NB	-2.77	1.34	1.37
23	C	511	CLA	C1C-C2C	2.77	1.50	1.44
23	a	405[B]	CLA	C3B-C4B	2.77	1.50	1.42
23	b	609	CLA	C4D-CHA	2.76	1.47	1.38
23	c	511	CLA	C4B-NB	-2.76	1.34	1.37
23	C	510	CLA	C3B-C2B	2.76	1.50	1.41
23	B	607	CLA	C1B-C2B	2.76	1.49	1.43
23	C	512	CLA	C1B-NB	-2.76	1.34	1.37
34	b	625	HTG	C1'-S1	-2.76	1.77	1.81
23	A	405[A]	CLA	C1B-C2B	2.76	1.49	1.43
23	b	615	CLA	C1B-C2B	2.75	1.49	1.43
23	B	614	CLA	C3D-C4D	-2.75	1.38	1.44
23	C	512	CLA	C4C-C3C	2.75	1.49	1.45
23	A	405[B]	CLA	C1B-C2B	2.75	1.49	1.43
23	C	506	CLA	C4B-NB	-2.75	1.34	1.37
23	c	506	CLA	C4D-CHA	2.75	1.47	1.38
23	A	406[B]	CLA	C3B-C4B	2.75	1.50	1.42
23	d	402	CLA	C1B-NB	-2.75	1.34	1.37
23	D	404[A]	CLA	C4B-NB	-2.74	1.34	1.37
28	d	404[B]	PL9	C6-C5	2.74	1.48	1.35
23	B	607	CLA	C4D-CHA	2.74	1.47	1.38
23	C	510	CLA	C4D-CHA	2.74	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	OBD-CAD	2.73	1.27	1.22
23	a	407[A]	CLA	C1B-C2B	2.73	1.49	1.43
23	D	405	CLA	C1B-C2B	2.73	1.49	1.43
23	B	616	CLA	C1C-C2C	2.73	1.50	1.44
23	C	503	CLA	C1C-C2C	2.73	1.50	1.44
23	b	613	CLA	C4D-CHA	2.73	1.47	1.38
23	a	406[A]	CLA	C1B-C2B	2.73	1.49	1.43
23	B	609	CLA	C1C-C2C	2.72	1.50	1.44
23	b	608	CLA	C4D-CHA	2.72	1.47	1.38
23	C	510	CLA	C1B-NB	-2.72	1.34	1.37
23	a	405[B]	CLA	C4D-CHA	2.72	1.47	1.38
23	b	609	CLA	C1B-NB	-2.72	1.34	1.37
23	c	504	CLA	C3D-C4D	-2.72	1.38	1.44
23	b	607	CLA	C1C-C2C	2.72	1.50	1.44
23	b	602	CLA	C4B-NB	-2.71	1.34	1.37
23	A	406[A]	CLA	C3B-C4B	2.71	1.50	1.42
23	b	612	CLA	C1B-NB	-2.71	1.34	1.37
23	c	504	CLA	C4D-CHA	2.71	1.47	1.38
23	B	613	CLA	C4C-C3C	2.71	1.49	1.45
23	D	404[A]	CLA	C4D-CHA	2.71	1.47	1.38
23	B	610	CLA	C4D-CHA	2.71	1.47	1.38
23	b	606	CLA	C4D-CHA	2.71	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.71	1.47	1.38
23	B	606	CLA	C1B-NB	-2.70	1.34	1.37
23	d	401[B]	CLA	C4C-C3C	2.70	1.49	1.45
34	C	523	HTG	C1'-S1	-2.70	1.77	1.81
23	A	405[B]	CLA	C4D-CHA	2.70	1.47	1.38
23	B	606	CLA	C1C-C2C	2.70	1.50	1.44
23	A	404[B]	CLA	C3B-C4B	2.70	1.50	1.42
23	d	401[A]	CLA	C4D-CHA	2.70	1.47	1.38
23	C	505	CLA	C4D-CHA	2.69	1.47	1.38
23	b	607	CLA	C4D-CHA	2.69	1.47	1.38
23	c	502	CLA	C4D-CHA	2.69	1.47	1.38
23	C	507	CLA	C1B-NB	-2.69	1.34	1.37
37	D	402[B]	PHO	CHA-CBD	-2.69	1.48	1.51
23	C	514	CLA	C3B-C4B	2.69	1.50	1.42
23	c	507	CLA	C4D-CHA	2.69	1.47	1.38
23	B	604	CLA	C4B-NB	-2.69	1.34	1.37
23	B	605	CLA	C3B-C4B	2.69	1.50	1.42
23	b	612	CLA	C4C-C3C	2.68	1.49	1.45
23	b	604	CLA	C4B-NB	-2.68	1.34	1.37
23	b	616	CLA	C1C-C2C	2.68	1.50	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	C4B-NB	-2.68	1.34	1.37
23	b	603	CLA	C4D-CHA	2.68	1.47	1.38
23	c	507	CLA	C4C-C3C	2.68	1.49	1.45
23	C	504	CLA	C1C-C2C	2.68	1.50	1.44
23	B	602	CLA	C3D-C4D	-2.68	1.38	1.44
23	B	615	CLA	C4D-CHA	2.67	1.47	1.38
23	A	406[A]	CLA	C4D-CHA	2.67	1.47	1.38
23	c	511	CLA	C1C-C2C	2.67	1.49	1.44
23	A	404[B]	CLA	C1C-C2C	2.67	1.49	1.44
25	o	302	GOL	C1-C2	2.67	1.62	1.51
37	a	416[A]	PHO	C3A-C2A	-2.67	1.52	1.54
23	c	505	CLA	C4C-C3C	2.67	1.49	1.45
23	b	601	CLA	C4D-CHA	2.67	1.47	1.38
23	a	407[B]	CLA	C1C-C2C	2.67	1.49	1.44
34	b	625	HTG	C1-S1	-2.67	1.76	1.80
23	d	402	CLA	C4B-NB	-2.67	1.34	1.37
23	B	609	CLA	C4D-CHA	2.66	1.47	1.38
23	A	407	CLA	C1B-NB	-2.66	1.34	1.37
23	c	503	CLA	C1B-NB	-2.66	1.34	1.37
23	b	613	CLA	C1B-C2B	2.66	1.49	1.43
23	A	406[B]	CLA	C4B-NB	-2.66	1.34	1.37
23	b	602	CLA	C4D-CHA	2.66	1.47	1.38
25	D	414	GOL	C3-C2	2.66	1.61	1.51
23	b	606	CLA	C1B-C2B	2.66	1.49	1.43
28	D	407[A]	PL9	C6-C5	2.66	1.48	1.35
23	B	603	CLA	C4C-C3C	2.65	1.49	1.45
23	c	509	CLA	C1B-C2B	2.65	1.49	1.43
23	d	402	CLA	C4D-CHA	2.65	1.47	1.38
23	B	605	CLA	C4D-CHA	2.65	1.47	1.38
23	C	507	CLA	C4C-C3C	2.65	1.49	1.45
23	c	502	CLA	C4C-C3C	2.65	1.49	1.45
23	a	405[A]	CLA	C4D-CHA	2.65	1.47	1.38
23	b	603	CLA	C1B-C2B	2.65	1.49	1.43
23	d	401[B]	CLA	C1B-C2B	2.65	1.49	1.43
23	B	604	CLA	C3D-C4D	-2.64	1.38	1.44
23	B	613	CLA	C4B-NB	-2.64	1.34	1.37
23	a	407[B]	CLA	C4D-CHA	2.64	1.47	1.38
23	c	506	CLA	C4C-C3C	2.64	1.49	1.45
23	A	404[A]	CLA	C4D-CHA	2.64	1.47	1.38
23	b	607	CLA	C3D-C4D	-2.63	1.38	1.44
23	b	612	CLA	C4D-CHA	2.63	1.47	1.38
23	b	610	CLA	C4B-NB	-2.63	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C4D-CHA	2.63	1.47	1.38
23	C	504	CLA	C4B-NB	-2.63	1.34	1.37
23	C	510	CLA	C1C-C2C	2.63	1.49	1.44
23	c	507	CLA	C1B-C2B	2.63	1.49	1.43
23	a	407[A]	CLA	C4B-NB	-2.63	1.34	1.37
23	C	513	CLA	C1B-C2B	2.63	1.49	1.43
23	a	407[B]	CLA	C1B-NB	-2.63	1.34	1.37
37	D	402[B]	PHO	C3A-C2A	-2.63	1.52	1.54
23	A	404[B]	CLA	C4D-CHA	2.62	1.47	1.38
23	b	613	CLA	C1C-C2C	2.62	1.49	1.44
23	A	405[A]	CLA	C1C-C2C	2.62	1.49	1.44
23	c	514	CLA	C4D-CHA	2.62	1.47	1.38
23	b	601	CLA	C4B-NB	-2.62	1.34	1.37
23	C	508	CLA	C1B-C2B	2.62	1.49	1.43
23	c	504	CLA	C3B-C4B	2.62	1.50	1.42
23	B	602	CLA	C4C-C3C	2.62	1.49	1.45
23	A	406[B]	CLA	C4D-CHA	2.62	1.47	1.38
23	a	406[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	a	406[A]	CLA	C4B-NB	-2.61	1.34	1.37
23	b	607	CLA	C4C-C3C	2.61	1.49	1.45
23	b	611	CLA	C3D-C4D	-2.61	1.38	1.44
35	H	102	DGD	O5D-C1E	2.60	1.44	1.40
23	b	605	CLA	C1C-C2C	2.60	1.49	1.44
37	D	402[A]	PHO	C3D-C4D	-2.60	1.37	1.41
23	A	405[A]	CLA	C4B-NB	-2.60	1.34	1.37
23	D	404[B]	CLA	C4D-CHA	2.60	1.47	1.38
23	B	616	CLA	C4D-CHA	2.60	1.47	1.38
23	B	606	CLA	C1B-C2B	2.60	1.49	1.43
37	a	416[B]	PHO	C3A-C2A	-2.60	1.52	1.54
23	B	602	CLA	C4B-NB	-2.60	1.34	1.37
23	B	609	CLA	C1B-C2B	2.60	1.49	1.43
23	C	504	CLA	C1B-C2B	2.59	1.49	1.43
23	C	514	CLA	C4D-CHA	2.59	1.47	1.38
23	c	513	CLA	C1B-C2B	2.59	1.49	1.43
23	C	507	CLA	C4D-CHA	2.59	1.47	1.38
23	A	407	CLA	C4D-CHA	2.59	1.47	1.38
28	D	407[B]	PL9	C6-C5	2.59	1.48	1.35
23	a	407[B]	CLA	C1B-C2B	2.58	1.49	1.43
23	c	502	CLA	C4B-NB	-2.58	1.34	1.37
38	f	101	HEM	C1C-C2C	-2.58	1.40	1.45
23	a	406[B]	CLA	C1B-C2B	2.58	1.49	1.43
23	C	512	CLA	C4B-NB	-2.58	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	C1B-C2B	2.57	1.49	1.43
23	d	401[A]	CLA	C1B-C2B	2.57	1.49	1.43
23	B	608	CLA	C4D-CHA	2.57	1.47	1.38
23	B	611	CLA	MG-NB	2.57	2.10	2.05
23	d	402	CLA	C1C-C2C	2.57	1.49	1.44
23	C	515	CLA	C1C-C2C	2.57	1.49	1.44
23	C	504	CLA	C3B-C2B	2.56	1.49	1.41
23	c	506	CLA	C3B-C4B	2.56	1.50	1.42
23	C	515	CLA	C4D-CHA	2.56	1.47	1.38
23	A	405[A]	CLA	C3B-C4B	2.56	1.50	1.42
23	b	609	CLA	C3B-C4B	2.56	1.50	1.42
23	C	512	CLA	C4D-CHA	2.56	1.47	1.38
23	a	409	CLA	C4B-NB	-2.56	1.34	1.37
23	B	608	CLA	OBD-CAD	2.56	1.26	1.22
23	B	601	CLA	C4D-CHA	2.55	1.47	1.38
23	c	504	CLA	C4C-C3C	2.55	1.49	1.45
31	t	102	LMT	O3'-C3'	-2.55	1.36	1.43
23	d	402	CLA	C1B-C2B	2.55	1.49	1.43
23	c	511	CLA	C3D-C4D	-2.54	1.38	1.44
23	C	514	CLA	C1B-NB	-2.54	1.34	1.37
23	b	616	CLA	C4D-CHA	2.54	1.47	1.38
23	b	602	CLA	C4C-C3C	2.54	1.49	1.45
23	B	610	CLA	C1C-C2C	2.54	1.49	1.44
23	C	508	CLA	C1C-C2C	2.54	1.49	1.44
23	B	605	CLA	OBD-CAD	2.54	1.26	1.22
23	b	609	CLA	C1C-C2C	2.54	1.49	1.44
34	c	522	HTG	C1'-S1	-2.54	1.77	1.81
33	C	522	LMG	O1-C1	2.54	1.44	1.40
23	C	505	CLA	C3D-C4D	-2.54	1.38	1.44
23	C	505	CLA	C1B-C2B	2.54	1.49	1.43
23	B	606	CLA	C4D-CHA	2.54	1.47	1.38
23	B	601	CLA	C3B-C4B	2.54	1.50	1.42
23	b	610	CLA	C1C-C2C	2.54	1.49	1.44
23	a	409	CLA	C3B-C4B	2.53	1.50	1.42
23	a	405[A]	CLA	C1B-C2B	2.53	1.49	1.43
23	b	609	CLA	C1B-C2B	2.53	1.49	1.43
23	c	502	CLA	C1C-C2C	2.53	1.49	1.44
23	A	405[B]	CLA	C3B-C4B	2.53	1.50	1.42
23	c	508	CLA	C1C-C2C	2.53	1.49	1.44
23	C	503	CLA	C3D-C4D	-2.53	1.38	1.44
23	c	504	CLA	C1C-C2C	2.53	1.49	1.44
23	c	513	CLA	C1C-C2C	2.53	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C1B-NB	-2.53	1.34	1.37
23	c	505	CLA	C1C-C2C	2.53	1.49	1.44
23	C	506	CLA	C3B-C2B	2.52	1.49	1.41
23	A	407	CLA	C1B-C2B	2.52	1.49	1.43
38	f	101	HEM	C1D-ND	-2.52	1.33	1.38
23	B	607	CLA	C1C-C2C	2.52	1.49	1.44
23	a	405[B]	CLA	C1C-C2C	2.52	1.49	1.44
23	c	514	CLA	C1C-C2C	2.52	1.49	1.44
23	D	405	CLA	C4D-CHA	2.52	1.47	1.38
34	B	622	HTG	O5-C1	2.52	1.46	1.42
23	B	604	CLA	C4C-C3C	2.51	1.49	1.45
23	b	616	CLA	C3B-C4B	2.51	1.50	1.42
23	b	606	CLA	C4B-NB	-2.51	1.34	1.37
37	D	402[A]	PHO	C3A-C2A	-2.51	1.52	1.54
23	c	512	CLA	C1B-NB	-2.51	1.34	1.37
23	A	407	CLA	C3B-C2B	2.51	1.49	1.41
23	C	507	CLA	C3B-C4B	2.50	1.50	1.42
23	b	601	CLA	C3B-C4B	2.50	1.50	1.42
23	B	605	CLA	C3D-C4D	-2.50	1.38	1.44
31	t	101	LMT	O3'-C3'	-2.50	1.36	1.43
37	a	416[A]	PHO	C4B-NB	-2.50	1.34	1.38
23	c	509	CLA	C3D-C4D	-2.50	1.38	1.44
23	b	604	CLA	C1C-C2C	2.50	1.49	1.44
23	b	601	CLA	C1B-C2B	2.49	1.49	1.43
23	C	505	CLA	C4B-NB	-2.49	1.34	1.37
23	c	509	CLA	C1C-C2C	2.49	1.49	1.44
23	c	513	CLA	C4B-NB	-2.49	1.34	1.37
23	C	508	CLA	C4D-CHA	2.49	1.46	1.38
23	B	608	CLA	C1B-NB	-2.49	1.34	1.37
23	A	404[B]	CLA	C1B-C2B	2.49	1.49	1.43
23	B	614	CLA	C3B-C4B	2.49	1.50	1.42
23	c	514	CLA	C4C-C3C	2.49	1.49	1.45
37	a	408[A]	PHO	C4B-NB	-2.48	1.34	1.38
23	B	616	CLA	C3B-C2B	2.48	1.49	1.41
34	B	625	HTG	C1-S1	-2.48	1.76	1.80
24	B	619	BCR	C30-C25	-2.48	1.50	1.53
23	b	601	CLA	C1B-NB	-2.48	1.34	1.37
23	C	504	CLA	C1B-NB	-2.48	1.34	1.37
28	d	404[A]	PL9	C6-C5	2.48	1.47	1.35
23	c	513	CLA	C3B-C4B	2.48	1.49	1.42
23	A	405[B]	CLA	C4B-NB	-2.48	1.34	1.37
23	C	505	CLA	C4C-C3C	2.48	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404[B]	CLA	C3D-C4D	-2.47	1.38	1.44
31	T	101	LMT	O3'-C3'	-2.47	1.36	1.43
23	B	608	CLA	C3D-C4D	-2.47	1.38	1.44
23	b	603	CLA	C1C-C2C	2.47	1.49	1.44
37	D	402[A]	PHO	C4B-NB	-2.47	1.34	1.38
23	c	514	CLA	C3B-C4B	2.47	1.49	1.42
23	a	405[B]	CLA	C3B-C2B	2.47	1.49	1.41
23	b	612	CLA	C3B-C2B	2.47	1.49	1.41
23	B	606	CLA	C3D-C4D	-2.46	1.38	1.44
23	d	401[A]	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	505	CLA	C1C-C2C	2.46	1.49	1.44
23	d	401[A]	CLA	C1C-C2C	2.45	1.49	1.44
23	b	601	CLA	C1C-C2C	2.45	1.49	1.44
23	C	505	CLA	C3B-C4B	2.45	1.49	1.42
23	B	610	CLA	C4C-C3C	2.44	1.49	1.45
23	A	406[A]	CLA	C4B-NB	-2.44	1.34	1.37
23	c	511	CLA	C1B-NB	-2.44	1.34	1.37
23	c	510	CLA	C1C-C2C	2.44	1.49	1.44
23	D	404[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	608	CLA	C3B-C4B	2.44	1.49	1.42
23	c	512	CLA	C1C-C2C	2.44	1.49	1.44
25	D	403	GOL	O2-C2	-2.44	1.36	1.43
23	B	612	CLA	C3B-C2B	2.43	1.49	1.41
23	C	511	CLA	C3B-C2B	2.43	1.49	1.41
23	C	514	CLA	C1B-C2B	2.43	1.48	1.43
23	a	407[B]	CLA	C3B-C4B	2.43	1.49	1.42
23	B	603	CLA	C3B-C2B	2.43	1.49	1.41
23	b	611	CLA	C4D-CHA	2.43	1.46	1.38
23	C	511	CLA	C1B-C2B	2.43	1.48	1.43
23	b	606	CLA	C3D-C4D	-2.43	1.38	1.44
23	A	406[B]	CLA	C1C-C2C	2.43	1.49	1.44
37	a	416[B]	PHO	CHA-CBD	-2.43	1.48	1.51
37	a	408[B]	PHO	C4B-NB	-2.43	1.34	1.38
31	m	103	LMT	C3'-C2'	2.42	1.58	1.52
23	b	610	CLA	C1B-C2B	2.42	1.48	1.43
40	v	201	HEC	CMC-C2C	2.42	1.55	1.50
23	d	401[B]	CLA	C4D-CHA	2.42	1.46	1.38
23	b	605	CLA	C1B-C2B	2.42	1.48	1.43
35	h	102	DGD	O5D-C1E	2.42	1.44	1.40
23	c	503	CLA	C3B-C2B	2.42	1.49	1.41
23	C	506	CLA	C3D-C4D	-2.41	1.38	1.44
23	a	407[B]	CLA	C4C-C3C	2.41	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C4D-CHA	2.41	1.46	1.38
23	b	616	CLA	C4B-NB	-2.41	1.34	1.37
23	B	616	CLA	C1C-NC	-2.41	1.34	1.37
23	A	406[B]	CLA	C1B-C2B	2.41	1.48	1.43
23	C	513	CLA	C3D-C4D	-2.41	1.38	1.44
23	B	614	CLA	C1C-C2C	2.41	1.49	1.44
23	a	407[A]	CLA	C3B-C4B	2.41	1.49	1.42
23	c	506	CLA	C1C-C2C	2.40	1.49	1.44
37	D	401[B]	PHO	CBD-CGD	-2.40	1.49	1.52
23	D	404[A]	CLA	C3B-C2B	2.40	1.49	1.41
23	B	615	CLA	C3B-C4B	2.40	1.49	1.42
23	C	513	CLA	C3B-C2B	2.40	1.49	1.41
23	a	405[A]	CLA	C4C-C3C	2.39	1.49	1.45
31	B	628	LMT	C3'-C2'	2.39	1.58	1.52
23	b	616	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	512	CLA	C1C-C2C	2.39	1.49	1.44
25	D	403	GOL	C3-C2	2.39	1.60	1.51
23	B	607	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	611	CLA	C1C-C2C	2.39	1.49	1.44
23	a	409	CLA	C4D-CHA	2.39	1.46	1.38
23	C	504	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	515	CLA	C3B-C2B	2.39	1.49	1.41
23	C	510	CLA	C4C-C3C	2.39	1.49	1.45
23	b	614	CLA	C4D-CHA	2.38	1.46	1.38
23	B	604	CLA	C1A-CHA	2.38	1.52	1.43
23	a	407[A]	CLA	C3D-C4D	-2.38	1.38	1.44
23	a	405[A]	CLA	C1C-C2C	2.38	1.49	1.44
23	C	514	CLA	C3D-C4D	-2.38	1.38	1.44
23	C	513	CLA	C4C-C3C	2.38	1.49	1.45
23	b	605	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	616	CLA	C1B-C2B	2.37	1.48	1.43
37	a	416[B]	PHO	C4B-NB	-2.37	1.34	1.38
23	D	404[A]	CLA	C1C-C2C	2.37	1.49	1.44
23	B	608	CLA	C3B-C2B	2.37	1.49	1.41
23	B	603	CLA	C1C-C2C	2.37	1.49	1.44
23	D	404[B]	CLA	C1B-C2B	2.37	1.48	1.43
23	c	509	CLA	C3B-C2B	2.37	1.49	1.41
23	C	503	CLA	C3B-C4B	2.36	1.49	1.42
23	b	610	CLA	C4C-C3C	2.36	1.49	1.45
23	C	507	CLA	C3D-C4D	-2.36	1.38	1.44
31	B	630	LMT	O2'-C2'	-2.36	1.37	1.43
23	d	402	CLA	C3B-C4B	2.35	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	OBD-CAD	2.35	1.26	1.22
23	c	514	CLA	C3D-C4D	-2.35	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.35	1.38	1.44
23	b	614	CLA	C4B-NB	-2.35	1.34	1.37
23	c	512	CLA	C3B-C2B	2.35	1.49	1.41
38	F	102	HEM	C1C-C2C	-2.34	1.40	1.45
23	C	503	CLA	C4C-C3C	2.34	1.49	1.45
37	a	408[A]	PHO	C1D-ND	-2.34	1.34	1.38
23	A	404[B]	CLA	C3B-C2B	2.34	1.49	1.41
23	b	611	CLA	C4B-NB	-2.33	1.34	1.37
38	F	102	HEM	C3B-C4B	2.33	1.49	1.44
23	c	509	CLA	C3B-C4B	2.33	1.49	1.42
23	A	404[A]	CLA	C1C-C2C	2.33	1.49	1.44
23	c	502	CLA	C3D-C4D	-2.33	1.39	1.44
23	b	605	CLA	C4B-NB	-2.32	1.34	1.37
23	d	402	CLA	C4C-C3C	2.32	1.49	1.45
23	D	404[B]	CLA	C3B-C2B	2.32	1.49	1.41
23	c	511	CLA	C4C-C3C	2.32	1.49	1.45
23	B	612	CLA	C4C-C3C	2.32	1.49	1.45
23	a	405[B]	CLA	C1B-C2B	2.31	1.48	1.43
23	A	407	CLA	C4C-C3C	2.31	1.49	1.45
23	C	513	CLA	C1B-NB	-2.31	1.34	1.37
23	B	601	CLA	C4C-C3C	2.31	1.49	1.45
31	A	417	LMT	O3'-C3'	-2.31	1.37	1.43
23	B	611	CLA	C3D-C4D	-2.30	1.39	1.44
23	b	614	CLA	C4C-C3C	2.30	1.48	1.45
23	c	503	CLA	C4D-CHA	2.30	1.46	1.38
31	b	621	LMT	C3'-C2'	2.30	1.58	1.52
23	b	601	CLA	C3B-C2B	2.30	1.48	1.41
23	B	605	CLA	C4B-NB	-2.30	1.34	1.37
23	d	401[B]	CLA	C3B-C2B	2.30	1.48	1.41
23	A	406[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	b	604	CLA	C3B-C2B	2.30	1.48	1.41
25	b	624	GOL	C3-C2	2.30	1.60	1.51
37	D	402[B]	PHO	C4B-NB	-2.29	1.34	1.38
23	B	602	CLA	C3B-C2B	2.29	1.48	1.41
26	F	103	SQD	O6-C1	2.29	1.44	1.40
23	c	513	CLA	C4C-C3C	2.29	1.48	1.45
23	b	613	CLA	C3B-C2B	2.29	1.48	1.41
23	a	409	CLA	C1D-C2D	2.29	1.49	1.45
23	a	406[A]	CLA	C3B-C4B	2.29	1.49	1.42
23	c	512	CLA	C4C-C3C	2.29	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	408[B]	PHO	C3A-C2A	-2.29	1.52	1.54
40	V	202	HEC	CMB-C2B	2.28	1.55	1.50
23	C	512	CLA	C1D-C2D	2.28	1.49	1.45
24	C	517	BCR	C1-C6	-2.28	1.50	1.53
23	A	404[B]	CLA	C4C-C3C	2.28	1.48	1.45
23	c	510	CLA	C3B-C2B	2.28	1.48	1.41
23	A	405[B]	CLA	C3D-C4D	-2.28	1.39	1.44
23	d	401[B]	CLA	C3D-C4D	-2.27	1.39	1.44
37	a	416[B]	PHO	C1B-NB	-2.27	1.34	1.38
23	c	509	CLA	C1B-NB	-2.27	1.34	1.37
23	C	504	CLA	C4D-CHA	2.27	1.46	1.38
35	c	519	DGD	O5D-C1E	2.27	1.44	1.40
23	B	608	CLA	C4C-C3C	2.27	1.48	1.45
35	C	519[A]	DGD	O5D-C1E	2.27	1.44	1.40
23	b	603	CLA	C3B-C4B	2.27	1.49	1.42
23	b	611	CLA	C4C-C3C	2.27	1.48	1.45
23	C	511	CLA	C3B-C4B	2.27	1.49	1.42
23	A	405[A]	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	604	CLA	MG-NA	2.26	2.11	2.06
23	d	401[B]	CLA	C1C-C2C	2.26	1.49	1.44
37	D	402[A]	PHO	C1D-ND	-2.26	1.34	1.38
23	C	508	CLA	C3D-C4D	-2.26	1.39	1.44
23	a	405[B]	CLA	C4C-C3C	2.26	1.48	1.45
23	D	405	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	603	CLA	C3B-C2B	2.26	1.48	1.41
23	b	606	CLA	C3B-C2B	2.26	1.48	1.41
31	M	101	LMT	O2'-C2'	-2.26	1.37	1.43
23	B	613	CLA	C3D-C4D	-2.26	1.39	1.44
35	c	519	DGD	O2G-C2G	-2.26	1.41	1.46
23	B	603	CLA	C1B-C2B	2.26	1.48	1.43
23	b	610	CLA	C3B-C4B	2.26	1.49	1.42
23	b	614	CLA	C3B-C2B	2.26	1.48	1.41
23	c	509	CLA	C4C-C3C	2.26	1.48	1.45
31	t	102	LMT	O2'-C2'	-2.26	1.37	1.43
23	C	512	CLA	C3B-C2B	2.25	1.48	1.41
23	B	606	CLA	C3B-C4B	2.25	1.49	1.42
23	B	609	CLA	C3D-C4D	-2.25	1.39	1.44
23	b	608	CLA	C3B-C2B	2.25	1.48	1.41
23	a	406[B]	CLA	C3B-C4B	2.24	1.49	1.42
23	b	602	CLA	C3D-C4D	-2.24	1.39	1.44
23	c	511	CLA	C3B-C4B	2.24	1.49	1.42
23	C	509	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	b	608	CLA	C1B-C2B	2.24	1.48	1.43
23	C	514	CLA	C3B-C2B	2.24	1.48	1.41
23	a	407[B]	CLA	C3D-C4D	-2.24	1.39	1.44
37	D	402[B]	PHO	C1D-ND	-2.23	1.34	1.38
23	B	610	CLA	C3D-C4D	-2.23	1.39	1.44
37	D	401[B]	PHO	CHA-CBD	-2.23	1.49	1.51
23	b	614	CLA	C1C-C2C	2.23	1.49	1.44
23	c	508	CLA	C3D-C4D	-2.23	1.39	1.44
37	D	402[B]	PHO	C3D-C4D	-2.22	1.38	1.41
28	a	414[A]	PL9	C2-C3	2.22	1.40	1.34
23	a	406[B]	CLA	C4B-NB	-2.22	1.34	1.37
23	c	503	CLA	C3D-C4D	-2.22	1.39	1.44
25	c	527	GOL	C3-C2	2.22	1.60	1.51
23	A	404[A]	CLA	C3B-C2B	2.22	1.48	1.41
37	D	401[B]	PHO	C1D-ND	-2.22	1.34	1.38
23	A	406[B]	CLA	C3D-C4D	-2.22	1.39	1.44
23	D	404[A]	CLA	C4C-C3C	2.21	1.48	1.45
23	B	608	CLA	C1C-C2C	2.21	1.49	1.44
23	b	608	CLA	C3B-C4B	2.21	1.49	1.42
23	b	615	CLA	C3B-C4B	2.21	1.49	1.42
23	d	402	CLA	C1D-C2D	2.21	1.49	1.45
35	c	518[A]	DGD	O2G-C2G	-2.21	1.41	1.46
23	B	614	CLA	C3B-C2B	2.20	1.48	1.41
23	c	511	CLA	C3B-C2B	2.20	1.48	1.41
23	B	607	CLA	C3B-C2B	2.20	1.48	1.41
28	a	414[B]	PL9	C2-C3	2.20	1.40	1.34
23	C	508	CLA	C1D-C2D	2.20	1.49	1.45
23	B	606	CLA	C4C-C3C	2.19	1.48	1.45
24	B	618	BCR	C19-C18	2.19	1.50	1.46
25	a	418	GOL	C1-C2	2.19	1.60	1.51
23	c	505	CLA	C1C-NC	-2.19	1.34	1.37
23	C	512	CLA	C3D-C4D	-2.19	1.39	1.44
23	c	505	CLA	C3D-C4D	-2.19	1.39	1.44
37	D	401[B]	PHO	C1B-NB	-2.19	1.34	1.38
23	b	608	CLA	C4C-C3C	2.19	1.48	1.45
23	B	604	CLA	MG-NA	2.19	2.11	2.06
25	a	418	GOL	C3-C2	2.19	1.60	1.51
23	c	507	CLA	C3D-C4D	-2.18	1.39	1.44
23	b	608	CLA	C3D-C4D	-2.18	1.39	1.44
23	b	602	CLA	C1B-NB	-2.18	1.35	1.37
23	c	512	CLA	MG-NA	2.18	2.11	2.06
23	b	606	CLA	C3B-C4B	2.18	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	a	408[B]	PHO	C1D-ND	-2.18	1.34	1.38
31	c	501	LMT	O2'-C2'	-2.18	1.37	1.43
23	c	514	CLA	C3B-C2B	2.18	1.48	1.41
23	b	602	CLA	C1B-C2B	2.18	1.48	1.43
40	v	201	HEC	CMD-C2D	2.18	1.55	1.50
23	b	609	CLA	C3D-C4D	-2.18	1.39	1.44
23	a	405[A]	CLA	C3B-C2B	2.18	1.48	1.41
23	C	514	CLA	C4B-NB	-2.18	1.35	1.37
23	C	507	CLA	C4B-NB	-2.17	1.35	1.37
23	b	611	CLA	C3B-C2B	2.17	1.48	1.41
23	a	406[B]	CLA	C1C-C2C	2.17	1.48	1.44
32	d	405[B]	LHG	O7-C5	-2.17	1.41	1.46
31	M	101	LMT	C1B-C2B	2.17	1.58	1.52
31	B	628	LMT	O3'-C3'	-2.17	1.37	1.43
23	b	611	CLA	C3B-C4B	2.17	1.49	1.42
23	b	614	CLA	C3B-C4B	2.17	1.49	1.42
37	a	416[A]	PHO	C1B-NB	-2.16	1.34	1.38
23	b	614	CLA	C3D-C4D	-2.16	1.39	1.44
23	B	614	CLA	C4C-C3C	2.16	1.48	1.45
23	A	407	CLA	C1C-NC	-2.16	1.34	1.37
37	D	401[B]	PHO	C4B-NB	-2.16	1.34	1.38
23	B	601	CLA	C3D-C4D	-2.16	1.39	1.44
23	C	503	CLA	C3B-C2B	2.16	1.48	1.41
23	c	513	CLA	C3D-C4D	-2.16	1.39	1.44
24	a	410	BCR	C19-C18	2.16	1.50	1.46
23	c	503	CLA	C3B-C4B	2.16	1.49	1.42
23	C	509	CLA	C4C-C3C	2.15	1.48	1.45
23	C	515	CLA	C3D-C4D	-2.15	1.39	1.44
31	e	101	LMT	O3'-C3'	-2.15	1.37	1.43
23	B	606	CLA	C4B-NB	-2.15	1.35	1.37
23	b	612	CLA	C3D-C4D	-2.15	1.39	1.44
23	c	507	CLA	C3B-C2B	2.15	1.48	1.41
23	C	509	CLA	C3D-C4D	-2.14	1.39	1.44
23	b	604	CLA	C4C-C3C	2.14	1.48	1.45
23	B	601	CLA	C1C-NC	-2.14	1.34	1.37
23	A	405[B]	CLA	C1C-C2C	2.14	1.48	1.44
23	B	601	CLA	C3B-C2B	2.14	1.48	1.41
23	a	405[B]	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	602	CLA	C3B-C4B	2.13	1.49	1.42
23	C	511	CLA	C4C-C3C	2.13	1.48	1.45
23	c	503	CLA	C4C-C3C	2.13	1.48	1.45
26	B	620	SQD	O6-C1	2.13	1.43	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	101	BCR	C30-C25	-2.13	1.51	1.53
23	C	504	CLA	C4C-C3C	2.13	1.48	1.45
23	a	407[A]	CLA	C4C-C3C	2.13	1.48	1.45
24	B	617	BCR	C1-C6	-2.13	1.51	1.53
23	A	406[A]	CLA	C3D-C4D	-2.12	1.39	1.44
23	a	406[B]	CLA	C3D-C4D	-2.12	1.39	1.44
37	D	401[A]	PHO	C1B-NB	-2.12	1.34	1.38
23	c	514	CLA	C1D-C2D	2.12	1.49	1.45
23	D	404[B]	CLA	C4C-C3C	2.12	1.48	1.45
23	c	502	CLA	C3B-C4B	2.12	1.48	1.42
32	d	411[A]	LHG	O7-C5	-2.12	1.41	1.46
28	A	412[B]	PL9	C2-C3	2.12	1.39	1.34
28	A	412[A]	PL9	C2-C1	-2.12	1.39	1.44
38	F	102	HEM	C3C-C4C	-2.12	1.42	1.46
23	b	615	CLA	C4B-NB	-2.11	1.35	1.37
23	b	616	CLA	C3B-C2B	2.11	1.48	1.41
23	B	610	CLA	C3B-C4B	2.11	1.48	1.42
23	A	406[B]	CLA	C4C-C3C	2.11	1.48	1.45
23	a	405[A]	CLA	C3D-C4D	-2.11	1.39	1.44
37	a	408[B]	PHO	C1B-NB	-2.11	1.34	1.38
23	C	508	CLA	C3B-C2B	2.11	1.48	1.41
23	B	613	CLA	C3B-C2B	2.11	1.48	1.41
23	c	505	CLA	C3B-C2B	2.11	1.48	1.41
23	B	607	CLA	C4C-C3C	2.11	1.48	1.45
31	M	101	LMT	O3'-C3'	-2.10	1.37	1.43
34	B	623	HTG	C1'-S1	-2.10	1.78	1.81
23	d	401[A]	CLA	C3B-C2B	2.10	1.48	1.41
37	D	401[B]	PHO	C3D-C4D	-2.09	1.38	1.41
23	B	606	CLA	C3B-C2B	2.09	1.48	1.41
23	a	406[B]	CLA	C3B-C2B	2.09	1.48	1.41
23	b	607	CLA	C3B-C2B	2.09	1.48	1.41
23	B	607	CLA	C1C-NC	-2.09	1.34	1.37
23	b	612	CLA	C3B-C4B	2.09	1.48	1.42
23	C	513	CLA	C3B-C4B	2.09	1.48	1.42
23	b	613	CLA	C4C-C3C	2.09	1.48	1.45
23	D	404[B]	CLA	C1C-C2C	2.09	1.48	1.44
40	v	201	HEC	C3B-C2B	-2.08	1.34	1.41
32	D	408[A]	LHG	O7-C5	-2.08	1.41	1.46
23	C	510	CLA	C1C-NC	-2.08	1.34	1.37
23	a	409	CLA	C3B-C2B	2.08	1.48	1.41
37	D	401[A]	PHO	C4B-NB	-2.08	1.34	1.38
23	C	515	CLA	C3B-C4B	2.07	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	202	HEC	CMA-C3A	2.07	1.55	1.50
23	A	406[A]	CLA	C1C-NC	-2.07	1.34	1.37
23	b	602	CLA	C1D-C2D	2.07	1.49	1.45
23	b	603	CLA	C4C-C3C	2.07	1.48	1.45
32	L	101[B]	LHG	O7-C5	-2.07	1.41	1.46
23	B	615	CLA	C4B-NB	-2.06	1.35	1.37
23	b	606	CLA	C1C-C2C	2.06	1.48	1.44
23	A	407	CLA	C3D-C4D	-2.06	1.39	1.44
35	C	519[B]	DGD	O5D-C1E	2.06	1.43	1.40
31	m	103	LMT	O2B-C2B	-2.05	1.37	1.43
23	A	407	CLA	C3B-C4B	2.05	1.48	1.42
23	A	405[B]	CLA	C4C-C3C	2.05	1.48	1.45
23	b	607	CLA	C1A-CHA	2.05	1.51	1.43
23	A	404[B]	CLA	C3D-C4D	-2.05	1.39	1.44
28	A	412[A]	PL9	C2-C3	2.05	1.39	1.34
23	d	402	CLA	C3D-C4D	-2.05	1.39	1.44
31	F	101	LMT	O3'-C3'	-2.05	1.37	1.43
38	F	102	HEM	C1D-ND	-2.05	1.34	1.38
24	b	617	BCR	C19-C18	2.04	1.50	1.46
24	d	403	BCR	C30-C25	-2.04	1.51	1.53
23	A	404[A]	CLA	C3D-C4D	-2.04	1.39	1.44
32	l	802[A]	LHG	O7-C5	-2.04	1.41	1.46
23	C	506	CLA	C3B-C4B	2.04	1.48	1.42
23	b	605	CLA	C3B-C4B	2.04	1.48	1.42
23	C	508	CLA	C3B-C4B	2.04	1.48	1.42
25	V	204[A]	GOL	C1-C2	2.04	1.59	1.51
23	B	616	CLA	C3D-C4D	-2.04	1.39	1.44
23	a	406[A]	CLA	C1C-C2C	2.04	1.48	1.44
25	c	528	GOL	C3-C2	2.04	1.59	1.51
23	B	607	CLA	C1A-CHA	2.04	1.51	1.43
28	D	407[B]	PL9	C2-C3	2.04	1.39	1.34
23	b	604	CLA	C3B-C4B	2.04	1.48	1.42
23	B	610	CLA	C4B-NB	-2.04	1.35	1.37
23	B	615	CLA	C4C-C3C	2.04	1.48	1.45
23	A	406[B]	CLA	C1D-C2D	2.04	1.49	1.45
34	b	622	HTG	C1-C2	2.03	1.56	1.53
37	a	408[A]	PHO	CHA-CBD	-2.03	1.49	1.51
23	b	609	CLA	C3B-C2B	2.03	1.48	1.41
23	B	608	CLA	C1C-NC	-2.03	1.34	1.37
31	B	630	LMT	O3B-C3B	-2.03	1.37	1.43
23	b	608	CLA	C1C-NC	-2.03	1.34	1.37
23	b	605	CLA	C3B-C2B	2.03	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	C3B-C2B	2.03	1.48	1.41
37	a	408[B]	PHO	CBD-CGD	-2.03	1.50	1.52
23	b	603	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	604	CLA	C3B-C4B	2.03	1.48	1.42
37	a	416[A]	PHO	C1D-ND	-2.03	1.35	1.38
37	a	416[B]	PHO	C1D-ND	-2.03	1.35	1.38
32	L	101[A]	LHG	O7-C5	-2.02	1.41	1.46
23	c	510	CLA	C1C-NC	-2.02	1.34	1.37
23	C	511	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	608	CLA	C1C-C2C	2.02	1.48	1.44
31	A	417	LMT	O2'-C2'	-2.02	1.38	1.43
31	B	628	LMT	O5'-C5'	-2.02	1.39	1.44
23	c	502	CLA	C1C-NC	-2.01	1.34	1.37
23	c	506	CLA	C4B-NB	-2.01	1.35	1.37
23	c	502	CLA	C3B-C2B	2.01	1.48	1.41
23	c	504	CLA	MG-NA	2.01	2.11	2.06
23	c	513	CLA	C3B-C2B	2.01	1.47	1.41
23	A	405[B]	CLA	C1D-C2D	2.01	1.49	1.45
31	b	627	LMT	O3'-C3'	-2.01	1.38	1.43
23	B	612	CLA	C3D-C4D	-2.01	1.39	1.44
23	c	507	CLA	C1D-C2D	2.00	1.49	1.45
31	c	501	LMT	O3'-C3'	-2.00	1.38	1.43
37	a	416[A]	PHO	CHA-CBD	-2.00	1.49	1.51
23	c	512	CLA	C1A-CHA	2.00	1.51	1.43
24	A	408	BCR	C1-C6	-2.00	1.51	1.53

All (3430) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C3B-C2B-C1B	-13.46	91.30	107.17
37	D	401[A]	PHO	C2D-C1D-ND	11.49	117.73	109.43
23	B	611	CLA	C1D-ND-C4D	-11.26	98.41	106.31
23	a	409	CLA	C1D-ND-C4D	-11.25	98.42	106.31
37	a	416[A]	PHO	C2D-C1D-ND	10.99	117.38	109.43
37	a	416[B]	PHO	C2D-C1D-ND	10.90	117.31	109.43
37	D	401[B]	PHO	C2D-C1D-ND	10.89	117.30	109.43
37	a	408[A]	PHO	C2D-C1D-ND	10.81	117.24	109.43
37	D	402[B]	PHO	C2D-C1D-ND	10.59	117.09	109.43
37	D	402[A]	PHO	C2D-C1D-ND	10.58	117.08	109.43
23	b	605	CLA	C1D-ND-C4D	-10.47	98.97	106.31
37	a	408[B]	PHO	C2D-C1D-ND	10.31	116.88	109.43
23	B	611	CLA	C2B-C1B-NB	10.31	121.02	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	C1D-ND-C4D	-10.17	99.18	106.31
23	B	606	CLA	C1D-ND-C4D	-10.15	99.19	106.31
23	a	407[B]	CLA	C1D-ND-C4D	-10.12	99.21	106.31
23	A	407	CLA	C1D-ND-C4D	-10.00	99.30	106.31
23	B	601	CLA	C1D-ND-C4D	-10.00	99.30	106.31
23	c	504	CLA	C1D-ND-C4D	-9.94	99.34	106.31
23	d	401[B]	CLA	C1D-ND-C4D	-9.82	99.42	106.31
23	C	512	CLA	C1D-ND-C4D	-9.81	99.43	106.31
23	A	406[B]	CLA	C1D-ND-C4D	-9.77	99.45	106.31
40	V	202	HEC	CBB-CAB-C3B	-9.75	107.95	127.43
23	c	512	CLA	C1D-ND-C4D	-9.73	99.48	106.31
23	c	506	CLA	C1D-ND-C4D	-9.73	99.48	106.31
23	b	602	CLA	C1D-ND-C4D	-9.71	99.50	106.31
23	b	614	CLA	C1D-ND-C4D	-9.69	99.52	106.31
23	B	610	CLA	C1D-ND-C4D	-9.66	99.54	106.31
23	C	515	CLA	C1D-ND-C4D	-9.65	99.54	106.31
23	b	601	CLA	C1D-ND-C4D	-9.65	99.54	106.31
23	a	405[B]	CLA	C1D-ND-C4D	-9.62	99.56	106.31
23	C	505	CLA	C1D-ND-C4D	-9.59	99.58	106.31
23	D	404[B]	CLA	C1D-ND-C4D	-9.56	99.60	106.31
23	B	614	CLA	C1D-ND-C4D	-9.56	99.61	106.31
23	c	510	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	C	507	CLA	C1D-ND-C4D	-9.55	99.61	106.31
23	B	612	CLA	C1D-ND-C4D	-9.54	99.62	106.31
23	A	405[B]	CLA	C1D-ND-C4D	-9.53	99.62	106.31
23	b	603	CLA	C1D-ND-C4D	-9.53	99.63	106.31
23	A	404[B]	CLA	C1D-ND-C4D	-9.52	99.63	106.31
23	b	609	CLA	C1D-ND-C4D	-9.49	99.65	106.31
37	a	408[A]	PHO	O2D-CGD-CBD	9.43	121.31	110.95
23	b	611	CLA	C1D-ND-C4D	-9.39	99.73	106.31
23	B	605	CLA	C1D-ND-C4D	-9.37	99.74	106.31
23	d	402	CLA	C1D-ND-C4D	-9.36	99.74	106.31
23	c	514	CLA	C1D-ND-C4D	-9.34	99.76	106.31
23	C	506	CLA	C1D-ND-C4D	-9.33	99.77	106.31
23	b	606	CLA	C1D-ND-C4D	-9.33	99.77	106.31
23	B	607	CLA	C1D-ND-C4D	-9.30	99.78	106.31
23	a	407[A]	CLA	C1D-ND-C4D	-9.26	99.82	106.31
23	b	610	CLA	C1D-ND-C4D	-9.25	99.82	106.31
23	D	404[A]	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	d	401[A]	CLA	C1D-ND-C4D	-9.17	99.88	106.31
23	A	406[A]	CLA	C1D-ND-C4D	-9.16	99.89	106.31
37	a	408[B]	PHO	O2D-CGD-CBD	9.13	120.98	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	402[B]	PHO	O2D-CGD-CBD	9.12	120.97	110.95
23	a	406[A]	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	C	511	CLA	C1D-ND-C4D	-9.12	99.91	106.31
23	B	608	CLA	C1D-ND-C4D	-9.07	99.95	106.31
37	a	416[A]	PHO	O2D-CGD-CBD	9.07	120.91	110.95
37	D	401[B]	PHO	O2D-CGD-CBD	9.07	120.91	110.95
23	C	508	CLA	C1D-ND-C4D	-9.06	99.95	106.31
23	b	616	CLA	C1D-ND-C4D	-9.03	99.98	106.31
23	b	615	CLA	C1D-ND-C4D	-9.02	99.98	106.31
23	a	406[B]	CLA	C1D-ND-C4D	-9.00	100.00	106.31
23	A	405[A]	CLA	C1D-ND-C4D	-8.99	100.01	106.31
23	B	609	CLA	C1D-ND-C4D	-8.98	100.01	106.31
23	B	603	CLA	C1D-ND-C4D	-8.95	100.03	106.31
37	a	416[B]	PHO	O2D-CGD-CBD	8.92	120.75	110.95
23	B	602	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	a	405[A]	CLA	C1D-ND-C4D	-8.91	100.06	106.31
23	c	502	CLA	C1D-ND-C4D	-8.90	100.06	106.31
23	c	513	CLA	C1D-ND-C4D	-8.83	100.11	106.31
23	C	503	CLA	C1D-ND-C4D	-8.80	100.14	106.31
23	C	509	CLA	C1D-ND-C4D	-8.80	100.14	106.31
23	B	613	CLA	C1D-ND-C4D	-8.79	100.15	106.31
37	D	401[B]	PHO	C3B-C4B-NB	8.76	113.17	107.46
37	D	401[A]	PHO	C3B-C4B-NB	8.75	113.17	107.46
23	b	612	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	C	514	CLA	C1D-ND-C4D	-8.68	100.22	106.31
23	b	607	CLA	C1D-ND-C4D	-8.66	100.23	106.31
37	D	402[A]	PHO	O2D-CGD-CBD	8.64	120.44	110.95
40	v	201	HEC	CBB-CAB-C3B	-8.63	110.18	127.43
23	c	507	CLA	C1D-ND-C4D	-8.62	100.26	106.31
23	A	404[A]	CLA	C1D-ND-C4D	-8.57	100.30	106.31
23	c	508	CLA	C1D-ND-C4D	-8.55	100.31	106.31
23	c	503	CLA	C1D-ND-C4D	-8.48	100.36	106.31
23	C	510	CLA	C1D-ND-C4D	-8.46	100.38	106.31
23	b	608	CLA	C1D-ND-C4D	-8.45	100.38	106.31
23	C	504	CLA	C1D-ND-C4D	-8.44	100.39	106.31
23	b	613	CLA	C1D-ND-C4D	-8.38	100.43	106.31
23	c	511	CLA	C1D-ND-C4D	-8.36	100.45	106.31
23	B	616	CLA	C1D-ND-C4D	-8.29	100.50	106.31
23	c	505	CLA	C1D-ND-C4D	-8.23	100.54	106.31
37	a	408[A]	PHO	C3B-C4B-NB	8.10	112.75	107.46
23	c	509	CLA	C1D-ND-C4D	-8.09	100.64	106.31
23	b	602	CLA	C4A-NA-C1A	-8.08	102.99	106.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	a	416[B]	PHO	C3B-C4B-NB	7.94	112.64	107.46
37	a	416[A]	PHO	C3B-C4B-NB	7.89	112.61	107.46
23	D	404[B]	CLA	C4A-NA-C1A	-7.85	103.10	106.68
23	C	513	CLA	C1D-ND-C4D	-7.83	100.82	106.31
23	B	609	CLA	C4A-NA-C1A	-7.70	103.17	106.68
37	D	402[A]	PHO	C3B-C4B-NB	7.61	112.43	107.46
23	a	409	CLA	C2D-C1D-ND	7.61	117.66	110.13
23	C	512	CLA	CMD-C2D-C1D	7.60	138.12	124.73
23	C	509	CLA	O2D-CGD-CBD	7.59	124.49	111.23
23	B	611	CLA	CHD-C4C-C3C	-7.56	113.75	124.77
23	D	405	CLA	C1D-ND-C4D	-7.55	101.02	106.31
37	a	408[B]	PHO	C3B-C4B-NB	7.51	112.36	107.46
23	b	604	CLA	C1D-ND-C4D	-7.50	101.05	106.31
23	c	504	CLA	CMD-C2D-C1D	7.38	137.72	124.73
23	B	604	CLA	C1D-ND-C4D	-7.37	101.14	106.31
23	B	610	CLA	C2D-C1D-ND	7.36	117.41	110.13
23	B	611	CLA	CHB-C1B-NB	-7.34	113.03	124.05
23	B	611	CLA	CMB-C2B-C1B	7.32	136.56	125.42
23	b	616	CLA	O2D-CGD-CBD	7.30	123.99	111.23
23	B	616	CLA	O2D-CGD-CBD	7.29	123.97	111.23
23	b	605	CLA	CHD-C4C-C3C	-7.28	114.16	124.77
37	D	402[A]	PHO	C2B-C1B-NB	7.26	114.68	109.43
23	b	605	CLA	C2D-C1D-ND	7.24	117.29	110.13
23	c	504	CLA	C4A-NA-C1A	-7.24	103.38	106.68
37	D	401[A]	PHO	O2D-CGD-CBD	7.23	118.89	110.95
23	C	506	CLA	C2D-C1D-ND	7.17	117.22	110.13
23	B	615	CLA	C2D-C1D-ND	7.15	117.20	110.13
23	C	505	CLA	C4A-NA-C1A	-7.15	103.42	106.68
23	c	508	CLA	O2D-CGD-CBD	7.15	123.72	111.23
23	D	405	CLA	C4A-NA-C1A	-7.15	103.42	106.68
23	B	610	CLA	O2D-CGD-CBD	7.14	123.72	111.23
23	C	509	CLA	CMD-C2D-C1D	7.14	137.30	124.73
23	B	605	CLA	CHD-C4C-C3C	-7.07	114.46	124.77
23	B	614	CLA	CMD-C2D-C1D	7.06	137.17	124.73
23	D	404[A]	CLA	C4A-NA-C1A	-7.05	103.46	106.68
23	B	616	CLA	CHD-C4C-C3C	-7.04	114.50	124.77
26	F	103	SQD	O6-C1-C2	7.03	118.95	108.27
23	b	615	CLA	C4A-NA-C1A	-7.01	103.48	106.68
23	d	402	CLA	CMD-C2D-C1D	6.99	137.04	124.73
23	B	603	CLA	O2D-CGD-CBD	6.96	123.40	111.23
23	B	606	CLA	CMD-C2D-C1D	6.92	136.91	124.73
23	c	514	CLA	CMD-C2D-C1D	6.91	136.90	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	C2D-C1D-ND	6.91	116.96	110.13
23	B	611	CLA	C2D-C1D-ND	6.91	116.96	110.13
37	D	402[B]	PHO	C2B-C1B-NB	6.90	114.42	109.43
23	b	616	CLA	C4A-NA-C1A	-6.88	103.54	106.68
23	b	610	CLA	CHD-C4C-C3C	-6.86	114.77	124.77
23	C	503	CLA	O2D-CGD-CBD	6.85	123.20	111.23
23	C	508	CLA	CMD-C2D-C1D	6.81	136.73	124.73
23	b	614	CLA	C2D-C1D-ND	6.80	116.86	110.13
23	c	508	CLA	CMD-C2D-C1D	6.80	136.70	124.73
23	b	605	CLA	CMD-C2D-C1D	6.78	136.67	124.73
23	C	514	CLA	CHD-C4C-C3C	-6.78	114.89	124.77
23	d	401[B]	CLA	CMD-C2D-C1D	6.77	136.65	124.73
23	A	407	CLA	C2D-C1D-ND	6.76	116.81	110.13
23	B	607	CLA	C2D-C1D-ND	6.76	116.81	110.13
23	b	601	CLA	CHD-C4C-C3C	-6.75	114.93	124.77
23	b	616	CLA	CHD-C4C-C3C	-6.74	114.94	124.77
37	a	416[A]	PHO	C2B-C1B-NB	6.74	114.30	109.43
23	b	601	CLA	O2D-CGD-CBD	6.71	122.95	111.23
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.73
23	A	404[B]	CLA	CMD-C2D-C1D	6.70	136.52	124.73
34	b	623	HTG	C1'-S1-C1	6.64	114.79	100.45
26	C	501[A]	SQD	O6-C1-C2	6.64	118.36	108.27
23	B	612	CLA	C2D-C1D-ND	6.64	116.69	110.13
23	B	603	CLA	C2D-C1D-ND	6.63	116.69	110.13
23	a	406[A]	CLA	CHD-C4C-C3C	-6.62	115.12	124.77
23	B	605	CLA	C2D-C1D-ND	6.62	116.67	110.13
23	b	611	CLA	CMD-C2D-C1D	6.61	136.38	124.73
23	b	606	CLA	CHD-C4C-C3C	-6.61	115.13	124.77
37	D	402[B]	PHO	C3B-C4B-NB	6.59	111.76	107.46
23	b	602	CLA	O2D-CGD-CBD	6.59	122.75	111.23
23	b	606	CLA	C4A-NA-C1A	-6.58	103.67	106.68
23	b	609	CLA	CHD-C4C-C3C	-6.57	115.19	124.77
23	b	603	CLA	CHD-C4C-C3C	-6.56	115.21	124.77
23	B	611	CLA	CMD-C2D-C1D	6.53	136.22	124.73
23	b	601	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	a	406[A]	CLA	C2D-C1D-ND	6.50	116.56	110.13
23	B	606	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	D	404[B]	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	b	607	CLA	CMD-C2D-C1D	6.47	136.12	124.73
37	a	408[B]	PHO	C2B-C1B-NB	6.46	114.10	109.43
23	B	614	CLA	C2D-C1D-ND	6.45	116.51	110.13
23	A	406[B]	CLA	CMD-C2D-C1D	6.43	136.06	124.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	CHD-C4C-C3C	-6.43	115.40	124.77
23	a	407[A]	CLA	C2D-C1D-ND	6.42	116.48	110.13
23	D	404[B]	CLA	CMD-C2D-C1D	6.42	136.03	124.73
23	b	613	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
23	B	615	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
23	a	407[A]	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
37	a	416[B]	PHO	C2B-C1B-NB	6.41	114.06	109.43
23	c	502	CLA	CMD-C2D-C1D	6.40	136.00	124.73
23	C	507	CLA	CHD-C4C-C3C	-6.40	115.44	124.77
23	B	616	CLA	C2D-C1D-ND	6.39	116.45	110.13
23	B	603	CLA	CHD-C4C-C3C	-6.38	115.47	124.77
23	b	610	CLA	O2D-CGD-CBD	6.38	122.38	111.23
23	B	601	CLA	CHD-C4C-C3C	-6.38	115.47	124.77
23	B	613	CLA	CMD-C2D-C1D	6.37	135.95	124.73
23	B	610	CLA	CMD-C2D-C1D	6.37	135.94	124.73
23	B	605	CLA	CMD-C2D-C1D	6.36	135.93	124.73
23	C	509	CLA	CHD-C4C-C3C	-6.35	115.51	124.77
23	c	512	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
23	c	512	CLA	C2D-C1D-ND	6.34	116.40	110.13
37	a	408[A]	PHO	C2B-C1B-NB	6.33	114.01	109.43
23	c	510	CLA	C2D-C1D-ND	6.31	116.38	110.13
23	C	510	CLA	O2D-CGD-CBD	6.31	122.26	111.23
23	D	404[A]	CLA	C2D-C1D-ND	6.30	116.37	110.13
23	B	606	CLA	O2D-CGD-CBD	6.30	122.25	111.23
23	b	603	CLA	C2D-C1D-ND	6.29	116.36	110.13
23	C	514	CLA	C4A-NA-C1A	-6.29	103.81	106.68
23	A	404[A]	CLA	C4A-NA-C1A	-6.29	103.81	106.68
23	a	409	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
23	c	513	CLA	CHD-C4C-C3C	-6.28	115.61	124.77
37	D	401[A]	PHO	C4D-ND-C1D	-6.28	101.35	108.87
23	b	605	CLA	O2D-CGD-CBD	6.27	122.18	111.23
23	a	407[B]	CLA	C2D-C1D-ND	6.26	116.32	110.13
23	B	601	CLA	C2D-C1D-ND	6.26	116.32	110.13
23	A	404[B]	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	A	405[B]	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	B	609	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	a	406[B]	CLA	C2D-C1D-ND	6.22	116.28	110.13
23	b	611	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	B	608	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	a	406[B]	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
23	b	606	CLA	CMD-C2D-C1D	6.21	135.66	124.73
26	F	103	SQD	O47-C7-C8	6.21	124.91	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	CHD-C4C-C3C	-6.20	115.73	124.77
23	c	511	CLA	C4A-NA-C1A	-6.20	103.85	106.68
26	B	620	SQD	O6-C1-C2	6.20	117.69	108.27
23	C	515	CLA	C2D-C1D-ND	6.20	116.26	110.13
23	b	611	CLA	C2D-C1D-ND	6.20	116.26	110.13
23	C	515	CLA	CHD-C4C-C3C	-6.19	115.75	124.77
23	b	616	CLA	C2D-C1D-ND	6.19	116.25	110.13
23	C	504	CLA	CHD-C4C-C3C	-6.18	115.76	124.77
23	C	513	CLA	CHD-C4C-C3C	-6.18	115.76	124.77
23	b	612	CLA	CHD-C4C-C3C	-6.17	115.77	124.77
23	c	511	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	B	613	CLA	C2D-C1D-ND	6.17	116.23	110.13
23	d	401[B]	CLA	C4A-NA-C1A	-6.16	103.87	106.68
23	B	604	CLA	CMD-C2D-C1D	6.16	135.57	124.73
23	B	602	CLA	CHD-C4C-C3C	-6.15	115.81	124.77
23	a	407[B]	CLA	CMD-C2D-C1D	6.15	135.55	124.73
23	C	505	CLA	CMD-C2D-C1D	6.14	135.55	124.73
23	b	610	CLA	CMD-C2D-C1D	6.14	135.54	124.73
23	c	508	CLA	C2D-C1D-ND	6.14	116.20	110.13
23	A	405[A]	CLA	C2D-C1D-ND	6.12	116.18	110.13
23	B	601	CLA	CMD-C2D-C1D	6.11	135.49	124.73
23	c	511	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	c	509	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	C	511	CLA	CMD-C2D-C1D	6.10	135.47	124.73
23	C	505	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	b	609	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	D	404[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.73
23	A	407	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
23	C	510	CLA	C2D-C1D-ND	6.10	116.16	110.13
23	b	605	CLA	C4A-NA-C1A	-6.09	103.90	106.68
37	D	401[B]	PHO	C2B-C1B-NB	6.09	113.83	109.43
23	c	510	CLA	C1-C2-C3	-6.09	116.22	126.20
23	D	405	CLA	CMD-C2D-C1D	6.08	135.43	124.73
23	c	506	CLA	C4A-NA-C1A	-6.08	103.91	106.68
23	a	405[B]	CLA	CHD-C4C-C3C	-6.08	115.91	124.77
23	b	606	CLA	C2D-C1D-ND	6.07	116.14	110.13
23	B	608	CLA	C2D-C1D-ND	6.07	116.13	110.13
23	a	405[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.73
23	B	609	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	a	407[B]	CLA	CHD-C4C-C3C	-6.06	115.94	124.77
23	B	609	CLA	CMD-C2D-C1D	6.05	135.38	124.73
23	A	406[A]	CLA	C2D-C1D-ND	6.05	116.11	110.13

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C2D-C1D-ND	6.05	116.11	110.13
23	d	402	CLA	C2D-C1D-ND	6.05	116.11	110.13
23	b	601	CLA	CMD-C2D-C1D	6.03	135.35	124.73
23	a	405[A]	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	a	407[A]	CLA	C4A-NA-C1A	-6.02	103.93	106.68
23	C	511	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
23	C	509	CLA	C2D-C1D-ND	6.00	116.07	110.13
23	b	602	CLA	CMD-C2D-C1D	6.00	135.30	124.73
37	D	401[A]	PHO	C2B-C1B-NB	6.00	113.77	109.43
23	B	614	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
23	a	405[B]	CLA	CMD-C2D-C1D	5.99	135.28	124.73
23	D	404[B]	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
23	c	505	CLA	CMD-C2D-C1D	5.99	135.27	124.73
23	A	404[B]	CLA	C2D-C1D-ND	5.98	116.05	110.13
23	c	503	CLA	C2D-C1D-ND	5.97	116.03	110.13
23	c	513	CLA	C2D-C1D-ND	5.97	116.03	110.13
23	c	508	CLA	CHD-C4C-C3C	-5.96	116.08	124.77
23	c	505	CLA	C2D-C1D-ND	5.96	116.03	110.13
23	B	602	CLA	O2D-CGD-CBD	5.95	121.64	111.23
23	B	604	CLA	O2D-CGD-CBD	5.95	121.64	111.23
23	B	601	CLA	O2D-CGD-CBD	5.95	121.63	111.23
23	b	608	CLA	C4A-NA-C1A	-5.95	103.97	106.68
23	C	511	CLA	C2D-C1D-ND	5.95	116.01	110.13
23	b	609	CLA	CMD-C2D-C1D	5.94	135.20	124.73
23	C	505	CLA	CHD-C4C-C3C	-5.93	116.13	124.77
23	a	406[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.73
37	D	401[B]	PHO	C4D-ND-C1D	-5.92	101.78	108.87
23	b	602	CLA	CHD-C4C-C3C	-5.91	116.15	124.77
23	B	607	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
23	A	406[B]	CLA	C2D-C1D-ND	5.89	115.96	110.13
23	C	510	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.73
23	b	607	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	B	614	CLA	C4A-NA-C1A	-5.87	104.00	106.68
26	a	411[A]	SQD	O6-C1-C2	5.87	117.19	108.27
23	B	608	CLA	CMD-C2D-C1D	5.87	135.06	124.73
23	b	611	CLA	O2D-CGD-CBD	5.87	121.48	111.23
23	b	609	CLA	C4A-NA-C1A	-5.86	104.00	106.68
23	c	504	CLA	C2D-C1D-ND	5.86	115.93	110.13
23	c	509	CLA	C4A-NA-C1A	-5.86	104.01	106.68
23	B	603	CLA	C4A-NA-C1A	-5.85	104.01	106.68
26	C	501[B]	SQD	O6-C1-C2	5.85	117.16	108.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
23	c	503	CLA	C2C-C1C-NC	5.85	116.12	109.98
23	B	610	CLA	C3D-C2D-C1D	-5.84	97.86	105.83
23	B	615	CLA	C4A-NA-C1A	-5.84	104.02	106.68
26	b	620	SQD	O6-C1-C2	5.83	117.12	108.27
23	c	510	CLA	O2D-CGD-CBD	5.83	121.42	111.23
23	A	407	CLA	CMD-C2D-C1D	5.82	134.99	124.73
23	b	614	CLA	O2D-CGD-CBD	5.82	121.41	111.23
23	C	507	CLA	CMD-C2D-C1D	5.82	134.97	124.73
23	b	610	CLA	C2D-C1D-ND	5.81	115.88	110.13
23	d	401[B]	CLA	C2D-C1D-ND	5.81	115.88	110.13
23	B	611	CLA	O2D-CGD-CBD	5.81	121.38	111.23
23	C	511	CLA	C4A-NA-C1A	-5.80	104.03	106.68
23	d	401[A]	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	c	509	CLA	C2D-C1D-ND	5.79	115.86	110.13
23	b	616	CLA	CMD-C2D-C1D	5.79	134.93	124.73
23	a	405[B]	CLA	C2D-C1D-ND	5.79	115.86	110.13
23	B	602	CLA	CMD-C2D-C1D	5.79	134.92	124.73
37	a	416[A]	PHO	C1-C2-C3	-5.78	116.72	126.20
23	d	401[A]	CLA	C2C-C1C-NC	5.78	116.05	109.98
23	b	614	CLA	CHD-C4C-C3C	-5.77	116.35	124.77
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	c	507	CLA	CMD-C2D-C1D	5.77	134.89	124.73
23	B	612	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	A	406[A]	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	A	406[B]	CLA	C4A-NA-C1A	-5.77	104.05	106.68
23	A	406[B]	CLA	CHD-C4C-C3C	-5.77	116.37	124.77
23	c	502	CLA	C2D-C1D-ND	5.76	115.83	110.13
23	C	503	CLA	CHD-C4C-C3C	-5.76	116.37	124.77
23	c	512	CLA	CMD-C2D-C1D	5.76	134.87	124.73
23	B	605	CLA	O2D-CGD-CBD	5.75	121.28	111.23
37	a	416[A]	PHO	C4D-ND-C1D	-5.74	101.99	108.87
23	b	602	CLA	C2D-C1D-ND	5.74	115.81	110.13
23	c	506	CLA	O2D-CGD-CBD	5.74	121.26	111.23
23	b	604	CLA	O2D-CGD-CBD	5.73	121.25	111.23
23	a	409	CLA	O2D-CGD-CBD	5.72	121.24	111.23
23	b	615	CLA	CMD-C2D-C1D	5.72	134.80	124.73
23	c	509	CLA	CMD-C2D-C1D	5.71	134.78	124.73
23	c	504	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
23	c	510	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
23	C	512	CLA	CHD-C4C-C3C	-5.70	116.46	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C1-C2-C3	-5.70	116.86	126.20
23	C	507	CLA	O2D-CGD-CBD	5.69	121.19	111.23
23	C	503	CLA	C2D-C1D-ND	5.69	115.76	110.13
26	C	501[A]	SQD	C1-O5-C5	-5.69	102.61	113.72
37	D	401[A]	PHO	C3D-C4D-ND	5.69	115.00	107.71
23	C	503	CLA	C4A-NA-C1A	-5.69	104.08	106.68
23	c	503	CLA	CHD-C4C-C3C	-5.69	116.48	124.77
23	C	513	CLA	C2D-C1D-ND	5.68	115.75	110.13
23	C	510	CLA	C2C-C1C-NC	5.67	115.94	109.98
23	A	405[B]	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
23	A	404[A]	CLA	C2D-C1D-ND	5.67	115.73	110.13
23	c	514	CLA	C2D-C1D-ND	5.66	115.73	110.13
23	C	504	CLA	C2D-C1D-ND	5.66	115.73	110.13
23	C	515	CLA	CMD-C2D-C1D	5.66	134.69	124.73
23	c	506	CLA	C2D-C1D-ND	5.65	115.72	110.13
23	B	612	CLA	O2D-CGD-CBD	5.65	121.11	111.23
37	a	416[B]	PHO	C4D-ND-C1D	-5.64	102.11	108.87
23	c	507	CLA	C2C-C1C-NC	5.64	115.91	109.98
23	C	512	CLA	C2D-C1D-ND	5.64	115.71	110.13
23	B	604	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
23	b	605	CLA	C3D-C2D-C1D	-5.64	98.14	105.83
23	C	507	CLA	C2D-C1D-ND	5.64	115.70	110.13
23	b	614	CLA	CMD-C2D-C1D	5.63	134.64	124.73
24	D	406	BCR	C7-C8-C9	-5.63	117.91	126.23
23	B	602	CLA	C2D-C1D-ND	5.63	115.69	110.13
23	c	513	CLA	O2D-CGD-CBD	5.62	121.05	111.23
23	C	504	CLA	CMD-C2D-C1D	5.62	134.62	124.73
23	b	604	CLA	C2C-C1C-NC	5.61	115.88	109.98
23	b	615	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
23	b	606	CLA	O2D-CGD-CBD	5.61	121.03	111.23
23	c	510	CLA	CMD-C2D-C1D	5.60	134.59	124.73
23	A	405[B]	CLA	CMD-C2D-C1D	5.60	134.59	124.73
37	a	416[B]	PHO	C1-C2-C3	-5.60	117.02	126.20
34	b	622	HTG	C1-O5-C5	5.59	122.59	112.56
23	c	503	CLA	C3B-C2B-C1B	-5.57	100.60	107.17
23	B	603	CLA	C2C-C1C-NC	5.57	115.83	109.98
23	C	508	CLA	C2C-C1C-NC	5.55	115.81	109.98
26	B	620	SQD	O47-C7-C8	5.55	123.49	111.48
23	D	405	CLA	O2D-CGD-CBD	5.55	120.93	111.23
23	c	510	CLA	C2C-C1C-NC	5.55	115.81	109.98
23	b	607	CLA	C4A-NA-C1A	-5.55	104.15	106.68
23	b	613	CLA	C3D-C2D-C1D	-5.54	98.26	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C4A-NA-C1A	-5.54	104.15	106.68
23	D	404[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
23	d	402	CLA	CHD-C4C-C3C	-5.53	116.70	124.77
37	D	401[B]	PHO	C3D-C4D-ND	5.53	114.80	107.71
23	a	405[A]	CLA	C2C-C1C-NC	5.53	115.79	109.98
37	a	416[A]	PHO	C3D-C4D-ND	5.52	114.79	107.71
23	B	603	CLA	CMD-C2D-C1D	5.52	134.46	124.73
23	C	514	CLA	CMD-C2D-C1D	5.52	134.45	124.73
23	c	506	CLA	CMD-C2D-C1D	5.52	134.45	124.73
23	B	607	CLA	C2C-C1C-NC	5.51	115.77	109.98
23	a	405[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
23	c	507	CLA	C4A-NA-C1A	-5.50	104.17	106.68
23	C	508	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
37	a	416[B]	PHO	C3D-C4D-ND	5.50	114.75	107.71
23	C	506	CLA	C2C-C1C-NC	5.49	115.75	109.98
23	d	401[A]	CLA	CHD-C4C-C3C	-5.49	116.76	124.77
37	D	402[A]	PHO	C4D-ND-C1D	-5.49	102.29	108.87
23	a	407[A]	CLA	CMD-C2D-C1D	5.48	134.38	124.73
23	b	611	CLA	C4A-NA-C1A	-5.48	104.18	106.68
23	a	407[B]	CLA	C4A-NA-C1A	-5.47	104.18	106.68
23	C	508	CLA	C2D-C1D-ND	5.46	115.53	110.13
23	B	604	CLA	C2C-C1C-NC	5.46	115.71	109.98
23	b	604	CLA	C2D-C1D-ND	5.45	115.52	110.13
23	C	506	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
23	b	613	CLA	CMD-C2D-C1D	5.45	134.33	124.73
23	B	611	CLA	C3D-C2D-C1D	-5.45	98.40	105.83
24	Y	101	BCR	C33-C5-C6	-5.44	118.55	124.48
23	B	606	CLA	C4A-NA-C1A	-5.44	104.20	106.68
23	c	507	CLA	C2D-C1D-ND	5.43	115.50	110.13
23	b	608	CLA	CMD-C2D-C1D	5.43	134.30	124.73
23	d	401[A]	CLA	CMD-C2D-C1D	5.43	134.30	124.73
23	d	402	CLA	O2D-CGD-CBD	5.43	120.73	111.23
26	a	411[B]	SQD	O47-C7-C8	5.43	123.22	111.48
23	a	405[A]	CLA	C2D-C1D-ND	5.43	115.50	110.13
37	a	408[B]	PHO	C4D-ND-C1D	-5.43	102.37	108.87
23	C	514	CLA	C2D-C1D-ND	5.42	115.49	110.13
23	b	603	CLA	O2D-CGD-CBD	5.42	120.70	111.23
23	C	506	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
23	b	607	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
23	D	405	CLA	CHD-C4C-C3C	-5.40	116.91	124.77
23	C	515	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
23	b	604	CLA	CHD-C4C-C3C	-5.39	116.91	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403	BCR	C7-C8-C9	-5.39	118.26	126.23
23	c	509	CLA	O2D-CGD-CBD	5.38	120.64	111.23
23	C	513	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
23	c	505	CLA	CHD-C4C-C3C	-5.38	116.94	124.77
23	b	602	CLA	C3B-C2B-C1B	-5.37	100.83	107.17
23	c	514	CLA	C4A-NA-C1A	-5.37	104.23	106.68
23	b	608	CLA	C2D-C1D-ND	5.37	115.44	110.13
23	C	513	CLA	O2D-CGD-CBD	5.37	120.62	111.23
23	B	614	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
24	y	101	BCR	C33-C5-C6	-5.37	118.63	124.48
23	b	601	CLA	C4A-NA-C1A	-5.36	104.23	106.68
23	b	604	CLA	C1-C2-C3	-5.35	117.43	126.20
23	B	605	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
23	d	401[B]	CLA	CHD-C4C-C3C	-5.35	116.98	124.77
23	C	512	CLA	C2C-C1C-NC	5.34	115.59	109.98
23	a	406[B]	CLA	CMD-C2D-C1D	5.34	134.14	124.73
23	c	505	CLA	O2D-CGD-CBD	5.34	120.56	111.23
23	c	504	CLA	O2D-CGD-CBD	5.33	120.55	111.23
37	D	402[B]	PHO	C4D-ND-C1D	-5.32	102.49	108.87
23	a	405[B]	CLA	C4A-NA-C1A	-5.32	104.25	106.68
23	C	503	CLA	CMD-C2D-C1D	5.32	134.09	124.73
23	b	608	CLA	C2C-C1C-NC	5.32	115.57	109.98
23	c	514	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
37	a	408[B]	PHO	C3D-C4D-ND	5.31	114.51	107.71
23	B	616	CLA	C3C-C4C-NC	5.31	117.23	110.43
23	A	407	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
23	B	614	CLA	O2D-CGD-CBD	5.30	120.50	111.23
23	C	512	CLA	O2D-CGD-CBD	5.30	120.50	111.23
26	C	501[A]	SQD	C1-C2-C3	-5.30	98.86	110.01
23	c	508	CLA	C4A-NA-C1A	-5.29	104.27	106.68
37	D	402[A]	PHO	C3D-C4D-ND	5.28	114.48	107.71
23	a	405[B]	CLA	C2B-C1B-NB	5.28	115.80	110.33
23	B	613	CLA	CHD-C4C-C3C	-5.28	117.07	124.77
23	b	612	CLA	C2D-C1D-ND	5.28	115.35	110.13
40	v	201	HEC	CBC-CAC-C3C	-5.27	116.90	127.43
23	C	509	CLA	C3B-C2B-C1B	-5.26	100.96	107.17
23	b	607	CLA	C2C-C1C-NC	5.24	115.49	109.98
23	A	405[A]	CLA	C4A-NA-C1A	-5.24	104.29	106.68
23	B	612	CLA	CMD-C2D-C1D	5.24	133.96	124.73
23	C	505	CLA	O2D-CGD-CBD	5.24	120.39	111.23
23	B	603	CLA	C3D-C2D-C1D	-5.23	98.69	105.83
23	c	502	CLA	CHD-C4C-C3C	-5.23	117.14	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	t	103	BCR	C33-C5-C6	-5.23	118.78	124.48
23	D	404[A]	CLA	C2C-C1C-NC	5.23	115.48	109.98
23	A	406[B]	CLA	C2B-C1B-NB	5.23	115.75	110.33
23	c	513	CLA	C3B-C2B-C1B	-5.23	101.01	107.17
23	c	509	CLA	C2C-C1C-NC	5.23	115.47	109.98
34	D	412	HTG	C1'-S1-C1	5.23	111.74	100.45
23	C	506	CLA	O2D-CGD-CBD	5.22	120.36	111.23
34	B	623	HTG	C1'-S1-C1	5.22	111.73	100.45
34	c	522	HTG	C1'-S1-C1	5.21	111.70	100.45
23	A	404[A]	CLA	C2C-C1C-NC	5.20	115.44	109.98
23	c	512	CLA	O2D-CGD-CBD	5.20	120.31	111.23
23	b	613	CLA	C2C-C1C-NC	5.19	115.44	109.98
23	B	608	CLA	O2D-CGD-CBD	5.19	120.31	111.23
33	C	502	LMG	C7-O1-C1	-5.19	102.67	113.80
23	b	614	CLA	C4A-NA-C1A	-5.19	104.31	106.68
23	c	511	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
23	B	602	CLA	C4A-NA-C1A	-5.18	104.31	106.68
23	d	401[B]	CLA	O2D-CGD-CBD	5.18	120.28	111.23
23	C	510	CLA	C1-C2-C3	-5.18	117.72	126.20
23	B	616	CLA	C3B-C4B-NB	5.17	115.15	110.53
23	C	513	CLA	CMD-C2D-C1D	5.17	133.84	124.73
37	a	408[A]	PHO	C4D-ND-C1D	-5.17	102.68	108.87
26	b	620	SQD	O47-C7-C8	5.17	122.66	111.48
23	B	614	CLA	C2C-C1C-NC	5.17	115.41	109.98
23	b	611	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	b	612	CLA	CMD-C2D-C1D	5.16	133.81	124.73
23	A	405[B]	CLA	O2D-CGD-CBD	5.15	120.23	111.23
23	b	602	CLA	C2B-C1B-NB	5.15	115.66	110.33
23	b	609	CLA	C1-C2-C3	-5.15	117.76	126.20
37	D	402[B]	PHO	C3D-C4D-ND	5.13	114.29	107.71
23	a	407[B]	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
23	b	616	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	b	608	CLA	CHD-C4C-C3C	-5.13	117.29	124.77
23	B	606	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.77
23	B	607	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
23	d	401[B]	CLA	C2C-C1C-NC	5.12	115.36	109.98
23	B	614	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
23	B	612	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
23	b	611	CLA	C1-C2-C3	-5.12	117.81	126.20
23	C	506	CLA	CMD-C2D-C1D	5.12	133.74	124.73
23	b	614	CLA	C3B-C2B-C1B	-5.11	101.14	107.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	101	HEM	CHC-C4B-NB	5.11	129.93	124.42
23	A	405[A]	CLA	O2D-CGD-CBD	5.11	120.17	111.23
23	b	614	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	C	514	CLA	O2D-CGD-CBD	5.11	120.16	111.23
23	a	407[B]	CLA	O2D-CGD-CBD	5.10	120.14	111.23
23	B	613	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	c	512	CLA	C2C-C1C-NC	5.10	115.34	109.98
23	c	514	CLA	C2B-C1B-NB	5.10	115.61	110.33
23	A	407	CLA	C2C-C1C-NC	5.09	115.33	109.98
23	B	607	CLA	O2D-CGD-CBD	5.09	120.14	111.23
23	c	505	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
23	b	604	CLA	CMD-C2D-C1D	5.09	133.69	124.73
23	c	511	CLA	C2D-C1D-ND	5.09	115.16	110.13
23	B	615	CLA	CMD-C2D-C1D	5.09	133.69	124.73
23	B	615	CLA	C3D-C2D-C1D	-5.09	98.89	105.83
23	c	511	CLA	O2D-CGD-CBD	5.09	120.12	111.23
23	b	603	CLA	CMD-C2D-C1D	5.08	133.68	124.73
23	C	507	CLA	C2C-C1C-NC	5.08	115.32	109.98
23	C	508	CLA	C4A-NA-C1A	-5.08	104.36	106.68
23	a	406[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	C	503	CLA	O2D-CGD-O1D	-5.08	113.97	123.85
23	C	512	CLA	C1-C2-C3	-5.07	117.89	126.20
26	a	411[A]	SQD	O47-C7-C8	5.07	122.45	111.48
23	D	404[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	c	513	CLA	C4A-NA-C1A	-5.06	104.37	106.68
23	c	513	CLA	C2B-C1B-NB	5.06	115.57	110.33
23	b	608	CLA	O2D-CGD-CBD	5.06	120.07	111.23
23	c	514	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
23	C	515	CLA	O2D-CGD-CBD	5.06	120.07	111.23
23	c	511	CLA	C1-C2-C3	-5.05	117.92	126.20
23	c	508	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
23	b	610	CLA	C4A-NA-C1A	-5.05	104.38	106.68
23	B	616	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	A	405[B]	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
23	b	606	CLA	C2B-C1B-NB	5.03	115.54	110.33
23	d	402	CLA	C4A-NA-C1A	-5.03	104.38	106.68
23	D	404[B]	CLA	C2C-C1C-NC	5.03	115.27	109.98
23	a	406[B]	CLA	C2C-C1C-NC	5.03	115.26	109.98
23	c	505	CLA	C2C-C1C-NC	5.02	115.25	109.98
23	b	603	CLA	C3B-C2B-C1B	-5.02	101.26	107.17
23	c	513	CLA	CMD-C2D-C1D	5.01	133.55	124.73
23	B	613	CLA	C1-C2-C3	-5.01	117.99	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	508	CLA	C3D-C2D-C1D	-5.00	99.00	105.83
23	C	514	CLA	C2B-C1B-NB	5.00	115.51	110.33
23	D	404[B]	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
23	C	506	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
23	b	603	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	C	513	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	c	504	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	c	514	CLA	O2D-CGD-CBD	4.98	119.94	111.23
23	c	509	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	c	505	CLA	C3D-C2D-C1D	-4.98	99.03	105.83
23	C	514	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
23	b	603	CLA	C4A-NA-C1A	-4.97	104.41	106.68
23	d	402	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	a	407[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	C	511	CLA	C1-C2-C3	-4.96	118.07	126.20
23	D	404[B]	CLA	C3B-C2B-C1B	-4.96	101.32	107.17
26	a	411[A]	SQD	C1-O5-C5	-4.95	104.05	113.72
23	C	515	CLA	C2B-C1B-NB	4.95	115.46	110.33
23	c	503	CLA	CMD-C2D-C1D	4.94	133.44	124.73
37	a	408[A]	PHO	C3D-C4D-ND	4.94	114.04	107.71
24	b	617	BCR	C33-C5-C6	-4.94	119.09	124.48
23	A	407	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	A	405[A]	CLA	C2C-C1C-NC	4.93	115.17	109.98
23	C	511	CLA	C3B-C2B-C1B	-4.92	101.36	107.17
23	a	406[B]	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
23	a	407[B]	CLA	C2B-C1B-NB	4.92	115.43	110.33
23	C	511	CLA	C2C-C1C-NC	4.92	115.15	109.98
23	c	508	CLA	C2C-C1C-NC	4.92	115.15	109.98
23	A	405[B]	CLA	C2C-C1C-NC	4.92	115.15	109.98
23	C	504	CLA	C2C-C1C-NC	4.91	115.14	109.98
23	A	404[B]	CLA	C4A-NA-C1A	-4.91	104.44	106.68
23	b	604	CLA	C4A-NA-C1A	-4.91	104.44	106.68
23	a	406[A]	CLA	C2C-C1C-NC	4.90	115.13	109.98
23	B	613	CLA	C2C-C1C-NC	4.89	115.12	109.98
23	D	405	CLA	C2D-C1D-ND	4.89	114.97	110.13
23	b	602	CLA	C3D-C4D-ND	4.89	117.94	109.99
23	a	409	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	A	406[B]	CLA	C3D-C4D-ND	4.89	117.93	109.99
23	B	616	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
23	a	407[B]	CLA	C3D-C4D-ND	4.89	117.93	109.99
23	c	507	CLA	CHD-C4C-C3C	-4.88	117.65	124.77
26	f	102	SQD	O47-C7-C8	4.88	122.03	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	b	612	CLA	C2C-C1C-NC	4.87	115.10	109.98
23	a	409	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
23	a	409	CLA	C3D-C4D-ND	4.87	117.90	109.99
23	A	407	CLA	C2B-C1B-NB	4.87	115.37	110.33
23	B	608	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	C	507	CLA	C4A-NA-C1A	-4.85	104.47	106.68
23	B	603	CLA	O2D-CGD-O1D	-4.85	114.41	123.85
23	c	502	CLA	O2D-CGD-CBD	4.84	119.70	111.23
23	b	611	CLA	C2C-C1C-NC	4.84	115.07	109.98
23	c	503	CLA	O2D-CGD-CBD	4.84	119.70	111.23
23	b	607	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
23	c	506	CLA	C3D-C4D-ND	4.84	117.86	109.99
23	b	605	CLA	CHD-C1D-ND	-4.84	117.99	124.80
28	a	414[A]	PL9	C7-C8-C9	-4.84	118.50	126.83
23	C	515	CLA	C2C-C1C-NC	4.83	115.06	109.98
23	c	511	CLA	C2C-C1C-NC	4.83	115.06	109.98
23	b	601	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
23	a	405[A]	CLA	C3B-C2B-C1B	-4.83	101.47	107.17
23	B	602	CLA	C2C-C1C-NC	4.83	115.06	109.98
23	b	606	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	b	615	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	a	406[B]	CLA	C4A-NA-C1A	-4.82	104.48	106.68
23	B	601	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
23	b	606	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
23	d	402	CLA	C3B-C2B-C1B	-4.81	101.49	107.17
23	c	510	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
23	B	616	CLA	C4A-NA-C1A	-4.81	104.48	106.68
23	C	509	CLA	C4A-NA-C1A	-4.81	104.48	106.68
23	c	503	CLA	C1C-C2C-C3C	-4.81	101.92	106.98
23	C	512	CLA	C3D-C4D-ND	4.81	117.80	109.99
23	c	506	CLA	C2C-C1C-NC	4.81	115.03	109.98
23	b	605	CLA	O2D-CGD-O1D	-4.81	114.50	123.85
33	C	502	LMG	O1-C1-C2	4.80	115.57	108.27
23	b	613	CLA	C1-C2-C3	-4.80	118.33	126.20
23	B	616	CLA	C2C-C1C-NC	4.80	115.03	109.98
38	F	102	HEM	CAD-CBD-CGD	4.80	126.40	113.67
23	c	512	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
28	A	412[A]	PL9	C7-C8-C9	-4.80	118.56	126.83
23	C	504	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	B	604	CLA	C3C-C4C-NC	4.80	116.58	110.43
23	c	503	CLA	C3D-C2D-C1D	-4.79	99.29	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	402[B]	PHO	C1-C2-C3	-4.79	118.35	126.20
23	C	510	CLA	C3C-C4C-NC	4.79	116.56	110.43
23	C	510	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
23	C	504	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	c	502	CLA	C2C-C1C-NC	4.77	114.99	109.98
23	A	407	CLA	O2D-CGD-CBD	4.77	119.57	111.23
23	A	406[A]	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	d	401[B]	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
23	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.73
23	d	402	CLA	C2B-C1B-NB	4.76	115.27	110.33
23	d	401[A]	CLA	C4A-NA-C1A	-4.76	104.51	106.68
23	B	611	CLA	C1D-CHD-C4C	-4.76	115.90	126.02
26	b	620	SQD	C1-O5-C5	-4.76	104.43	113.72
23	C	505	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	B	607	CLA	C1C-C2C-C3C	-4.75	101.99	106.98
23	B	615	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	C	504	CLA	O2D-CGD-CBD	4.74	119.51	111.23
23	b	612	CLA	C4A-NA-C1A	-4.73	104.52	106.68
23	a	406[A]	CLA	O2D-CGD-CBD	4.73	119.49	111.23
23	B	614	CLA	C2B-C1B-NB	4.73	115.23	110.33
23	c	502	CLA	C4A-NA-C1A	-4.72	104.52	106.68
23	c	513	CLA	C3D-C2D-C1D	-4.72	99.40	105.83
23	B	611	CLA	CMC-C2C-C1C	4.71	132.40	125.03
23	C	510	CLA	CMD-C2D-C1D	4.71	133.03	124.73
23	c	503	CLA	C2B-C1B-NB	4.71	115.21	110.33
23	B	609	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	B	605	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
23	b	612	CLA	C1-C2-C3	-4.71	118.48	126.20
23	B	604	CLA	C4A-NA-C1A	-4.71	104.53	106.68
24	a	410	BCR	C38-C26-C25	-4.70	119.35	124.48
23	C	508	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	b	603	CLA	C1D-CHD-C4C	-4.70	116.03	126.02
23	d	401[B]	CLA	C3D-C4D-ND	4.69	117.61	109.99
23	A	404[A]	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	B	604	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	B	601	CLA	C4A-NA-C1A	-4.69	104.54	106.68
23	c	510	CLA	C4A-NA-C1A	-4.69	104.54	106.68
23	A	405[B]	CLA	C3D-C4D-ND	4.68	117.60	109.99
23	B	602	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
24	k	101	BCR	C29-C30-C25	4.68	117.24	110.44
23	a	409	CLA	C2B-C1B-NB	4.68	115.18	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C3B-C2B-C1B	-4.68	101.66	107.17
23	A	407	CLA	C3D-C4D-ND	4.68	117.59	109.99
23	B	610	CLA	O2A-CGA-CBA	4.67	126.08	111.83
23	B	601	CLA	C3D-C4D-ND	4.67	117.58	109.99
23	b	603	CLA	C2B-C1B-NB	4.67	115.17	110.33
23	c	502	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	c	511	CLA	C2B-C1B-NB	4.67	115.17	110.33
23	B	601	CLA	C2B-C1B-NB	4.67	115.17	110.33
23	B	607	CLA	CMD-C2D-C1D	4.67	132.95	124.73
23	c	514	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	a	406[B]	CLA	O2D-CGD-CBD	4.66	119.38	111.23
23	A	406[A]	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	C	508	CLA	C3D-C4D-ND	4.66	117.56	109.99
23	C	512	CLA	C3D-C2D-C1D	-4.66	99.48	105.83
23	C	512	CLA	C1C-C2C-C3C	-4.66	102.08	106.98
23	a	405[B]	CLA	C3D-C4D-ND	4.65	117.55	109.99
23	c	504	CLA	C2B-C1B-NB	4.65	115.15	110.33
34	d	408	HTG	C1'-S1-C1	4.64	110.47	100.45
23	C	504	CLA	C4A-NA-C1A	-4.64	104.56	106.68
23	C	515	CLA	C3D-C2D-C1D	-4.64	99.51	105.83
23	C	508	CLA	CHD-C1D-ND	-4.63	118.28	124.80
24	H	101	BCR	C38-C26-C25	-4.63	119.43	124.48
23	b	612	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
23	A	404[B]	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	C	512	CLA	CHD-C1D-ND	-4.62	118.30	124.80
23	d	401[A]	CLA	C3D-C4D-ND	4.62	117.50	109.99
23	b	606	CLA	C2C-C1C-NC	4.62	114.84	109.98
23	a	407[B]	CLA	CHD-C1D-ND	-4.62	118.30	124.80
23	c	510	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
33	m	101	LMG	O7-C10-C11	4.62	121.47	111.48
23	c	508	CLA	CHD-C1D-ND	-4.61	118.31	124.80
23	d	402	CLA	CHD-C1D-ND	-4.61	118.31	124.80
23	A	406[A]	CLA	O2D-CGD-CBD	4.61	119.28	111.23
23	C	515	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	B	615	CLA	CMB-C2B-C1B	4.60	132.43	125.42
23	B	616	CLA	O2D-CGD-O1D	-4.60	114.89	123.85
23	D	404[B]	CLA	C1-C2-C3	-4.60	118.66	126.20
23	B	608	CLA	C2C-C1C-NC	4.60	114.81	109.98
23	b	612	CLA	CAC-C3C-C4C	4.59	130.77	124.79
23	b	610	CLA	C3B-C2B-C1B	-4.59	101.75	107.17
23	A	404[B]	CLA	C2B-C1B-NB	4.59	115.09	110.33
23	b	607	CLA	C3C-C4C-NC	4.59	116.31	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C2C-C1C-NC	4.59	114.81	109.98
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	A	405[A]	CLA	C1C-C2C-C3C	-4.59	102.15	106.98
28	A	412[B]	PL9	C32-C33-C34	-4.59	117.12	127.62
23	b	605	CLA	C3B-C2B-C1B	-4.59	101.76	107.17
23	b	613	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	c	504	CLA	C3D-C4D-ND	4.58	117.44	109.99
23	A	406[B]	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	a	407[B]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	502	CLA	C3B-C2B-C1B	-4.58	101.77	107.17
23	C	513	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
26	F	103	SQD	C1-O5-C5	-4.57	104.79	113.72
23	b	615	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	B	608	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
23	B	612	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	B	611	CLA	C3D-C4D-ND	4.56	117.39	109.99
23	C	513	CLA	C3C-C4C-NC	4.56	116.27	110.43
23	c	512	CLA	C3B-C2B-C1B	-4.56	101.80	107.17
23	b	613	CLA	C4A-NA-C1A	-4.55	104.60	106.68
23	b	616	CLA	C2B-C1B-NB	4.55	115.04	110.33
23	c	505	CLA	C4A-NA-C1A	-4.55	104.61	106.68
23	C	510	CLA	C3B-C4B-NB	4.54	114.59	110.53
23	b	614	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	b	614	CLA	C2C-C1C-NC	4.54	114.75	109.98
23	a	407[A]	CLA	O2D-CGD-CBD	4.54	119.17	111.23
28	a	414[B]	PL9	C32-C33-C34	-4.54	117.24	127.62
23	c	504	CLA	C2C-C1C-NC	4.54	114.75	109.98
23	B	612	CLA	O2D-CGD-O1D	-4.54	115.02	123.85
23	b	603	CLA	C3D-C4D-ND	4.54	117.36	109.99
23	A	406[B]	CLA	C3D-C2D-C1D	-4.53	99.64	105.83
23	B	612	CLA	C3C-C4C-NC	4.53	116.24	110.43
23	A	405[A]	CLA	C2B-C1B-NB	4.53	115.03	110.33
23	b	614	CLA	C2B-C1B-NB	4.53	115.03	110.33
23	C	510	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	C	507	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	B	601	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	A	404[B]	CLA	O2D-CGD-CBD	4.53	119.14	111.23
23	a	406[B]	CLA	C1C-C2C-C3C	-4.52	102.22	106.98
23	C	508	CLA	C2B-C1B-NB	4.52	115.02	110.33
23	b	609	CLA	C3D-C4D-ND	4.52	117.34	109.99
23	b	616	CLA	O2D-CGD-O1D	-4.52	115.04	123.85
23	b	610	CLA	C3D-C2D-C1D	-4.52	99.66	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C2D-C1D-ND	4.52	114.60	110.13
23	a	409	CLA	CMD-C2D-C1D	4.52	132.69	124.73
23	b	607	CLA	CHD-C1D-ND	-4.52	118.44	124.80
23	C	507	CLA	C3D-C4D-ND	4.52	117.33	109.99
23	C	512	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
23	B	606	CLA	C2C-C1C-NC	4.52	114.73	109.98
23	b	610	CLA	C3D-C4D-ND	4.51	117.32	109.99
23	A	406[B]	CLA	O2D-CGD-CBD	4.51	119.12	111.23
23	B	603	CLA	C3C-C4C-NC	4.51	116.21	110.43
23	b	605	CLA	C2B-C1B-NB	4.51	115.00	110.33
28	A	412[A]	PL9	C32-C33-C34	-4.51	117.31	127.62
23	A	405[B]	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
28	A	412[B]	PL9	C7-C8-C9	-4.50	119.08	126.83
23	A	406[A]	CLA	CMB-C2B-C1B	4.50	132.27	125.42
23	b	604	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
23	A	405[A]	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	C	505	CLA	C3D-C4D-ND	4.50	117.30	109.99
23	C	511	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	d	402	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	b	605	CLA	C3D-C4D-ND	4.49	117.29	109.99
33	B	621	LMG	O7-C10-C11	4.49	121.20	111.48
23	b	616	CLA	C1D-CHD-C4C	-4.49	116.47	126.02
23	D	404[A]	CLA	C3C-C4C-NC	4.49	116.18	110.43
23	C	503	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
23	b	601	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	c	514	CLA	C3D-C4D-ND	4.49	117.28	109.99
23	b	611	CLA	C3B-C4B-NB	4.49	114.54	110.53
23	b	608	CLA	C3D-C4D-ND	4.48	117.27	109.99
23	B	613	CLA	O2D-CGD-CBD	4.48	119.06	111.23
23	b	604	CLA	C3B-C4B-NB	4.48	114.53	110.53
23	c	514	CLA	CHD-C1D-ND	-4.48	118.50	124.80
34	C	523	HTG	C1'-S1-C1	4.48	110.12	100.45
23	b	616	CLA	C3B-C2B-C1B	-4.48	101.89	107.17
23	b	610	CLA	O2A-CGA-CBA	4.47	125.47	111.83
23	c	502	CLA	O2D-CGD-O1D	-4.47	115.15	123.85
23	a	407[A]	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
23	a	405[B]	CLA	C1D-CHD-C4C	-4.46	116.54	126.02
23	b	609	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	C	505	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	b	608	CLA	C2B-C1B-NB	4.46	114.95	110.33
23	c	510	CLA	C1D-CHD-C4C	-4.46	116.55	126.02
23	b	601	CLA	C3B-C2B-C1B	-4.45	101.92	107.17

