Full wwPDB X-ray Structure Validation Report (i)

Aug 13, 2026 – 10:22 PM JST

PDB ID	:	8IR5 / pdb_00008ir5
Title	:	XFEL structure of cyanobacterial photosystem II under dark conditions
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

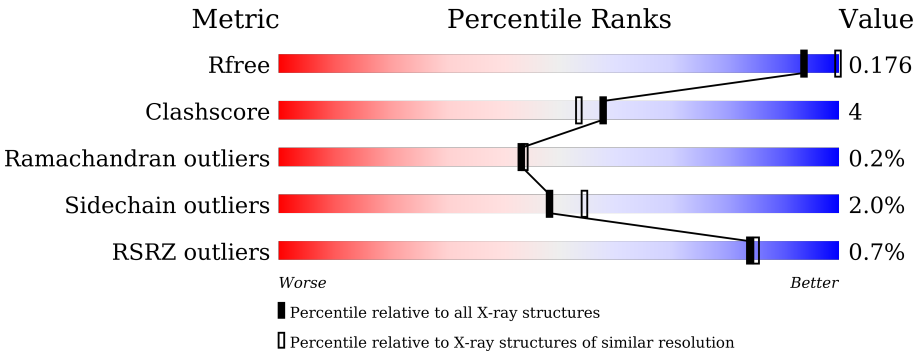
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	92%
1	a	344	90% 7%
2	B	505	93% 6%
2	b	505	93% 7%
3	C	455	91% 8%
3	c	455	93% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	342	92% 8%
4	d	342	93% 7%
5	E	84	2% 86% 11%
5	e	84	86% 8% 6%
6	F	44	64% 14% 23%
6	f	44	5% 61% 9% 30%
7	H	65	3% 94% 5%
7	h	65	2% 92% 6%
8	I	38	3% 76% 16% 8%
8	i	38	3% 95% 5%
9	J	39	87% 10%
9	j	39	3% 92% 8%
10	K	37	70% 24% 5%
10	k	37	78% 16% 5%
11	L	37	95%
11	l	37	5% 86% 11%
12	M	36	78% 11% 8%
12	m	36	81% 11% 6%
13	O	244	89% 10%
13	o	244	92% 7%
14	T	32	78% 12% 6%
14	t	32	3% 81% 12% 6%
15	U	104	85% 8% 8%
15	u	104	90% 7%
16	V	137	97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	v	137	93% 6%
17	X	40	85% 10% 5%
17	x	40	2% 92% 5%
18	Y	30	3% 83% 13%
18	y	30	70% 27%
19	Z	62	87% 11%
19	z	62	76% 24%
20	R	34	9% 71% 29%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	GOL	a	420	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 52978 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	1	0
			2628	1722	432	459	15			
1	a	334	Total	C	N	O	S	0	2	0
			2629	1721	432	461	15			

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	7	0
			4029	2639	674	703	13			
2	b	504	Total	C	N	O	S	0	6	0
			4017	2636	669	699	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	1	0
			3497	2287	588	609	13			
3	c	455	Total	C	N	O	S	0	5	0
			3555	2327	595	620	13			

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	1	0
			2732	1808	446	466	12			
4	d	341	Total	C	N	O	S	0	2	0
			2732	1808	447	465	12			

- 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	0	0
			296	197	47	52			
11	l	36	Total	C	N	O	0	0	0
			296	197	47	52			

- 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	3	0
			1894	1181	321	388	4			
13	o	243	Total	C	N	O	S	0	0	0
			1865	1165	315	381	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	1	0
			267	186	37	42	2			
14	t	30	Total	C	N	O	S	0	0	0
			258	181	36	39	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	1	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	1	0
			781	496	130	155			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	2	0
			1082	685	179	214	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	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 1	Fe 1	0	0
21	a	1	Total 1	Fe 1	0	0

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

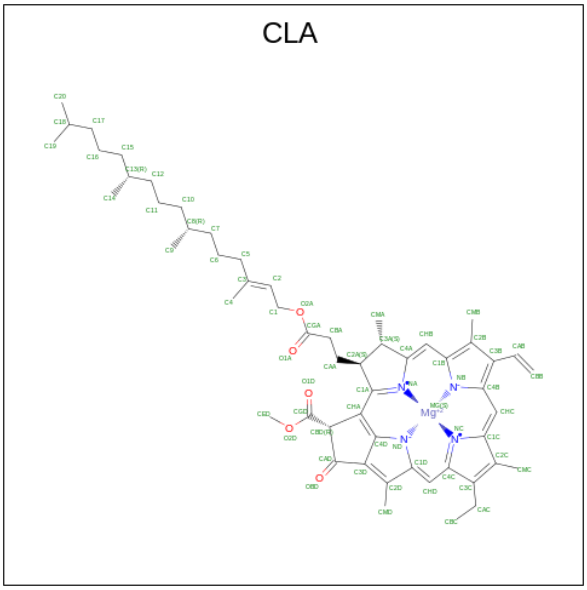
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 2	Cl 2	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

Continued on next page...

Continued from previous page...

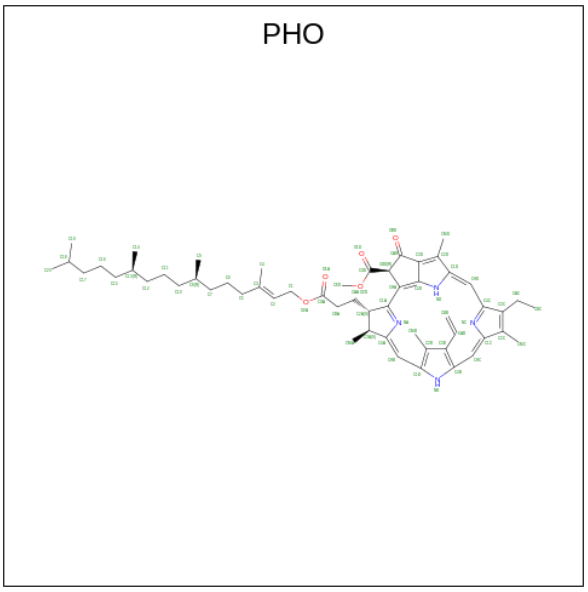
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

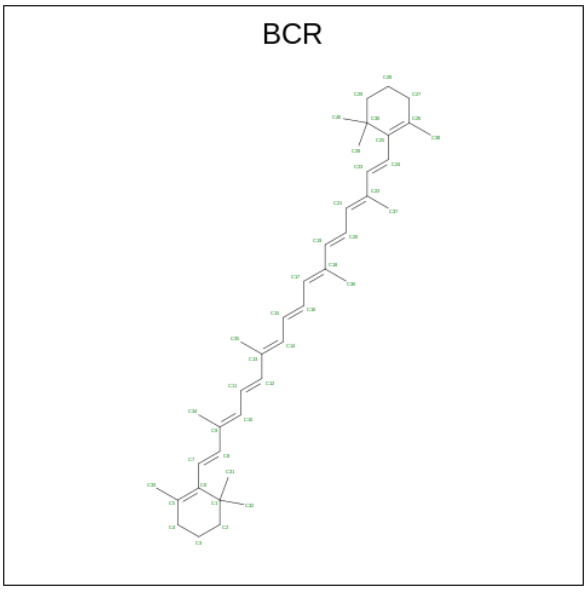
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



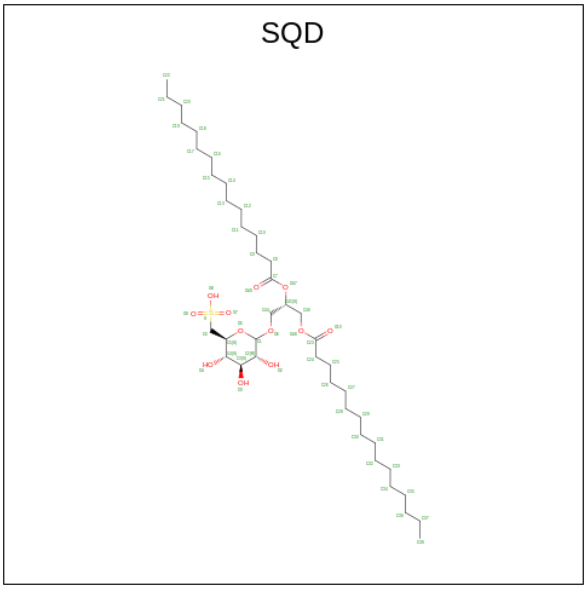
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

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



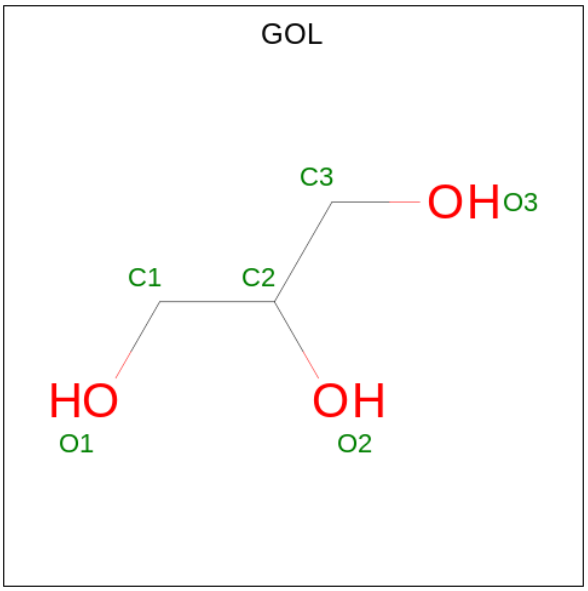
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



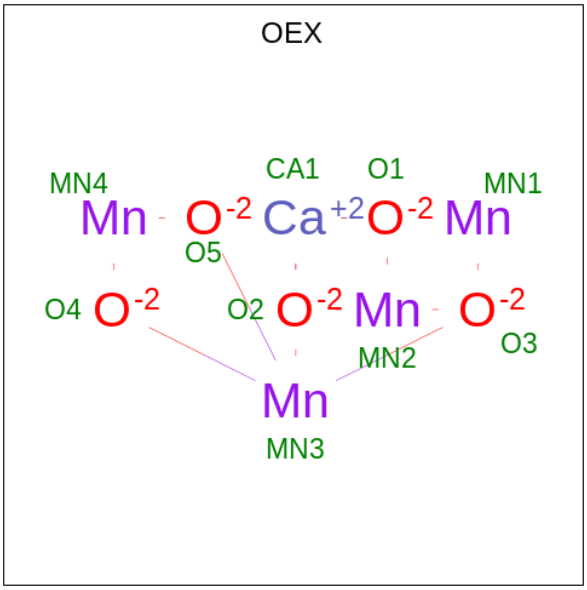
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

Continued on next page...

Continued from previous page...

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

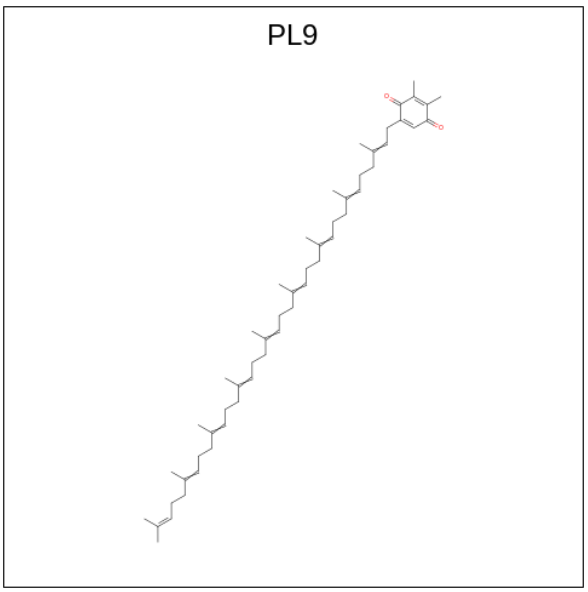
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 55 53 2	0	0
29	D	1	Total C O 55 53 2	0	0
29	a	1	Total C O 55 53 2	0	0
29	d	1	Total C O 55 53 2	0	0

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

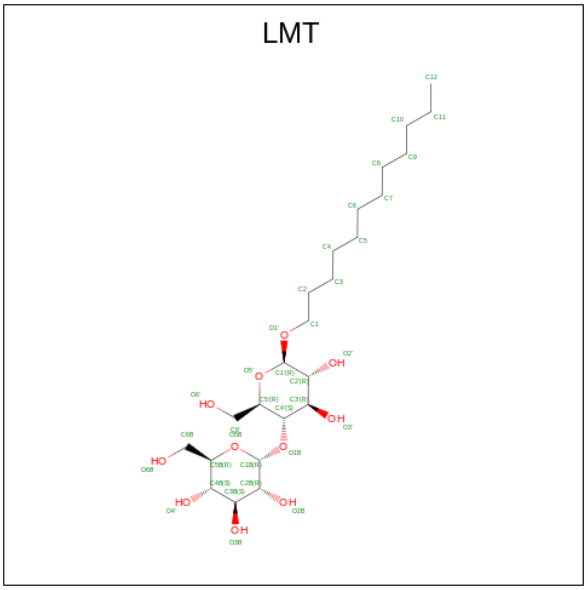
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 34 29 5	0	0
30	X	1	Total C O 18 16 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 32 27 5	0	0
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

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



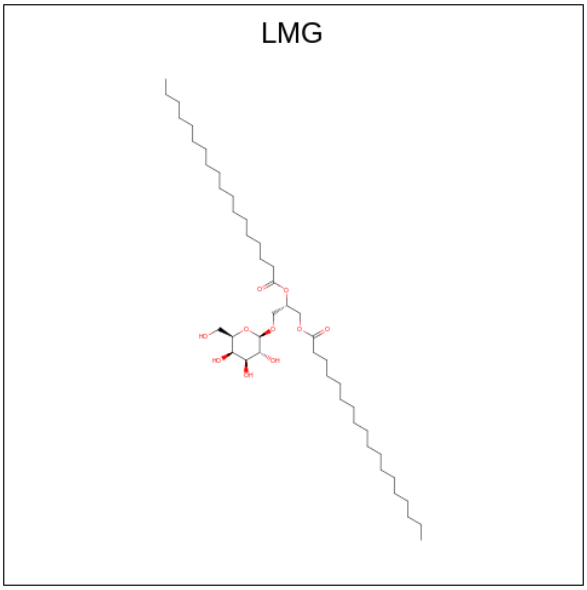
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0
31	A	1	Total C O 35 24 11	0	0

Continued on next page...

Continued from previous page...

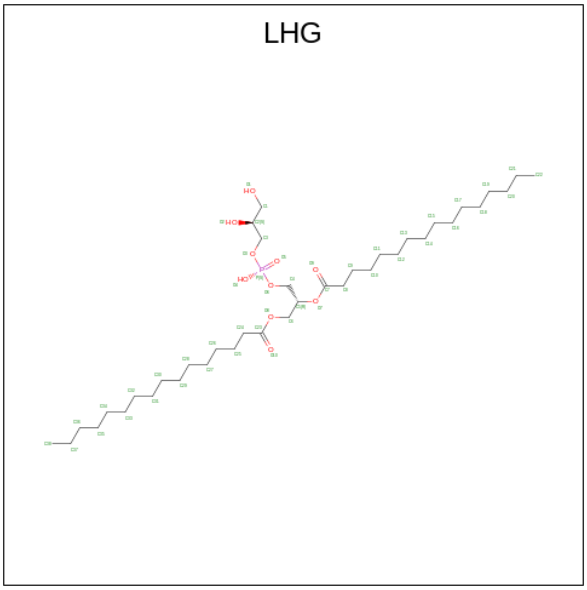
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 25 19 6	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	T	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 6	0	0
31	c	1	Total C O 35 24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

- Molecule 32 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



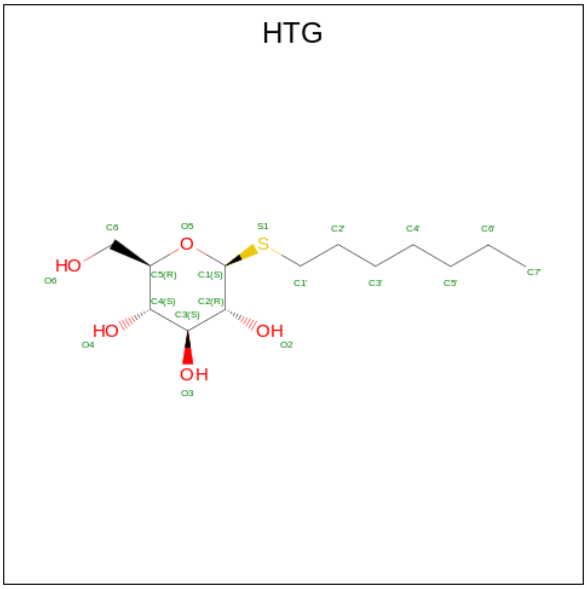
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	a	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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



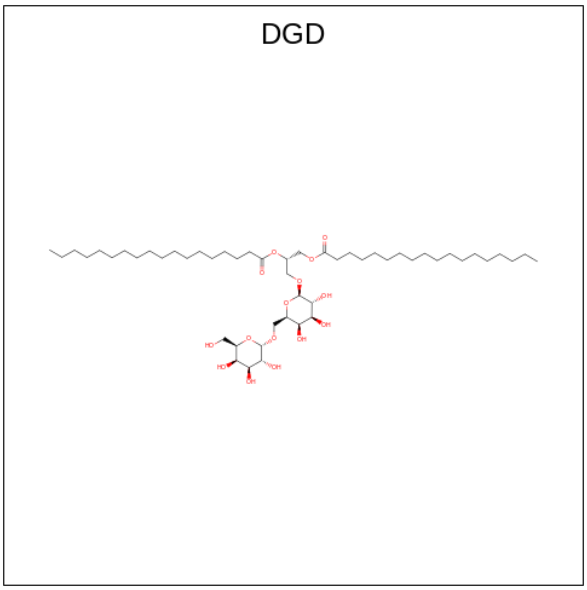
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
34	B	1	Total	C	O	S	0	0
			19	13	5	1		
34	B	1	Total	C	O	S	0	0
			19	13	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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 62 47 15	0	0
35	C	1	Total C O 62 47 15	0	0

Continued on next page...

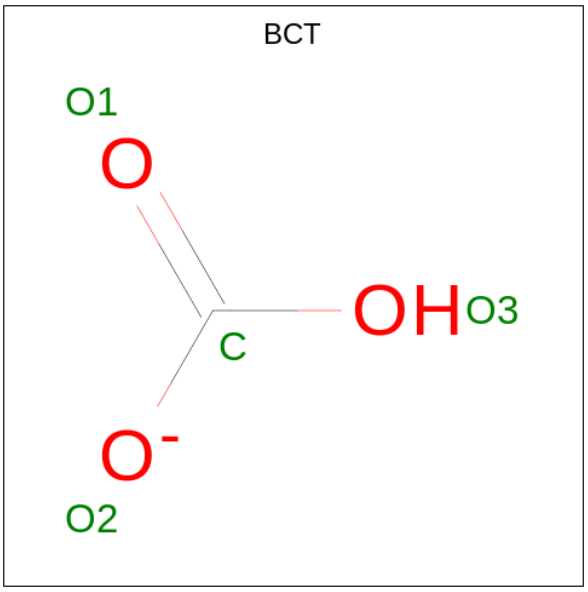
Continued from previous page...

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

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

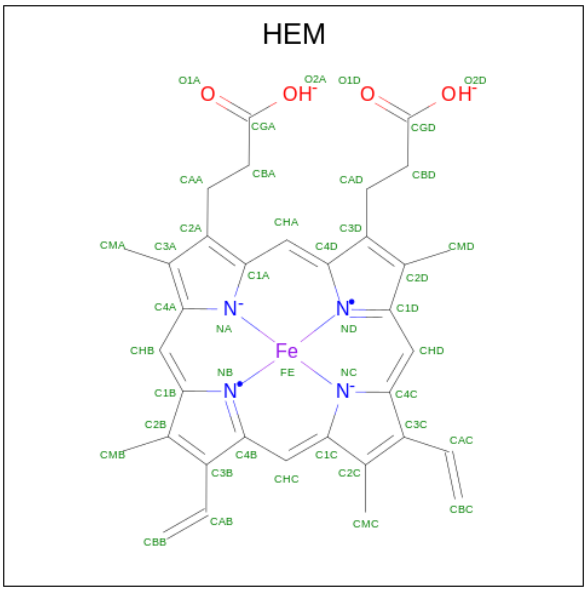
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
37	D	1	Total	C	O	0	0
			4	1	3		
37	a	1	Total	C	O	0	0
			4	1	3		

- 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		

Continued on next page...

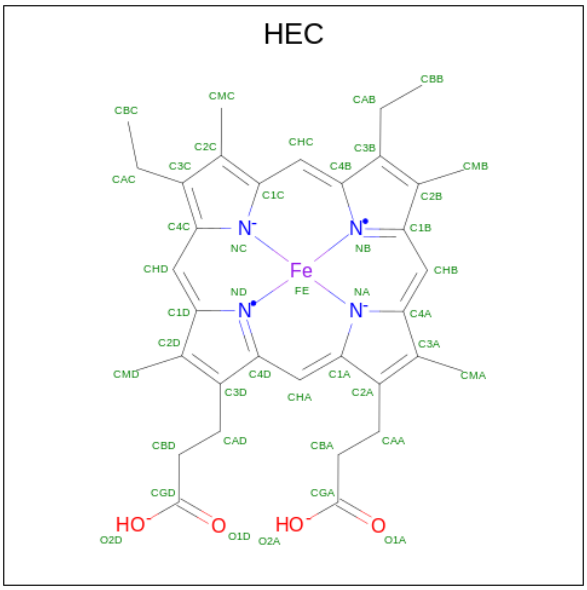
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	139	Total	O	0	1
			140	140		
41	B	188	Total	O	0	0
			188	188		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	167	Total O 167 167	0	0
41	D	123	Total O 123 123	0	0
41	E	13	Total O 13 13	0	0
41	F	7	Total O 7 7	0	0
41	H	21	Total O 21 21	0	0
41	I	5	Total O 5 5	0	0
41	J	8	Total O 8 8	0	0
41	K	5	Total O 5 5	0	0
41	L	9	Total O 9 9	0	0
41	M	5	Total O 5 5	0	0
41	O	105	Total O 105 105	0	0
41	T	10	Total O 10 10	0	0
41	U	44	Total O 44 44	0	0
41	V	82	Total O 82 82	0	0
41	X	7	Total O 7 7	0	0
41	a	130	Total O 130 130	0	0
41	b	202	Total O 202 202	0	0
41	c	161	Total O 161 161	0	0
41	d	111	Total O 111 111	0	0
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0

Continued on next page...

Continued from previous page...

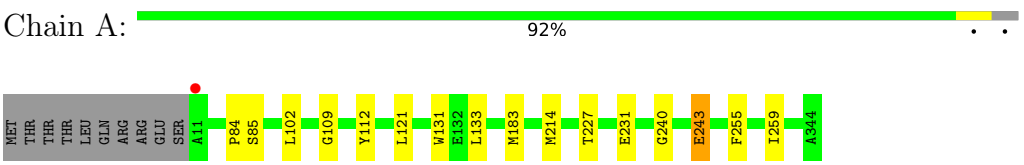
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	17	Total O 17 17	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 8 8	0	0
41	m	13	Total O 13 13	0	0
41	o	103	Total O 103 103	0	0
41	t	7	Total O 7 7	0	0
41	u	49	Total O 49 49	0	0
41	v	57	Total O 57 57	0	0
41	x	8	Total O 8 8	0	0
41	y	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

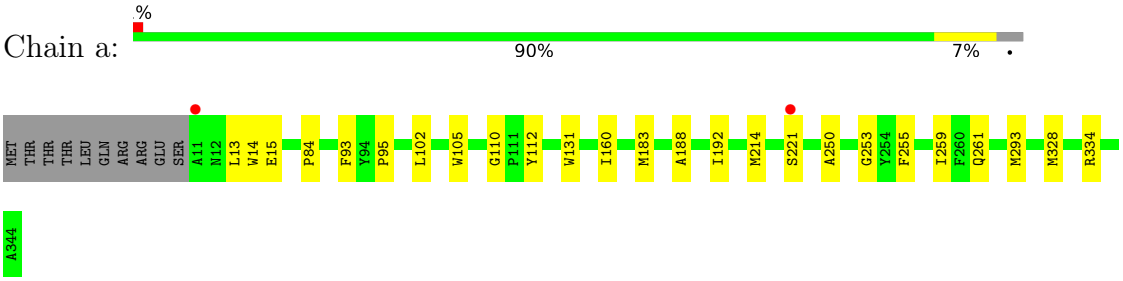
• Molecule 1: Photosystem II protein D1

Chain A:



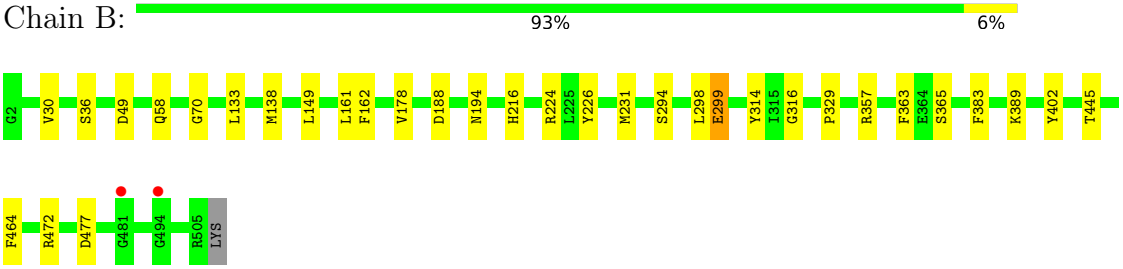
• Molecule 1: Photosystem II protein D1

Chain a:



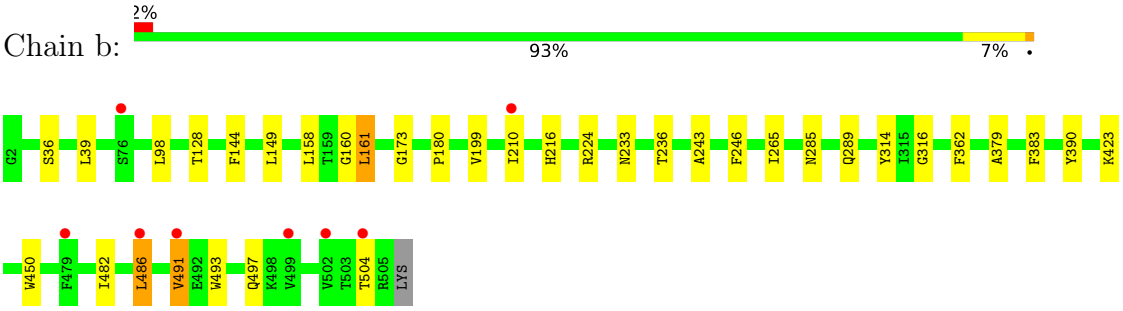
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



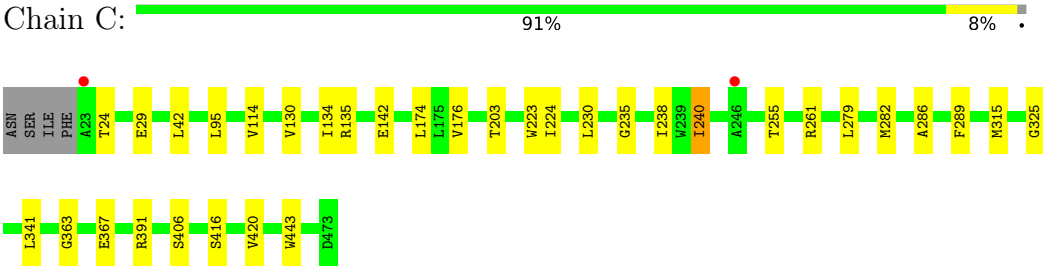
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



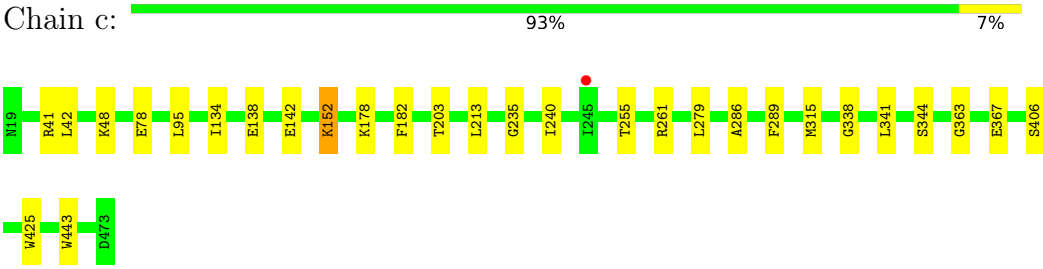
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



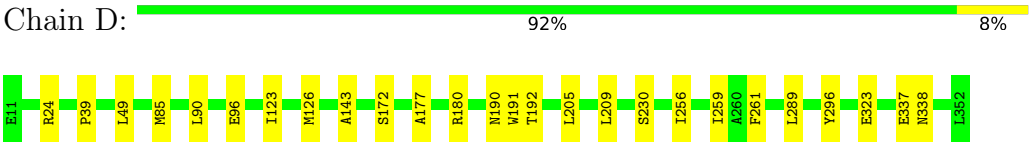
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



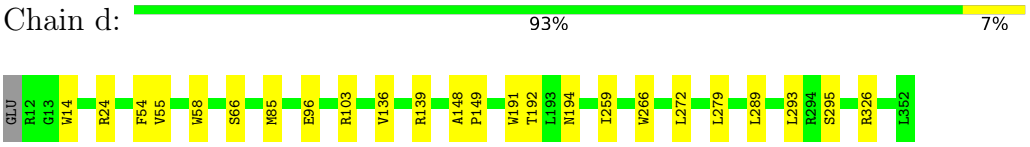
• Molecule 4: Photosystem II D2 protein

Chain D:



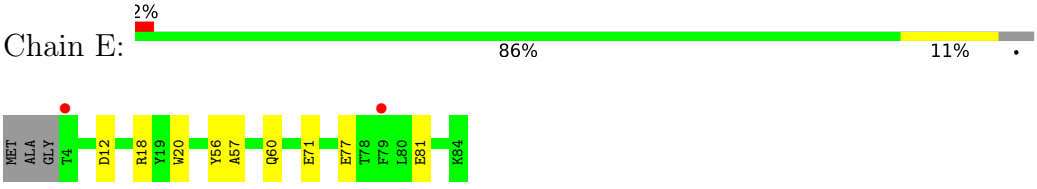
• Molecule 4: Photosystem II D2 protein

Chain d:



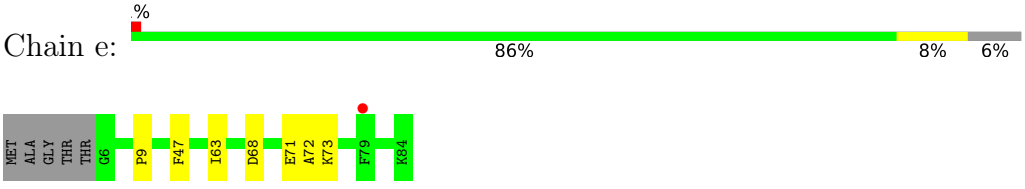
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

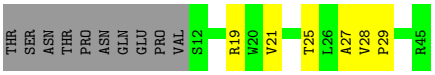
Chain e:



• Molecule 6: Cytochrome b559 subunit beta

Chain F:

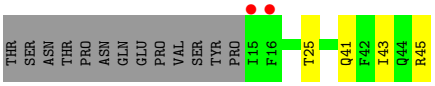




• Molecule 6: Cytochrome b559 subunit beta

Chain f:





• Molecule 7: Photosystem II reaction center protein H

Chain H:

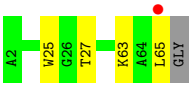




• Molecule 7: Photosystem II reaction center protein H

Chain h:

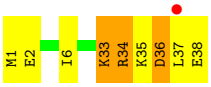




• Molecule 8: Photosystem II reaction center protein I

Chain I:

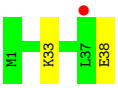




• Molecule 8: Photosystem II reaction center protein I

Chain i:





• Molecule 9: Photosystem II reaction center protein J

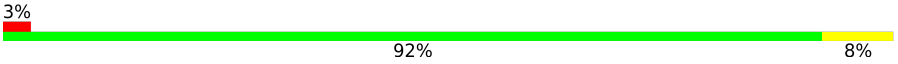
Chain J:

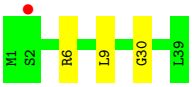




• Molecule 9: Photosystem II reaction center protein J

Chain j:

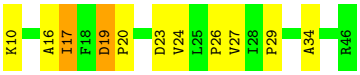




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

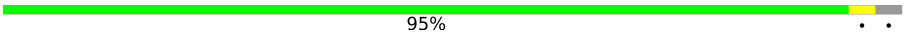
Chain k:

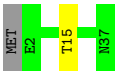




• Molecule 11: Photosystem II reaction center protein L

Chain L:

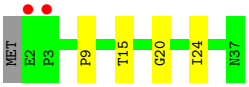




• Molecule 11: Photosystem II reaction center protein L

Chain l:

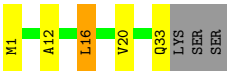




• Molecule 12: Photosystem II reaction center protein M

Chain M:

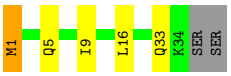




• Molecule 12: Photosystem II reaction center protein M

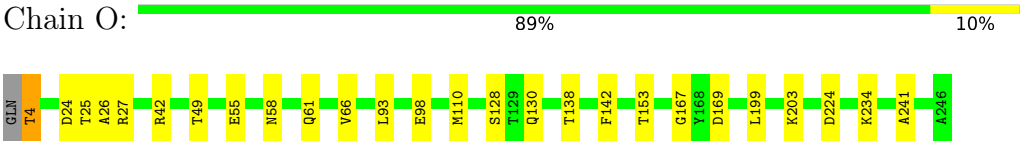
Chain m:





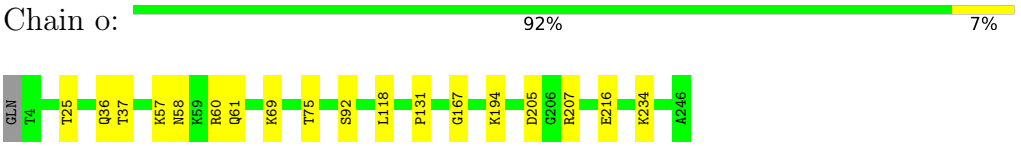
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



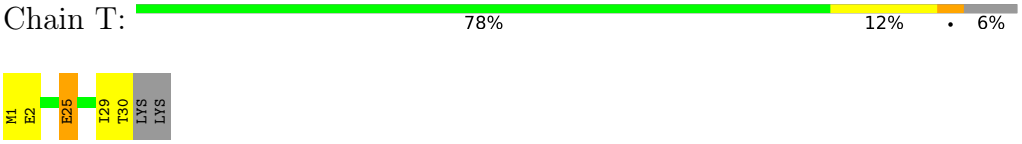
• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:



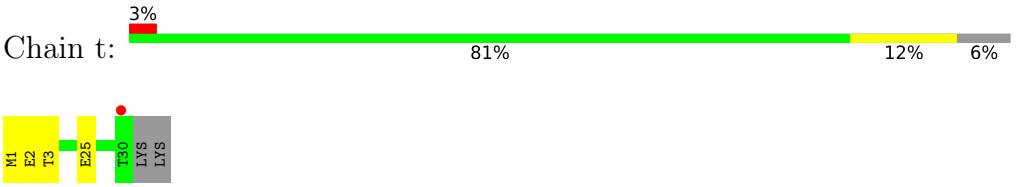
• Molecule 14: Photosystem II reaction center protein T

Chain T:



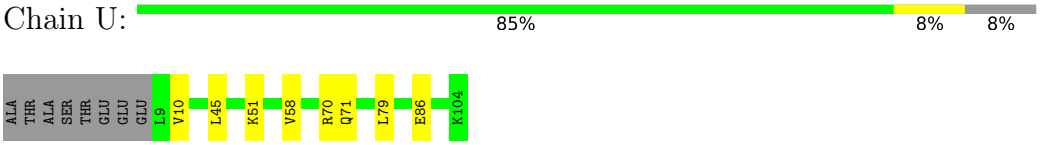
• Molecule 14: Photosystem II reaction center protein T

Chain t:



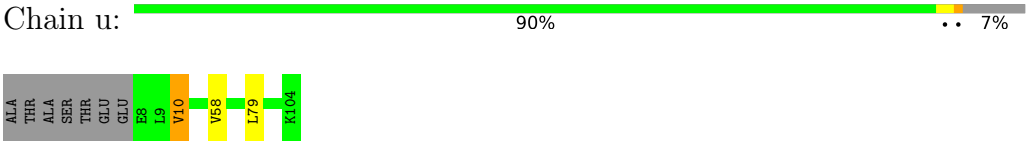
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:



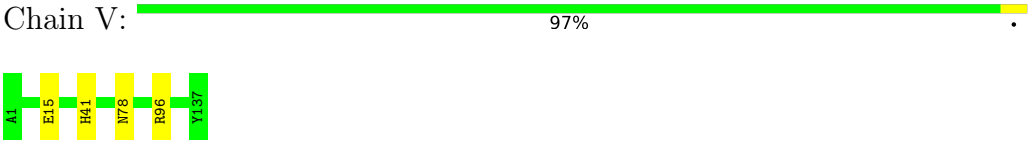
• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain u:



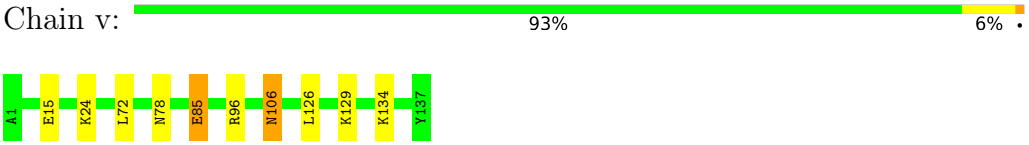
• Molecule 16: Cytochrome c-550

Chain V:



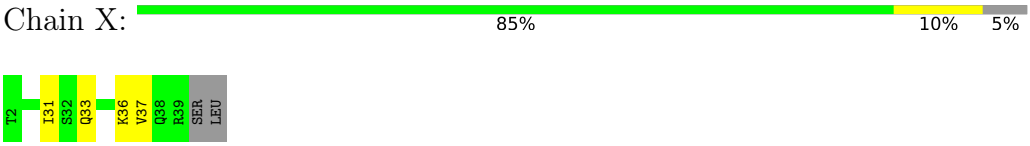
• Molecule 16: Cytochrome c-550

Chain v:



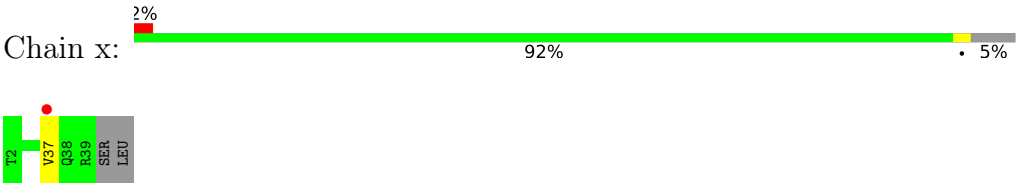
• Molecule 17: Photosystem II reaction center protein X

Chain X:



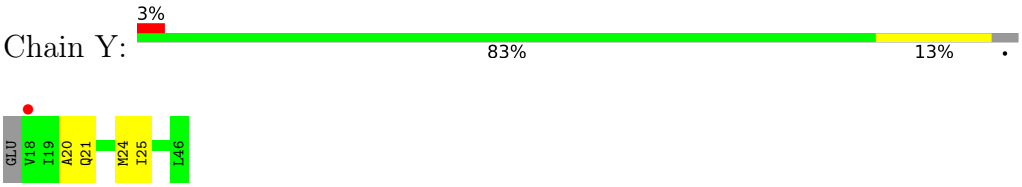
• Molecule 17: Photosystem II reaction center protein X

Chain x:



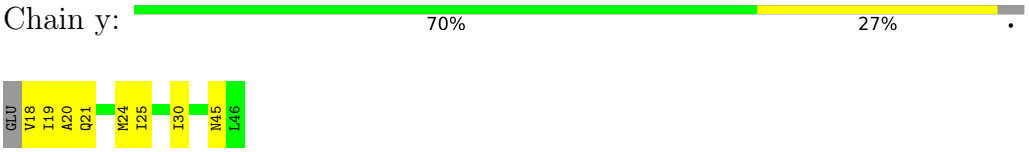
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



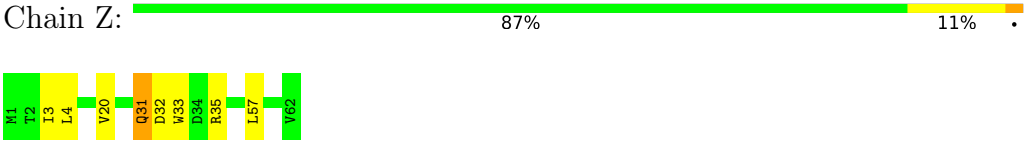
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



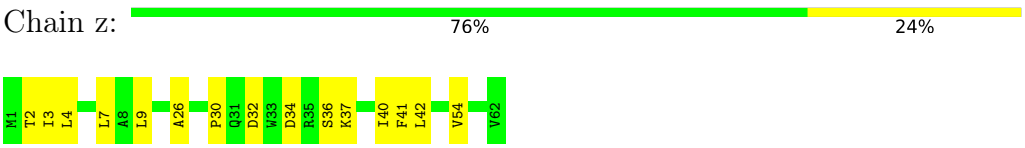
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

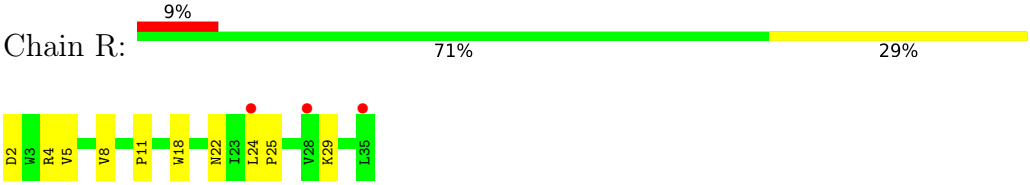


• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.15) 99.7 (19.98-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.15Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.144 , 0.175 0.146 , 0.176	Depositor DCC
R_{free} test set	22666 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	52978	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: HEC, LHG, LMT, CA, FME, GOL, PL9, OEX, MG, BCR, BCT, CL, HEM, HTG, LMG, CLA, PHO, DGD, SQD, UNL, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.36	0/2713	0.53	0/3700
1	a	0.33	0/2717	0.49	0/3705
2	B	0.32	0/4169	0.47	0/5679
2	b	0.29	0/4161	0.47	0/5669
3	C	0.29	0/3610	0.45	0/4914
3	c	0.28	0/3675	0.43	0/5002
4	D	0.35	0/2827	0.50	0/3852
4	d	0.34	0/2827	0.48	0/3852
5	E	0.27	0/681	0.46	0/928
5	e	0.25	0/690	0.42	0/939
6	F	0.27	0/284	0.41	0/387
6	f	0.23	0/269	0.40	0/365
7	H	0.26	0/519	0.43	0/708
7	h	0.25	0/530	0.44	0/722
8	I	0.25	0/311	0.40	0/419
8	i	0.29	0/311	0.44	0/419
9	J	0.25	0/278	0.34	0/376
9	j	0.23	0/283	0.38	0/383
10	K	0.28	0/303	0.43	0/416
10	k	0.27	0/303	0.41	0/416
11	L	0.31	0/303	0.44	0/412
11	l	0.33	0/303	0.46	0/412
12	M	0.32	0/261	0.48	0/357
12	m	0.30	0/279	0.43	0/380
13	O	0.30	0/1925	0.47	0/2609
13	o	0.28	0/1896	0.46	0/2571
14	T	0.32	0/266	0.40	0/362
14	t	0.31	0/257	0.40	0/349
15	U	0.32	0/785	0.52	0/1064
15	u	0.31	0/792	0.51	0/1074
16	V	0.32	0/1103	0.46	0/1497

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.27	0/1085	0.42	0/1473
17	X	0.21	0/292	0.31	0/395
17	x	0.20	0/284	0.33	0/384
18	Y	0.23	0/216	0.40	0/289
18	y	0.19	0/216	0.35	0/289
19	Z	0.18	0/490	0.33	0/669
19	z	0.19	0/490	0.35	0/669
20	R	0.21	0/279	0.34	0/383
All	All	0.30	0/42983	0.46	0/58489

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	2628	0	2527	10	0
1	a	2629	0	2526	18	0
2	B	4029	0	3880	26	0
2	b	4017	0	3872	29	0
3	C	3497	0	3419	21	0
3	c	3555	0	3480	21	0
4	D	2732	0	2631	20	0
4	d	2732	0	2632	18	0
5	E	662	0	648	6	0
5	e	670	0	655	5	0
6	F	275	0	282	4	0
6	f	261	0	269	4	0
7	H	506	0	529	3	0
7	h	517	0	541	2	0
8	I	314	0	328	5	0
8	i	314	0	328	1	0
9	J	272	0	279	4	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	7	0
10	k	293	0	305	7	0
11	L	296	0	304	1	0
11	l	296	0	304	3	0
12	M	268	0	285	3	0
12	m	286	0	305	7	0
13	O	1894	0	1860	15	0
13	o	1865	0	1838	9	0
14	T	267	0	267	3	0
14	t	258	0	261	3	0
15	U	774	0	772	5	0
15	u	781	0	781	2	0
16	V	1082	0	1083	2	0
16	v	1064	0	1073	6	0
17	X	289	0	322	3	0
17	x	281	0	312	1	0
18	Y	215	0	246	3	0
18	y	215	0	246	6	0
19	Z	479	0	516	3	0
19	z	479	0	516	5	0
20	R	273	0	305	4	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	260	0	288	13	0
23	B	1040	0	1152	29	0
23	C	845	0	936	28	0
23	D	130	0	144	3	0
23	a	260	0	288	9	0
23	b	1040	0	1152	21	0
23	c	845	0	936	33	0
23	d	130	0	144	3	0
24	A	128	0	148	3	0
24	a	128	0	148	2	0
25	A	40	0	56	2	0
25	B	120	0	168	5	0
25	C	40	0	56	1	0
25	D	40	0	56	3	0
25	H	40	0	56	2	0
25	K	80	0	112	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	7	0
25	Y	40	0	56	2	0
25	a	40	0	56	2	0
25	b	120	0	168	7	0
25	c	80	0	112	6	0
25	d	40	0	56	2	0
25	h	40	0	56	3	0
25	k	40	0	56	0	0
25	t	40	0	56	5	0
25	y	40	0	56	2	0
26	A	108	0	155	3	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	108	0	155	5	0
26	b	54	0	78	2	0
26	f	43	0	53	1	0
27	A	12	0	15	3	0
27	B	18	0	24	5	0
27	C	6	0	8	0	0
27	O	12	0	16	3	0
27	V	6	0	8	0	0
27	a	18	0	24	6	0
27	b	18	0	24	3	0
27	c	12	0	16	0	0
27	l	6	0	8	1	0
27	o	12	0	16	0	0
27	v	6	0	8	1	0
28	A	10	0	0	0	0
28	a	10	0	0	0	0
29	A	55	0	80	10	0
29	D	55	0	80	0	0
29	a	55	0	80	4	0
29	d	55	0	80	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	34	0	0	0	0
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	c	32	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	2	0
31	B	95	0	127	3	0
31	F	35	0	46	0	0
31	M	35	0	46	1	0
31	T	35	0	46	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	45	0	0
31	t	26	0	33	2	0
32	A	51	0	72	0	0
32	B	51	0	72	1	0
32	C	102	0	144	4	0
32	D	51	0	72	0	0
32	Z	37	0	44	2	0
32	a	51	0	72	0	0
32	c	102	0	144	2	0
32	d	51	0	72	2	0
32	m	51	0	72	0	0
32	z	39	0	48	2	0
33	A	49	0	74	2	0
33	D	98	0	148	7	0
33	E	42	0	57	4	0
33	L	49	0	74	0	0
33	a	42	0	57	4	0
33	b	49	0	74	0	0
33	d	147	0	222	12	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	3	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	186	0	246	5	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	186	0	246	4	0
35	h	62	0	82	1	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	4	0	0	0	0
37	a	4	0	0	0	0
38	F	43	0	30	1	0
38	f	43	0	30	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	140	0	0	1	0
41	B	188	0	0	1	0
41	C	167	0	0	1	0
41	D	123	0	0	1	0
41	E	13	0	0	0	0
41	F	7	0	0	0	0
41	H	21	0	0	0	0
41	I	5	0	0	0	0
41	J	8	0	0	1	0
41	K	5	0	0	1	0
41	L	9	0	0	1	0
41	M	5	0	0	0	0
41	O	105	0	0	2	0
41	T	10	0	0	0	0
41	U	44	0	0	0	0
41	V	82	0	0	0	0
41	X	7	0	0	0	0
41	a	130	0	0	2	0
41	b	202	0	0	0	0
41	c	161	0	0	2	0
41	d	111	0	0	1	0
41	e	9	0	0	0	0
41	f	3	0	0	1	0
41	h	17	0	0	0	0
41	i	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	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	103	0	0	0	0
41	t	7	0	0	1	0
41	u	49	0	0	1	0
41	v	57	0	0	1	0
41	x	8	0	0	0	0
41	y	2	0	0	0	0
All	All	52978	0	52086	462	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 4.

All (462) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:418:GOL:H11	12:M:1:FME:HG2	1.44	0.99
23:B:604:CLA:H42	23:B:605:CLA:H2	1.53	0.91
1:a:250:ALA:HA	2:b:491:VAL:HG11	1.53	0.88
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.62	0.82
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.62	0.81
4:d:192:THR:HG23	23:d:401:CLA:HBC2	1.64	0.80
23:C:503:CLA:HBB1	23:C:512:CLA:H41	1.64	0.78
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.67	0.77
23:A:406:CLA:H152	29:A:414:PL9:H252	1.67	0.76
23:C:501:CLA:H193	23:C:507:CLA:HBB1	1.68	0.76
23:B:601:CLA:H12	23:B:601:CLA:H71	1.65	0.75
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.72	0.71
33:D:407:LHG:H112	33:D:407:LHG:H382	1.74	0.70
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.73	0.70
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.74	0.69
1:a:253:GLY:HA3	2:b:491:VAL:HG12	1.74	0.69
27:a:420:GOL:O2	41:a:501:HOH:O	2.10	0.69
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.24	0.68
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.77	0.67
27:a:419:GOL:H32	12:m:1:FME:HG3	1.77	0.67
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	1.78	0.65
23:C:506:CLA:H142	35:C:515:DGD:HAF2	1.79	0.65
23:C:513:CLA:H202	32:C:519:LMG:H402	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:418:GOL:O2	41:A:501:HOH:O	2.15	0.64
29:A:414:PL9:H262	33:E:101:LHG:H223	1.80	0.64
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.80	0.64
23:a:409:CLA:H152	23:c:507:CLA:H142	1.79	0.63
23:a:409:CLA:H192	23:c:506:CLA:H142	1.79	0.63
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.79	0.63
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.28	0.63
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.29	0.63
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.81	0.63
10:K:17:ILE:H	10:K:17:ILE:HD13	1.64	0.62
2:b:482:ILE:HD12	2:b:486:LEU:HD12	1.82	0.62
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.82	0.62
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.81	0.62
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.83	0.61
23:C:505:CLA:CMD	23:C:507:CLA:HAB	2.30	0.61
32:z:101:LMG:H302	32:z:101:LMG:H141	1.82	0.61
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.33	0.61
16:v:134:LYS:HE2	27:v:202:GOL:H32	1.83	0.60
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.83	0.60
2:b:285:ASN:O	2:b:289:GLN:HG2	2.01	0.59
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.85	0.59
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.82	0.59
23:A:408:CLA:H193	23:C:506:CLA:H101	1.85	0.58
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.85	0.58
23:a:406:CLA:HHC	23:a:406:CLA:HBB1	1.85	0.58
26:a:411:SQD:H152	33:d:406:LHG:H172	1.86	0.58
27:a:420:GOL:O3	14:t:2:GLU:OE1	2.22	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.68	0.58
3:C:286:ALA:HB2	23:C:502:CLA:HMD1	1.85	0.57
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.87	0.57
23:b:601:CLA:H72	23:b:601:CLA:H2	1.87	0.57
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.85	0.57
23:c:512:CLA:H191	32:z:101:LMG:H241	1.87	0.57
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.38	0.57
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.13	0.56
23:c:503:CLA:H61	23:c:513:CLA:H42	1.88	0.56
23:C:510:CLA:HBC3	23:C:510:CLA:H192	1.87	0.56
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.06	0.56
26:a:411:SQD:H141	33:d:406:LHG:H152	1.86	0.56
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.87	0.56
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.13	0.55
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.88	0.55
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.88	0.55
26:F:103:SQD:H102	17:X:31:ILE:HD11	1.88	0.55
6:F:27:ALA:HB1	38:F:102:HEM:HAC	1.89	0.55
1:a:334:ARG:NH2	41:a:503:HOH:O	2.40	0.55
27:b:628:GOL:O3	27:b:628:GOL:O1	2.18	0.54
2:B:357[A]:ARG:HH12	27:B:624:GOL:H32	1.72	0.54
23:a:407:CLA:H191	33:a:421:LHG:H111	1.88	0.54
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.54
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.41	0.54
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.88	0.54
1:a:183:MET:HA	23:a:405:CLA:HMD1	1.90	0.54
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.42	0.54
3:c:338:GLY:HA3	3:c:341:LEU:O	2.08	0.53
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.90	0.53
4:D:192:THR:HG23	23:D:402:CLA:HBC2	1.90	0.53
3:C:325:GLY:O	15:U:51:LYS:NZ	2.35	0.53
23:b:604:CLA:H42	23:b:605:CLA:H2	1.90	0.53
23:c:505:CLA:H151	23:c:509:CLA:H143	1.91	0.53
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.42	0.53
10:K:23:ASP:OD2	41:K:201:HOH:O	2.19	0.53
27:a:420:GOL:H31	12:m:1:FME:HG2	1.92	0.52
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.91	0.52
23:C:505:CLA:HBB1	23:C:505:CLA:HHC	1.91	0.52
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.42	0.52
25:b:619:BCR:H331	25:b:619:BCR:C8	2.40	0.52
23:C:508:CLA:HBC3	23:C:510:CLA:H71	1.92	0.52
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.92	0.52
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.10	0.52
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.92	0.52
2:B:226:TYR:HA	2:B:231:MET:HG3	1.91	0.51
1:a:84:PRO:HA	1:a:112:TYR:CG	2.45	0.51
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.39	0.51
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.75	0.51
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.91	0.51
24:A:407:PHO:HAB	4:D:205:LEU:HD13	1.91	0.51
13:O:42:ARG:O	13:O:241:ALA:HA	2.11	0.51
25:T:102:BCR:H19C	25:b:618:BCR:H363	1.93	0.51
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.45	0.51
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.46	0.51
29:a:415:PL9:H28	33:a:421:LHG:H222	1.92	0.51
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.92	0.51
33:a:421:LHG:HC31	5:e:9:PRO:HA	1.92	0.51
2:b:497:GLN:HB2	2:b:504:THR:HB	1.93	0.51
5:E:77:GLU:O	5:E:81:GLU:HG2	2.11	0.50
29:a:415:PL9:H351	6:f:25:THR:OG1	2.11	0.50
15:u:10[A]:VAL:HG12	41:u:242:HOH:O	2.11	0.50
26:A:412:SQD:H301	23:b:606:CLA:H202	1.93	0.50
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.24	0.50
9:J:2:SER:N	41:J:201:HOH:O	2.43	0.50
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.40	0.50
29:A:414:PL9:H253	23:D:402:CLA:H141	1.92	0.50
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.92	0.50
33:d:405:LHG:HC62	11:l:15:THR:HG23	1.94	0.50
34:B:625:HTG:H61	1:a:102:LEU:HD12	1.93	0.50
27:B:629:GOL:O2	4:D:323:GLU:O	2.30	0.50
27:l:102:GOL:H32	14:t:25:GLU:HB2	1.92	0.50
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.46	0.50
23:C:501:CLA:C3D	23:C:503:CLA:H2	2.42	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	2.41	0.50
4:D:230:SER:HB2	41:D:551:HOH:O	2.11	0.50
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.12	0.50
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.42	0.49
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.94	0.49
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.92	0.49
32:C:519:LMG:H352	25:K:101:BCR:H352	1.94	0.49
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.94	0.49
25:T:102:BCR:HC8	25:T:102:BCR:H311	1.93	0.49
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.95	0.49
1:A:227:THR:HB	1:A:231:GLU:HG3	1.94	0.49
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.94	0.49
23:a:405:CLA:H201	33:d:405:LHG:H161	1.95	0.49
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.13	0.49
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.94	0.48
29:A:414:PL9:H503	26:F:103:SQD:H341	1.95	0.48
23:B:606:CLA:H202	26:a:413:SQD:H302	1.95	0.48
13:O:224:ASP:OD2	41:O:402:HOH:O	2.20	0.48
33:d:406:LHG:H331	33:d:406:LHG:H361	1.55	0.48
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.78	0.48
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:D:407:LHG:H382	33:D:407:LHG:H132	1.96	0.48
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.96	0.48
27:a:420:GOL:H11	12:m:1:FME:HE3	1.95	0.48
18:y:20:ALA:O	18:y:24:MET:HG2	2.14	0.48
33:d:406:LHG:H122	33:d:406:LHG:C38	2.44	0.48
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.78	0.48
2:B:49:ASP:OD2	13:o:57:LYS:NZ	2.44	0.47
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.94	0.47
3:c:41:ARG:NH1	23:c:512:CLA:HMD1	2.29	0.47
32:c:520:LMG:H181	10:k:27:VAL:HG11	1.95	0.47
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.95	0.47
23:A:405:CLA:H203	23:A:405:CLA:H162	1.74	0.47
27:A:418:GOL:H12	14:T:2:GLU:OE1	2.14	0.47
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.14	0.47
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.96	0.47
3:C:174:LEU:HB3	23:C:502:CLA:H152	1.94	0.47
31:t:101:LMT:H112	31:t:101:LMT:H81	1.67	0.47
1:A:240:GLY:HA3	14:T:29:ILE:HG23	1.96	0.47
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.49	0.47
2:b:36:SER:OG	25:b:618:BCR:H362	2.13	0.47
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.50	0.47
27:O:303:GOL:O1	41:O:401:HOH:O	2.19	0.47
1:a:160:ILE:HD11	35:c:517:DGD:HBT1	1.96	0.47
23:b:615:CLA:H61	23:b:615:CLA:H92	1.66	0.47
26:A:410:SQD:H152	26:A:410:SQD:H122	1.54	0.47
31:A:417:LMT:H71	2:b:39:LEU:HD13	1.96	0.47
23:B:613:CLA:H162	23:B:613:CLA:H121	1.60	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.40	0.47
6:F:21:VAL:O	6:F:25:THR:HG23	2.14	0.47
32:d:410:LMG:H221	32:d:410:LMG:H191	1.61	0.47
25:h:101:BCR:C8	25:h:101:BCR:H331	2.44	0.47
23:A:408:CLA:H18	23:C:505:CLA:H142	1.97	0.47
23:C:501:CLA:HHC	23:C:501:CLA:HBB1	1.96	0.47
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.97	0.47
1:a:15:GLU:HB2	31:c:501:LMT:H6'2	1.96	0.47
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.49	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.47
23:C:513:CLA:H161	32:C:519:LMG:H421	1.97	0.47
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.15	0.47
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.97	0.47
13:o:58:ASN:C	13:o:60:ARG:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:z:32:ASP:O	19:z:36:SER:OG	2.18	0.47
33:d:406:LHG:H332	33:d:406:LHG:H302	1.77	0.47
26:B:620:SQD:H1	26:B:620:SQD:H462	1.97	0.46
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.96	0.46
32:c:521:LMG:H232	32:c:521:LMG:H391	1.97	0.46
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.96	0.46
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.96	0.46
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.46
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.97	0.46
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.98	0.46
8:I:35:LYS:O	8:I:37:LEU:N	2.48	0.46
29:a:415:PL9:H171	29:a:415:PL9:H151	1.57	0.46
13:O:25:THR:O	13:O:27:ARG:N	2.48	0.46
25:t:102:BCR:H11C	25:t:102:BCR:H341	1.83	0.46
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.14	0.46
19:Z:33:TRP:HZ2	32:Z:101:LMG:HC61	1.81	0.46
20:R:18:TRP:O	20:R:22:ASN:ND2	2.41	0.46
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.98	0.46
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.47	0.46
25:K:103:BCR:H24C	25:K:103:BCR:H371	1.70	0.46
23:c:505:CLA:H62	35:c:519:DGD:HB62	1.97	0.46
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.61	0.46
23:A:408:CLA:H41	23:A:408:CLA:H61	1.58	0.46
3:C:130:VAL:O	3:C:134:ILE:HG12	2.16	0.46
25:T:102:BCR:HC7	25:T:102:BCR:H331	1.60	0.46
23:C:504:CLA:H62	23:C:504:CLA:H41	1.74	0.46
23:C:510:CLA:H112	23:C:510:CLA:H152	1.43	0.46
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.70	0.46
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.16	0.45
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.45
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.79	0.45
23:a:406:CLA:HBA1	23:a:406:CLA:C4A	2.45	0.45
3:c:182:PHE:HA	34:c:522:HTG:H61	1.99	0.45
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.31	0.45
2:B:133:LEU:HB2	27:B:627:GOL:H31	1.99	0.45
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.98	0.45
23:b:602:CLA:HHC	23:b:602:CLA:HBB1	1.97	0.45
23:A:408:CLA:H171	23:C:506:CLA:H121	1.98	0.45
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.72	0.45
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.98	0.45
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.76	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:403:BCR:C8	25:d:403:BCR:H331	2.47	0.45
3:C:443:TRP:CE2	23:C:508:CLA:HMD2	2.52	0.45
26:a:411:SQD:H271	33:d:406:LHG:H141	1.98	0.45
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.98	0.45
33:d:406:LHG:H342	33:d:406:LHG:H151	1.99	0.45
25:t:102:BCR:H382	25:t:102:BCR:H23C	1.98	0.45
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.99	0.45
23:b:605:CLA:H62	23:b:605:CLA:H41	1.68	0.45
35:h:102:DGD:HB61	35:h:102:DGD:HB91	1.87	0.45
26:A:410:SQD:H361	10:K:34:ALA:HA	1.99	0.45
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.99	0.45
13:O:130:GLN:H	13:O:130:GLN:CD	2.20	0.45
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.52	0.45
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.52	0.45
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.99	0.45
20:R:8:VAL:O	20:R:11:PRO:HD2	2.17	0.45
23:a:407:CLA:H203	32:d:410:LMG:H412	1.98	0.44
32:B:621:LMG:H112	32:B:621:LMG:H141	1.78	0.44
25:H:101:BCR:H331	25:H:101:BCR:C8	2.47	0.44
23:B:610:CLA:H162	23:B:612:CLA:O1A	2.17	0.44
23:a:405:CLA:H203	23:a:405:CLA:H162	1.80	0.44
23:b:601:CLA:H92	25:h:101:BCR:H403	1.99	0.44
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.82	0.44
3:C:406:SER:HA	3:C:420:VAL:HG23	1.99	0.44
4:D:261:PHE:CZ	33:D:406:LHG:HC81	2.52	0.44
25:T:102:BCR:H24C	25:T:102:BCR:H371	1.82	0.44
3:c:203:THR:O	3:c:235:GLY:HA3	2.18	0.44
4:d:266:TRP:CD1	33:d:405:LHG:HC31	2.52	0.44
34:B:622:HTG:H4'1	31:B:630:LMT:H52	1.99	0.44
31:B:628:LMT:H91	31:B:628:LMT:H62	1.54	0.44
8:I:36:ASP:OD1	8:I:36:ASP:N	2.51	0.44
3:c:406:SER:HA	3:c:420:VAL:HG23	2.00	0.44
4:d:85:MET:CE	4:d:96:GLU:HG2	2.46	0.44
33:E:101:LHG:H241	33:E:101:LHG:HC61	1.85	0.44
41:L:206:HOH:O	14:T:25[A]:GLU:HG3	2.18	0.44
23:c:513:CLA:HMB2	23:c:513:CLA:H192	2.00	0.44
4:d:14:TRP:CD1	34:d:409:HTG:H61	2.52	0.44
23:d:402:CLA:H41	23:d:402:CLA:H61	1.72	0.44
26:b:620:SQD:H462	26:b:620:SQD:H1	1.99	0.44
23:c:510:CLA:H91	23:c:510:CLA:H111	1.84	0.44
29:A:414:PL9:H322	29:A:414:PL9:H301	1.77	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414:PL9:H472	4:D:39:PRO:HD3	2.00	0.44
23:B:612:CLA:H61	23:B:612:CLA:H102	1.85	0.44
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.00	0.44
1:a:14:TRP:HD1	31:c:501:LMT:H6'1	1.83	0.44
24:a:417:PHO:HBC3	4:d:279:LEU:HD22	1.99	0.44
3:c:95:LEU:HD21	23:c:502:CLA:OBD	2.18	0.44
23:c:513:CLA:H121	23:c:514:CLA:H142	1.99	0.44
23:d:401:CLA:HAA2	23:d:401:CLA:HBD	2.00	0.44
13:o:92:SER:HB3	13:o:131:PRO:HA	1.98	0.44
10:K:16:ALA:O	10:K:19:ASP:HB2	2.17	0.43
35:c:517:DGD:HG11	41:c:605:HOH:O	2.18	0.43
25:d:403:BCR:H15C	25:d:403:BCR:H351	1.79	0.43
25:b:618:BCR:H24C	25:b:618:BCR:H371	1.84	0.43
27:b:628:GOL:H11	41:d:502:HOH:O	2.17	0.43
3:C:223:TRP:CG	3:C:224:ILE:H	2.36	0.43
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.18	0.43
23:C:505:CLA:H93	23:C:505:CLA:H111	1.77	0.43
23:A:404:CLA:H143	24:A:407:PHO:H61	2.01	0.43
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.69	0.43
23:B:610:CLA:H161	23:B:615:CLA:CAD	2.48	0.43
3:C:279:LEU:HA	3:C:282:MET:HE3	2.01	0.43
23:c:506:CLA:HMD2	23:c:508:CLA:HAB	2.00	0.43
35:c:518:DGD:HAT1	35:c:519:DGD:HBF2	2.01	0.43
33:d:406:LHG:H242	33:d:406:LHG:H272	1.86	0.43
11:l:20:GLY:O	11:l:24:ILE:HG12	2.17	0.43
3:C:114:VAL:HG22	32:C:519:LMG:H182	2.00	0.43
33:D:406:LHG:HC62	11:L:15:THR:HG23	2.00	0.43
1:a:105:TRP:CE2	1:a:110:GLY:HA3	2.53	0.43
23:A:404:CLA:HBB1	23:A:404:CLA:HMB3	2.01	0.43
25:C:514:BCR:H11C	25:C:514:BCR:H341	1.90	0.43
35:C:515:DGD:HG11	41:C:601:HOH:O	2.18	0.43
34:D:410:HTG:H1'2	7:H:25:TRP:CZ3	2.54	0.43
23:b:615:CLA:H91	23:b:615:CLA:H112	1.78	0.43
5:e:68:ASP:O	5:e:72:ALA:HB2	2.19	0.43
14:t:3:THR:OG1	41:t:201:HOH:O	2.21	0.43
16:v:85:GLU:OE2	41:v:301:HOH:O	2.21	0.43
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.91	0.43
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.84	0.43
23:A:405:CLA:HHC	23:A:405:CLA:HBB1	2.01	0.43
24:A:416:PHO:H3A	23:D:402:CLA:H142	1.99	0.43
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:601:CLA:H72	23:B:601:CLA:C4D	2.48	0.43
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.01	0.43
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.77	0.43
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.88	0.43
35:C:516:DGD:HAT1	35:C:517:DGD:HBE1	2.00	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.68	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.19	0.43
23:b:607:CLA:H91	23:b:607:CLA:H112	1.66	0.43
23:b:614:CLA:H112	23:b:614:CLA:H72	1.59	0.43
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	2.00	0.43
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.80	0.43
3:C:176:VAL:HG21	3:C:238:ILE:HG13	2.01	0.42
23:c:506:CLA:H93	23:c:506:CLA:H111	1.86	0.42
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.83	0.42
23:B:605:CLA:H62	23:B:605:CLA:H41	1.85	0.42
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.19	0.42
2:b:491:VAL:HG13	4:d:136:VAL:HG13	2.02	0.42
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.01	0.42
33:a:421:LHG:H241	33:a:421:LHG:HC61	1.89	0.42
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.54	0.42
23:b:601:CLA:H91	23:b:601:CLA:H111	1.86	0.42
25:c:516:BCR:H24C	25:c:516:BCR:H371	1.85	0.42
25:h:101:BCR:H24C	25:h:101:BCR:H371	1.69	0.42
10:k:24:VAL:HG21	18:y:25:ILE:HB	2.01	0.42
25:T:102:BCR:HC8	25:T:102:BCR:H321	2.01	0.42
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.86	0.42
29:A:414:PL9:H171	29:A:414:PL9:H151	1.53	0.42
2:B:357[A]:ARG:HH12	27:B:624:GOL:C3	2.32	0.42
23:B:614:CLA:H8	25:B:617:BCR:H362	2.01	0.42
17:X:33:GLN:O	17:X:36:LYS:NZ	2.50	0.42
23:c:513:CLA:HBA2	23:c:513:CLA:H3A	1.80	0.42
23:c:514:CLA:H171	25:c:515:BCR:H373	2.02	0.42
19:z:26:ALA:HB3	19:z:40:ILE:HD11	2.02	0.42
31:A:421:LMT:H6'2	31:A:421:LMT:O3'	2.20	0.42
2:B:445:THR:HA	41:B:705:HOH:O	2.18	0.42
23:B:603:CLA:H102	23:B:603:CLA:H61	1.84	0.42
3:C:338:GLY:HA3	3:C:341:LEU:O	2.20	0.42
23:C:505:CLA:HAA1	23:C:505:CLA:HBD	2.01	0.42
25:a:410:BCR:H11C	25:a:410:BCR:H341	1.86	0.42
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.55	0.42
23:B:602:CLA:H162	23:B:602:CLA:H203	1.65	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:B:622:HTG:H6'2	34:B:622:HTG:H3'1	1.88	0.42
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.95	0.42
33:D:407:LHG:H332	33:D:407:LHG:H302	1.85	0.42
32:Z:101:LMG:H141	32:Z:101:LMG:H111	1.88	0.42
1:A:183:MET:HA	23:A:404:CLA:HMD1	2.01	0.42
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.55	0.42
3:C:42:LEU:HD21	23:C:511:CLA:H2A	2.01	0.42
23:C:506:CLA:H18	23:C:506:CLA:H152	1.50	0.42
35:C:517:DGD:HBE2	35:C:517:DGD:HB81	1.82	0.42
23:A:405:CLA:C4A	23:A:405:CLA:HBA1	2.50	0.42
33:D:407:LHG:H382	33:D:407:LHG:C11	2.45	0.42
2:b:450:TRP:HB3	23:b:607:CLA:HMB1	2.02	0.42
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.02	0.42
3:c:363:GLY:O	3:c:367:GLU:HG2	2.20	0.42
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.55	0.42
2:B:363:PHE:HB3	2:B:365:SER:O	2.19	0.41
4:D:126:MET:HE3	4:D:143:ALA:O	2.20	0.41
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.41
16:V:41:HIS:CD2	40:V:201:HEC:NB	2.88	0.41
2:b:233:ASN:O	2:b:236:THR:HG22	2.20	0.41
23:A:404:CLA:H192	23:A:404:CLA:H161	1.80	0.41
33:A:420:LHG:H361	23:B:613:CLA:H51	2.02	0.41
3:C:363:GLY:O	3:C:367:GLU:HG2	2.21	0.41
33:D:407:LHG:H362	33:D:407:LHG:H331	1.86	0.41
15:U:45:LEU:HD23	15:U:45:LEU:HA	1.94	0.41
25:a:410:BCR:H24C	25:a:410:BCR:H371	1.72	0.41
2:b:149[B]:LEU:HD21	23:b:604:CLA:H171	2.02	0.41
3:c:425:TRP:CD1	23:c:505:CLA:HMA3	2.55	0.41
4:d:58:TRP:CH2	5:e:63:ILE:HD12	2.55	0.41
33:A:420:LHG:H252	2:B:464:PHE:CZ	2.55	0.41
2:B:58:GLN:C	2:B:329:PRO:HB3	2.46	0.41
1:a:261:GLN:HG3	2:b:493:TRP:CH2	2.56	0.41
26:a:411:SQD:H321	23:c:509:CLA:H102	2.02	0.41
13:O:4:THR:O	13:O:4:THR:OG1	2.33	0.41
1:a:214:MET:HB3	29:a:415:PL9:H103	2.01	0.41
24:a:417:PHO:H42	24:a:417:PHO:H11	1.92	0.41
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.50	0.41
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.03	0.41
33:d:406:LHG:H372	33:d:406:LHG:H142	2.03	0.41
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.51	0.41
25:K:101:BCR:H15C	25:K:101:BCR:H351	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:152:LYS:HD2	41:c:742:HOH:O	2.21	0.41
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.97	0.41
20:R:2:ASP:HB3	20:R:5:VAL:HG23	2.02	0.41
1:A:85:SER:HA	1:A:109:GLY:HA3	2.03	0.41
23:C:508:CLA:H122	23:C:508:CLA:H162	1.87	0.41
23:C:508:CLA:H142	23:C:508:CLA:H111	1.83	0.41
13:O:24:ASP:HA	13:O:203:LYS:HE2	2.03	0.41
13:O:110:MET:HE2	13:O:110:MET:HB3	1.92	0.41
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.21	0.41
1:a:93:PHE:CD2	1:a:95:PRO:HD3	2.55	0.41
23:c:509:CLA:H162	23:c:509:CLA:H122	1.73	0.41
25:c:516:BCR:H11C	25:c:516:BCR:H341	1.96	0.41
6:f:45:ARG:HG2	41:f:201:HOH:O	2.20	0.41
10:k:20:PRO:HB3	18:y:21:GLN:HG3	2.03	0.41
20:R:24:LEU:N	20:R:25:PRO:HD2	2.34	0.41
31:B:631:LMT:H6E	31:t:101:LMT:H6D	2.03	0.41
5:E:18:ARG:H	9:J:2:SER:N	2.18	0.41
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.85	0.41
33:E:101:LHG:H291	33:E:101:LHG:H261	1.75	0.41
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.55	0.41
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.79	0.41
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	2.03	0.41
2:B:365:SER:OG	27:B:629:GOL:H32	2.21	0.41
4:D:209:LEU:HD23	4:D:209:LEU:C	2.46	0.41
13:O:93:LEU:O	13:O:128:SER:HA	2.20	0.41
23:c:508:CLA:HAA2	23:c:508:CLA:HBD	2.01	0.41
23:B:604:CLA:HMD2	23:B:612:CLA:H203	2.02	0.41
23:B:606:CLA:H151	23:B:616:CLA:H122	2.03	0.41
8:I:2:GLU:O	8:I:6:ILE:HG12	2.20	0.41
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.84	0.41
1:a:131:TRP:CH2	23:c:506:CLA:HAA2	2.56	0.41
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.89	0.41
23:b:614:CLA:H62	23:b:614:CLA:H41	1.74	0.41
3:c:344:SER:O	13:o:75:THR:HG22	2.21	0.41
1:A:243:GLU:CD	1:A:243:GLU:H	2.27	0.40
23:A:404:CLA:CBD	23:A:405:CLA:HAC2	2.51	0.40
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.88	0.40
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.57	0.40
10:K:20:PRO:HB3	18:Y:21:GLN:HG3	2.03	0.40
25:T:102:BCR:H351	26:b:620:SQD:H211	2.03	0.40
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414:PL9:H121	29:A:414:PL9:HC8	1.78	0.40
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.90	0.40
2:B:477:ASP:OD1	2:B:477:ASP:N	2.54	0.40
25:D:404:BCR:H11C	25:D:404:BCR:H341	1.99	0.40
25:D:404:BCR:H20C	25:D:404:BCR:H361	1.91	0.40
25:K:101:BCR:H24C	25:K:101:BCR:H371	1.81	0.40
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.03	0.40
27:b:629:GOL:H12	4:d:326:ARG:HB2	2.03	0.40
15:u:58:VAL:HG12	15:u:79:LEU:HD22	2.02	0.40
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.90	0.40
2:B:162:PHE:O	23:B:606:CLA:HHD	2.22	0.40
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.94	0.40
33:E:101:LHG:O2	6:F:19:ARG:NH1	2.54	0.40
4:d:55:VAL:O	4:d:66:SER:HB3	2.22	0.40
1:A:131:TRP:CD2	1:A:131:TRP:C	2.98	0.40
29:A:414:PL9:HC8	29:A:414:PL9:HC2	1.71	0.40
25:T:102:BCR:H11C	25:T:102:BCR:H341	1.83	0.40
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.53	0.40
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.84	0.40
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.36	0.40
29:A:414:PL9:H221	29:A:414:PL9:H201	1.86	0.40
35:C:516:DGD:HAE2	35:C:516:DGD:HA81	1.86	0.40
4:D:49:LEU:HD13	25:D:404:BCR:C15	2.51	0.40
27:a:420:GOL:C3	12:m:1:FME:HG2	2.51	0.40
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.57	0.40
3:c:48:LYS:HG3	3:c:138:GLU:HG3	2.04	0.40
3:c:443:TRP:CZ2	23:c:509:CLA:HMD1	2.56	0.40
26:f:102:SQD:H462	26:f:102:SQD:O7	2.22	0.40
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.96	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	333/344 (97%)	328 (98%)	4 (1%)	1 (0%)	36	34
1	a	334/344 (97%)	327 (98%)	6 (2%)	1 (0%)	36	34
2	B	509/505 (101%)	501 (98%)	8 (2%)	0	100	100
2	b	508/505 (101%)	496 (98%)	12 (2%)	0	100	100
3	C	450/455 (99%)	443 (98%)	6 (1%)	1 (0%)	43	44
3	c	458/455 (101%)	449 (98%)	8 (2%)	1 (0%)	43	44
4	D	341/342 (100%)	327 (96%)	14 (4%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
7	h	63/65 (97%)	60 (95%)	2 (3%)	1 (2%)	7	3
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	1
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	34/37 (92%)	34 (100%)	0	0	100	100
11	l	34/37 (92%)	34 (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	244/244 (100%)	237 (97%)	5 (2%)	2 (1%)	16	10
13	o	241/244 (99%)	237 (98%)	4 (2%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	28/32 (88%)	28 (100%)	0	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	94 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	133 (97%)	4 (3%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100 100
17	x	36/40 (90%)	36 (100%)	0	0	100 100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100 100
18	y	27/30 (90%)	27 (100%)	0	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7 2
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 2
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	5252/5384 (98%)	5138 (98%)	104 (2%)	10 (0%)	43 44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
13	O	138	THR
7	h	63	LYS
1	a	259	ILE
1	A	259	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	270/279 (97%)	268 (99%)	2 (1%)	76 82
1	a	271/279 (97%)	270 (100%)	1 (0%)	84 89
2	B	409/403 (102%)	404 (99%)	5 (1%)	63 70
2	b	408/403 (101%)	403 (99%)	5 (1%)	63 70
3	C	353/356 (99%)	346 (98%)	7 (2%)	48 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	c	361/356 (101%)	355 (98%)	6 (2%)	53 60
4	D	278/277 (100%)	276 (99%)	2 (1%)	76 82
4	d	278/277 (100%)	276 (99%)	2 (1%)	76 82
5	E	72/73 (99%)	71 (99%)	1 (1%)	59 66
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 66
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30 30
7	h	55/54 (102%)	54 (98%)	1 (2%)	51 58
8	I	34/34 (100%)	32 (94%)	2 (6%)	18 13
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 39
9	J	26/27 (96%)	25 (96%)	1 (4%)	29 29
9	j	26/27 (96%)	25 (96%)	1 (4%)	29 29
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 1
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 3
11	L	34/35 (97%)	34 (100%)	0	100 100
11	l	34/35 (97%)	34 (100%)	0	100 100
12	M	30/32 (94%)	27 (90%)	3 (10%)	7 3
12	m	32/32 (100%)	29 (91%)	3 (9%)	8 4
13	O	209/207 (101%)	203 (97%)	6 (3%)	37 39
13	o	206/207 (100%)	200 (97%)	6 (3%)	37 39
14	T	27/28 (96%)	24 (89%)	3 (11%)	6 3
14	t	26/28 (93%)	26 (100%)	0	100 100
15	U	84/89 (94%)	82 (98%)	2 (2%)	43 47
15	u	85/89 (96%)	83 (98%)	2 (2%)	43 47
16	V	119/117 (102%)	118 (99%)	1 (1%)	73 79
16	v	117/117 (100%)	113 (97%)	4 (3%)	32 33
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%)	19 (86%)	3 (14%)	3 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 14
19	z	52/52 (100%)	46 (88%)	6 (12%)	5 2
20	R	29/29 (100%)	27 (93%)	2 (7%)	14 9
All	All	4358/4403 (99%)	4267 (98%)	91 (2%)	48 52

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	243	GLU
2	B	161	LEU
2	B	294	SER
2	B	299	GLU
2	B	389	LYS
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	142	GLU
3	C	240	ILE
3	C	255	THR
3	C	289	PHE
3	C	315	MET
4	D	259	ILE
4	D	338	ASN
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
12	M	20	VAL
13	O	4	THR
13	O	49	THR
13	O	55	GLU
13	O	98[A]	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	O	98[B]	GLU
13	O	234	LYS
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
1	a	13	LEU
2	b	128	THR
2	b	161	LEU
2	b	362	PHE
2	b	486	LEU
2	b	491	VAL
3	c	142	GLU
3	c	152	LYS
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315	MET
4	d	259	ILE
4	d	272	LEU
5	e	71	GLU
7	h	65	LEU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
12	m	9	ILE
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	v	85	GLU
16	v	106	ASN
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	20	VAL
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	34	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	296	ASN
4	D	142	ASN
4	D	186	GLN
4	D	250	ASN
4	D	301	GLN
5	E	60	GLN
11	L	8	GLN
12	M	28	GLN
13	O	155	ASN
13	O	231	HIS
15	U	78	ASN
1	a	165	GLN
1	a	296	ASN
2	b	14	ASN
2	b	331	ASN
3	c	201	ASN
4	d	186	GLN
11	l	8	GLN
13	o	58	ASN
13	o	88	ASN
15	u	78	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	v	86	GLN
18	y	45	ASN

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	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	0.66	0	7,9,11	1.24	0
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.28	0
14	FME	T	1	14	8,9,10	0.71	0	7,9,11	1.68	2 (28%)
8	FME	I	1	8	8,9,10	0.55	0	7,9,11	1.24	1 (14%)
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.38	1 (14%)
14	FME	t	1	14	8,9,10	0.62	0	7,9,11	1.63	2 (28%)