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	-4.45	116.56	126.02
23	b	613	CLA	C3C-C4C-NC	4.45	116.13	110.43
23	B	613	CLA	C4A-NA-C1A	-4.45	104.65	106.68
23	b	607	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	c	506	CLA	C3C-C4C-NC	4.45	116.13	110.43
23	C	509	CLA	C3C-C4C-NC	4.45	116.13	110.43
23	B	615	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	D	404[B]	CLA	CHD-C1D-ND	-4.45	118.54	124.80
23	C	508	CLA	O2D-CGD-CBD	4.45	119.00	111.23
23	b	612	CLA	C3C-C4C-NC	4.45	116.13	110.43
23	B	602	CLA	O2D-CGD-O1D	-4.45	115.19	123.85
23	B	605	CLA	C2B-C1B-NB	4.44	114.93	110.33
23	c	502	CLA	C3D-C4D-ND	4.44	117.21	109.99
23	c	507	CLA	C3D-C4D-ND	4.44	117.20	109.99
23	c	507	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
23	c	510	CLA	C3D-C4D-ND	4.43	117.19	109.99
23	b	603	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
23	A	406[B]	CLA	C2C-C1C-NC	4.43	114.63	109.98
23	b	615	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	a	406[B]	CLA	C3D-C4D-ND	4.43	117.18	109.99
26	f	102	SQD	C1-O5-C5	4.43	122.36	113.72
23	a	407[A]	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	c	504	CLA	C3B-C2B-C1B	-4.42	101.96	107.17
23	A	405[B]	CLA	C2B-C1B-NB	4.42	114.91	110.33
23	C	513	CLA	C1D-CHD-C4C	-4.42	116.63	126.02
23	a	405[A]	CLA	C3D-C4D-ND	4.42	117.17	109.99
23	C	506	CLA	C3B-C2B-C1B	-4.42	101.97	107.17
23	c	507	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	a	405[A]	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	b	607	CLA	C3B-C2B-C1B	-4.41	101.97	107.17
23	b	612	CLA	C3D-C4D-ND	4.41	117.16	109.99
23	a	406[A]	CLA	C1C-C2C-C3C	-4.41	102.34	106.98
23	a	409	CLA	C4A-NA-C1A	-4.41	104.67	106.68
23	B	602	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
23	c	508	CLA	C1C-C2C-C3C	-4.40	102.35	106.98
23	C	507	CLA	C3C-C4C-NC	4.40	116.07	110.43
23	b	611	CLA	C3C-C4C-NC	4.40	116.06	110.43
23	a	407[A]	CLA	C2B-C1B-NB	4.40	114.89	110.33
23	B	609	CLA	C3D-C4D-ND	4.39	117.13	109.99
23	a	406[A]	CLA	C2B-C1B-NB	4.39	114.88	110.33
23	c	502	CLA	C2B-C1B-NB	4.39	114.88	110.33
23	b	609	CLA	C3C-C4C-NC	4.39	116.06	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C2C-C1C-NC	4.39	114.59	109.98
23	C	515	CLA	C4A-NA-C1A	-4.39	104.68	106.68
37	D	402[A]	PHO	C1-C2-C3	-4.39	119.00	126.20
23	A	405[A]	CLA	C3B-C2B-C1B	-4.39	102.00	107.17
23	A	406[B]	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	c	504	CLA	CHD-C1D-ND	-4.39	118.63	124.80
23	c	514	CLA	C2C-C1C-NC	4.39	114.59	109.98
24	K	102	BCR	C7-C8-C9	-4.38	119.75	126.23
24	C	517	BCR	C32-C1-C6	-4.38	103.37	110.24
23	B	616	CLA	CMD-C2D-C1D	4.38	132.44	124.73
23	B	606	CLA	C3D-C4D-ND	4.38	117.11	109.99
23	C	503	CLA	C2B-C1B-NB	4.38	114.87	110.33
23	b	604	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	C	504	CLA	C3C-C4C-NC	4.37	116.03	110.43
23	B	606	CLA	CHD-C1D-ND	-4.37	118.65	124.80
23	C	512	CLA	C4A-NA-C1A	-4.37	104.69	106.68
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	D	405	CLA	C2C-C1C-NC	4.37	114.57	109.98
23	c	510	CLA	C3B-C4B-NB	4.37	114.43	110.53
23	C	513	CLA	C2B-C1B-NB	4.36	114.85	110.33
23	A	405[B]	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
23	d	401[A]	CLA	C1C-C2C-C3C	-4.36	102.39	106.98
23	C	511	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	C	509	CLA	C2C-C1C-NC	4.36	114.56	109.98
23	C	510	CLA	O2D-CGD-O1D	-4.36	115.36	123.85
23	A	404[B]	CLA	C2C-C1C-NC	4.36	114.56	109.98
23	b	605	CLA	C2C-C1C-NC	4.36	114.56	109.98
33	a	417	LMG	O7-C10-C11	4.36	120.90	111.48
33	C	522	LMG	O6-C5-C4	4.35	117.55	109.70
23	b	603	CLA	CAA-C2A-C3A	-4.35	101.23	113.00
32	E	101[A]	LHG	O7-C7-C8	4.35	120.90	111.48
23	b	614	CLA	O2D-CGD-O1D	-4.35	115.37	123.85
23	B	603	CLA	C3B-C2B-C1B	-4.35	102.04	107.17
23	b	602	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
28	A	412[B]	PL9	C7-C3-C4	4.35	120.49	116.91
23	b	610	CLA	C1-C2-C3	-4.34	119.08	126.20
23	C	511	CLA	C3D-C4D-ND	4.34	117.05	109.99
23	C	514	CLA	C3D-C4D-ND	4.34	117.05	109.99
23	b	615	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
23	C	508	CLA	C3D-C2D-C1D	-4.34	99.91	105.83
38	F	102	HEM	CHC-C4B-NB	4.34	129.09	124.42
23	c	510	CLA	C2B-C1B-NB	4.33	114.82	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C3D-C4D-ND	4.33	117.03	109.99
23	C	511	CLA	CHD-C1D-ND	-4.33	118.71	124.80
23	b	604	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
23	C	504	CLA	C3D-C4D-ND	4.33	117.02	109.99
23	b	601	CLA	C2B-C1B-NB	4.32	114.81	110.33
23	B	602	CLA	C3C-C4C-NC	4.32	115.97	110.43
23	B	614	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	c	502	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	a	409	CLA	C3C-C4C-NC	4.32	115.96	110.43
23	D	405	CLA	C2B-C1B-NB	4.32	114.80	110.33
23	B	607	CLA	C3D-C4D-ND	4.32	117.00	109.99
23	C	503	CLA	C2C-C1C-NC	4.31	114.51	109.98
23	B	612	CLA	CAC-C3C-C4C	4.31	130.40	124.79
23	C	514	CLA	C1D-CHD-C4C	-4.31	116.85	126.02
23	a	405[B]	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.38	110.53
23	C	510	CLA	C2B-C1B-NB	4.31	114.80	110.33
24	d	403	BCR	C29-C30-C25	4.31	116.70	110.44
23	c	512	CLA	C1D-CHD-C4C	-4.31	116.87	126.02
23	B	609	CLA	CHD-C1D-ND	-4.31	118.74	124.80
23	c	507	CLA	O2D-CGD-CBD	4.31	118.76	111.23
23	b	604	CLA	C3C-C4C-NC	4.30	115.94	110.43
32	E	101[B]	LHG	O7-C7-C8	4.30	120.79	111.48
23	B	607	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
23	B	607	CLA	C4A-NA-C1A	-4.30	104.72	106.68
23	c	512	CLA	C3B-C4B-NB	4.30	114.37	110.53
23	B	616	CLA	C2B-C1B-NB	4.30	114.79	110.33
23	C	507	CLA	CMB-C2B-C1B	4.30	131.97	125.42
23	A	406[A]	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	b	602	CLA	CHD-C1D-ND	-4.30	118.76	124.80
23	B	613	CLA	C3B-C4B-NB	4.29	114.36	110.53
23	a	407[A]	CLA	C2C-C1C-NC	4.29	114.49	109.98
23	b	611	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	B	610	CLA	C2C-C1C-NC	4.29	114.49	109.98
23	b	606	CLA	CHD-C1D-ND	-4.29	118.77	124.80
23	c	512	CLA	C3D-C4D-ND	4.28	116.95	109.99
23	B	608	CLA	C2B-C1B-NB	4.28	114.77	110.33
23	b	606	CLA	O2D-CGD-O1D	-4.28	115.52	123.85
23	B	605	CLA	C1-C2-C3	-4.28	119.19	126.20
33	C	526	LMG	O7-C10-C11	4.28	120.74	111.48
23	B	605	CLA	CHD-C1D-ND	-4.28	118.78	124.80
23	b	608	CLA	C1-C2-C3	-4.28	119.19	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	CLA	C2C-C1C-NC	4.28	114.47	109.98
23	b	610	CLA	C2C-C1C-NC	4.27	114.47	109.98
23	C	515	CLA	CHD-C1D-ND	-4.27	118.79	124.80
26	a	411[A]	SQD	C1-C2-C3	-4.27	101.02	110.01
23	D	404[B]	CLA	C3D-C4D-ND	4.27	116.93	109.99
23	B	614	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
23	B	609	CLA	C3C-C4C-NC	4.27	115.90	110.43
23	a	405[A]	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	b	610	CLA	C2B-C1B-NB	4.26	114.75	110.33
23	a	405[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	B	608	CLA	C4A-NA-C1A	-4.26	104.73	106.68
23	A	406[A]	CLA	CHD-C1D-ND	-4.26	118.81	124.80
23	C	514	CLA	C1-C2-C3	-4.26	119.22	126.20
23	a	406[A]	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	A	406[A]	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	D	405	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	C	508	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
23	c	509	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	a	406[A]	CLA	C4A-NA-C1A	-4.25	104.74	106.68
23	a	407[A]	CLA	CHD-C1D-ND	-4.25	118.81	124.80
23	B	605	CLA	C3C-C4C-NC	4.25	115.88	110.43
23	D	404[A]	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	d	401[B]	CLA	CHD-C1D-ND	-4.25	118.82	124.80
23	b	609	CLA	O2D-CGD-CBD	4.25	118.66	111.23
23	b	604	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	A	404[B]	CLA	C4B-C3B-C2B	-4.25	102.02	107.30
23	B	611	CLA	C3C-C4C-NC	4.25	115.87	110.43
23	C	503	CLA	C3D-C4D-ND	4.25	116.89	109.99
23	C	509	CLA	CHD-C1D-ND	-4.24	118.83	124.80
23	b	608	CLA	C3B-C4B-NB	4.24	114.32	110.53
23	A	404[A]	CLA	CHD-C1D-ND	-4.24	118.83	124.80
23	a	405[B]	CLA	C2C-C1C-NC	4.24	114.43	109.98
32	A	416[A]	LHG	O8-C23-O10	-4.23	113.04	123.63
23	A	407	CLA	C3C-C4C-NC	4.23	115.85	110.43
23	C	514	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	a	406[B]	CLA	C2B-C1B-NB	4.23	114.71	110.33
23	b	603	CLA	C3C-C4C-NC	4.23	115.85	110.43
23	a	406[A]	CLA	CAA-C2A-C3A	-4.22	101.59	113.00
23	d	401[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
28	a	414[A]	PL9	C32-C33-C34	-4.22	117.96	127.62
23	A	405[B]	CLA	CHD-C1D-ND	-4.22	118.86	124.80
23	b	609	CLA	C2C-C1C-NC	4.22	114.41	109.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	C3C-C4C-NC	4.22	115.83	110.43
23	B	615	CLA	C3C-C4C-NC	4.22	115.83	110.43
24	C	516	BCR	C33-C5-C6	-4.21	119.89	124.48
23	B	602	CLA	C3D-C4D-ND	4.21	116.84	109.99
23	b	606	CLA	C3D-C4D-ND	4.21	116.84	109.99
28	a	414[A]	PL9	C7-C3-C2	-4.21	118.42	123.39
23	C	509	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	B	605	CLA	C2C-C1C-NC	4.21	114.40	109.98
23	A	404[A]	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	A	404[B]	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	D	404[A]	CLA	C3D-C4D-ND	4.21	116.82	109.99
23	C	503	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
33	c	521	LMG	O6-C5-C4	4.20	117.27	109.70
23	B	607	CLA	C3C-C4C-NC	4.20	115.81	110.43
23	a	405[A]	CLA	CAA-C2A-C3A	-4.20	101.65	113.00
23	b	601	CLA	C2C-C1C-NC	4.20	114.39	109.98
23	d	401[A]	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
23	B	608	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	a	405[A]	CLA	C1D-CHD-C4C	-4.19	117.12	126.02
23	c	512	CLA	O2D-CGD-O1D	-4.19	115.70	123.85
28	A	412[B]	PL9	C7-C3-C2	-4.19	118.45	123.39
23	b	610	CLA	C3C-C4C-NC	4.18	115.79	110.43
23	b	613	CLA	C2B-C1B-NB	4.18	114.66	110.33
24	c	515	BCR	C11-C10-C9	-4.18	121.42	127.28
23	c	508	CLA	CMC-C2C-C1C	4.18	131.57	125.03
23	c	514	CLA	C1D-CHD-C4C	-4.18	117.14	126.02
23	B	613	CLA	C3B-C2B-C1B	-4.18	102.24	107.17
23	d	401[A]	CLA	O2D-CGD-CBD	4.18	118.53	111.23
23	C	506	CLA	C3D-C4D-ND	4.18	116.78	109.99
23	B	605	CLA	C3D-C4D-ND	4.18	116.77	109.99
23	c	511	CLA	C1D-CHD-C4C	-4.17	117.15	126.02
23	C	512	CLA	C3B-C4B-NB	4.17	114.26	110.53
24	B	618	BCR	C29-C30-C25	4.17	116.50	110.44
23	C	515	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
23	d	401[B]	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	b	602	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
23	C	511	CLA	C3C-C4C-NC	4.17	115.77	110.43
23	B	615	CLA	CHD-C1D-ND	-4.17	118.94	124.80
23	c	509	CLA	C3C-C4C-NC	4.17	115.77	110.43
23	a	406[A]	CLA	C3B-C2B-C1B	-4.17	102.26	107.17
23	A	404[A]	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	C	511	CLA	C1C-C2C-C3C	-4.16	102.60	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	C3C-C4C-NC	4.16	115.76	110.43
23	D	405	CLA	O2D-CGD-O1D	-4.16	115.75	123.85
23	C	509	CLA	O2D-CGD-O1D	-4.16	115.75	123.85
23	b	616	CLA	C3D-C4D-ND	4.16	116.75	109.99
23	A	404[B]	CLA	C3B-C4B-NB	4.16	114.24	110.53
33	d	409	LMG	O7-C10-C11	4.16	120.47	111.48
23	D	404[A]	CLA	O2D-CGD-CBD	4.15	118.49	111.23
23	b	601	CLA	CHD-C1D-ND	-4.15	118.96	124.80
23	b	602	CLA	CMC-C2C-C1C	4.15	131.52	125.03
23	C	514	CLA	C3C-C4C-NC	4.15	115.75	110.43
23	c	509	CLA	C1-C2-C3	-4.15	119.40	126.20
23	B	615	CLA	C3B-C2B-C1B	-4.15	102.28	107.17
23	B	612	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	b	608	CLA	C3B-C2B-C1B	-4.14	102.29	107.17
24	C	516	BCR	C15-C14-C13	-4.14	121.47	127.28
23	B	614	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	c	508	CLA	C2B-C1B-NB	4.14	114.62	110.33
23	c	511	CLA	C3D-C2D-C1D	-4.14	100.19	105.83
23	A	404[B]	CLA	CHD-C1D-ND	-4.13	118.98	124.80
23	D	405	CLA	CAC-C3C-C4C	4.13	130.17	124.79
23	b	611	CLA	C2B-C1B-NB	4.13	114.61	110.33
24	d	403	BCR	C15-C14-C13	-4.12	121.50	127.28
23	b	606	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
23	B	601	CLA	C3C-C4C-NC	4.12	115.71	110.43
23	c	513	CLA	C1D-CHD-C4C	-4.12	117.26	126.02
23	c	503	CLA	C4A-NA-C1A	-4.12	104.80	106.68
24	Y	101	BCR	C15-C14-C13	-4.12	121.50	127.28
23	B	615	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
23	D	404[B]	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
23	C	506	CLA	C3C-C4C-NC	4.12	115.70	110.43
23	B	604	CLA	C2B-C1B-NB	4.12	114.59	110.33
23	B	612	CLA	C2C-C1C-NC	4.12	114.31	109.98
23	A	407	CLA	CHD-C1D-ND	-4.12	119.01	124.80
23	b	608	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	D	404[A]	CLA	CHD-C1D-ND	-4.11	119.02	124.80
23	a	406[B]	CLA	C3B-C2B-C1B	-4.11	102.33	107.17
31	t	102	LMT	C3'-C4'-C5'	-4.11	101.82	110.93
23	b	613	CLA	C1C-C2C-C3C	-4.11	102.66	106.98
23	b	601	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
23	C	509	CLA	C3D-C4D-ND	4.10	116.66	109.99
24	T	102	BCR	C15-C16-C17	-4.10	115.13	123.52
23	a	406[A]	CLA	C1D-CHD-C4C	-4.10	117.30	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	404[B]	CLA	C2B-C1B-NB	4.10	114.58	110.33
23	A	405[B]	CLA	C4A-NA-C1A	-4.10	104.81	106.68
23	c	504	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
23	c	508	CLA	CMB-C2B-C1B	4.09	131.65	125.42
23	B	614	CLA	CAC-C3C-C4C	4.09	130.11	124.79
23	c	505	CLA	C2B-C1B-NB	4.08	114.56	110.33
23	B	613	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	d	401[A]	CLA	C3C-C4C-NC	4.08	115.66	110.43
23	b	612	CLA	O2D-CGD-CBD	4.08	118.37	111.23
23	c	511	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
23	c	507	CLA	CHD-C1D-ND	-4.08	119.06	124.80
23	c	513	CLA	C3D-C4D-ND	4.08	116.61	109.99
37	D	401[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
23	b	610	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
23	b	602	CLA	CAA-C2A-C3A	-4.07	101.99	113.00
38	F	102	HEM	CHD-C4C-NC	4.07	128.88	124.45
23	A	407	CLA	C4A-NA-C1A	-4.07	104.82	106.68
23	a	405[B]	CLA	C3B-C4B-NB	4.07	114.16	110.53
23	C	510	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
23	C	512	CLA	C2B-C1B-NB	4.07	114.54	110.33
23	c	507	CLA	C1C-C2C-C3C	-4.06	102.70	106.98
23	B	602	CLA	C1D-CHD-C4C	-4.06	117.38	126.02
23	D	404[A]	CLA	C1-C2-C3	-4.06	119.54	126.20
23	c	509	CLA	C3D-C4D-ND	4.06	116.59	109.99
23	B	601	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
23	a	406[A]	CLA	CMB-C2B-C1B	4.06	131.60	125.42
23	a	405[B]	CLA	C3B-C2B-C1B	-4.06	102.39	107.17
23	D	404[B]	CLA	O2D-CGD-CBD	4.06	118.32	111.23
23	b	608	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
23	B	603	CLA	CHD-C1D-ND	-4.05	119.10	124.80
23	c	511	CLA	C3D-C4D-ND	4.05	116.57	109.99
23	b	609	CLA	CHD-C1D-ND	-4.04	119.11	124.80
23	C	508	CLA	C1-C2-C3	-4.04	119.57	126.20
23	B	608	CLA	CHD-C1D-ND	-4.04	119.12	124.80
28	a	414[A]	PL9	C7-C3-C4	4.04	120.24	116.91
33	c	521	LMG	O7-C10-C11	4.04	120.22	111.48
23	c	507	CLA	C2B-C1B-NB	4.04	114.51	110.33
23	B	603	CLA	C1C-C2C-C3C	-4.04	102.74	106.98
23	B	608	CLA	C3B-C4B-NB	4.03	114.13	110.53
28	A	412[A]	PL9	C7-C3-C2	-4.03	118.63	123.39
23	c	503	CLA	C3D-C4D-ND	4.03	116.55	109.99
23	c	509	CLA	C1C-C2C-C3C	-4.03	102.74	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[B]	CLA	C4B-C3B-C2B	-4.03	102.29	107.30
23	B	616	CLA	C4C-C3C-C2C	-4.03	101.02	106.89
23	b	614	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	d	401[B]	CLA	C2B-C1B-NB	4.03	114.50	110.33
23	C	507	CLA	C2B-C1B-NB	4.03	114.50	110.33
24	C	516	BCR	C7-C8-C9	-4.03	120.28	126.23
23	A	404[A]	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
23	c	513	CLA	C2C-C1C-NC	4.03	114.21	109.98
23	C	510	CLA	C3D-C4D-ND	4.02	116.53	109.99
23	b	616	CLA	C3C-C4C-NC	4.02	115.58	110.43
23	c	506	CLA	C2B-C1B-NB	4.02	114.50	110.33
23	a	406[B]	CLA	CHD-C1D-ND	-4.02	119.15	124.80
23	B	606	CLA	C3C-C4C-NC	4.01	115.57	110.43
32	l	802[B]	LHG	O7-C7-C8	4.01	120.16	111.48
33	C	502	LMG	O7-C10-C11	4.01	120.16	111.48
23	b	613	CLA	O2A-CGA-O1A	-4.01	113.60	123.63
23	b	606	CLA	C4-C3-C5	4.01	122.18	115.23
23	b	609	CLA	C2B-C1B-NB	4.01	114.48	110.33
23	B	602	CLA	C2B-C1B-NB	4.00	114.48	110.33
23	b	607	CLA	C2B-C1B-NB	4.00	114.47	110.33
23	C	514	CLA	C2C-C1C-NC	4.00	114.18	109.98
23	C	507	CLA	C3D-C2D-C1D	-4.00	100.38	105.83
35	C	519[A]	DGD	O2G-C1B-C2B	3.99	120.12	111.48
23	C	505	CLA	CHD-C1D-ND	-3.99	119.18	124.80
23	D	405	CLA	C3C-C4C-NC	3.99	115.55	110.43
23	c	505	CLA	CHD-C1D-ND	-3.99	119.19	124.80
23	B	615	CLA	C2B-C1B-NB	3.99	114.46	110.33
23	A	405[B]	CLA	CBC-CAC-C3C	-3.98	101.62	112.42
23	c	507	CLA	C3B-C4B-NB	3.98	114.09	110.53
23	d	402	CLA	C2C-C1C-NC	3.98	114.17	109.98
23	b	613	CLA	C3B-C4B-NB	3.98	114.08	110.53
28	a	414[B]	PL9	C7-C8-C9	-3.98	119.98	126.83
26	A	410	SQD	O47-C7-C8	3.98	120.08	111.48
24	h	101	BCR	C38-C26-C25	-3.98	120.15	124.48
40	V	202	HEC	CBC-CAC-C3C	-3.98	119.49	127.43
33	c	521	LMG	C3-C4-C5	3.97	117.44	110.23
23	A	406[B]	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
23	B	611	CLA	O2D-CGD-O1D	-3.97	116.12	123.85
34	V	203	HTG	C1-O5-C5	3.97	117.50	112.19
23	B	613	CLA	C3D-C4D-ND	3.97	116.44	109.99
23	B	611	CLA	CHD-C4C-NC	3.97	130.38	124.23
23	B	603	CLA	C2B-C1B-NB	3.97	114.44	110.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	520	LMG	O7-C10-C11	3.97	120.06	111.48
23	a	405[A]	CLA	O2D-CGD-CBD	3.96	118.16	111.23
23	a	407[B]	CLA	C2C-C1C-NC	3.96	114.14	109.98
35	C	518[A]	DGD	O2G-C1B-C2B	3.96	120.05	111.48
23	B	610	CLA	C3B-C2B-C1B	-3.96	102.50	107.17
23	A	404[A]	CLA	CAA-C2A-C3A	-3.96	102.30	113.00
23	B	601	CLA	C2C-C1C-NC	3.96	114.14	109.98
23	c	503	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
28	A	412[B]	PL9	C22-C23-C24	-3.95	118.58	127.62
23	B	611	CLA	C1-C2-C3	-3.95	119.72	126.20
23	D	405	CLA	C3D-C4D-ND	3.95	116.40	109.99
23	B	606	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
23	B	604	CLA	C3B-C4B-NB	3.94	114.05	110.53
23	c	509	CLA	C1D-CHD-C4C	-3.94	117.65	126.02
23	b	601	CLA	C3C-C4C-NC	3.94	115.48	110.43
23	b	615	CLA	CHD-C1D-ND	-3.94	119.26	124.80
23	B	609	CLA	C2B-C1B-NB	3.94	114.41	110.33
23	c	505	CLA	C3D-C4D-ND	3.94	116.39	109.99
23	C	515	CLA	C3C-C4C-NC	3.94	115.47	110.43
23	B	601	CLA	CHD-C1D-ND	-3.94	119.26	124.80
23	B	610	CLA	C3D-C4D-ND	3.94	116.38	109.99
23	C	507	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
37	D	401[B]	PHO	C1A-C2A-C3A	-3.93	99.10	102.84
23	B	614	CLA	CMC-C2C-C1C	3.93	131.18	125.03
23	A	404[A]	CLA	O2A-CGA-CBA	3.93	123.81	111.83
23	A	407	CLA	CAA-C2A-C3A	-3.93	102.39	113.00
23	b	614	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
23	b	608	CLA	CAC-C3C-C4C	3.93	129.90	124.79
23	d	402	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
23	B	603	CLA	C3D-C4D-ND	3.92	116.36	109.99
23	c	513	CLA	C1-C2-C3	-3.92	119.77	126.20
23	a	407[A]	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	C	503	CLA	C3C-C4C-NC	3.92	115.45	110.43
23	c	507	CLA	C1-C2-C3	-3.92	119.78	126.20
23	B	616	CLA	C3D-C4D-ND	3.92	116.35	109.99
23	c	512	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
28	D	407[B]	PL9	C42-C43-C44	-3.91	118.67	127.62
23	A	406[A]	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
23	a	405[B]	CLA	CHD-C1D-ND	-3.91	119.30	124.80
23	b	607	CLA	O2D-CGD-CBD	3.91	118.06	111.23
23	b	610	CLA	O2A-CGA-O1A	-3.91	113.86	123.63
23	b	605	CLA	C1D-CHD-C4C	-3.91	117.72	126.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	501[B]	SQD	C1-O5-C5	-3.91	106.09	113.72
23	a	405[B]	CLA	CAA-C2A-C3A	-3.91	102.44	113.00
23	c	512	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	B	604	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
23	a	406[B]	CLA	C1D-CHD-C4C	-3.90	117.72	126.02
23	D	404[A]	CLA	C3B-C4B-NB	3.90	114.01	110.53
23	b	611	CLA	C3B-C2B-C1B	-3.90	102.58	107.17
23	b	612	CLA	C3B-C4B-NB	3.89	114.01	110.53
23	B	606	CLA	C1C-C2C-C3C	-3.89	102.89	106.98
23	B	608	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
24	d	403	BCR	C40-C30-C25	-3.89	104.14	110.24
23	C	503	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
23	C	511	CLA	O2D-CGD-CBD	3.89	118.02	111.23
23	b	606	CLA	C3C-C4C-NC	3.88	115.41	110.43
23	c	513	CLA	C3C-C4C-NC	3.88	115.41	110.43
24	A	408	BCR	C15-C14-C13	-3.88	121.83	127.28
23	D	404[B]	CLA	C3C-C4C-NC	3.88	115.41	110.43
23	C	505	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
23	C	513	CLA	C4A-NA-C1A	-3.88	104.91	106.68
23	b	608	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
23	a	409	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
23	b	615	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
23	b	614	CLA	C1-C2-C3	-3.87	119.85	126.20
23	C	509	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
23	c	505	CLA	C3B-C4B-NB	3.87	113.99	110.53
34	b	622	HTG	O2-C2-C1	3.87	117.17	110.30
23	B	614	CLA	O2D-CGD-O1D	-3.87	116.32	123.85
23	C	506	CLA	CHD-C1D-ND	-3.87	119.36	124.80
23	b	608	CLA	C4B-C3B-C2B	-3.87	102.49	107.30
33	C	521	LMG	O7-C10-C11	3.86	119.84	111.48
23	B	606	CLA	C3B-C2B-C1B	-3.86	102.61	107.17
23	C	504	CLA	C2B-C1B-NB	3.86	114.33	110.33
23	b	602	CLA	C3C-C4C-NC	3.86	115.38	110.43
35	C	518[B]	DGD	O2G-C1B-C2B	3.86	119.83	111.48
23	B	610	CLA	CHD-C1D-ND	-3.86	119.38	124.80
23	c	506	CLA	C3B-C2B-C1B	-3.86	102.62	107.17
23	b	612	CLA	C2B-C1B-NB	3.85	114.32	110.33
23	C	507	CLA	CMC-C2C-C1C	3.85	131.06	125.03
33	C	526	LMG	C1-C2-C3	3.85	118.11	110.01
23	b	613	CLA	O2A-CGA-CBA	3.85	123.57	111.83
23	B	613	CLA	CHD-C1D-ND	-3.85	119.39	124.80
23	A	405[A]	CLA	CMC-C2C-C1C	3.84	131.04	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	D	407[A]	PL9	C42-C43-C44	-3.84	118.83	127.62
23	b	612	CLA	CMC-C2C-C1C	3.84	131.04	125.03
23	d	401[B]	CLA	C3C-C4C-NC	3.84	115.35	110.43
23	c	509	CLA	C2B-C1B-NB	3.84	114.31	110.33
33	C	521	LMG	O8-C28-C29	3.84	123.53	111.83
23	b	602	CLA	C2C-C1C-NC	3.83	114.01	109.98
23	a	406[A]	CLA	CHD-C1D-ND	-3.83	119.41	124.80
23	c	504	CLA	C3C-C4C-NC	3.83	115.34	110.43
23	c	511	CLA	CMC-C2C-C1C	3.83	131.02	125.03
23	B	605	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
23	b	602	CLA	C1-C2-C3	-3.82	119.94	126.20
23	C	515	CLA	C3B-C4B-NB	3.82	113.94	110.53
34	b	625	HTG	C1-O5-C5	3.82	119.41	112.56
23	A	407	CLA	C1-C2-C3	-3.82	119.94	126.20
23	c	508	CLA	C3C-C4C-NC	3.82	115.32	110.43
33	C	522	LMG	O7-C10-C11	3.82	119.74	111.48
23	A	404[A]	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
23	C	505	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	B	608	CLA	O2D-CGD-O1D	-3.81	116.43	123.85
23	b	612	CLA	C4-C3-C5	3.81	121.84	115.23
23	A	405[B]	CLA	CAA-C2A-C3A	-3.81	102.71	113.00
23	A	405[A]	CLA	CBC-CAC-C3C	-3.81	102.10	112.42
26	a	411[B]	SQD	O6-C1-C2	3.81	114.05	108.27
23	b	606	CLA	C3B-C4B-NB	3.81	113.93	110.53
23	B	604	CLA	C3D-C2D-C1D	-3.81	100.64	105.83
23	C	504	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
23	C	509	CLA	CMB-C2B-C1B	3.80	131.21	125.42
23	c	505	CLA	C1-O2A-CGA	3.80	125.86	116.65
23	b	604	CLA	CMC-C2C-C1C	3.80	130.98	125.03
23	A	404[A]	CLA	O2D-CGD-CBD	3.80	117.88	111.23
23	B	612	CLA	C1-C2-C3	-3.80	119.97	126.20
23	b	608	CLA	CHD-C1D-ND	-3.80	119.46	124.80
23	d	401[A]	CLA	C2B-C1B-NB	3.80	114.26	110.33
23	a	406[A]	CLA	C3C-C4C-NC	3.80	115.29	110.43
23	b	609	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
24	c	516	BCR	C7-C8-C9	-3.79	120.63	126.23
23	B	610	CLA	CAA-C2A-C3A	-3.79	102.76	113.00
23	B	606	CLA	O2D-CGD-O1D	-3.78	116.48	123.85
28	a	414[B]	PL9	C7-C3-C4	3.78	120.03	116.91
23	b	616	CLA	O2A-CGA-CBA	3.78	123.37	111.83
23	C	507	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
28	a	414[B]	PL9	C7-C3-C2	-3.78	118.93	123.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	411[A]	LHG	O8-C23-O10	-3.78	114.17	123.63
23	A	405[A]	CLA	CHD-C1D-ND	-3.78	119.48	124.80
24	D	406	BCR	C29-C30-C25	3.77	115.92	110.44
23	c	505	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
23	C	506	CLA	C1-O2A-CGA	3.77	125.78	116.65
23	b	607	CLA	C3B-C4B-NB	3.77	113.90	110.53
23	a	409	CLA	CHD-C1D-ND	-3.77	119.49	124.80
23	b	616	CLA	C2C-C1C-NC	3.77	113.94	109.98
23	B	609	CLA	O2D-CGD-CBD	3.77	117.82	111.23
26	B	620	SQD	C3-C4-C5	3.77	117.07	110.23
23	a	405[B]	CLA	O2D-CGD-CBD	3.77	117.82	111.23
33	C	522	LMG	C3-C4-C5	3.77	117.06	110.23
23	b	612	CLA	C3D-C2D-C1D	-3.77	100.69	105.83
23	B	610	CLA	C1D-CHD-C4C	-3.76	118.02	126.02
23	b	614	CLA	C1D-CHD-C4C	-3.76	118.02	126.02
23	B	612	CLA	CHD-C1D-ND	-3.76	119.51	124.80
23	c	512	CLA	C3C-C4C-NC	3.76	115.25	110.43
23	c	502	CLA	CAC-C3C-C4C	3.76	129.68	124.79
23	c	508	CLA	C3D-C4D-ND	3.76	116.10	109.99
23	b	612	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
23	B	602	CLA	CAA-C2A-C3A	-3.76	102.84	113.00
28	d	404[A]	PL9	C42-C43-C44	-3.76	119.02	127.62
23	c	512	CLA	C4A-NA-C1A	-3.76	104.97	106.68
23	d	401[B]	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
23	b	611	CLA	C4B-C3B-C2B	-3.75	102.63	107.30
28	a	414[B]	PL9	C27-C28-C29	-3.75	119.04	127.62
26	C	501[B]	SQD	O47-C7-C8	3.75	119.59	111.48
23	C	513	CLA	C3D-C4D-ND	3.75	116.08	109.99
23	b	611	CLA	CHD-C1D-ND	-3.74	119.53	124.80
28	A	412[A]	PL9	C22-C23-C24	-3.74	119.05	127.62
23	B	608	CLA	C3C-C4C-NC	3.74	115.22	110.43
23	C	513	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
23	C	506	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
38	F	102	HEM	CBD-CAD-C3D	-3.74	102.19	112.53
23	B	614	CLA	C1-C2-C3	-3.74	120.07	126.20
23	C	507	CLA	C1-C2-C3	-3.74	120.08	126.20
28	A	412[A]	PL9	C7-C3-C4	3.74	119.99	116.91
23	b	607	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
23	C	507	CLA	CAC-C3C-C4C	3.73	129.65	124.79
23	a	405[A]	CLA	CHD-C1D-ND	-3.73	119.55	124.80
23	b	603	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
23	a	406[B]	CLA	CAA-C2A-C3A	-3.73	102.91	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
23	C	508	CLA	C3B-C4B-NB	3.73	113.86	110.53
32	d	411[A]	LHG	O8-C23-C24	3.73	123.21	111.83
37	a	408[A]	PHO	O1D-CGD-CBD	-3.73	119.07	124.72
23	b	610	CLA	CHD-C1D-ND	-3.73	119.56	124.80
23	c	505	CLA	C3C-C4C-NC	3.73	115.20	110.43
23	c	506	CLA	CHD-C1D-ND	-3.73	119.56	124.80
23	D	405	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
23	B	615	CLA	CMC-C2C-C1C	3.73	130.85	125.03
23	b	605	CLA	CHD-C4C-NC	3.72	130.01	124.23
23	c	506	CLA	C3D-C2D-C1D	-3.72	100.75	105.83
23	B	603	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
23	B	613	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
28	d	404[B]	PL9	C7-C8-C9	-3.72	120.42	126.83
23	B	609	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
23	c	506	CLA	C4C-C3C-C2C	-3.72	101.48	106.89
23	B	614	CLA	C3B-C4B-NB	3.72	113.85	110.53
23	B	605	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
23	A	404[B]	CLA	C3C-C4C-NC	3.71	115.19	110.43
23	B	616	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
26	a	411[A]	SQD	C44-O6-C1	-3.71	105.84	113.80
23	c	514	CLA	C3B-C4B-NB	3.71	113.84	110.53
32	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.48
31	A	415	LMT	O5B-C5B-C4B	3.71	116.38	109.70
24	b	617	BCR	C7-C8-C9	-3.71	120.75	126.23
23	c	510	CLA	C1C-C2C-C3C	-3.70	103.08	106.98
23	a	409	CLA	C1C-C2C-C3C	-3.70	103.08	106.98
23	B	615	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
23	B	604	CLA	C3D-C4D-ND	3.70	116.00	109.99
23	B	607	CLA	CHD-C1D-ND	-3.70	119.60	124.80
23	b	604	CLA	CAC-C3C-C4C	3.69	129.59	124.79
23	C	508	CLA	C3C-C4C-NC	3.69	115.15	110.43
24	B	617	BCR	C33-C5-C6	-3.69	120.46	124.48
23	B	603	CLA	CAA-C2A-C3A	-3.69	103.04	113.00
23	D	404[A]	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
23	c	510	CLA	C3C-C4C-NC	3.68	115.15	110.43
23	c	511	CLA	C3C-C4C-NC	3.68	115.14	110.43
40	V	202	HEC	CBD-CAD-C3D	-3.68	102.37	112.53
23	c	508	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
23	A	407	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
28	a	414[A]	PL9	C15-C14-C16	3.67	121.60	115.23
23	D	405	CLA	CMB-C2B-C1B	3.67	131.01	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	B	613	CLA	C2B-C1B-NB	3.67	114.13	110.33
23	A	404[B]	CLA	CAA-C2A-C3A	-3.67	103.09	113.00
23	a	407[A]	CLA	C1D-CHD-C4C	-3.67	118.23	126.02
23	c	502	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	b	603	CLA	O2D-CGD-O1D	-3.66	116.72	123.85
23	a	405[A]	CLA	O2A-CGA-O1A	-3.66	114.47	123.63
23	B	615	CLA	C4-C3-C5	3.66	121.58	115.23
23	a	407[A]	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	B	614	CLA	C3C-C4C-NC	3.66	115.11	110.43
28	a	414[B]	PL9	C15-C14-C16	3.65	121.57	115.23
23	a	406[B]	CLA	C3C-C4C-NC	3.65	115.11	110.43
23	b	606	CLA	C1-C2-C3	-3.65	120.21	126.20
23	A	405[A]	CLA	CAA-C2A-C3A	-3.65	103.13	113.00
23	B	613	CLA	C4-C3-C5	3.65	121.56	115.23
23	A	406[B]	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
23	B	607	CLA	O2D-CGD-O1D	-3.65	116.75	123.85
35	C	519[B]	DGD	O2G-C1B-C2B	3.65	119.37	111.48
23	c	507	CLA	CAC-C3C-C4C	3.65	129.53	124.79
23	C	504	CLA	CHD-C1D-ND	-3.64	119.68	124.80
35	c	518[B]	DGD	O2G-C1B-C2B	3.64	119.35	111.48
23	C	506	CLA	C2B-C1B-NB	3.64	114.10	110.33
23	a	405[A]	CLA	C3C-C4C-NC	3.64	115.09	110.43
31	B	628	LMT	C1'-O5'-C5'	-3.64	106.62	113.72
35	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.48
23	c	504	CLA	CMB-C2B-C1B	3.63	130.95	125.42
23	d	401[A]	CLA	CHD-C1D-ND	-3.63	119.69	124.80
23	c	509	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
28	d	404[A]	PL9	C37-C38-C39	-3.63	119.33	127.62
23	B	609	CLA	CMB-C2B-C1B	3.62	130.94	125.42
38	f	101	HEM	CHA-C4D-ND	3.62	128.85	124.37
24	k	101	BCR	C7-C8-C9	-3.62	120.88	126.23
23	b	615	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
23	b	606	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
23	a	405[A]	CLA	C1-C2-C3	-3.61	120.28	126.20
23	B	610	CLA	O2A-CGA-O1A	-3.61	114.59	123.63
23	C	515	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
23	B	612	CLA	C4C-C3C-C2C	-3.61	101.64	106.89
23	c	510	CLA	CAC-C3C-C4C	3.61	129.49	124.79
23	b	613	CLA	CHD-C1D-ND	-3.61	119.72	124.80
23	c	507	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
23	d	401[A]	CLA	O2A-CGA-CBA	3.61	122.83	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	C1C-C2C-C3C	-3.61	103.19	106.98
23	c	504	CLA	C3B-C4B-NB	3.60	113.75	110.53
23	b	605	CLA	O2A-CGA-O1A	-3.60	114.62	123.63
33	B	621	LMG	O8-C28-C29	3.60	122.81	111.83
23	B	610	CLA	C2B-C1B-NB	3.60	114.06	110.33
23	B	610	CLA	C1C-C2C-C3C	-3.60	103.19	106.98
23	B	604	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
28	A	412[B]	PL9	C37-C38-C39	-3.60	119.39	127.62
23	A	405[A]	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
23	d	401[A]	CLA	C3B-C4B-NB	3.59	113.73	110.53
23	b	604	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
23	C	506	CLA	C3B-C4B-NB	3.59	113.73	110.53
23	a	407[B]	CLA	C1C-C2C-C3C	-3.59	103.21	106.98
23	A	404[B]	CLA	C3B-C2B-C1B	-3.58	102.95	107.17
28	a	414[A]	PL9	C30-C29-C31	3.58	121.44	115.23
23	A	406[A]	CLA	C3C-C4C-NC	3.58	115.02	110.43
23	b	604	CLA	C3D-C4D-ND	3.58	115.81	109.99
23	c	506	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
23	b	611	CLA	C1D-CHD-C4C	-3.58	118.42	126.02
23	A	406[A]	CLA	C1D-CHD-C4C	-3.57	118.42	126.02
23	B	605	CLA	O2D-CGD-O1D	-3.57	116.89	123.85
23	b	612	CLA	C4C-C3C-C2C	-3.57	101.69	106.89
38	F	102	HEM	C1B-NB-C4B	3.57	109.43	105.21
23	c	503	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
23	c	504	CLA	C1-C2-C3	-3.57	120.35	126.20
23	B	612	CLA	C2B-C1B-NB	3.57	114.02	110.33
23	c	502	CLA	C3B-C4B-NB	3.57	113.71	110.53
35	c	518[A]	DGD	O2G-C1B-C2B	3.56	119.19	111.48
23	A	407	CLA	C4C-C3C-C2C	-3.56	101.70	106.89
28	A	412[A]	PL9	C15-C14-C16	3.56	121.41	115.23
32	d	411[B]	LHG	O7-C7-C8	3.56	119.19	111.48
32	D	409[B]	LHG	O7-C7-C8	3.56	119.19	111.48
23	C	503	CLA	CHD-C1D-ND	-3.56	119.79	124.80
38	f	101	HEM	CHD-C1D-ND	3.56	128.25	124.42
23	c	512	CLA	C2B-C1B-NB	3.56	114.02	110.33
23	C	503	CLA	C1-C2-C3	-3.56	120.37	126.20
23	C	507	CLA	CHD-C1D-ND	-3.55	119.80	124.80
23	B	607	CLA	CAA-C2A-C3A	-3.55	103.40	113.00
23	B	616	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
24	A	408	BCR	C24-C23-C22	-3.55	120.98	126.23
23	D	405	CLA	C4-C3-C5	3.55	121.39	115.23
23	A	404[A]	CLA	C3C-C4C-NC	3.55	114.98	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	501[A]	SQD	O47-C7-C8	3.55	119.16	111.48
33	D	413	LMG	O7-C10-C11	3.55	119.16	111.48
23	c	510	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
23	b	611	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
23	C	503	CLA	C3B-C4B-NB	3.55	113.70	110.53
23	D	405	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
23	A	404[B]	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
23	a	405[B]	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
23	c	511	CLA	C3B-C4B-NB	3.54	113.69	110.53
32	L	101[B]	LHG	O7-C7-C8	3.54	119.14	111.48
28	a	414[A]	PL9	C27-C28-C29	-3.54	119.53	127.62
23	B	602	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
28	A	412[A]	PL9	C37-C38-C39	-3.53	119.54	127.62
23	C	515	CLA	C1-C2-C3	-3.53	120.41	126.20
23	D	405	CLA	C3B-C2B-C1B	-3.53	103.00	107.17
23	B	601	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
23	C	510	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
26	F	103	SQD	O8-S-C6	3.53	112.78	105.97
38	F	102	HEM	CHD-C1D-ND	3.53	128.22	124.42
23	b	610	CLA	CAA-C2A-C3A	-3.53	103.47	113.00
24	A	408	BCR	C40-C30-C25	-3.52	104.72	110.24
23	d	402	CLA	C3C-C4C-NC	3.52	114.94	110.43
28	A	412[A]	PL9	C27-C28-C29	-3.52	119.56	127.62
23	b	615	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	a	407[B]	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
26	a	411[A]	SQD	O9-S-C6	3.52	112.01	106.76
23	d	401[A]	CLA	C1-C2-C3	-3.52	120.43	126.20
23	B	605	CLA	O2A-CGA-O1A	-3.52	114.83	123.63
23	a	409	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
23	a	407[B]	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	B	609	CLA	C3B-C2B-C1B	-3.51	103.03	107.17
23	C	506	CLA	CMC-C2C-C1C	3.51	130.52	125.03
23	c	504	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
28	D	407[B]	PL9	C25-C24-C26	3.51	121.31	115.23
23	c	510	CLA	CHD-C1D-ND	-3.50	119.87	124.80
23	c	514	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	b	605	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
23	B	615	CLA	O2D-CGD-CBD	3.50	117.35	111.23
23	B	605	CLA	CHD-C4C-NC	3.50	129.66	124.23
23	A	407	CLA	C3B-C4B-NB	3.50	113.65	110.53
23	A	404[A]	CLA	O2A-CGA-O1A	-3.50	114.89	123.63
23	c	513	CLA	CMB-C2B-C1B	3.49	130.74	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[A]	CLA	C3B-C4B-NB	3.49	113.65	110.53
32	A	416[A]	LHG	O7-C7-C8	3.49	119.04	111.48
23	A	405[B]	CLA	C1D-CHD-C4C	-3.49	118.60	126.02
23	b	601	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
23	b	603	CLA	CHD-C1D-ND	-3.49	119.89	124.80
23	b	607	CLA	C4C-C3C-C2C	-3.49	101.81	106.89
23	c	505	CLA	C1D-CHD-C4C	-3.49	118.60	126.02
23	b	610	CLA	O2D-CGD-O1D	-3.49	117.06	123.85
26	a	412	SQD	O47-C7-C8	3.49	119.03	111.48
23	C	509	CLA	CBC-CAC-C3C	-3.49	102.97	112.42
28	d	404[A]	PL9	C40-C39-C41	3.49	121.28	115.23
24	d	403	BCR	C37-C22-C23	3.48	123.41	118.09
23	C	515	CLA	CMC-C2C-C1C	3.48	130.48	125.03
26	B	620	SQD	O7-S-C6	3.48	111.96	106.76
23	a	405[A]	CLA	O2A-CGA-CBA	3.48	122.45	111.83
23	C	512	CLA	C4-C3-C5	3.48	121.27	115.23
28	A	412[B]	PL9	C15-C14-C16	3.48	121.26	115.23
23	b	613	CLA	C3D-C4D-ND	3.48	115.64	109.99
23	b	604	CLA	C4B-C3B-C2B	-3.48	102.98	107.30
23	d	401[B]	CLA	C1-C2-C3	-3.48	120.50	126.20
23	D	405	CLA	CAA-C2A-C3A	-3.47	103.61	113.00
23	C	514	CLA	CHD-C1D-ND	-3.47	119.92	124.80
32	D	408[B]	LHG	O7-C7-C8	3.47	118.99	111.48
23	C	510	CLA	C4A-NA-C1A	-3.47	105.10	106.68
23	b	614	CLA	C3C-C4C-NC	3.47	114.87	110.43
23	B	602	CLA	C3B-C4B-NB	3.47	113.63	110.53
37	D	402[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
26	A	410	SQD	O8-S-C6	3.46	112.65	105.97
23	B	610	CLA	CAA-CBA-CGA	-3.46	103.39	113.21
23	A	405[A]	CLA	C3C-C4C-NC	3.46	114.86	110.43
23	b	609	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
28	a	414[A]	PL9	C37-C38-C39	-3.46	119.71	127.62
40	v	201	HEC	C4D-ND-C1D	3.46	111.46	105.82
23	b	601	CLA	CHD-C4C-NC	3.46	129.59	124.23
23	b	613	CLA	O2D-CGD-CBD	3.46	117.27	111.23
23	b	615	CLA	O2D-CGD-CBD	3.46	117.27	111.23
24	B	617	BCR	C7-C8-C9	-3.45	121.12	126.23
23	c	503	CLA	CBC-CAC-C3C	-3.45	103.06	112.42
37	a	416[B]	PHO	O2D-CGD-O1D	-3.45	117.13	123.85
37	a	408[B]	PHO	CMA-C3A-C4A	-3.45	107.17	114.61
23	a	406[A]	CLA	CHD-C4C-NC	3.45	129.58	124.23
23	B	611	CLA	CHB-C4A-NA	3.45	129.38	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	CMB-C2B-C1B	3.45	130.67	125.42
23	B	606	CLA	C2B-C1B-NB	3.45	113.90	110.33
23	c	513	CLA	O2A-CGA-CBA	3.45	122.35	111.83
32	A	416[B]	LHG	C5-O7-C7	-3.45	109.55	117.80
34	b	622	HTG	O5-C5-C4	3.45	115.91	109.70
23	D	405	CLA	CMC-C2C-C1C	3.44	130.42	125.03
23	D	404[A]	CLA	C2B-C1B-NB	3.44	113.90	110.33
23	C	509	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
23	C	510	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
23	c	503	CLA	CMB-C2B-C1B	3.44	130.65	125.42
23	B	611	CLA	C4C-C3C-C2C	-3.43	101.90	106.89
23	a	405[B]	CLA	C3C-C4C-NC	3.43	114.83	110.43
37	a	408[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
23	b	612	CLA	O2A-CGA-CBA	3.43	122.28	111.83
32	A	416[A]	LHG	O8-C23-C24	3.42	122.28	111.83
23	b	612	CLA	O2A-CGA-O1A	-3.42	115.06	123.63
37	D	402[B]	PHO	C1A-C2A-C3A	-3.42	99.58	102.84
35	c	517[B]	DGD	O2G-C1B-C2B	3.42	118.88	111.48
23	b	616	CLA	CMB-C2B-C1B	3.42	130.63	125.42
23	B	611	CLA	CHD-C1D-ND	-3.42	119.99	124.80
23	b	610	CLA	C4C-C3C-C2C	-3.42	101.92	106.89
23	d	401[B]	CLA	C1D-CHD-C4C	-3.42	118.76	126.02
28	A	412[B]	PL9	C17-C18-C19	-3.42	119.80	127.62
23	b	615	CLA	CMB-C2B-C1B	3.41	130.62	125.42
32	d	406[A]	LHG	O7-C7-C8	3.41	118.86	111.48
23	a	405[A]	CLA	C3B-C4B-NB	3.41	113.58	110.53
23	A	406[A]	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
23	d	401[B]	CLA	O2D-CGD-O1D	-3.41	117.21	123.85
23	a	409	CLA	O2A-CGA-CBA	3.41	122.22	111.83
24	y	101	BCR	C15-C14-C13	-3.41	122.50	127.28
26	C	501[B]	SQD	C1-C2-C3	-3.40	102.86	110.01
23	A	406[A]	CLA	C3B-C4B-NB	3.40	113.56	110.53
23	B	616	CLA	CAC-C3C-C4C	3.40	129.21	124.79
23	A	404[A]	CLA	C1-C2-C3	-3.40	120.63	126.20
23	C	508	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
23	B	609	CLA	C1D-CHD-C4C	-3.40	118.80	126.02
23	B	610	CLA	C4C-C3C-C2C	-3.39	101.95	106.89
23	c	506	CLA	CMB-C2B-C1B	3.39	130.59	125.42
23	c	511	CLA	CHD-C1D-ND	-3.39	120.03	124.80
26	a	412	SQD	O48-C23-C24	3.39	122.17	111.83
23	b	604	CLA	C1D-CHD-C4C	-3.39	118.82	126.02
23	b	616	CLA	CMC-C2C-C1C	3.39	130.33	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C1D-CHD-C4C	-3.39	118.82	126.02
24	c	515	BCR	C15-C14-C13	-3.39	122.53	127.28
23	B	610	CLA	CMB-C2B-C1B	3.38	130.57	125.42
23	C	515	CLA	CBC-CAC-C3C	-3.38	103.24	112.42
34	b	622	HTG	C1'-S1-C1	3.38	107.76	100.45
23	b	616	CLA	CHD-C4C-NC	3.38	129.48	124.23
23	B	609	CLA	CBC-CAC-C3C	-3.38	103.25	112.42
23	b	611	CLA	C1C-C2C-C3C	-3.38	103.42	106.98
35	C	520	DGD	O1G-C1A-C2A	3.38	122.14	111.83
23	C	510	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
28	d	404[B]	PL9	C37-C38-C39	-3.38	119.89	127.62
23	D	404[B]	CLA	O2A-CGA-CBA	3.38	122.13	111.83
23	B	613	CLA	CAC-C3C-C4C	3.37	129.18	124.79
23	D	405	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
23	c	507	CLA	C1D-CHD-C4C	-3.37	118.85	126.02
23	D	405	CLA	CHD-C1D-ND	-3.37	120.06	124.80
26	C	501[A]	SQD	C44-O6-C1	-3.37	106.57	113.80
23	c	507	CLA	CHC-C1C-C2C	-3.37	117.37	126.95
23	b	616	CLA	CHD-C1D-ND	-3.37	120.06	124.80
23	C	514	CLA	C1C-C2C-C3C	-3.37	103.44	106.98
23	b	606	CLA	CHD-C4C-NC	3.37	129.46	124.23
23	B	610	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
23	c	506	CLA	C1D-CHD-C4C	-3.37	118.86	126.02
23	B	607	CLA	C4-C3-C5	3.37	121.07	115.23
23	b	609	CLA	C1C-C2C-C3C	-3.37	103.44	106.98
23	a	406[B]	CLA	C1-C2-C3	-3.36	120.68	126.20
23	c	503	CLA	C3C-C4C-NC	3.36	114.74	110.43
23	C	511	CLA	C3B-C4B-NB	3.36	113.53	110.53
23	C	513	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
23	b	610	CLA	CHD-C4C-NC	3.36	129.44	124.23
23	C	512	CLA	CHD-C4C-NC	3.36	129.44	124.23
23	c	509	CLA	CHD-C1D-ND	-3.36	120.08	124.80
28	a	414[A]	PL9	C17-C18-C19	-3.36	119.94	127.62
23	B	608	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
23	c	505	CLA	CMB-C2B-C1B	3.36	130.53	125.42
23	B	613	CLA	C4B-C3B-C2B	-3.36	103.13	107.30
23	B	604	CLA	C4C-C3C-C2C	-3.36	102.01	106.89
31	b	627	LMT	C3'-C4'-C5'	-3.36	103.49	110.93
23	D	404[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
23	B	604	CLA	CMB-C2B-C1B	3.35	130.53	125.42
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.79
24	C	517	BCR	C7-C8-C9	-3.35	121.28	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	408	BCR	C16-C17-C18	-3.35	122.58	127.28
23	C	513	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
23	B	615	CLA	CED-O2D-CGD	3.35	123.51	115.92
23	C	505	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
28	D	407[A]	PL9	C17-C18-C19	-3.35	119.96	127.62
23	A	406[B]	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
33	C	526	LMG	O6-C1-C2	3.35	117.24	110.37
23	b	601	CLA	C1C-C2C-C3C	-3.34	103.46	106.98
32	l	802[A]	LHG	O7-C7-C8	3.34	118.72	111.48
35	c	519	DGD	O2G-C1B-C2B	3.34	118.71	111.48
23	B	614	CLA	O2A-CGA-CBA	3.34	122.02	111.83
23	a	406[B]	CLA	C3B-C4B-NB	3.34	113.51	110.53
23	c	510	CLA	C4B-C3B-C2B	-3.34	103.15	107.30
23	B	614	CLA	O2A-CGA-O1A	-3.34	115.28	123.63
23	B	612	CLA	C1D-CHD-C4C	-3.34	118.93	126.02
23	A	405[B]	CLA	O2D-CGD-O1D	-3.33	117.36	123.85
24	D	406	BCR	C38-C26-C25	-3.33	120.85	124.48
23	c	503	CLA	C1-C2-C3	-3.33	120.73	126.20
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
23	C	505	CLA	CMB-C2B-C1B	3.33	130.49	125.42
23	A	404[B]	CLA	O2A-CGA-CBA	3.33	121.99	111.83
23	B	601	CLA	CAC-C3C-C4C	3.33	129.12	124.79
32	A	416[B]	LHG	O7-C7-C8	3.33	118.68	111.48
31	B	630	LMT	O1'-C1'-C2'	3.33	113.33	108.27
23	c	510	CLA	CHC-C1C-C2C	-3.33	117.50	126.95
23	B	607	CLA	CBC-CAC-C3C	-3.33	103.40	112.42
23	d	401[A]	CLA	C1D-CHD-C4C	-3.33	118.95	126.02
23	C	510	CLA	CAC-C3C-C4C	3.32	129.12	124.79
32	d	411[B]	LHG	O8-C23-C24	3.32	121.97	111.83
23	A	407	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
23	b	615	CLA	C3B-C4B-NB	3.32	113.49	110.53
23	b	614	CLA	CMB-C2B-C1B	3.32	130.47	125.42
23	a	405[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	b	603	CLA	C3B-C4B-NB	3.32	113.49	110.53
23	b	607	CLA	C4B-C3B-C2B	-3.32	103.18	107.30
23	C	511	CLA	O2A-CGA-O1A	-3.32	115.33	123.63
23	b	613	CLA	C1D-CHD-C4C	-3.32	118.97	126.02
23	B	605	CLA	C4-C3-C5	3.31	120.98	115.23
23	b	611	CLA	C4C-C3C-C2C	-3.31	102.07	106.89
23	C	514	CLA	CHD-C4C-NC	3.31	129.37	124.23
23	b	612	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
23	B	603	CLA	O2A-CGA-O1A	-3.31	115.35	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	C4-C3-C5	3.31	120.97	115.23
26	a	411[A]	SQD	C45-O47-C7	-3.31	109.88	117.80
32	d	406[B]	LHG	O7-C7-C8	3.31	118.63	111.48
23	c	512	CLA	C1-O2A-CGA	3.30	124.65	116.65
23	d	402	CLA	C1D-CHD-C4C	-3.30	119.00	126.02
23	C	504	CLA	C1-C2-C3	-3.30	120.79	126.20
23	B	603	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
23	b	612	CLA	C2A-C1A-CHA	-3.30	118.14	123.87
23	B	602	CLA	CHD-C1D-ND	-3.30	120.16	124.80
23	a	405[A]	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
24	C	517	BCR	C33-C5-C6	-3.30	120.89	124.48
23	D	404[B]	CLA	O2A-CGA-O1A	-3.29	115.39	123.63
23	c	508	CLA	C1D-CHD-C4C	-3.29	119.02	126.02
23	C	510	CLA	CHD-C1D-ND	-3.29	120.18	124.80
24	y	101	BCR	C38-C26-C25	-3.29	120.90	124.48
23	B	609	CLA	O2A-CGA-CBA	3.29	121.85	111.83
23	A	406[B]	CLA	C3C-C4C-NC	3.28	114.64	110.43
26	F	103	SQD	C44-O6-C1	-3.28	106.75	113.80
23	c	511	CLA	CAC-C3C-C4C	3.28	129.06	124.79
23	A	405[B]	CLA	CMB-C2B-C1B	3.28	130.41	125.42
23	C	506	CLA	C1D-CHD-C4C	-3.28	119.06	126.02
23	c	513	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
23	b	610	CLA	CMB-C2B-C1B	3.27	130.40	125.42
23	D	404[B]	CLA	C1D-CHD-C4C	-3.27	119.06	126.02
23	B	612	CLA	CMC-C2C-C1C	3.27	130.15	125.03
26	C	501[A]	SQD	O9-S-C6	3.27	111.64	106.76
23	A	406[A]	CLA	O2A-CGA-O1A	-3.27	115.45	123.63
23	C	504	CLA	C1D-CHD-C4C	-3.27	119.07	126.02
37	a	416[A]	PHO	C4-C3-C5	3.27	120.90	115.23
26	a	411[B]	SQD	C45-O47-C7	-3.27	109.98	117.80
23	B	609	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
23	D	405	CLA	C3B-C4B-NB	3.27	113.45	110.53
23	B	607	CLA	CMC-C2C-C1C	3.26	130.13	125.03
23	d	401[A]	CLA	C4-C3-C5	3.26	120.89	115.23
23	C	503	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
28	A	412[B]	PL9	C27-C28-C29	-3.26	120.17	127.62
28	a	414[B]	PL9	C17-C18-C19	-3.26	120.17	127.62
23	b	601	CLA	C4C-C3C-C2C	-3.26	102.15	106.89
23	d	401[B]	CLA	O2A-CGA-CBA	3.26	121.76	111.83
23	b	608	CLA	CHC-C1C-C2C	-3.26	117.70	126.95
28	d	404[B]	PL9	C10-C9-C11	3.25	120.87	115.23
23	B	612	CLA	O2A-CGA-CBA	3.25	121.75	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	101	BCR	C28-C27-C26	-3.25	108.26	114.06
38	f	101	HEM	CAD-CBD-CGD	3.25	122.28	113.67
37	D	402[B]	PHO	O2D-CGD-O1D	-3.25	117.52	123.85
23	c	507	CLA	C3C-C4C-NC	3.25	114.59	110.43
37	a	408[A]	PHO	O2A-CGA-O1A	-3.25	115.51	123.63
23	c	509	CLA	C3B-C4B-NB	3.24	113.42	110.53
23	c	504	CLA	C1C-C2C-C3C	-3.24	103.57	106.98
23	C	512	CLA	CHC-C1C-C2C	-3.24	117.75	126.95
23	c	514	CLA	C3C-C4C-NC	3.24	114.58	110.43
23	c	513	CLA	CHD-C1D-ND	-3.24	120.25	124.80
23	a	406[B]	CLA	C4B-C3B-C2B	-3.24	103.28	107.30
23	b	602	CLA	CAC-C3C-C4C	3.24	129.00	124.79
23	c	506	CLA	C1C-C2C-C3C	-3.24	103.58	106.98
23	B	603	CLA	C4B-C3B-C2B	-3.23	103.28	107.30
23	C	511	CLA	C1D-CHD-C4C	-3.23	119.15	126.02
23	A	405[B]	CLA	C3B-C4B-NB	3.23	113.42	110.53
24	D	406	BCR	C11-C10-C9	-3.23	122.75	127.28
23	a	405[B]	CLA	CHD-C4C-NC	3.23	129.24	124.23
33	c	521	LMG	C9-C8-C7	-3.23	104.26	111.78
23	c	513	CLA	C4C-C3C-C2C	-3.23	102.20	106.89
23	c	510	CLA	O2A-CGA-CBA	3.23	121.67	111.83
23	b	605	CLA	C4C-C3C-C2C	-3.23	102.20	106.89
23	b	605	CLA	C4-C3-C5	3.23	120.83	115.23
23	c	508	CLA	C4-C3-C5	3.22	120.83	115.23
23	A	406[A]	CLA	C4B-C3B-C2B	-3.22	103.29	107.30
23	B	608	CLA	C1-C2-C3	-3.22	120.92	126.20
23	b	609	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
23	B	613	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
31	M	101	LMT	C3'-C4'-C5'	-3.22	103.79	110.93
23	b	610	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
23	d	401[A]	CLA	O2A-CGA-O1A	-3.22	115.57	123.63
23	C	504	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
23	C	514	CLA	CMC-C2C-C1C	3.22	130.06	125.03
23	c	512	CLA	CHD-C4C-NC	3.22	129.22	124.23
23	c	507	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
23	d	401[B]	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
28	D	407[A]	PL9	C25-C24-C26	3.22	120.81	115.23
23	a	407[A]	CLA	CAA-C2A-C3A	-3.22	104.31	113.00
23	A	404[B]	CLA	C1-C2-C3	-3.21	120.93	126.20
33	m	101	LMG	C8-O7-C10	-3.21	110.11	117.80
37	a	408[A]	PHO	O2A-CGA-CBA	3.21	121.63	111.83
23	d	402	CLA	C1C-C2C-C3C	-3.21	103.60	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	407	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
28	a	414[B]	PL9	C42-C43-C44	-3.21	120.27	127.62
37	D	402[B]	PHO	C4-C3-C5	3.21	120.80	115.23
31	B	628	LMT	C4B-C3B-C2B	3.21	116.46	110.83
23	B	608	CLA	C4B-C3B-C2B	-3.21	103.31	107.30
23	a	409	CLA	CAA-C2A-C3A	-3.21	104.33	113.00
23	c	513	CLA	C4-C3-C5	3.21	120.79	115.23
23	b	608	CLA	C3C-C4C-NC	3.20	114.53	110.43
24	b	619	BCR	C24-C23-C22	-3.20	121.50	126.23
23	C	511	CLA	O2A-CGA-CBA	3.20	121.60	111.83
23	b	602	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
23	b	613	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
26	f	102	SQD	O5-C1-C2	3.20	116.95	110.37
28	a	414[B]	PL9	C30-C29-C31	3.20	120.78	115.23
23	c	505	CLA	CAC-C3C-C4C	3.20	128.95	124.79
23	D	404[A]	CLA	C4B-C3B-C2B	-3.20	103.33	107.30
23	A	406[B]	CLA	CBC-CAC-C3C	-3.20	103.75	112.42
28	D	407[B]	PL9	C7-C8-C9	-3.20	121.32	126.83
23	a	405[B]	CLA	C1-C2-C3	-3.20	120.96	126.20
23	a	407[B]	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
23	b	609	CLA	CBC-CAC-C3C	-3.19	103.76	112.42
23	c	510	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
34	b	625	HTG	O5-C5-C4	3.19	115.45	109.70
23	b	603	CLA	O2A-CGA-CBA	3.19	121.56	111.83
33	c	520	LMG	O1-C7-C8	-3.19	103.06	110.82
23	C	503	CLA	CAC-C3C-C4C	3.19	128.94	124.79
28	A	412[A]	PL9	O1-C4-C3	-3.19	117.37	120.73
23	B	608	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	C	509	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
24	d	403	BCR	C21-C20-C19	-3.19	113.97	123.20
23	a	406[B]	CLA	CHD-C4C-NC	3.18	129.17	124.23
23	B	605	CLA	CMB-C2B-C1B	3.18	130.27	125.42
23	c	504	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	D	406	BCR	C10-C11-C12	-3.18	113.98	123.20
33	m	101	LMG	O8-C28-C29	3.18	121.53	111.83
23	b	604	CLA	CHD-C1D-ND	-3.18	120.33	124.80
23	b	603	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
33	C	522	LMG	O8-C28-C29	3.18	121.53	111.83
23	C	514	CLA	C4C-C3C-C2C	-3.18	102.27	106.89
23	C	509	CLA	O2A-CGA-CBA	3.18	121.53	111.83
23	a	407[A]	CLA	C3B-C4B-NB	3.18	113.37	110.53
24	Y	101	BCR	C16-C17-C18	-3.18	122.82	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
23	b	616	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
23	B	603	CLA	O2A-CGA-CBA	3.17	121.50	111.83
23	c	503	CLA	CHD-C1D-ND	-3.17	120.34	124.80
23	C	507	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
23	a	406[A]	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
23	c	503	CLA	C3B-C4B-NB	3.17	113.36	110.53
37	a	416[B]	PHO	C4-C3-C5	3.17	120.72	115.23
24	a	410	BCR	C7-C8-C9	-3.17	121.55	126.23
24	T	102	BCR	C11-C10-C9	-3.17	122.84	127.28
23	B	607	CLA	C1D-CHD-C4C	-3.17	119.29	126.02
23	c	511	CLA	C4-C3-C5	3.16	120.72	115.23
28	D	407[B]	PL9	C27-C28-C29	-3.16	120.39	127.62
23	b	611	CLA	CHC-C1C-C2C	-3.16	117.97	126.95
23	d	401[A]	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
32	D	409[A]	LHG	O8-C23-C24	3.16	121.46	111.83
23	A	404[A]	CLA	C4B-C3B-C2B	-3.16	103.38	107.30
28	D	407[B]	PL9	C17-C18-C19	-3.16	120.40	127.62
38	f	101	HEM	CBD-CAD-C3D	-3.16	103.80	112.53
23	B	605	CLA	C4C-C3C-C2C	-3.16	102.30	106.89
26	a	411[B]	SQD	C1-O5-C5	-3.15	107.56	113.72
33	z	101	LMG	O8-C28-C29	3.15	121.45	111.83
23	C	506	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
23	a	409	CLA	C4-C3-C5	3.15	120.70	115.23
23	b	612	CLA	CHD-C1D-ND	-3.15	120.36	124.80
23	A	404[B]	CLA	CHD-C4C-NC	3.15	129.12	124.23
23	a	407[A]	CLA	CHD-C4C-NC	3.15	129.12	124.23
37	D	401[B]	PHO	C1-C2-C3	-3.15	121.04	126.20
23	b	612	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
23	b	604	CLA	C6-C5-C3	-3.15	105.80	113.47
23	C	503	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
23	c	506	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
23	a	407[B]	CLA	CHD-C4C-NC	3.15	129.11	124.23
23	b	608	CLA	CMC-C2C-C1C	3.14	129.95	125.03
23	C	507	CLA	C4C-C3C-C2C	-3.14	102.32	106.89
26	b	620	SQD	C3-C4-C5	3.14	115.93	110.23
23	b	605	CLA	C1-C2-C3	-3.14	121.05	126.20
23	B	606	CLA	CMC-C2C-C1C	3.14	129.94	125.03
28	d	404[A]	PL9	C22-C23-C24	-3.14	120.44	127.62
23	A	406[B]	CLA	CMB-C2B-C1B	3.14	130.20	125.42
23	D	404[A]	CLA	C1D-CHD-C4C	-3.13	119.36	126.02
23	c	514	CLA	CAC-C3C-C4C	3.13	128.87	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	O2A-CGA-O1A	-3.13	115.79	123.63
23	d	401[B]	CLA	C4-C3-C5	3.13	120.67	115.23
28	A	412[A]	PL9	C17-C18-C19	-3.13	120.45	127.62
32	d	405[B]	LHG	O7-C7-C8	3.13	118.25	111.48
24	Y	101	BCR	C10-C11-C12	-3.13	114.13	123.20
23	A	405[A]	CLA	CMB-C2B-C1B	3.13	130.18	125.42
24	d	403	BCR	C38-C26-C25	-3.13	121.07	124.48
24	D	406	BCR	C37-C22-C23	3.13	122.87	118.09
23	B	613	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
23	A	405[A]	CLA	CAC-C3C-C4C	3.13	128.86	124.79
23	d	401[B]	CLA	C3B-C4B-NB	3.13	113.32	110.53
37	a	416[B]	PHO	C1A-C2A-C3A	-3.13	99.87	102.84
23	A	405[B]	CLA	CHD-C4C-NC	3.13	129.08	124.23
23	C	506	CLA	CBC-CAC-C3C	-3.13	103.95	112.42
28	a	414[A]	PL9	C25-C24-C26	3.12	120.65	115.23
23	A	405[A]	CLA	C3B-C4B-NB	3.12	113.32	110.53
23	c	503	CLA	CHC-C1C-C2C	-3.12	118.07	126.95
32	D	408[A]	LHG	O8-C23-O10	-3.12	115.82	123.63
23	B	608	CLA	CHD-C4C-NC	3.12	129.07	124.23
23	B	616	CLA	C1C-C2C-C3C	-3.12	103.70	106.98
37	D	402[A]	PHO	C4-C3-C5	3.12	120.64	115.23
23	b	609	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
23	B	610	CLA	C3B-C4B-NB	3.11	113.31	110.53
23	a	406[B]	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
23	C	506	CLA	C4A-NA-C1A	-3.11	105.26	106.68
23	a	407[B]	CLA	C1-C2-C3	-3.11	121.10	126.20
23	A	405[B]	CLA	C3C-C4C-NC	3.11	114.42	110.43
23	b	608	CLA	CBC-CAC-C3C	-3.11	103.99	112.42
28	a	414[A]	PL9	C42-C43-C44	-3.11	120.50	127.62
23	A	406[B]	CLA	CAA-C2A-C3A	-3.11	104.60	113.00
28	a	414[B]	PL9	C37-C38-C39	-3.11	120.51	127.62
37	D	401[B]	PHO	CBC-CAC-C3C	-3.11	108.42	112.87
23	c	506	CLA	CAC-C3C-C4C	3.11	128.83	124.79
23	a	409	CLA	C3B-C4B-NB	3.11	113.30	110.53
23	C	503	CLA	C4C-C3C-C2C	-3.10	102.37	106.89
32	D	409[A]	LHG	O7-C7-C8	3.10	118.19	111.48
23	c	509	CLA	C4C-C3C-C2C	-3.10	102.38	106.89
23	b	614	CLA	CMC-C2C-C1C	3.10	129.88	125.03
23	C	511	CLA	C4B-C3B-C2B	-3.10	103.45	107.30
23	b	601	CLA	C1-O2A-CGA	3.09	124.14	116.65
23	a	407[A]	CLA	CMB-C2B-C1B	3.09	130.12	125.42
23	a	406[A]	CLA	CMA-C3A-C2A	-3.09	102.03	113.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
23	a	406[B]	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
23	B	612	CLA	C3B-C4B-NB	3.09	113.29	110.53
23	B	606	CLA	CHD-C4C-NC	3.09	129.02	124.23
23	B	602	CLA	C4B-C3B-C2B	-3.09	103.47	107.30
23	b	601	CLA	C4-C3-C5	3.08	120.58	115.23
23	b	606	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	C	508	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
23	a	405[B]	CLA	O2A-CGA-CBA	3.08	121.22	111.83
33	C	526	LMG	C4-C3-C2	3.08	116.23	110.83
23	a	405[A]	CLA	C4-C3-C5	3.08	120.57	115.23
23	a	407[B]	CLA	CMC-C2C-C1C	3.08	129.84	125.03
23	A	406[B]	CLA	C4B-C3B-C2B	-3.08	103.48	107.30
23	b	613	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
23	C	508	CLA	CAC-C3C-C4C	3.08	128.79	124.79
23	B	606	CLA	O2A-CGA-O1A	-3.08	115.94	123.63
23	B	603	CLA	C3B-C4B-NB	3.07	113.28	110.53
26	f	102	SQD	C4-C3-C2	-3.07	105.43	110.83
28	a	414[B]	PL9	C25-C24-C26	3.07	120.56	115.23
23	A	406[B]	CLA	CHD-C4C-NC	3.07	129.00	124.23
23	C	505	CLA	C4-C3-C5	3.07	120.56	115.23
40	V	202	HEC	C4D-ND-C1D	3.07	110.83	105.82
26	C	501[B]	SQD	C44-O6-C1	-3.07	107.22	113.80
23	b	607	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
23	C	508	CLA	C4-C3-C5	3.07	120.55	115.23
23	c	511	CLA	CHD-C4C-NC	3.06	128.98	124.23
23	B	603	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
23	c	513	CLA	CHD-C4C-NC	3.06	128.98	124.23
35	C	518[A]	DGD	C2G-O2G-C1B	-3.06	110.47	117.80
23	B	608	CLA	CMA-C3A-C4A	-3.06	103.55	111.77
23	b	612	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	C	511	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
35	C	518[B]	DGD	C2G-O2G-C1B	-3.05	110.49	117.80
32	D	409[A]	LHG	O8-C23-O10	-3.05	115.99	123.63
32	a	420[A]	LHG	O7-C7-C8	3.05	118.08	111.48
23	B	601	CLA	CMB-C2B-C1B	3.05	130.07	125.42
23	d	402	CLA	CAC-C3C-C4C	3.05	128.76	124.79
23	B	607	CLA	C3B-C4B-NB	3.05	113.25	110.53
23	B	610	CLA	C4A-NA-C1A	-3.05	105.29	106.68
28	D	407[B]	PL9	C10-C9-C11	3.05	120.52	115.23
23	B	615	CLA	C3B-C4B-NB	3.05	113.25	110.53
23	a	406[B]	CLA	CMB-C2B-C1B	3.05	130.06	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	502	CLA	C4C-C3C-C2C	-3.05	102.46	106.89
23	c	503	CLA	CMC-C2C-C1C	3.04	129.79	125.03
23	c	505	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	c	502	CLA	C1D-CHD-C4C	-3.04	119.56	126.02
23	c	513	CLA	C1C-C2C-C3C	-3.04	103.79	106.98
23	a	405[B]	CLA	CHC-C1C-C2C	-3.03	118.32	126.95
28	a	414[A]	PL9	C35-C34-C36	3.03	120.49	115.23
23	B	601	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
34	B	622	HTG	C1'-S1-C1	3.03	107.00	100.45
32	d	411[A]	LHG	O7-C7-C8	3.03	118.04	111.48
23	A	406[A]	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
23	A	405[B]	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
23	c	509	CLA	O2A-CGA-CBA	3.03	121.07	111.83
23	d	402	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
35	h	102	DGD	O1G-C1A-C2A	3.03	121.07	111.83
23	b	603	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	C	514	CLA	C4-C3-C5	3.03	120.48	115.23
32	E	101[A]	LHG	O8-C23-C24	3.03	121.06	111.83
23	b	614	CLA	C3B-C4B-NB	3.02	113.23	110.53
23	C	512	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
35	h	102	DGD	O2G-C1B-C2B	3.02	118.02	111.48
23	A	404[B]	CLA	CMC-C2C-C1C	3.02	129.75	125.03
23	B	614	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
23	B	610	CLA	CMA-C3A-C4A	-3.02	103.66	111.77
24	Y	101	BCR	C37-C22-C23	3.02	122.70	118.09
34	B	622	HTG	O5-C1-C2	3.02	114.47	110.32
23	A	405[B]	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	C	505	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
23	b	614	CLA	CBC-CAC-C3C	-3.01	104.26	112.42
23	D	404[A]	CLA	O2A-CGA-CBA	3.01	121.00	111.83
23	c	509	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
33	a	417	LMG	C8-O7-C10	-3.01	110.60	117.80
23	a	407[B]	CLA	CMB-C2B-C1B	3.01	130.00	125.42
23	b	615	CLA	C11-C10-C8	-3.00	105.98	115.97
31	e	101	LMT	O1'-C1'-C2'	3.00	112.84	108.27
37	D	401[B]	PHO	O1D-CGD-CBD	-3.00	120.17	124.72
28	D	407[B]	PL9	C53-C6-C1	3.00	121.43	115.28
23	b	615	CLA	C4-C3-C5	3.00	120.44	115.23
23	D	404[A]	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
23	d	401[A]	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
23	a	409	CLA	CMB-C2B-C1B	3.00	129.99	125.42
23	a	405[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	O2A-CGA-O1A	-3.00	116.13	123.63
23	a	407[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
23	c	507	CLA	O2A-CGA-O1A	-3.00	116.13	123.63
23	C	513	CLA	CAC-C3C-C4C	3.00	128.69	124.79
23	B	607	CLA	C2B-C1B-NB	3.00	113.43	110.33
33	z	101	LMG	O7-C10-C11	3.00	117.96	111.48
23	c	503	CLA	O2A-CGA-CBA	2.99	120.96	111.83
23	c	504	CLA	C4-C3-C5	2.99	120.42	115.23
23	a	406[B]	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
23	C	505	CLA	O2A-CGA-O1A	-2.99	116.14	123.63
23	c	512	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
23	B	611	CLA	C2A-C1A-CHA	-2.99	118.68	123.87
23	b	609	CLA	CMC-C2C-C1C	2.99	129.71	125.03
28	a	414[B]	PL9	C35-C34-C36	2.99	120.42	115.23
38	f	101	HEM	CHD-C4C-NC	2.99	127.71	124.45
35	h	102	DGD	O1G-C1A-O1A	-2.99	116.16	123.63
23	C	503	CLA	O2A-CGA-CBA	2.99	120.94	111.83
23	b	614	CLA	CAC-C3C-C4C	2.98	128.67	124.79
37	a	416[A]	PHO	O2D-CGD-O1D	-2.98	118.05	123.85
37	a	416[A]	PHO	CBA-CAA-C2A	-2.98	105.00	113.78
23	a	405[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
24	d	403	BCR	C10-C11-C12	-2.98	114.57	123.20
24	h	101	BCR	C16-C15-C14	-2.97	117.43	123.52
28	a	414[A]	PL9	C10-C9-C11	2.97	120.39	115.23
23	B	611	CLA	C3B-C4B-NB	2.97	113.18	110.53
28	d	404[B]	PL9	C40-C39-C41	2.97	120.39	115.23
26	a	411[A]	SQD	O47-C7-O49	-2.97	116.75	123.70
23	d	401[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
23	A	404[A]	CLA	CMC-C2C-C1C	2.97	129.68	125.03
24	b	619	BCR	C15-C14-C13	-2.97	123.11	127.28
23	a	409	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
23	D	404[A]	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
28	A	412[A]	PL9	C20-C19-C21	2.97	120.38	115.23
23	b	606	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
23	c	510	CLA	C4-C3-C5	2.97	120.38	115.23
23	A	404[B]	CLA	C2A-C1A-CHA	-2.97	118.72	123.87
28	d	404[B]	PL9	C42-C43-C44	-2.97	120.83	127.62
24	k	101	BCR	C15-C14-C13	-2.96	123.12	127.28
23	b	602	CLA	C1C-C2C-C3C	-2.96	103.86	106.98
23	b	609	CLA	CAC-C3C-C4C	2.96	128.65	124.79
24	t	103	BCR	C11-C10-C9	-2.96	123.12	127.28
24	T	102	BCR	C7-C8-C9	-2.96	121.85	126.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	515	CLA	CMB-C2B-C1B	2.96	129.93	125.42
23	b	615	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
24	H	101	BCR	C16-C15-C14	-2.96	117.47	123.52
28	D	407[A]	PL9	C37-C38-C39	-2.96	120.85	127.62
23	B	601	CLA	CHD-C4C-NC	2.96	128.82	124.23
33	c	520	LMG	O8-C28-C29	2.96	120.85	111.83
23	b	608	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
23	c	512	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
23	A	407	CLA	O2A-CGA-CBA	2.96	120.84	111.83
23	B	613	CLA	C1D-CHD-C4C	-2.95	119.74	126.02
28	d	404[B]	PL9	C17-C18-C19	-2.95	120.86	127.62
28	A	412[B]	PL9	C53-C6-C1	2.95	121.33	115.28
23	c	514	CLA	O2A-CGA-CBA	2.95	120.84	111.83
28	a	414[B]	PL9	C22-C23-C24	-2.95	120.87	127.62
23	C	510	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
23	B	614	CLA	CBC-CAC-C3C	-2.95	104.42	112.42
32	A	416[A]	LHG	C5-O7-C7	-2.95	110.73	117.80
23	B	609	CLA	CMC-C2C-C1C	2.95	129.65	125.03
32	a	420[B]	LHG	O7-C7-C8	2.95	117.86	111.48
31	t	101	LMT	C3'-C4'-C5'	-2.95	104.39	110.93
23	A	406[B]	CLA	C1-C2-C3	-2.95	121.37	126.20
23	B	614	CLA	CHD-C4C-NC	2.95	128.80	124.23
23	c	504	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
26	C	501[A]	SQD	O48-C23-C24	2.95	120.82	111.83
38	f	101	HEM	CHB-C1B-NB	2.95	128.01	124.37
23	A	405[A]	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
23	D	405	CLA	C1C-C2C-C3C	-2.94	103.88	106.98
23	C	514	CLA	O2A-CGA-CBA	2.94	120.81	111.83
28	A	412[B]	PL9	C35-C34-C36	2.94	120.33	115.23
23	A	406[A]	CLA	O2A-CGA-CBA	2.94	120.80	111.83
23	B	601	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
23	c	505	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
23	b	602	CLA	C2A-C1A-CHA	-2.94	118.77	123.87
23	A	404[A]	CLA	C2A-C1A-CHA	-2.94	118.77	123.87
23	C	511	CLA	CMC-C2C-C1C	2.94	129.62	125.03
23	a	407[B]	CLA	C4-C3-C5	2.94	120.32	115.23
32	E	101[B]	LHG	O8-C23-C24	2.94	120.79	111.83
23	b	616	CLA	C1C-C2C-C3C	-2.94	103.89	106.98
23	C	503	CLA	O2A-CGA-O1A	-2.93	116.29	123.63
23	b	602	CLA	CMB-C2B-C1B	2.93	129.88	125.42
23	C	515	CLA	CHD-C4C-NC	2.93	128.78	124.23
23	A	405[A]	CLA	CHD-C4C-NC	2.93	128.78	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	CHD-C4C-NC	2.93	128.78	124.23
28	a	414[A]	PL9	C22-C23-C24	-2.93	120.92	127.62
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	c	512	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
23	b	614	CLA	CHD-C4C-NC	2.93	128.77	124.23
26	B	620	SQD	O48-C23-C24	2.93	120.76	111.83
38	f	101	HEM	C4D-ND-C1D	2.93	108.67	105.21
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	B	614	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
23	C	515	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
23	A	406[B]	CLA	C3B-C4B-NB	2.92	113.14	110.53
37	a	408[B]	PHO	C1A-C2A-C3A	-2.92	100.06	102.84
32	L	101[A]	LHG	O8-C23-C24	2.92	120.75	111.83
23	C	513	CLA	CHD-C1D-ND	-2.92	120.69	124.80
23	A	404[B]	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	B	602	CLA	CMC-C2C-C1C	2.92	129.60	125.03
23	B	606	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
23	c	506	CLA	C3B-C4B-NB	2.92	113.14	110.53
24	H	101	BCR	C7-C8-C9	-2.92	121.92	126.23
33	C	502	LMG	C8-O7-C10	-2.92	110.81	117.80
23	B	601	CLA	C1-O2A-CGA	2.92	123.71	116.65
23	b	614	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
23	C	512	CLA	CMB-C2B-C1B	2.91	129.85	125.42
26	F	103	SQD	O48-C23-C24	2.91	120.72	111.83
23	b	609	CLA	CHD-C4C-NC	2.91	128.75	124.23
23	c	502	CLA	CHC-C1C-C2C	-2.91	118.68	126.95
23	B	615	CLA	CHD-C4C-NC	2.91	128.74	124.23
23	B	609	CLA	O2A-CGA-O1A	-2.91	116.36	123.63
23	B	616	CLA	CHD-C1D-ND	-2.90	120.72	124.80
23	A	406[A]	CLA	CHD-C4C-NC	2.90	128.73	124.23
23	A	406[A]	CLA	CMC-C2C-C1C	2.90	129.57	125.03
23	c	512	CLA	CMB-C2B-C1B	2.90	129.84	125.42
28	d	404[A]	PL9	C10-C9-C11	2.90	120.27	115.23
31	A	417	LMT	O5B-C5B-C4B	2.90	114.93	109.70
23	C	504	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	B	608	CLA	O2A-CGA-O1A	-2.90	116.37	123.63
23	d	401[A]	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
23	a	405[A]	CLA	CMC-C2C-C1C	2.90	129.56	125.03
23	b	606	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
37	D	401[A]	PHO	C1-C2-C3	-2.90	121.45	126.20
23	c	514	CLA	CAA-C2A-C3A	-2.90	105.17	113.00
23	A	407	CLA	CHC-C1C-C2C	-2.90	118.72	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	409[B]	LHG	O8-C23-C24	2.89	120.66	111.83
23	C	508	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
23	b	615	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
23	C	508	CLA	CMC-C2C-C1C	2.89	129.55	125.03
23	b	610	CLA	CMC-C2C-C1C	2.89	129.55	125.03
37	D	402[A]	PHO	O2D-CGD-O1D	-2.89	118.22	123.85
24	y	101	BCR	C34-C9-C8	2.89	122.50	118.09
23	b	616	CLA	CAC-C3C-C4C	2.89	128.55	124.79
23	D	404[B]	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
28	A	412[B]	PL9	C20-C19-C21	2.89	120.24	115.23
32	A	416[B]	LHG	O8-C23-C24	2.89	120.64	111.83
33	C	521	LMG	O8-C28-O10	-2.89	116.41	123.63
23	a	405[B]	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
23	C	513	CLA	C3B-C4B-NB	2.88	113.10	110.53
35	C	518[A]	DGD	O6D-C1D-O3G	-2.88	103.24	110.04
32	d	405[A]	LHG	O7-C7-C8	2.88	117.71	111.48
23	B	607	CLA	O2A-CGA-O1A	-2.88	116.42	123.63
24	h	101	BCR	C20-C21-C22	-2.88	123.24	127.28
23	c	505	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
37	a	416[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	d	402	CLA	C3B-C4B-NB	2.88	113.10	110.53
23	D	404[B]	CLA	CAA-C2A-C3A	-2.88	105.23	113.00
23	a	405[A]	CLA	CAC-C3C-C4C	2.88	128.53	124.79
23	A	407	CLA	C1-O2A-CGA	2.87	123.61	116.65
23	B	606	CLA	O2A-CGA-CBA	2.87	120.59	111.83
23	c	514	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
23	c	509	CLA	C4-C3-C5	2.87	120.21	115.23
31	B	628	LMT	O1'-C1'-C2'	2.87	112.64	108.27
24	t	103	BCR	C36-C18-C19	2.87	122.47	118.09
23	B	601	CLA	CMC-C2C-C1C	2.87	129.52	125.03
23	a	407[B]	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
23	D	404[B]	CLA	C4-C3-C5	2.87	120.21	115.23
24	D	406	BCR	C28-C27-C26	-2.87	108.94	114.06
23	c	506	CLA	CHC-C1C-C2C	-2.87	118.79	126.95
24	h	101	BCR	C7-C8-C9	-2.87	121.99	126.23
38	F	102	HEM	O2A-CGA-CBA	2.87	123.06	114.00
23	C	506	CLA	CAC-C3C-C4C	2.87	128.52	124.79
23	d	401[B]	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
23	C	509	CLA	O2A-CGA-O1A	-2.87	116.45	123.63
23	a	406[A]	CLA	O2A-CGA-CBA	2.87	120.58	111.83
23	b	602	CLA	C1-O2A-CGA	2.87	123.59	116.65
35	H	102	DGD	O1G-C1A-C2A	2.87	120.58	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
28	D	407[A]	PL9	C10-C9-C11	2.87	120.20	115.23
23	B	616	CLA	C1-O2A-CGA	2.87	123.59	116.65
33	a	417	LMG	C7-O1-C1	-2.86	107.65	113.80
32	d	405[B]	LHG	O8-C23-O10	-2.86	116.46	123.63
23	a	406[A]	CLA	CHC-C1C-C2C	-2.86	118.81	126.95
33	D	413	LMG	O8-C28-O10	-2.86	116.46	123.63
23	C	513	CLA	CMC-C2C-C1C	2.86	129.51	125.03
23	C	512	CLA	C3C-C4C-NC	2.86	114.09	110.43
23	b	609	CLA	C3B-C4B-NB	2.86	113.08	110.53
28	D	407[A]	PL9	C53-C6-C1	2.86	121.13	115.28
23	D	404[B]	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
23	C	507	CLA	C4-C3-C5	2.86	120.19	115.23
23	B	609	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
23	a	409	CLA	CMC-C2C-C1C	2.85	129.49	125.03
23	a	407[A]	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	b	607	CLA	CBC-CAC-C3C	-2.85	104.69	112.42
23	a	409	CLA	O2A-CGA-O1A	-2.85	116.50	123.63
23	C	504	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
23	b	609	CLA	C16-C15-C13	-2.85	106.50	115.97
23	B	610	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
23	D	404[A]	CLA	C4-C3-C5	2.85	120.17	115.23
32	A	416[B]	LHG	O8-C23-O10	-2.85	116.50	123.63
23	b	601	CLA	C4B-C3B-C2B	-2.85	103.76	107.30
28	d	404[A]	PL9	C27-C28-C29	-2.85	121.11	127.62
37	D	401[B]	PHO	CMA-C3A-C4A	-2.85	108.48	114.61
24	k	101	BCR	C39-C30-C25	-2.85	105.78	110.24
23	C	515	CLA	C4-C3-C5	2.84	120.16	115.23
23	B	609	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
23	c	511	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
28	d	404[B]	PL9	C15-C14-C16	2.84	120.16	115.23
23	B	613	CLA	O2A-CGA-CBA	2.84	120.49	111.83
23	d	402	CLA	O2A-CGA-CBA	2.84	120.49	111.83
23	D	405	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
37	a	416[B]	PHO	CMB-C2B-C3B	2.84	130.35	124.68
35	C	518[B]	DGD	O3G-C3G-C2G	-2.84	103.92	110.82
32	d	406[B]	LHG	O8-C23-C24	2.84	120.48	111.83
32	d	411[B]	LHG	O8-C23-O10	-2.84	116.53	123.63
28	A	412[B]	PL9	C42-C43-C44	-2.83	121.14	127.62
24	t	103	BCR	C21-C20-C19	-2.83	114.99	123.20
23	b	616	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
23	B	604	CLA	CHC-C1C-C2C	-2.83	118.90	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	601	CLA	C3B-C4B-NB	2.83	113.06	110.53
23	a	407[A]	CLA	C4B-C3B-C2B	-2.83	103.78	107.30
23	C	513	CLA	C4-C3-C5	2.83	120.14	115.23
23	c	509	CLA	CAA-C2A-C3A	-2.83	105.35	113.00
38	f	101	HEM	C1B-NB-C4B	2.83	108.56	105.21
23	A	404[A]	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
23	C	509	CLA	C4-C3-C5	2.83	120.13	115.23
23	C	504	CLA	CAC-C3C-C4C	2.83	128.47	124.79
23	A	404[A]	CLA	CHC-C1C-C2C	-2.83	118.92	126.95
23	C	505	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
35	C	519[B]	DGD	C2G-O2G-C1B	-2.82	111.04	117.80
23	C	511	CLA	C16-C15-C13	-2.82	106.59	115.97
38	F	102	HEM	CHB-C1B-NB	2.82	127.86	124.37
28	A	412[B]	PL9	C30-C29-C31	2.82	120.12	115.23
24	T	102	BCR	C33-C5-C6	-2.82	121.41	124.48
23	b	609	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
23	C	507	CLA	C3B-C4B-NB	2.82	113.04	110.53
24	H	101	BCR	C10-C11-C12	-2.81	115.04	123.20
23	B	602	CLA	O2A-CGA-CBA	2.81	120.42	111.83
24	k	101	BCR	C10-C11-C12	-2.81	115.05	123.20
23	B	607	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
23	c	510	CLA	CMB-C2B-C1B	2.81	129.70	125.42
23	c	508	CLA	CHD-C4C-NC	2.81	128.59	124.23
37	a	416[A]	PHO	CMB-C2B-C3B	2.81	130.30	124.68
24	C	516	BCR	C16-C17-C18	-2.81	123.33	127.28
37	D	401[A]	PHO	O1D-CGD-CBD	-2.81	120.46	124.72
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
24	Y	101	BCR	C34-C9-C8	2.81	122.38	118.09
23	B	610	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
23	A	405[A]	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
23	c	514	CLA	C4C-C3C-C2C	-2.81	102.81	106.89
23	c	514	CLA	CBC-CAC-C3C	-2.80	104.82	112.42
23	a	407[A]	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
34	b	622	HTG	O5-C1-C2	2.80	114.18	110.32
26	C	501[B]	SQD	O48-C23-C24	2.80	120.38	111.83
23	a	405[B]	CLA	CMA-C3A-C4A	-2.80	104.25	111.77
23	a	407[A]	CLA	O2A-CGA-O1A	-2.80	116.62	123.63
23	B	612	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
23	b	615	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
24	B	619	BCR	C21-C20-C19	-2.80	115.10	123.20
23	A	406[B]	CLA	O2A-CGA-CBA	2.80	120.36	111.83
23	D	405	CLA	O2A-CGA-CBA	2.80	120.36	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	f	102	SQD	O48-C23-C24	2.80	120.36	111.83
23	b	605	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
23	b	607	CLA	C4-C3-C5	2.80	120.08	115.23
31	T	101	LMT	C3'-C4'-C5'	-2.79	104.73	110.93
23	d	401[B]	CLA	CAC-C3C-C4C	2.79	128.43	124.79
23	C	505	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
23	A	404[B]	CLA	C4-C3-C5	2.79	120.07	115.23
23	A	406[B]	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
37	a	408[B]	PHO	O2D-CGD-O1D	-2.79	118.41	123.85
24	K	102	BCR	C29-C30-C25	2.79	114.49	110.44
23	c	514	CLA	CMB-C2B-C1B	2.79	129.67	125.42
23	b	603	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
23	b	613	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
23	D	404[B]	CLA	CHD-C4C-NC	2.79	128.56	124.23
23	A	405[A]	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
23	a	409	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
23	C	507	CLA	CHC-C1C-C2C	-2.79	119.03	126.95
23	B	604	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
23	c	502	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
23	c	511	CLA	O2A-CGA-O1A	-2.78	116.66	123.63
32	l	802[A]	LHG	O8-C23-C24	2.78	120.32	111.83
23	c	514	CLA	CHC-C1C-C2C	-2.78	119.04	126.95
23	C	505	CLA	CHD-C4C-NC	2.78	128.54	124.23
23	b	615	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
23	B	615	CLA	C4C-C3C-C2C	-2.78	102.85	106.89
23	B	604	CLA	CAC-C3C-C4C	2.78	128.41	124.79
24	a	410	BCR	C29-C30-C25	2.77	114.47	110.44
23	C	515	CLA	C2A-C1A-CHA	-2.77	119.05	123.87
26	A	410	SQD	C4-C3-C2	-2.77	105.97	110.83
31	T	101	LMT	C1'-O5'-C5'	-2.77	108.31	113.72
23	C	506	CLA	O2A-CGA-CBA	2.77	120.28	111.83
23	C	503	CLA	CHC-C1C-C2C	-2.77	119.08	126.95
26	a	411[B]	SQD	C1-C2-C3	-2.77	104.19	110.01
23	a	406[B]	CLA	C4-C3-C5	2.77	120.03	115.23
23	B	616	CLA	O2A-CGA-CBA	2.77	120.27	111.83
23	b	607	CLA	C1D-CHD-C4C	-2.77	120.14	126.02
24	b	618	BCR	C29-C30-C25	2.77	114.46	110.44
28	d	404[B]	PL9	C22-C23-C24	-2.76	121.30	127.62
23	B	615	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
32	a	420[A]	LHG	O8-C23-C24	2.76	120.25	111.83
23	B	610	CLA	CHD-C4C-NC	2.76	128.51	124.23
38	F	102	HEM	CBA-CAA-C2A	-2.76	104.91	112.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	412[A]	PL9	C35-C34-C36	2.76	120.01	115.23
23	B	611	CLA	CAC-C3C-C4C	2.76	128.38	124.79
23	c	504	CLA	CAC-C3C-C4C	2.75	128.37	124.79
23	b	604	CLA	C4C-C3C-C2C	-2.75	102.88	106.89
23	A	405[A]	CLA	CMA-C3A-C2A	-2.75	103.33	113.98
32	D	408[A]	LHG	O7-C7-C8	2.75	117.44	111.48
23	C	503	CLA	CMB-C2B-C1B	2.75	129.61	125.42
23	b	609	CLA	O2A-CGA-O1A	-2.75	116.74	123.63
26	f	102	SQD	O5-C5-C4	2.75	114.66	109.70
23	D	404[B]	CLA	C3B-C4B-NB	2.75	112.99	110.53
23	b	603	CLA	C2A-C1A-CHA	-2.75	119.09	123.87
28	D	407[A]	PL9	C51-C49-C50	2.75	120.92	114.59
23	d	401[B]	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
23	B	604	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
24	y	101	BCR	C24-C23-C22	-2.75	122.17	126.23
34	B	622	HTG	C1-O5-C5	2.75	117.49	112.56
23	A	407	CLA	CMA-C3A-C2A	-2.75	103.36	113.98
23	A	406[A]	CLA	C4-C3-C5	2.75	119.99	115.23
28	A	412[A]	PL9	C30-C29-C31	2.75	119.99	115.23
32	D	408[A]	LHG	O8-C23-C24	2.74	120.20	111.83
31	B	628	LMT	C2'-C3'-C4'	2.74	115.91	109.68
23	c	505	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
23	d	402	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
23	C	512	CLA	CBC-CAC-C3C	-2.74	104.99	112.42
23	c	513	CLA	CHC-C1C-C2C	-2.74	119.16	126.95
24	C	517	BCR	C11-C10-C9	-2.74	123.43	127.28
23	C	507	CLA	CHD-C4C-NC	2.74	128.48	124.23
26	F	103	SQD	C1-C2-C3	-2.74	104.25	110.01
23	b	607	CLA	O2A-CGA-O1A	-2.74	116.77	123.63
23	b	616	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
23	B	612	CLA	C4B-C3B-C2B	-2.74	103.90	107.30
23	C	509	CLA	C1-C2-C3	-2.74	121.71	126.20
23	C	507	CLA	O2A-CGA-CBA	2.74	120.18	111.83
24	c	515	BCR	C16-C17-C18	-2.74	123.44	127.28
23	C	508	CLA	CGD-CBD-CAD	-2.74	101.99	110.85
23	A	407	CLA	C4-C3-C5	2.73	119.97	115.23
24	b	618	BCR	C37-C22-C21	-2.73	118.39	122.82
23	C	508	CLA	C2A-C1A-CHA	-2.73	119.12	123.87
23	b	615	CLA	CHD-C4C-NC	2.73	128.47	124.23
23	B	610	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
23	b	602	CLA	CHD-C4C-NC	2.73	128.47	124.23
24	k	101	BCR	C11-C10-C9	-2.73	123.45	127.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403	BCR	C16-C17-C18	-2.73	123.45	127.28
23	b	603	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
32	L	101[A]	LHG	O8-C23-O10	-2.73	116.80	123.63
23	b	605	CLA	CMB-C2B-C1B	2.73	129.57	125.42
37	a	408[B]	PHO	O1D-CGD-CBD	-2.73	120.59	124.72
23	C	508	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
34	B	625	HTG	C1'-S1-C1	2.73	106.34	100.45
24	b	617	BCR	C29-C30-C25	2.73	114.40	110.44
31	M	101	LMT	C1'-O5'-C5'	-2.73	108.40	113.72
23	D	405	CLA	C1-C2-C3	-2.72	121.73	126.20
28	d	404[A]	PL9	C36-C34-C33	-2.72	115.05	121.17
23	A	404[B]	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
28	d	404[B]	PL9	C12-C13-C14	-2.72	121.39	127.62
23	c	513	CLA	CAC-C3C-C4C	2.72	128.33	124.79
23	b	605	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
32	a	420[B]	LHG	O8-C23-C24	2.72	120.13	111.83
23	b	604	CLA	C4-C3-C5	2.72	119.95	115.23
23	a	405[A]	CLA	C2A-C1A-CHA	-2.72	119.15	123.87
35	H	102	DGD	O3G-C3G-C2G	-2.72	104.21	110.82
24	t	103	BCR	C28-C27-C26	-2.72	109.21	114.06
24	T	102	BCR	C12-C13-C14	-2.72	114.73	119.01
23	b	604	CLA	CMB-C2B-C1B	2.71	129.55	125.42
23	b	605	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
23	B	604	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
23	b	613	CLA	CHD-C4C-NC	2.71	128.44	124.23
23	b	607	CLA	CAC-C3C-C4C	2.71	128.32	124.79
31	c	501	LMT	C3'-C4'-C5'	-2.71	104.92	110.93
23	a	407[A]	CLA	O2A-CGA-CBA	2.71	120.10	111.83
23	A	406[B]	CLA	C2A-C1A-CHA	-2.71	119.16	123.87
24	K	102	BCR	C36-C18-C19	2.71	122.23	118.09
28	d	404[B]	PL9	C25-C24-C26	2.71	119.93	115.23
24	T	102	BCR	C2-C1-C6	2.71	114.37	110.44
32	d	406[A]	LHG	O8-C23-C24	2.71	120.09	111.83
28	D	407[A]	PL9	C2-C1-C6	2.71	122.22	119.00
23	B	602	CLA	OBD-CAD-C3D	-2.71	122.09	128.42
23	B	608	CLA	O2A-CGA-CBA	2.71	120.09	111.83
28	a	414[A]	PL9	C53-C6-C1	2.71	120.82	115.28
23	a	407[B]	CLA	CAA-C2A-C3A	-2.71	105.69	113.00
23	B	608	CLA	CHB-C4A-NA	2.70	128.30	124.40
37	a	416[B]	PHO	O2A-CGA-CBA	2.70	120.08	111.83
23	b	607	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
23	B	606	CLA	C3B-C4B-NB	2.70	112.94	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	O2A-CGA-CBA	2.70	120.07	111.83
23	a	409	CLA	CHD-C4C-NC	2.70	128.42	124.23
23	C	504	CLA	C4-C3-C5	2.70	119.92	115.23
23	d	402	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
23	b	614	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
23	B	607	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
23	D	404[B]	CLA	C2A-C1A-CHA	-2.70	119.19	123.87
23	B	607	CLA	CMB-C2B-C1B	2.70	129.53	125.42
23	D	404[A]	CLA	CAC-C3C-C4C	2.70	128.30	124.79
23	c	511	CLA	CBC-CAC-C3C	-2.70	105.11	112.42
23	C	515	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
23	C	503	CLA	C4-C3-C5	2.70	119.91	115.23
23	B	606	CLA	C4C-C3C-C2C	-2.70	102.97	106.89
23	b	613	CLA	CED-O2D-CGD	2.70	122.03	115.92
37	D	401[A]	PHO	O2A-CGA-CBA	2.69	120.05	111.83
23	B	612	CLA	C6-C5-C3	-2.69	106.91	113.47
23	c	514	CLA	C2A-C1A-CHA	-2.69	119.19	123.87
24	D	406	BCR	C16-C17-C18	-2.69	123.50	127.28
23	b	608	CLA	O2A-CGA-CBA	2.69	120.04	111.83
23	A	404[B]	CLA	CAC-C3C-C4C	2.69	128.29	124.79
28	A	412[A]	PL9	C2-C1-C6	2.69	122.20	119.00
26	a	411[B]	SQD	O47-C7-O49	-2.69	117.42	123.70
23	B	608	CLA	C11-C12-C13	-2.69	107.03	115.97
35	C	519[A]	DGD	O1G-C1A-O1A	-2.69	116.90	123.63
23	c	502	CLA	C1-C2-C3	-2.69	121.79	126.20
23	A	404[B]	CLA	O2A-CGA-O1A	-2.69	116.91	123.63
23	d	401[B]	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
28	a	414[B]	PL9	C53-C6-C1	2.69	120.78	115.28
24	H	101	BCR	C16-C17-C18	-2.69	123.51	127.28
32	A	416[B]	LHG	O7-C7-O9	-2.69	117.43	123.70
23	b	616	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
23	B	609	CLA	CHD-C4C-NC	2.68	128.39	124.23
26	F	103	SQD	O47-C7-O49	-2.68	117.43	123.70
23	b	608	CLA	CMA-C3A-C4A	-2.68	104.56	111.77
23	b	604	CLA	O2A-CGA-O1A	-2.68	116.92	123.63
23	c	514	CLA	CHD-C4C-NC	2.68	128.39	124.23
23	c	508	CLA	O2A-CGA-CBA	2.68	120.01	111.83
23	c	510	CLA	CHD-C4C-NC	2.68	128.39	124.23
24	k	101	BCR	C2-C1-C6	2.68	114.33	110.44
24	B	619	BCR	C7-C8-C9	-2.68	122.27	126.23
23	c	502	CLA	CMC-C2C-C1C	2.68	129.22	125.03
33	c	521	LMG	O8-C28-C29	2.68	120.00	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	BCR	C20-C21-C22	-2.68	123.52	127.28
24	A	408	BCR	C33-C5-C6	-2.68	121.56	124.48
23	B	606	CLA	CHC-C1C-C2C	-2.68	119.34	126.95
23	C	508	CLA	CAA-C2A-C3A	-2.68	105.76	113.00
23	B	602	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
28	D	407[B]	PL9	C20-C19-C21	2.68	119.88	115.23
23	C	504	CLA	C2A-C1A-CHA	-2.68	119.22	123.87
35	c	517[B]	DGD	C3G-C2G-C1G	-2.68	105.55	111.78
26	B	620	SQD	C4-C3-C2	2.68	115.53	110.83
23	b	608	CLA	O2A-CGA-O1A	-2.67	116.94	123.63
23	b	604	CLA	CHC-C1C-C2C	-2.67	119.35	126.95
23	d	401[A]	CLA	C2A-C1A-CHA	-2.67	119.23	123.87
23	B	612	CLA	C4A-NA-C1A	-2.67	105.46	106.68
23	A	406[B]	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
23	c	507	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
23	D	404[A]	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	c	507	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
23	b	609	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	D	404[A]	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
23	c	509	CLA	CHD-C4C-NC	2.67	128.37	124.23
23	a	406[A]	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
23	B	608	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
23	a	406[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
32	d	405[B]	LHG	C6-C5-C4	-2.66	105.57	111.78
24	B	619	BCR	C24-C23-C22	-2.66	122.29	126.23
24	T	102	BCR	C15-C14-C13	2.66	131.01	127.28
28	a	414[B]	PL9	C40-C39-C41	2.66	119.85	115.23
28	D	407[B]	PL9	C12-C13-C14	-2.66	121.53	127.62
35	c	519	DGD	O1G-C1A-C2A	2.66	119.95	111.83
23	d	401[A]	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
23	d	402	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
23	a	405[B]	CLA	C4-C3-C5	2.66	119.84	115.23
23	D	404[B]	CLA	CBC-CAC-C3C	-2.66	105.21	112.42
23	C	509	CLA	CHD-C4C-NC	2.66	128.35	124.23
23	d	401[A]	CLA	CAC-C3C-C4C	2.66	128.25	124.79
23	B	604	CLA	CHD-C1D-ND	-2.66	121.06	124.80
23	B	601	CLA	O2A-CGA-CBA	2.66	119.94	111.83
28	D	407[B]	PL9	C40-C39-C41	2.66	119.84	115.23
28	D	407[B]	PL9	C45-C44-C46	2.66	119.84	115.23
23	d	402	CLA	CHD-C4C-NC	2.66	128.35	124.23
33	D	413	LMG	O8-C28-C29	2.65	119.93	111.83
28	a	414[B]	PL9	C20-C19-C21	2.65	119.83	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	CHC-C1C-C2C	-2.65	119.41	126.95
24	Y	101	BCR	C29-C30-C25	2.65	114.29	110.44
23	d	402	CLA	CMB-C2B-C1B	2.65	129.46	125.42
23	b	610	CLA	CAA-CBA-CGA	-2.65	105.68	113.21
24	c	516	BCR	C32-C1-C6	-2.65	106.09	110.24
23	B	606	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
23	A	405[B]	CLA	CMC-C2C-C1C	2.65	129.17	125.03
23	B	604	CLA	C4-C3-C5	2.65	119.82	115.23
23	A	406[A]	CLA	C1-C2-C3	-2.65	121.86	126.20
23	C	506	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
23	C	504	CLA	CMC-C2C-C1C	2.65	129.17	125.03
23	c	511	CLA	O2A-CGA-CBA	2.65	119.90	111.83
23	C	515	CLA	C4B-C3B-C2B	-2.64	104.01	107.30
23	B	616	CLA	CMC-C2C-C1C	2.64	129.17	125.03
28	a	414[A]	PL9	C47-C48-C49	-2.64	118.83	127.64
28	d	404[B]	PL9	C20-C19-C21	2.64	119.81	115.23
33	c	520	LMG	C8-O7-C10	-2.64	111.47	117.80
23	b	609	CLA	C7-C6-C5	-2.64	106.22	113.26
26	B	620	SQD	C1-O5-C5	-2.64	108.56	113.72
26	b	620	SQD	O7-S-C6	2.64	110.70	106.76
23	b	615	CLA	O2A-CGA-CBA	2.64	119.89	111.83
23	A	407	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
23	C	514	CLA	CMB-C2B-C1B	2.64	129.44	125.42
23	b	611	CLA	CAC-C3C-C4C	2.64	128.22	124.79
35	C	520	DGD	O2G-C1B-C2B	2.64	117.19	111.48
23	B	603	CLA	C4-C3-C5	2.64	119.81	115.23
23	B	603	CLA	CHD-C4C-NC	2.64	128.32	124.23
23	B	604	CLA	C11-C12-C13	-2.64	107.20	115.97
23	A	405[B]	CLA	C4-C3-C5	2.64	119.80	115.23
23	C	504	CLA	C3B-C4B-NB	2.63	112.88	110.53
23	a	409	CLA	CMA-C3A-C2A	-2.63	103.80	113.98
26	f	102	SQD	O47-C7-O49	-2.63	117.55	123.70
26	b	620	SQD	O48-C23-C24	2.63	119.86	111.83
23	b	614	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
35	H	102	DGD	O1G-C1A-O1A	-2.63	117.05	123.63
23	b	605	CLA	C3B-C4B-NB	2.63	112.88	110.53
24	b	619	BCR	C16-C17-C18	-2.63	123.59	127.28
23	c	513	CLA	O2A-CGA-O1A	-2.63	117.05	123.63
23	A	407	CLA	CAC-C3C-C4C	2.63	128.21	124.79
23	d	402	CLA	C4-C3-C5	2.63	119.79	115.23
23	B	614	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
23	B	604	CLA	C6-C7-C8	-2.63	107.24	115.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[A]	CLA	O2A-CGA-O1A	-2.63	117.06	123.63
28	A	412[B]	PL9	C40-C39-C41	2.63	119.78	115.23
26	A	410	SQD	O48-C23-C24	2.62	119.84	111.83
24	B	617	BCR	C37-C22-C23	2.62	122.09	118.09
23	b	601	CLA	C2A-C1A-CHA	-2.62	119.32	123.87
23	B	609	CLA	C16-C15-C13	-2.62	107.26	115.97
23	b	606	CLA	C1-O2A-CGA	2.62	122.99	116.65
24	K	102	BCR	C24-C23-C22	-2.62	122.36	126.23
23	B	612	CLA	C11-C12-C13	-2.62	107.27	115.97
24	C	517	BCR	C36-C18-C19	2.62	122.09	118.09
32	D	408[B]	LHG	O8-C23-C24	2.62	119.81	111.83
23	B	614	CLA	CMA-C3A-C2A	-2.62	103.87	113.98
23	C	515	CLA	O2A-CGA-CBA	2.62	119.81	111.83
23	C	512	CLA	O2A-CGA-O1A	-2.62	117.09	123.63
31	m	103	LMT	C3'-C4'-C5'	-2.62	105.13	110.93
23	c	510	CLA	C1-O2A-CGA	2.61	122.98	116.65
37	a	408[B]	PHO	O2A-CGA-CBA	2.61	119.80	111.83
25	b	628	GOL	C3-C2-C1	-2.61	102.22	111.80
23	a	405[B]	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
23	D	404[A]	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
26	B	620	SQD	O5-C1-C2	-2.61	105.01	110.37
24	D	406	BCR	C40-C30-C25	-2.61	106.15	110.24
23	c	512	CLA	C1-C2-C3	-2.61	121.92	126.20
23	a	405[A]	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
33	C	502	LMG	C6-C5-C4	2.61	119.42	113.02
23	b	609	CLA	CMB-C2B-C1B	2.61	129.39	125.42
26	C	501[A]	SQD	O48-C23-O10	-2.61	117.11	123.63
23	B	608	CLA	C2A-C1A-CHA	-2.61	119.35	123.87
35	c	518[B]	DGD	O1G-C1A-C2A	2.61	119.78	111.83
28	A	412[B]	PL9	C12-C13-C14	-2.60	121.66	127.62
23	b	609	CLA	O2A-CGA-CBA	2.60	119.78	111.83
37	D	401[A]	PHO	O2A-CGA-O1A	-2.60	117.12	123.63
23	a	407[B]	CLA	CAC-C3C-C4C	2.60	128.18	124.79
23	a	406[A]	CLA	CAA-CBA-CGA	2.60	120.59	113.21
23	c	505	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
24	b	619	BCR	C16-C15-C14	-2.60	118.20	123.52
23	c	509	CLA	CMB-C2B-C1B	2.60	129.38	125.42
23	c	507	CLA	C4-C3-C5	2.60	119.74	115.23
23	A	405[A]	CLA	C2A-C1A-CHA	-2.60	119.35	123.87
24	d	403	BCR	C28-C27-C26	-2.60	109.42	114.06
23	B	608	CLA	CAC-C3C-C4C	2.60	128.17	124.79
23	B	609	CLA	CHC-C1C-C2C	-2.60	119.56	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	h	101	BCR	C24-C23-C22	-2.60	122.39	126.23
35	c	517[B]	DGD	O3G-C3G-C2G	-2.60	104.50	110.82
23	A	407	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	c	504	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
23	C	503	CLA	CMC-C2C-C1C	2.60	129.09	125.03
23	A	406[A]	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
23	c	509	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
32	d	405[B]	LHG	O8-C23-C24	2.60	119.75	111.83
23	B	616	CLA	CHD-C4C-NC	2.60	128.26	124.23
23	a	409	CLA	C4B-C3B-C2B	-2.60	104.08	107.30
23	B	611	CLA	C4B-C3B-C2B	2.59	110.53	107.30
23	C	509	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
35	c	518[A]	DGD	O1G-C1A-C2A	2.59	119.74	111.83
23	B	615	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
23	A	405[A]	CLA	C4-C3-C5	2.59	119.73	115.23
37	D	401[B]	PHO	O2A-CGA-CBA	2.59	119.74	111.83
37	a	408[A]	PHO	CMB-C2B-C3B	2.59	129.86	124.68
28	a	414[A]	PL9	C40-C39-C41	2.59	119.72	115.23
24	K	102	BCR	C15-C14-C13	-2.59	123.65	127.28
23	B	603	CLA	CMA-C3A-C2A	-2.59	103.98	113.98
35	h	102	DGD	O3G-C1D-C2D	2.59	112.20	108.27
23	B	605	CLA	C3B-C4B-NB	2.59	112.84	110.53
23	b	615	CLA	CAC-C3C-C4C	2.59	128.16	124.79
23	B	601	CLA	C3B-C4B-NB	2.59	112.84	110.53
23	C	512	CLA	C4-C3-C2	-2.59	116.99	123.63
23	b	616	CLA	C4-C3-C5	2.58	119.71	115.23
23	b	601	CLA	CHC-C1C-C2C	-2.58	119.61	126.95
23	b	616	CLA	OBD-CAD-C3D	-2.58	122.38	128.42
23	B	601	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
23	A	405[A]	CLA	O2A-CGA-O1A	-2.58	117.17	123.63
23	b	611	CLA	CHD-C4C-NC	2.58	128.23	124.23
23	C	511	CLA	CHD-C4C-NC	2.58	128.23	124.23
31	m	103	LMT	C1'-O5'-C5'	-2.58	108.68	113.72
24	b	619	BCR	C11-C10-C9	-2.58	123.66	127.28
23	A	407	CLA	CMB-C2B-C1B	2.58	129.35	125.42
28	a	414[A]	PL9	C10-C9-C8	-2.58	117.01	123.63
23	c	514	CLA	CMC-C2C-C1C	2.58	129.06	125.03
28	A	412[A]	PL9	C40-C39-C41	2.58	119.70	115.23
23	a	407[A]	CLA	C1-C2-C3	-2.58	121.98	126.20
28	A	412[A]	PL9	C47-C48-C49	-2.58	119.05	127.64
23	b	602	CLA	CMA-C3A-C2A	-2.58	104.03	113.98
23	B	608	CLA	CMC-C2C-C1C	2.58	129.06	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	519	DGD	O2G-C1B-O1B	-2.57	117.69	123.70
23	B	602	CLA	CHD-C4C-NC	2.57	128.22	124.23
23	A	404[B]	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	a	407[B]	CLA	CBC-CAC-C3C	-2.57	105.45	112.42
23	A	406[B]	CLA	O2A-CGA-O1A	-2.57	117.20	123.63
31	A	417	LMT	O5'-C5'-C6'	2.57	112.80	106.44
23	c	506	CLA	O2A-CGA-CBA	2.57	119.66	111.83
23	a	407[B]	CLA	C2A-C1A-CHA	-2.57	119.41	123.87
24	B	618	BCR	C2-C1-C6	2.57	114.17	110.44
23	B	613	CLA	CMC-C2C-C1C	2.57	129.04	125.03
23	B	605	CLA	CHC-C1C-C2C	-2.57	119.66	126.95
23	B	613	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
23	a	407[B]	CLA	O2A-CGA-CBA	2.56	119.65	111.83
28	d	404[B]	PL9	C7-C3-C4	2.56	119.02	116.91
23	a	407[B]	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
23	C	504	CLA	CHD-C4C-NC	2.56	128.20	124.23
23	c	504	CLA	CHD-C4C-NC	2.56	128.20	124.23
33	m	101	LMG	O7-C10-O9	-2.56	117.72	123.70
23	C	508	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
23	A	405[B]	CLA	C2A-C1A-CHA	-2.56	119.43	123.87
37	D	401[A]	PHO	CMA-C3A-C4A	-2.56	109.11	114.61
23	c	511	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
26	a	411[B]	SQD	C44-O6-C1	-2.55	108.32	113.80
24	t	103	BCR	C29-C28-C27	-2.55	105.66	111.28
32	D	409[B]	LHG	O8-C23-O10	-2.55	117.25	123.63
23	a	405[B]	CLA	CAA-C2A-C1A	-2.55	103.61	111.97
24	c	516	BCR	C21-C20-C19	-2.55	115.81	123.20
26	b	620	SQD	O47-C7-O49	-2.55	117.75	123.70
23	a	407[B]	CLA	C3B-C4B-NB	2.55	112.81	110.53
24	b	618	BCR	C37-C22-C23	2.55	121.98	118.09
33	B	621	LMG	O8-C28-O10	-2.55	117.26	123.63
28	D	407[A]	PL9	C42-C41-C39	-2.55	104.75	113.19
35	c	517[A]	DGD	C2G-O2G-C1B	-2.55	111.70	117.80
23	b	610	CLA	C4-C3-C5	2.54	119.64	115.23
28	d	404[B]	PL9	C27-C28-C29	-2.54	121.80	127.62
23	C	513	CLA	C1-C2-C3	-2.54	122.03	126.20
23	b	608	CLA	CHD-C4C-NC	2.54	128.17	124.23
24	t	103	BCR	C1-C6-C7	2.54	122.54	115.65
23	C	503	CLA	CHD-C4C-NC	2.54	128.17	124.23
23	c	508	CLA	C3B-C4B-NB	2.54	112.80	110.53
31	A	417	LMT	O1'-C1'-C2'	2.54	112.13	108.27
23	b	612	CLA	CHC-C1C-C2C	-2.54	119.73	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	CBC-CAC-C3C	-2.54	105.53	112.42
23	B	610	CLA	CAC-C3C-C4C	2.54	128.09	124.79
28	A	412[A]	PL9	C10-C9-C8	-2.54	117.11	123.63
24	k	101	BCR	C24-C23-C22	-2.54	122.48	126.23
26	F	103	SQD	O7-S-C6	2.54	110.54	106.76
24	D	406	BCR	C21-C20-C19	-2.53	115.86	123.20
34	b	622	HTG	O2-C2-C3	-2.53	104.40	110.38
23	c	508	CLA	CBC-CAC-C3C	-2.53	105.55	112.42
23	a	405[B]	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
23	a	407[A]	CLA	CMC-C2C-C1C	2.53	128.99	125.03
23	c	509	CLA	CMC-C2C-C1C	2.53	128.99	125.03
37	D	401[B]	PHO	O2D-CGD-O1D	-2.53	118.92	123.85
23	c	508	CLA	O1D-CGD-CBD	-2.53	119.52	124.52
23	d	402	CLA	CMA-C3A-C2A	-2.53	104.19	113.98
23	b	613	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
23	A	406[A]	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
23	a	405[A]	CLA	CHD-C4C-NC	2.53	128.15	124.23
23	B	612	CLA	C7-C6-C5	-2.53	106.52	113.26
23	B	602	CLA	CAC-C3C-C4C	2.53	128.08	124.79
32	l	802[B]	LHG	O8-C23-C24	2.53	119.55	111.83
23	B	608	CLA	CMA-C3A-C2A	-2.53	104.20	113.98
23	C	513	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
34	B	625	HTG	O5-C5-C4	2.53	114.26	109.70
37	D	402[B]	PHO	C6-C5-C3	-2.53	107.31	113.47
24	t	103	BCR	C35-C13-C12	2.53	121.95	118.09
23	a	406[B]	CLA	O2A-CGA-CBA	2.53	119.54	111.83
23	a	409	CLA	C2A-C1A-CHA	-2.53	119.48	123.87
23	a	406[B]	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
23	a	405[A]	CLA	CMA-C3A-C2A	-2.53	104.22	113.98
23	c	507	CLA	O2A-CGA-CBA	2.53	119.53	111.83
35	C	519[B]	DGD	O1G-C1A-C2A	2.53	119.53	111.83
28	a	414[B]	PL9	C10-C9-C11	2.52	119.61	115.23
23	b	613	CLA	CMA-C3A-C4A	-2.52	104.99	111.77
23	B	611	CLA	C2C-C1C-NC	2.52	112.63	109.98
23	C	507	CLA	O2A-CGA-O1A	-2.52	117.32	123.63
24	Y	101	BCR	C1-C6-C7	2.52	122.49	115.65
23	a	406[A]	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
37	D	402[B]	PHO	CED-O2D-CGD	2.52	121.63	115.92
31	B	630	LMT	O5'-C5'-C6'	2.52	112.68	106.44
23	B	606	CLA	C1-C2-C3	-2.52	122.07	126.20
23	B	616	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
23	D	405	CLA	CHC-C1C-C2C	-2.51	119.81	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	515	BCR	C38-C26-C25	-2.51	121.74	124.48
28	A	412[B]	PL9	C10-C9-C11	2.51	119.59	115.23
23	c	504	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
23	b	606	CLA	CMB-C2B-C1B	2.51	129.24	125.42
23	A	405[A]	CLA	CAA-CBA-CGA	2.51	120.34	113.21
23	b	602	CLA	CHB-C1B-C2B	-2.51	120.14	127.43
23	C	513	CLA	O2A-CGA-CBA	2.51	119.49	111.83
23	a	405[B]	CLA	C2A-C1A-CHA	-2.51	119.51	123.87
23	b	603	CLA	C4-C3-C5	2.51	119.58	115.23
24	c	516	BCR	C33-C5-C6	-2.51	121.75	124.48
23	B	607	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
28	d	404[A]	PL9	C17-C18-C19	-2.51	121.89	127.62
23	A	404[A]	CLA	CAA-CBA-CGA	-2.51	106.09	113.21
24	H	101	BCR	C20-C21-C22	-2.50	123.77	127.28
24	T	102	BCR	C16-C17-C18	-2.50	123.77	127.28
32	L	101[B]	LHG	O8-C23-C24	2.50	119.47	111.83
31	B	630	LMT	O5'-C5'-C4'	2.50	114.90	109.72
23	A	407	CLA	CBC-CAC-C3C	-2.50	105.63	112.42
24	C	517	BCR	C15-C14-C13	-2.50	123.77	127.28
23	B	607	CLA	C2A-C1A-CHA	-2.50	119.52	123.87
31	b	621	LMT	C1'-O5'-C5'	-2.50	108.83	113.72
24	B	618	BCR	C38-C26-C25	-2.50	121.75	124.48
23	A	407	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
23	b	607	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
23	C	504	CLA	CMB-C2B-C1B	2.50	129.23	125.42
28	D	407[B]	PL9	C22-C23-C24	-2.50	121.90	127.62
23	c	513	CLA	CBA-CAA-C2A	-2.50	106.36	113.79
32	A	416[A]	LHG	O7-C7-O9	-2.50	117.87	123.70
31	M	101	LMT	O1B-C1B-C2B	2.50	114.23	108.09
23	b	603	CLA	O2A-CGA-O1A	-2.50	117.39	123.63
24	d	403	BCR	C16-C15-C14	-2.49	118.42	123.52
23	B	609	CLA	C3B-C4B-NB	2.49	112.76	110.53
23	a	405[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	C	507	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
23	a	405[B]	CLA	C7-C6-C5	-2.49	106.62	113.26
24	H	101	BCR	C37-C22-C21	-2.49	118.78	122.82
23	B	605	CLA	O2A-CGA-CBA	2.49	119.43	111.83
24	y	101	BCR	C1-C6-C7	2.49	122.40	115.65
23	b	602	CLA	CAA-CBA-CGA	-2.49	106.14	113.21
23	B	607	CLA	CMA-C3A-C2A	-2.49	104.36	113.98
31	F	101	LMT	C1'-O5'-C5'	-2.49	108.86	113.72
23	b	612	CLA	CHD-C4C-NC	2.49	128.09	124.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
23	c	508	CLA	O2A-CGA-O1A	-2.49	117.41	123.63
23	C	508	CLA	CHD-C4C-NC	2.49	128.09	124.23
24	b	619	BCR	C7-C6-C5	2.49	127.28	121.56
23	b	605	CLA	O2A-CGA-CBA	2.49	119.41	111.83
23	B	611	CLA	C1C-C2C-C3C	-2.49	104.37	106.98
33	z	101	LMG	C8-O7-C10	-2.49	111.85	117.80
33	C	502	LMG	O6-C1-O1	-2.48	104.17	110.04
23	c	505	CLA	CED-O2D-CGD	2.48	121.55	115.92
23	b	608	CLA	C4C-C3C-C2C	-2.48	103.28	106.89
23	B	602	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
23	A	406[A]	CLA	CMA-C3A-C2A	-2.48	104.38	113.98
23	B	604	CLA	C6-C5-C3	-2.48	107.42	113.47
23	C	512	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
24	k	101	BCR	C20-C21-C22	-2.48	123.80	127.28
35	C	520	DGD	O3G-C3G-C2G	-2.48	104.78	110.82
24	c	516	BCR	C2-C1-C6	2.48	114.04	110.44
23	C	508	CLA	O2A-CGA-CBA	2.48	119.40	111.83
23	a	406[B]	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
34	C	523	HTG	C1-O5-C5	2.48	117.01	112.56
28	d	404[B]	PL9	C51-C49-C50	2.48	120.30	114.59
23	B	612	CLA	CHC-C1C-C2C	-2.48	119.90	126.95
23	C	511	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
23	d	402	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
23	b	615	CLA	C1-C2-C3	-2.48	122.14	126.20
23	C	512	CLA	CMC-C2C-C1C	2.48	128.90	125.03
23	c	502	CLA	C1-O2A-CGA	2.48	122.64	116.65
23	D	404[B]	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
23	C	503	CLA	C2A-C1A-CHA	-2.47	119.57	123.87
23	B	602	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
31	t	101	LMT	O1'-C1'-C2'	2.47	112.03	108.27
23	c	508	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
28	D	407[B]	PL9	C51-C49-C50	2.47	120.28	114.59
24	c	516	BCR	C20-C21-C22	-2.47	123.81	127.28
23	b	616	CLA	C3B-C4B-NB	2.47	112.74	110.53
23	c	506	CLA	C1-C2-C3	-2.47	122.15	126.20
28	D	407[B]	PL9	C37-C38-C39	-2.47	121.97	127.62
23	A	405[B]	CLA	C1-C2-C3	-2.47	122.15	126.20
23	b	612	CLA	CMA-C3A-C2A	-2.47	104.44	113.98
23	C	504	CLA	C4B-C3B-C2B	-2.46	104.24	107.30
24	B	617	BCR	C29-C30-C25	2.46	114.02	110.44
28	d	404[A]	PL9	C12-C13-C14	-2.46	121.99	127.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	b	611	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
23	c	512	CLA	CMC-C2C-C1C	2.46	128.88	125.03
23	B	605	CLA	C2A-C1A-CHA	-2.46	119.60	123.87
26	a	411[B]	SQD	C3-C4-C5	2.46	114.69	110.23
23	C	515	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
23	b	615	CLA	CBC-CAC-C3C	-2.46	105.76	112.42
23	B	607	CLA	CHD-C4C-NC	2.45	128.03	124.23
23	C	515	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
23	d	401[A]	CLA	CMC-C2C-C1C	2.45	128.86	125.03
24	K	102	BCR	C38-C26-C25	-2.45	121.81	124.48
23	b	613	CLA	CMC-C2C-C1C	2.45	128.85	125.03
24	K	102	BCR	C20-C21-C22	-2.45	123.85	127.28
23	C	510	CLA	CMB-C2B-C1B	2.44	129.14	125.42
28	A	412[A]	PL9	C42-C43-C44	-2.44	122.03	127.62
26	a	411[B]	SQD	O48-C23-C24	2.44	119.28	111.83
23	b	601	CLA	CMB-C2B-C1B	2.44	129.14	125.42
23	c	502	CLA	CBC-CAC-C3C	-2.44	105.80	112.42
23	c	503	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
23	c	510	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
23	B	606	CLA	CMB-C2B-C1B	2.44	129.13	125.42
24	y	101	BCR	C21-C20-C19	-2.44	116.14	123.20
32	l	802[A]	LHG	O8-C23-O10	-2.44	117.53	123.63
28	D	407[B]	PL9	C7-C3-C2	-2.44	120.52	123.39
23	C	513	CLA	C1-O2A-CGA	2.44	122.55	116.65
32	d	406[A]	LHG	O8-C23-O10	-2.43	117.54	123.63
24	b	618	BCR	C33-C5-C6	-2.43	121.83	124.48
28	A	412[B]	PL9	C45-C44-C46	2.43	119.45	115.23
23	b	611	CLA	OBD-CAD-C3D	-2.43	122.73	128.42
23	b	603	CLA	C7-C6-C5	-2.43	106.78	113.26
23	b	605	CLA	CMC-C2C-C1C	2.43	128.83	125.03
37	a	416[A]	PHO	O1D-CGD-CBD	-2.43	121.04	124.72
24	K	102	BCR	C2-C1-C6	2.43	113.97	110.44
24	Y	101	BCR	C3-C4-C5	-2.43	109.73	114.06
24	h	101	BCR	C11-C10-C9	-2.43	123.88	127.28
23	b	606	CLA	C2A-C1A-CHA	-2.42	119.66	123.87
23	C	514	CLA	CHB-C4A-NA	2.42	127.90	124.40
28	D	407[A]	PL9	C20-C19-C21	2.42	119.43	115.23
26	C	501[B]	SQD	O7-S-C6	2.42	110.37	106.76
23	D	404[B]	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
23	B	601	CLA	C2A-C1A-CHA	-2.42	119.67	123.87
23	b	610	CLA	CHC-C1C-C2C	-2.42	120.07	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
23	B	603	CLA	C7-C6-C5	-2.42	106.82	113.26
24	c	515	BCR	C33-C5-C6	-2.42	121.84	124.48
23	b	610	CLA	C4B-C3B-C2B	-2.42	104.30	107.30
24	b	618	BCR	C15-C14-C13	-2.42	123.89	127.28
23	b	615	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
23	C	514	CLA	CHC-C1C-C2C	-2.42	120.08	126.95
24	D	406	BCR	C39-C30-C25	-2.42	106.45	110.24
23	D	405	CLA	C2A-C1A-CHA	-2.41	119.68	123.87
23	B	609	CLA	C7-C6-C5	-2.41	106.83	113.26
23	B	607	CLA	CED-O2D-CGD	2.41	121.39	115.92
35	H	102	DGD	C3E-C4E-C5E	-2.41	105.85	110.23
23	C	509	CLA	O1D-CGD-CBD	-2.41	119.76	124.52
23	A	407	CLA	CHB-C4A-NA	2.41	127.88	124.40
23	b	614	CLA	O2A-CGA-CBA	2.41	119.18	111.83
23	C	513	CLA	CHD-C4C-NC	2.41	127.97	124.23
23	b	613	CLA	C4-C3-C5	2.41	119.41	115.23
23	b	601	CLA	O2A-CGA-CBA	2.41	119.17	111.83
23	b	614	CLA	C4B-C3B-C2B	-2.41	104.31	107.30
24	B	618	BCR	C15-C14-C13	-2.41	123.90	127.28
35	C	519[B]	DGD	O1G-C1A-O1A	-2.41	117.61	123.63
23	A	404[B]	CLA	CAA-CBA-CGA	-2.41	106.38	113.21
23	d	401[B]	CLA	O2A-CGA-O1A	-2.40	117.61	123.63
23	c	514	CLA	C1-O2A-CGA	2.40	122.47	116.65
38	F	102	HEM	C3B-C4B-NB	-2.40	107.74	109.47
32	D	408[B]	LHG	O8-C23-O10	-2.40	117.62	123.63
23	b	604	CLA	O2A-CGA-CBA	2.40	119.16	111.83
24	k	101	BCR	C36-C18-C19	2.40	121.76	118.09
23	c	511	CLA	CED-O2D-CGD	2.40	121.36	115.92
23	B	610	CLA	CMA-C3A-C2A	-2.40	104.71	113.98
28	d	404[B]	PL9	C7-C3-C2	-2.40	120.56	123.39
23	B	610	CLA	CHB-C4A-NA	2.40	127.86	124.40
23	B	611	CLA	O2A-CGA-O1A	-2.40	117.63	123.63
37	a	408[A]	PHO	CMA-C3A-C4A	-2.40	109.45	114.61
28	D	407[A]	PL9	C40-C39-C41	2.40	119.39	115.23
23	c	503	CLA	C4C-C3C-C2C	-2.40	103.40	106.89
26	b	620	SQD	O8-S-C6	2.40	110.60	105.97
23	b	607	CLA	O2D-CGD-O1D	-2.40	119.19	123.85
37	a	408[B]	PHO	C4A-C3A-C2A	-2.40	100.56	102.84
35	c	519	DGD	O3G-C1D-C2D	-2.39	104.64	108.27
23	C	506	CLA	CAA-C2A-C3A	-2.39	106.53	113.00
23	b	616	CLA	CBC-CAC-C3C	-2.39	105.93	112.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	CMB-C2B-C1B	2.39	129.06	125.42
23	B	615	CLA	C2A-C1A-CHA	-2.39	119.72	123.87
35	c	517[A]	DGD	C3G-C2G-C1G	-2.39	106.21	111.78
23	b	609	CLA	CMA-C3A-C4A	-2.39	105.35	111.77
23	b	607	CLA	C1-O2A-CGA	2.39	122.44	116.65
23	C	504	CLA	O2A-CGA-CBA	2.39	119.12	111.83
23	c	508	CLA	C4C-C3C-C2C	-2.39	103.42	106.89
26	a	411[A]	SQD	O48-C23-C24	2.39	119.11	111.83
23	A	406[B]	CLA	C4-C3-C5	2.39	119.37	115.23
24	Y	101	BCR	C36-C18-C19	2.38	121.73	118.09
23	b	606	CLA	CAA-C2A-C3A	-2.38	106.56	113.00
24	B	617	BCR	C15-C14-C13	-2.38	123.94	127.28
26	F	103	SQD	O48-C23-O10	-2.38	117.67	123.63
24	B	617	BCR	C16-C17-C18	-2.38	123.94	127.28
23	A	406[A]	CLA	CAC-C3C-C4C	2.38	127.89	124.79
40	v	201	HEC	CBD-CAD-C3D	-2.38	105.95	112.53
24	h	101	BCR	C16-C17-C18	-2.38	123.94	127.28
23	a	407[B]	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
23	c	514	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
28	A	412[B]	PL9	C10-C9-C8	-2.38	117.52	123.63
24	c	516	BCR	C37-C22-C23	2.38	121.72	118.09
23	C	508	CLA	CMB-C2B-C1B	2.38	129.04	125.42
23	b	615	CLA	CMC-C2C-C1C	2.38	128.75	125.03
23	B	603	CLA	C2A-C1A-CHA	-2.38	119.74	123.87
23	C	514	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
35	C	519[A]	DGD	C2G-O2G-C1B	-2.38	112.11	117.80
23	B	611	CLA	CMB-C2B-C3B	2.37	132.13	126.55
26	a	412	SQD	O5-C5-C4	2.37	113.97	109.70
35	C	518[B]	DGD	O1G-C1A-O1A	-2.37	117.70	123.63
24	B	617	BCR	C21-C20-C19	-2.37	116.33	123.20
23	b	602	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
24	d	403	BCR	C39-C30-C25	-2.37	106.53	110.24
40	v	201	HEC	CHA-C1A-NA	2.37	127.03	124.45
23	b	601	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
32	d	405[A]	LHG	C6-C5-C4	-2.37	106.27	111.78
38	F	102	HEM	CHA-C4D-ND	2.36	127.29	124.37
28	a	414[B]	PL9	C45-C44-C46	2.36	119.33	115.23
33	C	522	LMG	O1-C1-C2	2.36	111.86	108.27
37	a	416[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	b	606	CLA	CMC-C2C-C1C	2.36	128.72	125.03
23	c	511	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
24	c	515	BCR	C28-C27-C26	-2.36	109.85	114.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	402[A]	PHO	C4D-CHA-CBD	2.36	109.59	108.45
23	a	406[B]	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
37	a	416[A]	PHO	O2A-CGA-CBA	2.36	119.03	111.83
23	B	609	CLA	C1-C2-C3	-2.36	122.33	126.20
28	D	407[A]	PL9	C7-C8-C9	-2.36	122.77	126.83
23	b	602	CLA	C11-C12-C13	-2.36	108.13	115.97
33	m	101	LMG	C1-O6-C5	-2.35	109.12	113.72
23	c	513	CLA	CMC-C2C-C1C	2.35	128.71	125.03
23	A	404[B]	CLA	CAA-C2A-C1A	-2.35	104.26	111.97
24	B	618	BCR	C37-C22-C23	2.35	121.68	118.09
23	a	405[B]	CLA	CHB-C1B-C2B	-2.35	120.59	127.43
23	b	611	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
23	c	513	CLA	CMA-C3A-C4A	-2.35	105.45	111.77
24	y	101	BCR	C10-C11-C12	-2.35	116.39	123.20
23	a	406[B]	CLA	CMA-C3A-C2A	-2.35	104.89	113.98
23	d	401[A]	CLA	CMB-C2B-C1B	2.35	129.00	125.42
28	d	404[B]	PL9	C53-C6-C1	2.35	120.09	115.28
37	D	401[B]	PHO	C4-C3-C5	2.35	119.31	115.23
23	A	406[B]	CLA	CMC-C2C-C1C	2.35	128.70	125.03
33	C	521	LMG	C8-O7-C10	-2.35	112.18	117.80
23	b	611	CLA	CMB-C2B-C1B	2.34	128.99	125.42
35	H	102	DGD	O2G-C1B-C2B	2.34	116.55	111.48
32	E	101[B]	LHG	O7-C7-O9	-2.34	118.23	123.70
33	d	409	LMG	O8-C28-C29	2.34	118.98	111.83
23	B	611	CLA	C4A-NA-C1A	-2.34	105.61	106.68
23	B	601	CLA	CHC-C1C-C2C	-2.34	120.29	126.95
23	c	505	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
23	b	608	CLA	C11-C12-C13	-2.34	108.18	115.97
23	c	505	CLA	CHD-C4C-NC	2.34	127.86	124.23
26	a	412	SQD	O7-S-C6	2.34	110.25	106.76
35	C	519[A]	DGD	O2G-C1B-O1B	-2.34	118.24	123.70
35	C	518[B]	DGD	O1G-C1A-C2A	2.34	118.96	111.83
23	C	506	CLA	C2A-C1A-CHA	-2.34	119.81	123.87
23	B	615	CLA	C11-C10-C8	-2.34	108.20	115.97
28	d	404[A]	PL9	C7-C8-C9	-2.34	122.81	126.83
37	D	401[B]	PHO	C4A-C3A-C2A	-2.34	100.62	102.84
23	B	602	CLA	C11-C12-C13	-2.33	108.20	115.97
24	C	516	BCR	C29-C30-C25	2.33	113.83	110.44
23	C	509	CLA	CMC-C2C-C1C	2.33	128.68	125.03
24	T	102	BCR	C21-C20-C19	-2.33	116.44	123.20
24	t	103	BCR	C7-C6-C5	-2.33	116.18	121.56
23	A	407	CLA	O2A-CGA-O1A	-2.33	117.79	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	414[A]	PL9	C20-C19-C21	2.33	119.28	115.23
23	B	604	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
23	C	506	CLA	C4C-C3C-C2C	-2.33	103.50	106.89
37	a	408[B]	PHO	CMB-C2B-C3B	2.33	129.34	124.68
23	b	603	CLA	CMA-C3A-C2A	-2.33	104.98	113.98
23	C	503	CLA	C11-C12-C13	-2.33	108.22	115.97
26	C	501[A]	SQD	O9-S-O7	-2.33	106.25	113.82
23	c	511	CLA	C4-C3-C2	-2.33	117.65	123.63
26	C	501[A]	SQD	O8-S-C6	2.33	110.46	105.97
23	D	404[A]	CLA	CMC-C2C-C1C	2.33	128.67	125.03
28	A	412[A]	PL9	C12-C13-C14	-2.33	122.30	127.62
26	F	103	SQD	O5-C1-O6	2.32	115.54	110.04
23	B	607	CLA	OBD-CAD-C3D	-2.32	122.99	128.42
23	C	505	CLA	C3B-C4B-NB	2.32	112.60	110.53
32	d	406[B]	LHG	O8-C23-O10	-2.32	117.82	123.63
38	F	102	HEM	C4C-CHD-C1D	-2.32	121.09	126.02
35	C	518[A]	DGD	O6E-C5E-C4E	2.32	113.88	109.70
35	C	518[A]	DGD	C3G-C2G-C1G	-2.32	106.38	111.78
23	d	402	CLA	CMC-C2C-C1C	2.32	128.66	125.03
26	a	412	SQD	C1-O5-C5	2.32	118.25	113.72
23	d	401[B]	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
24	y	101	BCR	C16-C17-C18	-2.32	124.03	127.28
23	c	507	CLA	CMC-C2C-C1C	2.32	128.65	125.03
23	C	506	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
23	b	606	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
33	d	409	LMG	O7-C10-O9	-2.32	118.29	123.70
31	m	103	LMT	C3B-C4B-C5B	-2.32	106.03	110.23
23	A	405[B]	CLA	O2A-CGA-CBA	2.31	118.89	111.83
23	c	509	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
24	b	617	BCR	C32-C1-C6	-2.31	106.62	110.24
26	a	412	SQD	C3-C4-C5	2.31	114.42	110.23
24	h	101	BCR	C37-C22-C21	-2.31	119.07	122.82
23	b	613	CLA	CBC-CAC-C3C	-2.31	106.16	112.42
23	A	406[B]	CLA	CAC-C3C-C4C	2.31	127.80	124.79
33	m	101	LMG	O8-C28-O10	-2.31	117.85	123.63
23	c	511	CLA	C2A-C1A-CHA	-2.31	119.86	123.87
24	Y	101	BCR	C7-C6-C5	-2.31	116.24	121.56
23	B	608	CLA	C11-C10-C8	-2.31	108.29	115.97
31	A	415	LMT	O1'-C1'-C2'	2.31	111.78	108.27
24	b	619	BCR	C21-C20-C19	-2.31	116.52	123.20
23	c	504	CLA	O2A-CGA-CBA	2.30	118.86	111.83
23	b	616	CLA	CHC-C1C-C2C	-2.30	120.40	126.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	401[A]	PHO	CMB-C2B-C3B	2.30	129.29	124.68
24	C	516	BCR	C40-C30-C25	-2.30	106.63	110.24
23	C	512	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
24	A	408	BCR	C8-C7-C6	-2.30	120.85	127.00
32	E	101[B]	LHG	C5-O7-C7	-2.30	112.29	117.80
28	A	412[A]	PL9	C45-C44-C46	2.30	119.22	115.23
26	a	411[A]	SQD	O9-S-O7	-2.30	106.34	113.82
26	B	620	SQD	O48-C23-O10	-2.30	117.87	123.63
23	c	508	CLA	CAC-C3C-C4C	2.30	127.78	124.79
23	a	409	CLA	CHB-C4A-NA	2.30	127.72	124.40
23	D	404[A]	CLA	CMB-C2B-C1B	2.30	128.92	125.42
24	D	406	BCR	C15-C16-C17	-2.30	118.82	123.52
33	m	101	LMG	O3-C3-C2	-2.30	104.96	110.38
24	C	516	BCR	C38-C26-C25	-2.30	121.98	124.48
34	c	522	HTG	O5-C1-C2	2.30	113.48	110.32
23	C	512	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
23	c	505	CLA	O2A-CGA-CBA	2.29	118.83	111.83
23	b	611	CLA	CBC-CAC-C3C	-2.29	106.20	112.42
32	D	408[B]	LHG	C5-O7-C7	-2.29	112.31	117.80
23	c	511	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
23	b	601	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
24	y	101	BCR	C37-C22-C23	2.29	121.59	118.09
24	y	101	BCR	C11-C10-C9	-2.29	124.06	127.28
23	C	510	CLA	C2A-C1A-CHA	-2.29	119.89	123.87
23	C	512	CLA	CHB-C4A-NA	2.29	127.70	124.40
26	F	103	SQD	C46-C45-C44	-2.29	106.45	111.78
31	t	101	LMT	O5'-C5'-C4'	2.29	114.45	109.72
28	d	404[A]	PL9	C20-C19-C21	2.29	119.20	115.23
33	B	621	LMG	C8-O7-C10	-2.29	112.32	117.80
24	K	102	BCR	C10-C11-C12	-2.29	116.58	123.20
23	C	505	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
23	a	405[B]	CLA	CMA-C3A-C2A	-2.28	105.15	113.98
37	D	402[B]	PHO	CMA-C3A-C4A	-2.28	109.69	114.61
23	C	513	CLA	CMB-C2B-C1B	2.28	128.90	125.42
34	B	625	HTG	C3-C4-C5	2.28	114.37	110.23
32	E	101[A]	LHG	O7-C7-O9	-2.28	118.37	123.70
23	C	505	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
23	c	505	CLA	CMC-C2C-C1C	2.28	128.60	125.03
23	c	512	CLA	CAC-C3C-C4C	2.28	127.76	124.79
24	b	619	BCR	C38-C26-C25	-2.28	122.00	124.48
23	B	610	CLA	C1-C2-C3	-2.28	122.46	126.20
23	C	510	CLA	O2A-CGA-CBA	2.28	118.78	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
28	d	404[B]	PL9	C45-C44-C46	2.28	119.18	115.23
23	B	616	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
23	C	510	CLA	C4-C3-C5	2.27	119.18	115.23
31	M	101	LMT	O5B-C5B-C6B	2.27	112.07	106.44
23	c	507	CLA	CHD-C4C-NC	2.27	127.76	124.23
23	a	405[A]	CLA	C7-C6-C5	-2.27	107.20	113.26
31	A	417	LMT	O5'-C5'-C4'	2.27	114.42	109.72
23	a	406[A]	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
23	c	512	CLA	CMA-C3A-C4A	2.27	117.88	111.77
23	b	612	CLA	C6-C7-C8	-2.27	108.42	115.97
23	b	615	CLA	C6-C7-C8	-2.27	108.42	115.97
23	b	614	CLA	CMA-C3A-C2A	-2.27	105.20	113.98
24	d	403	BCR	C40-C30-C39	2.27	115.13	108.63
23	B	605	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
24	T	102	BCR	C7-C6-C5	-2.27	116.33	121.56
23	a	405[B]	CLA	CMC-C2C-C1C	2.27	128.58	125.03
32	l	802[B]	LHG	O7-C7-O9	-2.27	118.40	123.70
28	d	404[A]	PL9	C47-C48-C49	-2.27	120.08	127.64
23	A	404[B]	CLA	CHB-C1B-C2B	-2.27	120.85	127.43
23	b	610	CLA	C2A-C1A-CHA	-2.27	119.94	123.87
37	a	416[B]	PHO	C4A-C3A-C2A	-2.26	100.68	102.84
23	B	606	CLA	CBC-CAC-C3C	-2.26	106.28	112.42
37	a	416[B]	PHO	O2A-CGA-O1A	-2.26	117.97	123.63
35	C	520	DGD	O1G-C1A-O1A	-2.26	117.97	123.63
33	B	621	LMG	C12-C11-C10	-2.26	105.41	113.69
23	B	602	CLA	CMA-C3A-C2A	-2.26	105.24	113.98
33	C	502	LMG	C9-C8-C7	-2.26	106.51	111.78
32	A	416[A]	LHG	O4-P-O5	2.26	122.96	112.44
23	C	511	CLA	CAC-C3C-C4C	2.26	127.73	124.79
23	C	514	CLA	CAC-C3C-C4C	2.26	127.73	124.79
24	b	618	BCR	C2-C1-C6	2.26	113.72	110.44
23	b	610	CLA	CHB-C4A-NA	2.26	127.66	124.40
23	D	404[B]	CLA	CMC-C2C-C1C	2.26	128.56	125.03
23	c	512	CLA	C4-C3-C2	-2.26	117.83	123.63
38	F	102	HEM	CHA-C1A-NA	2.26	127.95	123.86
23	c	502	CLA	CHD-C4C-NC	2.26	127.73	124.23
23	b	605	CLA	OBD-CAD-C3D	-2.26	123.14	128.42
23	b	606	CLA	CBC-CAC-C3C	-2.26	106.30	112.42
23	B	609	CLA	C2A-C1A-CHA	-2.26	119.95	123.87
28	D	407[B]	PL9	C7-C3-C4	2.26	118.77	116.91
23	b	611	CLA	O2A-CGA-CBA	2.26	118.71	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	D	401[B]	PHO	CMB-C2B-C3B	2.26	129.19	124.68
23	a	406[A]	CLA	CMC-C2C-C1C	2.26	128.56	125.03
24	h	101	BCR	C36-C18-C19	2.25	121.53	118.09
24	k	101	BCR	C34-C9-C8	2.25	121.53	118.09
23	D	404[A]	CLA	CED-O2D-CGD	2.25	121.03	115.92
23	d	401[B]	CLA	CMB-C2B-C1B	2.25	128.85	125.42
32	d	405[A]	LHG	O8-C23-O10	-2.25	117.99	123.63
31	B	630	LMT	O5B-C5B-C6B	2.25	112.02	106.44
23	A	404[B]	CLA	CMA-C3A-C2A	-2.25	105.28	113.98
23	B	602	CLA	CAA-CBA-CGA	-2.25	106.82	113.21
26	B	620	SQD	O9-S-C6	2.25	110.11	106.76
23	c	513	CLA	CHB-C4A-NA	2.25	127.64	124.40
37	a	408[A]	PHO	C1-C2-C3	-2.25	122.51	126.20
23	C	511	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
23	b	615	CLA	C2A-C1A-CHA	-2.25	119.97	123.87
28	D	407[A]	PL9	C12-C13-C14	-2.25	122.48	127.62
33	D	413	LMG	O7-C10-O9	-2.25	118.45	123.70
23	A	405[A]	CLA	O2A-CGA-CBA	2.25	118.68	111.83
24	C	517	BCR	C2-C1-C6	2.25	113.70	110.44
28	A	412[A]	PL9	C35-C34-C33	-2.25	117.86	123.63
23	a	406[B]	CLA	C1-O2A-CGA	2.24	122.08	116.65
32	l	802[B]	LHG	C5-O7-C7	-2.24	112.42	117.80
23	a	409	CLA	CHC-C1C-C2C	-2.24	120.58	126.95
23	A	404[A]	CLA	CHD-C4C-NC	2.24	127.71	124.23
23	d	401[A]	CLA	CMA-C3A-C2A	-2.24	105.31	113.98
37	D	402[A]	PHO	O1D-CGD-CBD	-2.24	121.33	124.72
33	C	526	LMG	C1-O6-C5	2.24	118.09	113.72
23	c	503	CLA	CAC-C3C-C4C	2.24	127.70	124.79
23	b	612	CLA	CMB-C2B-C1B	2.24	128.83	125.42
23	b	605	CLA	C1-O2A-CGA	2.24	122.07	116.65
23	C	505	CLA	O2A-CGA-CBA	2.24	118.66	111.83
24	H	101	BCR	C31-C1-C6	-2.24	106.73	110.24
23	B	608	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
23	B	613	CLA	O2D-CGD-O1D	-2.24	119.50	123.85
37	a	408[B]	PHO	C1-C2-C3	-2.24	122.53	126.20
33	z	101	LMG	C7-O1-C1	-2.24	109.00	113.80
23	c	509	CLA	C2A-C1A-CHA	-2.24	119.99	123.87
35	H	102	DGD	O6E-C5E-C6E	2.23	111.98	106.44
23	B	604	CLA	CMC-C2C-C1C	2.23	128.52	125.03
23	b	610	CLA	C3B-C4B-NB	2.23	112.52	110.53
24	B	619	BCR	C39-C30-C25	-2.23	106.74	110.24
35	h	102	DGD	C3B-C2B-C1B	-2.23	105.52	113.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	619	BCR	C29-C30-C25	2.23	113.68	110.44
35	C	518[B]	DGD	C3G-C2G-C1G	-2.23	106.58	111.78
35	H	102	DGD	C3G-C2G-C1G	-2.23	106.58	111.78
33	C	502	LMG	C12-C11-C10	-2.23	105.52	113.69
23	C	512	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
23	C	514	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
23	B	601	CLA	CHB-C4A-NA	2.23	127.61	124.40
37	D	402[A]	PHO	CED-O2D-CGD	2.23	120.97	115.92
37	a	408[B]	PHO	CBA-CAA-C2A	-2.23	107.22	113.78
35	c	518[A]	DGD	O1G-C1A-O1A	-2.23	118.06	123.63
23	c	504	CLA	CMC-C2C-C1C	2.23	128.51	125.03
23	B	616	CLA	CBC-CAC-C3C	-2.22	106.39	112.42
23	C	505	CLA	CAC-C3C-C4C	2.22	127.68	124.79
23	c	512	CLA	O2A-CGA-O1A	-2.22	118.06	123.63
32	d	411[A]	LHG	O7-C7-O9	-2.22	118.51	123.70
23	c	508	CLA	OBD-CAD-C3D	-2.22	123.22	128.42
32	D	408[B]	LHG	O7-C7-O9	-2.22	118.51	123.70
24	B	619	BCR	C10-C11-C12	-2.22	116.77	123.20
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.89
28	A	412[B]	PL9	C47-C48-C49	-2.22	120.24	127.64
23	B	615	CLA	O2A-CGA-CBA	2.22	118.60	111.83
24	A	408	BCR	C31-C1-C6	-2.22	106.77	110.24
33	c	521	LMG	O8-C28-O10	-2.22	118.08	123.63
38	F	102	HEM	C4C-NC-C1C	2.22	109.43	105.82
26	f	102	SQD	O8-S-C6	2.22	110.25	105.97
23	B	602	CLA	C11-C10-C8	-2.21	108.60	115.97
32	d	405[A]	LHG	O8-C23-C24	2.21	118.59	111.83
23	d	401[B]	CLA	CHD-C4C-NC	2.21	127.67	124.23
28	A	412[B]	PL9	C35-C34-C33	-2.21	117.94	123.63
24	h	101	BCR	C10-C11-C12	-2.21	116.78	123.20
23	B	609	CLA	CHA-C1A-NA	-2.21	121.38	126.39
23	D	404[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
24	c	515	BCR	C37-C22-C21	-2.21	119.23	122.82
38	F	102	HEM	O2D-CGD-CBD	2.21	120.99	114.00
37	D	402[B]	PHO	O2A-CGA-CBA	2.21	118.58	111.83
24	a	410	BCR	C40-C30-C25	-2.21	106.77	110.24
23	c	512	CLA	O2A-CGA-CBA	2.21	118.58	111.83
31	B	628	LMT	C1B-C2B-C3B	2.21	114.66	110.01
23	c	507	CLA	CBC-CAC-C3C	-2.21	106.43	112.42
23	C	513	CLA	C4B-C3B-C2B	-2.21	104.55	107.30
28	a	414[A]	PL9	C35-C34-C33	-2.21	117.95	123.63
23	b	616	CLA	C1-C2-C3	-2.21	122.58	126.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	C3B-C4B-NB	2.21	112.50	110.53
37	D	401[A]	PHO	C4-C3-C5	2.21	119.06	115.23
23	b	607	CLA	CAA-CBA-CGA	2.21	119.48	113.21
23	C	514	CLA	C4B-C3B-C2B	-2.21	104.56	107.30
23	B	606	CLA	C4-C3-C5	2.21	119.06	115.23
23	A	405[B]	CLA	C4C-C3C-C2C	-2.21	103.68	106.89
23	c	507	CLA	CMB-C2B-C1B	2.21	128.78	125.42
32	L	101[B]	LHG	O8-C23-O10	-2.21	118.11	123.63
23	B	612	CLA	CMB-C2B-C1B	2.20	128.77	125.42
34	B	622	HTG	O5-C5-C6	2.20	111.90	106.44
23	B	612	CLA	C4-C3-C5	2.20	119.05	115.23
23	B	614	CLA	OBD-CAD-C3D	-2.20	123.27	128.42
23	C	510	CLA	CMC-C2C-C1C	2.20	128.47	125.03
23	c	503	CLA	C4B-C3B-C2B	-2.20	104.57	107.30
23	c	502	CLA	O2A-CGA-CBA	2.20	118.54	111.83
23	C	504	CLA	CBC-CAC-C3C	-2.20	106.46	112.42
23	C	514	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
23	b	606	CLA	CMA-C3A-C2A	-2.20	105.48	113.98
23	B	615	CLA	C1-O2A-CGA	2.20	121.97	116.65
24	T	102	BCR	C1-C6-C7	2.20	121.61	115.65
23	a	405[B]	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
35	C	519[A]	DGD	O1G-C1A-C2A	2.19	118.53	111.83
23	b	608	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
23	C	512	CLA	C4C-C3C-C2C	-2.19	103.70	106.89
24	C	517	BCR	C38-C26-C25	-2.19	122.09	124.48
35	c	517[A]	DGD	O3G-C3G-C2G	-2.19	105.48	110.82
23	c	504	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
33	C	502	LMG	C1-O6-C5	-2.19	109.44	113.72
28	d	404[A]	PL9	C51-C49-C50	2.19	119.63	114.59
23	c	508	CLA	C1-C2-C3	-2.19	122.61	126.20
23	b	602	CLA	O2A-CGA-CBA	2.19	118.51	111.83
23	C	507	CLA	CHA-C1A-NA	-2.19	121.43	126.39
23	B	613	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
23	b	608	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
23	c	506	CLA	CHD-C4C-NC	2.19	127.62	124.23
23	B	612	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
26	a	412	SQD	O48-C23-O10	-2.19	118.16	123.63
23	c	512	CLA	C2A-C1A-CHA	-2.19	120.07	123.87
23	b	602	CLA	C4-C3-C5	2.19	119.02	115.23
23	b	603	CLA	CMB-C2B-C1B	2.18	128.75	125.42
28	A	412[A]	PL9	C25-C24-C26	2.18	119.02	115.23
33	d	409	LMG	O8-C28-O10	-2.18	118.17	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	C4-C3-C2	-2.18	118.02	123.63
24	b	617	BCR	C16-C17-C18	-2.18	124.22	127.28
24	a	410	BCR	C8-C7-C6	-2.18	121.18	127.00
33	C	522	LMG	C9-C8-C7	-2.18	106.71	111.78
23	B	606	CLA	CAA-C2A-C3A	-2.18	107.11	113.00
24	c	515	BCR	C21-C20-C19	-2.18	116.89	123.20
23	B	616	CLA	CMB-C2B-C3B	2.18	131.67	126.55
24	C	517	BCR	C24-C23-C22	-2.18	123.02	126.23
25	B	624	GOL	C3-C2-C1	-2.18	103.82	111.80
28	a	414[B]	PL9	C47-C48-C49	-2.17	120.39	127.64
23	A	406[B]	CLA	CHB-C1B-C2B	-2.17	121.11	127.43
26	f	102	SQD	O48-C23-O10	-2.17	118.19	123.63
37	a	408[A]	PHO	O2D-CGD-O1D	-2.17	119.62	123.85
23	B	606	CLA	CAC-C3C-C4C	2.17	127.61	124.79
24	D	406	BCR	C30-C25-C24	2.17	121.54	115.65
23	a	407[B]	CLA	C4B-C3B-C2B	-2.17	104.60	107.30
23	B	611	CLA	OBD-CAD-C3D	-2.17	123.34	128.42
24	c	515	BCR	C31-C1-C6	-2.17	106.84	110.24
23	C	507	CLA	C11-C10-C8	-2.17	108.76	115.97
23	A	405[B]	CLA	CED-O2D-CGD	2.17	120.83	115.92
23	C	505	CLA	C1-C2-C3	-2.17	122.65	126.20
23	B	603	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
26	f	102	SQD	O6-C1-C2	2.17	111.56	108.27
23	C	515	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
35	c	517[A]	DGD	O6D-C1D-O3G	-2.16	104.93	110.04
37	a	416[A]	PHO	C4-C3-C2	-2.16	118.07	123.63
28	d	404[A]	PL9	O2-C1-C6	-2.16	117.04	120.48
23	c	513	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
31	t	102	LMT	C1-O1'-C1'	2.16	117.38	113.68
37	D	402[A]	PHO	OBD-CAD-C3D	-2.16	124.52	127.89
24	a	410	BCR	C24-C23-C22	-2.16	123.04	126.23
23	c	514	CLA	C4-C3-C5	2.16	118.98	115.23
23	b	614	CLA	CAA-C2A-C3A	-2.16	107.16	113.00
23	d	402	CLA	C1-O2A-CGA	2.16	121.88	116.65
23	c	506	CLA	C2A-C1A-CHA	-2.16	120.12	123.87
23	D	404[A]	CLA	OBD-CAD-C3D	-2.16	123.37	128.42
32	L	101[B]	LHG	C5-O7-C7	-2.16	112.63	117.80
23	b	615	CLA	C6-C5-C3	-2.16	108.21	113.47
23	a	407[A]	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
23	B	605	CLA	CMC-C2C-C1C	2.16	128.40	125.03
23	C	505	CLA	CMC-C2C-C1C	2.16	128.40	125.03
23	A	405[B]	CLA	CHB-C4A-NA	2.16	127.51	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	H	101	BCR	C11-C10-C9	-2.15	124.26	127.28
23	B	616	CLA	C2A-C1A-CHA	-2.15	120.13	123.87
34	b	623	HTG	O5-C5-C6	2.15	111.78	106.44
35	C	518[A]	DGD	O3G-C3G-C2G	-2.15	105.59	110.82
24	K	102	BCR	C16-C17-C18	-2.15	124.26	127.28
23	B	615	CLA	CAC-C3C-C4C	2.15	127.59	124.79
25	O	303	GOL	C3-C2-C1	-2.15	103.91	111.80
28	D	407[A]	PL9	C27-C28-C29	-2.15	122.71	127.62
23	B	601	CLA	C4-C3-C5	2.15	118.96	115.23
23	A	407	CLA	C11-C12-C13	-2.15	108.83	115.97
33	C	526	LMG	C9-C8-C7	-2.15	106.78	111.78
26	b	620	SQD	C44-O6-C1	-2.15	109.19	113.80
33	c	520	LMG	O7-C10-O9	-2.15	118.69	123.70
35	c	517[A]	DGD	O1G-C1A-O1A	-2.15	118.26	123.63
23	b	614	CLA	CED-O2D-CGD	2.15	120.78	115.92
23	b	601	CLA	CAC-C3C-C2C	2.15	131.50	127.56
31	T	101	LMT	C3B-C4B-C5B	-2.14	106.34	110.23
23	c	513	CLA	C3B-C4B-NB	2.14	112.44	110.53
24	B	619	BCR	C31-C1-C6	-2.14	106.88	110.24
23	b	606	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
38	f	101	HEM	CMD-C2D-C1D	2.14	128.38	125.03
35	c	517[B]	DGD	O1G-C1A-C2A	2.14	118.37	111.83
23	B	613	CLA	C7-C6-C5	-2.14	107.56	113.26
23	b	604	CLA	CHA-C1A-NA	-2.14	121.54	126.39
23	B	603	CLA	CMC-C2C-C1C	2.14	128.38	125.03
23	c	510	CLA	C4-C3-C2	-2.14	118.13	123.63
23	d	401[A]	CLA	CHD-C4C-NC	2.14	127.55	124.23
35	H	102	DGD	C3B-C2B-C1B	-2.14	105.86	113.69
23	c	506	CLA	C4-C3-C5	2.14	118.94	115.23
34	d	408	HTG	C4-C3-C2	-2.14	107.08	110.83
34	c	522	HTG	C1-O5-C5	2.14	116.40	112.56
33	a	417	LMG	O7-C10-O9	-2.14	118.71	123.70
24	c	516	BCR	C15-C16-C17	-2.14	119.15	123.52
23	B	606	CLA	CHB-C1B-C2B	-2.14	121.23	127.43
23	D	405	CLA	CHD-C4C-NC	2.14	127.54	124.23
23	C	508	CLA	CBC-CAC-C3C	-2.13	106.63	112.42
35	c	518[B]	DGD	C2G-O2G-C1B	-2.13	112.69	117.80
35	C	519[B]	DGD	C6D-C5D-C4D	2.13	116.54	112.07
23	b	613	CLA	CAC-C3C-C4C	2.13	127.56	124.79
37	a	408[B]	PHO	CBC-CAC-C3C	-2.13	109.82	112.87
24	H	101	BCR	C24-C23-C22	-2.13	123.08	126.23
23	A	405[B]	CLA	CAC-C3C-C4C	2.13	127.56	124.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	406	BCR	C3-C4-C5	-2.13	110.25	114.06
28	a	414[B]	PL9	C51-C49-C50	2.13	119.49	114.59
34	b	623	HTG	O5-C1-C2	2.13	113.25	110.32
23	C	514	CLA	CHB-C1B-C2B	-2.13	121.24	127.43
23	B	614	CLA	CMB-C2B-C1B	2.13	128.66	125.42
32	L	101[A]	LHG	O4-P-O5	2.13	122.36	112.44
37	D	402[A]	PHO	C6-C5-C3	-2.13	108.28	113.47
23	A	407	CLA	CMC-C2C-C1C	2.13	128.36	125.03
23	c	514	CLA	C1-C2-C3	-2.13	122.71	126.20
24	Y	101	BCR	C39-C30-C25	-2.13	106.90	110.24
23	a	407[A]	CLA	C4-C3-C5	2.13	118.92	115.23
23	B	611	CLA	C7-C6-C5	-2.13	107.59	113.26
23	c	507	CLA	CAA-CBA-CGA	2.13	119.25	113.21
23	B	601	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
23	b	615	CLA	CHA-C1A-NA	-2.13	121.57	126.39
28	A	412[B]	PL9	C37-C36-C34	-2.13	106.13	113.19
32	d	406[B]	LHG	C5-O7-C7	-2.13	112.70	117.80
23	B	604	CLA	CHA-C1A-NA	-2.13	121.58	126.39
33	a	417	LMG	O8-C28-C29	2.13	118.32	111.83
23	c	506	CLA	C1-O2A-CGA	2.12	121.79	116.65
28	D	407[B]	PL9	C30-C29-C31	2.12	118.91	115.23
37	D	402[B]	PHO	O1D-CGD-CBD	-2.12	121.50	124.72
31	b	627	LMT	C1'-O5'-C5'	-2.12	109.58	113.72
28	a	414[A]	PL9	C45-C44-C46	2.12	118.91	115.23
34	B	622	HTG	C2'-C1'-S1	-2.12	105.21	112.36
23	a	405[A]	CLA	CMB-C2B-C3B	2.12	131.54	126.55
23	C	506	CLA	C4-C3-C5	2.12	118.91	115.23
31	b	621	LMT	C2'-C3'-C4'	2.12	114.49	109.68
23	b	603	CLA	CMC-C2C-C1C	2.12	128.35	125.03
24	Y	101	BCR	C21-C20-C19	-2.12	117.06	123.20
23	A	406[A]	CLA	CHB-C4A-NA	2.12	127.46	124.40
40	V	202	HEC	CMD-C2D-C1D	2.12	128.64	125.42
31	F	101	LMT	C2'-C3'-C4'	2.12	114.49	109.68
23	c	509	CLA	CHA-C1A-NA	-2.12	121.60	126.39
24	D	406	BCR	C40-C30-C39	2.12	114.69	108.63
24	C	517	BCR	C37-C22-C23	2.12	121.32	118.09
28	a	414[B]	PL9	C12-C13-C14	-2.11	122.78	127.62
24	t	103	BCR	C37-C22-C23	2.11	121.32	118.09
35	c	517[B]	DGD	O6D-C1D-O3G	-2.11	105.05	110.04
26	C	501[B]	SQD	O48-C23-O10	-2.11	118.34	123.63
24	b	618	BCR	C8-C7-C6	-2.11	121.36	127.00
23	B	605	CLA	CAC-C3C-C2C	2.11	131.44	127.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	516	BCR	C38-C26-C25	-2.11	122.18	124.48
40	V	202	HEC	CAD-CBD-CGD	-2.11	108.07	113.67
23	A	405[A]	CLA	CHB-C4A-NA	2.11	127.44	124.40
32	l	802[A]	LHG	O7-C7-O9	-2.11	118.77	123.70
33	C	502	LMG	O8-C28-C29	2.11	118.27	111.83
23	A	406[B]	CLA	CMA-C3A-C2A	-2.11	105.83	113.98
37	a	416[B]	PHO	C4-C3-C2	-2.11	118.22	123.63
23	c	510	CLA	CMC-C2C-C1C	2.11	128.32	125.03
23	D	404[A]	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
23	A	404[A]	CLA	C7-C6-C5	-2.11	107.65	113.26
23	A	405[B]	CLA	CMA-C3A-C2A	-2.11	105.84	113.98
23	C	508	CLA	CED-O2D-CGD	2.11	120.69	115.92
26	a	411[B]	SQD	O9-S-C6	2.11	109.90	106.76
38	f	101	HEM	C4C-NC-C1C	2.10	109.25	105.82
23	d	401[B]	CLA	CMA-C3A-C2A	-2.10	105.85	113.98
24	c	516	BCR	C15-C14-C13	-2.10	124.33	127.28
23	C	509	CLA	CAC-C3C-C4C	2.10	127.53	124.79
34	B	622	HTG	O2-C2-C3	-2.10	105.42	110.38
23	a	406[A]	CLA	CHB-C4A-NA	2.10	127.43	124.40
24	b	618	BCR	C15-C16-C17	-2.10	119.22	123.52
28	d	404[A]	PL9	C45-C44-C46	2.10	118.87	115.23
26	B	620	SQD	O9-S-O7	-2.10	107.00	113.82
23	c	508	CLA	CHA-C1A-NA	-2.10	121.64	126.39
24	b	619	BCR	C1-C6-C5	-2.10	119.77	122.64
23	C	511	CLA	CMB-C2B-C3B	2.10	131.48	126.55
26	C	501[B]	SQD	O8-S-C6	2.10	110.02	105.97
23	C	509	CLA	CHA-C1A-NA	-2.10	121.64	126.39
35	c	517[A]	DGD	O1G-C1A-C2A	2.10	118.23	111.83
23	C	514	CLA	CBA-CAA-C2A	-2.10	107.56	113.79
24	t	103	BCR	C2-C1-C6	2.10	113.48	110.44
23	b	604	CLA	C1-O2A-CGA	2.09	121.72	116.65
23	a	407[A]	CLA	CAC-C3C-C4C	2.09	127.52	124.79
35	c	519	DGD	C6B-C5B-C4B	-2.09	103.78	114.37
26	b	620	SQD	C1-C2-C3	-2.09	105.60	110.01
23	A	405[B]	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
24	K	102	BCR	C33-C5-C6	-2.09	122.20	124.48
23	B	615	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
23	c	511	CLA	C11-C10-C8	-2.09	109.01	115.97
23	d	401[A]	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
26	F	103	SQD	O5-C1-C2	-2.09	106.08	110.37
26	F	103	SQD	C3-C4-C5	2.09	114.02	110.23
23	B	612	CLA	OBD-CAD-C3D	-2.09	123.53	128.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	BCR	C28-C27-C26	-2.09	110.33	114.06
26	C	501[B]	SQD	O6-C44-C45	-2.09	105.74	110.82
26	f	102	SQD	O7-S-C6	2.09	109.87	106.76
23	B	615	CLA	CHA-C1A-NA	-2.09	121.67	126.39
33	z	101	LMG	O8-C28-O10	-2.09	118.41	123.63
28	d	404[A]	PL9	C2-C1-C6	2.08	121.48	119.00
34	b	622	HTG	C6-C5-C4	-2.08	107.90	113.02
40	V	202	HEC	CBA-CAA-C2A	-2.08	106.77	112.53
24	H	101	BCR	C37-C22-C23	2.08	121.27	118.09
23	c	505	CLA	C2A-C1A-CHA	-2.08	120.25	123.87
23	C	510	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
24	t	103	BCR	C15-C16-C17	-2.08	119.26	123.52
28	A	412[A]	PL9	C53-C6-C1	2.08	119.54	115.28
26	a	411[A]	SQD	C3-C4-C5	2.08	114.00	110.23
26	b	620	SQD	C4-C3-C2	2.08	114.48	110.83
31	M	101	LMT	O6'-C6'-C5'	-2.08	104.26	111.33
23	a	405[B]	CLA	CHB-C4A-NA	2.08	127.40	124.40
24	c	516	BCR	C39-C30-C25	-2.08	106.99	110.24
23	B	613	CLA	CMA-C3A-C4A	-2.08	106.19	111.77
24	a	410	BCR	C33-C5-C6	-2.08	122.22	124.48
23	B	601	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
23	D	404[A]	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
23	A	406[A]	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
23	C	515	CLA	CAC-C3C-C4C	2.07	127.49	124.79
23	b	611	CLA	C7-C6-C5	-2.07	107.73	113.26
23	B	607	CLA	O2A-CGA-CBA	2.07	118.16	111.83
37	a	416[A]	PHO	O2A-CGA-O1A	-2.07	118.44	123.63
35	C	519[B]	DGD	O2G-C1B-O1B	-2.07	118.86	123.70
28	A	412[B]	PL9	C25-C24-C26	2.07	118.82	115.23
35	c	518[B]	DGD	O1G-C1A-O1A	-2.07	118.45	123.63
23	c	505	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
25	a	419	GOL	C3-C2-C1	-2.07	104.21	111.80
23	A	407	CLA	CMA-C3A-C4A	-2.07	106.22	111.77
33	C	526	LMG	O7-C10-O9	-2.07	118.88	123.70
26	f	102	SQD	C44-O6-C1	-2.06	109.37	113.80
28	A	412[B]	PL9	C51-C49-C50	2.06	119.34	114.59
23	b	609	CLA	CGD-CBD-CAD	-2.06	104.16	110.85
28	a	414[B]	PL9	C35-C34-C33	-2.06	118.33	123.63
23	a	407[A]	CLA	CAA-CBA-CGA	2.06	119.06	113.21
24	Y	101	BCR	C15-C16-C17	-2.06	119.30	123.52
23	C	512	CLA	CAC-C3C-C4C	2.06	127.47	124.79
23	C	503	CLA	CAA-C2A-C3A	-2.06	107.43	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	517	BCR	C29-C30-C25	2.06	113.43	110.44
24	c	516	BCR	C29-C30-C25	2.06	113.43	110.44
23	b	603	CLA	C5-C3-C2	-2.06	116.54	121.17
23	C	510	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
23	B	607	CLA	C6-C7-C8	-2.06	109.12	115.97
24	c	515	BCR	C29-C30-C25	2.06	113.43	110.44
33	a	417	LMG	O6-C5-C4	2.06	113.41	109.70
23	c	511	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
23	b	606	CLA	C4-C3-C2	-2.06	118.34	123.63
32	L	101[B]	LHG	O4-P-O5	2.06	122.02	112.44
23	A	405[A]	CLA	C1-C2-C3	-2.06	122.82	126.20
23	B	606	CLA	C7-C6-C5	-2.06	107.78	113.26
24	b	617	BCR	C21-C20-C19	-2.06	117.24	123.20
34	b	623	HTG	C1-C2-C3	2.05	114.57	110.55
37	D	402[A]	PHO	O2A-CGA-CBA	2.05	118.10	111.83
33	C	526	LMG	C3-C4-C5	2.05	113.95	110.23
24	d	403	BCR	C29-C28-C27	-2.05	106.76	111.28
23	C	511	CLA	C11-C12-C13	-2.05	109.14	115.97
38	f	101	HEM	O2A-CGA-CBA	2.05	120.48	114.00
28	D	407[A]	PL9	C47-C48-C49	-2.05	120.81	127.64
28	d	404[A]	PL9	C40-C39-C38	-2.05	118.37	123.63
23	c	513	CLA	CHA-C1A-NA	-2.05	121.75	126.39
23	a	407[B]	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
24	D	406	BCR	C29-C28-C27	-2.05	106.78	111.28
23	D	405	CLA	CHB-C4A-NA	2.05	127.35	124.40
23	B	603	CLA	C6-C7-C8	-2.05	109.16	115.97
35	H	102	DGD	C1E-O6E-C5E	-2.05	109.72	113.72
23	a	405[B]	CLA	CBB-CAB-C3B	-2.05	117.31	127.53
32	d	411[B]	LHG	O7-C7-O9	-2.04	118.92	123.70
23	B	612	CLA	CHD-C4C-NC	2.04	127.40	124.23
24	a	410	BCR	C10-C11-C12	-2.04	117.28	123.20
24	c	515	BCR	C36-C18-C19	2.04	121.21	118.09
23	C	509	CLA	C6-C7-C8	-2.04	109.17	115.97
23	B	616	CLA	C4-C3-C2	-2.04	118.38	123.63
23	d	401[A]	CLA	CBB-CAB-C3B	-2.04	117.32	127.53
28	A	412[B]	PL9	C32-C31-C29	-2.04	106.42	113.19
28	d	404[B]	PL9	C35-C34-C36	2.04	118.77	115.23
23	B	616	CLA	OBD-CAD-C3D	-2.04	123.65	128.42
23	a	407[A]	CLA	CHA-C1A-NA	-2.04	121.77	126.39
24	b	619	BCR	C34-C9-C8	2.04	121.20	118.09
28	A	412[A]	PL9	C10-C9-C11	2.04	118.77	115.23
23	c	508	CLA	C4B-C3B-C2B	-2.04	104.77	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	414[A]	PL9	C47-C46-C44	-2.04	106.43	113.19
23	C	514	CLA	CBC-CAC-C3C	-2.04	106.90	112.42
24	d	403	BCR	C3-C4-C5	-2.04	110.43	114.06
34	B	625	HTG	C1-O5-C5	2.04	116.21	112.56
23	b	613	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
35	c	519	DGD	O4D-C4D-C3D	-2.03	105.58	110.38
33	c	520	LMG	O8-C28-O10	-2.03	118.54	123.63
23	c	509	CLA	CAC-C3C-C4C	2.03	127.44	124.79
24	a	410	BCR	C38-C26-C27	2.03	117.93	113.60
34	b	625	HTG	C1-C2-C3	-2.03	106.58	110.55
23	c	510	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
23	C	506	CLA	CHD-C4C-NC	2.03	127.38	124.23
23	B	602	CLA	CMB-C2B-C1B	2.03	128.51	125.42
25	l	801[A]	GOL	C3-C2-C1	-2.03	104.36	111.80
23	b	602	CLA	C11-C10-C8	-2.03	109.22	115.97
23	d	401[B]	CLA	CMC-C2C-C1C	2.03	128.20	125.03
23	B	614	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
31	m	103	LMT	O5B-C5B-C6B	2.03	111.47	106.44
34	B	623	HTG	C1-C2-C3	2.03	114.51	110.55
24	A	408	BCR	C11-C10-C9	-2.03	124.44	127.28
35	c	518[A]	DGD	O6E-C1E-O5D	-2.03	105.26	110.04
35	c	518[B]	DGD	C1D-O6D-C5D	2.02	117.67	113.72
28	a	414[A]	PL9	C51-C49-C50	2.02	119.25	114.59
23	C	505	CLA	C2A-C1A-CHA	-2.02	120.36	123.87
23	c	504	CLA	CBC-CAC-C3C	-2.02	106.94	112.42
23	b	615	CLA	C11-C12-C13	-2.02	109.25	115.97
23	C	506	CLA	OBD-CAD-C3D	-2.02	123.70	128.42
35	C	520	DGD	O2G-C1B-O1B	-2.02	118.98	123.70
23	b	612	CLA	CHB-C1B-NB	-2.02	121.02	124.05
37	a	416[B]	PHO	C4D-CHA-CBD	2.02	109.42	108.45
32	D	409[A]	LHG	O4-P-O5	2.01	121.82	112.44
23	B	608	CLA	C6-C7-C8	-2.01	109.27	115.97
28	A	412[A]	PL9	C51-C49-C50	2.01	119.22	114.59
35	C	518[B]	DGD	O6E-C5E-C4E	2.01	113.33	109.70
23	D	404[B]	CLA	CBB-CAB-C3B	-2.01	117.46	127.53
33	d	409	LMG	O3-C3-C2	-2.01	105.63	110.38
24	y	101	BCR	C16-C15-C14	-2.01	119.40	123.52
26	C	501[B]	SQD	O9-S-O7	-2.01	107.28	113.82
23	b	610	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
34	b	622	HTG	C3-C4-C5	2.01	113.88	110.23
33	m	101	LMG	C3-C4-C5	2.01	113.88	110.23
28	D	407[A]	PL9	C45-C44-C46	2.01	118.72	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
24	D	406	BCR	C30-C25-C26	-2.01	119.89	122.64
23	b	603	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
24	D	406	BCR	C31-C1-C6	-2.01	107.09	110.24
23	b	616	CLA	C11-C12-C13	-2.01	109.29	115.97
24	B	617	BCR	C11-C10-C9	-2.01	124.46	127.28
35	c	517[A]	DGD	O2G-C1B-O1B	-2.01	119.01	123.70
23	a	406[B]	CLA	CAC-C3C-C2C	2.01	131.25	127.56
23	C	510	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	c	510	CLA	CHB-C4A-NA	2.00	127.29	124.40
37	D	402[B]	PHO	OBD-CAD-C3D	-2.00	124.77	127.89
31	F	101	LMT	O1'-C1'-C2'	2.00	111.32	108.27
23	c	502	CLA	C2A-C1A-CHA	-2.00	120.39	123.87
28	D	407[A]	PL9	C22-C23-C24	-2.00	123.04	127.62
24	h	101	BCR	C34-C9-C8	2.00	121.15	118.09

All (69) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND
23	A	405[A]	CLA	ND
23	A	405[B]	CLA	ND
23	A	407	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	506	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	C	515	CLA	ND
23	D	404[A]	CLA	ND
23	D	404[B]	CLA	ND
23	D	405	CLA	ND
23	a	405[A]	CLA	ND
23	a	405[B]	CLA	ND
23	a	406[A]	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
23	c	514	CLA	ND
23	d	401[A]	CLA	ND
23	d	401[B]	CLA	ND
23	d	402	CLA	ND

All (1636) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	509	CLA	C2B-C3B-CAB-CBB
23	C	509	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	a	405[B]	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C4B-C3B-CAB-CBB
23	a	407[B]	CLA	C2B-C3B-CAB-CBB
23	a	407[B]	CLA	C4B-C3B-CAB-CBB
23	a	409	CLA	C4-C3-C5-C6
23	b	604	CLA	C6-C7-C8-C9
23	b	606	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
24	T	102	BCR	C13-C14-C15-C16
24	Y	101	BCR	C5-C6-C7-C8
24	b	619	BCR	C5-C6-C7-C8
24	y	101	BCR	C1-C6-C7-C8
24	y	101	BCR	C5-C6-C7-C8
25	A	409	GOL	O1-C1-C2-O2
25	A	409	GOL	O1-C1-C2-C3
25	B	624	GOL	C1-C2-C3-O3
25	B	629	GOL	O1-C1-C2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	B	629	GOL	C1-C2-C3-O3
25	D	403	GOL	O1-C1-C2-C3
25	D	414	GOL	C1-C2-C3-O3
25	V	204[A]	GOL	C1-C2-C3-O3
25	V	204[B]	GOL	C1-C2-C3-O3
25	a	418	GOL	O1-C1-C2-O2
25	a	418	GOL	O1-C1-C2-C3
25	b	624	GOL	C1-C2-C3-O3
25	c	527	GOL	C1-C2-C3-O3
25	c	528	GOL	C1-C2-C3-O3
25	o	302	GOL	C1-C2-C3-O3
25	v	202[B]	GOL	O1-C1-C2-O2
26	A	410	SQD	O6-C44-C45-O47
26	B	620	SQD	O5-C1-O6-C44
26	B	620	SQD	O49-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
26	C	501[B]	SQD	C8-C7-O47-C45
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	a	412	SQD	O6-C44-C45-O47
26	a	412	SQD	C5-C6-S-O7
26	a	412	SQD	C5-C6-S-O8
26	a	412	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
28	A	412[A]	PL9	C9-C11-C12-C13
28	a	414[A]	PL9	C23-C24-C26-C27
28	a	414[A]	PL9	C25-C24-C26-C27
31	A	415	LMT	O5'-C1'-O1'-C1
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
31	t	102	LMT	O5'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	D	408[A]	LHG	O2-C2-C3-O3
32	D	408[A]	LHG	C3-O3-P-O4
32	D	408[A]	LHG	C3-O3-P-O5
32	D	408[A]	LHG	C3-O3-P-O6
32	D	408[A]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	C3-O3-P-O4
32	D	408[B]	LHG	C3-O3-P-O6
32	D	408[B]	LHG	C4-O6-P-O3
32	D	408[B]	LHG	C4-O6-P-O4
32	D	408[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C3-O3-P-O4
32	a	420[A]	LHG	C3-O3-P-O6
32	a	420[A]	LHG	C4-O6-P-O3
32	a	420[A]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	O10-C23-O8-C6
32	a	420[A]	LHG	C24-C23-O8-C6
32	a	420[B]	LHG	C3-O3-P-O4
32	a	420[B]	LHG	C3-O3-P-O6
32	a	420[B]	LHG	C4-O6-P-O3
32	a	420[B]	LHG	C4-O6-P-O4
32	a	420[B]	LHG	C4-O6-P-O5
32	a	420[B]	LHG	O10-C23-O8-C6
32	a	420[B]	LHG	C24-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	d	405[A]	LHG	C3-O3-P-O4
32	d	405[A]	LHG	C3-O3-P-O5
32	d	405[A]	LHG	C3-O3-P-O6
32	d	405[A]	LHG	C4-O6-P-O4
32	d	405[B]	LHG	O2-C2-C3-O3
32	d	405[B]	LHG	C3-O3-P-O4
32	d	405[B]	LHG	C3-O3-P-O6
32	d	405[B]	LHG	C4-O6-P-O3
32	d	405[B]	LHG	C4-O6-P-O4
32	d	411[A]	LHG	C3-O3-P-O5
32	d	411[B]	LHG	C1-C2-C3-O3
32	d	411[B]	LHG	C3-O3-P-O5
32	l	802[A]	LHG	C4-O6-P-O3
32	l	802[A]	LHG	C4-O6-P-O4
32	l	802[A]	LHG	C4-O6-P-O5
32	l	802[B]	LHG	C4-O6-P-O3
32	l	802[B]	LHG	C4-O6-P-O4
32	l	802[B]	LHG	C4-O6-P-O5
33	C	522	LMG	C11-C10-O7-C8
33	C	526	LMG	O9-C10-O7-C8
33	C	526	LMG	C11-C10-O7-C8
33	c	521	LMG	O9-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	C11-C10-O7-C8
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
40	V	202	HEC	C2B-C3B-CAB-CBB
40	V	202	HEC	C4B-C3B-CAB-CBB
40	V	202	HEC	C2C-C3C-CAC-CBC
40	V	202	HEC	C4C-C3C-CAC-CBC
40	v	201	HEC	C2B-C3B-CAB-CBB
40	v	201	HEC	C4B-C3B-CAB-CBB
40	v	201	HEC	C2C-C3C-CAC-CBC
40	v	201	HEC	C4C-C3C-CAC-CBC
31	A	417	LMT	O5B-C1B-O1B-C4'
26	C	501[A]	SQD	O49-C7-O47-C45
26	C	501[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
33	z	101	LMG	O9-C10-O7-C8
23	D	405	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	d	402	CLA	C3-C5-C6-C7
23	D	405	CLA	CBD-CGD-O2D-CED
23	A	407	CLA	C4-C3-C5-C6
23	C	506	CLA	C4-C3-C5-C6
23	C	509	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
28	A	412[A]	PL9	C15-C14-C16-C17
28	a	414[B]	PL9	C25-C24-C26-C27
28	a	414[B]	PL9	C30-C29-C31-C32
23	A	407	CLA	C2-C3-C5-C6
23	C	506	CLA	C2-C3-C5-C6
23	a	409	CLA	C2-C3-C5-C6
23	d	402	CLA	C2-C3-C5-C6
28	a	414[B]	PL9	C23-C24-C26-C27
23	B	614	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
31	B	630	LMT	C4'-C5'-C6'-O6'
34	B	625	HTG	S1-C1'-C2'-C3'
33	C	522	LMG	O9-C10-O7-C8
31	F	101	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	C4B-C5B-C6B-O6B
32	d	405[A]	LHG	O2-C2-C3-O3
31	B	630	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O5B-C5B-C6B-O6B
31	b	627	LMT	O5'-C5'-C6'-O6'
33	C	522	LMG	O6-C5-C6-O5
34	D	412	HTG	C4-C5-C6-O6
26	C	501[A]	SQD	C8-C7-O47-C45
34	D	412	HTG	O5-C5-C6-O6
31	A	417	LMT	O5B-C5B-C6B-O6B
23	B	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
28	A	412[A]	PL9	C20-C19-C21-C22
28	A	412[B]	PL9	C15-C14-C16-C17
28	A	412[B]	PL9	C20-C19-C21-C22
28	A	412[B]	PL9	C30-C29-C31-C32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	a	414[A]	PL9	C15-C14-C16-C17
28	a	414[A]	PL9	C30-C29-C31-C32
23	B	605	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
28	A	412[A]	PL9	C13-C14-C16-C17
28	A	412[A]	PL9	C18-C19-C21-C22
28	A	412[B]	PL9	C13-C14-C16-C17
28	a	414[A]	PL9	C13-C14-C16-C17
28	a	414[A]	PL9	C28-C29-C31-C32
28	a	414[B]	PL9	C13-C14-C16-C17
28	a	414[B]	PL9	C28-C29-C31-C32
34	b	625	HTG	O5-C5-C6-O6
28	A	412[A]	PL9	C14-C16-C17-C18
28	A	412[A]	PL9	C44-C46-C47-C48
28	A	412[B]	PL9	C9-C11-C12-C13
28	A	412[B]	PL9	C14-C16-C17-C18
28	D	407[A]	PL9	C39-C41-C42-C43
28	a	414[A]	PL9	C9-C11-C12-C13
28	a	414[A]	PL9	C14-C16-C17-C18
28	a	414[B]	PL9	C9-C11-C12-C13
28	a	414[B]	PL9	C14-C16-C17-C18
31	T	101	LMT	C4'-C5'-C6'-O6'
23	c	502	CLA	CBD-CGD-O2D-CED
31	T	101	LMT	O5B-C5B-C6B-O6B
31	b	621	LMT	C4'-C5'-C6'-O6'
31	e	101	LMT	C4'-C5'-C6'-O6'
31	m	103	LMT	C4B-C5B-C6B-O6B
23	B	605	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
31	A	417	LMT	O5'-C5'-C6'-O6'
31	B	628	LMT	O5B-C5B-C6B-O6B
31	t	101	LMT	O5'-C5'-C6'-O6'
31	B	628	LMT	C4'-C5'-C6'-O6'
33	c	521	LMG	C4-C5-C6-O5
23	c	514	CLA	CBD-CGD-O2D-CED
34	b	625	HTG	S1-C1'-C2'-C3'
32	d	405[A]	LHG	C1-C2-C3-O3
32	d	405[B]	LHG	C1-C2-C3-O3
23	c	510	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	621	LMG	C39-C40-C41-C42
31	B	630	LMT	C4B-C5B-C6B-O6B
31	c	501	LMT	C4B-C5B-C6B-O6B
23	b	603	CLA	C4-C3-C5-C6
28	a	414[B]	PL9	C15-C14-C16-C17
23	C	509	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
28	A	412[B]	PL9	C18-C19-C21-C22
23	A	407	CLA	C3-C5-C6-C7
23	B	602	CLA	C6-C7-C8-C9
23	C	508	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	513	CLA	C6-C7-C8-C9
31	F	101	LMT	C4'-C5'-C6'-O6'
31	b	627	LMT	C4'-C5'-C6'-O6'
31	t	101	LMT	C4'-C5'-C6'-O6'
31	A	415	LMT	C2'-C1'-O1'-C1
31	b	621	LMT	C2'-C1'-O1'-C1
31	t	102	LMT	C2'-C1'-O1'-C1
24	b	619	BCR	C7-C8-C9-C34
31	A	415	LMT	O5B-C5B-C6B-O6B
24	b	619	BCR	C7-C8-C9-C10
31	B	628	LMT	C4B-C5B-C6B-O6B
31	m	103	LMT	O5B-C5B-C6B-O6B
23	b	614	CLA	C8-C10-C11-C12
31	A	417	LMT	C4B-C5B-C6B-O6B
23	a	405[B]	CLA	CBD-CGD-O2D-CED
31	B	628	LMT	O5'-C5'-C6'-O6'
23	C	510	CLA	C10-C11-C12-C13
31	B	628	LMT	C5'-C4'-O1B-C1B
31	B	628	LMT	C6-C7-C8-C9
23	b	611	CLA	C8-C10-C11-C12
31	M	101	LMT	O5'-C5'-C6'-O6'
25	O	302	GOL	O1-C1-C2-O2
23	B	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C12-C13-C15-C16
34	b	622	HTG	S1-C1'-C2'-C3'
28	A	412[A]	PL9	C30-C29-C31-C32
26	B	620	SQD	C7-C8-C9-C10
28	A	412[B]	PL9	C44-C46-C47-C48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
28	D	407[B]	PL9	C39-C41-C42-C43
28	d	404[A]	PL9	C39-C41-C42-C43
28	d	404[B]	PL9	C39-C41-C42-C43
31	e	101	LMT	O5'-C5'-C6'-O6'
33	C	526	LMG	C10-C11-C12-C13
35	c	518[A]	DGD	C1B-C2B-C3B-C4B
23	C	505	CLA	CBD-CGD-O2D-CED
23	A	407	CLA	C5-C6-C7-C8
23	b	611	CLA	C15-C16-C17-C18
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	615	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
26	F	103	SQD	C23-C24-C25-C26
32	E	101[A]	LHG	C23-C24-C25-C26
35	c	518[B]	DGD	C1B-C2B-C3B-C4B
23	C	513	CLA	C3-C5-C6-C7
26	F	103	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
26	b	620	SQD	C18-C19-C20-C21
35	h	102	DGD	C6B-C7B-C8B-C9B
23	B	601	CLA	C5-C6-C7-C8
23	B	602	CLA	C13-C15-C16-C17
23	B	606	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	b	614	CLA	C10-C11-C12-C13
23	c	510	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	C15-C16-C17-C18
31	c	501	LMT	C4'-C5'-C6'-O6'
31	c	501	LMT	O5'-C5'-C6'-O6'
31	A	415	LMT	O1'-C1-C2-C3
32	D	409[B]	LHG	C24-C23-O8-C6
31	c	501	LMT	O1'-C1-C2-C3
31	A	417	LMT	C5'-C4'-O1B-C1B
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
26	b	620	SQD	C31-C32-C33-C34
23	a	405[A]	CLA	C15-C16-C17-C18
23	c	514	CLA	C10-C11-C12-C13
32	D	408[A]	LHG	C1-C2-C3-O3
23	b	606	CLA	C2A-CAA-CBA-CGA
23	a	409	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	D	409[A]	LHG	C33-C34-C35-C36
23	A	405[B]	CLA	C15-C16-C17-C18
23	D	405	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	606	CLA	C15-C16-C17-C18
31	A	417	LMT	O1'-C1-C2-C3
32	D	409[B]	LHG	C33-C34-C35-C36
23	D	405	CLA	O1D-CGD-O2D-CED
23	C	509	CLA	C5-C6-C7-C8
31	A	417	LMT	C4'-C5'-C6'-O6'
34	D	412	HTG	S1-C1'-C2'-C3'
23	B	614	CLA	C10-C11-C12-C13
23	c	513	CLA	C13-C15-C16-C17
33	B	621	LMG	O9-C10-O7-C8
31	e	101	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
35	C	519[A]	DGD	C2E-C1E-O5D-C6D
33	B	621	LMG	C15-C16-C17-C18
26	C	501[A]	SQD	C7-C8-C9-C10
23	c	510	CLA	C3-C5-C6-C7
33	c	520	LMG	C4-C5-C6-O5
24	c	516	BCR	C7-C8-C9-C34
35	C	520	DGD	C6B-C7B-C8B-C9B
31	e	101	LMT	O5B-C5B-C6B-O6B
35	C	518[B]	DGD	O6D-C5D-C6D-O5D
23	b	610	CLA	C2A-CAA-CBA-CGA
25	B	627	GOL	C1-C2-C3-O3
25	D	414	GOL	O1-C1-C2-C3
25	O	302	GOL	O1-C1-C2-C3
25	O	303	GOL	O1-C1-C2-C3
25	v	202[A]	GOL	O1-C1-C2-C3
25	v	202[B]	GOL	O1-C1-C2-C3
33	B	621	LMG	C37-C38-C39-C40
23	a	409	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C20
31	t	101	LMT	O1'-C1-C2-C3
23	B	616	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	t	102	LMT	C11-C10-C9-C8
35	C	520	DGD	C2B-C3B-C4B-C5B
33	B	621	LMG	C11-C10-O7-C8
34	B	622	HTG	C1'-C2'-C3'-C4'
35	c	517[B]	DGD	C4D-C5D-C6D-O5D
26	C	501[A]	SQD	C12-C13-C14-C15
31	c	501	LMT	C1-C2-C3-C4
37	a	416[B]	PHO	C2C-C3C-CAC-CBC
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
23	B	608	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
34	B	625	HTG	O5-C5-C6-O6
26	f	102	SQD	C32-C33-C34-C35
32	L	101[A]	LHG	C15-C16-C17-C18
32	L	101[A]	LHG	C17-C18-C19-C20
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
35	c	519	DGD	CBB-CCB-CDB-CEB
26	A	410	SQD	C17-C18-C19-C20
26	F	103	SQD	C30-C31-C32-C33
31	b	627	LMT	C7-C8-C9-C10
31	e	101	LMT	C4-C5-C6-C7
32	D	408[B]	LHG	C12-C13-C14-C15
32	L	101[B]	LHG	C17-C18-C19-C20
33	C	502	LMG	C17-C18-C19-C20
33	C	522	LMG	C18-C19-C20-C21
33	c	520	LMG	C34-C35-C36-C37
23	c	502	CLA	O1D-CGD-O2D-CED
23	c	507	CLA	C15-C16-C17-C18
23	a	409	CLA	O1A-CGA-O2A-C1
32	D	409[B]	LHG	O10-C23-O8-C6
35	c	517[A]	DGD	O6D-C5D-C6D-O5D
31	A	417	LMT	C1-C2-C3-C4
26	a	412	SQD	C25-C26-C27-C28
31	b	627	LMT	C3-C4-C5-C6
32	D	409[B]	LHG	C32-C33-C34-C35
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
25	B	624	GOL	O2-C2-C3-O3
25	B	629	GOL	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	D	403	GOL	O1-C1-C2-O2
25	D	414	GOL	O2-C2-C3-O3
25	O	303	GOL	O1-C1-C2-O2
25	V	204[A]	GOL	O2-C2-C3-O3
25	V	204[B]	GOL	O2-C2-C3-O3
25	b	624	GOL	O2-C2-C3-O3
25	o	302	GOL	O2-C2-C3-O3
31	T	101	LMT	C2-C1-O1'-C1'
31	t	102	LMT	C2-C1-O1'-C1'
31	B	628	LMT	C5-C6-C7-C8
33	D	413	LMG	C19-C20-C21-C22
35	C	518[B]	DGD	C4D-C5D-C6D-O5D
23	B	602	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
33	c	520	LMG	C10-C11-C12-C13
26	C	501[B]	SQD	C15-C16-C17-C18
32	d	411[A]	LHG	C16-C17-C18-C19
23	B	608	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	a	409	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C19
32	D	408[B]	LHG	C16-C17-C18-C19
23	A	405[A]	CLA	C15-C16-C17-C18
33	m	101	LMG	C11-C10-O7-C8
23	A	407	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C10-C8-C7
23	C	512	CLA	C11-C12-C13-C15
33	B	621	LMG	C17-C18-C19-C20
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
35	h	102	DGD	C7B-C8B-C9B-CAB
23	B	614	CLA	C5-C6-C7-C8
26	B	620	SQD	C30-C31-C32-C33
26	C	501[B]	SQD	C11-C10-C9-C8
32	d	411[A]	LHG	C32-C33-C34-C35
33	C	502	LMG	C12-C13-C14-C15
33	a	417	LMG	C34-C35-C36-C37
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
31	B	628	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	420[A]	LHG	C26-C27-C28-C29
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
31	e	101	LMT	C1-C2-C3-C4
32	D	408[A]	LHG	C16-C17-C18-C19
23	B	614	CLA	C8-C10-C11-C12
23	B	615	CLA	C13-C15-C16-C17
23	b	615	CLA	C16-C17-C18-C19
23	d	401[A]	CLA	C16-C17-C18-C20
35	C	518[A]	DGD	O6D-C5D-C6D-O5D
31	A	417	LMT	C5-C6-C7-C8
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
32	D	409[A]	LHG	C32-C33-C34-C35
32	a	420[B]	LHG	C26-C27-C28-C29
33	m	101	LMG	C35-C36-C37-C38
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
34	b	623	HTG	C1'-C2'-C3'-C4'
33	C	502	LMG	C10-C11-C12-C13
33	a	417	LMG	C10-C11-C12-C13
23	B	605	CLA	O1D-CGD-O2D-CED
31	t	101	LMT	C11-C10-C9-C8
32	L	101[A]	LHG	C12-C13-C14-C15
32	L	101[A]	LHG	C13-C14-C15-C16
32	l	802[A]	LHG	C16-C17-C18-C19
34	b	622	HTG	C2'-C3'-C4'-C5'
35	C	518[A]	DGD	C4B-C5B-C6B-C7B
35	C	519[A]	DGD	CCB-CDB-CEB-CFB
35	h	102	DGD	C9A-CAA-CBA-CCA
26	C	501[A]	SQD	C15-C16-C17-C18
31	e	101	LMT	C5-C6-C7-C8
32	E	101[A]	LHG	C24-C25-C26-C27
32	d	411[A]	LHG	C29-C30-C31-C32
33	C	521	LMG	C16-C17-C18-C19
33	D	413	LMG	C12-C13-C14-C15
33	a	417	LMG	C30-C31-C32-C33
35	H	102	DGD	C9B-CAB-CBB-CCB
32	l	802[B]	LHG	C17-C18-C19-C20
23	B	603	CLA	C16-C17-C18-C19
23	c	502	CLA	C2B-C3B-CAB-CBB
24	Y	101	BCR	C1-C6-C7-C8
24	b	617	BCR	C1-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
24	b	617	BCR	C5-C6-C7-C8
24	b	619	BCR	C1-C6-C7-C8
33	c	521	LMG	C29-C28-O8-C9
35	C	519[B]	DGD	CCB-CDB-CEB-CFB
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
26	a	412	SQD	C16-C17-C18-C19
32	E	101[B]	LHG	C24-C25-C26-C27
32	d	411[B]	LHG	C32-C33-C34-C35
32	l	802[B]	LHG	C12-C13-C14-C15
31	B	630	LMT	C2-C3-C4-C5
32	L	101[A]	LHG	C25-C26-C27-C28
33	B	621	LMG	C34-C35-C36-C37
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
26	A	410	SQD	C26-C27-C28-C29
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
23	c	506	CLA	C4-C3-C5-C6
33	D	413	LMG	C35-C36-C37-C38
23	B	610	CLA	C16-C17-C18-C19
26	F	103	SQD	C24-C25-C26-C27
23	b	610	CLA	C11-C12-C13-C14
31	t	101	LMT	C3-C4-C5-C6
33	C	522	LMG	C13-C14-C15-C16
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
35	C	519[A]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
33	C	522	LMG	C17-C18-C19-C20
23	A	406[B]	CLA	C13-C15-C16-C17
32	l	802[A]	LHG	C14-C15-C16-C17
32	A	416[B]	LHG	C34-C35-C36-C37
33	C	502	LMG	C36-C37-C38-C39
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	411[B]	LHG	O2-C2-C3-O3
26	B	620	SQD	C11-C10-C9-C8
31	b	621	LMT	C11-C10-C9-C8
32	L	101[B]	LHG	C12-C13-C14-C15
32	d	411[B]	LHG	C16-C17-C18-C19
35	H	102	DGD	C5B-C6B-C7B-C8B
23	B	610	CLA	C16-C17-C18-C20
35	H	102	DGD	C7A-C8A-C9A-CAA
32	E	101[B]	LHG	C23-C24-C25-C26
33	c	520	LMG	C30-C31-C32-C33
33	C	522	LMG	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	c	519	DGD	CBA-CCA-CDA-CEA
37	D	402[B]	PHO	C2C-C3C-CAC-CBC
33	C	522	LMG	C10-C11-C12-C13
31	t	102	LMT	C7-C8-C9-C10
33	C	521	LMG	C17-C18-C19-C20
35	c	517[A]	DGD	C7A-C8A-C9A-CAA
32	D	408[B]	LHG	C10-C11-C12-C13
33	m	101	LMG	C39-C40-C41-C42
23	B	603	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C20
32	L	101[B]	LHG	C13-C14-C15-C16
38	f	101	HEM	C2C-C3C-CAC-CBC
26	b	620	SQD	C28-C29-C30-C31
31	t	102	LMT	C4-C5-C6-C7
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
23	a	405[B]	CLA	C15-C16-C17-C18
23	c	511	CLA	C10-C11-C12-C13
32	d	406[A]	LHG	C29-C30-C31-C32
35	C	518[B]	DGD	C4B-C5B-C6B-C7B
31	A	417	LMT	C3'-C4'-O1B-C1B
26	b	620	SQD	C27-C28-C29-C30
33	C	502	LMG	C39-C40-C41-C42
33	m	101	LMG	O9-C10-O7-C8
33	d	409	LMG	O6-C5-C6-O5
26	a	412	SQD	C31-C32-C33-C34
32	A	416[A]	LHG	C12-C13-C14-C15
35	C	518[A]	DGD	C9A-CAA-CBA-CCA
32	d	406[A]	LHG	C27-C28-C29-C30
35	H	102	DGD	CCA-CDA-CEA-CFA
33	c	521	LMG	O10-C28-O8-C9
33	c	521	LMG	O6-C5-C6-O5
26	b	620	SQD	C14-C15-C16-C17
31	t	101	LMT	C4-C5-C6-C7
33	a	417	LMG	C29-C30-C31-C32
35	C	520	DGD	CAA-CBA-CCA-CDA
23	C	513	CLA	C8-C10-C11-C12
23	c	507	CLA	C10-C11-C12-C13
26	a	411[B]	SQD	C12-C13-C14-C15
32	d	406[A]	LHG	C25-C26-C27-C28
32	d	406[B]	LHG	C27-C28-C29-C30
33	m	101	LMG	C38-C39-C40-C41
31	b	621	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	501[A]	SQD	O6-C44-C45-O47
26	C	501[B]	SQD	O6-C44-C45-O47
32	d	411[A]	LHG	C24-C25-C26-C27
33	c	520	LMG	C31-C32-C33-C34
33	C	526	LMG	O6-C5-C6-O5
31	T	101	LMT	C3-C4-C5-C6
32	l	802[A]	LHG	C27-C28-C29-C30
35	c	517[A]	DGD	C4D-C5D-C6D-O5D
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
26	b	620	SQD	C13-C14-C15-C16
32	D	408[A]	LHG	C12-C13-C14-C15
32	l	802[B]	LHG	C27-C28-C29-C30
23	d	401[A]	CLA	C16-C17-C18-C19
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	CCB-CDB-CEB-CFB
31	m	103	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	C5-C6-C7-C8
23	D	405	CLA	C4-C3-C5-C6
23	c	514	CLA	C4-C3-C5-C6
35	c	519	DGD	C1A-C2A-C3A-C4A
23	C	512	CLA	C2-C3-C5-C6
37	a	408[B]	PHO	C2-C3-C5-C6
32	D	409[A]	LHG	C15-C16-C17-C18
33	C	502	LMG	C11-C12-C13-C14
33	C	502	LMG	C19-C20-C21-C22
23	B	604	CLA	CBD-CGD-O2D-CED
26	b	620	SQD	C24-C23-O48-C46
33	c	520	LMG	C33-C34-C35-C36
33	d	409	LMG	C29-C30-C31-C32
23	C	508	CLA	C15-C16-C17-C18
31	B	630	LMT	C6-C7-C8-C9
32	A	416[A]	LHG	C34-C35-C36-C37
32	D	409[B]	LHG	C17-C18-C19-C20
23	c	511	CLA	O1D-CGD-O2D-CED
25	B	629	GOL	O2-C2-C3-O3
25	D	414	GOL	O1-C1-C2-O2
25	c	528	GOL	O2-C2-C3-O3
23	b	607	CLA	C3-C5-C6-C7
32	d	406[A]	LHG	C34-C35-C36-C37
26	F	103	SQD	C29-C30-C31-C32
26	f	102	SQD	C25-C26-C27-C28
23	C	503	CLA	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	512	CLA	CBD-CGD-O2D-CED
35	C	518[B]	DGD	C3B-C4B-C5B-C6B
35	c	518[A]	DGD	C6A-C7A-C8A-C9A
23	B	611	CLA	C8-C10-C11-C12
23	B	615	CLA	C5-C6-C7-C8
34	b	623	HTG	O5-C5-C6-O6
32	d	405[A]	LHG	C34-C35-C36-C37
33	C	521	LMG	C34-C35-C36-C37
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
23	C	507	CLA	C11-C12-C13-C15
23	C	515	CLA	C11-C10-C8-C7
23	D	405	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	A	406[A]	CLA	C13-C15-C16-C17
35	c	518[A]	DGD	C4A-C5A-C6A-C7A
23	C	504	CLA	C15-C16-C17-C18
31	m	103	LMT	C7-C8-C9-C10
28	a	414[A]	PL9	C12-C11-C9-C10
28	d	404[B]	PL9	C15-C14-C16-C17
23	c	506	CLA	C2-C3-C5-C6
23	B	606	CLA	C11-C10-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	B	611	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	508	CLA	C6-C7-C8-C9
23	D	405	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
35	h	102	DGD	CAB-CBB-CCB-CDB
23	b	601	CLA	C13-C15-C16-C17
33	D	413	LMG	O6-C5-C6-O5
32	d	406[B]	LHG	C34-C35-C36-C37
31	t	102	LMT	O1'-C1-C2-C3
26	A	410	SQD	C2-C1-O6-C44
26	A	410	SQD	O6-C44-C45-C46
26	C	501[B]	SQD	O6-C44-C45-C46
26	a	411[A]	SQD	O6-C44-C45-C46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	a	412	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	E	101[A]	LHG	C4-C5-C6-O8
32	a	420[B]	LHG	C4-C5-C6-O8
32	D	409[A]	LHG	C13-C14-C15-C16
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
32	d	411[B]	LHG	C33-C34-C35-C36
35	c	518[B]	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	CAA-CBA-CCA-CDA
32	A	416[A]	LHG	O2-C2-C3-O3
35	c	517[A]	DGD	C2A-C1A-O1G-C1G
35	C	518[A]	DGD	O6E-C5E-C6E-O5E
35	C	518[B]	DGD	O6E-C5E-C6E-O5E
35	c	517[A]	DGD	O6E-C5E-C6E-O5E
31	M	101	LMT	C3-C4-C5-C6
23	a	406[B]	CLA	C2C-C3C-CAC-CBC
31	b	627	LMT	C1-C2-C3-C4
33	a	417	LMG	C4-C5-C6-O5
26	f	102	SQD	C34-C35-C36-C37
35	c	519	DGD	O6D-C5D-C6D-O5D
23	B	605	CLA	C5-C6-C7-C8
35	c	518[B]	DGD	C4A-C5A-C6A-C7A
33	C	522	LMG	C19-C20-C21-C22
23	C	512	CLA	C4-C3-C5-C6
28	a	414[B]	PL9	C12-C11-C9-C10
37	a	408[B]	PHO	C4-C3-C5-C6
23	C	510	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	C2-C3-C5-C6
31	b	627	LMT	C5-C6-C7-C8
31	b	621	LMT	C3-C4-C5-C6
32	D	409[B]	LHG	C13-C14-C15-C16
32	d	411[A]	LHG	C25-C26-C27-C28
35	c	517[B]	DGD	O6E-C5E-C6E-O5E
32	D	409[A]	LHG	C29-C30-C31-C32
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
23	B	602	CLA	C15-C16-C17-C18
32	L	101[B]	LHG	C24-C25-C26-C27
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
25	l	801[A]	GOL	O1-C1-C2-C3
23	d	402	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	a	406[A]	CLA	C2C-C3C-CAC-CBC
23	c	514	CLA	O1D-CGD-O2D-CED
26	a	411[A]	SQD	C9-C10-C11-C12
32	A	416[A]	LHG	C26-C27-C28-C29
35	C	520	DGD	C8A-C9A-CAA-CBA
35	H	102	DGD	CAB-CBB-CCB-CDB
26	F	103	SQD	C34-C35-C36-C37
31	e	101	LMT	C3-C4-C5-C6
35	h	102	DGD	C9B-CAB-CBB-CCB
26	b	620	SQD	C11-C10-C9-C8
23	b	610	CLA	C15-C16-C17-C18
32	d	406[A]	LHG	C28-C29-C30-C31
33	a	417	LMG	C21-C22-C23-C24
23	b	616	CLA	CBA-CGA-O2A-C1
23	c	513	CLA	CBA-CGA-O2A-C1
34	B	625	HTG	C4'-C5'-C6'-C7'
23	B	616	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
28	D	407[B]	PL9	C15-C14-C16-C17
31	b	627	LMT	O1'-C1-C2-C3
31	A	417	LMT	C3-C4-C5-C6
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
35	C	519[A]	DGD	CDA-CEA-CFA-CGA
35	C	519[B]	DGD	CDA-CEA-CFA-CGA
35	C	520	DGD	CDB-CEB-CFB-CGB
26	a	411[A]	SQD	C12-C13-C14-C15
32	D	408[A]	LHG	C10-C11-C12-C13
32	l	802[B]	LHG	C13-C14-C15-C16
33	z	101	LMG	C13-C14-C15-C16
35	C	518[B]	DGD	C9A-CAA-CBA-CCA
31	B	628	LMT	C7-C8-C9-C10
35	C	520	DGD	C7B-C8B-C9B-CAB
32	l	802[A]	LHG	C9-C10-C11-C12
23	a	405[B]	CLA	O1D-CGD-O2D-CED
32	d	406[B]	LHG	C9-C10-C11-C12
32	E	101[A]	LHG	C25-C26-C27-C28
34	B	622	HTG	C2'-C3'-C4'-C5'
26	b	620	SQD	O10-C23-O48-C46
35	h	102	DGD	CDB-CEB-CFB-CGB
23	B	601	CLA	CBA-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	512	CLA	CBA-CGA-O2A-C1
35	c	519	DGD	C2A-C1A-O1G-C1G
34	b	622	HTG	C1'-C2'-C3'-C4'
32	d	411[A]	LHG	C33-C34-C35-C36
33	m	101	LMG	C11-C12-C13-C14
23	C	514	CLA	C10-C11-C12-C13
23	b	606	CLA	C16-C17-C18-C20
23	d	401[B]	CLA	C16-C17-C18-C20
28	D	407[A]	PL9	C45-C44-C46-C47
28	d	404[B]	PL9	C45-C44-C46-C47
28	d	404[A]	PL9	C13-C14-C16-C17
23	C	514	CLA	CBA-CGA-O2A-C1
26	A	410	SQD	C24-C23-O48-C46
23	C	508	CLA	C5-C6-C7-C8
23	b	615	CLA	C5-C6-C7-C8
32	A	416[B]	LHG	C12-C13-C14-C15
32	E	101[B]	LHG	C25-C26-C27-C28
26	C	501[A]	SQD	C11-C10-C9-C8
33	z	101	LMG	C14-C15-C16-C17
25	c	527	GOL	O2-C2-C3-O3
25	v	202[A]	GOL	O1-C1-C2-O2
31	A	417	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
23	C	507	CLA	C11-C12-C13-C14
23	C	515	CLA	C11-C10-C8-C9
33	C	521	LMG	C11-C12-C13-C14
23	C	512	CLA	C10-C11-C12-C13
23	c	504	CLA	C8-C10-C11-C12
31	t	102	LMT	O5'-C5'-C6'-O6'
23	D	404[B]	CLA	C4B-C3B-CAB-CBB
23	a	407[A]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
32	d	406[A]	LHG	C33-C34-C35-C36
32	D	409[B]	LHG	C15-C16-C17-C18
32	E	101[B]	LHG	C17-C18-C19-C20
23	A	404[A]	CLA	C13-C15-C16-C17
23	b	604	CLA	C15-C16-C17-C18
23	b	616	CLA	C5-C6-C7-C8
32	L	101[B]	LHG	C25-C26-C27-C28
35	c	517[B]	DGD	C2A-C1A-O1G-C1G
23	d	402	CLA	O1A-CGA-O2A-C1
32	D	409[A]	LHG	C17-C18-C19-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	d	409	LMG	C35-C36-C37-C38
35	C	519[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
23	c	513	CLA	C10-C11-C12-C13
31	b	621	LMT	C7-C8-C9-C10
31	c	501	LMT	C2-C3-C4-C5
32	D	409[B]	LHG	C27-C28-C29-C30
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
35	C	520	DGD	C6A-C7A-C8A-C9A
32	L	101[B]	LHG	O6-C4-C5-C6
35	C	518[A]	DGD	C4D-C5D-C6D-O5D
33	D	413	LMG	C30-C31-C32-C33
33	z	101	LMG	C20-C21-C22-C23
35	h	102	DGD	CBA-CCA-CDA-CEA
23	C	508	CLA	C6-C7-C8-C10
23	C	512	CLA	C12-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
35	c	517[A]	DGD	O1A-C1A-O1G-C1G
32	d	411[B]	LHG	C25-C26-C27-C28
32	A	416[B]	LHG	O2-C2-C3-O3
32	E	101[A]	LHG	C13-C14-C15-C16
23	C	507	CLA	C4-C3-C5-C6
23	c	507	CLA	C3A-C2A-CAA-CBA
23	C	505	CLA	O1D-CGD-O2D-CED
35	c	519	DGD	C2B-C3B-C4B-C5B
28	A	412[A]	PL9	C12-C11-C9-C8
28	A	412[B]	PL9	C12-C11-C9-C8
28	D	407[A]	PL9	C13-C14-C16-C17
28	d	404[B]	PL9	C28-C29-C31-C32
32	d	405[B]	LHG	C34-C35-C36-C37
33	C	502	LMG	C20-C21-C22-C23
33	C	522	LMG	C35-C36-C37-C38
33	m	101	LMG	C37-C38-C39-C40
23	a	406[B]	CLA	C15-C16-C17-C18
26	A	410	SQD	C27-C28-C29-C30
35	h	102	DGD	C2B-C3B-C4B-C5B
26	F	103	SQD	C7-C8-C9-C10
33	d	409	LMG	C10-C11-C12-C13
31	c	501	LMT	C3-C4-C5-C6
35	c	517[B]	DGD	C8B-C9B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
26	C	501[A]	SQD	O6-C44-C45-C46
32	E	101[B]	LHG	C4-C5-C6-O8
32	a	420[A]	LHG	C4-C5-C6-O8
33	a	417	LMG	C7-C8-C9-O8
32	D	409[B]	LHG	C10-C11-C12-C13
35	c	518[A]	DGD	CBB-CCB-CDB-CEB
26	a	412	SQD	C18-C19-C20-C21
35	c	519	DGD	O6E-C5E-C6E-O5E
28	A	412[A]	PL9	C45-C44-C46-C47
32	a	420[A]	LHG	C23-C24-C25-C26
28	D	407[A]	PL9	C43-C44-C46-C47
28	d	404[B]	PL9	C13-C14-C16-C17
33	m	101	LMG	C14-C15-C16-C17
32	A	416[B]	LHG	C11-C12-C13-C14
23	b	606	CLA	C16-C17-C18-C19
23	a	407[A]	CLA	C2B-C3B-CAB-CBB
24	a	410	BCR	C23-C24-C25-C30
35	C	518[A]	DGD	CCA-CDA-CEA-CFA
23	b	616	CLA	O1A-CGA-O2A-C1
32	a	420[A]	LHG	C10-C11-C12-C13
32	l	802[B]	LHG	C14-C15-C16-C17
33	C	526	LMG	C11-C12-C13-C14
26	a	411[A]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
32	L	101[A]	LHG	C27-C28-C29-C30
35	C	520	DGD	CBA-CCA-CDA-CEA
23	b	608	CLA	C13-C15-C16-C17
28	D	407[B]	PL9	C13-C14-C16-C17
28	a	414[B]	PL9	C12-C11-C9-C8
32	d	411[B]	LHG	C24-C25-C26-C27
32	L	101[B]	LHG	C26-C27-C28-C29
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
35	C	518[A]	DGD	C3B-C4B-C5B-C6B
26	C	501[B]	SQD	C7-C8-C9-C10
32	a	420[B]	LHG	C23-C24-C25-C26
26	a	411[B]	SQD	C35-C36-C37-C38
23	C	512	CLA	C14-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C9
33	B	621	LMG	C21-C22-C23-C24
33	d	409	LMG	C19-C20-C21-C22
26	A	410	SQD	O5-C1-O6-C44
35	c	517[A]	DGD	O6E-C1E-O5D-C6D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	b	625	HTG	C4-C5-C6-O6
32	L	101[B]	LHG	C27-C28-C29-C30
31	B	628	LMT	C1-C2-C3-C4
26	B	620	SQD	C34-C35-C36-C37
28	A	412[A]	PL9	C39-C41-C42-C43
28	a	414[A]	PL9	C24-C26-C27-C28
26	b	620	SQD	C26-C27-C28-C29
32	l	802[B]	LHG	C25-C26-C27-C28
35	C	518[A]	DGD	C1B-C2B-C3B-C4B
25	B	627	GOL	O1-C1-C2-O2
25	c	527	GOL	O1-C1-C2-O2
35	H	102	DGD	O2G-C1B-C2B-C3B
23	A	406[A]	CLA	C16-C17-C18-C20
35	c	517[B]	DGD	C4B-C5B-C6B-C7B
32	d	406[B]	LHG	C25-C26-C27-C28
23	c	510	CLA	C8-C10-C11-C12
32	A	416[A]	LHG	C1-C2-C3-O3
32	A	416[B]	LHG	C1-C2-C3-O3
32	d	411[B]	LHG	C29-C30-C31-C32
23	C	512	CLA	O1A-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
26	a	411[B]	SQD	C27-C28-C29-C30
32	D	408[B]	LHG	O6-C4-C5-C6
31	B	630	LMT	C3-C4-C5-C6
24	y	101	BCR	C37-C22-C23-C24
23	B	614	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7
23	c	506	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	d	401[B]	CLA	C11-C12-C13-C15
32	D	409[A]	LHG	C27-C28-C29-C30
32	l	802[A]	LHG	C34-C35-C36-C37
33	B	621	LMG	O8-C28-C29-C30
26	a	412	SQD	C15-C16-C17-C18
33	c	521	LMG	C39-C40-C41-C42
24	D	406	BCR	C21-C22-C23-C24
24	c	516	BCR	C7-C8-C9-C10
24	d	403	BCR	C21-C22-C23-C24
24	y	101	BCR	C21-C22-C23-C24
26	a	411[B]	SQD	C9-C10-C11-C12
32	D	409[B]	LHG	C29-C30-C31-C32
23	B	601	CLA	O1A-CGA-O2A-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	c	519	DGD	O1A-C1A-O1G-C1G
35	C	519[A]	DGD	C2G-C3G-O3G-C1D
35	C	519[B]	DGD	C5D-C6D-O5D-C1E
35	c	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	518[B]	DGD	C5D-C6D-O5D-C1E
31	e	101	LMT	C9-C10-C11-C12
32	L	101[A]	LHG	C11-C10-C9-C8
35	c	518[B]	DGD	CBB-CCB-CDB-CEB
28	d	404[A]	PL9	C45-C44-C46-C47
23	C	514	CLA	O1A-CGA-O2A-C1
23	c	513	CLA	O1A-CGA-O2A-C1
28	a	414[A]	PL9	C12-C11-C9-C8
38	F	102	HEM	C2B-C3B-CAB-CBB
38	f	101	HEM	C2B-C3B-CAB-CBB
26	b	620	SQD	C35-C36-C37-C38
25	d	410	GOL	O1-C1-C2-C3
34	b	622	HTG	C3'-C4'-C5'-C6'
26	A	410	SQD	O10-C23-O48-C46
26	C	501[A]	SQD	C18-C19-C20-C21
32	d	406[B]	LHG	C29-C30-C31-C32
35	C	519[A]	DGD	C5B-C6B-C7B-C8B
23	A	404[B]	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
32	d	405[B]	LHG	C13-C14-C15-C16
32	l	802[A]	LHG	C13-C14-C15-C16
35	C	519[A]	DGD	C8B-C9B-CAB-CBB
31	A	415	LMT	C9-C10-C11-C12
35	c	517[B]	DGD	O1A-C1A-O1G-C1G
23	C	509	CLA	C13-C15-C16-C17
32	D	408[A]	LHG	C11-C10-C9-C8
35	c	517[A]	DGD	CCB-CDB-CEB-CFB
33	D	413	LMG	C36-C37-C38-C39
32	E	101[A]	LHG	O6-C4-C5-O7
32	L	101[A]	LHG	O6-C4-C5-O7
32	L	101[B]	LHG	O6-C4-C5-O7
26	a	411[A]	SQD	C27-C28-C29-C30
32	a	420[B]	LHG	C10-C11-C12-C13
33	C	526	LMG	C29-C28-O8-C9
35	C	519[B]	DGD	O6E-C1E-O5D-C6D
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
26	B	620	SQD	C44-C45-C46-O48
33	C	502	LMG	C7-C8-C9-O8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	f	101	HEM	C4C-C3C-CAC-CBC
32	L	101[A]	LHG	C24-C25-C26-C27
35	C	518[B]	DGD	CCA-CDA-CEA-CFA
32	d	405[A]	LHG	C13-C14-C15-C16
23	a	405[B]	CLA	C2A-CAA-CBA-CGA
23	D	405	CLA	C2-C3-C5-C6
28	d	404[B]	PL9	C43-C44-C46-C47
32	D	409[A]	LHG	C10-C11-C12-C13
35	C	519[A]	DGD	C7A-C8A-C9A-CAA
26	a	411[A]	SQD	C34-C35-C36-C37
35	c	517[B]	DGD	CAB-CBB-CCB-CDB
32	d	405[B]	LHG	C16-C17-C18-C19
26	B	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
32	E	101[B]	LHG	O7-C5-C6-O8
32	a	420[A]	LHG	O7-C5-C6-O8
32	a	420[B]	LHG	O7-C5-C6-O8
33	C	502	LMG	O7-C8-C9-O8
23	b	605	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
23	d	402	CLA	C11-C12-C13-C14
23	d	401[B]	CLA	C16-C17-C18-C19
33	a	417	LMG	C35-C36-C37-C38
31	F	101	LMT	C4-C5-C6-C7
33	c	520	LMG	C29-C30-C31-C32
23	b	601	CLA	O1A-CGA-O2A-C1
23	b	604	CLA	C10-C11-C12-C13
32	a	420[A]	LHG	C7-C8-C9-C10
23	B	601	CLA	C15-C16-C17-C18
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
23	b	601	CLA	C8-C10-C11-C12
31	c	501	LMT	C9-C10-C11-C12
23	c	511	CLA	C4-C3-C5-C6
23	B	602	CLA	C3-C5-C6-C7
32	A	416[A]	LHG	C32-C33-C34-C35
32	D	408[B]	LHG	O2-C2-C3-O3
32	d	405[B]	LHG	C9-C10-C11-C12
32	d	406[A]	LHG	C9-C10-C11-C12
26	C	501[A]	SQD	C34-C35-C36-C37
35	c	518[B]	DGD	C9B-CAB-CBB-CCB
32	d	405[A]	LHG	C11-C10-C9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	A	406[B]	CLA	C16-C17-C18-C20
25	B	627	GOL	O2-C2-C3-O3
31	M	101	LMT	O1'-C1-C2-C3
26	B	620	SQD	C12-C13-C14-C15
33	C	502	LMG	C13-C14-C15-C16
24	D	406	BCR	C37-C22-C23-C24
28	a	414[B]	PL9	C24-C26-C27-C28
23	B	604	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C1A-C2A-CAA-CBA
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
23	a	406[B]	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C4B-C3B-CAB-CBB
28	D	407[B]	PL9	C45-C44-C46-C47
26	b	620	SQD	C30-C31-C32-C33
26	a	411[A]	SQD	C35-C36-C37-C38
33	c	520	LMG	O6-C5-C6-O5
23	C	511	CLA	C3-C5-C6-C7
33	C	522	LMG	C4-C5-C6-O5
35	C	520	DGD	C4A-C5A-C6A-C7A
23	B	610	CLA	C2A-CAA-CBA-CGA
32	L	101[A]	LHG	O6-C4-C5-C6
32	d	411[A]	LHG	C18-C19-C20-C21
32	d	406[B]	LHG	C28-C29-C30-C31
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	601	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	C	509	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	d	401[A]	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C4C-C3C-CAC-CBC
26	F	103	SQD	C32-C33-C34-C35
32	d	405[A]	LHG	C16-C17-C18-C19
26	B	620	SQD	C9-C10-C11-C12
31	F	101	LMT	C2-C3-C4-C5
33	C	521	LMG	C37-C38-C39-C40
32	D	409[B]	LHG	C2-C3-O3-P
23	C	503	CLA	C16-C17-C18-C20
32	D	408[B]	LHG	O6-C4-C5-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	607	CLA	C3-C5-C6-C7
23	B	601	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C14-C13-C15-C16
23	D	405	CLA	C11-C10-C8-C9
23	a	409	CLA	C11-C10-C8-C9
23	d	401[B]	CLA	C11-C12-C13-C14
23	b	601	CLA	CAA-CBA-CGA-O2A
33	m	101	LMG	C28-C29-C30-C31
35	C	518[A]	DGD	C6A-C7A-C8A-C9A
23	B	602	CLA	C8-C10-C11-C12
31	c	501	LMT	C7-C8-C9-C10
32	L	101[A]	LHG	C26-C27-C28-C29
35	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	B	604	CLA	C3-C5-C6-C7
32	D	408[B]	LHG	O10-C23-O8-C6
26	F	103	SQD	O47-C45-C46-O48
32	E	101[A]	LHG	O7-C5-C6-O8
33	a	417	LMG	O7-C8-C9-O8
23	C	504	CLA	C13-C15-C16-C17
32	d	411[B]	LHG	C18-C19-C20-C21
28	a	414[B]	PL9	C45-C44-C46-C47
31	b	627	LMT	C6-C7-C8-C9
28	a	414[A]	PL9	C43-C44-C46-C47
28	a	414[B]	PL9	C43-C44-C46-C47
23	C	510	CLA	O1D-CGD-O2D-CED
32	d	406[B]	LHG	C33-C34-C35-C36
33	C	522	LMG	C38-C39-C40-C41
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	607	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	C	506	CLA	CAD-CBD-CGD-O2D
23	b	601	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
26	C	501[A]	SQD	C13-C14-C15-C16
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
32	D	408[A]	LHG	C34-C35-C36-C37
35	C	519[A]	DGD	C8A-C9A-CAA-CBA
31	B	628	LMT	C9-C10-C11-C12
33	d	409	LMG	C11-C12-C13-C14
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
32	D	408[A]	LHG	C4-O6-P-O3
32	D	408[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	a	420[A]	LHG	C4-O6-P-O4
32	d	405[B]	LHG	C4-O6-P-O5
35	H	102	DGD	CDB-CEB-CFB-CGB
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
23	c	511	CLA	O1A-CGA-O2A-C1
33	B	621	LMG	C36-C37-C38-C39
23	B	602	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C1-C6-C7-C8
23	c	511	CLA	C2-C3-C5-C6
23	c	514	CLA	C2-C3-C5-C6
28	A	412[A]	PL9	C28-C29-C31-C32
31	A	415	LMT	C7-C8-C9-C10
32	D	409[A]	LHG	C2-C3-O3-P
32	d	406[A]	LHG	C2-C3-O3-P
32	d	406[B]	LHG	C2-C3-O3-P
32	d	406[A]	LHG	C32-C33-C34-C35
23	b	602	CLA	C10-C11-C12-C13
35	C	520	DGD	CDA-CEA-CFA-CGA
32	D	408[A]	LHG	C26-C27-C28-C29
32	L	101[B]	LHG	C33-C34-C35-C36
28	A	412[B]	PL9	C4-C3-C7-C8
28	a	414[A]	PL9	C4-C3-C7-C8
28	a	414[B]	PL9	C4-C3-C7-C8
28	d	404[B]	PL9	C4-C3-C7-C8
32	A	416[A]	LHG	O1-C1-C2-C3
35	C	519[B]	DGD	C1A-C2A-C3A-C4A
23	c	505	CLA	C5-C6-C7-C8
23	c	510	CLA	C15-C16-C17-C18
32	d	411[A]	LHG	C34-C35-C36-C37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C4-C3-C5-C6
33	d	409	LMG	C40-C41-C42-C43
23	B	612	CLA	C10-C11-C12-C13
23	D	404[B]	CLA	C8-C10-C11-C12
23	C	508	CLA	C16-C17-C18-C20
32	d	411[A]	LHG	C11-C12-C13-C14
32	E	101[A]	LHG	O6-C4-C5-C6
26	a	411[B]	SQD	C34-C35-C36-C37
35	C	519[A]	DGD	C7B-C8B-C9B-CAB
23	C	506	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	d	401[A]	CLA	C11-C12-C13-C14
23	B	602	CLA	C11-C12-C13-C15
23	D	405	CLA	C11-C10-C8-C7
26	f	102	SQD	C7-C8-C9-C10
26	a	411[B]	SQD	C11-C12-C13-C14
33	C	502	LMG	C18-C19-C20-C21
33	C	502	LMG	C29-C30-C31-C32
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
28	D	407[A]	PL9	C15-C14-C16-C17
32	D	409[B]	LHG	C28-C29-C30-C31
23	c	511	CLA	CBA-CGA-O2A-C1
32	D	408[B]	LHG	C24-C23-O8-C6
32	D	408[A]	LHG	C13-C14-C15-C16
32	d	406[B]	LHG	C11-C10-C9-C8
23	b	612	CLA	C10-C11-C12-C13
32	d	406[A]	LHG	C10-C11-C12-C13
32	l	802[A]	LHG	C28-C29-C30-C31
23	B	613	CLA	C13-C15-C16-C17
32	l	802[B]	LHG	C16-C17-C18-C19
26	A	410	SQD	C30-C31-C32-C33
31	A	417	LMT	C4-C5-C6-C7
32	D	408[B]	LHG	C13-C14-C15-C16
33	z	101	LMG	C19-C20-C21-C22
23	a	406[A]	CLA	C15-C16-C17-C18
28	A	412[B]	PL9	C39-C41-C42-C43
23	B	601	CLA	CAA-CBA-CGA-O2A
35	h	102	DGD	C3B-C4B-C5B-C6B
33	C	522	LMG	C11-C12-C13-C14
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
35	c	518[A]	DGD	C2G-C3G-O3G-C1D
26	C	501[B]	SQD	C12-C13-C14-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	B	622	HTG	C4'-C5'-C6'-C7'
23	C	512	CLA	C8-C10-C11-C12
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
28	a	414[A]	PL9	C45-C44-C46-C47
23	c	508	CLA	C5-C6-C7-C8
28	A	412[B]	PL9	C28-C29-C31-C32
26	C	501[A]	SQD	C16-C17-C18-C19
32	d	406[B]	LHG	O10-C23-O8-C6
31	B	628	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
23	b	608	CLA	C16-C17-C18-C20
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C14
23	c	507	CLA	C11-C10-C8-C9
32	D	408[A]	LHG	C28-C29-C30-C31
37	a	408[A]	PHO	C2C-C3C-CAC-CBC
35	h	102	DGD	C6A-C7A-C8A-C9A
23	B	610	CLA	C4B-C3B-CAB-CBB
23	D	404[A]	CLA	C4B-C3B-CAB-CBB
23	B	610	CLA	C13-C15-C16-C17
23	b	603	CLA	C5-C6-C7-C8
35	C	520	DGD	O6D-C5D-C6D-O5D
31	F	101	LMT	C6-C7-C8-C9
32	d	406[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C23-C24-C25-C26
23	b	610	CLA	C13-C15-C16-C17
23	b	601	CLA	C4-C3-C5-C6
23	B	616	CLA	C2-C3-C5-C6
28	D	407[B]	PL9	C43-C44-C46-C47
28	d	404[A]	PL9	C43-C44-C46-C47
35	C	520	DGD	C7A-C8A-C9A-CAA
32	D	409[A]	LHG	O10-C23-O8-C6
38	F	102	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4B-C3B-CAB-CBB
23	B	604	CLA	O1D-CGD-O2D-CED
23	a	406[A]	CLA	C4C-C3C-CAC-CBC
32	D	408[B]	LHG	C11-C10-C9-C8
23	B	613	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C10-C8-C7
23	C	515	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C12-C13-C15-C16
23	c	510	CLA	C13-C15-C16-C17
23	c	513	CLA	O1D-CGD-O2D-CED
32	E	101[B]	LHG	C13-C14-C15-C16
33	D	413	LMG	C18-C19-C20-C21
32	D	409[A]	LHG	C24-C23-O8-C6
26	a	412	SQD	C19-C20-C21-C22
26	B	620	SQD	C29-C30-C31-C32
23	C	508	CLA	C3A-C2A-CAA-CBA
32	D	408[B]	LHG	C23-C24-C25-C26
33	B	621	LMG	C18-C19-C20-C21
33	m	101	LMG	C32-C33-C34-C35
35	C	518[B]	DGD	CDB-CEB-CFB-CGB
23	C	510	CLA	C5-C6-C7-C8
26	a	411[A]	SQD	C11-C12-C13-C14
23	c	512	CLA	C8-C10-C11-C12
26	f	102	SQD	C11-C10-C9-C8
31	M	101	LMT	C2-C3-C4-C5
33	B	621	LMG	O6-C5-C6-O5
35	h	102	DGD	O2G-C1B-C2B-C3B
32	d	411[A]	LHG	C1-C2-C3-O3
33	d	409	LMG	C36-C37-C38-C39
23	c	507	CLA	C13-C15-C16-C17
23	A	407	CLA	C11-C12-C13-C14
23	B	601	CLA	C11-C12-C13-C14
23	B	610	CLA	C11-C12-C13-C14
23	B	613	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	a	407[A]	CLA	C14-C13-C15-C16
23	b	602	CLA	C6-C7-C8-C9
23	b	603	CLA	C11-C10-C8-C9
23	b	608	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
26	a	412	SQD	C28-C29-C30-C31
25	B	627	GOL	O1-C1-C2-C3
31	t	102	LMT	C2-C3-C4-C5
32	a	420[B]	LHG	C24-C25-C26-C27
35	c	517[A]	DGD	C4B-C5B-C6B-C7B
23	c	512	CLA	O1D-CGD-O2D-CED
24	t	103	BCR	C13-C14-C15-C16
26	f	102	SQD	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	406[B]	CLA	C4C-C3C-CAC-CBC
33	c	520	LMG	C32-C33-C34-C35
23	A	405[B]	CLA	CBD-CGD-O2D-CED
33	C	521	LMG	C36-C37-C38-C39
32	E	101[A]	LHG	C12-C13-C14-C15
23	C	503	CLA	C2A-CAA-CBA-CGA
26	a	411[A]	SQD	C10-C11-C12-C13
23	B	608	CLA	C13-C15-C16-C17
32	d	405[A]	LHG	C9-C10-C11-C12
23	B	611	CLA	C1A-C2A-CAA-CBA
23	a	407[A]	CLA	C1A-C2A-CAA-CBA
35	C	519[B]	DGD	C8A-C9A-CAA-CBA
23	C	510	CLA	C13-C15-C16-C17
33	C	521	LMG	C29-C30-C31-C32
37	D	402[A]	PHO	C2C-C3C-CAC-CBC
23	B	610	CLA	C2B-C3B-CAB-CBB
23	D	404[A]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
24	D	406	BCR	C23-C24-C25-C30
24	H	101	BCR	C23-C24-C25-C30
24	a	410	BCR	C23-C24-C25-C26
24	d	403	BCR	C23-C24-C25-C30
32	D	408[A]	LHG	C17-C18-C19-C20
33	B	621	LMG	C20-C21-C22-C23
23	A	406[A]	CLA	C16-C17-C18-C19
32	l	802[B]	LHG	O6-C4-C5-C6
33	a	417	LMG	C33-C34-C35-C36
32	l	802[B]	LHG	C11-C12-C13-C14
33	C	521	LMG	O6-C5-C6-O5
32	A	416[A]	LHG	C29-C30-C31-C32
23	B	602	CLA	C6-C7-C8-C10
23	C	505	CLA	C6-C7-C8-C10
23	C	506	CLA	C12-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C7
23	b	604	CLA	C11-C12-C13-C15
23	b	616	CLA	C6-C7-C8-C10
23	c	513	CLA	C6-C7-C8-C10
32	l	802[A]	LHG	C10-C11-C12-C13
23	A	407	CLA	C16-C17-C18-C19
26	a	411[B]	SQD	O6-C44-C45-O47
33	c	521	LMG	O1-C7-C8-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
40	V	202	HEC	CAD-CBD-CGD-O1D
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
23	c	513	CLA	CBD-CGD-O2D-CED
28	A	412[A]	PL9	C4-C3-C7-C8
23	C	515	CLA	C8-C10-C11-C12
26	B	620	SQD	C33-C34-C35-C36
33	m	101	LMG	C29-C30-C31-C32
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
23	b	605	CLA	C3-C5-C6-C7
23	b	605	CLA	C13-C15-C16-C17
24	K	102	BCR	C7-C8-C9-C34
24	d	403	BCR	C37-C22-C23-C24
35	C	520	DGD	O1A-C1A-O1G-C1G
28	D	407[A]	PL9	C35-C34-C36-C37
23	C	508	CLA	C2-C3-C5-C6
23	b	601	CLA	C2-C3-C5-C6
34	B	623	HTG	C1'-C2'-C3'-C4'
32	L	101[A]	LHG	C10-C11-C12-C13
35	C	519[B]	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C15-C16-C17-C18
35	C	520	DGD	C2A-C1A-O1G-C1G
26	a	411[B]	SQD	C10-C11-C12-C13
23	b	603	CLA	C2A-CAA-CBA-CGA
23	C	514	CLA	C11-C10-C8-C9
35	c	517[B]	DGD	C7B-C8B-C9B-CAB
35	c	519	DGD	C4D-C5D-C6D-O5D
33	c	521	LMG	C30-C31-C32-C33
32	a	420[A]	LHG	C24-C25-C26-C27
23	b	616	CLA	C4-C3-C5-C6
28	A	412[A]	PL9	C25-C24-C26-C27
28	a	414[B]	PL9	C35-C34-C36-C37
40	V	202	HEC	CAD-CBD-CGD-O2D
23	b	616	CLA	C2-C3-C5-C6
35	h	102	DGD	CCA-CDA-CEA-CFA
33	B	621	LMG	C2-C1-O1-C7
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
23	D	405	CLA	C8-C10-C11-C12
23	a	409	CLA	C15-C16-C17-C18
35	H	102	DGD	O1G-C1G-C2G-C3G
35	c	517[B]	DGD	C7A-C8A-C9A-CAA
23	c	508	CLA	C2A-CAA-CBA-CGA
32	A	416[B]	LHG	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	416[A]	LHG	O1-C1-C2-O2
32	d	411[A]	LHG	C27-C28-C29-C30
32	d	411[A]	LHG	C17-C18-C19-C20
33	m	101	LMG	C30-C31-C32-C33
23	B	612	CLA	C13-C15-C16-C17
31	t	101	LMT	C1-C2-C3-C4
35	C	519[B]	DGD	C7A-C8A-C9A-CAA
23	c	505	CLA	C4B-C3B-CAB-CBB
23	c	512	CLA	O1A-CGA-O2A-C1
32	d	405[A]	LHG	C25-C26-C27-C28
23	C	504	CLA	C3-C5-C6-C7
23	C	512	CLA	C15-C16-C17-C18
35	c	518[B]	DGD	C7B-C8B-C9B-CAB
31	e	101	LMT	C2B-C1B-O1B-C4'
23	b	610	CLA	C16-C17-C18-C20
23	B	615	CLA	C8-C10-C11-C12
37	a	408[A]	PHO	CHA-CBD-CGD-O1D
23	C	505	CLA	C5-C6-C7-C8
33	a	417	LMG	O8-C28-C29-C30
31	A	417	LMT	C7-C8-C9-C10
31	t	101	LMT	C2-C3-C4-C5
32	L	101[B]	LHG	C11-C10-C9-C8
33	C	526	LMG	C21-C22-C23-C24
26	A	410	SQD	C16-C17-C18-C19
35	C	520	DGD	CCA-CDA-CEA-CFA
28	D	407[B]	PL9	C28-C29-C31-C32
33	B	621	LMG	O6-C1-O1-C7
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
23	B	612	CLA	C8-C10-C11-C12
26	f	102	SQD	C26-C27-C28-C29
32	D	408[B]	LHG	C33-C34-C35-C36
32	d	411[A]	LHG	C9-C10-C11-C12
32	d	411[B]	LHG	C34-C35-C36-C37
32	E	101[B]	LHG	O2-C2-C3-O3
35	C	520	DGD	C3B-C4B-C5B-C6B
32	A	416[A]	LHG	C17-C18-C19-C20
38	F	102	HEM	CAD-CBD-CGD-O1D
23	B	616	CLA	C14-C13-C15-C16
23	a	407[A]	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C11-C12-C13-C14
23	c	506	CLA	C14-C13-C15-C16
33	C	522	LMG	C8-C7-O1-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
35	c	517[A]	DGD	CDB-CEB-CFB-CGB
33	B	621	LMG	C14-C15-C16-C17
40	v	201	HEC	CAD-CBD-CGD-O2D
23	b	614	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C16-C17-C18-C19
31	A	415	LMT	C4B-C5B-C6B-O6B
33	C	502	LMG	C31-C32-C33-C34
23	D	405	CLA	O1A-CGA-O2A-C1
23	B	614	CLA	C2-C3-C5-C6
32	d	411[B]	LHG	C27-C28-C29-C30
35	C	520	DGD	C2A-C3A-C4A-C5A
33	z	101	LMG	O7-C10-C11-C12
23	b	604	CLA	C13-C15-C16-C17
37	a	408[A]	PHO	O2A-C1-C2-C3
26	a	412	SQD	C24-C25-C26-C27
31	T	101	LMT	C7-C8-C9-C10
38	f	101	HEM	CAA-CBA-CGA-O2A
23	c	512	CLA	C3-C5-C6-C7
26	A	410	SQD	C7-C8-C9-C10
32	E	101[B]	LHG	C12-C13-C14-C15
32	l	802[A]	LHG	C25-C26-C27-C28
23	b	610	CLA	C16-C17-C18-C19
28	d	404[B]	PL9	C30-C29-C31-C32
33	C	526	LMG	O10-C28-O8-C9
37	D	401[B]	PHO	C2-C3-C5-C6
34	B	623	HTG	C2'-C3'-C4'-C5'
40	v	201	HEC	CAD-CBD-CGD-O1D
26	F	103	SQD	C44-C45-C46-O48
33	B	621	LMG	O1-C7-C8-C9
31	B	630	LMT	C7-C8-C9-C10
38	f	101	HEM	CAA-CBA-CGA-O1A
32	A	416[B]	LHG	C18-C19-C20-C21
32	L	101[A]	LHG	C11-C12-C13-C14
33	C	502	LMG	C38-C39-C40-C41
23	C	514	CLA	CAA-CBA-CGA-O2A
26	a	411[B]	SQD	O47-C7-C8-C9
32	A	416[B]	LHG	C27-C28-C29-C30
35	C	520	DGD	C5B-C6B-C7B-C8B
23	C	512	CLA	C11-C12-C13-C14
23	C	515	CLA	C6-C7-C8-C9
23	D	405	CLA	C6-C7-C8-C9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	601	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	c	507	CLA	C16-C17-C18-C19
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
26	B	620	SQD	C14-C15-C16-C17
35	C	520	DGD	CCB-CDB-CEB-CFB
23	B	613	CLA	CAA-CBA-CGA-O2A
32	A	416[A]	LHG	O8-C23-C24-C25
32	l	802[B]	LHG	O7-C7-C8-C9
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
24	K	102	BCR	C7-C8-C9-C10
33	m	101	LMG	O6-C5-C6-O5
28	A	412[B]	PL9	C45-C44-C46-C47
23	c	511	CLA	CAA-CBA-CGA-O2A
35	C	520	DGD	O1G-C1A-C2A-C3A
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
32	d	411[B]	LHG	C11-C10-C9-C8
23	C	509	CLA	C2A-CAA-CBA-CGA
23	C	508	CLA	C12-C13-C15-C16
23	a	407[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C7
23	c	505	CLA	C12-C13-C15-C16
23	c	513	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
32	E	101[B]	LHG	C11-C10-C9-C8
23	C	506	CLA	C2B-C3B-CAB-CBB
23	D	404[B]	CLA	C2B-C3B-CAB-CBB
23	b	612	CLA	C2B-C3B-CAB-CBB
24	B	617	BCR	C5-C6-C7-C8
24	C	516	BCR	C1-C6-C7-C8
24	D	406	BCR	C23-C24-C25-C26
24	H	101	BCR	C23-C24-C25-C26
24	d	403	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C26
24	h	101	BCR	C23-C24-C25-C30
24	y	101	BCR	C23-C24-C25-C30
23	b	613	CLA	CAA-CBA-CGA-O2A
32	a	420[A]	LHG	O8-C23-C24-C25
32	a	420[B]	LHG	O8-C23-C24-C25
33	a	417	LMG	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2-C1-O2A-CGA
37	D	401[B]	PHO	CBA-CGA-O2A-C1
26	b	620	SQD	C12-C13-C14-C15
23	c	513	CLA	CAA-CBA-CGA-O2A
23	C	515	CLA	CBD-CGD-O2D-CED
32	E	101[B]	LHG	O7-C7-C8-C9
37	a	408[A]	PHO	C2-C3-C5-C6
38	F	102	HEM	CAD-CBD-CGD-O2D
35	C	520	DGD	C9A-CAA-CBA-CCA
34	B	622	HTG	C2'-C1'-S1-C1
23	c	502	CLA	C2A-CAA-CBA-CGA
23	c	504	CLA	C2A-CAA-CBA-CGA
23	c	504	CLA	C5-C6-C7-C8
32	L	101[A]	LHG	O7-C7-C8-C9
32	l	802[A]	LHG	O7-C7-C8-C9
23	C	508	CLA	C16-C17-C18-C19
23	b	612	CLA	C13-C15-C16-C17
32	L	101[B]	LHG	O7-C7-C8-C9
35	c	519	DGD	C3B-C4B-C5B-C6B
37	D	401[B]	PHO	C4-C3-C5-C6
37	a	408[A]	PHO	C4-C3-C5-C6
32	d	411[B]	LHG	C7-C8-C9-C10
33	C	526	LMG	O7-C10-C11-C12
31	T	101	LMT	C9-C10-C11-C12
32	l	802[B]	LHG	C9-C10-C11-C12
23	C	503	CLA	C16-C17-C18-C19
38	f	101	HEM	CAD-CBD-CGD-O1D
23	b	615	CLA	C13-C15-C16-C17
34	b	623	HTG	C4'-C5'-C6'-C7'
33	c	520	LMG	O7-C10-C11-C12
34	c	522	HTG	C4'-C5'-C6'-C7'
33	B	621	LMG	O10-C28-C29-C30
34	b	622	HTG	O5-C5-C6-O6
31	b	627	LMT	C2-C1-O1'-C1'
23	C	513	CLA	O1A-CGA-O2A-C1
32	d	411[A]	LHG	C30-C31-C32-C33
35	c	517[B]	DGD	C6B-C7B-C8B-C9B
33	B	621	LMG	C30-C31-C32-C33
38	f	101	HEM	CAD-CBD-CGD-O2D
23	C	509	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	604	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C10-C8-C9
26	A	410	SQD	C15-C16-C17-C18
32	A	416[B]	LHG	C30-C31-C32-C33
23	b	602	CLA	C8-C10-C11-C12
32	L	101[B]	LHG	C15-C16-C17-C18
37	a	416[A]	PHO	C2C-C3C-CAC-CBC
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	C	514	CLA	C4B-C3B-CAB-CBB
23	b	601	CLA	C3-C5-C6-C7
31	e	101	LMT	C2-C3-C4-C5
33	z	101	LMG	C15-C16-C17-C18
33	B	621	LMG	O1-C7-C8-O7
28	D	407[B]	PL9	C11-C12-C13-C14
24	Y	101	BCR	C21-C22-C23-C24
24	a	410	BCR	C19-C20-C21-C22
31	m	103	LMT	C11-C10-C9-C8
33	m	101	LMG	C40-C41-C42-C43
32	A	416[B]	LHG	O8-C23-C24-C25
33	D	413	LMG	O7-C10-C11-C12
32	d	405[B]	LHG	C11-C10-C9-C8
23	B	602	CLA	C2A-CAA-CBA-CGA
37	a	408[B]	PHO	C8-C10-C11-C12
34	b	625	HTG	C4'-C5'-C6'-C7'
23	C	512	CLA	CAA-CBA-CGA-O2A
32	L	101[B]	LHG	C11-C12-C13-C14
31	A	415	LMT	C2B-C1B-O1B-C4'
23	a	405[A]	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
35	C	520	DGD	C8B-C9B-CAB-CBB
23	B	616	CLA	C11-C12-C13-C15
23	C	504	CLA	C12-C13-C15-C16
23	C	510	CLA	C12-C13-C15-C16
23	c	511	CLA	C11-C10-C8-C7
28	a	414[B]	PL9	C33-C34-C36-C37
23	b	615	CLA	C10-C11-C12-C13
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
23	B	602	CLA	O2A-C1-C2-C3
37	a	408[B]	PHO	O2A-C1-C2-C3
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
33	a	417	LMG	C31-C32-C33-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	C	518[B]	DGD	C6A-C7A-C8A-C9A
32	A	416[A]	LHG	C18-C19-C20-C21
32	d	406[A]	LHG	C30-C31-C32-C33
35	C	519[B]	DGD	C3B-C4B-C5B-C6B
26	f	102	SQD	C28-C29-C30-C31
28	d	404[A]	PL9	C34-C36-C37-C38
32	D	408[B]	LHG	C26-C27-C28-C29
32	d	405[B]	LHG	C25-C26-C27-C28
32	E	101[A]	LHG	O7-C7-C8-C9
31	M	101	LMT	C4'-C5'-C6'-O6'
32	L	101[B]	LHG	O9-C7-C8-C9
32	l	802[A]	LHG	O9-C7-C8-C9
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
28	a	414[B]	PL9	C21-C22-C23-C24
32	d	406[A]	LHG	O10-C23-O8-C6
32	D	408[B]	LHG	C31-C32-C33-C34
31	b	621	LMT	C5'-C4'-O1B-C1B
23	b	607	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16
23	c	513	CLA	CAA-CBA-CGA-O1A
32	L	101[A]	LHG	O9-C7-C8-C9
35	C	520	DGD	O1A-C1A-C2A-C3A
23	c	512	CLA	CBA-CGA-O2A-C1
34	d	408	HTG	S1-C1'-C2'-C3'
26	f	102	SQD	O5-C5-C6-S
37	D	401[B]	PHO	O1A-CGA-O2A-C1
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
23	c	511	CLA	CAA-CBA-CGA-O1A
32	E	101[B]	LHG	O9-C7-C8-C9
25	l	801[A]	GOL	O1-C1-C2-O2
26	B	620	SQD	C11-C12-C13-C14
32	A	416[A]	LHG	C30-C31-C32-C33
32	A	416[A]	LHG	O10-C23-C24-C25
32	a	420[A]	LHG	O10-C23-C24-C25
32	a	420[B]	LHG	O10-C23-C24-C25
23	B	601	CLA	C13-C15-C16-C17
32	D	409[A]	LHG	C28-C29-C30-C31
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	C	519[A]	DGD	C5D-C6D-O5D-C1E
35	c	517[A]	DGD	C5D-C6D-O5D-C1E
35	H	102	DGD	O1G-C1G-C2G-O2G
26	C	501[B]	SQD	C18-C19-C20-C21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	E	101[A]	LHG	C11-C10-C9-C8
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	514	CLA	CAA-CBA-CGA-O1A
32	l	802[B]	LHG	O9-C7-C8-C9
33	c	520	LMG	O9-C10-C11-C12
35	C	519[A]	DGD	O2G-C1B-C2B-C3B
33	D	413	LMG	C38-C39-C40-C41
23	C	504	CLA	C16-C17-C18-C19
26	A	410	SQD	C25-C26-C27-C28
35	C	518[A]	DGD	CBA-CCA-CDA-CEA
33	z	101	LMG	C17-C18-C19-C20
23	b	613	CLA	CAA-CBA-CGA-O1A
33	C	526	LMG	O9-C10-C11-C12
28	A	412[B]	PL9	C46-C47-C48-C49
28	d	404[A]	PL9	C11-C12-C13-C14
23	b	612	CLA	C8-C10-C11-C12
37	a	416[B]	PHO	C8-C10-C11-C12
35	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	b	612	CLA	O1A-CGA-O2A-C1
23	B	609	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	609	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
37	a	408[A]	PHO	CAD-CBD-CGD-O2D
32	L	101[A]	LHG	C32-C33-C34-C35
32	d	406[B]	LHG	O8-C23-C24-C25
32	d	406[B]	LHG	C32-C33-C34-C35
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	A	407	CLA	C2-C1-O2A-CGA
23	a	405[B]	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
32	A	416[B]	LHG	O10-C23-C24-C25
23	c	502	CLA	CAA-CBA-CGA-O2A
32	E	101[A]	LHG	O8-C23-C24-C25
33	C	521	LMG	O7-C10-C11-C12
23	C	504	CLA	C16-C17-C18-C20
31	T	101	LMT	C11-C10-C9-C8
32	l	802[A]	LHG	C17-C18-C19-C20
23	C	512	CLA	CAA-CBA-CGA-O1A
33	C	521	LMG	O9-C10-C11-C12
26	a	412	SQD	O48-C23-C24-C25
32	D	409[A]	LHG	O8-C23-C24-C25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	B	621	LMG	O7-C10-C11-C12
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[B]	LHG	O8-C23-C24-C25
33	C	502	LMG	O8-C28-C29-C30
33	D	413	LMG	O9-C10-C11-C12
33	a	417	LMG	C13-C14-C15-C16