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

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

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-2.69	118.69	122.82
14	T	1	FME	CG-CB-CA	2.51	119.91	112.95
14	T	1	FME	CA-N-CN	2.43	126.55	122.82
14	t	1	FME	O-C-CA	-2.42	118.42	124.78
12	m	1	FME	O1-CN-N	-2.26	119.31	125.27
8	I	1	FME	O-C-CA	-2.19	119.04	124.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	M	1	FME	1	0
12	m	1	FME	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 225 ligands modelled in this entry, 15 are monoatomic and 18 are unknown - leaving 192 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	$\#\|Z\|>2$
27	GOL	C	521	-	5,5,5	1.18	0	5,5,5	0.83	0
27	GOL	b	628	-	5,5,5	0.40	0	5,5,5	1.38	1 (20%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.57	10 (19%)
23	CLA	c	514	3	69,73,73	2.10	21 (30%)	83,113,113	2.84	30 (36%)
27	GOL	O	303	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)
23	CLA	C	507	41	69,73,73	1.99	19 (27%)	83,113,113	2.80	29 (34%)
23	CLA	c	504	3	69,73,73	2.04	19 (27%)	83,113,113	2.85	28 (33%)
23	CLA	B	607	41	69,73,73	1.94	20 (28%)	83,113,113	2.80	29 (34%)
23	CLA	C	502	3	69,73,73	2.02	20 (28%)	83,113,113	2.71	28 (33%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.32	8 (14%)
32	LMG	z	101	-	39,39,55	1.08	2 (5%)	47,47,63	1.07	3 (6%)
31	LMT	e	101	-	36,36,36	1.04	4 (11%)	47,47,47	0.97	1 (2%)
35	DGD	C	516	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.93	30 (36%)
40	HEC	v	201	16	50,50,50	1.74	6 (12%)	68,82,82	1.45	10 (14%)
23	CLA	B	604	2	69,73,73	1.97	22 (31%)	83,113,113	2.74	31 (37%)
23	CLA	C	511	3	69,73,73	2.01	20 (28%)	83,113,113	2.79	26 (31%)
23	CLA	d	401	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
25	BCR	B	617	-	41,41,41	1.04	1 (2%)	56,56,56	1.25	3 (5%)
25	BCR	K	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	6 (10%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.61	11 (17%)
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.07	6 (7%)
25	BCR	D	404	-	41,41,41	1.07	1 (2%)	56,56,56	1.80	15 (26%)
23	CLA	C	508	3	69,73,73	2.06	19 (27%)	83,113,113	2.78	28 (33%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.72	14 (25%)
33	LHG	L	101	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
31	LMT	t	101	-	26,26,36	0.93	2 (7%)	31,31,47	1.31	2 (6%)
23	CLA	a	406	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
23	CLA	A	404	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
31	LMT	B	631	-	25,25,36	0.90	2 (8%)	30,30,47	1.12	3 (10%)
23	CLA	c	512	3	69,73,73	2.07	20 (28%)	83,113,113	2.79	33 (39%)
34	HTG	c	522	-	19,19,19	0.97	2 (10%)	23,24,24	1.54	2 (8%)
26	SQD	B	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.75	14 (22%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.29	6 (10%)
23	CLA	C	512	3	69,73,73	2.05	20 (28%)	83,113,113	2.87	34 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	616	2	69,73,73	2.00	18 (26%)	83,113,113	2.97	29 (34%)
25	BCR	t	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	12 (21%)
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	83,113,113	2.81	30 (36%)
23	CLA	D	403	4	69,73,73	2.08	18 (26%)	83,113,113	2.80	32 (38%)
23	CLA	C	505	3	69,73,73	2.01	19 (27%)	83,113,113	2.81	31 (37%)
33	LHG	A	420	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
23	CLA	b	609	2	69,73,73	2.01	19 (27%)	83,113,113	2.76	32 (38%)
23	CLA	C	506	3	69,73,73	2.03	21 (30%)	83,113,113	2.78	31 (37%)
23	CLA	B	605	2	69,73,73	2.00	18 (26%)	83,113,113	2.93	30 (36%)
24	PHO	A	407	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
25	BCR	B	619	-	41,41,41	1.06	1 (2%)	56,56,56	1.30	7 (12%)
25	BCR	T	102	-	41,41,41	1.02	1 (2%)	56,56,56	1.55	12 (21%)
23	CLA	b	608	2	69,73,73	1.96	19 (27%)	83,113,113	2.86	32 (38%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.33	5 (8%)
27	GOL	a	419	-	5,5,5	1.02	0	5,5,5	0.97	0
33	LHG	d	411	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	616	2	69,73,73	1.97	20 (28%)	83,113,113	2.86	26 (31%)
23	CLA	B	614	2	69,73,73	2.02	19 (27%)	83,113,113	2.98	32 (38%)
27	GOL	o	302	-	5,5,5	0.94	0	5,5,5	0.95	0
40	HEC	V	201	16	50,50,50	1.75	8 (16%)	68,82,82	1.50	8 (11%)
23	CLA	B	610	41	69,73,73	2.06	19 (27%)	83,113,113	2.92	31 (37%)
23	CLA	b	615	2	69,73,73	1.99	18 (26%)	83,113,113	2.82	31 (37%)
32	LMG	Z	101	-	37,37,55	0.99	2 (5%)	45,45,63	1.42	5 (11%)
37	BCT	D	401	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
24	PHO	A	416	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.16	6 (9%)
23	CLA	A	406	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
31	LMT	m	103	-	36,36,36	1.10	4 (11%)	47,47,47	1.06	3 (6%)
32	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.43	8 (13%)
31	LMT	A	421	-	36,36,36	1.06	4 (11%)	47,47,47	1.14	4 (8%)
23	CLA	b	613	2	69,73,73	1.94	19 (27%)	83,113,113	2.82	32 (38%)
23	CLA	c	503	3	69,73,73	1.97	19 (27%)	83,113,113	2.77	27 (32%)
27	GOL	V	203	-	5,5,5	1.22	0	5,5,5	0.91	0
35	DGD	H	102	-	63,63,67	0.85	4 (6%)	77,77,81	0.97	6 (7%)
33	LHG	D	406	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HTG	V	202	-	11,11,19	0.23	0	15,15,24	1.08	1 (6%)
25	BCR	d	403	-	41,41,41	1.11	1 (2%)	56,56,56	1.89	18 (32%)
23	CLA	b	607	41	69,73,73	1.95	21 (30%)	83,113,113	2.77	29 (34%)
33	LHG	d	406	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	C	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.81	31 (37%)
23	CLA	C	504	41	69,73,73	1.98	20 (28%)	83,113,113	2.75	30 (36%)
26	SQD	A	410	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
27	GOL	A	418	-	5,5,5	1.58	2 (40%)	5,5,5	1.02	1 (20%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.02	0
27	GOL	c	527	-	5,5,5	0.97	0	5,5,5	0.98	0
34	HTG	b	625	-	19,19,19	1.01	2 (10%)	23,24,24	1.61	5 (21%)
32	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	6 (10%)
26	SQD	a	411	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
27	GOL	b	629	-	5,5,5	1.07	0	5,5,5	0.91	0
23	CLA	c	513	3	69,73,73	2.06	20 (28%)	83,113,113	2.85	32 (38%)
23	CLA	c	506	3	69,73,73	2.00	19 (27%)	83,113,113	2.77	30 (36%)
23	CLA	c	505	41	69,73,73	2.05	21 (30%)	83,113,113	2.82	30 (36%)
31	LMT	b	627	-	25,25,36	0.89	2 (8%)	30,30,47	1.10	1 (3%)
23	CLA	C	501	3	69,73,73	1.98	20 (28%)	83,113,113	2.82	30 (36%)
28	OEX	A	413	1,41,3	0,14,14	-	-	-		
23	CLA	A	405	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
35	DGD	c	517	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
31	LMT	F	101	-	36,36,36	1.08	3 (8%)	47,47,47	1.02	2 (4%)
23	CLA	c	510	3	69,73,73	2.04	19 (27%)	83,113,113	2.85	31 (37%)
37	BCT	a	404	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	c	511	3	69,73,73	1.99	20 (28%)	83,113,113	2.85	31 (37%)
31	LMT	M	101	-	36,36,36	1.15	3 (8%)	47,47,47	1.21	4 (8%)
31	LMT	b	621	-	25,25,36	0.97	2 (8%)	30,30,47	1.17	1 (3%)
35	DGD	C	515	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
23	CLA	B	608	2	69,73,73	1.90	20 (28%)	83,113,113	2.85	34 (40%)
33	LHG	E	101	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
32	LMG	C	518	-	51,51,55	0.93	2 (3%)	59,59,63	1.11	4 (6%)
32	LMG	c	521	-	51,51,55	0.99	2 (3%)	59,59,63	1.36	7 (11%)
23	CLA	C	503	3	69,73,73	2.00	19 (27%)	83,113,113	2.89	30 (36%)
27	GOL	B	627	-	5,5,5	0.95	0	5,5,5	0.99	0
32	LMG	B	621	-	51,51,55	0.91	2 (3%)	59,59,63	1.28	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMG	a	418	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	4 (6%)
25	BCR	c	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.61	12 (21%)
31	LMT	c	501	-	36,36,36	1.03	1 (2%)	47,47,47	1.02	1 (2%)
31	LMT	B	630	-	36,36,36	1.00	3 (8%)	47,47,47	1.14	3 (6%)
27	GOL	o	303	-	5,5,5	1.04	0	5,5,5	1.04	0
23	CLA	B	602	2	69,73,73	2.02	20 (28%)	83,113,113	2.86	29 (34%)
23	CLA	b	611	2	69,73,73	1.93	20 (28%)	83,113,113	2.91	30 (36%)
34	HTG	b	623	-	19,19,19	1.05	1 (5%)	23,24,24	1.87	2 (8%)
23	CLA	B	612	2	69,73,73	2.00	19 (27%)	83,113,113	2.82	31 (37%)
26	SQD	a	413	-	53,54,54	1.05	3 (5%)	62,65,65	1.19	8 (12%)
23	CLA	b	603	2	69,73,73	1.96	19 (27%)	83,113,113	2.88	30 (36%)
23	CLA	B	613	2	69,73,73	1.99	19 (27%)	83,113,113	2.80	30 (36%)
31	LMT	A	417	-	36,36,36	0.96	3 (8%)	47,47,47	1.01	1 (2%)
23	CLA	B	611	2	69,73,73	2.51	20 (28%)	83,113,113	3.98	30 (36%)
23	CLA	c	502	3	69,73,73	2.00	21 (30%)	83,113,113	2.84	30 (36%)
23	CLA	B	606	2	69,73,73	1.98	20 (28%)	83,113,113	2.94	32 (38%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.66	12 (21%)
27	GOL	c	526	-	5,5,5	0.94	0	5,5,5	0.95	0
28	OEX	a	414	1,41,3	0,14,14	-	-	-		
32	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.22	5 (8%)
35	DGD	c	519	-	63,63,67	0.87	3 (4%)	77,77,81	1.00	5 (6%)
31	LMT	B	628	-	36,36,36	1.17	4 (11%)	47,47,47	1.30	5 (10%)
23	CLA	b	602	2	69,73,73	2.06	19 (27%)	83,113,113	2.93	36 (43%)
23	CLA	c	509	3	69,73,73	2.09	20 (28%)	83,113,113	2.80	29 (34%)
25	BCR	K	103	-	41,41,41	1.03	1 (2%)	56,56,56	1.44	9 (16%)
35	DGD	c	518	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	b	612	2	69,73,73	1.97	19 (27%)	83,113,113	2.81	29 (34%)
34	HTG	B	623	-	19,19,19	0.79	1 (5%)	23,24,24	1.47	2 (8%)
23	CLA	C	510	3	69,73,73	2.07	20 (28%)	83,113,113	2.91	33 (39%)
34	HTG	C	520	-	19,19,19	0.89	1 (5%)	23,24,24	1.33	2 (8%)
26	SQD	F	103	-	42,43,54	1.19	4 (9%)	51,54,65	2.02	12 (23%)
33	LHG	b	630	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
27	GOL	B	629	-	5,5,5	1.32	1 (20%)	5,5,5	0.90	0
34	HTG	B	622	-	19,19,19	1.16	2 (10%)	23,24,24	1.52	5 (21%)
32	LMG	d	410	39	51,51,55	0.90	2 (3%)	59,59,63	1.10	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	HEM	F	102	5,6	50,50,50	1.53	7 (14%)	66,82,82	1.85	16 (24%)
24	PHO	a	408	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
27	GOL	A	411	-	5,5,5	1.14	0	5,5,5	0.71	0
27	GOL	b	624	-	5,5,5	1.15	1 (20%)	5,5,5	0.81	0
29	PL9	D	405	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
32	LMG	C	519	-	51,51,55	1.05	3 (5%)	59,59,63	1.31	5 (8%)
27	GOL	O	302	-	5,5,5	0.92	0	5,5,5	0.95	0
33	LHG	a	421	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
34	HTG	B	625	-	19,19,19	1.04	2 (10%)	23,24,24	1.22	3 (13%)
29	PL9	A	414	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
23	CLA	B	601	41	69,73,73	2.08	21 (30%)	83,113,113	2.84	29 (34%)
32	LMG	D	411	39	51,51,55	0.84	2 (3%)	59,59,63	1.01	3 (5%)
33	LHG	d	405	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
27	GOL	v	202	-	5,5,5	1.27	0	5,5,5	0.72	0
25	BCR	k	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.52	12 (21%)
31	LMT	T	101	-	36,36,36	1.09	3 (8%)	47,47,47	1.07	2 (4%)
25	BCR	a	410	-	41,41,41	1.03	1 (2%)	56,56,56	1.39	9 (16%)
33	LHG	D	407	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
25	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.23	7 (12%)
27	GOL	l	102	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	c	508	41	69,73,73	2.03	18 (26%)	83,113,113	2.83	29 (34%)
29	PL9	d	404	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
34	HTG	b	622	-	19,19,19	1.20	2 (10%)	23,24,24	1.94	7 (30%)
25	BCR	B	618	-	41,41,41	0.97	1 (2%)	56,56,56	1.33	7 (12%)
25	BCR	C	514	-	41,41,41	1.03	1 (2%)	56,56,56	1.38	8 (14%)
23	CLA	D	402	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	b	605	2	69,73,73	1.96	19 (27%)	83,113,113	3.03	28 (33%)
23	CLA	a	405	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)
23	CLA	c	507	3	69,73,73	2.02	21 (30%)	83,113,113	2.78	30 (36%)
23	CLA	a	407	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
27	GOL	a	420	-	5,5,5	1.26	1 (20%)	5,5,5	0.87	0
23	CLA	a	409	1	69,73,73	1.97	19 (27%)	83,113,113	2.87	30 (36%)
25	BCR	c	516	-	41,41,41	1.03	1 (2%)	56,56,56	1.35	11 (19%)
35	DGD	C	517	-	63,63,67	0.87	3 (4%)	77,77,81	0.93	3 (3%)
24	PHO	a	417	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HTG	d	409	-	16,16,19	0.98	1 (6%)	20,21,24	1.59	1 (5%)
23	CLA	b	614	2	69,73,73	1.99	20 (28%)	83,113,113	2.94	31 (37%)
38	HEM	f	101	5,6	50,50,50	1.50	6 (12%)	66,82,82	1.71	12 (18%)
23	CLA	B	609	2	69,73,73	2.02	18 (26%)	83,113,113	2.79	29 (34%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	9 (16%)
34	HTG	D	410	-	16,16,19	1.08	2 (12%)	20,21,24	1.50	1 (5%)
23	CLA	b	606	2	69,73,73	1.99	19 (27%)	83,113,113	2.89	32 (38%)
23	CLA	B	603	2	69,73,73	2.00	19 (27%)	83,113,113	2.96	28 (33%)
29	PL9	a	415	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
23	CLA	B	615	2	69,73,73	2.04	20 (28%)	83,113,113	2.84	29 (34%)
23	CLA	d	402	4	69,73,73	2.03	20 (28%)	83,113,113	2.87	32 (38%)
23	CLA	b	604	2	69,73,73	2.01	19 (27%)	83,113,113	2.75	28 (33%)
23	CLA	A	408	1	69,73,73	1.97	20 (28%)	83,113,113	2.93	37 (44%)
27	GOL	B	624	-	5,5,5	0.88	0	5,5,5	1.13	1 (20%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.36	8 (14%)
23	CLA	b	610	41	69,73,73	2.00	20 (28%)	83,113,113	2.83	30 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	C	521	-	-	0/4/4/4	-
27	GOL	b	628	-	-	0/4/4/4	-
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	c	514	3	-	10/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
23	CLA	C	507	41	-	8/39/115/115	-
23	CLA	c	504	3	-	1/39/115/115	-
23	CLA	B	607	41	-	5/39/115/115	-
23	CLA	C	502	3	-	9/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
40	HEC	v	201	16	1/1/3/7	5/14/54/54	-
31	LMT	e	101	-	-	14/21/61/61	0/2/2/2
32	LMG	z	101	-	-	9/34/54/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	509	3	-	2/39/115/115	-
35	DGD	C	516	-	-	15/51/91/95	0/2/2/2
23	CLA	B	604	2	-	2/39/115/115	-
23	CLA	C	511	3	-	3/39/115/115	-
23	CLA	d	401	4	-	2/39/115/115	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
25	BCR	K	101	-	-	1/29/63/63	0/2/2/2
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	C	508	3	-	3/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
33	LHG	L	101	-	-	19/53/53/53	-
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
23	CLA	a	406	41	-	8/39/115/115	-
23	CLA	A	404	1	-	5/39/115/115	-
31	LMT	B	631	-	-	10/17/37/61	0/1/1/2
23	CLA	c	512	3	-	4/39/115/115	-
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
25	BCR	b	619	-	-	3/29/63/63	0/2/2/2
23	CLA	C	512	3	-	13/39/115/115	-
23	CLA	b	616	2	-	10/39/115/115	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	601	41	-	19/39/115/115	-
23	CLA	D	403	4	-	14/39/115/115	-
23	CLA	C	505	3	-	6/39/115/115	-
33	LHG	A	420	-	-	10/53/53/53	-
23	CLA	b	609	2	-	3/39/115/115	-
23	CLA	C	506	3	-	11/39/115/115	-
23	CLA	B	605	2	-	6/39/115/115	-
24	PHO	A	407	-	-	3/37/103/103	0/5/6/6
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	608	2	-	5/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	GOL	a	419	-	-	2/4/4/4	-
33	LHG	d	411	-	-	13/53/53/53	-
23	CLA	B	616	2	-	5/39/115/115	-
23	CLA	B	614	2	-	14/39/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
23	CLA	B	610	41	-	7/39/115/115	-
23	CLA	b	615	2	-	7/39/115/115	-
32	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
24	PHO	A	416	-	-	1/37/103/103	0/5/6/6
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
23	CLA	A	406	41	-	7/39/115/115	-
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2
32	LMG	A	419	-	-	13/46/66/70	0/1/1/1
31	LMT	A	421	-	-	15/21/61/61	0/2/2/2
23	CLA	b	613	2	-	3/39/115/115	-
23	CLA	c	503	3	-	8/39/115/115	-
27	GOL	V	203	-	-	2/4/4/4	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
33	LHG	D	406	-	-	16/53/53/53	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
25	BCR	d	403	-	-	5/29/63/63	0/2/2/2
23	CLA	b	607	41	-	2/39/115/115	-
33	LHG	d	406	-	-	11/53/53/53	-
23	CLA	C	513	3	-	7/39/115/115	-
23	CLA	C	504	41	-	8/39/115/115	-
26	SQD	A	410	-	-	12/49/69/69	0/1/1/1
27	GOL	A	418	-	-	2/4/4/4	-
27	GOL	a	412	-	-	4/4/4/4	-
27	GOL	c	527	-	-	4/4/4/4	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
32	LMG	c	520	-	-	11/46/66/70	0/1/1/1
26	SQD	a	411	-	-	10/49/69/69	0/1/1/1
27	GOL	b	629	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	513	3	-	13/39/115/115	-
23	CLA	c	506	3	-	8/39/115/115	-
23	CLA	c	505	41	-	9/39/115/115	-
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	C	501	3	-	6/39/115/115	-
23	CLA	A	405	41	-	4/39/115/115	-
35	DGD	c	517	-	-	20/51/91/95	0/2/2/2
31	LMT	F	101	-	-	9/21/61/61	0/2/2/2
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	c	511	3	-	11/39/115/115	-
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
35	DGD	C	515	-	-	11/51/91/95	0/2/2/2
23	CLA	B	608	2	-	3/39/115/115	-
33	LHG	E	101	-	-	22/46/46/53	-
32	LMG	C	518	-	-	8/46/66/70	0/1/1/1
32	LMG	c	521	-	-	7/46/66/70	0/1/1/1
23	CLA	C	503	3	-	3/39/115/115	-
27	GOL	B	627	-	-	2/4/4/4	-
32	LMG	B	621	-	-	19/46/66/70	0/1/1/1
32	LMG	a	418	-	-	13/46/66/70	0/1/1/1
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
31	LMT	c	501	-	-	11/21/61/61	0/2/2/2
31	LMT	B	630	-	-	11/21/61/61	0/2/2/2
27	GOL	o	303	-	-	4/4/4/4	-
23	CLA	B	602	2	-	10/39/115/115	-
23	CLA	b	611	2	-	3/39/115/115	-
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
23	CLA	B	612	2	-	5/39/115/115	-
26	SQD	a	413	-	-	15/49/69/69	0/1/1/1
23	CLA	b	603	2	-	5/39/115/115	-
23	CLA	B	613	2	-	8/39/115/115	-
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2
23	CLA	B	611	2	-	3/39/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	502	3	-	3/39/115/115	-
23	CLA	B	606	2	-	10/39/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
27	GOL	c	526	-	-	0/4/4/4	-
35	DGD	c	519	-	-	8/51/91/95	0/2/2/2
32	LMG	m	101	-	-	10/46/66/70	0/1/1/1
31	LMT	B	628	-	-	11/21/61/61	0/2/2/2
23	CLA	b	602	2	-	5/39/115/115	-
23	CLA	c	509	3	-	5/39/115/115	-
25	BCR	K	103	-	-	2/29/63/63	0/2/2/2
35	DGD	c	518	-	-	17/51/91/95	0/2/2/2
23	CLA	b	612	2	-	2/39/115/115	-
34	HTG	B	623	-	-	1/10/30/30	0/1/1/1
23	CLA	C	510	3	-	13/39/115/115	-
34	HTG	C	520	-	-	0/10/30/30	0/1/1/1
26	SQD	F	103	-	-	15/38/58/69	0/1/1/1
33	LHG	b	630	-	-	20/53/53/53	-
27	GOL	B	629	-	-	4/4/4/4	-
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
32	LMG	d	410	39	-	11/46/66/70	0/1/1/1
38	HEM	F	102	5,6	-	6/14/54/54	-
24	PHO	a	408	-	-	5/37/103/103	0/5/6/6
27	GOL	A	411	-	-	2/4/4/4	-
27	GOL	b	624	-	-	2/4/4/4	-
29	PL9	D	405	-	-	8/53/73/73	0/1/1/1
32	LMG	C	519	-	-	11/46/66/70	0/1/1/1
27	GOL	O	302	-	-	2/4/4/4	-
33	LHG	a	421	-	-	16/46/46/53	-
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
29	PL9	A	414	-	-	15/53/73/73	0/1/1/1
23	CLA	B	601	41	-	12/39/115/115	-
32	LMG	D	411	39	-	10/46/66/70	0/1/1/1
33	LHG	d	405	-	-	13/53/53/53	-
27	GOL	v	202	-	-	1/4/4/4	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	T	101	-	-	8/21/61/61	0/2/2/2
25	BCR	a	410	-	-	1/29/63/63	0/2/2/2
33	LHG	D	407	-	-	14/53/53/53	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
27	GOL	l	102	-	-	2/4/4/4	-
23	CLA	c	508	41	-	9/39/115/115	-
29	PL9	d	404	-	-	6/53/73/73	0/1/1/1
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	C	514	-	-	0/29/63/63	0/2/2/2
23	CLA	D	402	4	-	0/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
23	CLA	a	405	1	-	3/39/115/115	-
23	CLA	c	507	3	-	8/39/115/115	-
23	CLA	a	407	41	-	7/39/115/115	-
27	GOL	a	420	-	-	0/4/4/4	-
23	CLA	a	409	1	-	9/39/115/115	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
35	DGD	C	517	-	-	16/51/91/95	0/2/2/2
24	PHO	a	417	-	-	1/37/103/103	0/5/6/6
34	HTG	d	409	-	-	1/7/27/30	0/1/1/1
23	CLA	b	614	2	-	15/39/115/115	-
38	HEM	f	101	5,6	-	5/14/54/54	-
23	CLA	B	609	2	-	1/39/115/115	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	B	603	2	-	8/39/115/115	-
29	PL9	a	415	-	-	14/53/73/73	0/1/1/1
23	CLA	B	615	2	-	5/39/115/115	-
23	CLA	d	402	4	-	8/39/115/115	-
23	CLA	b	604	2	-	10/39/115/115	-
23	CLA	A	408	1	-	8/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	b	610	41	-	7/39/115/115	-

All (1628) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	C1D-C2D	9.11	1.49	1.39
24	a	408	PHO	C1B-C2B	8.96	1.49	1.39
24	a	417	PHO	C1B-C2B	8.77	1.49	1.39
24	A	416	PHO	C1D-C2D	8.71	1.49	1.39
24	a	417	PHO	C1D-C2D	8.58	1.49	1.39
24	a	408	PHO	C1D-C2D	8.45	1.48	1.39
24	A	407	PHO	C1B-C2B	8.30	1.48	1.39
24	A	416	PHO	C1B-C2B	8.26	1.48	1.39
40	v	201	HEC	C3D-C2D	7.72	1.53	1.36
40	V	201	HEC	C3D-C2D	7.34	1.52	1.36
24	a	417	PHO	C3B-C4B	7.11	1.49	1.41
23	B	611	CLA	CMB-C2B	7.10	1.65	1.50
23	B	611	CLA	C1B-C2B	6.72	1.59	1.43
24	A	416	PHO	C3B-C4B	6.61	1.49	1.41
24	a	408	PHO	C3B-C4B	6.52	1.49	1.41
24	A	407	PHO	C3B-C4B	6.43	1.48	1.41
24	a	408	PHO	C3B-C2B	6.36	1.49	1.40
24	A	416	PHO	C4D-CHA	6.36	1.49	1.39
24	A	407	PHO	C4D-CHA	6.35	1.49	1.39
24	a	408	PHO	C4D-CHA	6.34	1.49	1.39
24	A	407	PHO	C3B-C2B	6.19	1.49	1.40
23	B	611	CLA	C1D-ND	6.14	1.45	1.37
24	A	416	PHO	C3B-C2B	6.12	1.48	1.40
24	a	417	PHO	C4D-CHA	6.09	1.49	1.39
24	A	416	PHO	C3C-C2C	6.07	1.49	1.36
24	a	417	PHO	C3C-C2C	5.98	1.49	1.36
24	a	417	PHO	C3B-C2B	5.90	1.48	1.40
23	C	510	CLA	C1D-ND	5.89	1.45	1.37
23	B	611	CLA	CHC-C1C	5.63	1.50	1.38
23	B	610	CLA	C3C-C2C	5.59	1.48	1.36
24	A	407	PHO	C3C-C2C	5.58	1.48	1.36
23	B	611	CLA	C3C-C2C	5.57	1.48	1.36
23	d	402	CLA	C1D-ND	5.55	1.44	1.37
23	C	503	CLA	C3C-C2C	5.53	1.48	1.36
23	c	509	CLA	C3C-C2C	5.53	1.48	1.36
23	c	510	CLA	C3C-C2C	5.53	1.48	1.36
23	c	513	CLA	C3C-C2C	5.51	1.48	1.36
23	c	512	CLA	C1D-ND	5.50	1.44	1.37
24	a	408	PHO	C3C-C2C	5.49	1.48	1.36
23	b	605	CLA	C3C-C2C	5.47	1.48	1.36
23	b	601	CLA	C1D-ND	5.45	1.44	1.37
23	A	404	CLA	C3C-C2C	5.45	1.48	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C3C-C2C	5.42	1.48	1.36
23	C	512	CLA	C3C-C2C	5.42	1.48	1.36
24	a	408	PHO	C3D-C2D	5.41	1.49	1.39
23	C	510	CLA	C3C-C2C	5.40	1.48	1.36
23	c	506	CLA	C3C-C2C	5.40	1.48	1.36
23	C	508	CLA	C3C-C2C	5.39	1.48	1.36
23	c	504	CLA	C3C-C2C	5.36	1.48	1.36
23	a	406	CLA	C3C-C2C	5.35	1.48	1.36
23	a	407	CLA	C3C-C2C	5.34	1.48	1.36
23	D	403	CLA	C1D-ND	5.32	1.44	1.37
23	c	509	CLA	O2D-CGD	5.32	1.46	1.33
23	B	614	CLA	C3C-C2C	5.31	1.48	1.36
23	c	514	CLA	C1D-ND	5.30	1.44	1.37
23	d	402	CLA	C3C-C2C	5.30	1.48	1.36
23	B	610	CLA	C1D-ND	5.30	1.44	1.37
23	B	616	CLA	C3C-C2C	5.30	1.48	1.36
23	b	607	CLA	C3C-C2C	5.30	1.48	1.36
23	b	601	CLA	C3C-C2C	5.30	1.48	1.36
23	B	605	CLA	C3C-C2C	5.28	1.48	1.36
24	a	417	PHO	C3D-C2D	5.28	1.48	1.39
23	b	616	CLA	C3C-C2C	5.27	1.47	1.36
23	B	601	CLA	C3C-C2C	5.27	1.47	1.36
23	C	509	CLA	C3C-C2C	5.27	1.47	1.36
23	c	502	CLA	C1D-ND	5.27	1.44	1.37
23	C	502	CLA	C3C-C2C	5.26	1.47	1.36
23	A	408	CLA	C3C-C2C	5.25	1.47	1.36
24	A	416	PHO	C3D-C2D	5.25	1.48	1.39
23	c	505	CLA	O2D-CGD	5.24	1.46	1.33
23	b	606	CLA	C3C-C2C	5.23	1.47	1.36
23	d	401	CLA	C3C-C2C	5.23	1.47	1.36
23	b	614	CLA	C3C-C2C	5.23	1.47	1.36
23	c	514	CLA	C3C-C2C	5.23	1.47	1.36
23	B	609	CLA	O2D-CGD	5.23	1.46	1.33
23	C	507	CLA	C3C-C2C	5.23	1.47	1.36
23	D	402	CLA	C3C-C2C	5.22	1.47	1.36
23	a	405	CLA	C3C-C2C	5.22	1.47	1.36
23	b	615	CLA	C3C-C2C	5.21	1.47	1.36
23	b	609	CLA	O2D-CGD	5.21	1.45	1.33
23	b	603	CLA	C3C-C2C	5.21	1.47	1.36
23	c	510	CLA	O2D-CGD	5.19	1.45	1.33
23	b	610	CLA	C3C-C2C	5.18	1.47	1.36
23	B	601	CLA	C1D-ND	5.18	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	C1D-ND	5.18	1.44	1.37
23	C	502	CLA	C1D-ND	5.17	1.44	1.37
40	V	201	HEC	FE-ND	5.17	2.10	1.94
23	c	505	CLA	C3C-C2C	5.16	1.47	1.36
23	a	406	CLA	C1D-ND	5.16	1.44	1.37
23	B	612	CLA	C3C-C2C	5.16	1.47	1.36
23	b	604	CLA	C1D-ND	5.15	1.44	1.37
23	c	502	CLA	C3C-C2C	5.14	1.47	1.36
23	B	614	CLA	C1D-ND	5.14	1.44	1.37
23	C	508	CLA	C1D-ND	5.14	1.44	1.37
23	c	507	CLA	O2D-CGD	5.14	1.45	1.33
23	b	616	CLA	C1D-ND	5.14	1.44	1.37
23	b	602	CLA	C3C-C2C	5.14	1.47	1.36
23	c	507	CLA	C1D-ND	5.13	1.44	1.37
23	b	603	CLA	O2D-CGD	5.13	1.45	1.33
23	c	513	CLA	C1D-ND	5.13	1.44	1.37
23	C	501	CLA	C3C-C2C	5.12	1.47	1.36
23	b	612	CLA	C3C-C2C	5.12	1.47	1.36
23	c	509	CLA	C1D-ND	5.11	1.44	1.37
23	b	602	CLA	O2D-CGD	5.11	1.45	1.33
23	B	605	CLA	C1D-ND	5.10	1.44	1.37
23	c	507	CLA	C3C-C2C	5.10	1.47	1.36
23	B	609	CLA	C3C-C2C	5.09	1.47	1.36
23	c	514	CLA	O2D-CGD	5.09	1.45	1.33
23	c	503	CLA	C3C-C2C	5.08	1.47	1.36
23	B	606	CLA	C3C-C2C	5.08	1.47	1.36
23	B	602	CLA	C3C-C2C	5.08	1.47	1.36
23	C	504	CLA	C3C-C2C	5.08	1.47	1.36
23	C	509	CLA	C1D-ND	5.08	1.44	1.37
23	C	506	CLA	O2D-CGD	5.07	1.45	1.33
23	C	512	CLA	C1D-ND	5.06	1.44	1.37
23	c	508	CLA	C1D-ND	5.06	1.44	1.37
23	B	613	CLA	O2D-CGD	5.05	1.45	1.33
23	A	406	CLA	C3C-C2C	5.05	1.47	1.36
23	C	513	CLA	C1D-ND	5.05	1.44	1.37
23	b	613	CLA	C1D-ND	5.05	1.44	1.37
23	b	610	CLA	O2D-CGD	5.05	1.45	1.33
23	B	612	CLA	CHC-C1C	5.05	1.48	1.38
23	C	513	CLA	C3C-C2C	5.04	1.47	1.36
23	C	511	CLA	O2D-CGD	5.04	1.45	1.33
23	c	512	CLA	C3C-C2C	5.04	1.47	1.36
25	K	101	BCR	C23-C22	-5.03	1.35	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	O2D-CGD	5.03	1.45	1.33
23	B	603	CLA	C3C-C2C	5.03	1.47	1.36
25	d	403	BCR	C23-C22	-5.03	1.35	1.45
23	B	613	CLA	C1D-ND	5.02	1.44	1.37
23	B	601	CLA	O2D-CGD	5.02	1.45	1.33
23	c	504	CLA	C1D-ND	5.02	1.44	1.37
23	c	511	CLA	C3C-C2C	5.02	1.47	1.36
23	B	604	CLA	C3C-C2C	5.02	1.47	1.36
23	C	508	CLA	O2D-CGD	5.00	1.45	1.33
23	B	616	CLA	CHC-C1C	5.00	1.48	1.38
23	a	409	CLA	C3C-C2C	4.99	1.47	1.36
23	b	606	CLA	C1D-ND	4.98	1.43	1.37
23	a	406	CLA	O2D-CGD	4.98	1.45	1.33
23	b	615	CLA	O2D-CGD	4.97	1.45	1.33
25	k	101	BCR	C23-C22	-4.97	1.35	1.45
23	C	512	CLA	CHC-C1C	4.96	1.48	1.38
23	c	505	CLA	C1D-ND	4.96	1.43	1.37
23	C	502	CLA	O2D-CGD	4.96	1.45	1.33
23	b	613	CLA	O2D-CGD	4.95	1.45	1.33
23	b	602	CLA	CHC-C1C	4.95	1.48	1.38
23	B	601	CLA	O2A-CGA	4.95	1.47	1.33
24	a	417	PHO	O2D-CGD	4.95	1.45	1.33
23	C	509	CLA	O2D-CGD	4.95	1.45	1.33
23	B	613	CLA	CHC-C1C	4.94	1.48	1.38
23	C	504	CLA	O2D-CGD	4.94	1.45	1.33
23	c	508	CLA	O2D-CGD	4.94	1.45	1.33
23	c	511	CLA	O2D-CGD	4.94	1.45	1.33
23	c	508	CLA	C3C-C2C	4.93	1.47	1.36
23	B	615	CLA	O2D-CGD	4.93	1.45	1.33
38	f	101	HEM	FE-NB	4.93	2.10	1.94
23	C	506	CLA	C3C-C2C	4.92	1.47	1.36
23	B	615	CLA	C3C-C2C	4.92	1.47	1.36
23	c	513	CLA	CHC-C1C	4.92	1.48	1.38
23	B	606	CLA	C1D-ND	4.92	1.43	1.37
23	b	609	CLA	C3C-C2C	4.92	1.47	1.36
23	b	613	CLA	C3C-C2C	4.92	1.47	1.36
23	b	608	CLA	C3C-C2C	4.91	1.47	1.36
23	b	601	CLA	O2D-CGD	4.91	1.45	1.33
23	D	403	CLA	O2D-CGD	4.91	1.45	1.33
24	A	416	PHO	O2D-CGD	4.91	1.45	1.33
23	c	511	CLA	C1D-ND	4.90	1.43	1.37
23	B	603	CLA	C1D-ND	4.90	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407	PHO	O2D-CGD	4.90	1.45	1.33
23	A	406	CLA	O2D-CGD	4.90	1.45	1.33
23	C	505	CLA	C3C-C2C	4.89	1.47	1.36
23	b	616	CLA	CHC-C1C	4.89	1.48	1.38
23	C	503	CLA	CHC-C1C	4.89	1.48	1.38
24	A	407	PHO	C3D-C2D	4.88	1.48	1.39
25	T	102	BCR	C23-C22	-4.88	1.35	1.45
38	F	102	HEM	FE-NB	4.87	2.10	1.94
23	c	514	CLA	CHC-C1C	4.87	1.48	1.38
23	c	512	CLA	O2D-CGD	4.87	1.45	1.33
23	A	405	CLA	C3C-C2C	4.87	1.47	1.36
23	C	513	CLA	O2D-CGD	4.87	1.45	1.33
23	B	610	CLA	CHC-C1C	4.86	1.48	1.38
23	c	503	CLA	O2D-CGD	4.86	1.45	1.33
23	C	505	CLA	CHC-C1C	4.86	1.48	1.38
23	a	409	CLA	O2D-CGD	4.85	1.45	1.33
23	b	604	CLA	C3C-C2C	4.84	1.47	1.36
23	b	614	CLA	C1D-ND	4.84	1.43	1.37
24	a	417	PHO	OBD-CAD	4.84	1.29	1.22
23	B	602	CLA	C1D-ND	4.84	1.43	1.37
25	b	617	BCR	C23-C22	-4.84	1.35	1.45
23	D	403	CLA	CHC-C1C	4.84	1.48	1.38
23	a	409	CLA	CHC-C1C	4.83	1.48	1.38
23	C	507	CLA	CHC-C1C	4.82	1.48	1.38
23	B	605	CLA	O2D-CGD	4.82	1.45	1.33
23	B	613	CLA	C3C-C2C	4.82	1.47	1.36
25	K	103	BCR	C23-C22	-4.82	1.35	1.45
25	c	516	BCR	C23-C22	-4.81	1.35	1.45
23	C	510	CLA	O2D-CGD	4.80	1.44	1.33
23	B	604	CLA	O2D-CGD	4.80	1.44	1.33
23	D	402	CLA	O2D-CGD	4.80	1.44	1.33
23	C	501	CLA	C1D-ND	4.79	1.43	1.37
23	c	504	CLA	CHC-C1C	4.79	1.48	1.38
23	b	611	CLA	C3C-C2C	4.79	1.46	1.36
23	b	605	CLA	O2D-CGD	4.79	1.44	1.33
23	C	505	CLA	O2D-CGD	4.78	1.44	1.33
25	C	514	BCR	C23-C22	-4.78	1.35	1.45
23	C	512	CLA	O2D-CGD	4.78	1.44	1.33
23	C	511	CLA	C3C-C2C	4.78	1.46	1.36
23	b	616	CLA	O2D-CGD	4.78	1.44	1.33
23	B	610	CLA	O2D-CGD	4.77	1.44	1.33
23	b	605	CLA	C1D-ND	4.77	1.43	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C3C-C2C	4.77	1.46	1.36
23	d	402	CLA	CHC-C1C	4.76	1.48	1.38
23	B	603	CLA	O2D-CGD	4.76	1.44	1.33
25	D	404	BCR	C23-C22	-4.76	1.35	1.45
23	A	408	CLA	O2D-CGD	4.76	1.44	1.33
23	c	513	CLA	O2D-CGD	4.75	1.44	1.33
23	C	510	CLA	CHC-C1C	4.75	1.48	1.38
26	F	103	SQD	O47-C7	4.75	1.47	1.34
23	b	601	CLA	O2A-CGA	4.75	1.47	1.33
23	B	611	CLA	CHC-C4B	4.75	1.50	1.39
23	b	614	CLA	O2D-CGD	4.75	1.44	1.33
23	c	503	CLA	C1D-ND	4.74	1.43	1.37
23	c	509	CLA	CHC-C1C	4.73	1.48	1.38
23	b	602	CLA	CHD-C1D	4.73	1.47	1.38
23	A	404	CLA	O2D-CGD	4.73	1.44	1.33
23	b	614	CLA	CHC-C1C	4.73	1.48	1.38
23	A	406	CLA	CHC-C1C	4.72	1.48	1.38
25	c	515	BCR	C23-C22	-4.72	1.35	1.45
23	B	606	CLA	CHC-C1C	4.71	1.48	1.38
23	B	615	CLA	CHC-C1C	4.71	1.48	1.38
23	B	601	CLA	CHC-C1C	4.71	1.48	1.38
23	b	611	CLA	O2D-CGD	4.71	1.44	1.33
25	t	102	BCR	C23-C22	-4.71	1.35	1.45
23	C	503	CLA	C1D-ND	4.70	1.43	1.37
23	C	501	CLA	CHC-C1C	4.70	1.48	1.38
23	C	505	CLA	C1D-ND	4.70	1.43	1.37
23	b	603	CLA	CHC-C1C	4.69	1.48	1.38
23	B	611	CLA	O2D-CGD	4.69	1.44	1.33
23	b	601	CLA	CHC-C1C	4.68	1.48	1.38
23	b	615	CLA	C1D-ND	4.68	1.43	1.37
25	b	619	BCR	C23-C22	-4.67	1.35	1.45
25	B	619	BCR	C23-C22	-4.67	1.35	1.45
23	d	401	CLA	O2D-CGD	4.66	1.44	1.33
25	A	409	BCR	C23-C22	-4.66	1.35	1.45
23	C	504	CLA	C1D-ND	4.66	1.43	1.37
23	B	609	CLA	CHC-C1C	4.66	1.48	1.38
23	c	506	CLA	CHC-C1C	4.66	1.48	1.38
23	C	506	CLA	C1D-ND	4.65	1.43	1.37
23	b	612	CLA	O2D-CGD	4.65	1.44	1.33
23	B	608	CLA	C1D-ND	4.64	1.43	1.37
23	B	602	CLA	CHC-C1C	4.64	1.48	1.38
23	b	609	CLA	CHC-C1C	4.64	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CHC-C1C	4.64	1.47	1.38
23	b	608	CLA	O2D-CGD	4.64	1.44	1.33
23	c	510	CLA	C1D-ND	4.63	1.43	1.37
23	b	604	CLA	CHC-C1C	4.62	1.47	1.38
23	c	502	CLA	CHC-C1C	4.62	1.47	1.38
23	C	506	CLA	CHD-C1D	4.62	1.47	1.38
23	a	405	CLA	C1D-ND	4.62	1.43	1.37
23	B	616	CLA	O2D-CGD	4.62	1.44	1.33
25	y	101	BCR	C23-C22	-4.61	1.36	1.45
23	B	606	CLA	O2D-CGD	4.61	1.44	1.33
23	b	613	CLA	CHC-C1C	4.60	1.47	1.38
23	b	606	CLA	O2D-CGD	4.60	1.44	1.33
23	b	609	CLA	C1D-ND	4.60	1.43	1.37
23	C	508	CLA	CHC-C1C	4.60	1.47	1.38
25	a	410	BCR	C23-C22	-4.60	1.36	1.45
23	b	610	CLA	CHC-C1C	4.60	1.47	1.38
23	B	602	CLA	O2D-CGD	4.59	1.44	1.33
32	c	521	LMG	O7-C10	4.58	1.47	1.34
23	C	507	CLA	O2D-CGD	4.58	1.44	1.33
23	a	407	CLA	CHC-C1C	4.58	1.47	1.38
23	B	608	CLA	C3C-C2C	4.56	1.46	1.36
23	C	507	CLA	C1D-ND	4.55	1.43	1.37
23	B	614	CLA	O2D-CGD	4.55	1.44	1.33
23	b	605	CLA	CHC-C1C	4.55	1.47	1.38
23	A	405	CLA	CHC-C1C	4.55	1.47	1.38
32	C	519	LMG	O7-C10	4.54	1.47	1.34
23	C	513	CLA	CHC-C1C	4.54	1.47	1.38
23	a	405	CLA	O2D-CGD	4.54	1.44	1.33
23	B	605	CLA	CHC-C1C	4.53	1.47	1.38
23	c	514	CLA	CHD-C1D	4.52	1.47	1.38
23	B	609	CLA	C1D-ND	4.52	1.43	1.37
23	b	607	CLA	O2D-CGD	4.51	1.44	1.33
23	b	606	CLA	CHC-C1C	4.51	1.47	1.38
23	C	511	CLA	C1D-ND	4.51	1.43	1.37
23	c	505	CLA	CHC-C1C	4.51	1.47	1.38
23	B	604	CLA	CHD-C1D	4.50	1.47	1.38
23	b	607	CLA	CHC-C1C	4.50	1.47	1.38
23	B	615	CLA	CHD-C1D	4.50	1.47	1.38
23	a	407	CLA	O2D-CGD	4.50	1.44	1.33
26	A	412	SQD	O48-C23	4.49	1.46	1.33
32	C	519	LMG	O8-C28	4.49	1.46	1.33
23	c	504	CLA	CHD-C1D	4.49	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	CHC-C1C	4.49	1.47	1.38
23	B	604	CLA	CHC-C1C	4.48	1.47	1.38
25	h	101	BCR	C23-C22	-4.48	1.36	1.45
25	H	101	BCR	C23-C22	-4.48	1.36	1.45
25	B	617	BCR	C23-C22	-4.48	1.36	1.45
33	E	101	LHG	O8-C23	4.48	1.46	1.33
23	b	604	CLA	O2D-CGD	4.47	1.44	1.33
26	f	102	SQD	O47-C7	4.47	1.46	1.34
23	b	601	CLA	CHD-C1D	4.46	1.47	1.38
26	a	413	SQD	O48-C23	4.46	1.46	1.33
23	B	612	CLA	C1B-NB	-4.46	1.32	1.37
23	B	611	CLA	C4B-NB	-4.46	1.32	1.37
23	b	612	CLA	C1D-ND	4.45	1.43	1.37
26	B	620	SQD	O47-C7	4.44	1.46	1.34
23	B	607	CLA	O2D-CGD	4.44	1.44	1.33
23	B	612	CLA	CHB-C1B	4.44	1.49	1.39
23	d	402	CLA	O2A-CGA	4.43	1.46	1.33
23	A	408	CLA	O2A-CGA	4.43	1.46	1.33
23	c	513	CLA	O2A-CGA	4.42	1.46	1.33
32	z	101	LMG	O8-C28	4.42	1.46	1.33
23	c	506	CLA	O2D-CGD	4.42	1.44	1.33
23	B	603	CLA	CHC-C1C	4.41	1.47	1.38
23	b	615	CLA	CHC-C1C	4.41	1.47	1.38
23	b	611	CLA	CHC-C1C	4.41	1.47	1.38
23	B	609	CLA	CHD-C1D	4.40	1.46	1.38
23	a	406	CLA	CHC-C1C	4.40	1.47	1.38
23	b	602	CLA	C1D-ND	4.40	1.43	1.37
33	a	421	LHG	O8-C23	4.39	1.46	1.33
23	D	403	CLA	CHD-C1D	4.38	1.46	1.38
23	B	614	CLA	CHC-C1C	4.38	1.47	1.38
23	a	406	CLA	C3D-C2D	4.38	1.51	1.39
23	B	610	CLA	OBD-CAD	4.38	1.30	1.22
23	c	512	CLA	CHD-C1D	4.37	1.46	1.38
23	b	608	CLA	CHC-C1C	4.37	1.47	1.38
23	C	512	CLA	CHD-C1D	4.37	1.46	1.38
23	c	506	CLA	C1D-ND	4.36	1.43	1.37
23	a	405	CLA	CHC-C1C	4.36	1.47	1.38
24	a	408	PHO	OBD-CAD	4.36	1.28	1.22
23	B	616	CLA	C1D-ND	4.35	1.43	1.37
23	A	405	CLA	O2D-CGD	4.35	1.43	1.33
23	C	511	CLA	CHC-C1C	4.34	1.47	1.38
23	b	611	CLA	O2A-CGA	4.34	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C1D-ND	4.34	1.43	1.37
23	c	514	CLA	O2A-CGA	4.34	1.46	1.33
32	C	518	LMG	O8-C28	4.33	1.46	1.33
23	c	507	CLA	CHC-C1C	4.33	1.47	1.38
32	B	621	LMG	O8-C28	4.33	1.46	1.33
23	b	608	CLA	C1D-ND	4.32	1.43	1.37
23	c	513	CLA	CHD-C1D	4.31	1.46	1.38
23	C	513	CLA	CHD-C1D	4.31	1.46	1.38
24	A	416	PHO	OBD-CAD	4.31	1.28	1.22
23	B	602	CLA	CHD-C1D	4.31	1.46	1.38
25	Y	101	BCR	C23-C22	-4.31	1.36	1.45
38	F	102	HEM	FE-NC	4.31	2.09	1.95
23	A	404	CLA	CHC-C1C	4.31	1.47	1.38
23	c	511	CLA	CHC-C1C	4.31	1.47	1.38
26	b	620	SQD	O48-C23	4.31	1.45	1.33
23	A	408	CLA	CHC-C1C	4.31	1.47	1.38
33	d	406	LHG	O8-C23	4.31	1.45	1.33
26	b	620	SQD	O47-C7	4.31	1.46	1.34
23	C	502	CLA	CHD-C1D	4.31	1.46	1.38
23	B	608	CLA	O2D-CGD	4.30	1.43	1.33
23	C	503	CLA	O2D-CGD	4.30	1.43	1.33
23	B	607	CLA	CHC-C1C	4.30	1.47	1.38
23	c	506	CLA	CHD-C1D	4.30	1.46	1.38
23	a	409	CLA	O2A-CGA	4.29	1.45	1.33
26	B	620	SQD	O48-C23	4.28	1.45	1.33
23	d	402	CLA	CHD-C1D	4.28	1.46	1.38
23	c	502	CLA	O2D-CGD	4.27	1.43	1.33
35	c	519	DGD	O1G-C1A	4.27	1.45	1.33
23	C	502	CLA	CHC-C1C	4.27	1.47	1.38
23	C	509	CLA	CHD-C1D	4.27	1.46	1.38
23	D	402	CLA	C1D-ND	4.27	1.43	1.37
23	c	512	CLA	O2A-CGA	4.27	1.45	1.33
23	C	504	CLA	CHC-C1C	4.26	1.47	1.38
23	c	508	CLA	O2A-CGA	4.26	1.45	1.33
23	b	609	CLA	CHD-C1D	4.26	1.46	1.38
23	C	508	CLA	C3D-C2D	4.25	1.50	1.39
23	b	614	CLA	CHD-C1D	4.25	1.46	1.38
23	D	402	CLA	CHC-C1C	4.25	1.47	1.38
26	f	102	SQD	O48-C23	4.25	1.45	1.33
25	b	618	BCR	C23-C22	-4.24	1.36	1.45
32	c	521	LMG	O8-C28	4.23	1.45	1.33
23	c	510	CLA	CHD-C1D	4.23	1.46	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	m	101	LMG	O8-C28	4.23	1.45	1.33
23	b	611	CLA	C1D-ND	4.23	1.43	1.37
23	B	604	CLA	C1D-ND	4.22	1.43	1.37
23	A	404	CLA	C1D-ND	4.22	1.43	1.37
23	D	402	CLA	O2A-CGA	4.22	1.45	1.33
26	A	412	SQD	O47-C7	4.22	1.46	1.34
23	c	505	CLA	C3D-C2D	4.21	1.50	1.39
23	C	509	CLA	CHC-C1C	4.20	1.47	1.38
23	b	607	CLA	CHD-C1D	4.20	1.46	1.38
23	C	508	CLA	O2A-CGA	4.19	1.45	1.33
23	b	602	CLA	CHC-C4B	4.19	1.48	1.39
23	C	504	CLA	CHB-C1B	4.19	1.48	1.39
33	E	101	LHG	O7-C7	4.19	1.46	1.34
34	B	622	HTG	C1'-S1	-4.19	1.76	1.81
23	A	406	CLA	CHD-C1D	4.18	1.46	1.38
23	c	503	CLA	O2A-CGA	4.18	1.45	1.33
26	F	103	SQD	O48-C23	4.18	1.45	1.33
23	b	602	CLA	CHD-C4C	4.18	1.48	1.39
23	C	513	CLA	O2A-CGA	4.18	1.45	1.33
23	c	507	CLA	O2A-CGA	4.18	1.45	1.33
23	C	506	CLA	CHC-C1C	4.17	1.47	1.38
23	C	511	CLA	CHD-C1D	4.17	1.46	1.38
34	b	622	HTG	C1'-S1	-4.17	1.76	1.81
23	B	611	CLA	CHB-C1B	4.17	1.48	1.39
23	D	403	CLA	CHC-C4B	4.17	1.48	1.39
23	C	512	CLA	O2A-CGA	4.17	1.45	1.33
23	c	512	CLA	CHB-C1B	4.16	1.48	1.39
23	C	505	CLA	CHD-C1D	4.16	1.46	1.38
23	b	603	CLA	C1D-ND	4.16	1.42	1.37
23	b	612	CLA	CHC-C1C	4.16	1.47	1.38
23	b	601	CLA	C3D-C2D	4.16	1.50	1.39
23	b	616	CLA	O2A-CGA	4.15	1.45	1.33
23	a	407	CLA	C1D-ND	4.15	1.42	1.37
23	c	509	CLA	O2A-CGA	4.15	1.45	1.33
23	d	402	CLA	O2D-CGD	4.15	1.43	1.33
32	Z	101	LMG	O7-C10	4.15	1.46	1.34
23	C	501	CLA	CHD-C1D	4.15	1.46	1.38
23	B	601	CLA	CHD-C1D	4.15	1.46	1.38
23	c	510	CLA	C1B-NB	-4.15	1.32	1.37
40	v	201	HEC	FE-ND	4.15	2.07	1.94
24	A	407	PHO	OBD-CAD	4.14	1.28	1.22
23	c	514	CLA	CHD-C4C	4.14	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	CHD-C1D	4.13	1.46	1.38
33	a	421	LHG	O7-C7	4.13	1.46	1.34
38	f	101	HEM	FE-NC	4.13	2.09	1.95
23	b	606	CLA	CHD-C1D	4.13	1.46	1.38
23	c	509	CLA	CHD-C1D	4.13	1.46	1.38
23	d	401	CLA	CHC-C1C	4.13	1.46	1.38
23	c	503	CLA	CHD-C1D	4.13	1.46	1.38
23	b	601	CLA	CHD-C4C	4.12	1.48	1.39
23	a	407	CLA	O2A-CGA	4.12	1.45	1.33
23	C	510	CLA	CHD-C4C	4.12	1.48	1.39
23	b	610	CLA	C1D-ND	4.12	1.42	1.37
23	c	504	CLA	O2D-CGD	4.11	1.43	1.33
23	b	615	CLA	CHD-C1D	4.11	1.46	1.38
23	d	401	CLA	CHB-C1B	4.11	1.48	1.39
23	C	503	CLA	CHD-C1D	4.11	1.46	1.38
23	c	510	CLA	O2A-CGA	4.11	1.45	1.33
23	b	604	CLA	CHD-C1D	4.11	1.46	1.38
23	B	605	CLA	CHC-C4B	4.10	1.48	1.39
23	C	512	CLA	CHC-C4B	4.10	1.48	1.39
23	c	510	CLA	CHC-C1C	4.10	1.46	1.38
32	z	101	LMG	O7-C10	4.10	1.45	1.34
23	b	607	CLA	C1D-ND	4.10	1.42	1.37
23	B	611	CLA	C3B-C2B	4.10	1.55	1.41
23	C	507	CLA	O2A-CGA	4.10	1.45	1.33
32	d	410	LMG	O8-C28	4.10	1.45	1.33
32	c	520	LMG	O7-C10	4.09	1.45	1.34
23	c	508	CLA	CHD-C1D	4.09	1.46	1.38
35	c	517	DGD	O2G-C1B	4.09	1.45	1.34
23	B	612	CLA	O2D-CGD	4.09	1.43	1.33
23	c	504	CLA	CHC-C4B	4.09	1.48	1.39
23	B	609	CLA	O2A-CGA	4.08	1.45	1.33
23	C	503	CLA	CHD-C4C	4.08	1.48	1.39
23	B	608	CLA	C3D-C2D	4.08	1.50	1.39
23	B	608	CLA	CHD-C1D	4.08	1.46	1.38
23	a	406	CLA	O2A-CGA	4.08	1.45	1.33
23	B	615	CLA	O2A-CGA	4.08	1.45	1.33
23	C	511	CLA	O2A-CGA	4.08	1.45	1.33
35	C	517	DGD	O1G-C1A	4.08	1.45	1.33
32	a	418	LMG	O8-C28	4.07	1.45	1.33
23	c	513	CLA	CHD-C4C	4.07	1.48	1.39
23	B	606	CLA	CHD-C1D	4.07	1.46	1.38
23	C	501	CLA	O2D-CGD	4.07	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	CHB-C1B	4.07	1.48	1.39
26	a	411	SQD	O47-C7	4.07	1.45	1.34
23	c	504	CLA	O2A-CGA	4.06	1.45	1.33
23	c	504	CLA	CHD-C4C	4.06	1.48	1.39
23	b	608	CLA	CHD-C1D	4.06	1.46	1.38
35	C	515	DGD	O2G-C1B	4.06	1.45	1.34
32	c	520	LMG	O8-C28	4.06	1.45	1.33
23	D	402	CLA	CHB-C1B	4.06	1.48	1.39
32	a	418	LMG	O7-C10	4.05	1.45	1.34
23	B	607	CLA	C1B-NB	-4.05	1.32	1.37
23	A	405	CLA	C3D-C2D	4.05	1.50	1.39
23	C	506	CLA	CHD-C4C	4.05	1.48	1.39
23	d	401	CLA	O2A-CGA	4.05	1.45	1.33
23	B	607	CLA	CHB-C1B	4.05	1.48	1.39
23	C	502	CLA	O2A-CGA	4.05	1.45	1.33
23	C	508	CLA	CHD-C1D	4.04	1.46	1.38
32	A	419	LMG	O7-C10	4.04	1.45	1.34
23	A	404	CLA	CHD-C1D	4.03	1.46	1.38
23	c	502	CLA	O2A-CGA	4.03	1.45	1.33
23	C	502	CLA	C3D-C2D	4.03	1.50	1.39
23	B	611	CLA	O2A-CGA	4.03	1.45	1.33
23	c	507	CLA	CHD-C1D	4.03	1.46	1.38
23	c	503	CLA	CHC-C1C	4.03	1.46	1.38
23	A	406	CLA	C1D-ND	4.02	1.42	1.37
23	C	513	CLA	CHD-C4C	4.02	1.48	1.39
26	a	413	SQD	O47-C7	4.01	1.45	1.34
23	c	507	CLA	CHD-C4C	4.01	1.48	1.39
23	b	609	CLA	CHB-C1B	4.01	1.48	1.39
23	A	408	CLA	CHD-C1D	4.01	1.46	1.38
23	C	506	CLA	O2A-CGA	4.01	1.45	1.33
23	B	616	CLA	O2A-CGA	4.01	1.45	1.33
23	B	610	CLA	CHD-C1D	4.00	1.46	1.38
32	A	419	LMG	O8-C28	4.00	1.45	1.33
23	C	511	CLA	CHD-C4C	4.00	1.48	1.39
23	b	607	CLA	C1B-NB	-4.00	1.32	1.37
23	c	509	CLA	C3D-C2D	3.99	1.50	1.39
23	B	609	CLA	C3D-C2D	3.99	1.50	1.39
23	c	502	CLA	CHB-C1B	3.99	1.48	1.39
23	a	405	CLA	CHD-C1D	3.99	1.46	1.38
23	b	608	CLA	O2A-CGA	3.99	1.45	1.33
23	B	605	CLA	CHB-C1B	3.99	1.48	1.39
32	C	518	LMG	O7-C10	3.99	1.45	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	OBD-CAD	3.99	1.29	1.22
23	C	501	CLA	O2A-CGA	3.98	1.45	1.33
23	B	605	CLA	O2A-CGA	3.98	1.45	1.33
33	D	407	LHG	O7-C7	3.98	1.45	1.34
26	a	411	SQD	O48-C23	3.98	1.45	1.33
23	B	614	CLA	O2A-CGA	3.97	1.44	1.33
23	B	602	CLA	CHD-C4C	3.97	1.48	1.39
23	b	615	CLA	O2A-CGA	3.97	1.44	1.33
23	c	510	CLA	C3D-C2D	3.97	1.50	1.39
23	c	512	CLA	CHD-C4C	3.96	1.48	1.39
23	C	513	CLA	C3D-C2D	3.96	1.49	1.39
23	c	506	CLA	CHC-C4B	3.96	1.48	1.39
23	C	510	CLA	CHD-C1D	3.96	1.46	1.38
23	b	606	CLA	O2A-CGA	3.96	1.44	1.33
23	c	508	CLA	CHC-C4B	3.96	1.48	1.39
23	B	603	CLA	C1B-NB	-3.96	1.32	1.37
23	C	504	CLA	C3D-C2D	3.96	1.49	1.39
32	d	410	LMG	O7-C10	3.96	1.45	1.34
23	a	405	CLA	CHD-C4C	3.96	1.48	1.39
23	B	614	CLA	CHD-C4C	3.95	1.48	1.39
23	c	511	CLA	C3D-C2D	3.95	1.49	1.39
23	b	615	CLA	CHD-C4C	3.95	1.48	1.39
23	c	503	CLA	C3D-C2D	3.95	1.49	1.39
23	c	505	CLA	CHD-C1D	3.95	1.46	1.38
23	B	611	CLA	OBD-CAD	3.95	1.29	1.22
23	c	504	CLA	CHB-C1B	3.95	1.48	1.39
23	B	613	CLA	C3D-C2D	3.95	1.49	1.39
23	c	503	CLA	CHD-C4C	3.94	1.48	1.39
23	B	614	CLA	CHD-C1D	3.93	1.46	1.38
23	b	612	CLA	CHB-C1B	3.93	1.48	1.39
23	c	505	CLA	O2A-CGA	3.93	1.44	1.33
23	B	601	CLA	CHD-C4C	3.93	1.48	1.39
23	b	609	CLA	C3D-C2D	3.93	1.49	1.39
23	b	616	CLA	CHD-C1D	3.93	1.46	1.38
40	v	201	HEC	FE-NB	3.92	2.07	1.94
23	d	402	CLA	C3D-C2D	3.92	1.49	1.39
23	c	508	CLA	CHD-C4C	3.92	1.48	1.39
23	B	611	CLA	CHD-C1D	3.92	1.46	1.38
23	B	610	CLA	CHB-C1B	3.92	1.48	1.39
23	D	402	CLA	CHD-C1D	3.92	1.46	1.38
23	c	508	CLA	C3D-C2D	3.92	1.49	1.39
23	b	616	CLA	CHC-C4B	3.92	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CHB-C1B	3.92	1.48	1.39
23	B	609	CLA	CHD-C4C	3.92	1.48	1.39
23	C	505	CLA	CHB-C1B	3.92	1.48	1.39
23	b	612	CLA	C3D-C2D	3.91	1.49	1.39
23	c	502	CLA	CHC-C4B	3.91	1.48	1.39
23	B	613	CLA	CHD-C1D	3.91	1.46	1.38
23	b	603	CLA	CHD-C1D	3.91	1.46	1.38
33	D	407	LHG	O8-C23	3.90	1.44	1.33
23	B	616	CLA	C3D-C2D	3.90	1.49	1.39
35	h	102	DGD	O2G-C1B	3.90	1.45	1.34
23	a	407	CLA	C3D-C2D	3.90	1.49	1.39
23	D	402	CLA	CHD-C4C	3.89	1.48	1.39
23	C	509	CLA	C4B-NB	-3.89	1.33	1.37
25	B	618	BCR	C23-C22	-3.89	1.37	1.45
23	C	509	CLA	O2A-CGA	3.89	1.44	1.33
23	A	405	CLA	C1D-ND	3.89	1.42	1.37
23	B	615	CLA	CHD-C4C	3.89	1.48	1.39
23	B	606	CLA	O2A-CGA	3.89	1.44	1.33
23	C	512	CLA	CHD-C4C	3.89	1.48	1.39
23	B	601	CLA	CHC-C4B	3.88	1.48	1.39
32	B	621	LMG	O7-C10	3.88	1.45	1.34
23	c	502	CLA	CHD-C1D	3.88	1.45	1.38
23	b	614	CLA	CHD-C4C	3.88	1.48	1.39
23	C	504	CLA	CHD-C1D	3.88	1.45	1.38
23	b	604	CLA	CHC-C4B	3.88	1.48	1.39
23	B	609	CLA	CHC-C4B	3.87	1.48	1.39
23	a	409	CLA	CHB-C1B	3.87	1.48	1.39
23	B	615	CLA	CHB-C1B	3.87	1.48	1.39
23	C	501	CLA	CHC-C4B	3.87	1.48	1.39
23	b	602	CLA	C3D-C2D	3.87	1.49	1.39
23	c	506	CLA	CHD-C4C	3.87	1.48	1.39
23	b	610	CLA	CHD-C4C	3.87	1.48	1.39
23	c	507	CLA	C3D-C2D	3.87	1.49	1.39
23	C	512	CLA	C3D-C2D	3.87	1.49	1.39
23	d	401	CLA	C1B-NB	-3.87	1.33	1.37
23	c	503	CLA	CHB-C1B	3.87	1.48	1.39
23	B	610	CLA	C3D-C2D	3.87	1.49	1.39
23	C	509	CLA	CHD-C4C	3.86	1.48	1.39
23	c	513	CLA	CHC-C4B	3.86	1.48	1.39
23	b	614	CLA	CHC-C4B	3.86	1.48	1.39
24	A	416	PHO	O2A-CGA	3.86	1.44	1.33
23	C	507	CLA	CHC-C4B	3.86	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	h	102	DGD	O1G-C1A	3.86	1.44	1.33
23	B	616	CLA	CHB-C1B	3.86	1.48	1.39
23	C	505	CLA	O2A-CGA	3.85	1.44	1.33
23	B	603	CLA	CHD-C1D	3.85	1.45	1.38
23	b	615	CLA	C3D-C2D	3.85	1.49	1.39
35	C	516	DGD	O2G-C1B	3.85	1.45	1.34
23	B	615	CLA	C3D-C2D	3.85	1.49	1.39
23	C	505	CLA	CHD-C4C	3.85	1.48	1.39
26	A	410	SQD	O48-C23	3.85	1.44	1.33
23	A	408	CLA	CHD-C4C	3.84	1.48	1.39
23	b	609	CLA	OBD-CAD	3.84	1.29	1.22
23	C	503	CLA	CHC-C4B	3.84	1.48	1.39
23	c	510	CLA	CHB-C1B	3.84	1.48	1.39
33	L	101	LHG	O8-C23	3.84	1.44	1.33
23	C	511	CLA	CHB-C1B	3.84	1.48	1.39
23	A	406	CLA	C3D-C2D	3.84	1.49	1.39
35	c	518	DGD	O1G-C1A	3.83	1.44	1.33
23	B	610	CLA	CHD-C4C	3.83	1.48	1.39
23	A	405	CLA	O2A-CGA	3.83	1.44	1.33
24	a	417	PHO	O2A-CGA	3.83	1.44	1.33
23	b	611	CLA	CHD-C1D	3.83	1.45	1.38
23	D	403	CLA	CHB-C1B	3.83	1.48	1.39
23	c	514	CLA	C3D-C2D	3.82	1.49	1.39
23	B	602	CLA	CHB-C1B	3.82	1.48	1.39
23	b	610	CLA	CHB-C1B	3.82	1.48	1.39
33	L	101	LHG	O7-C7	3.82	1.45	1.34
23	B	607	CLA	CHD-C1D	3.82	1.45	1.38
23	B	603	CLA	C3D-C2D	3.82	1.49	1.39
23	D	403	CLA	OBD-CAD	3.82	1.29	1.22
23	B	604	CLA	CHD-C4C	3.82	1.47	1.39
23	D	403	CLA	O2A-CGA	3.82	1.44	1.33
23	B	606	CLA	CHB-C1B	3.82	1.48	1.39
23	c	502	CLA	C3D-C2D	3.81	1.49	1.39
23	b	604	CLA	C3D-C2D	3.81	1.49	1.39
23	b	610	CLA	CHC-C4B	3.81	1.48	1.39
23	b	610	CLA	C3D-C2D	3.81	1.49	1.39
23	C	507	CLA	C3D-C2D	3.81	1.49	1.39
35	C	517	DGD	O2G-C1B	3.81	1.45	1.34
23	d	401	CLA	CHD-C1D	3.81	1.45	1.38
23	b	612	CLA	CHD-C1D	3.80	1.45	1.38
23	C	509	CLA	C3D-C2D	3.80	1.49	1.39
23	C	507	CLA	CHB-C1B	3.80	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	OBD-CAD	3.80	1.29	1.22
23	B	611	CLA	C3B-C4B	3.80	1.51	1.42
23	A	406	CLA	O2A-CGA	3.80	1.44	1.33
23	c	511	CLA	CHD-C4C	3.80	1.47	1.39
23	b	613	CLA	C3D-C2D	3.80	1.49	1.39
23	C	502	CLA	CHB-C1B	3.80	1.47	1.39
23	c	511	CLA	CHD-C1D	3.80	1.45	1.38
23	A	406	CLA	CHC-C4B	3.80	1.47	1.39
23	a	406	CLA	CHD-C1D	3.80	1.45	1.38
23	C	503	CLA	O2A-CGA	3.79	1.44	1.33
23	B	603	CLA	CHB-C1B	3.79	1.47	1.39
23	b	605	CLA	C1B-NB	-3.79	1.33	1.37
23	b	616	CLA	C3D-C2D	3.79	1.49	1.39
23	C	511	CLA	C3D-C2D	3.79	1.49	1.39
23	c	509	CLA	CHD-C4C	3.79	1.47	1.39
23	B	605	CLA	C3D-C2D	3.79	1.49	1.39
23	b	608	CLA	CHD-C4C	3.78	1.47	1.39
23	b	604	CLA	CHD-C4C	3.78	1.47	1.39
23	A	405	CLA	CHB-C1B	3.78	1.47	1.39
23	C	505	CLA	CHC-C4B	3.78	1.47	1.39
23	B	602	CLA	O2A-CGA	3.78	1.44	1.33
23	c	509	CLA	OBD-CAD	3.78	1.29	1.22
23	B	604	CLA	CHB-C1B	3.78	1.47	1.39
23	c	511	CLA	O2A-CGA	3.78	1.44	1.33
23	C	507	CLA	CHD-C1D	3.77	1.45	1.38
23	a	406	CLA	OBD-CAD	3.77	1.29	1.22
23	c	512	CLA	OBD-CAD	3.77	1.29	1.22
23	c	509	CLA	CHC-C4B	3.77	1.47	1.39
23	D	403	CLA	C3D-C2D	3.77	1.49	1.39
23	B	607	CLA	C1D-ND	3.76	1.42	1.37
23	B	610	CLA	CHC-C4B	3.76	1.47	1.39
23	B	612	CLA	C1D-ND	3.76	1.42	1.37
23	c	510	CLA	CHD-C4C	3.76	1.47	1.39
23	C	508	CLA	CHB-C1B	3.76	1.47	1.39
23	B	614	CLA	C4B-NB	-3.76	1.33	1.37
23	b	605	CLA	CHD-C1D	3.75	1.45	1.38
23	B	611	CLA	C1C-C2C	3.75	1.51	1.44
23	c	506	CLA	O2A-CGA	3.75	1.44	1.33
23	a	407	CLA	CHB-C1B	3.75	1.47	1.39
34	b	623	HTG	C1'-S1	-3.75	1.76	1.81
23	b	614	CLA	C3D-C2D	3.75	1.49	1.39
23	C	501	CLA	CHD-C4C	3.75	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	CHB-C1B	3.75	1.47	1.39
33	d	411	LHG	O8-C23	3.75	1.44	1.33
23	b	606	CLA	CHD-C4C	3.75	1.47	1.39
23	c	512	CLA	C3D-C2D	3.74	1.49	1.39
23	b	603	CLA	CHD-C4C	3.74	1.47	1.39
23	c	513	CLA	C3D-C2D	3.74	1.49	1.39
23	C	504	CLA	O2A-CGA	3.74	1.44	1.33
23	B	608	CLA	CHC-C1C	3.74	1.46	1.38
23	A	406	CLA	OBD-CAD	3.74	1.28	1.22
23	b	607	CLA	C3D-C2D	3.73	1.49	1.39
23	C	510	CLA	O2A-CGA	3.73	1.44	1.33
23	b	610	CLA	OBD-CAD	3.73	1.28	1.22
23	A	404	CLA	CHD-C4C	3.73	1.47	1.39
23	C	506	CLA	C3D-C2D	3.73	1.49	1.39
23	b	605	CLA	CHD-C4C	3.73	1.47	1.39
23	B	603	CLA	O2A-CGA	3.73	1.44	1.33
23	D	402	CLA	C1B-NB	-3.72	1.33	1.37
23	d	402	CLA	CHD-C4C	3.72	1.47	1.39
23	b	605	CLA	CHB-C1B	3.72	1.47	1.39
33	d	405	LHG	O7-C7	3.72	1.44	1.34
23	C	510	CLA	CHB-C1B	3.72	1.47	1.39
23	A	405	CLA	CHD-C1D	3.72	1.45	1.38
23	B	601	CLA	C3D-C2D	3.72	1.49	1.39
23	b	606	CLA	CHB-C1B	3.72	1.47	1.39
23	a	409	CLA	C1D-ND	3.72	1.42	1.37
23	c	505	CLA	CHD-C4C	3.72	1.47	1.39
23	c	507	CLA	CHB-C1B	3.71	1.47	1.39
35	C	516	DGD	O1G-C1A	3.71	1.44	1.33
23	B	613	CLA	CHB-C1B	3.71	1.47	1.39
23	c	514	CLA	CHB-C1B	3.71	1.47	1.39
23	B	605	CLA	CHD-C1D	3.70	1.45	1.38
23	b	608	CLA	C3D-C2D	3.70	1.49	1.39
23	C	510	CLA	C3D-C2D	3.70	1.49	1.39
23	b	615	CLA	OBD-CAD	3.70	1.28	1.22
23	b	611	CLA	CHB-C1B	3.70	1.47	1.39
23	B	601	CLA	OBD-CAD	3.70	1.28	1.22
23	b	604	CLA	CHB-C1B	3.70	1.47	1.39
23	B	614	CLA	CHC-C4B	3.70	1.47	1.39
23	B	611	CLA	CHD-C4C	3.70	1.47	1.39
23	d	402	CLA	CHC-C4B	3.69	1.47	1.39
23	a	405	CLA	CHB-C1B	3.69	1.47	1.39
23	C	508	CLA	CHC-C4B	3.69	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	OBD-CAD	3.69	1.28	1.22
23	B	602	CLA	C3D-C2D	3.69	1.49	1.39
23	b	613	CLA	O2A-CGA	3.68	1.44	1.33
23	C	503	CLA	CHB-C1B	3.68	1.47	1.39
23	c	513	CLA	OBD-CAD	3.68	1.28	1.22
26	A	410	SQD	O47-C7	3.68	1.44	1.34
23	a	407	CLA	OBD-CAD	3.68	1.28	1.22
23	b	603	CLA	CHC-C4B	3.68	1.47	1.39
23	b	612	CLA	O2A-CGA	3.68	1.44	1.33
23	C	513	CLA	CHB-C1B	3.68	1.47	1.39
23	C	504	CLA	CHD-C4C	3.68	1.47	1.39
23	A	404	CLA	C4B-NB	-3.68	1.33	1.37
23	b	601	CLA	OBD-CAD	3.68	1.28	1.22
32	m	101	LMG	O7-C10	3.67	1.44	1.34
23	b	616	CLA	CHD-C4C	3.67	1.47	1.39
23	A	406	CLA	C1B-NB	-3.67	1.33	1.37
23	b	609	CLA	CHD-C4C	3.67	1.47	1.39
23	A	406	CLA	CHD-C4C	3.67	1.47	1.39
23	c	506	CLA	CHB-C1B	3.67	1.47	1.39
35	H	102	DGD	O1G-C1A	3.66	1.44	1.33
23	B	612	CLA	O2A-CGA	3.66	1.44	1.33
23	b	611	CLA	CHD-C4C	3.66	1.47	1.39
23	a	405	CLA	C3D-C2D	3.66	1.49	1.39
23	a	409	CLA	CHC-C4B	3.66	1.47	1.39
23	B	613	CLA	OBD-CAD	3.66	1.28	1.22
23	b	605	CLA	CHC-C4B	3.66	1.47	1.39
23	c	511	CLA	CHC-C4B	3.66	1.47	1.39
33	d	406	LHG	O7-C7	3.66	1.44	1.34
23	b	606	CLA	OBD-CAD	3.66	1.28	1.22
23	A	405	CLA	C1B-NB	-3.66	1.33	1.37
23	C	502	CLA	CHD-C4C	3.65	1.47	1.39
23	c	506	CLA	OBD-CAD	3.65	1.28	1.22
23	B	612	CLA	CHD-C1D	3.65	1.45	1.38
23	b	601	CLA	CHC-C4B	3.65	1.47	1.39
23	a	409	CLA	CHD-C1D	3.65	1.45	1.38
23	C	501	CLA	C3D-C2D	3.65	1.49	1.39
23	c	502	CLA	CHD-C4C	3.65	1.47	1.39
23	C	502	CLA	OBD-CAD	3.65	1.28	1.22
23	C	501	CLA	CHB-C1B	3.65	1.47	1.39
23	C	513	CLA	OBD-CAD	3.65	1.28	1.22
23	b	609	CLA	O2A-CGA	3.65	1.44	1.33
23	b	615	CLA	CHB-C1B	3.65	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	O2A-CGA	3.65	1.44	1.33
23	a	409	CLA	C1B-NB	-3.64	1.33	1.37
24	A	407	PHO	O2A-CGA	3.64	1.44	1.33
23	c	506	CLA	C3D-C2D	3.64	1.49	1.39
23	D	403	CLA	CHD-C4C	3.64	1.47	1.39
23	b	603	CLA	C3D-C2D	3.64	1.49	1.39
23	c	508	CLA	OBD-CAD	3.64	1.28	1.22
23	A	404	CLA	C3D-C2D	3.63	1.49	1.39
23	B	604	CLA	O2A-CGA	3.63	1.43	1.33
23	b	611	CLA	C3D-C2D	3.63	1.49	1.39
23	d	402	CLA	CHB-C1B	3.63	1.47	1.39
23	B	607	CLA	CHD-C4C	3.63	1.47	1.39
23	B	604	CLA	OBD-CAD	3.62	1.28	1.22
23	b	613	CLA	CHC-C4B	3.62	1.47	1.39
23	C	504	CLA	CHC-C4B	3.62	1.47	1.39
35	c	517	DGD	O1G-C1A	3.62	1.43	1.33
23	B	606	CLA	C3D-C2D	3.62	1.49	1.39
23	B	613	CLA	CHD-C4C	3.62	1.47	1.39
23	c	514	CLA	CHC-C4B	3.62	1.47	1.39
23	a	406	CLA	CHD-C4C	3.62	1.47	1.39
33	b	630	LHG	O7-C7	3.62	1.44	1.34
23	a	405	CLA	OBD-CAD	3.61	1.28	1.22
23	B	606	CLA	CHD-C4C	3.61	1.47	1.39
32	D	411	LMG	O8-C28	3.61	1.43	1.33
23	b	614	CLA	O2A-CGA	3.61	1.43	1.33
23	B	606	CLA	CHC-C4B	3.61	1.47	1.39
23	C	506	CLA	CHB-C1B	3.61	1.47	1.39
23	B	603	CLA	CHD-C4C	3.60	1.47	1.39
23	B	602	CLA	CHC-C4B	3.60	1.47	1.39
23	B	612	CLA	C3D-C2D	3.60	1.49	1.39
23	b	606	CLA	C3D-C2D	3.60	1.48	1.39
33	D	406	LHG	O7-C7	3.60	1.44	1.34
23	a	409	CLA	C3D-C2D	3.60	1.48	1.39
23	C	510	CLA	C1B-NB	-3.60	1.33	1.37
23	C	508	CLA	CHD-C4C	3.60	1.47	1.39
23	b	611	CLA	CHC-C4B	3.59	1.47	1.39
32	D	411	LMG	O7-C10	3.58	1.44	1.34
23	a	407	CLA	CHD-C4C	3.58	1.47	1.39
34	B	625	HTG	C1'-S1	-3.58	1.76	1.81
23	b	608	CLA	CHB-C1B	3.58	1.47	1.39
23	b	615	CLA	C1B-NB	-3.58	1.33	1.37
23	C	510	CLA	CHC-C4B	3.57	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	O2A-CGA	3.57	1.43	1.33
23	b	608	CLA	C1B-NB	-3.57	1.33	1.37
23	d	401	CLA	CHD-C4C	3.57	1.47	1.39
23	b	604	CLA	OBD-CAD	3.57	1.28	1.22
23	c	505	CLA	CHC-C4B	3.57	1.47	1.39
23	c	509	CLA	CHB-C1B	3.56	1.47	1.39
23	c	513	CLA	CHB-C1B	3.56	1.47	1.39
23	A	405	CLA	CHD-C4C	3.56	1.47	1.39
23	A	405	CLA	CHC-C4B	3.56	1.47	1.39
23	b	602	CLA	OBD-CAD	3.56	1.28	1.22
23	C	507	CLA	CHD-C4C	3.56	1.47	1.39
23	A	404	CLA	CHB-C1B	3.55	1.47	1.39
23	b	612	CLA	CHC-C4B	3.55	1.47	1.39
35	C	515	DGD	O1G-C1A	3.55	1.43	1.33
23	b	614	CLA	CHB-C1B	3.55	1.47	1.39
23	b	612	CLA	OBD-CAD	3.55	1.28	1.22
23	d	401	CLA	C3D-C2D	3.55	1.48	1.39
23	B	613	CLA	CHC-C4B	3.55	1.47	1.39
23	B	607	CLA	CHC-C4B	3.54	1.47	1.39
23	B	614	CLA	C3D-C2D	3.54	1.48	1.39
23	a	407	CLA	CHD-C1D	3.54	1.45	1.38
35	c	518	DGD	O2G-C1B	3.53	1.44	1.34
23	A	408	CLA	C3D-C2D	3.53	1.48	1.39
23	c	507	CLA	OBD-CAD	3.53	1.28	1.22
33	d	405	LHG	O8-C23	3.53	1.43	1.33
33	D	406	LHG	O8-C23	3.53	1.43	1.33
23	C	509	CLA	CHC-C4B	3.52	1.47	1.39
23	B	603	CLA	C4B-NB	-3.52	1.33	1.37
23	B	612	CLA	C4B-NB	-3.52	1.33	1.37
33	A	420	LHG	O8-C23	3.52	1.43	1.33
23	c	505	CLA	C1B-NB	-3.52	1.33	1.37
23	C	512	CLA	OBD-CAD	3.52	1.28	1.22
23	c	514	CLA	OBD-CAD	3.52	1.28	1.22
23	b	607	CLA	CHB-C1B	3.52	1.47	1.39
35	c	519	DGD	O2G-C1B	3.51	1.44	1.34
23	B	605	CLA	CHD-C4C	3.51	1.47	1.39
23	B	609	CLA	CHB-C1B	3.51	1.47	1.39
23	b	606	CLA	CHC-C4B	3.51	1.47	1.39
23	b	602	CLA	O2A-CGA	3.51	1.43	1.33
23	C	503	CLA	C3D-C2D	3.51	1.48	1.39
23	b	601	CLA	CHB-C1B	3.50	1.47	1.39
33	d	411	LHG	O7-C7	3.50	1.44	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	506	CLA	OBD-CAD	3.50	1.28	1.22
23	C	512	CLA	CHB-C1B	3.50	1.47	1.39
23	c	508	CLA	CHB-C1B	3.50	1.47	1.39
33	A	420	LHG	O7-C7	3.49	1.44	1.34
33	b	630	LHG	O8-C23	3.49	1.43	1.33
23	c	505	CLA	CHB-C1B	3.49	1.47	1.39
23	b	609	CLA	CHC-C4B	3.49	1.47	1.39
23	B	616	CLA	CHD-C1D	3.48	1.45	1.38
23	B	608	CLA	CHB-C1B	3.48	1.47	1.39
23	a	406	CLA	CHB-C1B	3.48	1.47	1.39
23	b	605	CLA	OBD-CAD	3.48	1.28	1.22
23	c	503	CLA	OBD-CAD	3.48	1.28	1.22
23	b	613	CLA	CHD-C1D	3.47	1.45	1.38
23	C	506	CLA	C1B-NB	-3.47	1.33	1.37
23	a	406	CLA	CHC-C4B	3.47	1.47	1.39
23	B	601	CLA	CHB-C1B	3.46	1.47	1.39
23	b	613	CLA	CHB-C1B	3.46	1.47	1.39
23	b	605	CLA	C3D-C2D	3.46	1.48	1.39
23	b	608	CLA	OBD-CAD	3.45	1.28	1.22
23	B	610	CLA	O2A-CGA	3.45	1.43	1.33
23	b	605	CLA	O2A-CGA	3.44	1.43	1.33
23	B	602	CLA	C1B-NB	-3.44	1.33	1.37
23	B	609	CLA	C1B-NB	-3.44	1.33	1.37
23	b	602	CLA	CHB-C1B	3.44	1.47	1.39
23	c	507	CLA	CHC-C4B	3.44	1.47	1.39
23	B	616	CLA	CHC-C4B	3.44	1.47	1.39
23	C	509	CLA	C1B-NB	-3.43	1.33	1.37
23	C	513	CLA	C4B-NB	-3.43	1.33	1.37
23	D	402	CLA	C3D-C2D	3.43	1.48	1.39
23	C	505	CLA	OBD-CAD	3.43	1.28	1.22
23	c	503	CLA	CHC-C4B	3.43	1.47	1.39
23	A	406	CLA	CHB-C1B	3.43	1.47	1.39
23	B	611	CLA	C3D-C2D	3.42	1.48	1.39
23	d	401	CLA	CHC-C4B	3.42	1.47	1.39
23	c	510	CLA	C4B-NB	-3.42	1.33	1.37
23	B	612	CLA	CHC-C4B	3.41	1.47	1.39
23	d	401	CLA	OBD-CAD	3.41	1.28	1.22
23	A	408	CLA	CHB-C1B	3.41	1.47	1.39
23	B	608	CLA	CHD-C4C	3.41	1.47	1.39
23	c	510	CLA	OBD-CAD	3.41	1.28	1.22
23	B	608	CLA	OBD-CAD	3.40	1.28	1.22
23	C	505	CLA	C3D-C2D	3.40	1.48	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C4B-NB	-3.40	1.33	1.37
23	c	504	CLA	C3D-C2D	3.40	1.48	1.39
23	c	505	CLA	OBD-CAD	3.40	1.28	1.22
23	C	501	CLA	C1B-NB	-3.40	1.33	1.37
23	C	501	CLA	OBD-CAD	3.39	1.28	1.22
23	b	613	CLA	C1B-NB	-3.39	1.33	1.37
24	a	408	PHO	O2A-CGA	3.39	1.43	1.33
23	b	607	CLA	CHC-C4B	3.39	1.47	1.39
23	C	502	CLA	CHC-C4B	3.39	1.47	1.39
23	b	607	CLA	CHD-C4C	3.39	1.47	1.39
23	b	603	CLA	OBD-CAD	3.39	1.28	1.22
23	C	505	CLA	C1B-NB	-3.39	1.33	1.37
23	b	603	CLA	CHB-C1B	3.39	1.47	1.39
38	f	101	HEM	C4D-ND	-3.39	1.34	1.40
23	B	607	CLA	OBD-CAD	3.38	1.28	1.22
23	c	512	CLA	CHC-C4B	3.38	1.47	1.39
23	B	612	CLA	OBD-CAD	3.37	1.28	1.22
23	B	608	CLA	O2A-CGA	3.37	1.43	1.33
35	H	102	DGD	O2G-C1B	3.37	1.43	1.34
34	D	410	HTG	C1'-S1	-3.36	1.77	1.81
23	B	603	CLA	CHC-C4B	3.36	1.47	1.39
23	b	604	CLA	C1B-NB	-3.36	1.33	1.37
23	a	405	CLA	CHC-C4B	3.36	1.46	1.39
23	a	406	CLA	C1B-NB	-3.36	1.33	1.37
23	b	616	CLA	OBD-CAD	3.36	1.28	1.22
23	C	513	CLA	CHC-C4B	3.36	1.46	1.39
23	c	514	CLA	C1B-NB	-3.35	1.33	1.37
23	C	511	CLA	CHC-C4B	3.35	1.46	1.39
23	B	613	CLA	O2A-CGA	3.35	1.43	1.33
23	C	507	CLA	C1B-NB	-3.34	1.33	1.37
23	b	607	CLA	C1B-C2B	3.34	1.51	1.43
23	A	404	CLA	OBD-CAD	3.34	1.28	1.22
23	B	604	CLA	CHC-C4B	3.34	1.46	1.39
23	B	607	CLA	C3D-C2D	3.34	1.48	1.39
23	D	402	CLA	CHC-C4B	3.33	1.46	1.39
23	b	610	CLA	O2A-CGA	3.33	1.43	1.33
23	A	408	CLA	CHC-C4B	3.33	1.46	1.39
23	C	510	CLA	OBD-CAD	3.33	1.28	1.22
23	b	602	CLA	C3B-C4B	3.33	1.50	1.42
23	b	616	CLA	C3B-C4B	3.32	1.50	1.42
23	b	615	CLA	CHC-C4B	3.32	1.46	1.39
23	B	612	CLA	CHD-C4C	3.32	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1B-NB	-3.32	1.33	1.37
23	b	603	CLA	O2A-CGA	3.31	1.43	1.33
23	c	507	CLA	C1B-NB	-3.31	1.33	1.37
23	B	609	CLA	C3B-C4B	3.31	1.50	1.42
23	b	610	CLA	C1B-NB	-3.31	1.33	1.37
23	C	507	CLA	OBD-CAD	3.30	1.28	1.22
23	a	405	CLA	C1B-NB	-3.30	1.33	1.37
38	F	102	HEM	C1B-NB	-3.30	1.34	1.40
23	C	504	CLA	OBD-CAD	3.29	1.28	1.22
23	C	506	CLA	CHC-C4B	3.29	1.46	1.39
23	b	612	CLA	C4B-NB	-3.29	1.33	1.37
23	B	616	CLA	CHD-C4C	3.29	1.46	1.39
23	B	608	CLA	C1B-NB	-3.28	1.33	1.37
38	f	101	HEM	C1B-NB	-3.28	1.34	1.40
23	c	506	CLA	C3B-C4B	3.28	1.50	1.42
23	d	401	CLA	C1D-ND	3.27	1.41	1.37
34	c	522	HTG	C1'-S1	-3.27	1.77	1.81
23	b	612	CLA	C1B-NB	-3.27	1.33	1.37
23	D	402	CLA	OBD-CAD	3.26	1.28	1.22
23	A	408	CLA	C1B-NB	-3.26	1.33	1.37
23	B	603	CLA	OBD-CAD	3.26	1.28	1.22
23	B	604	CLA	C3D-C2D	3.26	1.48	1.39
38	F	102	HEM	C4D-ND	-3.26	1.34	1.40
23	B	601	CLA	C3B-C4B	3.25	1.50	1.42
23	B	613	CLA	C1B-NB	-3.25	1.33	1.37
23	b	608	CLA	CHC-C4B	3.24	1.46	1.39
23	B	610	CLA	C1B-NB	-3.24	1.33	1.37
23	b	601	CLA	C1B-NB	-3.24	1.33	1.37
23	b	616	CLA	CHB-C1B	3.24	1.46	1.39
23	b	607	CLA	O2A-CGA	3.24	1.42	1.33
23	d	402	CLA	OBD-CAD	3.24	1.28	1.22
23	a	407	CLA	CHC-C4B	3.24	1.46	1.39
23	C	507	CLA	C4B-NB	-3.22	1.33	1.37
23	C	505	CLA	C3B-C4B	3.22	1.50	1.42
23	b	606	CLA	C1B-NB	-3.21	1.33	1.37
23	c	504	CLA	C3B-C4B	3.21	1.50	1.42
23	a	409	CLA	CHD-C4C	3.21	1.46	1.39
23	B	615	CLA	CHC-C4B	3.21	1.46	1.39
23	c	512	CLA	C1B-C2B	3.20	1.50	1.43
23	A	405	CLA	C3B-C4B	3.20	1.50	1.42
23	b	613	CLA	CHD-C4C	3.20	1.46	1.39
23	C	506	CLA	C4B-NB	-3.20	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C1B-NB	-3.19	1.33	1.37
23	C	513	CLA	C1B-NB	-3.19	1.33	1.37
23	A	404	CLA	O2A-CGA	3.19	1.42	1.33
34	b	625	HTG	C1'-S1	-3.19	1.77	1.81
23	b	608	CLA	C4B-NB	-3.19	1.33	1.37
23	B	609	CLA	OBD-CAD	3.18	1.28	1.22
23	D	403	CLA	C1C-C2C	3.18	1.50	1.44
23	b	614	CLA	C1B-NB	-3.18	1.33	1.37
23	C	503	CLA	OBD-CAD	3.18	1.28	1.22
23	B	612	CLA	C1C-C2C	3.17	1.50	1.44
23	D	402	CLA	C4B-NB	-3.17	1.33	1.37
23	b	602	CLA	C1B-NB	-3.17	1.33	1.37
23	a	405	CLA	C4B-NB	-3.17	1.33	1.37
23	b	611	CLA	OBD-CAD	3.17	1.27	1.22
23	c	502	CLA	OBD-CAD	3.17	1.27	1.22
23	c	511	CLA	OBD-CAD	3.16	1.27	1.22
23	b	612	CLA	CHD-C4C	3.16	1.46	1.39
23	B	606	CLA	OBD-CAD	3.15	1.27	1.22
23	A	404	CLA	CHC-C4B	3.15	1.46	1.39
34	d	409	HTG	C1'-S1	-3.15	1.77	1.81
23	c	514	CLA	C4B-NB	-3.15	1.33	1.37
23	C	503	CLA	C3B-C4B	3.14	1.50	1.42
23	B	602	CLA	OBD-CAD	3.14	1.27	1.22
23	B	605	CLA	C1B-C2B	3.13	1.50	1.43
23	C	501	CLA	C3B-C4B	3.13	1.50	1.42
23	b	609	CLA	C1B-NB	-3.13	1.33	1.37
23	A	406	CLA	C3B-C4B	3.13	1.50	1.42
23	b	611	CLA	C1B-NB	-3.12	1.33	1.37
23	B	605	CLA	C1B-NB	-3.12	1.33	1.37
23	A	405	CLA	OBD-CAD	3.12	1.27	1.22
23	C	508	CLA	C4B-NB	-3.12	1.33	1.37
23	C	512	CLA	C3B-C4B	3.12	1.50	1.42
23	c	506	CLA	C1B-NB	-3.11	1.34	1.37
24	A	416	PHO	CHA-CBD	-3.10	1.47	1.51
23	b	604	CLA	C1B-C2B	3.10	1.50	1.43
23	b	612	CLA	C1B-C2B	3.10	1.50	1.43
23	A	404	CLA	C1B-NB	-3.09	1.34	1.37
23	a	407	CLA	C1B-NB	-3.09	1.34	1.37
23	B	608	CLA	C4B-NB	-3.09	1.34	1.37
23	D	403	CLA	C3B-C4B	3.08	1.50	1.42
23	b	613	CLA	C4B-NB	-3.07	1.34	1.37
23	a	405	CLA	O2A-CGA	3.07	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	C1B-NB	-3.07	1.34	1.37
23	b	614	CLA	OBD-CAD	3.07	1.27	1.22
23	c	503	CLA	C4B-NB	-3.07	1.34	1.37
23	B	615	CLA	C3B-C4B	3.06	1.49	1.42
34	C	520	HTG	C1'-S1	-3.06	1.77	1.81
23	c	513	CLA	C3B-C4B	3.06	1.49	1.42
23	B	605	CLA	C3B-C4B	3.06	1.49	1.42
23	C	502	CLA	C4B-NB	-3.05	1.34	1.37
23	C	505	CLA	C1B-C2B	3.05	1.50	1.43
23	a	409	CLA	C1C-C2C	3.05	1.50	1.44
23	C	511	CLA	OBD-CAD	3.05	1.27	1.22
23	a	407	CLA	C3B-C4B	3.05	1.49	1.42
23	c	514	CLA	C3B-C4B	3.04	1.49	1.42
23	b	611	CLA	C1B-C2B	3.04	1.50	1.43
40	V	201	HEC	FE-NB	3.04	2.04	1.94
23	a	409	CLA	OBD-CAD	3.04	1.27	1.22
23	C	510	CLA	C4B-NB	-3.03	1.34	1.37
23	c	505	CLA	C1B-C2B	3.03	1.50	1.43
23	b	601	CLA	C3B-C4B	3.03	1.49	1.42
23	B	607	CLA	C4B-NB	-3.02	1.34	1.37
23	B	616	CLA	OBD-CAD	3.02	1.27	1.22
23	B	616	CLA	C1B-C2B	3.02	1.50	1.43
40	V	201	HEC	FE-NC	3.01	2.05	1.95
23	B	614	CLA	C1B-NB	-3.01	1.34	1.37
23	B	607	CLA	C1B-C2B	3.00	1.50	1.43
23	B	602	CLA	C1C-C2C	2.99	1.50	1.44
23	d	401	CLA	C4B-NB	-2.99	1.34	1.37
23	B	614	CLA	OBD-CAD	2.98	1.27	1.22
23	b	603	CLA	C1B-C2B	2.98	1.50	1.43
23	c	504	CLA	C1B-NB	-2.98	1.34	1.37
23	B	606	CLA	C1B-NB	-2.98	1.34	1.37
23	c	512	CLA	C1B-NB	-2.98	1.34	1.37
23	d	402	CLA	C3B-C4B	2.98	1.49	1.42
23	B	606	CLA	C3B-C4B	2.97	1.49	1.42
23	b	614	CLA	C1B-C2B	2.97	1.50	1.43
23	b	603	CLA	C3B-C4B	2.96	1.49	1.42
23	B	616	CLA	C1B-NB	-2.96	1.34	1.37
23	C	502	CLA	C1B-NB	-2.96	1.34	1.37
23	A	404	CLA	C4C-C3C	2.96	1.50	1.45
23	a	409	CLA	C1B-C2B	2.96	1.50	1.43
23	a	406	CLA	C3B-C4B	2.96	1.49	1.42
23	A	408	CLA	OBD-CAD	2.95	1.27	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	C4B-NB	-2.95	1.34	1.37
23	B	605	CLA	OBD-CAD	2.95	1.27	1.22
23	c	506	CLA	C1B-C2B	2.94	1.50	1.43
23	c	504	CLA	OBD-CAD	2.94	1.27	1.22
23	c	504	CLA	C4B-NB	-2.94	1.34	1.37
23	c	509	CLA	C3B-C4B	2.94	1.49	1.42
23	a	409	CLA	C3B-C4B	2.93	1.49	1.42
23	A	408	CLA	C4B-NB	-2.93	1.34	1.37
40	v	201	HEC	FE-NC	2.93	2.05	1.95
23	B	608	CLA	CHC-C4B	2.93	1.46	1.39
23	c	503	CLA	C1B-C2B	2.93	1.50	1.43
23	c	502	CLA	C3B-C4B	2.92	1.49	1.42
23	C	511	CLA	C1B-C2B	2.92	1.50	1.43
23	C	503	CLA	C4B-NB	-2.92	1.34	1.37
23	C	512	CLA	C1B-NB	-2.92	1.34	1.37
23	B	604	CLA	C1B-NB	-2.91	1.34	1.37
23	b	602	CLA	C1C-C2C	2.91	1.50	1.44
23	b	607	CLA	OBD-CAD	2.91	1.27	1.22
23	B	610	CLA	C3B-C4B	2.90	1.49	1.42
23	B	601	CLA	C4B-NB	-2.90	1.34	1.37
23	b	603	CLA	C1B-NB	-2.90	1.34	1.37
23	c	508	CLA	C1C-C2C	2.90	1.50	1.44
23	C	511	CLA	C4D-CHA	2.90	1.48	1.38
23	C	501	CLA	C1C-C2C	2.90	1.50	1.44
23	c	504	CLA	C1C-C2C	2.89	1.50	1.44
23	c	508	CLA	C4B-NB	-2.89	1.34	1.37
23	B	608	CLA	C1B-C2B	2.88	1.50	1.43
23	B	607	CLA	C4D-CHA	2.88	1.48	1.38
23	c	508	CLA	C1B-NB	-2.88	1.34	1.37
23	C	512	CLA	C1C-C2C	2.87	1.50	1.44
23	A	406	CLA	C4B-NB	-2.87	1.34	1.37
23	b	609	CLA	C3B-C4B	2.87	1.49	1.42
23	b	604	CLA	C4D-CHA	2.86	1.48	1.38
23	c	507	CLA	C4B-NB	-2.85	1.34	1.37
23	B	616	CLA	C4B-NB	-2.84	1.34	1.37
23	C	502	CLA	C1B-C2B	2.83	1.49	1.43
23	C	504	CLA	C1B-C2B	2.83	1.49	1.43
23	D	402	CLA	C1B-C2B	2.83	1.49	1.43
23	b	610	CLA	C3B-C4B	2.83	1.49	1.42
24	A	407	PHO	CBD-CGD	-2.83	1.48	1.52
23	b	606	CLA	C3B-C4B	2.83	1.49	1.42
23	b	612	CLA	C3B-C4B	2.83	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C1B-C2B	2.83	1.49	1.43
23	c	510	CLA	CHC-C4B	2.82	1.45	1.39
23	C	513	CLA	C1B-C2B	2.82	1.49	1.43
23	B	601	CLA	C1B-NB	-2.82	1.34	1.37
23	B	614	CLA	C1B-C2B	2.82	1.49	1.43
23	B	604	CLA	C1B-C2B	2.82	1.49	1.43
23	C	507	CLA	C4D-CHA	2.81	1.48	1.38
35	H	102	DGD	O5D-C1E	2.81	1.45	1.40
23	B	614	CLA	C4D-CHA	2.80	1.48	1.38
23	B	615	CLA	C1B-C2B	2.80	1.49	1.43
23	B	604	CLA	C4B-NB	-2.80	1.34	1.37
23	b	611	CLA	C4B-NB	-2.80	1.34	1.37
23	B	613	CLA	C4D-CHA	2.80	1.48	1.38
23	c	509	CLA	C4B-NB	-2.80	1.34	1.37
23	C	504	CLA	C4D-CHA	2.79	1.48	1.38
23	C	503	CLA	C1B-NB	-2.79	1.34	1.37
23	c	504	CLA	C1B-C2B	2.78	1.49	1.43
23	c	511	CLA	C1B-C2B	2.78	1.49	1.43
23	c	511	CLA	C4B-NB	-2.78	1.34	1.37
23	c	505	CLA	C4B-NB	-2.78	1.34	1.37
23	B	602	CLA	C1B-C2B	2.78	1.49	1.43
23	c	508	CLA	C1B-C2B	2.78	1.49	1.43
23	b	612	CLA	C1C-C2C	2.78	1.49	1.44
23	b	614	CLA	C3B-C4B	2.77	1.49	1.42
23	B	615	CLA	C1B-NB	-2.77	1.34	1.37
23	c	512	CLA	C4B-NB	-2.77	1.34	1.37
23	b	613	CLA	C4D-CHA	2.77	1.48	1.38
29	A	414	PL9	C6-C5	2.76	1.49	1.35
23	b	609	CLA	C4D-CHA	2.76	1.48	1.38
23	c	510	CLA	C1B-C2B	2.76	1.49	1.43
23	B	602	CLA	C3B-C4B	2.76	1.49	1.42
23	B	610	CLA	C4D-CHA	2.75	1.48	1.38
29	a	415	PL9	C6-C5	2.75	1.49	1.35
23	B	610	CLA	C1B-C2B	2.75	1.49	1.43
23	B	606	CLA	C1B-C2B	2.75	1.49	1.43
23	A	404	CLA	C1B-C2B	2.75	1.49	1.43
23	c	502	CLA	C4B-NB	-2.75	1.34	1.37
23	c	509	CLA	C1B-C2B	2.75	1.49	1.43
23	C	504	CLA	C4B-NB	-2.75	1.34	1.37
23	b	613	CLA	C1B-C2B	2.74	1.49	1.43
23	b	605	CLA	C3B-C4B	2.74	1.49	1.42
23	c	509	CLA	C4D-CHA	2.74	1.48	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3B-C4B	2.74	1.49	1.42
34	b	625	HTG	C1-S1	-2.74	1.76	1.80
23	B	609	CLA	C1B-C2B	2.73	1.49	1.43
26	a	411	SQD	C6-S	-2.73	1.67	1.77
23	c	513	CLA	C4D-CHA	2.73	1.48	1.38
23	A	405	CLA	C4B-NB	-2.73	1.34	1.37
23	c	505	CLA	C1C-C2C	2.73	1.49	1.44
23	c	506	CLA	C1C-C2C	2.73	1.49	1.44
26	A	410	SQD	C6-S	-2.73	1.67	1.77
23	A	406	CLA	C4D-CHA	2.72	1.48	1.38
23	a	407	CLA	C1C-C2C	2.72	1.49	1.44
23	a	406	CLA	C1B-C2B	2.72	1.49	1.43
23	c	508	CLA	C4D-CHA	2.72	1.48	1.38
23	c	512	CLA	C4D-CHA	2.72	1.48	1.38
23	b	615	CLA	C4D-CHA	2.72	1.48	1.38
23	D	402	CLA	C4D-CHA	2.71	1.48	1.38
23	c	514	CLA	C1C-C2C	2.71	1.49	1.44
23	c	506	CLA	C4C-C3C	2.71	1.49	1.45
23	c	510	CLA	C4D-CHA	2.71	1.48	1.38
23	c	513	CLA	C1B-NB	-2.70	1.34	1.37
23	B	613	CLA	C4C-C3C	2.70	1.49	1.45
23	C	508	CLA	C3B-C4B	2.70	1.49	1.42
26	A	412	SQD	C6-S	-2.70	1.67	1.77
23	c	511	CLA	C4D-CHA	2.70	1.48	1.38
23	c	511	CLA	C3B-C4B	2.70	1.49	1.42
23	c	507	CLA	C1B-C2B	2.70	1.49	1.43
23	b	603	CLA	C4B-NB	-2.70	1.34	1.37
23	b	616	CLA	C1B-NB	-2.70	1.34	1.37
26	f	102	SQD	C6-S	-2.70	1.67	1.77
23	B	616	CLA	C3B-C4B	2.70	1.49	1.42
23	C	510	CLA	C1B-C2B	2.70	1.49	1.43
23	B	605	CLA	C1C-C2C	2.69	1.49	1.44
23	c	511	CLA	C1C-C2C	2.69	1.49	1.44
23	C	501	CLA	C4D-CHA	2.69	1.48	1.38
23	B	610	CLA	C1C-C2C	2.69	1.49	1.44
23	A	405	CLA	C4D-CHA	2.68	1.47	1.38
23	b	611	CLA	C3B-C4B	2.68	1.49	1.42
23	B	612	CLA	C4D-CHA	2.68	1.47	1.38
23	B	612	CLA	C1B-C2B	2.68	1.49	1.43
23	c	502	CLA	C1B-C2B	2.68	1.49	1.43
23	a	407	CLA	C1B-C2B	2.68	1.49	1.43
32	Z	101	LMG	O8-C28	2.68	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	509	CLA	C1C-C2C	2.68	1.49	1.44
23	B	608	CLA	C4C-C3C	2.67	1.49	1.45
23	B	606	CLA	C1C-C2C	2.67	1.49	1.44
23	B	615	CLA	C1C-C2C	2.67	1.49	1.44
23	A	408	CLA	C4D-CHA	2.67	1.47	1.38
23	C	510	CLA	C1C-C2C	2.66	1.49	1.44
23	B	601	CLA	C1C-C2C	2.66	1.49	1.44
23	B	616	CLA	C4D-CHA	2.66	1.47	1.38
23	b	604	CLA	C3B-C4B	2.66	1.49	1.42
23	a	405	CLA	C1B-C2B	2.66	1.49	1.43
23	b	609	CLA	C4B-NB	-2.66	1.34	1.37
23	C	506	CLA	C3B-C4B	2.65	1.49	1.42
26	a	413	SQD	C6-S	-2.65	1.67	1.77
23	C	504	CLA	C1C-C2C	2.65	1.49	1.44
23	d	401	CLA	C1B-C2B	2.65	1.49	1.43
23	C	506	CLA	C4C-C3C	2.65	1.49	1.45
23	D	403	CLA	C1B-C2B	2.64	1.49	1.43
23	b	610	CLA	C1C-C2C	2.64	1.49	1.44
23	C	509	CLA	C3B-C4B	2.64	1.48	1.42
23	C	505	CLA	C4D-CHA	2.64	1.47	1.38
23	C	507	CLA	C1C-C2C	2.64	1.49	1.44
23	c	502	CLA	C1C-C2C	2.64	1.49	1.44
31	t	101	LMT	O3'-C3'	-2.64	1.36	1.43
23	B	613	CLA	C1B-C2B	2.63	1.49	1.43
23	c	504	CLA	C4D-CHA	2.63	1.47	1.38
23	c	503	CLA	C1B-NB	-2.63	1.34	1.37
23	a	407	CLA	C4B-NB	-2.63	1.34	1.37
23	c	509	CLA	C4C-C3C	2.62	1.49	1.45
23	a	407	CLA	C4D-CHA	2.62	1.47	1.38
23	c	502	CLA	C4D-CHA	2.62	1.47	1.38
27	A	418	GOL	O2-C2	-2.62	1.35	1.43
23	b	608	CLA	C3B-C4B	2.62	1.48	1.42
23	A	405	CLA	C1B-C2B	2.62	1.49	1.43
23	b	616	CLA	C1C-C2C	2.62	1.49	1.44
23	C	506	CLA	C4D-CHA	2.62	1.47	1.38
23	B	614	CLA	C3B-C4B	2.61	1.48	1.42
23	b	607	CLA	C4D-CHA	2.61	1.47	1.38
23	B	607	CLA	C4C-C3C	2.61	1.49	1.45
23	C	503	CLA	C1C-C2C	2.61	1.49	1.44
23	B	603	CLA	C3B-C4B	2.61	1.48	1.42
23	D	403	CLA	C4C-C3C	2.61	1.49	1.45
23	C	508	CLA	C1B-C2B	2.61	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C4C-C3C	2.61	1.49	1.45
23	c	505	CLA	C4D-CHA	2.61	1.47	1.38
23	c	514	CLA	C1B-C2B	2.60	1.49	1.43
23	C	511	CLA	C3D-C4D	-2.60	1.38	1.44
23	c	509	CLA	C1B-NB	-2.60	1.34	1.37
23	C	508	CLA	C4D-CHA	2.60	1.47	1.38
23	d	402	CLA	C4B-NB	-2.60	1.34	1.37
23	B	604	CLA	C4D-CHA	2.60	1.47	1.38
23	C	505	CLA	C1C-C2C	2.60	1.49	1.44
23	C	513	CLA	C4D-CHA	2.59	1.47	1.38
23	c	504	CLA	C3D-C4D	-2.59	1.38	1.44
31	m	103	LMT	O2B-C2B	-2.59	1.36	1.43
23	B	603	CLA	C4D-CHA	2.59	1.47	1.38
23	b	608	CLA	C1B-C2B	2.58	1.49	1.43
23	B	609	CLA	C1C-C2C	2.58	1.49	1.44
23	c	513	CLA	C4B-NB	-2.58	1.34	1.37
23	b	610	CLA	C4D-CHA	2.58	1.47	1.38
23	C	512	CLA	C4D-CHA	2.58	1.47	1.38
23	C	508	CLA	C1B-NB	-2.58	1.34	1.37
23	C	509	CLA	C1C-C2C	2.57	1.49	1.44
23	a	405	CLA	C3B-C4B	2.57	1.48	1.42
23	A	404	CLA	C4D-CHA	2.57	1.47	1.38
23	C	501	CLA	C1B-C2B	2.57	1.49	1.43
34	B	623	HTG	C1'-S1	-2.57	1.78	1.81
23	b	614	CLA	C4C-C3C	2.57	1.49	1.45
23	B	607	CLA	C1C-C2C	2.56	1.49	1.44
23	C	509	CLA	C4D-CHA	2.56	1.47	1.38
23	C	509	CLA	C1B-C2B	2.56	1.49	1.43
23	b	615	CLA	C1B-C2B	2.56	1.49	1.43
23	d	401	CLA	C4C-C3C	2.56	1.49	1.45
23	a	409	CLA	C4D-CHA	2.55	1.47	1.38
23	b	615	CLA	C3B-C4B	2.55	1.48	1.42
34	b	622	HTG	O5-C1	2.55	1.46	1.42
23	d	402	CLA	C4D-CHA	2.55	1.47	1.38
31	A	421	LMT	O3'-C3'	-2.55	1.37	1.43
23	B	607	CLA	C3D-C4D	-2.55	1.38	1.44
23	B	608	CLA	C4D-CHA	2.55	1.47	1.38
24	a	417	PHO	C3A-C2A	-2.55	1.52	1.54
23	b	606	CLA	C1B-C2B	2.55	1.49	1.43
23	d	402	CLA	C1C-C2C	2.55	1.49	1.44
23	C	513	CLA	C3B-C4B	2.54	1.48	1.42
23	b	607	CLA	C1C-C2C	2.54	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1B-C2B	2.54	1.49	1.43
23	c	506	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	C4C-C3C	2.54	1.49	1.45
23	B	615	CLA	C4D-CHA	2.54	1.47	1.38
23	b	606	CLA	C4D-CHA	2.54	1.47	1.38
23	C	505	CLA	C4B-NB	-2.54	1.34	1.37
23	c	503	CLA	C4D-CHA	2.54	1.47	1.38
38	f	101	HEM	C1C-C2C	-2.54	1.40	1.45
23	C	510	CLA	C4D-CHA	2.54	1.47	1.38
23	B	602	CLA	C4D-CHA	2.53	1.47	1.38
23	C	511	CLA	C4C-C3C	2.53	1.49	1.45
23	B	604	CLA	C4C-C3C	2.53	1.49	1.45
23	C	512	CLA	C1B-C2B	2.53	1.49	1.43
23	b	609	CLA	C1B-C2B	2.53	1.49	1.43
23	B	605	CLA	C4D-CHA	2.53	1.47	1.38
23	b	601	CLA	C4D-CHA	2.53	1.47	1.38
23	d	402	CLA	C1B-C2B	2.53	1.49	1.43
23	B	602	CLA	C4B-NB	-2.52	1.34	1.37
26	b	620	SQD	C6-S	-2.52	1.68	1.77
23	B	606	CLA	C4D-CHA	2.52	1.47	1.38
26	B	620	SQD	C6-S	-2.52	1.68	1.77
23	B	609	CLA	C4D-CHA	2.52	1.47	1.38
31	e	101	LMT	O3'-C3'	-2.52	1.37	1.43
23	b	616	CLA	C1B-C2B	2.52	1.49	1.43
23	B	604	CLA	C3B-C4B	2.52	1.48	1.42
34	B	625	HTG	C1-S1	-2.52	1.76	1.80
23	C	510	CLA	C4C-C3C	2.52	1.49	1.45
40	V	201	HEC	CAC-C3C	2.52	1.57	1.51
23	b	608	CLA	C4D-CHA	2.52	1.47	1.38
31	c	501	LMT	O3'-C3'	-2.51	1.37	1.43
31	B	631	LMT	O3'-C3'	-2.51	1.37	1.43
31	M	101	LMT	O2'-C2'	-2.51	1.37	1.43
23	b	613	CLA	C4C-C3C	2.51	1.49	1.45
23	c	502	CLA	C1B-NB	-2.51	1.34	1.37
23	B	616	CLA	C1C-C2C	2.51	1.49	1.44
23	C	511	CLA	C1C-C2C	2.51	1.49	1.44
23	b	603	CLA	C1C-C2C	2.51	1.49	1.44
23	C	506	CLA	C1B-C2B	2.50	1.49	1.43
23	b	614	CLA	C4D-CHA	2.50	1.47	1.38
23	C	505	CLA	C4C-C3C	2.50	1.49	1.45
23	c	507	CLA	C3B-C4B	2.50	1.48	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	C3D-C4D	-2.50	1.38	1.44
23	b	612	CLA	C4D-CHA	2.50	1.47	1.38
23	A	404	CLA	C1C-C2C	2.49	1.49	1.44
23	a	405	CLA	C4C-C3C	2.49	1.49	1.45
23	C	502	CLA	C3B-C4B	2.49	1.48	1.42
23	c	508	CLA	C3B-C4B	2.49	1.48	1.42
23	b	616	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	503	CLA	C3D-C4D	-2.48	1.38	1.44
23	c	510	CLA	C3B-C4B	2.48	1.48	1.42
23	c	507	CLA	C4D-CHA	2.48	1.47	1.38
23	B	616	CLA	C3B-C2B	2.48	1.49	1.41
23	a	405	CLA	C4D-CHA	2.48	1.47	1.38
23	B	613	CLA	C4B-NB	-2.48	1.34	1.37
23	a	406	CLA	C4D-CHA	2.48	1.47	1.38
23	c	514	CLA	C4D-CHA	2.47	1.47	1.38
23	B	603	CLA	C1C-C2C	2.47	1.49	1.44
23	c	512	CLA	C1C-C2C	2.47	1.49	1.44
23	c	513	CLA	C1B-C2B	2.47	1.49	1.43
23	B	612	CLA	C3B-C2B	2.47	1.49	1.41
26	F	103	SQD	C6-S	-2.47	1.68	1.77
23	B	615	CLA	C4B-NB	-2.46	1.34	1.37
23	B	611	CLA	MG-NB	2.46	2.10	2.05
23	b	602	CLA	C3D-C4D	-2.46	1.38	1.44
23	C	502	CLA	C4D-CHA	2.46	1.47	1.38
23	c	502	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	616	CLA	C4D-CHA	2.46	1.47	1.38
23	C	513	CLA	C1C-C2C	2.46	1.49	1.44
23	B	613	CLA	C1C-C2C	2.45	1.49	1.44
23	b	610	CLA	C4B-NB	-2.45	1.34	1.37
23	c	502	CLA	C4C-C3C	2.45	1.49	1.45
23	b	612	CLA	C3B-C2B	2.45	1.49	1.41
23	C	506	CLA	C1C-C2C	2.45	1.49	1.44
23	B	606	CLA	C3D-C4D	-2.45	1.38	1.44
23	b	602	CLA	C4B-NB	-2.45	1.34	1.37
23	C	508	CLA	C3B-C2B	2.44	1.49	1.41
23	b	607	CLA	C4C-C3C	2.44	1.49	1.45
23	B	602	CLA	C3D-C4D	-2.44	1.38	1.44
23	C	506	CLA	C3D-C4D	-2.44	1.38	1.44
23	a	407	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	607	CLA	C4B-NB	-2.44	1.34	1.37
23	C	510	CLA	C3B-C4B	2.44	1.48	1.42
23	A	406	CLA	C1B-C2B	2.44	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C4C-C3C	2.44	1.49	1.45
23	B	608	CLA	C3B-C4B	2.44	1.48	1.42
23	b	609	CLA	C1C-C2C	2.44	1.49	1.44
31	T	101	LMT	O3'-C3'	-2.43	1.37	1.43
23	B	601	CLA	C4D-CHA	2.43	1.47	1.38
23	d	402	CLA	C1B-NB	-2.43	1.34	1.37
31	M	101	LMT	O3'-C3'	-2.43	1.37	1.43
23	C	503	CLA	C4D-CHA	2.43	1.47	1.38
23	b	614	CLA	C4B-NB	-2.43	1.34	1.37
23	C	509	CLA	C4C-C3C	2.43	1.49	1.45
23	A	408	CLA	C3D-C4D	-2.43	1.38	1.44
23	A	404	CLA	C3B-C4B	2.43	1.48	1.42
23	c	505	CLA	C3B-C4B	2.43	1.48	1.42
23	b	602	CLA	C4D-CHA	2.42	1.47	1.38
23	c	504	CLA	C4C-C3C	2.42	1.49	1.45
23	b	606	CLA	C4B-NB	-2.42	1.34	1.37
31	F	101	LMT	O3'-C3'	-2.42	1.37	1.43
31	M	101	LMT	O2B-C2B	-2.42	1.37	1.43
23	b	613	CLA	C3B-C4B	2.42	1.48	1.42
23	b	614	CLA	C3D-C4D	-2.41	1.38	1.44
23	b	605	CLA	C1B-C2B	2.41	1.48	1.43
23	A	405	CLA	C1C-C2C	2.41	1.49	1.44
23	b	604	CLA	C1C-C2C	2.41	1.49	1.44
40	v	201	HEC	CAC-C3C	2.41	1.57	1.51
23	A	406	CLA	C1C-C2C	2.41	1.49	1.44
23	B	614	CLA	C4C-C3C	2.41	1.49	1.45
23	C	508	CLA	C1C-C2C	2.41	1.49	1.44
23	D	403	CLA	C4D-CHA	2.41	1.47	1.38
23	C	511	CLA	C1B-NB	-2.41	1.34	1.37
23	b	603	CLA	C3B-C2B	2.41	1.49	1.41
23	B	613	CLA	C3B-C4B	2.40	1.48	1.42
23	b	603	CLA	C4D-CHA	2.40	1.46	1.38
23	b	612	CLA	C4C-C3C	2.40	1.49	1.45
23	C	512	CLA	C4B-NB	-2.40	1.34	1.37
23	b	616	CLA	C4B-NB	-2.40	1.34	1.37
23	b	605	CLA	C1C-C2C	2.40	1.49	1.44
23	b	605	CLA	C4D-CHA	2.40	1.46	1.38
23	b	615	CLA	C3D-C4D	-2.40	1.38	1.44
23	D	402	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	608	CLA	C3D-C4D	-2.39	1.38	1.44
23	c	512	CLA	C3B-C4B	2.39	1.48	1.42
38	F	102	HEM	C1C-C2C	-2.39	1.40	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1B-C2B	2.38	1.48	1.43
23	b	610	CLA	C3D-C4D	-2.38	1.38	1.44
23	d	401	CLA	C4D-CHA	2.38	1.46	1.38
23	c	514	CLA	C3D-C4D	-2.38	1.38	1.44
23	C	513	CLA	C3B-C2B	2.37	1.49	1.41
23	c	503	CLA	C3B-C4B	2.37	1.48	1.42
23	B	611	CLA	C4D-CHA	2.37	1.46	1.38
23	c	503	CLA	C3B-C2B	2.37	1.49	1.41
23	b	606	CLA	C3D-C4D	-2.37	1.38	1.44
31	B	630	LMT	O2'-C2'	-2.36	1.37	1.43
23	C	510	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	601	CLA	C1C-C2C	2.36	1.49	1.44
32	C	519	LMG	O1-C1	2.36	1.44	1.40
23	c	505	CLA	C1C-NC	-2.36	1.34	1.37
23	B	605	CLA	C3D-C4D	-2.36	1.38	1.44
40	V	201	HEC	CMB-C2B	2.36	1.55	1.50
23	b	613	CLA	OBD-CAD	2.35	1.26	1.22
29	d	404	PL9	C6-C5	2.35	1.47	1.35
23	c	512	CLA	C4C-C3C	2.35	1.49	1.45
23	A	408	CLA	C3B-C4B	2.35	1.48	1.42
38	f	101	HEM	C1D-ND	-2.35	1.34	1.38
23	b	614	CLA	C1C-C2C	2.35	1.49	1.44
31	B	628	LMT	C3'-C2'	2.35	1.58	1.52
23	c	505	CLA	C4C-C3C	2.35	1.49	1.45
24	A	416	PHO	C3D-C4D	-2.35	1.37	1.41
24	A	416	PHO	C3A-C2A	-2.34	1.52	1.54
23	A	405	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	613	CLA	C1C-C2C	2.34	1.49	1.44
23	B	610	CLA	C4B-NB	-2.34	1.34	1.37
23	b	611	CLA	C4D-CHA	2.34	1.46	1.38
29	D	405	PL9	C6-C5	2.34	1.47	1.35
23	B	601	CLA	C1B-C2B	2.34	1.48	1.43
35	c	519	DGD	O2G-C2G	-2.34	1.40	1.46
23	c	512	CLA	C3B-C2B	2.34	1.49	1.41
23	C	503	CLA	C1B-C2B	2.34	1.48	1.43
23	B	604	CLA	C3D-C4D	-2.34	1.38	1.44
31	B	628	LMT	O3'-C3'	-2.34	1.37	1.43
23	B	603	CLA	C3B-C2B	2.33	1.49	1.41
24	a	408	PHO	CBD-CGD	-2.33	1.49	1.52
23	b	615	CLA	C4C-C3C	2.33	1.49	1.45
23	b	604	CLA	C4B-NB	-2.33	1.34	1.37
23	c	514	CLA	C4C-C3C	2.33	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	405	CLA	C3B-C2B	2.32	1.49	1.41
23	A	404	CLA	C3B-C2B	2.32	1.49	1.41
23	C	501	CLA	C3D-C4D	-2.32	1.38	1.44
40	v	201	HEC	CMC-C2C	2.32	1.55	1.50
23	A	408	CLA	C3B-C2B	2.31	1.49	1.41
23	c	507	CLA	C3D-C4D	-2.31	1.39	1.44
31	A	417	LMT	O3'-C3'	-2.31	1.37	1.43
23	C	502	CLA	C1C-C2C	2.31	1.49	1.44
23	C	509	CLA	C3B-C2B	2.31	1.49	1.41
23	C	512	CLA	C3D-C4D	-2.31	1.39	1.44
23	d	401	CLA	C1C-C2C	2.30	1.49	1.44
23	d	401	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	504	CLA	C3B-C2B	2.30	1.49	1.41
23	a	409	CLA	C4B-NB	-2.30	1.35	1.37
23	C	511	CLA	C3B-C2B	2.30	1.49	1.41
23	c	509	CLA	C3B-C2B	2.30	1.49	1.41
35	C	517	DGD	O2G-C2G	-2.30	1.40	1.46
23	B	614	CLA	C1C-C2C	2.29	1.49	1.44
31	m	103	LMT	O3'-C3'	-2.28	1.37	1.43
23	b	606	CLA	C1C-C2C	2.28	1.49	1.44
23	b	609	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	601	CLA	C1B-C2B	2.28	1.48	1.43
31	A	421	LMT	O2'-C2'	-2.27	1.37	1.43
23	B	604	CLA	C3B-C2B	2.27	1.48	1.41
23	d	402	CLA	C3D-C4D	-2.27	1.39	1.44
31	B	630	LMT	O2B-C2B	-2.27	1.37	1.43
23	C	513	CLA	C3D-C4D	-2.27	1.39	1.44
27	A	418	GOL	C3-C2	2.27	1.61	1.51
23	C	504	CLA	C3D-C4D	-2.26	1.39	1.44
23	B	601	CLA	C3D-C4D	-2.26	1.39	1.44
24	A	416	PHO	C4B-NB	-2.26	1.34	1.38
23	b	610	CLA	C3B-C2B	2.26	1.48	1.41
23	C	502	CLA	C3D-C4D	-2.26	1.39	1.44
23	c	513	CLA	C1C-C2C	2.26	1.48	1.44
23	B	613	CLA	C3B-C2B	2.26	1.48	1.41
23	B	608	CLA	C3B-C2B	2.25	1.48	1.41
31	T	101	LMT	O2'-C2'	-2.25	1.37	1.43
23	b	601	CLA	C4C-C3C	2.25	1.48	1.45
31	T	101	LMT	O3B-C3B	-2.25	1.37	1.43
23	a	405	CLA	C1C-C2C	2.25	1.48	1.44
27	a	420	GOL	C1-C2	2.25	1.61	1.51
23	c	510	CLA	C3B-C2B	2.25	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C3B-C2B	2.25	1.48	1.41
23	c	511	CLA	C4C-C3C	2.25	1.48	1.45
31	b	621	LMT	C3'-C2'	2.25	1.58	1.52
23	A	406	CLA	C3D-C4D	-2.24	1.39	1.44
23	B	612	CLA	C4C-C3C	2.24	1.48	1.45
31	B	630	LMT	O3'-C3'	-2.24	1.37	1.43
23	C	502	CLA	C4C-C3C	2.24	1.48	1.45
23	d	401	CLA	C3B-C4B	2.24	1.48	1.42
35	h	102	DGD	O5D-C1E	2.24	1.44	1.40
23	B	615	CLA	C4C-C3C	2.24	1.48	1.45
23	C	508	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	615	CLA	C4B-NB	-2.24	1.35	1.37
23	b	604	CLA	C3B-C2B	2.24	1.48	1.41
23	b	607	CLA	C3B-C4B	2.24	1.48	1.42
23	C	503	CLA	C4C-C3C	2.24	1.48	1.45
23	c	507	CLA	C3B-C2B	2.23	1.48	1.41
23	b	610	CLA	C1B-C2B	2.23	1.48	1.43
23	C	510	CLA	C3B-C2B	2.23	1.48	1.41
34	D	410	HTG	C1-S1	-2.23	1.77	1.80
23	B	616	CLA	C3D-C4D	-2.23	1.39	1.44
23	B	602	CLA	C3B-C2B	2.23	1.48	1.41
34	B	622	HTG	O5-C1	2.23	1.45	1.42
23	C	506	CLA	C3B-C2B	2.23	1.48	1.41
23	b	608	CLA	C3B-C2B	2.23	1.48	1.41
35	H	102	DGD	O2G-C2G	-2.23	1.41	1.46
23	C	505	CLA	C3D-C4D	-2.23	1.39	1.44
23	A	408	CLA	C4C-C3C	2.22	1.48	1.45
23	d	402	CLA	C4C-C3C	2.22	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.22	1.39	1.44
23	c	513	CLA	C4C-C3C	2.22	1.48	1.45
23	a	409	CLA	C3B-C2B	2.21	1.48	1.41
23	B	610	CLA	C4C-C3C	2.21	1.48	1.45
23	b	601	CLA	C3B-C2B	2.21	1.48	1.41
23	c	505	CLA	C3D-C4D	-2.21	1.39	1.44
23	c	513	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	606	CLA	C4B-NB	-2.21	1.35	1.37
35	C	516	DGD	O5D-C1E	2.21	1.44	1.40
23	D	402	CLA	C4C-C3C	2.21	1.48	1.45
23	B	604	CLA	C1A-CHA	2.21	1.52	1.43
31	A	417	LMT	O2'-C2'	-2.20	1.37	1.43
23	c	506	CLA	C4B-NB	-2.20	1.35	1.37
23	b	611	CLA	C4C-C3C	2.20	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	409	CLA	C4C-C3C	2.20	1.48	1.45
23	a	406	CLA	C4B-NB	-2.20	1.35	1.37
24	A	416	PHO	C1D-ND	-2.20	1.34	1.38
23	D	402	CLA	C3B-C2B	2.19	1.48	1.41
23	b	605	CLA	C4B-NB	-2.19	1.35	1.37
23	B	612	CLA	C3B-C4B	2.19	1.47	1.42
29	a	415	PL9	C2-C3	2.19	1.40	1.34
23	C	507	CLA	C3D-C4D	-2.19	1.39	1.44
23	c	509	CLA	C3D-C4D	-2.19	1.39	1.44
23	C	501	CLA	C4C-C3C	2.19	1.48	1.45
23	b	611	CLA	C3D-C4D	-2.19	1.39	1.44
23	c	510	CLA	C3D-C4D	-2.19	1.39	1.44
31	t	101	LMT	O2'-C2'	-2.19	1.37	1.43
23	C	502	CLA	C3B-C2B	2.18	1.48	1.41
23	c	505	CLA	C3B-C2B	2.18	1.48	1.41
31	B	628	LMT	O4'-C4B	-2.17	1.37	1.43
23	c	512	CLA	MG-NA	2.17	2.11	2.06
27	b	624	GOL	C3-C2	2.17	1.60	1.51
40	V	201	HEC	CMC-C2C	2.17	1.55	1.50
23	B	608	CLA	C3D-C4D	-2.17	1.39	1.44
23	c	508	CLA	C3D-C4D	-2.16	1.39	1.44
31	b	627	LMT	O3'-C3'	-2.16	1.37	1.43
23	D	402	CLA	C3B-C4B	2.16	1.47	1.42
23	c	511	CLA	C3B-C2B	2.16	1.48	1.41
23	b	606	CLA	C3B-C2B	2.16	1.48	1.41
23	b	611	CLA	C1C-C2C	2.16	1.48	1.44
23	C	506	CLA	C1D-C2D	2.16	1.49	1.45
23	B	601	CLA	C3B-C2B	2.15	1.48	1.41
23	B	605	CLA	C4B-NB	-2.15	1.35	1.37
23	b	602	CLA	C1B-C2B	2.15	1.48	1.43
23	B	610	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	609	CLA	C3D-C4D	-2.14	1.39	1.44
23	b	605	CLA	C1D-C2D	2.14	1.49	1.45
40	V	201	HEC	CMA-C3A	2.14	1.55	1.50
23	B	601	CLA	C4C-C3C	2.14	1.48	1.45
24	a	408	PHO	C4B-NB	-2.14	1.34	1.38
23	B	604	CLA	C1C-C2C	2.14	1.48	1.44
23	C	501	CLA	C4B-NB	-2.14	1.35	1.37
31	m	103	LMT	O3B-C3B	-2.14	1.37	1.43
23	C	504	CLA	C3B-C4B	2.14	1.47	1.42
23	c	511	CLA	C3D-C4D	-2.13	1.39	1.44
23	c	514	CLA	C3B-C2B	2.13	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	621	LMT	O3'-C3'	-2.13	1.38	1.43
24	a	417	PHO	C4B-NB	-2.13	1.34	1.38
23	C	512	CLA	C3B-C2B	2.13	1.48	1.41
23	b	614	CLA	C3B-C2B	2.13	1.48	1.41
23	b	608	CLA	C1C-C2C	2.13	1.48	1.44
24	A	407	PHO	C4B-NB	-2.12	1.34	1.38
29	A	414	PL9	C2-C1	-2.12	1.39	1.44
26	F	103	SQD	O6-C1	2.12	1.43	1.40
23	B	616	CLA	C1C-NC	-2.12	1.34	1.37
23	b	611	CLA	C3B-C2B	2.12	1.48	1.41
31	A	417	LMT	O2B-C2B	-2.12	1.38	1.43
23	a	406	CLA	C1C-C2C	2.12	1.48	1.44
23	b	607	CLA	C3D-C4D	-2.12	1.39	1.44
31	B	631	LMT	O2'-C2'	-2.11	1.38	1.43
23	D	403	CLA	C3D-C4D	-2.11	1.39	1.44
31	e	101	LMT	O2'-C2'	-2.11	1.38	1.43
23	B	604	CLA	MG-NA	2.11	2.11	2.06
31	e	101	LMT	O2B-C2B	-2.11	1.38	1.43
31	B	628	LMT	O5'-C5'	-2.11	1.39	1.44
31	b	627	LMT	O2'-C2'	-2.10	1.38	1.43
23	c	506	CLA	C3D-C4D	-2.10	1.39	1.44
23	c	507	CLA	C1C-NC	-2.10	1.34	1.37
24	A	407	PHO	C1B-NB	-2.09	1.34	1.38
23	B	615	CLA	C3D-C4D	-2.08	1.39	1.44
23	B	606	CLA	C3B-C2B	2.08	1.48	1.41
23	a	407	CLA	C4C-C3C	2.08	1.48	1.45
23	c	514	CLA	C1D-C2D	2.08	1.49	1.45
23	b	604	CLA	C1A-CHA	2.08	1.51	1.43
23	B	603	CLA	C4C-C3C	2.08	1.48	1.45
23	d	401	CLA	C3B-C2B	2.07	1.48	1.41
23	B	608	CLA	C1C-NC	-2.07	1.34	1.37
23	C	507	CLA	C3B-C2B	2.07	1.48	1.41
23	c	502	CLA	C1C-NC	-2.07	1.34	1.37
23	C	507	CLA	C3B-C4B	2.07	1.47	1.42
24	A	407	PHO	C1D-ND	-2.07	1.34	1.38
23	b	603	CLA	C4C-C3C	2.06	1.48	1.45
23	c	503	CLA	C3D-C4D	-2.06	1.39	1.44
31	e	101	LMT	O3B-C3B	-2.06	1.38	1.43
23	b	607	CLA	C1D-C2D	2.06	1.49	1.45
23	C	509	CLA	C3D-C4D	-2.05	1.39	1.44
23	C	501	CLA	C3B-C2B	2.05	1.48	1.41
38	F	102	HEM	C3B-C4B	2.05	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C3B-C4B	2.05	1.47	1.42
23	c	507	CLA	C4C-C3C	2.05	1.48	1.45
23	b	609	CLA	C1C-NC	-2.04	1.34	1.37
23	B	606	CLA	C4C-C3C	2.04	1.48	1.45
23	b	601	CLA	C3D-C4D	-2.04	1.39	1.44
34	c	522	HTG	C1-S1	-2.04	1.77	1.80
29	D	405	PL9	C2-C3	2.04	1.40	1.34
38	F	102	HEM	C1D-ND	-2.04	1.34	1.38
24	a	417	PHO	C1B-NB	-2.03	1.34	1.38
23	c	503	CLA	C1C-C2C	2.03	1.48	1.44
23	c	502	CLA	C3B-C2B	2.03	1.48	1.41
23	B	611	CLA	C3D-C4D	-2.03	1.39	1.44
23	c	507	CLA	C1C-C2C	2.03	1.48	1.44
31	F	101	LMT	O3B-C3B	-2.03	1.38	1.43
23	B	607	CLA	C3B-C2B	2.03	1.48	1.41
23	d	402	CLA	C3B-C2B	2.03	1.48	1.41
33	b	630	LHG	O7-C5	-2.02	1.41	1.46
23	B	609	CLA	C4C-C3C	2.02	1.48	1.45
31	m	103	LMT	C3'-C2'	2.02	1.57	1.52
23	c	513	CLA	C3B-C2B	2.02	1.48	1.41
23	b	607	CLA	C1A-CHA	2.02	1.51	1.43
23	A	408	CLA	C1C-C2C	2.02	1.48	1.44
23	A	404	CLA	C3D-C4D	-2.02	1.39	1.44
27	B	629	GOL	O2-C2	-2.02	1.37	1.43
23	B	615	CLA	C1C-NC	-2.01	1.34	1.37
23	C	512	CLA	C4C-C3C	2.01	1.48	1.45
31	A	421	LMT	O2B-C2B	-2.01	1.38	1.43
23	C	504	CLA	C4C-C3C	2.01	1.48	1.45
23	B	601	CLA	C1C-NC	-2.01	1.34	1.37
31	A	421	LMT	O3B-C3B	-2.00	1.38	1.43
31	F	101	LMT	O2B-C2B	-2.00	1.38	1.43
24	a	417	PHO	CBD-CGD	-2.00	1.49	1.52