There are no ring outliers.

183 monomers are involved in 358 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	a	407[B]	CLA	2	0
25	l	801[A]	GOL	1	0
23	c	510	CLA	1	0
25	O	302	GOL	1	0
23	b	604	CLA	1	0
31	t	101	LMT	1	0
32	D	409[B]	LHG	4	0
35	c	518[A]	DGD	3	0
26	C	501[A]	SQD	1	0
24	c	515	BCR	3	0
32	d	405[A]	LHG	2	0
23	C	505	CLA	4	0
28	A	412[A]	PL9	11	0
23	C	506	CLA	1	0
23	C	508	CLA	4	0
25	V	204[B]	GOL	1	0
37	D	401[B]	PHO	1	0
23	B	602	CLA	3	0
25	B	629	GOL	1	0
23	C	511	CLA	3	0
26	F	103	SQD	2	0
23	a	405[B]	CLA	3	0
37	a	416[A]	PHO	1	0
23	b	616	CLA	4	0
23	B	606	CLA	2	0
23	B	613	CLA	3	0
23	c	502	CLA	4	0
23	D	404[A]	CLA	3	0
24	d	403	BCR	2	0
28	d	404[B]	PL9	1	0
26	a	411[A]	SQD	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	512	CLA	5	0
23	c	508	CLA	2	0
25	c	526[B]	GOL	1	0
23	a	406[A]	CLA	3	0
32	E	101[A]	LHG	3	0
25	b	628	GOL	2	0
35	C	518[B]	DGD	4	0
31	t	102	LMT	2	0
23	B	612	CLA	3	0
23	b	612	CLA	2	0
35	C	520	DGD	2	0
23	A	404[B]	CLA	2	0
23	B	609	CLA	2	0
23	A	407	CLA	3	0
25	B	624	GOL	1	0
25	D	403	GOL	5	0
38	F	102	HEM	1	0
24	A	408	BCR	1	0
24	T	102	BCR	6	0
23	B	603	CLA	1	0
24	k	101	BCR	2	0
28	a	414[A]	PL9	5	0
24	b	619	BCR	5	0
25	B	627	GOL	1	0
35	H	102	DGD	1	0
23	C	509	CLA	2	0
23	b	614	CLA	2	0
24	t	103	BCR	3	0
23	b	613	CLA	1	0
26	f	102	SQD	1	0
23	a	407[A]	CLA	1	0
33	c	520	LMG	1	0
23	C	503	CLA	4	0
23	A	405[A]	CLA	1	0
37	a	408[B]	PHO	2	0
25	a	419	GOL	5	0
32	a	420[B]	LHG	3	0
38	f	101	HEM	1	0
33	C	526	LMG	1	0
34	b	622	HTG	1	0
23	A	406[B]	CLA	3	0
33	C	502	LMG	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	402	CLA	2	0
37	D	401[A]	PHO	1	0
23	b	609	CLA	5	0
23	c	504	CLA	4	0
23	a	405[A]	CLA	2	0
26	B	620	SQD	3	0
23	b	602	CLA	1	0
35	C	519[A]	DGD	1	0
32	d	406[B]	LHG	7	0
23	C	514	CLA	2	0
24	y	101	BCR	2	0
32	D	408[A]	LHG	2	0
34	D	412	HTG	1	0
35	c	518[B]	DGD	4	0
25	v	202[A]	GOL	1	0
26	A	410	SQD	1	0
26	C	501[B]	SQD	1	0
31	A	415	LMT	1	0
32	d	405[B]	LHG	1	0
25	O	303	GOL	1	0
23	C	512	CLA	5	0
25	D	414	GOL	3	0
28	A	412[B]	PL9	8	0
35	c	519	DGD	4	0
23	B	604	CLA	2	0
24	D	406	BCR	2	0
35	C	518[A]	DGD	1	0
33	z	101	LMG	2	0
31	B	630	LMT	2	0
31	b	621	LMT	1	0
23	d	401[B]	CLA	4	0
24	H	101	BCR	2	0
28	D	407[A]	PL9	1	0
26	b	620	SQD	2	0
25	C	524[B]	GOL	1	0
24	c	516	BCR	1	0
31	c	501	LMT	2	0
24	B	619	BCR	1	0
23	B	615	CLA	2	0
34	b	625	HTG	1	0
23	c	513	CLA	2	0
23	a	406[B]	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	409[A]	LHG	5	0
23	C	513	CLA	4	0
23	C	507	CLA	6	0
37	D	402[B]	PHO	2	0
23	c	509	CLA	6	0
35	c	517[B]	DGD	2	0
23	C	510	CLA	4	0
31	e	101	LMT	1	0
23	C	504	CLA	3	0
23	A	406[A]	CLA	1	0
23	b	603	CLA	1	0
24	h	101	BCR	5	0
28	a	414[B]	PL9	5	0
23	b	606	CLA	3	0
31	B	628	LMT	1	0
33	B	621	LMG	1	0
23	b	601	CLA	3	0
23	B	605	CLA	4	0
23	b	605	CLA	3	0
23	b	607	CLA	2	0
24	K	102	BCR	1	0
32	L	101[B]	LHG	1	0
24	Y	101	BCR	3	0
23	c	507	CLA	3	0
23	c	505	CLA	4	0
23	b	615	CLA	2	0
24	b	617	BCR	2	0
32	d	406[A]	LHG	11	0
23	c	503	CLA	2	0
24	a	410	BCR	1	0
23	A	405[B]	CLA	3	0
23	c	506	CLA	6	0
34	c	522	HTG	1	0
23	B	601	CLA	3	0
23	A	404[A]	CLA	2	0
33	a	417	LMG	1	0
23	B	607	CLA	1	0
37	a	416[B]	PHO	1	0
23	D	404[B]	CLA	4	0
23	d	401[A]	CLA	1	0
34	d	408	HTG	1	0
25	a	418	GOL	2	0

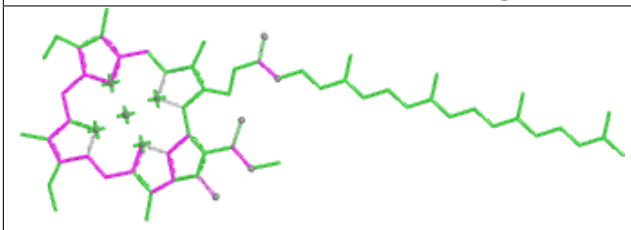
Continued on next page...

Continued from previous page...

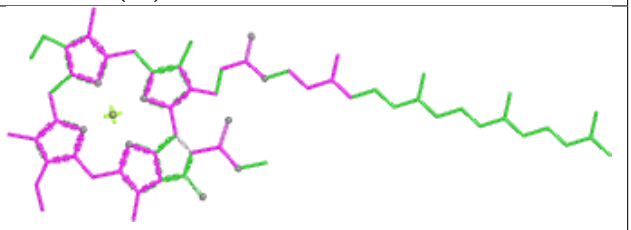
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	616	CLA	4	0
26	a	411[B]	SQD	4	0
35	C	519[B]	DGD	1	0
23	B	614	CLA	1	0
32	E	101[B]	LHG	3	0
32	D	408[B]	LHG	2	0
33	C	522	LMG	1	0
25	v	202[B]	GOL	1	0
26	a	412	SQD	1	0
25	A	409	GOL	1	0
33	c	521	LMG	1	0
32	A	416[A]	LHG	1	0
23	c	514	CLA	1	0
31	A	417	LMT	2	0
32	a	420[A]	LHG	5	0
34	B	625	HTG	1	0
34	B	622	HTG	2	0
23	a	409	CLA	2	0
37	D	402[A]	PHO	1	0
23	C	515	CLA	2	0
31	m	103	LMT	2	0
32	d	411[B]	LHG	3	0
35	c	517[A]	DGD	1	0
33	d	409	LMG	1	0
24	B	618	BCR	3	0
24	b	618	BCR	3	0

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

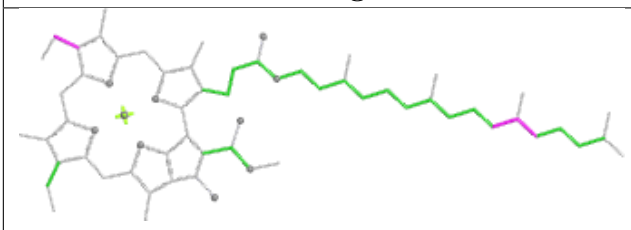
Ligand CLA a 407 (B)



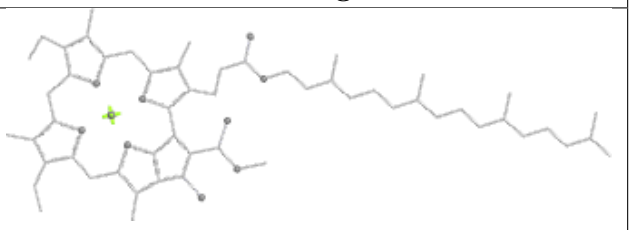
Bond lengths



Bond angles

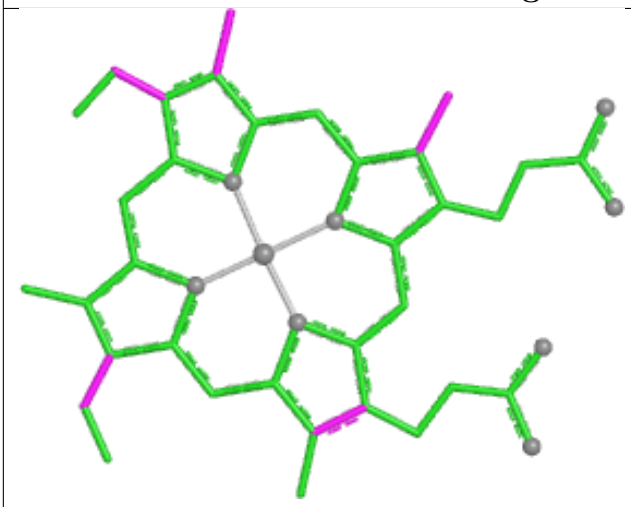


Torsions

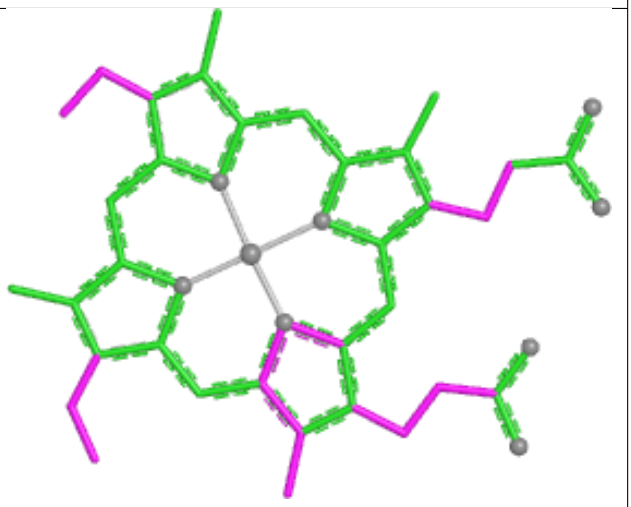


Rings

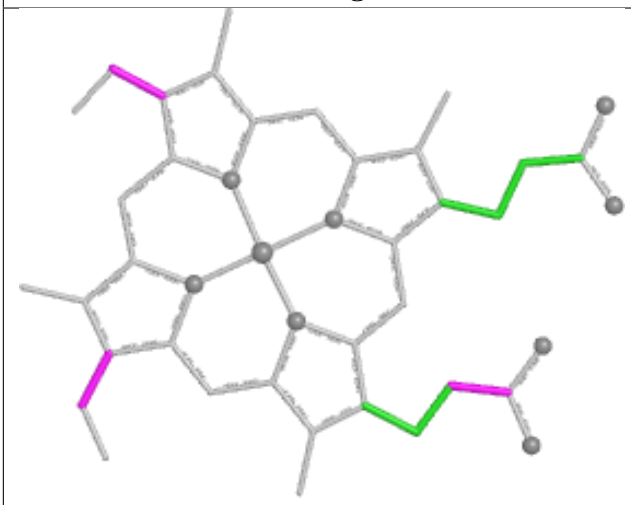
Ligand HEC V 202



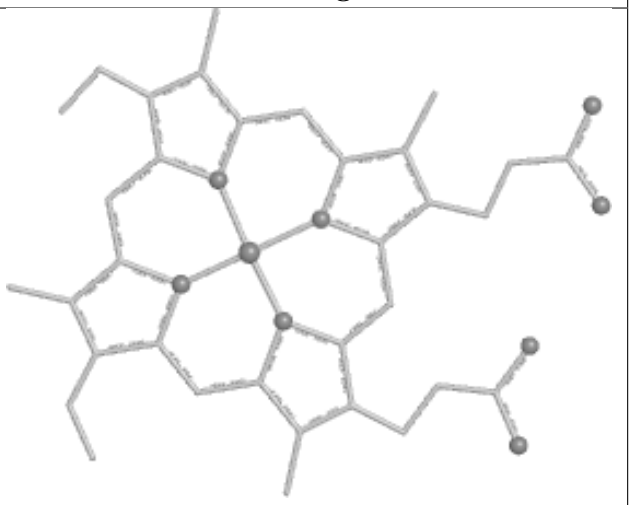
Bond lengths



Bond angles

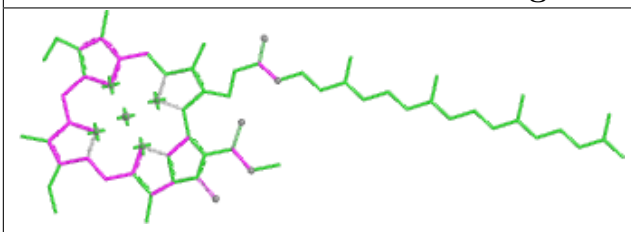


Torsions

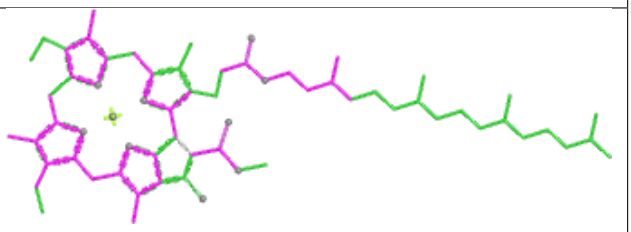


Rings

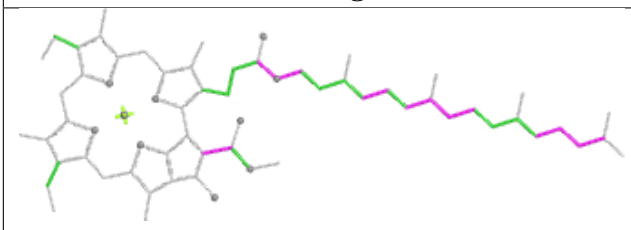
Ligand CLA c 510



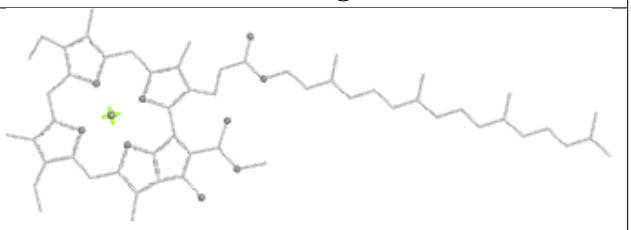
Bond lengths



Bond angles

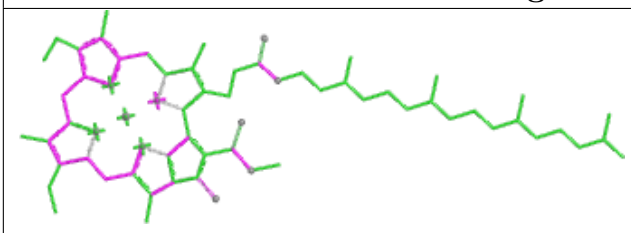


Torsions

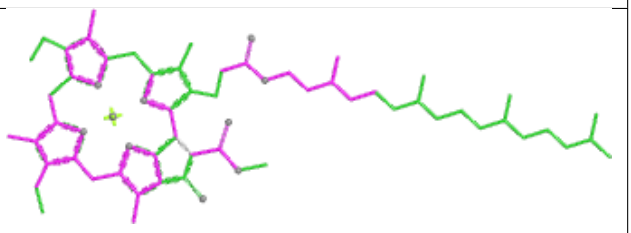


Rings

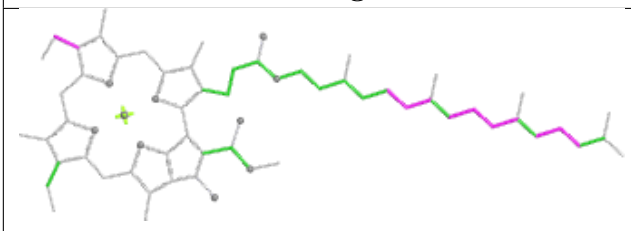
Ligand CLA b 604



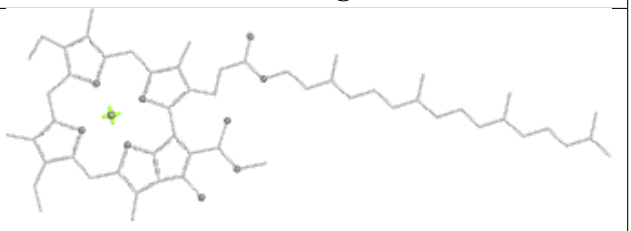
Bond lengths



Bond angles

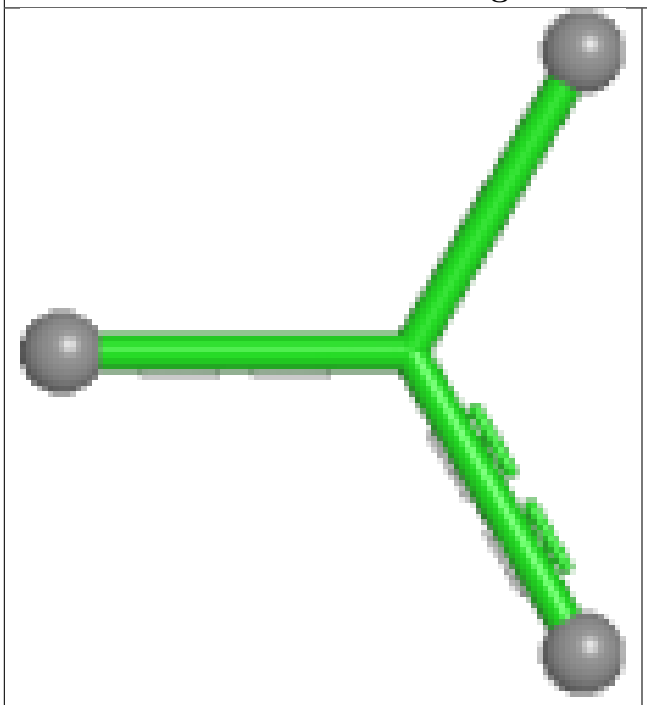


Torsions

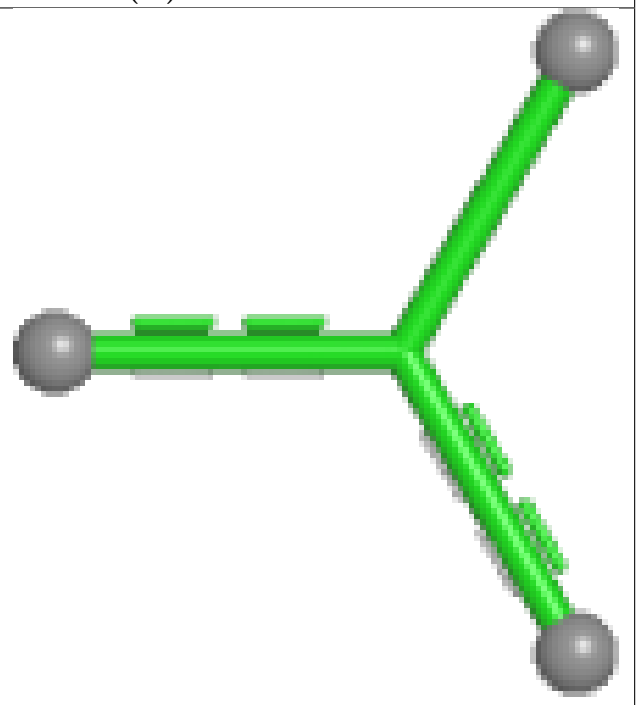


Rings

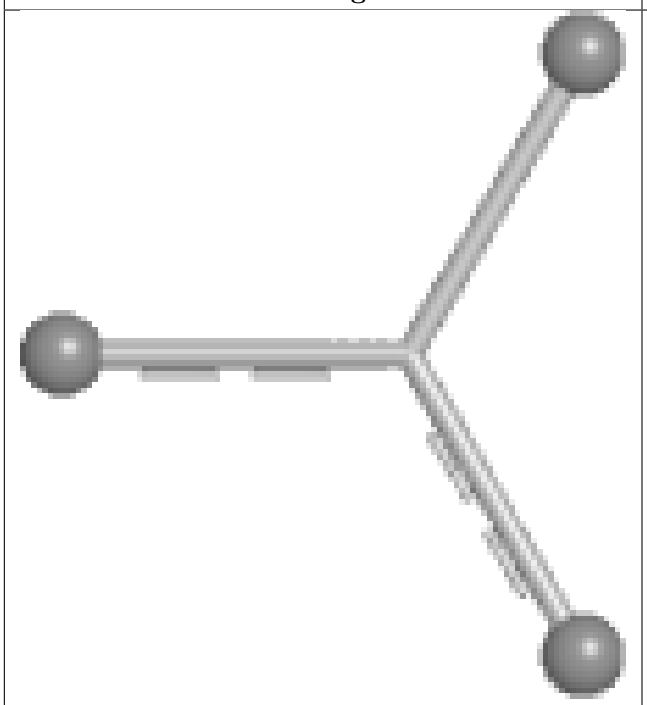
Ligand BCT A 414 (B)



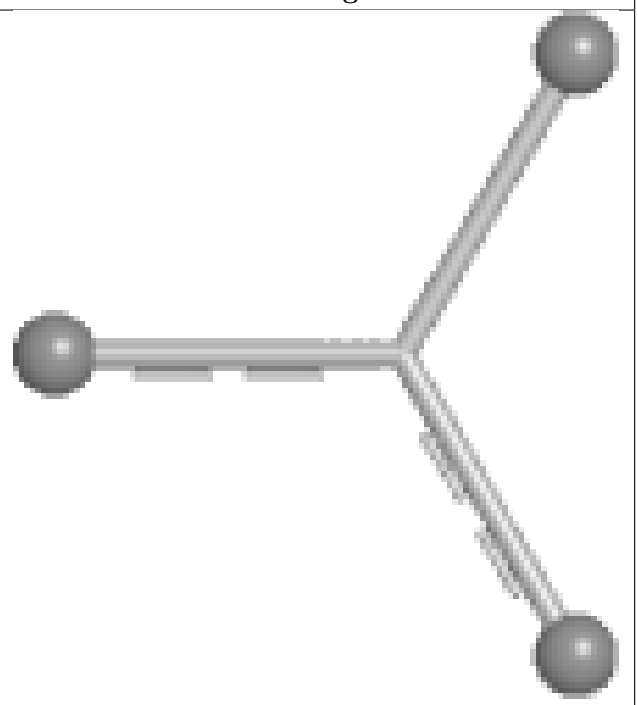
Bond lengths



Bond angles

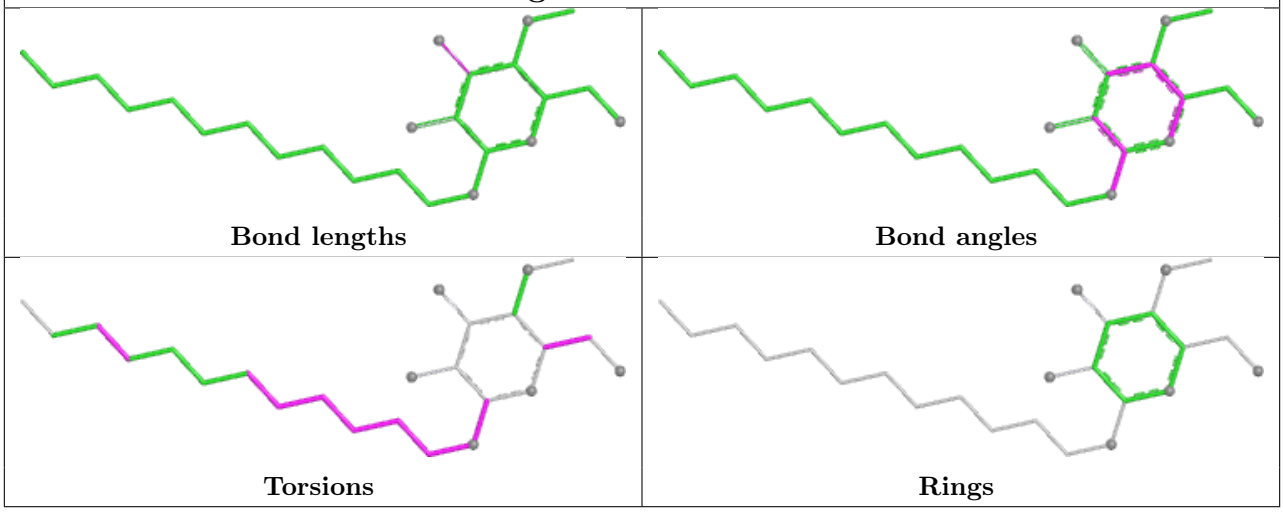


Torsions

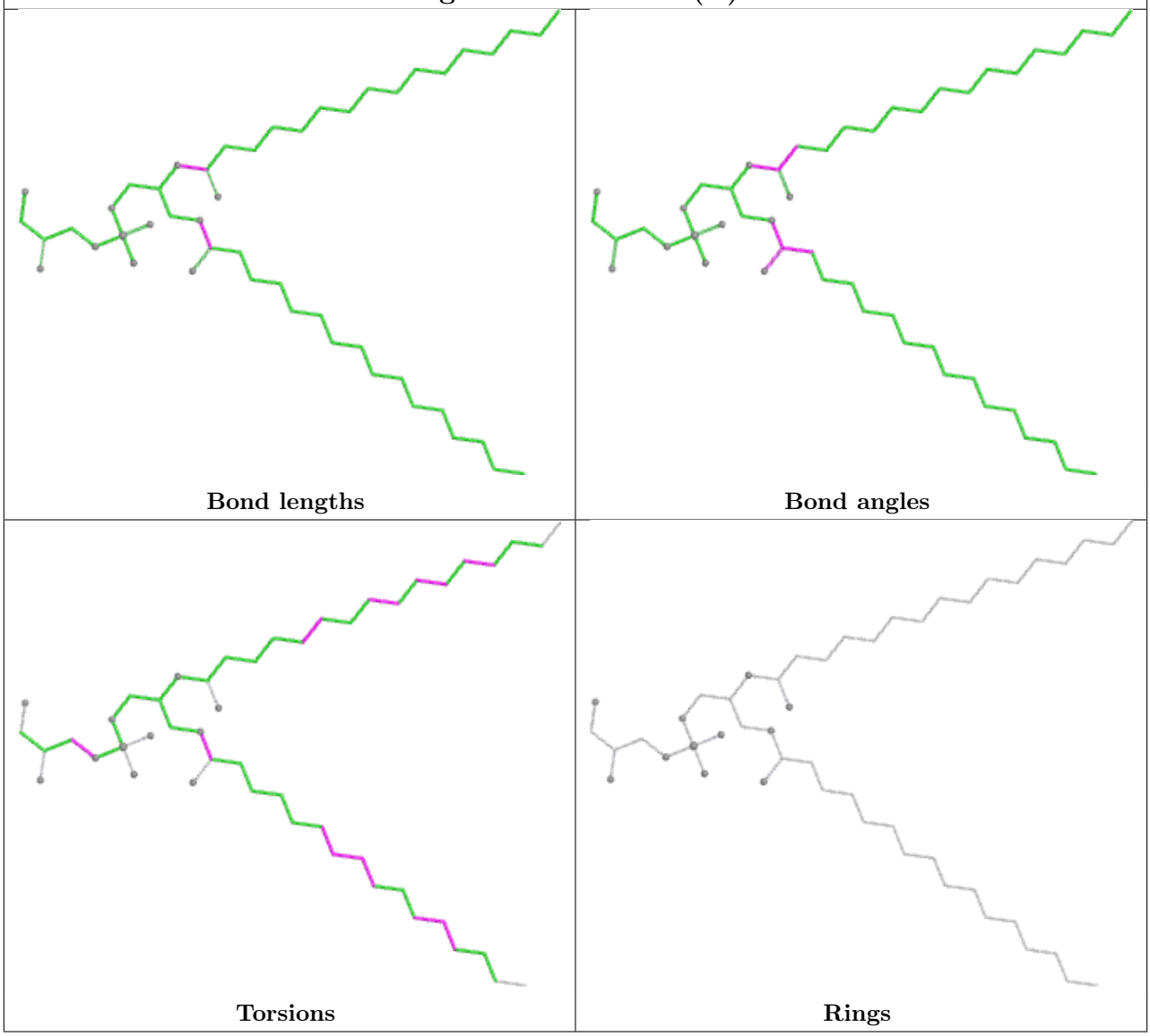


Rings

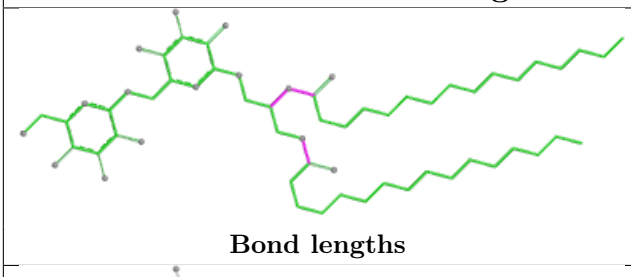
Ligand LMT t 101



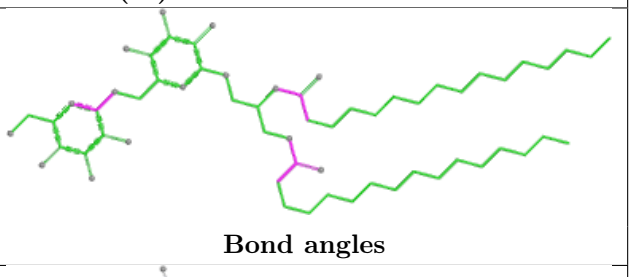
Ligand LHG D 409 (B)



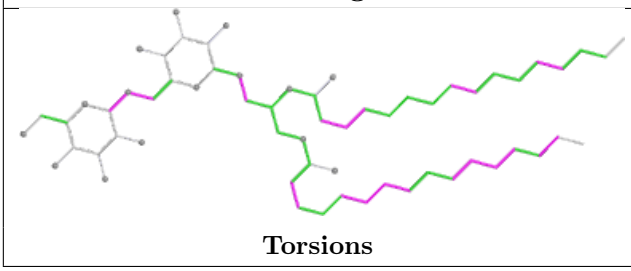
Ligand DGD c 518 (A)



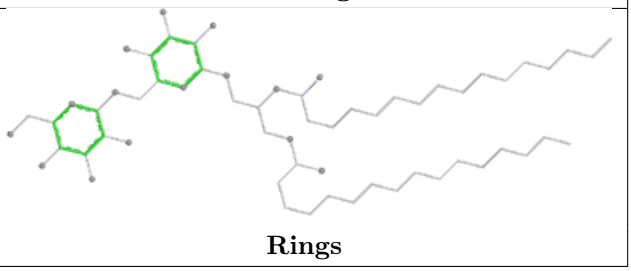
Bond lengths



Bond angles

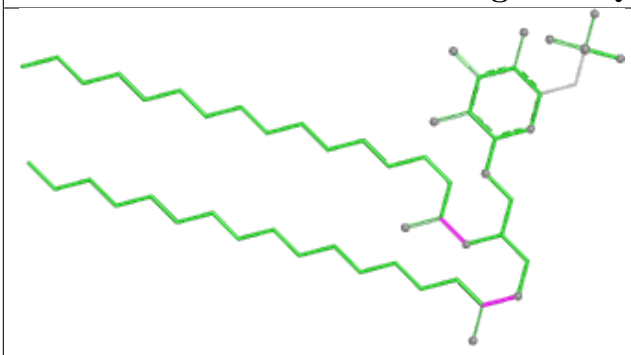


Torsions

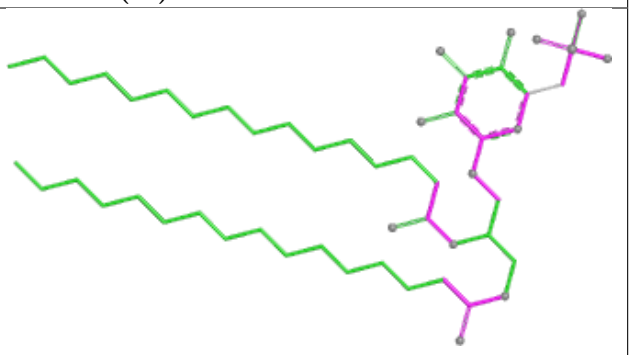


Rings

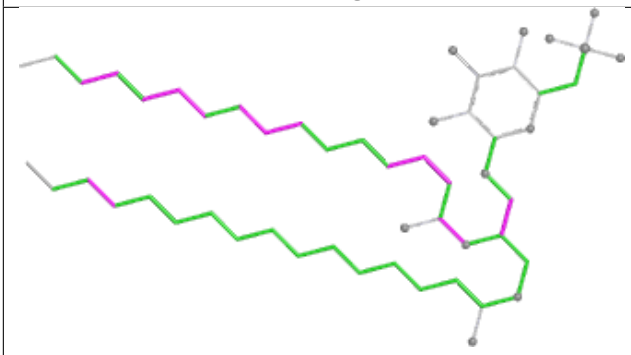
Ligand SQD C 501 (A)



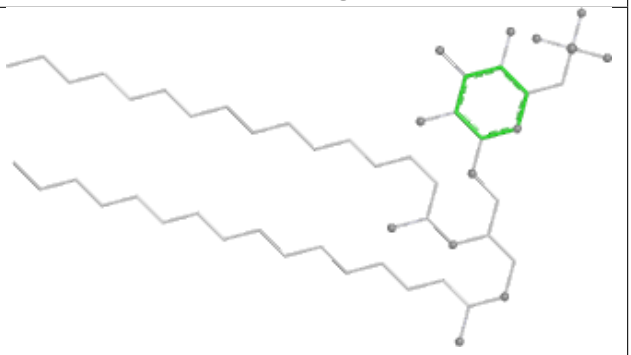
Bond lengths



Bond angles



Torsions

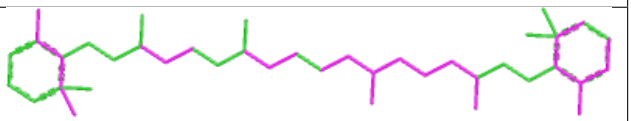


Rings

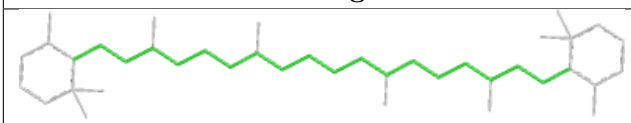
Ligand BCR c 515



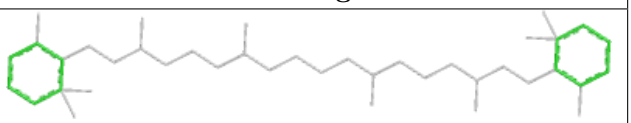
Bond lengths



Bond angles

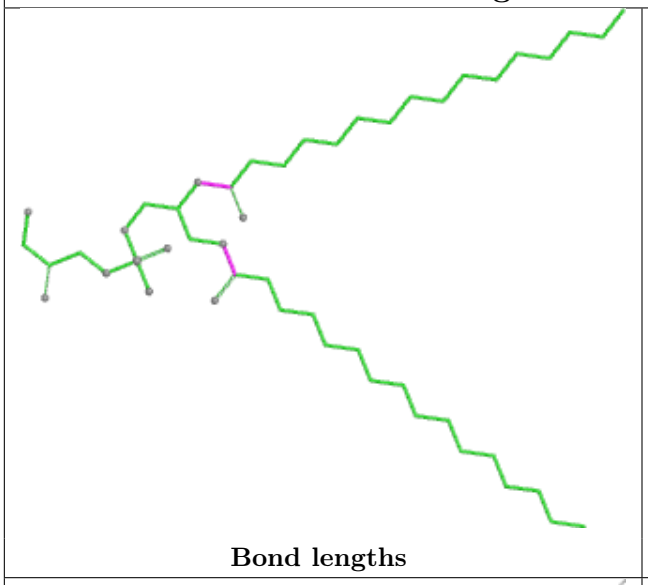


Torsions

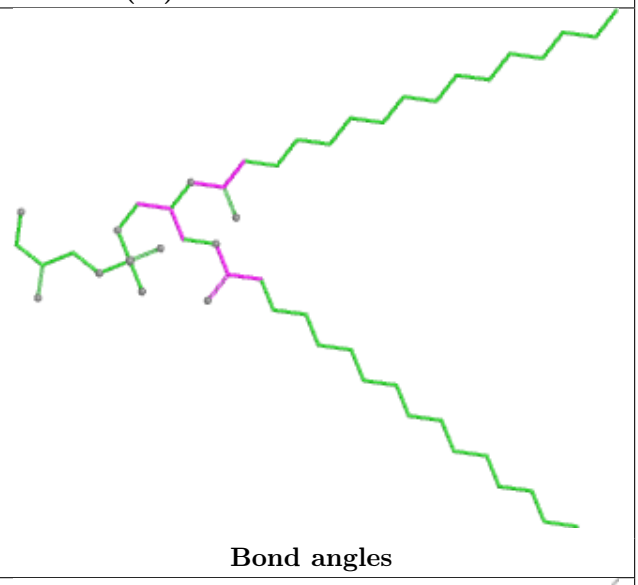


Rings

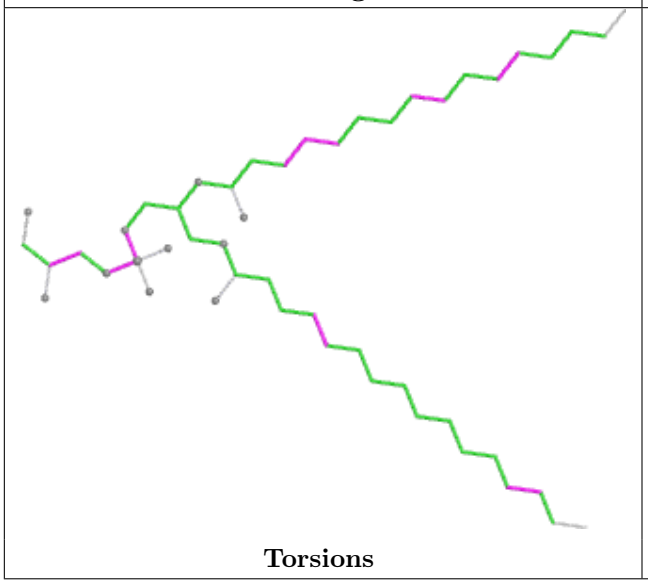
Ligand LHG d 405 (A)



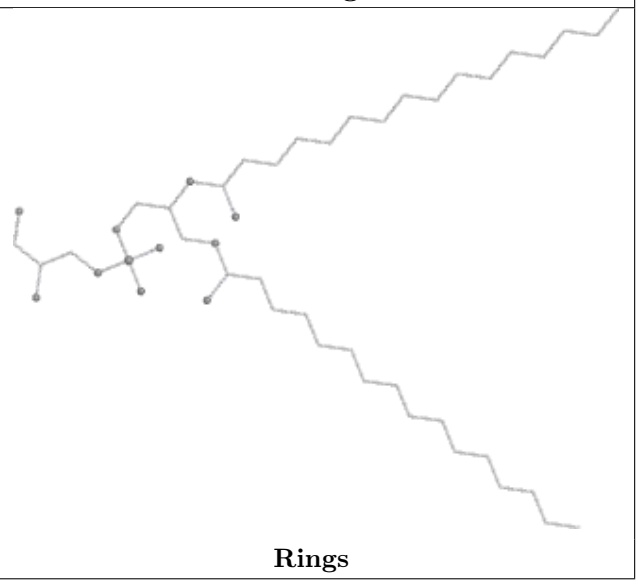
Bond lengths



Bond angles

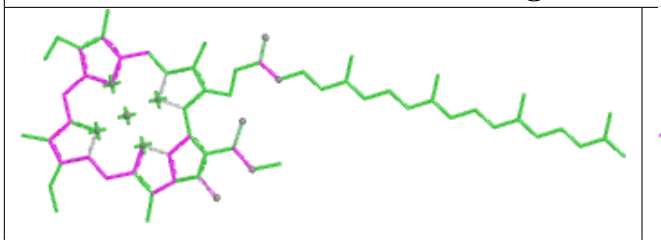


Torsions

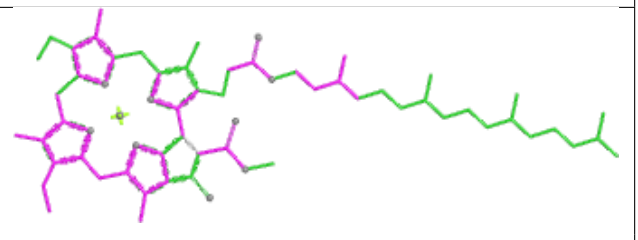


Rings

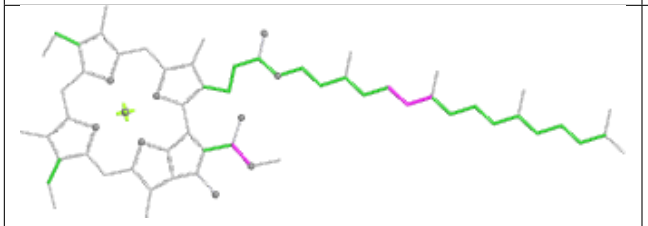
Ligand CLA C 505



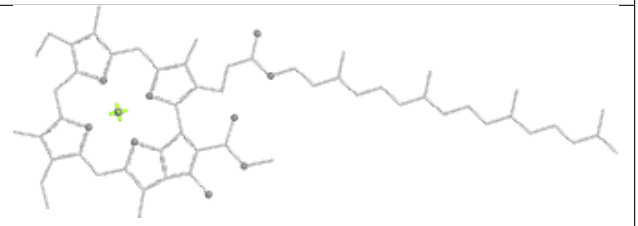
Bond lengths



Bond angles

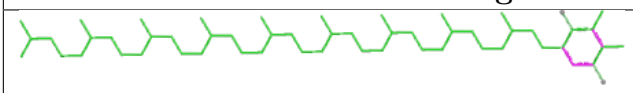


Torsions

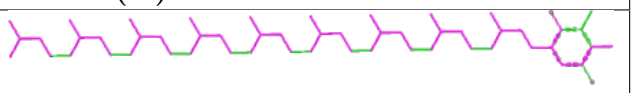


Rings

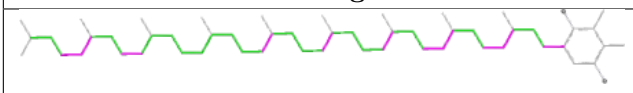
Ligand PL9 A 412 (A)



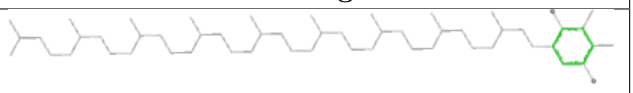
Bond lengths



Bond angles

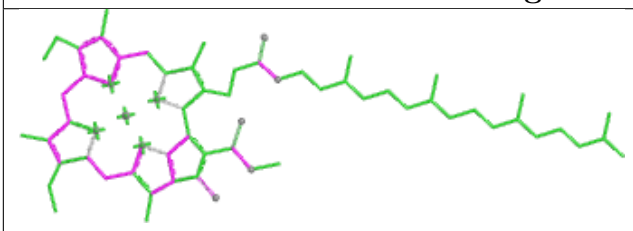


Torsions

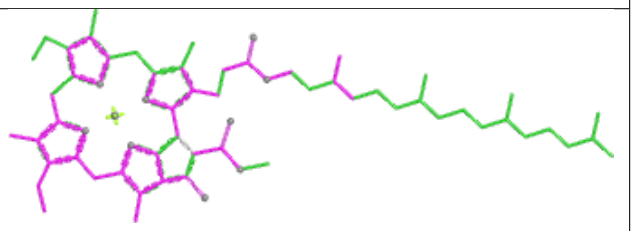


Rings

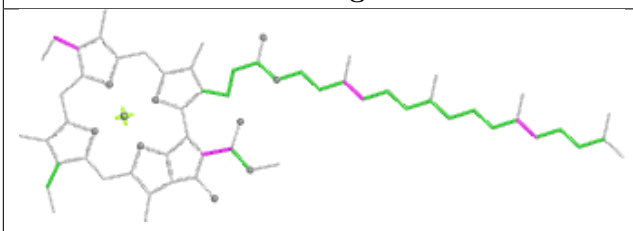
Ligand CLA C 506



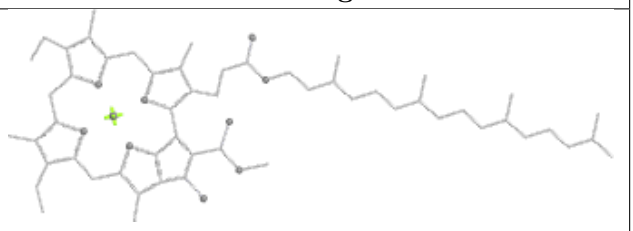
Bond lengths



Bond angles

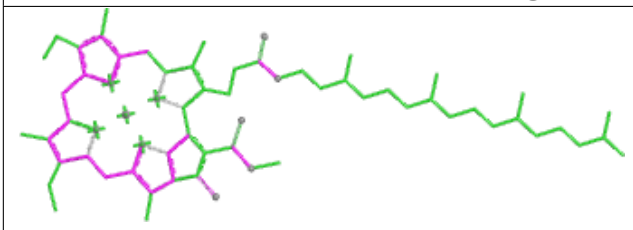


Torsions

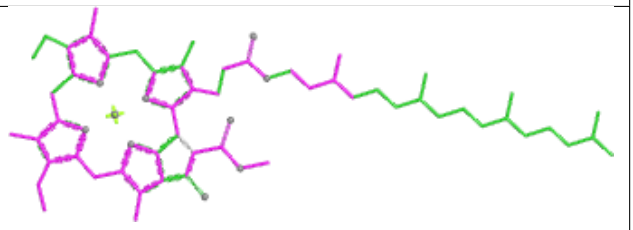


Rings

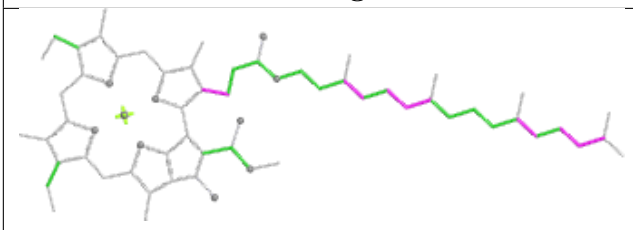
Ligand CLA C 508



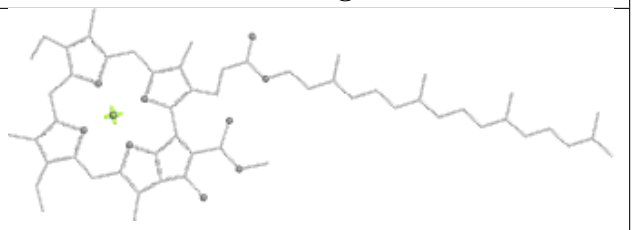
Bond lengths



Bond angles

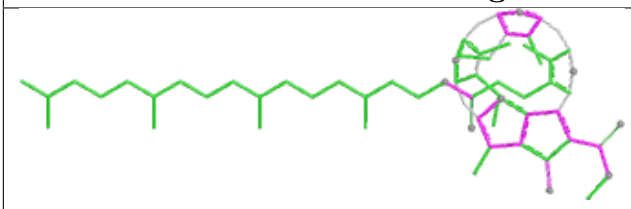


Torsions

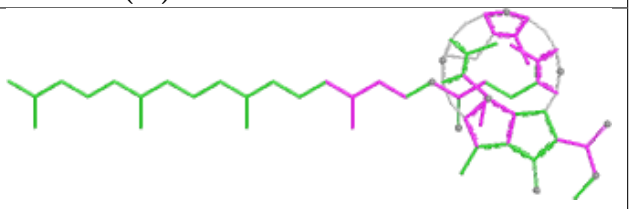


Rings

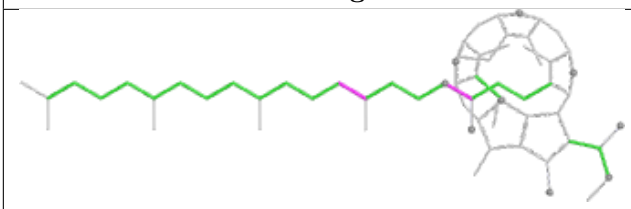
Ligand PHO D 401 (B)



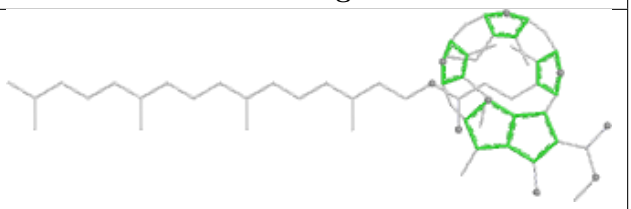
Bond lengths



Bond angles

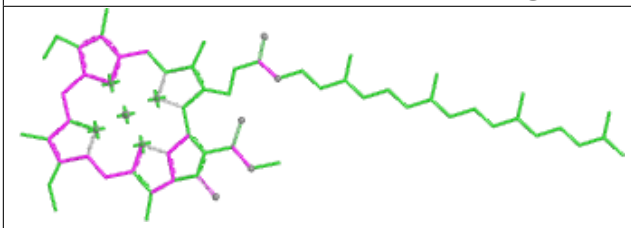


Torsions

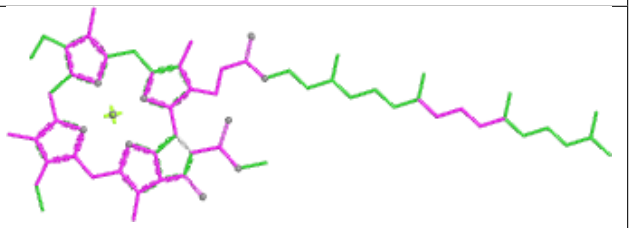


Rings

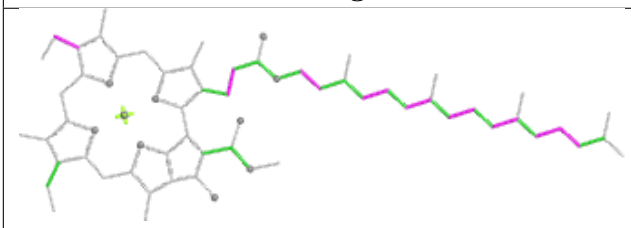
Ligand CLA B 602



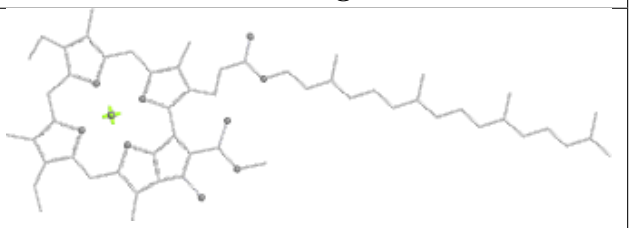
Bond lengths



Bond angles

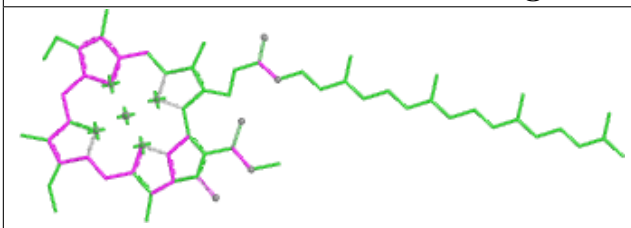


Torsions

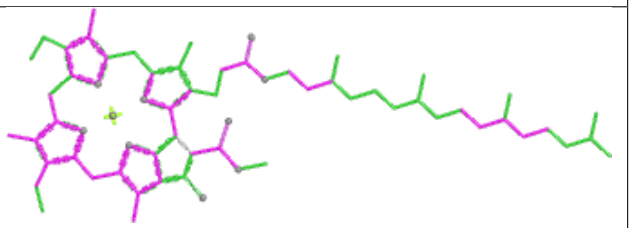


Rings

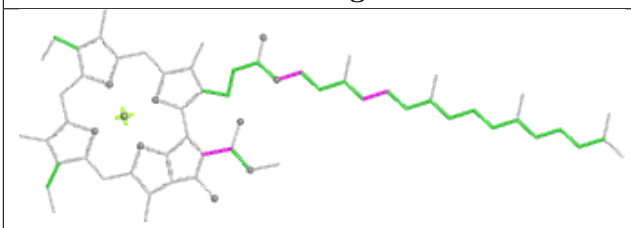
Ligand CLA C 511



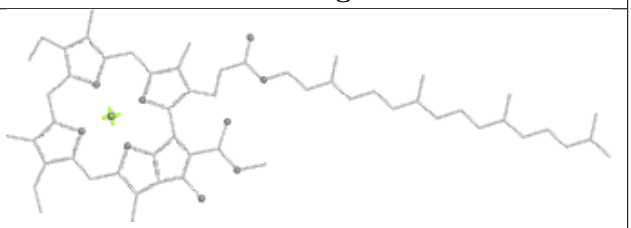
Bond lengths



Bond angles

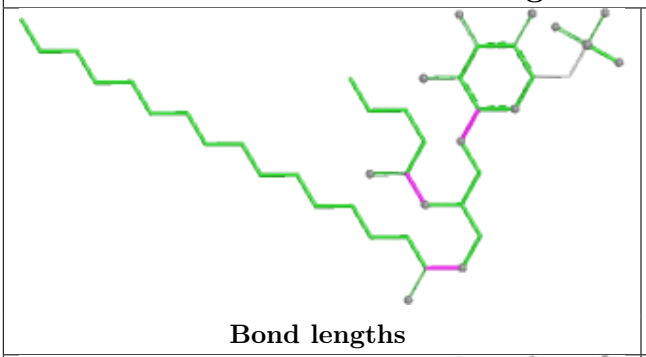


Torsions

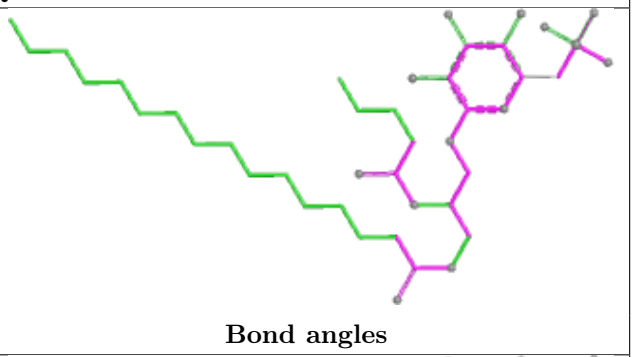


Rings

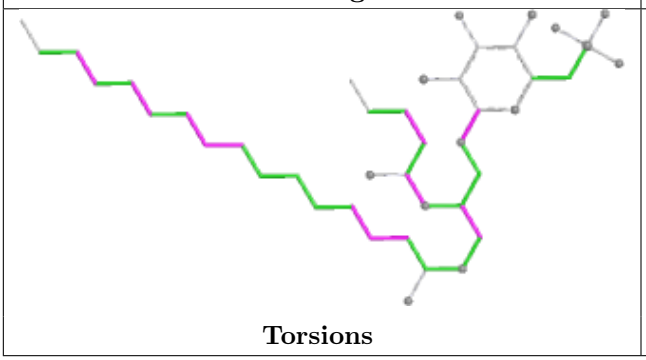
Ligand SQD F 103



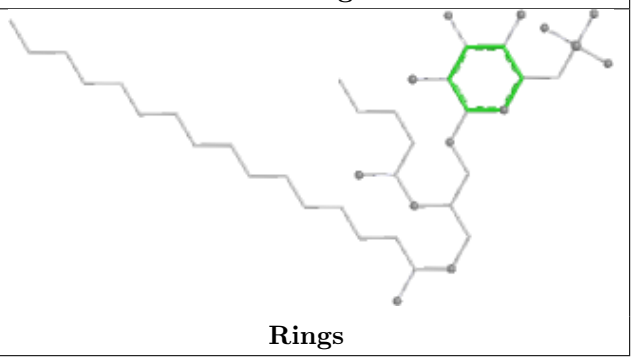
Bond lengths



Bond angles

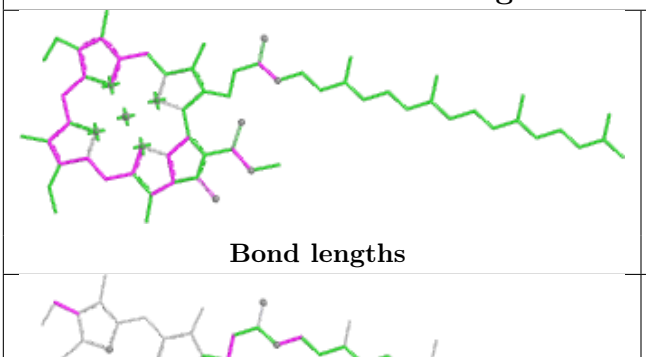


Torsions

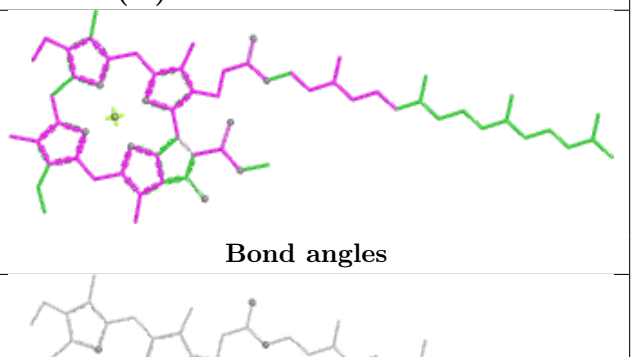


Rings

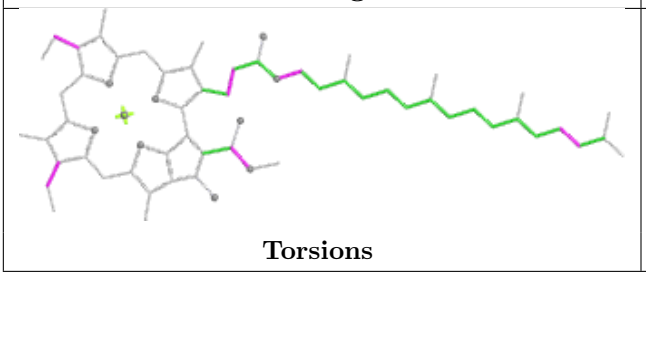
Ligand CLA a 405 (B)



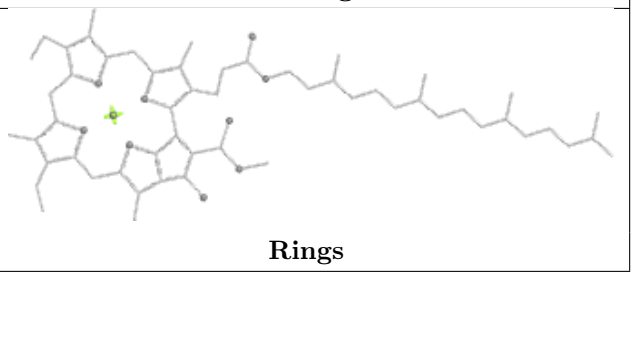
Bond lengths



Bond angles

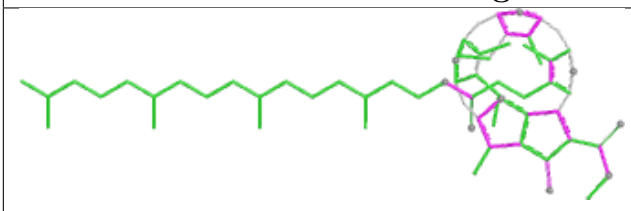


Torsions

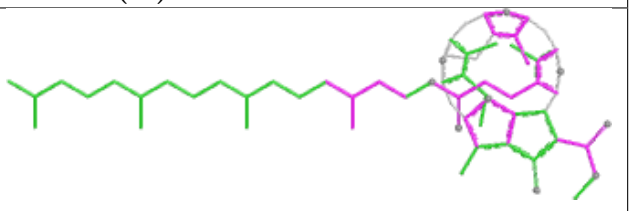


Rings

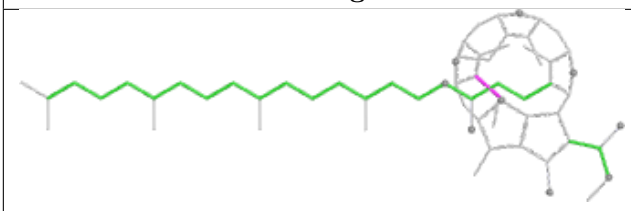
Ligand PHO a 416 (A)



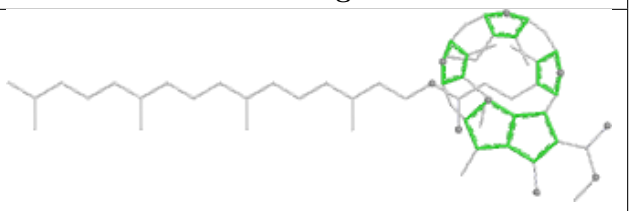
Bond lengths



Bond angles

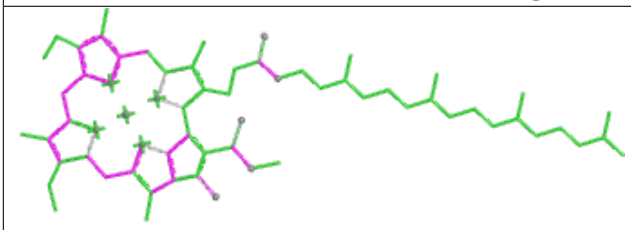


Torsions

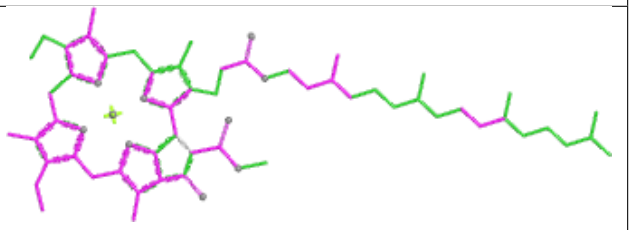


Rings

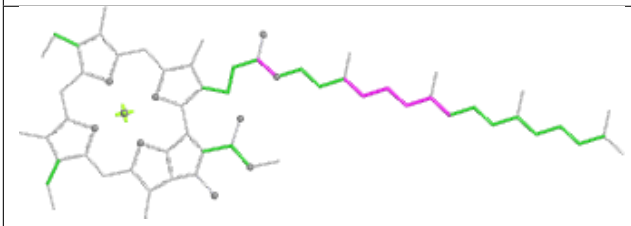
Ligand CLA b 616



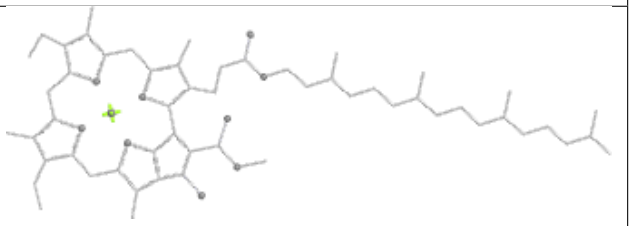
Bond lengths



Bond angles

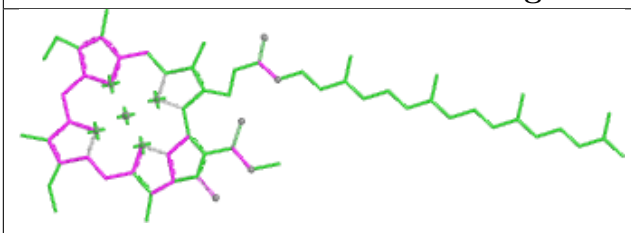


Torsions

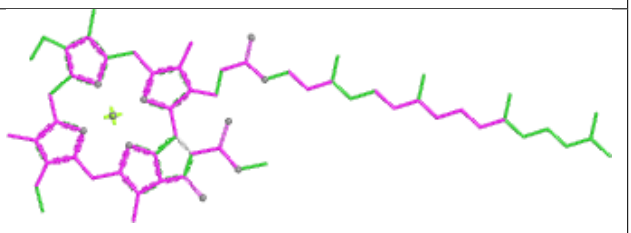


Rings

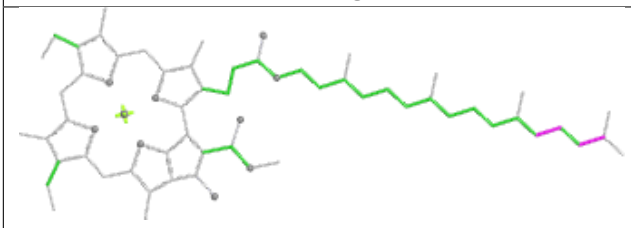
Ligand CLA B 608



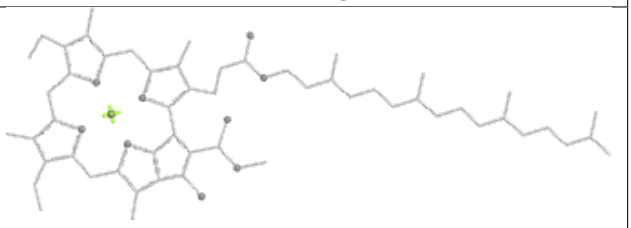
Bond lengths



Bond angles

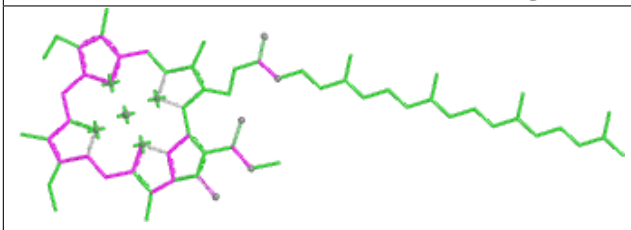


Torsions

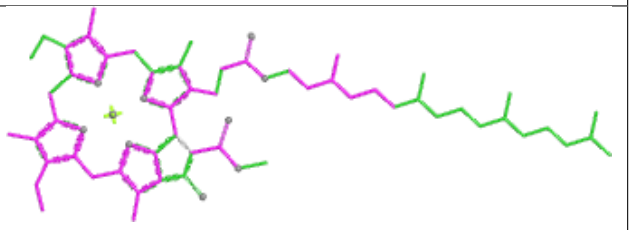


Rings

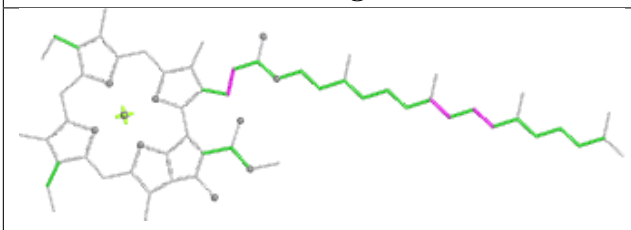
Ligand CLA B 606



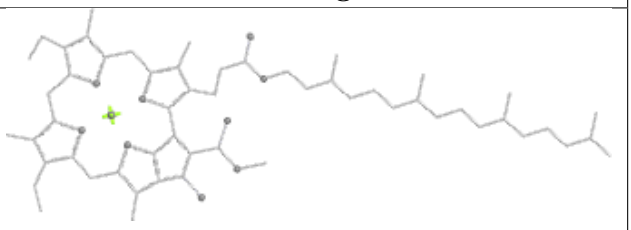
Bond lengths



Bond angles

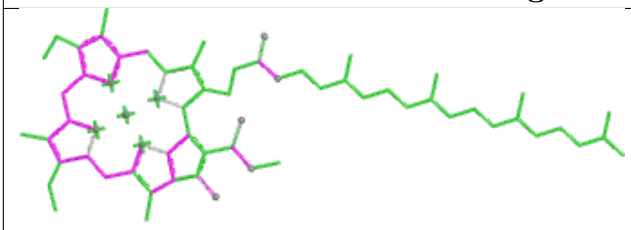


Torsions

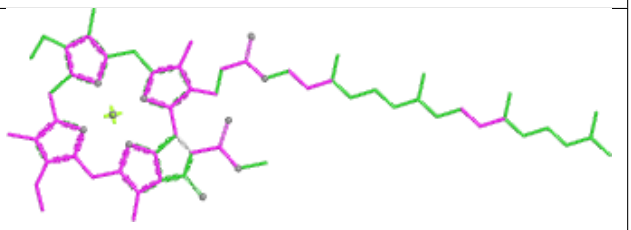


Rings

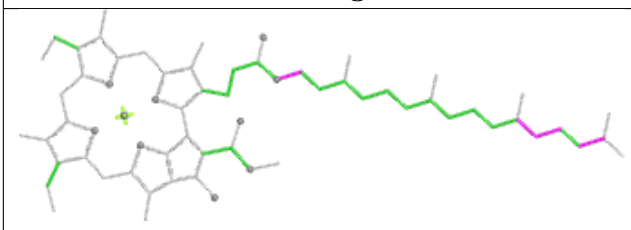
Ligand CLA b 608



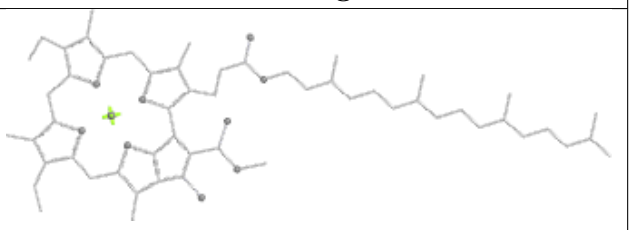
Bond lengths



Bond angles

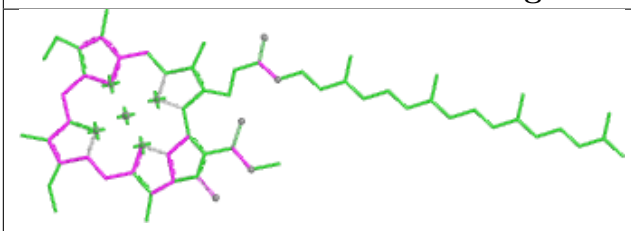


Torsions

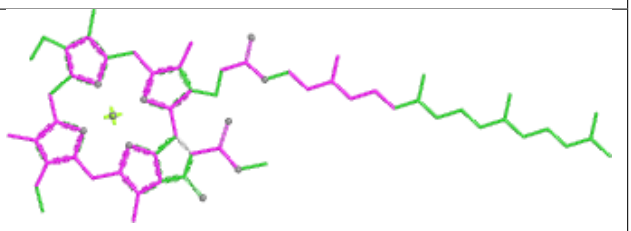


Rings

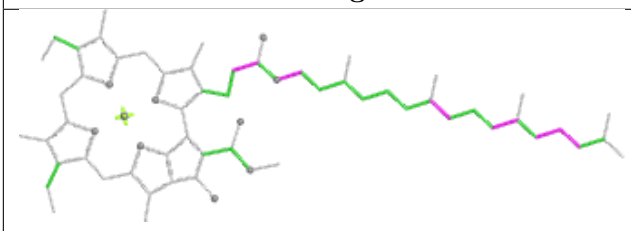
Ligand CLA B 613



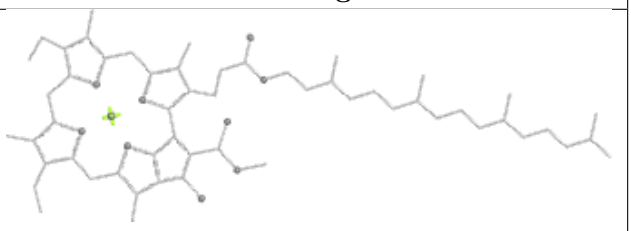
Bond lengths



Bond angles

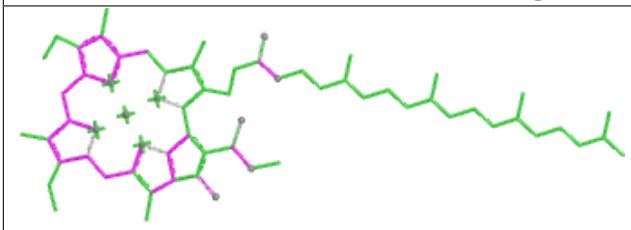


Torsions

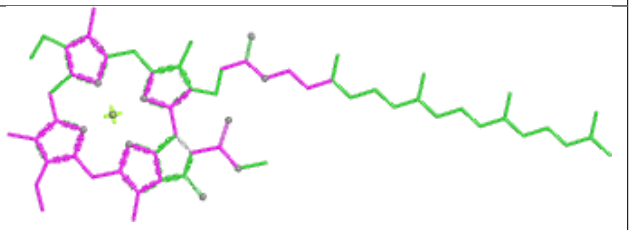


Rings

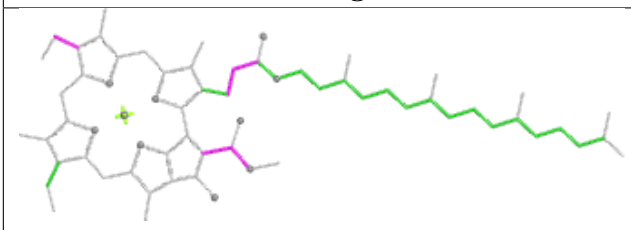
Ligand CLA c 502



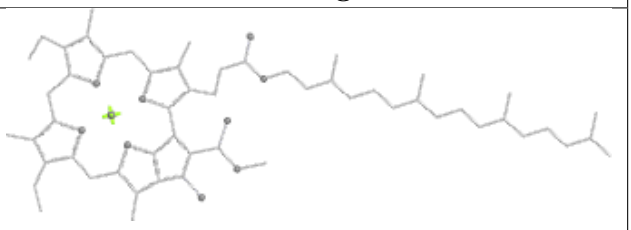
Bond lengths



Bond angles

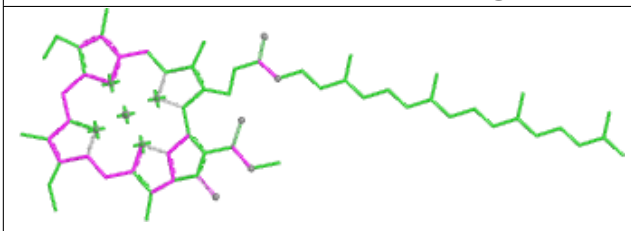


Torsions

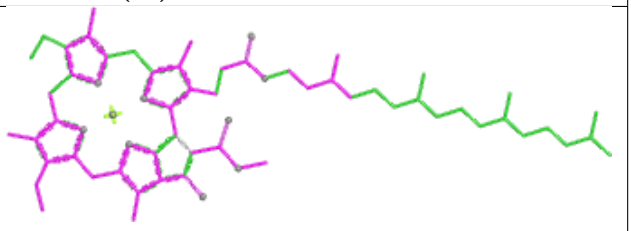


Rings

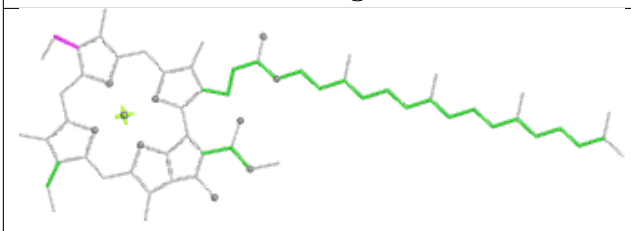
Ligand CLA D 404 (A)



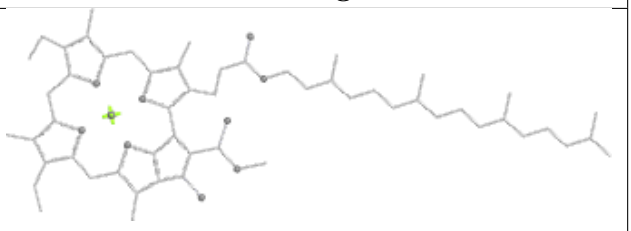
Bond lengths



Bond angles

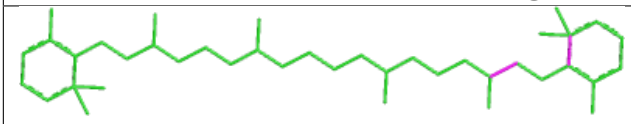


Torsions

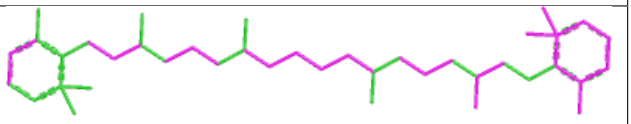


Rings

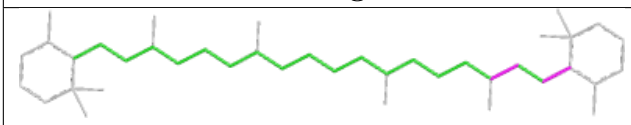
Ligand BCR d 403



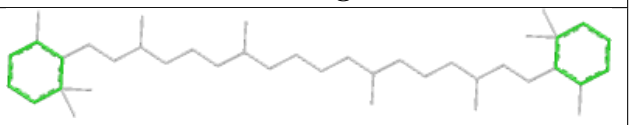
Bond lengths



Bond angles

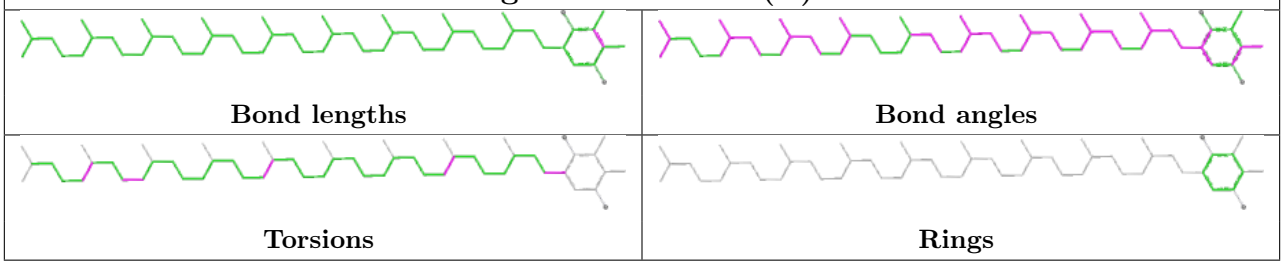


Torsions

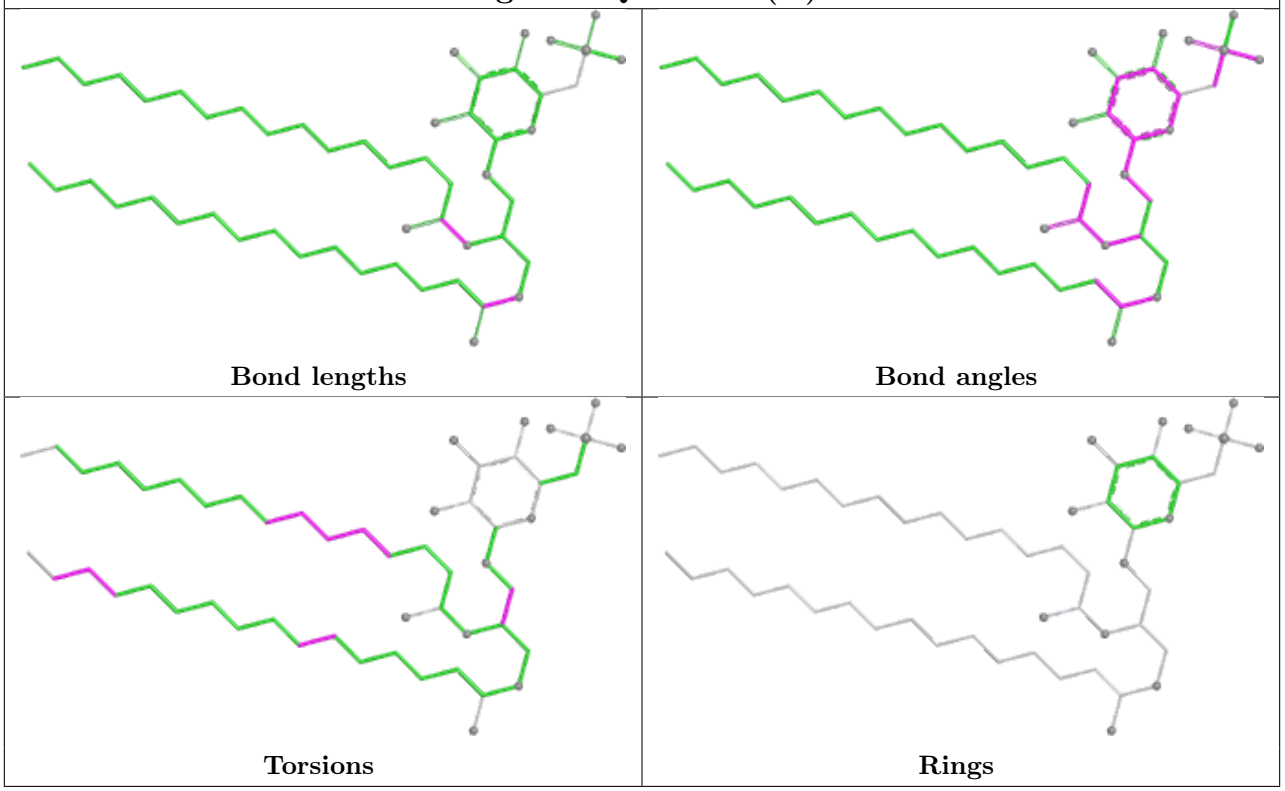


Rings

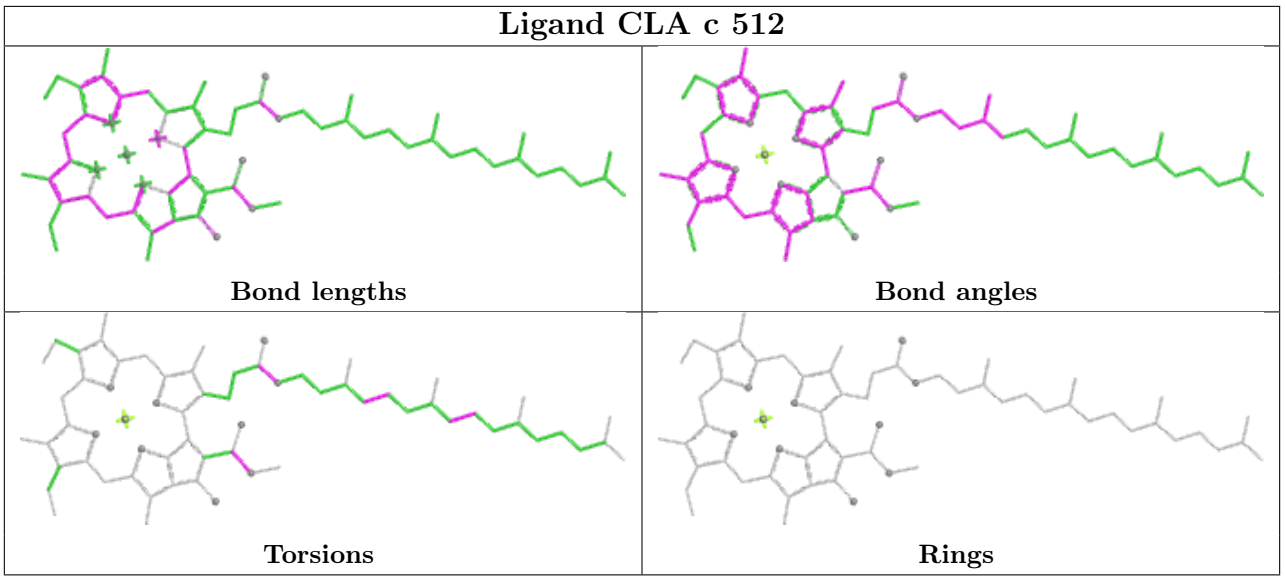
Ligand PL9 d 404 (B)



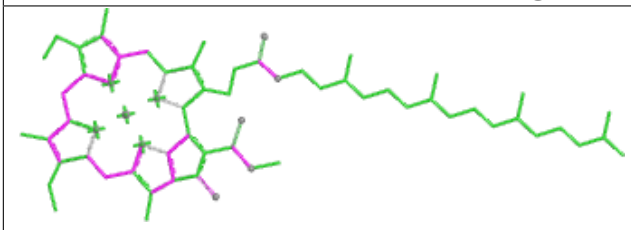
Ligand SQD a 411 (A)



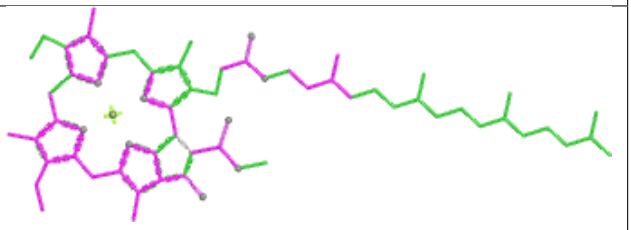
Ligand CLA c 512



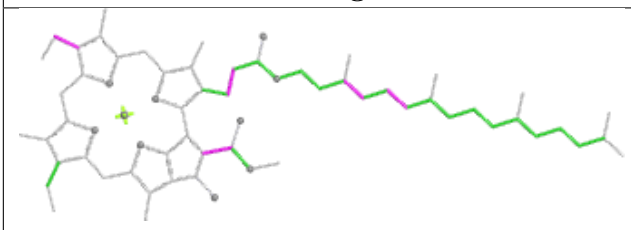
Ligand CLA c 508



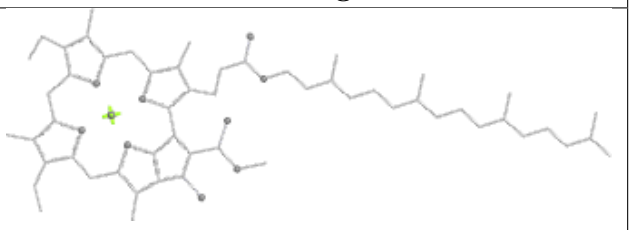
Bond lengths



Bond angles

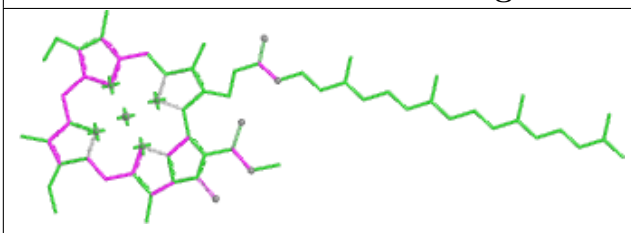


Torsions

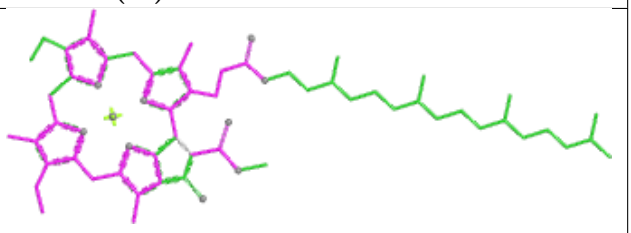


Rings

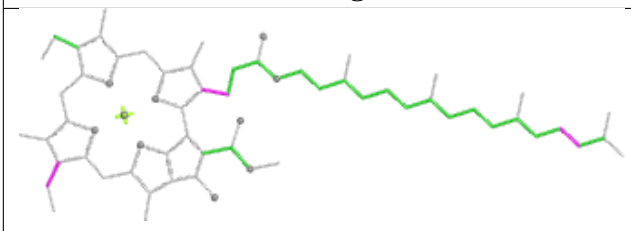
Ligand CLA a 406 (A)



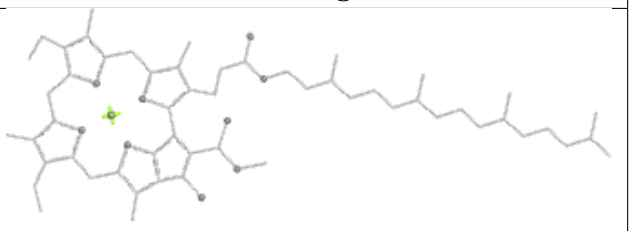
Bond lengths



Bond angles

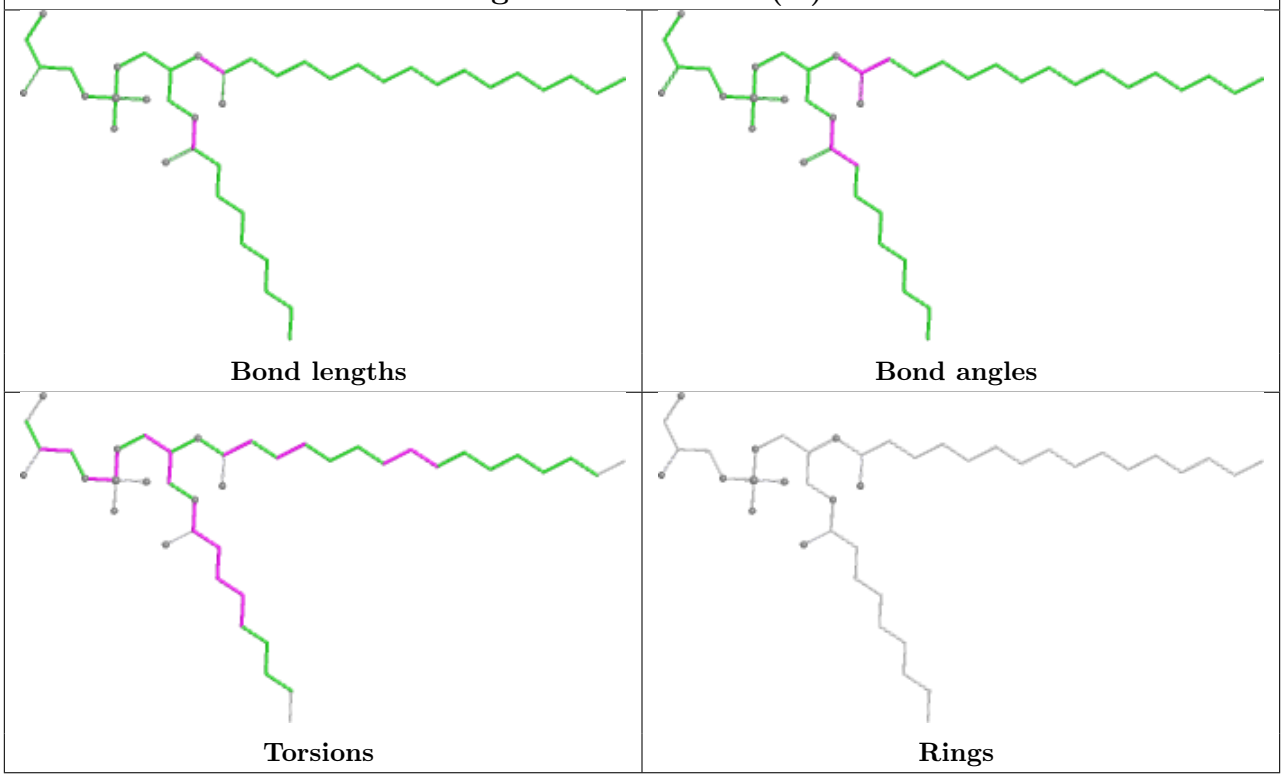


Torsions

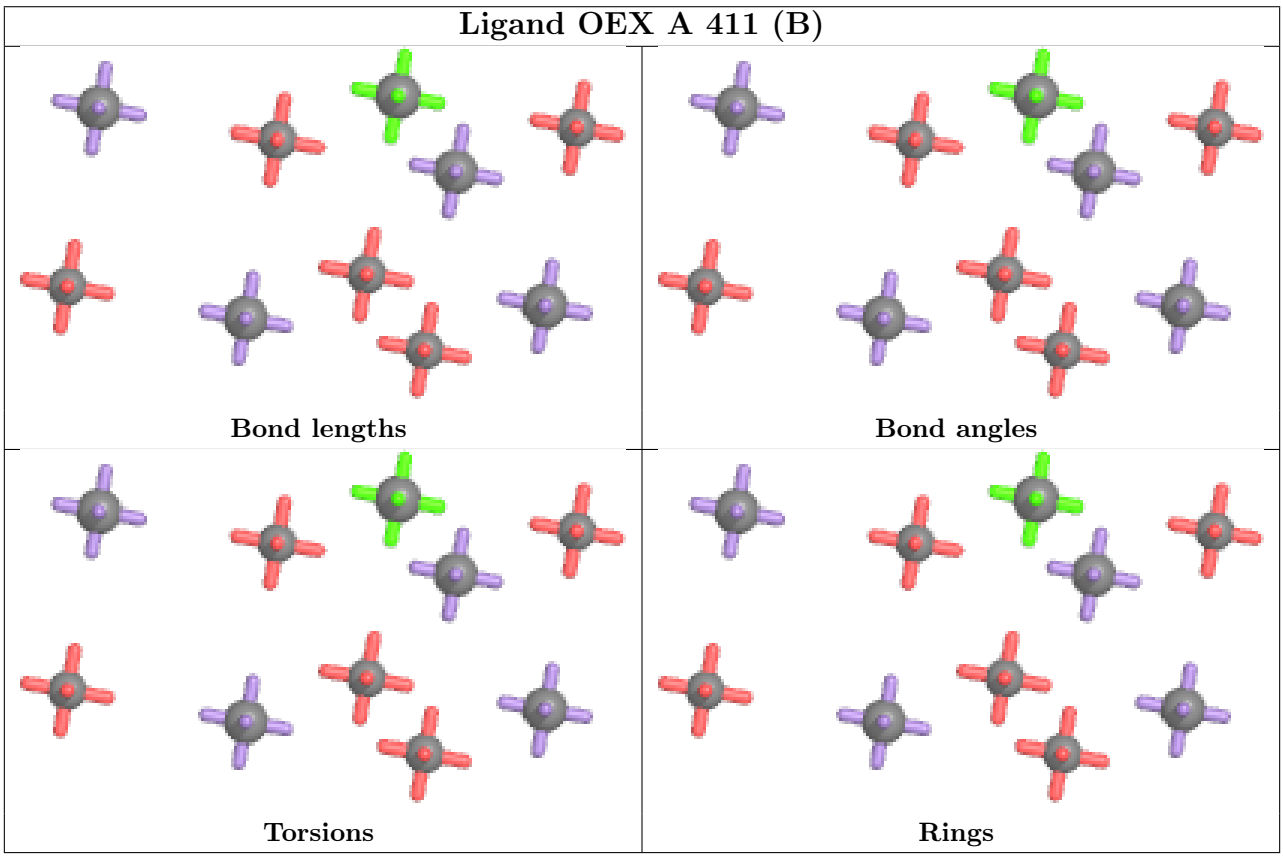


Rings

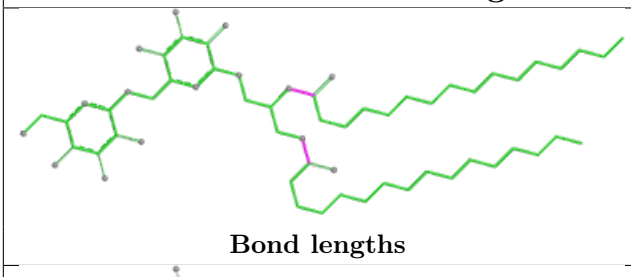
Ligand LHG E 101 (A)



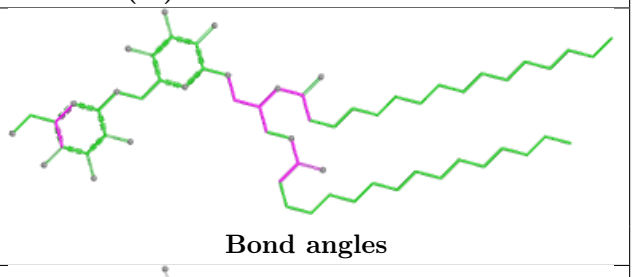
Ligand OEX A 411 (B)



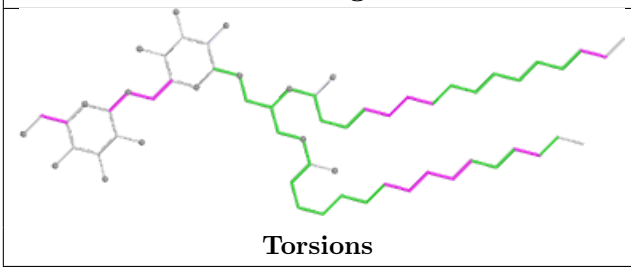
Ligand DGD C 518 (B)



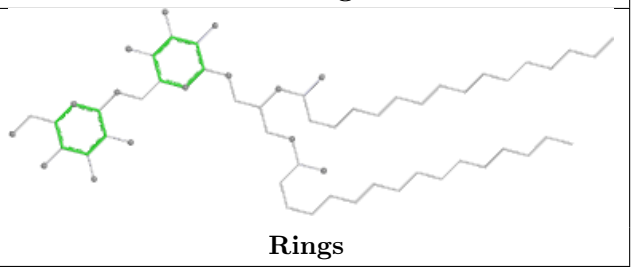
Bond lengths



Bond angles

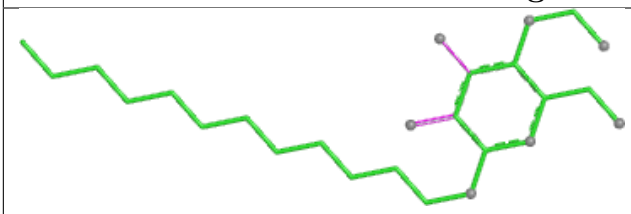


Torsions

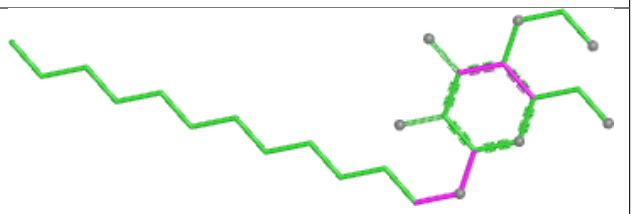


Rings

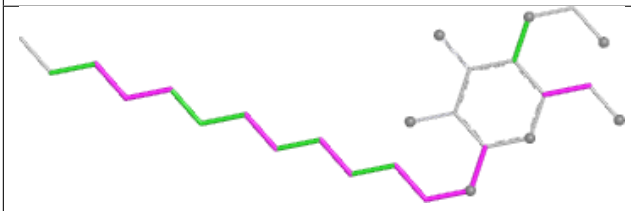
Ligand LMT t 102



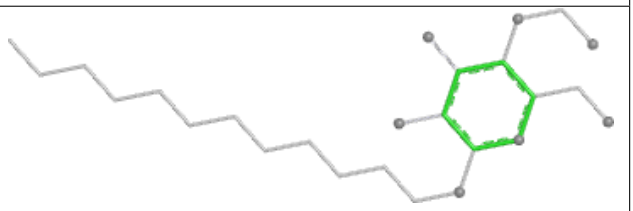
Bond lengths



Bond angles

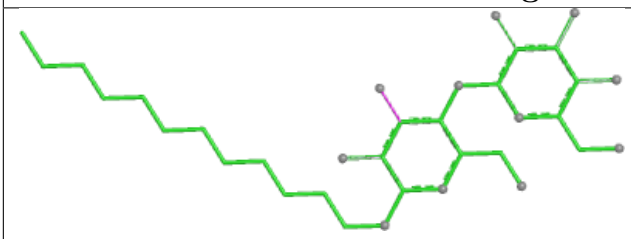


Torsions

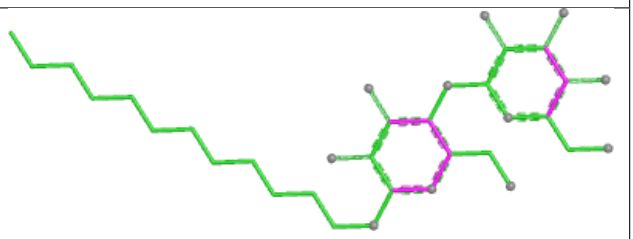


Rings

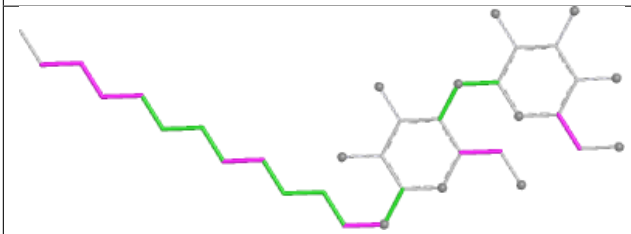
Ligand LMT T 101



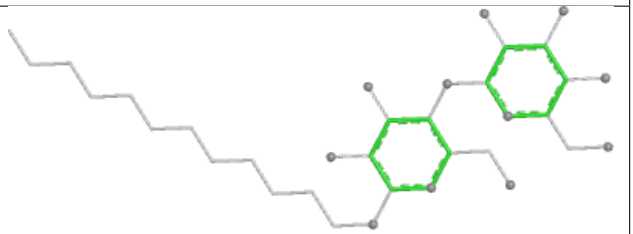
Bond lengths



Bond angles

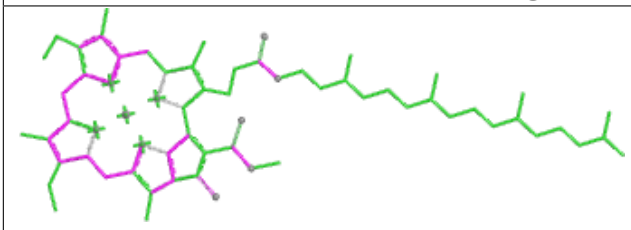


Torsions

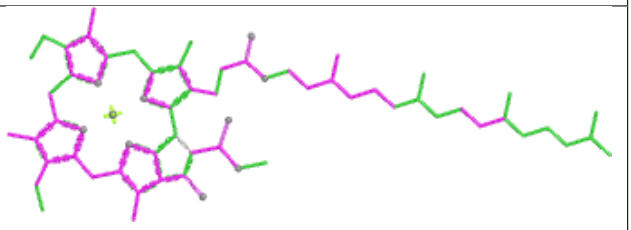


Rings

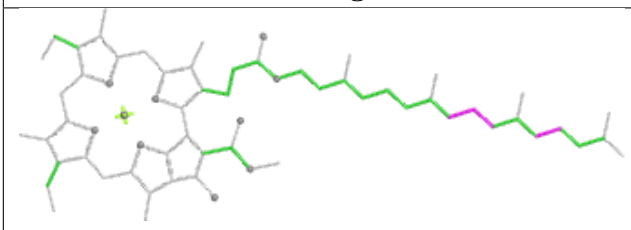
Ligand CLA B 612



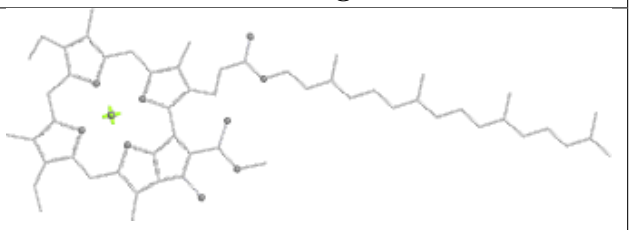
Bond lengths



Bond angles

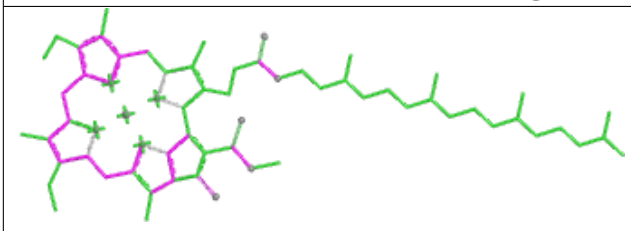


Torsions

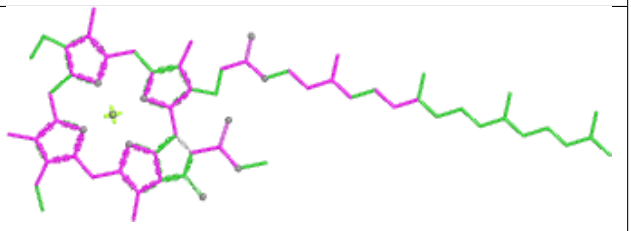


Rings

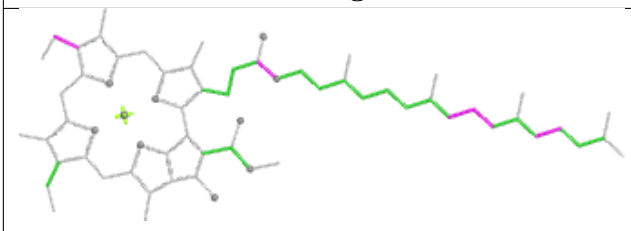
Ligand CLA b 612



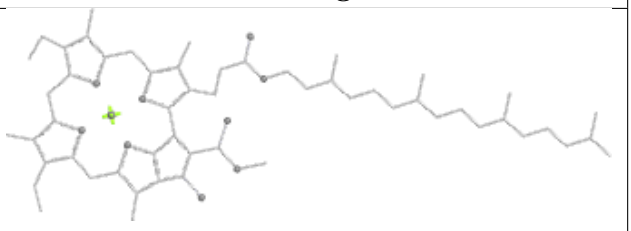
Bond lengths



Bond angles

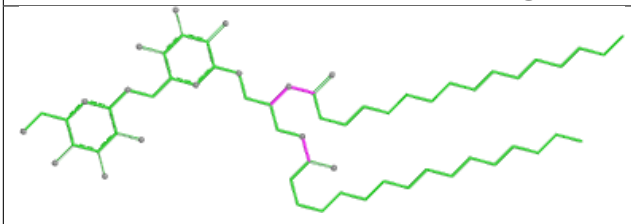


Torsions

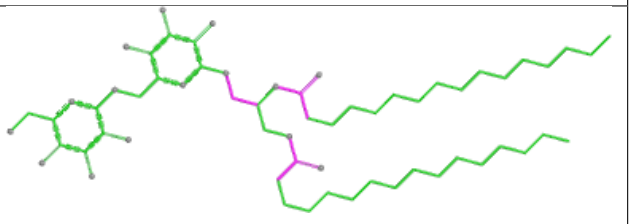


Rings

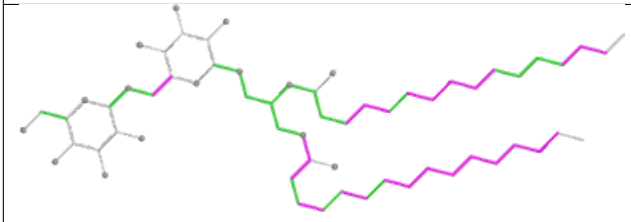
Ligand DGD C 520



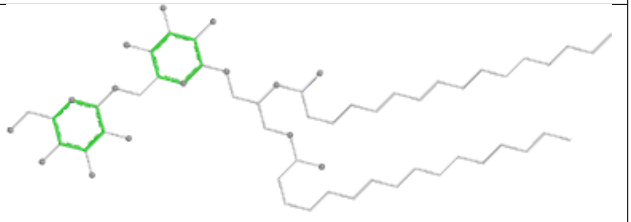
Bond lengths



Bond angles

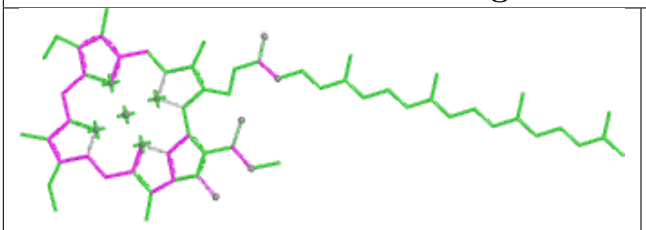


Torsions

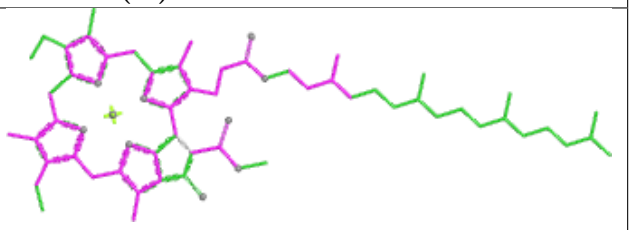


Rings

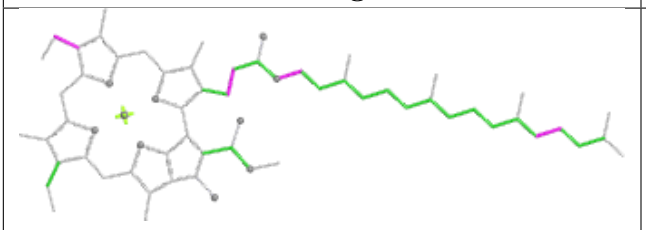
Ligand CLA A 404 (B)



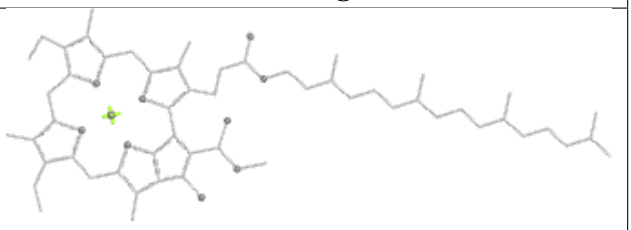
Bond lengths



Bond angles

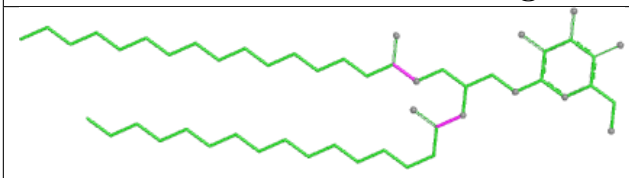


Torsions

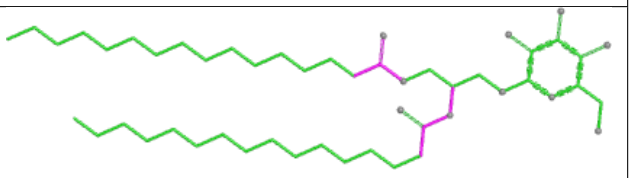


Rings

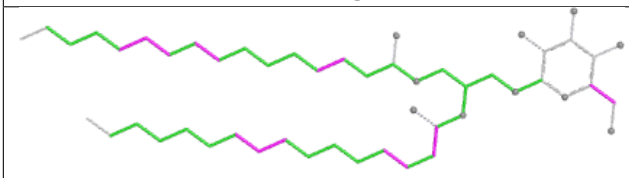
Ligand LMG C 521



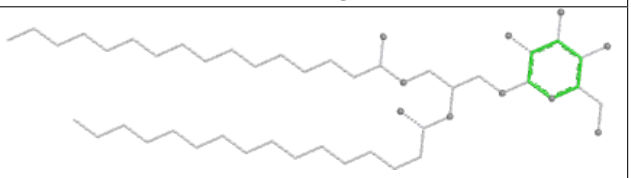
Bond lengths



Bond angles

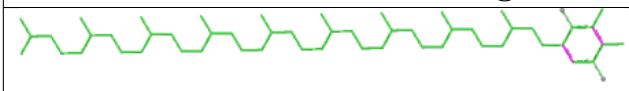


Torsions

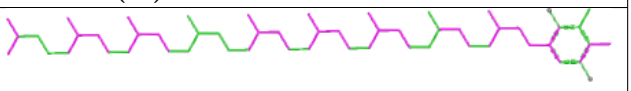


Rings

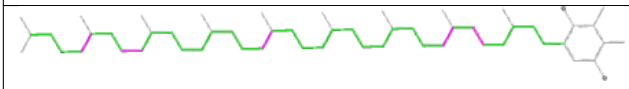
Ligand PL9 D 407 (B)



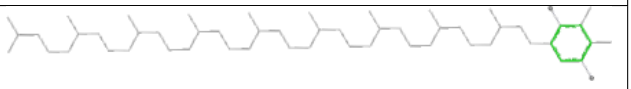
Bond lengths



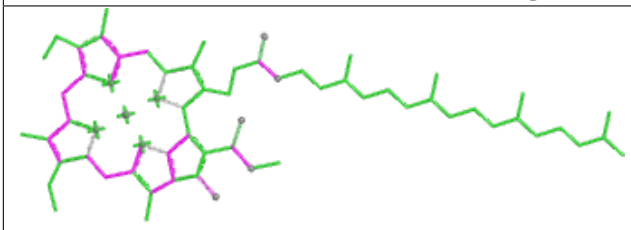
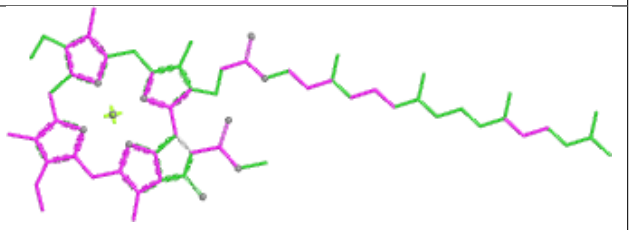
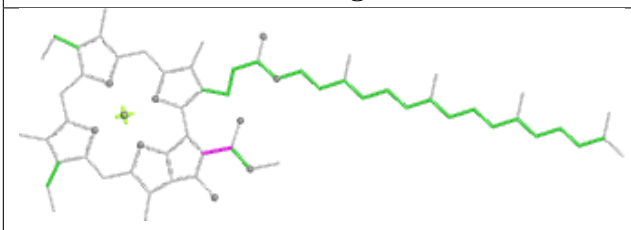
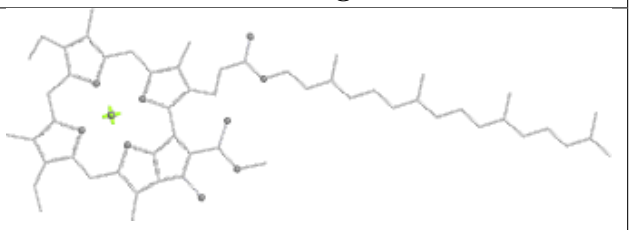
Bond angles

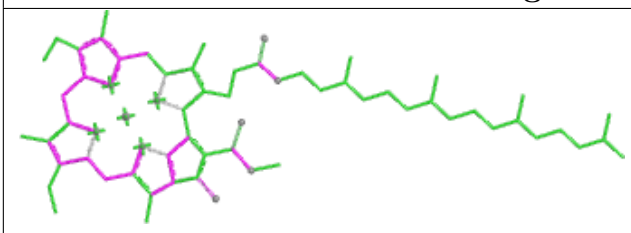
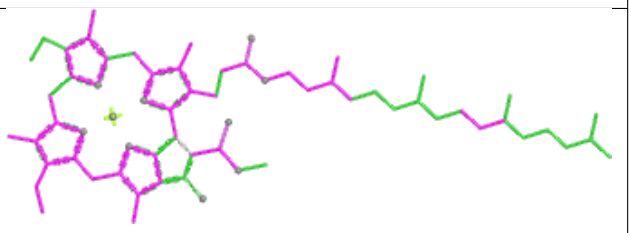
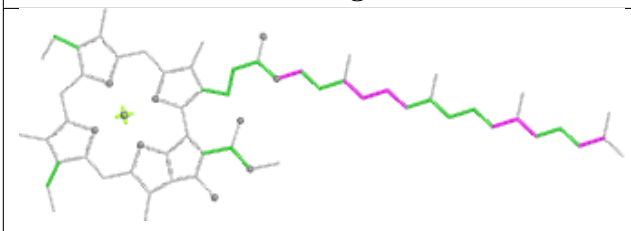
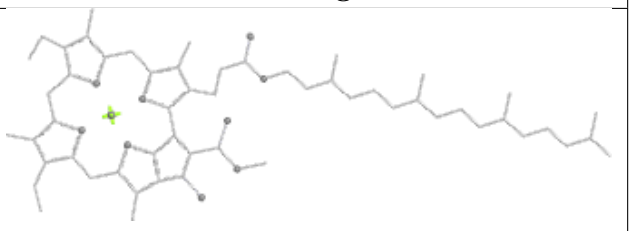


Torsions

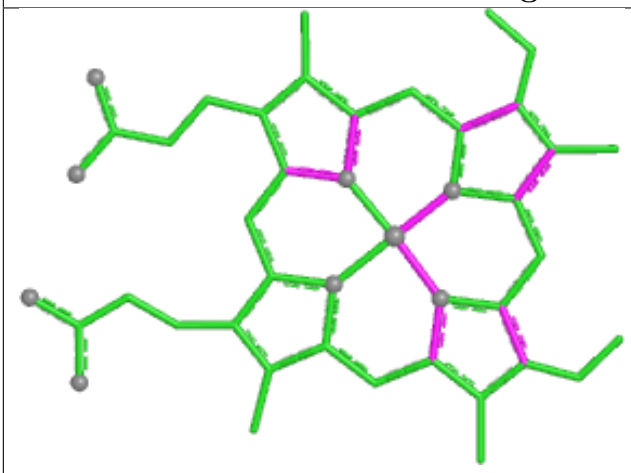


Rings

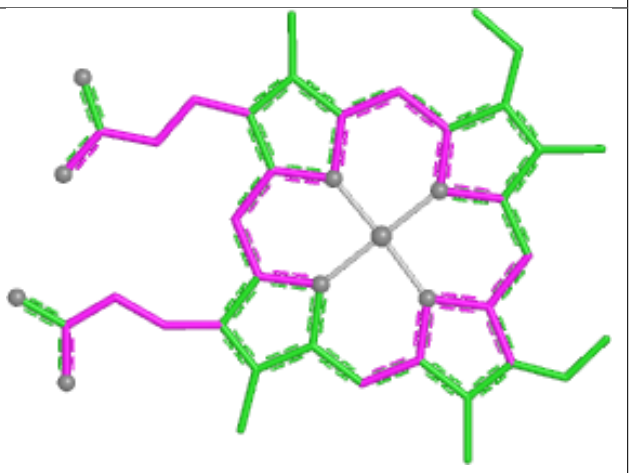
Ligand CLA B 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 407	
 Bond lengths	 Bond angles
 Torsions	 Rings

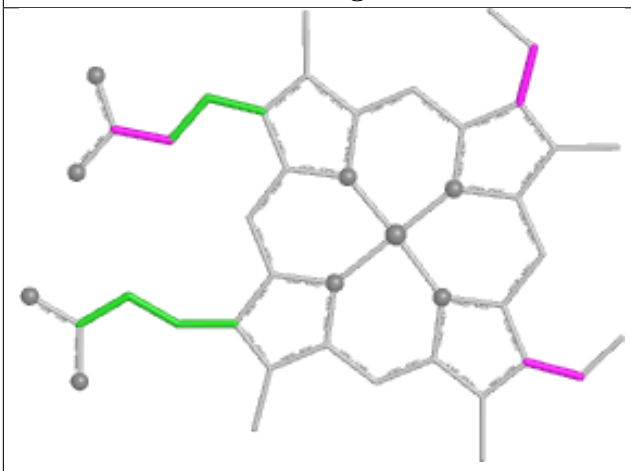
Ligand HEM F 102



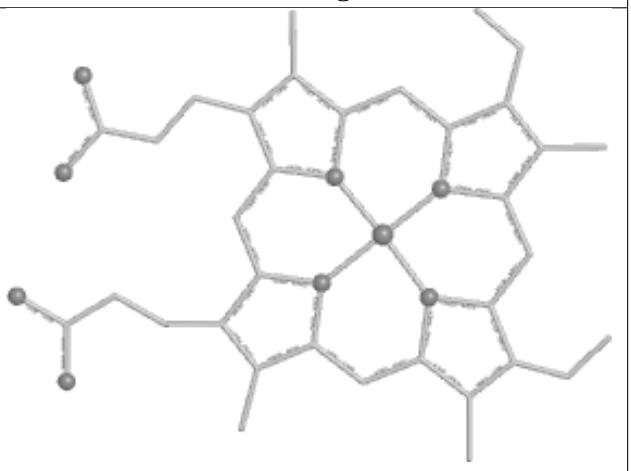
Bond lengths



Bond angles

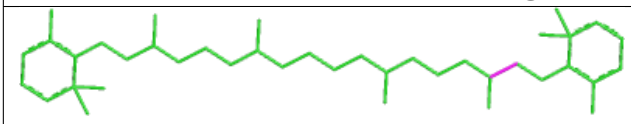


Torsions

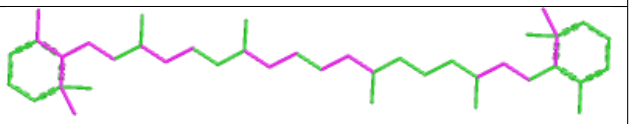


Rings

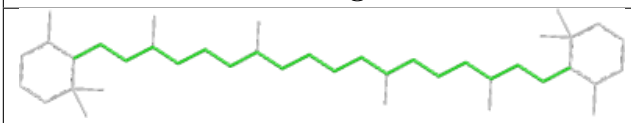
Ligand BCR A 408



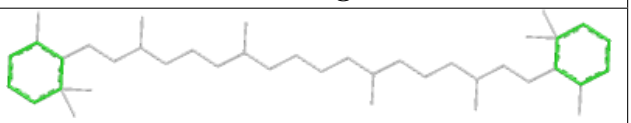
Bond lengths



Bond angles

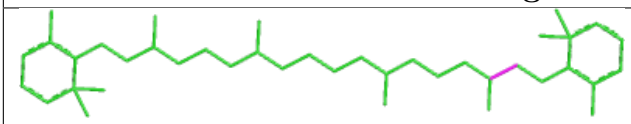


Torsions

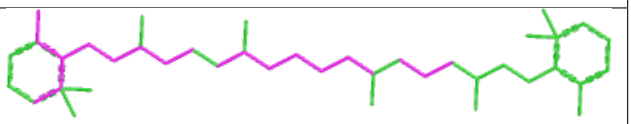


Rings

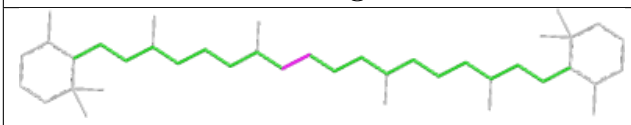
Ligand BCR T 102



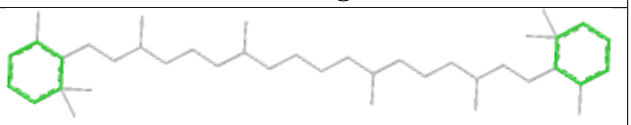
Bond lengths



Bond angles

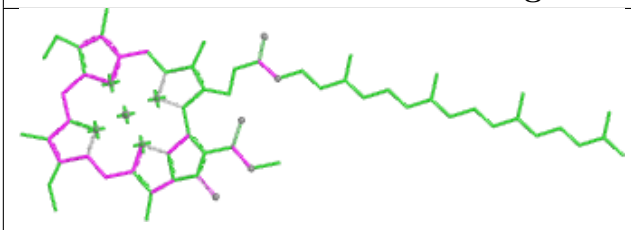


Torsions

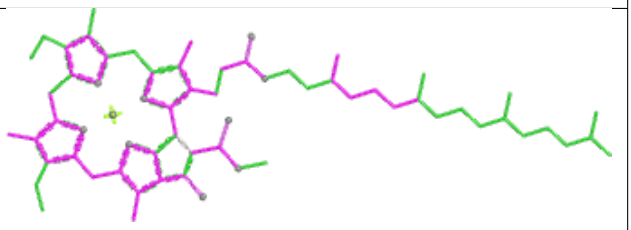


Rings

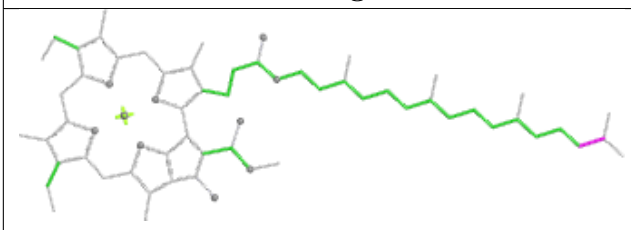
Ligand CLA B 603



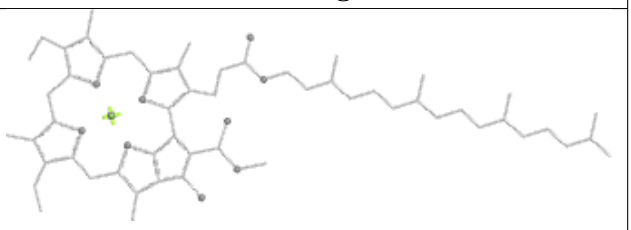
Bond lengths



Bond angles

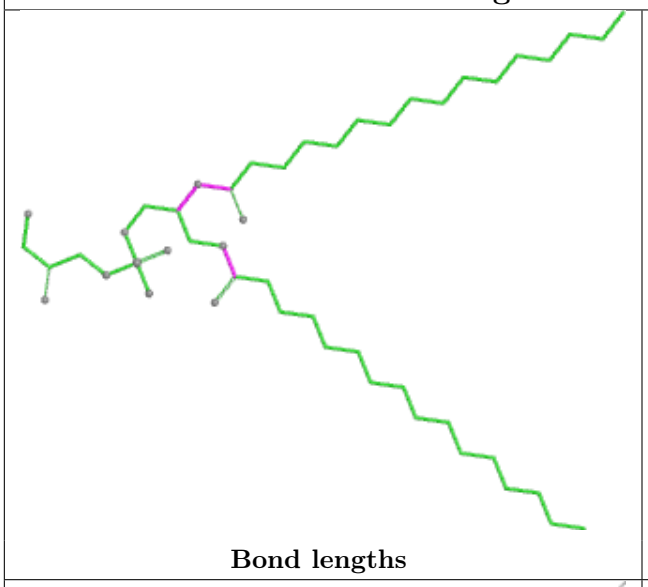


Torsions

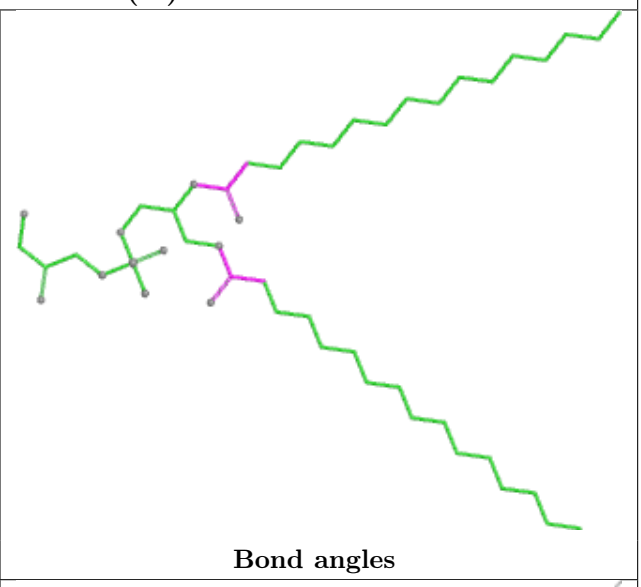


Rings

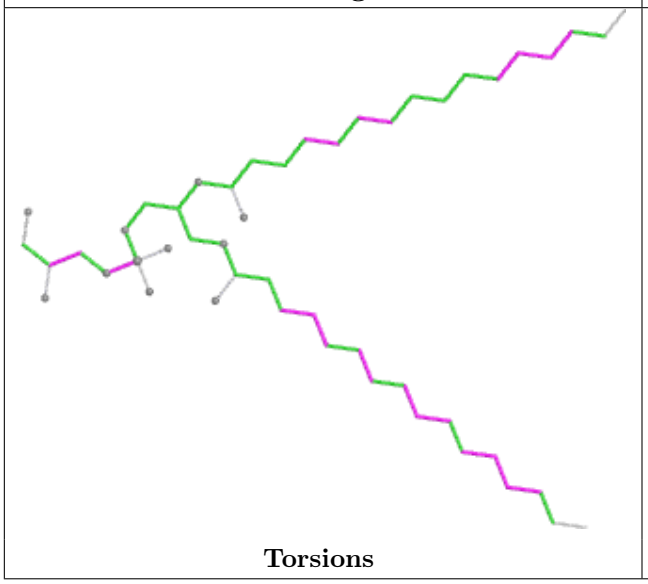
Ligand LHG d 411 (A)