All (2825) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	16.58	121.35	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.28	91.13	107.16
24	a	417	PHO	C2D-C1D-ND	11.91	117.75	109.53
23	B	611	CLA	C1D-ND-C4D	-11.66	98.05	106.33
24	A	407	PHO	C2D-C1D-ND	11.43	117.42	109.53
24	a	408	PHO	C2D-C1D-ND	11.21	117.26	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	416	PHO	C2D-C1D-ND	10.73	116.93	109.53
23	B	612	CLA	C1D-ND-C4D	-10.41	98.94	106.33
23	b	605	CLA	C1D-ND-C4D	-10.31	99.01	106.33
23	B	611	CLA	CHB-C1B-NB	-10.00	113.67	124.26
23	B	611	CLA	C2D-C1D-ND	9.92	117.42	110.10
23	a	409	CLA	C1D-ND-C4D	-9.84	99.34	106.33
23	C	503	CLA	C1D-ND-C4D	-9.77	99.40	106.33
23	B	615	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	a	407	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	B	605	CLA	C1D-ND-C4D	-9.66	99.47	106.33
23	b	611	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	B	606	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	B	612	CLA	C2D-C1D-ND	9.59	117.17	110.10
23	b	603	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	A	408	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	c	504	CLA	C1D-ND-C4D	-9.54	99.56	106.33
23	B	601	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	c	502	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	C	501	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	C	509	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	A	406	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	d	402	CLA	C1D-ND-C4D	-9.39	99.66	106.33
23	C	510	CLA	C1D-ND-C4D	-9.38	99.67	106.33
23	B	603	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	c	512	CLA	C1D-ND-C4D	-9.36	99.68	106.33
23	C	505	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	B	610	CLA	C1D-ND-C4D	-9.33	99.71	106.33
23	c	514	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	B	607	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	B	614	CLA	C1D-ND-C4D	-9.29	99.73	106.33
23	b	616	CLA	C1D-ND-C4D	-9.23	99.78	106.33
23	b	606	CLA	C1D-ND-C4D	-9.21	99.79	106.33
23	B	616	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	B	605	CLA	C2D-C1D-ND	9.16	116.85	110.10
23	a	409	CLA	C2D-C1D-ND	9.14	116.84	110.10
23	c	506	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	D	402	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	602	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	C	513	CLA	C1D-ND-C4D	-9.09	99.87	106.33
23	b	601	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	b	611	CLA	C2D-C1D-ND	9.09	116.80	110.10
23	A	405	CLA	C2D-C1D-ND	9.08	116.79	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	B	616	CLA	C2D-C1D-ND	9.06	116.78	110.10
23	b	615	CLA	C1D-ND-C4D	-9.05	99.91	106.33
23	d	401	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	c	507	CLA	C1D-ND-C4D	-9.02	99.93	106.33
23	D	403	CLA	C1D-ND-C4D	-9.01	99.93	106.33
23	B	602	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	b	614	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	b	608	CLA	C1D-ND-C4D	-9.01	99.94	106.33
23	a	405	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	605	CLA	C2D-C1D-ND	8.95	116.70	110.10
23	c	510	CLA	C1D-ND-C4D	-8.94	99.98	106.33
23	c	505	CLA	C1D-ND-C4D	-8.94	99.99	106.33
23	b	610	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	b	613	CLA	C2D-C1D-ND	8.88	116.65	110.10
23	c	513	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	C	512	CLA	C1D-ND-C4D	-8.86	100.04	106.33
23	A	408	CLA	C2D-C1D-ND	8.86	116.63	110.10
23	c	503	CLA	C1D-ND-C4D	-8.85	100.05	106.33
23	C	508	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	b	607	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	C	504	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	a	407	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	B	610	CLA	C2D-C1D-ND	8.78	116.58	110.10
23	b	609	CLA	C1D-ND-C4D	-8.78	100.10	106.33
23	B	603	CLA	C2D-C1D-ND	8.76	116.56	110.10
23	B	613	CLA	C2D-C1D-ND	8.76	116.56	110.10
23	B	608	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	C	504	CLA	C2D-C1D-ND	8.72	116.53	110.10
23	c	502	CLA	C2D-C1D-ND	8.72	116.53	110.10
23	B	606	CLA	C2D-C1D-ND	8.71	116.52	110.10
23	B	615	CLA	C2D-C1D-ND	8.67	116.49	110.10
23	a	406	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	b	612	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	B	607	CLA	C2D-C1D-ND	8.63	116.47	110.10
23	B	614	CLA	C2D-C1D-ND	8.63	116.47	110.10
23	c	511	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	A	406	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	B	608	CLA	C2D-C1D-ND	8.56	116.41	110.10
23	c	509	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	B	613	CLA	C1D-ND-C4D	-8.53	100.28	106.33
23	b	614	CLA	C2D-C1D-ND	8.53	116.39	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	C	511	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	D	402	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	509	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	507	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	C	503	CLA	C2D-C1D-ND	8.46	116.34	110.10
23	B	609	CLA	C1D-ND-C4D	-8.46	100.33	106.33
23	c	513	CLA	C2B-C1B-NB	8.45	115.90	110.23
23	c	509	CLA	C2D-C1D-ND	8.41	116.30	110.10
23	c	503	CLA	C2D-C1D-ND	8.37	116.27	110.10
23	C	506	CLA	C1D-ND-C4D	-8.36	100.39	106.33
23	b	603	CLA	C2D-C1D-ND	8.36	116.27	110.10
23	C	501	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	b	607	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	b	608	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	C	508	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	c	505	CLA	C2D-C1D-ND	8.28	116.21	110.10
23	b	613	CLA	C1D-ND-C4D	-8.28	100.45	106.33
23	d	402	CLA	C2D-C1D-ND	8.28	116.20	110.10
23	c	512	CLA	C2D-C1D-ND	8.26	116.19	110.10
23	b	610	CLA	C2D-C1D-ND	8.25	116.19	110.10
23	c	504	CLA	C2D-C1D-ND	8.22	116.16	110.10
23	C	502	CLA	C1D-ND-C4D	-8.21	100.50	106.33
23	b	612	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	b	604	CLA	C1D-ND-C4D	-8.15	100.55	106.33
23	b	615	CLA	C2D-C1D-ND	8.12	116.09	110.10
23	c	511	CLA	C2D-C1D-ND	8.12	116.09	110.10
23	c	508	CLA	C1D-ND-C4D	-8.12	100.57	106.33
23	b	616	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	C	507	CLA	C2D-C1D-ND	8.10	116.07	110.10
23	C	513	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	b	602	CLA	C4A-NA-C1A	-8.03	103.09	106.71
23	a	405	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	B	601	CLA	C2D-C1D-ND	7.98	115.98	110.10
23	b	609	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	507	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	d	401	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	C	511	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	B	601	CLA	C2B-C1B-NB	7.91	115.53	110.23
23	C	512	CLA	C2B-C1B-NB	7.90	115.53	110.23
23	c	510	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	D	403	CLA	C2D-C1D-ND	7.85	115.89	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	b	602	CLA	C2B-C1B-NB	7.84	115.49	110.23
23	B	602	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	b	601	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	C	512	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	C	503	CLA	C2B-C1B-NB	7.79	115.45	110.23
23	C	503	CLA	C4A-NA-C1A	-7.76	103.22	106.71
23	B	611	CLA	CHD-C4C-C3C	-7.75	113.45	124.84
23	C	513	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	C	505	CLA	C2D-C1D-ND	7.70	115.78	110.10
23	b	616	CLA	C2B-C1B-NB	7.70	115.39	110.23
23	A	404	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	B	604	CLA	C1D-ND-C4D	-7.68	100.88	106.33
23	c	513	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	c	508	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	c	506	CLA	C2D-C1D-ND	7.65	115.74	110.10
23	c	514	CLA	C2D-C1D-ND	7.64	115.74	110.10
23	c	514	CLA	C2B-C1B-NB	7.62	115.34	110.23
23	B	614	CLA	C2B-C1B-NB	7.61	115.33	110.23
23	b	614	CLA	C2B-C1B-NB	7.60	115.33	110.23
23	B	609	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	d	402	CLA	C2B-C1B-NB	7.55	115.29	110.23
23	b	604	CLA	C2D-C1D-ND	7.54	115.66	110.10
23	A	404	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	c	509	CLA	C2B-C1B-NB	7.52	115.28	110.23
23	b	601	CLA	C2B-C1B-NB	7.48	115.24	110.23
23	C	502	CLA	C2D-C1D-ND	7.47	115.61	110.10
23	b	606	CLA	C2B-C1B-NB	7.46	115.24	110.23
23	C	510	CLA	C2B-C1B-NB	7.46	115.23	110.23
23	C	510	CLA	C2D-C1D-ND	7.45	115.59	110.10
34	b	623	HTG	C1'-S1-C1	7.40	113.94	100.09
23	B	605	CLA	CHD-C4C-C3C	-7.39	113.97	124.84
23	b	602	CLA	C2D-C1D-ND	7.39	115.55	110.10
23	C	511	CLA	C2B-C1B-NB	7.38	115.18	110.23
24	A	416	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	A	408	CLA	C2B-C1B-NB	7.37	115.17	110.23
23	B	606	CLA	CMD-C2D-C1D	7.34	137.65	124.71
23	C	510	CLA	CMD-C2D-C1D	7.29	137.57	124.71
23	C	508	CLA	C2B-C1B-NB	7.27	115.11	110.23
23	C	509	CLA	C2B-C1B-NB	7.24	115.09	110.23
24	a	417	PHO	O2D-CGD-CBD	7.21	120.13	111.00
23	B	608	CLA	C2B-C1B-NB	7.20	115.06	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404	CLA	C2B-C1B-NB	7.20	115.06	110.23
23	B	609	CLA	C4A-NA-C1A	-7.20	103.47	106.71
23	c	506	CLA	C2B-C1B-NB	7.17	115.04	110.23
24	a	408	PHO	O2D-CGD-CBD	7.16	120.07	111.00
24	a	408	PHO	C1C-C2C-C3C	-7.15	102.67	108.61
23	B	614	CLA	CMD-C2D-C1D	7.13	137.28	124.71
23	c	508	CLA	O2D-CGD-CBD	7.13	123.93	111.27
24	A	416	PHO	C2B-C1B-NB	7.12	114.44	109.53
23	B	611	CLA	CMB-C2B-C1B	7.12	136.21	125.37
24	a	417	PHO	C2B-C1B-NB	7.11	114.44	109.53
23	A	406	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	c	505	CLA	C2B-C1B-NB	7.09	114.99	110.23
24	a	417	PHO	C4D-ND-C1D	-7.08	101.62	108.83
23	b	605	CLA	C2B-C1B-NB	7.08	114.98	110.23
23	b	611	CLA	C2B-C1B-NB	7.08	114.98	110.23
23	c	504	CLA	C2B-C1B-NB	7.06	114.97	110.23
23	c	510	CLA	C2B-C1B-NB	7.06	114.97	110.23
23	b	616	CLA	C4A-NA-C1A	-7.05	103.53	106.71
23	C	506	CLA	C2D-C1D-ND	7.00	115.27	110.10
23	a	405	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	C	506	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	B	610	CLA	CMD-C2D-C1D	6.98	137.02	124.71
23	B	604	CLA	C2D-C1D-ND	6.97	115.24	110.10
23	c	511	CLA	C2B-C1B-NB	6.97	114.90	110.23
23	B	606	CLA	CHD-C1D-ND	-6.96	118.06	124.45
26	F	103	SQD	O6-C1-C2	6.95	119.16	108.30
23	b	605	CLA	CHD-C1D-ND	-6.95	118.06	124.45
23	B	602	CLA	C2B-C1B-NB	6.95	114.89	110.23
23	C	505	CLA	C2B-C1B-NB	6.95	114.89	110.23
23	b	608	CLA	C2B-C1B-NB	6.94	114.89	110.23
23	b	605	CLA	CHD-C4C-C3C	-6.94	114.63	124.84
24	A	407	PHO	O2D-CGD-CBD	6.91	119.75	111.00
24	a	417	PHO	C1C-C2C-C3C	-6.90	102.87	108.61
23	B	613	CLA	C2B-C1B-NB	6.90	114.86	110.23
23	B	609	CLA	C2B-C1B-NB	6.90	114.86	110.23
23	C	502	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	b	613	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	a	407	CLA	C2B-C1B-NB	6.86	114.83	110.23
24	A	407	PHO	C4D-ND-C1D	-6.85	101.86	108.83
23	c	502	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	b	616	CLA	O2D-CGD-CBD	6.83	123.40	111.27
23	b	606	CLA	C4A-NA-C1A	-6.82	103.64	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	CMD-C2D-C1D	6.82	136.73	124.71
23	c	502	CLA	CMD-C2D-C1D	6.81	136.72	124.71
23	b	610	CLA	C2B-C1B-NB	6.80	114.79	110.23
23	B	616	CLA	CHD-C4C-C3C	-6.80	114.85	124.84
23	b	616	CLA	CHD-C4C-C3C	-6.79	114.86	124.84
23	D	403	CLA	C2B-C1B-NB	6.79	114.78	110.23
23	c	508	CLA	CMD-C2D-C1D	6.79	136.68	124.71
23	c	514	CLA	CMD-C2D-C1D	6.79	136.67	124.71
23	b	606	CLA	CMD-C2D-C1D	6.78	136.67	124.71
23	B	616	CLA	O2D-CGD-CBD	6.77	123.30	111.27
23	c	507	CLA	CMD-C2D-C1D	6.76	136.62	124.71
23	B	603	CLA	O2D-CGD-CBD	6.75	123.27	111.27
23	b	611	CLA	CMD-C2D-C1D	6.73	136.58	124.71
23	B	611	CLA	CMD-C2D-C1D	6.73	136.58	124.71
23	a	409	CLA	C2B-C1B-NB	6.72	114.74	110.23
23	d	402	CLA	CMD-C2D-C1D	6.72	136.56	124.71
23	A	405	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	C	507	CLA	CHD-C4C-C3C	-6.68	115.02	124.84
23	a	406	CLA	C2B-C1B-NB	6.67	114.71	110.23
40	V	201	HEC	C1D-ND-C4D	6.66	111.95	105.07
23	C	501	CLA	C2B-C1B-NB	6.66	114.70	110.23
23	C	509	CLA	CMD-C2D-C1D	6.65	136.43	124.71
23	b	615	CLA	C2B-C1B-NB	6.64	114.68	110.23
23	b	603	CLA	C2B-C1B-NB	6.63	114.68	110.23
23	A	404	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	c	504	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	C	512	CLA	C4A-NA-C1A	-6.62	103.73	106.71
23	B	604	CLA	C2B-C1B-NB	6.60	114.66	110.23
23	b	616	CLA	CMD-C2D-C1D	6.59	136.32	124.71
24	A	416	PHO	C1C-C2C-C3C	-6.58	103.14	108.61
23	B	603	CLA	C2B-C1B-NB	6.58	114.64	110.23
23	B	606	CLA	C4A-NA-C1A	-6.57	103.75	106.71
23	C	506	CLA	CMD-C2D-C1D	6.57	136.29	124.71
23	a	409	CLA	CHD-C4C-C3C	-6.56	115.19	124.84
23	b	606	CLA	CHD-C1D-ND	-6.55	118.44	124.45
23	B	615	CLA	C2B-C1B-NB	6.53	114.61	110.23
23	c	504	CLA	C4A-NA-C1A	-6.53	103.77	106.71
23	D	402	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	d	401	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	b	615	CLA	C4A-NA-C1A	-6.50	103.78	106.71
23	b	601	CLA	O2D-CGD-CBD	6.49	122.81	111.27
23	B	603	CLA	CHD-C4C-C3C	-6.49	115.30	124.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CMD-C2D-C1D	6.47	136.11	124.71
23	D	402	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	B	612	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	c	505	CLA	CHD-C1D-ND	-6.45	118.53	124.45
23	c	503	CLA	C2C-C1C-NC	6.45	116.01	109.97
23	C	503	CLA	CMD-C2D-C1D	6.44	136.07	124.71
23	C	512	CLA	CHD-C4C-C3C	-6.44	115.37	124.84
23	B	604	CLA	C2C-C1C-NC	6.43	116.00	109.97
23	c	514	CLA	CHD-C1D-ND	-6.43	118.54	124.45
23	B	601	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	B	616	CLA	C2B-C1B-NB	6.42	114.53	110.23
24	A	416	PHO	C4D-ND-C1D	-6.42	102.30	108.83
24	a	408	PHO	C2B-C1B-NB	6.41	113.95	109.53
23	c	513	CLA	C4A-NA-C1A	-6.41	103.83	106.71
23	c	503	CLA	C2B-C1B-NB	6.39	114.52	110.23
23	B	614	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	b	611	CLA	CHD-C1D-ND	-6.39	118.59	124.45
23	B	604	CLA	CMD-C2D-C1D	6.36	135.93	124.71
23	B	608	CLA	C2C-C1C-NC	6.36	115.93	109.97
23	c	508	CLA	CHD-C1D-ND	-6.35	118.61	124.45
24	a	408	PHO	C4D-ND-C1D	-6.34	102.38	108.83
23	c	507	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	a	407	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	b	609	CLA	C2B-C1B-NB	6.34	114.48	110.23
23	C	507	CLA	O2D-CGD-CBD	6.33	122.52	111.27
34	D	410	HTG	C1'-S1-C1	6.33	111.93	100.09
23	C	508	CLA	CHD-C4C-C3C	-6.32	115.55	124.84
23	C	503	CLA	CHD-C1D-ND	-6.32	118.65	124.45
23	b	610	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
23	a	407	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	b	607	CLA	C2C-C1C-NC	6.30	115.88	109.97
23	C	510	CLA	CHD-C1D-ND	-6.30	118.66	124.45
23	B	610	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
23	C	506	CLA	CHD-C1D-ND	-6.29	118.68	124.45
23	c	502	CLA	CHD-C1D-ND	-6.28	118.69	124.45
40	v	201	HEC	C1D-ND-C4D	6.27	111.55	105.07
23	b	614	CLA	CMD-C2D-C1D	6.27	135.76	124.71
23	D	402	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	b	612	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	a	405	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	c	512	CLA	C2B-C1B-NB	6.26	114.43	110.23
24	A	407	PHO	C2B-C1B-NB	6.25	113.84	109.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	C2B-C1B-NB	6.24	114.41	110.23
23	B	610	CLA	C2B-C1B-NB	6.23	114.41	110.23
23	b	614	CLA	O2D-CGD-CBD	6.22	122.32	111.27
23	b	601	CLA	CMD-C2D-C1D	6.22	135.67	124.71
23	a	406	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	B	605	CLA	CMD-C2D-C1D	6.20	135.65	124.71
23	b	613	CLA	CHD-C4C-C3C	-6.20	115.72	124.84
23	C	501	CLA	CMD-C2D-C1D	6.20	135.65	124.71
23	d	402	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	a	405	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	C	501	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
23	b	609	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	C	502	CLA	C2C-C1C-NC	6.17	115.76	109.97
23	c	503	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	c	507	CLA	C2B-C1B-NB	6.17	114.37	110.23
23	D	402	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	c	511	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
23	b	603	CLA	CHD-C4C-C3C	-6.16	115.78	124.84
24	A	407	PHO	C1C-C2C-C3C	-6.15	103.49	108.61
23	c	504	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
23	A	408	CLA	CHD-C1D-ND	-6.15	118.81	124.45
23	c	512	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
23	D	403	CLA	CMD-C2D-C1D	6.14	135.53	124.71
23	C	503	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	C	506	CLA	C2C-C1C-NC	6.13	115.72	109.97
23	b	612	CLA	C2B-C1B-NB	6.13	114.34	110.23
23	C	509	CLA	CHD-C1D-ND	-6.12	118.83	124.45
23	C	505	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	c	512	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	C	504	CLA	C2C-C1C-NC	6.12	115.70	109.97
23	B	610	CLA	O2D-CGD-CBD	6.10	122.11	111.27
23	b	607	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	A	404	CLA	C2C-C1C-NC	6.08	115.67	109.97
26	F	103	SQD	O47-C7-C8	6.08	124.60	111.50
23	b	601	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	A	408	CLA	C2C-C1C-NC	6.06	115.65	109.97
23	B	615	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	D	403	CLA	CHD-C4C-C3C	-6.05	115.94	124.84
23	c	506	CLA	O2D-CGD-CBD	6.05	122.02	111.27
23	b	601	CLA	C4A-NA-C1A	-6.05	103.99	106.71
23	b	615	CLA	CMD-C2D-C1D	6.04	135.36	124.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	c	522	HTG	C1'-S1-C1	6.04	111.39	100.09
26	A	410	SQD	O6-C1-C2	6.03	117.72	108.30
23	b	602	CLA	O2D-CGD-CBD	6.03	121.99	111.27
23	b	613	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	B	601	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	c	513	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	d	401	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	B	613	CLA	C2C-C1C-NC	6.02	115.61	109.97
23	b	606	CLA	CHD-C4C-C3C	-6.02	116.00	124.84
23	C	509	CLA	CHD-C4C-C3C	-6.01	116.00	124.84
23	b	604	CLA	O2D-CGD-CBD	6.01	121.95	111.27
23	A	408	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	B	611	CLA	CHD-C1D-ND	-6.01	118.93	124.45
23	B	609	CLA	CHD-C1D-ND	-6.00	118.94	124.45
23	B	602	CLA	CHD-C4C-C3C	-6.00	116.02	124.84
23	C	505	CLA	CHD-C4C-C3C	-5.99	116.03	124.84
23	B	606	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	b	604	CLA	C2B-C1B-NB	5.98	114.24	110.23
23	A	406	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
34	d	409	HTG	C1'-S1-C1	5.98	111.28	100.09
23	B	615	CLA	C4A-NA-C1A	-5.97	104.02	106.71
23	A	408	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
23	b	612	CLA	C2C-C1C-NC	5.96	115.56	109.97
23	b	604	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	C	510	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	c	508	CLA	C2B-C1B-NB	5.94	114.22	110.23
23	b	611	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	B	607	CLA	C2C-C1C-NC	5.93	115.53	109.97
23	c	505	CLA	CHD-C4C-C3C	-5.93	116.13	124.84
23	c	507	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	B	609	CLA	CMD-C2D-C1D	5.92	135.14	124.71
23	b	608	CLA	CMD-C2D-C1D	5.92	135.14	124.71
23	b	610	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	A	405	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414	PL9	C7-C8-C9	-5.89	116.99	126.79
23	A	404	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	B	613	CLA	CMD-C2D-C1D	5.89	135.09	124.71
23	c	505	CLA	CMD-C2D-C1D	5.88	135.08	124.71
23	A	406	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	C	509	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	603	CLA	C4A-NA-C1A	-5.88	104.06	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
23	b	615	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	D	402	CLA	C2B-C1B-NB	5.87	114.17	110.23
23	c	509	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	c	510	CLA	C2C-C1C-NC	5.86	115.46	109.97
23	D	403	CLA	C4A-NA-C1A	-5.85	104.07	106.71
23	b	608	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	B	601	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	C	511	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	c	511	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	B	613	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	b	607	CLA	CHD-C1D-ND	-5.84	119.09	124.45
23	c	508	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	C	510	CLA	O2D-CGD-CBD	5.83	121.63	111.27
23	b	608	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	C	513	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	b	613	CLA	CMD-C2D-C1D	5.82	134.97	124.71
23	b	614	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	A	404	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	c	506	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
23	C	511	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	C	511	CLA	CMD-C2D-C1D	5.79	134.93	124.71
23	C	509	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	c	509	CLA	C2C-C1C-NC	5.79	115.40	109.97
26	B	620	SQD	O6-C1-C2	5.79	117.35	108.30
23	B	601	CLA	O2D-CGD-CBD	5.78	121.55	111.27
23	d	402	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	c	504	CLA	CHD-C1D-ND	-5.77	119.16	124.45
23	B	615	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	B	602	CLA	C4A-NA-C1A	-5.76	104.12	106.71
23	C	501	CLA	O2D-CGD-CBD	5.75	121.49	111.27
23	B	607	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	a	405	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	a	406	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	C	512	CLA	CMD-C2D-C1D	5.74	134.83	124.71
23	B	615	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	A	406	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	c	507	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	b	604	CLA	CMD-C2D-C1D	5.71	134.78	124.71
23	B	602	CLA	O2D-CGD-CBD	5.71	121.42	111.27
23	b	601	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	B	602	CLA	C2C-C1C-NC	5.70	115.32	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	C	502	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
23	b	615	CLA	CHD-C4C-C3C	-5.69	116.47	124.84
23	B	606	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	b	602	CLA	CHD-C1D-ND	-5.69	119.22	124.45
23	c	513	CLA	CHD-C1D-ND	-5.68	119.23	124.45
23	d	401	CLA	C2B-C1B-NB	5.67	114.03	110.23
23	B	614	CLA	C2C-C1C-NC	5.66	115.27	109.97
23	b	603	CLA	CMD-C2D-C1D	5.65	134.67	124.71
23	B	605	CLA	C2B-C1B-NB	5.65	114.02	110.23
23	C	504	CLA	CHD-C1D-ND	-5.64	119.27	124.45
23	b	607	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	d	401	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	B	608	CLA	CHD-C4C-C3C	-5.64	116.56	124.84
23	B	603	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	c	506	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	b	602	CLA	CMD-C2D-C1D	5.63	134.64	124.71
23	c	513	CLA	CHD-C4C-C3C	-5.63	116.57	124.84
23	C	507	CLA	C2B-C1B-NB	5.61	113.99	110.23
23	b	611	CLA	O2D-CGD-CBD	5.61	121.23	111.27
23	a	406	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	B	602	CLA	CMD-C2D-C1D	5.60	134.58	124.71
23	b	616	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	B	610	CLA	CHD-C1D-ND	-5.59	119.31	124.45
23	b	615	CLA	CHD-C1D-ND	-5.59	119.32	124.45
26	a	411	SQD	O6-C1-C2	5.58	117.02	108.30
23	b	603	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	c	514	CLA	C4A-NA-C1A	-5.58	104.20	106.71
23	C	508	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	A	405	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	C	507	CLA	CHD-C1D-ND	-5.57	119.33	124.45
26	A	410	SQD	C1-O5-C5	-5.56	102.77	113.69
23	c	514	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
23	d	401	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	b	608	CLA	CHD-C4C-C3C	-5.56	116.67	124.84
23	a	407	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	C	502	CLA	CMD-C2D-C1D	5.55	134.50	124.71
23	d	401	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	b	603	CLA	C2C-C1C-NC	5.54	115.16	109.97
23	b	609	CLA	CHD-C1D-ND	-5.54	119.36	124.45
23	c	511	CLA	CHD-C1D-ND	-5.54	119.37	124.45