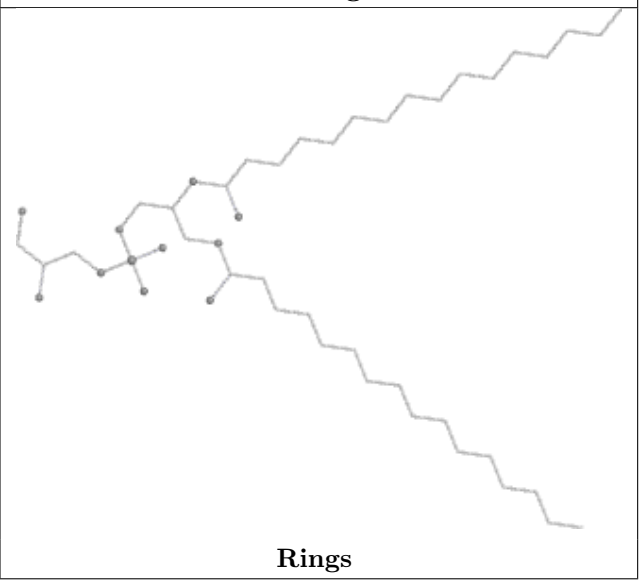
Bond lengths



Bond angles



Torsions



Rings

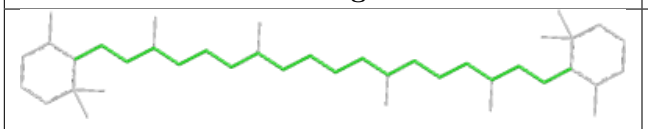
Ligand BCR k 101



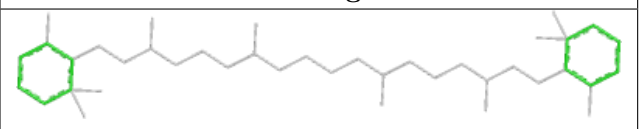
Bond lengths



Bond angles

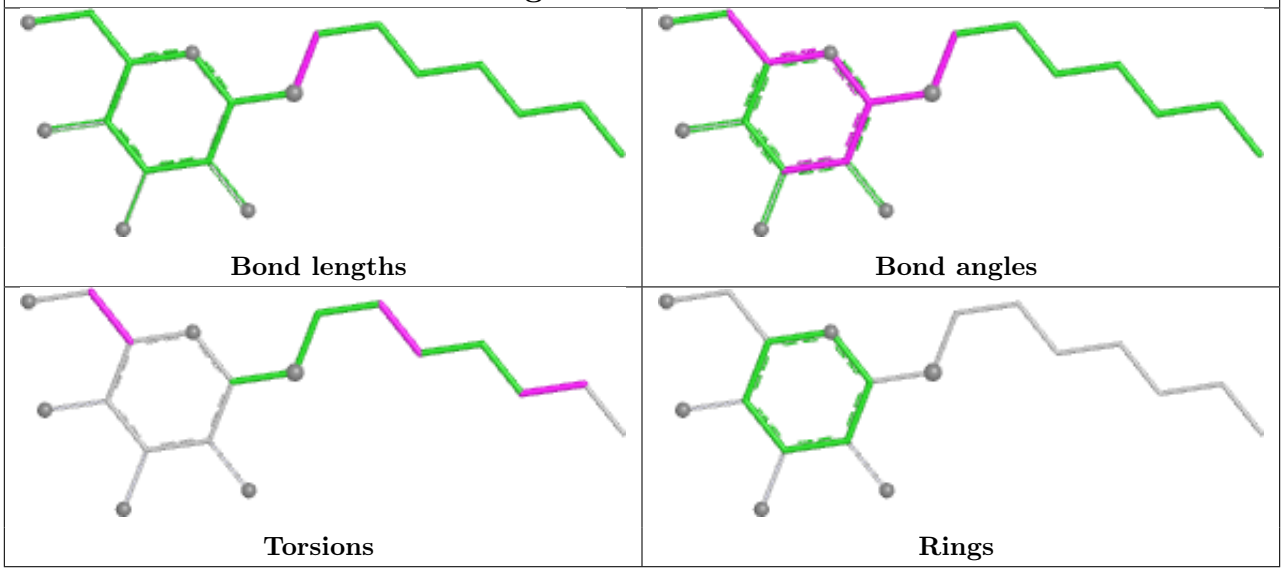


Torsions

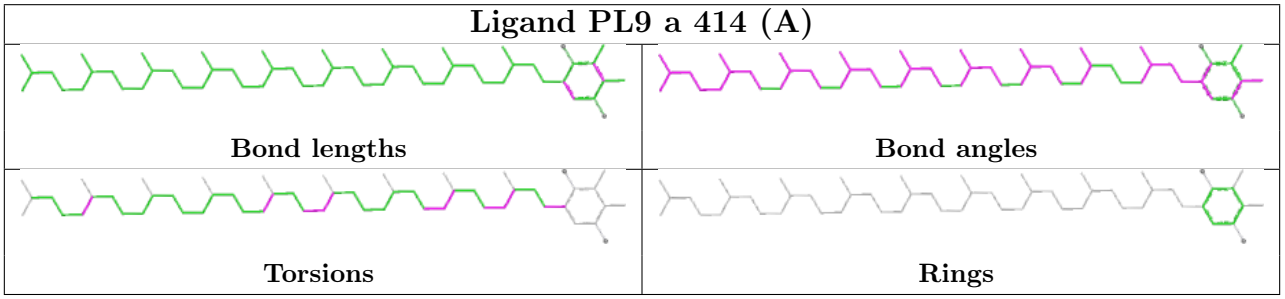


Rings

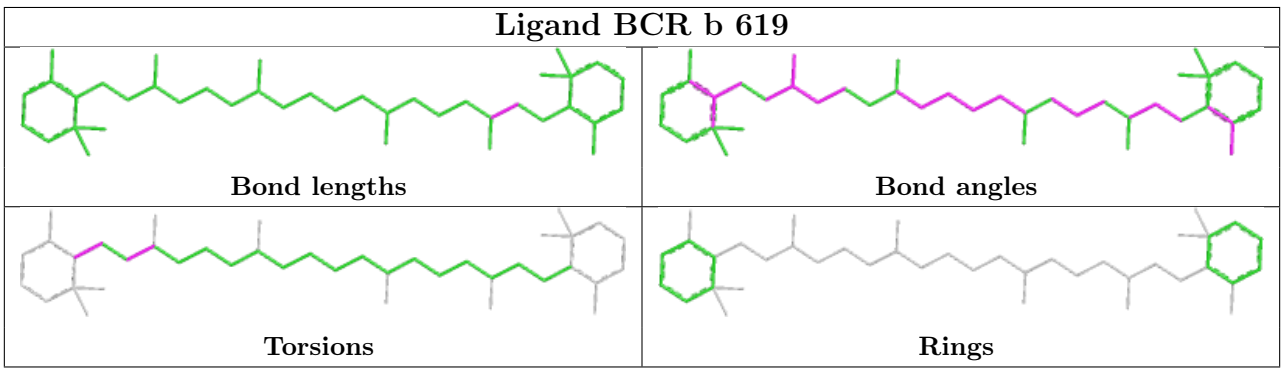
Ligand HTG b 623

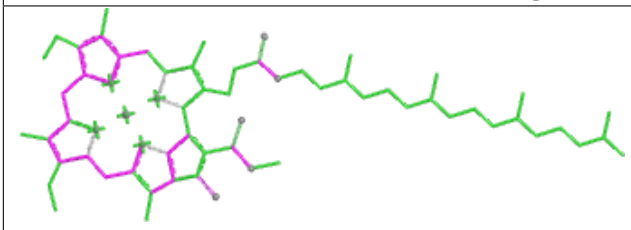
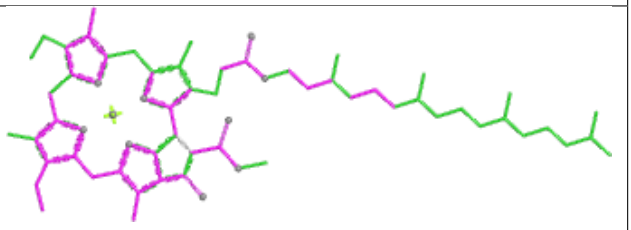
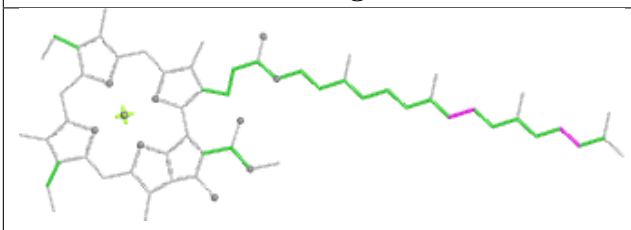
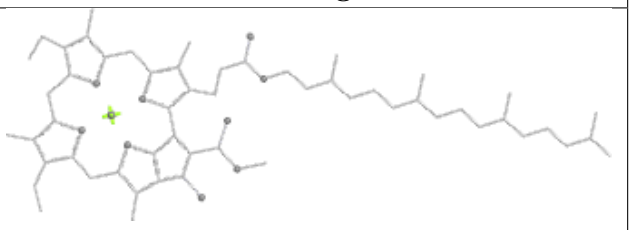


Ligand PL9 a 414 (A)

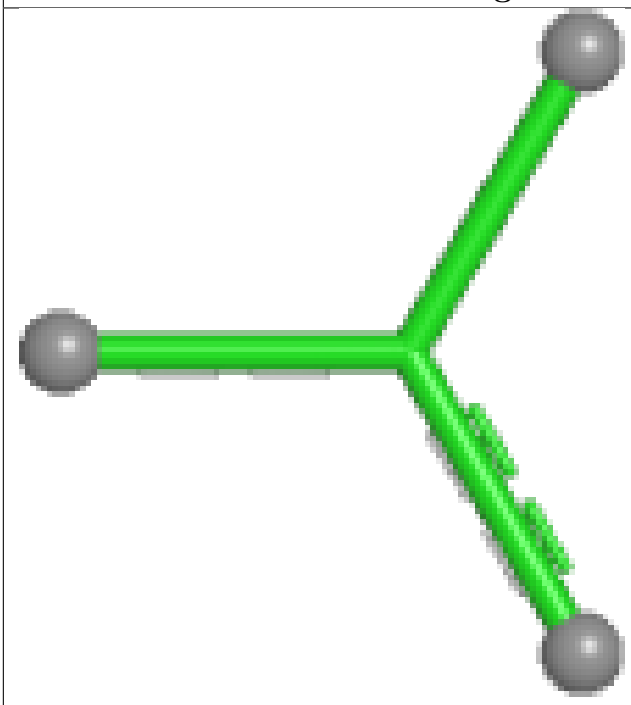


Ligand BCR b 619

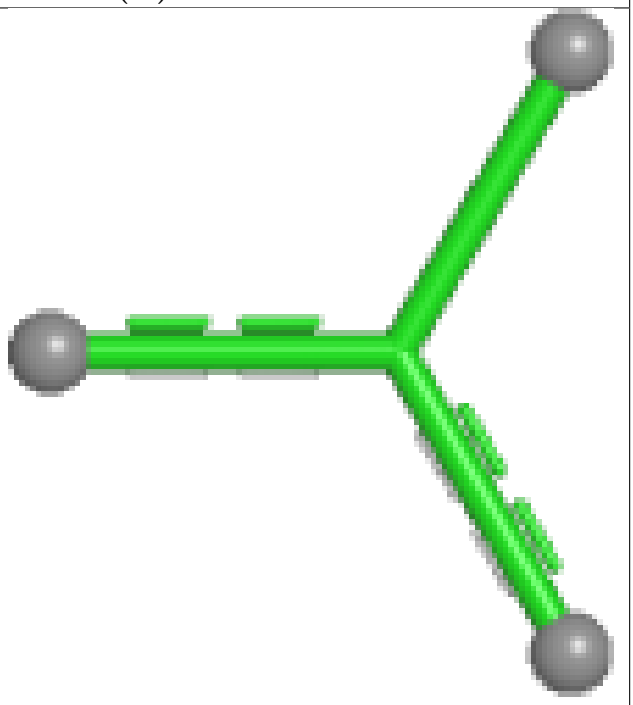


Ligand CLA b 611	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

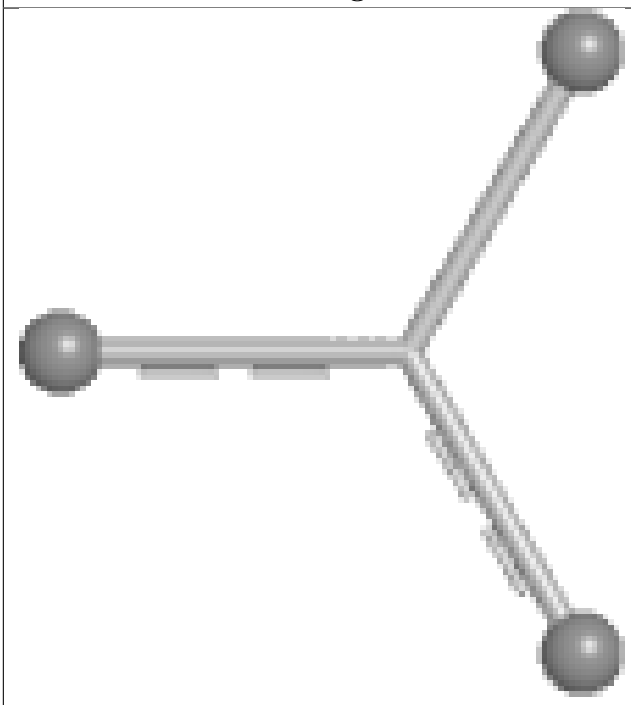
Ligand BCT a 404 (A)



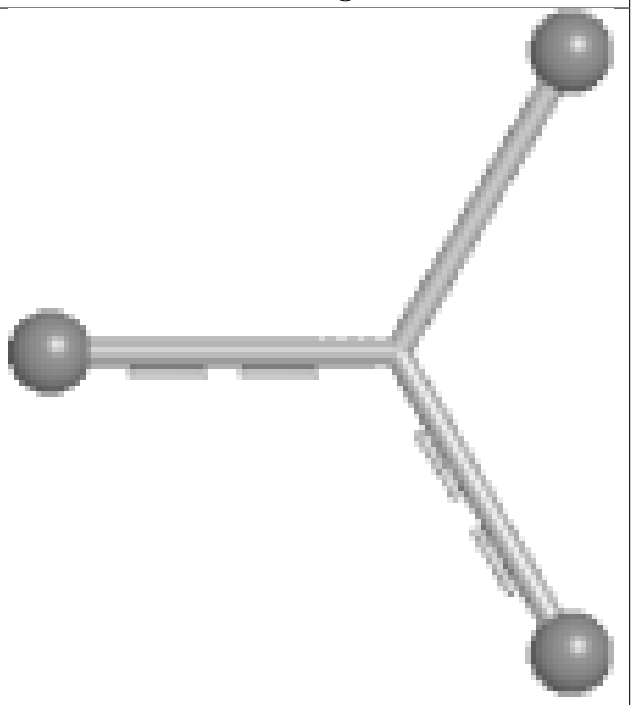
Bond lengths



Bond angles

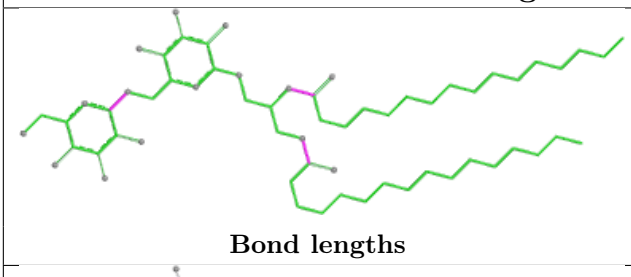


Torsions

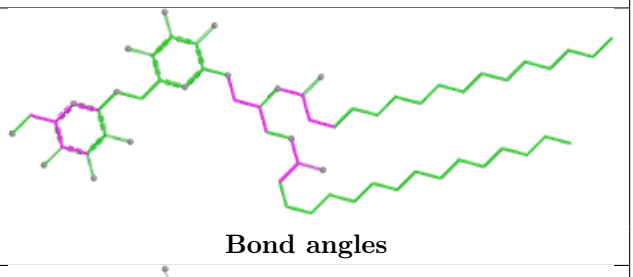


Rings

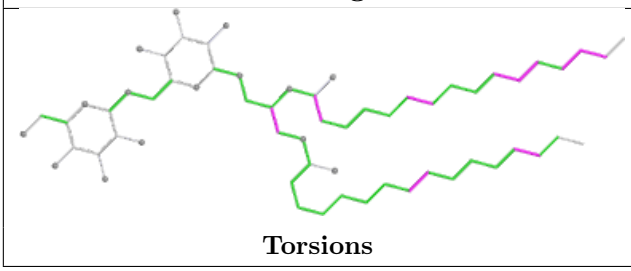
Ligand DGD H 102



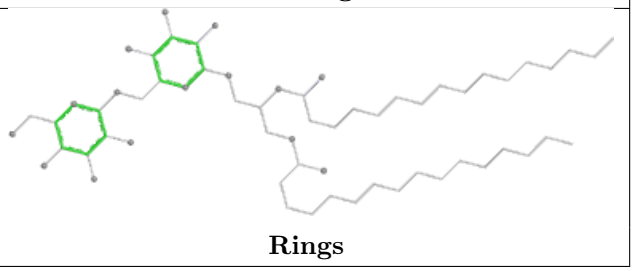
Bond lengths



Bond angles

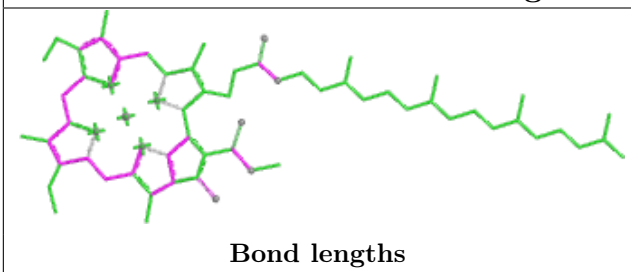


Torsions

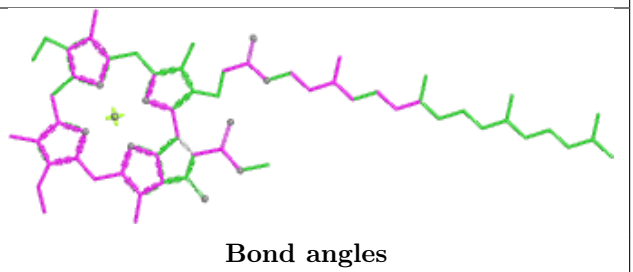


Rings

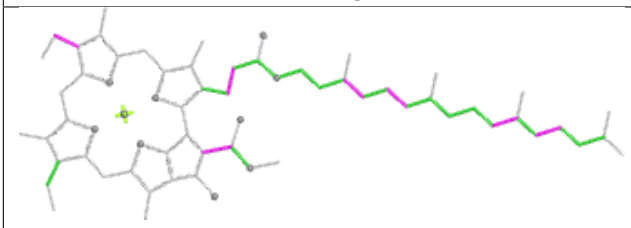
Ligand CLA C 509



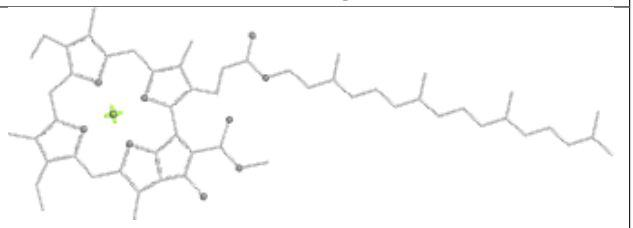
Bond lengths



Bond angles

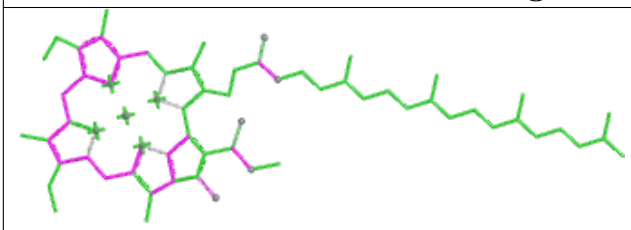


Torsions

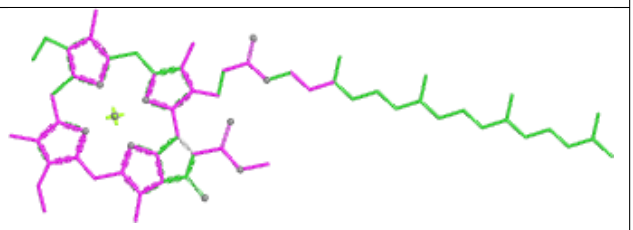


Rings

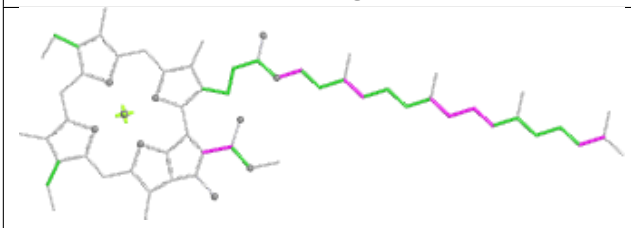
Ligand CLA b 614



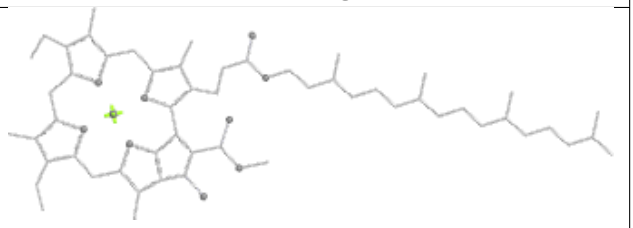
Bond lengths



Bond angles

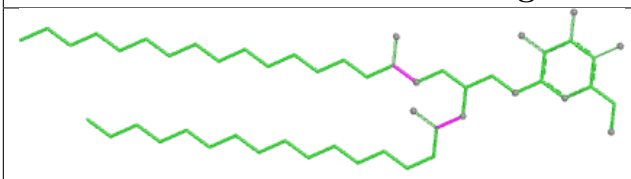


Torsions

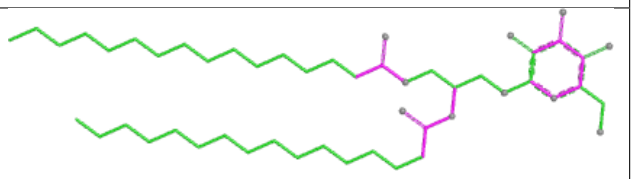


Rings

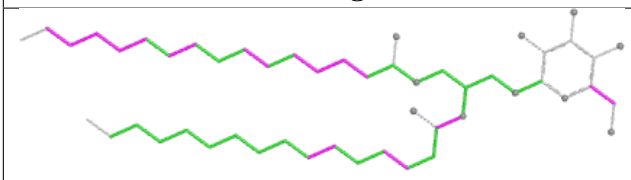
Ligand LMG m 101



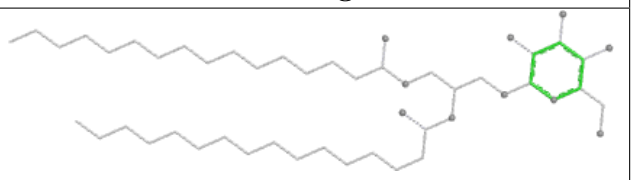
Bond lengths



Bond angles

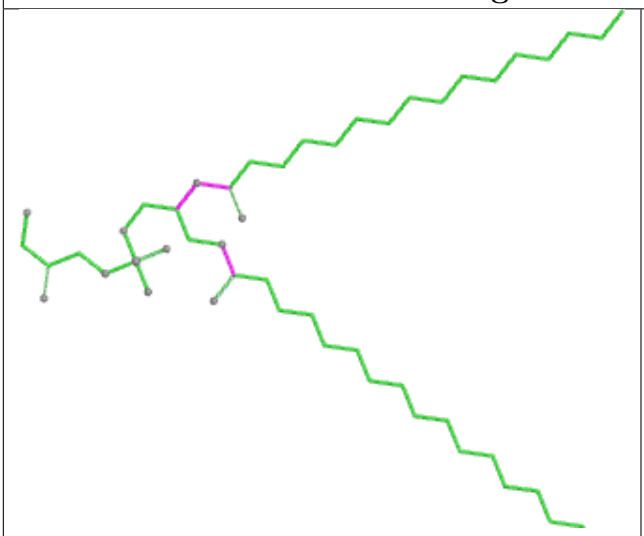


Torsions

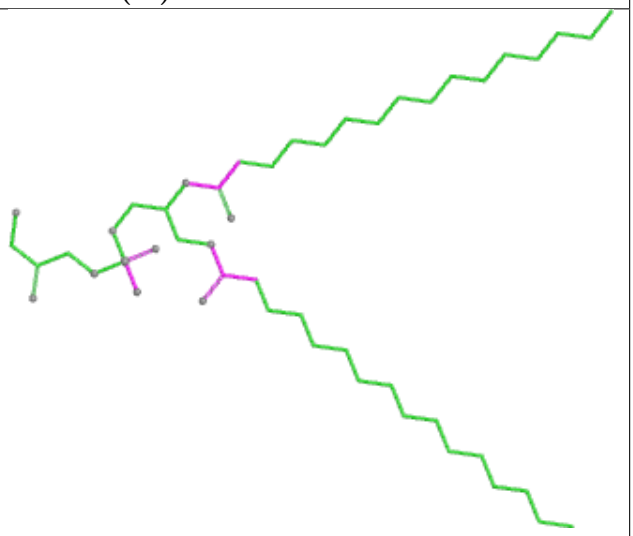


Rings

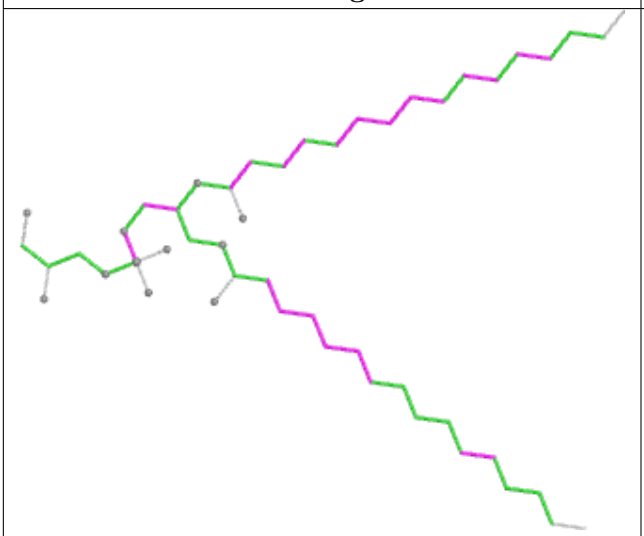
Ligand LHG L 101 (A)



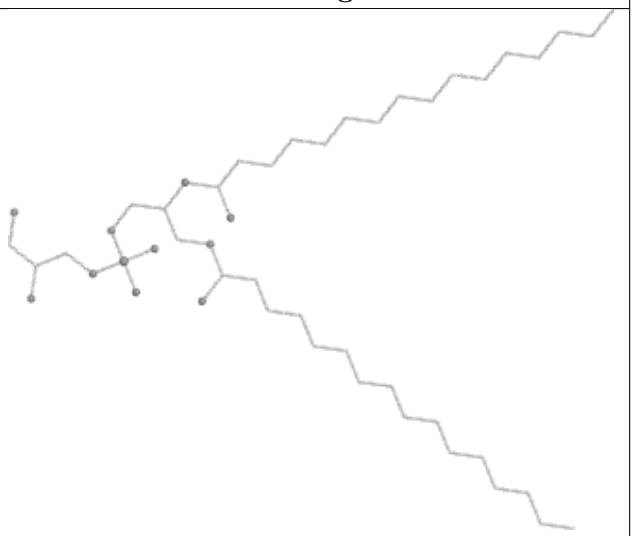
Bond lengths



Bond angles

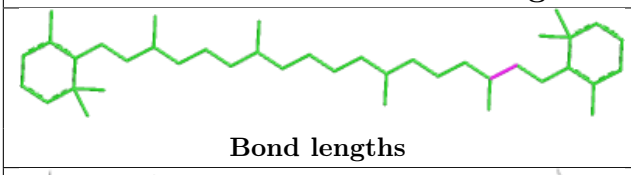


Torsions

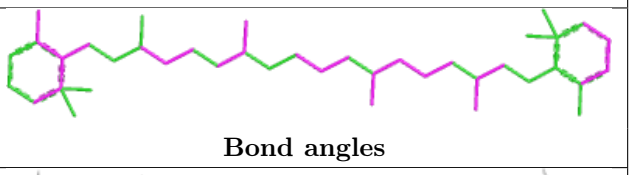


Rings

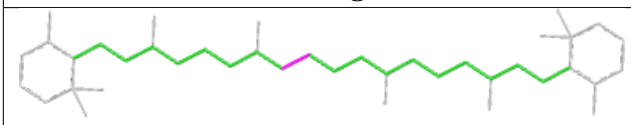
Ligand BCR t 103



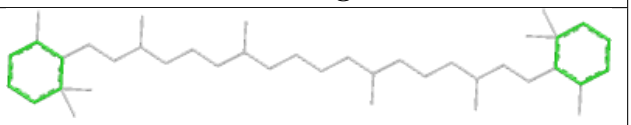
Bond lengths



Bond angles

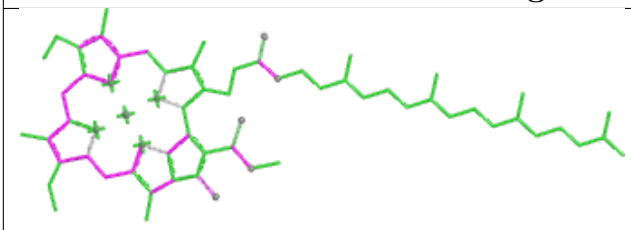


Torsions

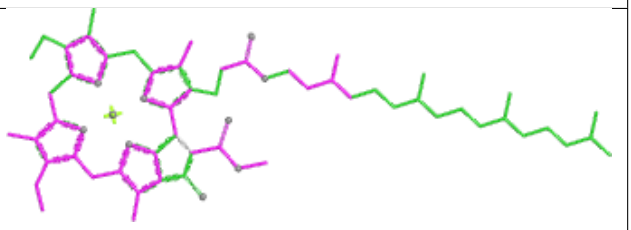


Rings

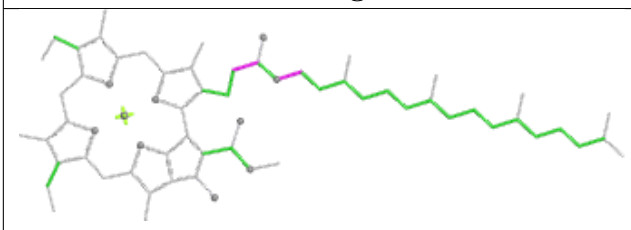
Ligand CLA b 613



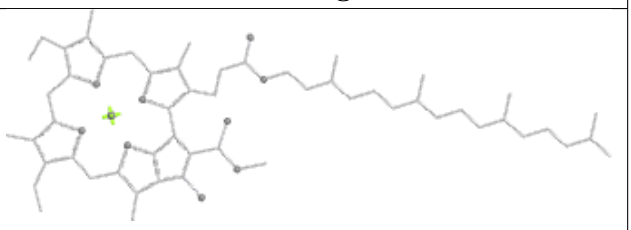
Bond lengths



Bond angles

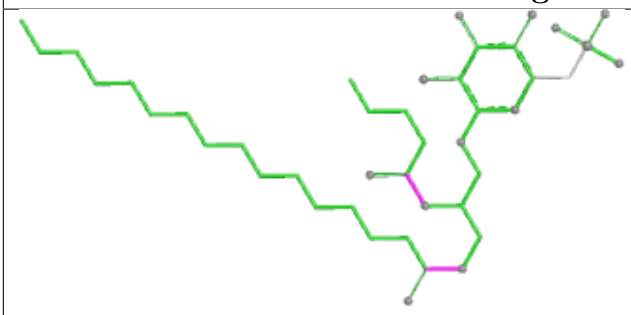


Torsions

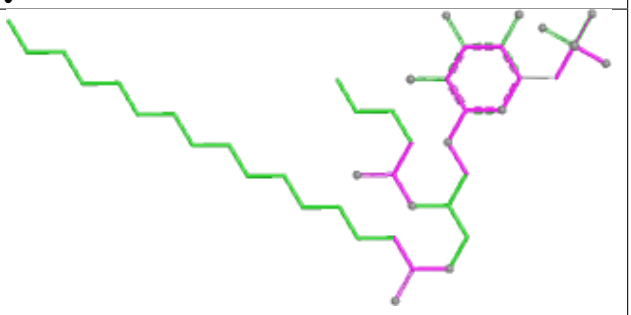


Rings

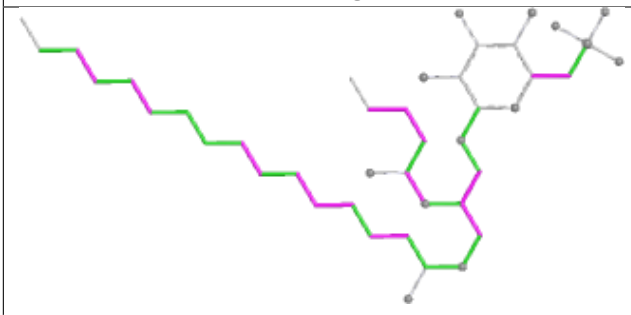
Ligand SQD f 102



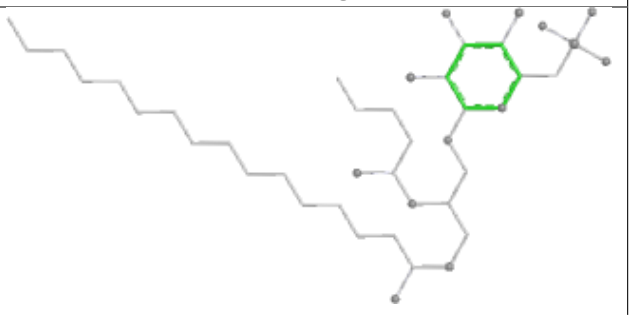
Bond lengths



Bond angles

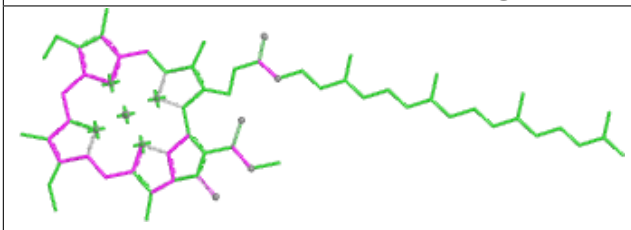


Torsions

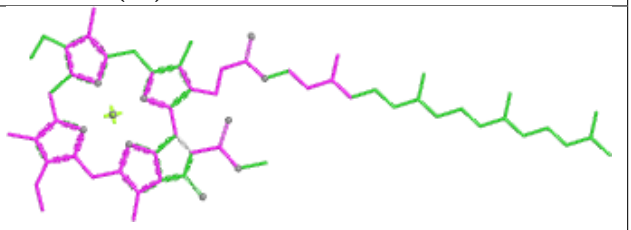


Rings

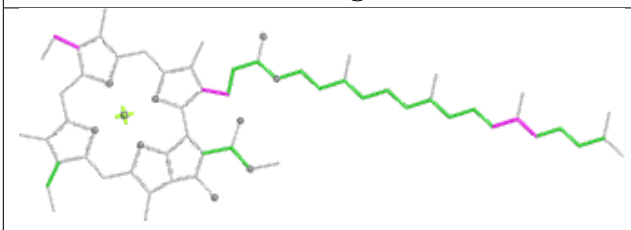
Ligand CLA a 407 (A)



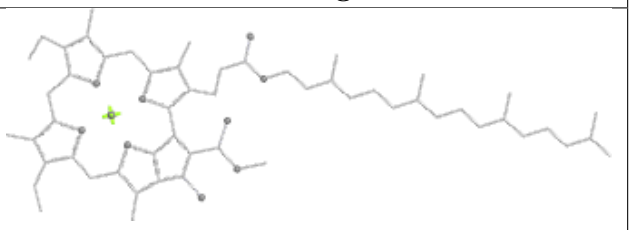
Bond lengths



Bond angles

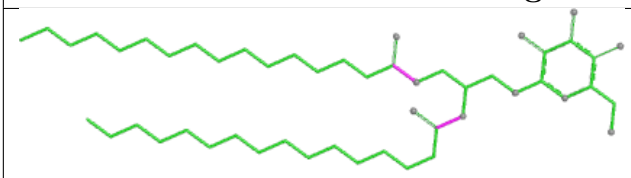


Torsions

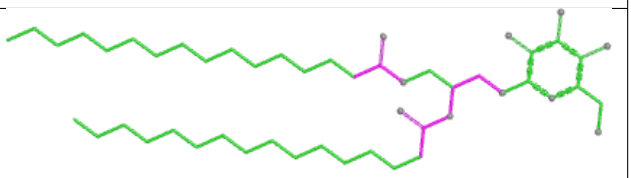


Rings

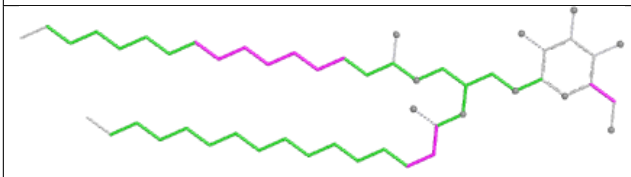
Ligand LMG c 520



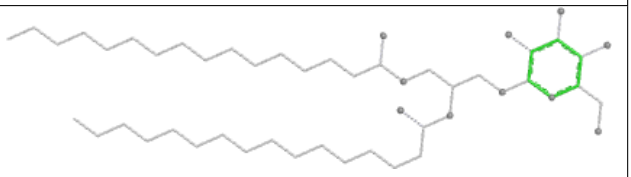
Bond lengths



Bond angles

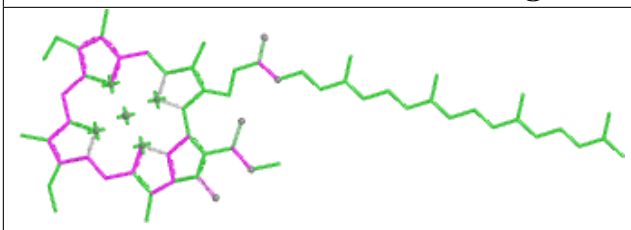


Torsions

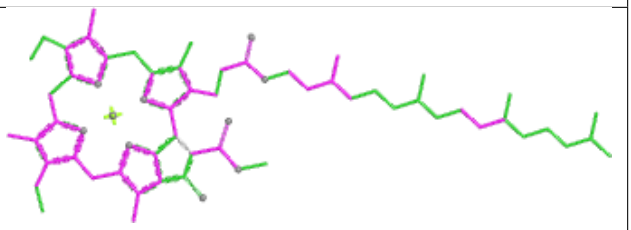


Rings

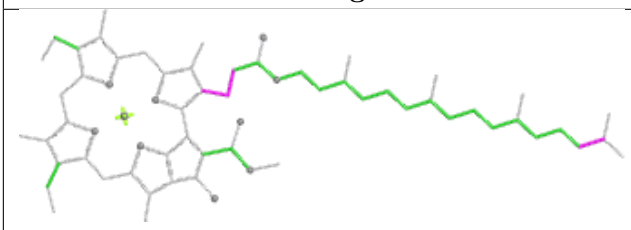
Ligand CLA C 503



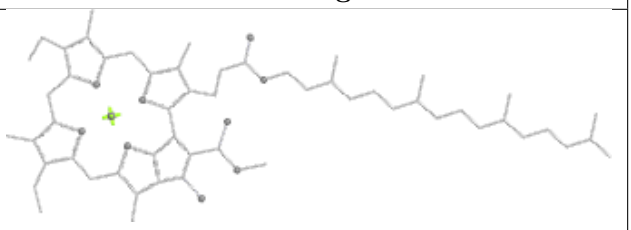
Bond lengths



Bond angles

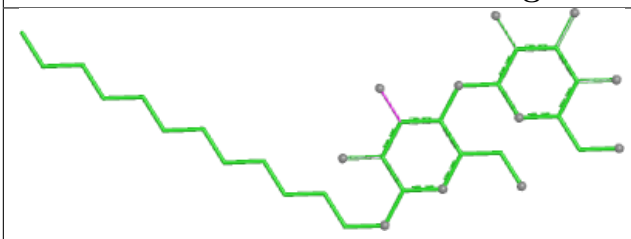


Torsions

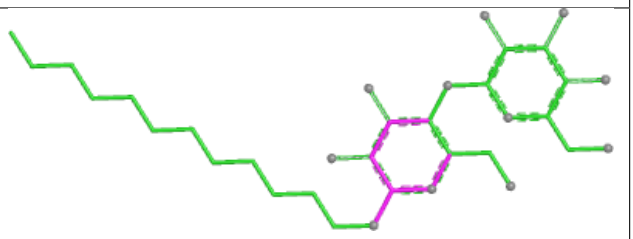


Rings

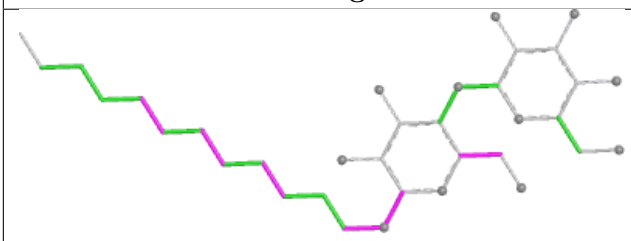
Ligand LMT F 101



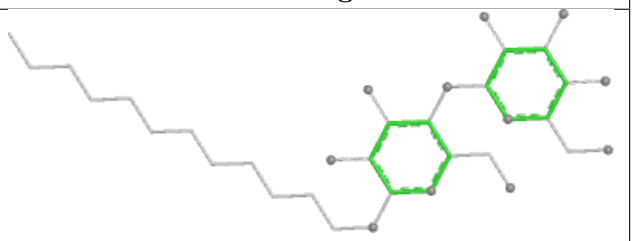
Bond lengths



Bond angles

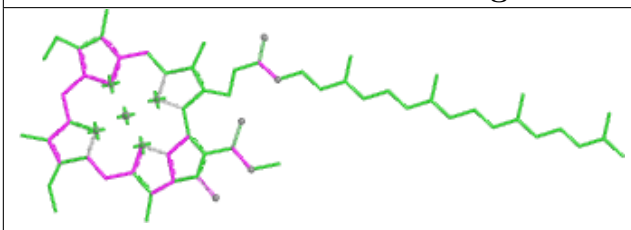


Torsions

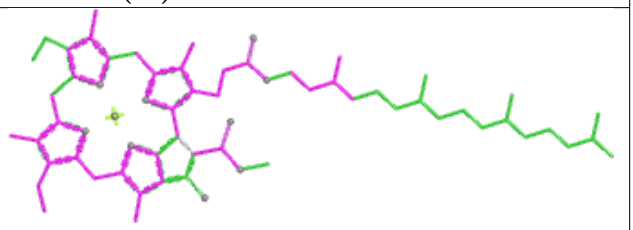


Rings

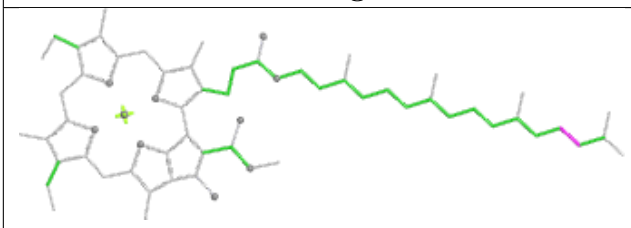
Ligand CLA A 405 (A)



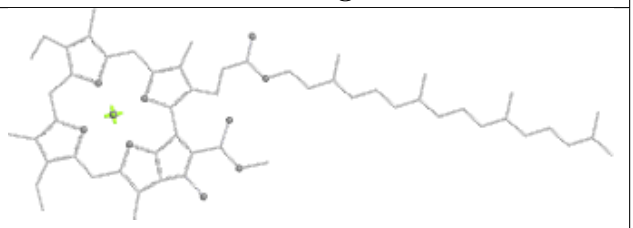
Bond lengths



Bond angles

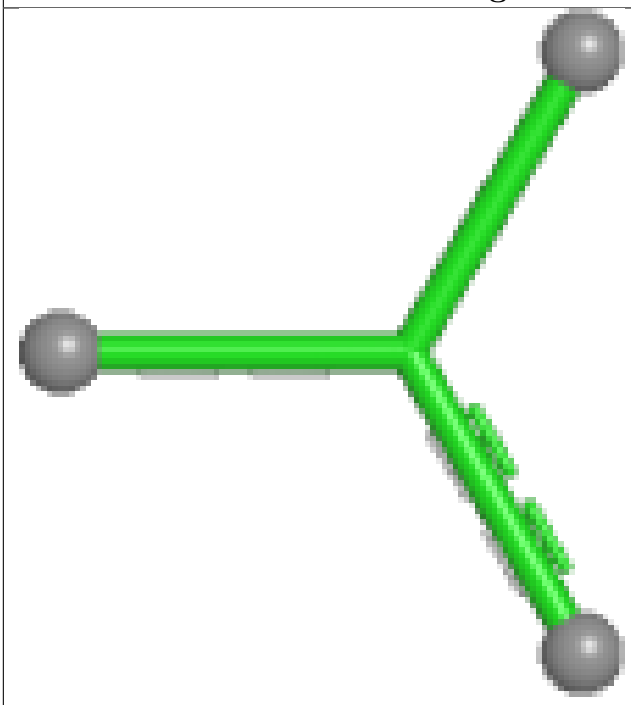


Torsions

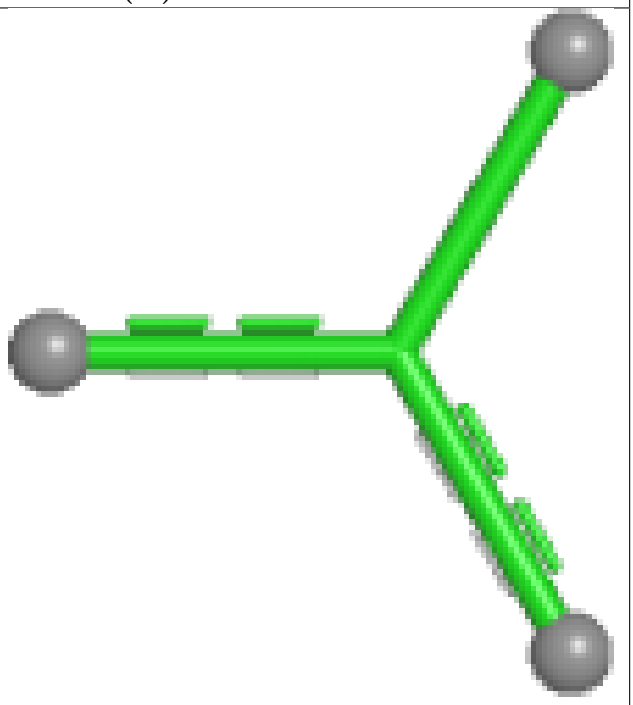


Rings

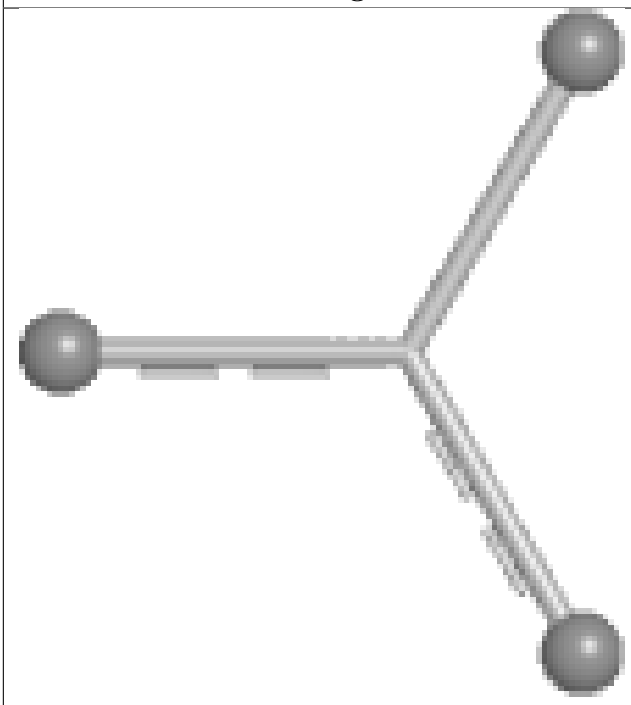
Ligand BCT A 414 (A)



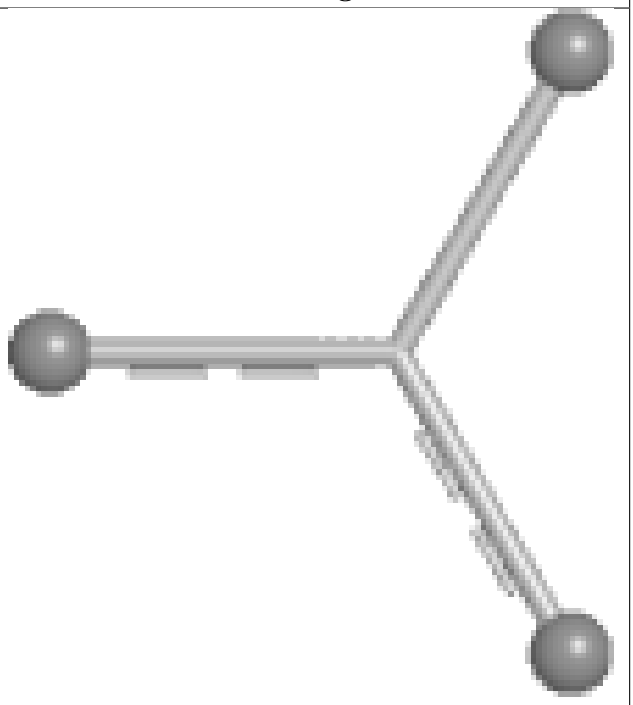
Bond lengths



Bond angles

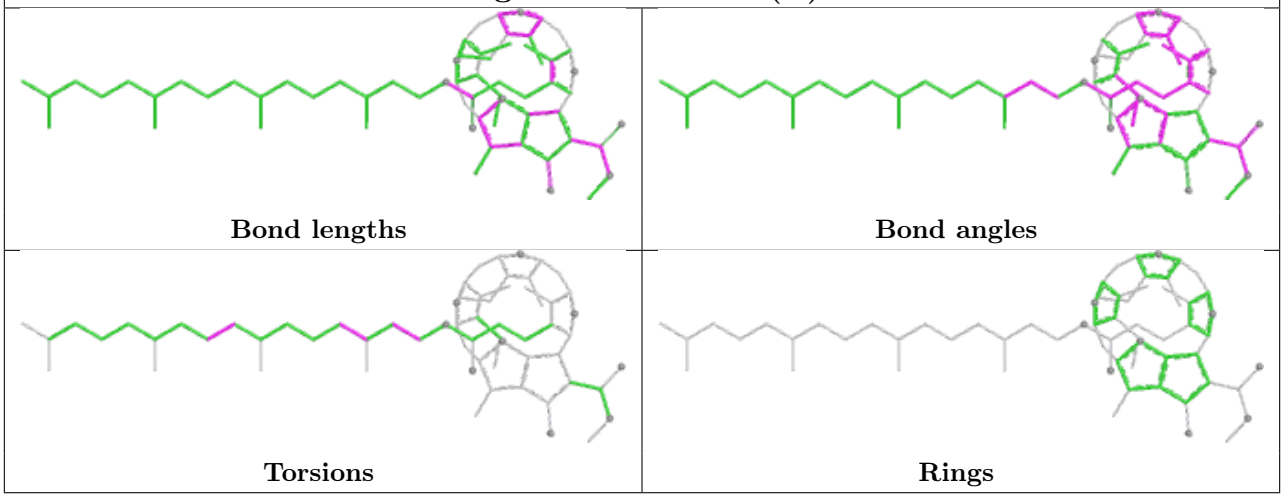


Torsions

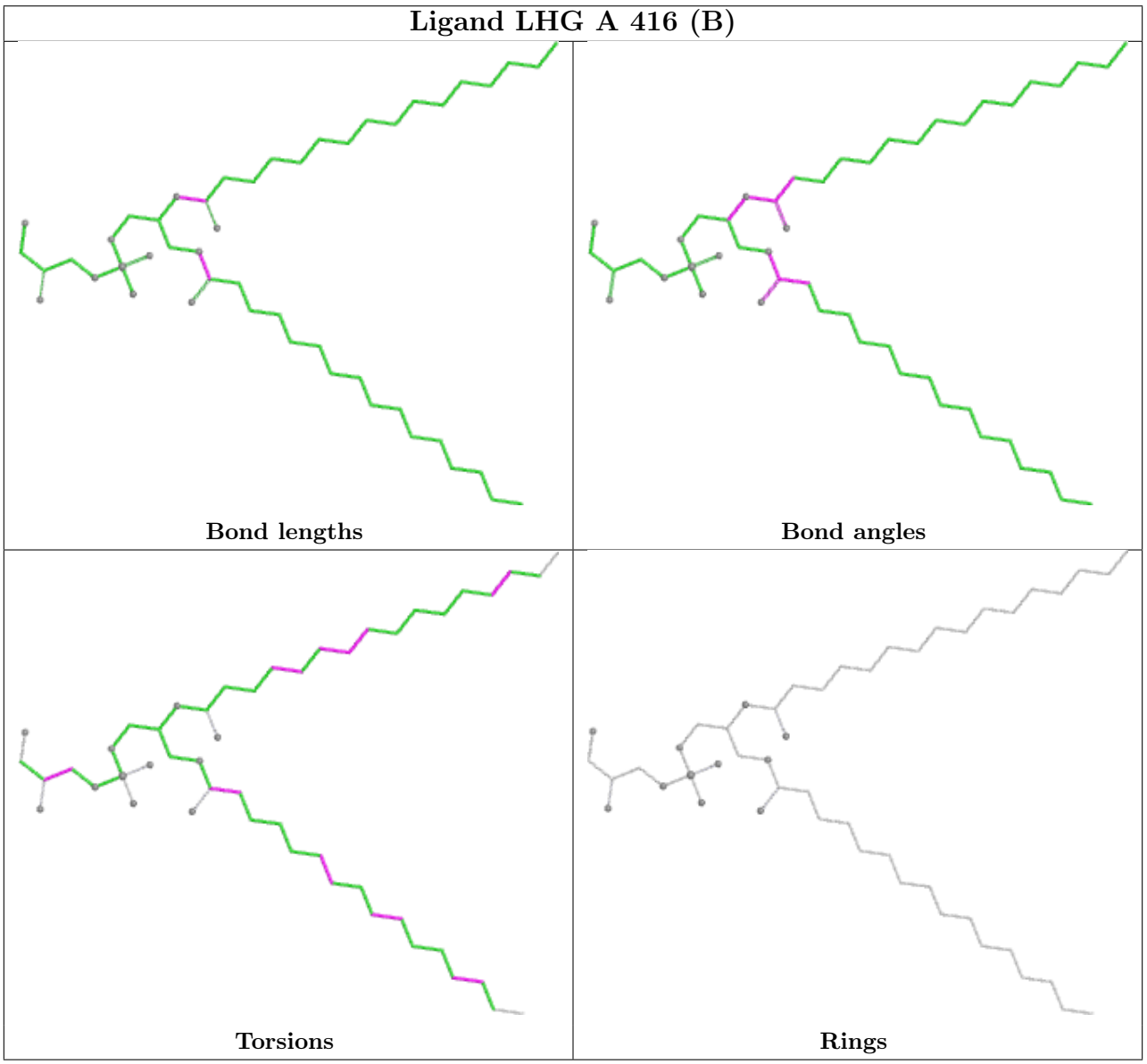


Rings

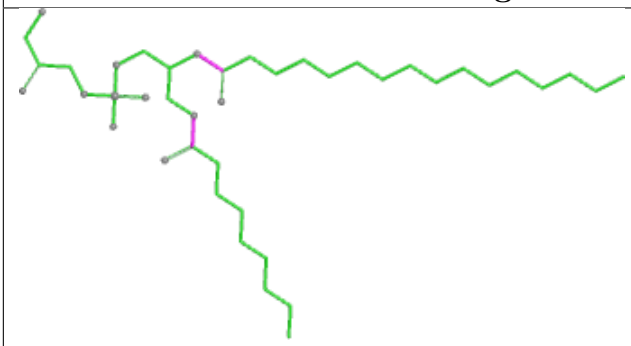
Ligand PHO a 408 (B)



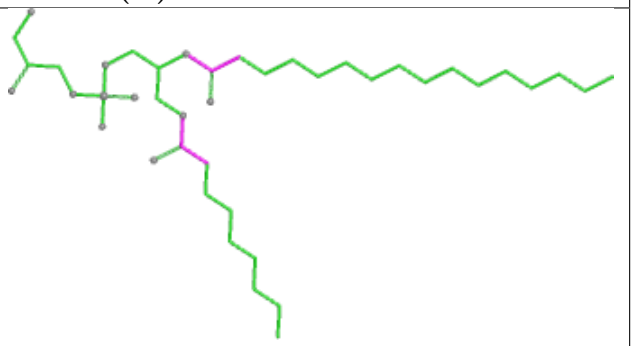
Ligand LHG A 416 (B)



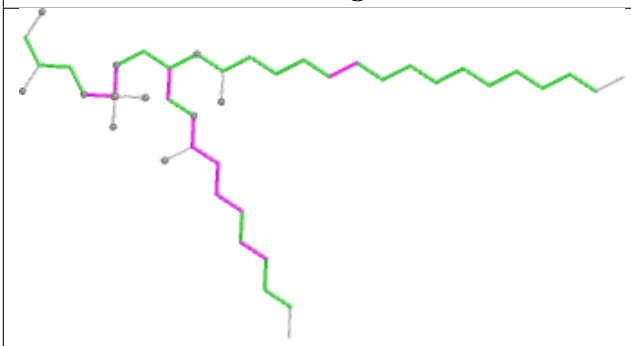
Ligand LHG a 420 (B)



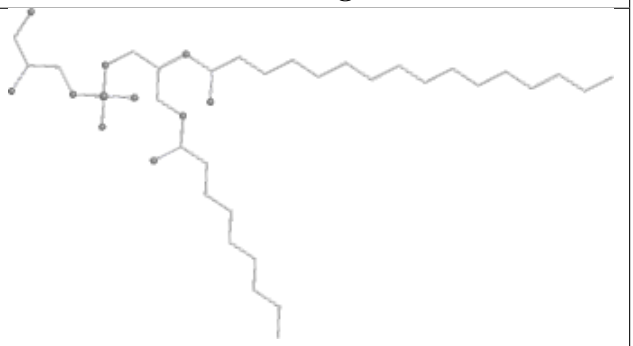
Bond lengths



Bond angles

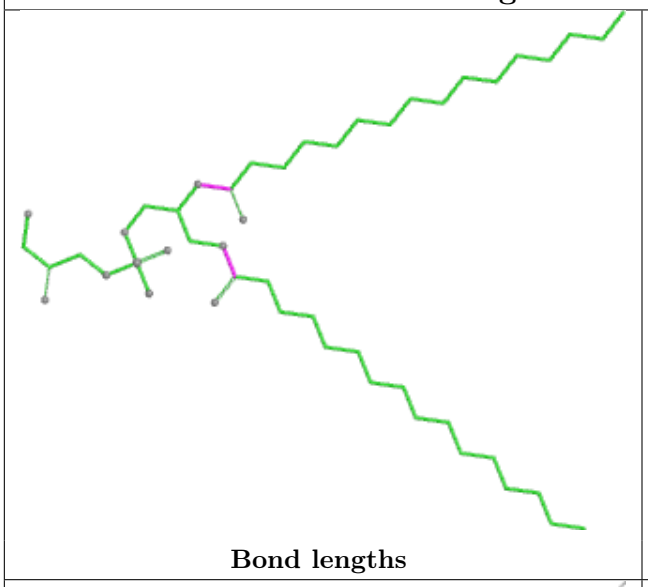


Torsions

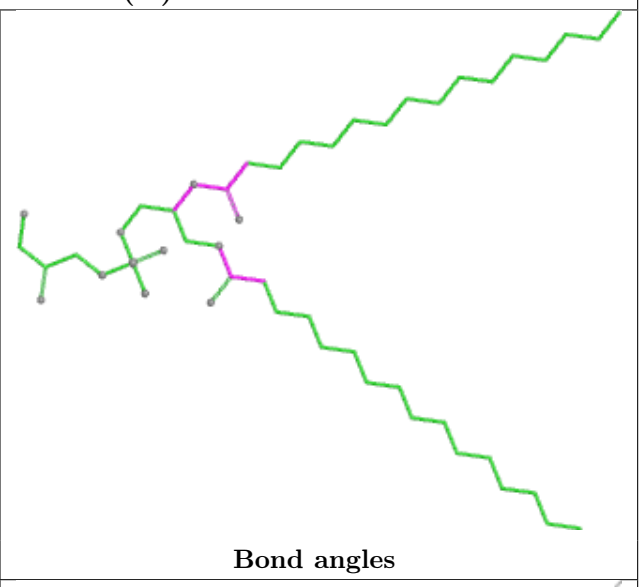


Rings

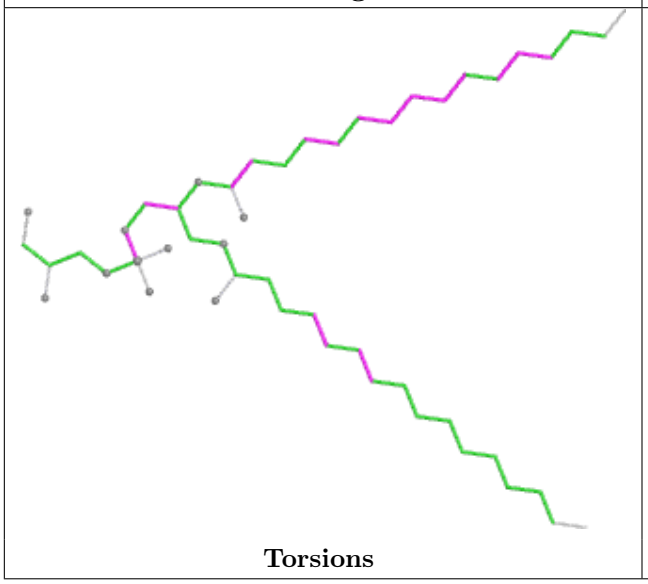
Ligand LHG l 802 (B)



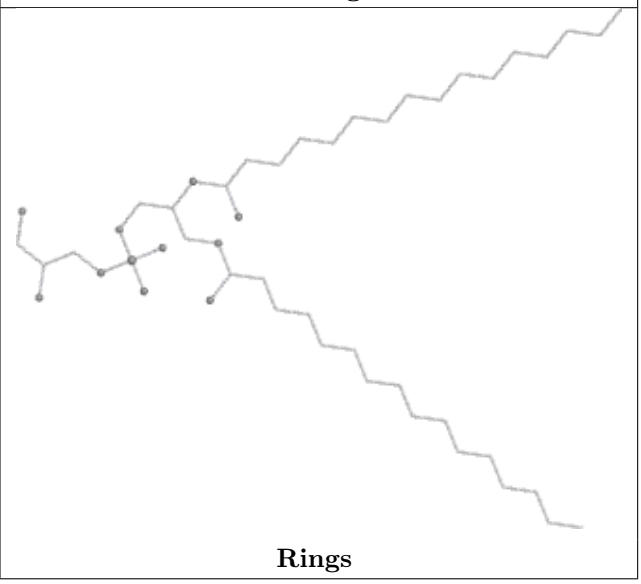
Bond lengths



Bond angles

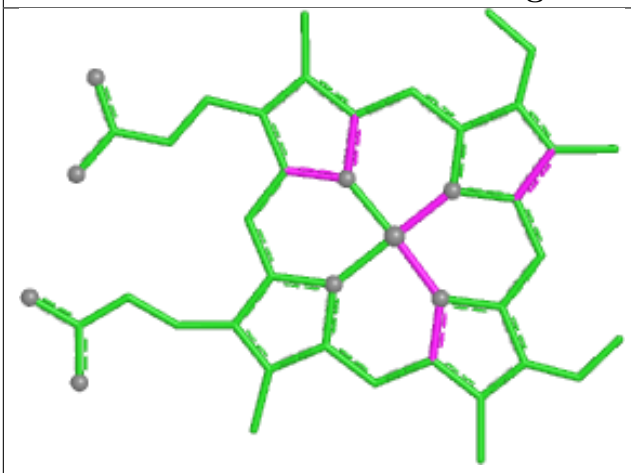


Torsions

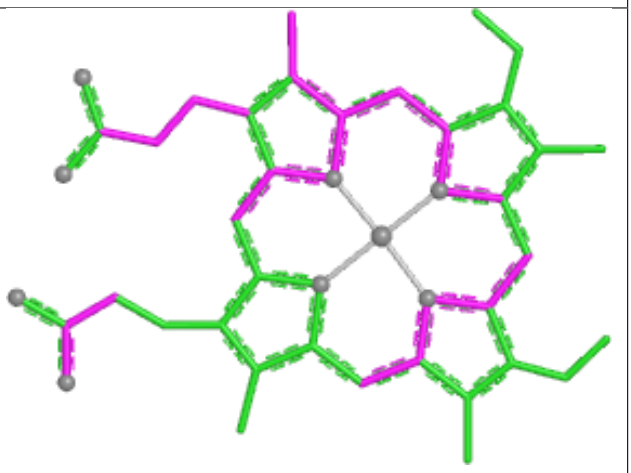


Rings

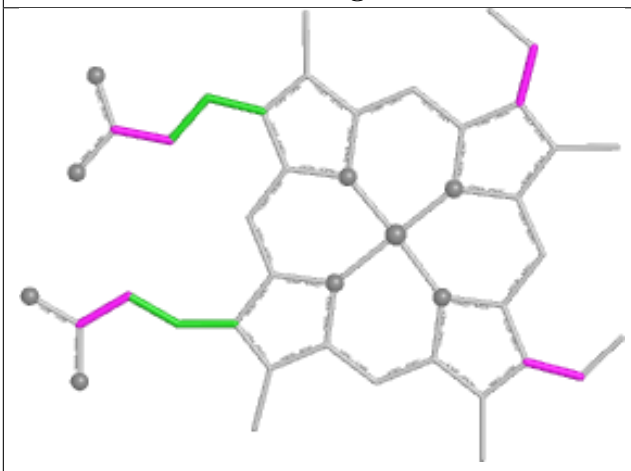
Ligand HEM f 101



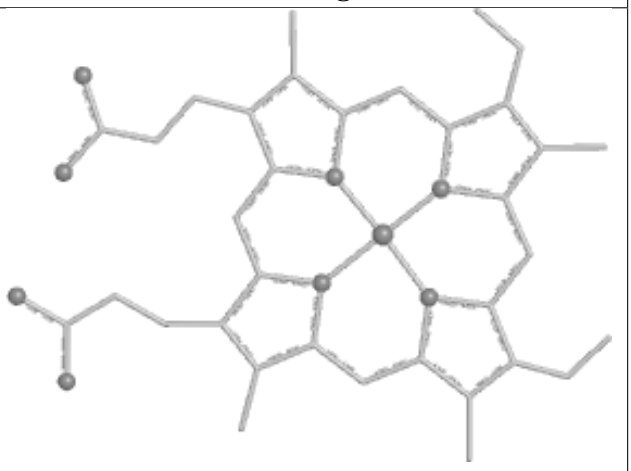
Bond lengths



Bond angles

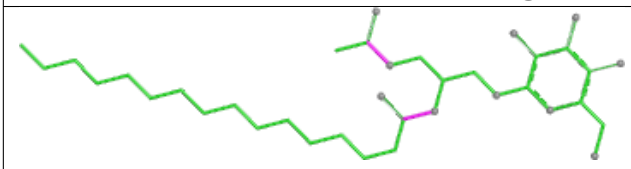


Torsions

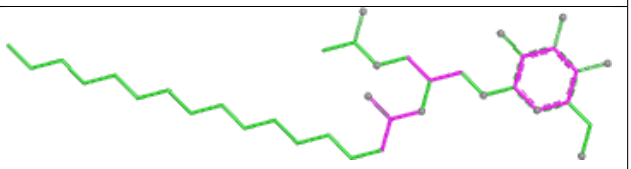


Rings

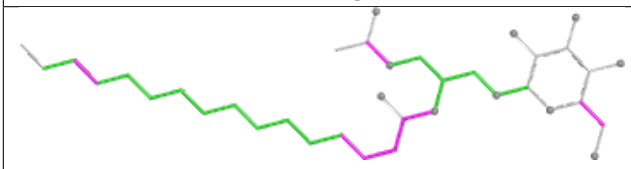
Ligand LMG C 526



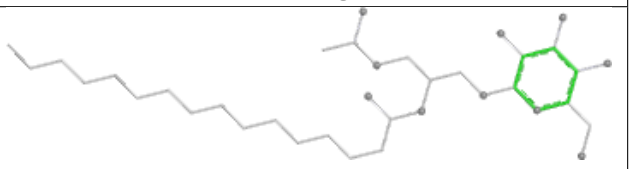
Bond lengths



Bond angles

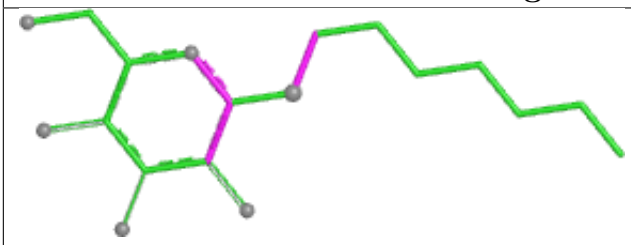


Torsions

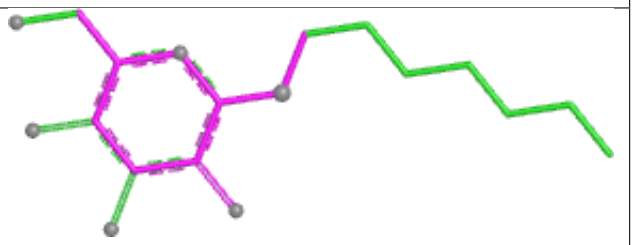


Rings

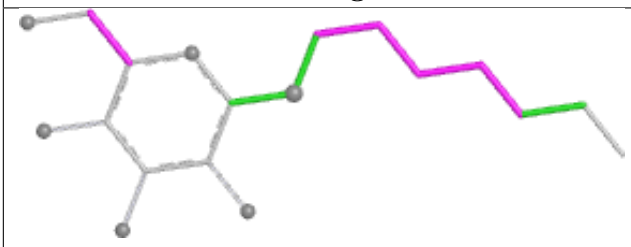
Ligand HTG b 622



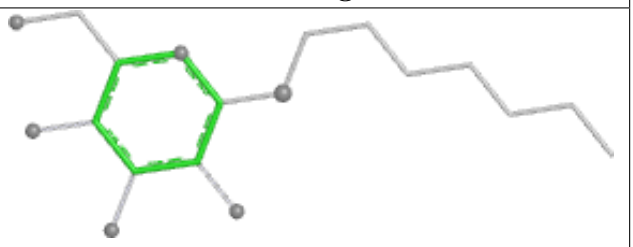
Bond lengths



Bond angles

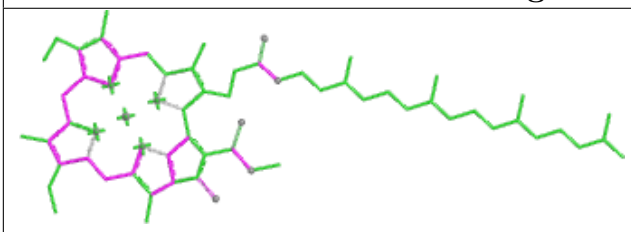


Torsions

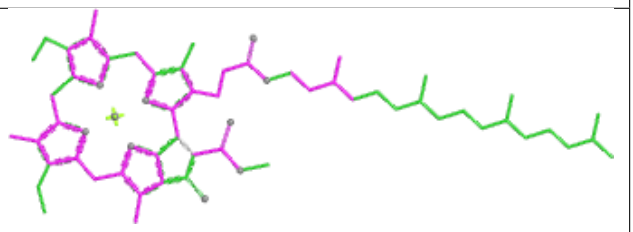


Rings

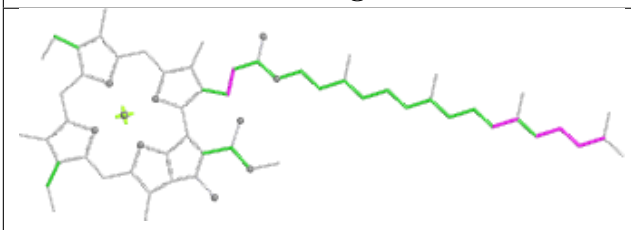
Ligand CLA b 610



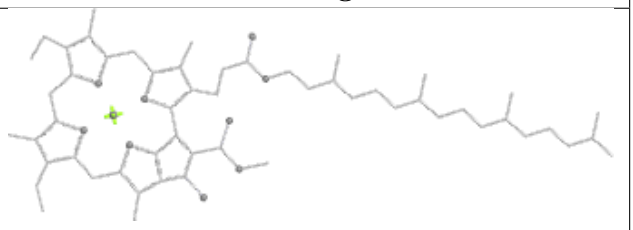
Bond lengths



Bond angles

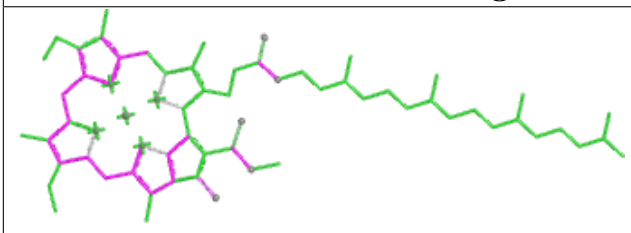


Torsions

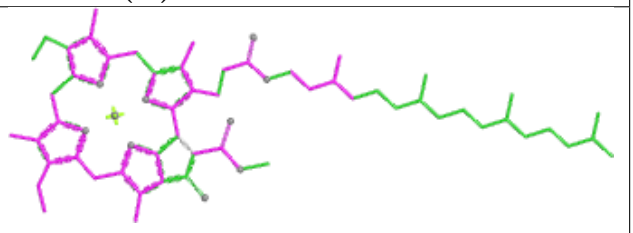


Rings

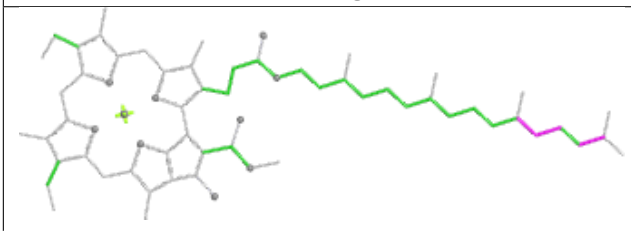
Ligand CLA A 406 (B)



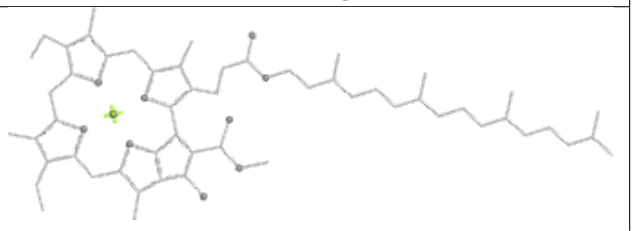
Bond lengths



Bond angles

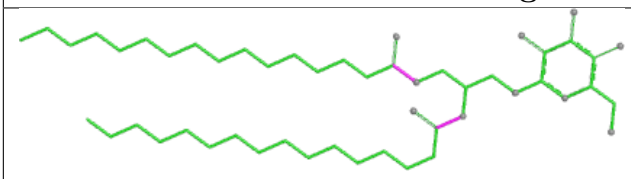


Torsions

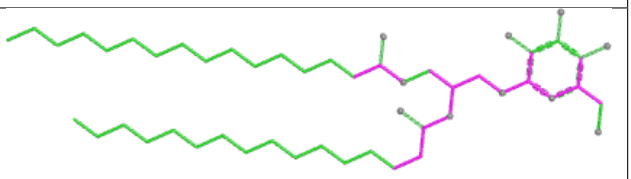


Rings

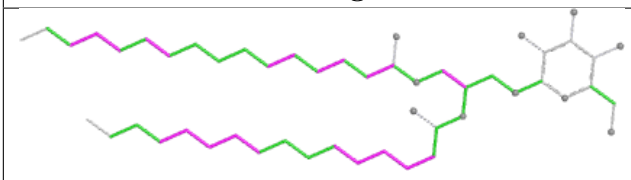
Ligand LMG C 502



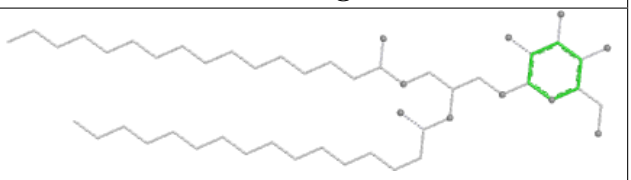
Bond lengths



Bond angles

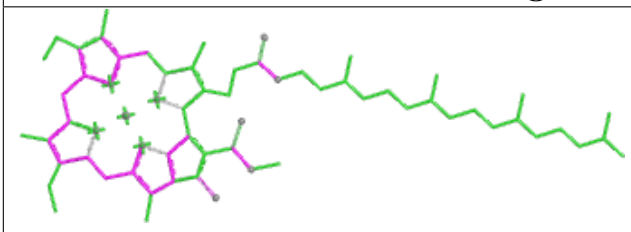


Torsions

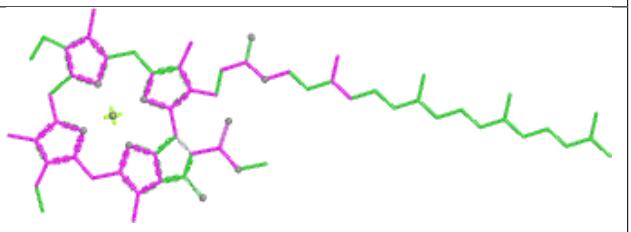


Rings

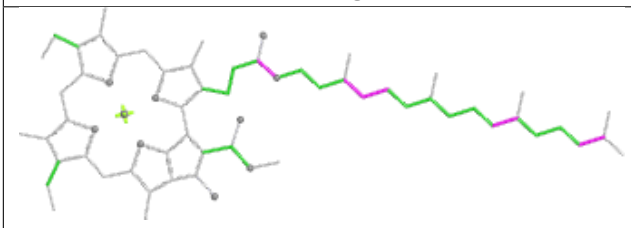
Ligand CLA d 402



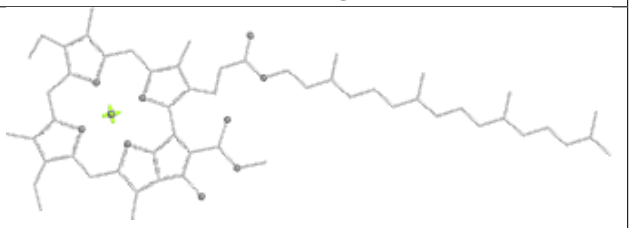
Bond lengths



Bond angles



Torsions

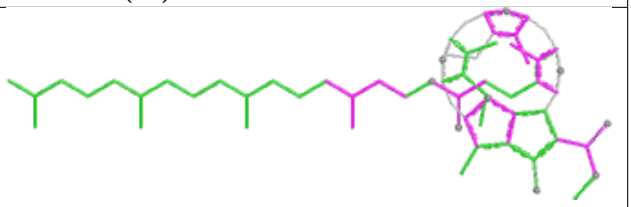


Rings

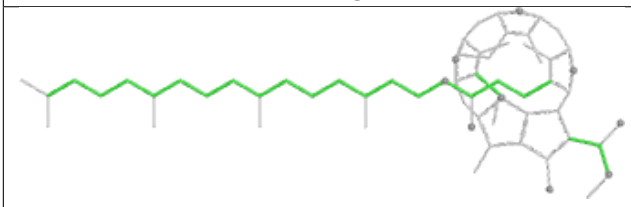
Ligand PHO D 401 (A)



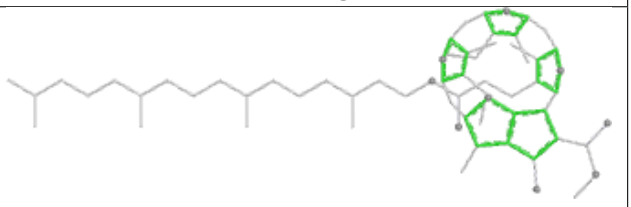
Bond lengths



Bond angles

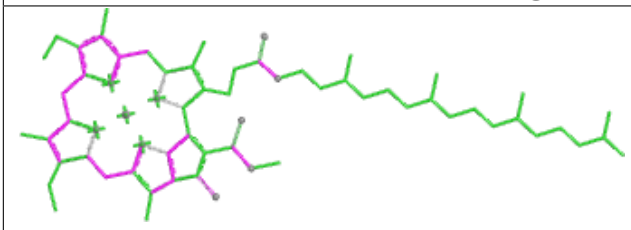


Torsions

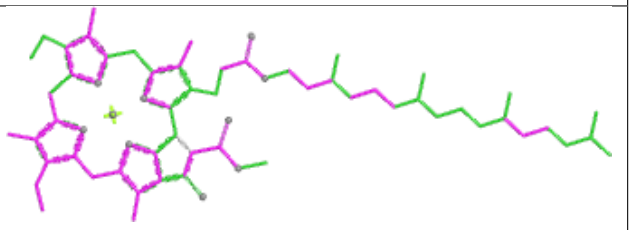


Rings

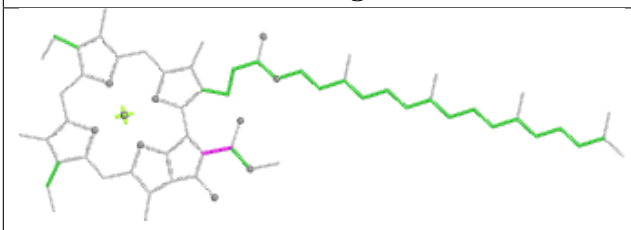
Ligand CLA b 609



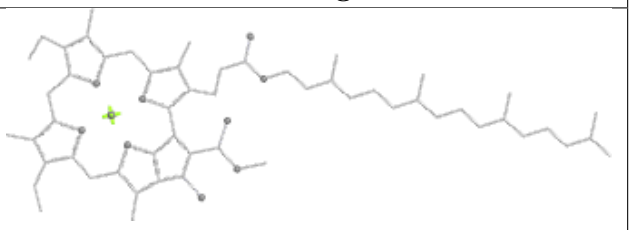
Bond lengths



Bond angles

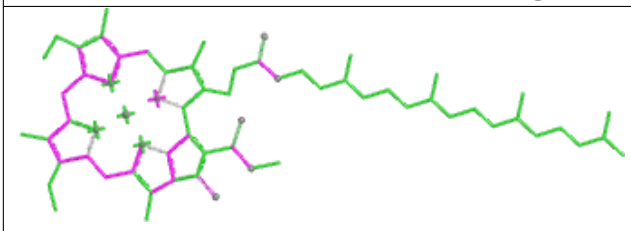


Torsions

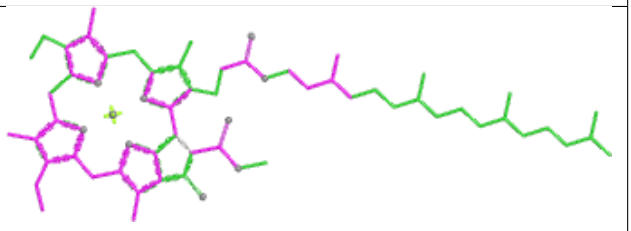


Rings

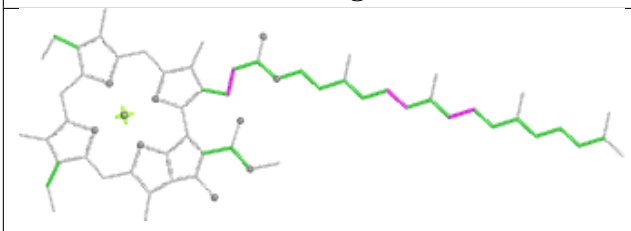
Ligand CLA c 504



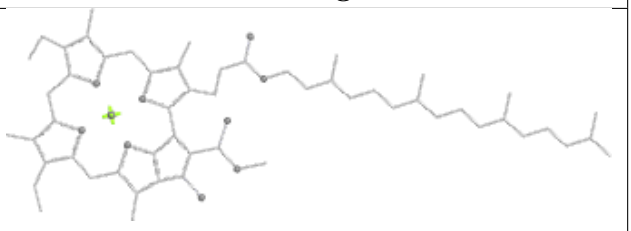
Bond lengths



Bond angles

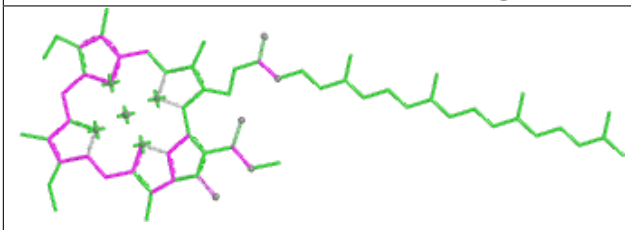


Torsions

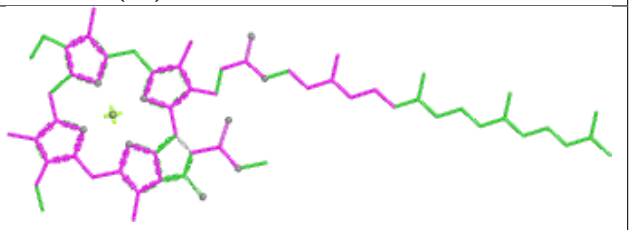


Rings

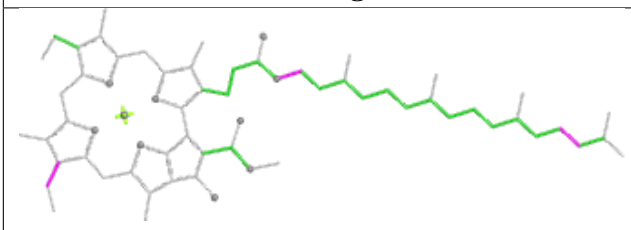
Ligand CLA a 405 (A)



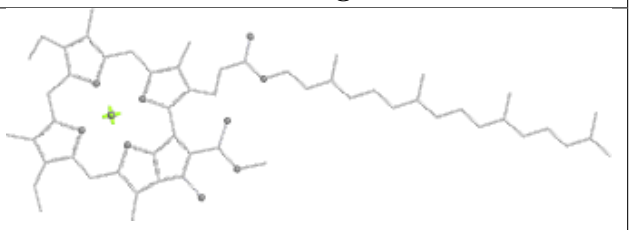
Bond lengths



Bond angles

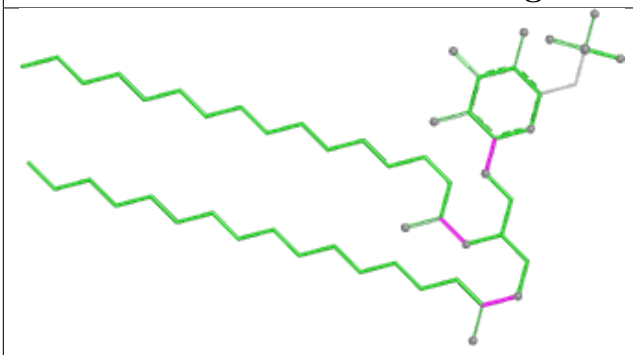


Torsions

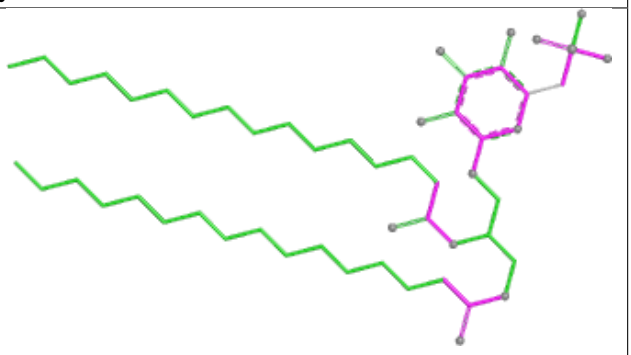


Rings

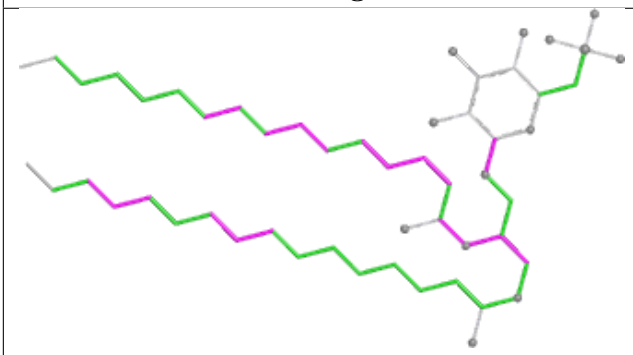
Ligand SQD B 620



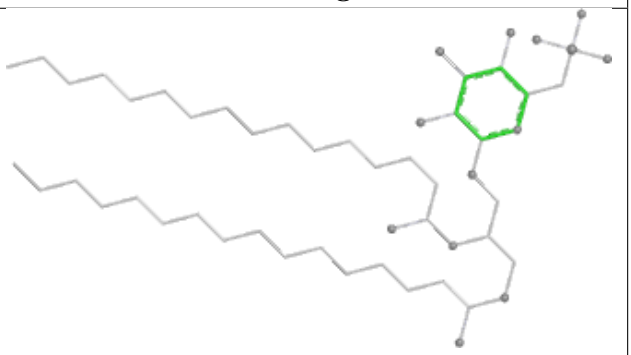
Bond lengths



Bond angles

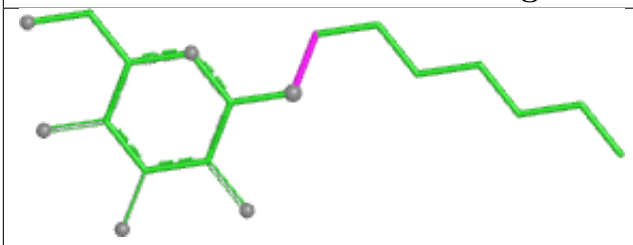


Torsions

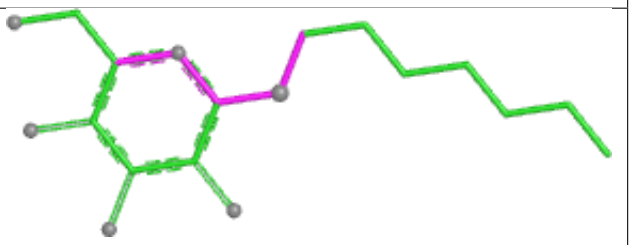


Rings

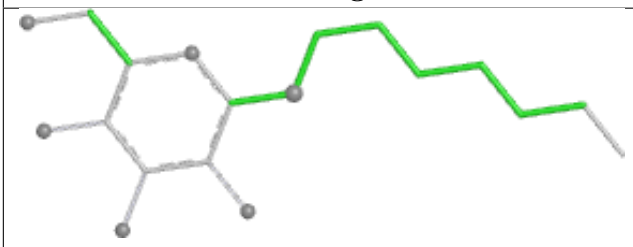
Ligand HTG C 523



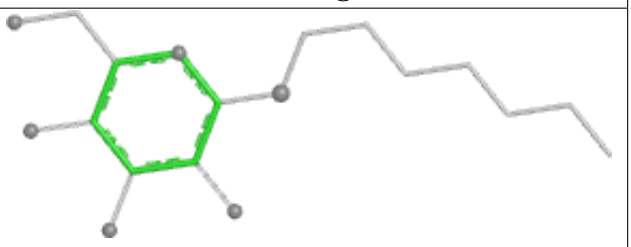
Bond lengths



Bond angles

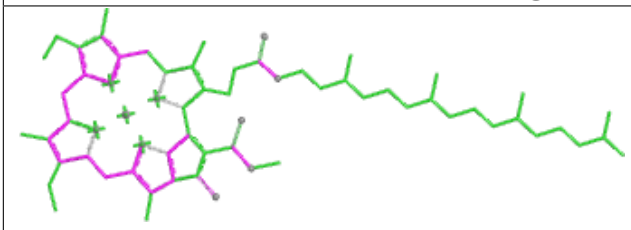


Torsions

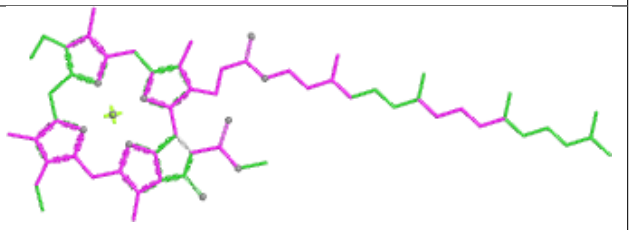


Rings

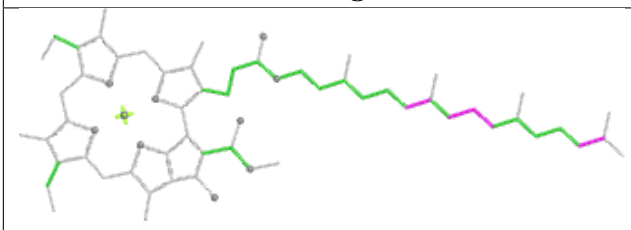
Ligand CLA b 602



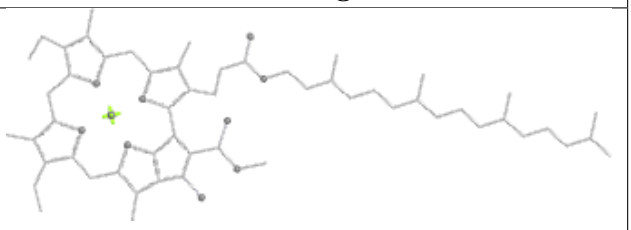
Bond lengths



Bond angles

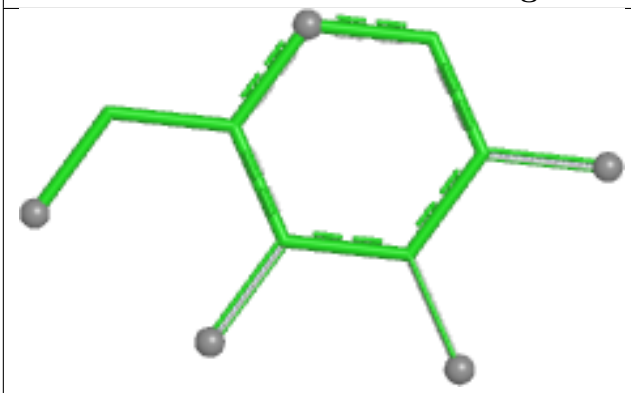


Torsions

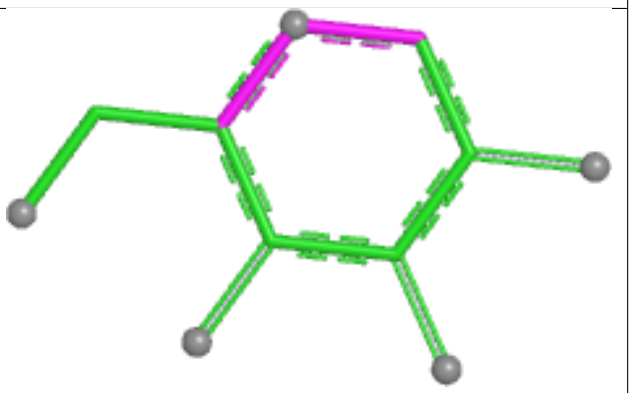


Rings

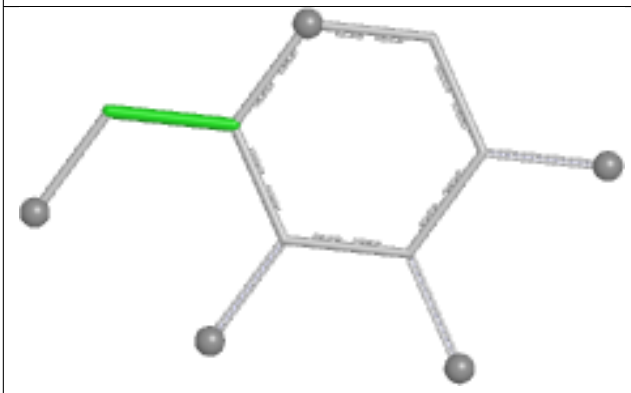
Ligand HTG V 203



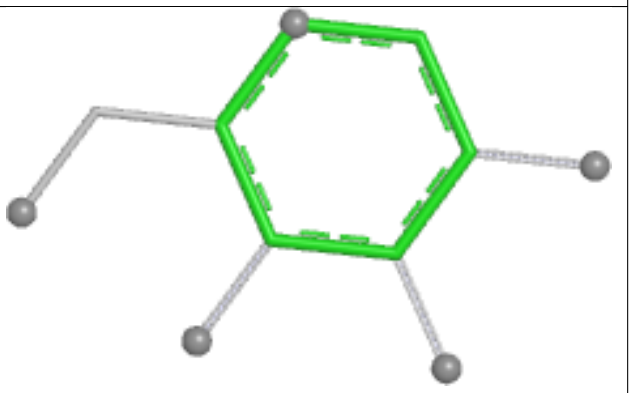
Bond lengths



Bond angles

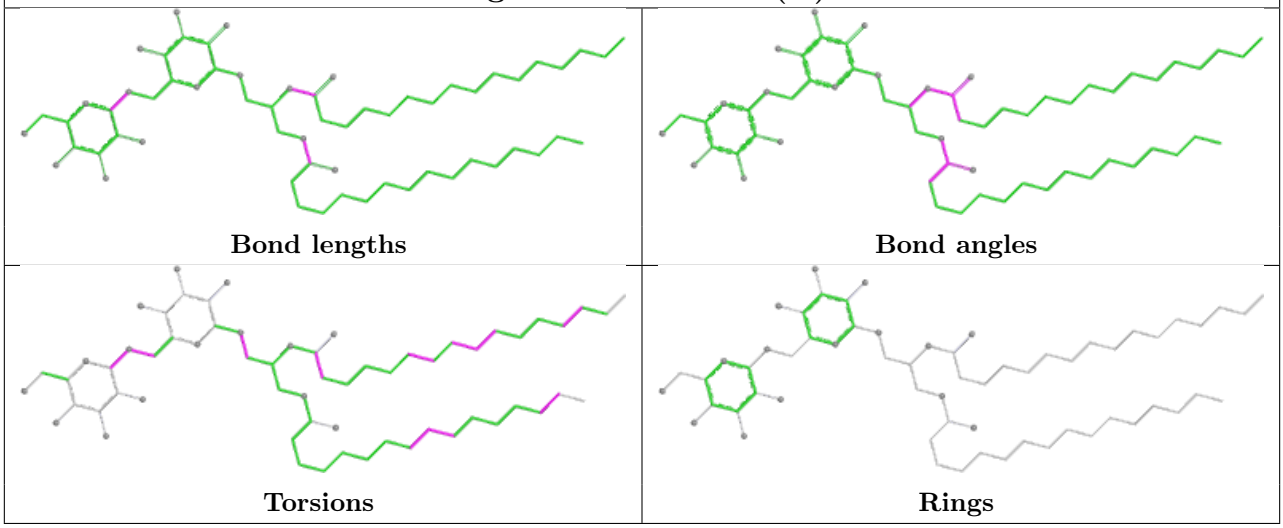


Torsions

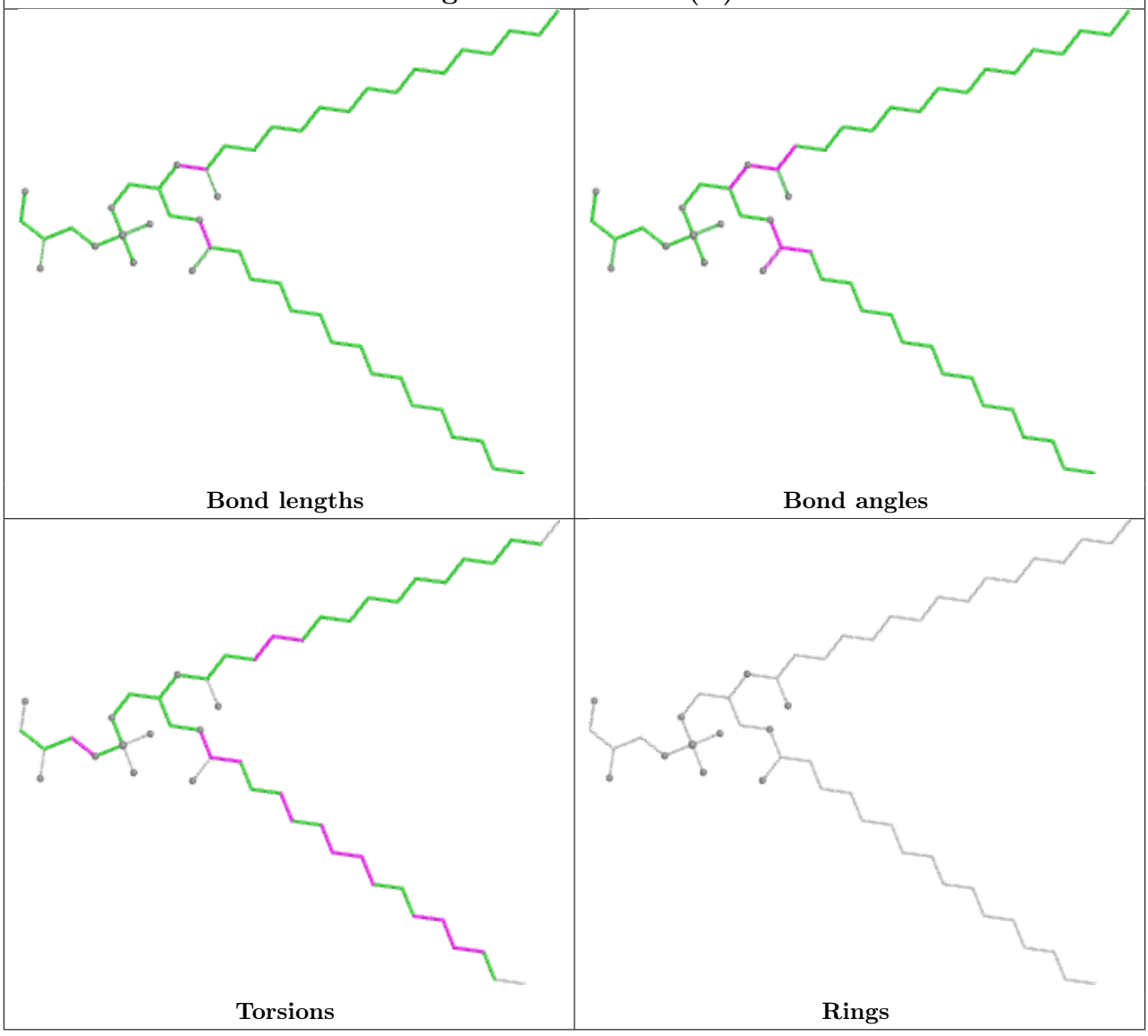


Rings

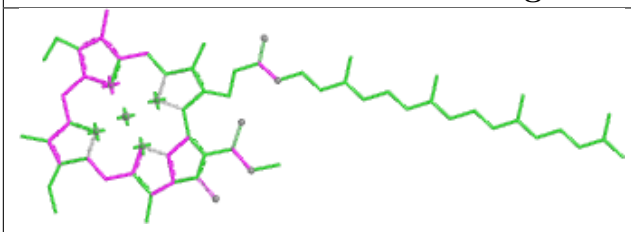
Ligand DGD C 519 (A)



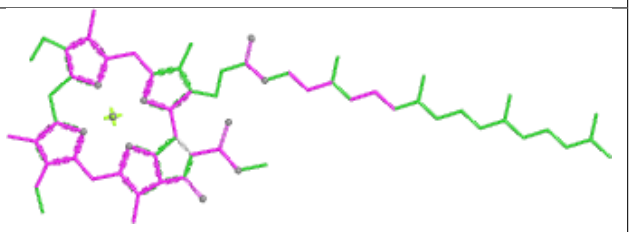
Ligand LHG d 406 (B)



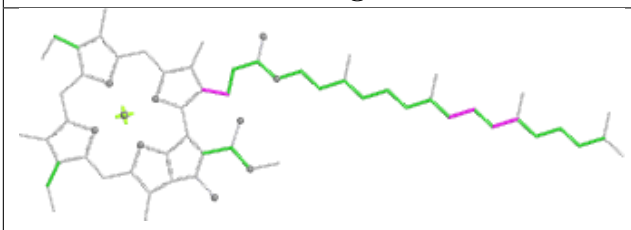
Ligand CLA B 611



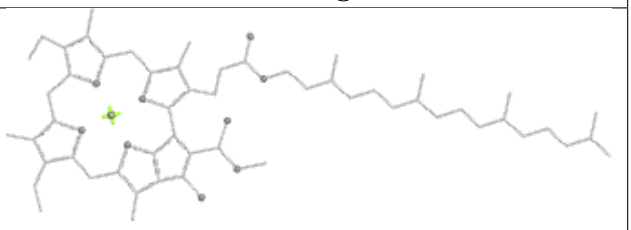
Bond lengths



Bond angles

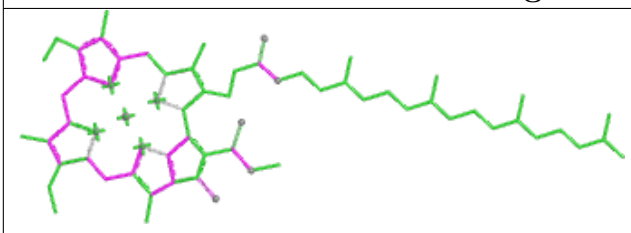


Torsions

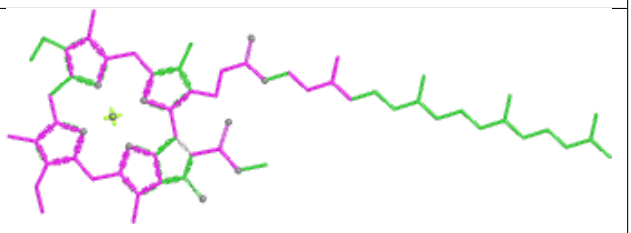


Rings

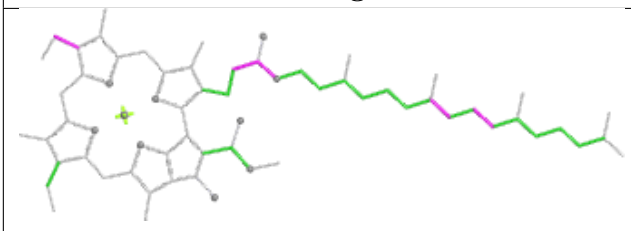
Ligand CLA C 514



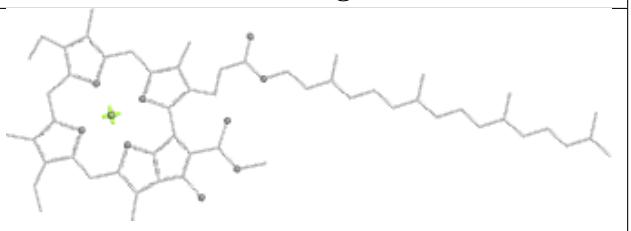
Bond lengths



Bond angles

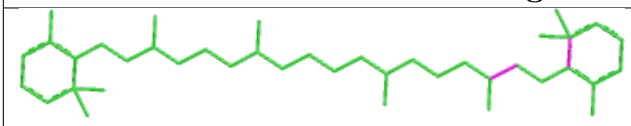


Torsions

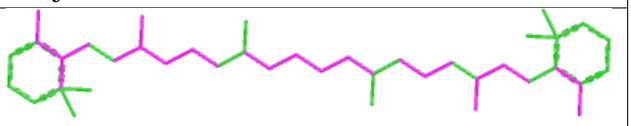


Rings

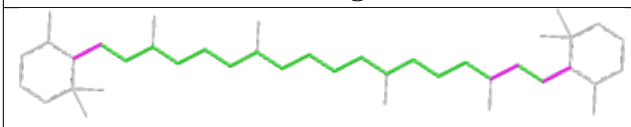
Ligand BCR y 101



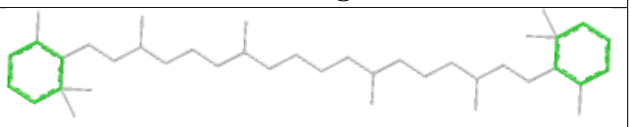
Bond lengths



Bond angles

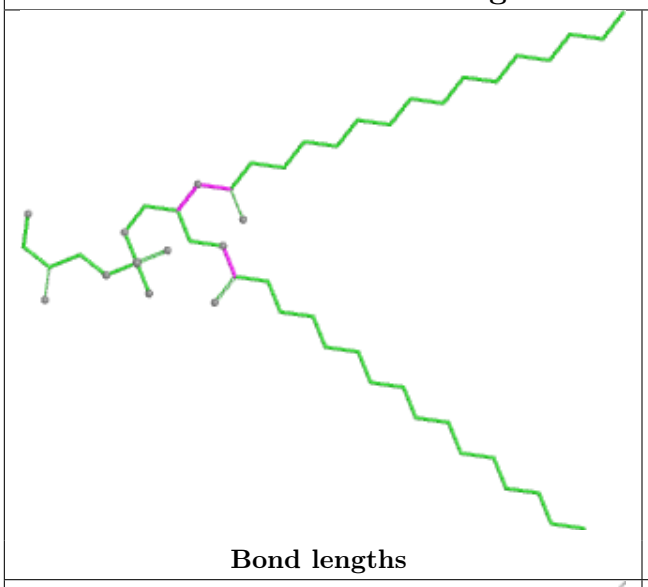


Torsions

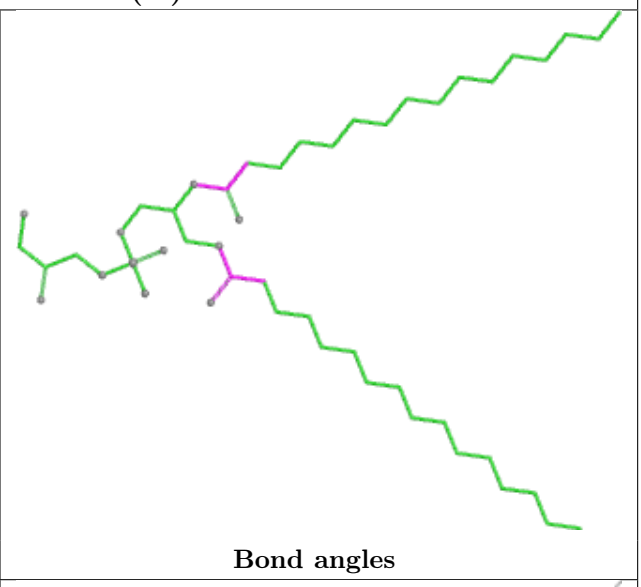


Rings

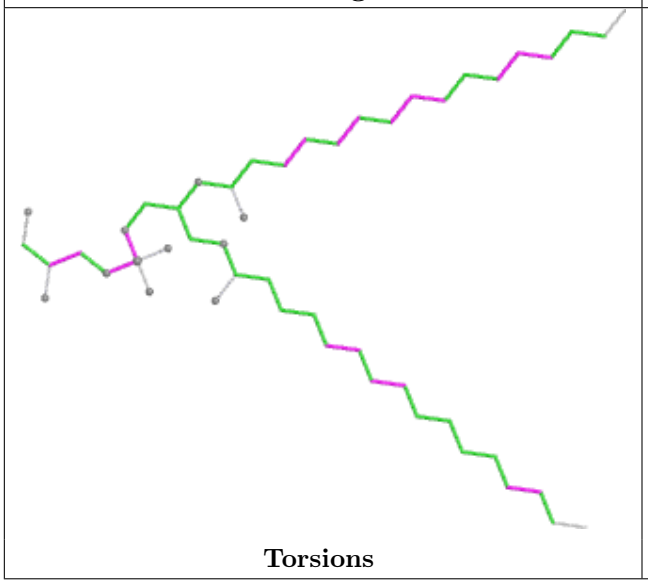
Ligand LHG D 408 (A)



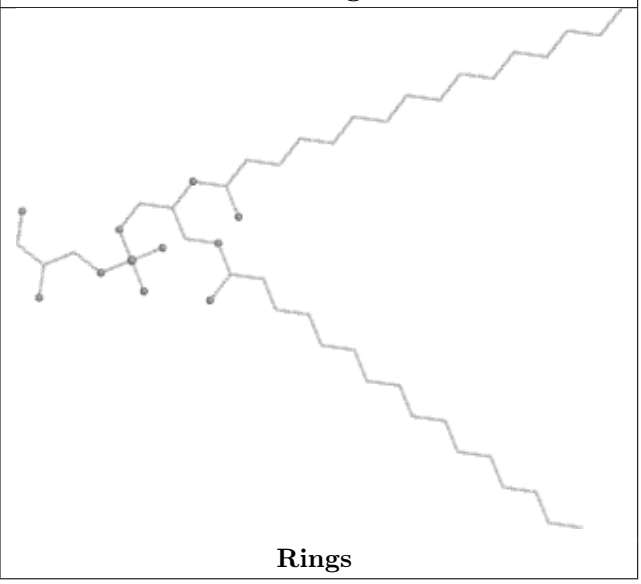
Bond lengths



Bond angles

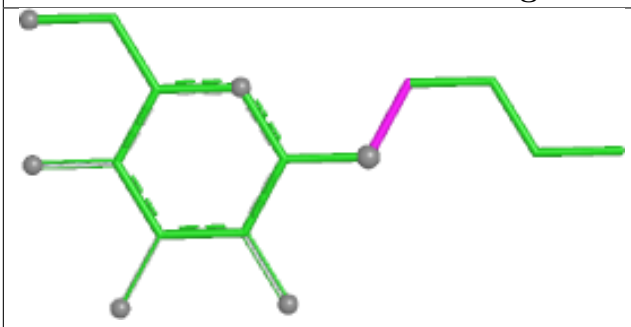


Torsions

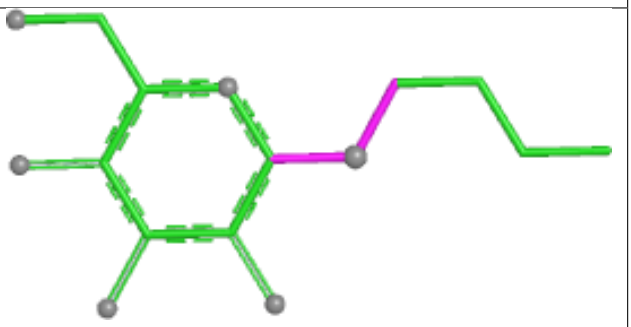


Rings

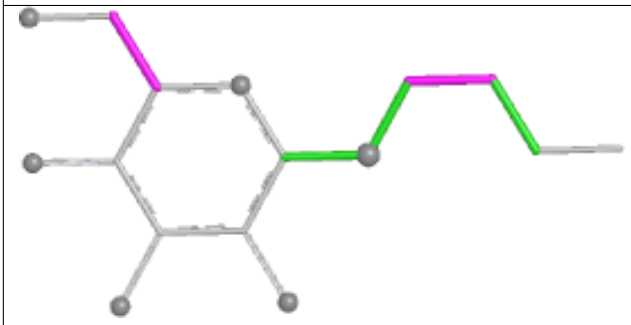
Ligand HTG D 412



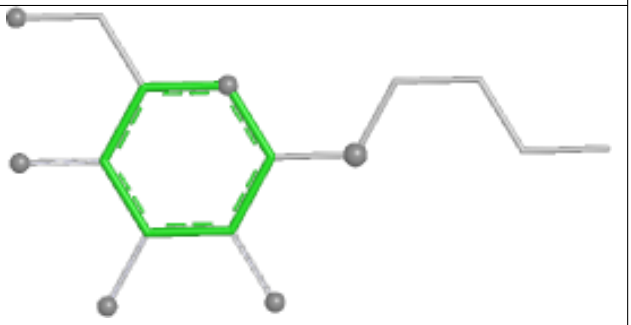
Bond lengths



Bond angles

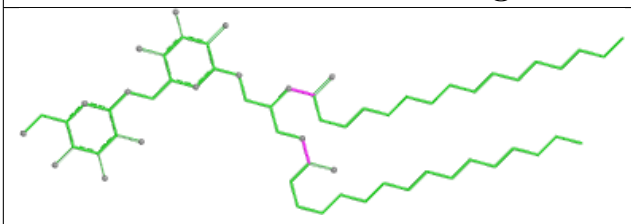


Torsions

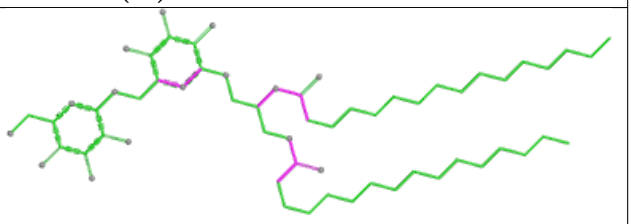


Rings

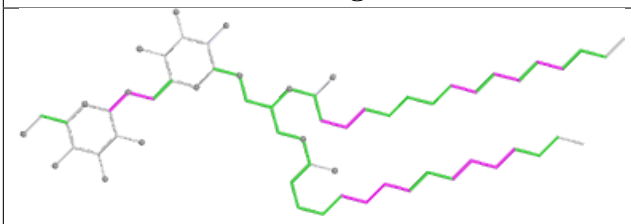
Ligand DGD c 518 (B)



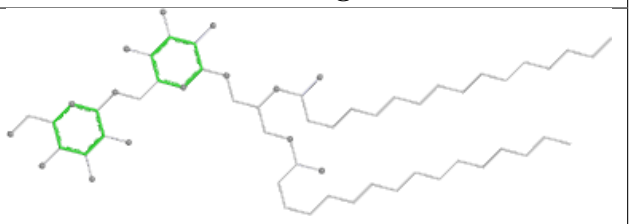
Bond lengths



Bond angles

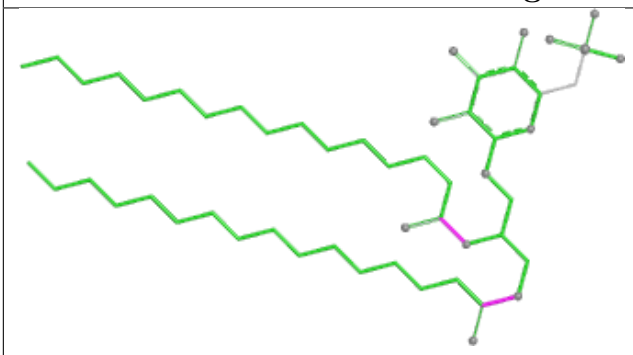


Torsions

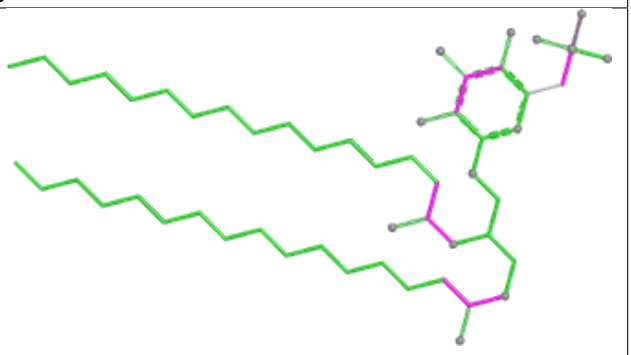


Rings

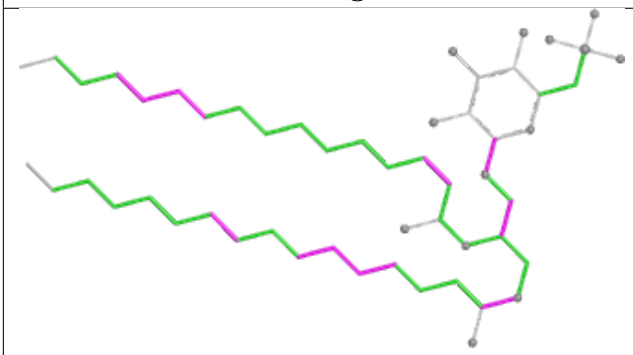
Ligand SQD A 410



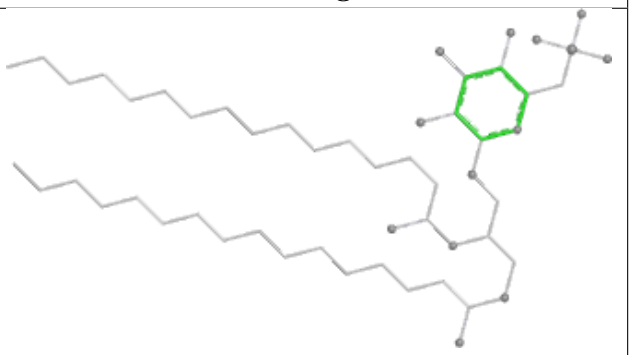
Bond lengths



Bond angles

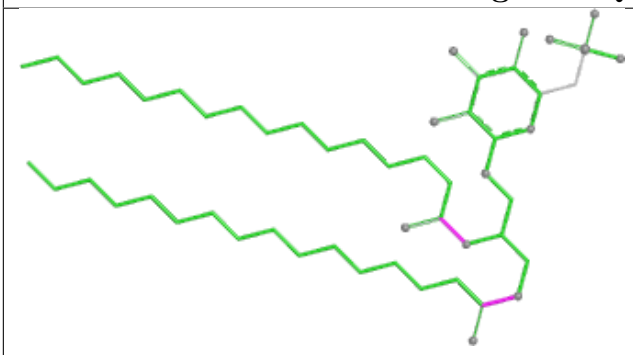


Torsions

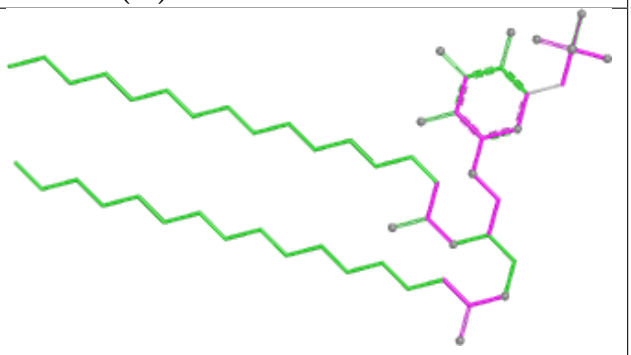


Rings

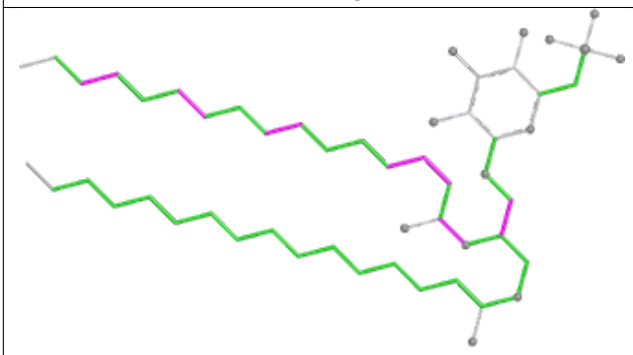
Ligand SQD C 501 (B)



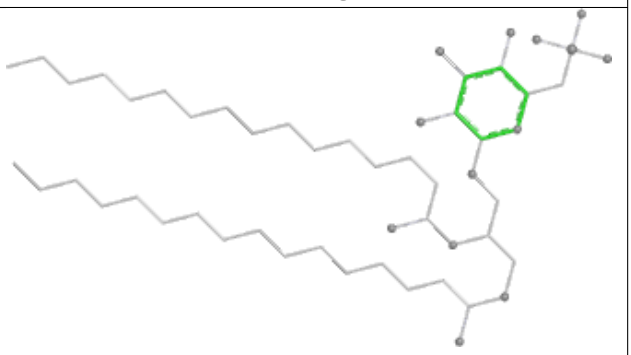
Bond lengths



Bond angles

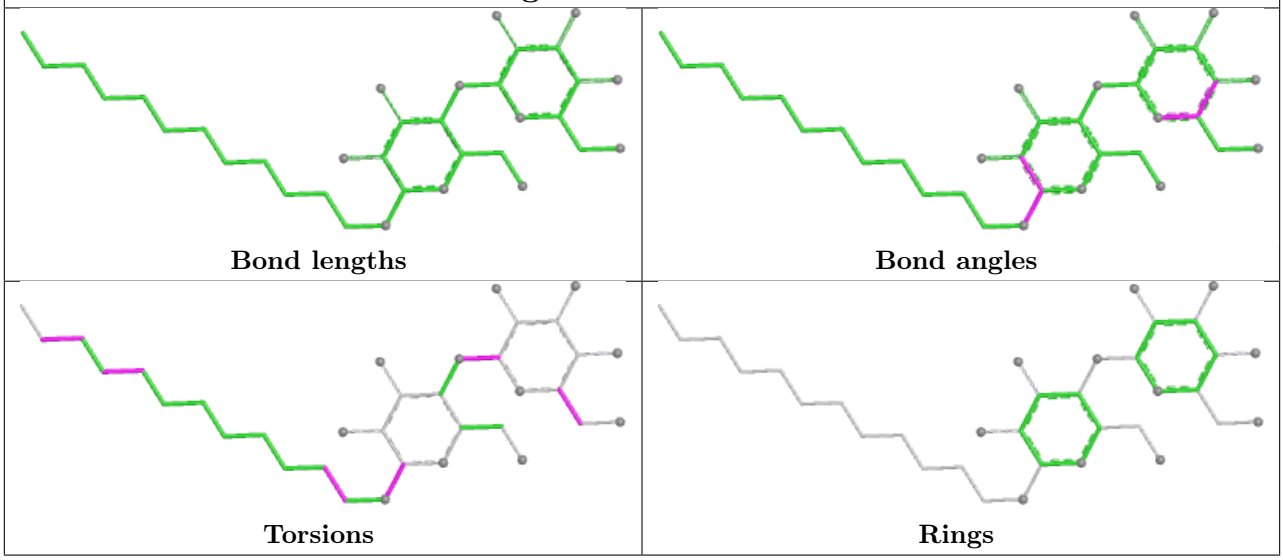


Torsions

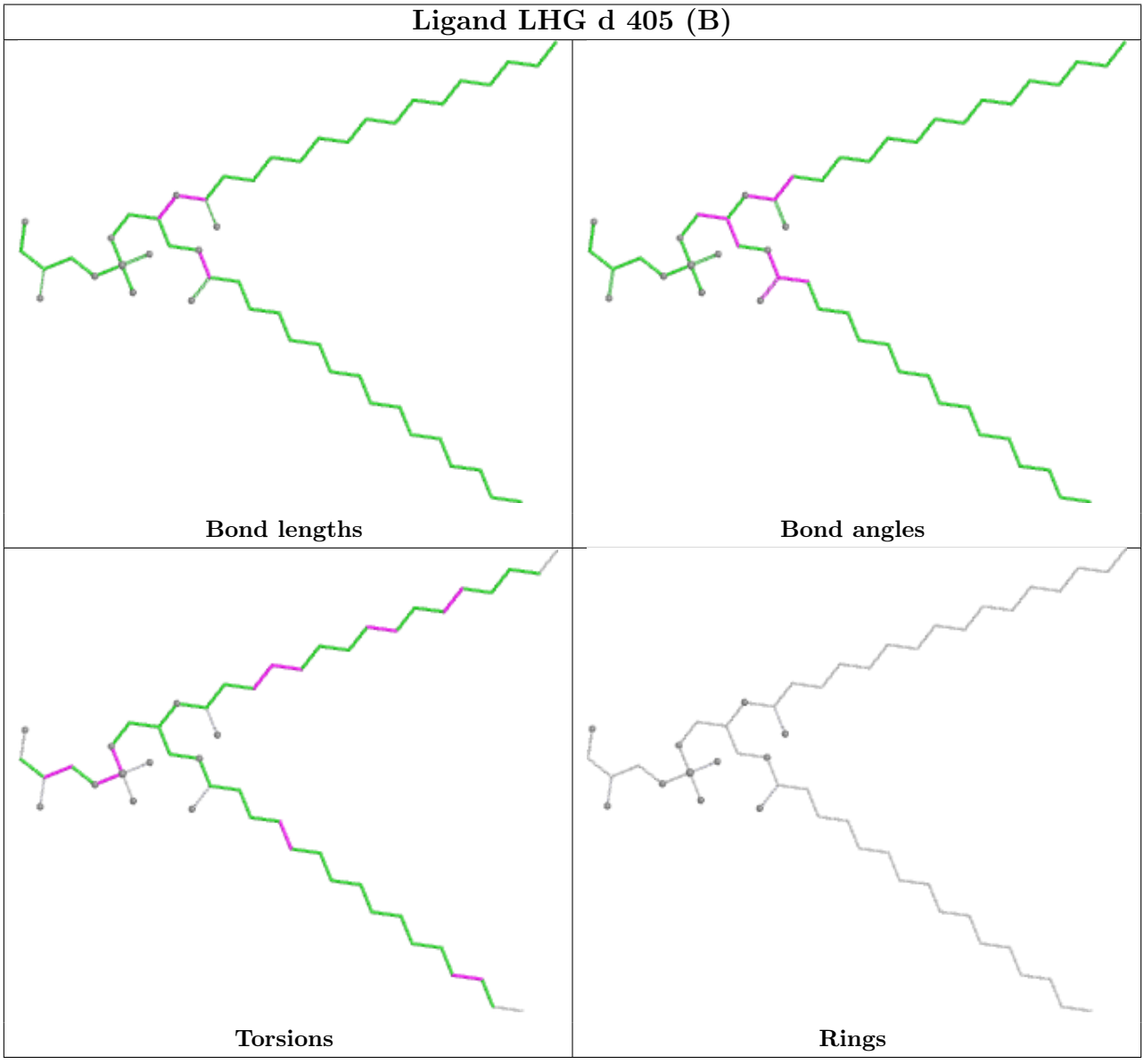


Rings

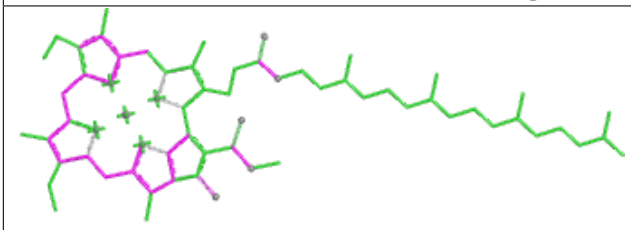
Ligand LMT A 415



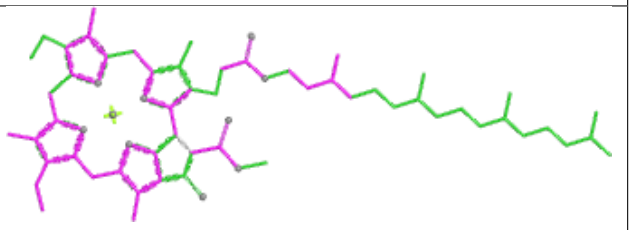
Ligand LHG d 405 (B)



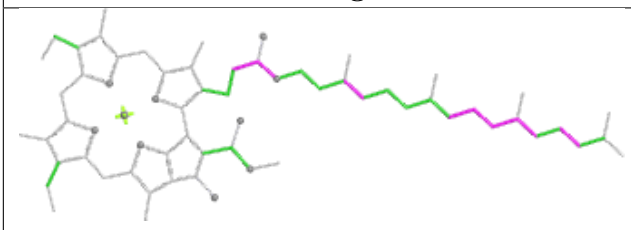
Ligand CLA C 512



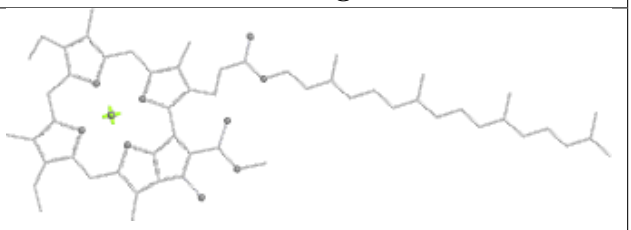
Bond lengths



Bond angles



Torsions

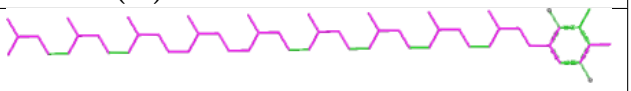


Rings

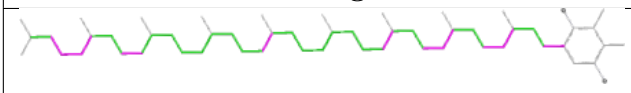
Ligand PL9 A 412 (B)



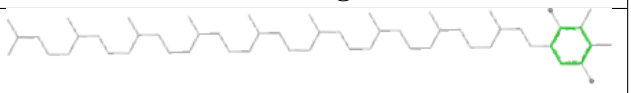
Bond lengths



Bond angles

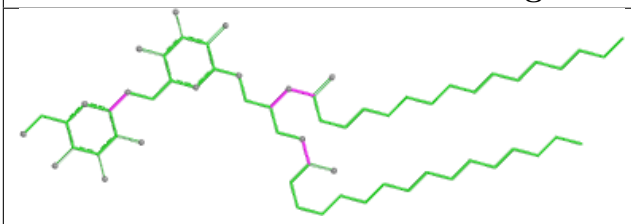


Torsions

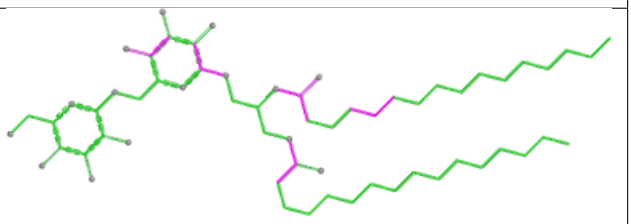


Rings

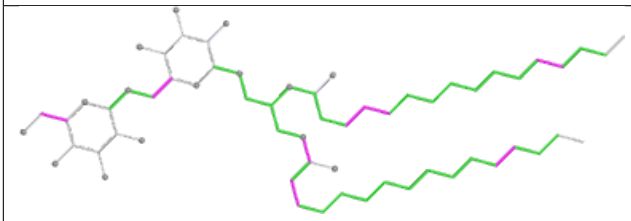
Ligand DGD c 519



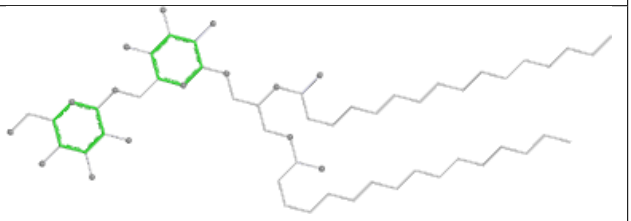
Bond lengths



Bond angles

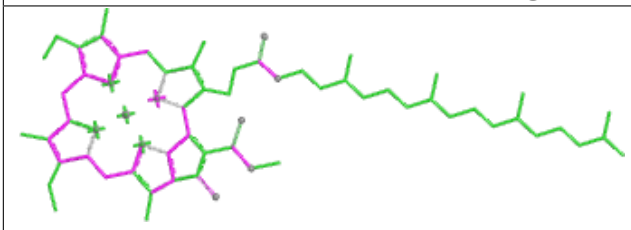


Torsions

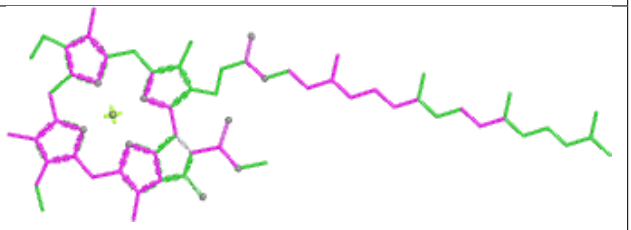


Rings

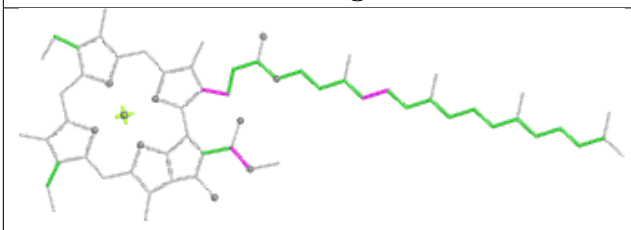
Ligand CLA B 604



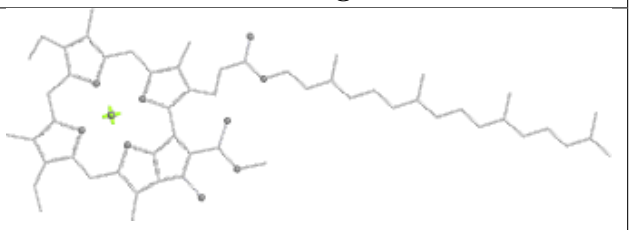
Bond lengths



Bond angles



Torsions

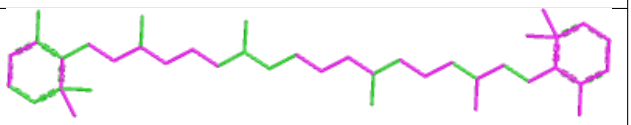


Rings

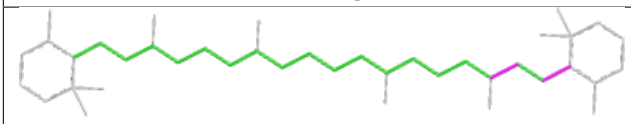
Ligand BCR D 406



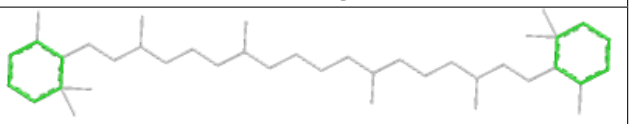
Bond lengths



Bond angles

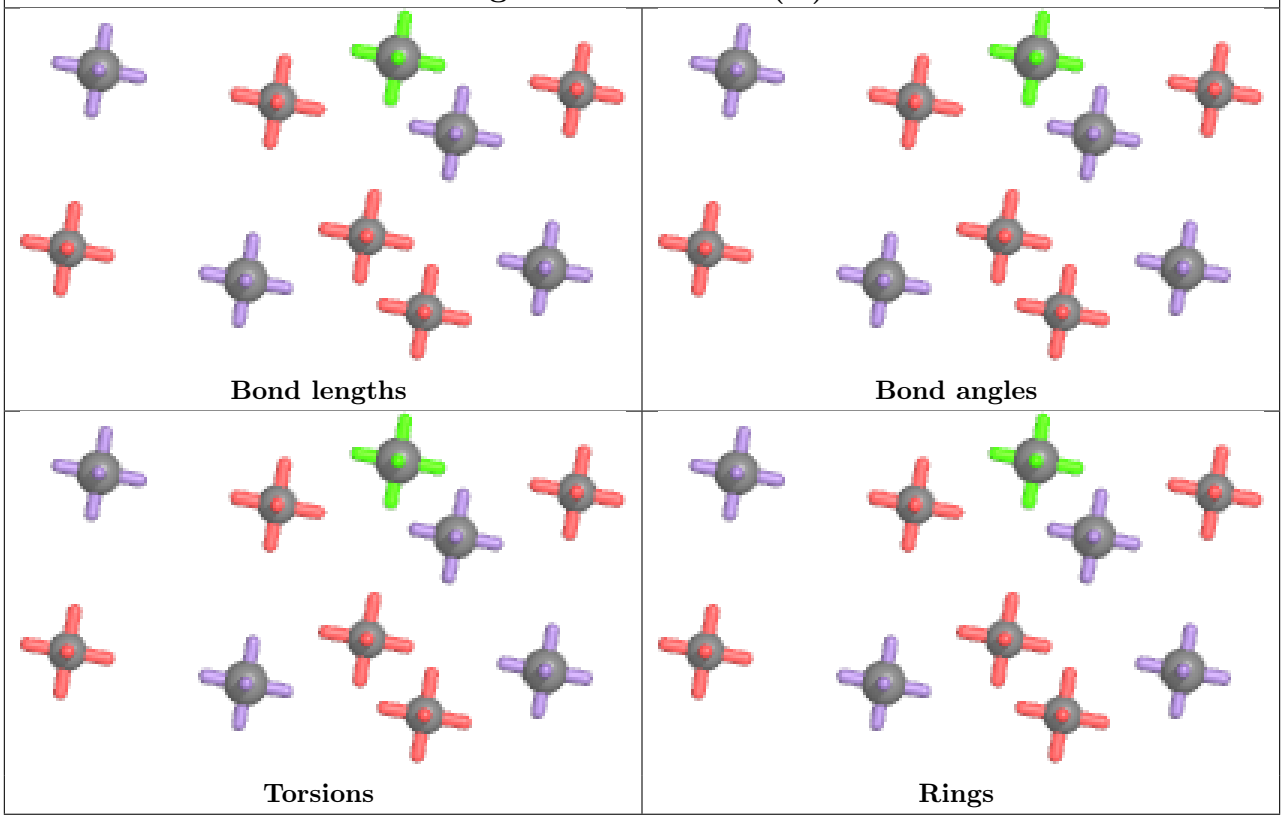


Torsions

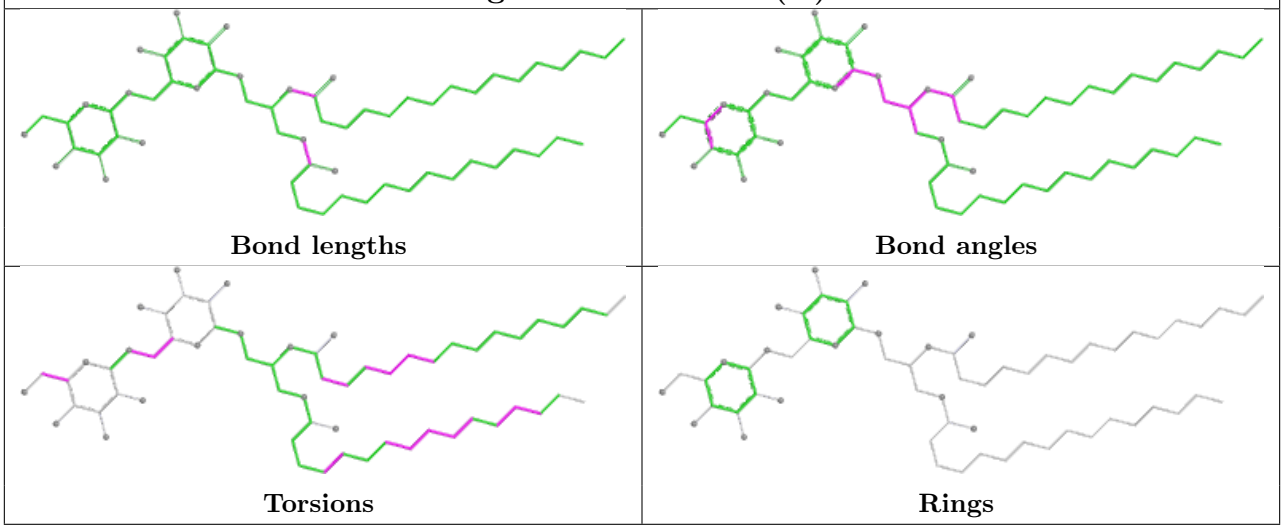


Rings

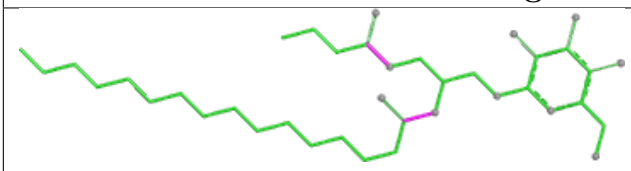
Ligand OEX A 411 (A)



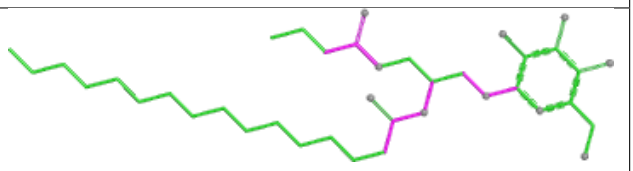
Ligand DGD C 518 (A)



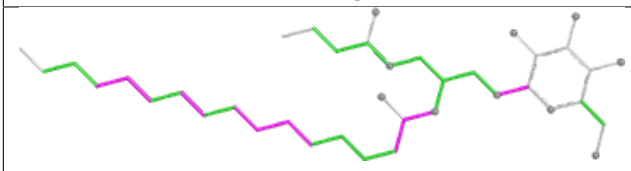
Ligand LMG z 101



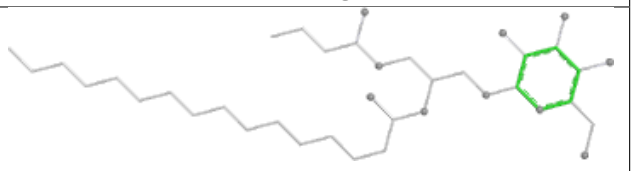
Bond lengths



Bond angles

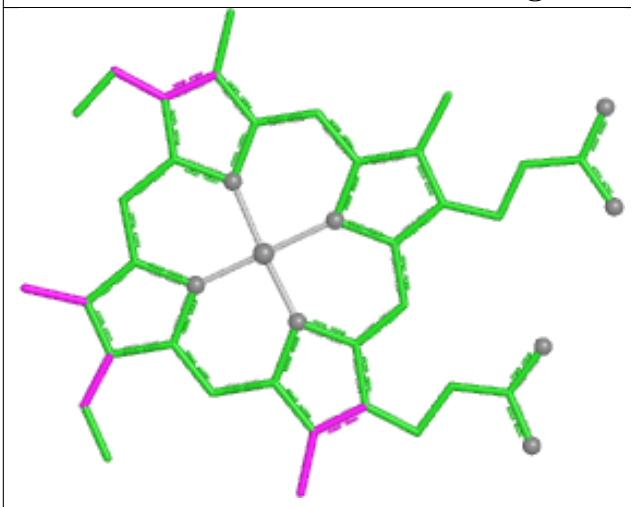


Torsions

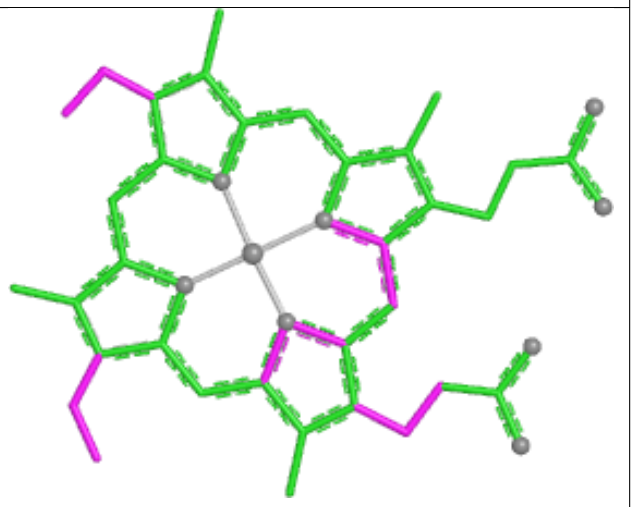


Rings

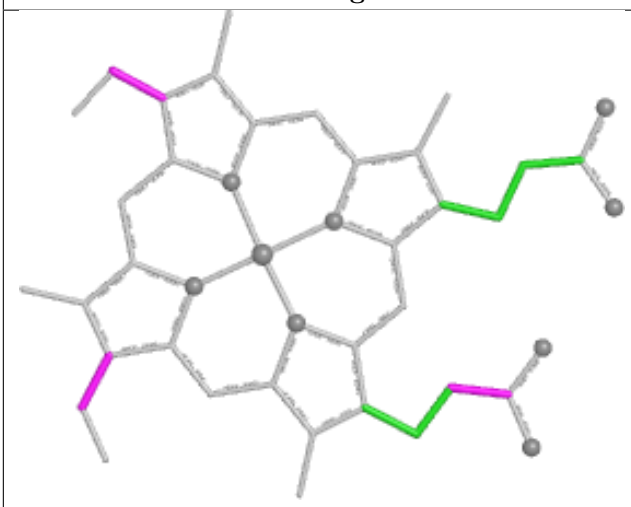
Ligand HEC v 201



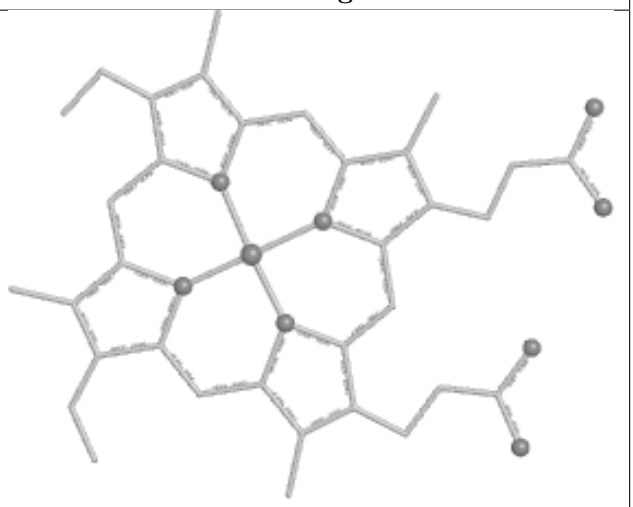
Bond lengths



Bond angles

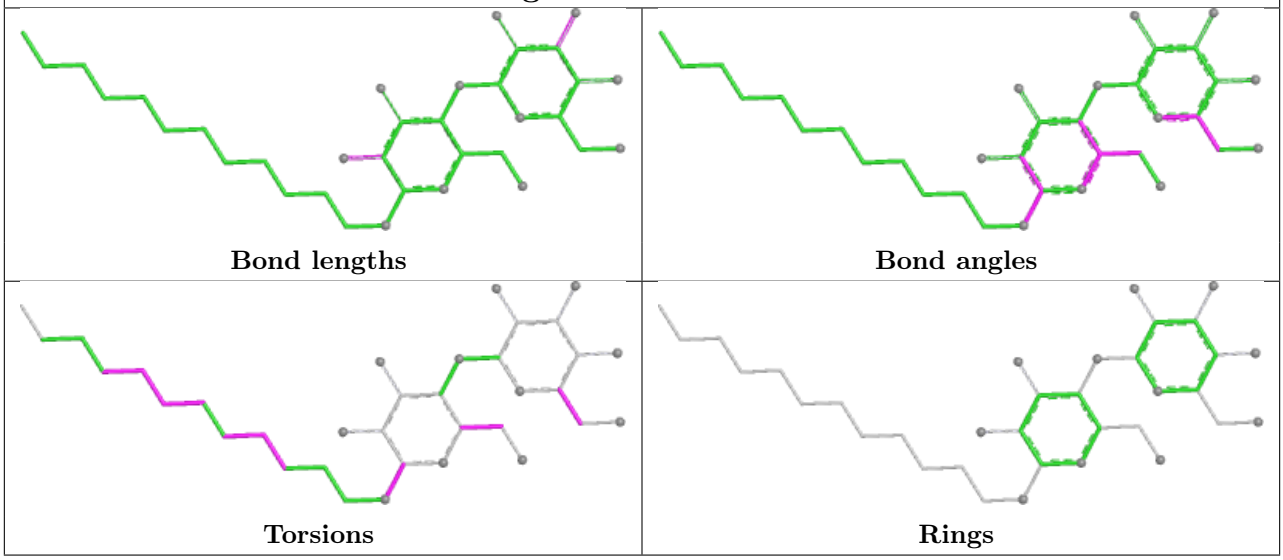


Torsions

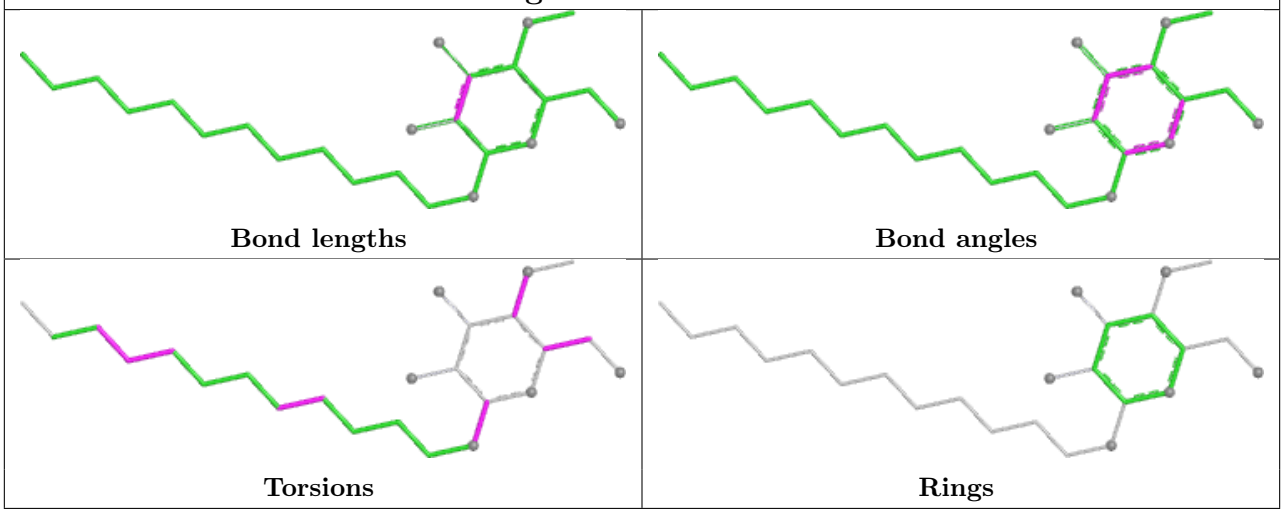


Rings

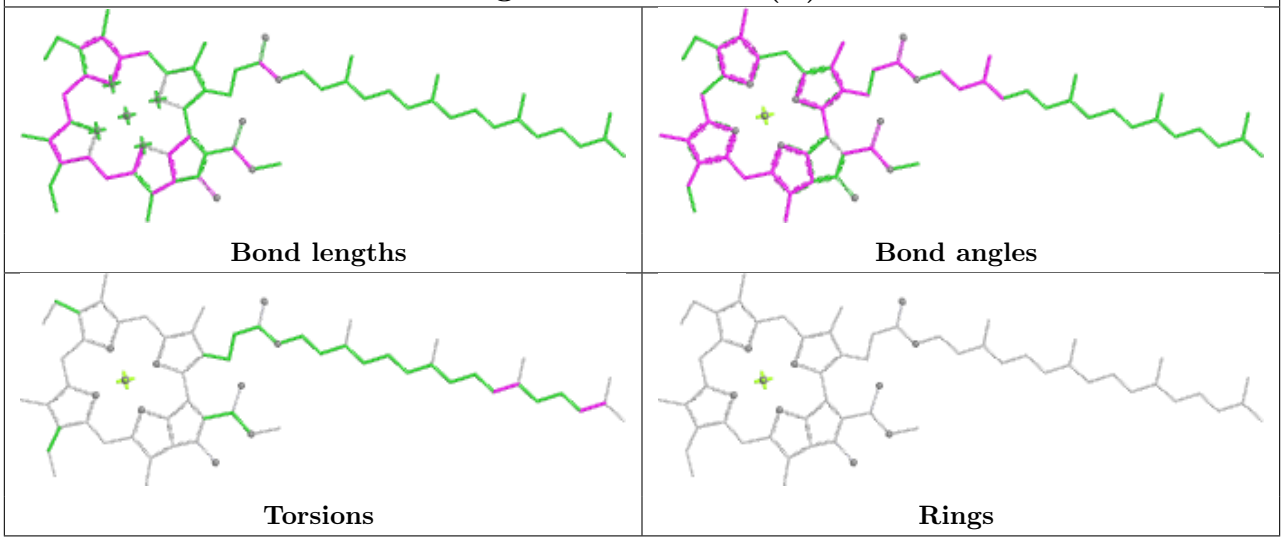
Ligand LMT B 630



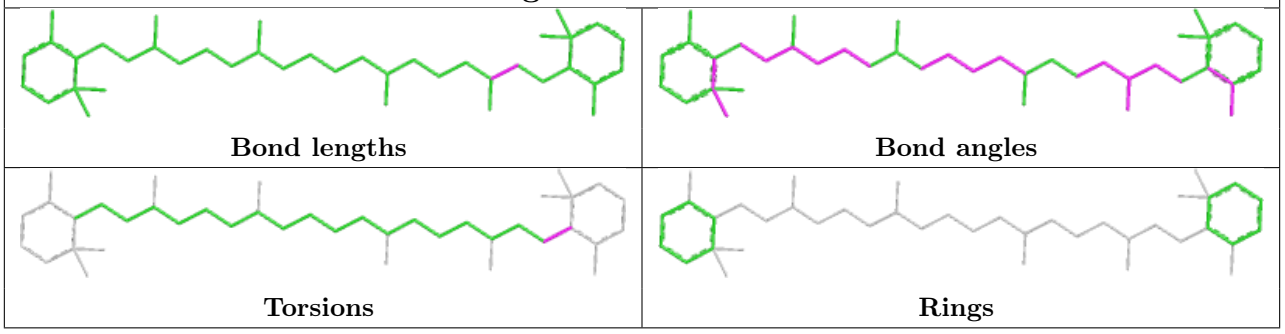
Ligand LMT b 621



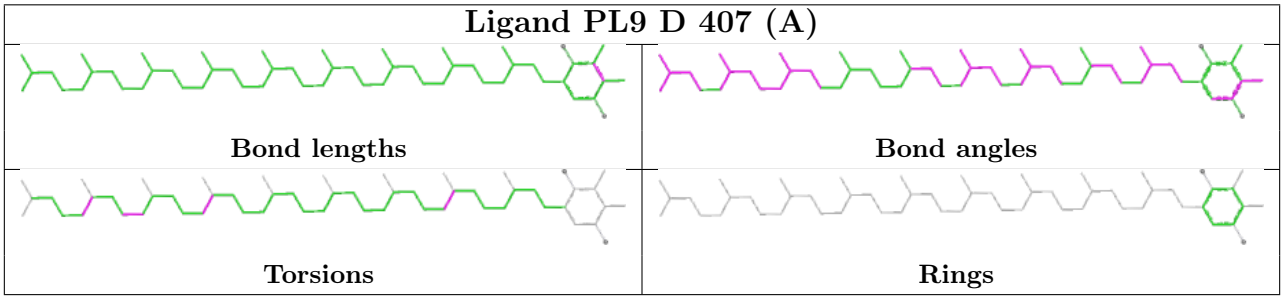
Ligand CLA d 401 (B)