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	104.22	106.71
23	B	607	CLA	O2D-CGD-CBD	5.53	121.10	111.27
23	D	402	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	B	614	CLA	C3D-C2D-C1D	-5.53	98.28	105.83
23	c	508	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	c	503	CLA	O2D-CGD-CBD	5.53	121.10	111.27
25	D	404	BCR	C7-C8-C9	-5.52	117.89	126.23
23	B	603	CLA	CMD-C2D-C1D	5.52	134.45	124.71
23	B	607	CLA	CMD-C2D-C1D	5.52	134.44	124.71
23	C	513	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	d	402	CLA	O2D-CGD-CBD	5.51	121.06	111.27
23	B	616	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	B	614	CLA	O2D-CGD-CBD	5.51	121.06	111.27
23	B	612	CLA	CHD-C1D-ND	-5.51	119.39	124.45
23	C	513	CLA	CMD-C2D-C1D	5.51	134.42	124.71
23	B	612	CLA	O2D-CGD-CBD	5.50	121.05	111.27
23	b	603	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	b	614	CLA	CHD-C1D-ND	-5.50	119.40	124.45
34	B	623	HTG	C1'-S1-C1	5.50	110.37	100.09
23	c	512	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	C	505	CLA	O2D-CGD-CBD	5.49	121.03	111.27
23	c	509	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	c	511	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	b	612	CLA	O2D-CGD-CBD	5.48	121.01	111.27
23	c	510	CLA	C1-C2-C3	-5.47	116.57	126.04
23	b	609	CLA	CMD-C2D-C1D	5.47	134.35	124.71
25	Y	101	BCR	C33-C5-C6	-5.47	118.39	124.53
23	c	510	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	C	501	CLA	C4A-NA-C1A	-5.46	104.25	106.71
23	B	609	CLA	C2C-C1C-NC	5.46	115.08	109.97
23	b	613	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
23	b	611	CLA	C4A-NA-C1A	-5.45	104.25	106.71
23	B	604	CLA	CHD-C4C-C3C	-5.45	116.84	124.84
23	b	607	CLA	C2B-C1B-NB	5.44	113.88	110.23
23	a	406	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	B	611	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
23	b	614	CLA	C2C-C1C-NC	5.42	115.05	109.97
23	C	504	CLA	CHD-C4C-C3C	-5.42	116.87	124.84
23	B	604	CLA	O2D-CGD-CBD	5.42	120.90	111.27
23	B	605	CLA	C3D-C2D-C1D	-5.42	98.43	105.83
23	B	605	CLA	CHD-C1D-ND	-5.42	119.47	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	C2C-C1C-NC	5.41	115.04	109.97
23	C	504	CLA	C2B-C1B-NB	5.40	113.85	110.23
23	C	505	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	c	510	CLA	CMD-C2D-C1D	5.40	134.23	124.71
23	b	605	CLA	O2D-CGD-CBD	5.39	120.85	111.27
23	a	405	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	c	512	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	B	603	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	B	607	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	C	512	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	C	504	CLA	CMD-C2D-C1D	5.37	134.17	124.71
24	a	417	PHO	C1-C2-C3	-5.37	116.76	126.04
23	b	603	CLA	O2D-CGD-CBD	5.37	120.80	111.27
38	F	102	HEM	CAD-CBD-CGD	5.36	125.14	113.60
23	B	616	CLA	C3C-C4C-NC	5.36	116.58	110.57
23	b	609	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	A	405	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	b	604	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	a	407	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	A	406	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	b	608	CLA	C4A-NA-C1A	-5.33	104.31	106.71
23	C	501	CLA	CHD-C1D-ND	-5.33	119.56	124.45
26	B	620	SQD	O47-C7-C8	5.32	122.97	111.50
23	C	510	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	c	504	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	C	506	CLA	C4A-NA-C1A	-5.32	104.32	106.71
23	b	610	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	B	611	CLA	O2D-CGD-CBD	5.31	120.70	111.27
23	b	609	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	c	511	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	a	409	CLA	C2C-C1C-NC	5.29	114.93	109.97
23	c	510	CLA	O2D-CGD-CBD	5.29	120.67	111.27
23	a	405	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	C	511	CLA	O2D-CGD-CBD	5.28	120.66	111.27
23	B	602	CLA	CHD-C1D-ND	-5.28	119.60	124.45
23	b	604	CLA	CHD-C1D-ND	-5.28	119.61	124.45
23	c	508	CLA	C4A-NA-C1A	-5.27	104.34	106.71
23	C	507	CLA	C2C-C1C-NC	5.27	114.91	109.97
23	A	408	CLA	C3D-C2D-C1D	-5.27	98.65	105.83
23	B	612	CLA	C3C-C4C-NC	5.26	116.47	110.57
23	c	513	CLA	O2D-CGD-CBD	5.25	120.60	111.27
26	A	410	SQD	C1-C2-C3	-5.25	99.07	110.00