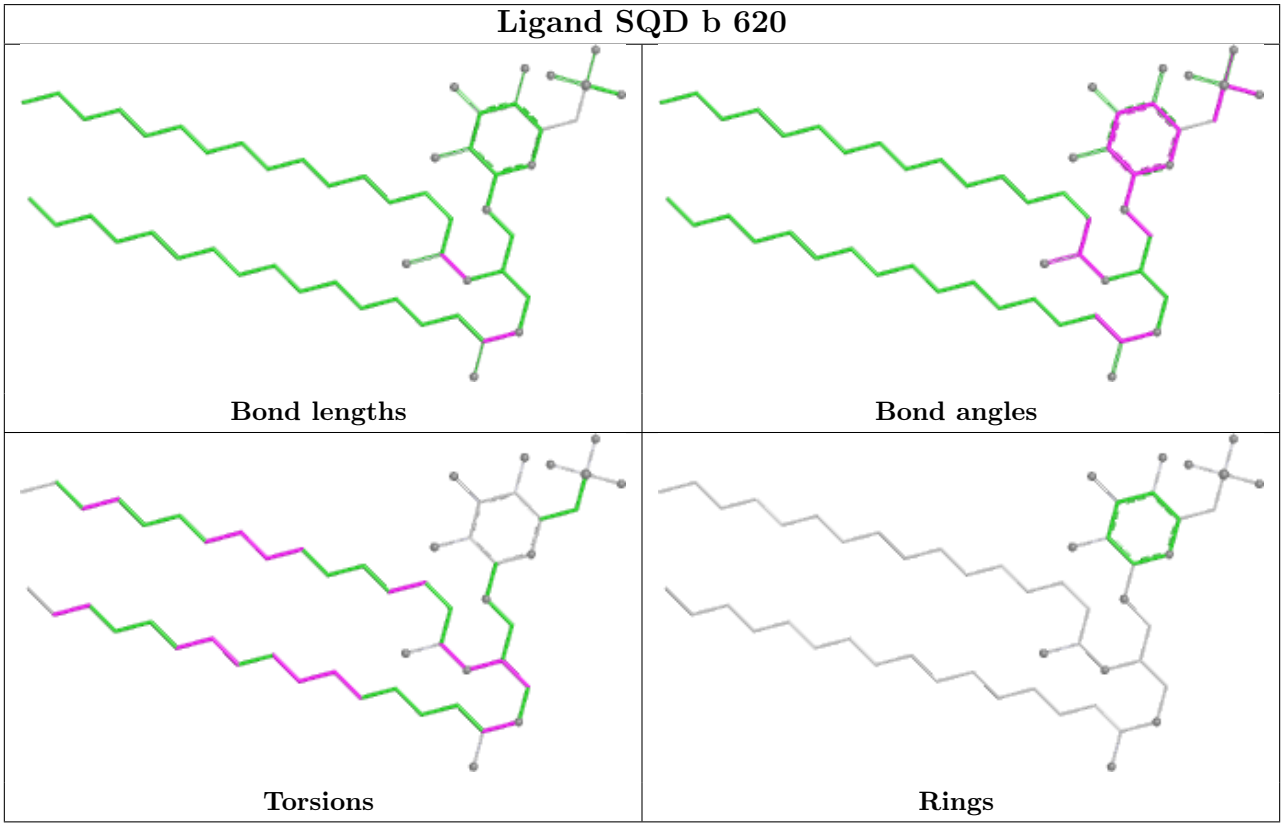
Ligand BCR H 101



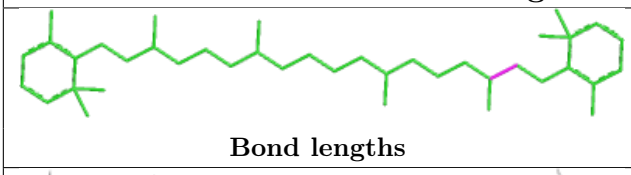
Ligand PL9 D 407 (A)

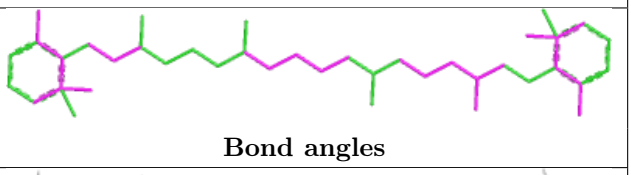


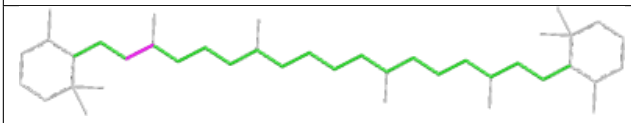
Ligand SQD b 620

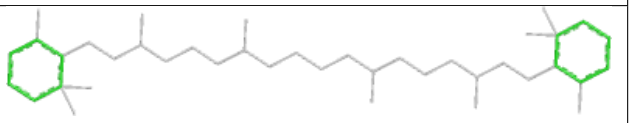


Ligand BCR c 516

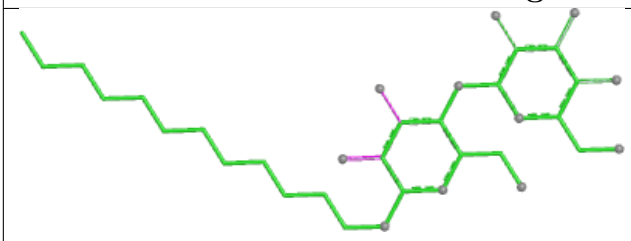

Bond lengths

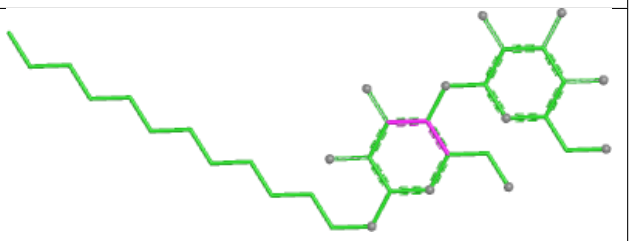

Bond angles

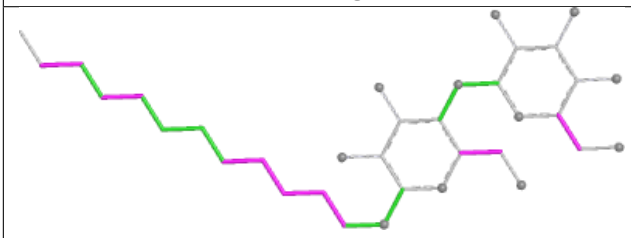

Torsions

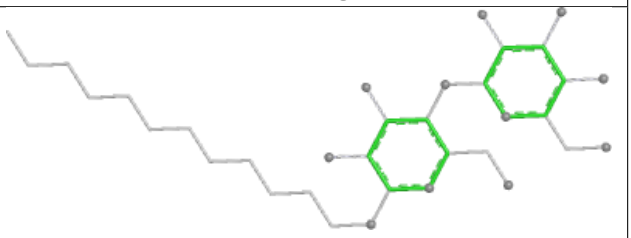

Rings

Ligand LMT c 501

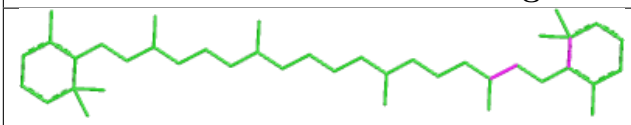

Bond lengths

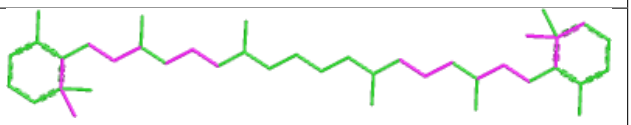

Bond angles

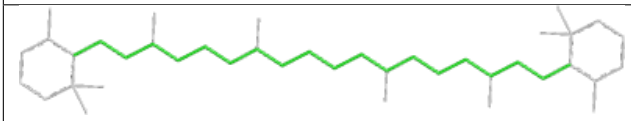

Torsions

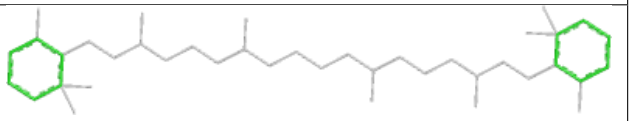

Rings

Ligand BCR B 619

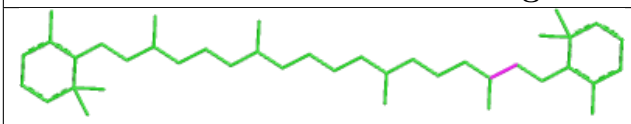

Bond lengths

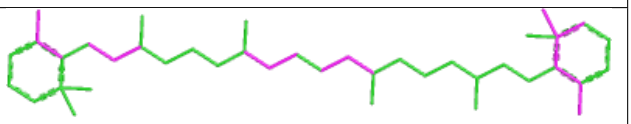

Bond angles


Torsions

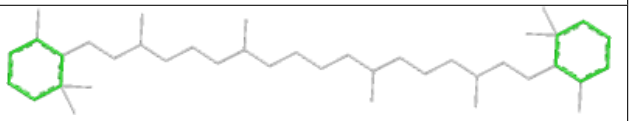

Rings

Ligand BCR C 516

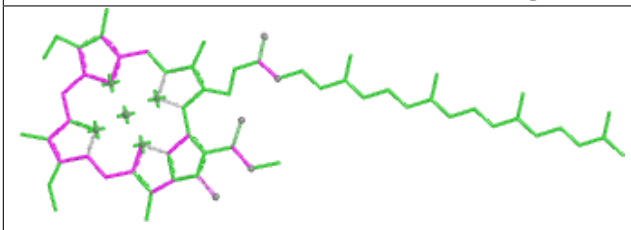

Bond lengths


Bond angles

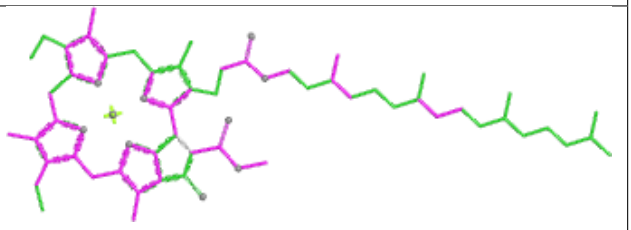

Torsions


Rings

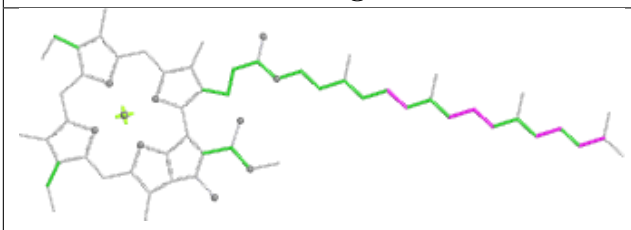
Ligand CLA B 615



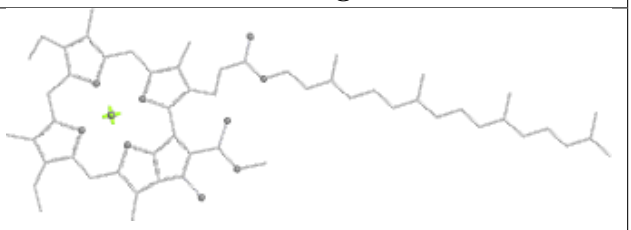
Bond lengths



Bond angles

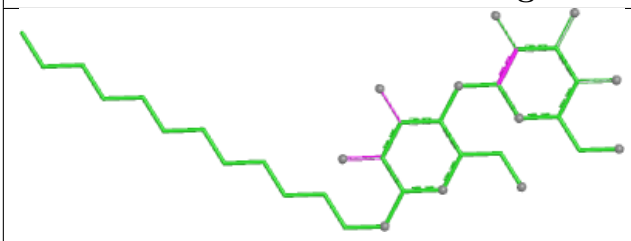


Torsions

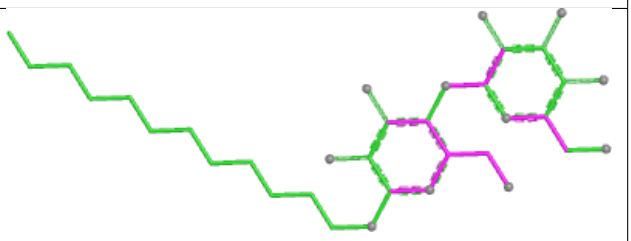


Rings

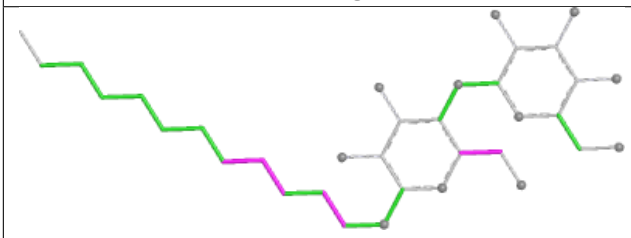
Ligand LMT M 101



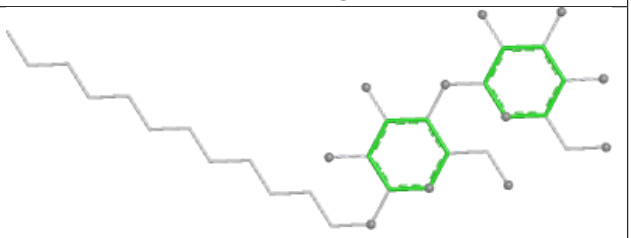
Bond lengths



Bond angles

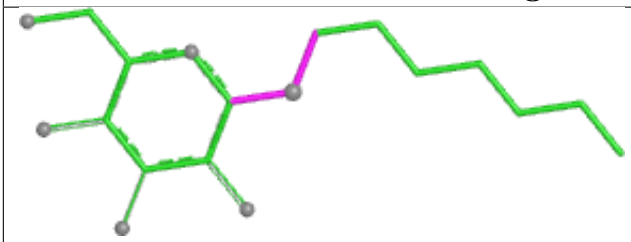


Torsions

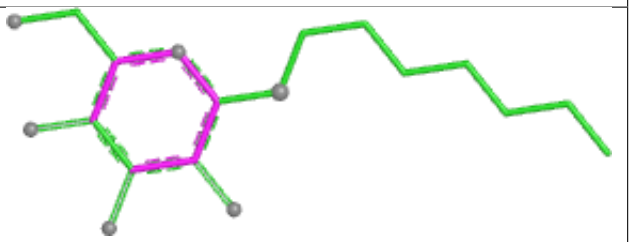


Rings

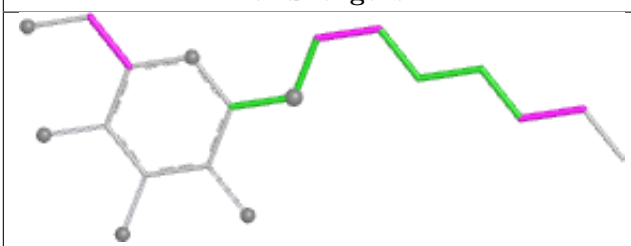
Ligand HTG b 625



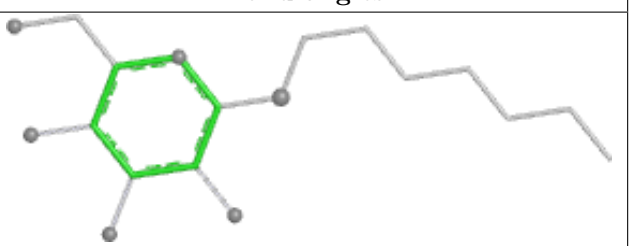
Bond lengths



Bond angles

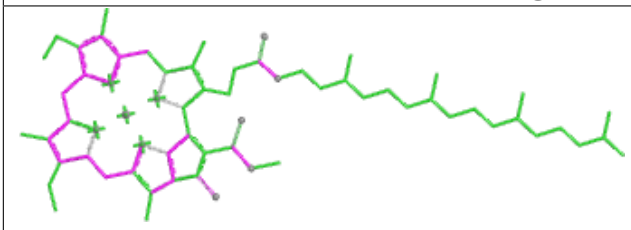


Torsions

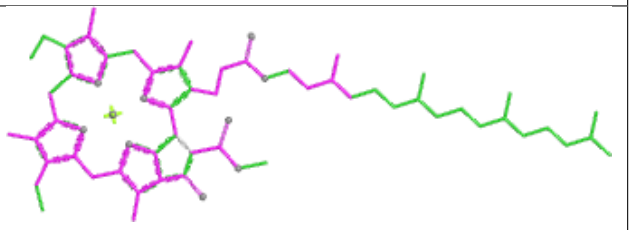


Rings

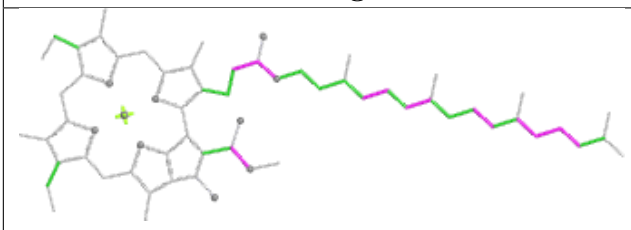
Ligand CLA c 513



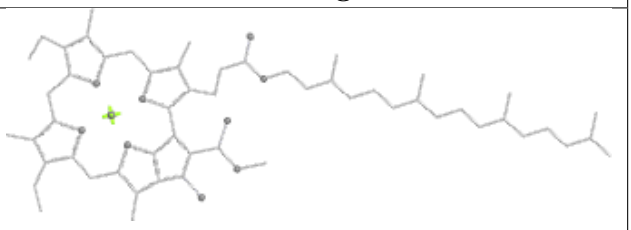
Bond lengths



Bond angles

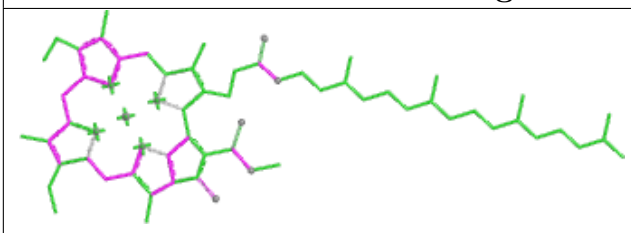


Torsions

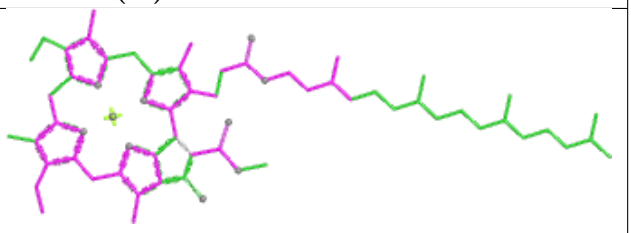


Rings

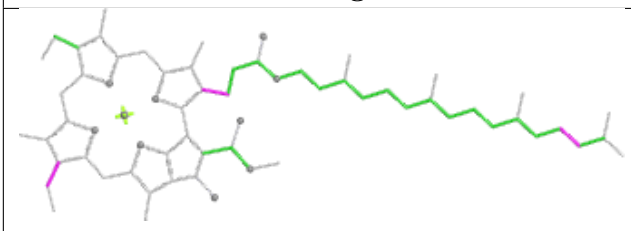
Ligand CLA a 406 (B)



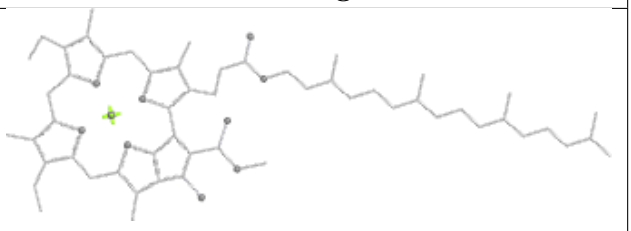
Bond lengths



Bond angles

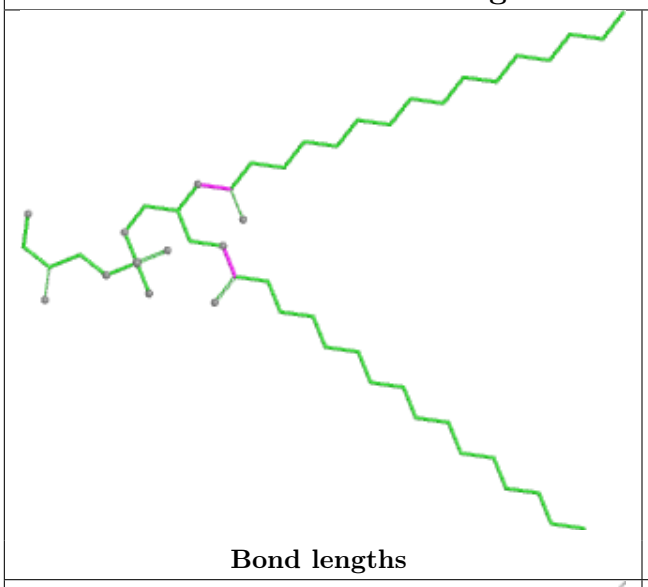


Torsions

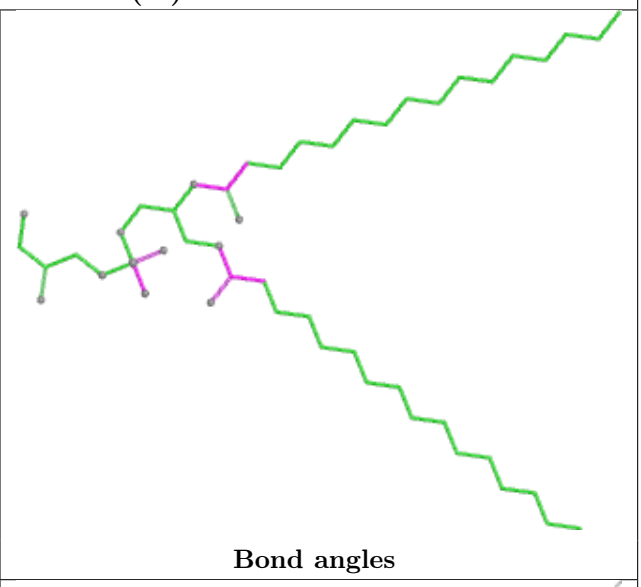


Rings

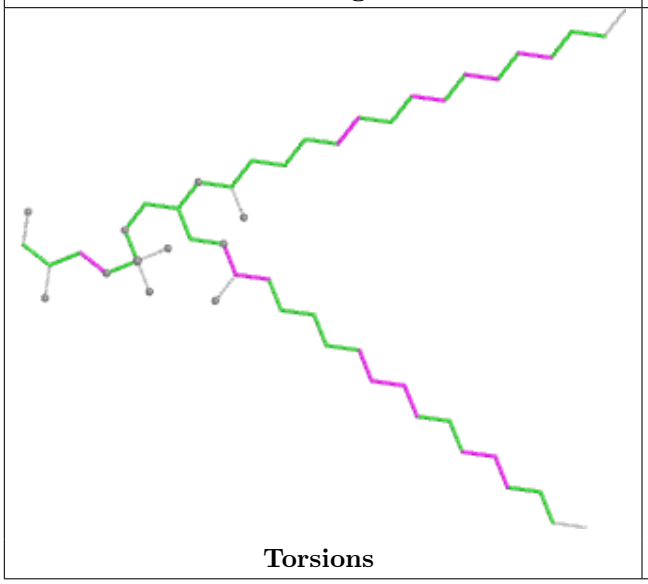
Ligand LHG D 409 (A)



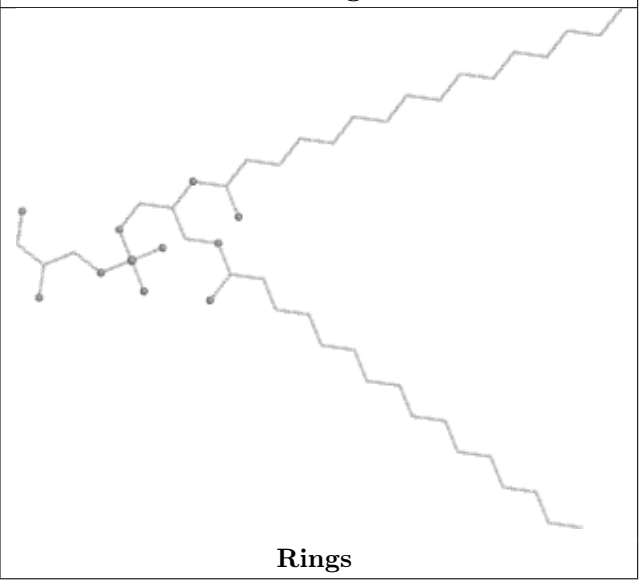
Bond lengths



Bond angles



Torsions

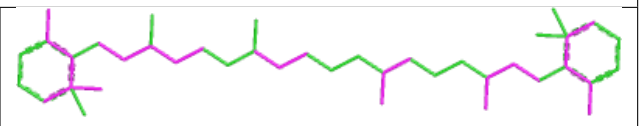


Rings

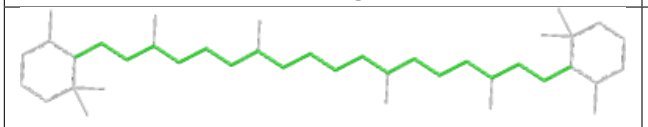
Ligand BCR C 517



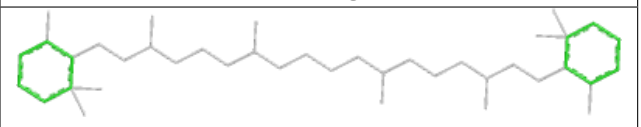
Bond lengths



Bond angles

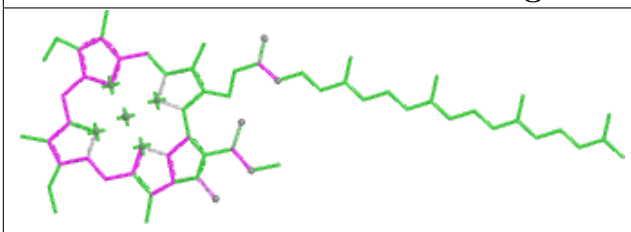


Torsions

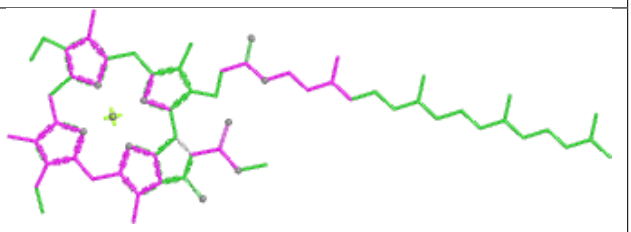


Rings

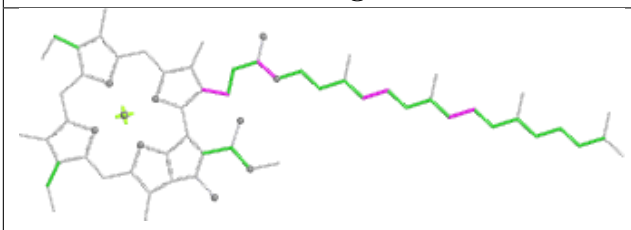
Ligand CLA C 513



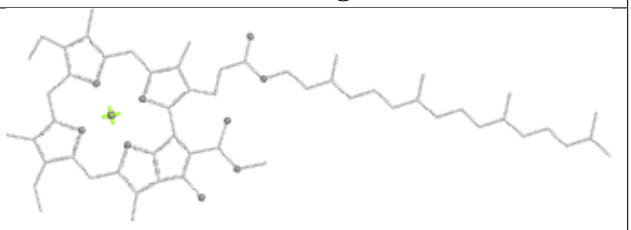
Bond lengths



Bond angles

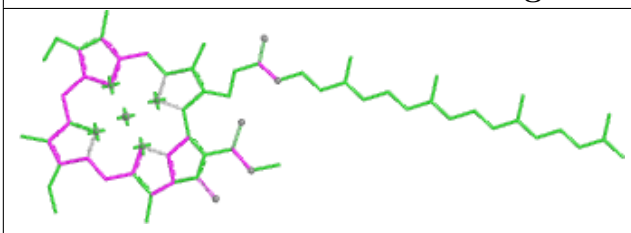


Torsions

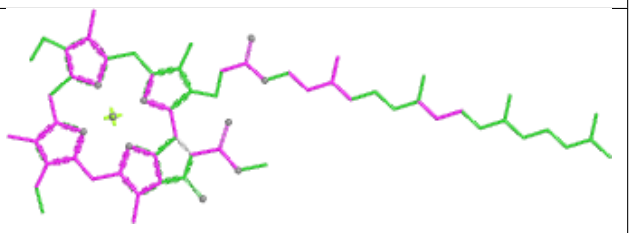


Rings

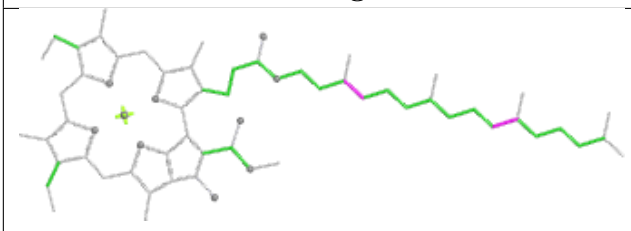
Ligand CLA C 507



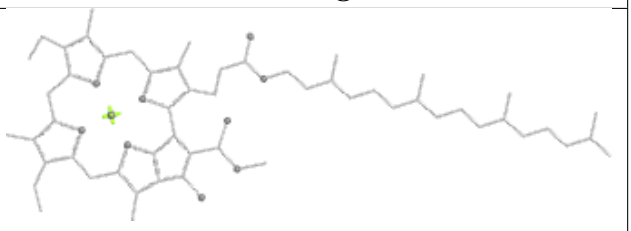
Bond lengths



Bond angles

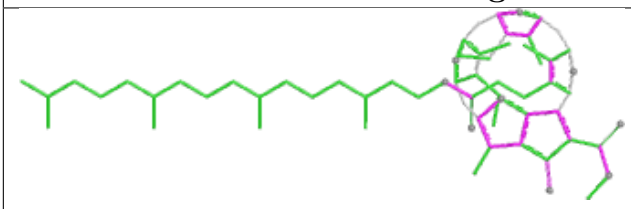


Torsions

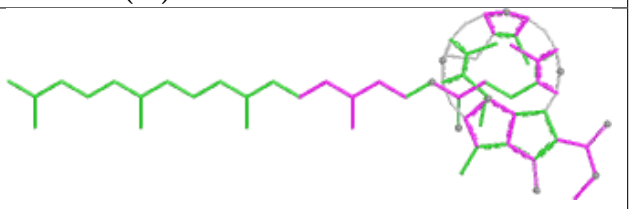


Rings

Ligand PHO D 402 (B)



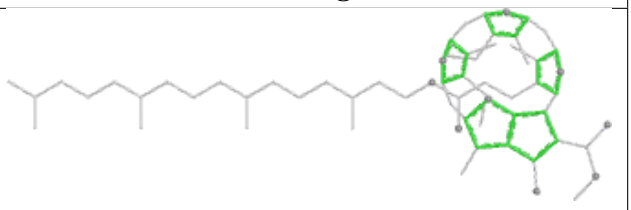
Bond lengths



Bond angles

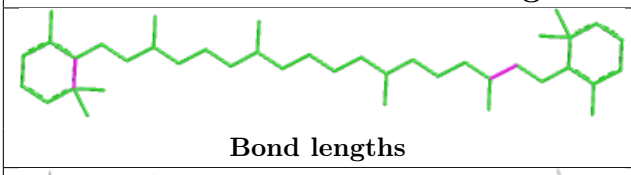


Torsions

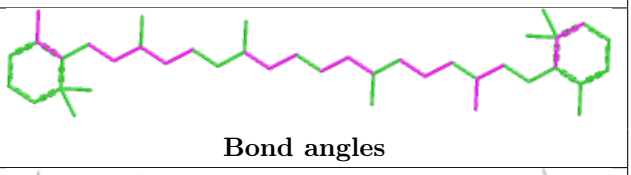


Rings

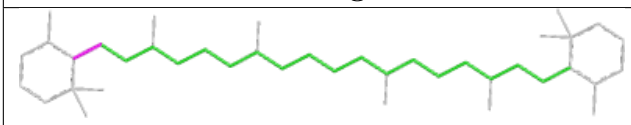
Ligand BCR B 617



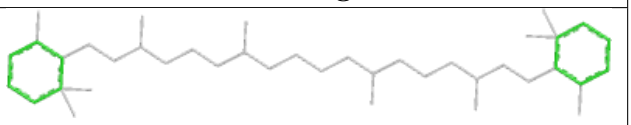
Bond lengths



Bond angles

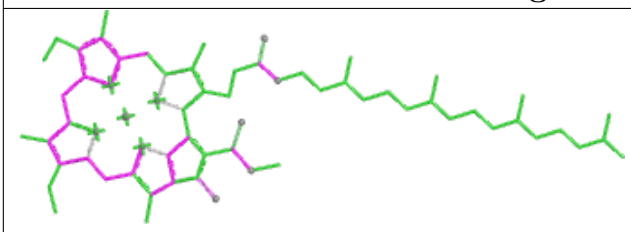


Torsions

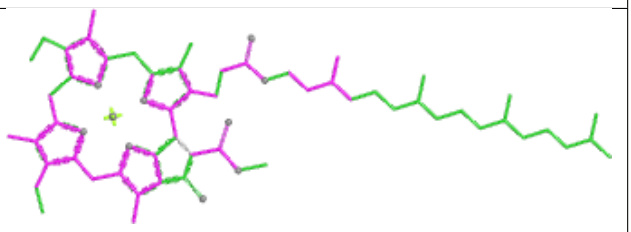


Rings

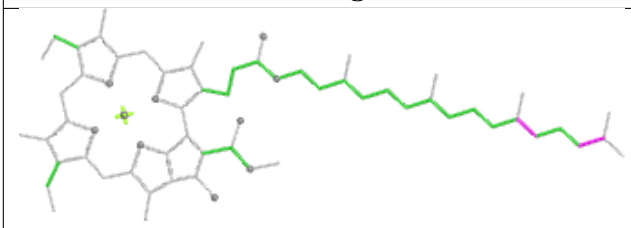
Ligand CLA c 509



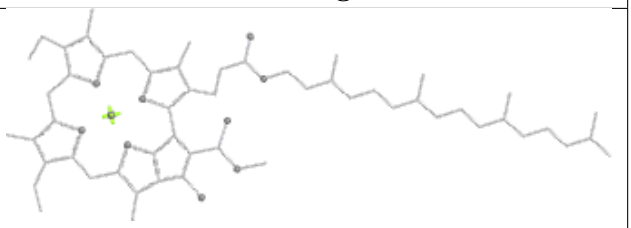
Bond lengths



Bond angles

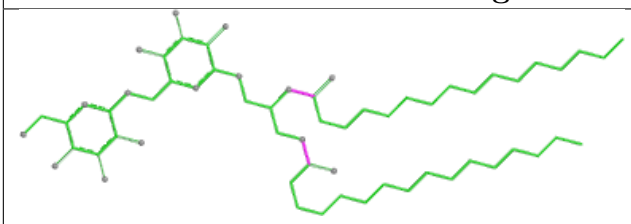


Torsions

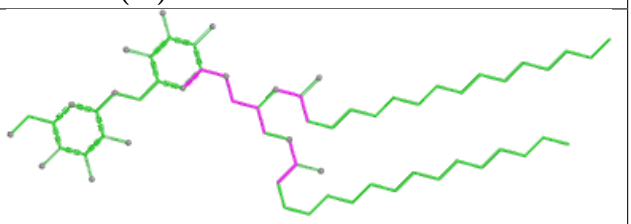


Rings

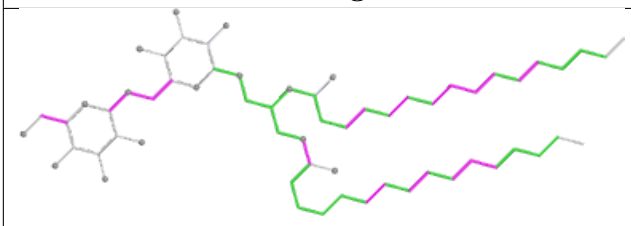
Ligand DGD c 517 (B)



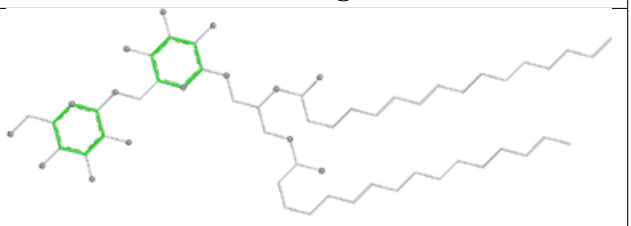
Bond lengths



Bond angles

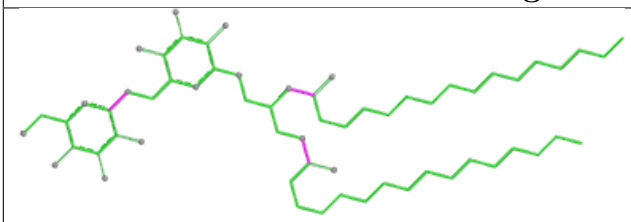


Torsions

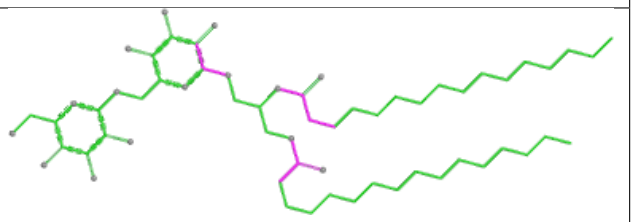


Rings

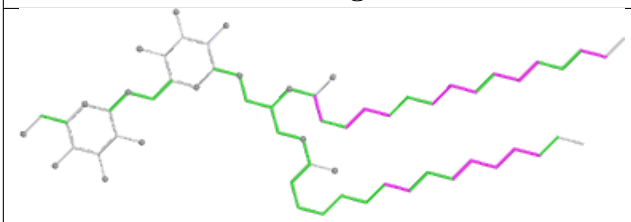
Ligand DGD h 102



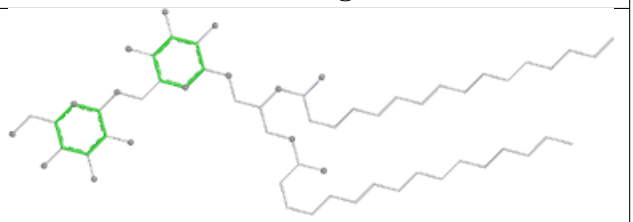
Bond lengths



Bond angles

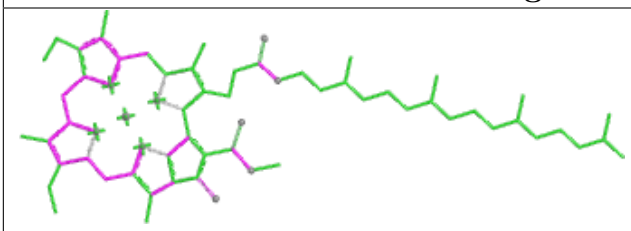


Torsions

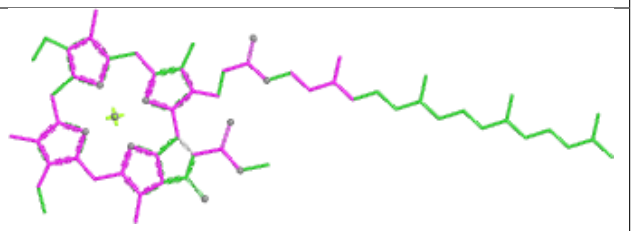


Rings

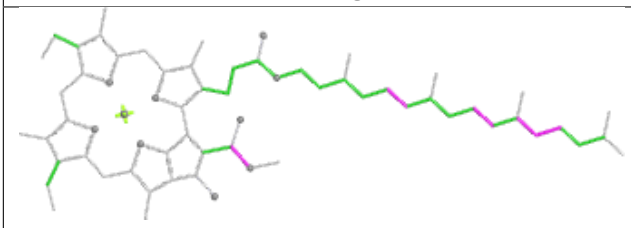
Ligand CLA C 510



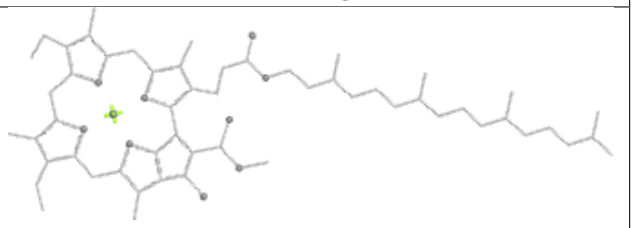
Bond lengths



Bond angles

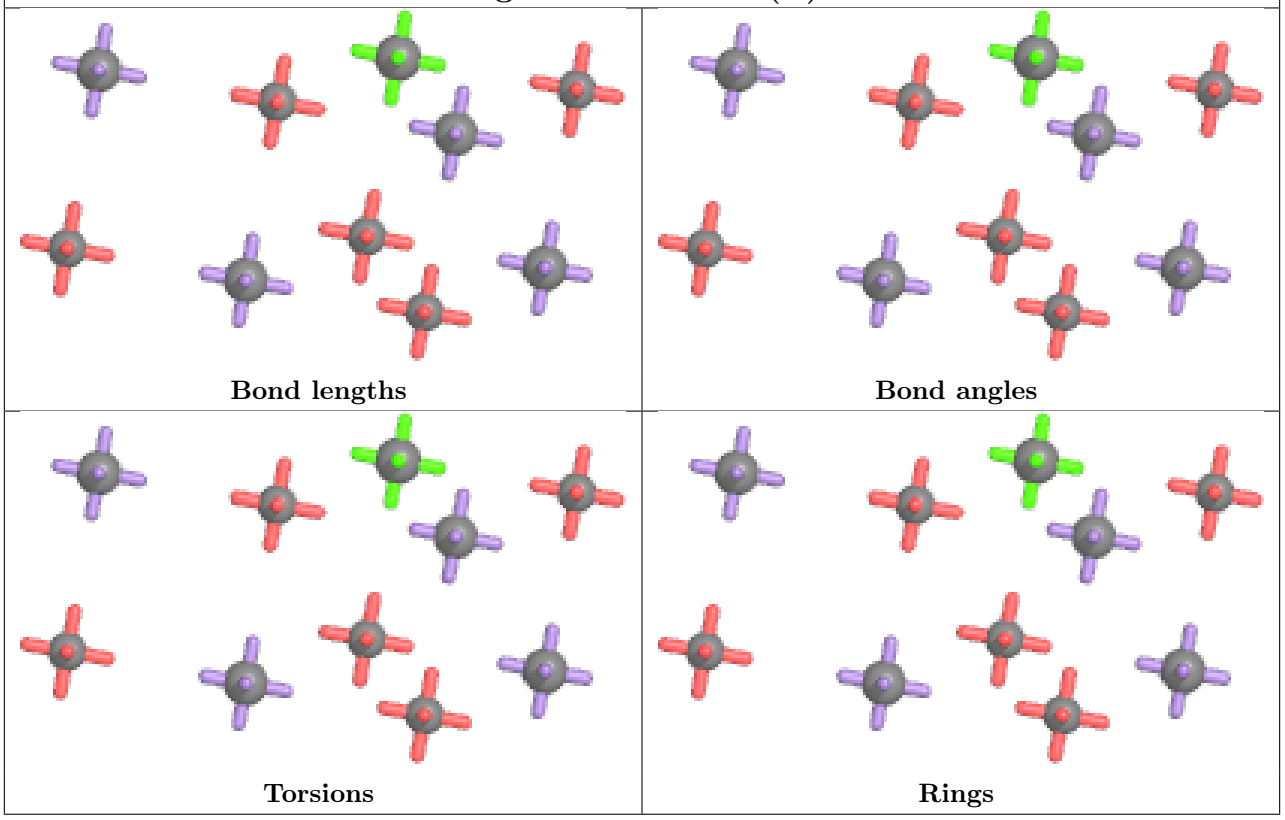


Torsions

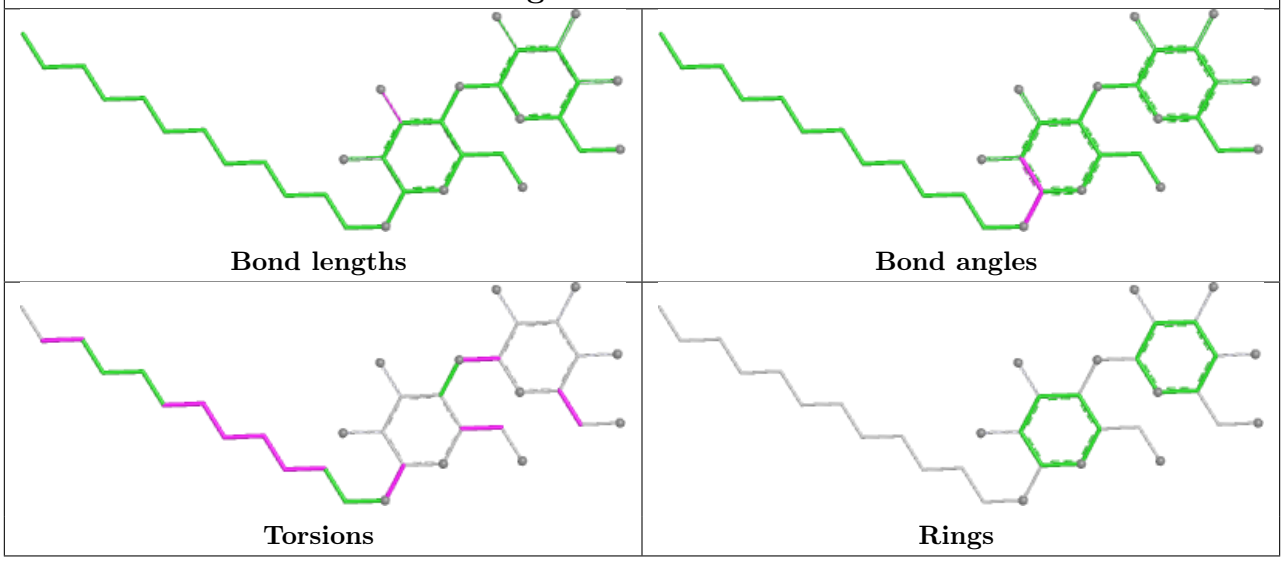


Rings

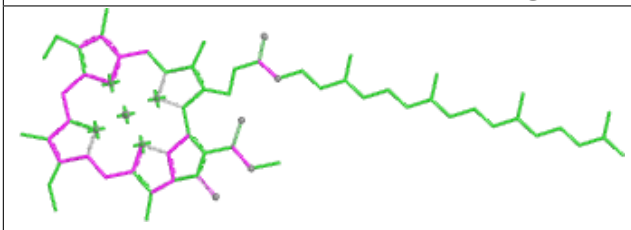
Ligand OEX a 413 (B)



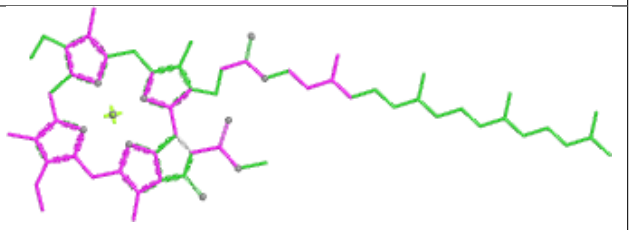
Ligand LMT e 101



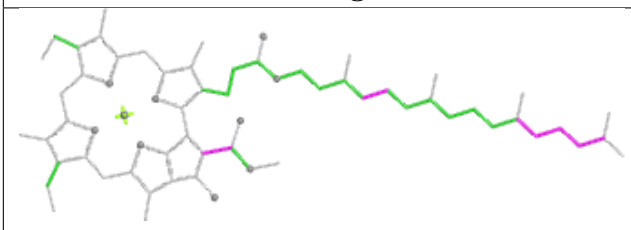
Ligand CLA C 504



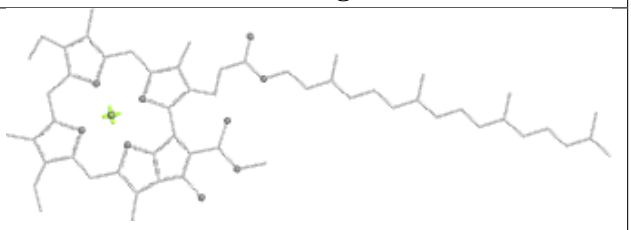
Bond lengths



Bond angles

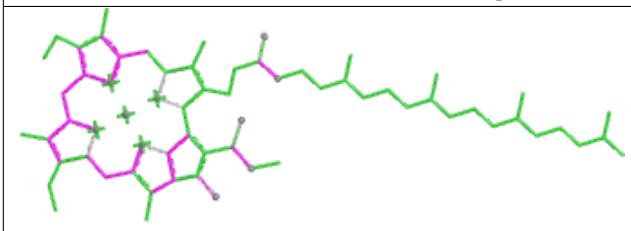


Torsions

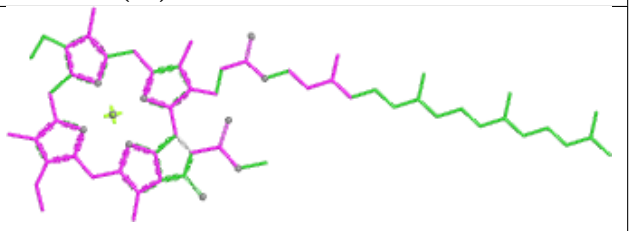


Rings

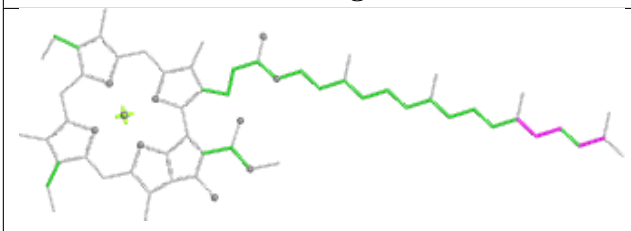
Ligand CLA A 406 (A)



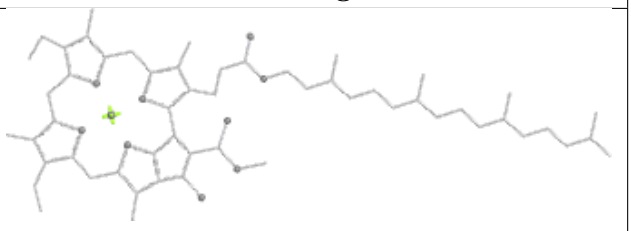
Bond lengths



Bond angles

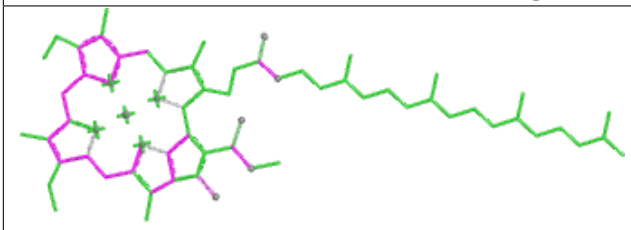


Torsions

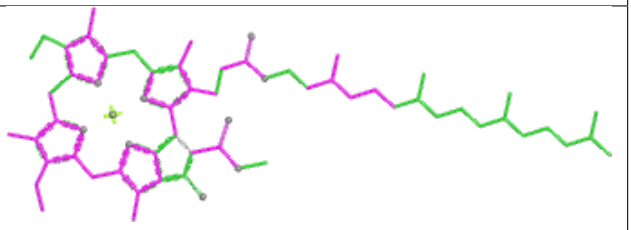


Rings

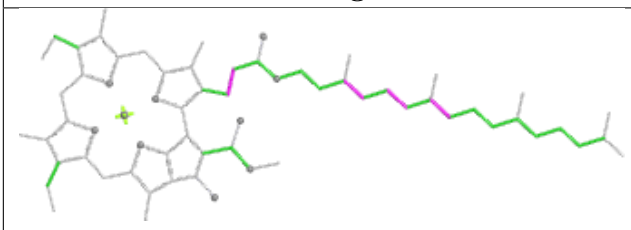
Ligand CLA b 603



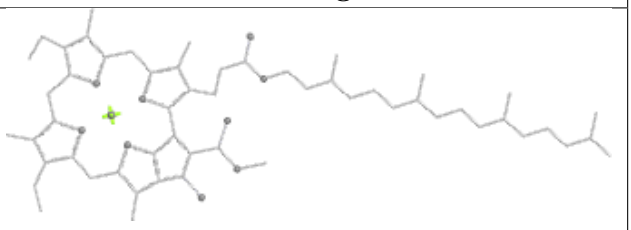
Bond lengths



Bond angles

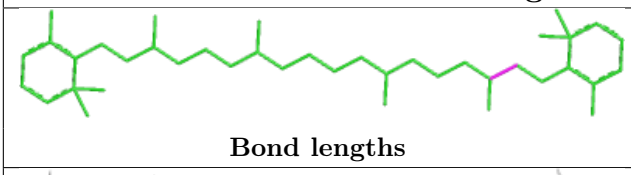


Torsions

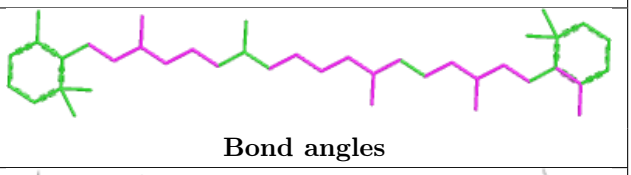


Rings

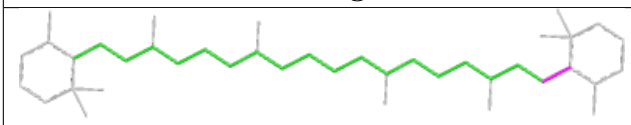
Ligand BCR h 101



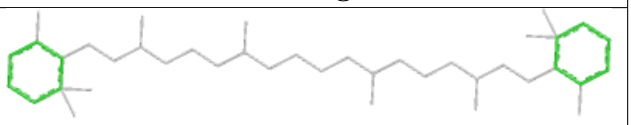
Bond lengths



Bond angles



Torsions



Rings

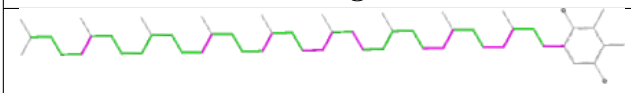
Ligand PL9 a 414 (B)



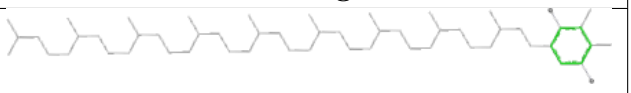
Bond lengths



Bond angles

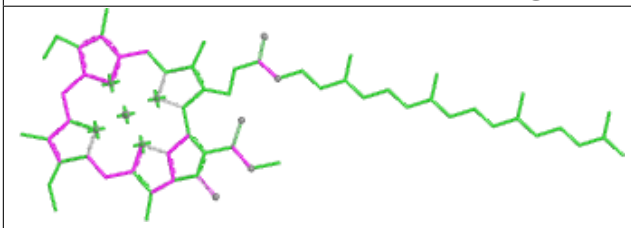


Torsions

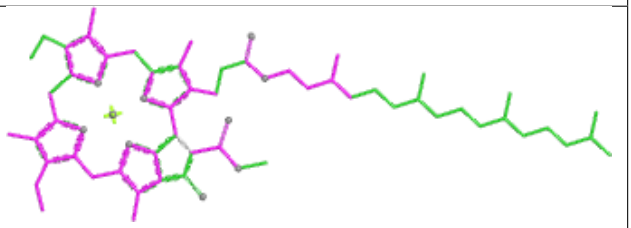


Rings

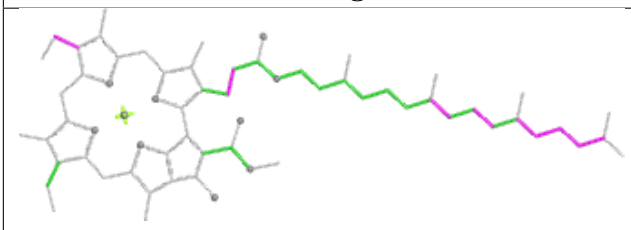
Ligand CLA b 606



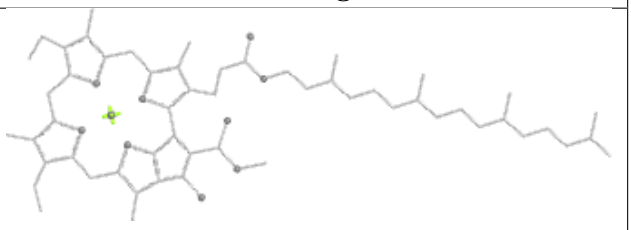
Bond lengths



Bond angles

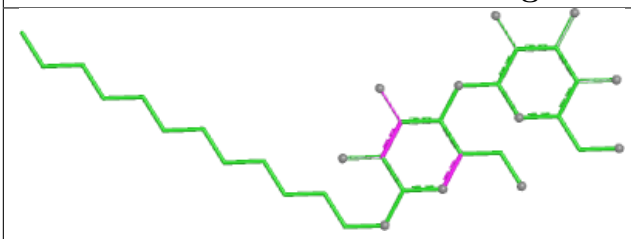


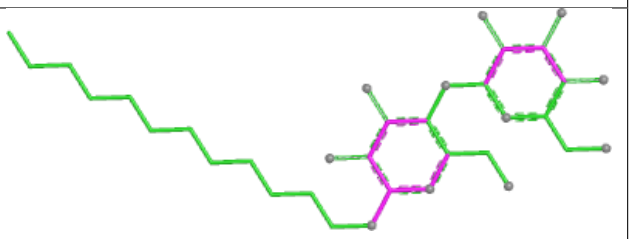
Torsions

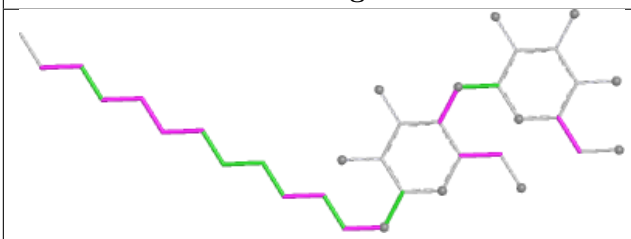


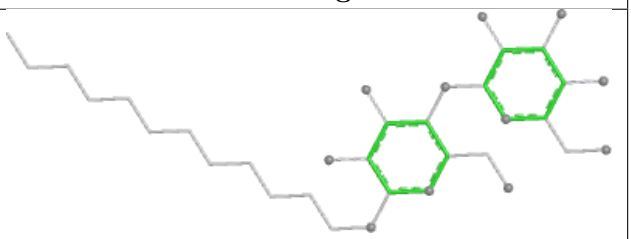
Rings

Ligand LMT B 628

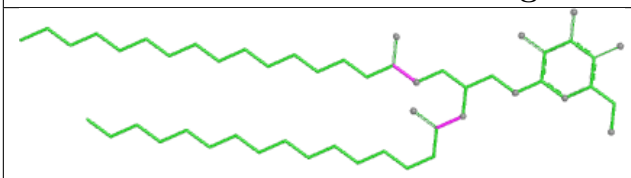

Bond lengths

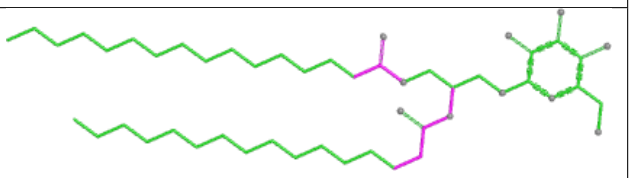

Bond angles

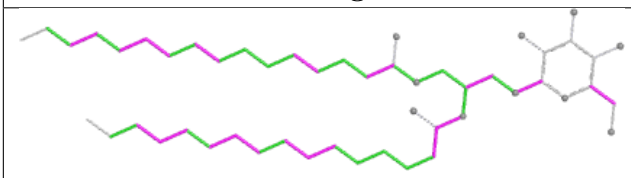

Torsions

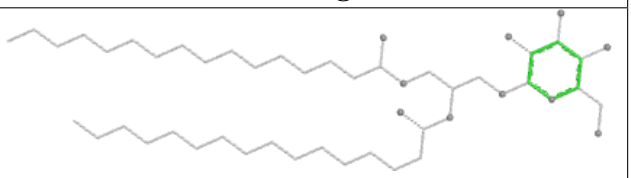

Rings

Ligand LMG B 621

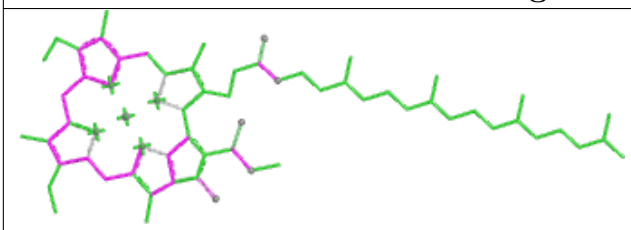

Bond lengths

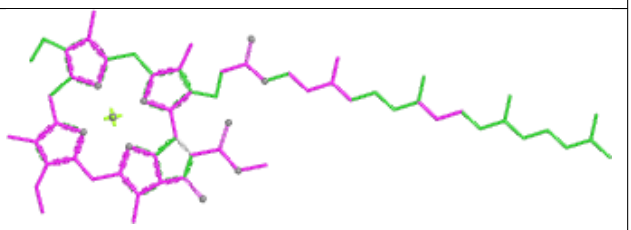

Bond angles

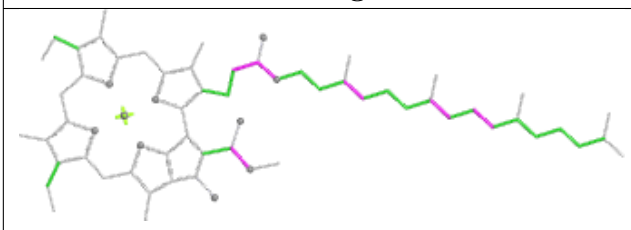

Torsions

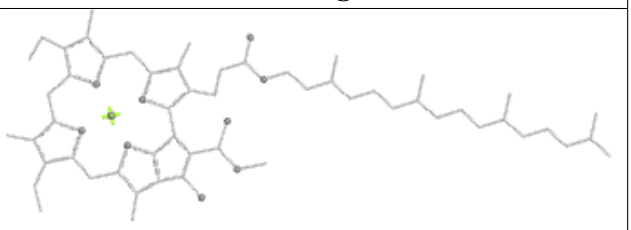

Rings

Ligand CLA c 511

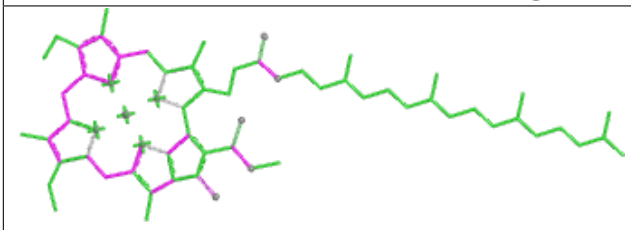

Bond lengths


Bond angles

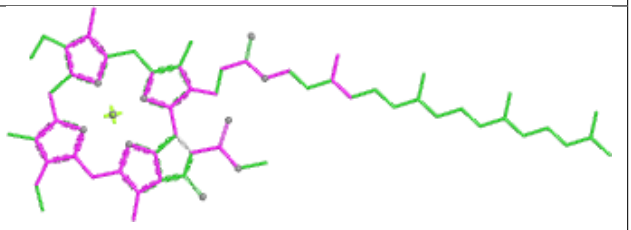

Torsions


Rings

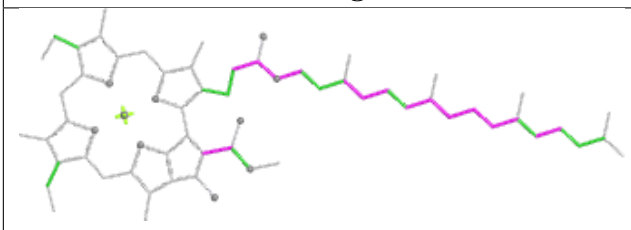
Ligand CLA b 601



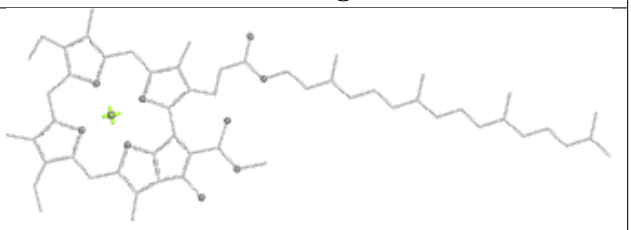
Bond lengths



Bond angles

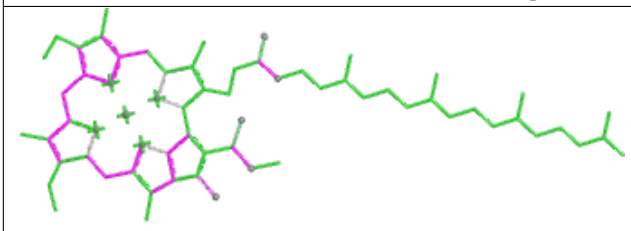


Torsions

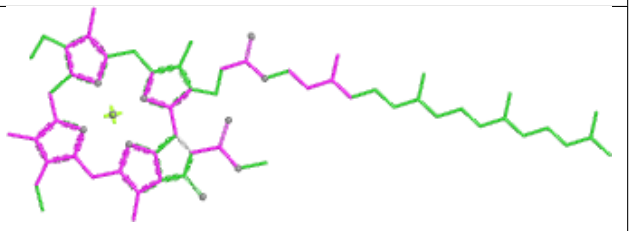


Rings

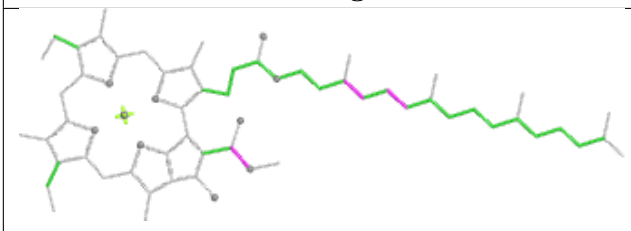
Ligand CLA B 605



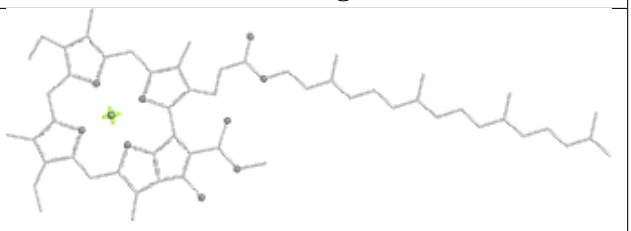
Bond lengths



Bond angles

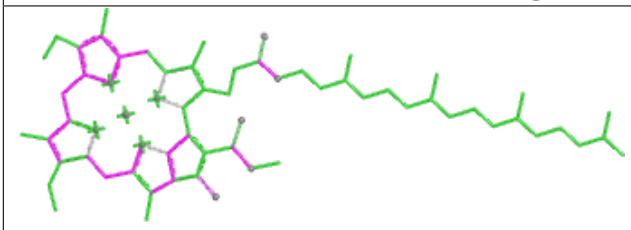


Torsions

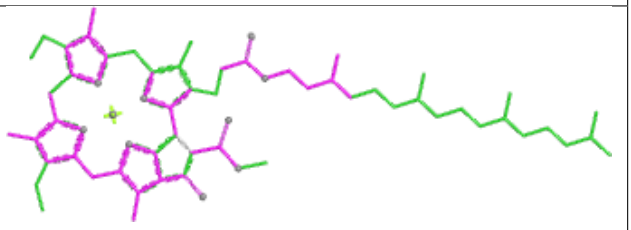


Rings

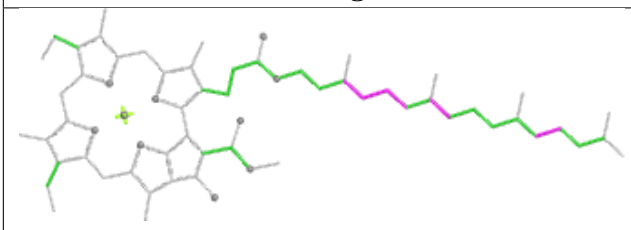
Ligand CLA b 605



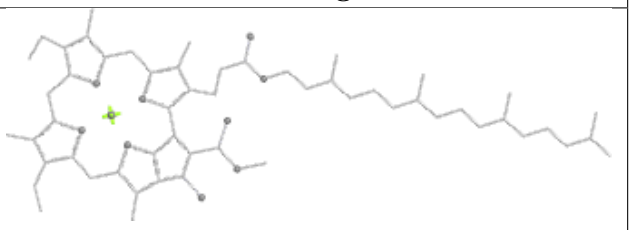
Bond lengths



Bond angles

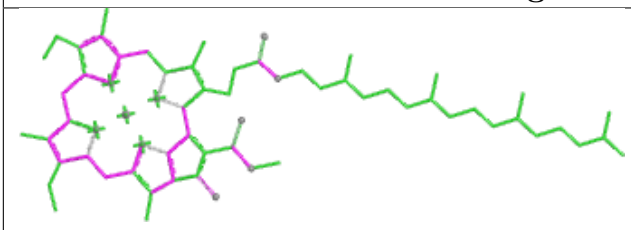


Torsions

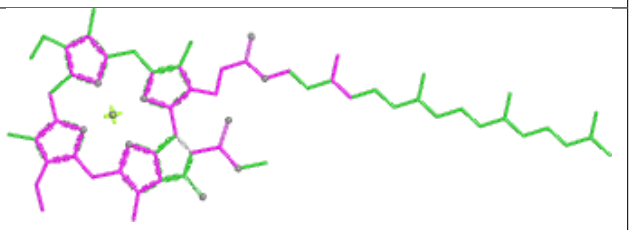


Rings

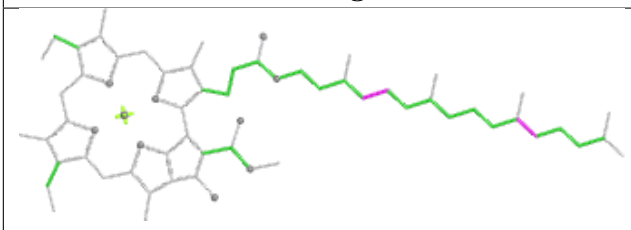
Ligand CLA b 607



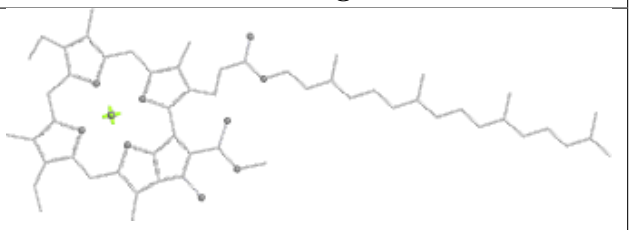
Bond lengths



Bond angles

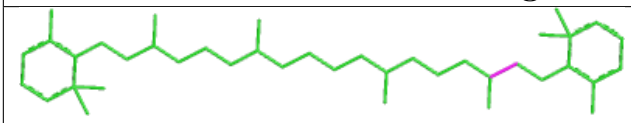


Torsions

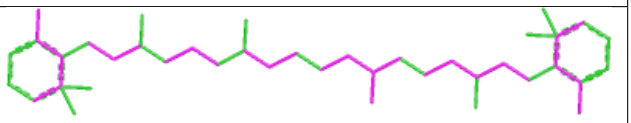


Rings

Ligand BCR K 102



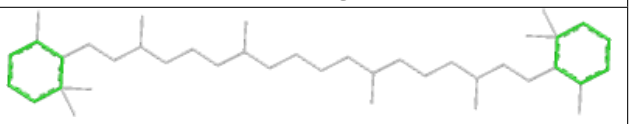
Bond lengths



Bond angles



Torsions

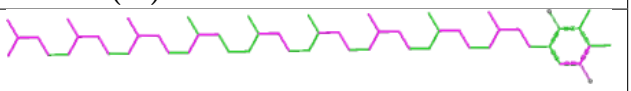


Rings

Ligand PL9 d 404 (A)



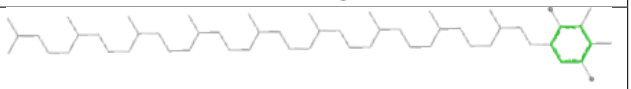
Bond lengths



Bond angles

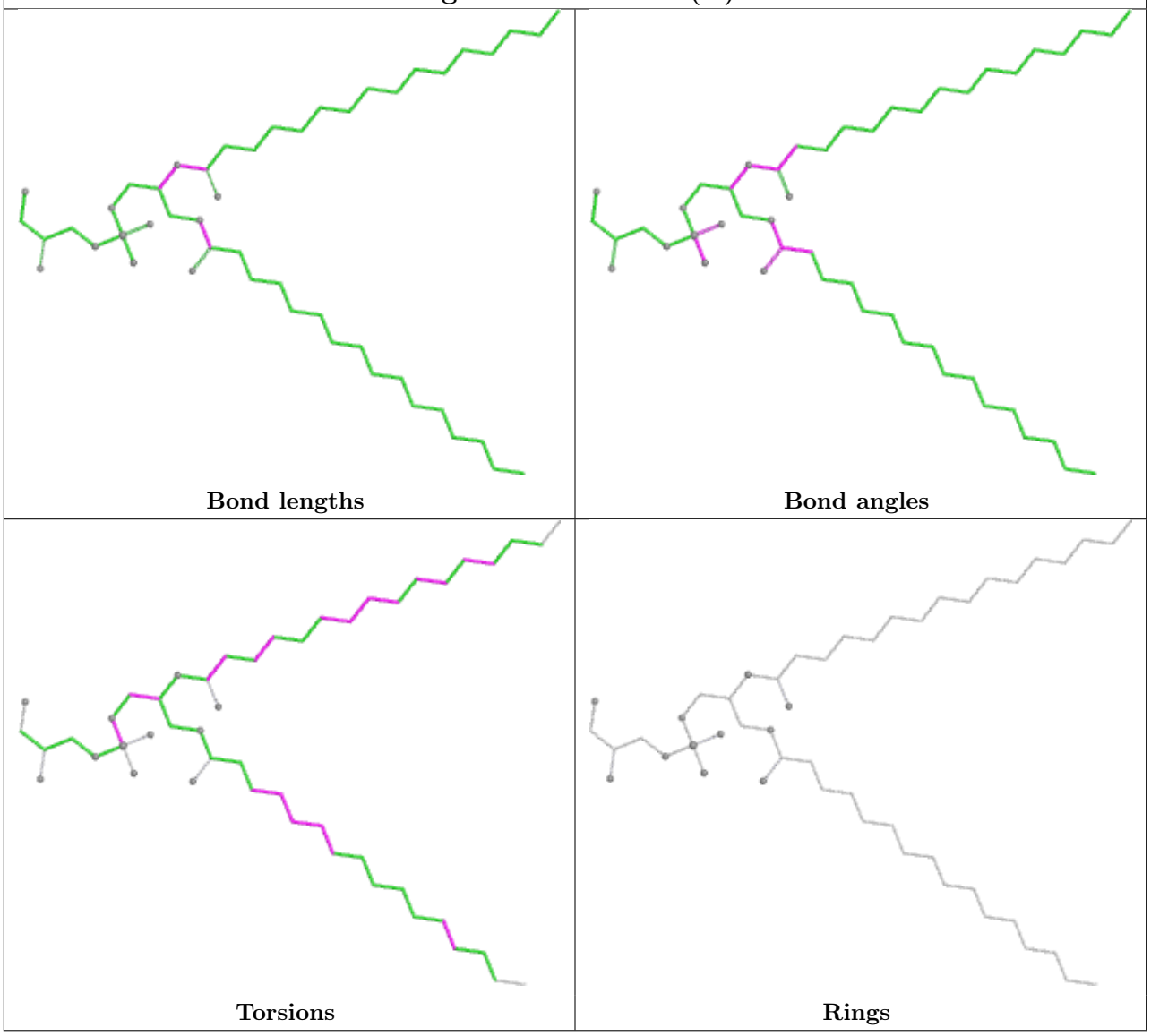


Torsions

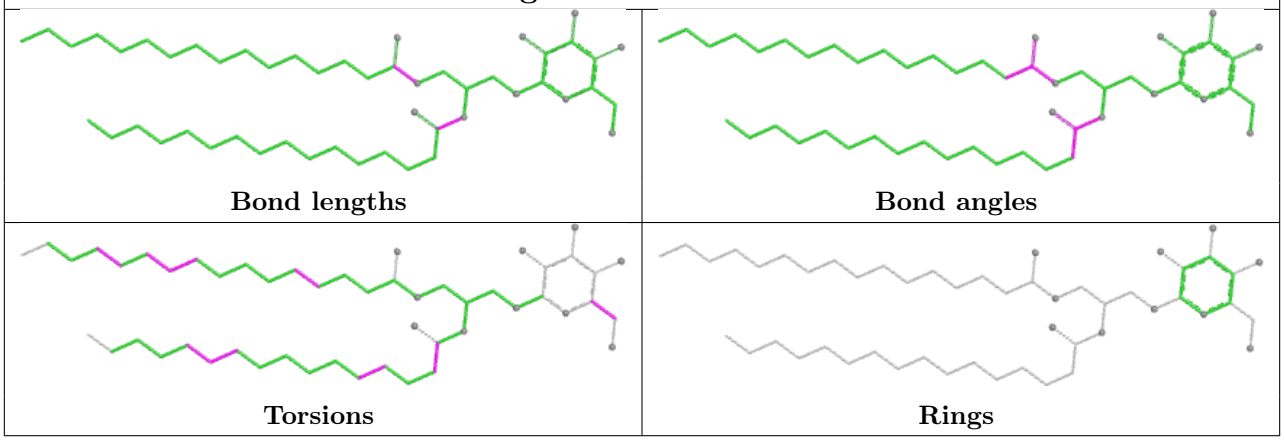


Rings

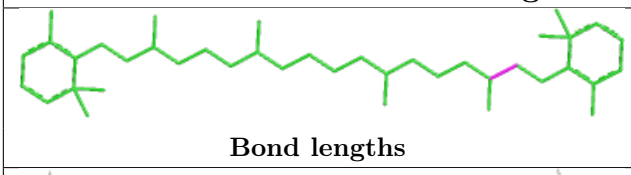
Ligand LHG L 101 (B)



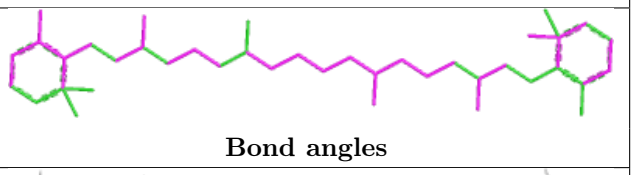
Ligand LMG D 413



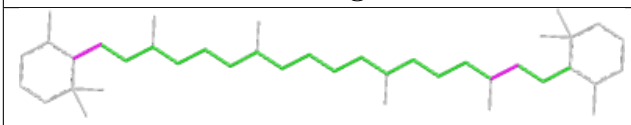
Ligand BCR Y 101



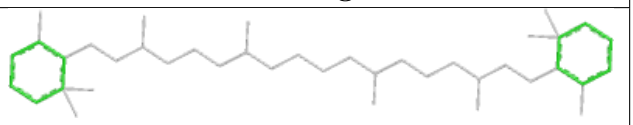
Bond lengths



Bond angles

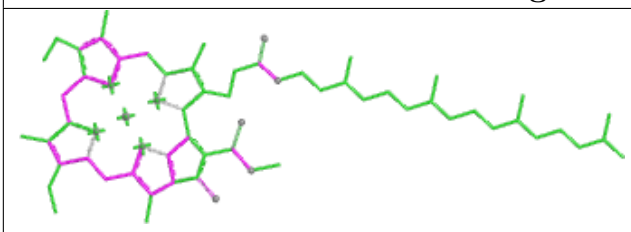


Torsions

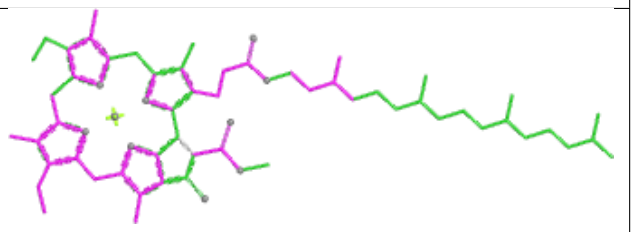


Rings

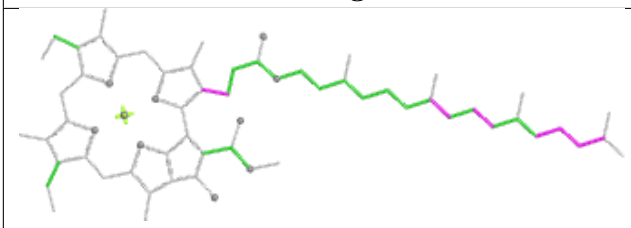
Ligand CLA c 507



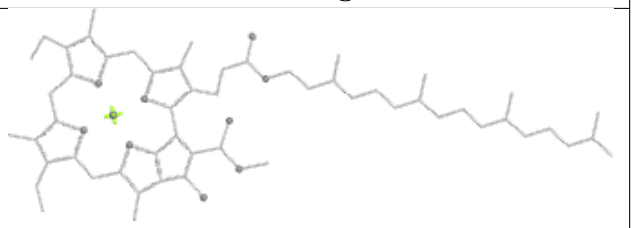
Bond lengths



Bond angles

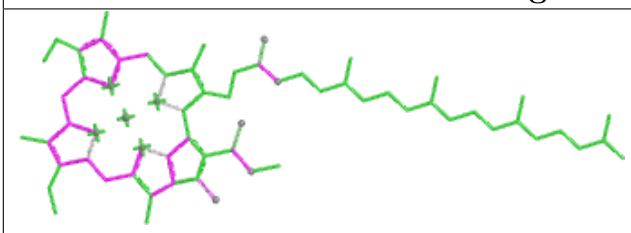


Torsions

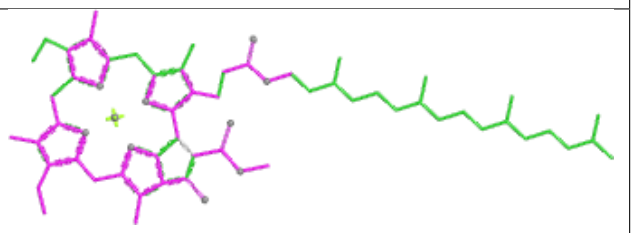


Rings

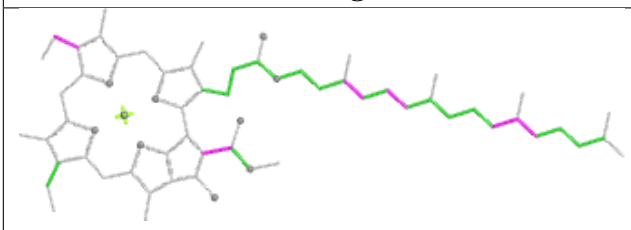
Ligand CLA c 505



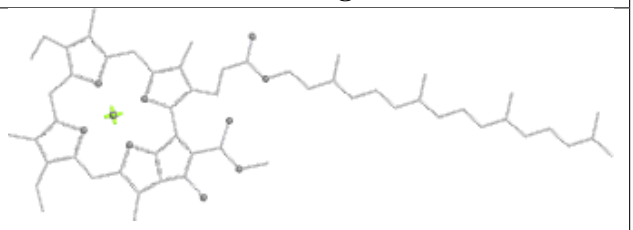
Bond lengths



Bond angles

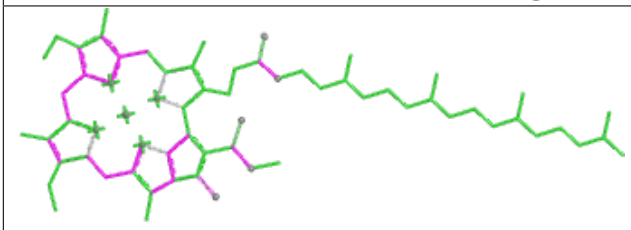


Torsions

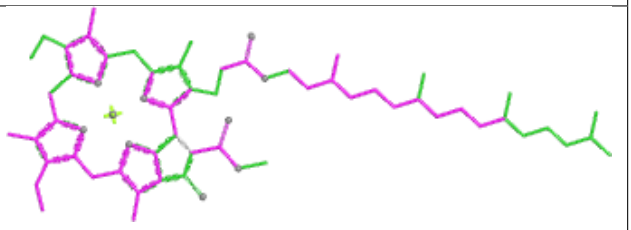


Rings

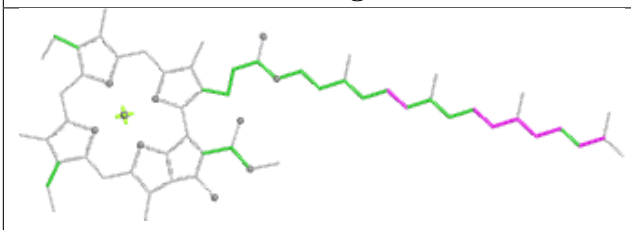
Ligand CLA b 615



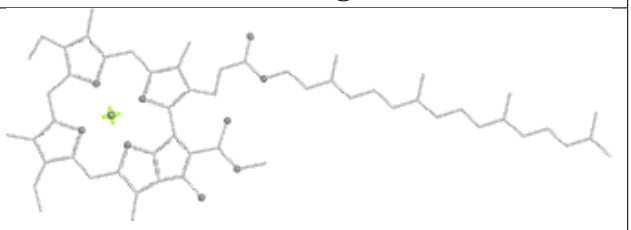
Bond lengths



Bond angles



Torsions

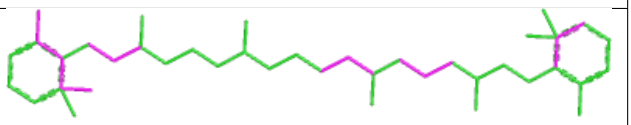


Rings

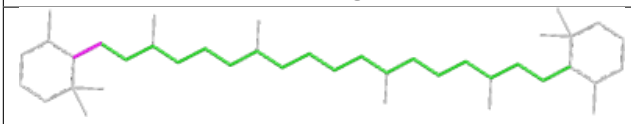
Ligand BCR b 617



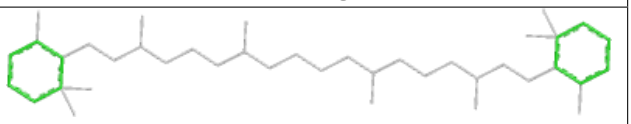
Bond lengths



Bond angles

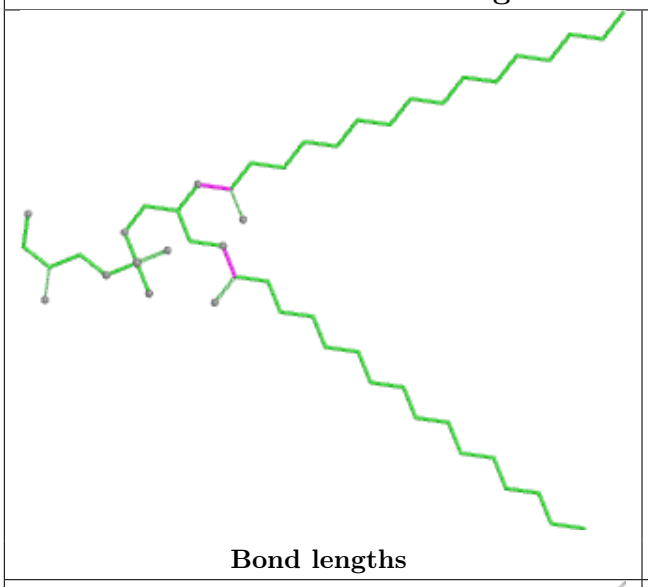


Torsions

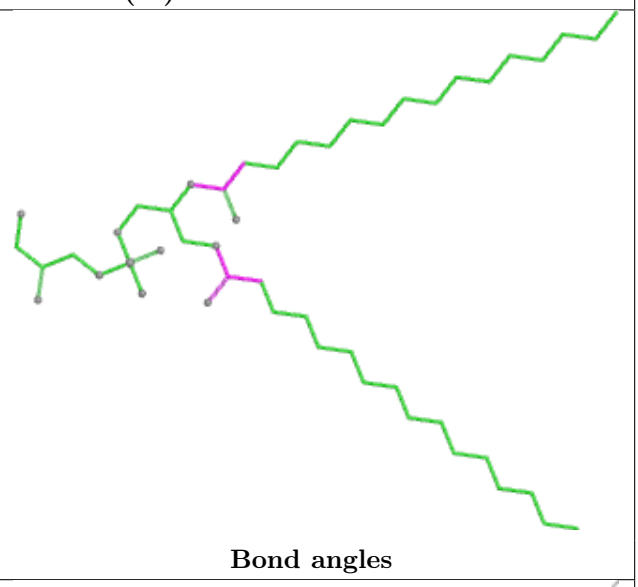


Rings

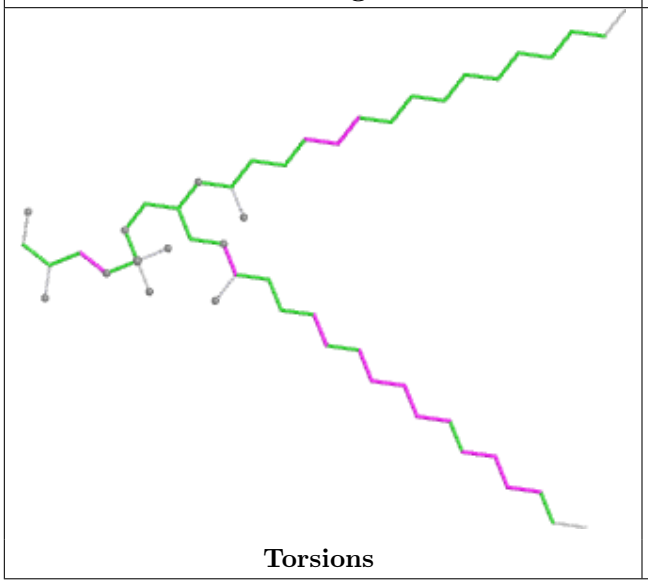
Ligand LHG d 406 (A)



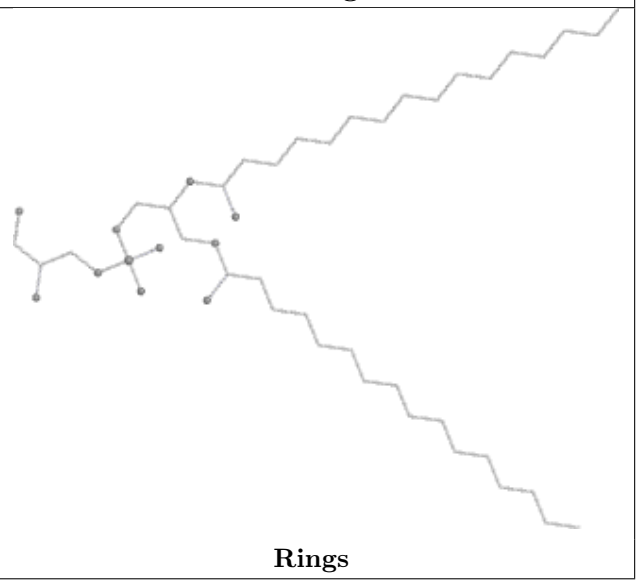
Bond lengths



Bond angles

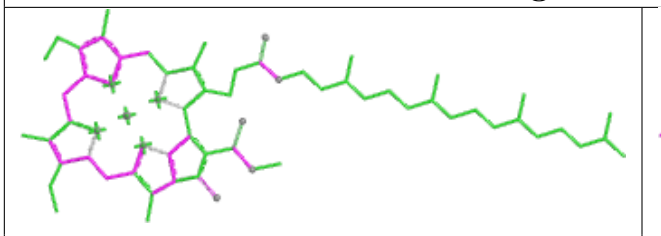


Torsions

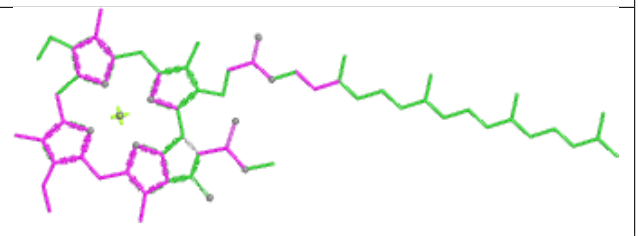


Rings

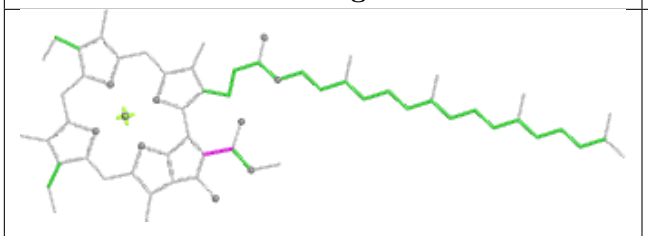
Ligand CLA c 503



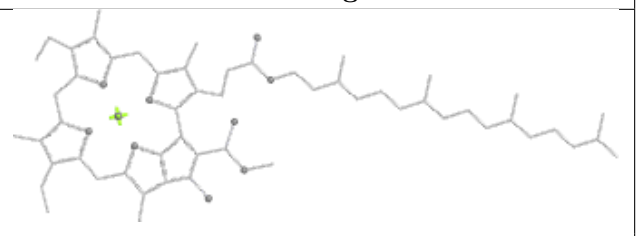
Bond lengths



Bond angles



Torsions

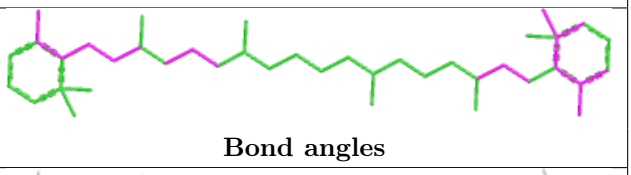


Rings

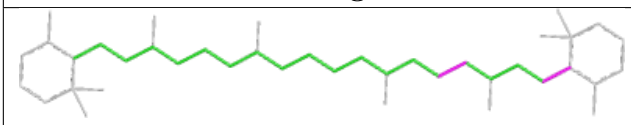
Ligand BCR a 410



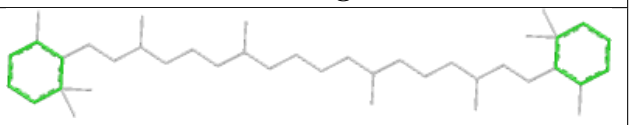
Bond lengths



Bond angles

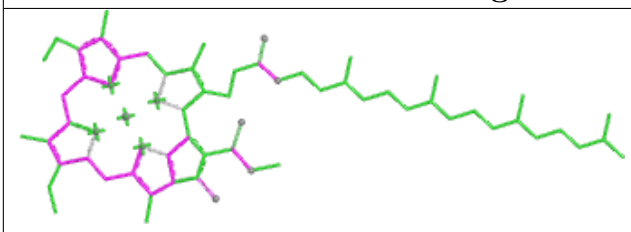


Torsions

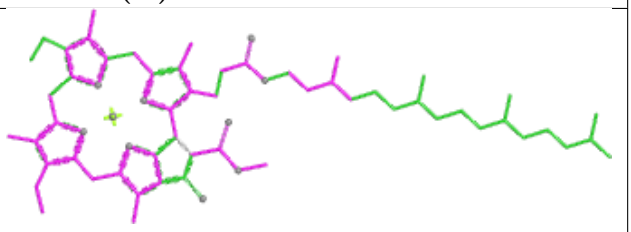


Rings

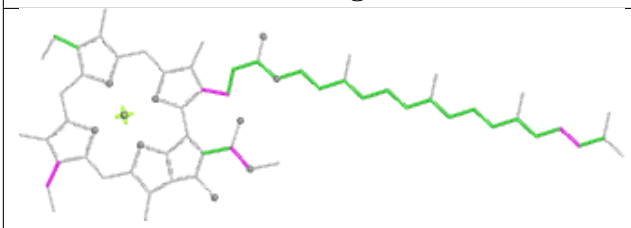
Ligand CLA A 405 (B)



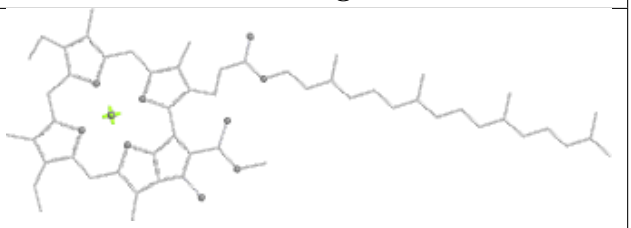
Bond lengths



Bond angles

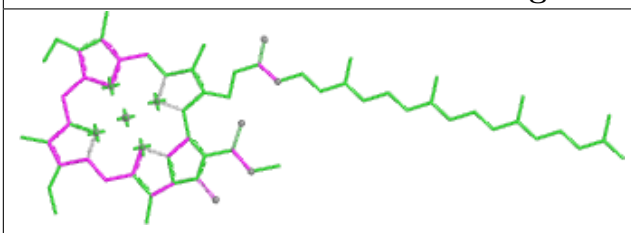


Torsions

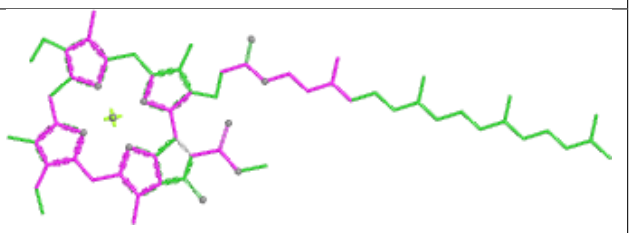


Rings

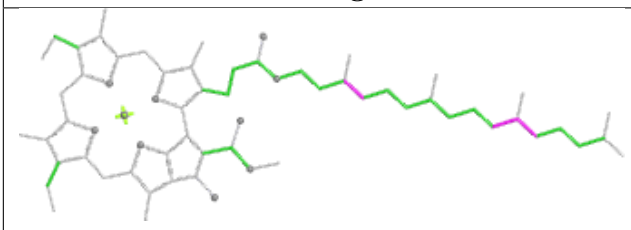
Ligand CLA c 506



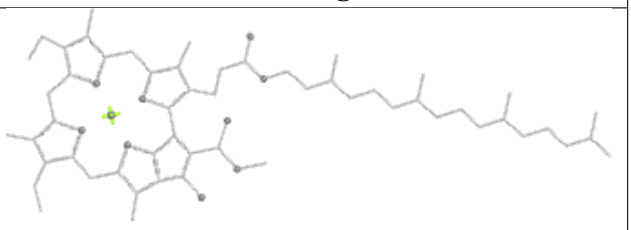
Bond lengths



Bond angles

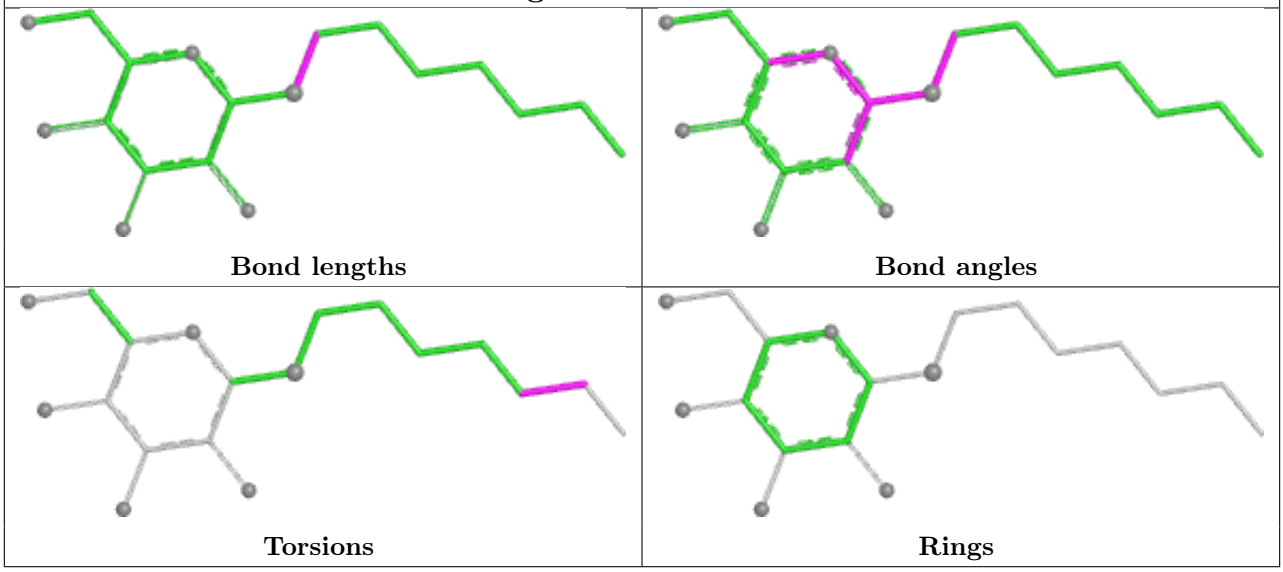


Torsions

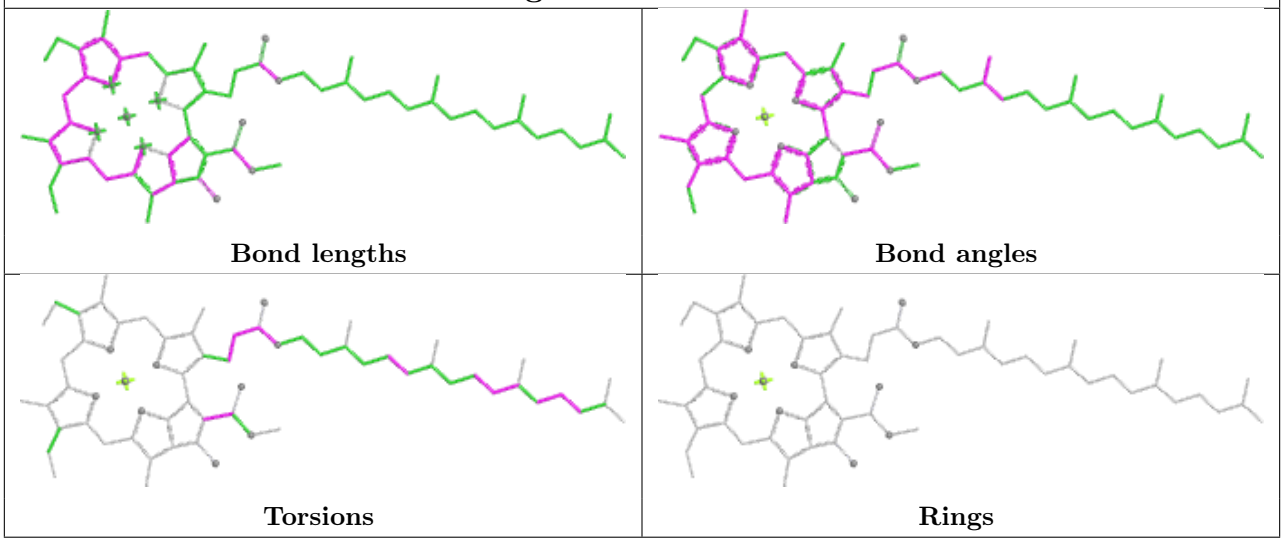


Rings

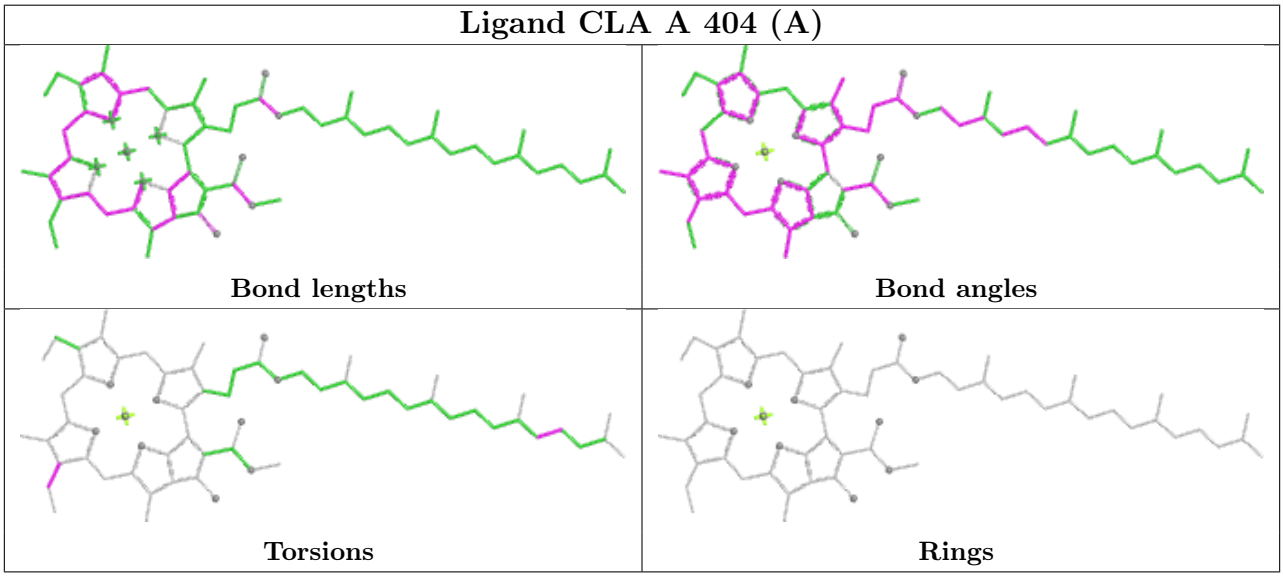
Ligand HTG c 522



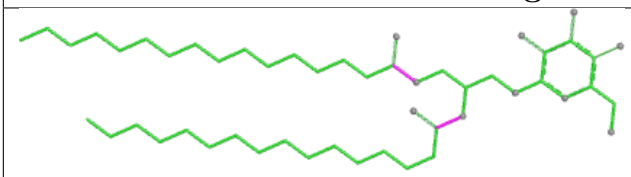
Ligand CLA B 601



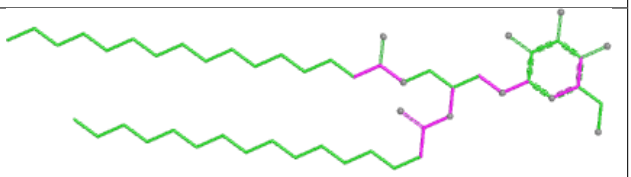
Ligand CLA A 404 (A)



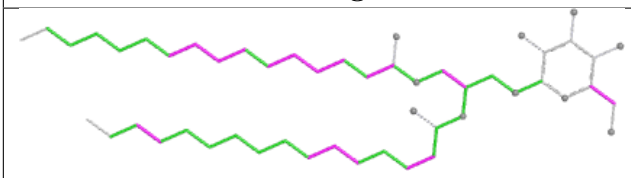
Ligand LMG a 417



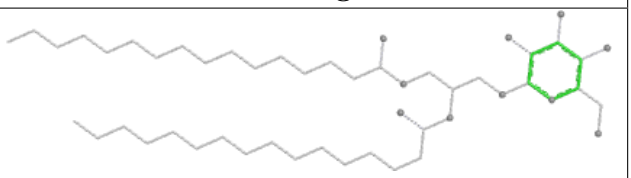
Bond lengths



Bond angles

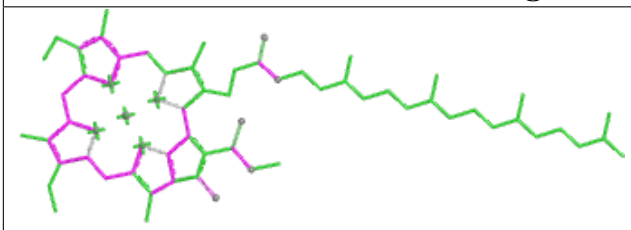


Torsions

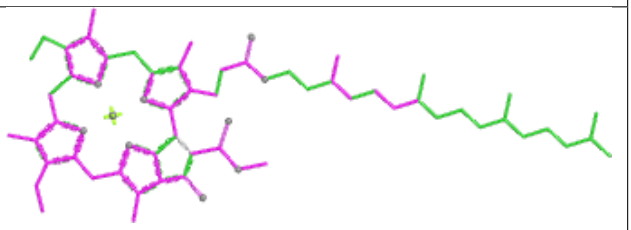


Rings

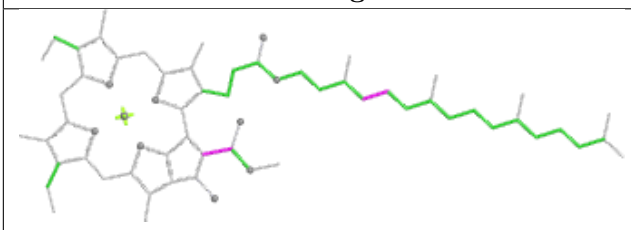
Ligand CLA B 607



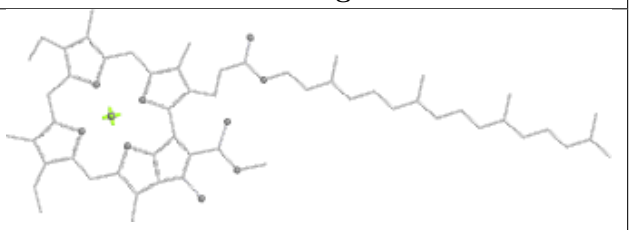
Bond lengths



Bond angles

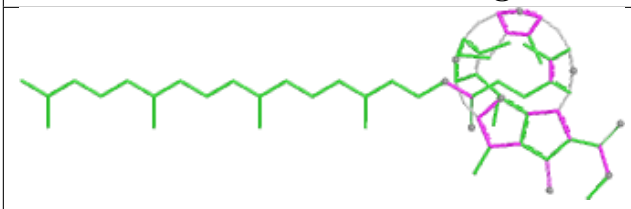


Torsions

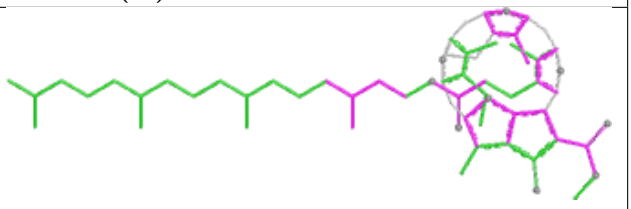


Rings

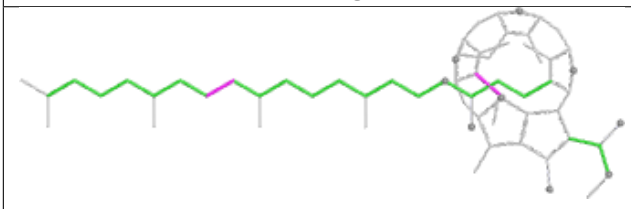
Ligand PHO a 416 (B)



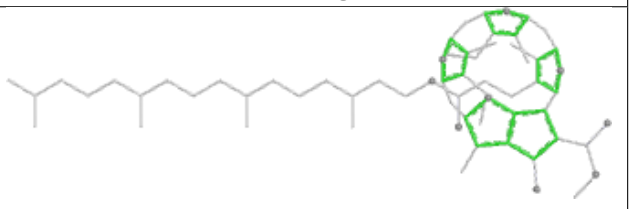
Bond lengths



Bond angles

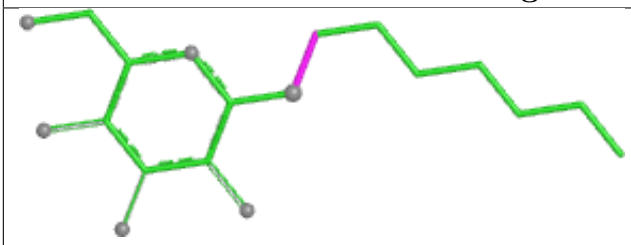


Torsions

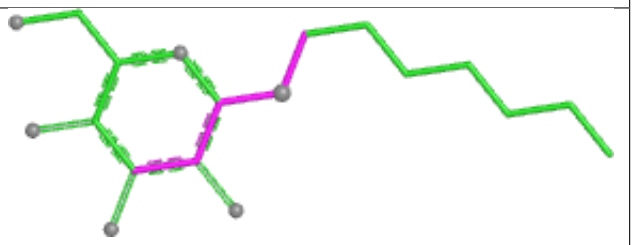


Rings

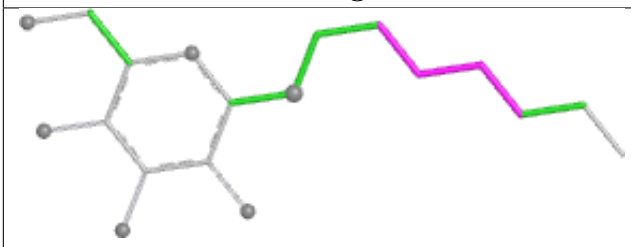
Ligand HTG B 623



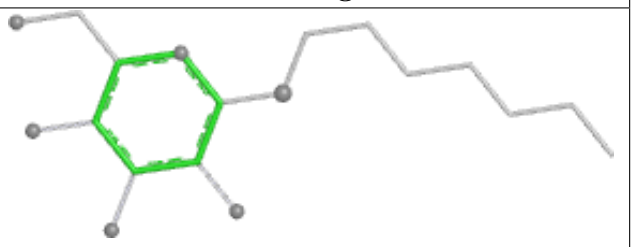
Bond lengths



Bond angles

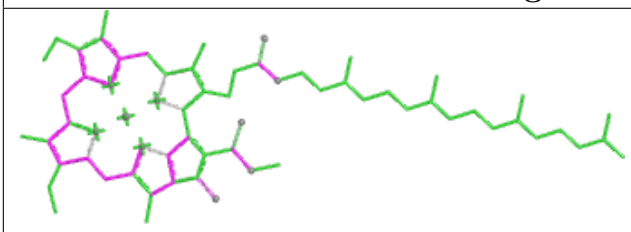


Torsions

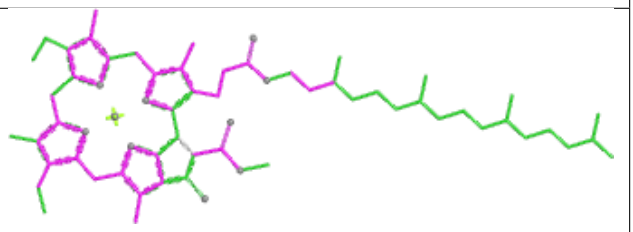


Rings

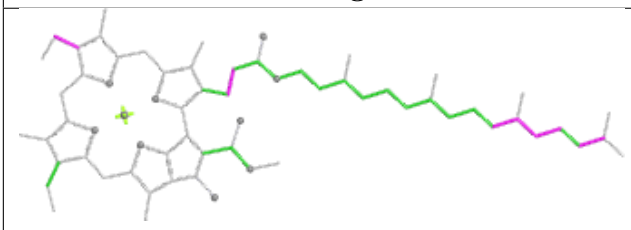
Ligand CLA B 610



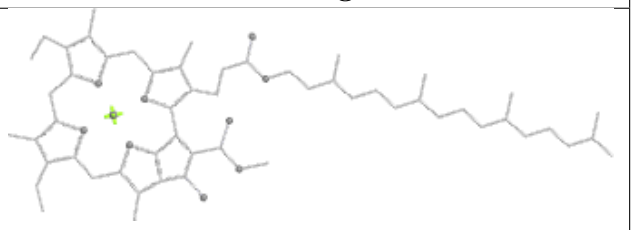
Bond lengths



Bond angles

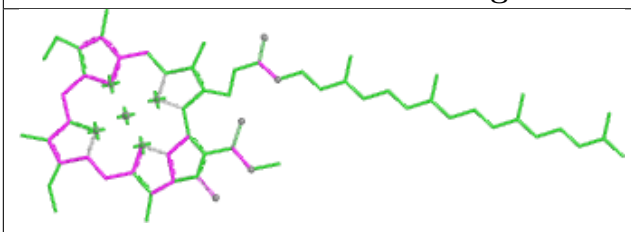


Torsions

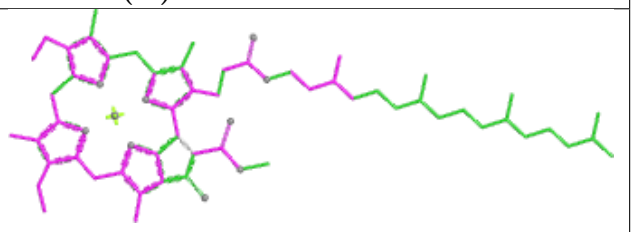


Rings

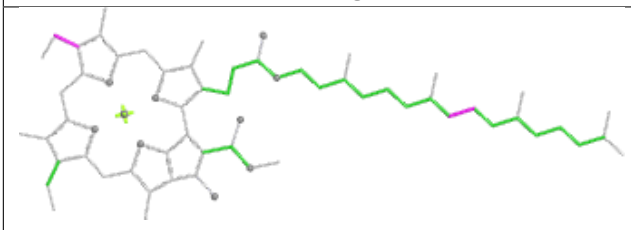
Ligand CLA D 404 (B)



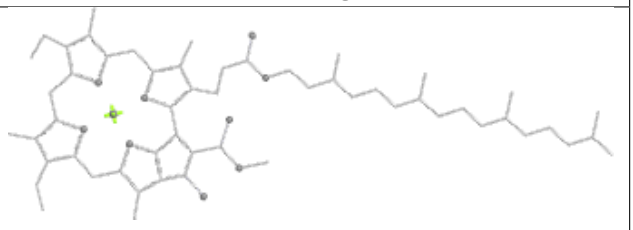
Bond lengths



Bond angles

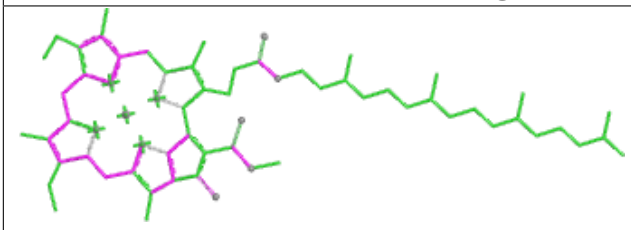


Torsions

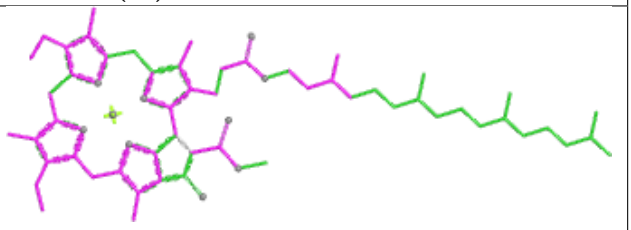


Rings

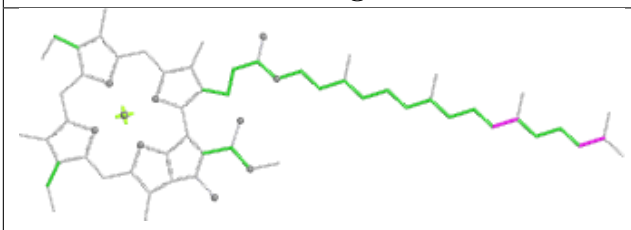
Ligand CLA d 401 (A)



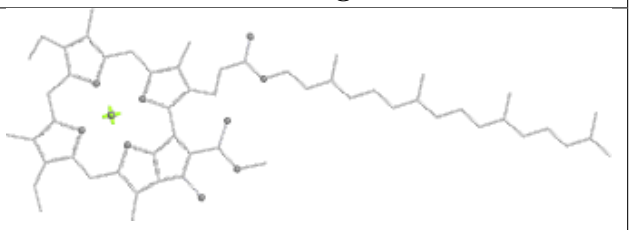
Bond lengths



Bond angles

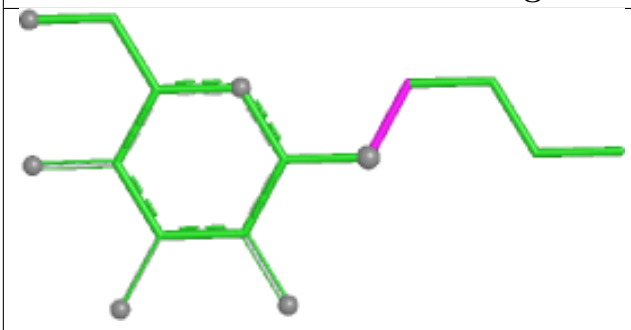


Torsions

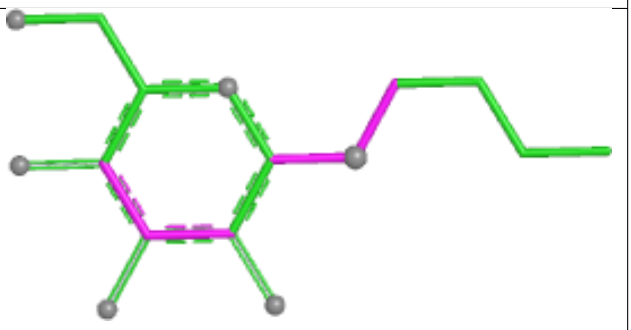


Rings

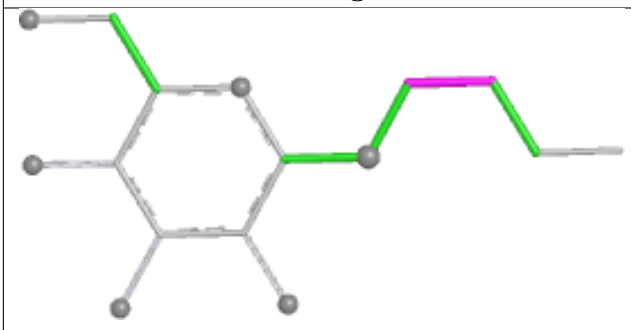
Ligand HTG d 408



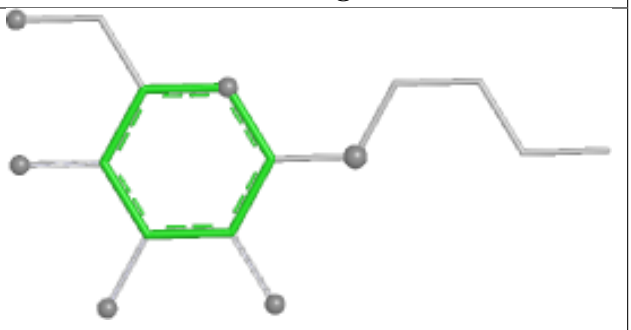
Bond lengths



Bond angles

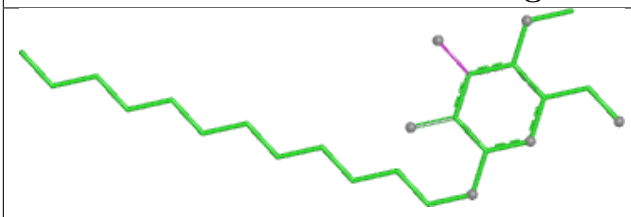


Torsions

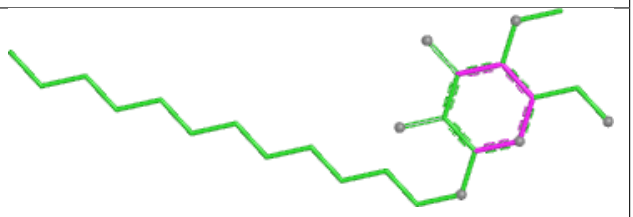


Rings

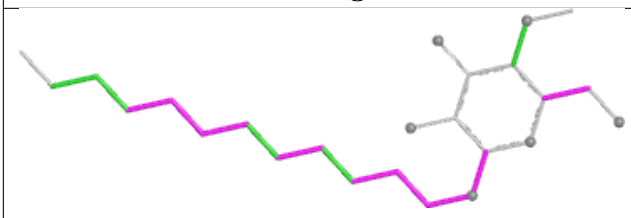
Ligand LMT b 627



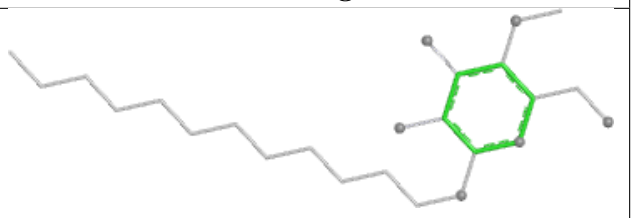
Bond lengths



Bond angles

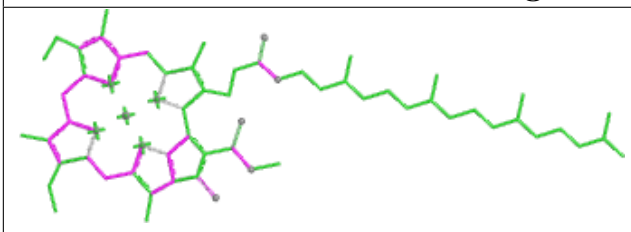


Torsions

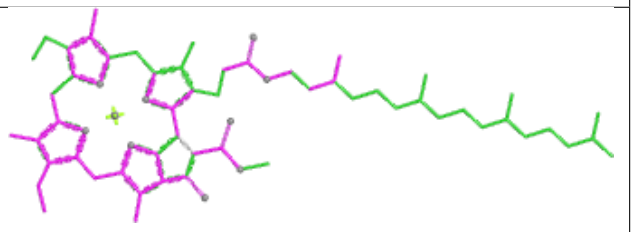


Rings

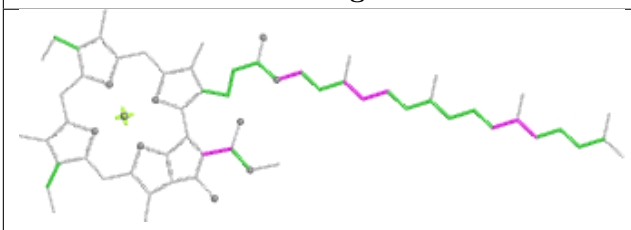
Ligand CLA B 616



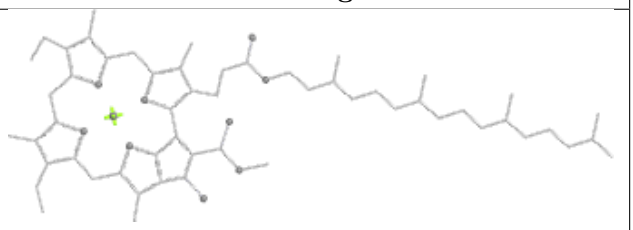
Bond lengths



Bond angles

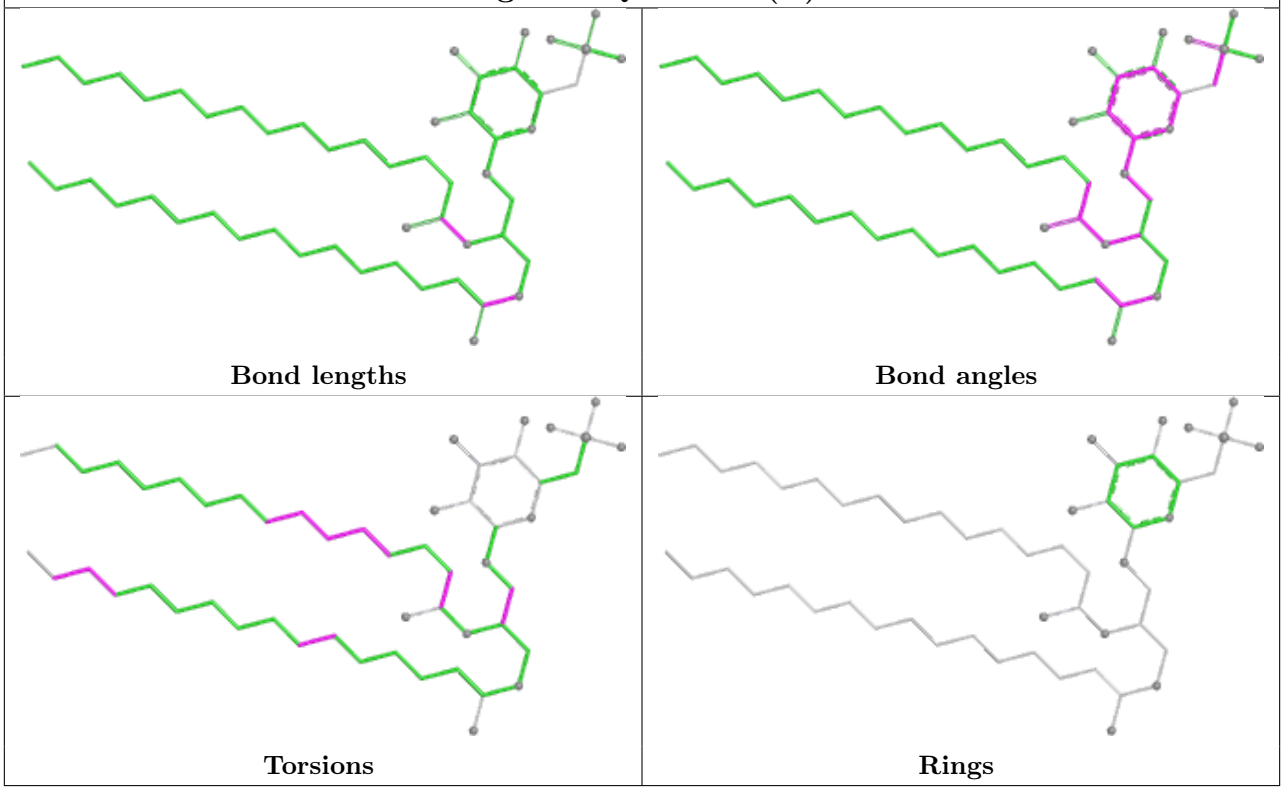


Torsions

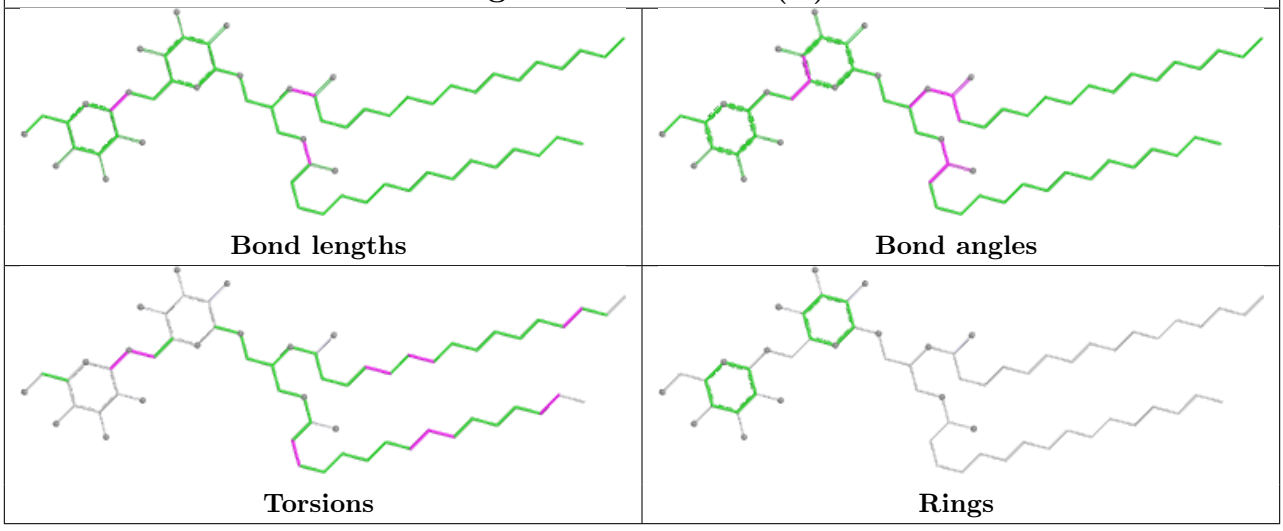


Rings

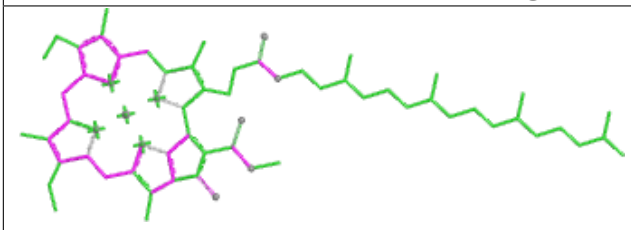
Ligand SQD a 411 (B)



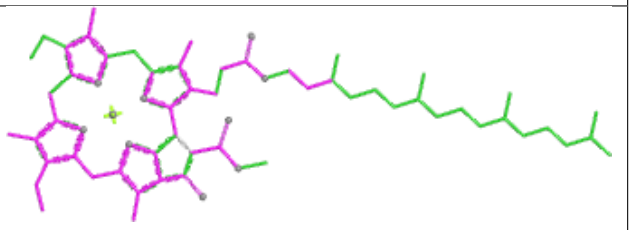
Ligand DGD C 519 (B)



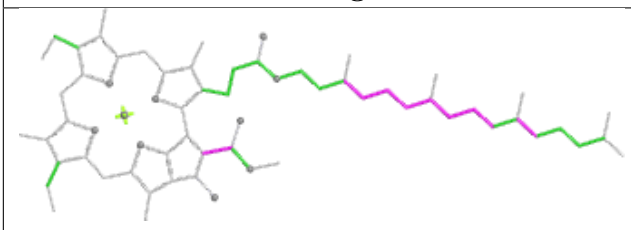
Ligand CLA B 614



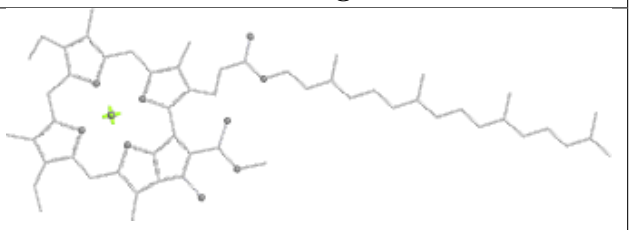
Bond lengths



Bond angles

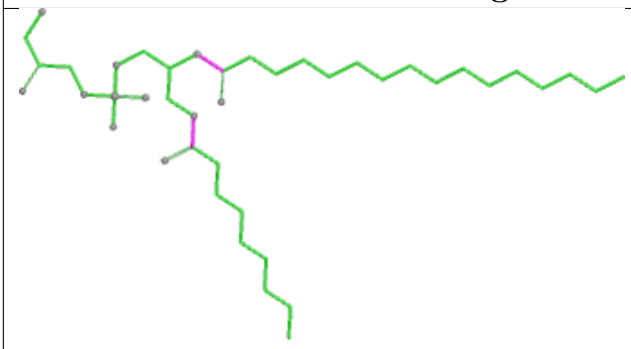


Torsions

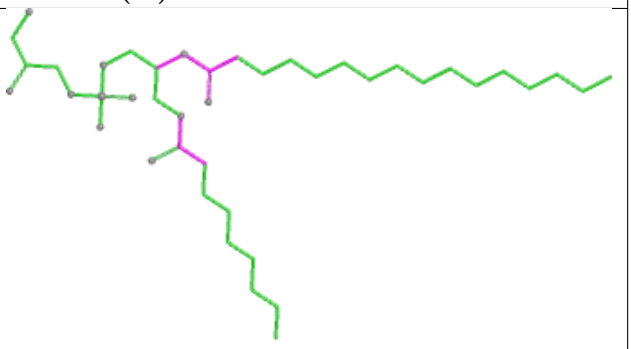


Rings

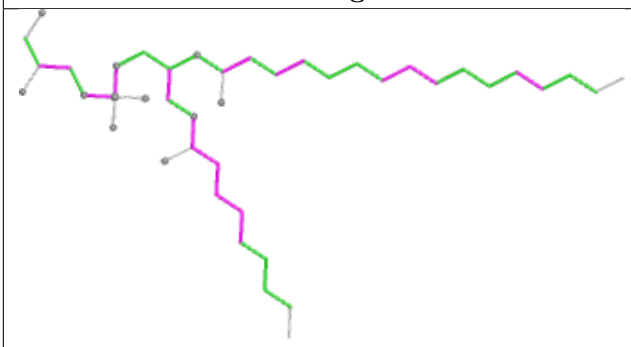
Ligand LHG E 101 (B)



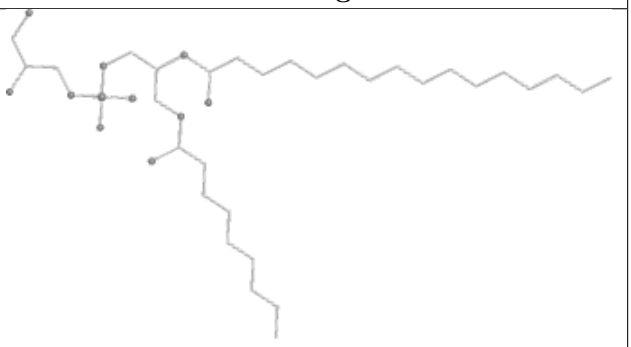
Bond lengths



Bond angles

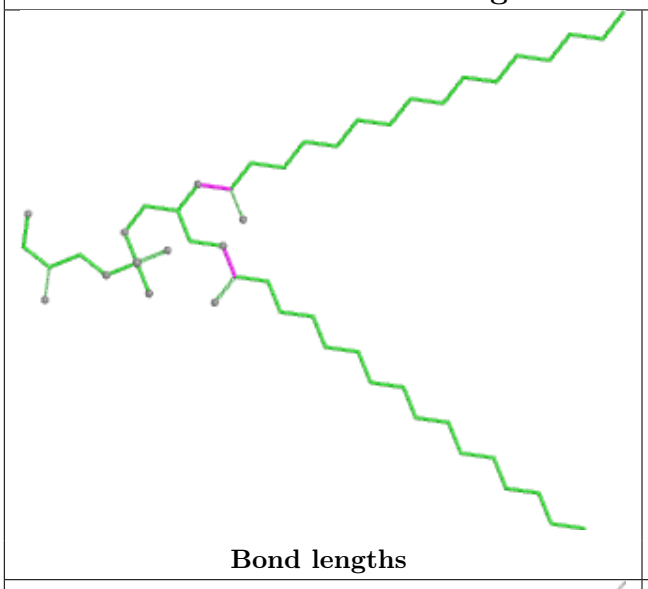


Torsions

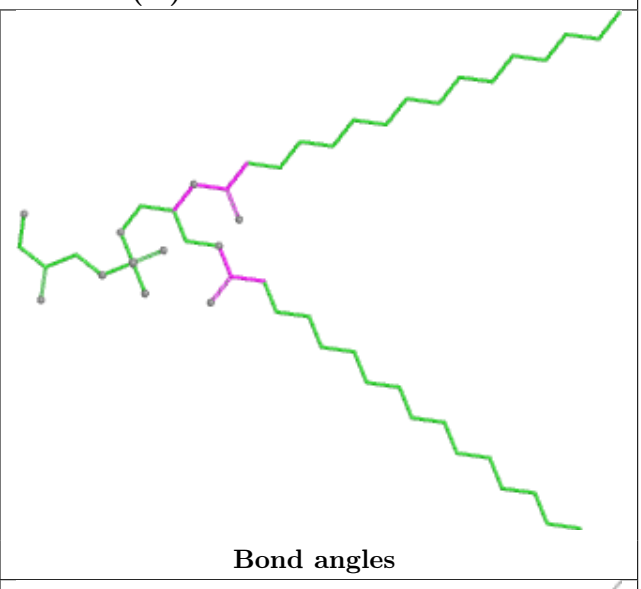


Rings

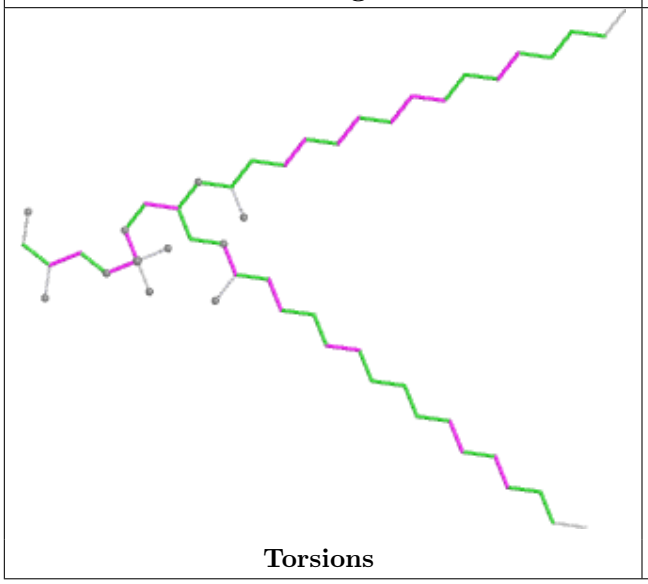
Ligand LHG D 408 (B)



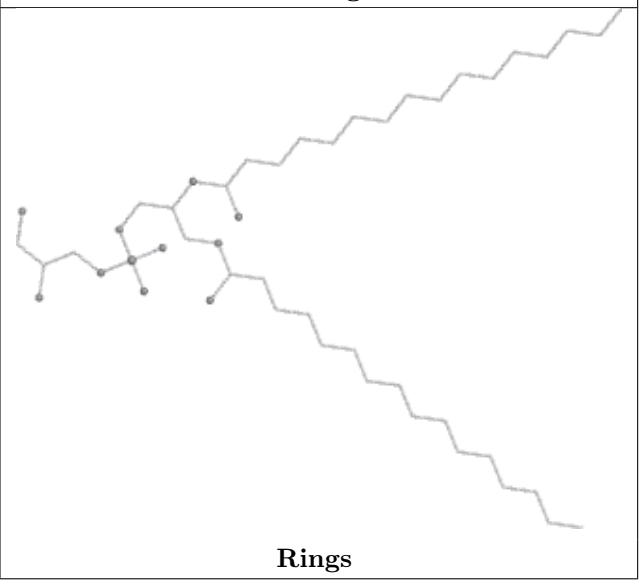
Bond lengths



Bond angles

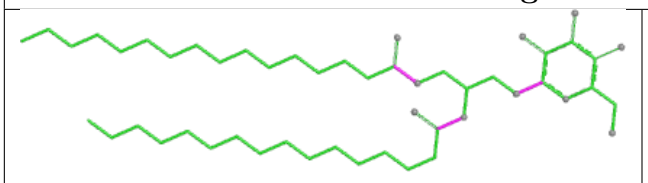


Torsions

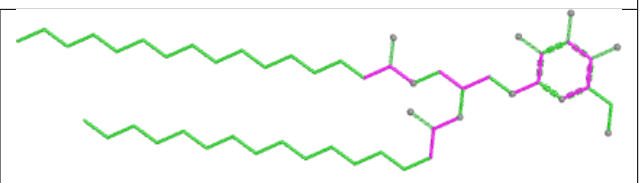


Rings

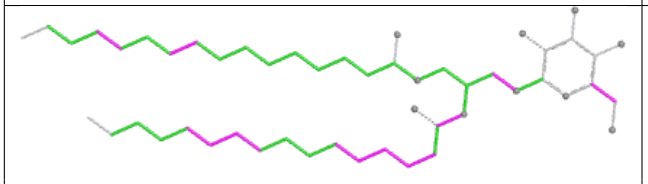
Ligand LMG C 522



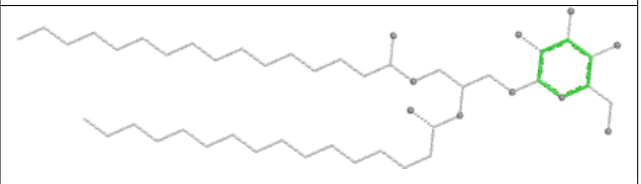
Bond lengths



Bond angles

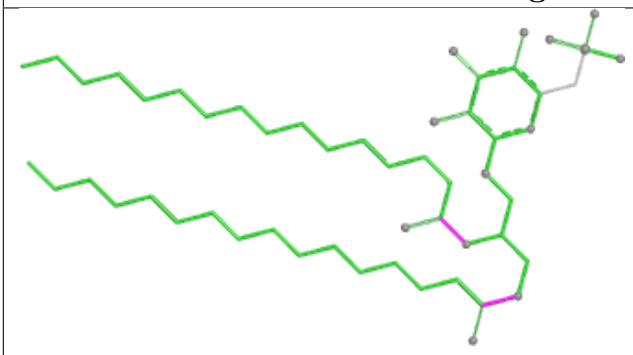


Torsions

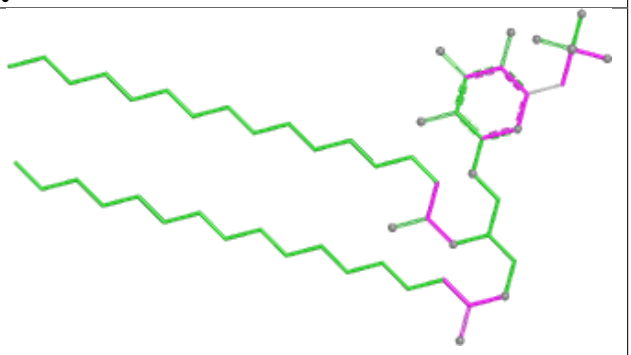


Rings

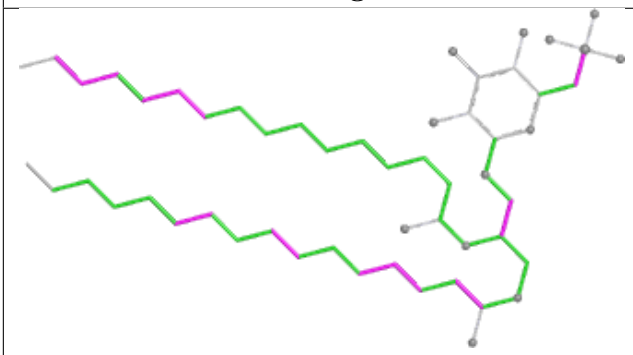
Ligand SQD a 412



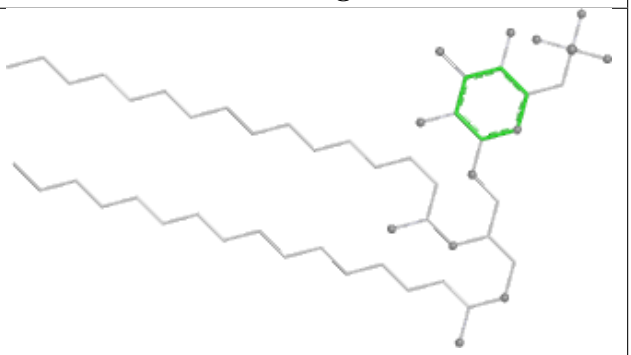
Bond lengths



Bond angles

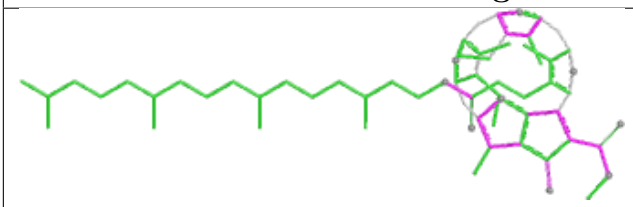


Torsions

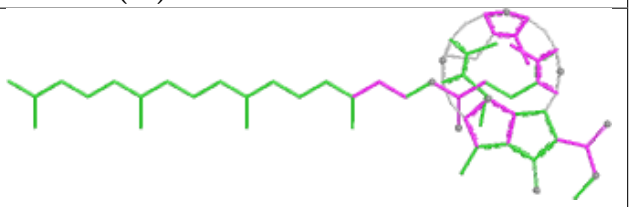


Rings

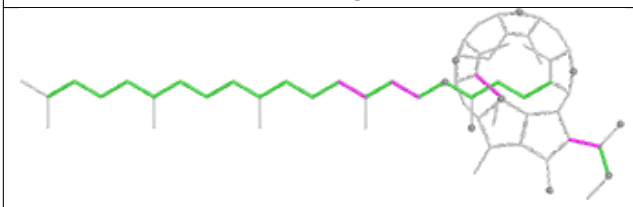
Ligand PHO a 408 (A)



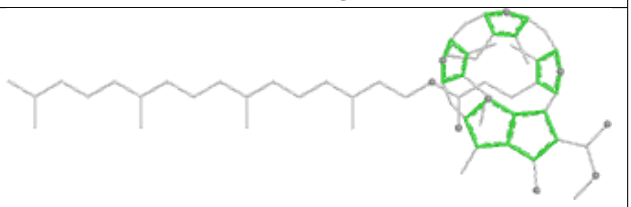
Bond lengths



Bond angles

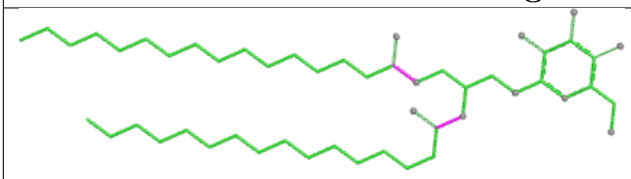


Torsions

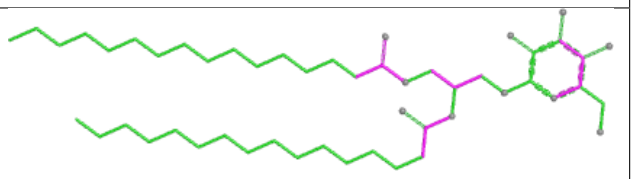


Rings

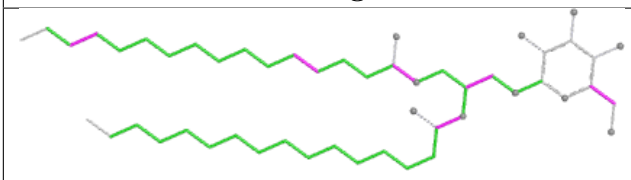
Ligand LMG c 521



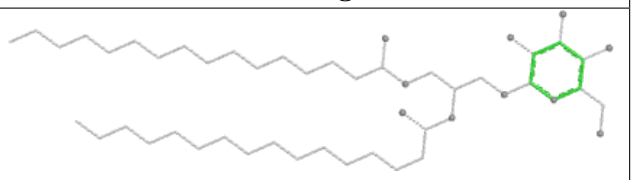
Bond lengths



Bond angles

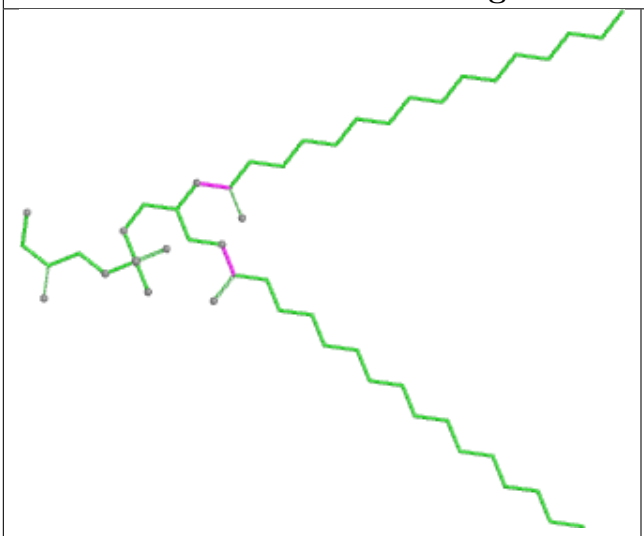


Torsions

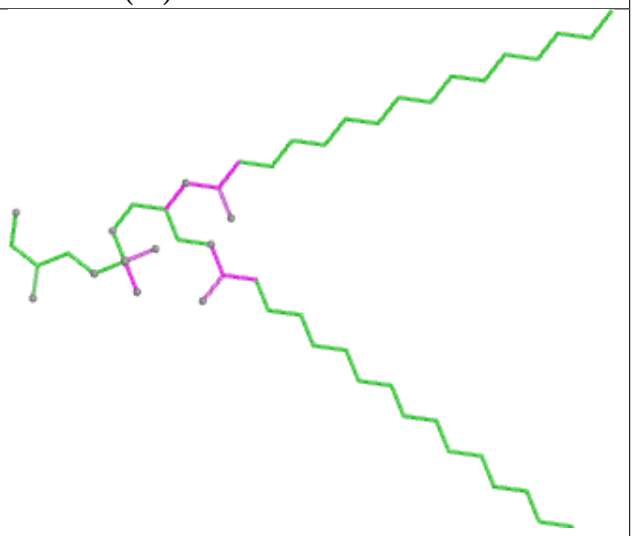


Rings

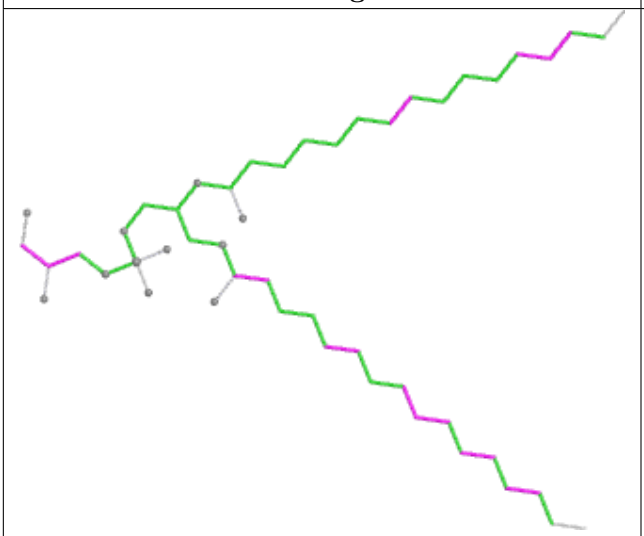
Ligand LHG A 416 (A)



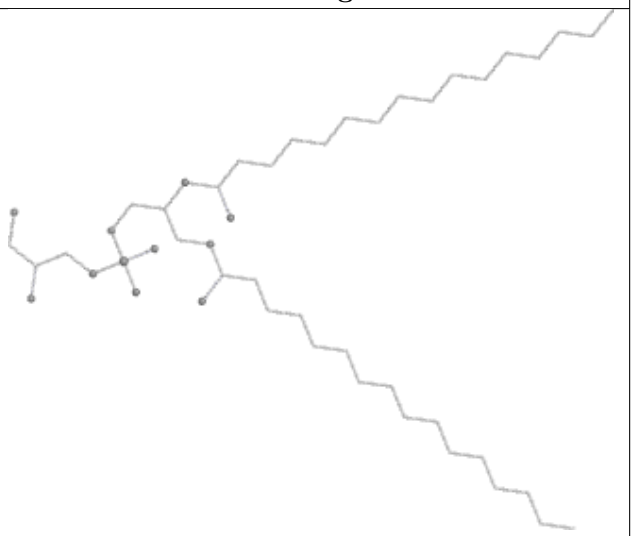
Bond lengths



Bond angles

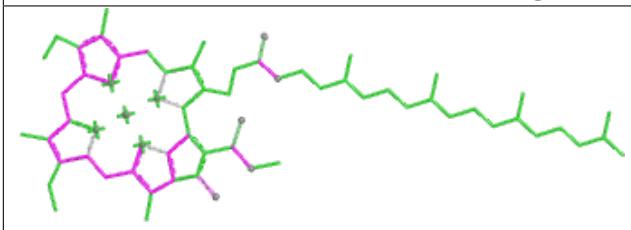


Torsions

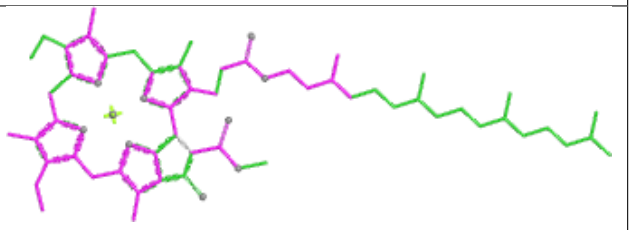


Rings

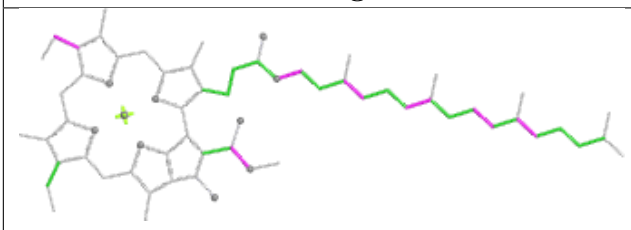
Ligand CLA c 514



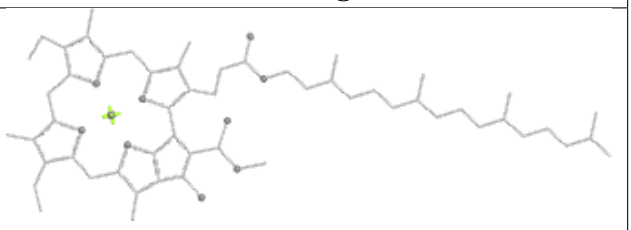
Bond lengths



Bond angles

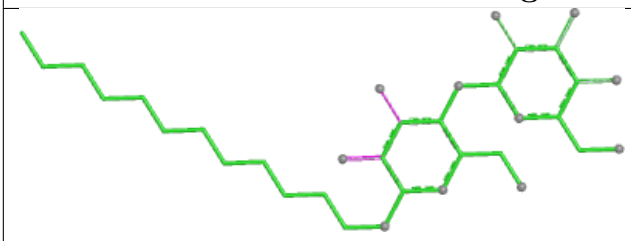


Torsions

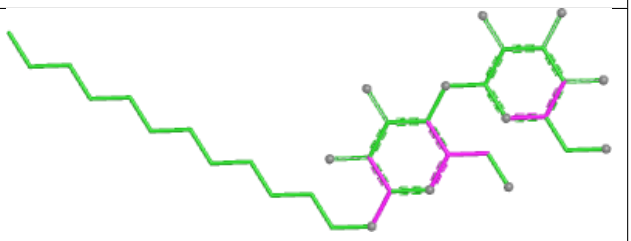


Rings

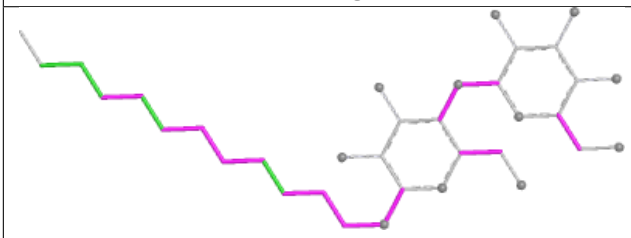
Ligand LMT A 417



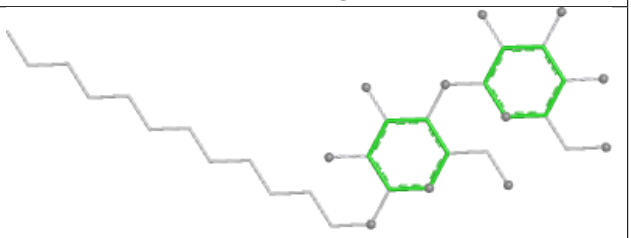
Bond lengths



Bond angles

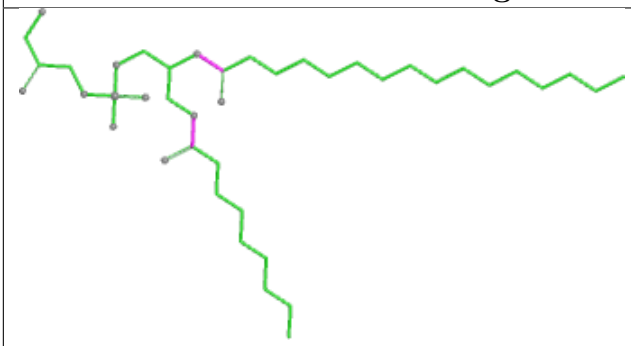


Torsions

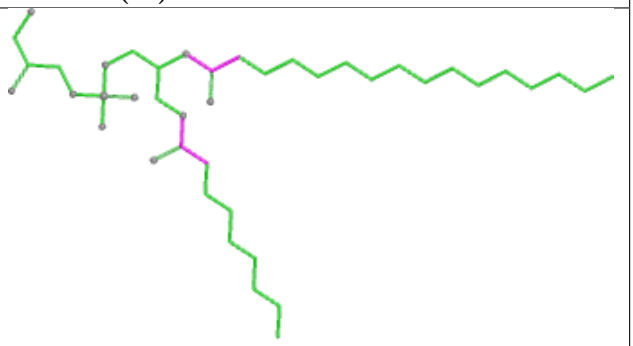


Rings

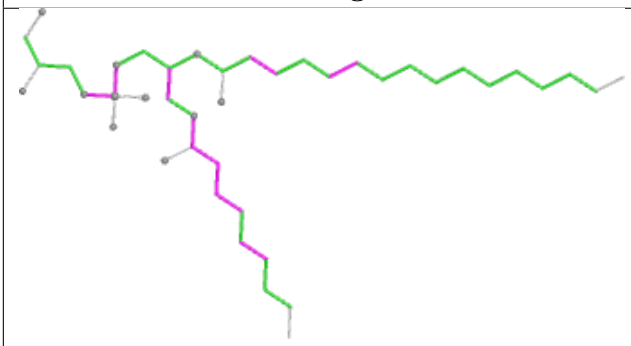
Ligand LHG a 420 (A)