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	-5.24	104.35	106.71
23	b	610	CLA	CMD-C2D-C1D	5.24	133.94	124.71
23	b	612	CLA	C3C-C4C-NC	5.24	116.44	110.57
23	B	608	CLA	CHD-C1D-ND	-5.23	119.64	124.45
23	C	506	CLA	CHD-C4C-C3C	-5.23	117.15	124.84
23	c	510	CLA	CHD-C1D-ND	-5.22	119.65	124.45
23	C	508	CLA	CMD-C2D-C1D	5.22	133.91	124.71
25	t	102	BCR	C33-C5-C6	-5.22	118.67	124.53
23	b	606	CLA	C2C-C1C-NC	5.21	114.86	109.97
23	b	611	CLA	C3D-C2D-C1D	-5.21	98.72	105.83
26	a	411	SQD	O47-C7-C8	5.21	122.73	111.50
23	C	504	CLA	C3D-C2D-C1D	-5.20	98.73	105.83
23	C	502	CLA	CHD-C1D-ND	-5.20	119.67	124.45
23	b	614	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	B	610	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
23	B	606	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	c	502	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	c	502	CLA	O2D-CGD-CBD	5.19	120.49	111.27
23	A	405	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	b	605	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	a	406	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	c	513	CLA	C3B-C2B-C1B	-5.18	100.90	107.16
23	C	505	CLA	CHD-C1D-ND	-5.18	119.69	124.45
24	A	407	PHO	C3D-C4D-ND	5.17	114.77	107.72
23	B	608	CLA	CMD-C2D-C1D	5.17	133.83	124.71
23	a	409	CLA	C3C-C4C-NC	5.16	116.35	110.57
23	B	614	CLA	C3B-C2B-C1B	-5.15	100.95	107.16
23	c	505	CLA	O2D-CGD-CBD	5.15	120.41	111.27
23	b	604	CLA	C4A-NA-C1A	-5.14	104.40	106.71
23	c	505	CLA	C2C-C1C-NC	5.14	114.78	109.97
23	B	616	CLA	C3D-C2D-C1D	-5.13	98.83	105.83
23	B	613	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	D	402	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	D	403	CLA	O2D-CGD-CBD	5.12	120.36	111.27
23	C	512	CLA	CHD-C1D-ND	-5.12	119.75	124.45
23	C	511	CLA	CHD-C1D-ND	-5.11	119.76	124.45
23	b	614	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	c	509	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	c	506	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	c	502	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	C	508	CLA	O2D-CGD-CBD	5.09	120.31	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	417	PHO	C3D-C4D-ND	5.09	114.66	107.72
23	C	508	CLA	C3C-C4C-NC	5.09	116.28	110.57
23	B	615	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	C	501	CLA	C2C-C1C-NC	5.08	114.73	109.97
23	B	607	CLA	C2B-C1B-NB	5.07	113.63	110.23
23	a	409	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	C	513	CLA	C3B-C2B-C1B	-5.07	101.04	107.16
23	b	607	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	B	613	CLA	C1-C2-C3	-5.06	117.30	126.04
26	b	620	SQD	O6-C1-C2	5.05	116.19	108.30
23	b	605	CLA	C2C-C1C-NC	5.05	114.70	109.97
23	b	608	CLA	O2D-CGD-CBD	5.04	120.22	111.27
23	b	613	CLA	C4A-NA-C1A	-5.04	104.44	106.71
23	D	403	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	C	511	CLA	C3B-C2B-C1B	-5.03	101.08	107.16
23	B	616	CLA	C2C-C1C-NC	5.03	114.69	109.97
23	a	409	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	C	509	CLA	C3B-C2B-C1B	-5.02	101.10	107.16
23	B	614	CLA	C4A-NA-C1A	-5.00	104.46	106.71
23	b	606	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	d	402	CLA	C3D-C2D-C1D	-4.99	99.02	105.83
23	B	606	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	B	605	CLA	C3C-C4C-NC	4.99	116.16	110.57
23	c	514	CLA	C2C-C1C-NC	4.98	114.64	109.97
23	B	608	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
32	A	419	LMG	C7-O1-C1	-4.97	104.02	113.74
23	B	605	CLA	C2C-C1C-NC	4.97	114.63	109.97
23	B	603	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
23	B	613	CLA	CHD-C1D-ND	-4.96	119.89	124.45
23	c	504	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	c	506	CLA	CHD-C1D-ND	-4.95	119.91	124.45
34	b	622	HTG	C1-O5-C5	4.94	121.69	112.58
23	a	407	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	c	505	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	b	611	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	b	607	CLA	C3C-C4C-NC	4.93	116.10	110.57
23	C	507	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	b	613	CLA	CHD-C1D-ND	-4.92	119.94	124.45
23	B	607	CLA	C3D-C2D-C1D	-4.92	99.12	105.83
23	a	407	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
24	A	416	PHO	C3D-C4D-ND	4.91	114.42	107.72
23	B	608	CLA	O2D-CGD-CBD	4.91	119.99	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	O2D-CGD-CBD	4.90	119.98	111.27
23	C	512	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
26	b	620	SQD	O47-C7-C8	4.90	122.05	111.50
23	C	507	CLA	C3C-C4C-NC	4.89	116.06	110.57
23	c	507	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	a	406	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	A	404	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
23	B	615	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	b	616	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
23	c	509	CLA	CHD-C1D-ND	-4.87	119.98	124.45
23	c	505	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
23	A	408	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
23	c	505	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	b	614	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
23	c	509	CLA	C4A-NA-C1A	-4.86	104.52	106.71
23	a	409	CLA	C3D-C2D-C1D	-4.86	99.21	105.83
26	f	102	SQD	O47-C7-C8	4.85	121.96	111.50
23	A	405	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	d	402	CLA	C2C-C1C-NC	4.85	114.51	109.97
23	C	502	CLA	C4A-NA-C1A	-4.84	104.53	106.71
23	C	507	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
23	A	404	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	B	610	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	C	504	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	c	509	CLA	O2D-CGD-CBD	4.83	119.85	111.27
23	C	503	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
23	b	613	CLA	C3C-C4C-NC	4.83	115.98	110.57
23	c	508	CLA	C3D-C2D-C1D	-4.83	99.25	105.83
23	b	608	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	C	510	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	C	509	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	B	603	CLA	C3C-C4C-NC	4.82	115.97	110.57
23	b	601	CLA	C2C-C1C-NC	4.82	114.48	109.97
23	c	507	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	b	604	CLA	C1-C2-C3	-4.81	117.72	126.04
23	C	503	CLA	C3D-C2D-C1D	-4.81	99.26	105.83
23	c	506	CLA	C3C-C4C-NC	4.81	115.97	110.57
23	C	507	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
23	C	511	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	B	601	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	a	409	CLA	C4A-NA-C1A	-4.80	104.55	106.71
23	C	504	CLA	C3C-C4C-NC	4.80	115.95	110.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	C	520	HTG	C1'-S1-C1	4.80	109.06	100.09
23	B	601	CLA	C2C-C1C-NC	4.80	114.47	109.97
23	B	611	CLA	CMC-C2C-C1C	4.78	132.33	125.04
26	f	102	SQD	C1-O5-C5	4.78	123.06	113.69
23	B	612	CLA	C2B-C1B-NB	4.77	113.43	110.23
23	b	612	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	b	610	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	c	509	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
23	B	601	CLA	C3B-C2B-C1B	-4.75	101.42	107.16
23	C	505	CLA	C3C-C4C-NC	4.75	115.90	110.57
38	f	101	HEM	CHC-C4B-NB	4.75	129.57	124.42
23	C	508	CLA	CHD-C1D-ND	-4.74	120.10	124.45
23	A	406	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	B	616	CLA	CMD-C2D-C1D	4.74	133.06	124.71
23	B	611	CLA	C3C-C4C-NC	4.74	115.88	110.57
23	C	502	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	B	610	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	C	510	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
23	c	510	CLA	C4A-NA-C1A	-4.73	104.58	106.71
23	C	501	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
23	c	503	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
23	B	612	CLA	CMD-C2D-C1D	4.72	133.04	124.71
23	c	508	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
23	C	508	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	b	602	CLA	C3D-C4D-ND	4.72	117.87	110.24
23	C	509	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	C	505	CLA	C4A-NA-C1A	-4.71	104.59	106.71
23	A	405	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
23	A	404	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	d	402	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
23	c	503	CLA	C1C-C2C-C3C	-4.70	102.02	106.96
23	b	615	CLA	C3D-C2D-C1D	-4.69	99.42	105.83
23	c	511	CLA	O2D-CGD-CBD	4.69	119.61	111.27
23	b	602	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	B	604	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	b	613	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	a	407	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	b	602	CLA	C2C-C1C-NC	4.68	114.35	109.97
23	B	608	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
25	d	403	BCR	C15-C14-C13	-4.67	120.64	127.31
23	b	611	CLA	C3B-C2B-C1B	-4.67	101.52	107.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	O2D-CGD-CBD	4.67	119.56	111.27
23	C	513	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	a	408	PHO	C3D-C4D-ND	4.67	114.08	107.72
23	d	401	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	b	610	CLA	C3C-C4C-NC	4.65	115.79	110.57
23	B	612	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	D	403	CLA	C2C-C1C-NC	4.64	114.32	109.97
23	b	605	CLA	C3D-C4D-ND	4.64	117.75	110.24
23	B	611	CLA	C3D-C4D-ND	4.64	117.74	110.24
23	b	614	CLA	O2D-CGD-O1D	-4.64	114.77	123.84
23	B	613	CLA	C3C-C4C-NC	4.63	115.77	110.57
23	b	606	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	b	610	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	D	403	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
23	c	502	CLA	O2D-CGD-O1D	-4.63	114.80	123.84
23	A	406	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	c	514	CLA	O2D-CGD-CBD	4.62	119.48	111.27
23	B	601	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	C	508	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
23	b	610	CLA	CHD-C1D-ND	-4.61	120.22	124.45
23	C	503	CLA	C2C-C1C-NC	4.60	114.29	109.97
29	a	415	PL9	C7-C8-C9	-4.60	119.13	126.79
23	B	608	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	511	CLA	C1-C2-C3	-4.60	118.08	126.04
23	c	509	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	B	609	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	c	513	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	c	514	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	B	602	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	c	503	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	C	502	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	b	603	CLA	C3D-C4D-ND	4.58	117.65	110.24
23	C	512	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	405	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	C	511	CLA	C4A-NA-C1A	-4.58	104.65	106.71
23	a	407	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	b	609	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	513	CLA	O2D-CGD-CBD	4.57	119.38	111.27
23	B	604	CLA	C1-C2-C3	-4.57	118.15	126.04
32	B	621	LMG	O7-C10-C11	4.56	121.34	111.50
23	B	612	CLA	C2C-C1C-NC	4.56	114.25	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	C3B-C2B-C1B	-4.56	101.66	107.16
23	D	403	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	c	504	CLA	C3C-C4C-NC	4.56	115.68	110.57
23	D	402	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	c	512	CLA	C3B-C2B-C1B	-4.55	101.66	107.16
23	A	406	CLA	C3D-C4D-ND	4.55	117.61	110.24
23	b	609	CLA	C3C-C4C-NC	4.55	115.68	110.57
23	A	405	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	b	601	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
23	C	506	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	C	506	CLA	C3B-C2B-C1B	-4.53	101.69	107.16
23	A	408	CLA	O2D-CGD-CBD	4.53	119.31	111.27
24	A	416	PHO	C1-C2-C3	-4.53	118.22	126.04
25	d	403	BCR	C7-C8-C9	-4.52	119.40	126.23
23	c	502	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
23	b	605	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	C	510	CLA	C3D-C2D-C1D	-4.51	99.67	105.83
23	B	616	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
32	c	521	LMG	O6-C5-C4	4.51	117.88	109.69
23	d	402	CLA	C4A-NA-C1A	-4.51	104.68	106.71
23	B	610	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	b	604	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	a	406	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	b	601	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	b	606	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	c	510	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	C	504	CLA	C4A-NA-C1A	-4.48	104.69	106.71
23	a	405	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	c	511	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	b	603	CLA	C3C-C4C-NC	4.48	115.59	110.57
23	B	613	CLA	O2D-CGD-CBD	4.48	119.22	111.27
23	B	604	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
23	B	612	CLA	C3D-C4D-ND	4.47	117.47	110.24
23	b	616	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
23	C	506	CLA	C1C-C2C-C3C	-4.47	102.26	106.96
23	a	409	CLA	C3D-C4D-ND	4.47	117.46	110.24
23	b	604	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	c	503	CLA	C1D-CHD-C4C	-4.45	116.45	126.06
32	d	410	LMG	O7-C10-C11	4.45	121.09	111.50
23	c	513	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	d	401	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	C	502	CLA	C3D-C2D-C1D	-4.45	99.76	105.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
26	B	620	SQD	C3-C4-C5	4.44	118.17	110.24
23	c	508	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	B	609	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	d	401	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	b	601	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	C	510	CLA	C1-C2-C3	-4.44	118.37	126.04
23	c	503	CLA	CMD-C2D-C1D	4.44	132.53	124.71
23	b	603	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
23	C	512	CLA	C2C-C1C-NC	4.43	114.12	109.97
23	b	607	CLA	O2D-CGD-CBD	4.42	119.13	111.27
23	B	603	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
23	c	514	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	B	615	CLA	C3D-C4D-ND	4.42	117.38	110.24
23	B	613	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
23	C	505	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
38	F	102	HEM	CHC-C4B-NB	4.41	129.21	124.42
23	c	510	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
26	F	103	SQD	C1-O5-C5	-4.41	105.03	113.69
23	c	503	CLA	CHD-C1D-ND	-4.41	120.40	124.45
31	t	101	LMT	C3'-C4'-C5'	-4.40	100.83	110.93
23	c	506	CLA	C3B-C2B-C1B	-4.40	101.84	107.16
23	B	613	CLA	C4A-NA-C1A	-4.40	104.73	106.71
23	b	608	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
23	C	510	CLA	C3D-C4D-ND	4.39	117.35	110.24
23	D	402	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
23	c	506	CLA	C3D-C4D-ND	4.39	117.34	110.24
23	a	406	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	B	610	CLA	O2A-CGA-CBA	4.39	125.67	111.91
23	B	601	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	c	504	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
29	a	415	PL9	C7-C3-C4	4.38	120.44	116.88
25	b	617	BCR	C33-C5-C6	-4.38	119.61	124.53
23	c	512	CLA	O2D-CGD-CBD	4.38	119.05	111.27
25	y	101	BCR	C33-C5-C6	-4.38	119.61	124.53
38	F	102	HEM	C1B-NB-C4B	4.37	109.59	105.07
32	A	419	LMG	O7-C10-C11	4.36	120.90	111.50
23	B	603	CLA	C1D-CHD-C4C	-4.36	116.66	126.06
23	b	611	CLA	C3D-C4D-ND	4.36	117.28	110.24
23	a	409	CLA	C3B-C2B-C1B	-4.35	101.91	107.16
23	B	602	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	506	CLA	O2D-CGD-CBD	4.34	118.99	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	418	LMG	O7-C10-C11	4.34	120.86	111.50
23	c	510	CLA	C3B-C4B-NB	4.34	114.54	110.52
23	b	616	CLA	C1D-CHD-C4C	-4.34	116.70	126.06
23	B	604	CLA	C4A-NA-C1A	-4.33	104.76	106.71
23	b	607	CLA	C3D-C4D-ND	4.33	117.25	110.24
23	C	511	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	C	512	CLA	C3C-C4C-NC	4.33	115.42	110.57
23	c	510	CLA	C3D-C4D-ND	4.33	117.23	110.24
33	E	101	LHG	O7-C7-C8	4.32	120.82	111.50
23	A	404	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	b	612	CLA	C1-C2-C3	-4.32	118.57	126.04
23	B	612	CLA	C3B-C2B-C1B	-4.32	101.94	107.16
23	B	607	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	C	502	CLA	C3C-C4C-NC	4.32	115.41	110.57
23	B	608	CLA	C3B-C4B-NB	4.32	114.52	110.52
23	a	409	CLA	CMD-C2D-C1D	4.32	132.32	124.71
23	B	616	CLA	CHD-C1D-ND	-4.32	120.49	124.45
23	b	605	CLA	C3B-C2B-C1B	-4.32	101.95	107.16
23	A	404	CLA	C3B-C4B-NB	4.31	114.52	110.52
23	D	402	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	b	603	CLA	C3D-C2D-C1D	-4.31	99.94	105.83
23	C	509	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	b	608	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	b	612	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
29	A	414	PL9	C32-C33-C34	-4.30	117.31	127.66
23	C	506	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	b	610	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
23	B	609	CLA	O2D-CGD-CBD	4.29	118.89	111.27
23	c	507	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	C	504	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	b	603	CLA	C1D-CHD-C4C	-4.29	116.81	126.06
23	a	405	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	C	505	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	b	616	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	C	503	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	b	607	CLA	C3B-C4B-NB	4.27	114.48	110.52
23	b	612	CLA	C3B-C2B-C1B	-4.27	102.00	107.16
38	F	102	HEM	C4C-NC-C1C	4.27	109.53	105.35
23	c	505	CLA	C3C-C4C-NC	4.27	115.36	110.57
23	d	402	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	c	505	CLA	C3D-C4D-ND	4.26	117.14	110.24
23	B	615	CLA	CMB-C2B-C1B	4.26	131.86	125.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	611	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	b	612	CLA	C4A-NA-C1A	-4.26	104.79	106.71
23	B	601	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	c	502	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	a	407	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	B	609	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	C	513	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	c	508	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	B	616	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
23	C	502	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	A	408	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	C	501	CLA	C3D-C4D-ND	4.25	117.11	110.24
23	B	605	CLA	C1D-CHD-C4C	-4.24	116.91	126.06
23	b	604	CLA	C1C-C2C-C3C	-4.24	102.50	106.96
23	B	602	CLA	C3D-C4D-ND	4.23	117.07	110.24
23	b	610	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	B	611	CLA	C1D-CHD-C4C	-4.22	116.95	126.06
23	a	405	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	b	606	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	407	CLA	C3B-C2B-C1B	-4.21	102.07	107.16
23	c	504	CLA	C1D-CHD-C4C	-4.21	116.97	126.06
25	H	101	BCR	C38-C26-C25	-4.21	119.80	124.53
23	b	614	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	a	405	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	B	606	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	501	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	B	615	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	c	511	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	509	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	C	513	CLA	C4A-NA-C1A	-4.20	104.82	106.71
23	b	607	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
23	b	612	CLA	CHD-C1D-ND	-4.19	120.60	124.45
23	b	602	CLA	C3C-C4C-NC	4.19	115.27	110.57
23	B	604	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	B	612	CLA	O2D-CGD-O1D	-4.19	115.65	123.84
26	a	411	SQD	C1-C2-C3	-4.19	101.27	110.00
23	B	603	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	b	602	CLA	C3D-C2D-C1D	-4.19	100.12	105.83
23	B	605	CLA	CMB-C2B-C1B	4.18	131.74	125.37
23	B	607	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	b	610	CLA	C1-C2-C3	-4.18	118.81	126.04
38	f	101	HEM	C4C-NC-C1C	4.18	109.44	105.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	O2D-CGD-CBD	4.18	118.69	111.27
23	a	405	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	C	505	CLA	CMB-C2B-C1B	4.17	131.73	125.37
23	b	615	CLA	C3D-C4D-ND	4.17	116.98	110.24
32	Z	101	LMG	O7-C10-C11	4.17	120.48	111.50
23	A	408	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	B	607	CLA	C3D-C4D-ND	4.16	116.97	110.24
25	b	617	BCR	C7-C8-C9	-4.16	119.95	126.23
23	A	406	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	b	616	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	A	408	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	B	610	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	C	512	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
23	C	505	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	C	503	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	c	512	CLA	C1D-CHD-C4C	-4.15	117.12	126.06
23	c	504	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	D	402	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	C	507	CLA	C1D-CHD-C4C	-4.14	117.14	126.06
23	b	609	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	B	605	CLA	C3D-C4D-ND	4.13	116.92	110.24
23	c	512	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	c	513	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	C	512	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	D	403	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	a	406	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	b	612	CLA	C3B-C4B-NB	4.12	114.34	110.52
29	A	414	PL9	C7-C3-C2	-4.12	117.89	123.30
23	d	401	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	C	508	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	C	513	CLA	C3C-C4C-NC	4.11	115.18	110.57
23	B	604	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
23	d	401	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	B	616	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	C	513	CLA	C3B-C4B-NB	4.11	114.33	110.52
23	B	608	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	B	611	CLA	C4A-NA-C1A	-4.10	104.86	106.71
23	B	611	CLA	CHD-C4C-NC	4.10	130.67	124.20
23	c	503	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	A	405	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	a	405	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	c	503	CLA	O2D-CGD-O1D	-4.09	115.84	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	C3D-C4D-ND	4.09	116.86	110.24
26	b	620	SQD	C1-O5-C5	-4.09	105.66	113.69
23	b	610	CLA	O2A-CGA-CBA	4.09	124.74	111.91
23	C	509	CLA	C1C-C2C-C3C	-4.09	102.66	106.96
32	c	521	LMG	O7-C10-C11	4.09	120.31	111.50
23	b	604	CLA	C3B-C4B-NB	4.08	114.30	110.52
23	c	507	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
23	A	404	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
23	A	405	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
35	C	515	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	D	403	CLA	C3B-C2B-C1B	-4.07	102.24	107.16
26	a	411	SQD	C1-O5-C5	-4.07	105.69	113.69
23	b	615	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
23	c	502	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	c	503	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	b	616	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	c	512	CLA	C3B-C4B-NB	4.07	114.29	110.52
23	C	508	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	D	402	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	A	406	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	b	616	CLA	C2C-C1C-NC	4.06	113.78	109.97
23	c	507	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	b	609	CLA	O2D-CGD-CBD	4.06	118.48	111.27
23	a	406	CLA	C3C-C4C-NC	4.06	115.12	110.57
25	Y	101	BCR	C16-C17-C18	-4.05	121.53	127.31
23	b	614	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	B	604	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	C	504	CLA	C3B-C2B-C1B	-4.05	102.27	107.16
23	b	613	CLA	C1C-C2C-C3C	-4.05	102.70	106.96
23	C	511	CLA	C1D-CHD-C4C	-4.05	117.33	126.06
23	b	608	CLA	C3D-C4D-ND	4.04	116.78	110.24
23	c	512	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	C	510	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	B	607	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
23	A	408	CLA	C3B-C4B-NB	4.04	114.26	110.52
23	B	605	CLA	C3B-C2B-C1B	-4.04	102.29	107.16
23	c	507	CLA	O2D-CGD-CBD	4.04	118.44	111.27
23	B	613	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	C	502	CLA	C3D-C4D-ND	4.03	116.76	110.24
23	c	506	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	b	608	CLA	C3B-C4B-NB	4.02	114.24	110.52
23	A	408	CLA	C4A-NA-C1A	-4.01	104.90	106.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	C3C-C4C-NC	4.01	115.07	110.57
32	C	519	LMG	O6-C5-C4	4.01	116.98	109.69
23	b	615	CLA	C3B-C2B-C1B	-4.01	102.32	107.16
23	a	406	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	C	501	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	C	512	CLA	C1-C2-C3	-4.00	119.12	126.04
32	C	519	LMG	O7-C10-C11	4.00	120.12	111.50
23	C	505	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
23	b	606	CLA	C3C-C4C-NC	4.00	115.05	110.57
23	c	514	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
23	C	508	CLA	C3B-C4B-NB	4.00	114.22	110.52
23	d	401	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
25	C	514	BCR	C7-C8-C9	-3.99	120.20	126.23
23	c	514	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	B	607	CLA	C4A-NA-C1A	-3.99	104.91	106.71
23	a	406	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
23	a	409	CLA	CMC-C2C-C1C	3.99	131.11	125.04
25	c	515	BCR	C11-C10-C9	-3.98	121.63	127.31
23	C	510	CLA	C3B-C4B-NB	3.98	114.21	110.52
23	B	615	CLA	C1D-CHD-C4C	-3.98	117.48	126.06
23	b	602	CLA	O2D-CGD-O1D	-3.97	116.07	123.84
23	c	503	CLA	C3C-C4C-NC	3.97	115.03	110.57
23	c	505	CLA	C1-O2A-CGA	3.97	126.86	116.44
23	C	513	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	C	502	CLA	C3B-C4B-NB	3.97	114.20	110.52
23	B	602	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
23	b	615	CLA	C1C-C2C-C3C	-3.97	102.79	106.96
23	C	501	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
23	B	610	CLA	C3B-C2B-C1B	-3.96	102.39	107.16
23	C	509	CLA	C1-C2-C3	-3.95	119.20	126.04
23	b	615	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	a	405	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	604	CLA	CAC-C3C-C4C	3.95	129.93	124.81
23	c	510	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	A	406	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
23	B	615	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
23	c	511	CLA	C3D-C4D-ND	3.95	116.62	110.24
23	B	603	CLA	O2D-CGD-O1D	-3.95	116.12	123.84
23	A	404	CLA	C3C-C4C-NC	3.95	115.00	110.57
32	c	520	LMG	O7-C10-C11	3.94	120.00	111.50
23	c	508	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
32	m	101	LMG	O7-C10-C11	3.94	120.00	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	b	607	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
23	B	606	CLA	C3B-C2B-C1B	-3.94	102.41	107.16
23	b	612	CLA	C3D-C4D-ND	3.94	116.61	110.24
29	d	404	PL9	C42-C43-C44	-3.93	118.19	127.66
38	f	101	HEM	CAD-CBD-CGD	3.93	122.07	113.60
23	b	601	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
23	D	402	CLA	C1-C2-C3	-3.93	119.25	126.04
23	B	614	CLA	C3D-C4D-ND	3.93	116.59	110.24
23	b	604	CLA	C3B-C2B-C1B	-3.93	102.42	107.16
23	a	407	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	c	502	CLA	C4A-NA-C1A	-3.93	104.94	106.71
25	d	403	BCR	C29-C30-C25	3.92	116.52	110.48
23	b	605	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	B	610	CLA	CAA-CBA-CGA	-3.92	101.80	113.25
23	C	504	CLA	C3B-C4B-NB	3.91	114.15	110.52
26	a	411	SQD	C44-O6-C1	-3.91	106.09	113.74
23	A	405	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
23	C	501	CLA	O2D-CGD-O1D	-3.91	116.19	123.84
29	A	414	PL9	C7-C3-C4	3.91	120.05	116.88
23	c	508	CLA	CMC-C2C-C1C	3.91	130.99	125.04
23	c	511	CLA	C1C-C2C-C3C	-3.91	102.85	106.96
23	b	610	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
34	b	625	HTG	C1-O5-C5	3.90	119.78	112.58
23	c	509	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	b	606	CLA	C1D-CHD-C4C	-3.90	117.65	126.06
29	a	415	PL9	C32-C33-C34	-3.89	118.28	127.66
23	B	602	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
23	B	604	CLA	CHD-C1D-ND	-3.89	120.88	124.45
23	b	609	CLA	C1-C2-C3	-3.89	119.31	126.04
31	B	628	LMT	C1'-O5'-C5'	-3.89	106.05	113.69
23	D	403	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	c	507	CLA	C3B-C4B-NB	3.89	114.12	110.52
23	c	510	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	B	608	CLA	CAC-C3C-C4C	3.89	129.85	124.81
33	A	420	LHG	O8-C23-O10	-3.88	113.79	123.59
35	c	517	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	b	605	CLA	C4-C3-C5	3.88	121.80	115.27
23	b	612	CLA	CAC-C3C-C4C	3.88	129.85	124.81
23	A	405	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	b	614	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
23	c	510	CLA	C1C-C2C-C3C	-3.88	102.88	106.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
24	A	407	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
32	c	521	LMG	C3-C4-C5	3.86	117.13	110.24
23	B	609	CLA	C3B-C2B-C1B	-3.86	102.50	107.16
23	B	602	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
23	C	510	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
23	b	612	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
23	C	503	CLA	C1D-CHD-C4C	-3.86	117.74	126.06
23	c	509	CLA	C1-C2-C3	-3.86	119.38	126.04
23	b	609	CLA	C3B-C2B-C1B	-3.85	102.51	107.16
23	A	405	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	c	509	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
23	B	609	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	C	511	CLA	C3B-C4B-NB	3.84	114.08	110.52
23	B	601	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
23	B	610	CLA	CAA-C2A-C3A	-3.84	102.26	112.78
23	b	607	CLA	C4A-NA-C1A	-3.84	104.98	106.71
29	a	415	PL9	C7-C3-C2	-3.84	118.25	123.30
23	b	603	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
23	c	507	CLA	C3C-C4C-NC	3.84	114.87	110.57
23	c	513	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	C	501	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	C	511	CLA	C3D-C4D-ND	3.83	116.43	110.24
23	B	616	CLA	C4C-C3C-C2C	-3.83	101.32	106.90
32	C	518	LMG	O7-C10-C11	3.83	119.75	111.50
23	C	511	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
23	B	614	CLA	O2D-CGD-O1D	-3.81	116.38	123.84
23	B	614	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	B	606	CLA	C1C-C2C-C3C	-3.81	102.96	106.96
23	B	602	CLA	CMC-C2C-C1C	3.80	130.83	125.04
23	a	406	CLA	CMB-C2B-C1B	3.80	131.16	125.37
25	k	101	BCR	C29-C30-C25	3.80	116.33	110.48
33	A	420	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	416	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
23	B	614	CLA	C1-C2-C3	-3.80	119.47	126.04
23	b	611	CLA	C3B-C4B-NB	3.79	114.03	110.52
23	d	402	CLA	C3C-C4C-NC	3.79	114.82	110.57
23	B	616	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	b	606	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
23	C	507	CLA	C3D-C4D-ND	3.78	116.35	110.24
26	A	410	SQD	C44-O6-C1	-3.78	106.36	113.74
23	B	606	CLA	C1D-CHD-C4C	-3.77	117.92	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	409	CLA	C1C-C2C-C3C	-3.77	102.99	106.96
23	b	606	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
23	A	405	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	c	502	CLA	CMB-C2B-C1B	3.77	131.11	125.37
23	B	610	CLA	CMB-C2B-C1B	3.76	131.10	125.37
24	a	417	PHO	C4-C3-C5	3.76	121.59	115.27
23	B	608	CLA	C4A-NA-C1A	-3.75	105.02	106.71
23	b	604	CLA	C3D-C4D-ND	3.75	116.31	110.24
23	B	607	CLA	C3B-C4B-NB	3.75	114.00	110.52
23	b	608	CLA	CMC-C2C-C1C	3.75	130.75	125.04
23	D	403	CLA	O2D-CGD-O1D	-3.75	116.51	123.84
23	b	604	CLA	CMC-C2C-C1C	3.75	130.75	125.04
23	c	512	CLA	C4A-NA-C1A	-3.75	105.02	106.71
23	b	608	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	C	508	CLA	C1-C2-C3	-3.75	119.56	126.04
23	c	504	CLA	CMB-C2B-C1B	3.75	131.07	125.37
23	B	604	CLA	C3B-C4B-NB	3.75	113.99	110.52
32	Z	101	LMG	C1-C2-C3	3.75	117.80	110.00
25	d	403	BCR	C38-C26-C25	-3.74	120.32	124.53
23	b	616	CLA	O2A-CGA-CBA	3.74	123.65	111.91
23	B	603	CLA	C1C-C2C-C3C	-3.74	103.02	106.96
26	A	410	SQD	O47-C7-C8	3.74	119.56	111.50
29	a	415	PL9	C15-C14-C16	3.74	121.56	115.27
26	F	103	SQD	O8-S-C6	3.74	111.69	105.74
23	A	406	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	b	612	CLA	CMC-C2C-C1C	3.73	130.72	125.04
23	b	612	CLA	C4-C3-C5	3.72	121.53	115.27
23	c	503	CLA	C3B-C4B-NB	3.72	113.97	110.52
23	A	404	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	C	513	CLA	C1D-CHD-C4C	-3.72	118.04	126.06
38	F	102	HEM	CHD-C4C-NC	3.71	128.46	124.44
23	b	612	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	B	615	CLA	O2D-CGD-CBD	3.71	117.87	111.27
23	c	512	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	B	613	CLA	C4-C3-C5	3.71	121.51	115.27
23	C	511	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
23	B	605	CLA	C4-C3-C5	3.71	121.50	115.27
23	B	616	CLA	C3B-C4B-NB	3.70	113.95	110.52
23	D	403	CLA	CAC-C3C-C4C	3.70	129.62	124.81
23	B	613	CLA	C3B-C4B-NB	3.70	113.95	110.52
35	C	516	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	c	508	CLA	C3D-C4D-ND	3.69	116.21	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	c	511	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	b	613	CLA	O2D-CGD-CBD	3.69	117.82	111.27
23	C	507	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
33	L	101	LHG	O7-C7-C8	3.68	119.43	111.50
26	A	412	SQD	O47-C7-C8	3.68	119.43	111.50
23	A	406	CLA	CMB-C2B-C1B	3.68	130.97	125.37
23	B	612	CLA	C4C-C3C-C2C	-3.67	101.55	106.90
23	c	505	CLA	C3B-C4B-NB	3.67	113.92	110.52
23	b	615	CLA	CMB-C2B-C1B	3.67	130.96	125.37
29	A	414	PL9	C37-C38-C39	-3.67	118.82	127.66
23	d	402	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
23	b	602	CLA	CMC-C2C-C1C	3.67	130.62	125.04
25	d	403	BCR	C40-C30-C25	-3.67	104.35	110.30
23	a	405	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	B	614	CLA	C3B-C4B-NB	3.66	113.91	110.52
23	b	616	CLA	CMB-C2B-C1B	3.66	130.94	125.37
23	b	614	CLA	C1-C2-C3	-3.65	119.73	126.04
23	b	602	CLA	CAA-C2A-C3A	-3.65	102.79	112.78
23	c	504	CLA	O2D-CGD-O1D	-3.65	116.71	123.84
23	b	604	CLA	CAC-C3C-C4C	3.64	129.54	124.81
23	B	611	CLA	C1-C2-C3	-3.64	119.75	126.04
23	b	603	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
23	B	603	CLA	CAA-C2A-C3A	-3.64	102.81	112.78
23	D	402	CLA	C3B-C4B-NB	3.64	113.89	110.52
23	d	402	CLA	C1D-CHD-C4C	-3.64	118.21	126.06
23	B	612	CLA	CMC-C2C-C1C	3.64	130.57	125.04
23	b	612	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	b	602	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	b	601	CLA	O2D-CGD-O1D	-3.63	116.74	123.84
26	a	411	SQD	O9-S-C6	3.63	111.25	106.94
23	b	608	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	c	508	CLA	CMB-C2B-C1B	3.63	130.89	125.37
25	Y	101	BCR	C15-C14-C13	-3.62	122.14	127.31
23	B	607	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	A	405	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
25	y	101	BCR	C15-C14-C13	-3.62	122.15	127.31
23	d	402	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	B	614	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
23	b	613	CLA	C3B-C4B-NB	3.61	113.86	110.52
26	F	103	SQD	C44-O6-C1	-3.61	106.69	113.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CAC-C3C-C4C	3.60	129.48	124.81
32	A	419	LMG	O1-C1-C2	3.60	113.92	108.30
23	B	610	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
23	C	506	CLA	C3C-C4C-NC	3.60	114.61	110.57
24	A	416	PHO	C4D-CHA-CBD	3.59	110.14	108.52
23	B	605	CLA	CHD-C4C-NC	3.59	129.86	124.20
23	C	510	CLA	C3C-C4C-NC	3.59	114.59	110.57
23	A	405	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	c	502	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
25	B	618	BCR	C29-C30-C25	3.58	116.00	110.48
34	b	625	HTG	O5-C5-C4	3.58	116.20	109.69
23	c	514	CLA	C1C-C2C-C3C	-3.58	103.19	106.96
23	d	401	CLA	C3B-C4B-NB	3.58	113.84	110.52
26	a	413	SQD	O47-C7-C8	3.58	119.22	111.50
25	T	102	BCR	C11-C10-C9	-3.58	122.20	127.31
25	h	101	BCR	C38-C26-C25	-3.58	120.51	124.53
23	B	611	CLA	C4C-C3C-C2C	-3.58	101.68	106.90
23	c	507	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	c	509	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
23	c	511	CLA	C3B-C4B-NB	3.57	113.83	110.52
23	B	613	CLA	C3D-C4D-ND	3.57	116.01	110.24
23	b	605	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	b	608	CLA	C1-C2-C3	-3.57	119.87	126.04
23	b	609	CLA	C1D-CHD-C4C	-3.57	118.36	126.06
23	c	513	CLA	C1-C2-C3	-3.57	119.87	126.04
25	B	617	BCR	C33-C5-C6	-3.57	120.52	124.53
23	C	508	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
25	K	101	BCR	C7-C8-C9	-3.56	120.85	126.23
23	B	615	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	d	401	CLA	C1-C2-C3	-3.56	119.89	126.04
23	C	505	CLA	CAC-C3C-C4C	3.56	129.42	124.81
23	B	611	CLA	C2A-C1A-CHA	-3.56	117.64	123.86
23	C	509	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
23	b	610	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
25	D	404	BCR	C28-C27-C26	-3.55	107.74	114.08
23	C	502	CLA	C1D-CHD-C4C	-3.55	118.41	126.06
29	d	404	PL9	C40-C39-C41	3.55	121.23	115.27
29	a	415	PL9	C27-C28-C29	-3.54	119.13	127.66
38	f	101	HEM	C1B-NB-C4B	3.54	108.73	105.07
23	C	502	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	b	616	CLA	CHD-C4C-NC	3.53	129.77	124.20
23	A	404	CLA	O2D-CGD-CBD	3.53	117.54	111.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	c	513	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	b	601	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	c	505	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	a	409	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	A	408	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	b	615	CLA	O2D-CGD-CBD	3.52	117.52	111.27
23	B	608	CLA	O2D-CGD-O1D	-3.52	116.96	123.84
23	C	507	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
29	A	414	PL9	C22-C23-C24	-3.52	119.19	127.66
23	c	514	CLA	C3B-C4B-NB	3.51	113.77	110.52
29	A	414	PL9	C15-C14-C16	3.51	121.18	115.27
23	B	608	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
23	A	404	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	b	605	CLA	CHD-C4C-NC	3.50	129.72	124.20
23	b	603	CLA	C3B-C4B-NB	3.50	113.77	110.52
25	K	101	BCR	C15-C14-C13	-3.50	122.31	127.31
23	c	508	CLA	C4-C3-C5	3.50	121.16	115.27
29	D	405	PL9	C53-C6-C1	3.50	122.15	114.99
23	c	509	CLA	C3B-C4B-NB	3.50	113.76	110.52
23	c	507	CLA	C1-C2-C3	-3.50	119.99	126.04
32	C	519	LMG	C3-C4-C5	3.50	116.48	110.24
23	c	504	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	a	407	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	c	505	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	C	508	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
34	B	622	HTG	C1'-S1-C1	3.49	106.61	100.09
29	a	415	PL9	C30-C29-C31	3.48	121.13	115.27
23	A	404	CLA	O2A-CGA-CBA	3.48	122.83	111.91
25	D	404	BCR	C38-C26-C25	-3.48	120.62	124.53
29	D	405	PL9	C42-C43-C44	-3.47	119.29	127.66
23	c	512	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	c	511	CLA	CMC-C2C-C1C	3.47	130.33	125.04
23	a	409	CLA	CAA-C2A-C3A	-3.47	103.27	112.78
23	b	608	CLA	CAC-C3C-C4C	3.47	129.31	124.81
23	a	405	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	B	607	CLA	C4-C3-C5	3.47	121.10	115.27
25	c	515	BCR	C15-C14-C13	-3.46	122.37	127.31
23	A	406	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	d	401	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	B	602	CLA	CAA-C2A-C3A	-3.46	103.31	112.78
23	B	607	CLA	C1D-CHD-C4C	-3.46	118.60	126.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
34	V	202	HTG	C1-O5-C5	3.45	116.87	112.19
23	B	606	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
34	b	622	HTG	O2-C2-C1	3.45	116.60	110.27
23	d	402	CLA	CMB-C2B-C1B	3.45	130.62	125.37
23	C	502	CLA	C1-C2-C3	-3.44	120.09	126.04
23	B	604	CLA	C3D-C4D-ND	3.44	115.81	110.24
25	T	102	BCR	C15-C16-C17	-3.44	116.42	123.47
23	c	506	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	B	610	CLA	C4C-C3C-C2C	-3.43	101.89	106.90
23	b	613	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
23	b	614	CLA	C3B-C4B-NB	3.43	113.69	110.52
34	b	622	HTG	C1'-S1-C1	3.42	106.50	100.09
23	c	503	CLA	CMB-C2B-C1B	3.42	130.58	125.37
23	c	511	CLA	C4-C3-C5	3.42	121.03	115.27
23	B	607	CLA	CBC-CAC-C3C	-3.42	103.00	112.43
23	b	603	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
23	b	610	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
23	B	611	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
23	c	506	CLA	CMB-C2B-C1B	3.42	130.57	125.37
23	D	403	CLA	CMB-C2B-C1B	3.41	130.57	125.37
40	V	201	HEC	CBD-CAD-C3D	-3.41	103.15	112.63
23	a	405	CLA	O2A-CGA-CBA	3.41	122.61	111.91
23	b	604	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
23	b	606	CLA	C4-C3-C5	3.41	121.01	115.27
29	a	415	PL9	C35-C34-C36	3.41	121.01	115.27
23	c	506	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	C	506	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	b	612	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
23	b	609	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	b	613	CLA	C3D-C4D-ND	3.39	115.73	110.24
23	b	609	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	c	506	CLA	O2D-CGD-O1D	-3.39	117.21	123.84
29	D	405	PL9	C25-C24-C26	3.39	120.97	115.27
23	C	506	CLA	C3B-C4B-NB	3.39	113.66	110.52
34	B	622	HTG	O5-C1-C2	3.39	114.57	110.31
23	B	613	CLA	C1D-CHD-C4C	-3.38	118.76	126.06
32	Z	101	LMG	O6-C1-C2	3.38	117.51	110.35
23	b	608	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
23	c	506	CLA	CAC-C3C-C4C	3.38	129.19	124.81
23	b	601	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
32	z	101	LMG	O7-C10-C11	3.37	118.77	111.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	518	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	b	615	CLA	C3B-C4B-NB	3.37	113.64	110.52
23	b	616	CLA	C4C-C3C-C2C	-3.37	101.99	106.90
23	B	601	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	c	506	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	C	512	CLA	C4-C3-C5	3.36	120.93	115.27
23	a	409	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
25	A	409	BCR	C24-C23-C22	-3.36	121.16	126.23
23	B	605	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	B	608	CLA	C1D-CHD-C4C	-3.36	118.81	126.06
23	b	610	CLA	C4C-C3C-C2C	-3.36	102.01	106.90
25	D	404	BCR	C29-C30-C25	3.35	115.64	110.48
25	D	404	BCR	C10-C11-C12	-3.35	112.76	123.22
23	B	602	CLA	C3B-C4B-NB	3.35	113.62	110.52
23	b	612	CLA	O2A-CGA-O1A	-3.35	115.14	123.59
23	C	508	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
25	B	617	BCR	C7-C8-C9	-3.34	121.19	126.23
23	b	609	CLA	C3B-C4B-NB	3.33	113.61	110.52
23	b	611	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
25	b	618	BCR	C15-C14-C13	-3.33	122.56	127.31
23	d	401	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	B	608	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
23	C	506	CLA	C1-C2-C3	-3.32	120.30	126.04
23	B	615	CLA	CED-O2D-CGD	3.32	123.45	115.94
23	D	403	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
23	C	510	CLA	C4-C3-C5	3.32	120.85	115.27
24	A	407	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	A	406	CLA	C3B-C4B-NB	3.32	113.59	110.52
23	b	615	CLA	C4-C3-C5	3.31	120.85	115.27
23	C	505	CLA	C1-C2-C3	-3.31	120.31	126.04
26	f	102	SQD	O5-C1-C2	3.31	117.36	110.35
23	C	507	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
25	t	102	BCR	C11-C10-C9	-3.31	122.58	127.31
23	C	506	CLA	CMC-C2C-C1C	3.31	130.08	125.04
23	B	610	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
23	C	509	CLA	CMC-C2C-C1C	3.30	130.07	125.04
35	h	102	DGD	O2G-C1B-C2B	3.30	118.61	111.50
26	F	103	SQD	C1-C2-C3	-3.30	103.13	110.00
23	B	615	CLA	C3B-C4B-NB	3.30	113.57	110.52
23	b	602	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
33	d	411	LHG	O8-C23-O10	-3.30	115.27	123.59
23	A	408	CLA	CAA-C2A-C3A	-3.30	103.75	112.78