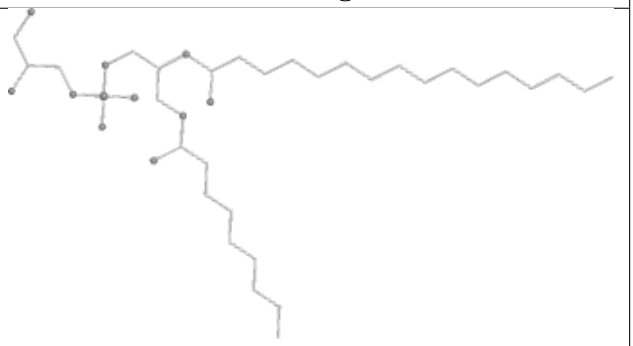
Bond lengths



Bond angles

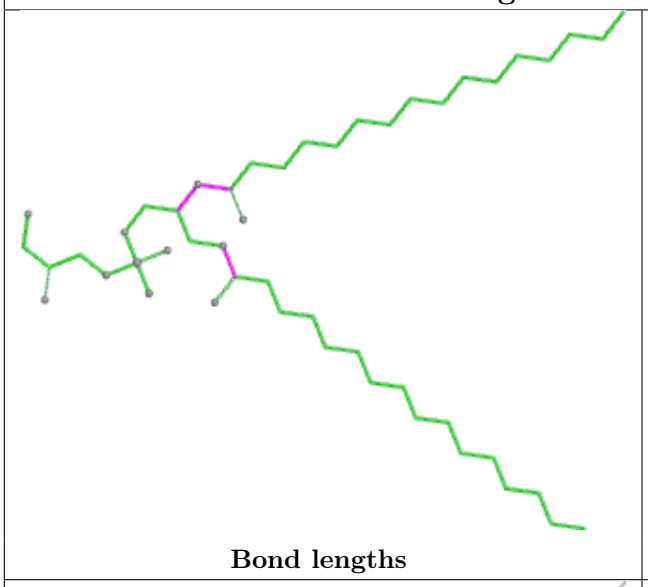


Torsions

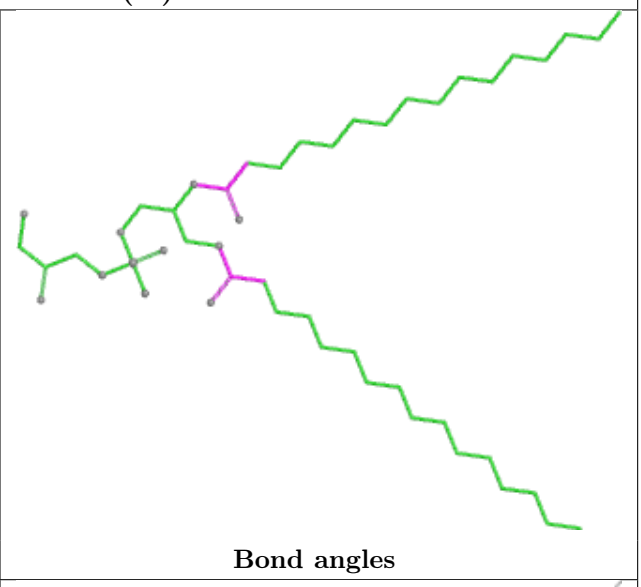


Rings

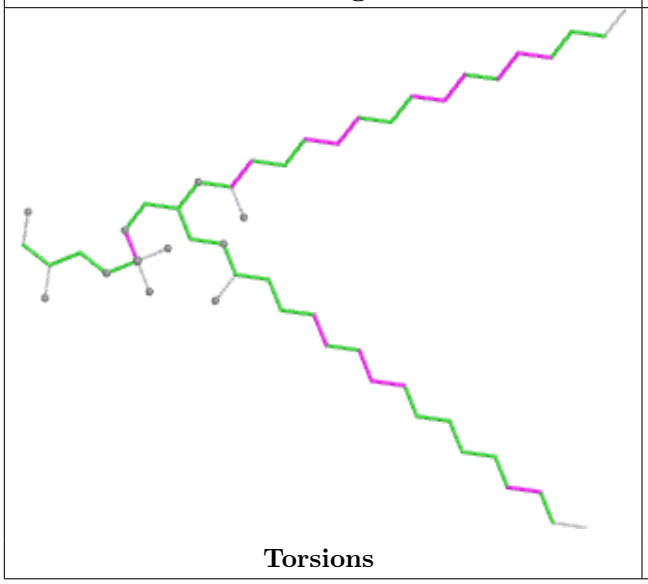
Ligand LHG l 802 (A)



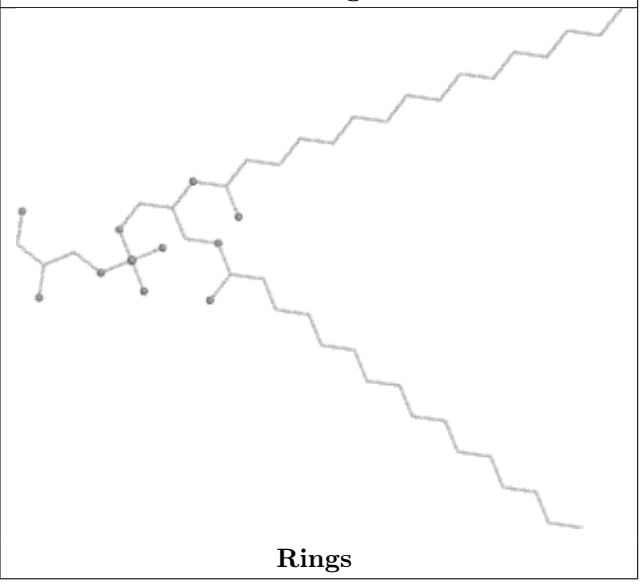
Bond lengths



Bond angles

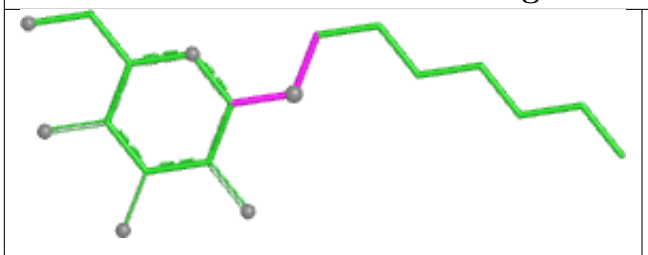


Torsions

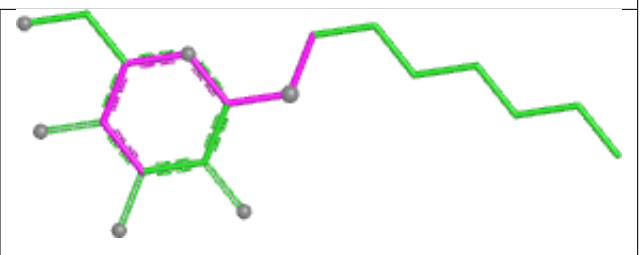


Rings

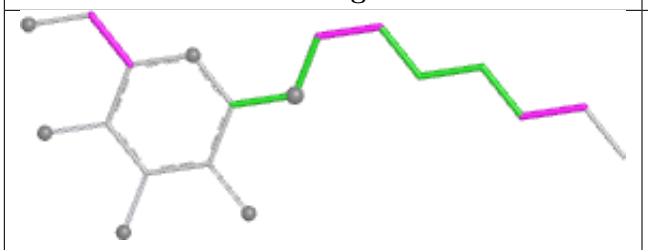
Ligand HTG B 625



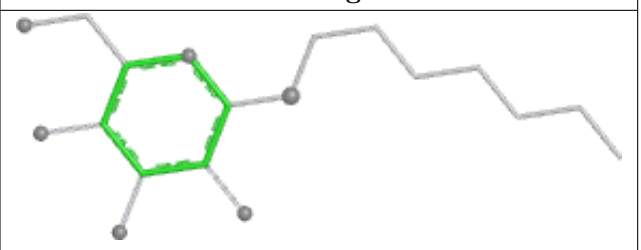
Bond lengths



Bond angles

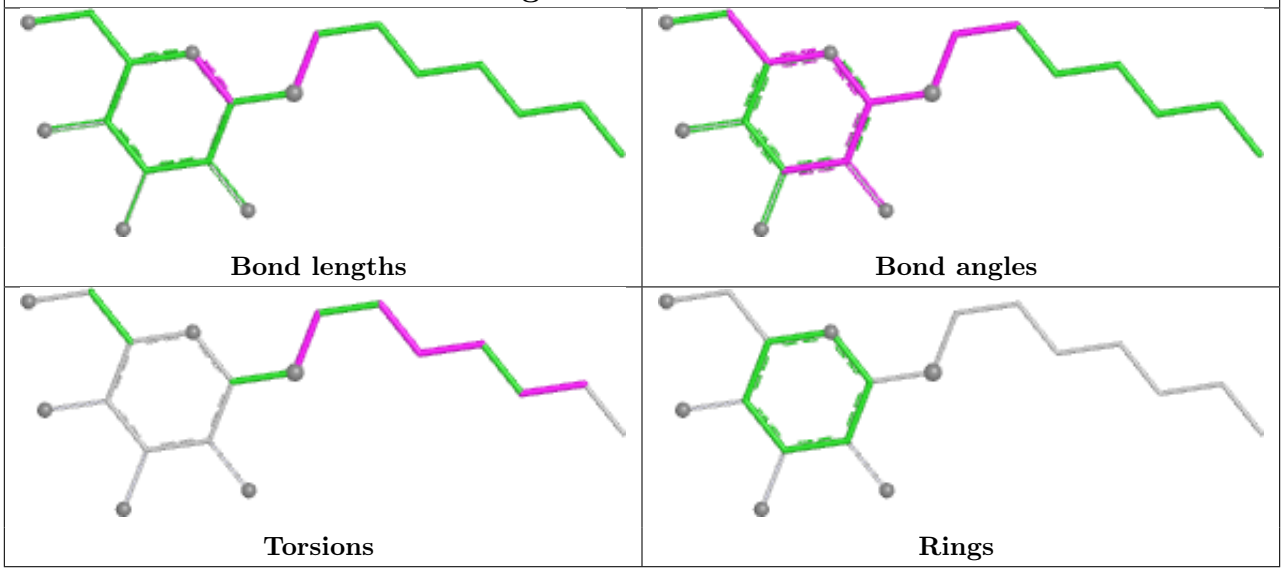


Torsions

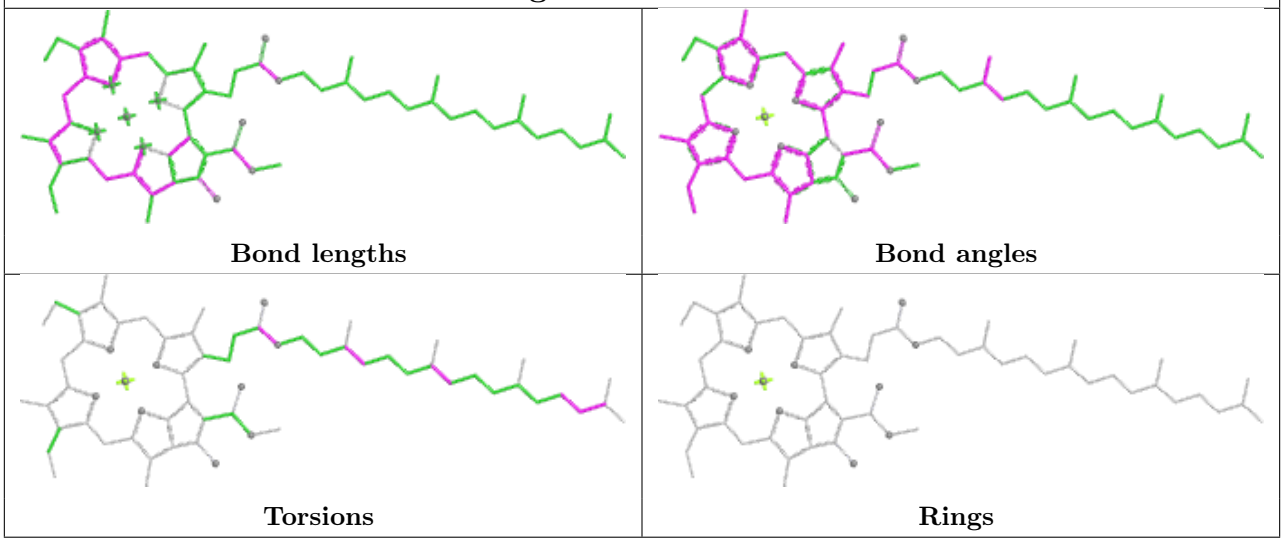


Rings

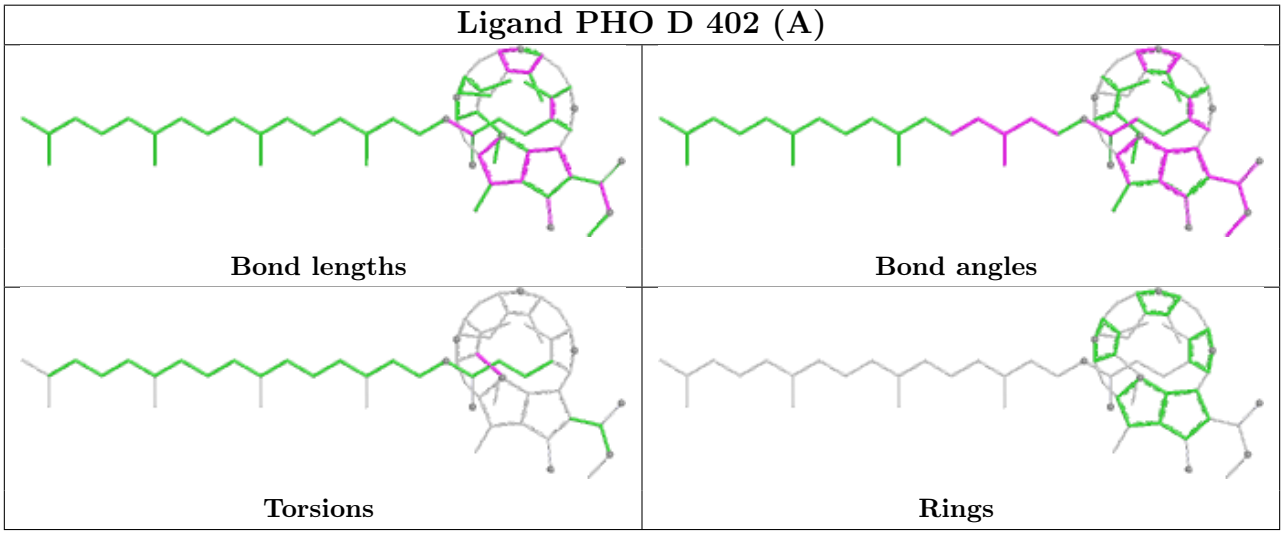
Ligand HTG B 622



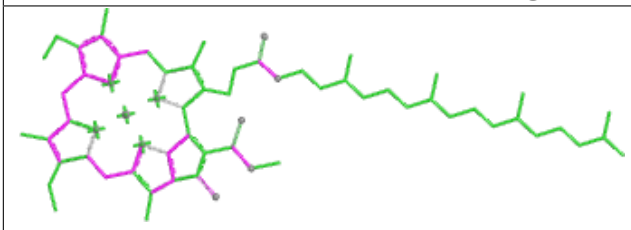
Ligand CLA a 409



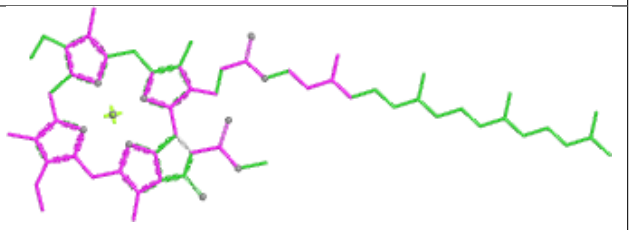
Ligand PHO D 402 (A)



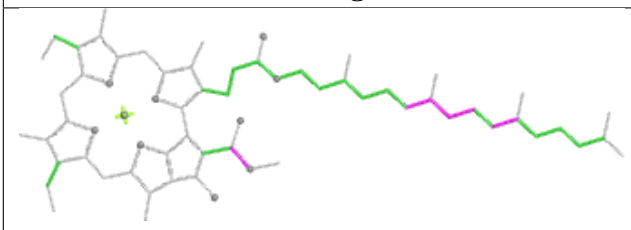
Ligand CLA C 515



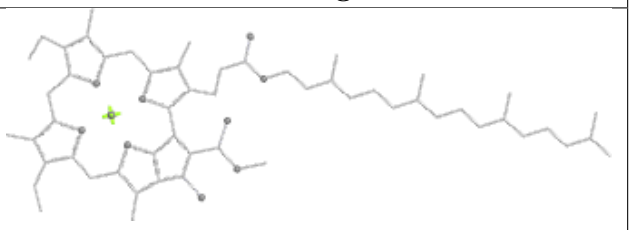
Bond lengths



Bond angles



Torsions

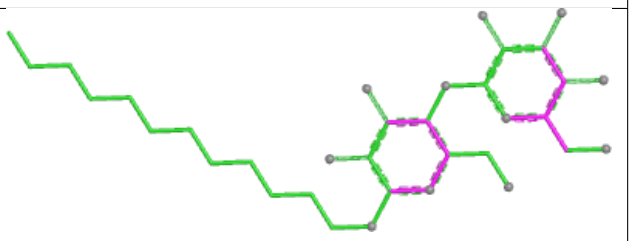


Rings

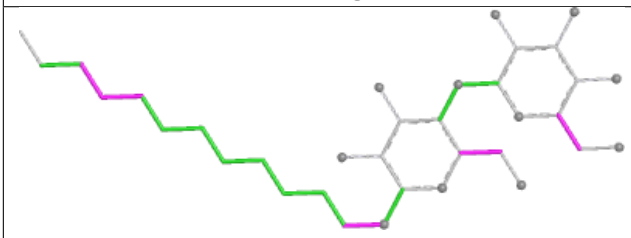
Ligand LMT m 103



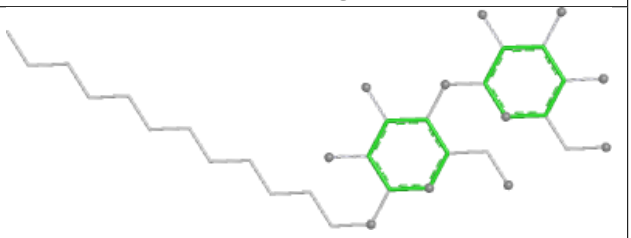
Bond lengths



Bond angles

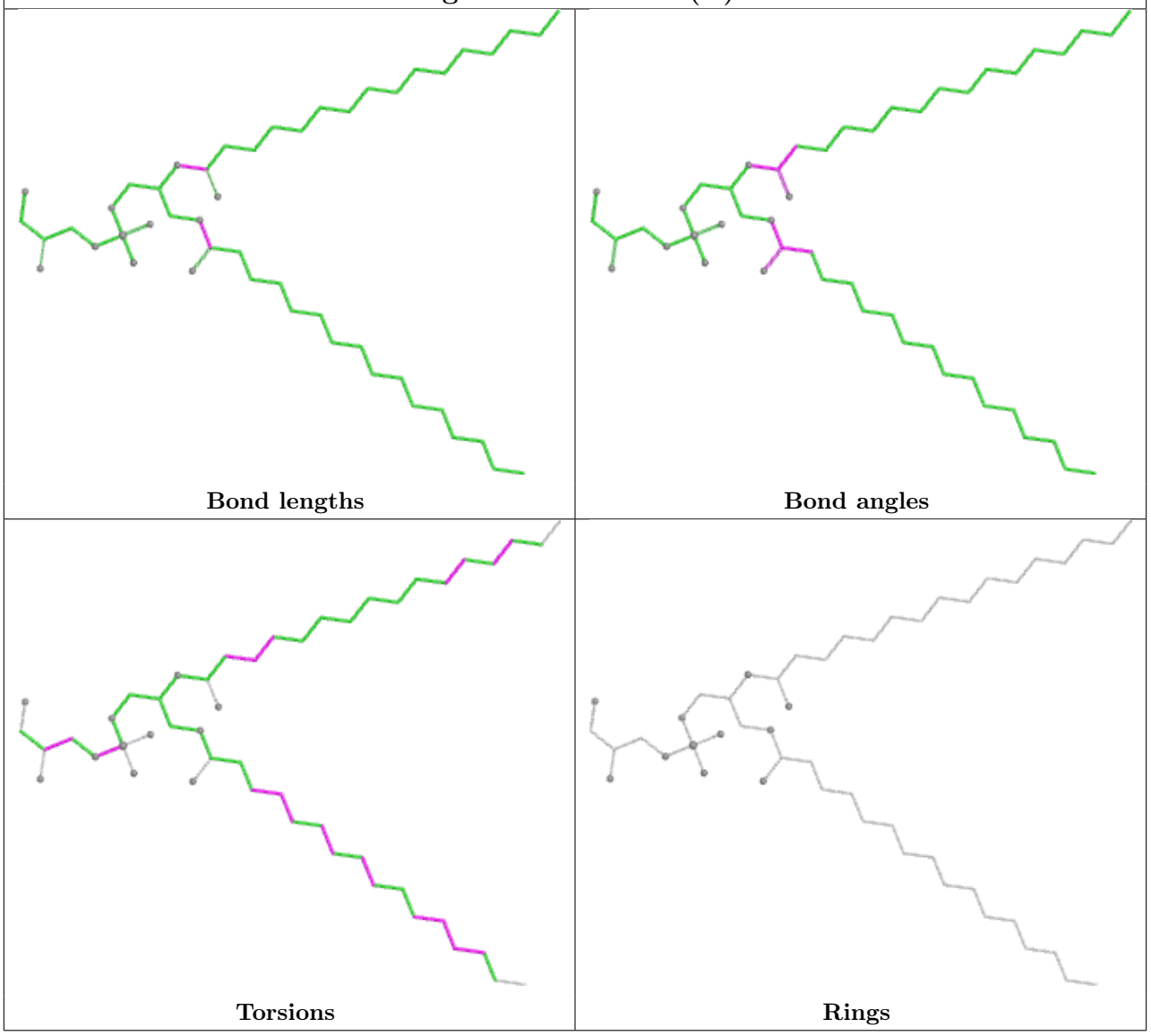


Torsions

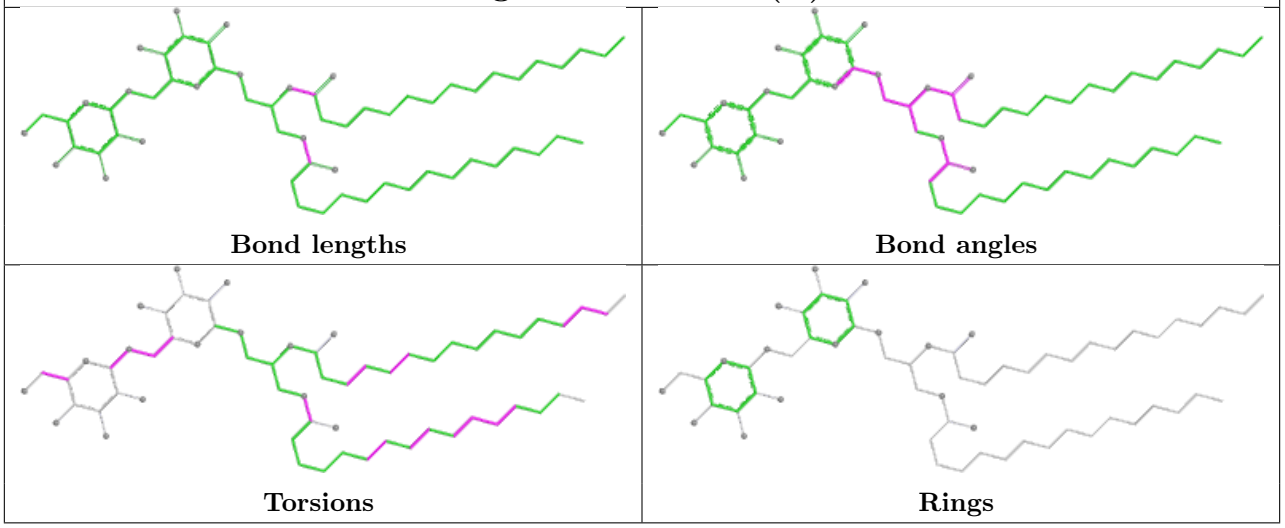


Rings

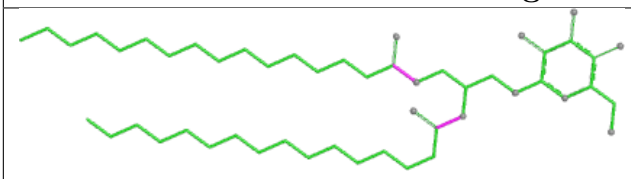
Ligand LHG d 411 (B)



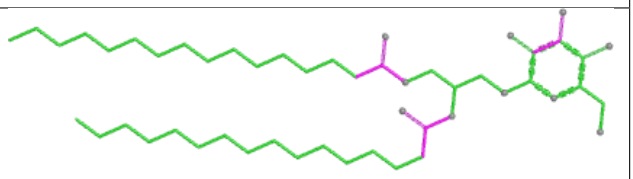
Ligand DGD c 517 (A)



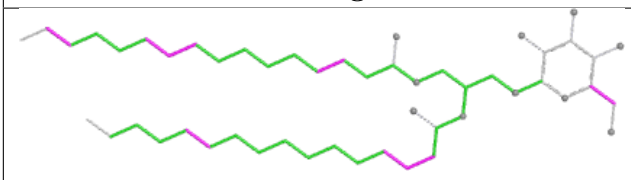
Ligand LMG d 409



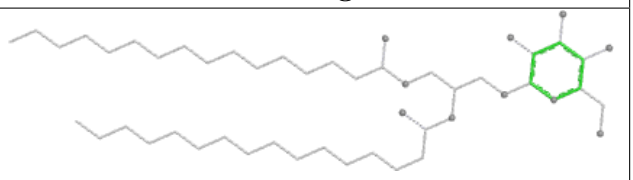
Bond lengths



Bond angles

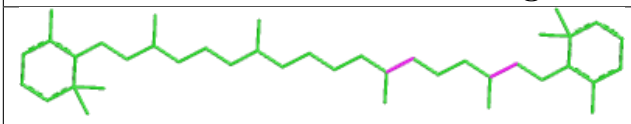


Torsions

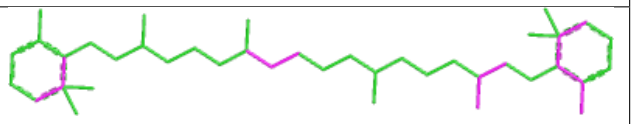


Rings

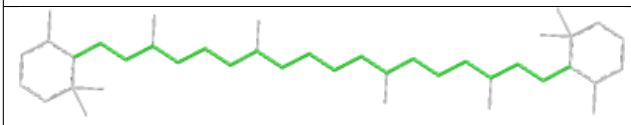
Ligand BCR B 618



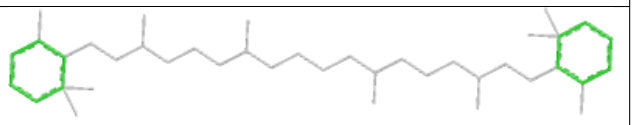
Bond lengths



Bond angles



Torsions

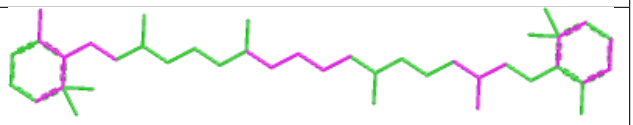


Rings

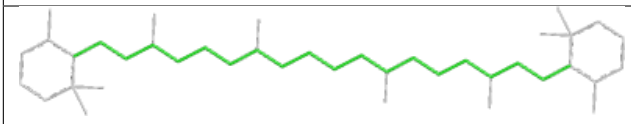
Ligand BCR b 618



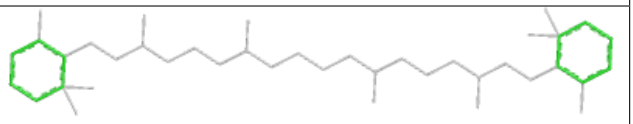
Bond lengths



Bond angles

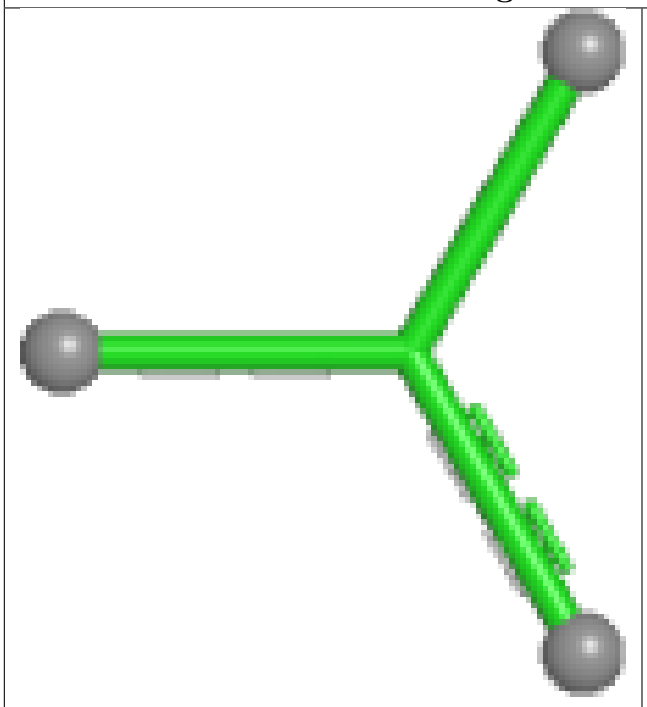


Torsions

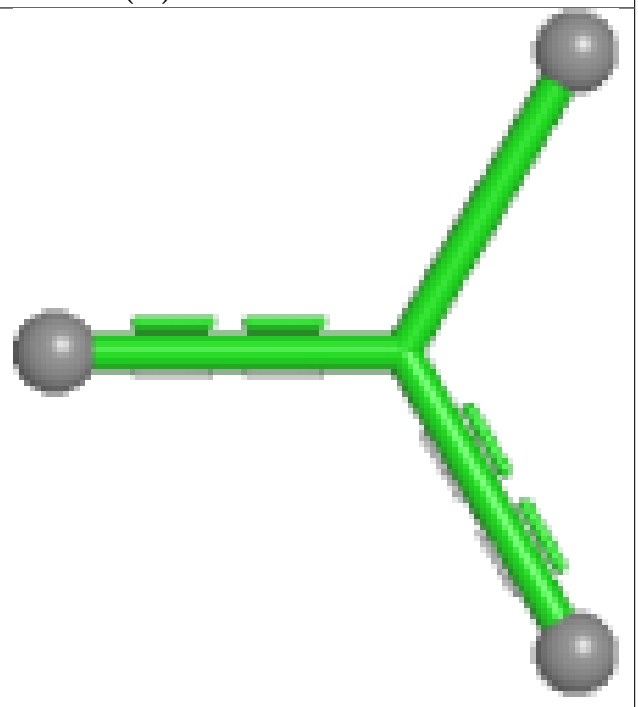


Rings

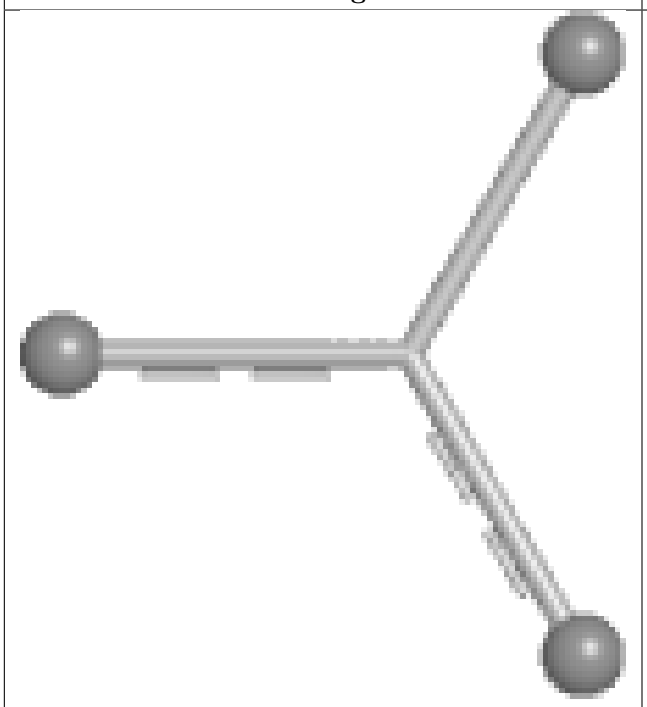
Ligand BCT a 404 (B)



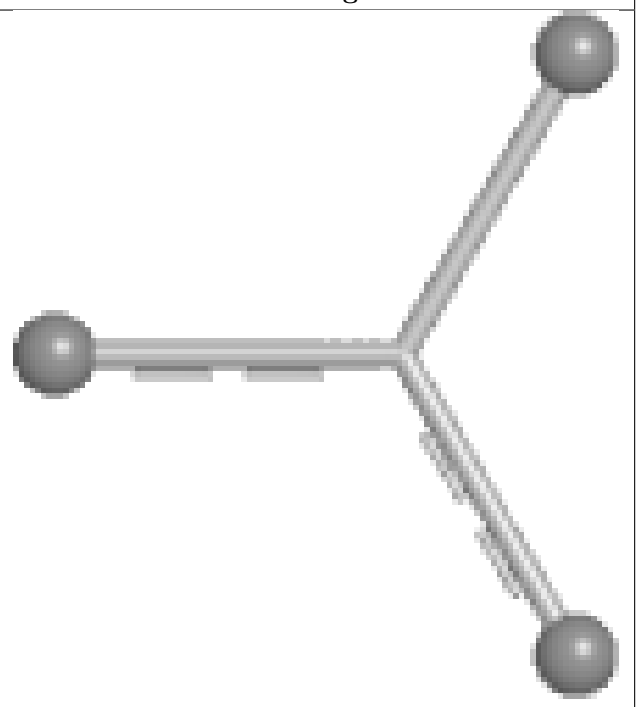
Bond lengths



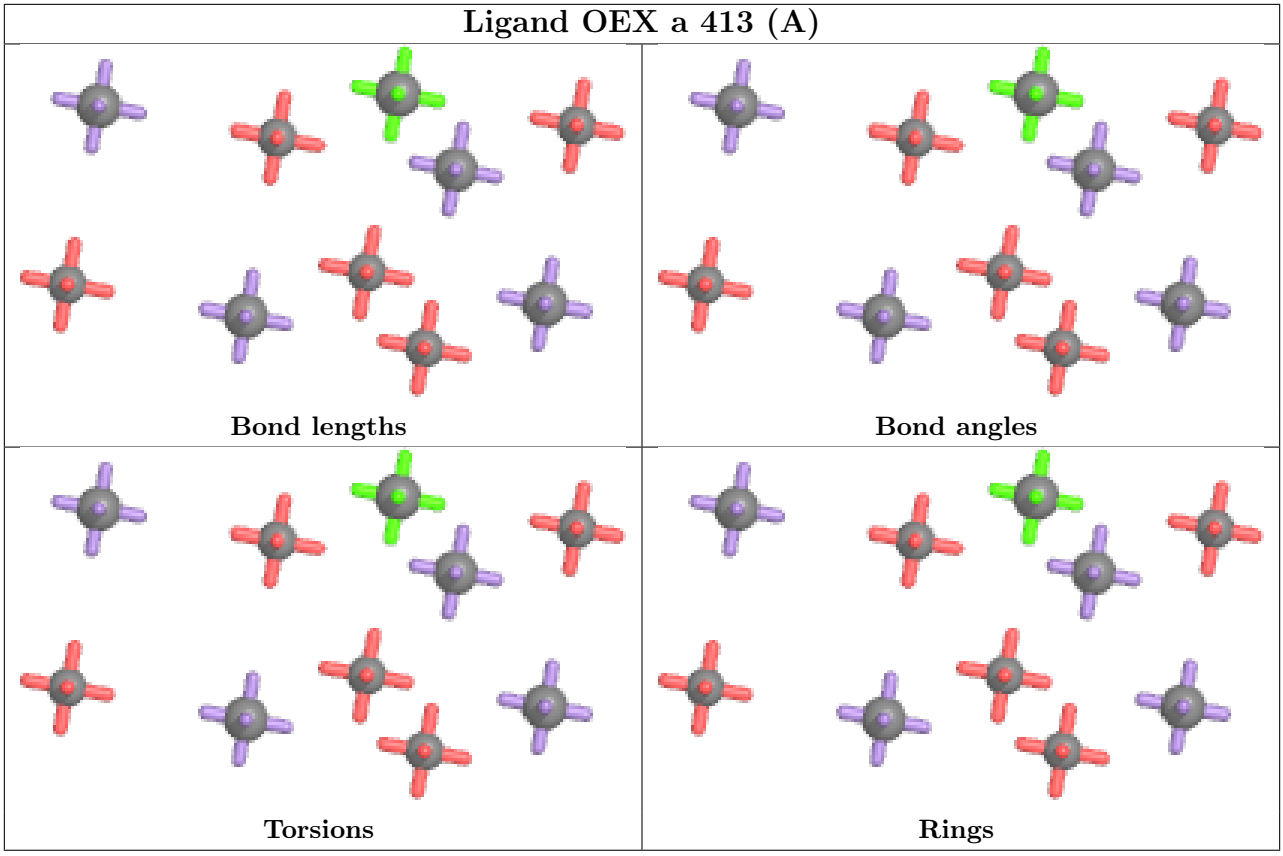
Bond angles

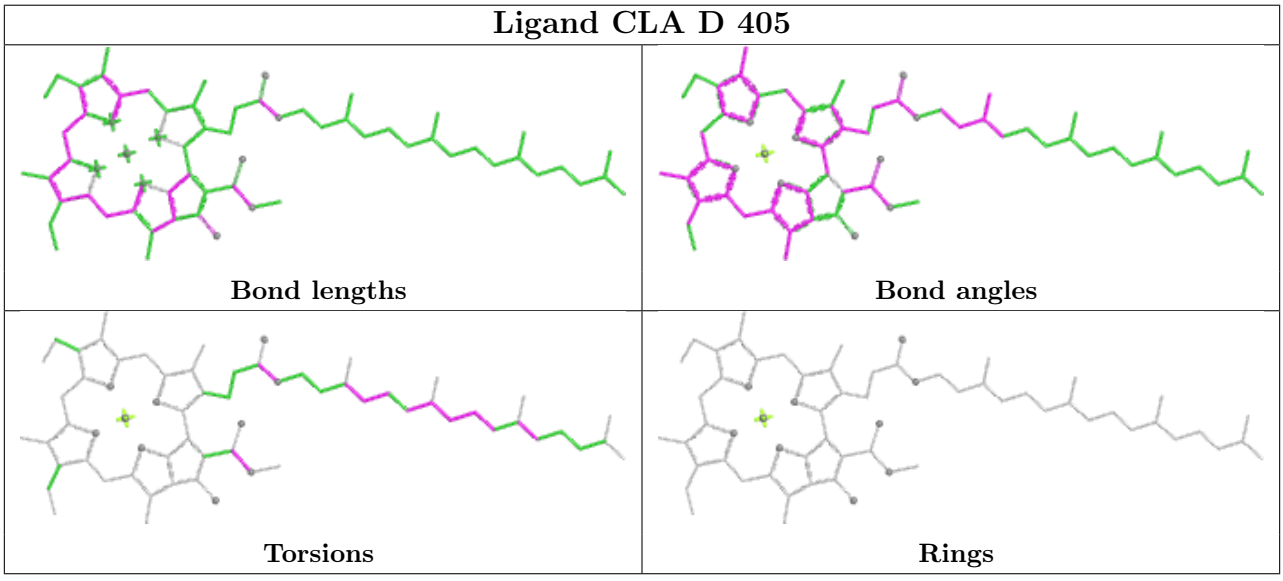


Torsions



Rings





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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.69	1 (0%) 90 90	20, 26, 61, 122	222 (66%)
1	a	334/344 (97%)	-0.63	0 100 100	21, 29, 65, 126	221 (66%)
2	B	504/505 (99%)	-0.61	1 (0%) 91 91	23, 54, 84, 113	20 (3%)
2	b	504/505 (99%)	-0.48	3 (0%) 85 86	24, 58, 95, 154	19 (3%)
3	C	451/455 (99%)	-0.56	0 100 100	22, 61, 84, 136	97 (21%)
3	c	455/455 (100%)	-0.47	1 (0%) 91 91	25, 67, 88, 125	100 (21%)
4	D	342/342 (100%)	-0.72	0 100 100	20, 46, 66, 129	114 (33%)
4	d	341/342 (99%)	-0.71	0 100 100	22, 51, 76, 130	116 (34%)
5	E	81/84 (96%)	-0.39	0 100 100	53, 71, 98, 147	0
5	e	79/84 (94%)	-0.32	1 (1%) 75 76	33, 76, 116, 143	2 (2%)
6	F	34/44 (77%)	-0.57	0 100 100	55, 61, 89, 113	0
6	f	31/44 (70%)	-0.35	1 (3%) 50 52	55, 69, 94, 138	1 (3%)
7	H	64/65 (98%)	-0.35	1 (1%) 70 72	54, 65, 89, 105	0
7	h	64/65 (98%)	-0.36	0 100 100	40, 73, 96, 101	1 (1%)
8	I	37/38 (97%)	-0.26	0 100 100	58, 66, 123, 146	0
8	i	37/38 (97%)	-0.29	0 100 100	56, 66, 115, 134	0
9	J	38/39 (97%)	-0.47	0 100 100	49, 70, 119, 153	0
9	j	39/39 (100%)	-0.30	0 100 100	58, 78, 129, 151	0
10	K	37/37 (100%)	-0.63	0 100 100	54, 68, 88, 110	0
10	k	37/37 (100%)	-0.52	0 100 100	65, 75, 98, 112	0
11	L	36/37 (97%)	-0.70	0 100 100	23, 46, 112, 127	2 (5%)
11	l	36/37 (97%)	-0.67	0 100 100	23, 47, 105, 115	2 (5%)
12	M	32/36 (88%)	-0.67	0 100 100	27, 50, 75, 131	1 (3%)
12	m	33/36 (91%)	-0.63	0 100 100	25, 49, 71, 140	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%)	-0.52	0 100 100	21, 66, 119, 161	10 (4%)
13	o	243/244 (99%)	-0.45	0 100 100	23, 68, 125, 155	8 (3%)
14	T	29/32 (90%)	-0.63	0 100 100	27, 47, 56, 66	6 (20%)
14	t	29/32 (90%)	-0.71	1 (3%) 48 50	27, 47, 61, 72	5 (17%)
15	U	96/104 (92%)	-0.63	0 100 100	25, 58, 93, 100	4 (4%)
15	u	97/104 (93%)	-0.68	0 100 100	28, 62, 81, 120	4 (4%)
16	V	137/137 (100%)	-0.75	0 100 100	24, 58, 81, 109	6 (4%)
16	v	137/137 (100%)	-0.55	0 100 100	27, 72, 102, 128	6 (4%)
17	X	38/40 (95%)	-0.20	0 100 100	37, 74, 97, 114	1 (2%)
17	x	38/40 (95%)	-0.04	0 100 100	69, 82, 131, 154	0
18	Y	29/30 (96%)	-0.08	0 100 100	68, 85, 113, 123	0
18	y	29/30 (96%)	-0.24	0 100 100	78, 91, 109, 115	0
19	Z	62/62 (100%)	-0.30	0 100 100	68, 83, 130, 153	0
19	z	62/62 (100%)	0.10	0 100 100	80, 95, 144, 168	0
20	R	34/34 (100%)	0.59	2 (5%) 28 30	85, 111, 136, 142	0
All	All	5283/5384 (98%)	-0.54	12 (0%) 91 91	20, 59, 101, 168	970 (18%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.4
5	e	79[A]	PHE	3.4
6	f	16[A]	PHE	3.2
20	R	19	ALA	2.5
1	A	11	ALA	2.5
20	R	28	VAL	2.5
3	c	245[A]	ILE	2.4
2	b	499	VAL	2.3
14	t	30[A]	THR	2.3
2	b	502	VAL	2.1
2	B	494	GLY	2.1
2	b	486[A]	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
8	FME	I	1	10/11	0.95	0.07	67,71,79,85	0
14	FME	T	1	10/11	0.95	0.07	43,53,62,73	0
8	FME	i	1	10/11	0.97	0.07	54,75,84,86	0
12	FME	m	1	10/11	0.97	0.07	48,63,87,111	0
14	FME	t	1	10/11	0.97	0.06	44,48,61,77	0
12	FME	M	1	10/11	0.98	0.06	46,62,94,98	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
25	GOL	a	418	6/6	0.59	0.17	74,98,100,102	0
29	UNL	A	413	28/-	0.67	0.15	80,110,132,143	0
31	LMT	A	417	35/35	0.68	0.13	97,127,153,163	0
31	LMT	F	101	35/35	0.68	0.15	88,126,165,171	0
31	LMT	e	101	35/35	0.68	0.15	98,140,176,179	0
31	LMT	B	630	35/35	0.69	0.15	65,111,140,146	0
29	UNL	J	101	10/-	0.70	0.22	69,80,87,101	0
29	UNL	K	101[A]	34/-	0.71	0.14	76,104,114,118	34
29	UNL	K	101[B]	34/-	0.71	0.14	75,104,114,118	34
29	UNL	a	415	30/-	0.71	0.12	85,113,133,140	0
31	LMT	A	415	35/35	0.71	0.13	61,109,130,134	0
29	UNL	m	102	10/-	0.72	0.20	68,75,102,103	0
34	HTG	C	523	19/19	0.73	0.13	100,124,139,139	0
31	LMT	c	501	35/35	0.74	0.13	103,128,147,150	0
29	UNL	I	101	40/-	0.74	0.15	73,102,150,162	0
34	HTG	B	623	19/19	0.74	0.16	61,95,108,117	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	SQD	f	102	43/54	0.74	0.13	101,124,167,183	0
25	GOL	o	302	6/6	0.75	0.16	82,89,96,104	0
25	GOL	O	302	6/6	0.76	0.12	81,90,105,109	0
34	HTG	D	412	16/19	0.76	0.12	93,103,134,149	0
29	UNL	j	101	10/-	0.77	0.15	73,90,97,98	0
32	LHG	a	420[A]	42/49	0.78	0.12	88,131,146,154	42
32	LHG	a	420[B]	42/49	0.78	0.12	87,131,146,154	42
29	UNL	c	525[B]	32/-	0.78	0.14	86,106,118,127	32
25	GOL	B	627	6/6	0.78	0.14	75,86,96,114	0
29	UNL	c	525[A]	32/-	0.78	0.14	86,106,118,127	32
34	HTG	c	522	19/19	0.78	0.10	109,124,142,145	0
33	LMG	C	522	51/55	0.79	0.11	61,115,156,161	0
29	UNL	M	102	10/-	0.80	0.15	63,77,98,100	0
29	UNL	B	631	40/-	0.80	0.13	74,103,154,159	0
29	UNL	b	626	33/-	0.80	0.13	67,98,162,171	0
29	UNL	D	411	40/-	0.80	0.13	63,88,138,150	0
29	UNL	b	629	36/-	0.81	0.11	68,96,134,143	0
25	GOL	c	528	6/6	0.81	0.16	82,104,109,121	0
36	CA	V	201	1/1	0.81	0.24	129,129,129,129	0
31	LMT	T	101	35/35	0.82	0.10	65,121,165,169	0
31	LMT	b	621	25/35	0.82	0.11	77,114,158,164	0
25	GOL	A	409	6/6	0.82	0.13	60,77,80,83	0
25	GOL	b	624	6/6	0.82	0.15	93,96,104,113	0
28	PL9	a	414[B]	55/55	0.83	0.14	75,97,111,114	55
25	GOL	d	410	6/6	0.83	0.23	51,69,79,86	0
28	PL9	A	412[A]	55/55	0.83	0.13	60,88,103,106	55
31	LMT	B	628	35/35	0.83	0.11	63,102,135,149	0
34	HTG	b	622	19/19	0.83	0.13	63,85,118,119	0
28	PL9	A	412[B]	55/55	0.83	0.13	60,88,103,106	55
28	PL9	a	414[A]	55/55	0.83	0.14	75,97,111,114	55
29	UNL	B	626	33/-	0.84	0.14	60,106,142,146	0
25	GOL	O	303	6/6	0.84	0.13	76,91,93,95	0
34	HTG	V	203	11/19	0.84	0.09	81,111,125,126	0
26	SQD	a	412	54/54	0.84	0.10	66,93,140,149	0
34	HTG	b	623	19/19	0.84	0.10	85,129,154,161	0
33	LMG	c	521	51/55	0.84	0.10	78,131,161,183	0
31	LMT	t	102	26/35	0.84	0.11	67,101,137,148	0
31	LMT	t	101	25/35	0.85	0.12	54,81,132,154	0
26	SQD	A	410	54/54	0.85	0.10	66,89,130,150	0
25	GOL	c	527	6/6	0.85	0.16	96,97,106,110	0
33	LMG	z	101	39/55	0.85	0.12	74,126,151,164	0
31	LMT	b	627	25/35	0.86	0.11	58,93,140,154	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	HTG	B	622	19/19	0.86	0.12	69,85,110,123	0
33	LMG	C	526	37/55	0.87	0.12	70,124,146,160	0
34	HTG	d	408	16/19	0.87	0.10	89,116,139,152	0
31	LMT	m	103	35/35	0.87	0.10	62,92,105,108	0
25	GOL	l	801[A]	6/6	0.88	0.17	67,93,96,98	6
25	GOL	l	801[B]	6/6	0.88	0.17	68,93,96,98	6
25	GOL	V	204[B]	6/6	0.88	0.13	59,70,77,78	6
31	LMT	M	101	35/35	0.88	0.10	59,96,115,122	0
25	GOL	v	202[A]	6/6	0.88	0.11	70,80,83,86	6
25	GOL	v	202[B]	6/6	0.88	0.11	70,80,83,86	6
25	GOL	V	204[A]	6/6	0.88	0.13	62,72,77,78	6
32	LHG	E	101[A]	42/49	0.89	0.11	74,100,113,119	42
32	LHG	E	101[B]	42/49	0.89	0.11	74,100,113,119	42
26	SQD	b	620	54/54	0.89	0.09	61,94,119,129	0
26	SQD	B	620	54/54	0.89	0.09	59,92,137,145	0
26	SQD	F	103	43/54	0.89	0.11	77,107,129,137	0
25	GOL	B	629	6/6	0.89	0.11	71,78,90,91	0
25	GOL	a	419	6/6	0.90	0.25	54,76,81,87	0
23	CLA	b	601	65/65	0.90	0.10	63,89,128,157	0
33	LMG	a	417	51/55	0.90	0.09	71,93,110,118	0
33	LMG	c	520	51/55	0.91	0.09	65,89,136,153	0
23	CLA	c	514	65/65	0.91	0.09	69,94,127,149	0
33	LMG	C	502	51/55	0.91	0.09	64,87,110,124	0
29	UNL	D	410	17/-	0.91	0.10	59,78,106,113	0
23	CLA	B	601	65/65	0.91	0.09	59,81,115,150	0
34	HTG	B	625	19/19	0.91	0.08	65,81,97,104	0
25	GOL	D	414	6/6	0.91	0.16	43,62,69,85	0
36	CA	f	103	1/1	0.91	0.13	120,120,120,120	0
36	CA	o	301	1/1	0.91	0.06	116,116,116,116	0
33	LMG	B	621	51/55	0.92	0.07	49,68,87,107	0
25	GOL	c	526[B]	6/6	0.92	0.09	68,70,75,77	6
33	LMG	C	521	51/55	0.92	0.09	55,85,119,129	0
33	LMG	m	101	51/55	0.92	0.09	51,73,100,110	0
25	GOL	D	403	6/6	0.92	0.28	50,72,82,83	0
25	GOL	c	526[A]	6/6	0.92	0.09	68,70,75,77	6
33	LMG	D	413	51/55	0.93	0.08	47,67,125,131	0
29	UNL	d	407	17/-	0.93	0.09	67,79,113,114	0
26	SQD	C	501[A]	54/54	0.93	0.09	57,79,116,121	54
26	SQD	C	501[B]	54/54	0.93	0.09	57,80,116,121	54
33	LMG	d	409	51/55	0.93	0.08	53,76,118,148	0
23	CLA	c	513	65/65	0.93	0.09	61,84,127,139	0
23	CLA	C	515	65/65	0.93	0.08	64,87,116,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LHG	A	416[A]	49/49	0.93	0.09	48,61,83,86	49
32	LHG	A	416[B]	49/49	0.93	0.09	48,61,83,86	49
24	BCR	T	102	40/40	0.93	0.07	48,59,70,75	0
23	CLA	B	614	65/65	0.94	0.08	39,52,102,126	0
24	BCR	Y	101	40/40	0.94	0.08	54,67,83,93	0
24	BCR	c	515	40/40	0.94	0.08	70,83,97,99	0
24	BCR	d	403	40/40	0.94	0.08	54,67,98,107	0
24	BCR	t	103	40/40	0.94	0.06	43,59,74,78	0
24	BCR	y	101	40/40	0.94	0.07	60,72,86,98	0
23	CLA	a	409	65/65	0.94	0.10	43,59,139,154	0
23	CLA	C	506	65/65	0.94	0.08	44,58,101,133	0
23	CLA	b	614	65/65	0.94	0.07	43,54,101,107	0
25	GOL	C	524[A]	6/6	0.94	0.09	59,62,66,70	6
25	GOL	C	524[B]	6/6	0.94	0.09	61,61,68,70	6
23	CLA	c	505	65/65	0.94	0.07	52,62,111,132	0
23	CLA	c	507	65/65	0.94	0.08	55,70,119,137	0
23	CLA	C	508	65/65	0.94	0.08	54,72,122,143	0
23	CLA	C	514	65/65	0.94	0.08	62,77,112,128	0
24	BCR	C	516	40/40	0.94	0.08	62,77,88,93	0
26	SQD	a	411[A]	54/54	0.94	0.09	61,81,115,120	54
32	LHG	D	409[A]	49/49	0.94	0.09	51,60,109,116	49
32	LHG	D	409[B]	49/49	0.94	0.09	51,61,109,116	49
26	SQD	a	411[B]	54/54	0.94	0.09	61,81,115,120	54
34	HTG	b	625	19/19	0.94	0.07	63,82,95,106	0
24	BCR	D	406	40/40	0.94	0.08	45,59,102,109	0
24	BCR	H	101	40/40	0.94	0.08	52,69,86,91	0
35	DGD	C	519[A]	62/66	0.94	0.08	48,66,110,113	62
35	DGD	C	519[B]	62/66	0.94	0.08	48,65,110,113	62
35	DGD	c	517[A]	62/66	0.94	0.08	51,66,102,113	62
35	DGD	c	517[B]	62/66	0.94	0.08	51,66,102,113	62
35	DGD	c	518[A]	62/66	0.94	0.08	53,70,120,136	62
35	DGD	c	518[B]	62/66	0.94	0.08	53,70,120,136	62
24	BCR	K	102	40/40	0.94	0.09	57,65,75,81	0
32	LHG	d	411[A]	49/49	0.94	0.08	51,66,80,89	49
32	LHG	d	411[B]	49/49	0.94	0.08	51,66,80,89	49
24	BCR	A	408	40/40	0.95	0.07	40,53,65,68	0
24	BCR	B	619	40/40	0.95	0.07	50,61,96,102	0
23	CLA	b	606	65/65	0.95	0.07	47,62,122,131	0
28	PL9	D	407[A]	55/55	0.95	0.06	36,49,57,68	55
28	PL9	D	407[B]	55/55	0.95	0.06	36,49,57,68	55
23	CLA	D	405	65/65	0.95	0.08	49,60,123,131	0
23	CLA	b	616	65/65	0.95	0.08	52,65,133,147	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	a	407[A]	65/65	0.95	0.07	41,52,121,129	65
32	LHG	d	406[A]	49/49	0.95	0.09	54,64,115,127	49
32	LHG	d	406[B]	49/49	0.95	0.09	54,64,115,127	49
23	CLA	a	407[B]	65/65	0.95	0.07	41,52,121,129	65
23	CLA	c	508	65/65	0.95	0.09	53,70,87,94	0
24	BCR	b	619	40/40	0.95	0.07	51,64,86,91	0
23	CLA	c	509	65/65	0.95	0.07	45,64,127,142	0
24	BCR	c	516	40/40	0.95	0.07	55,68,84,92	0
35	DGD	C	520	62/66	0.95	0.07	44,58,92,112	0
35	DGD	H	102	62/66	0.95	0.08	46,61,74,83	0
23	CLA	A	407	65/65	0.95	0.08	40,54,129,145	0
24	BCR	h	101	40/40	0.95	0.09	58,72,98,100	0
24	BCR	k	101	40/40	0.95	0.09	60,74,90,92	0
25	GOL	b	628	6/6	0.95	0.08	80,82,87,90	0
35	DGD	c	519	62/66	0.95	0.07	51,65,109,131	0
35	DGD	h	102	62/66	0.95	0.08	51,65,79,84	0
29	UNL	X	101	18/-	0.95	0.10	64,76,108,112	0
23	CLA	C	510	65/65	0.95	0.07	44,57,120,146	0
23	CLA	d	402	65/65	0.95	0.09	55,68,126,147	0
23	CLA	B	611	65/65	0.96	0.06	33,45,65,86	0
23	CLA	A	406[A]	65/65	0.96	0.06	38,47,111,118	65
24	BCR	B	617	40/40	0.96	0.05	42,52,64,65	0
29	UNL	x	101	18/-	0.96	0.10	68,81,119,137	0
24	BCR	B	618	40/40	0.96	0.05	37,57,69,76	0
23	CLA	B	616	65/65	0.96	0.08	45,61,131,138	0
23	CLA	b	602	65/65	0.96	0.07	52,63,84,91	0
24	BCR	C	517	40/40	0.96	0.07	52,67,79,90	0
23	CLA	C	503	65/65	0.96	0.07	50,62,76,89	0
23	CLA	b	607	65/65	0.96	0.06	39,48,84,93	0
23	CLA	b	612	65/65	0.96	0.07	47,56,66,78	0
23	CLA	A	406[B]	65/65	0.96	0.06	38,47,111,119	65
28	PL9	d	404[A]	55/55	0.96	0.06	39,51,61,68	55
28	PL9	d	404[B]	55/55	0.96	0.06	39,50,61,68	55
23	CLA	A	404[A]	65/65	0.96	0.06	38,42,60,67	65
24	BCR	a	410	40/40	0.96	0.06	46,54,66,68	0
24	BCR	b	617	40/40	0.96	0.06	44,54,66,67	0
24	BCR	b	618	40/40	0.96	0.06	43,59,78,89	0
23	CLA	c	502	65/65	0.96	0.07	54,69,80,87	0
23	CLA	c	504	65/65	0.96	0.07	55,71,85,90	0
32	LHG	D	408[A]	49/49	0.96	0.07	46,54,66,76	49
32	LHG	D	408[B]	49/49	0.96	0.07	46,55,66,77	49
23	CLA	C	509	65/65	0.96	0.07	52,66,83,93	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
35	DGD	C	518[A]	62/66	0.96	0.07	47,60,102,111	62
35	DGD	C	518[B]	62/66	0.96	0.07	47,60,102,111	62
23	CLA	c	506	65/65	0.96	0.06	51,65,94,103	0
23	CLA	A	404[B]	65/65	0.96	0.06	38,43,63,67	65
23	CLA	B	602	65/65	0.96	0.07	50,59,73,91	0
23	CLA	B	603	65/65	0.96	0.07	44,54,75,85	0
23	CLA	c	511	65/65	0.96	0.06	49,65,80,90	0
32	LHG	d	405[A]	49/49	0.96	0.07	48,55,70,76	49
32	LHG	d	405[B]	49/49	0.96	0.07	47,56,70,77	49
23	CLA	c	512	65/65	0.96	0.07	59,70,86,96	0
25	GOL	B	624	6/6	0.96	0.11	67,78,81,82	0
23	CLA	B	606	65/65	0.96	0.07	43,58,110,134	0
36	CA	O	301	1/1	0.96	0.04	105,105,105,105	0
23	CLA	B	609	65/65	0.96	0.07	46,61,72,83	0
32	LHG	l	802[A]	49/49	0.96	0.07	48,58,72,91	49
32	LHG	l	802[B]	49/49	0.96	0.07	48,57,72,91	49
37	PHO	D	402[A]	64/64	0.96	0.06	41,50,55,59	64
37	PHO	D	402[B]	64/64	0.96	0.06	40,50,55,60	64
37	PHO	a	416[A]	64/64	0.96	0.07	47,57,62,67	64
37	PHO	a	416[B]	64/64	0.96	0.07	47,57,62,66	64
23	CLA	a	406[B]	65/65	0.97	0.05	37,44,64,72	65
23	CLA	A	405[A]	65/65	0.97	0.05	35,43,53,64	65
23	CLA	d	401[A]	65/65	0.97	0.06	40,47,73,94	65
23	CLA	d	401[B]	65/65	0.97	0.06	40,47,73,94	65
23	CLA	B	607	65/65	0.97	0.06	33,48,76,83	0
23	CLA	C	505	65/65	0.97	0.06	48,65,73,84	0
23	CLA	A	405[B]	65/65	0.97	0.05	35,43,53,64	65
23	CLA	C	507	65/65	0.97	0.06	49,63,99,114	0
23	CLA	b	603	65/65	0.97	0.06	45,60,85,98	0
23	CLA	b	604	65/65	0.97	0.06	42,54,100,119	0
23	CLA	b	605	65/65	0.97	0.07	37,52,74,80	0
23	CLA	B	610	65/65	0.97	0.07	40,56,71,84	0
23	CLA	B	604	65/65	0.97	0.06	36,47,108,129	0
23	CLA	b	609	65/65	0.97	0.07	53,68,83,102	0
23	CLA	b	610	65/65	0.97	0.07	48,59,73,78	0
23	CLA	b	611	65/65	0.97	0.06	37,48,71,88	0
23	CLA	B	612	65/65	0.97	0.06	35,50,63,71	0
32	LHG	L	101[A]	49/49	0.97	0.06	47,55,68,87	49
32	LHG	L	101[B]	49/49	0.97	0.06	47,56,68,87	49
23	CLA	b	613	65/65	0.97	0.06	42,52,90,108	0
23	CLA	C	511	65/65	0.97	0.07	50,59,84,91	0
23	CLA	b	615	65/65	0.97	0.07	48,64,87,90	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	C	512	65/65	0.97	0.06	48,59,78,84	0
23	CLA	C	513	65/65	0.97	0.07	51,65,81,83	0
23	CLA	c	503	65/65	0.97	0.06	46,60,90,109	0
23	CLA	B	613	65/65	0.97	0.06	38,47,90,106	0
23	CLA	B	605	65/65	0.97	0.05	40,50,67,84	0
23	CLA	D	404[A]	65/65	0.97	0.06	36,44,67,75	65
36	CA	C	525	1/1	0.97	0.06	79,79,79,79	0
23	CLA	D	404[B]	65/65	0.97	0.06	36,44,67,76	65
30	BCT	a	404[A]	4/4	0.97	0.05	57,59,65,72	4
36	CA	c	523	1/1	0.97	0.05	78,78,78,78	0
30	BCT	a	404[B]	4/4	0.97	0.05	56,59,65,72	4
23	CLA	B	615	65/65	0.97	0.06	43,55,75,89	0
37	PHO	D	401[A]	64/64	0.97	0.04	39,46,52,56	64
37	PHO	D	401[B]	64/64	0.97	0.04	39,46,52,56	64
23	CLA	a	405[A]	65/65	0.97	0.06	36,46,63,76	65
23	CLA	c	510	65/65	0.97	0.07	45,62,86,94	0
37	PHO	a	408[A]	64/64	0.97	0.05	42,48,53,57	64
37	PHO	a	408[B]	64/64	0.97	0.05	42,48,53,57	64
23	CLA	a	405[B]	65/65	0.97	0.06	39,46,63,76	65
23	CLA	a	406[A]	65/65	0.97	0.05	37,43,63,72	65
23	CLA	B	608	65/65	0.98	0.05	41,52,70,84	0
22	CL	a	403[A]	1/1	0.98	0.09	53,53,53,53	1
22	CL	a	403[B]	1/1	0.98	0.09	53,53,53,53	1
30	BCT	A	414[A]	4/4	0.98	0.06	54,55,61,67	4
30	BCT	A	414[B]	4/4	0.98	0.06	54,55,61,67	4
22	CL	a	402[A]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	b	608	65/65	0.98	0.05	44,57,80,96	0
22	CL	a	402[B]	1/1	0.98	0.05	49,49,49,49	1
23	CLA	C	504	65/65	0.98	0.06	43,55,83,93	0
38	HEM	f	101	43/43	0.98	0.08	69,88,123,141	0
40	HEC	v	201	43/43	0.98	0.06	54,64,74,80	0
22	CL	A	403[B]	1/1	0.99	0.04	47,47,47,47	1
27	OEX	A	411[A]	10/10	0.99	0.03	39,46,50,51	10
27	OEX	A	411[B]	10/10	0.99	0.03	40,46,50,52	10
22	CL	A	402[A]	1/1	0.99	0.06	43,43,43,43	1
38	HEM	F	102	43/43	0.99	0.06	57,72,84,91	0
22	CL	A	402[B]	1/1	0.99	0.06	42,42,42,42	1
39	MG	J	102	1/1	0.99	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.99	0.03	67,67,67,67	0
40	HEC	V	202	43/43	0.99	0.06	37,51,58,60	0
22	CL	A	403[A]	1/1	0.99	0.04	48,48,48,48	1
27	OEX	a	413[B]	10/10	1.00	0.02	46,50,55,56	10

Continued on next page...

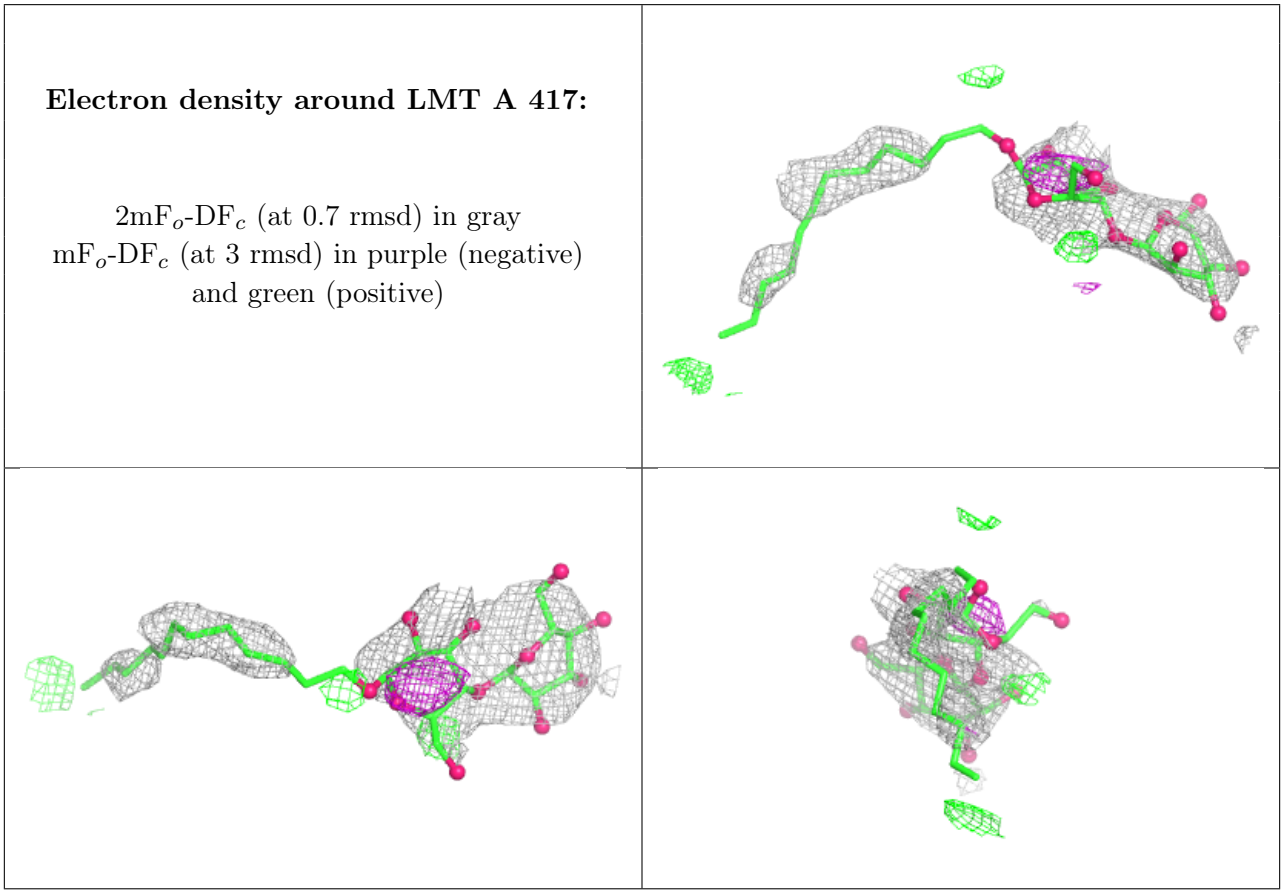
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	a	401[A]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	a	401[B]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	A	401[A]	1/1	1.00	0.01	51,51,51,51	1
36	CA	c	524	1/1	1.00	0.04	80,80,80,80	0
21	FE2	A	401[B]	1/1	1.00	0.01	51,51,51,51	1
27	OEX	a	413[A]	10/10	1.00	0.02	46,50,55,56	10

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.

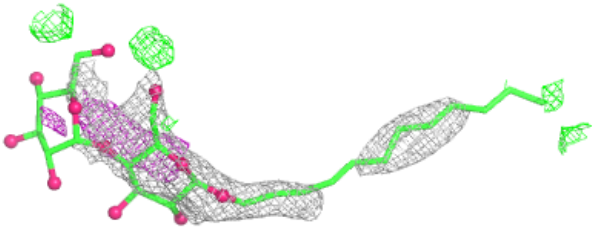
Electron density around LMT A 417:

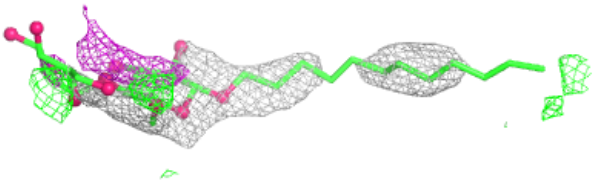
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

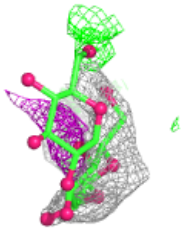


Electron density around LMT F 101:

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

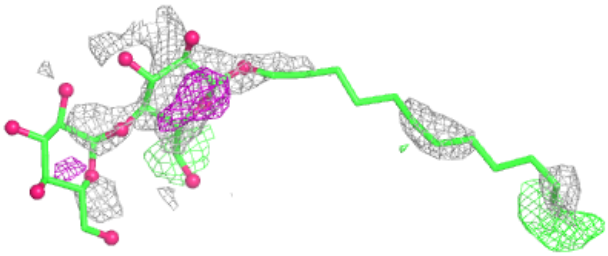


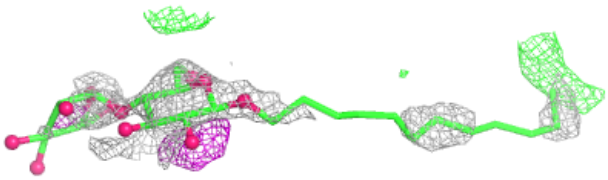


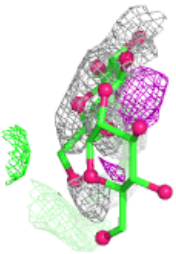


Electron density around LMT e 101:

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

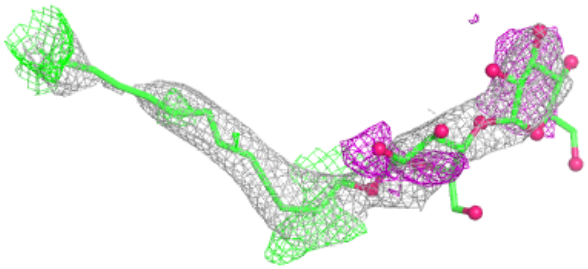


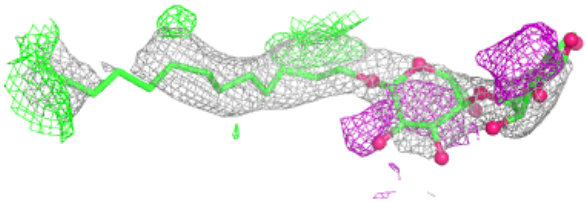


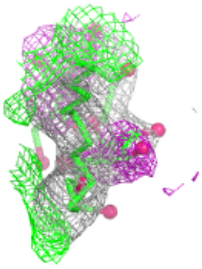


Electron density around LMT B 630:

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

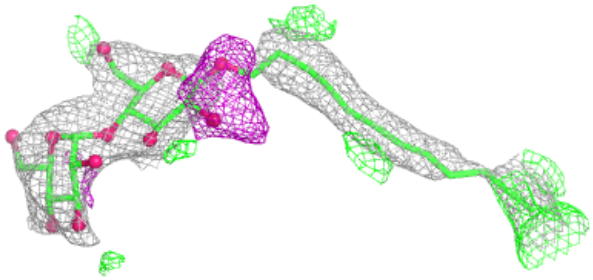


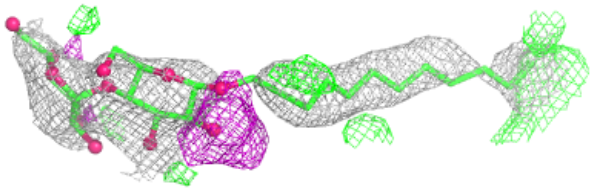


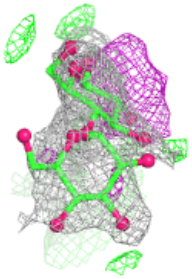


Electron density around LMT A 415:

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

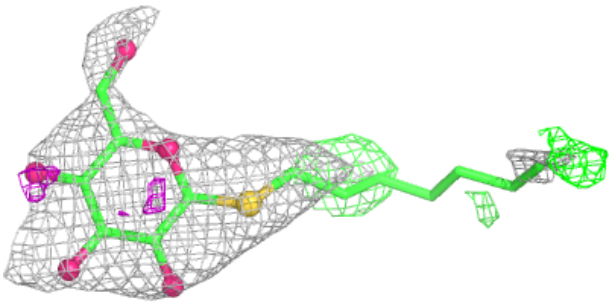


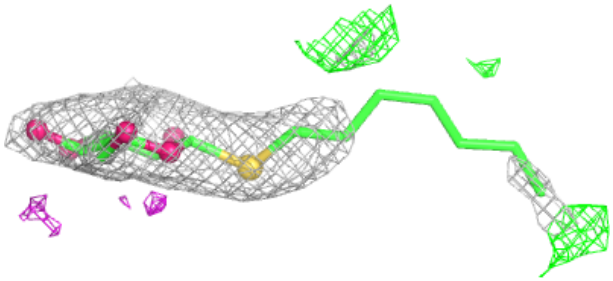


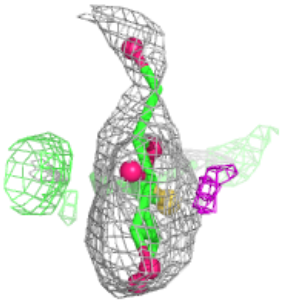


Electron density around HTG C 523:

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

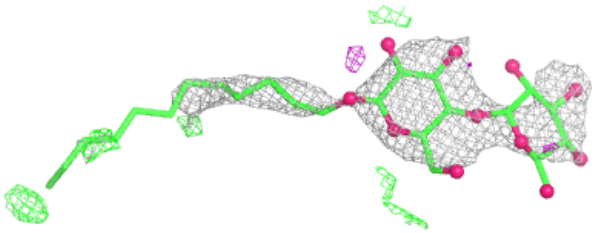


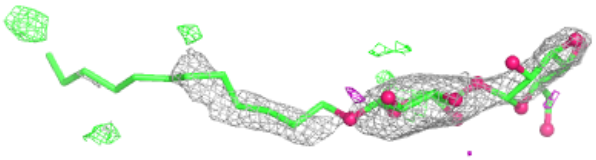


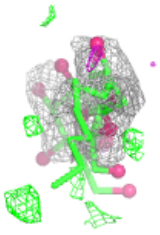


Electron density around LMT c 501:

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

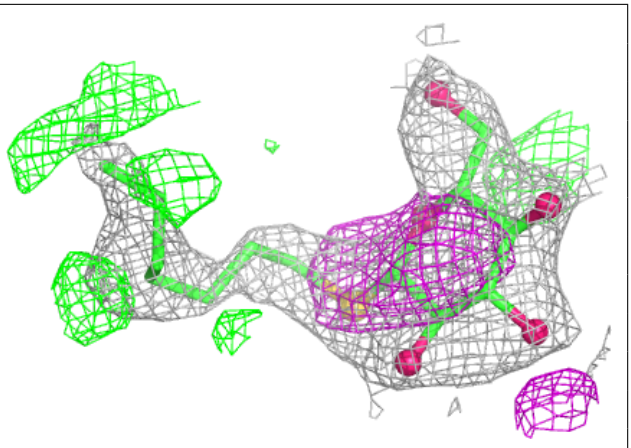


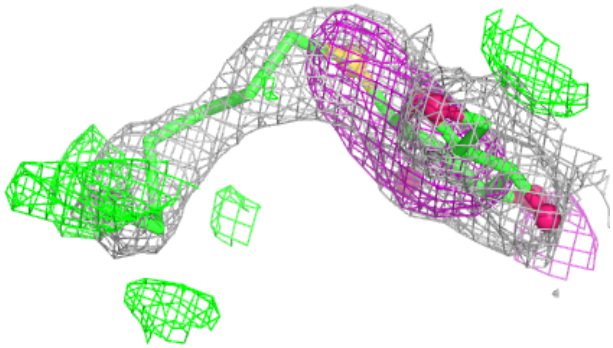


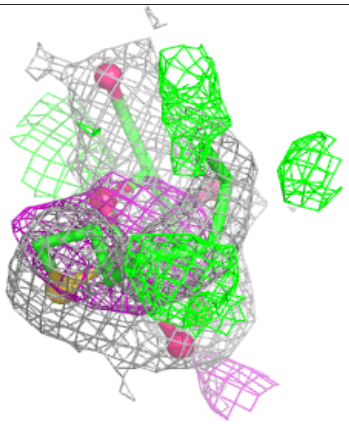


Electron density around HTG B 623:

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

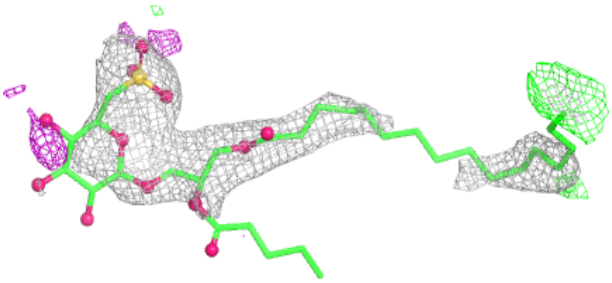


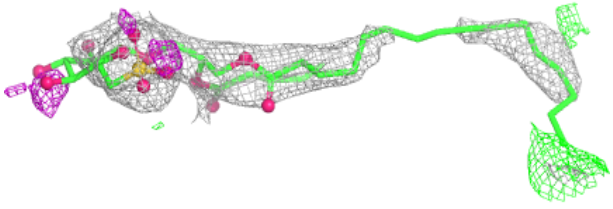


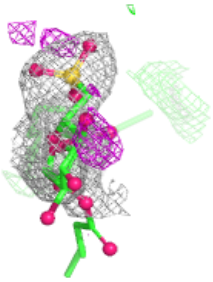


Electron density around SQD f 102:

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

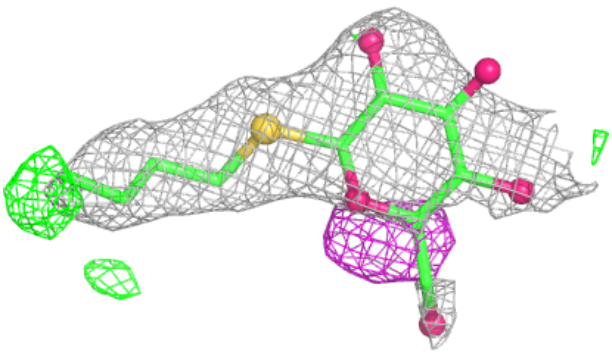


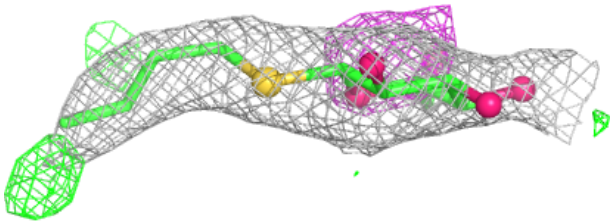


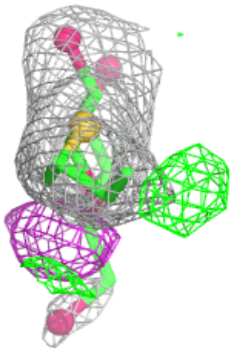


Electron density around HTG D 412:

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

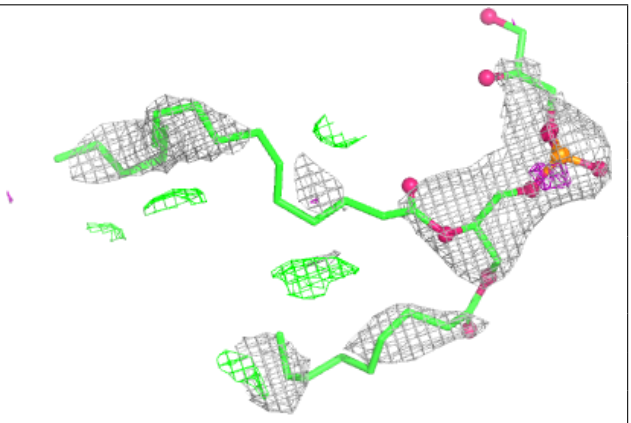


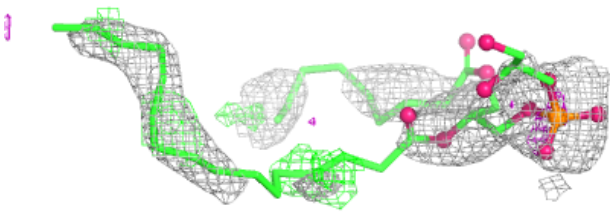


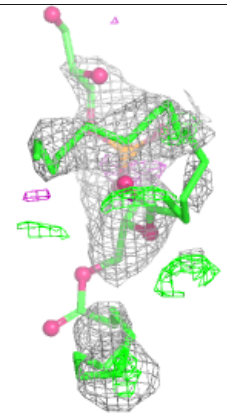


Electron density around LHG a 420 (A):

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

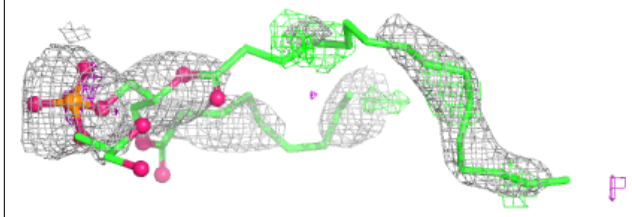


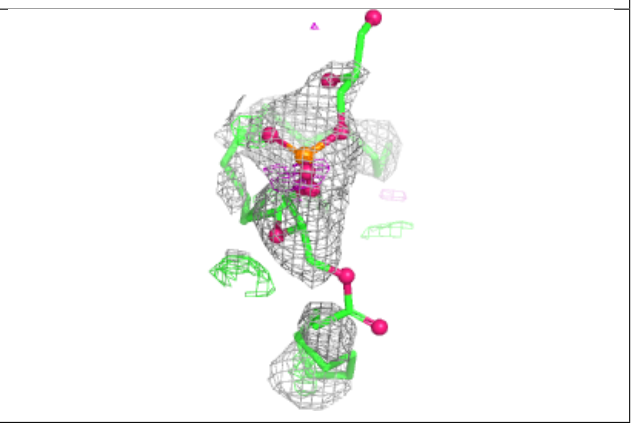




Electron density around LHG a 420 (B):

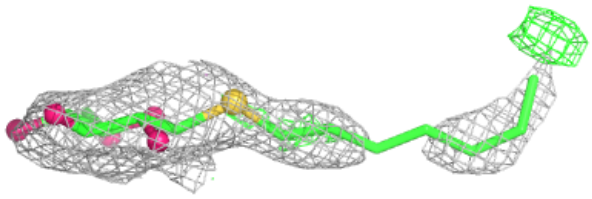
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

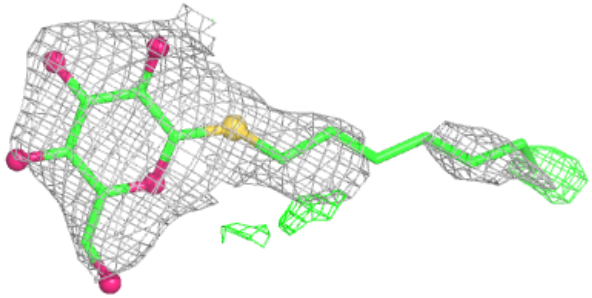




Electron density around HTG c 522:

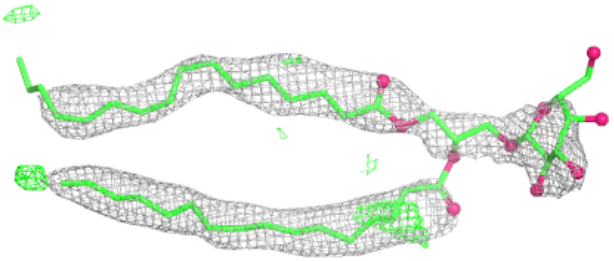
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

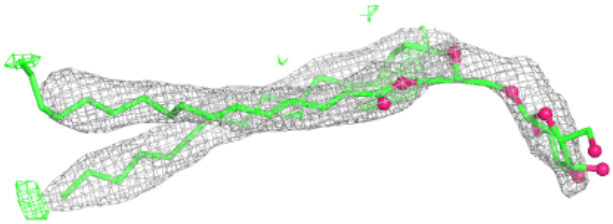


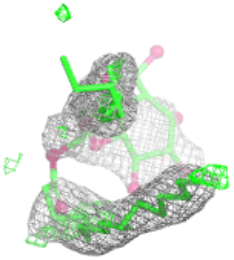


Electron density around LMG C 522:

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

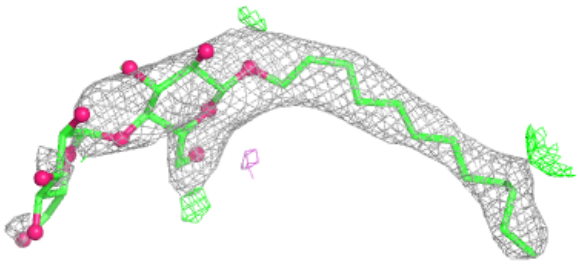


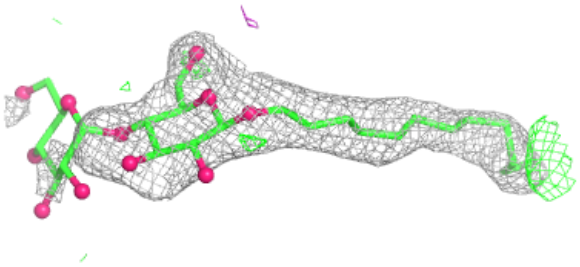




Electron density around LMT T 101:

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

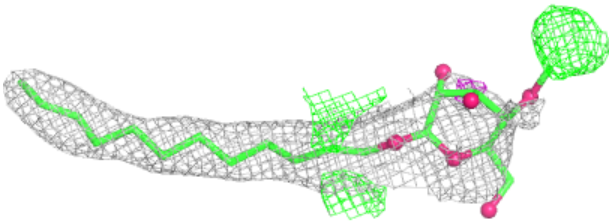


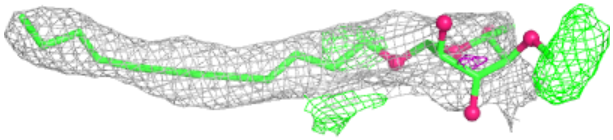


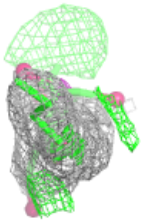


Electron density around LMT b 621:

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

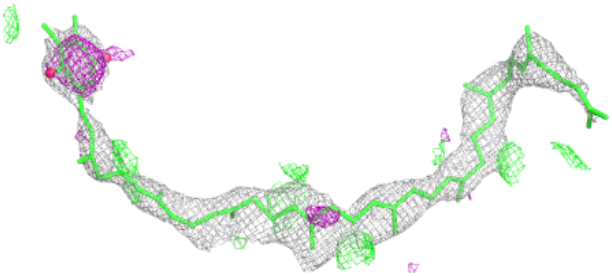


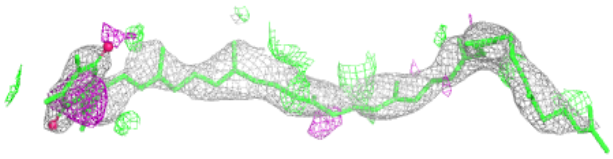


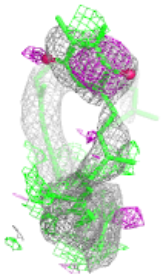


Electron density around PL9 a 414 (B):

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

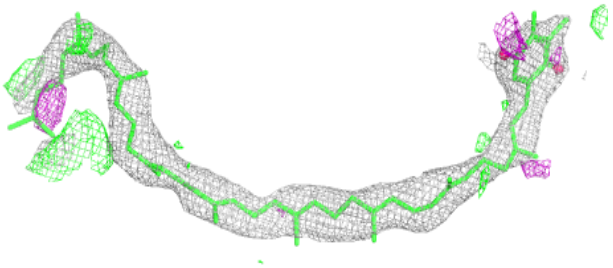


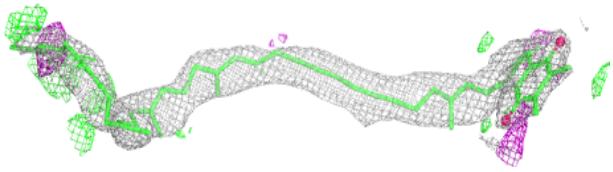


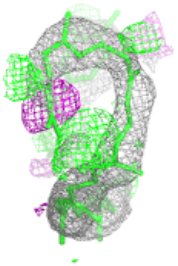


Electron density around PL9 A 412 (A):

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

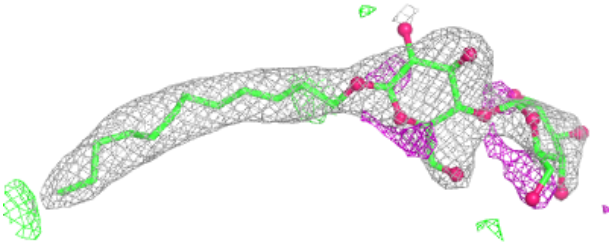


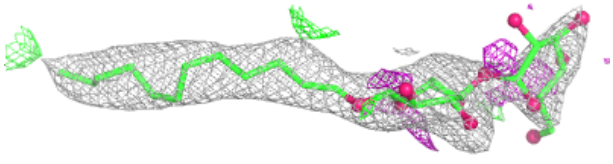


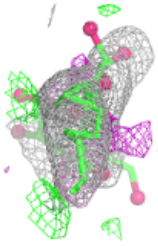


Electron density around LMT B 628:

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

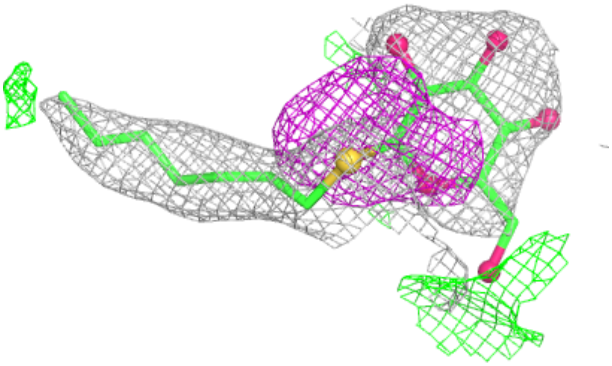


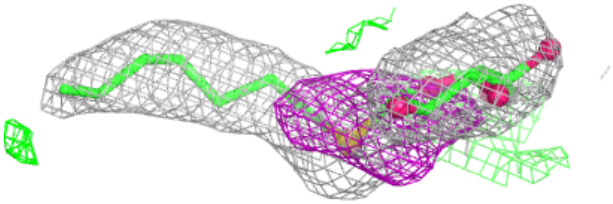


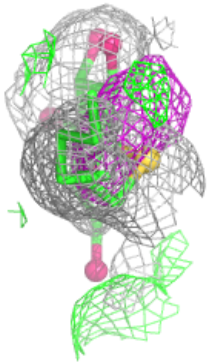


Electron density around HTG b 622:

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

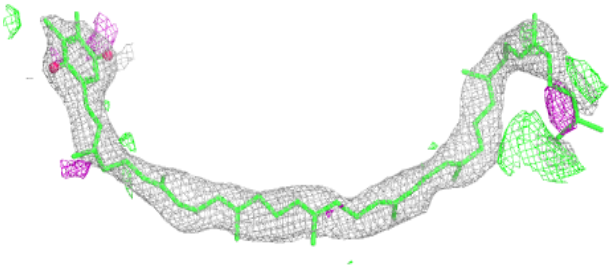


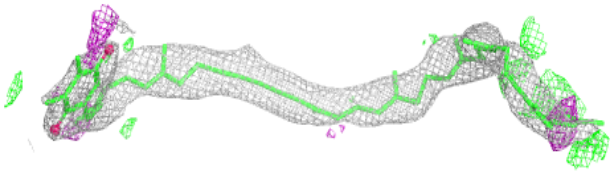


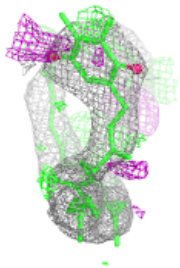


Electron density around PL9 A 412 (B):

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

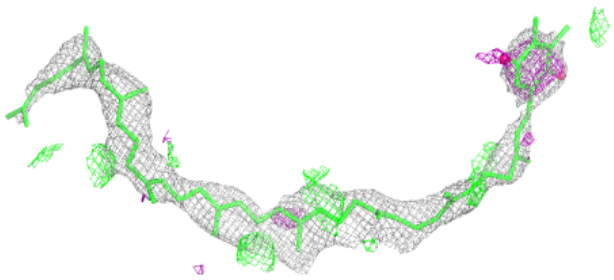


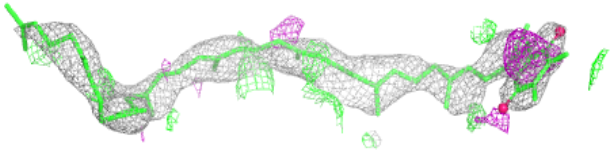


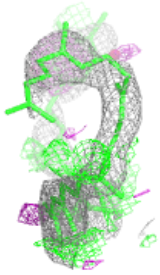


Electron density around PL9 a 414 (A):

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

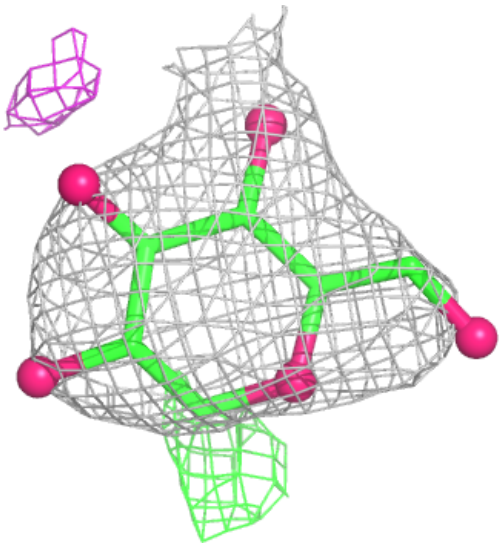


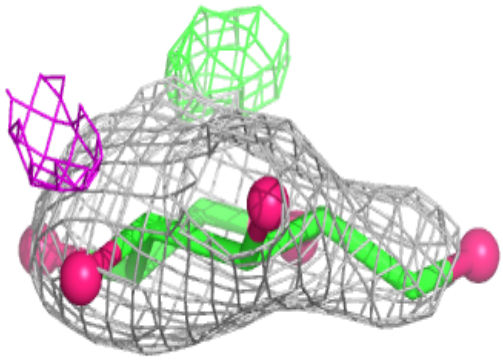


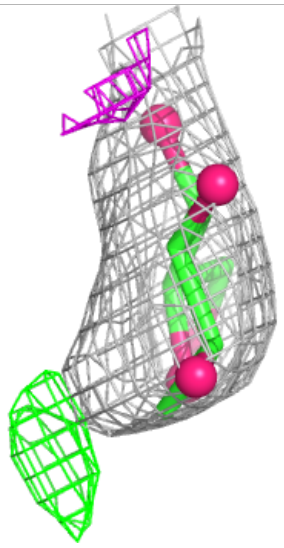


Electron density around HTG V 203:

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

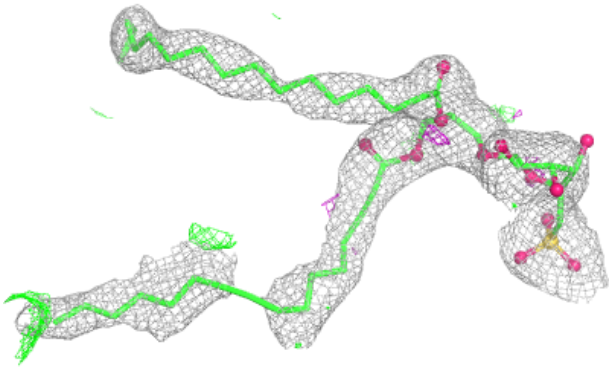


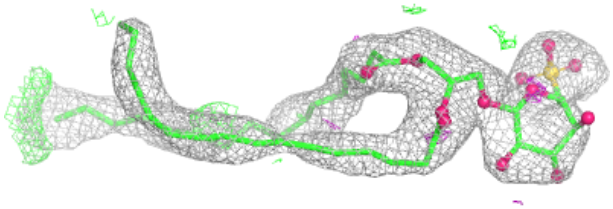


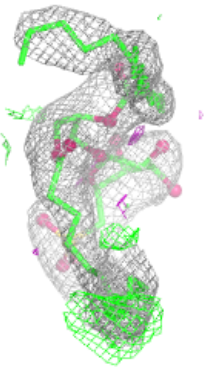


Electron density around SQD a 412:

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

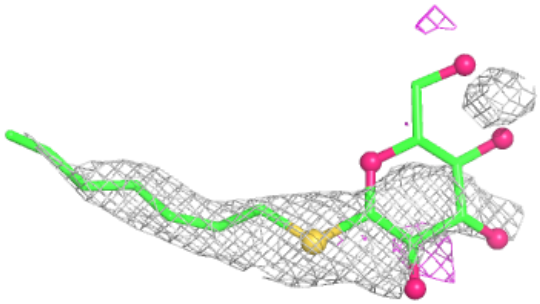


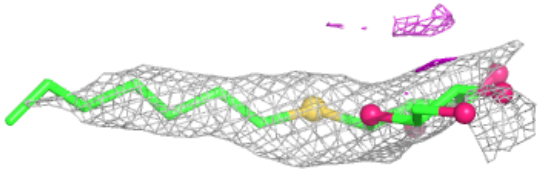


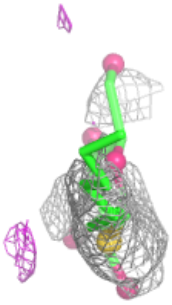


Electron density around HTG b 623:

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

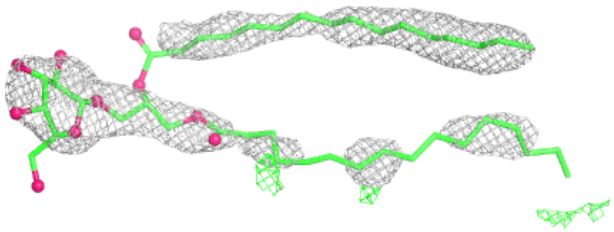


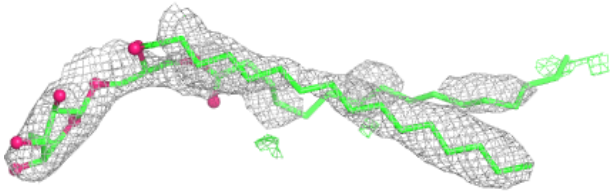


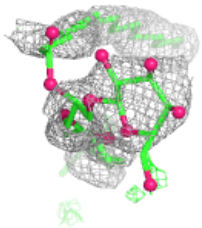


Electron density around LMG c 521:

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

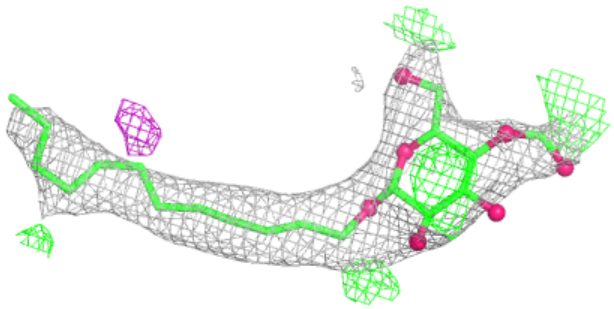


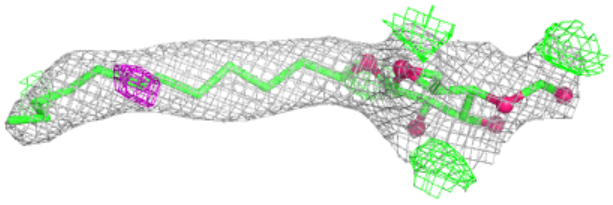


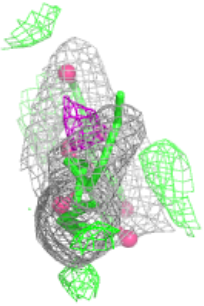


Electron density around LMT t 102:

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

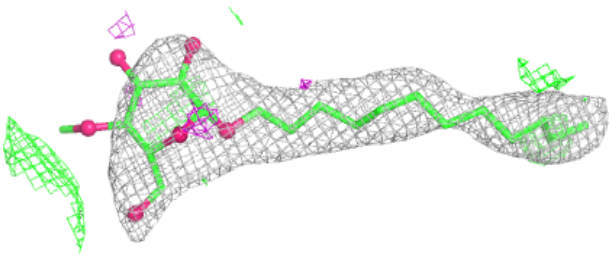


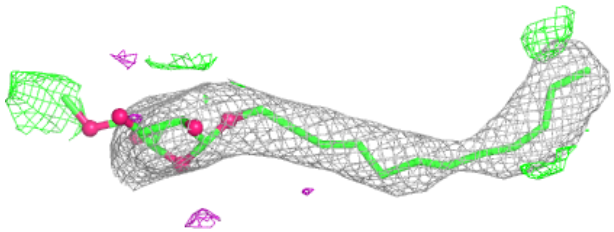


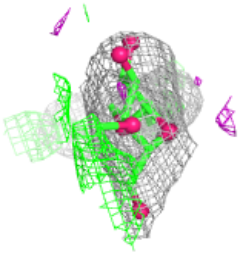


Electron density around LMT t 101:

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

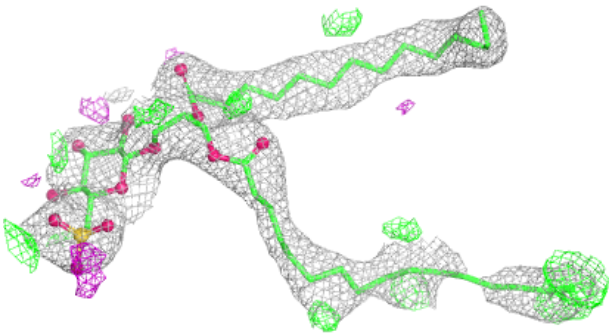


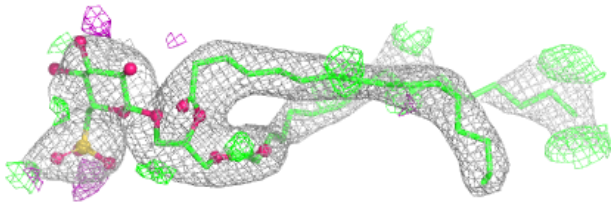


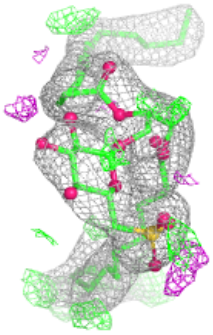


Electron density around SQD A 410:

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

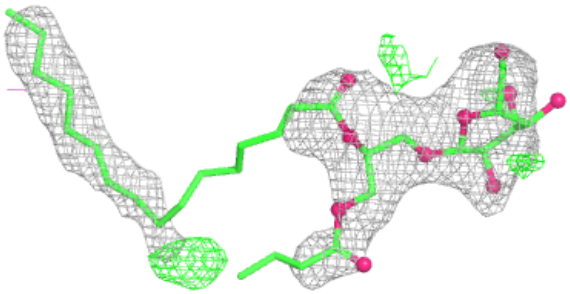


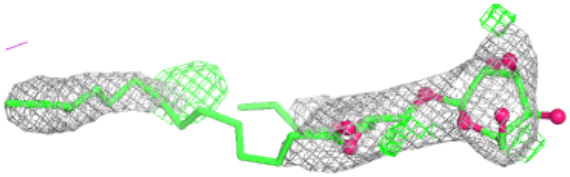


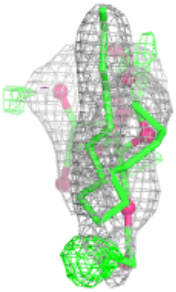


Electron density around LMG z 101:

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

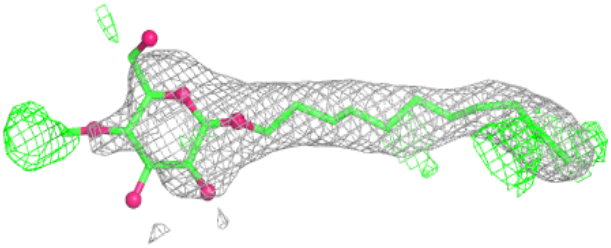


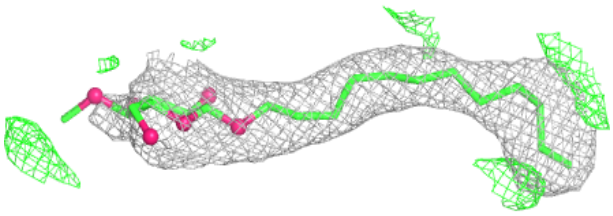


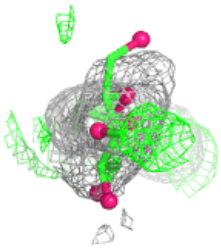


Electron density around LMT b 627:

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

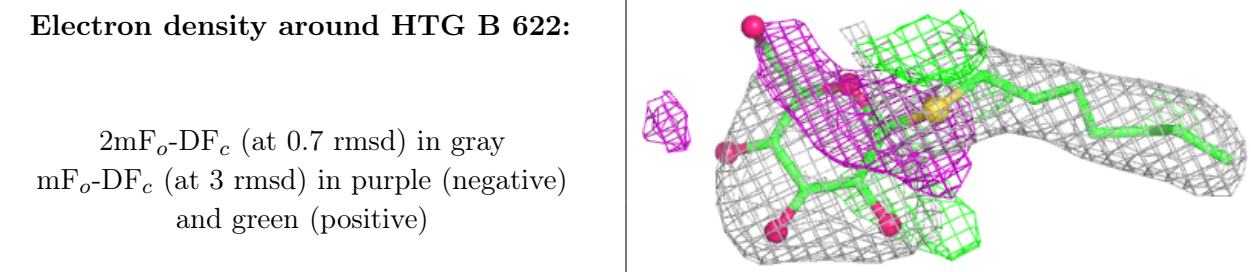


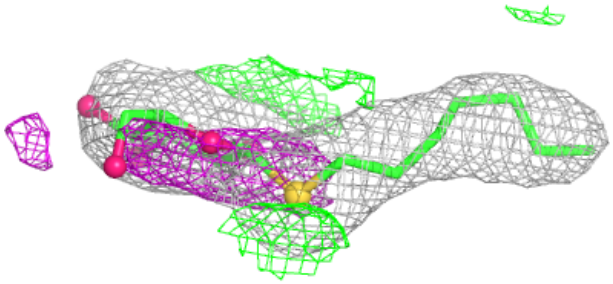


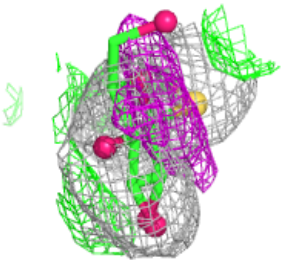


Electron density around HTG B 622:

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

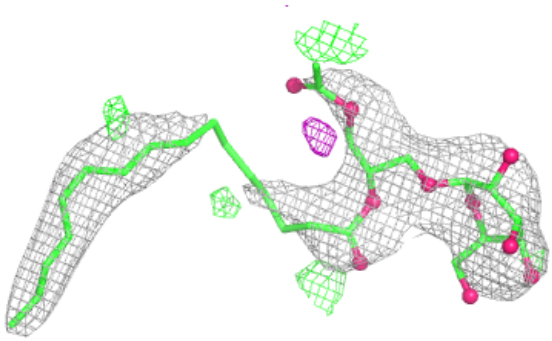


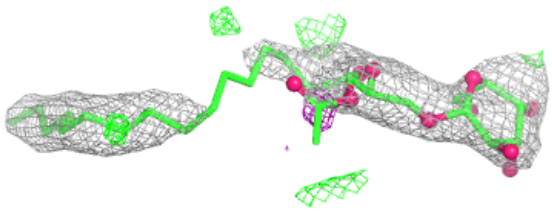


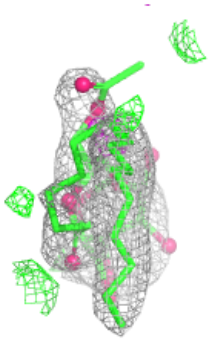


Electron density around LMG C 526:

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

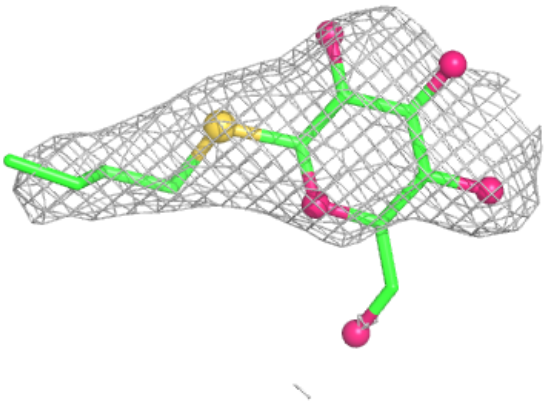


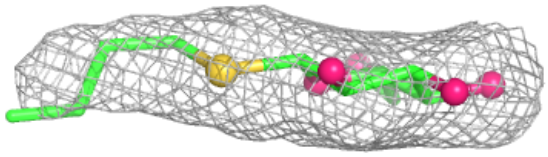


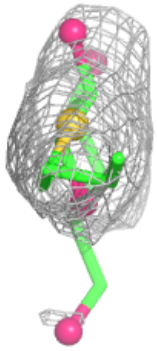


Electron density around HTG d 408:

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

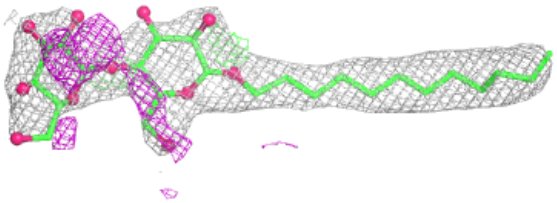


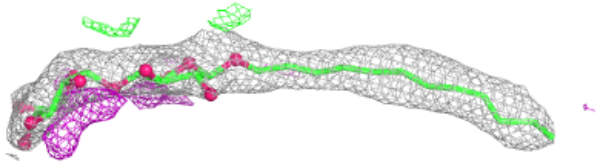


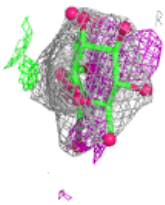


Electron density around LMT m 103:

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

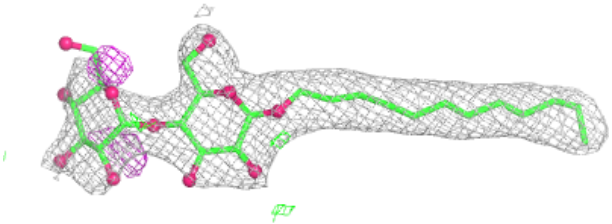


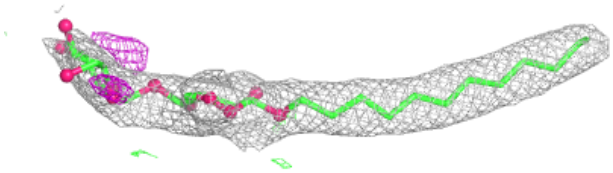


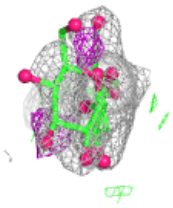


Electron density around LMT M 101:

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

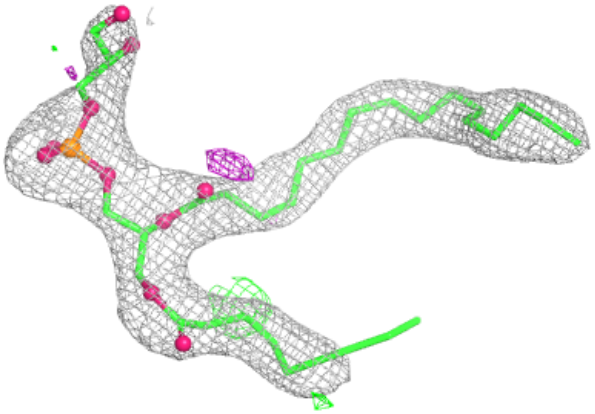


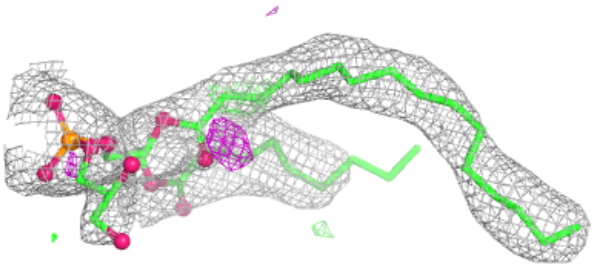


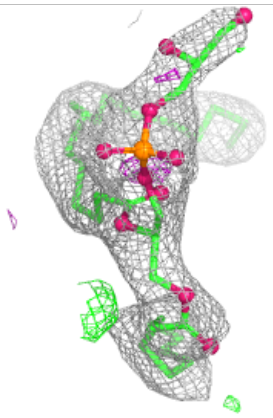


Electron density around LHG E 101 (A):

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

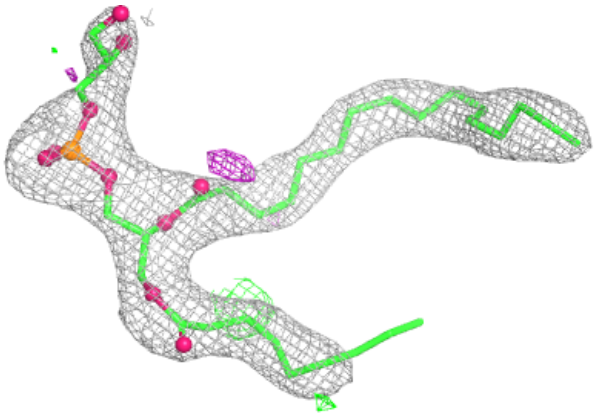


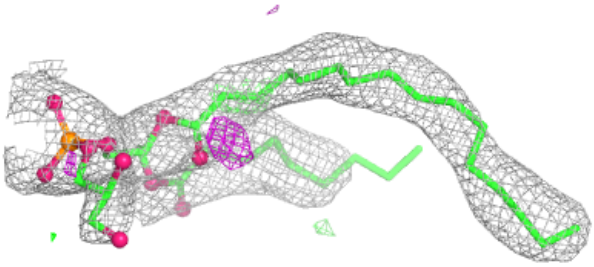


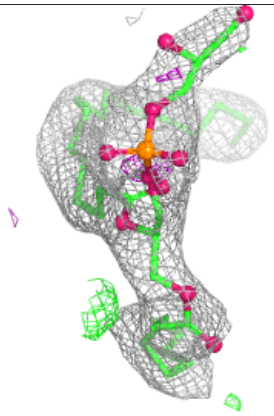


Electron density around LHG E 101 (B):

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

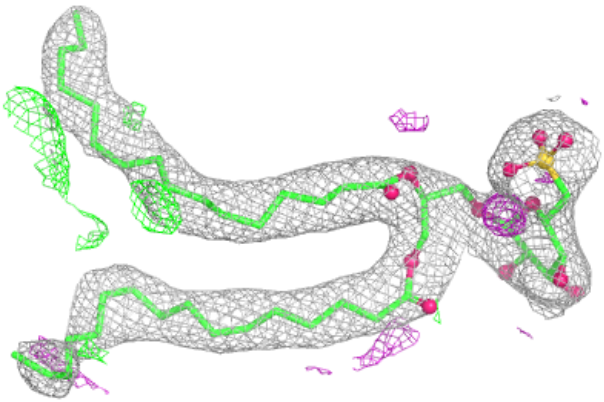


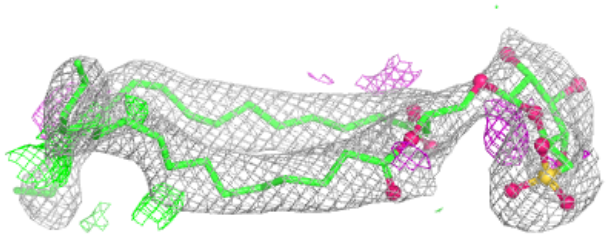


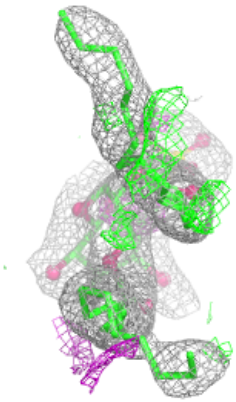


Electron density around SQD b 620:

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

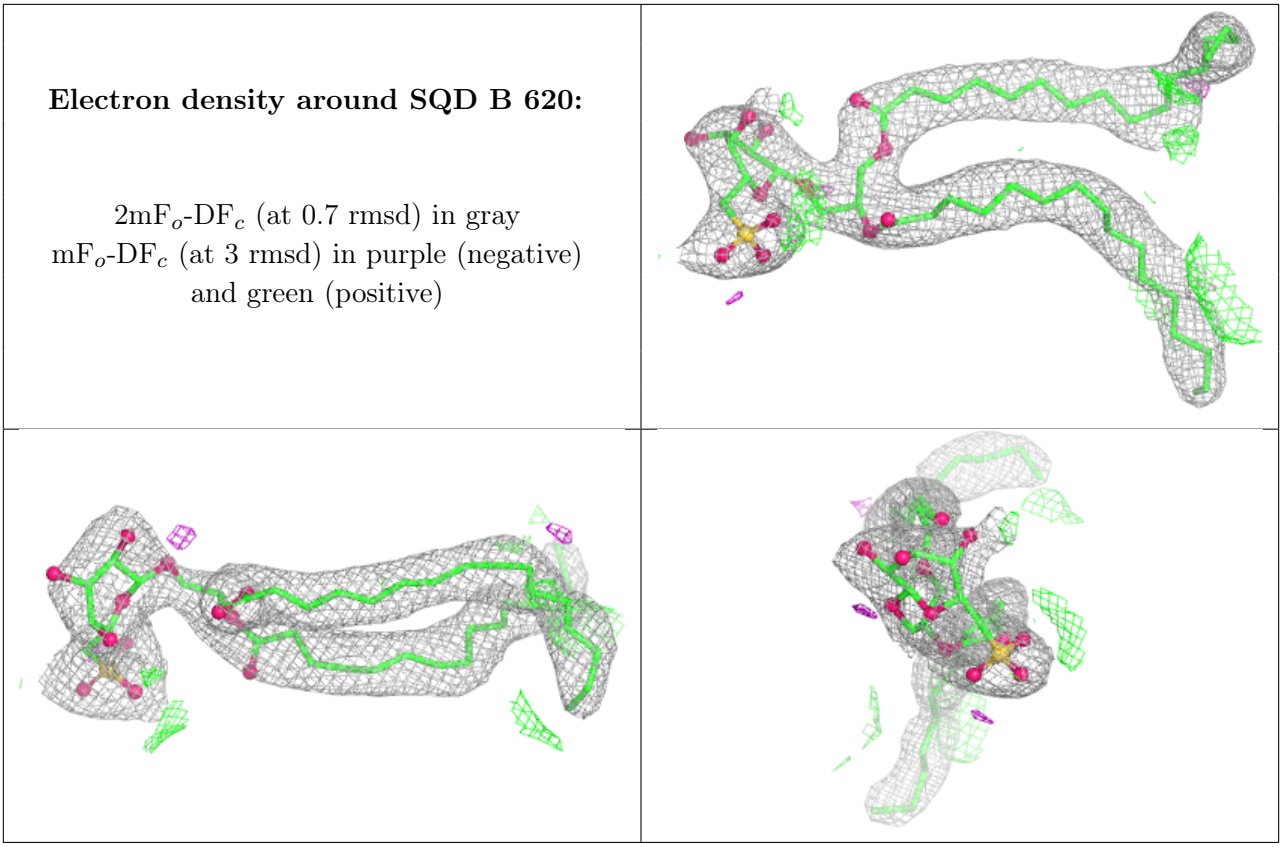






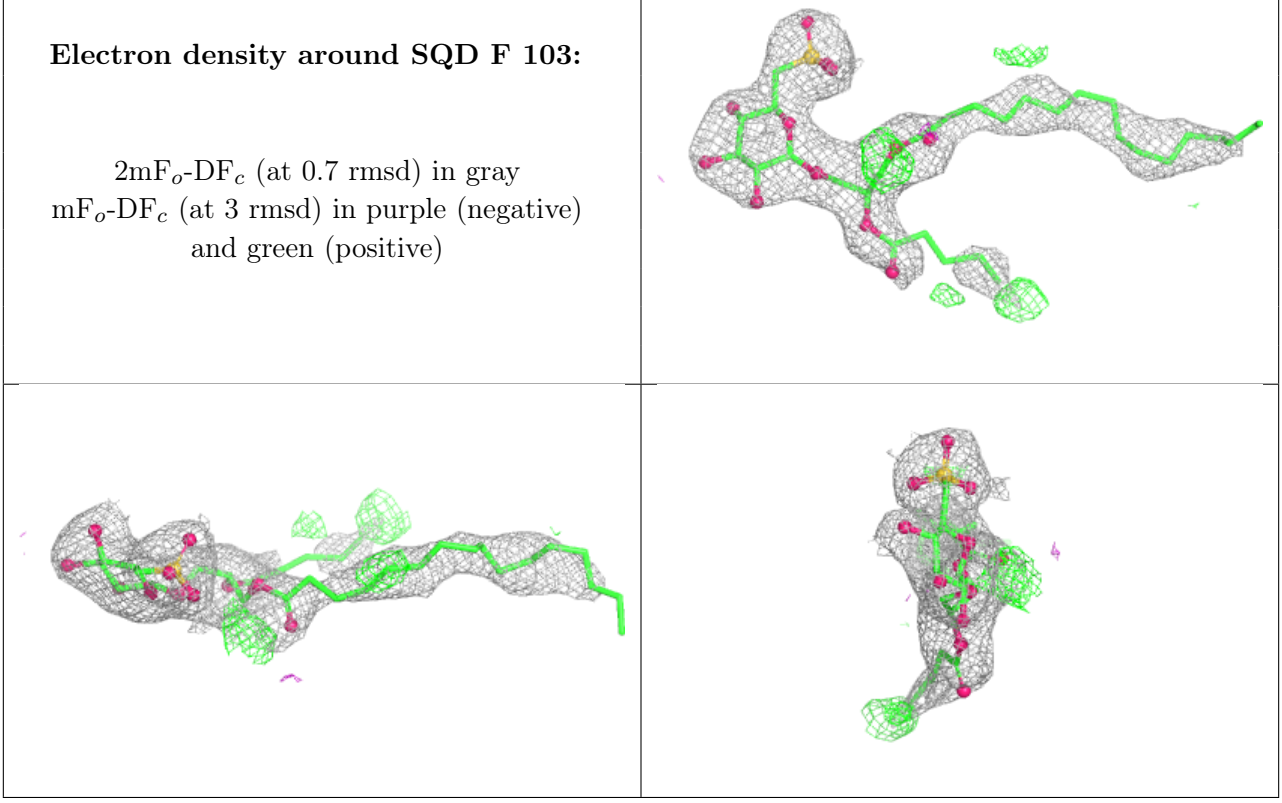
Electron density around SQD B 620:

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



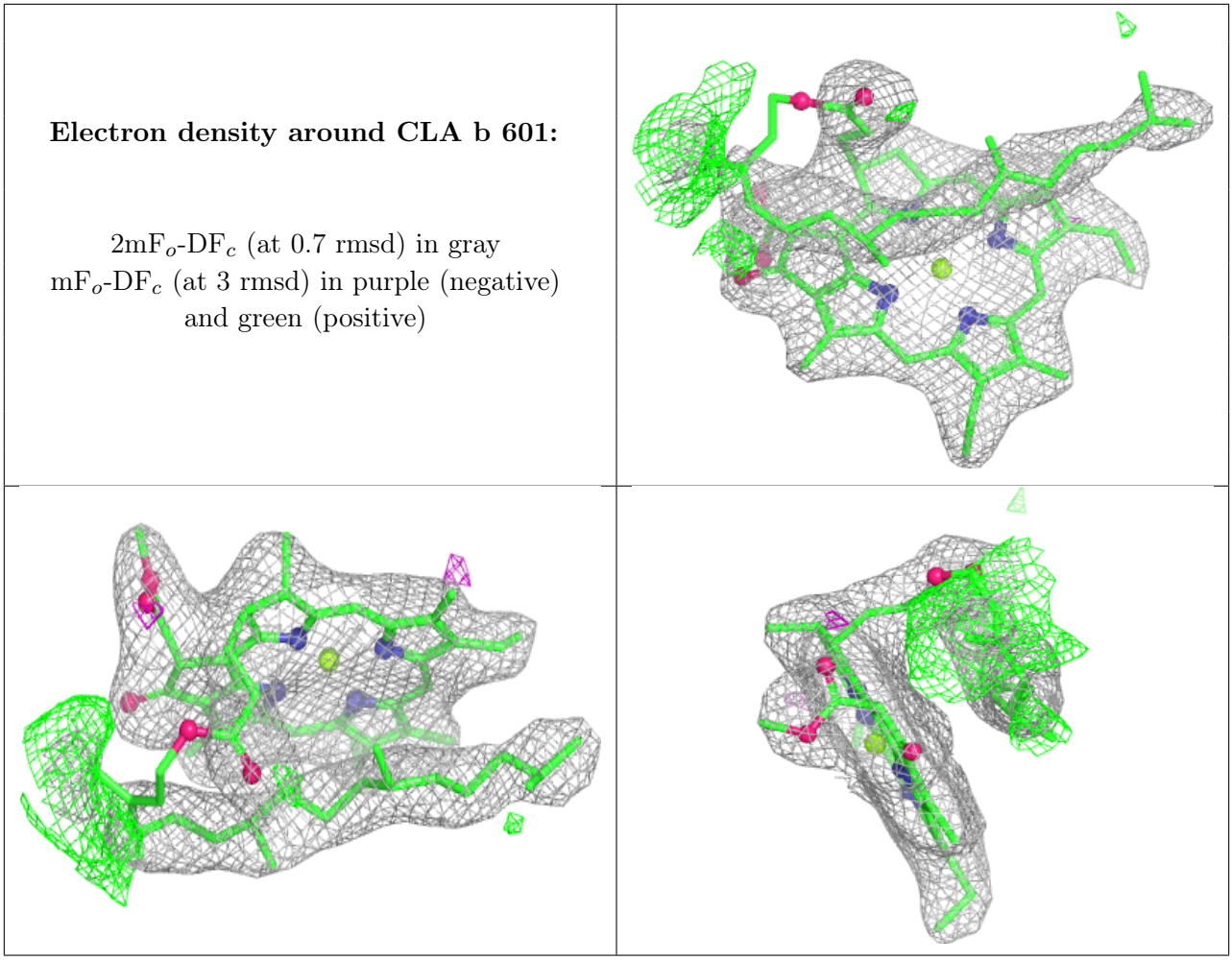
Electron density around SQD F 103:

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



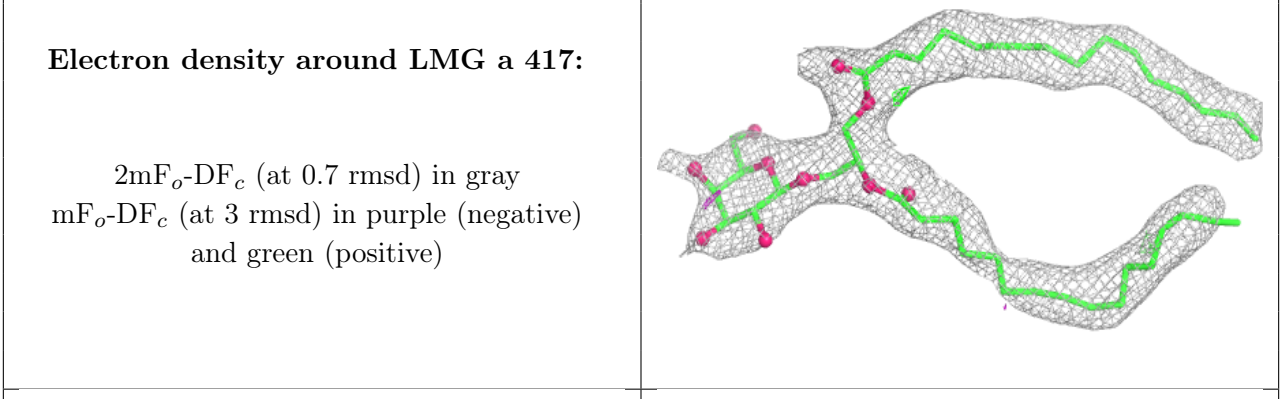
Electron density around CLA b 601:

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



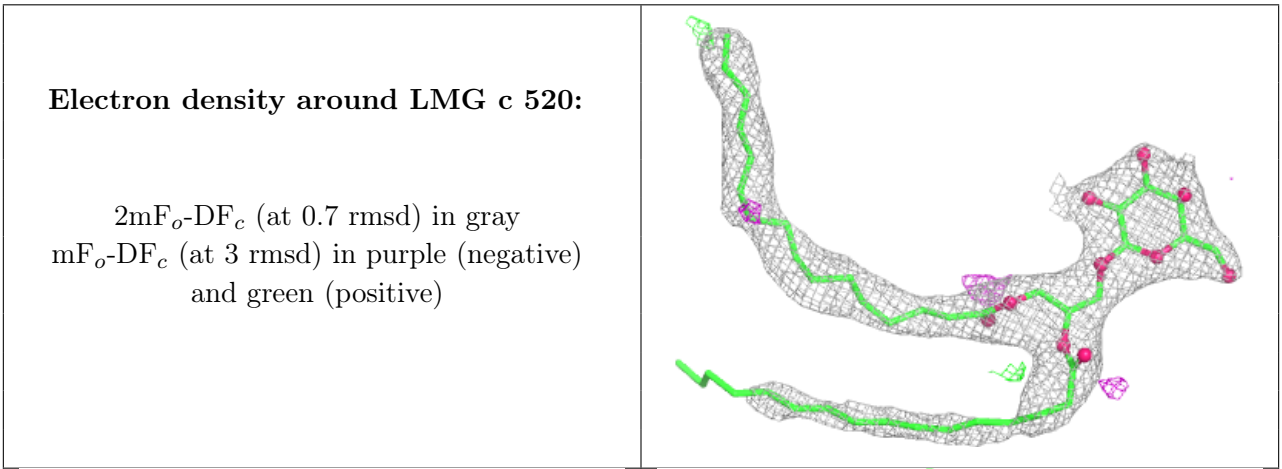
Electron density around LMG a 417:

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



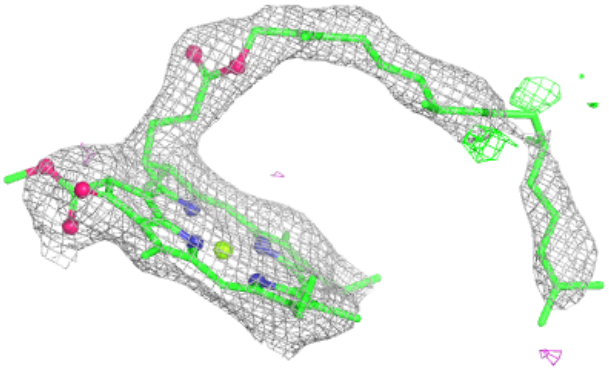
Electron density around LMG c 520:

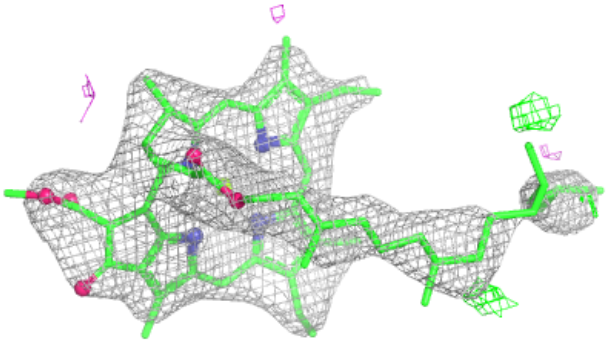
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

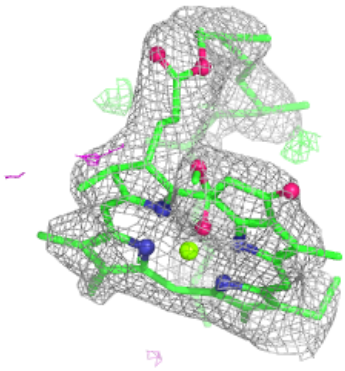


Electron density around CLA c 514:

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

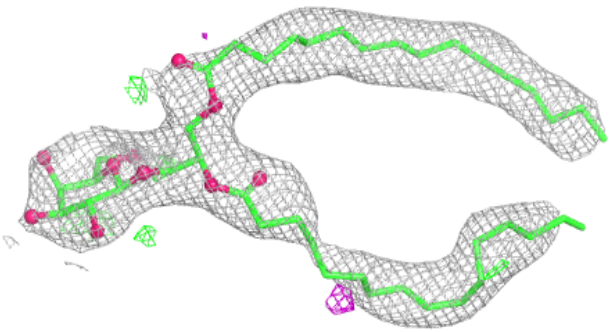


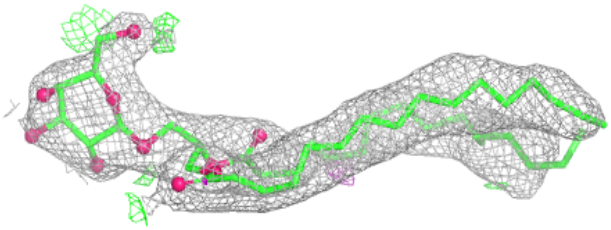




Electron density around LMG C 502:

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

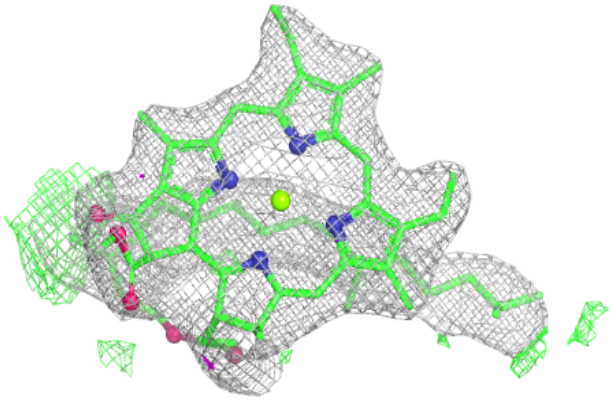


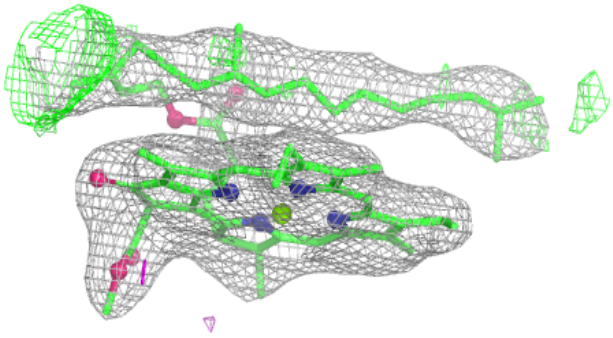


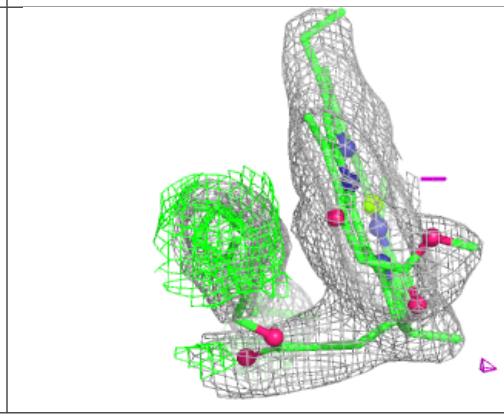


Electron density around CLA B 601:

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

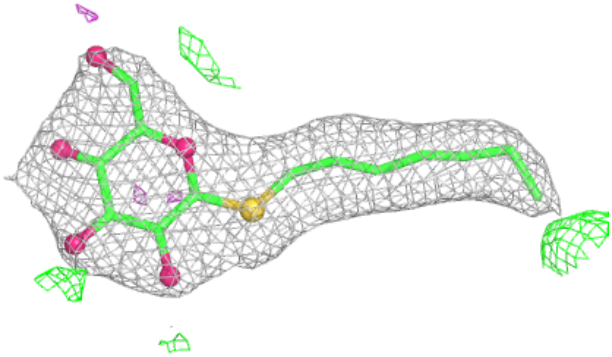


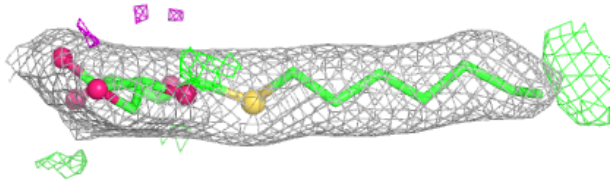


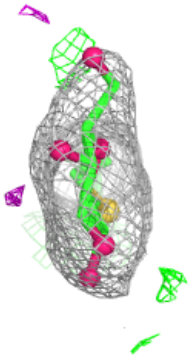


Electron density around HTG B 625:

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

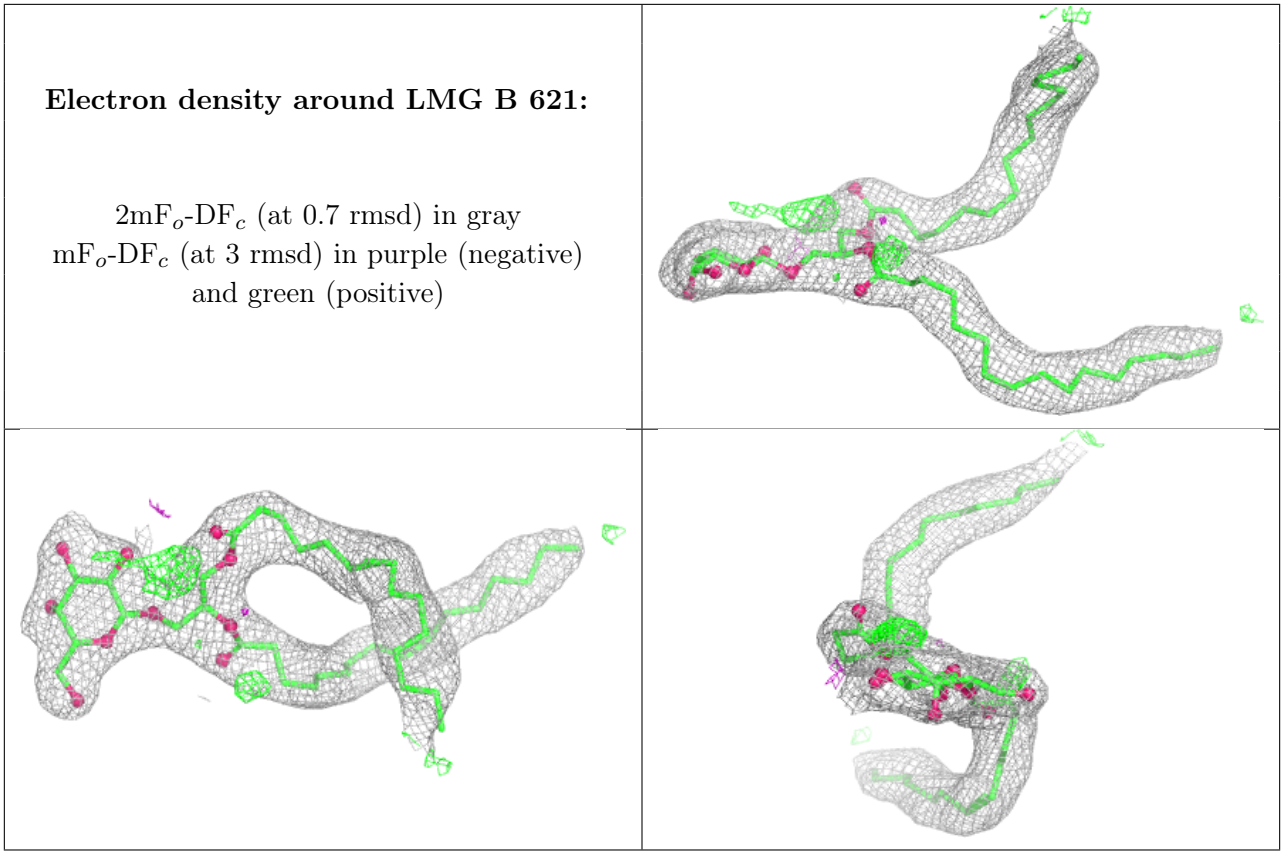






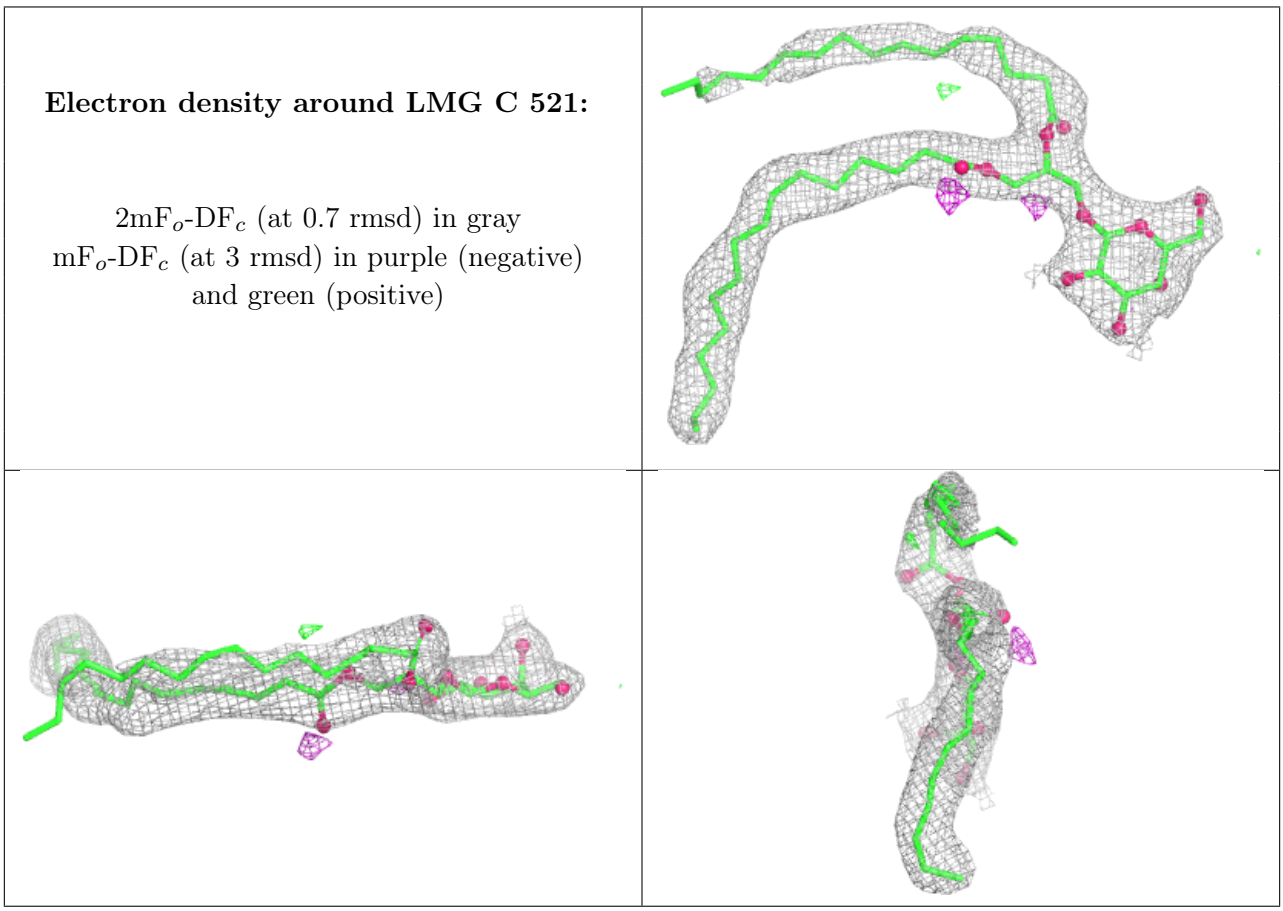
Electron density around LMG B 621:

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



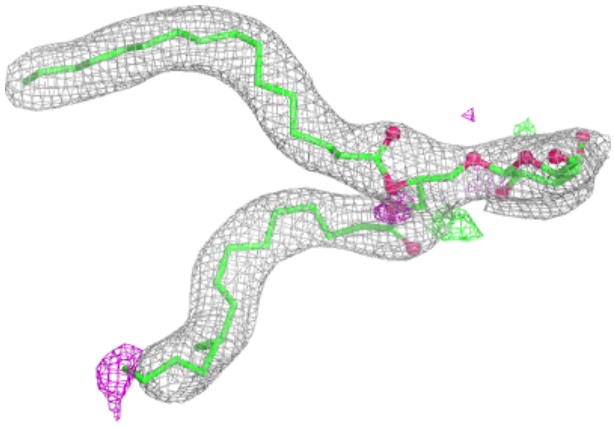
Electron density around LMG C 521:

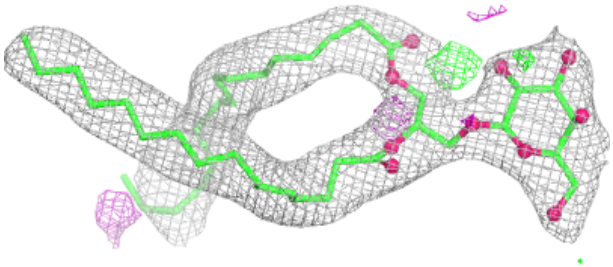
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

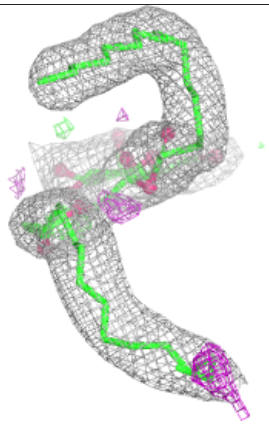


Electron density around LMG m 101:

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

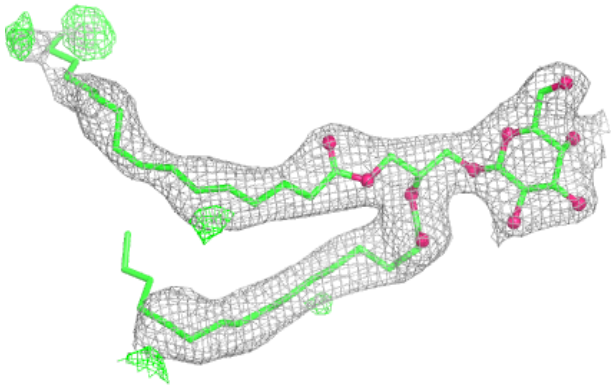


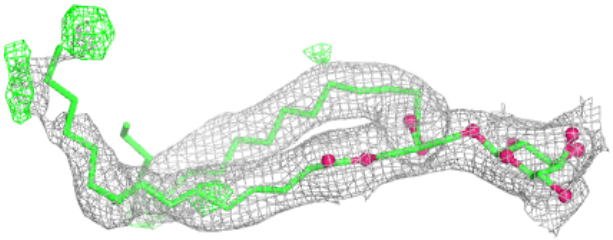


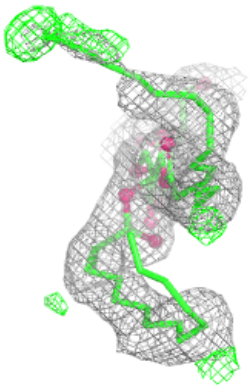


Electron density around LMG D 413:

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

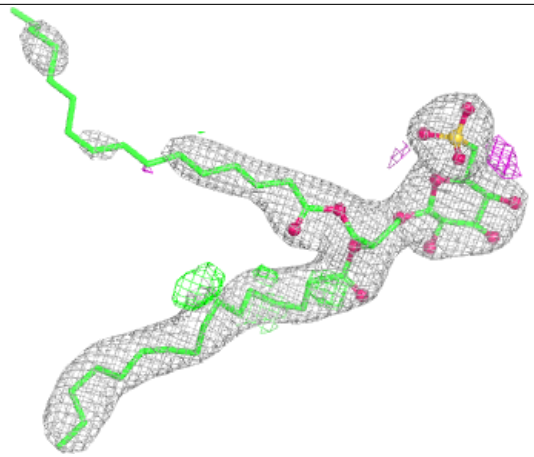


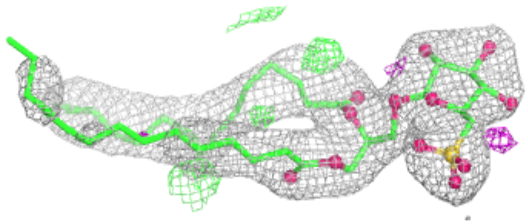


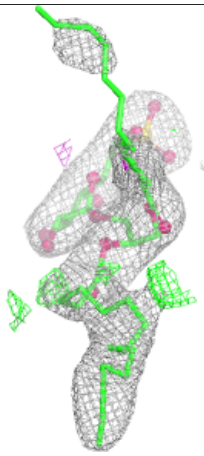


Electron density around SQD C 501 (A):

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

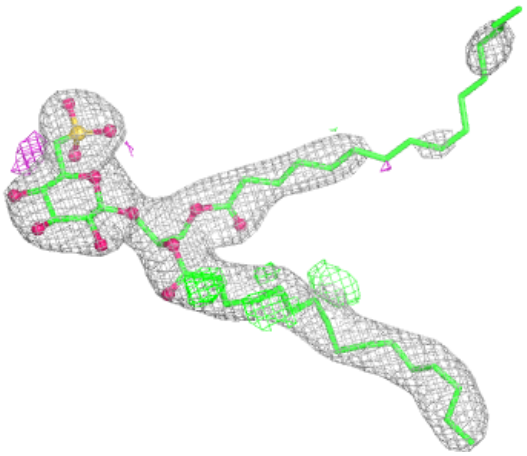


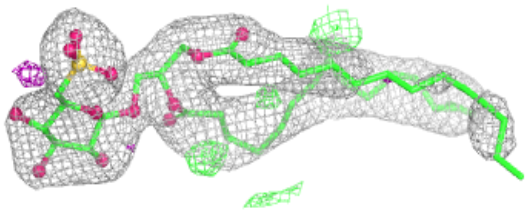


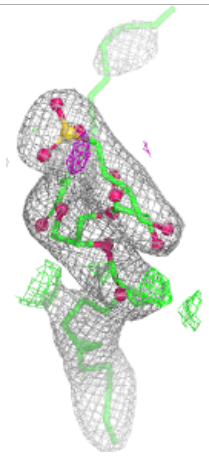


Electron density around SQD C 501 (B):

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

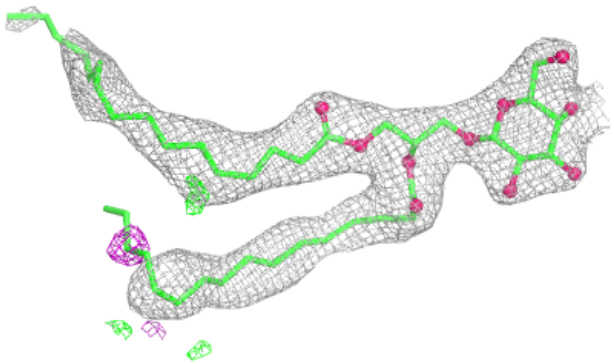


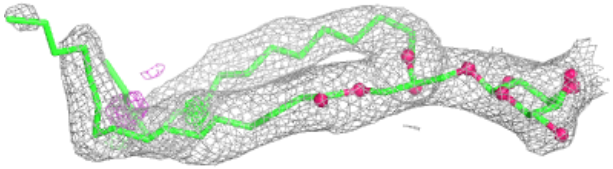


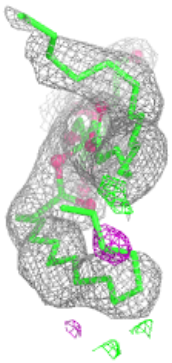


Electron density around LMG d 409:

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

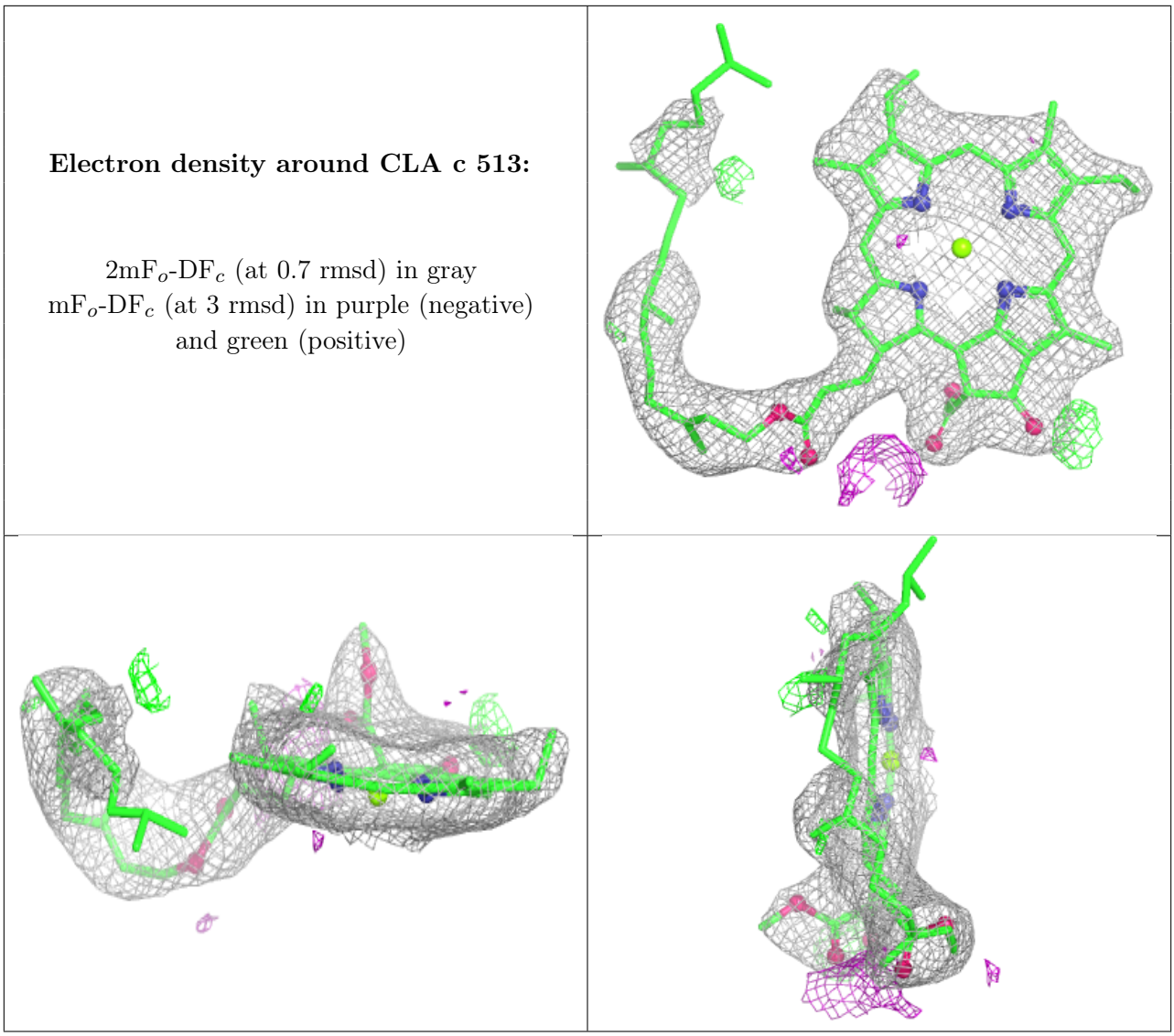






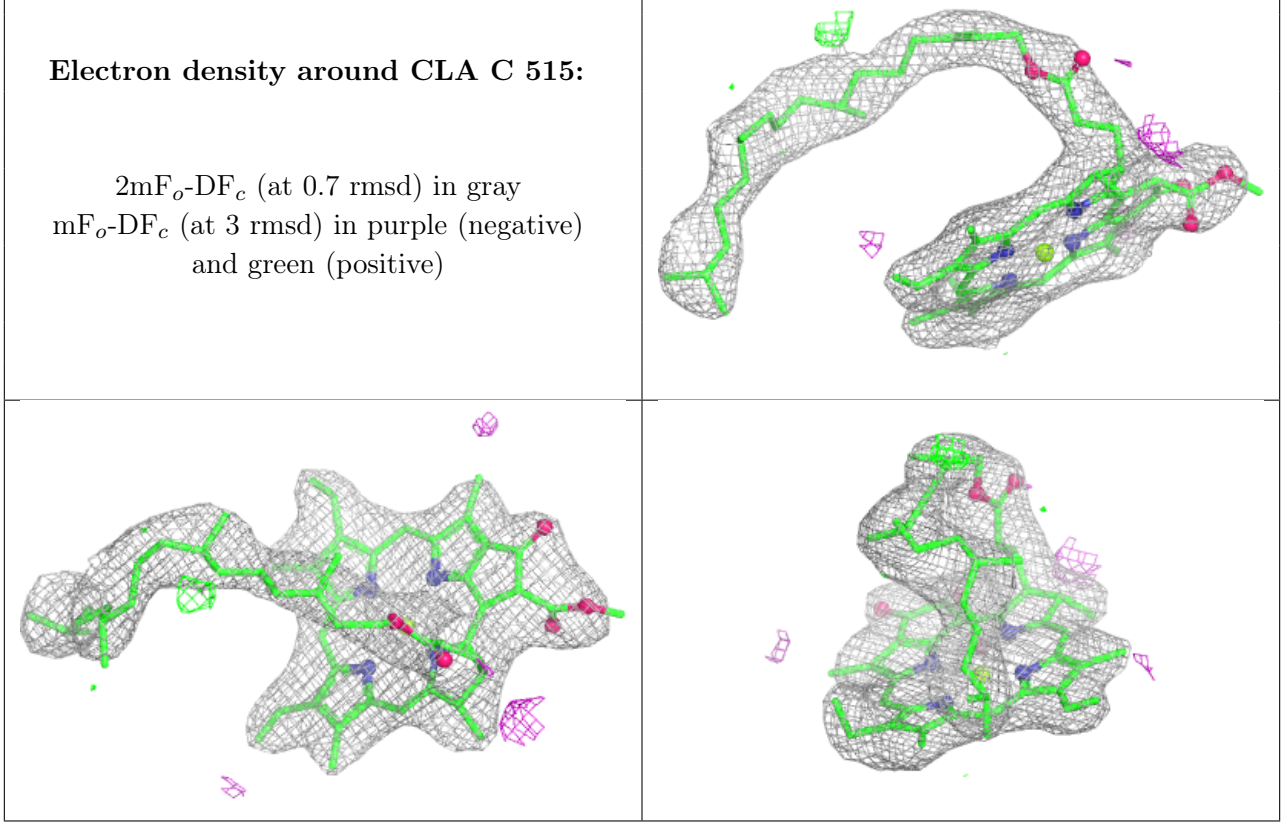
Electron density around CLA c 513:

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



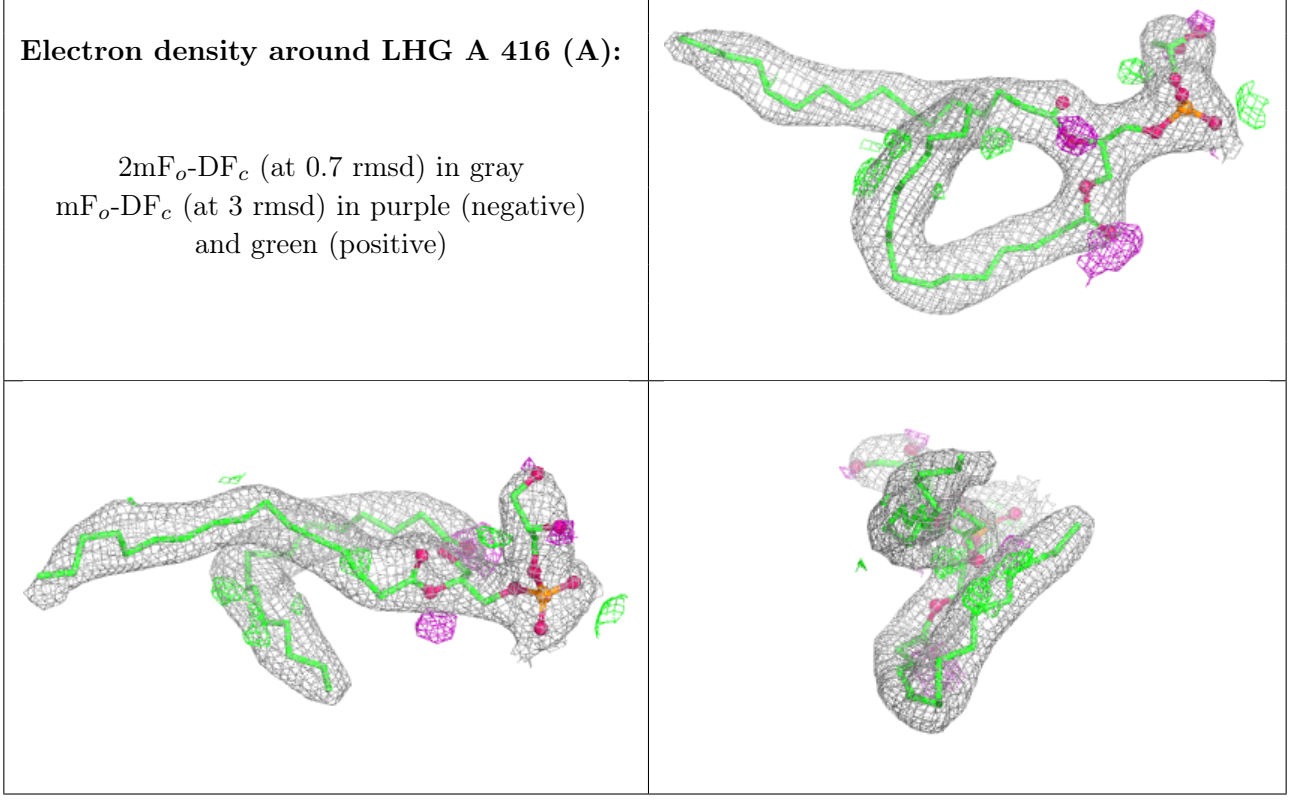
Electron density around CLA C 515:

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



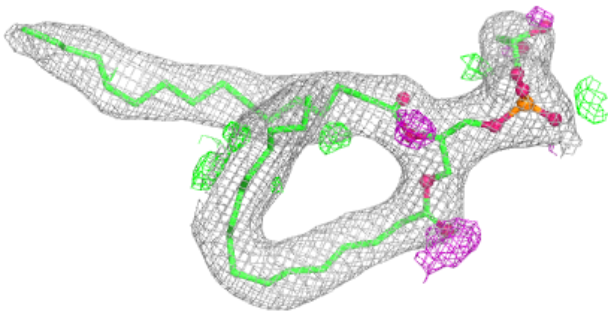
Electron density around LHG A 416 (A):

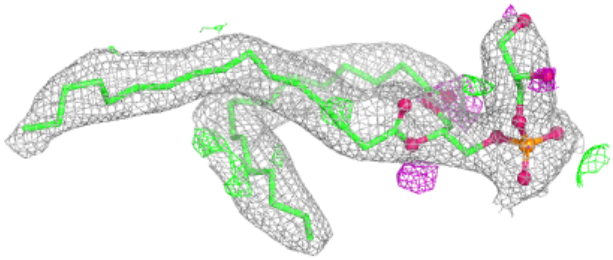
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

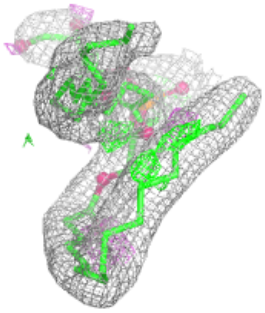


Electron density around LHG A 416 (B):

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

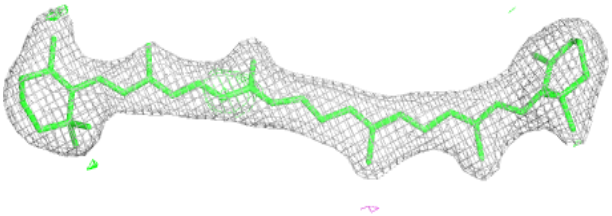


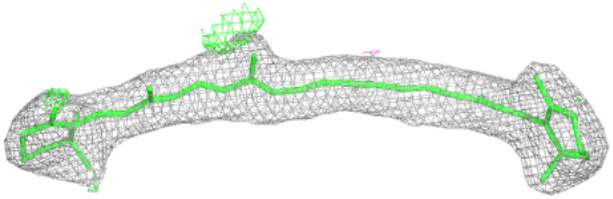


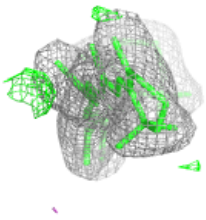


Electron density around BCR T 102:

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

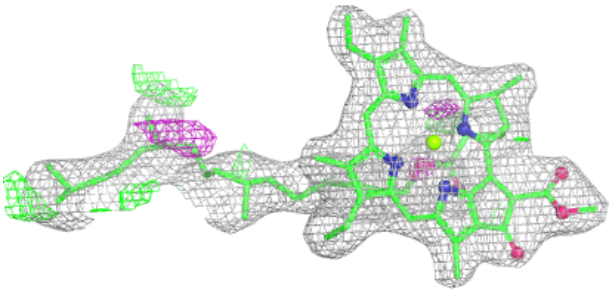


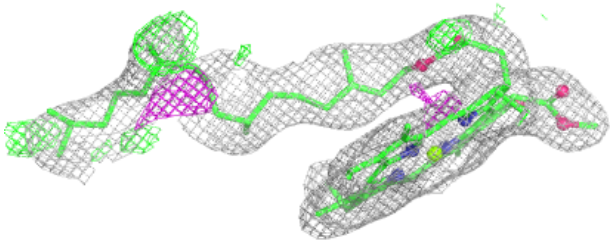


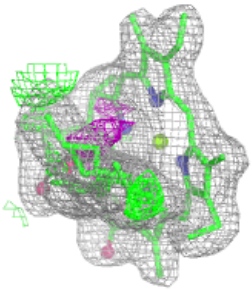


Electron density around CLA B 614:

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

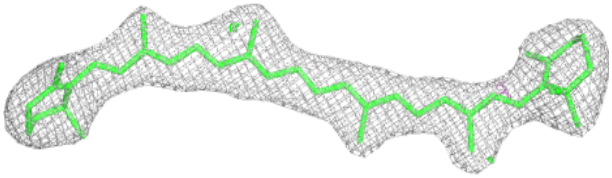


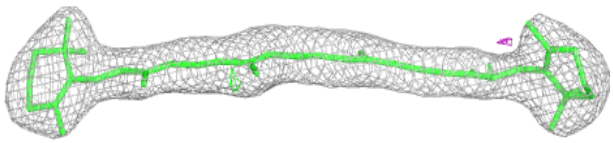


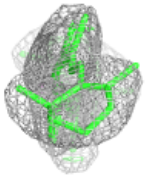


Electron density around BCR Y 101:

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

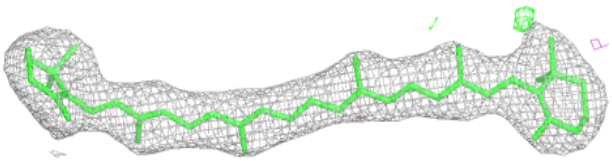


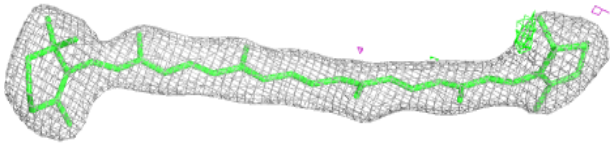


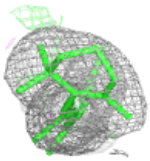


Electron density around BCR c 515:

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

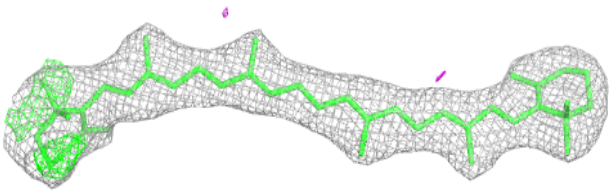


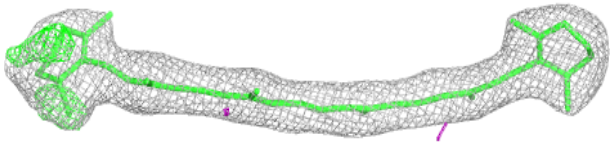


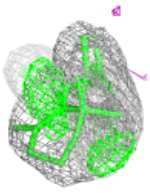


Electron density around BCR d 403:

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

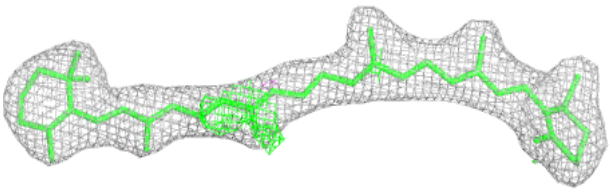


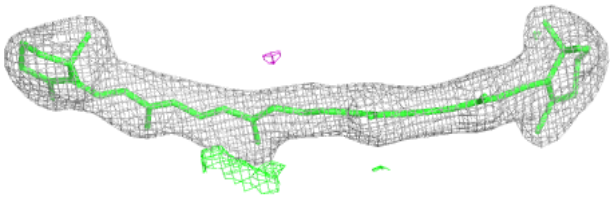


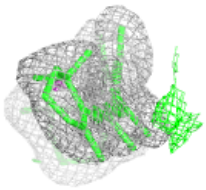


Electron density around BCR t 103:

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

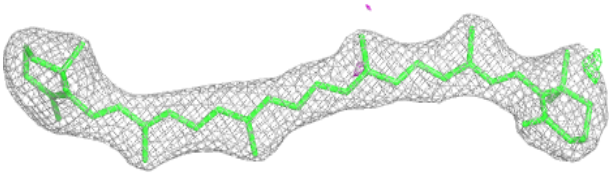


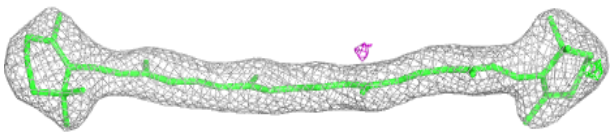


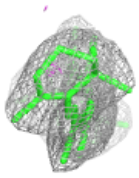


Electron density around BCR y 101:

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

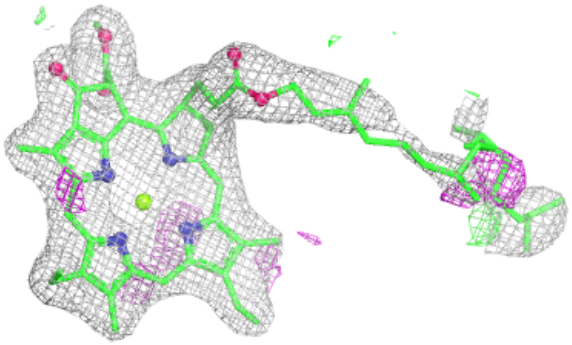


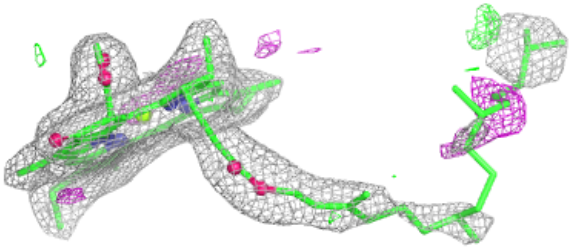


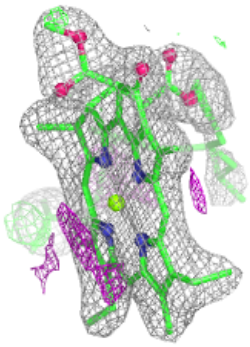


Electron density around CLA a 409:

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

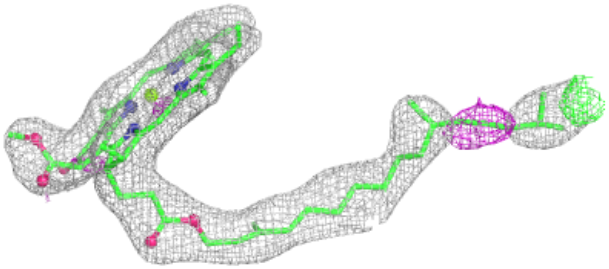


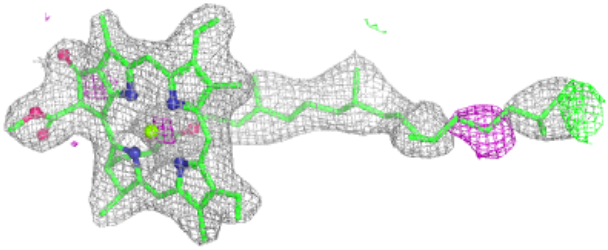


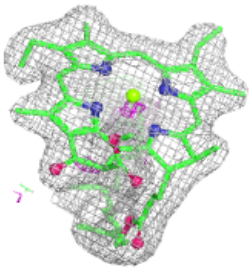


Electron density around CLA C 506:

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

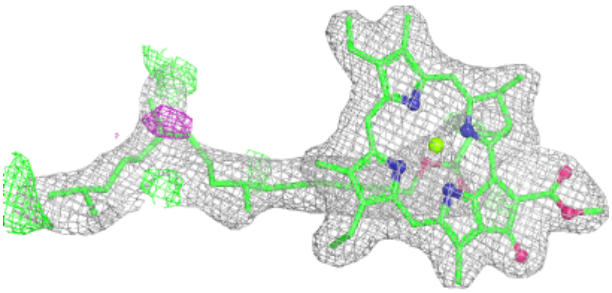


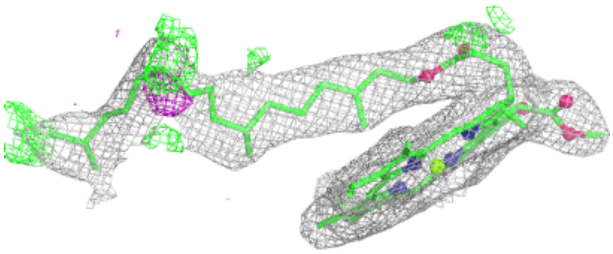


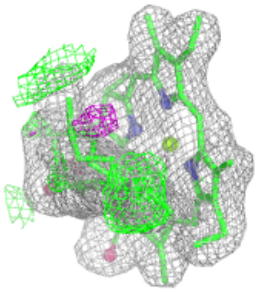


Electron density around CLA b 614:

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

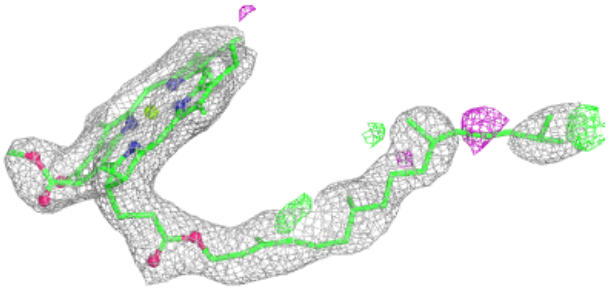


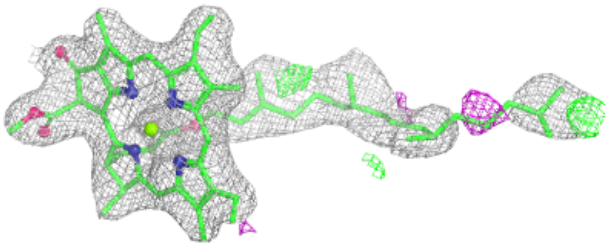


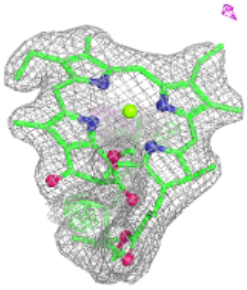


Electron density around CLA c 505:

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

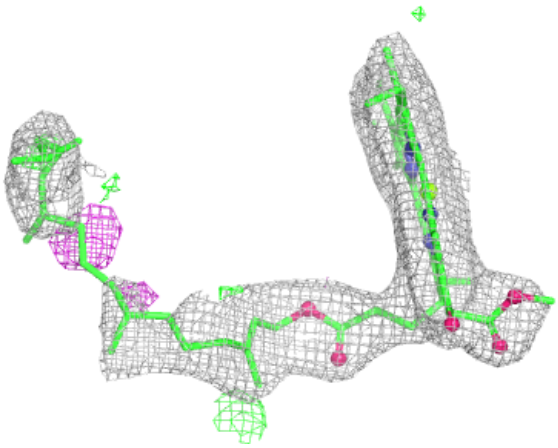


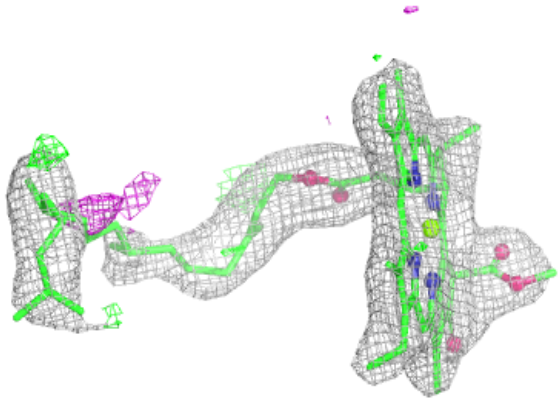


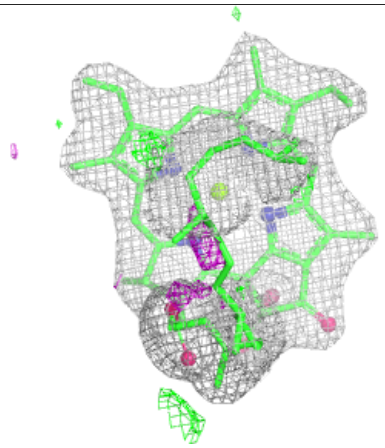


Electron density around CLA c 507:

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

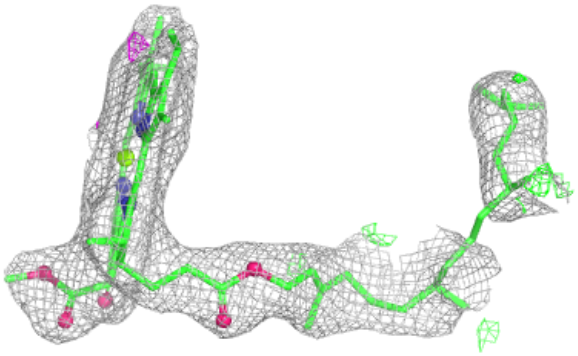


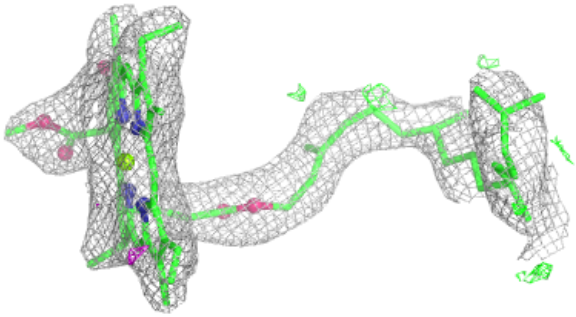


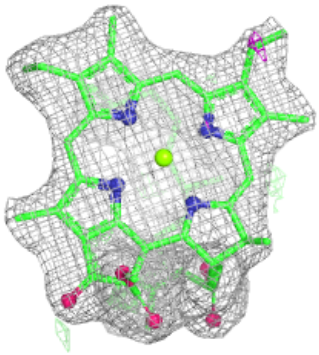


Electron density around CLA C 508:

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

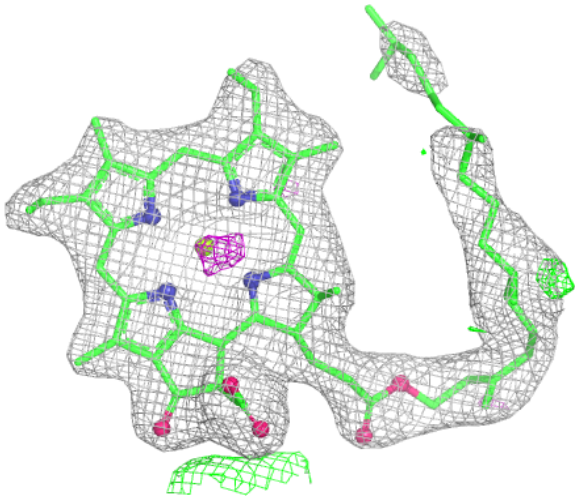


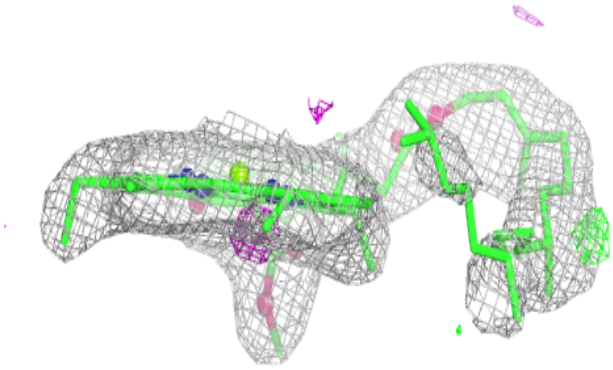


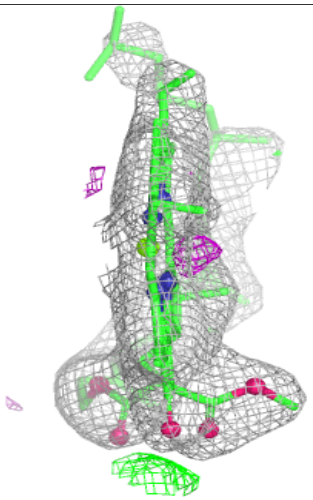


Electron density around CLA C 514:

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

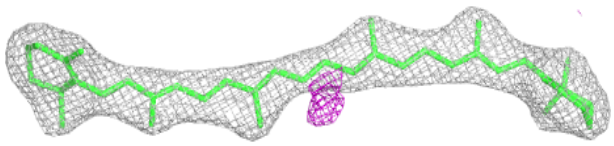


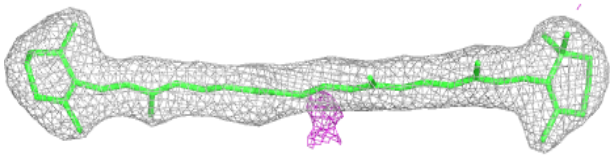


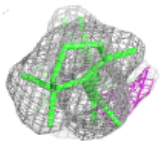


Electron density around BCR C 516:

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

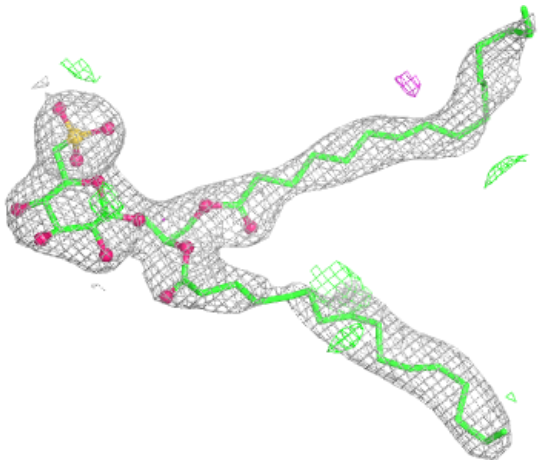


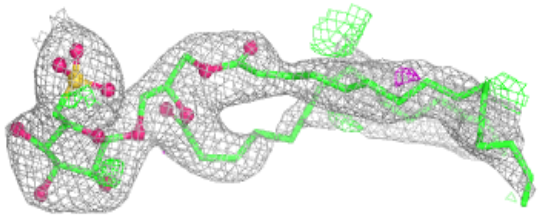


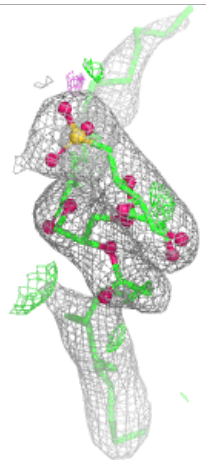


Electron density around SQD a 411 (A):

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

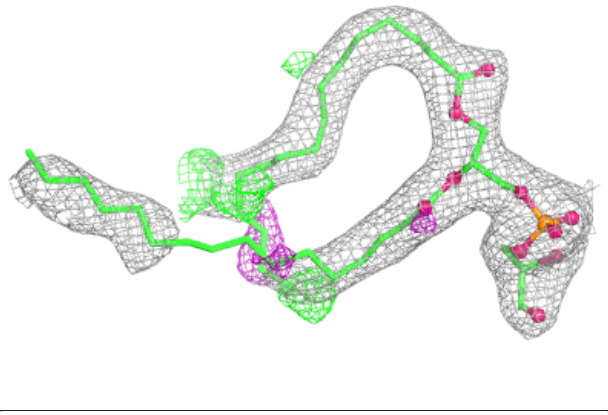


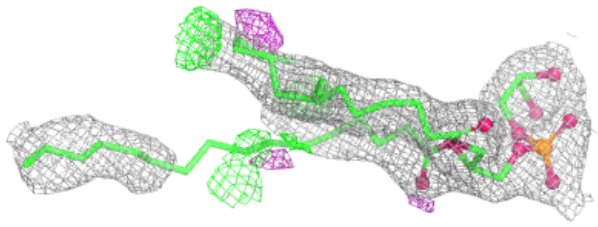


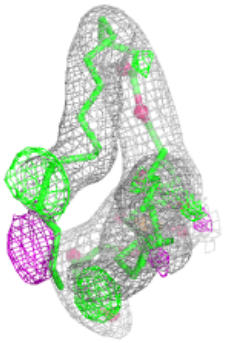


Electron density around LHG D 409 (A):

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

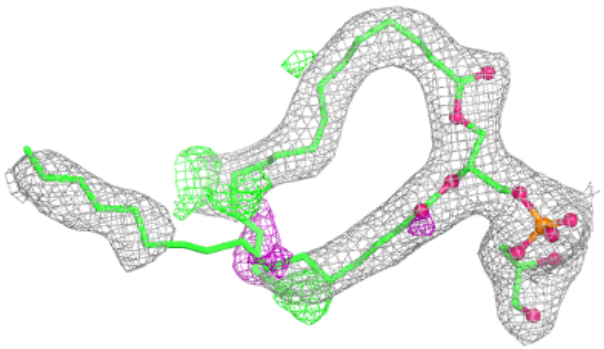


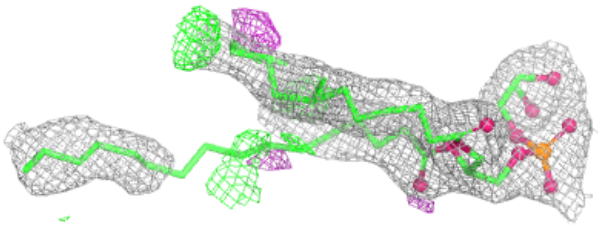


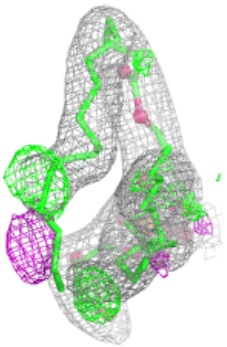


Electron density around LHG D 409 (B):

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

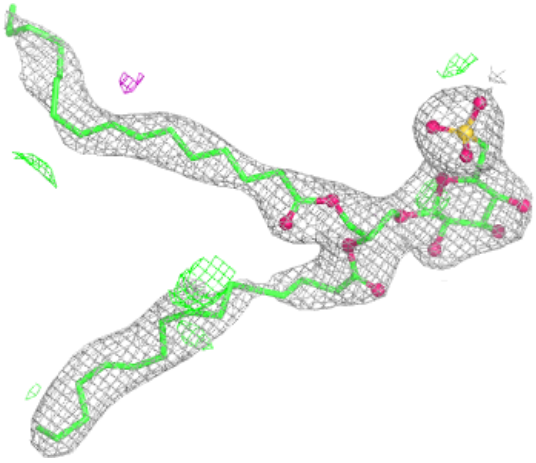


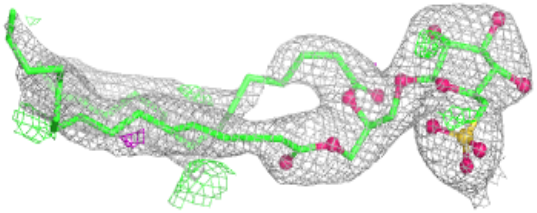




Electron density around SQD a 411 (B):

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

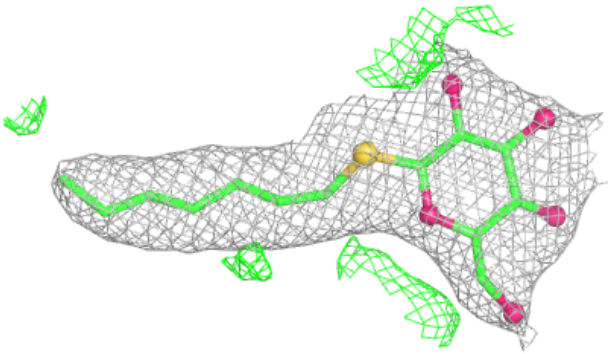


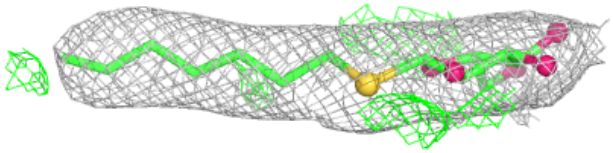


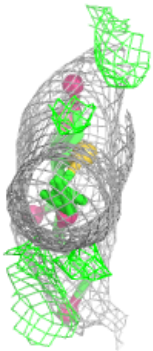


Electron density around HTG b 625:

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

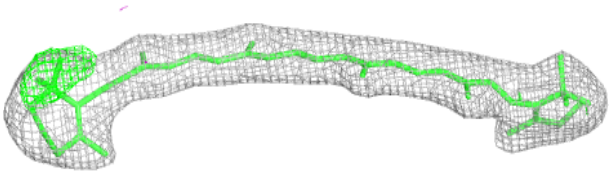


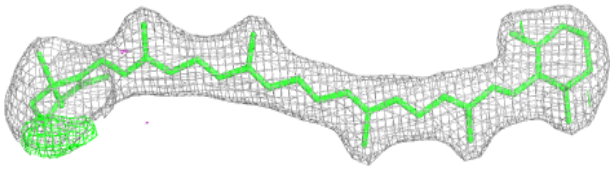


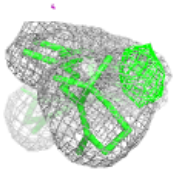


Electron density around BCR D 406:

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

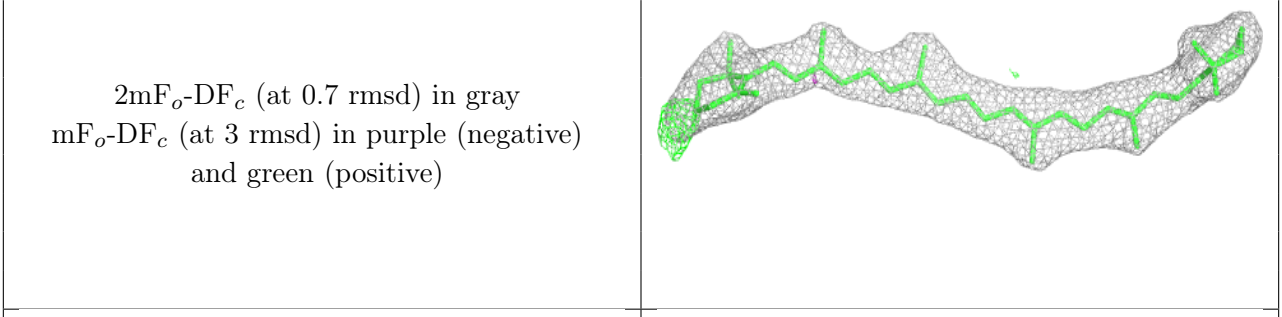


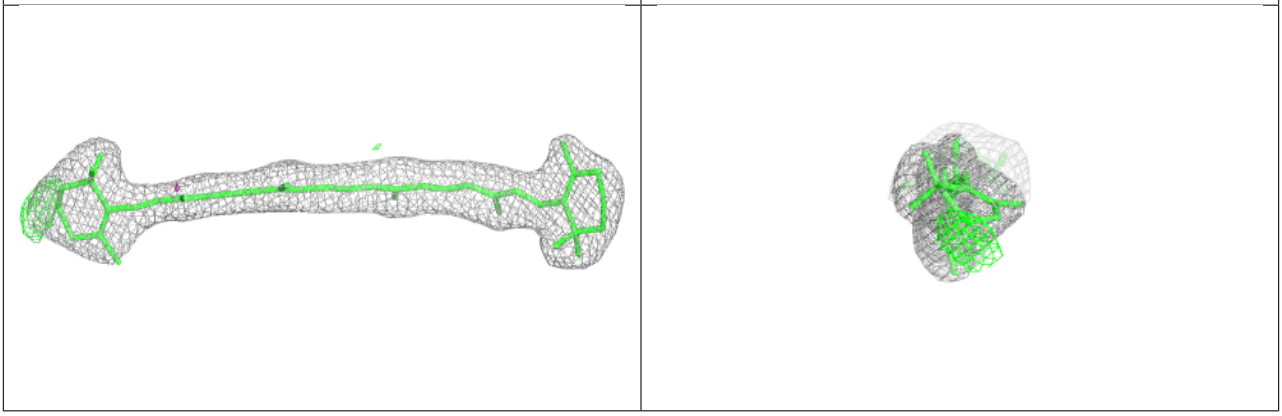




Electron density around BCR H 101:

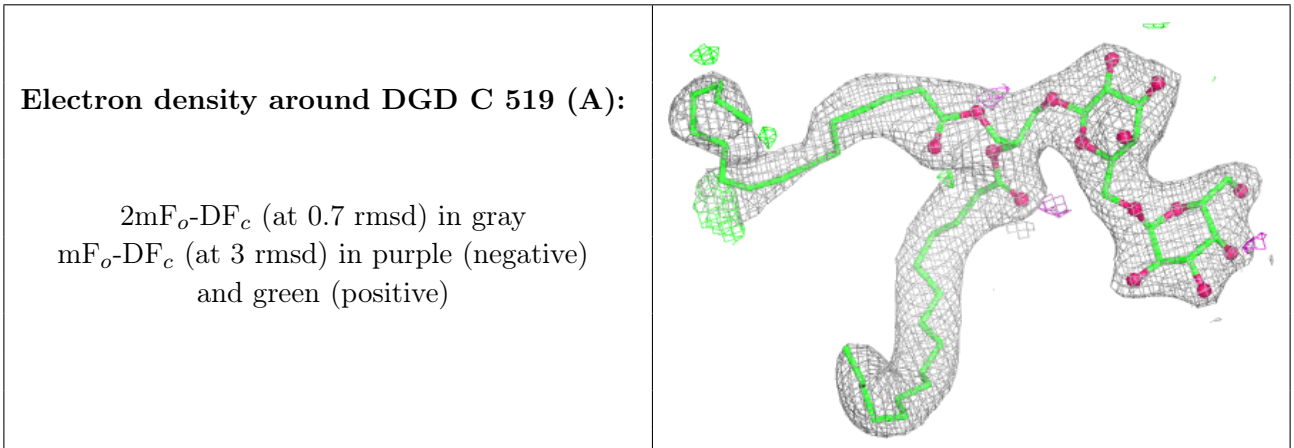
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

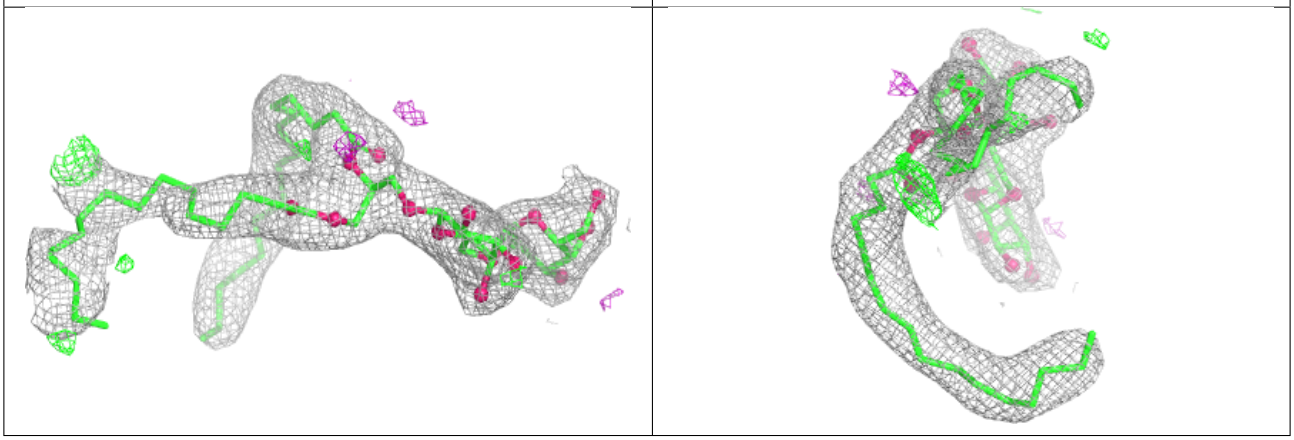




Electron density around DGD C 519 (A):

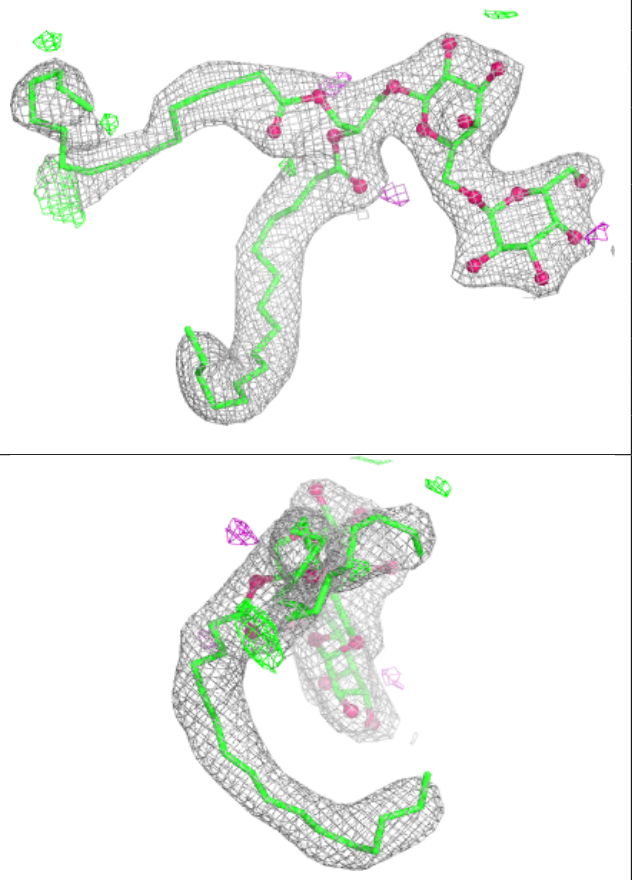
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





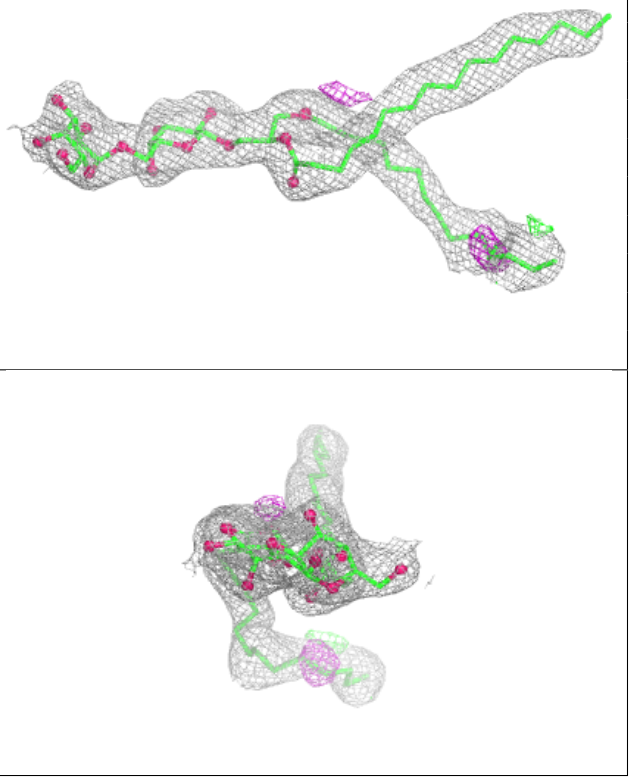
Electron density around DGD C 519 (B):

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



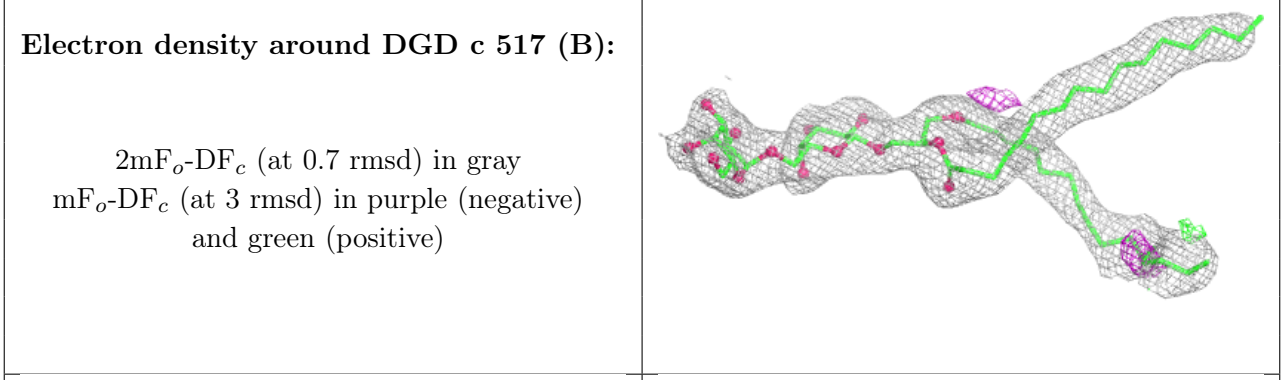
Electron density around DGD c 517 (A):

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



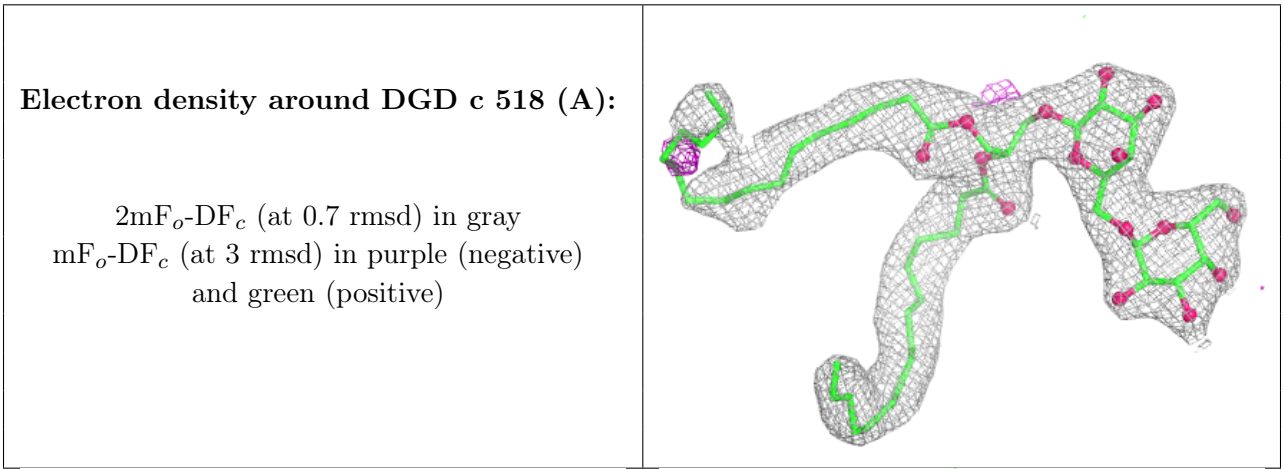
Electron density around DGD c 517 (B):

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



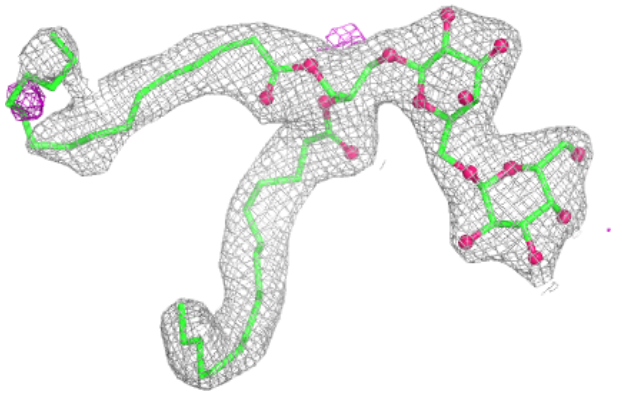
Electron density around DGD c 518 (A):

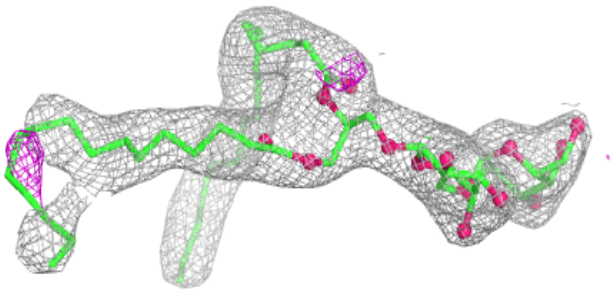
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

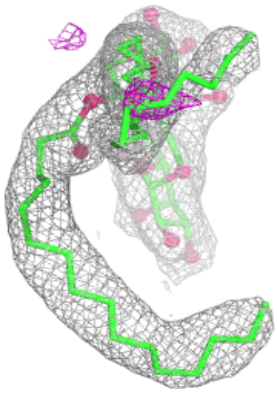


Electron density around DGD c 518 (B):

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

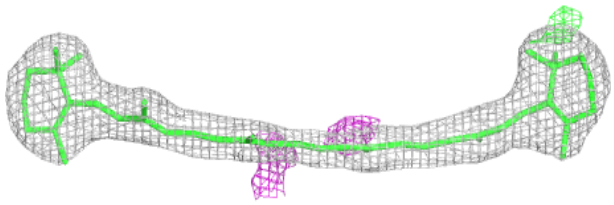


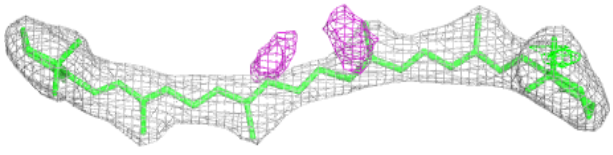


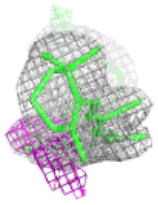


Electron density around BCR K 102:

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

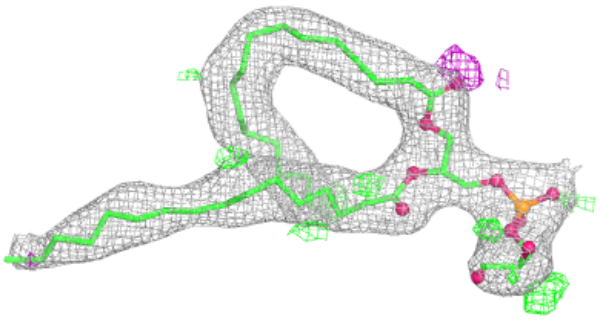


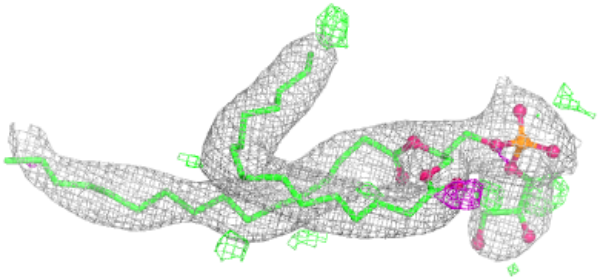


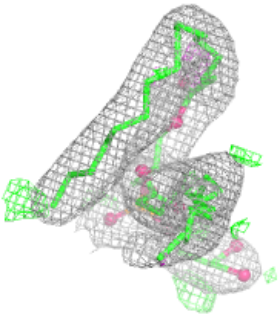


Electron density around LHG d 411 (A):

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

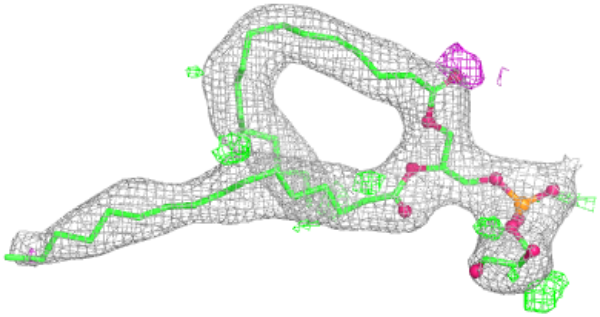


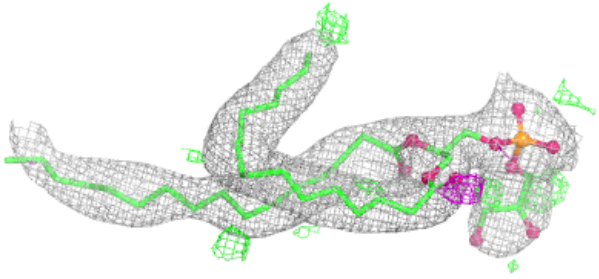


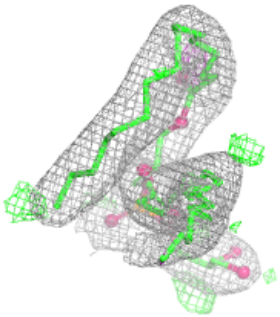


Electron density around LHG d 411 (B):

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

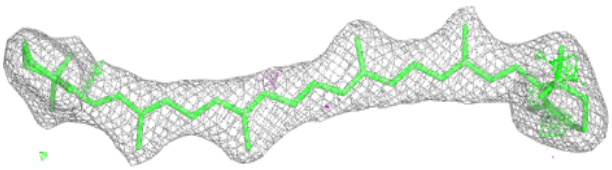


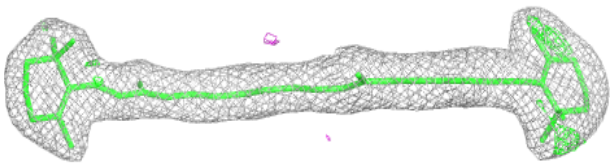


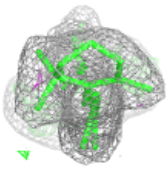


Electron density around BCR A 408:

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

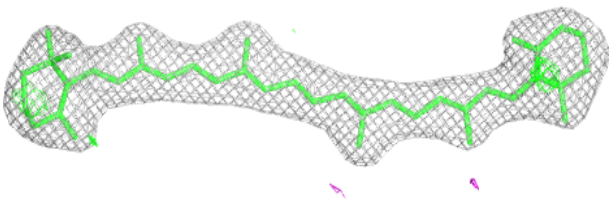


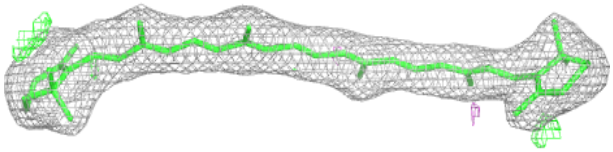


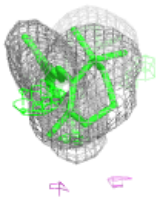


Electron density around BCR B 619:

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

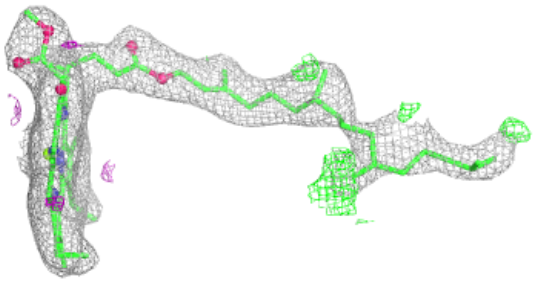


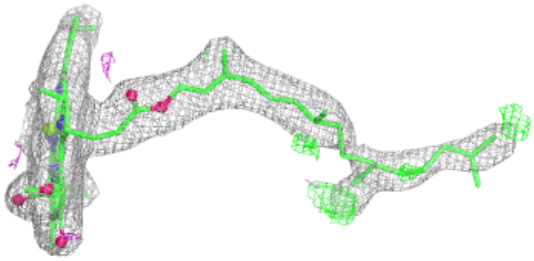


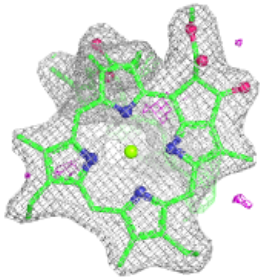


Electron density around CLA b 606:

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

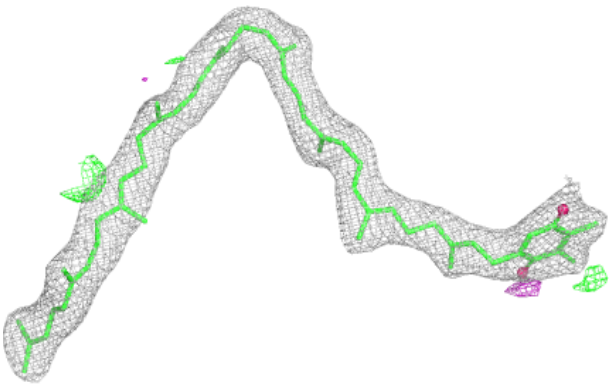


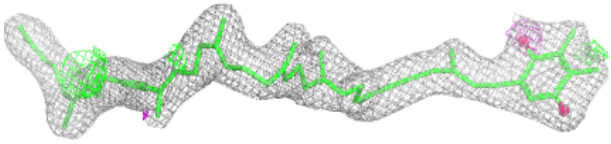


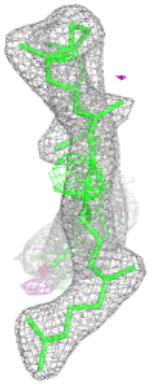


Electron density around PL9 D 407 (A):

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

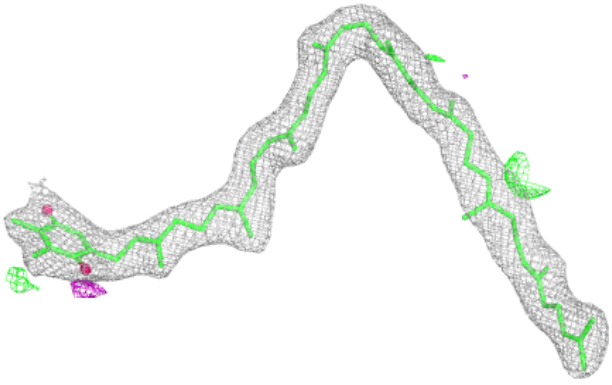


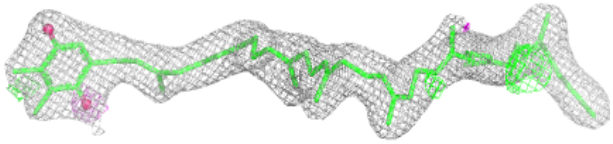




Electron density around PL9 D 407 (B):

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

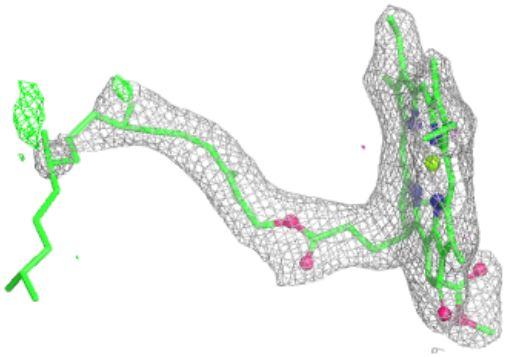


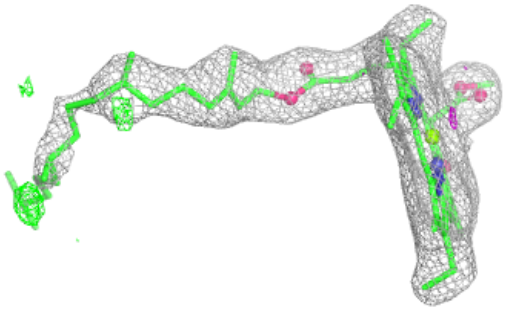


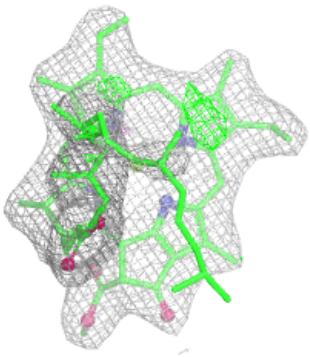


Electron density around CLA D 405:

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

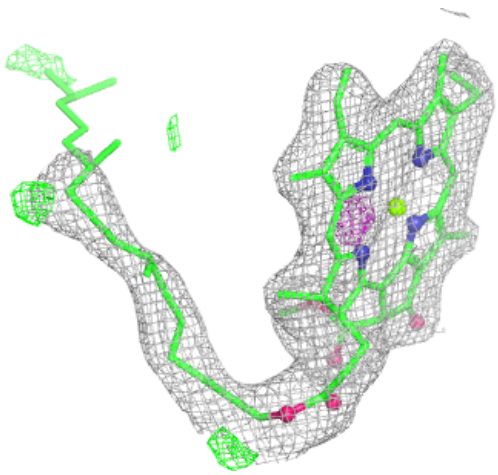


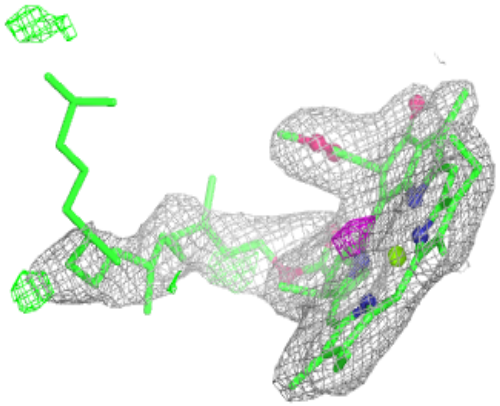


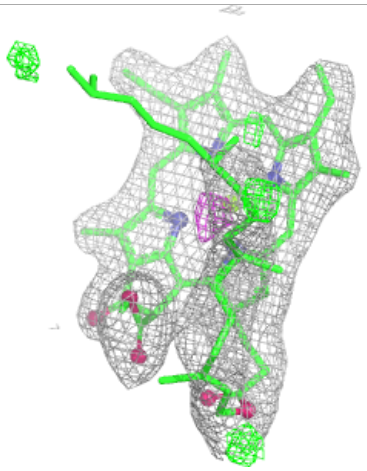


Electron density around CLA b 616:

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

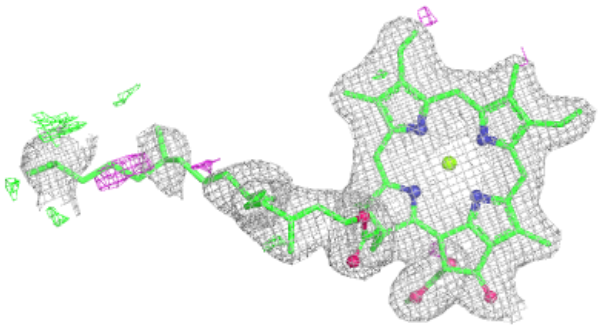


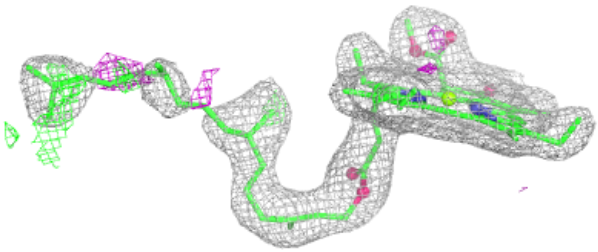


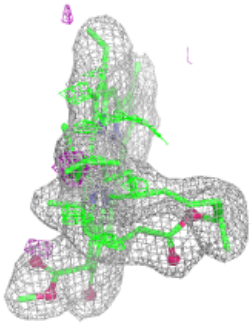


Electron density around CLA a 407 (A):

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

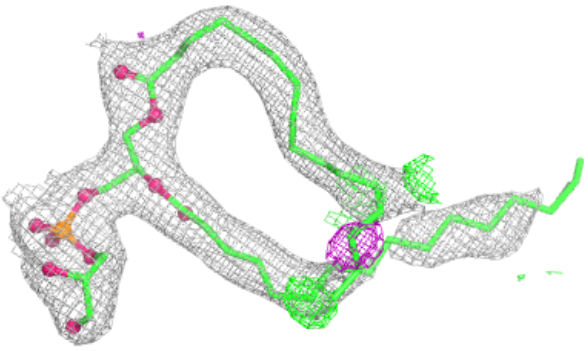


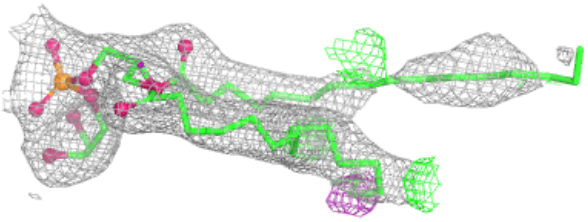


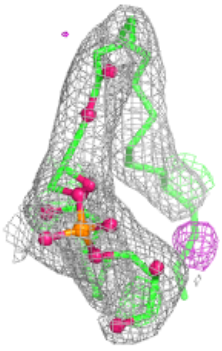


Electron density around LHG d 406 (A):

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

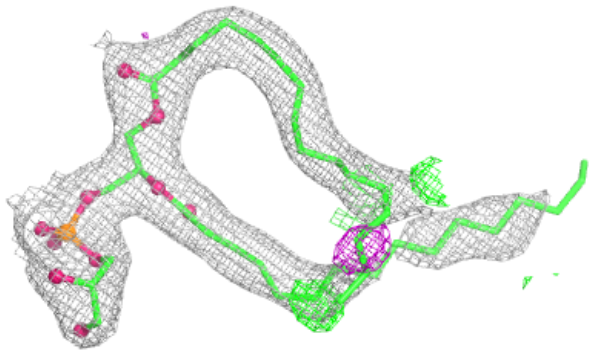


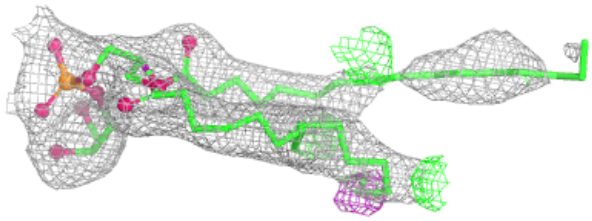


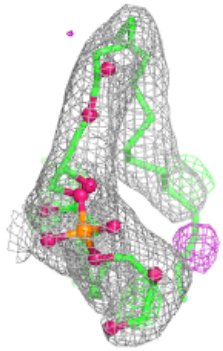


Electron density around LHG d 406 (B):

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

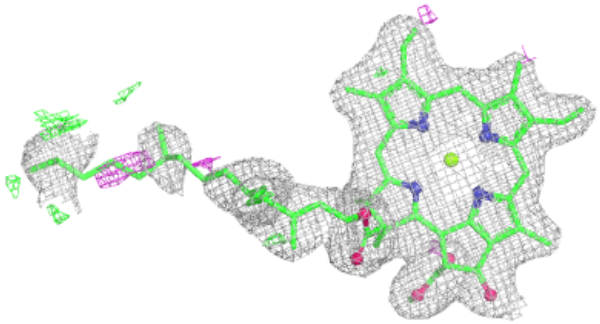


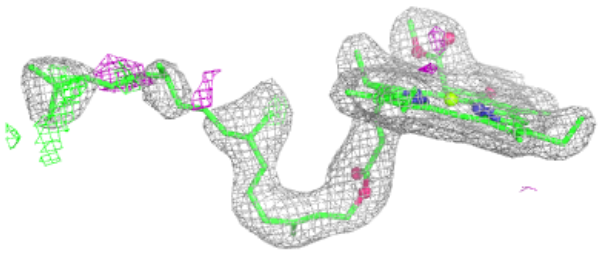


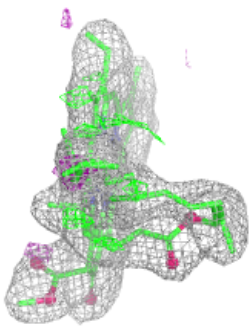


Electron density around CLA a 407 (B):

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

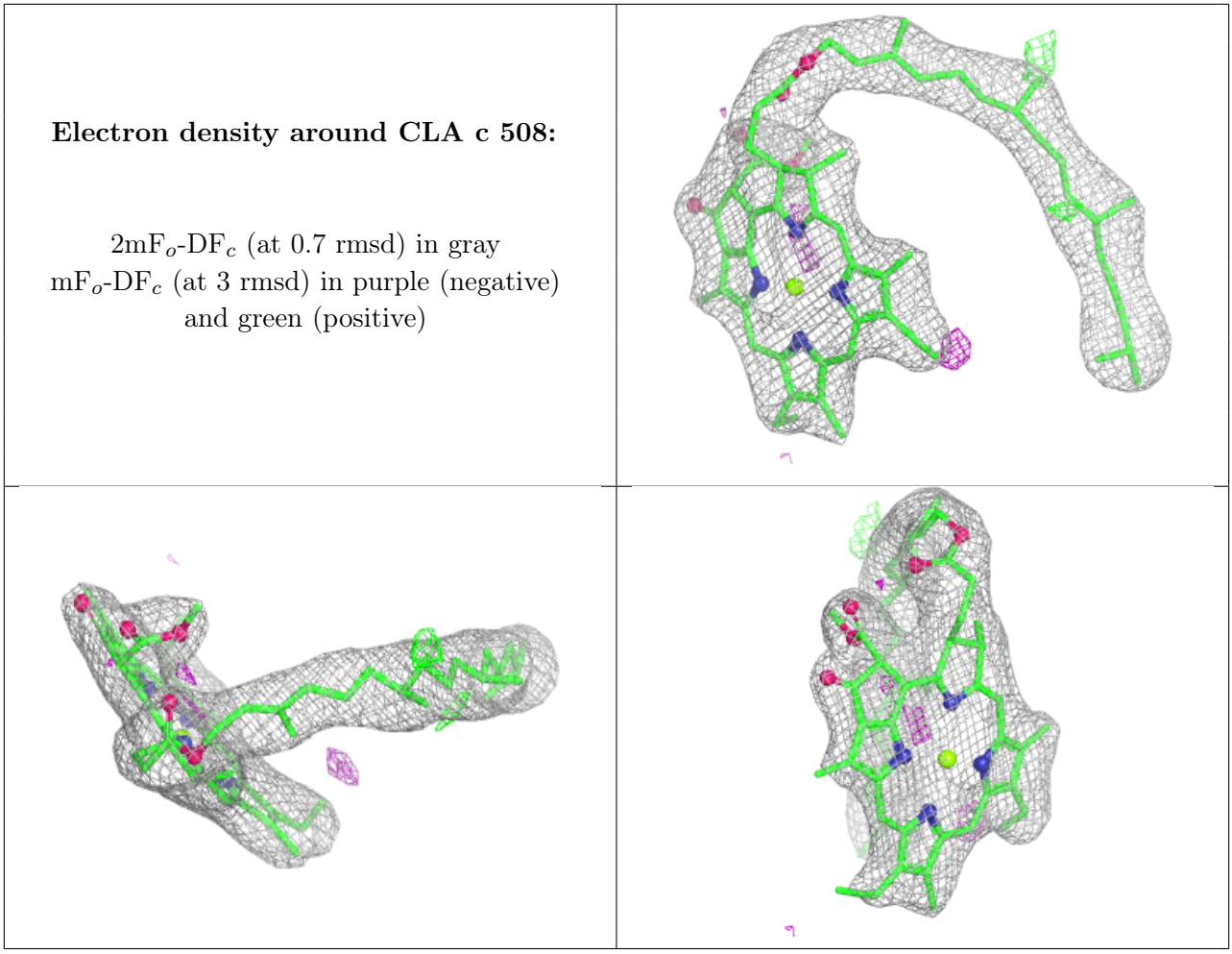






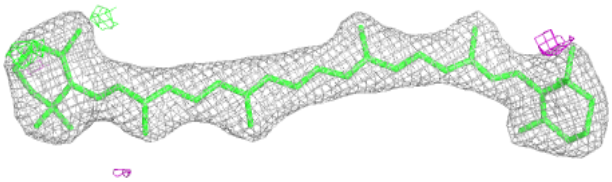
Electron density around CLA c 508:

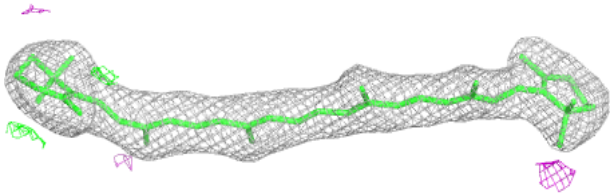
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

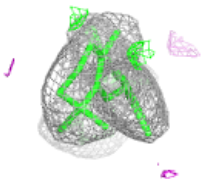


Electron density around BCR b 619:

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

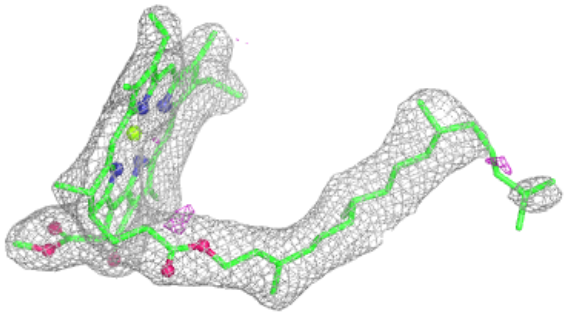


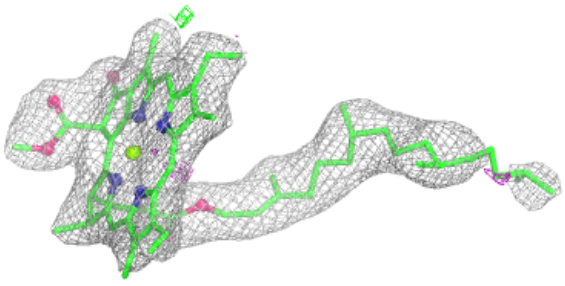


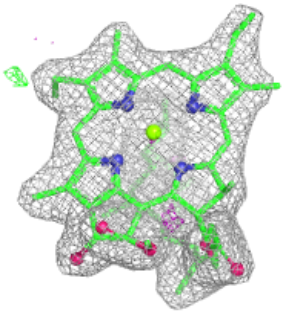


Electron density around CLA c 509:

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

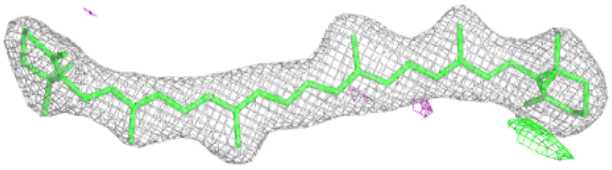


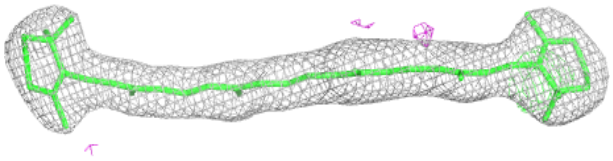


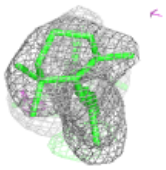


Electron density around BCR c 516:

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

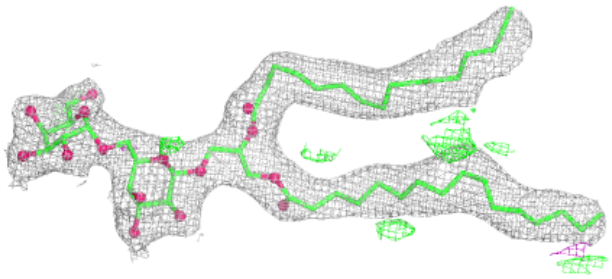


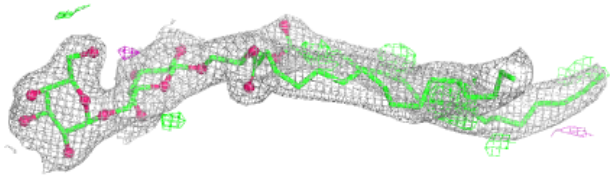


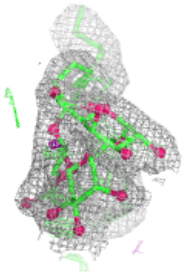


Electron density around DGD C 520:

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

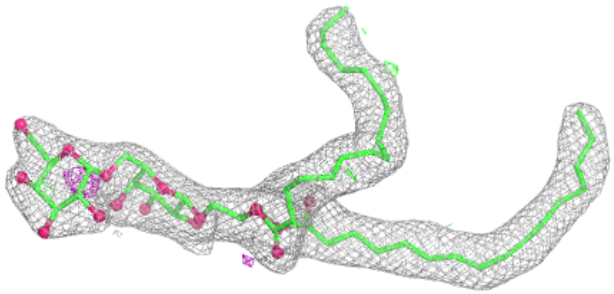


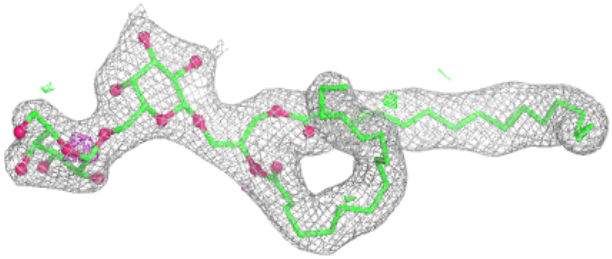


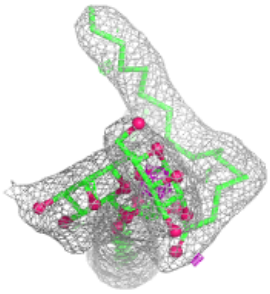


Electron density around DGD H 102:

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

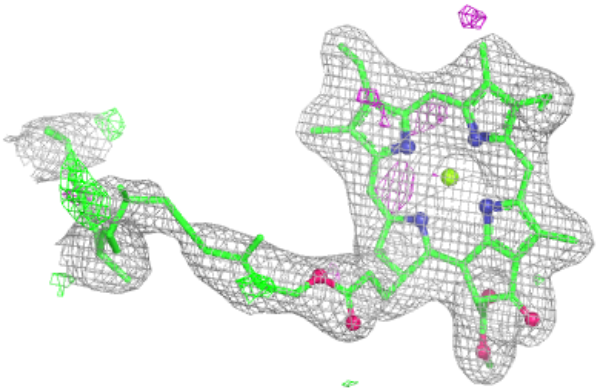


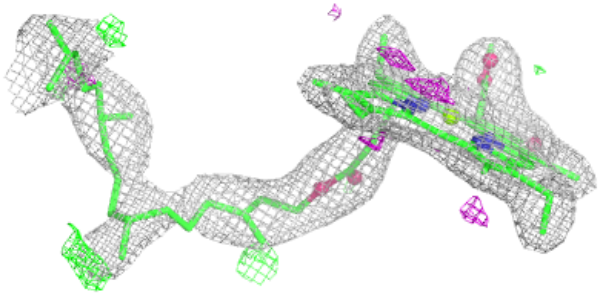


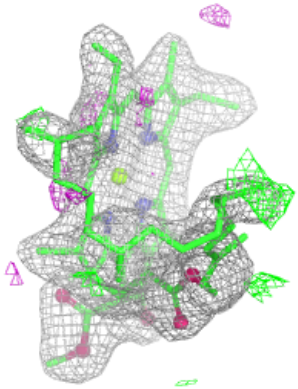


Electron density around CLA A 407:

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

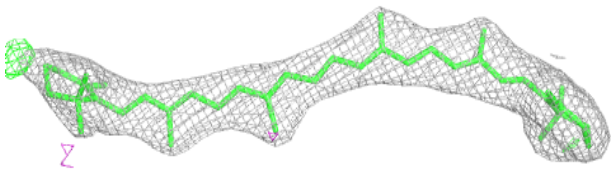


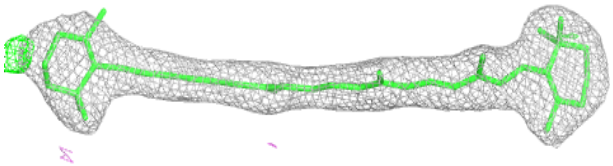


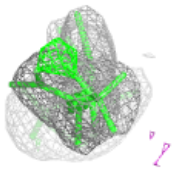


Electron density around BCR h 101:

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

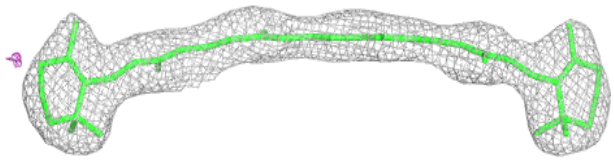


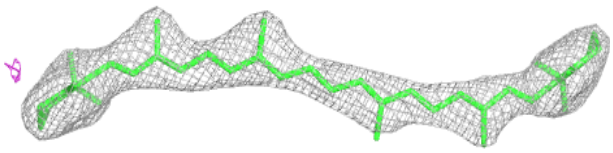


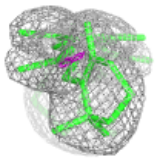


Electron density around BCR k 101:

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

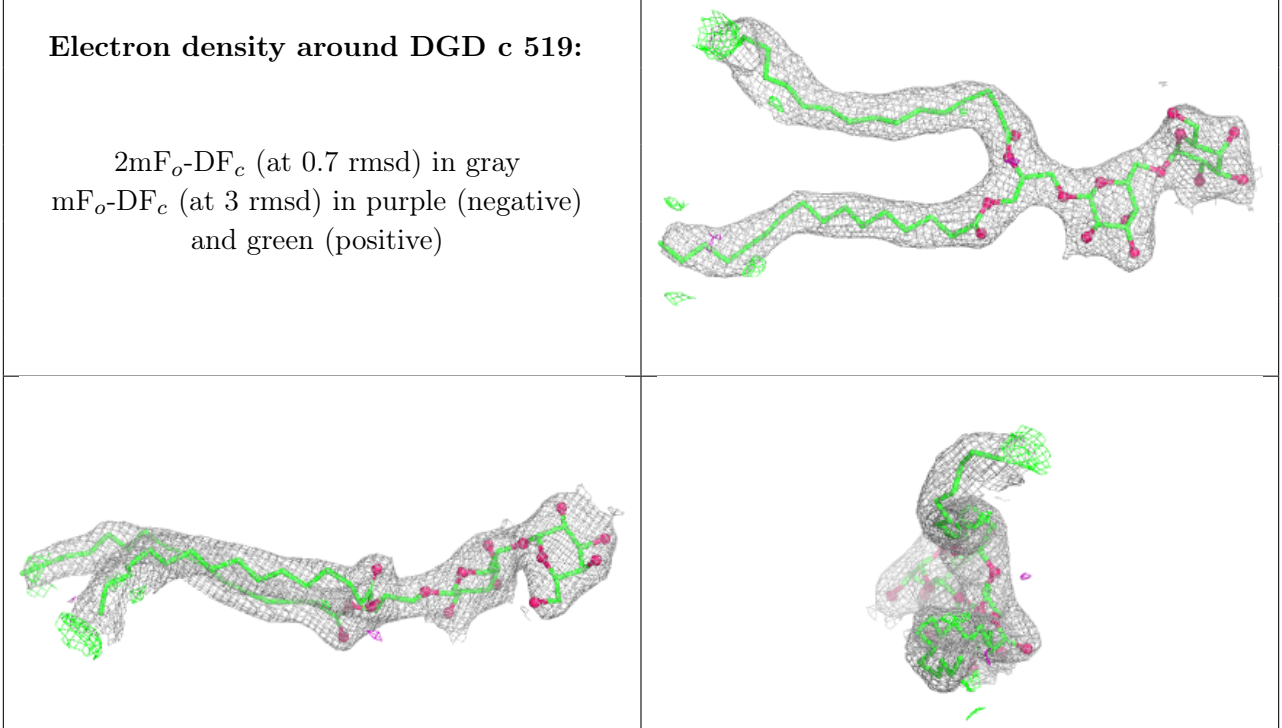






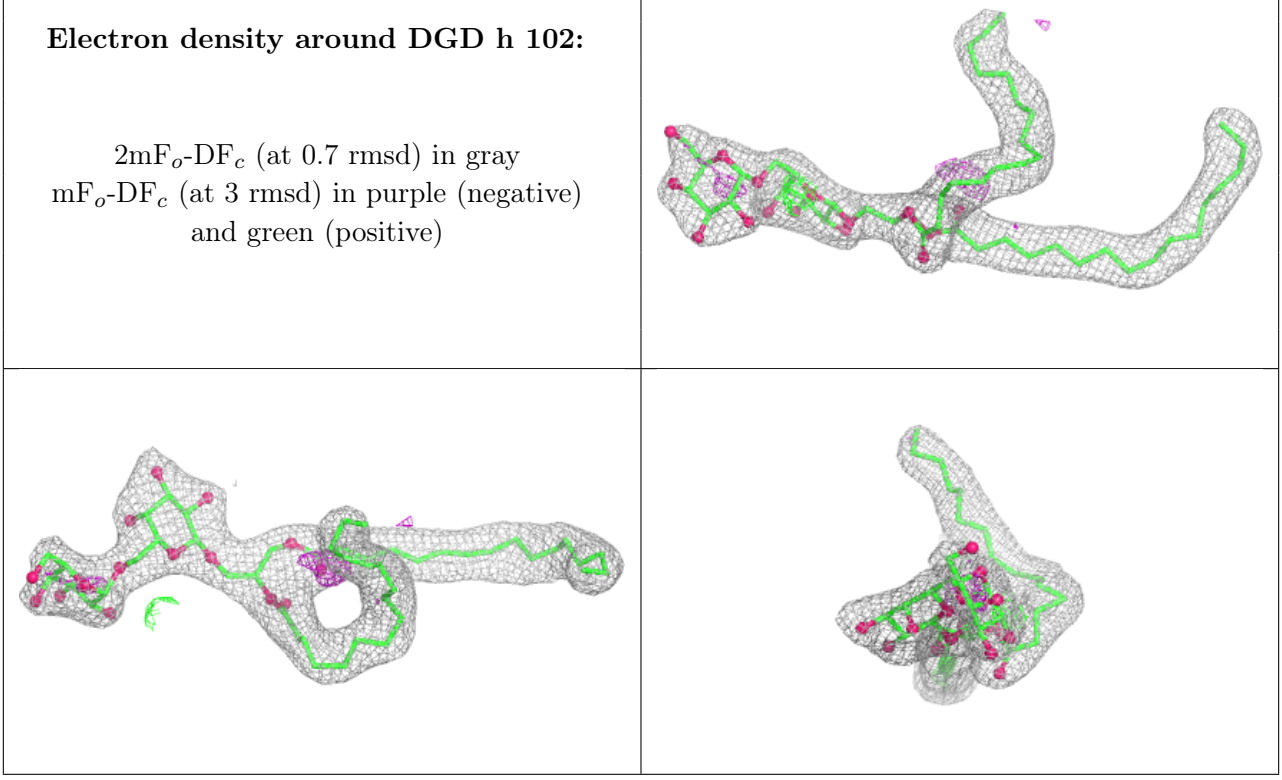
Electron density around DGD c 519:

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



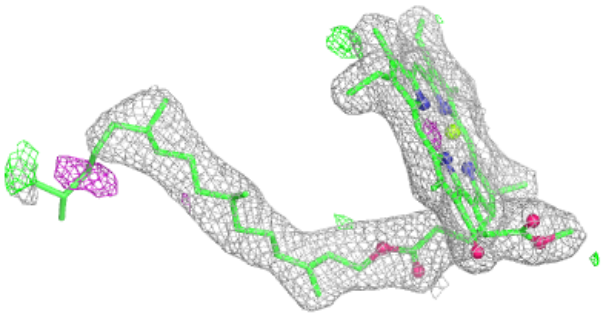
Electron density around DGD h 102:

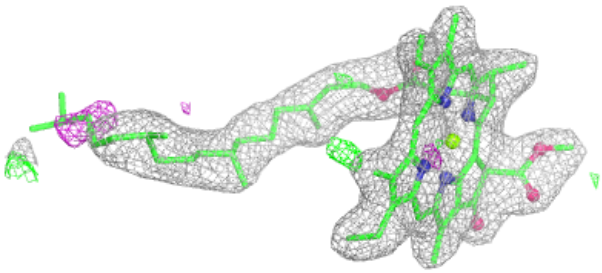
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

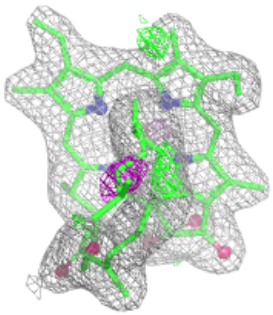


Electron density around CLA C 510:

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

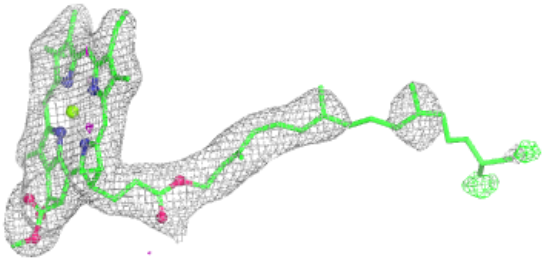


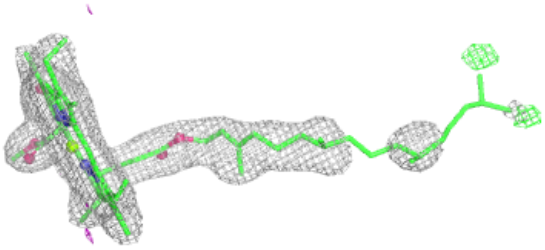


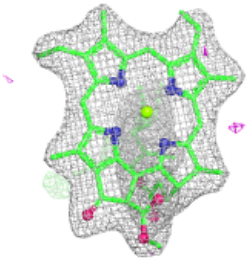


Electron density around CLA d 402:

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

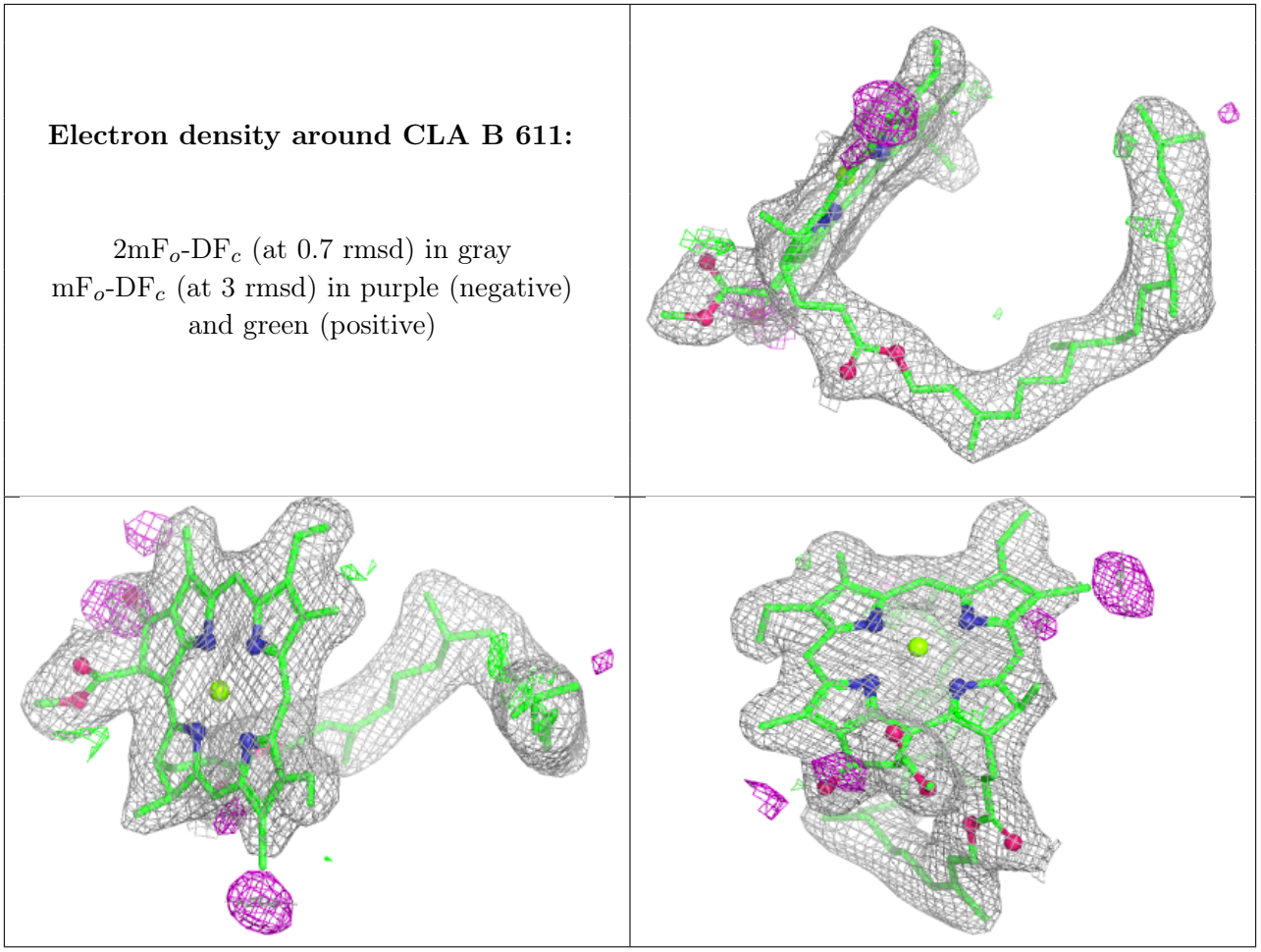






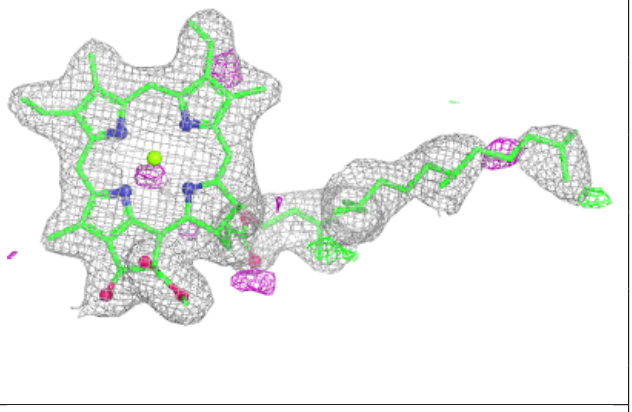
Electron density around CLA B 611:

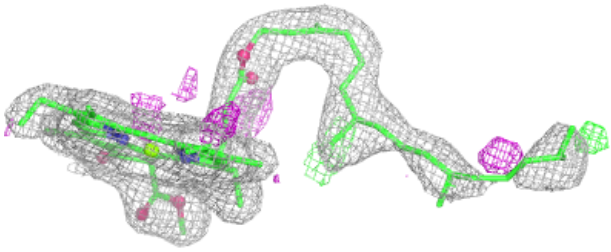
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

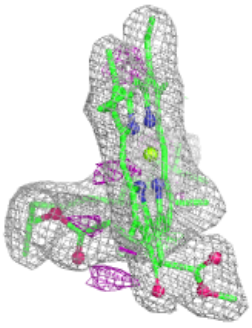


Electron density around CLA A 406 (A):

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

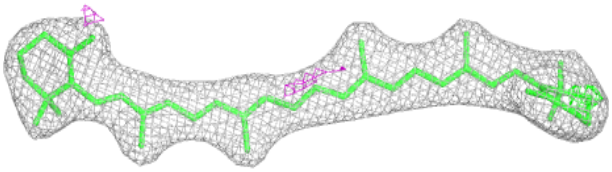


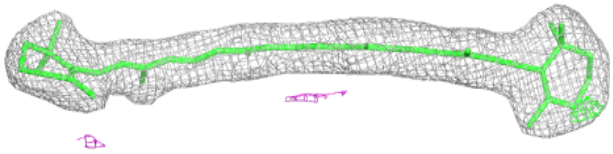


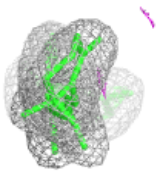


Electron density around BCR B 617:

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

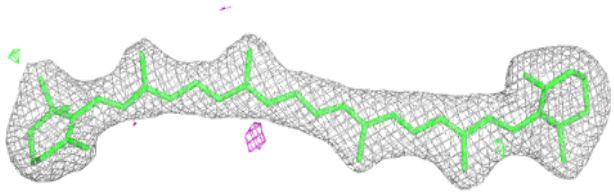


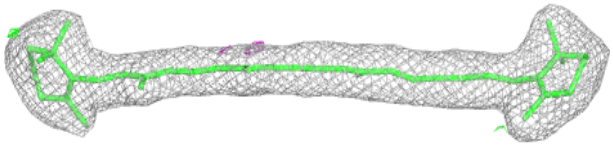


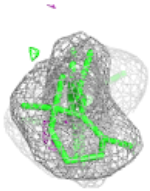


Electron density around BCR B 618:

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

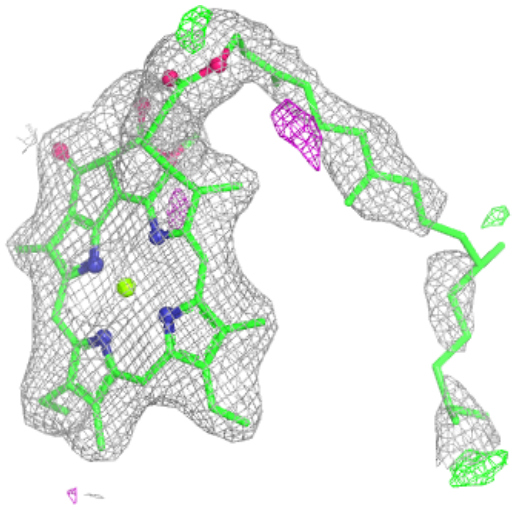


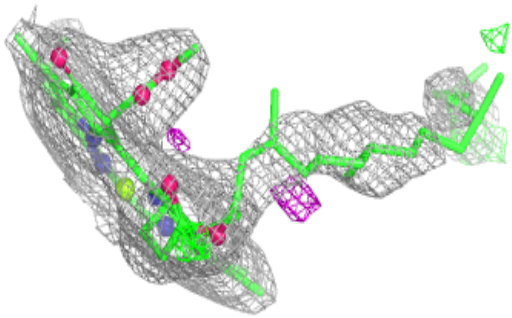


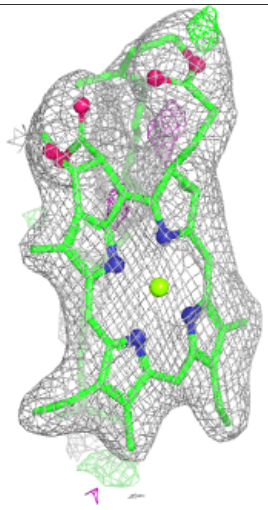


Electron density around CLA B 616:

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

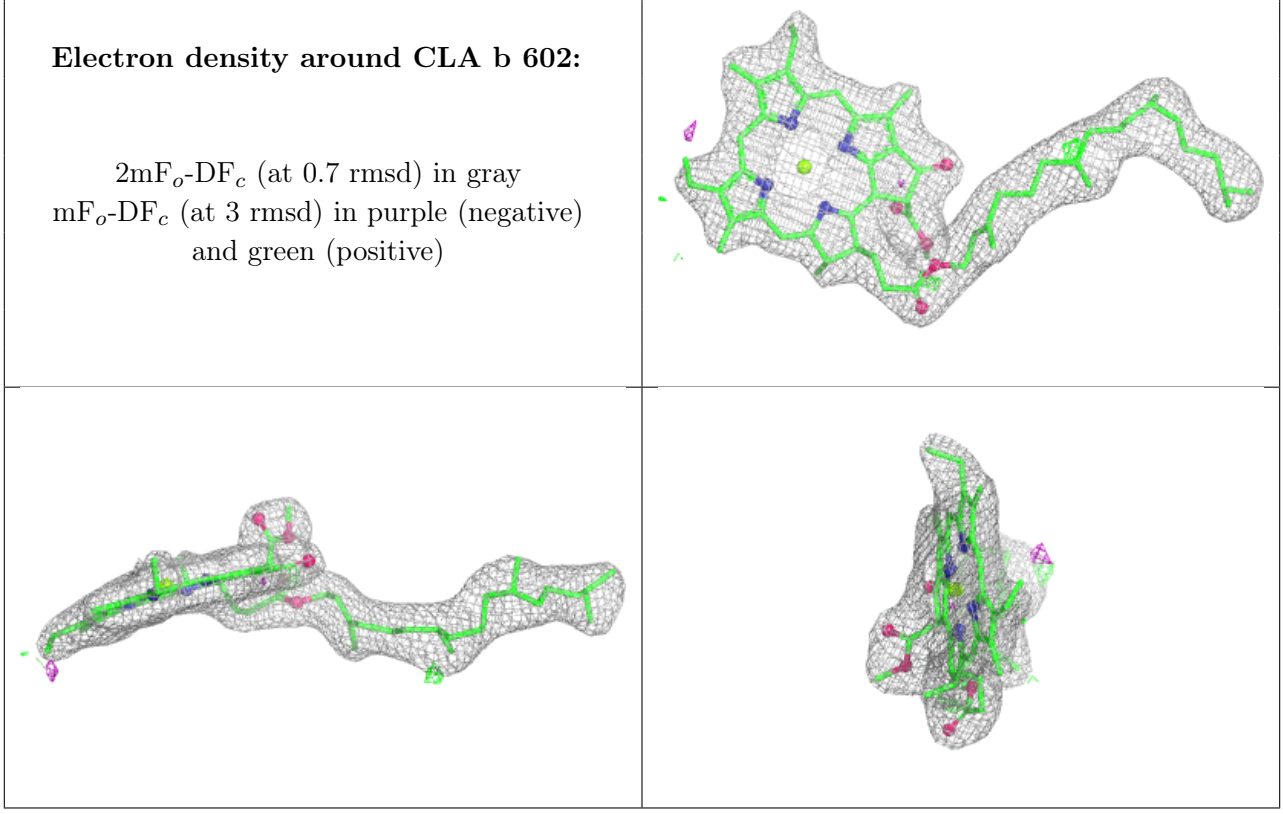






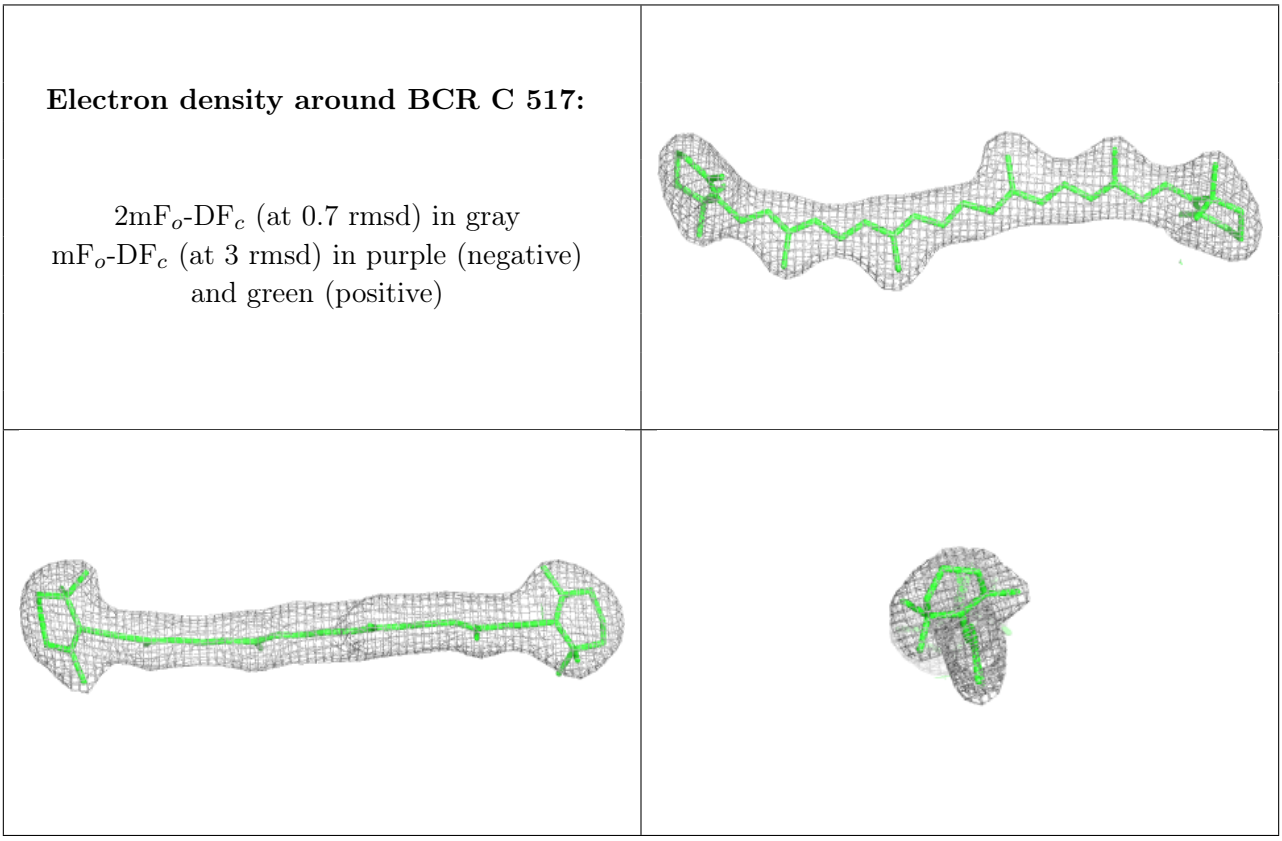
Electron density around CLA b 602:

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



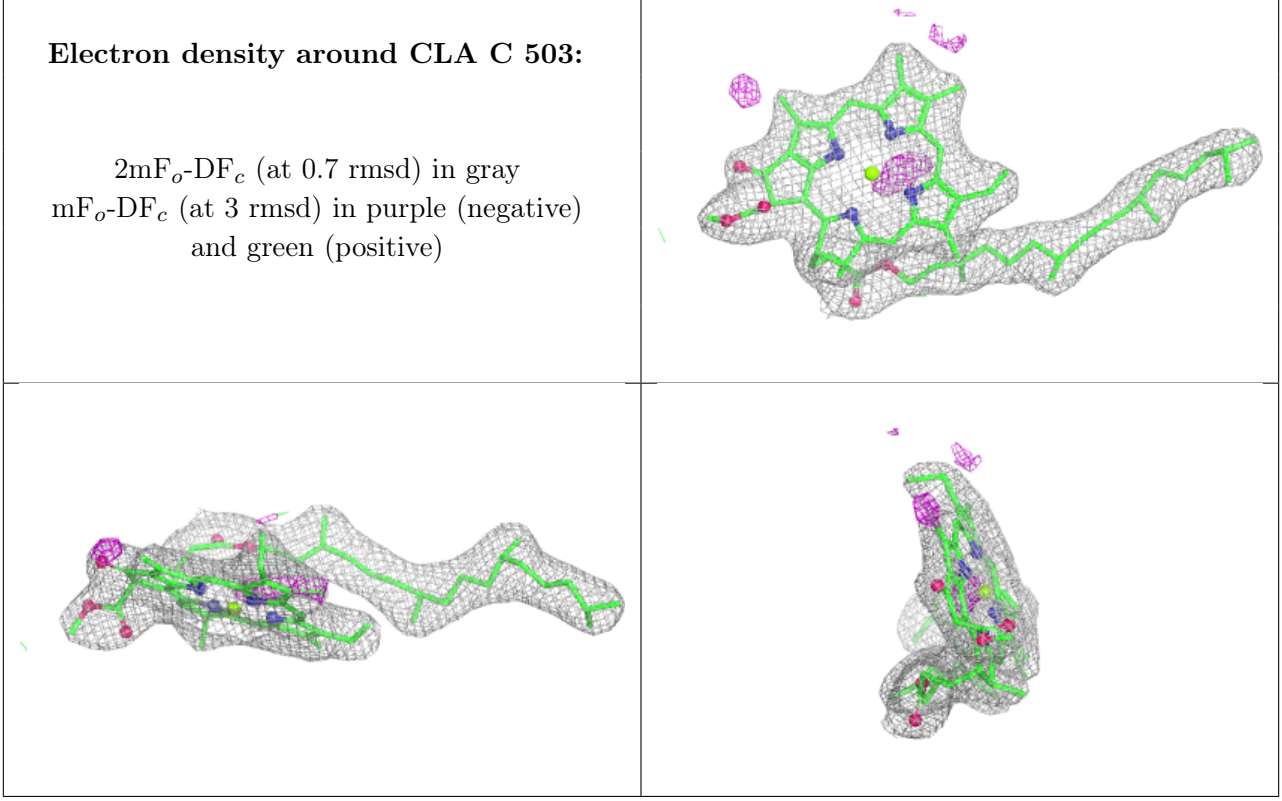
Electron density around BCR C 517:

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



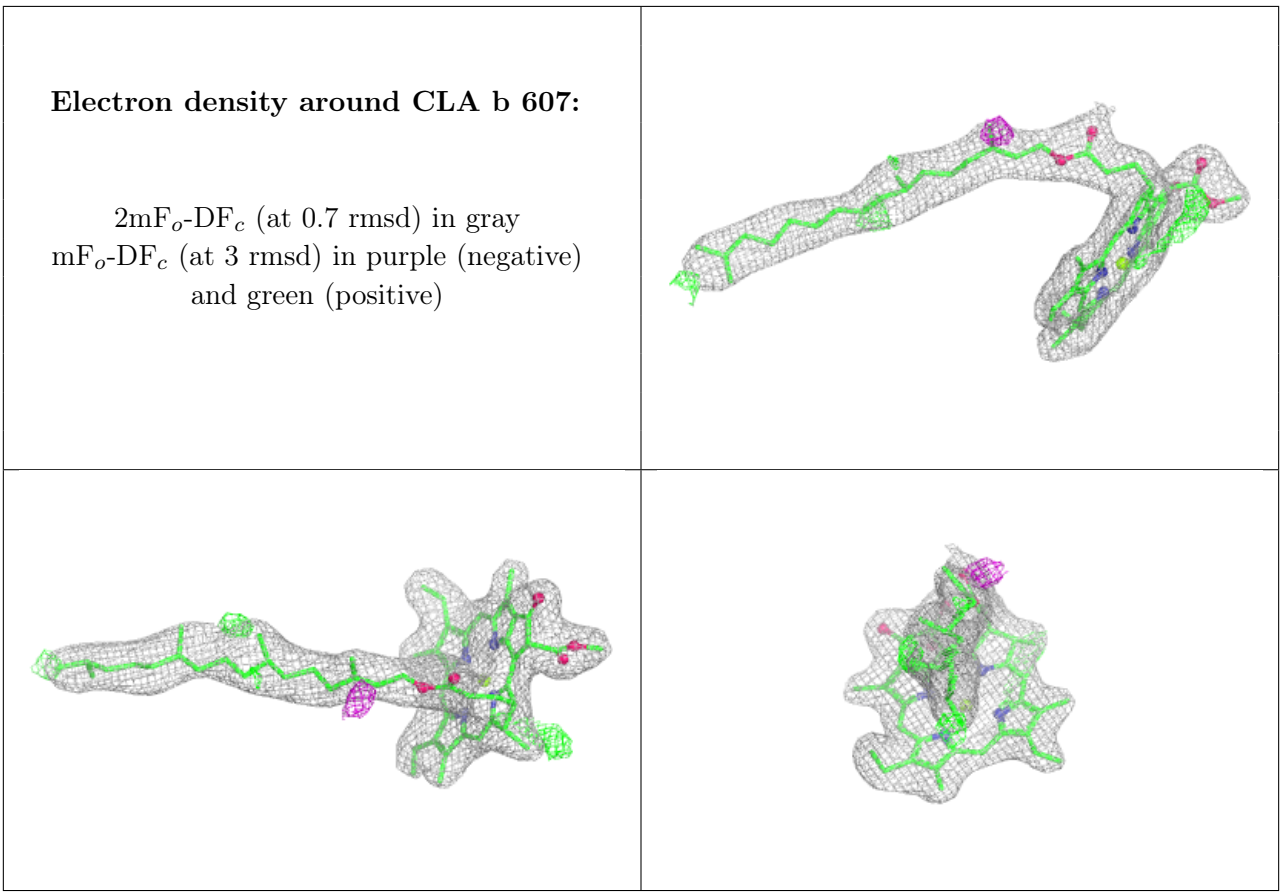
Electron density around CLA C 503:

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



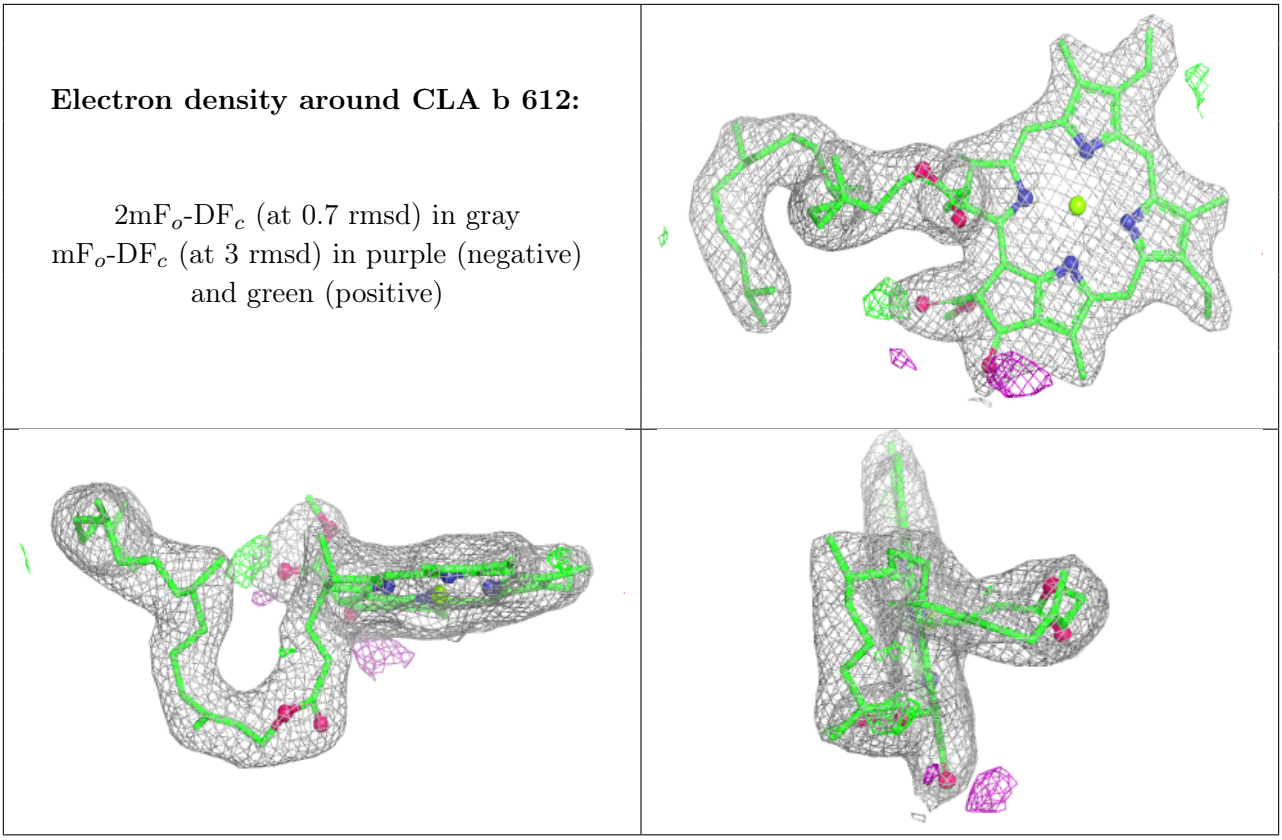
Electron density around CLA b 607:

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



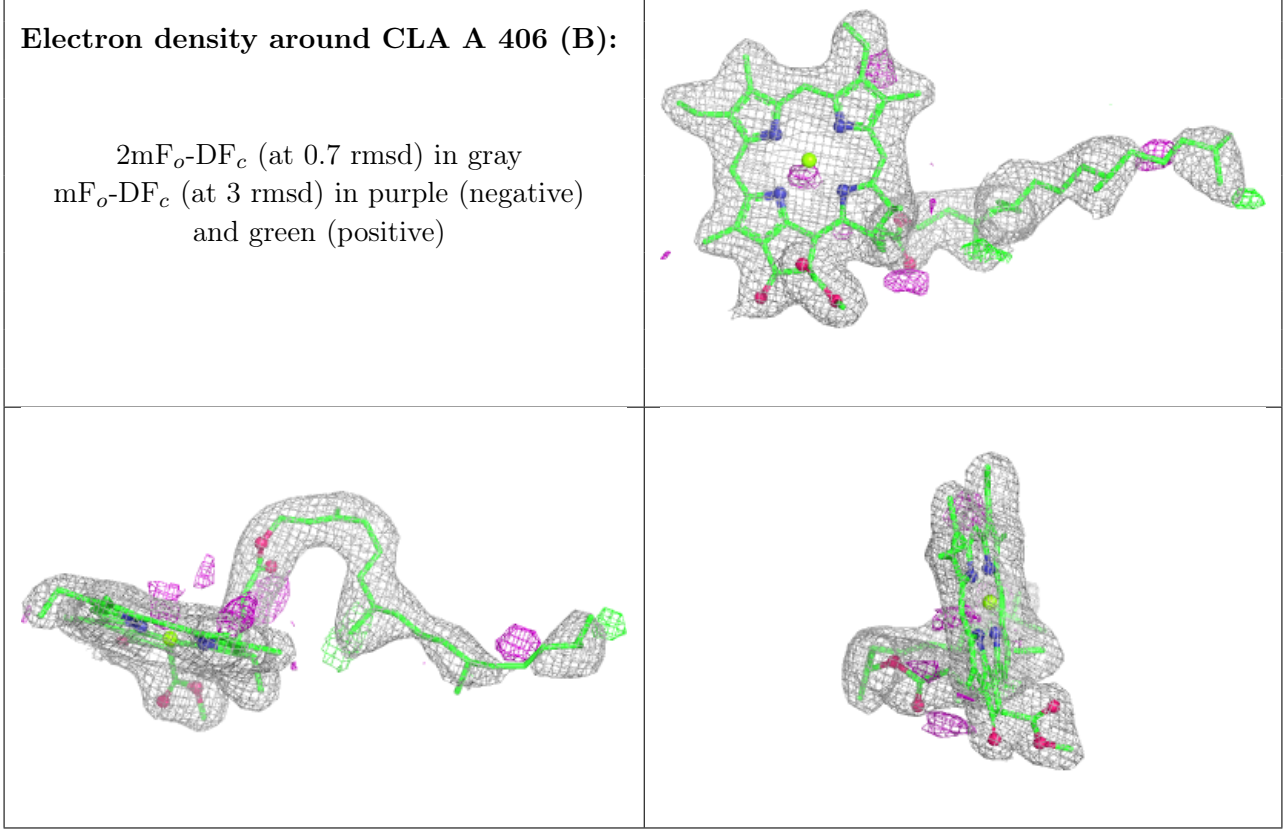
Electron density around CLA b 612:

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



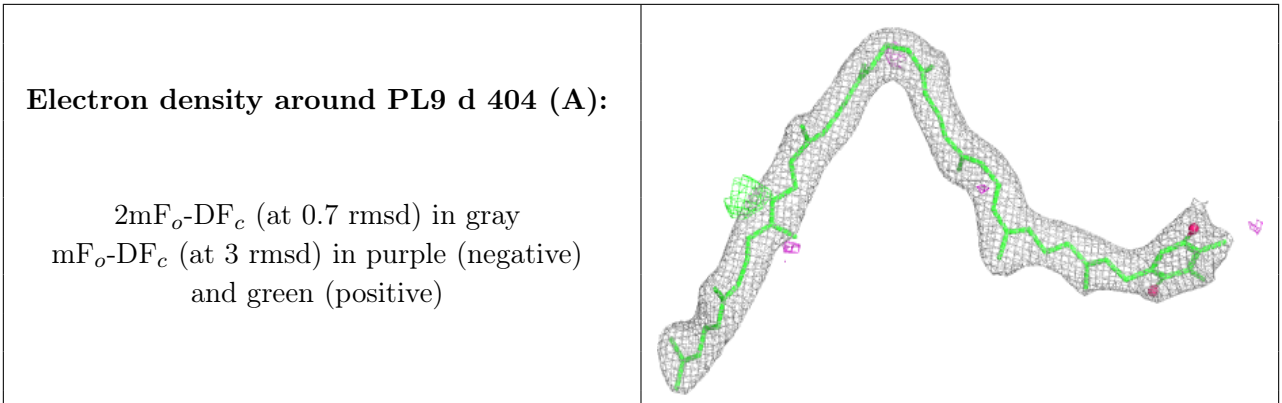
Electron density around CLA A 406 (B):

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



Electron density around PL9 d 404 (A):

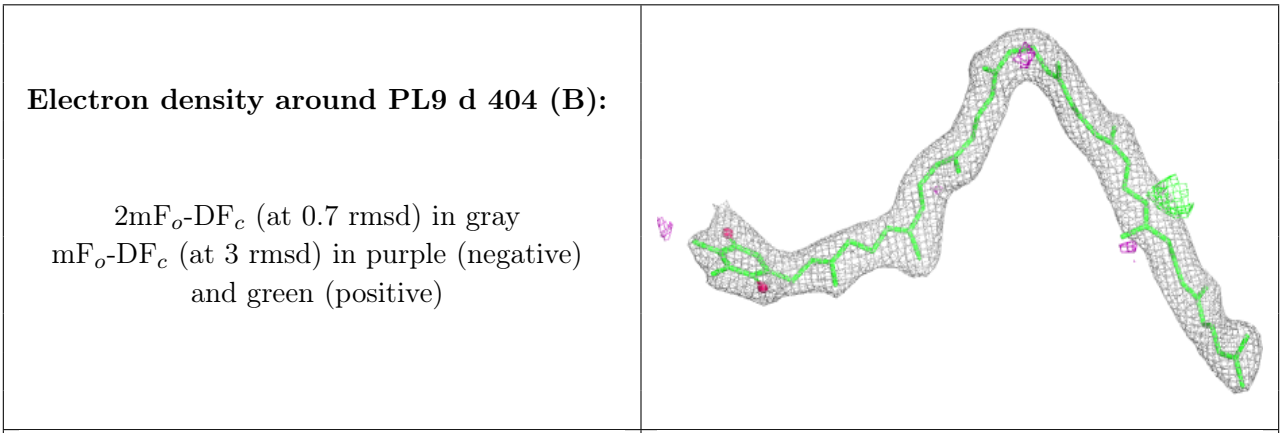
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

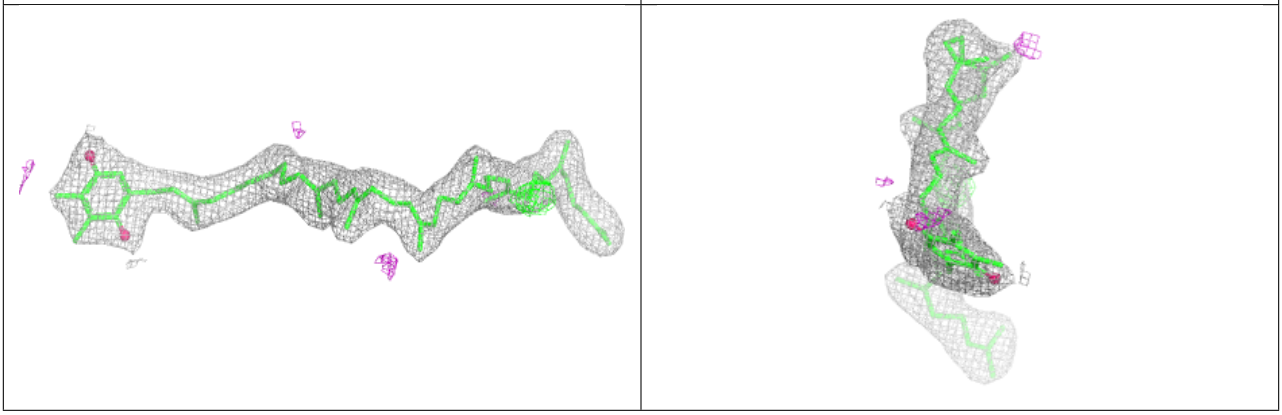




Electron density around PL9 d 404 (B):

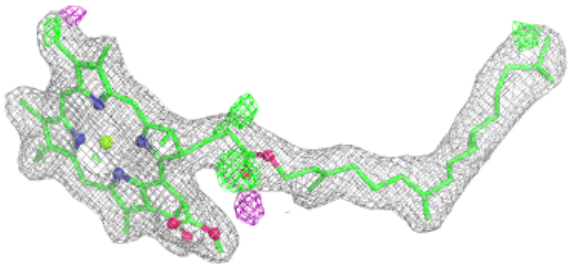
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

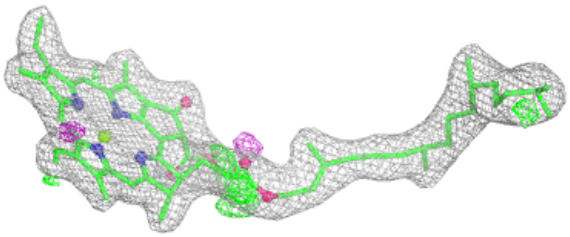


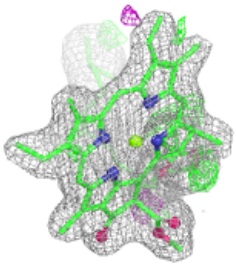


Electron density around CLA A 404 (A):

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

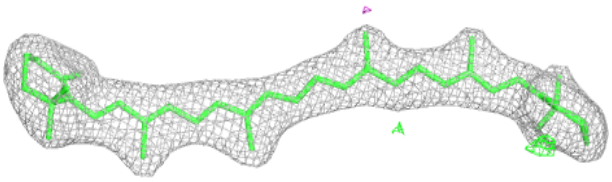


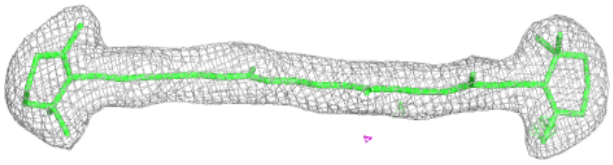


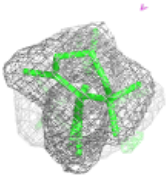


Electron density around BCR a 410:

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

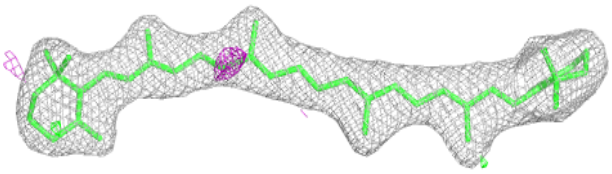


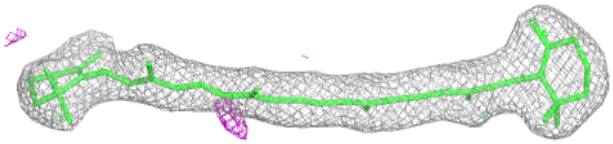


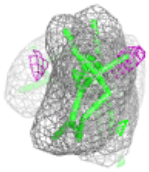


Electron density around BCR b 617:

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

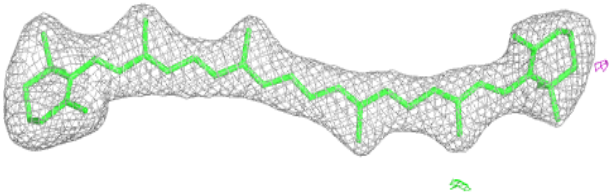


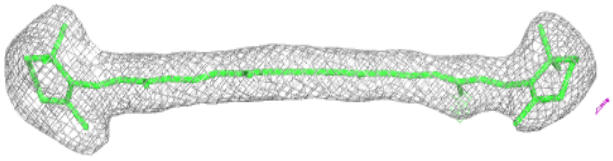


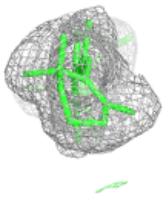


Electron density around BCR b 618:

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

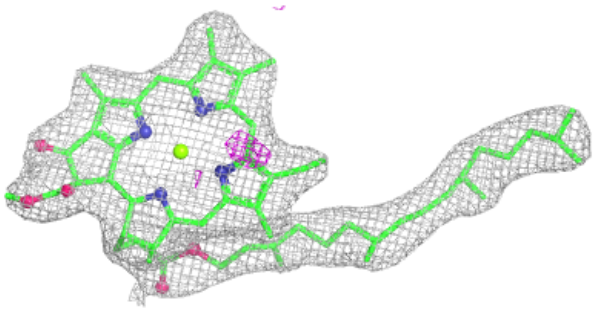


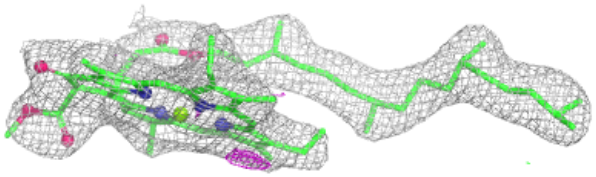


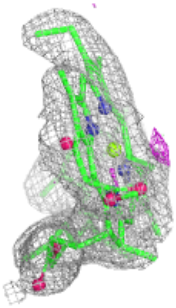


Electron density around CLA c 502:

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

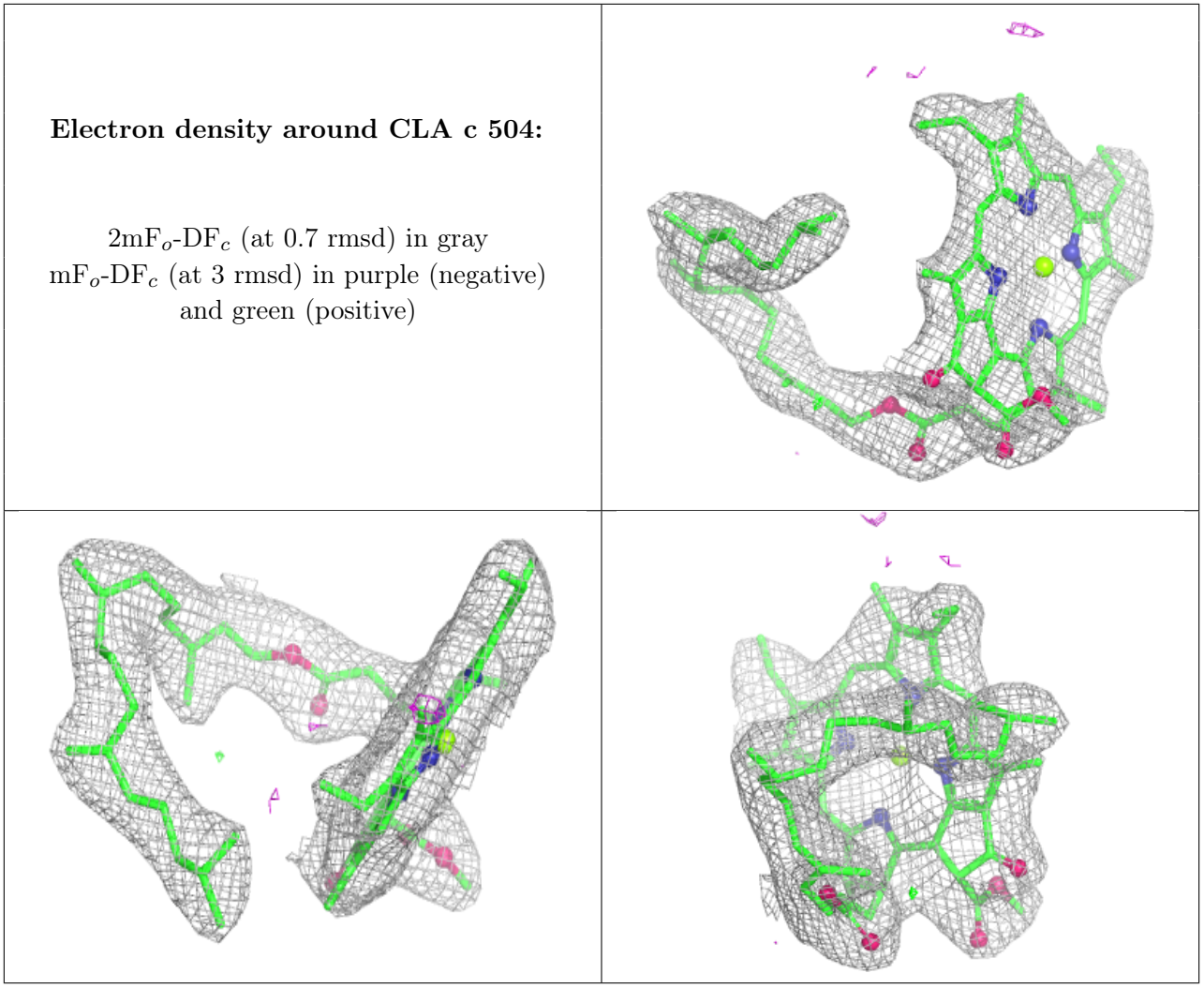






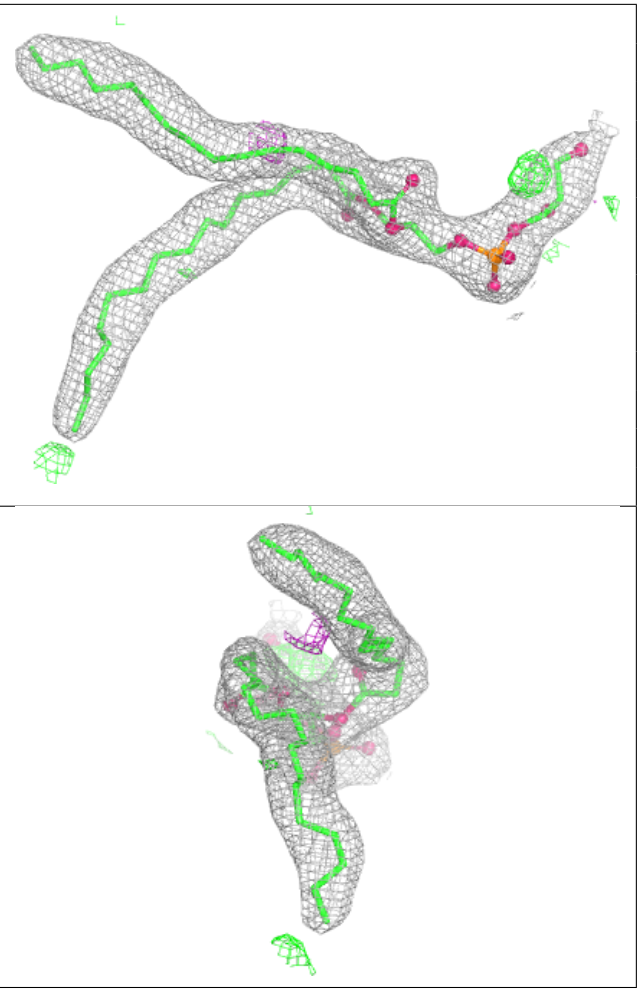
Electron density around CLA c 504:

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



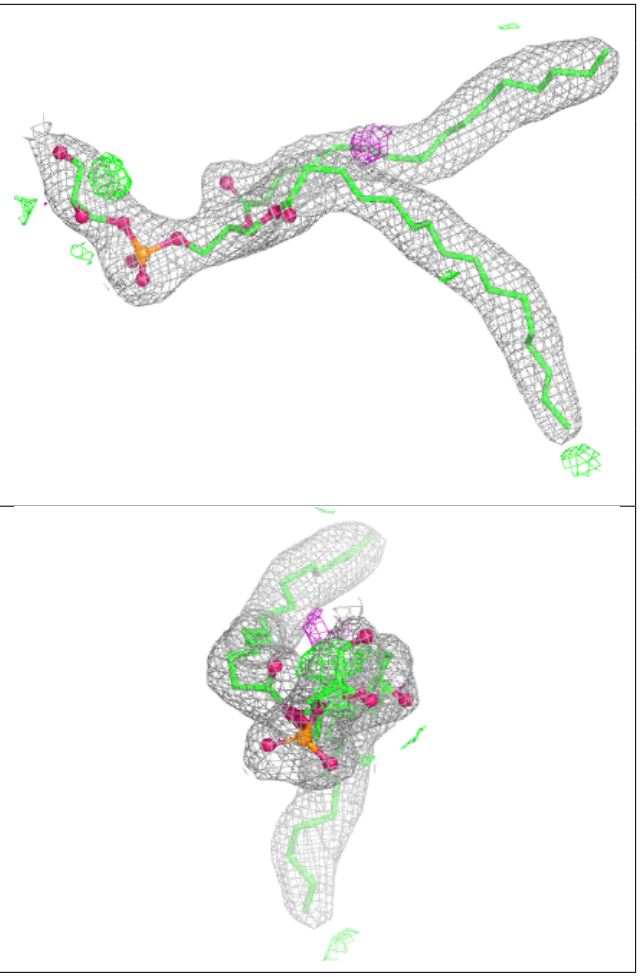
Electron density around LHG D 408 (A):

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



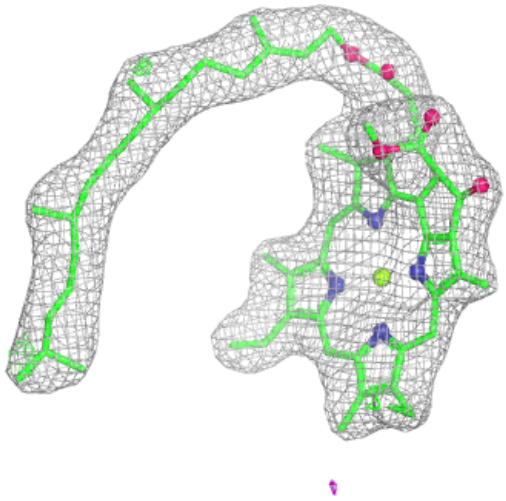
Electron density around LHG D 408 (B):

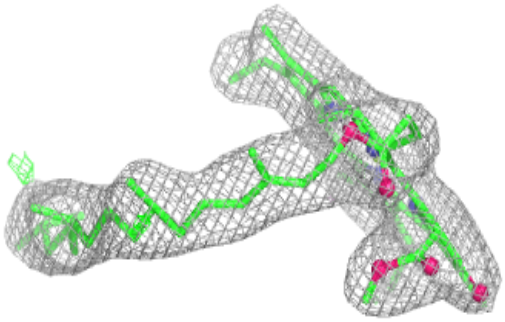
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

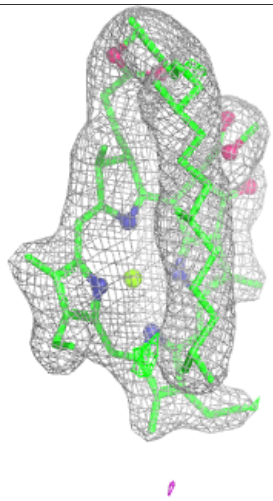


Electron density around CLA C 509:

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

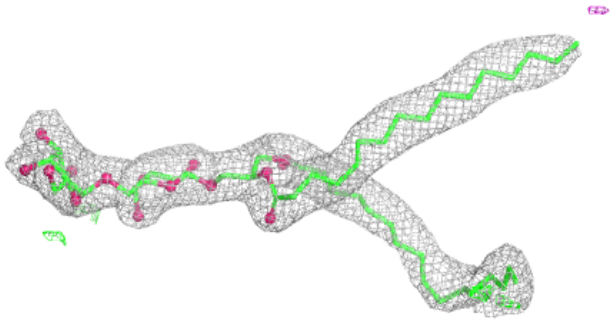


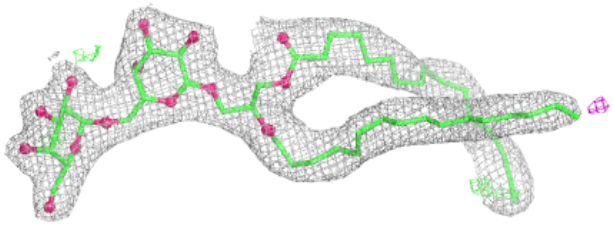


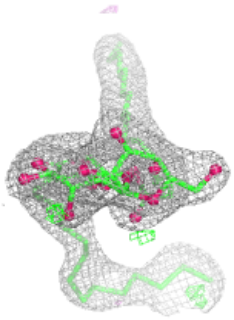


Electron density around DGD C 518 (A):

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

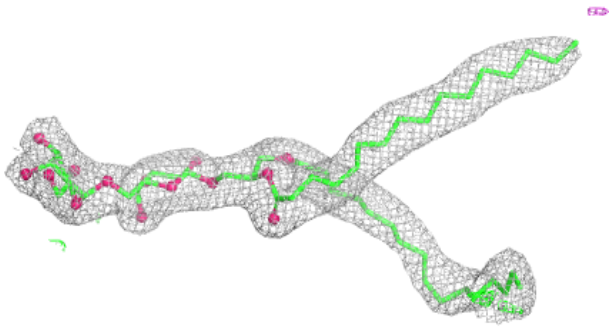


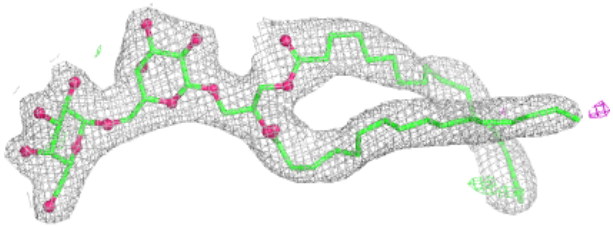


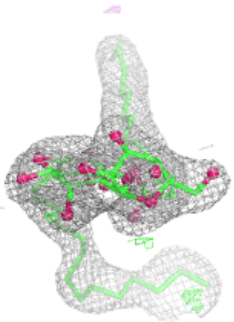


Electron density around DGD C 518 (B):

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

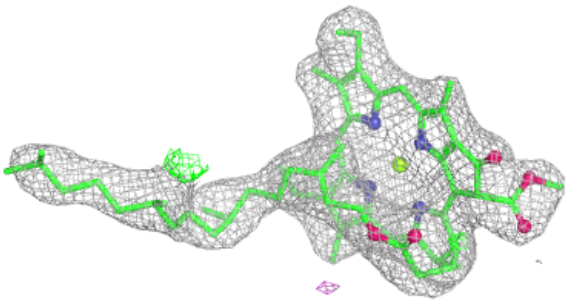


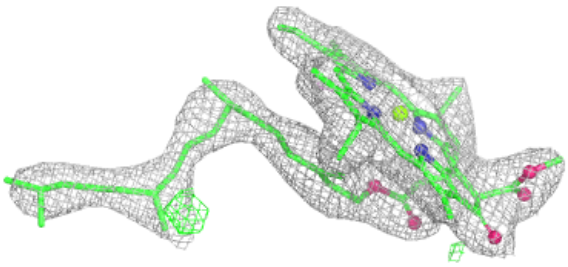


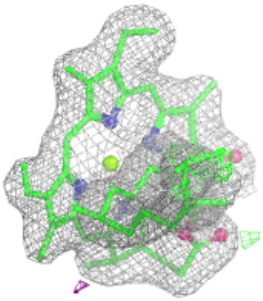


Electron density around CLA c 506:

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

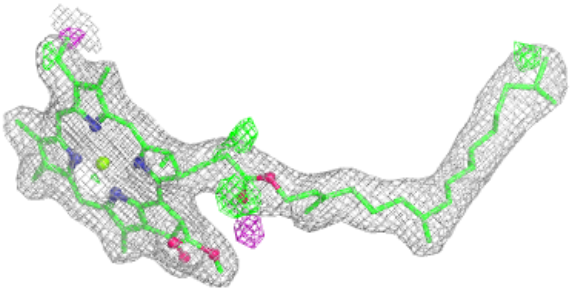


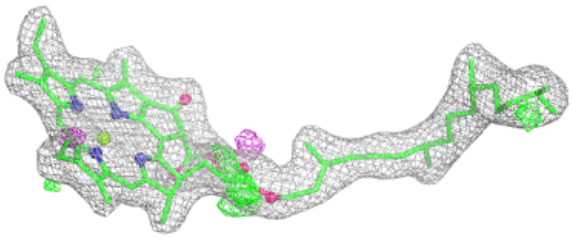




Electron density around CLA A 404 (B):

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

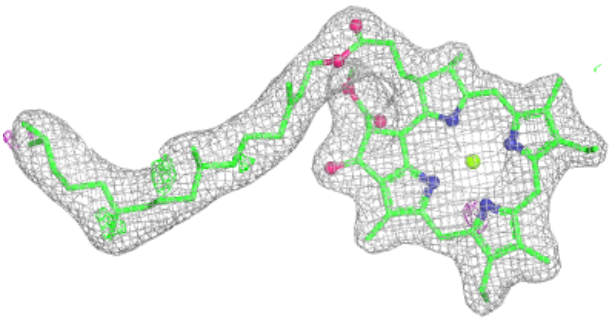


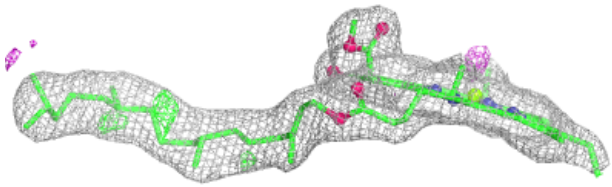


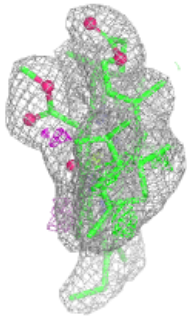


Electron density around CLA B 602:

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

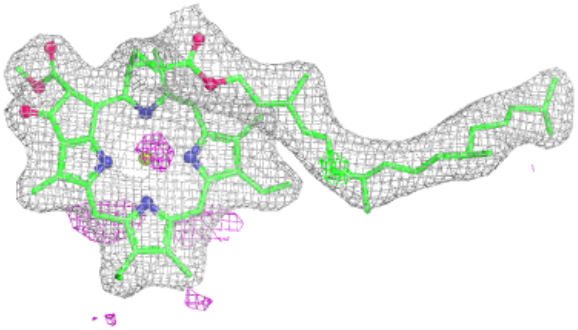


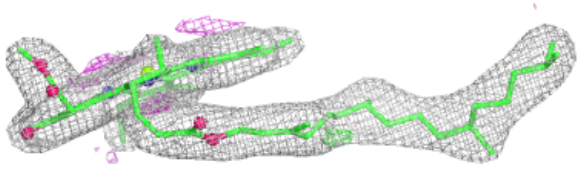


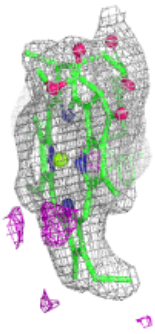


Electron density around CLA B 603:

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

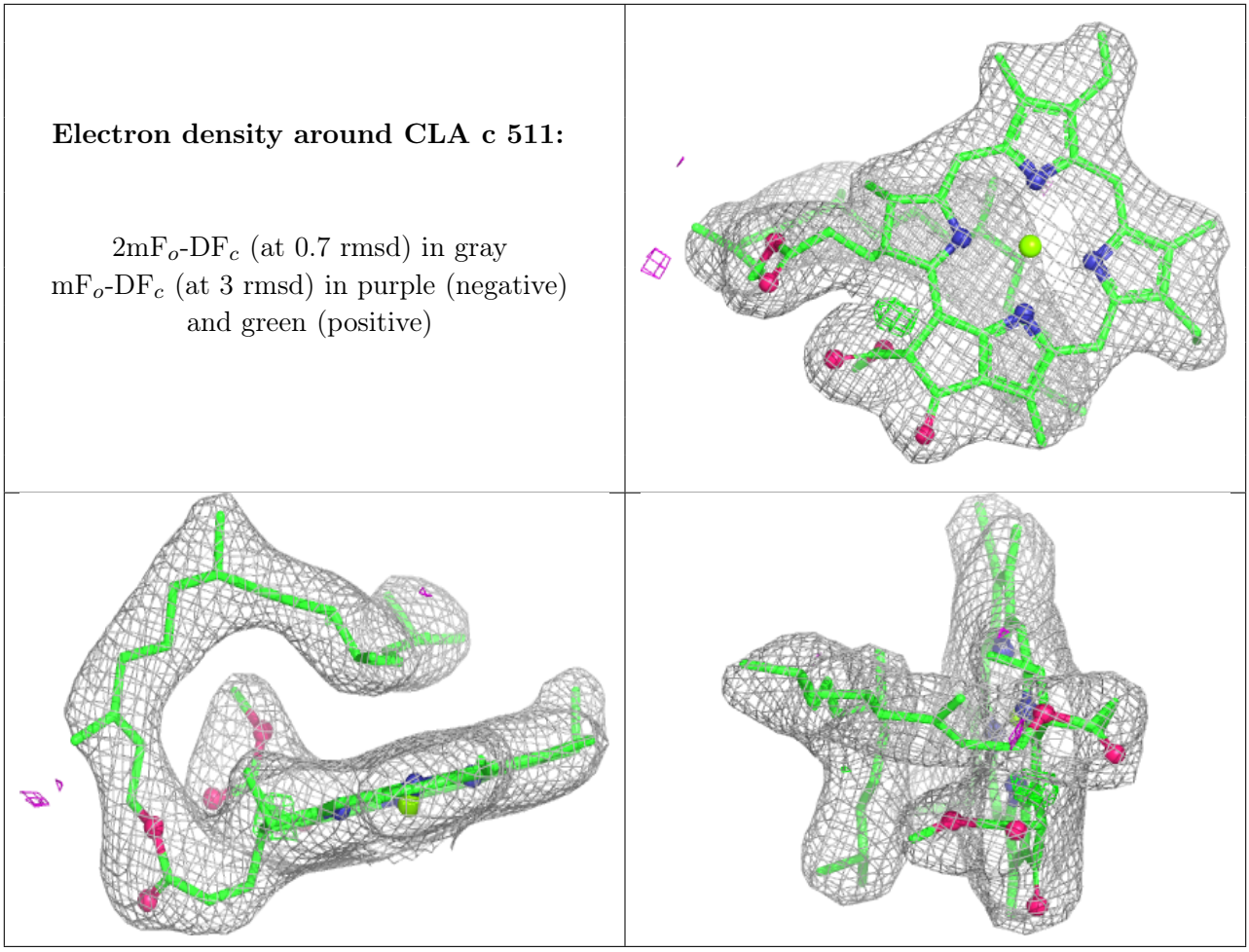






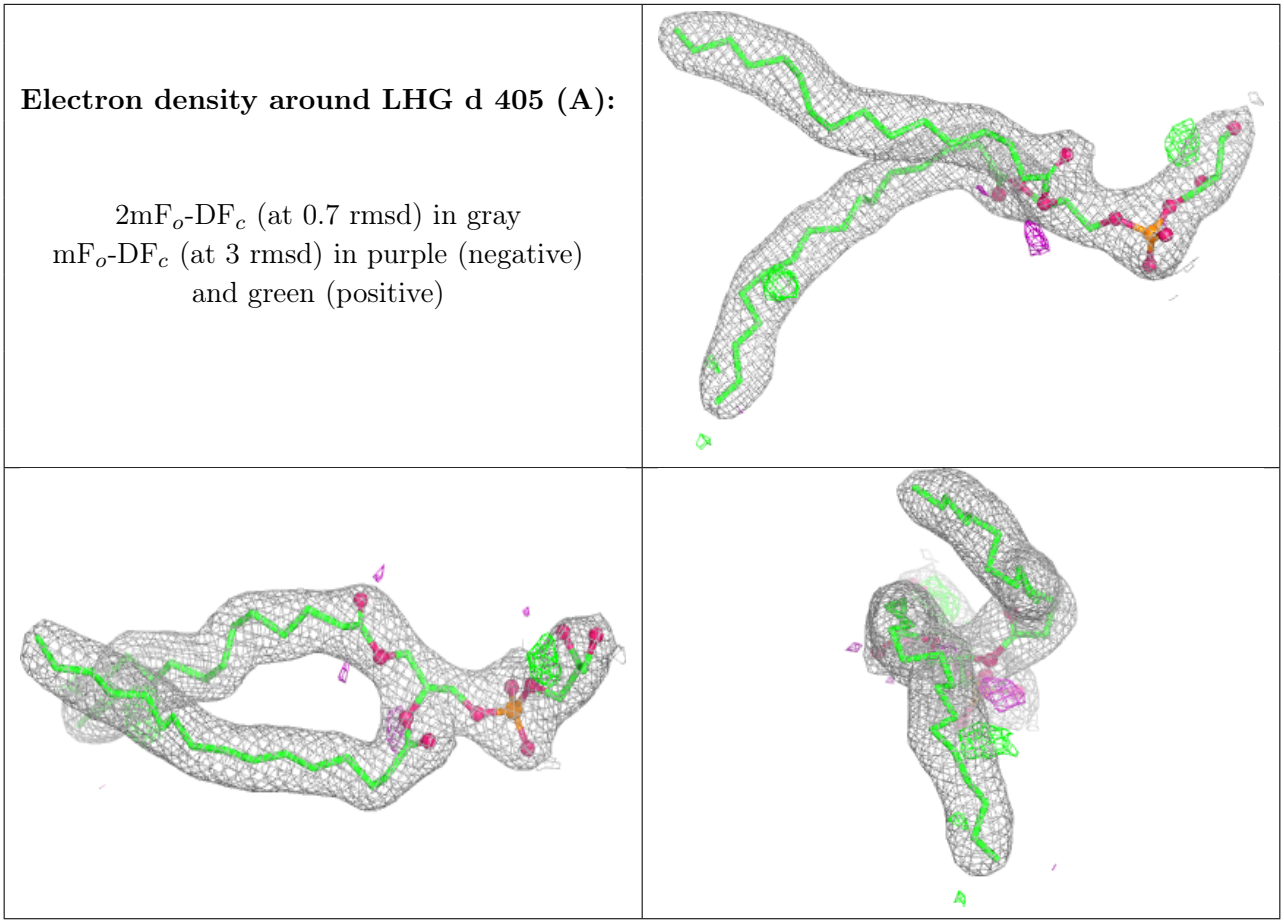
Electron density around CLA c 511:

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



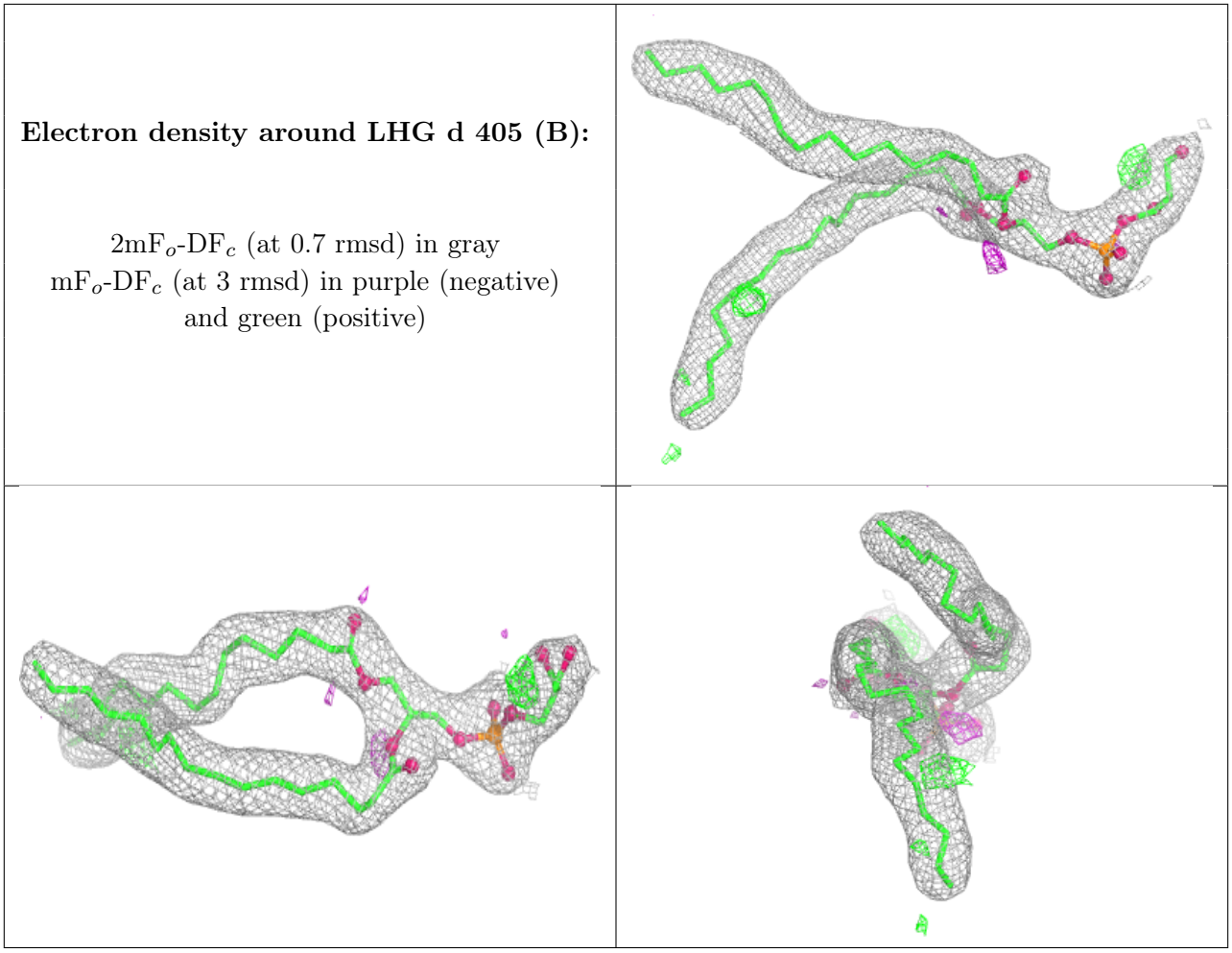
Electron density around LHG d 405 (A):

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



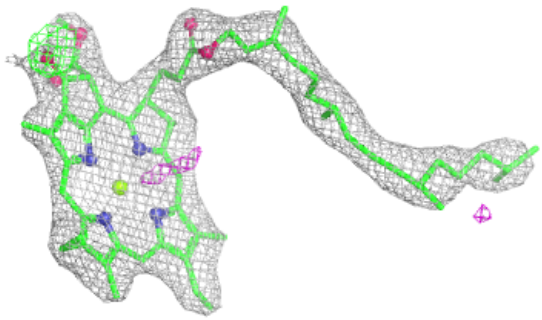
Electron density around LHG d 405 (B):

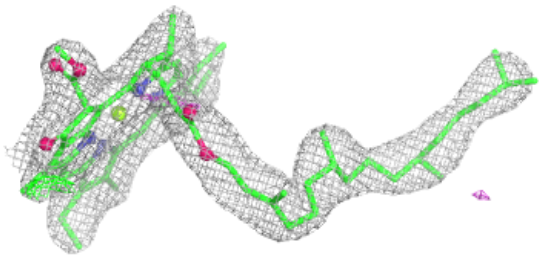
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

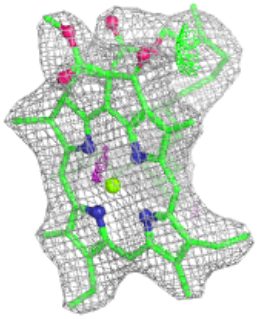


Electron density around CLA c 512:

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

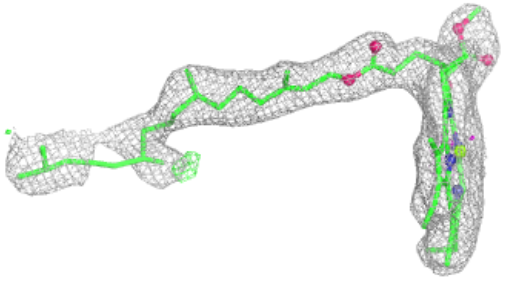


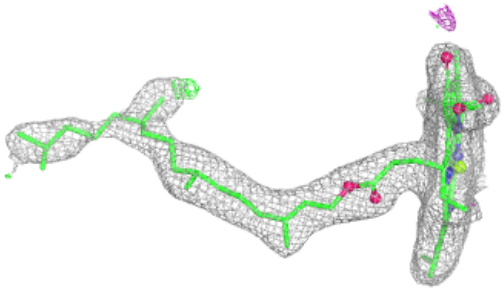


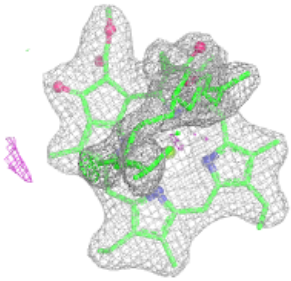


Electron density around CLA B 606:

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

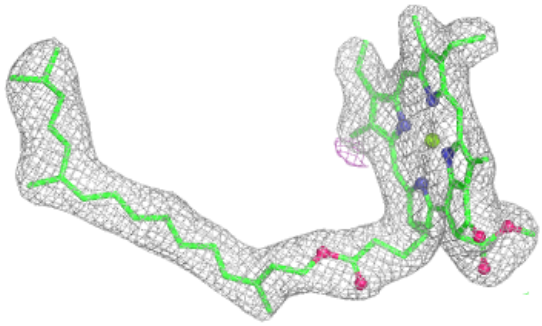


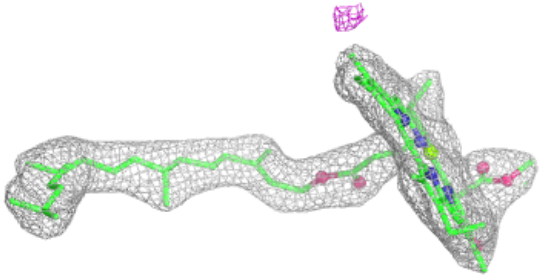


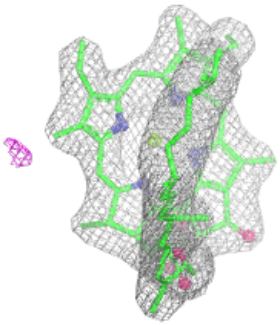


Electron density around CLA B 609:

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

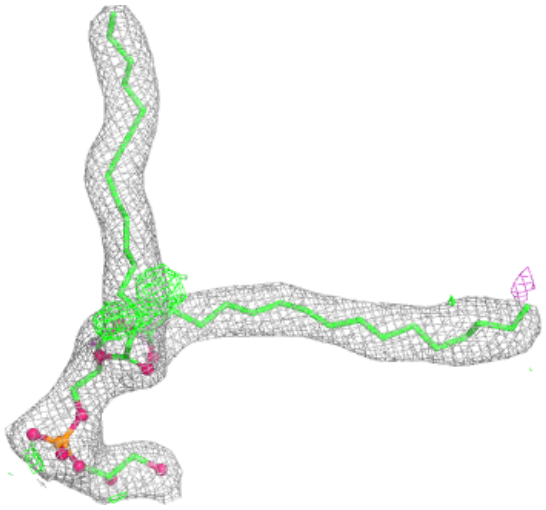


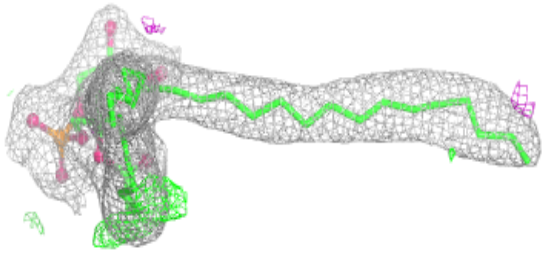


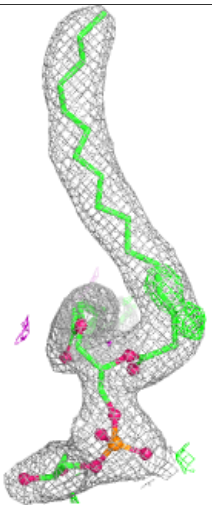


Electron density around LHG l 802 (A):

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

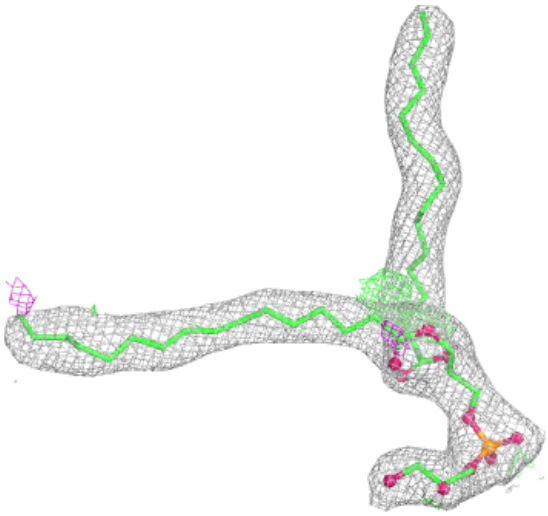


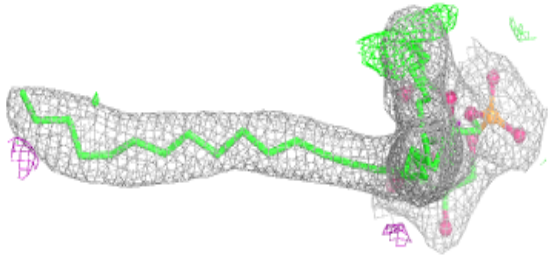


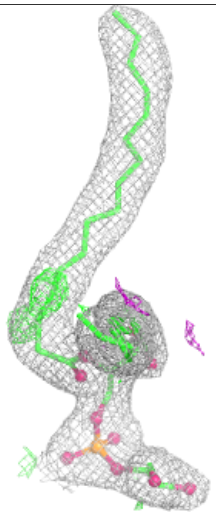


Electron density around LHG l 802 (B):

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

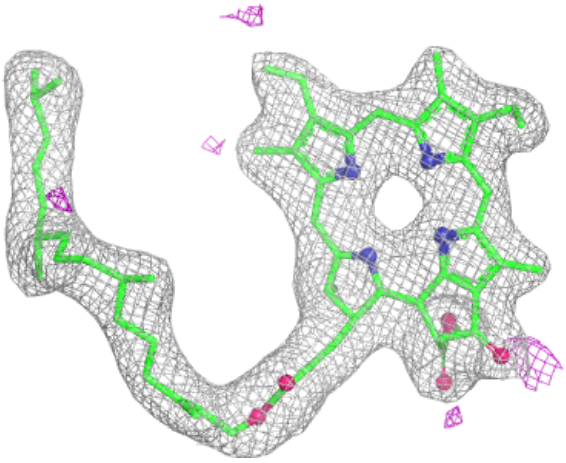


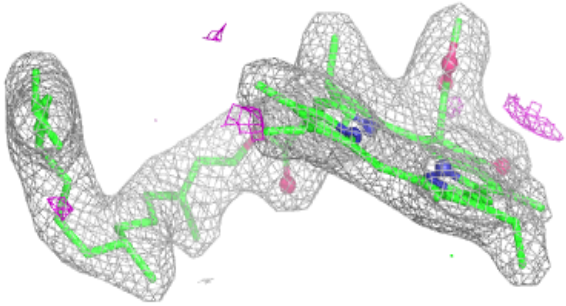


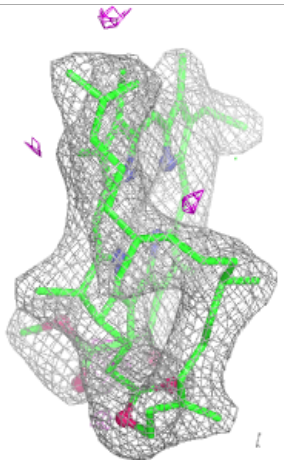


Electron density around PHO D 402 (A):

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

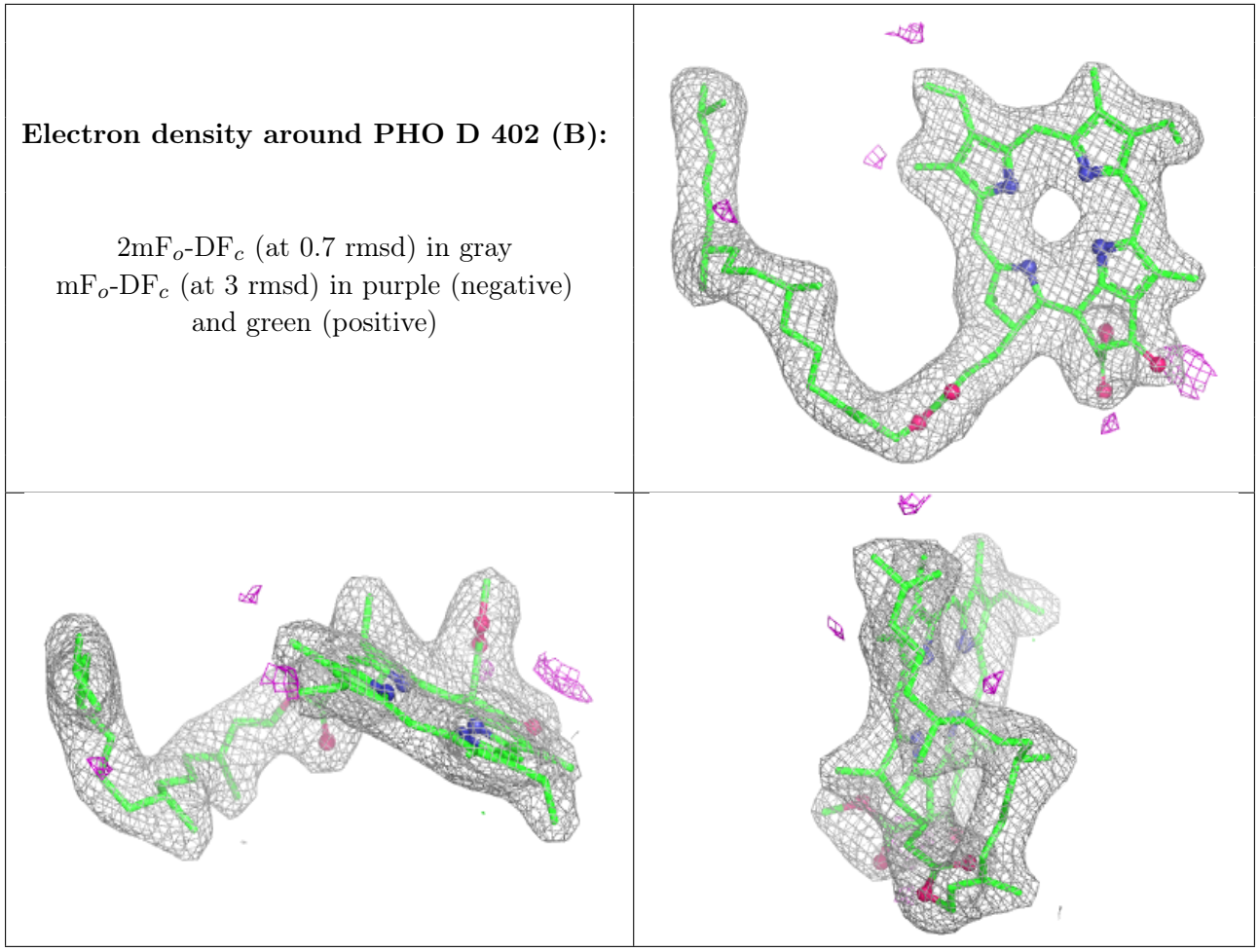






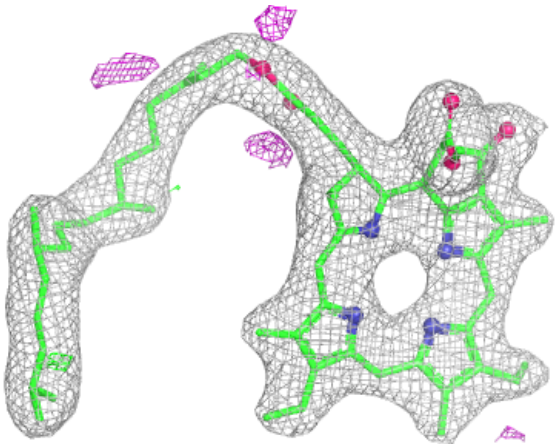
Electron density around PHO D 402 (B):

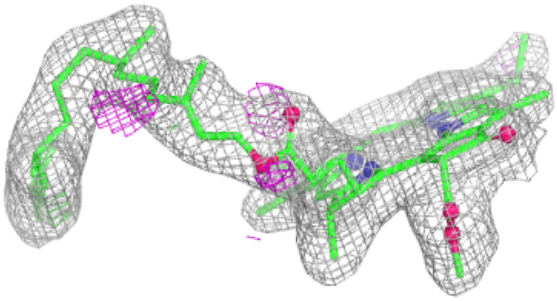
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO a 416 (A):

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

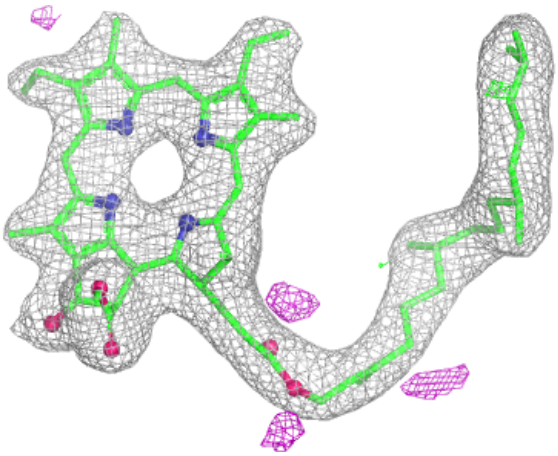


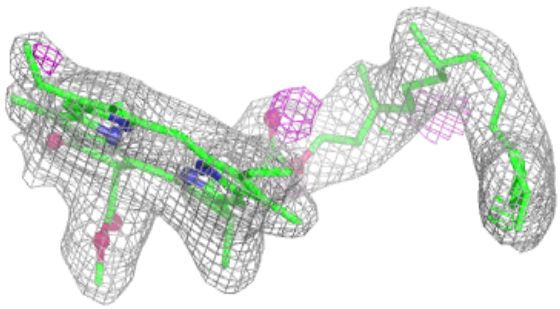


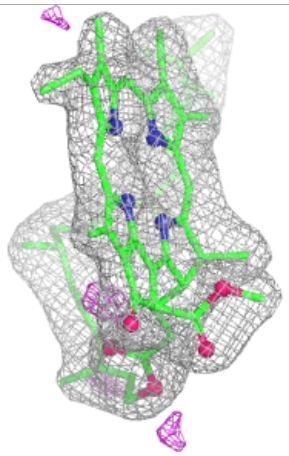


Electron density around PHO a 416 (B):

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

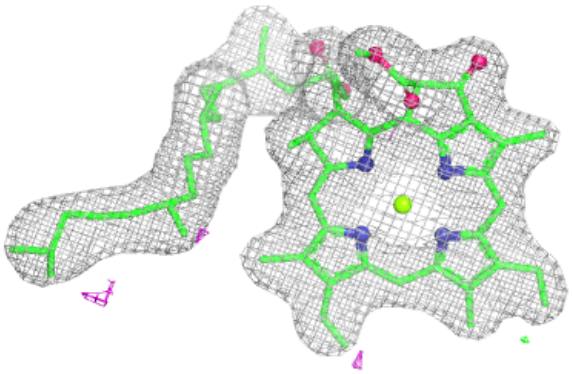


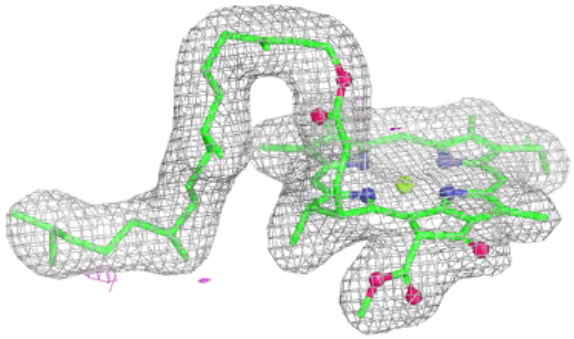


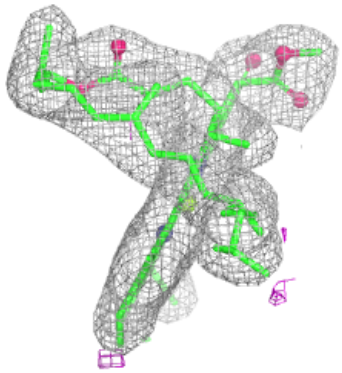


Electron density around CLA a 406 (B):

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

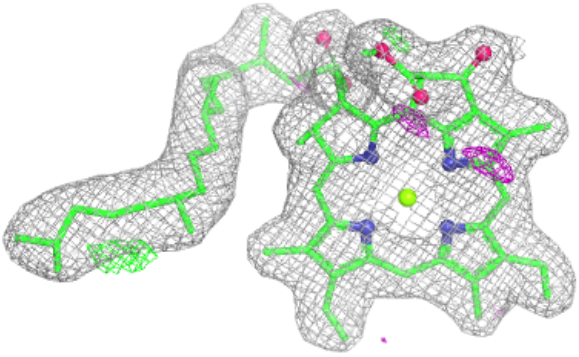


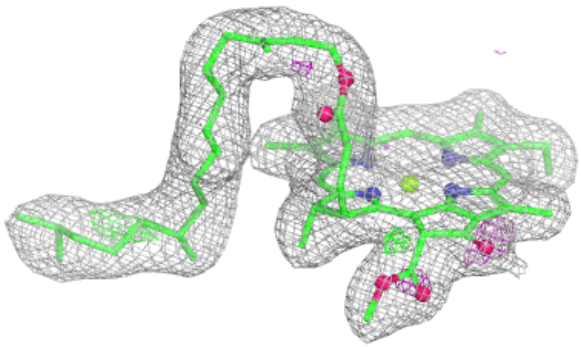


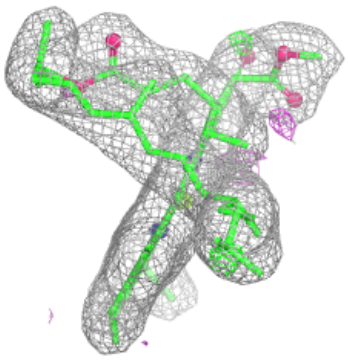


Electron density around CLA A 405 (A):

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

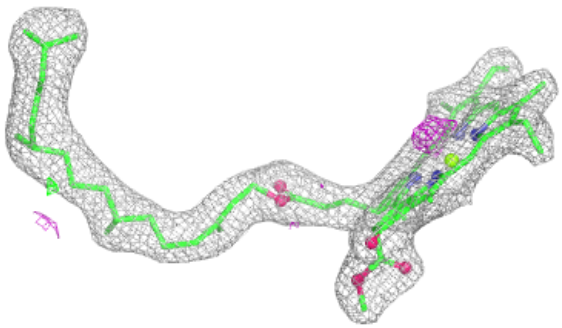


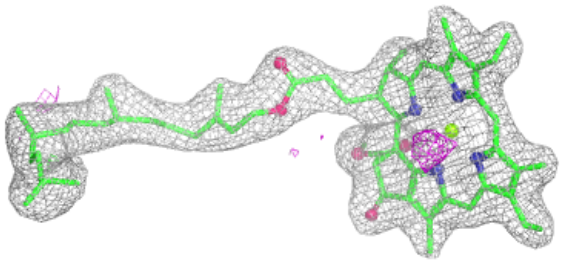


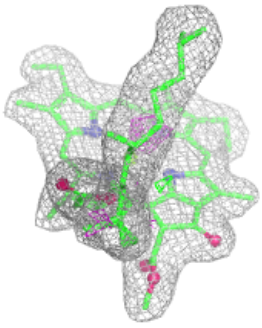


Electron density around CLA d 401 (A):

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

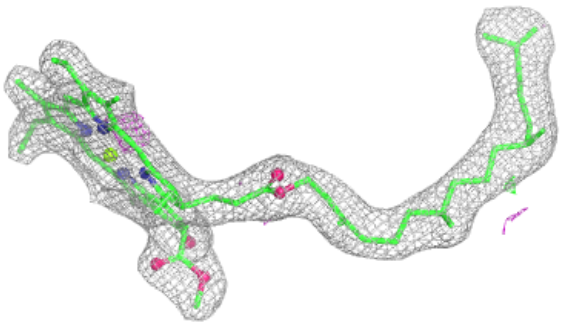


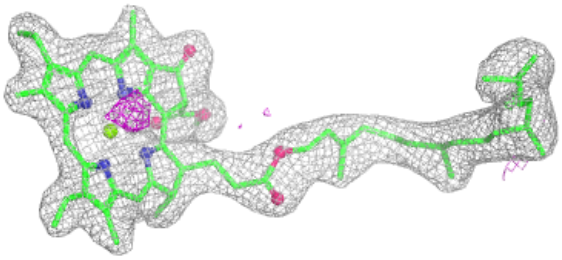


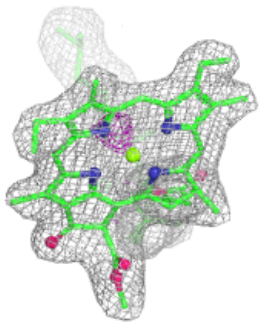


Electron density around CLA d 401 (B):

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

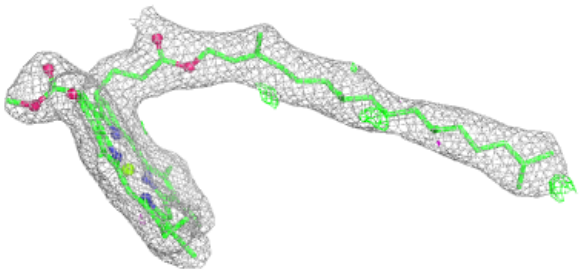


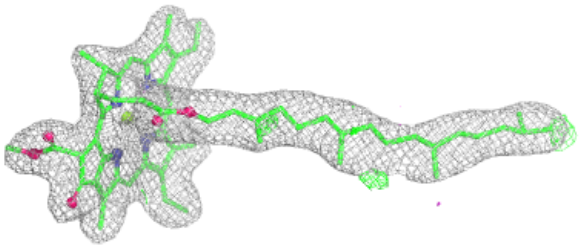


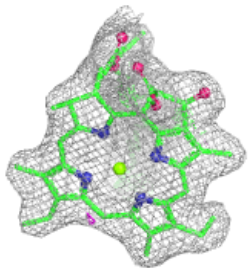


Electron density around CLA B 607:

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

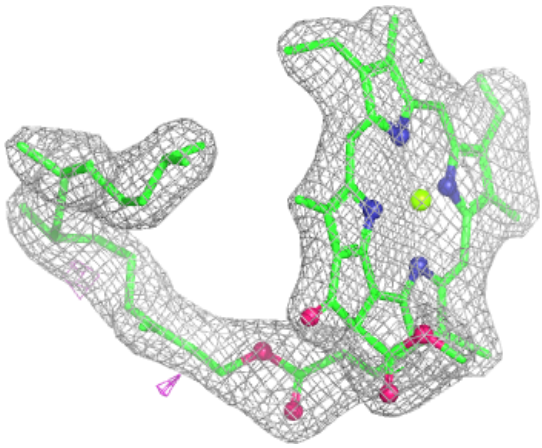


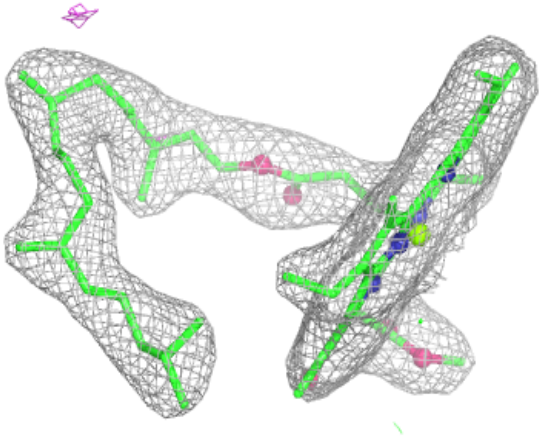


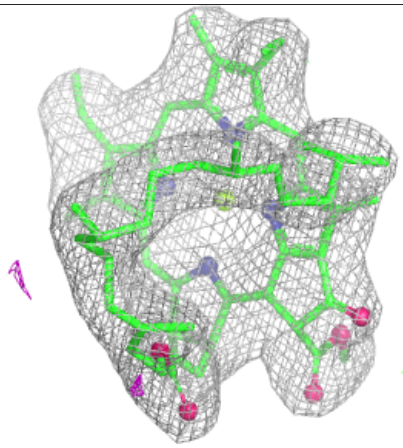


Electron density around CLA C 505:

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

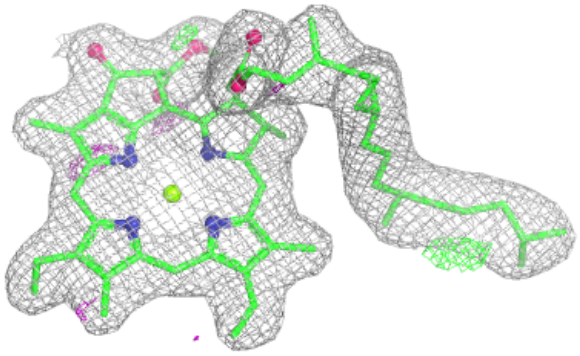


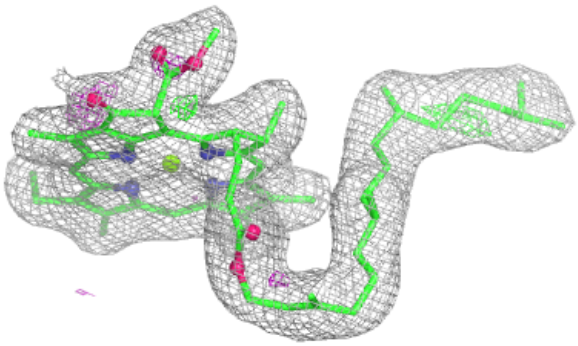


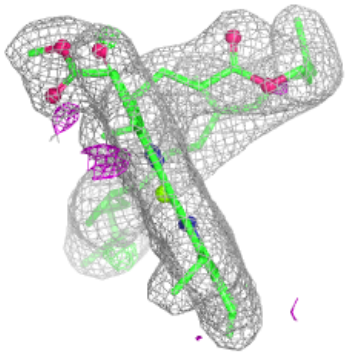


Electron density around CLA A 405 (B):

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

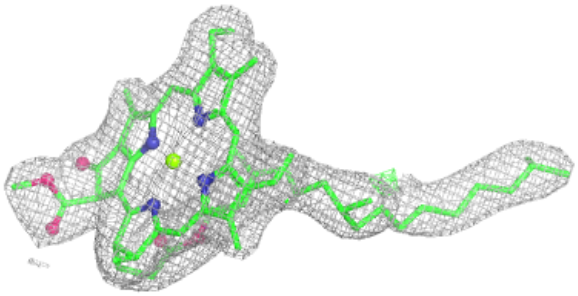


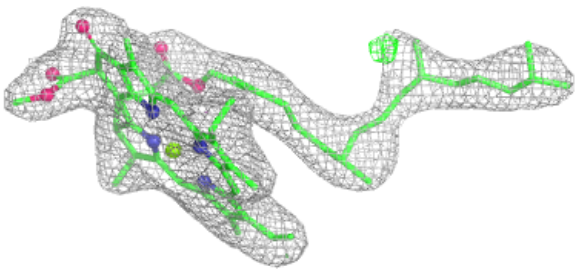


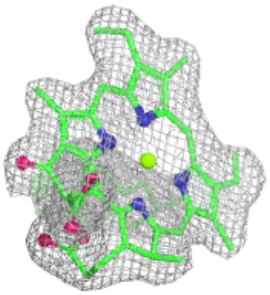


Electron density around CLA C 507:

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

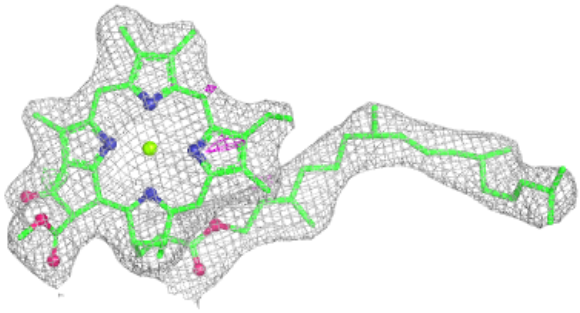


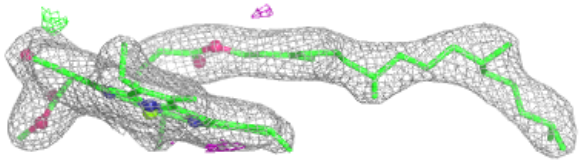


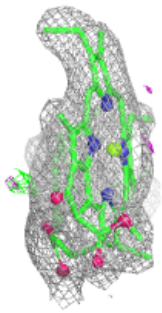


Electron density around CLA b 603:

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

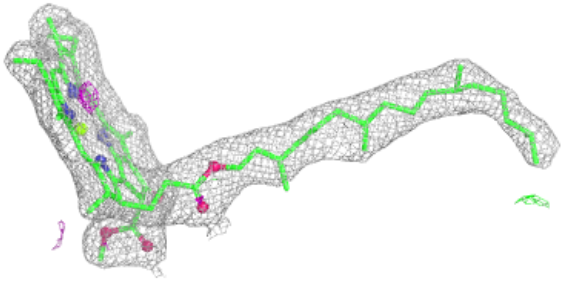


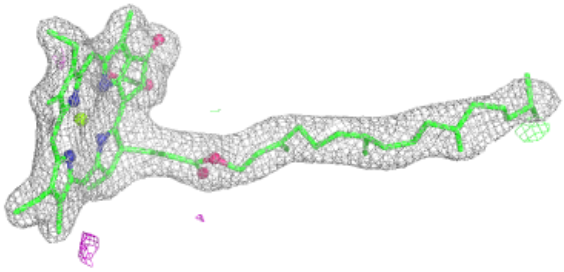


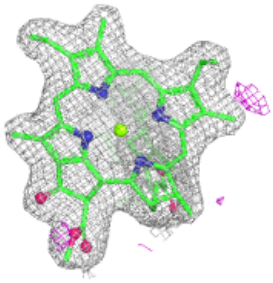


Electron density around CLA b 604:

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

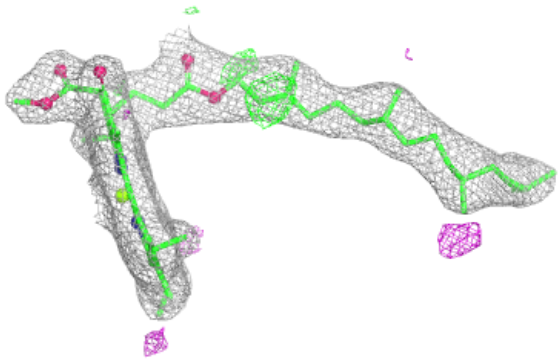


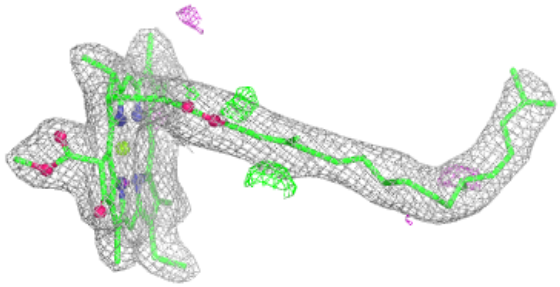


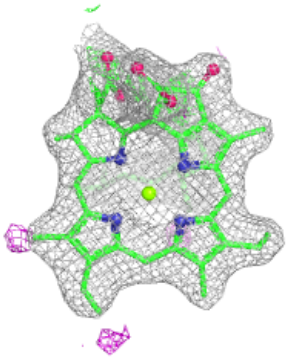


Electron density around CLA b 605:

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

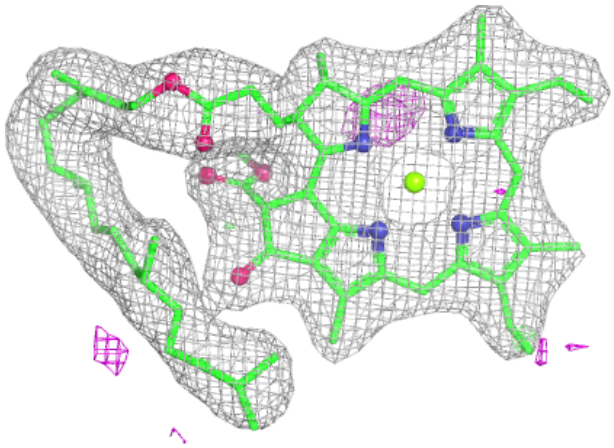


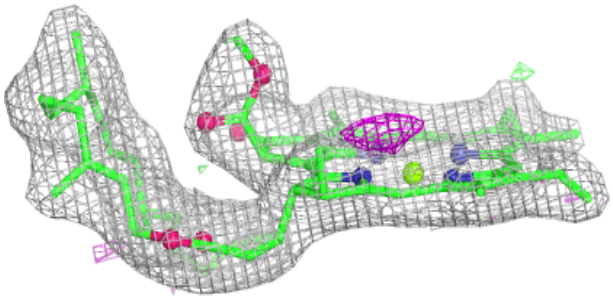


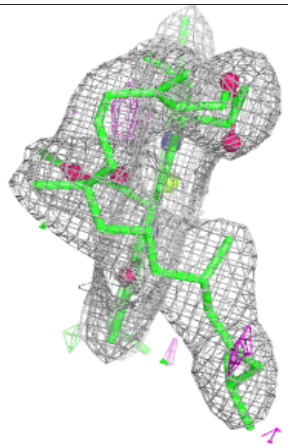


Electron density around CLA B 610:

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

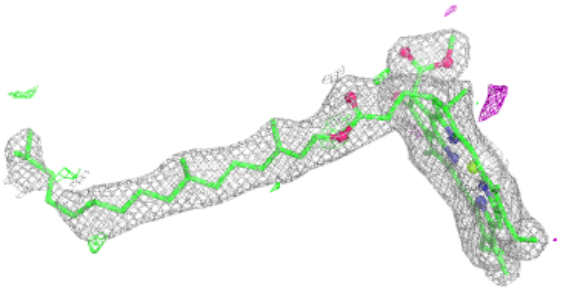


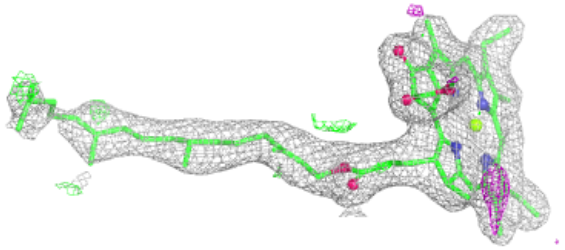


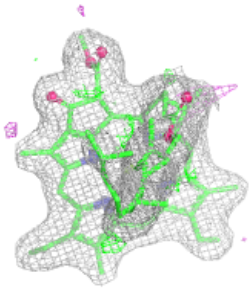


Electron density around CLA B 604:

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

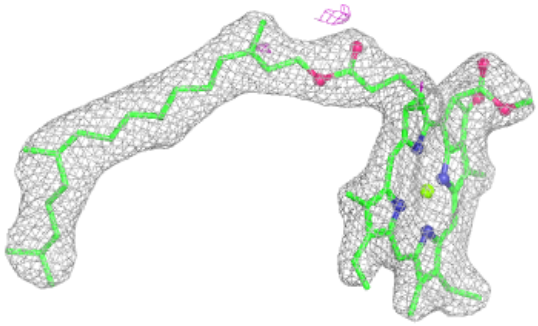


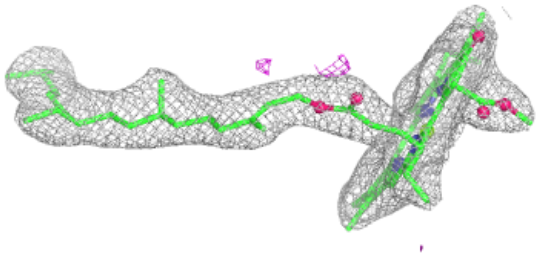


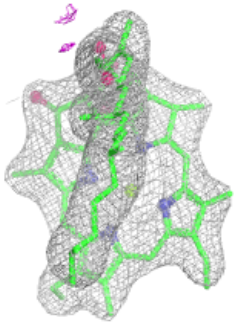


Electron density around CLA b 609:

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

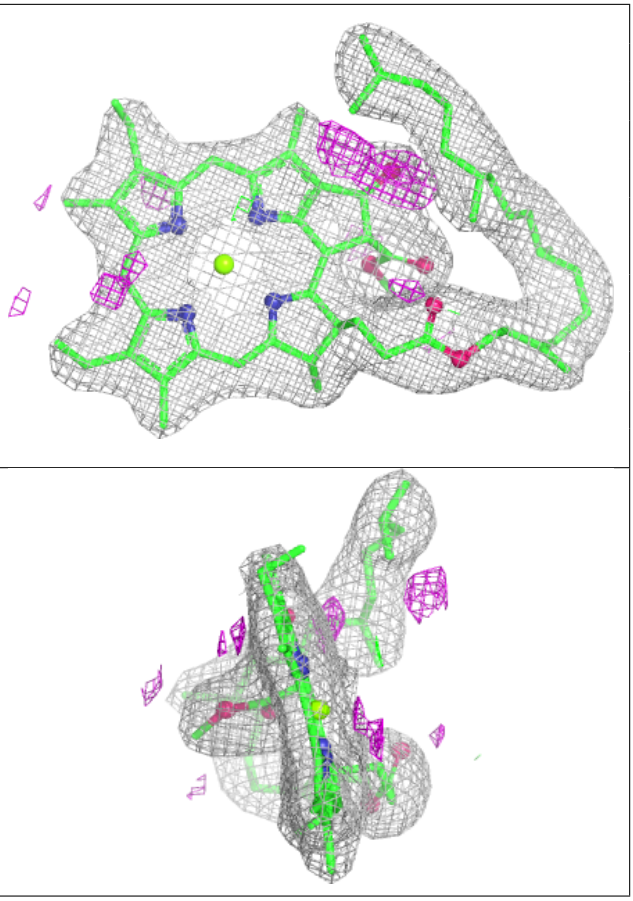


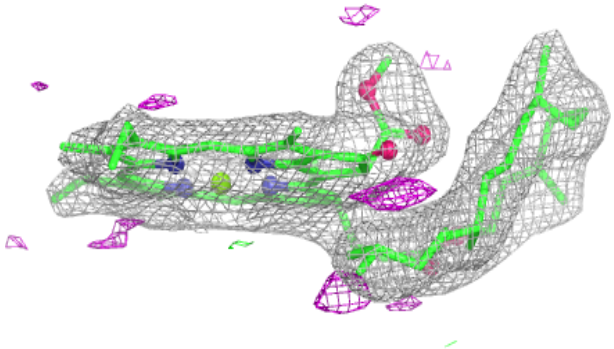




Electron density around CLA b 610:

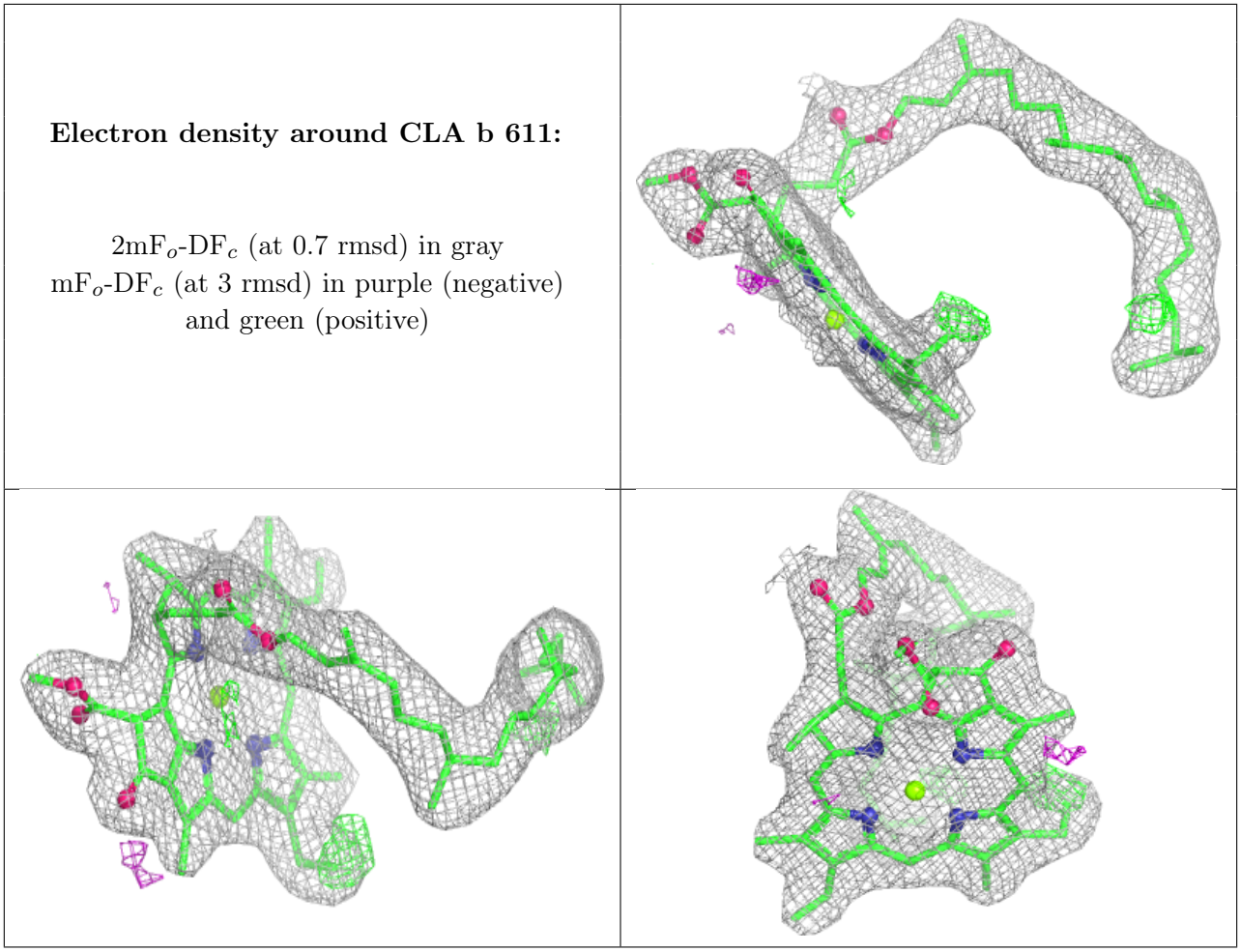
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





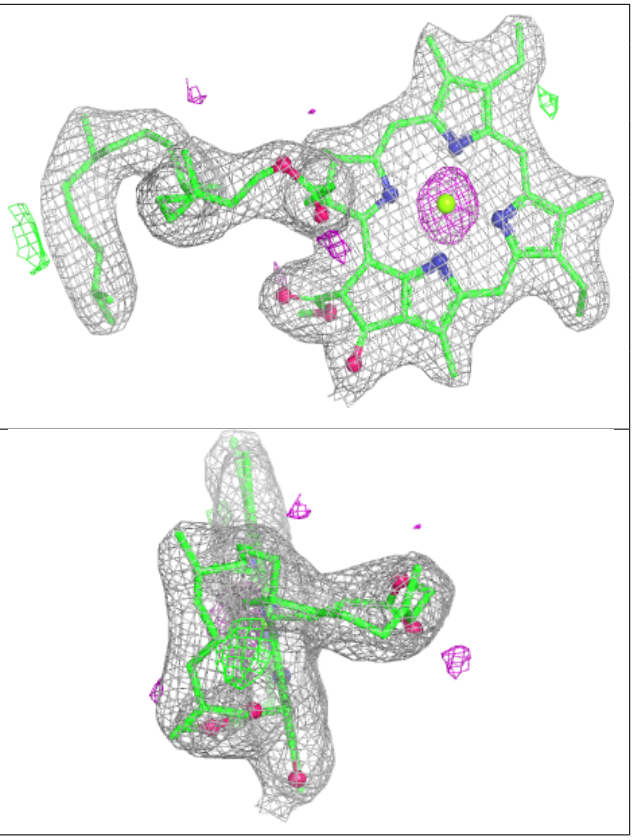
Electron density around CLA b 611:

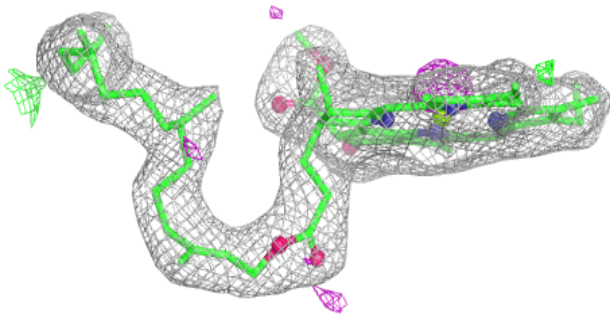
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 612:

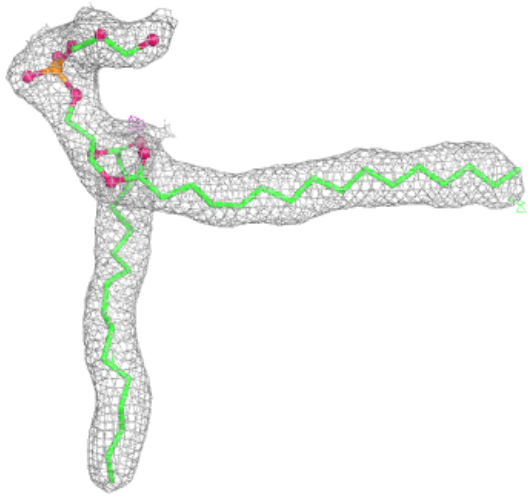
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

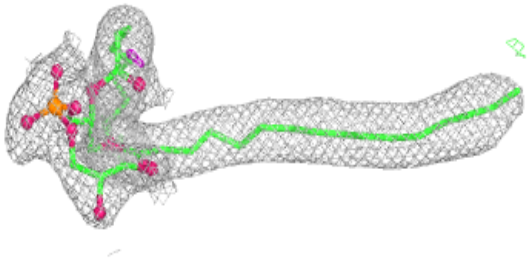


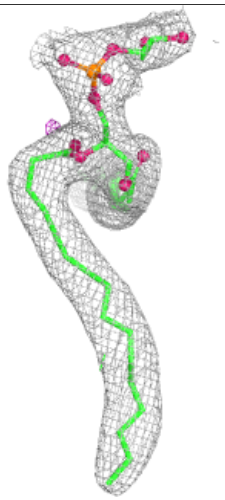


Electron density around LHG L 101 (A):

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

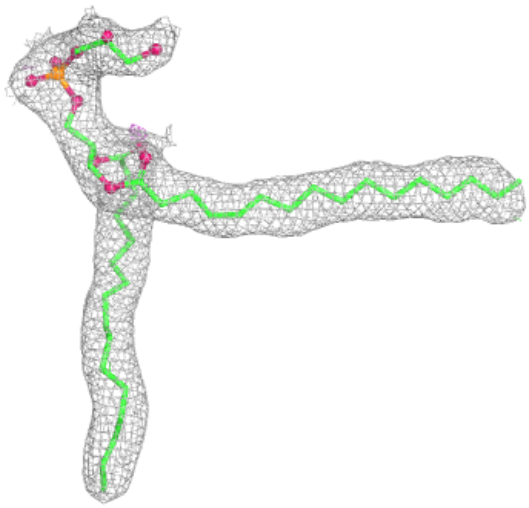


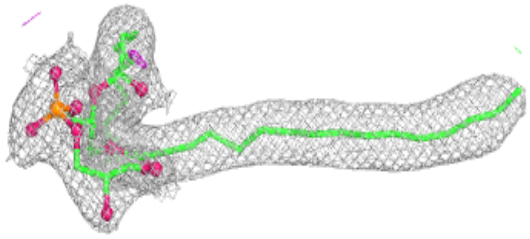


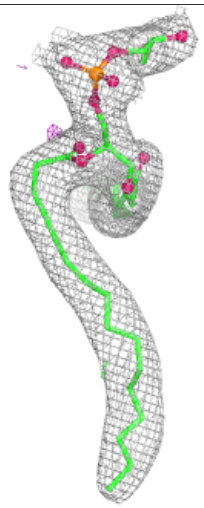


Electron density around LHG L 101 (B):

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

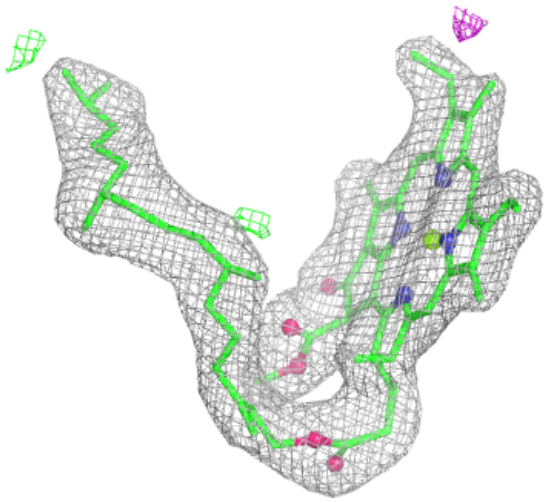


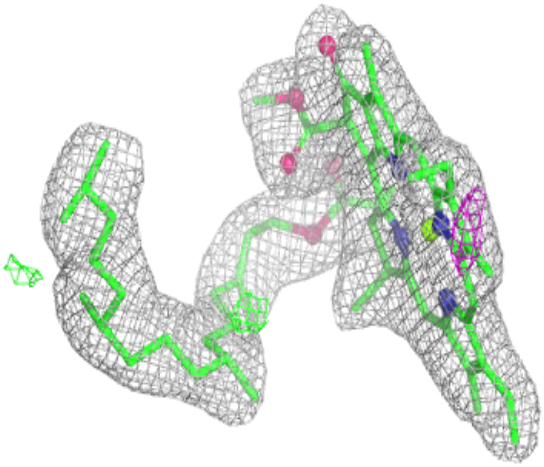


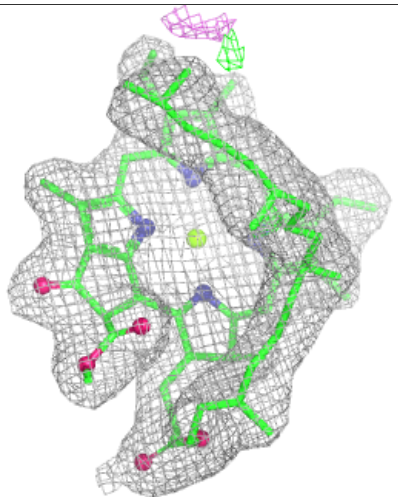


Electron density around CLA b 613:

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

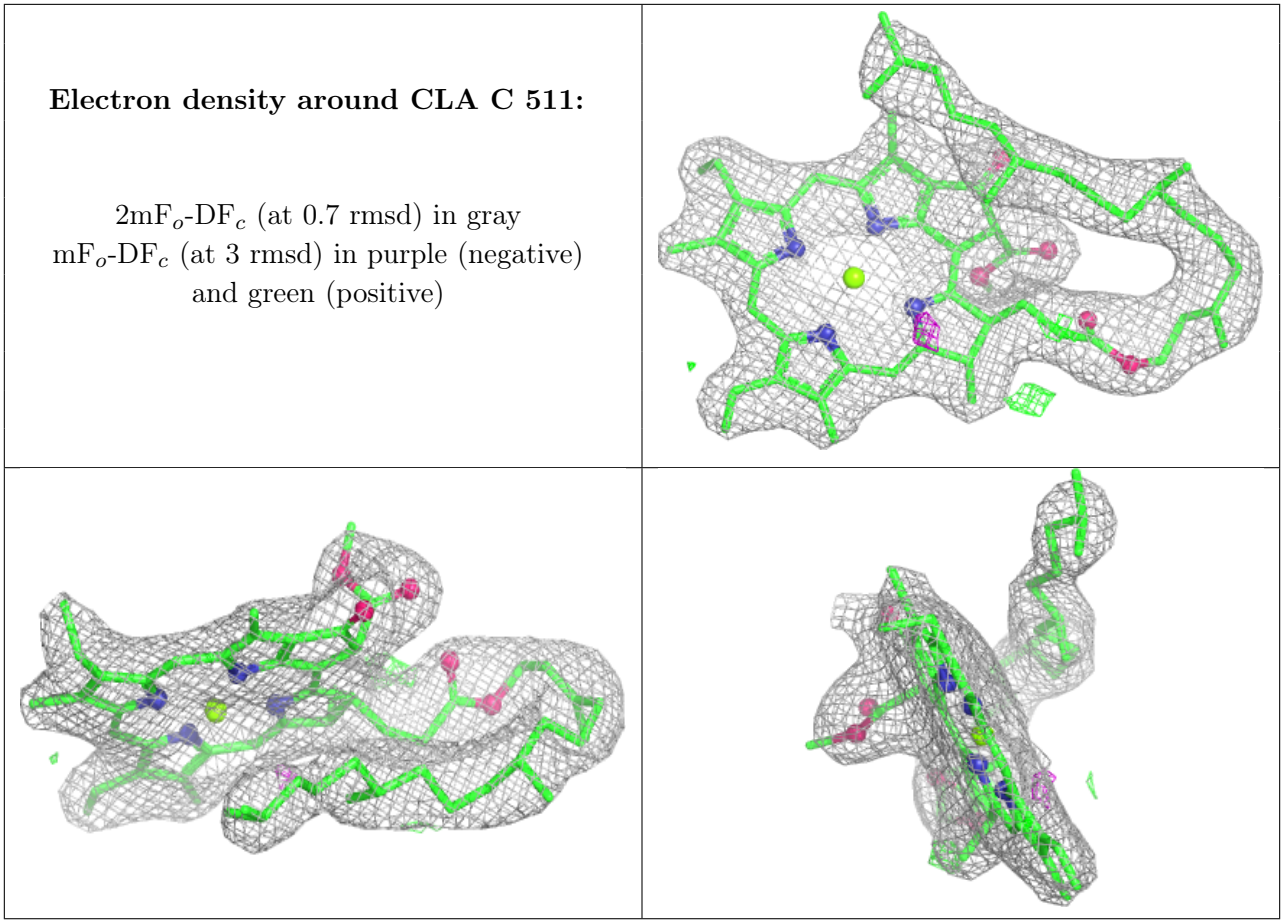






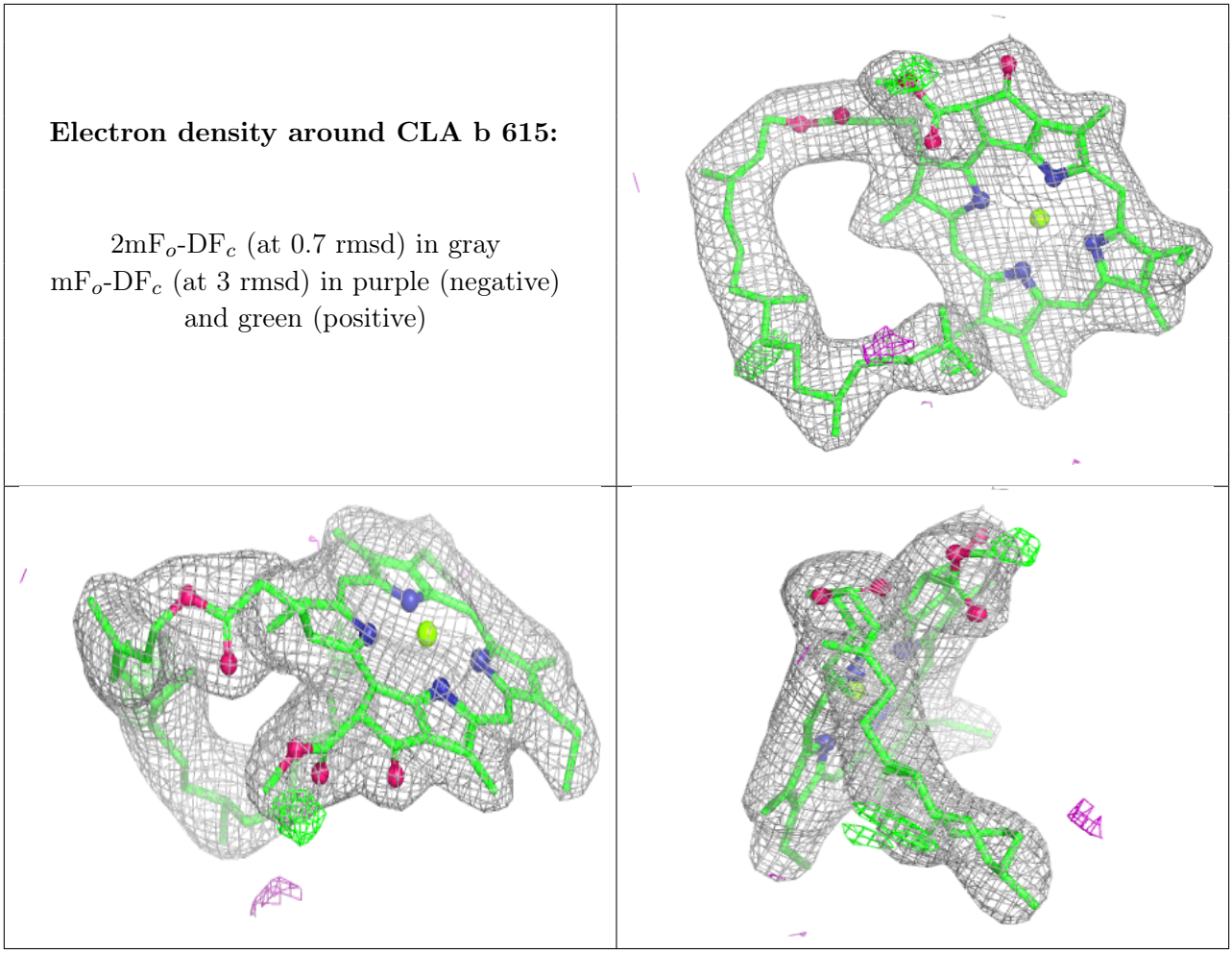
Electron density around CLA C 511:

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



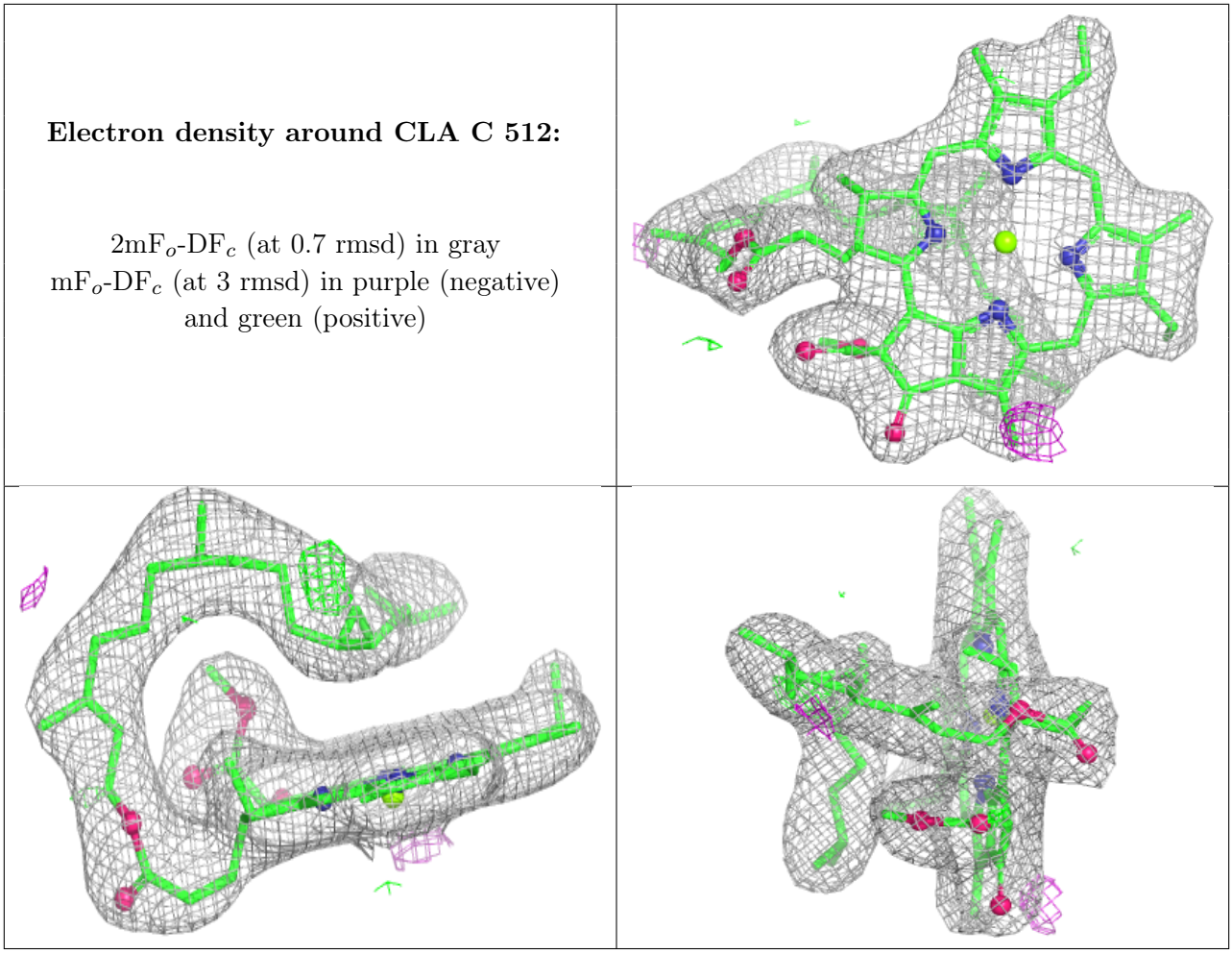
Electron density around CLA b 615:

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



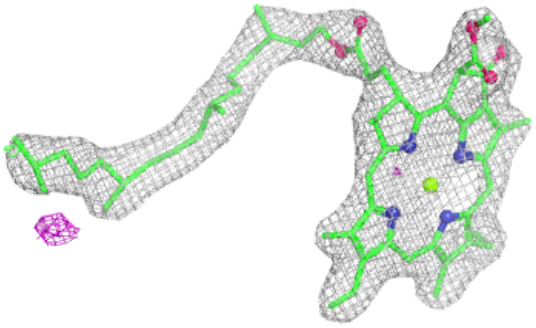
Electron density around CLA C 512:

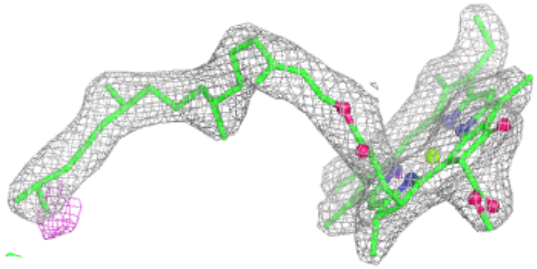
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

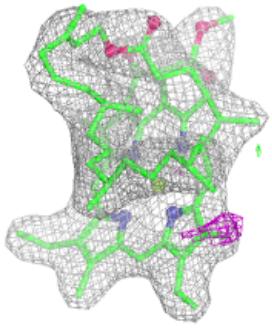


Electron density around CLA C 513:

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

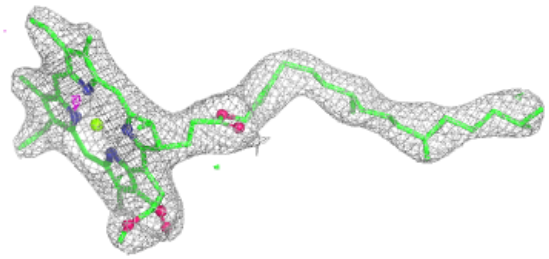


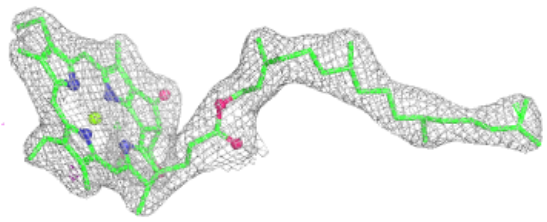


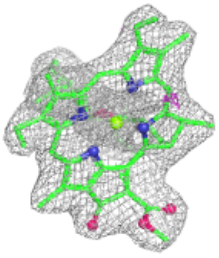


Electron density around CLA c 503:

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

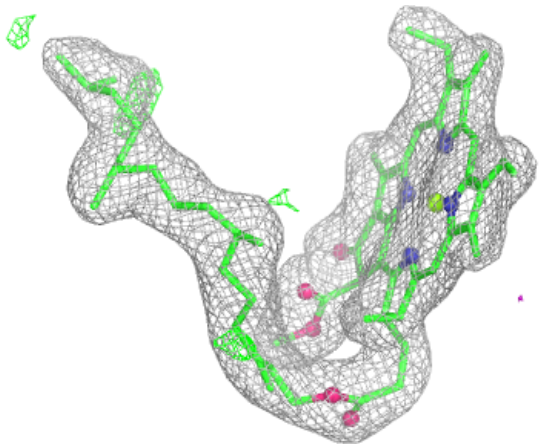


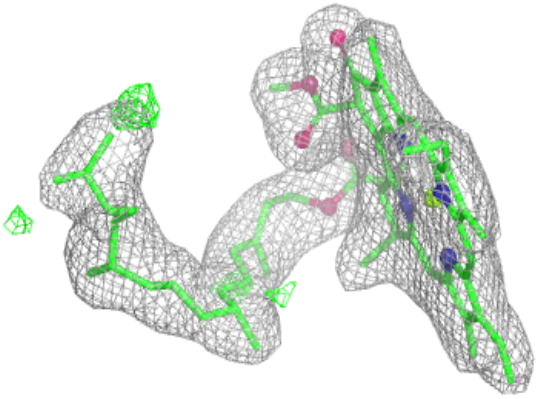


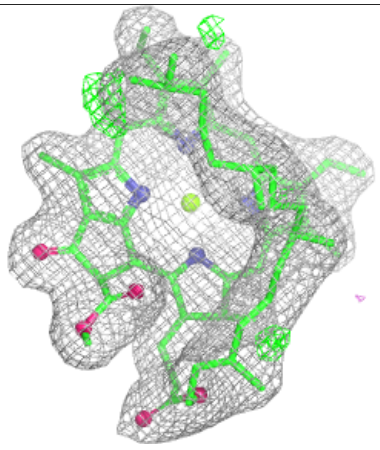


Electron density around CLA B 613:

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

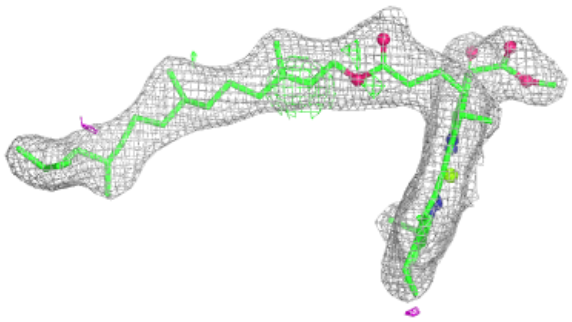


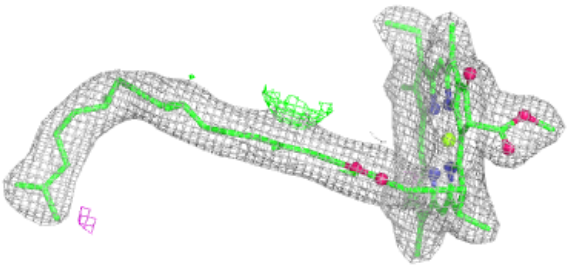


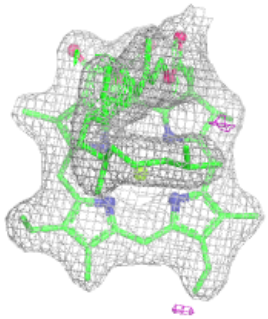


Electron density around CLA B 605:

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

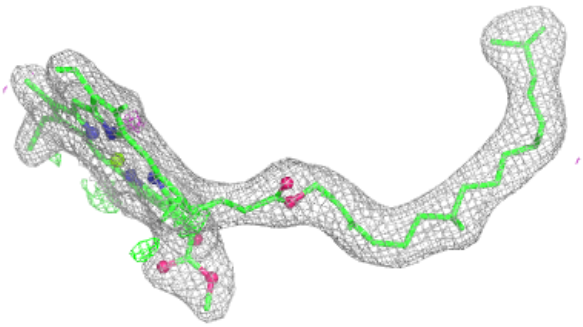


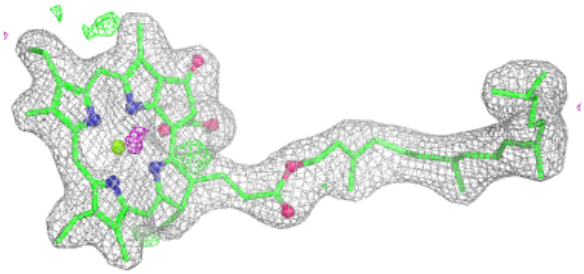


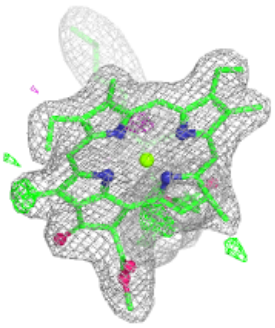


Electron density around CLA D 404 (A):

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

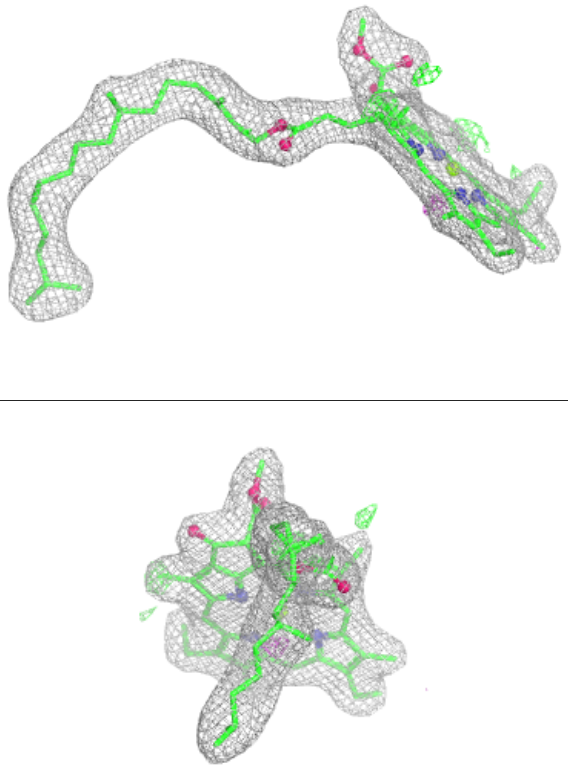


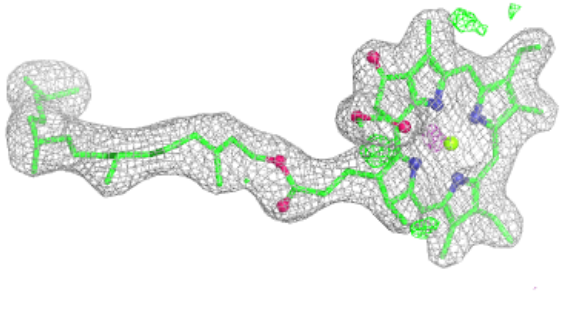




Electron density around CLA D 404 (B):

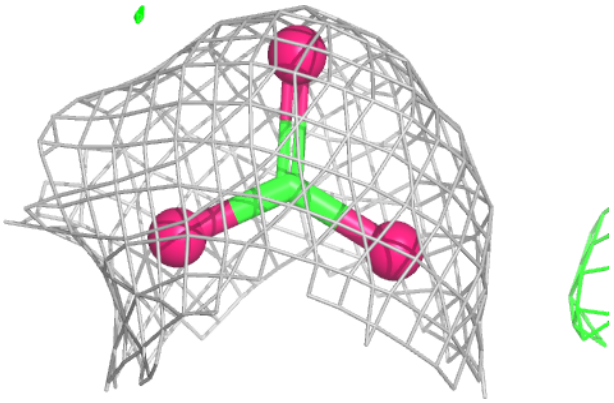
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

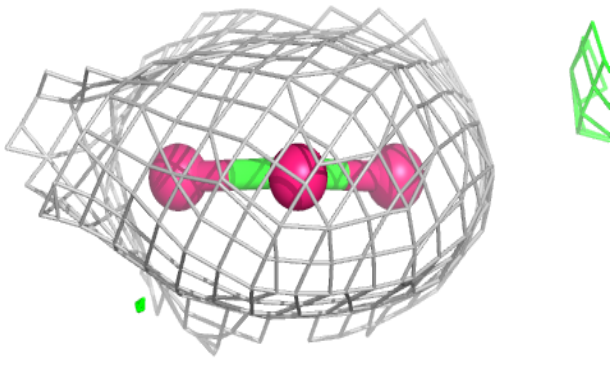


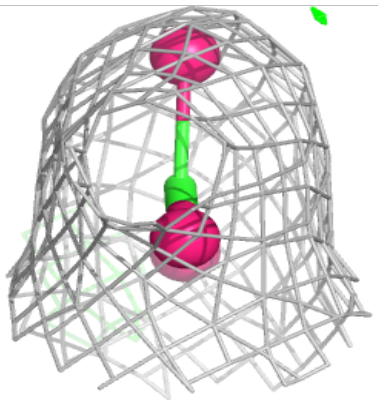


Electron density around BCT a 404 (A):

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

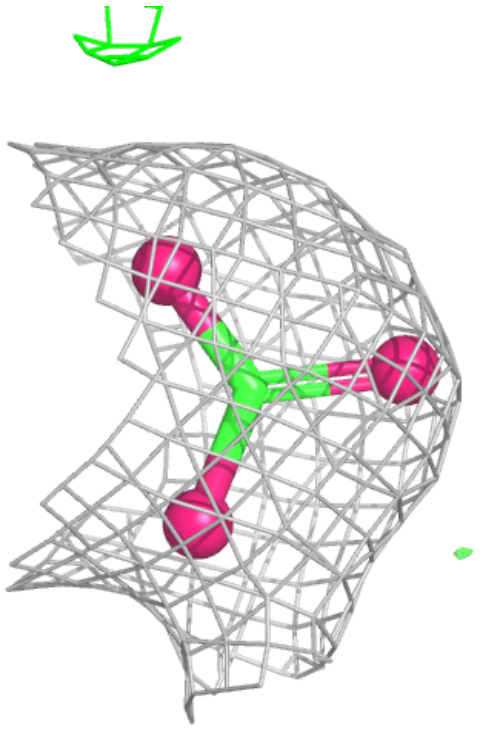


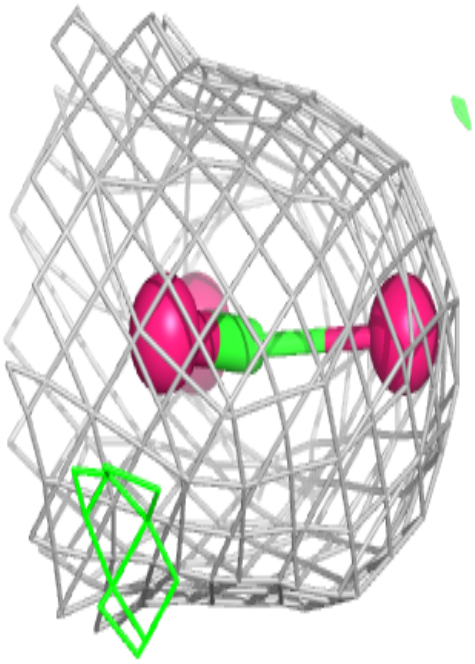


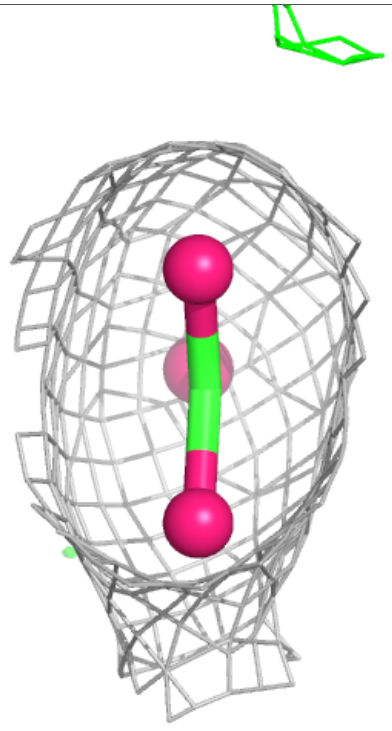


Electron density around BCT a 404 (B):

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

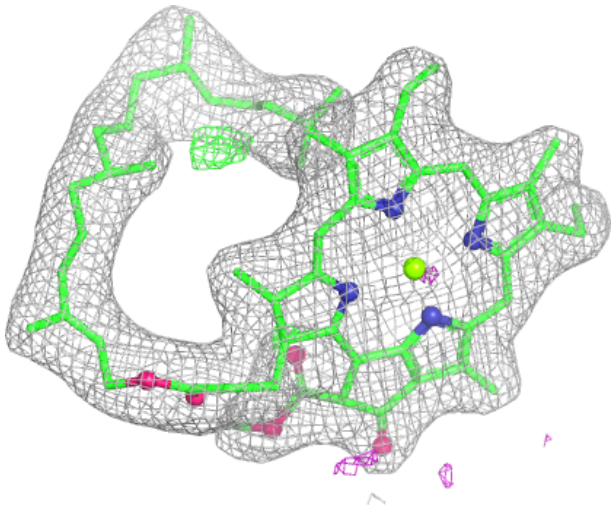


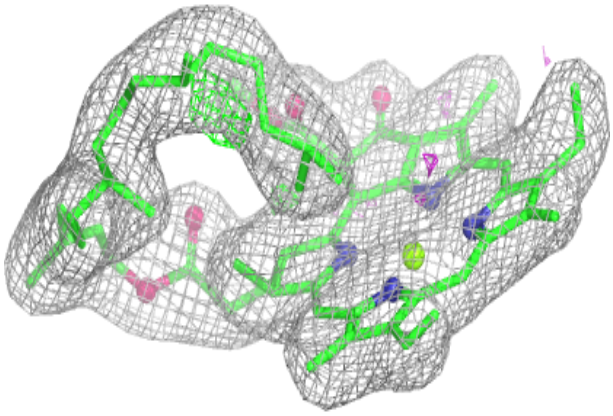


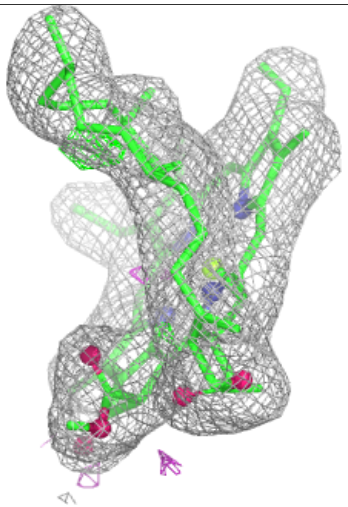


Electron density around CLA B 615:

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

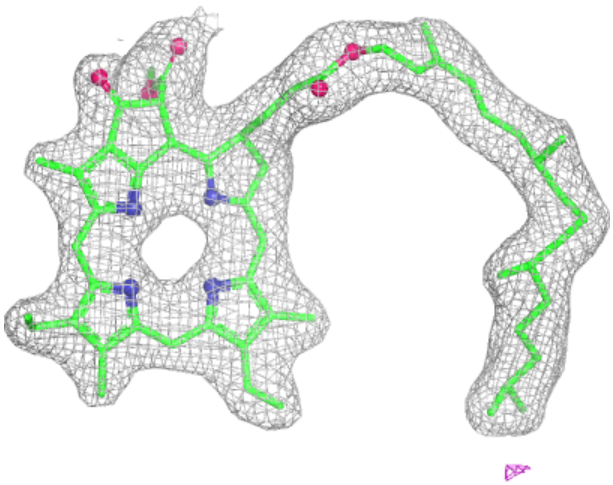


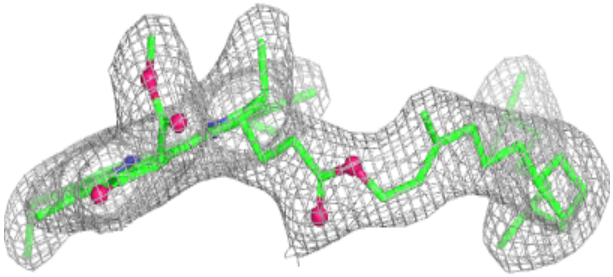


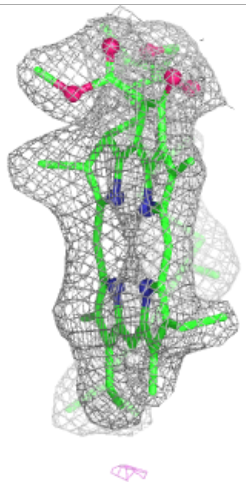


Electron density around PHO D 401 (A):

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

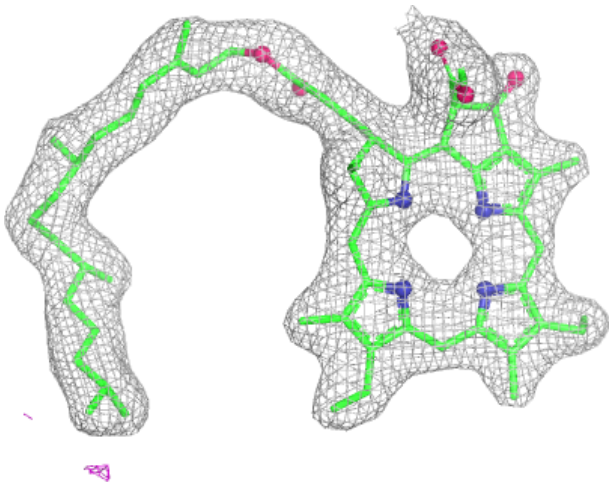


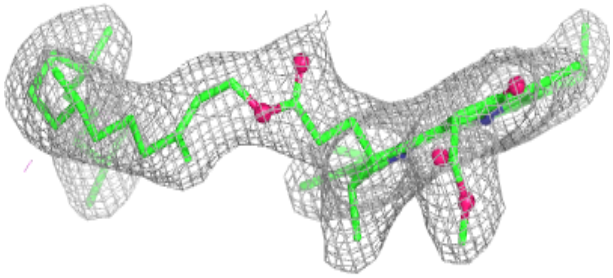


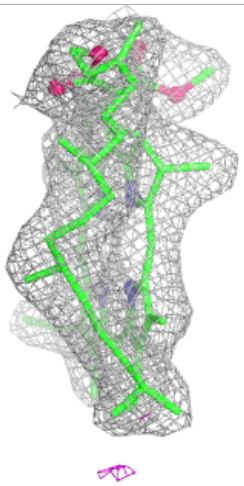


Electron density around PHO D 401 (B):

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

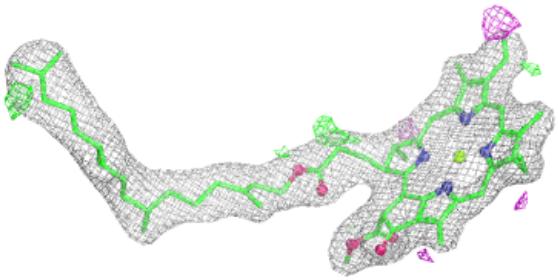


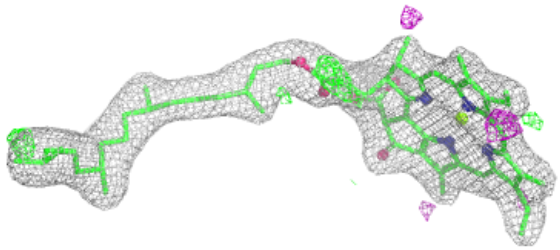


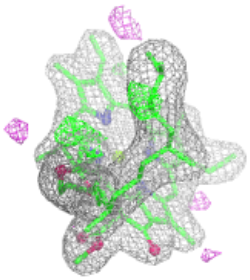


Electron density around CLA a 405 (A):

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

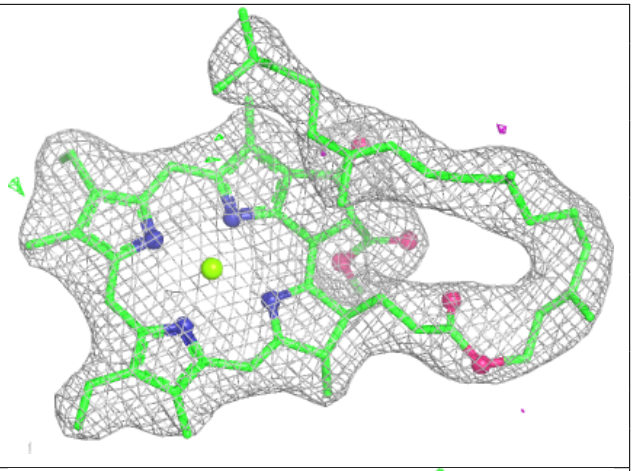


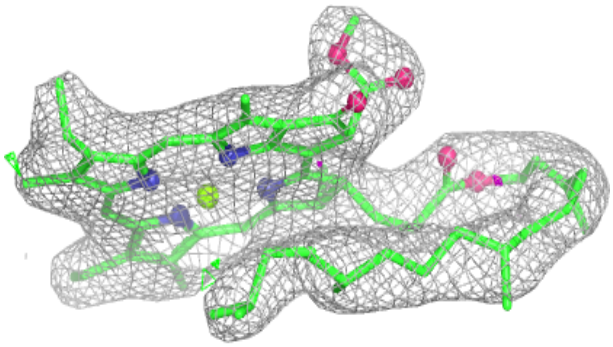


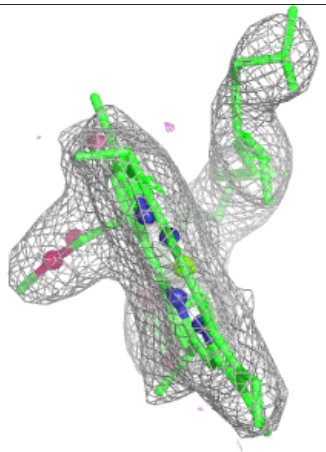


Electron density around CLA c 510:

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

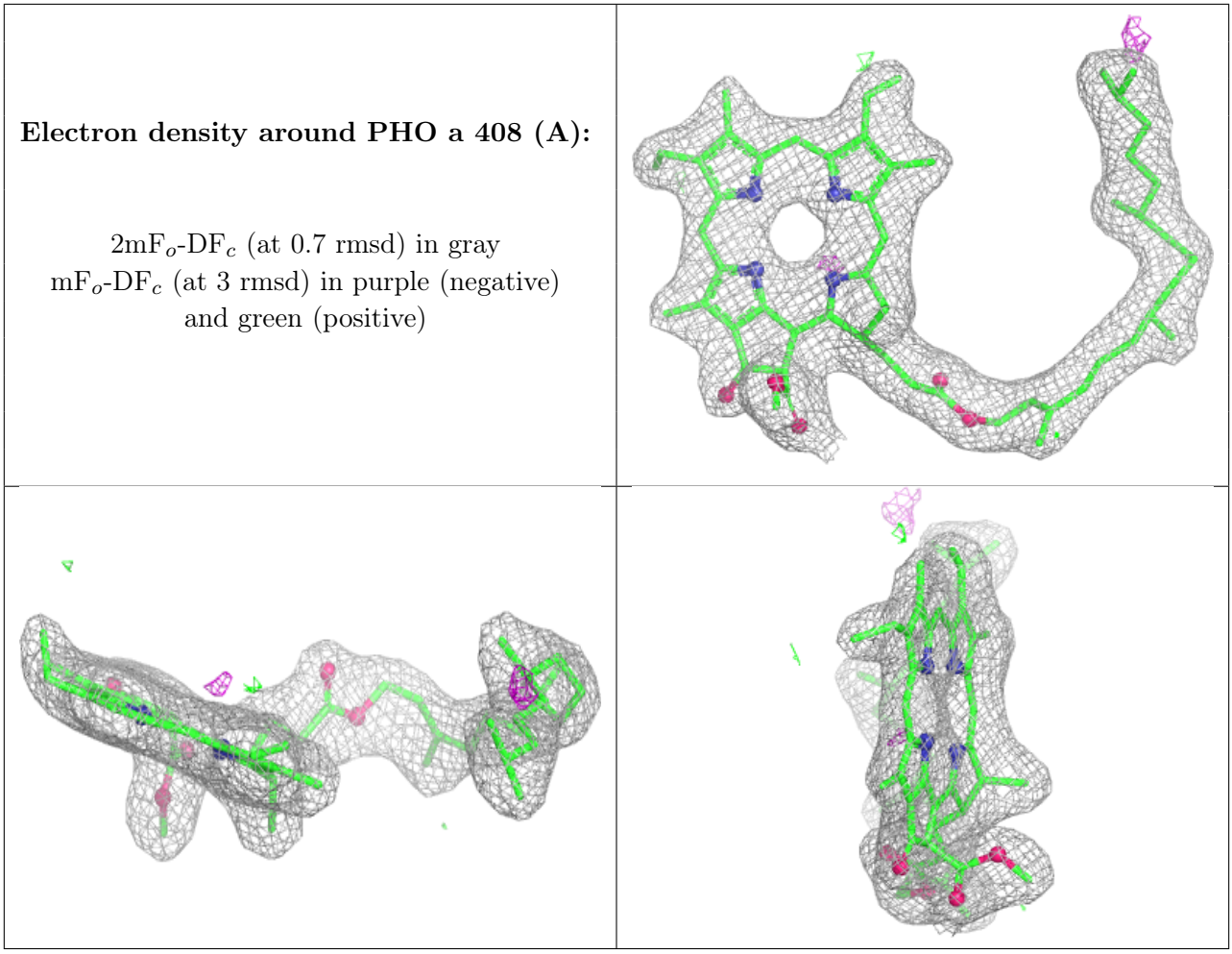






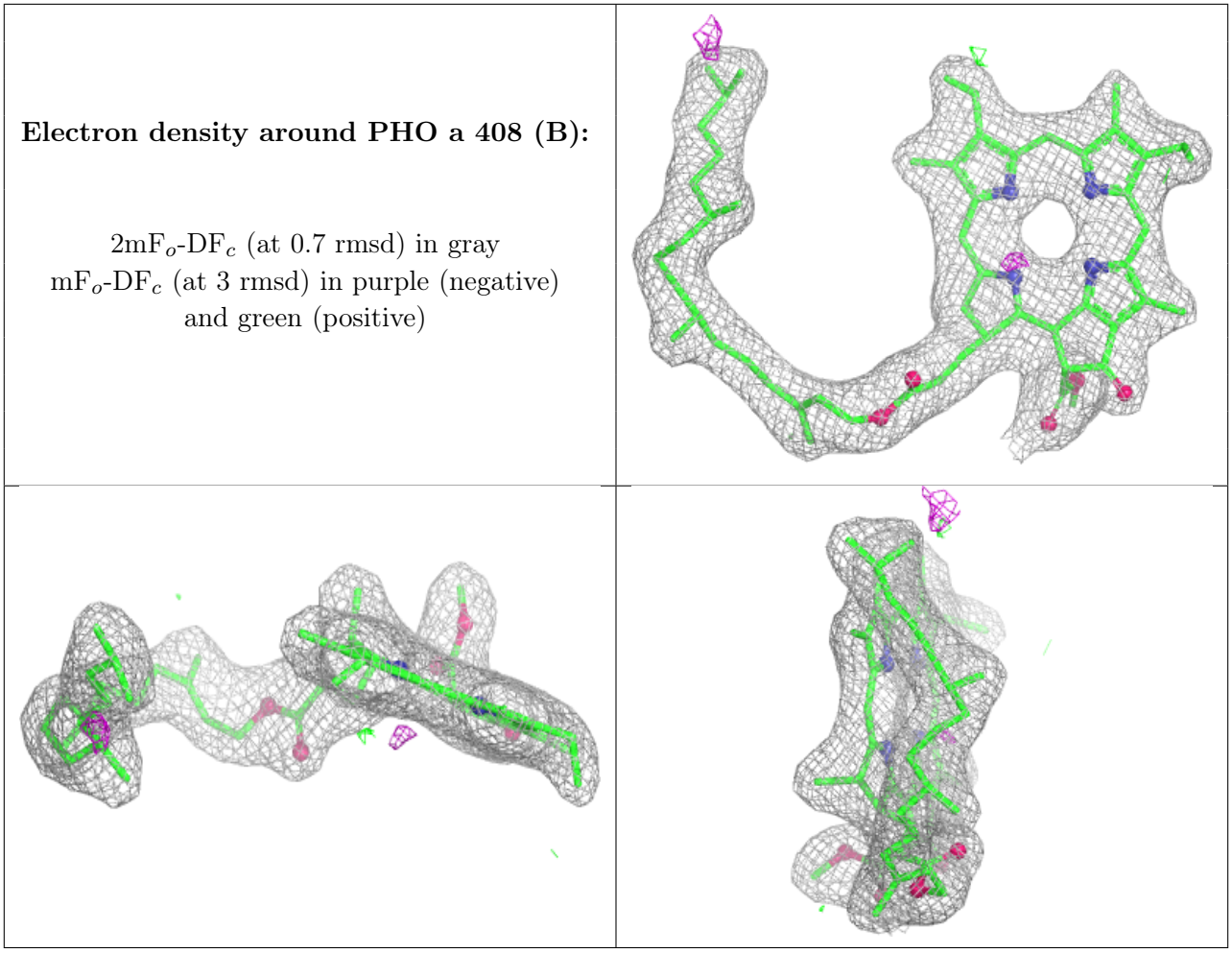
Electron density around PHO a 408 (A):

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



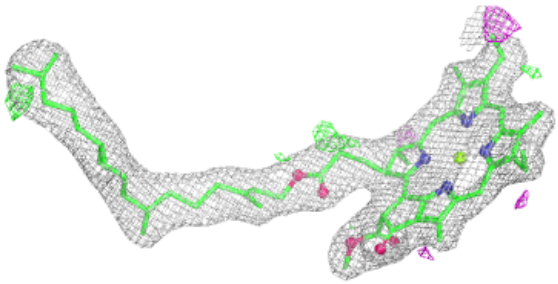
Electron density around PHO a 408 (B):

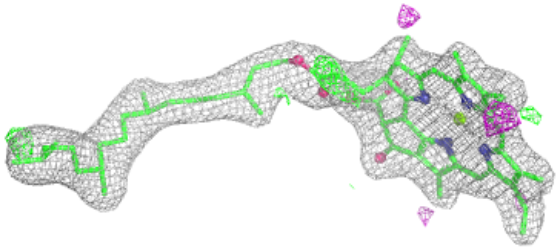
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

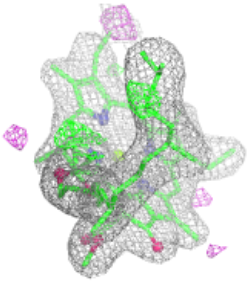


Electron density around CLA a 405 (B):

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

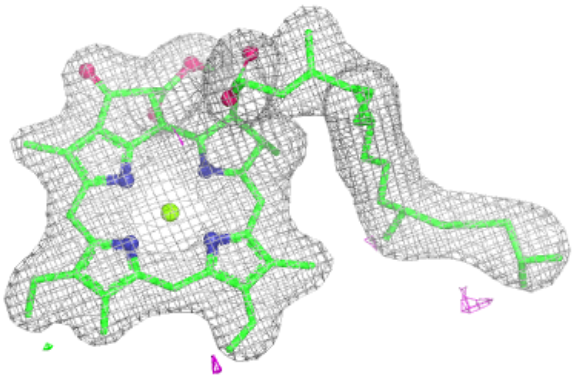


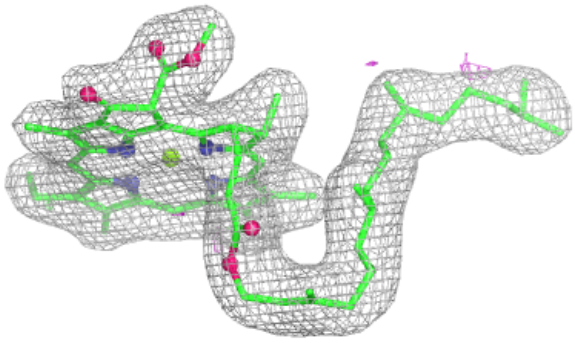




Electron density around CLA a 406 (A):

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

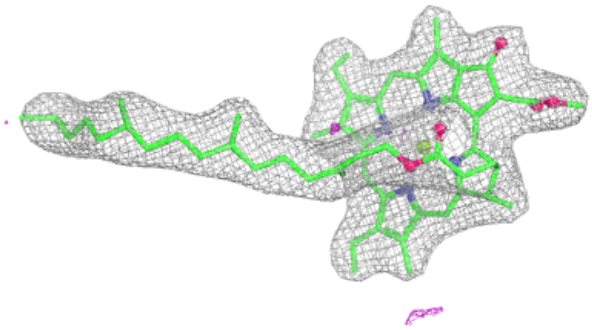


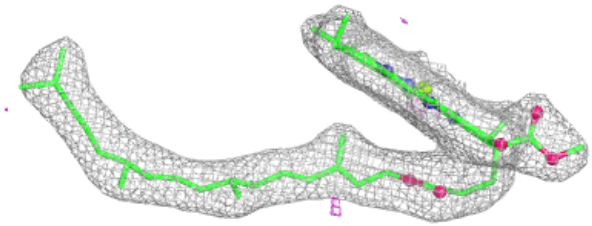


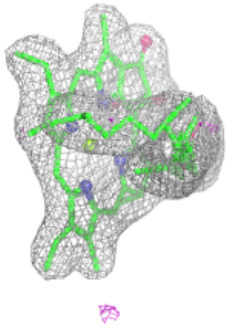


Electron density around CLA B 608:

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

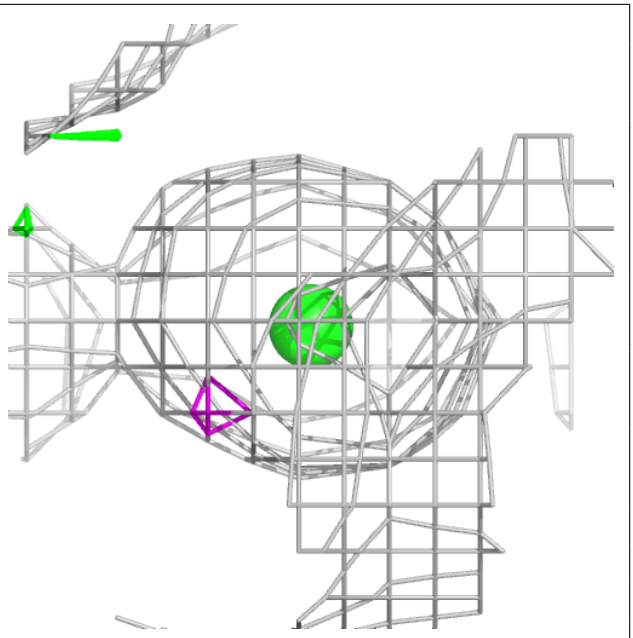


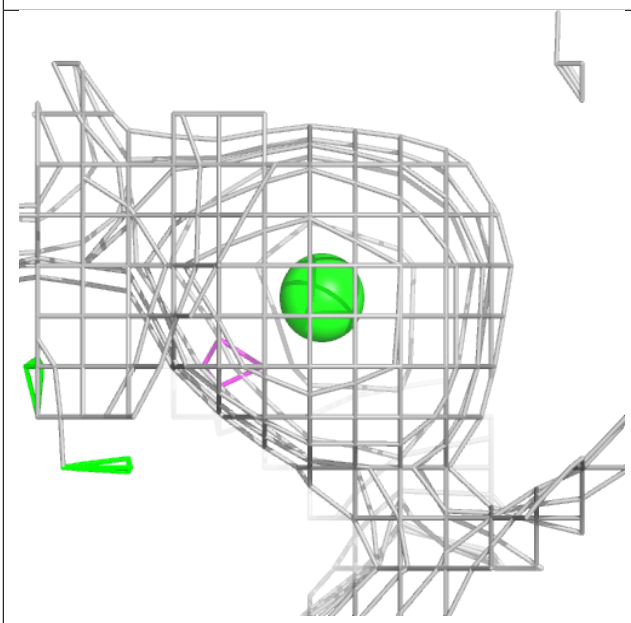


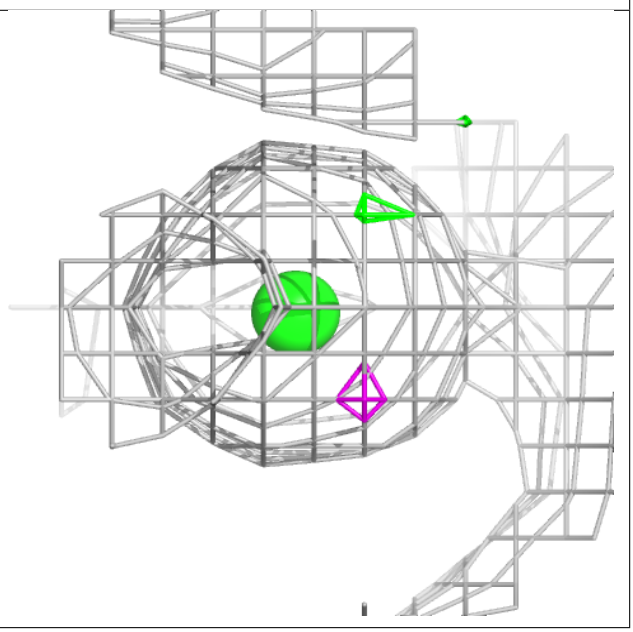


Electron density around CL a 403 (A):

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

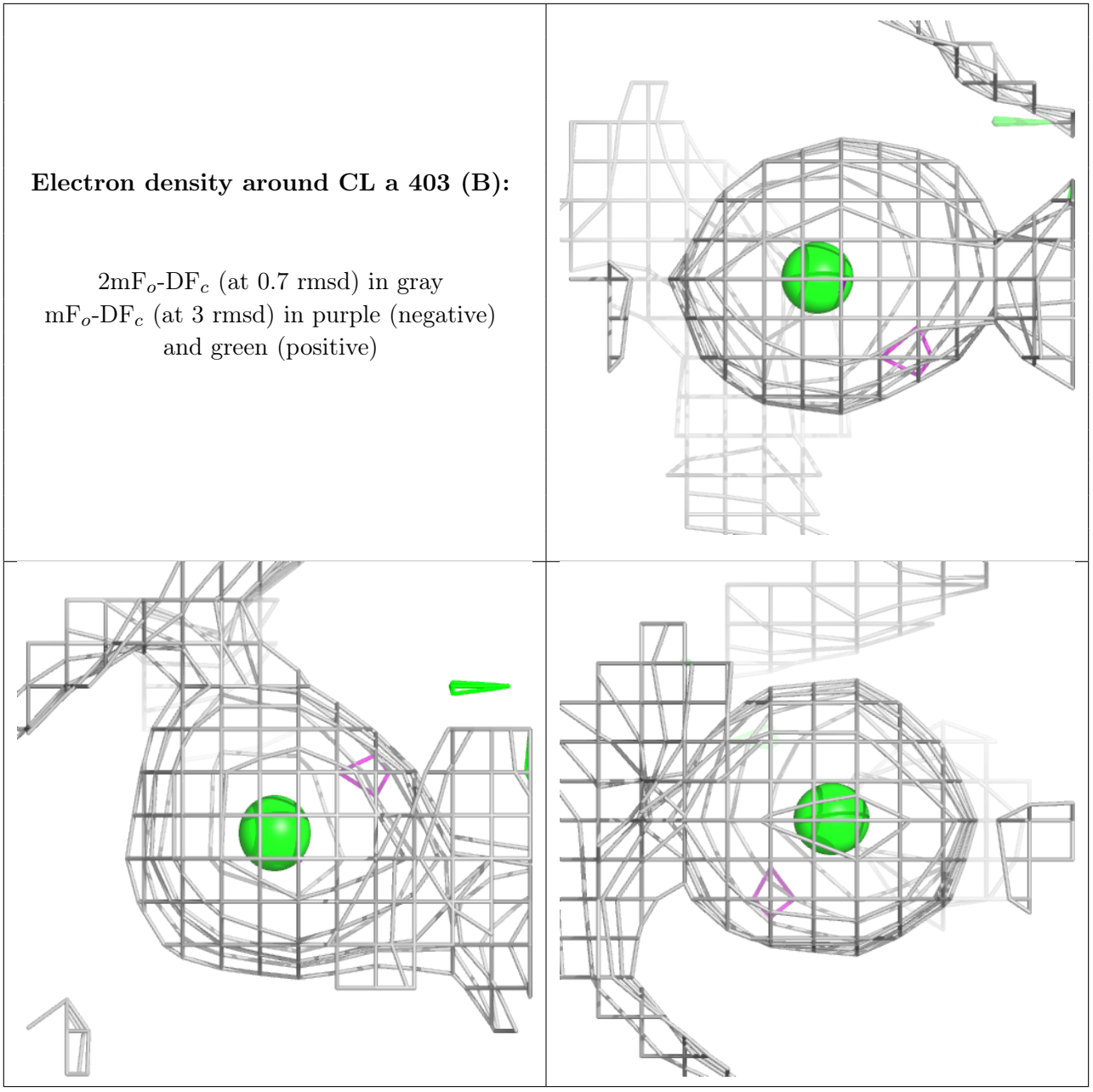






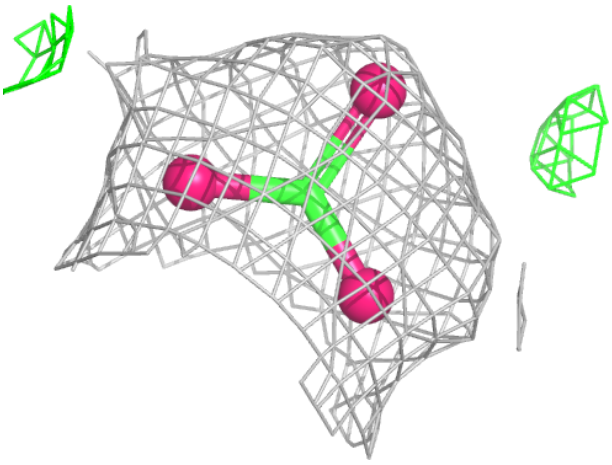
Electron density around CL a 403 (B):

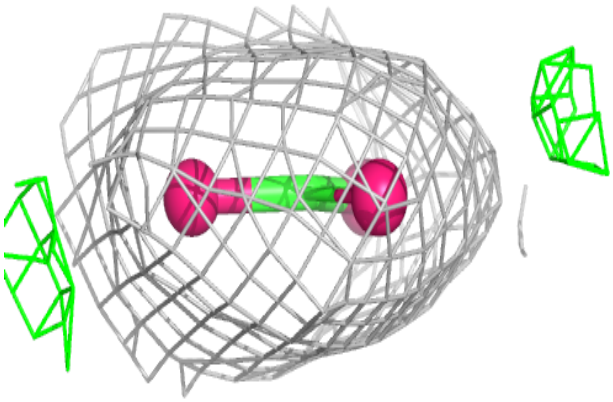
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

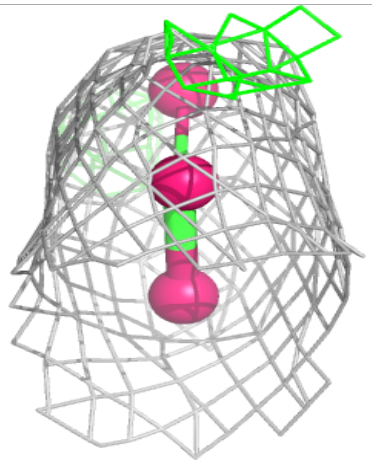


Electron density around BCT A 414 (A):

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

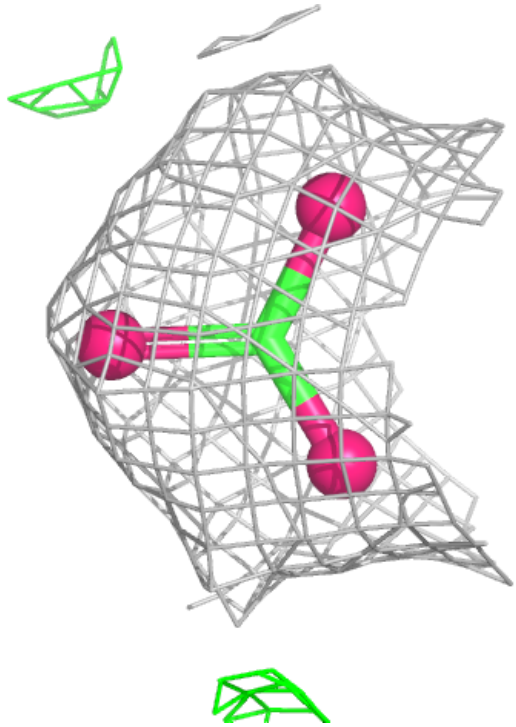


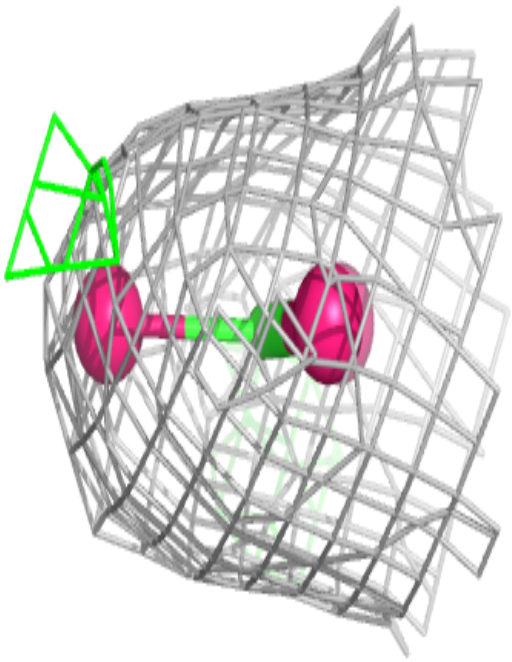


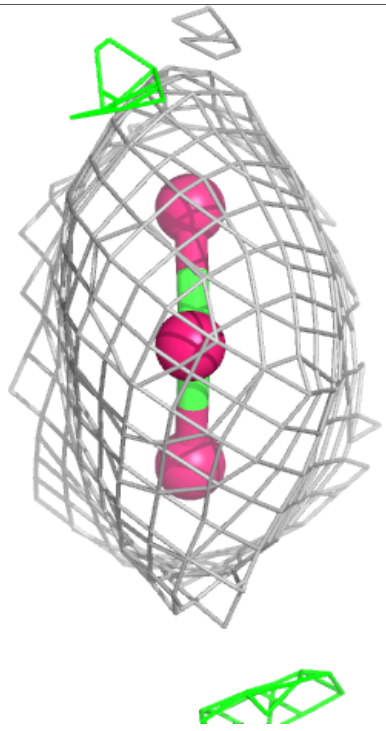


Electron density around BCT A 414 (B):

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

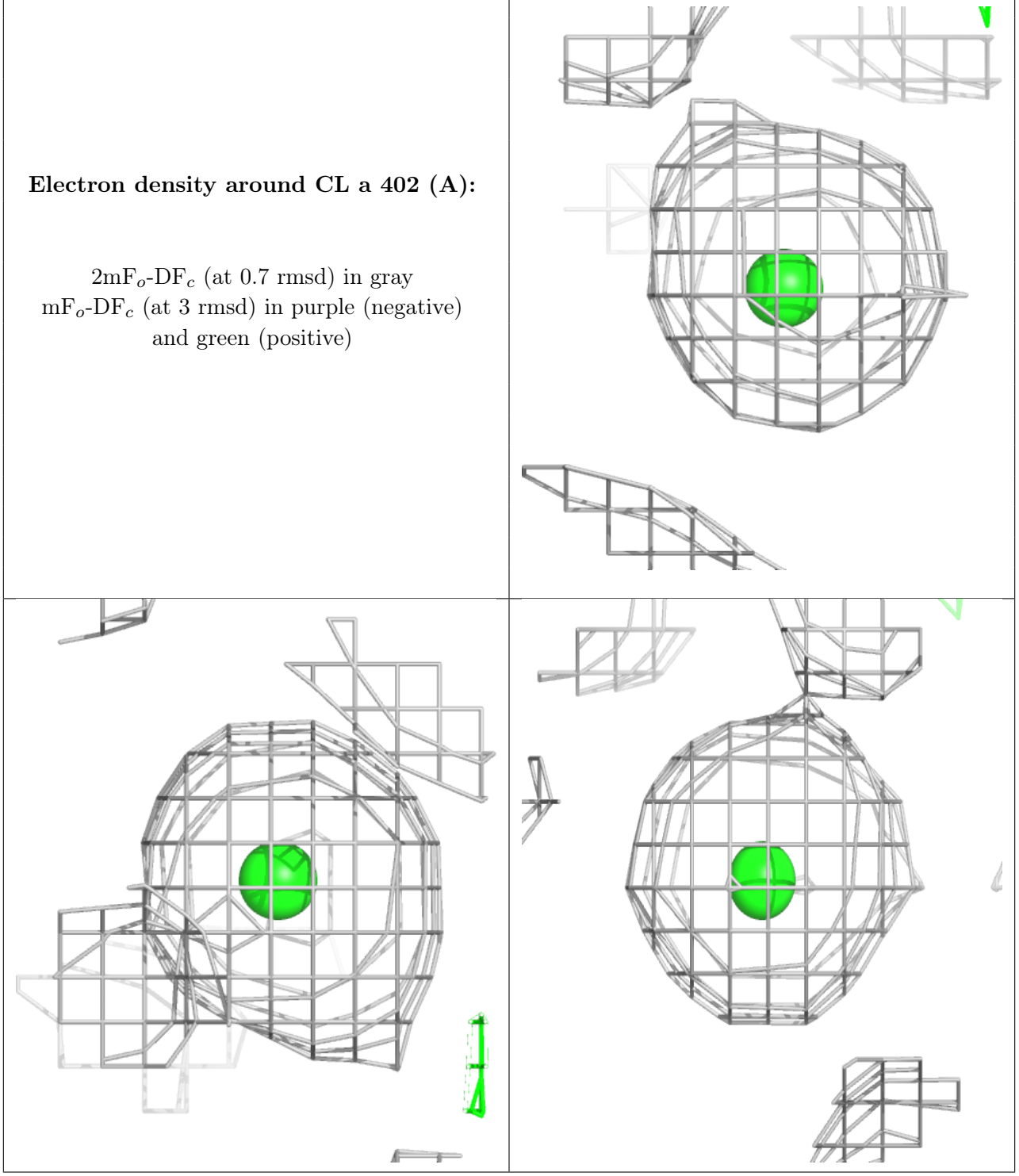






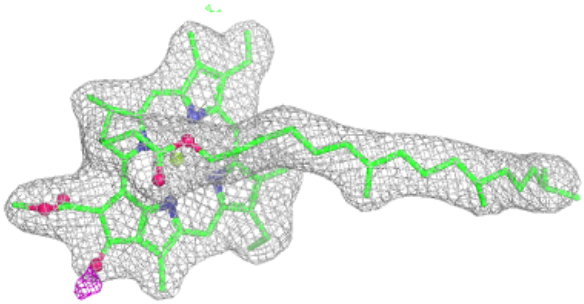
Electron density around CL a 402 (A):

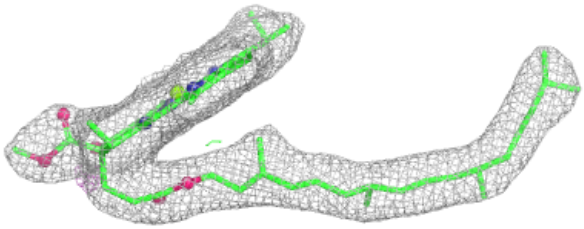
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

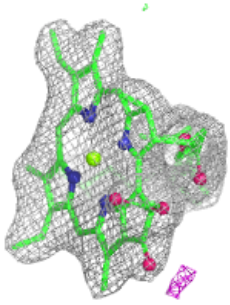


Electron density around CLA b 608:

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

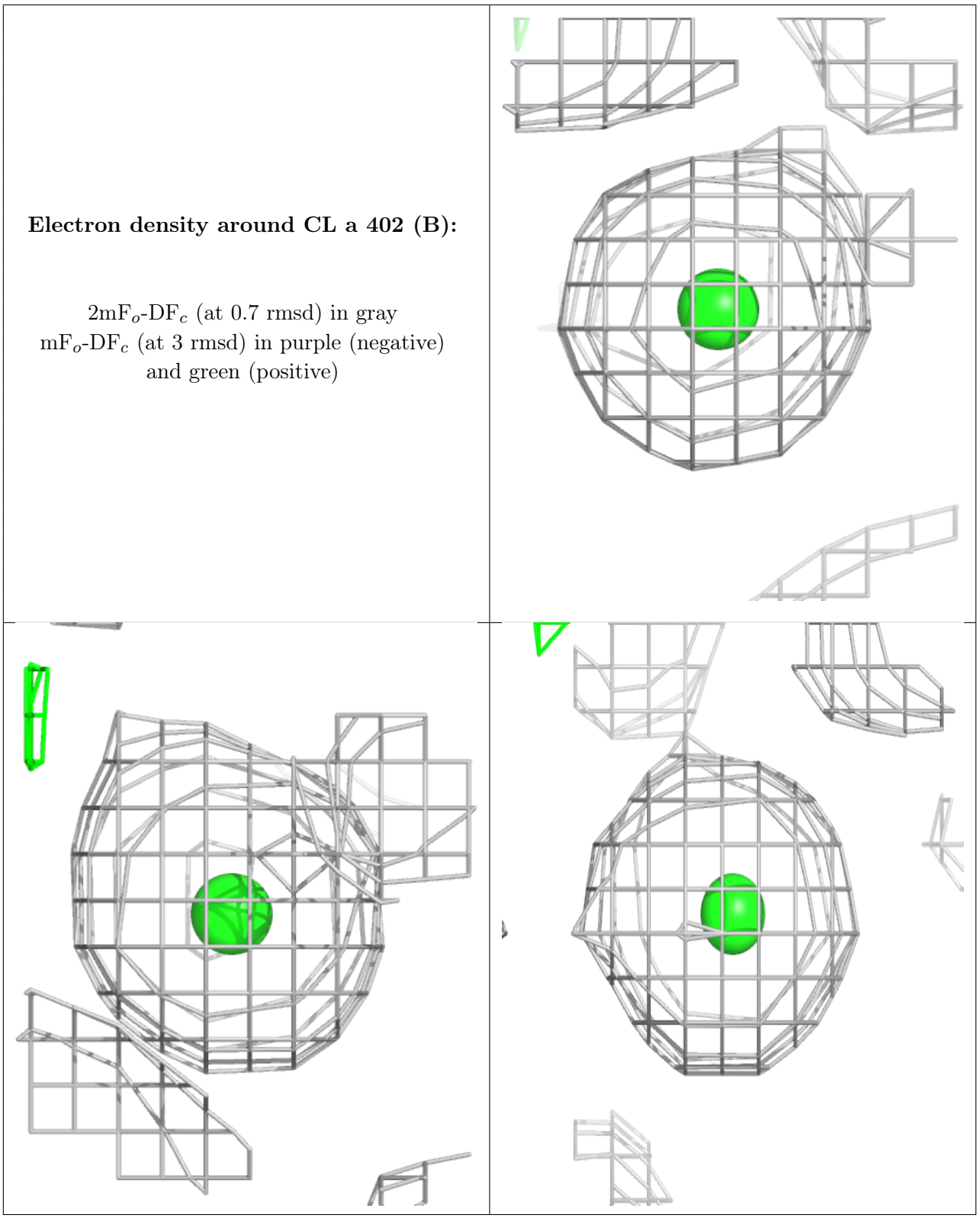






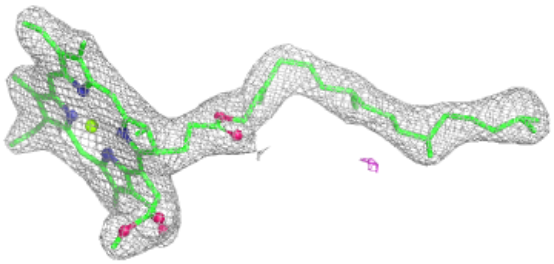
Electron density around CL a 402 (B):

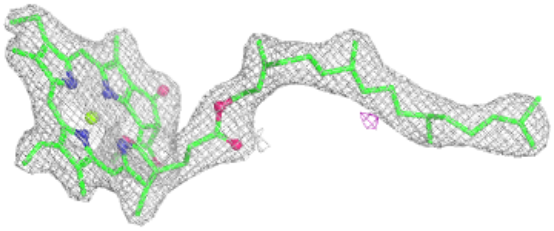
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

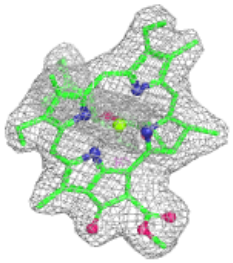


Electron density around CLA C 504:

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

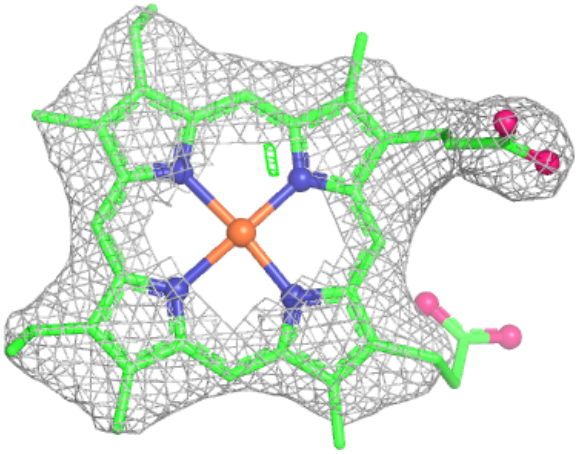


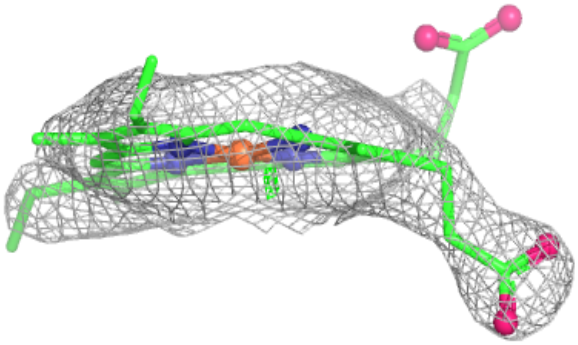


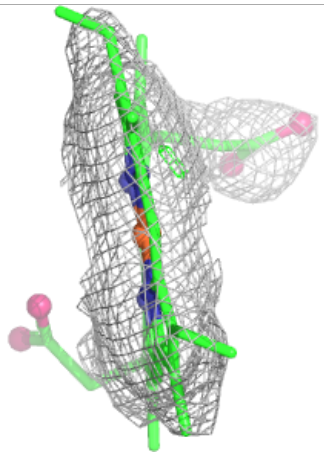


Electron density around HEM f 101:

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

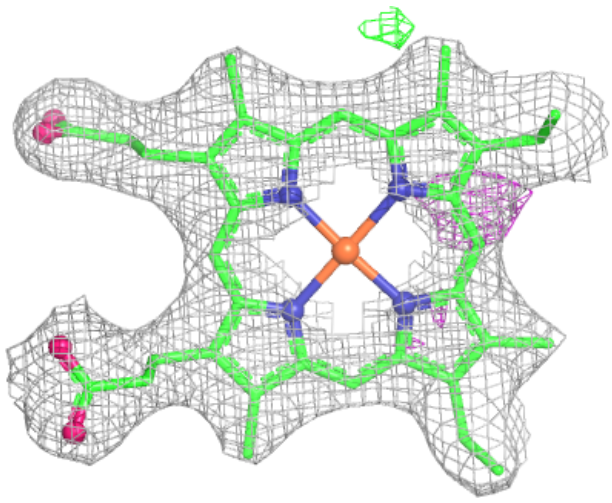


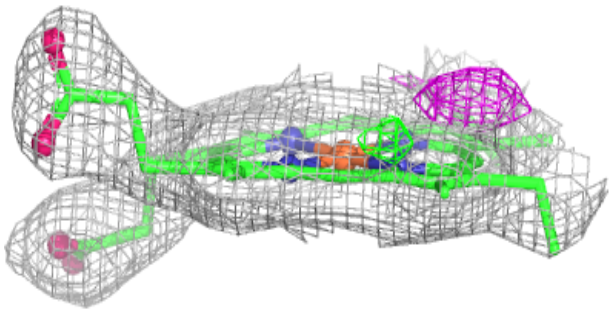




Electron density around HEC v 201:

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

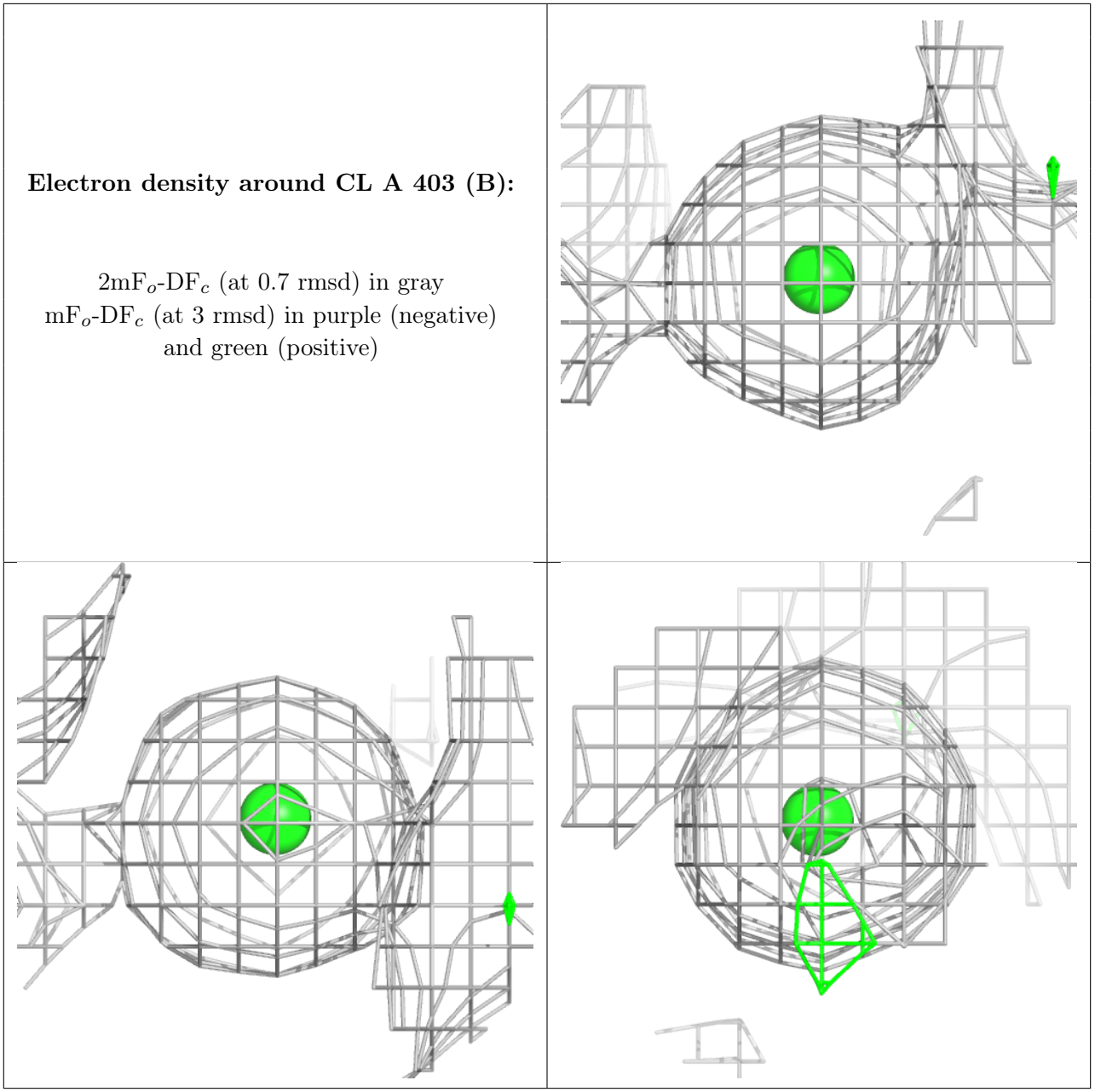






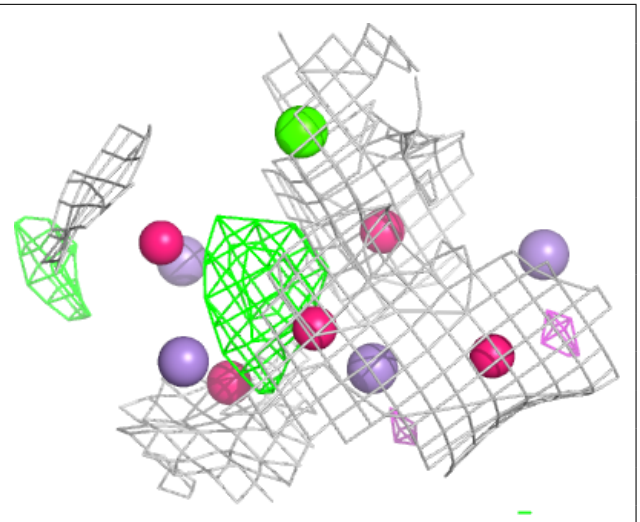
Electron density around CL A 403 (B):

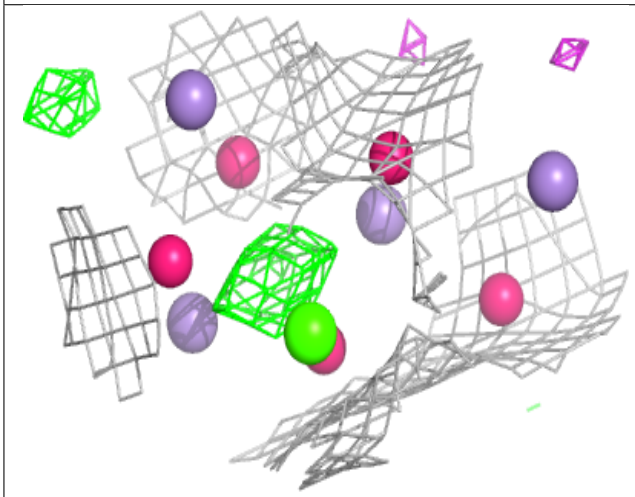
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

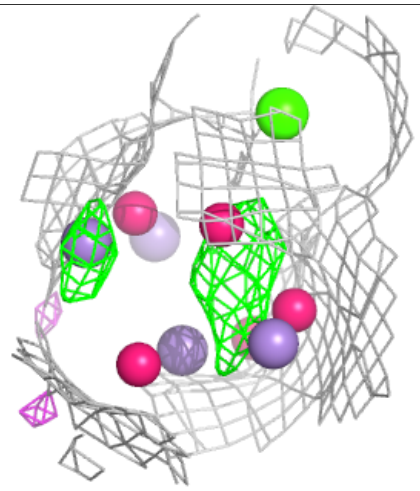


Electron density around OEX A 411 (A):

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

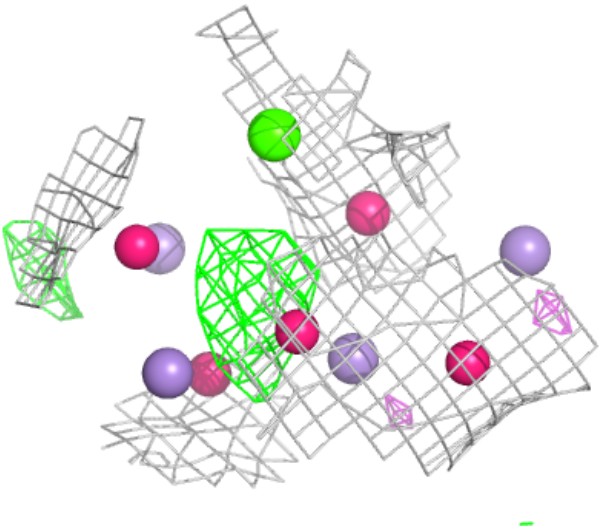


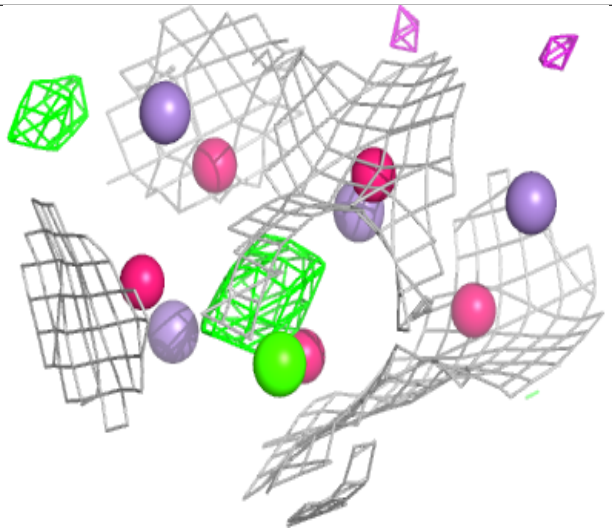


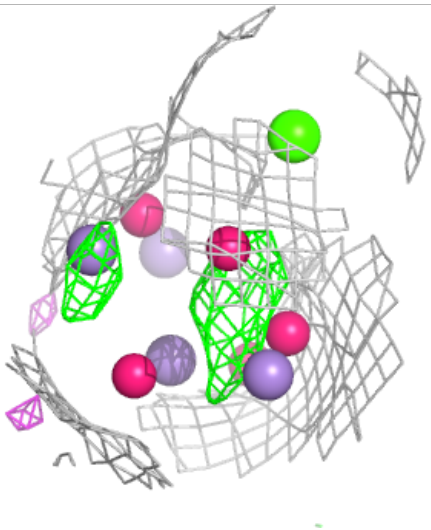


Electron density around OEX A 411 (B):

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

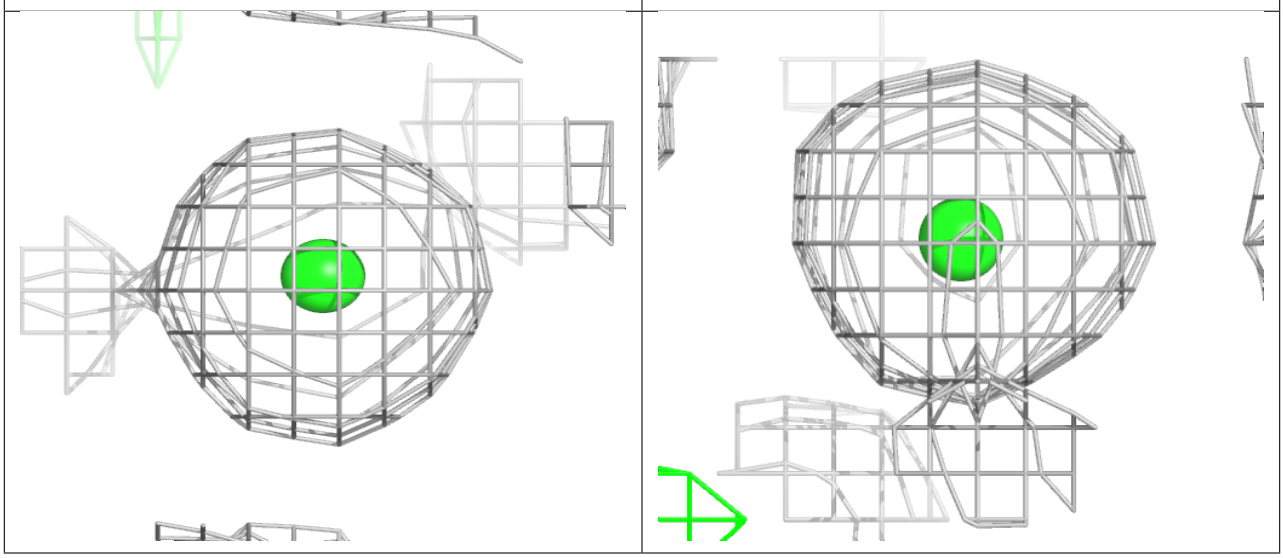






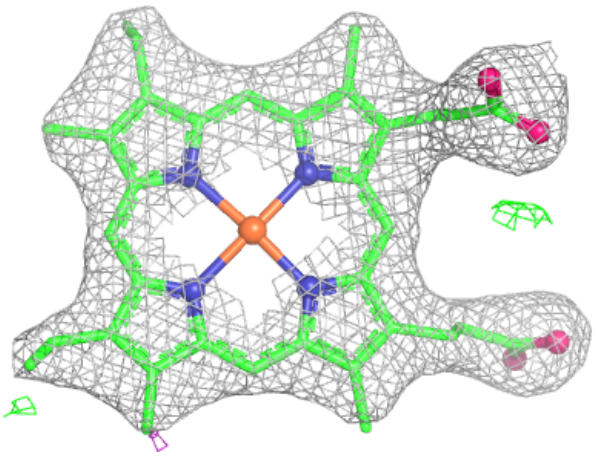
Electron density around CL A 402 (A):

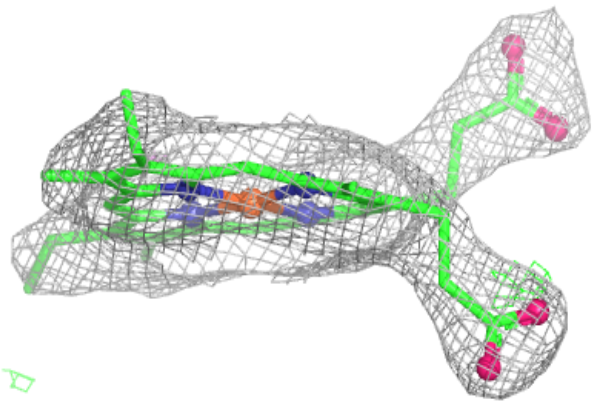
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

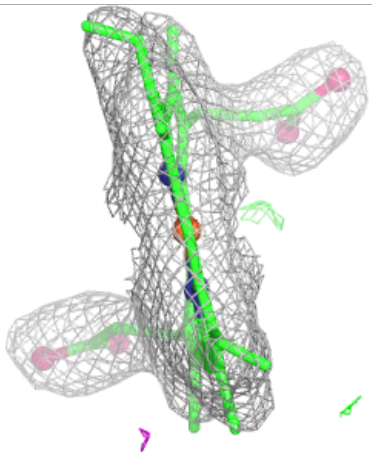


Electron density around HEM F 102:

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

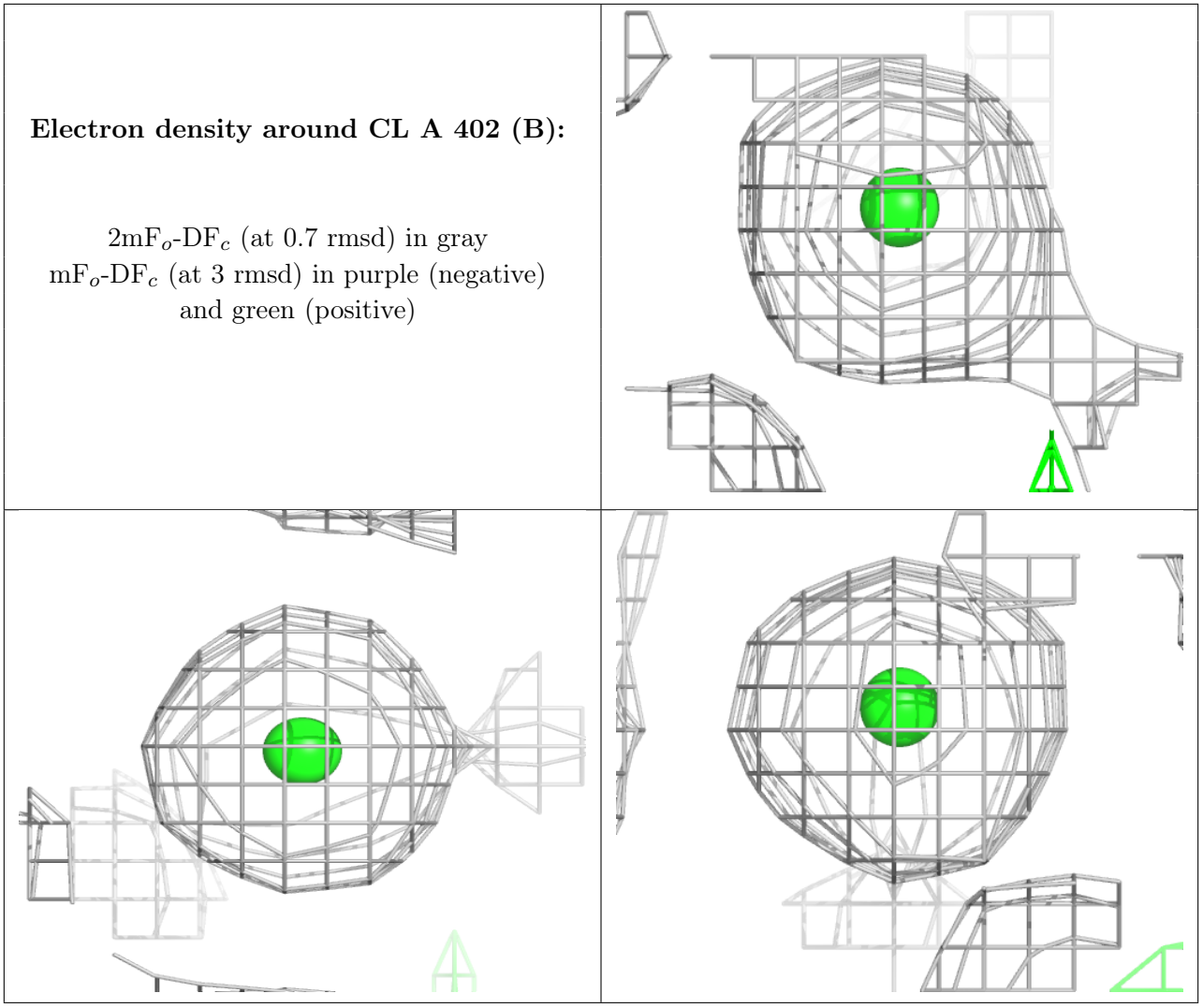






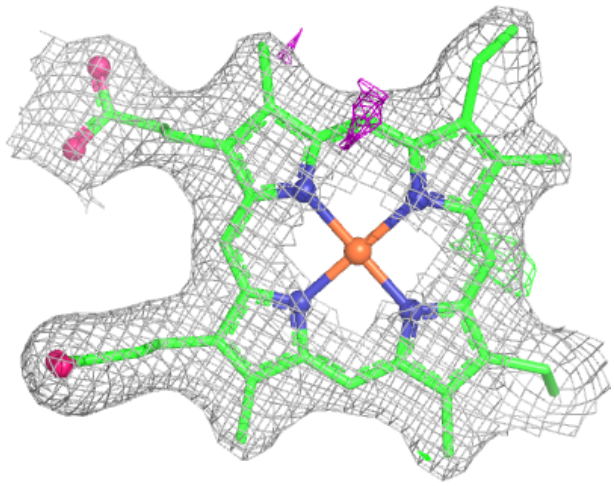
Electron density around CL A 402 (B):

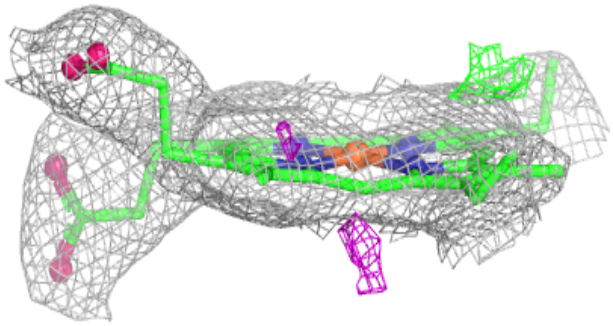
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

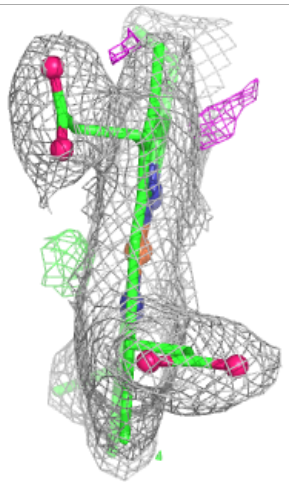


Electron density around HEC V 202:

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

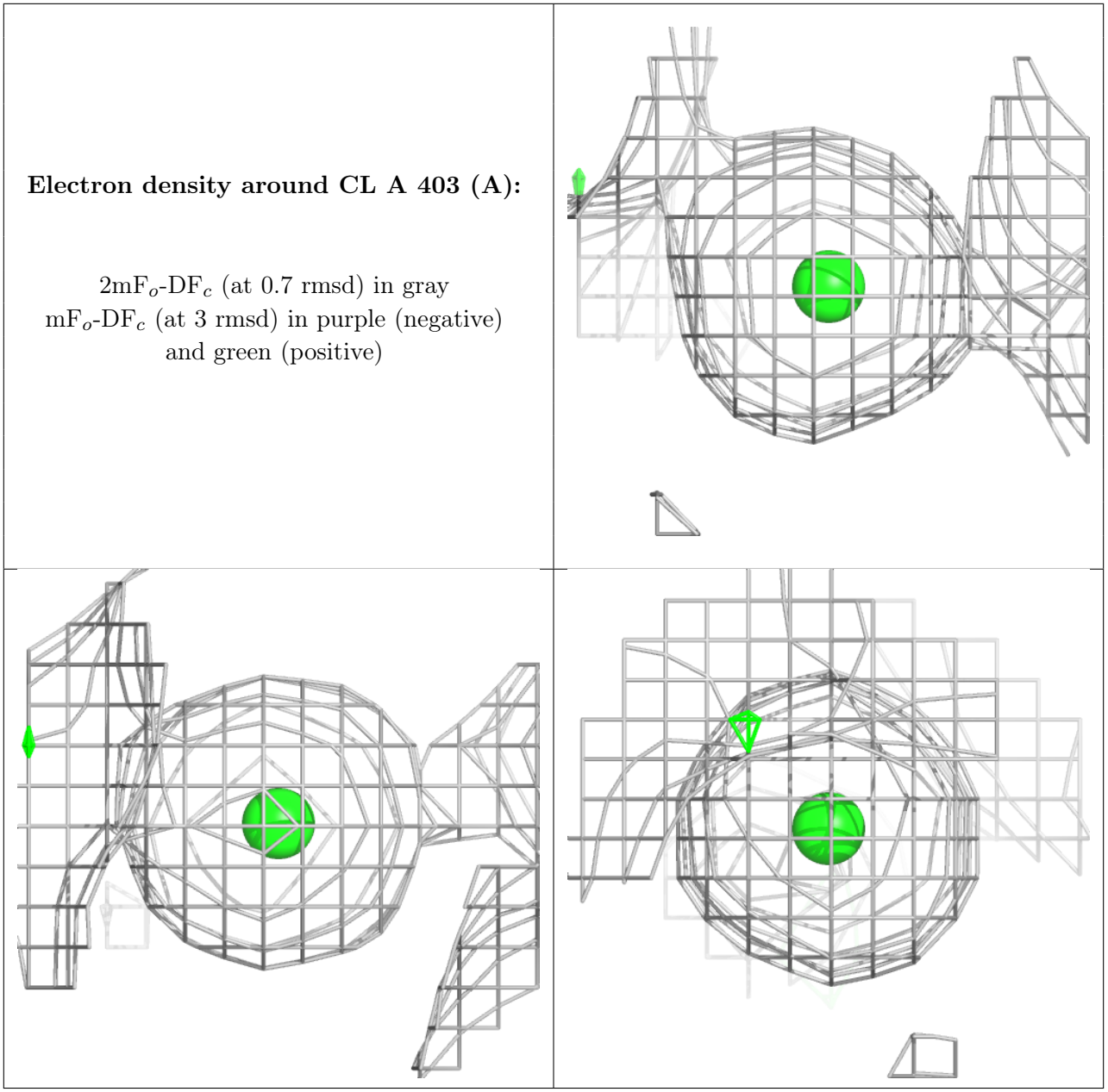






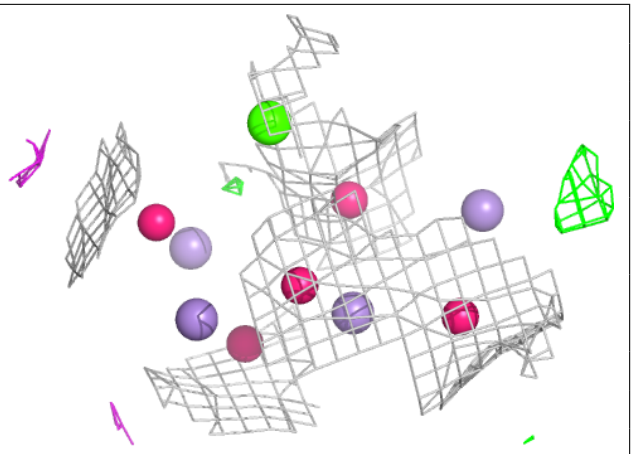
Electron density around CL A 403 (A):

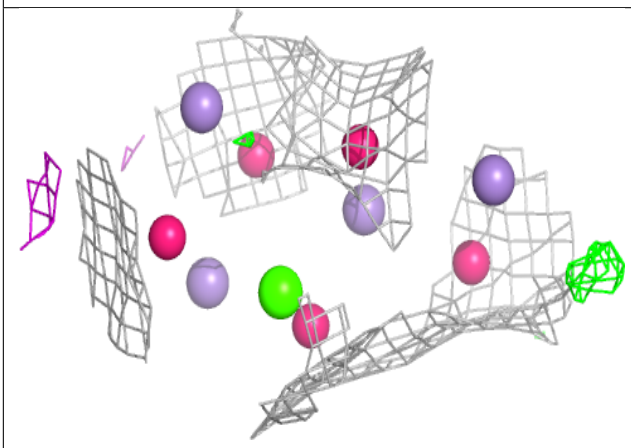
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

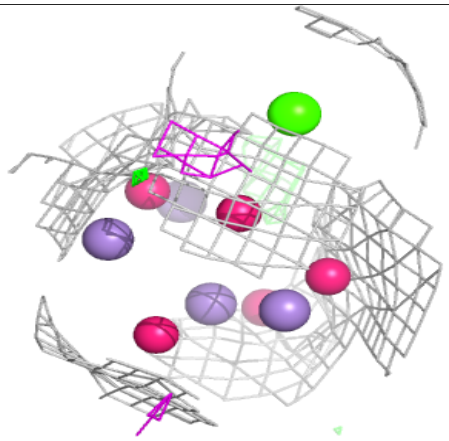


Electron density around OEX a 413 (B):

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

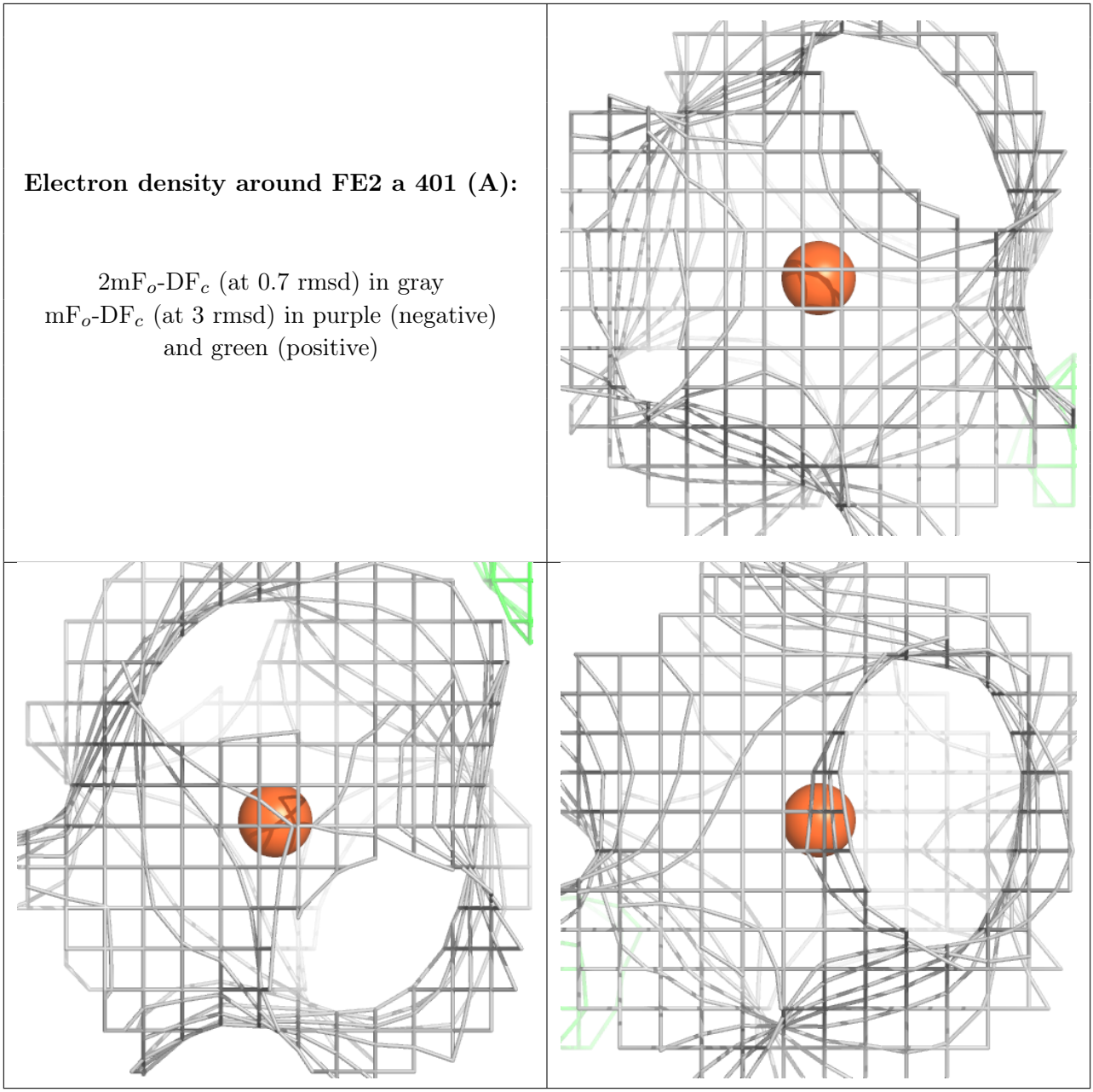






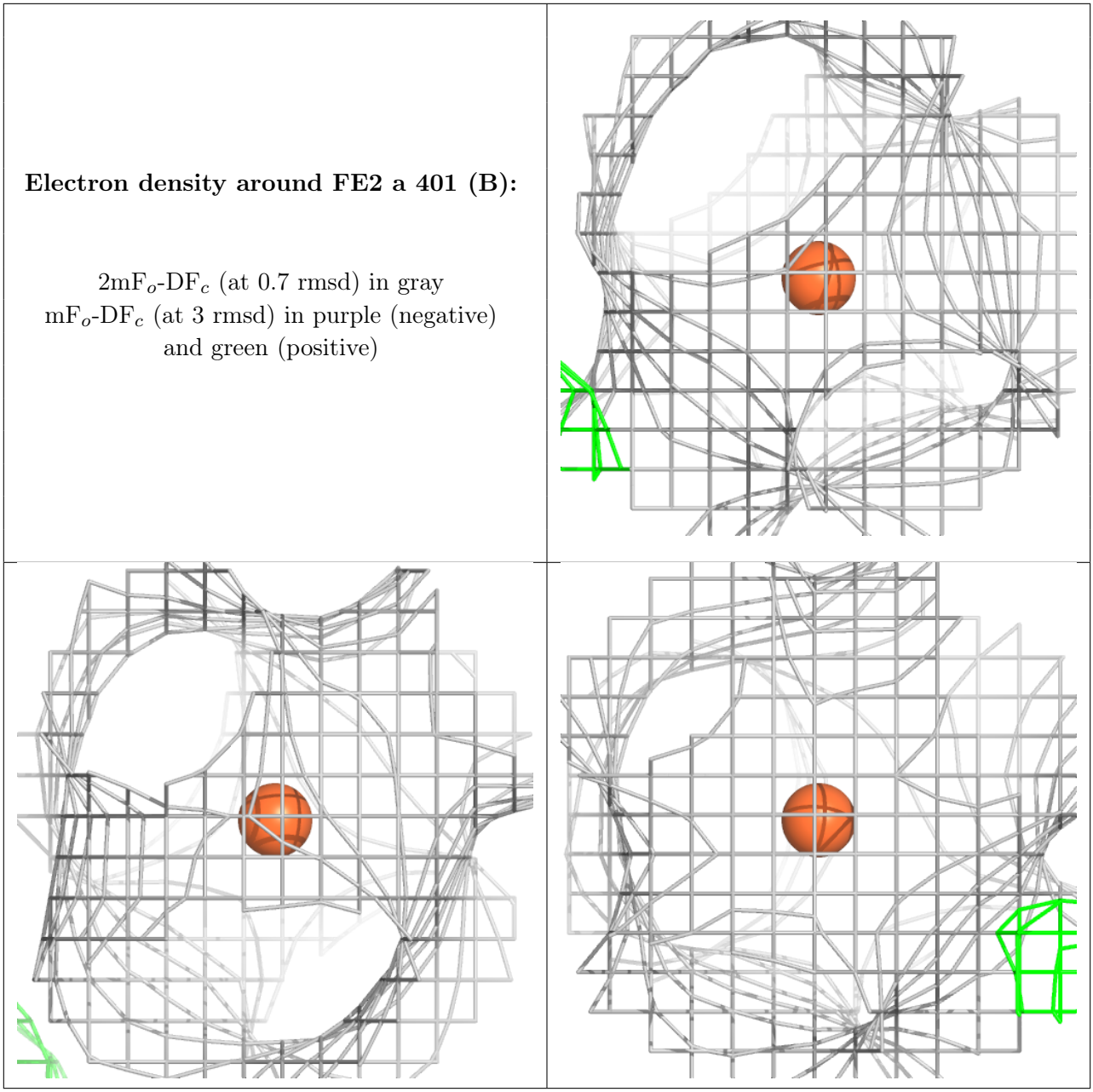
Electron density around FE2 a 401 (A):

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



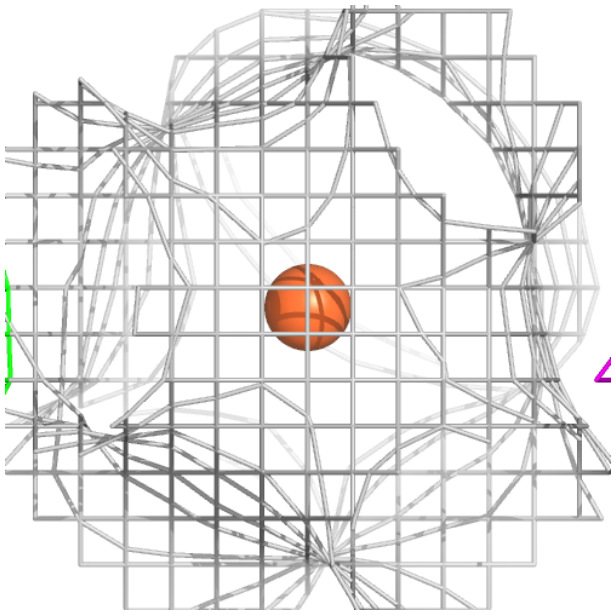
Electron density around FE2 a 401 (B):

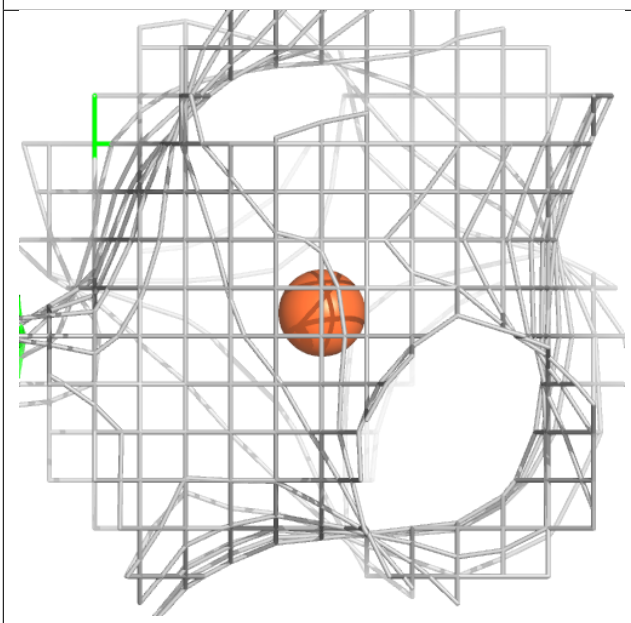
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

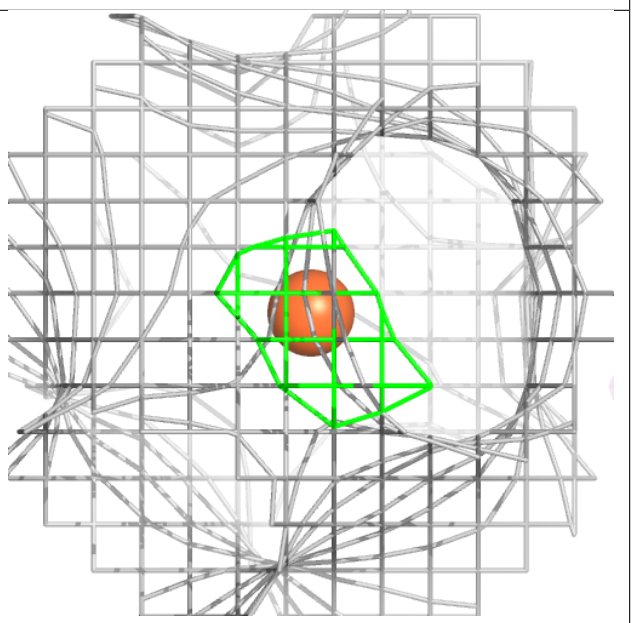


Electron density around FE2 A 401 (A):

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

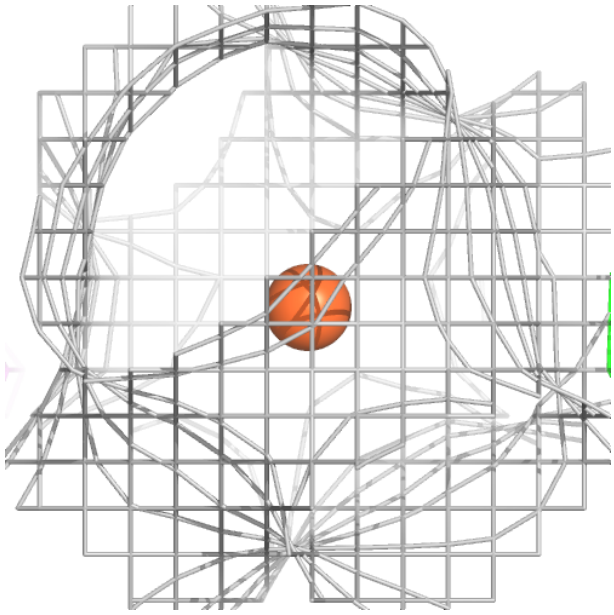


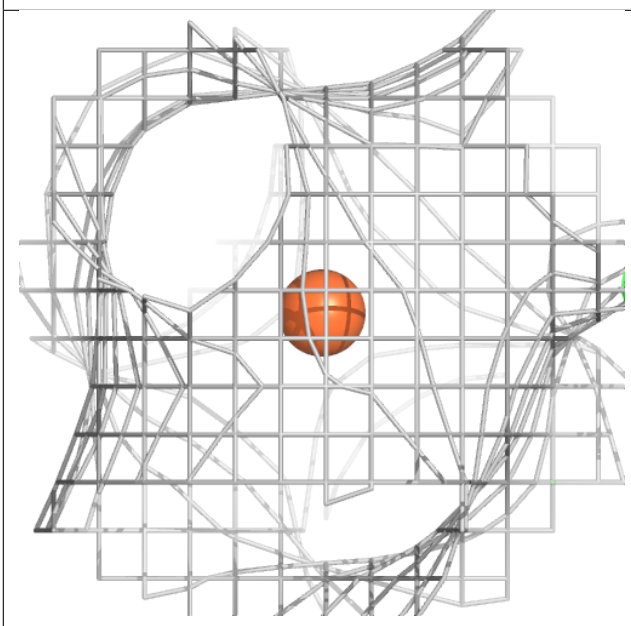


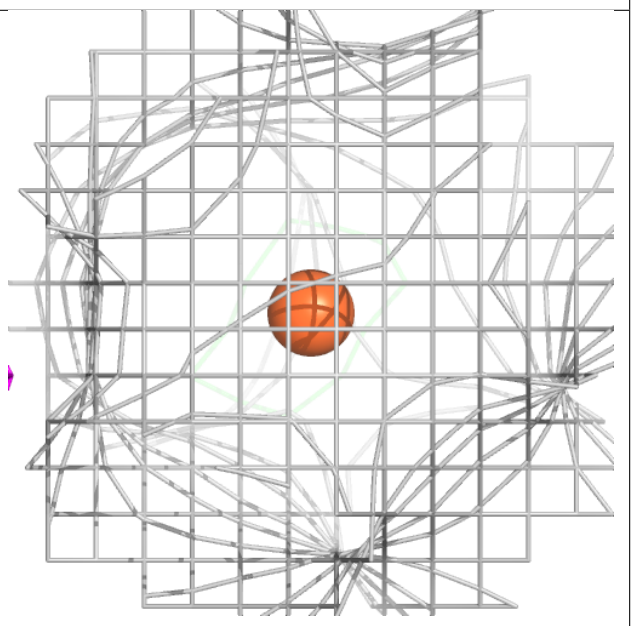


Electron density around FE2 A 401 (B):

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

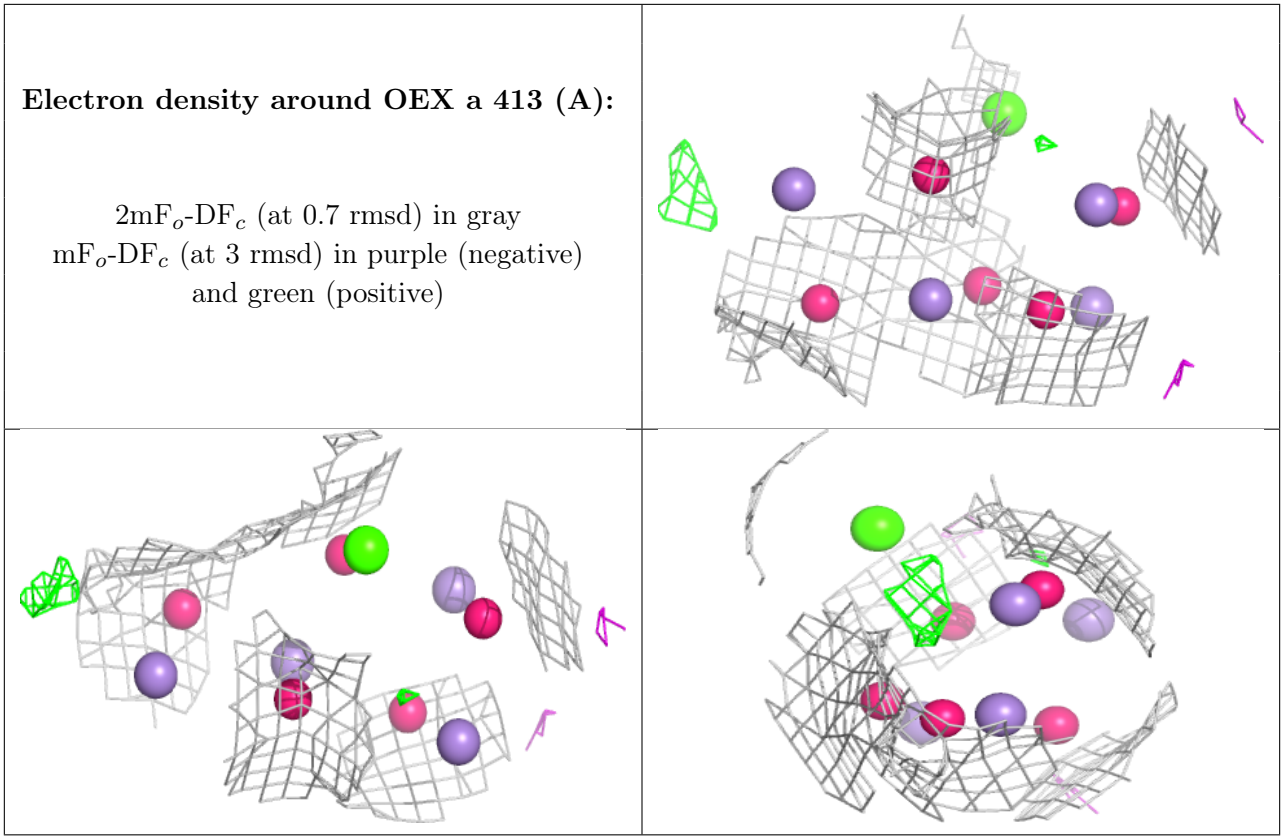






Electron density around OEX a 413 (A):

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



6.5 Other polymers

There are no such residues in this entry.