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	406	LHG	O7-C7-C8	3.29	118.59	111.50
23	b	615	CLA	C11-C10-C8	-3.29	105.29	115.92
25	b	619	BCR	C24-C23-C22	-3.29	121.27	126.23
23	C	510	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	B	605	CLA	C1C-C2C-C3C	-3.29	103.50	106.96
23	c	509	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
23	C	501	CLA	CMC-C2C-C1C	3.28	130.04	125.04
23	b	602	CLA	CAC-C3C-C4C	3.28	129.07	124.81
23	C	513	CLA	C1-C2-C3	-3.28	120.37	126.04
32	C	518	LMG	O8-C28-C29	3.28	122.20	111.91
23	C	511	CLA	C4-C3-C5	3.28	120.78	115.27
23	c	513	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	B	611	CLA	CHB-C4A-NA	3.28	129.04	124.51
23	B	612	CLA	CAC-C3C-C4C	3.27	129.06	124.81
26	b	620	SQD	C3-C4-C5	3.27	116.07	110.24
23	c	510	CLA	CAC-C3C-C4C	3.27	129.05	124.81
23	c	505	CLA	CMB-C2B-C1B	3.27	130.34	125.37
23	C	509	CLA	C3B-C4B-NB	3.27	113.55	110.52
23	C	505	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	b	613	CLA	C1-C2-C3	-3.26	120.40	126.04
23	b	604	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
23	b	611	CLA	C1D-CHD-C4C	-3.26	119.03	126.06
26	B	620	SQD	O7-S-C6	3.26	110.81	106.94
23	b	607	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	B	610	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	b	606	CLA	C3B-C4B-NB	3.25	113.53	110.52
23	b	603	CLA	C4-C3-C5	3.25	120.74	115.27
23	B	612	CLA	C4A-NA-C1A	-3.25	105.25	106.71
23	a	409	CLA	C4-C3-C5	3.25	120.74	115.27
33	d	411	LHG	O7-C7-C8	3.25	118.50	111.50
23	B	608	CLA	C1-C2-C3	-3.25	120.43	126.04
23	b	613	CLA	O2A-CGA-O1A	-3.25	115.40	123.59
32	B	621	LMG	O8-C28-C29	3.24	122.09	111.91
23	C	505	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	B	608	CLA	CHC-C1C-C2C	-3.24	117.72	126.73
32	a	418	LMG	C8-O7-C10	-3.24	109.81	117.79
25	a	410	BCR	C38-C26-C25	-3.24	120.89	124.53
23	C	503	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	C	510	CLA	CHD-C4C-NC	3.24	129.31	124.20
23	c	512	CLA	C4-C3-C5	3.24	120.72	115.27
23	B	614	CLA	CAC-C3C-C4C	3.24	129.01	124.81
23	B	608	CLA	CMA-C3A-C4A	-3.24	103.07	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	CHC-C1C-C2C	-3.23	117.75	126.73
23	c	505	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	b	613	CLA	O2A-CGA-CBA	3.23	122.05	111.91
23	B	607	CLA	CMC-C2C-C1C	3.23	129.96	125.04
23	A	405	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	A	408	CLA	C1-C2-C3	-3.22	120.47	126.04
25	k	101	BCR	C7-C8-C9	-3.22	121.36	126.23
24	a	417	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
25	h	101	BCR	C7-C8-C9	-3.22	121.38	126.23
33	d	411	LHG	O8-C23-C24	3.22	122.00	111.91
25	y	101	BCR	C38-C26-C25	-3.22	120.92	124.53
38	F	102	HEM	CBD-CAD-C3D	-3.21	103.70	112.63
23	c	502	CLA	C1D-CHD-C4C	-3.21	119.13	126.06
23	c	509	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
38	F	102	HEM	CHD-C1D-ND	3.21	127.90	124.42
23	B	601	CLA	O2D-CGD-O1D	-3.20	117.57	123.84
23	C	504	CLA	C1D-CHD-C4C	-3.20	119.15	126.06
23	B	603	CLA	C3B-C4B-NB	3.20	113.48	110.52
23	B	615	CLA	CMC-C2C-C1C	3.20	129.91	125.04
38	f	101	HEM	CHA-C4D-ND	3.20	128.32	124.37
23	b	609	CLA	CMB-C2B-C1B	3.20	130.24	125.37
23	b	607	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
23	C	504	CLA	CMC-C2C-C1C	3.19	129.90	125.04
23	a	405	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
23	a	405	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	B	601	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
23	B	614	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
29	a	415	PL9	C17-C18-C19	-3.19	119.99	127.66
23	B	603	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	c	503	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
23	A	408	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
23	b	615	CLA	CHC-C1C-C2C	-3.18	117.89	126.73
26	A	412	SQD	O8-S-C6	3.18	110.81	105.74
25	a	410	BCR	C40-C30-C25	-3.18	105.14	110.30
23	c	502	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
23	A	406	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	b	603	CLA	C2A-C1A-CHA	-3.18	118.30	123.86
23	C	512	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	A	414	PL9	C27-C28-C29	-3.18	120.01	127.66
23	C	512	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	B	609	CLA	CBC-CAC-C3C	-3.18	103.68	112.43
23	b	610	CLA	O2D-CGD-O1D	-3.17	117.63	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	415	PL9	C25-C24-C26	3.17	120.61	115.27
23	C	512	CLA	CMB-C2B-C1B	3.17	130.20	125.37
23	A	404	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	D	402	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	c	503	CLA	CHD-C4C-NC	3.17	129.20	124.20
25	b	619	BCR	C11-C10-C9	-3.17	122.79	127.31
23	b	614	CLA	CMB-C2B-C1B	3.17	130.19	125.37
23	C	504	CLA	CAC-C3C-C4C	3.16	128.92	124.81
31	A	417	LMT	O5B-C5B-C4B	3.16	115.44	109.69
23	C	502	CLA	CHC-C1C-C2C	-3.16	117.95	126.73
23	B	612	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
40	V	201	HEC	CAD-CBD-CGD	-3.16	106.81	113.60
25	H	101	BCR	C16-C17-C18	-3.16	122.80	127.31
23	b	609	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
23	b	613	CLA	C4C-C3C-C2C	-3.16	102.30	106.90
26	B	620	SQD	O9-S-C6	3.16	110.69	106.94
23	c	510	CLA	CHC-C1C-C2C	-3.16	117.96	126.73
25	c	516	BCR	C7-C8-C9	-3.16	121.47	126.23
23	a	409	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	C	506	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
24	A	416	PHO	C4-C3-C5	3.15	120.58	115.27
23	C	502	CLA	CMB-C2B-C1B	3.15	130.17	125.37
23	b	605	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	a	406	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	A	405	CLA	CMB-C2B-C1B	3.15	130.17	125.37
33	A	420	LHG	C5-O7-C7	-3.15	110.03	117.79
33	A	420	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405	PL9	C17-C18-C19	-3.15	120.08	127.66
25	c	515	BCR	C16-C17-C18	-3.14	122.82	127.31
23	B	606	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	b	611	CLA	C1-C2-C3	-3.14	120.61	126.04
23	b	616	CLA	O2A-CGA-O1A	-3.14	115.67	123.59
23	B	616	CLA	CMC-C2C-C1C	3.14	129.82	125.04
23	B	614	CLA	CMC-C2C-C1C	3.13	129.81	125.04
26	A	412	SQD	O48-C23-C24	3.13	121.74	111.91
23	B	604	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
23	C	506	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	B	606	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	b	605	CLA	CMB-C2B-C1B	3.13	130.14	125.37
23	b	611	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
23	a	406	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	a	407	CLA	CHD-C4C-NC	3.13	129.13	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
23	b	609	CLA	CBC-CAC-C3C	-3.13	103.81	112.43
23	a	407	CLA	C1-C2-C3	-3.13	120.64	126.04
23	d	401	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
26	a	413	SQD	O48-C23-C24	3.12	121.70	111.91
29	D	405	PL9	C51-C49-C50	3.12	121.49	114.60
23	C	503	CLA	C4C-C3C-C2C	-3.12	102.36	106.90
23	c	510	CLA	O2A-CGA-CBA	3.11	121.67	111.91
23	C	503	CLA	C1-C2-C3	-3.11	120.66	126.04
23	C	506	CLA	CBC-CAC-C3C	-3.11	103.86	112.43
23	C	509	CLA	O2A-CGA-CBA	3.11	121.66	111.91
25	y	101	BCR	C24-C23-C22	-3.11	121.54	126.23
23	B	603	CLA	C4-C3-C5	3.11	120.50	115.27
29	D	405	PL9	C10-C9-C11	3.11	120.50	115.27
23	B	603	CLA	CMC-C2C-C1C	3.11	129.77	125.04
38	F	102	HEM	CHB-C1B-NB	3.11	128.20	124.37
23	D	403	CLA	C1C-C2C-C3C	-3.10	103.69	106.96
23	a	409	CLA	C3B-C4B-NB	3.10	113.39	110.52
23	b	614	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
31	b	627	LMT	C3'-C4'-C5'	-3.10	103.81	110.93
23	D	403	CLA	CMC-C2C-C1C	3.10	129.76	125.04
23	c	513	CLA	CMB-C2B-C1B	3.10	130.09	125.37
23	c	513	CLA	O2A-CGA-CBA	3.10	121.64	111.91
23	c	512	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	B	612	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
23	b	611	CLA	C4C-C3C-C2C	-3.10	102.38	106.90
23	B	609	CLA	CMB-C2B-C1B	3.10	130.09	125.37
29	A	414	PL9	C10-C9-C11	3.10	120.48	115.27
23	B	613	CLA	O2A-CGA-O1A	-3.09	115.78	123.59
33	b	630	LHG	O7-C7-C8	3.09	118.16	111.50
23	b	609	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	b	610	CLA	O2A-CGA-O1A	-3.09	115.79	123.59
24	a	417	PHO	CMB-C2B-C3B	3.08	130.44	124.68
23	C	507	CLA	CMB-C2B-C1B	3.08	130.06	125.37
29	a	415	PL9	C10-C9-C11	3.08	120.45	115.27
23	b	614	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
25	K	101	BCR	C33-C5-C6	-3.08	121.07	124.53
23	b	601	CLA	C4-C3-C5	3.08	120.45	115.27
23	C	501	CLA	CMB-C2B-C1B	3.08	130.05	125.37
23	B	610	CLA	C3B-C4B-NB	3.07	113.37	110.52
23	C	513	CLA	CMC-C2C-C1C	3.07	129.72	125.04
25	K	103	BCR	C38-C26-C25	-3.07	121.08	124.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	C4-C3-C5	3.07	120.44	115.27
23	a	405	CLA	C1-C2-C3	-3.07	120.73	126.04
23	b	605	CLA	C1-C2-C3	-3.07	120.73	126.04
23	c	508	CLA	C1D-CHD-C4C	-3.07	119.44	126.06
23	C	506	CLA	CHC-C1C-C2C	-3.07	118.22	126.73
23	B	605	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
23	C	512	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
23	b	614	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
23	b	607	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
32	C	519	LMG	O8-C28-C29	3.06	121.52	111.91
23	B	604	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	b	601	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	B	605	CLA	CED-O2D-CGD	3.06	122.85	115.94
23	c	503	CLA	CMC-C2C-C1C	3.06	129.69	125.04
29	d	404	PL9	C10-C9-C11	3.05	120.41	115.27
23	C	505	CLA	CMC-C2C-C1C	3.05	129.69	125.04
32	a	418	LMG	C7-O1-C1	-3.05	107.77	113.74
23	a	405	CLA	C4-C3-C5	3.05	120.41	115.27
23	c	510	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	B	612	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	D	402	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	407	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	a	407	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	d	401	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	d	401	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	b	602	CLA	C2A-C1A-CHA	-3.04	118.54	123.86
38	f	101	HEM	CHD-C4C-NC	3.04	127.73	124.44
26	b	620	SQD	O8-S-C6	3.04	110.59	105.74
23	B	605	CLA	CMC-C2C-C1C	3.04	129.67	125.04
23	c	509	CLA	CHC-C1C-C2C	-3.04	118.28	126.73
23	C	509	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
25	d	403	BCR	C10-C11-C12	-3.04	113.73	123.22
29	A	414	PL9	C20-C19-C21	3.04	120.38	115.27
25	B	619	BCR	C24-C23-C22	-3.04	121.65	126.23
23	B	610	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	B	609	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	d	401	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	A	406	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	A	408	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
23	C	501	CLA	CHD-C4C-NC	3.03	128.97	124.20
26	B	620	SQD	O48-C23-C24	3.03	121.41	111.91
23	A	404	CLA	C1-C2-C3	-3.03	120.81	126.04

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	-3.02	102.49	106.90
23	d	401	CLA	C4-C3-C5	3.02	120.36	115.27
23	B	614	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
23	B	615	CLA	C4-C3-C5	3.02	120.36	115.27
23	b	607	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
29	d	404	PL9	C37-C38-C39	-3.02	120.38	127.66
25	K	103	BCR	C20-C21-C22	-3.02	123.00	127.31
34	B	625	HTG	C1'-S1-C1	3.02	105.74	100.09
25	A	409	BCR	C38-C26-C25	-3.02	121.14	124.53
23	A	404	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
23	C	504	CLA	O2D-CGD-O1D	-3.01	117.94	123.84
23	C	503	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	a	409	CLA	O2A-CGA-CBA	3.01	121.36	111.91
29	a	415	PL9	C42-C43-C44	-3.01	120.41	127.66
23	C	509	CLA	CAC-C3C-C4C	3.01	128.72	124.81
23	B	615	CLA	C4C-C3C-C2C	-3.01	102.51	106.90
23	b	606	CLA	CHD-C4C-NC	3.01	128.95	124.20
33	d	405	LHG	O7-C7-C8	3.01	117.99	111.50
25	K	103	BCR	C24-C23-C22	-3.01	121.69	126.23
23	D	402	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	b	613	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
23	c	502	CLA	C1-C2-C3	-3.01	120.84	126.04
23	C	510	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
23	D	403	CLA	C4-C3-C5	3.00	120.32	115.27
25	T	102	BCR	C15-C14-C13	3.00	131.59	127.31
23	c	511	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	C	511	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	B	604	CLA	CMB-C2B-C1B	3.00	129.94	125.37
23	A	405	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	411	SQD	C45-O47-C7	-3.00	110.42	117.79
25	C	514	BCR	C33-C5-C6	-2.99	121.17	124.53
23	C	507	CLA	CHD-C4C-NC	2.99	128.92	124.20
23	c	512	CLA	CMC-C2C-C1C	2.99	129.60	125.04
38	f	101	HEM	C4D-ND-C1D	2.99	108.16	105.07
23	A	404	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	b	606	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	c	509	CLA	CMB-C2B-C1B	2.99	129.92	125.37
32	Z	101	LMG	C4-C3-C2	2.99	116.04	110.82
23	c	513	CLA	CHD-C4C-NC	2.98	128.91	124.20
23	C	511	CLA	CAC-C3C-C4C	2.98	128.68	124.81
33	D	407	LHG	O8-C23-C24	2.98	121.27	111.91
23	b	608	CLA	CHC-C1C-C2C	-2.98	118.44	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	101	LMT	C1'-O5'-C5'	-2.98	107.84	113.69
32	c	521	LMG	C9-C8-C7	-2.98	104.75	111.79
26	a	413	SQD	O7-S-C6	2.97	110.47	106.94
33	E	101	LHG	O8-C23-C24	2.97	121.23	111.91
23	A	408	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
23	C	504	CLA	C1-O2A-CGA	2.97	124.23	116.44
23	B	602	CLA	CAC-C3C-C4C	2.97	128.66	124.81
23	B	609	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
38	f	101	HEM	CHD-C1D-ND	2.97	127.64	124.42
23	B	606	CLA	CMC-C2C-C1C	2.96	129.55	125.04
23	c	504	CLA	C3B-C4B-NB	2.96	113.26	110.52
23	b	605	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
23	b	613	CLA	CMA-C3A-C4A	-2.96	103.82	111.77
23	b	616	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
32	m	101	LMG	O8-C28-C29	2.96	121.20	111.91
40	V	201	HEC	CBC-CAC-C3C	2.96	120.58	112.43
24	A	407	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	C	503	CLA	C4-C3-C5	2.96	120.24	115.27
23	B	616	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
31	B	628	LMT	C4B-C3B-C2B	2.95	115.98	110.82
23	a	406	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
23	b	603	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	b	603	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	B	613	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	B	605	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
23	C	503	CLA	O2A-CGA-O1A	-2.95	116.16	123.59
26	A	410	SQD	O9-S-C6	2.95	110.44	106.94
23	b	612	CLA	O2A-CGA-CBA	2.95	121.15	111.91
23	C	511	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
23	B	606	CLA	O2A-CGA-CBA	2.94	121.14	111.91
29	A	414	PL9	C30-C29-C31	2.94	120.22	115.27
25	k	101	BCR	C24-C23-C22	-2.94	121.79	126.23
23	d	402	CLA	C4-C3-C5	2.94	120.22	115.27
25	c	516	BCR	C32-C1-C6	-2.94	105.53	110.30
23	d	402	CLA	CHD-C4C-NC	2.94	128.83	124.20
23	c	510	CLA	C1-O2A-CGA	2.94	124.15	116.44
33	a	421	LHG	O7-C7-C8	2.94	117.83	111.50
23	c	510	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
23	b	608	CLA	CBC-CAC-C3C	-2.94	104.34	112.43
23	A	406	CLA	CHD-C4C-NC	2.93	128.83	124.20
29	A	414	PL9	C17-C18-C19	-2.93	120.59	127.66
33	D	406	LHG	O8-C23-O10	-2.93	116.19	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	404	PL9	C22-C23-C24	-2.93	120.60	127.66
23	B	603	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
23	C	505	CLA	C4-C3-C5	2.93	120.20	115.27
25	C	514	BCR	C11-C10-C9	-2.93	123.13	127.31
29	d	404	PL9	C27-C28-C29	-2.93	120.61	127.66
23	d	402	CLA	CAA-C2A-C3A	-2.93	104.77	112.78
23	A	404	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	C	512	CLA	CMC-C2C-C1C	2.92	129.49	125.04
23	B	609	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	C	508	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
23	a	406	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	B	607	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
26	F	103	SQD	O7-S-C6	2.92	110.41	106.94
23	A	406	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
35	h	102	DGD	O1G-C1A-C2A	2.92	121.06	111.91
25	K	103	BCR	C7-C8-C9	-2.92	121.83	126.23
23	B	609	CLA	C3B-C4B-NB	2.92	113.22	110.52
29	d	404	PL9	C53-C6-C1	2.92	120.95	114.99
29	a	415	PL9	C22-C23-C24	-2.92	120.64	127.66
23	b	613	CLA	C4-C3-C5	2.91	120.17	115.27
23	A	408	CLA	O2A-CGA-CBA	2.91	121.05	111.91
23	c	511	CLA	CBC-CAC-C3C	-2.91	104.40	112.43
23	c	504	CLA	CMC-C2C-C1C	2.91	129.47	125.04
23	c	514	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
26	A	410	SQD	O48-C23-C24	2.91	121.04	111.91
33	D	407	LHG	O8-C23-O10	-2.91	116.25	123.59
23	B	615	CLA	CHD-C4C-NC	2.91	128.79	124.20
23	C	509	CLA	C4C-C3C-C2C	-2.91	102.66	106.90
23	A	405	CLA	C4-C3-C5	2.91	120.16	115.27
23	a	405	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	C	511	CLA	C1-O2A-CGA	2.90	124.06	116.44
23	a	407	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	B	604	CLA	CMC-C2C-C1C	2.90	129.46	125.04
35	c	519	DGD	O1G-C1A-C2A	2.90	121.00	111.91
23	a	406	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
23	B	614	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	c	502	CLA	C3B-C4B-NB	2.90	113.20	110.52
23	a	407	CLA	CMB-C2B-C1B	2.89	129.78	125.37
23	b	601	CLA	C3B-C4B-NB	2.89	113.20	110.52
23	C	505	CLA	C3B-C4B-NB	2.89	113.20	110.52
23	D	403	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
25	D	404	BCR	C37-C22-C23	2.89	122.63	118.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	c	506	CLA	CMC-C2C-C1C	2.88	129.43	125.04
23	A	405	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	D	402	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
25	T	102	BCR	C16-C17-C18	-2.88	123.20	127.31
25	b	619	BCR	C38-C26-C25	-2.88	121.29	124.53
23	C	501	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
23	B	612	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
24	a	408	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	D	402	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	B	603	CLA	CHD-C4C-NC	2.87	128.72	124.20
31	A	421	LMT	O5B-C5B-C4B	2.87	114.90	109.69
23	C	511	CLA	CMB-C2B-C1B	2.87	129.74	125.37
23	c	514	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	B	614	CLA	O2A-CGA-CBA	2.87	120.91	111.91
23	b	603	CLA	O2A-CGA-O1A	-2.87	116.36	123.59
29	a	415	PL9	C37-C38-C39	-2.86	120.77	127.66
23	B	606	CLA	C4-C3-C5	2.86	120.09	115.27
23	b	605	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
23	C	507	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
23	b	611	CLA	CHC-C1C-C2C	-2.86	118.79	126.73
23	c	514	CLA	C1-C2-C3	-2.86	121.10	126.04
23	B	616	CLA	O2A-CGA-CBA	2.86	120.87	111.91
23	c	513	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
24	a	408	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
34	b	622	HTG	O5-C5-C4	2.85	114.87	109.69
23	C	505	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
23	B	614	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	B	601	CLA	O2A-CGA-CBA	2.85	120.85	111.91
35	h	102	DGD	O1G-C1A-O1A	-2.85	116.40	123.59
23	c	507	CLA	CHD-C4C-NC	2.85	128.69	124.20
33	b	630	LHG	O8-C23-C24	2.85	120.84	111.91
23	B	613	CLA	O2A-CGA-CBA	2.84	120.83	111.91
23	b	601	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
23	C	511	CLA	C1-C2-C3	-2.84	121.13	126.04
23	b	607	CLA	C4-C3-C5	2.84	120.05	115.27
24	a	408	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
25	T	102	BCR	C33-C5-C6	-2.84	121.34	124.53
23	B	601	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	B	606	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	b	601	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	c	510	CLA	C4-C3-C5	2.84	120.05	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402	CLA	C4C-C3C-C2C	-2.84	102.77	106.90
23	c	504	CLA	C1-C2-C3	-2.83	121.14	126.04
23	c	513	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	c	510	CLA	CHB-C1B-NB	-2.83	121.26	124.26
23	c	512	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
23	d	402	CLA	C3B-C4B-NB	2.83	113.14	110.52
26	f	102	SQD	C4-C3-C2	-2.83	105.88	110.82
23	b	609	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
23	B	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	c	512	CLA	C4C-C3C-C2C	-2.83	102.78	106.90
23	b	602	CLA	CMB-C2B-C1B	2.82	129.67	125.37
23	C	502	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
25	T	102	BCR	C12-C13-C14	-2.82	114.61	118.94
23	b	610	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	B	609	CLA	CMC-C2C-C1C	2.82	129.33	125.04
38	f	101	HEM	CHB-C1B-NB	2.82	127.85	124.37
23	C	504	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	b	615	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
26	B	620	SQD	C4-C3-C2	2.82	115.74	110.82
23	c	502	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
35	c	517	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	c	505	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	B	615	CLA	CAC-C3C-C4C	2.81	128.45	124.81
23	B	604	CLA	C6-C7-C8	-2.81	106.84	115.92
23	c	511	CLA	O2A-CGA-O1A	-2.81	116.51	123.59
23	b	603	CLA	CHD-C4C-NC	2.80	128.62	124.20
23	B	603	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
23	c	514	CLA	O2A-CGA-CBA	2.80	120.70	111.91
25	D	404	BCR	C40-C30-C25	-2.80	105.76	110.30
23	B	616	CLA	C1-O2A-CGA	2.80	123.79	116.44
23	C	506	CLA	C4-C3-C5	2.80	119.98	115.27
23	b	603	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	C	512	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	c	514	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
23	c	507	CLA	CAC-C3C-C4C	2.80	128.44	124.81
23	d	401	CLA	CHC-C1C-C2C	-2.80	118.97	126.73
23	b	606	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
32	c	520	LMG	O8-C28-C29	2.79	120.68	111.91
32	z	101	LMG	O8-C28-C29	2.79	120.67	111.91
35	C	515	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
23	d	402	CLA	CMC-C2C-C1C	2.79	129.29	125.04
23	b	605	CLA	CHC-C1C-C2C	-2.79	118.98	126.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	T	101	LMT	C1'-O5'-C5'	-2.79	108.22	113.69
23	A	406	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
33	D	407	LHG	O7-C7-C8	2.79	117.50	111.50
23	c	511	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
23	c	512	CLA	CMB-C2B-C1B	2.78	129.61	125.37
23	A	408	CLA	CHD-C4C-NC	2.78	128.59	124.20
23	B	603	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	B	608	CLA	CMC-C2C-C1C	2.78	129.28	125.04
26	a	411	SQD	O47-C7-O49	-2.78	116.98	123.70
23	b	604	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
23	C	509	CLA	CHD-C4C-NC	2.78	128.58	124.20
23	A	404	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
25	A	409	BCR	C33-C5-C6	-2.78	121.41	124.53
35	C	517	DGD	O1G-C1A-C2A	2.78	120.62	111.91
23	b	602	CLA	CMA-C3A-C4A	-2.77	104.31	111.77
23	B	616	CLA	CHD-C4C-NC	2.77	128.57	124.20
25	K	101	BCR	C38-C26-C25	-2.77	121.41	124.53
23	C	504	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
25	B	618	BCR	C2-C1-C6	2.77	114.74	110.48
23	C	509	CLA	C16-C15-C13	-2.77	106.98	115.92
23	C	504	CLA	CHC-C1C-C2C	-2.77	119.05	126.73
25	b	618	BCR	C37-C22-C21	-2.77	119.05	122.92
23	c	513	CLA	C4C-C3C-C2C	-2.77	102.87	106.90
32	m	101	LMG	C8-O7-C10	-2.76	110.99	117.79
23	b	609	CLA	CHD-C4C-NC	2.76	128.56	124.20
29	a	415	PL9	C53-C6-C1	2.76	120.64	114.99
23	c	512	CLA	C1-C2-C3	-2.76	121.27	126.04
23	b	608	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	B	613	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
25	B	618	BCR	C15-C14-C13	-2.76	123.38	127.31
23	b	611	CLA	C2A-C1A-CHA	-2.75	119.04	123.86
23	b	611	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	d	402	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	c	514	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	c	509	CLA	C4-C3-C5	2.75	119.90	115.27
29	A	414	PL9	C40-C39-C41	2.75	119.90	115.27
23	C	513	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	c	512	CLA	CAC-C3C-C4C	2.75	128.38	124.81
23	b	610	CLA	CAA-CBA-CGA	-2.75	105.22	113.25
26	f	102	SQD	O8-S-C6	2.75	110.12	105.74
23	B	606	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
23	c	507	CLA	C4C-C3C-C2C	-2.75	102.89	106.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	CHD-C4C-NC	2.75	128.53	124.20
26	f	102	SQD	O48-C23-C24	2.74	120.52	111.91
23	C	509	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
23	A	408	CLA	CMC-C2C-C1C	2.74	129.22	125.04
23	c	508	CLA	O2A-CGA-CBA	2.74	120.52	111.91
23	B	610	CLA	CHD-C4C-NC	2.74	128.53	124.20
23	B	607	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
25	a	410	BCR	C11-C10-C9	-2.74	123.40	127.31
23	b	615	CLA	CHD-C4C-NC	2.74	128.52	124.20
23	B	602	CLA	C4C-C3C-C2C	-2.74	102.90	106.90
25	k	101	BCR	C15-C14-C13	-2.74	123.40	127.31
23	b	606	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
29	A	414	PL9	C10-C9-C8	-2.74	116.66	123.68
25	c	515	BCR	C20-C21-C22	-2.74	123.41	127.31
32	c	520	LMG	O1-C7-C8	-2.73	104.30	110.90
23	A	404	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	C	501	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
23	C	513	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
23	B	605	CLA	C1-C2-C3	-2.73	121.32	126.04
23	c	504	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	c	505	CLA	CHD-C4C-NC	2.73	128.51	124.20
23	A	406	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
35	C	515	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
23	C	501	CLA	C3B-C4B-NB	2.73	113.05	110.52
33	d	406	LHG	O8-C23-C24	2.73	120.46	111.91
23	c	506	CLA	C3B-C4B-NB	2.72	113.04	110.52
23	B	606	CLA	C4C-C3C-C2C	-2.72	102.93	106.90
23	a	406	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	b	603	CLA	CBC-CAC-C3C	-2.72	104.93	112.43
29	D	405	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	402	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	B	608	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	B	609	CLA	CHD-C4C-NC	2.72	128.49	124.20
34	b	623	HTG	O5-C1-C2	2.72	113.73	110.31
31	B	628	LMT	O1'-C1'-C2'	2.72	112.55	108.30
33	A	420	LHG	O7-C7-O9	-2.72	117.13	123.70
23	c	510	CLA	O2A-C1-C2	2.72	115.78	108.64
25	t	102	BCR	C15-C16-C17	-2.72	117.91	123.47
23	C	501	CLA	C1-O2A-CGA	2.71	123.57	116.44
23	c	506	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
23	c	502	CLA	CHD-C4C-NC	2.71	128.48	124.20
23	D	403	CLA	C3B-C4B-NB	2.71	113.03	110.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	404	PL9	C36-C34-C33	-2.71	115.63	121.12
23	C	510	CLA	O2A-CGA-O1A	-2.71	116.75	123.59
26	B	620	SQD	C1-O5-C5	-2.71	108.37	113.69
23	b	614	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
23	a	407	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
24	a	408	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	A	406	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	A	404	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
32	D	411	LMG	O8-C28-C29	2.70	120.39	111.91
32	A	419	LMG	C8-O7-C10	-2.70	111.13	117.79
23	B	615	CLA	C11-C10-C8	-2.70	107.18	115.92
23	c	513	CLA	CAC-C3C-C4C	2.70	128.32	124.81
23	d	402	CLA	CBC-CAC-C3C	-2.70	104.98	112.43
23	d	402	CLA	CHC-C1C-C2C	-2.70	119.23	126.73
23	c	511	CLA	O2A-CGA-CBA	2.70	120.38	111.91
25	y	101	BCR	C10-C11-C12	-2.70	114.80	123.22
31	c	501	LMT	C3'-C4'-C5'	-2.70	104.74	110.93
31	b	621	LMT	C1'-O5'-C5'	-2.70	108.39	113.69
35	C	516	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	a	409	CLA	CHD-C4C-NC	2.70	128.45	124.20
23	D	402	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	B	615	CLA	CHC-C1C-C2C	-2.70	119.24	126.73
32	c	521	LMG	O8-C28-C29	2.70	120.37	111.91
25	b	618	BCR	C29-C30-C25	2.70	114.63	110.48
23	B	609	CLA	O2A-CGA-O1A	-2.70	116.79	123.59
23	B	615	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
23	b	616	CLA	C3B-C4B-NB	2.69	113.01	110.52
23	a	405	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	B	604	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
23	B	606	CLA	CMB-C2B-C1B	2.68	129.46	125.37
25	k	101	BCR	C2-C1-C6	2.68	114.61	110.48
23	A	408	CLA	CBC-CAC-C3C	-2.68	105.04	112.43
23	A	406	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	A	405	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	b	610	CLA	C4-C3-C5	2.68	119.78	115.27
23	b	616	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
23	a	407	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
23	c	505	CLA	CAC-C3C-C4C	2.68	128.28	124.81
23	b	610	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
23	b	614	CLA	CHD-C4C-NC	2.68	128.42	124.20
25	H	101	BCR	C24-C23-C22	-2.68	122.19	126.23
33	a	421	LHG	O8-C23-C24	2.68	120.30	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	417	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
35	c	517	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	405	PL9	C37-C38-C39	-2.67	121.22	127.66
23	A	406	CLA	C1-C2-C3	-2.67	121.42	126.04
23	B	607	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
23	c	511	CLA	CAC-C3C-C4C	2.67	128.28	124.81
35	c	519	DGD	O2G-C1B-C2B	2.67	117.25	111.50
23	c	505	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	t	102	BCR	C35-C13-C12	2.67	122.28	118.08
23	b	611	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
23	B	608	CLA	C11-C12-C13	-2.67	107.30	115.92
23	b	607	CLA	C2A-C1A-CHA	-2.67	119.20	123.86
25	K	101	BCR	C16-C17-C18	-2.66	123.51	127.31
26	b	620	SQD	O9-S-C6	2.66	110.11	106.94
23	b	603	CLA	CHC-C1C-C2C	-2.66	119.33	126.73
23	c	514	CLA	CMC-C2C-C1C	2.66	129.09	125.04
23	b	607	CLA	CAC-C3C-C4C	2.66	128.26	124.81
23	C	503	CLA	CMB-C2B-C1B	2.66	129.42	125.37
23	b	607	CLA	C1-C2-C3	-2.66	121.44	126.04
23	a	407	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
38	F	102	HEM	CHA-C4D-ND	2.66	127.65	124.37
31	B	630	LMT	O1'-C1'-C2'	2.66	112.45	108.30
23	B	614	CLA	C4-C3-C5	2.66	119.74	115.27
34	b	622	HTG	O2-C2-C3	-2.66	104.21	110.35
23	c	508	CLA	CAC-C3C-C4C	2.65	128.25	124.81
26	A	410	SQD	O48-C23-O10	-2.65	116.89	123.59
23	c	504	CLA	C4-C3-C5	2.65	119.74	115.27
23	C	513	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	a	405	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	A	408	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	B	603	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	C	511	CLA	CMC-C2C-C1C	2.65	129.08	125.04
23	B	607	CLA	CMB-C2B-C1B	2.65	129.41	125.37
23	C	510	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
25	B	619	BCR	C38-C26-C25	-2.65	121.55	124.53
23	C	513	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	a	410	BCR	C29-C30-C25	2.65	114.56	110.48
29	D	405	PL9	C40-C39-C41	2.65	119.72	115.27
23	b	612	CLA	CHC-C1C-C2C	-2.65	119.38	126.73
32	c	520	LMG	C8-O7-C10	-2.65	111.28	117.79
23	D	403	CLA	CHD-C4C-NC	2.65	128.37	124.20
23	C	509	CLA	O2D-CGD-O1D	-2.65	118.67	123.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	CHC-C1C-C2C	-2.65	119.38	126.73
23	C	507	CLA	CHC-C1C-C2C	-2.64	119.38	126.73
23	C	513	CLA	CBC-CAC-C3C	-2.64	105.14	112.43
23	b	607	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
23	c	511	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	B	601	CLA	CMB-C2B-C1B	2.64	129.39	125.37
23	A	406	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	C	513	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	B	608	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
23	A	406	CLA	C4-C3-C5	2.63	119.70	115.27
31	T	101	LMT	C3'-C4'-C5'	-2.63	104.89	110.93
26	a	413	SQD	C3-C4-C5	2.63	114.94	110.24
24	A	416	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
23	B	612	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	b	606	CLA	CAA-C2A-C3A	-2.63	105.57	112.78
25	t	102	BCR	C21-C20-C19	-2.63	115.01	123.22
23	B	607	CLA	CHD-C4C-NC	2.63	128.35	124.20
26	f	102	SQD	O5-C5-C4	2.63	114.47	109.69
23	C	506	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	c	512	CLA	O2A-CGA-CBA	2.63	120.15	111.91
23	B	610	CLA	CHC-C1C-C2C	-2.62	119.44	126.73
23	c	503	CLA	CBC-CAC-C3C	-2.62	105.20	112.43
23	a	409	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	B	605	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	B	602	CLA	CHC-C1C-C2C	-2.62	119.45	126.73
23	b	612	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	d	401	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	B	607	CLA	C4C-C3C-C2C	-2.62	103.08	106.90
23	B	614	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	C	503	CLA	CMC-C2C-C1C	2.62	129.02	125.04
23	B	611	CLA	C3B-C4B-NB	2.61	112.94	110.52
23	D	403	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
23	C	506	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
23	B	606	CLA	CBC-CAC-C3C	-2.61	105.23	112.43
29	A	414	PL9	C53-C6-C1	2.61	120.33	114.99
23	C	505	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
33	D	406	LHG	O8-C23-C24	2.61	120.09	111.91
33	D	406	LHG	O7-C7-C8	2.61	117.12	111.50
23	c	508	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
23	B	613	CLA	CMC-C2C-C1C	2.60	129.01	125.04
23	b	605	CLA	CMC-C2C-C1C	2.60	129.00	125.04
23	C	513	CLA	O2A-CGA-CBA	2.60	120.08	111.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	CAC-C3C-C4C	2.60	128.19	124.81
23	C	510	CLA	CBC-CAC-C3C	-2.60	105.26	112.43
38	f	101	HEM	CBD-CAD-C3D	-2.60	105.40	112.63
32	D	411	LMG	O7-C10-C11	2.60	117.11	111.50
23	b	610	CLA	CMA-C3A-C4A	-2.60	104.79	111.77
33	L	101	LHG	O8-C23-C24	2.60	120.06	111.91
23	c	507	CLA	O2A-CGA-O1A	-2.60	117.04	123.59
23	b	613	CLA	CHD-C4C-NC	2.60	128.29	124.20
31	A	421	LMT	O5'-C5'-C6'	2.60	112.89	106.44
23	b	616	CLA	C4-C3-C5	2.60	119.64	115.27
23	b	613	CLA	CAC-C3C-C4C	2.60	128.18	124.81
23	b	615	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	a	406	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	b	613	CLA	CMC-C2C-C1C	2.59	128.99	125.04
23	A	405	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	C	501	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
23	C	513	CLA	C4-C3-C5	2.59	119.62	115.27
23	C	503	CLA	CHC-C1C-C2C	-2.59	119.54	126.73
23	C	501	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	B	603	CLA	CMA-C3A-C2A	-2.59	103.39	113.83
23	C	512	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
25	d	403	BCR	C28-C27-C26	-2.59	109.46	114.08
23	a	405	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
23	c	514	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	b	614	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
23	b	606	CLA	C1-O2A-CGA	2.59	123.23	116.44
32	D	411	LMG	O8-C28-O10	-2.59	117.07	123.59
23	c	509	CLA	O2A-CGA-CBA	2.59	120.02	111.91
23	b	615	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
23	B	612	CLA	C11-C12-C13	-2.58	107.57	115.92
23	b	603	CLA	CMA-C3A-C2A	-2.58	103.41	113.83
29	d	404	PL9	C36-C37-C38	-2.58	103.40	111.88
23	C	513	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
40	v	201	HEC	CMD-C2D-C1D	2.58	128.97	125.04
23	B	615	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	b	611	CLA	CAC-C3C-C4C	2.58	128.15	124.81
23	c	508	CLA	CBC-CAC-C3C	-2.57	105.33	112.43
23	d	402	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	B	601	CLA	C3B-C4B-NB	2.57	112.90	110.52
23	b	604	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	b	602	CLA	CHD-C4C-NC	2.57	128.26	124.20
23	C	511	CLA	CHD-C4C-NC	2.57	128.26	124.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	O2A-CGA-CBA	2.57	119.98	111.91
25	c	515	BCR	C37-C22-C21	-2.57	119.32	122.92
23	c	510	CLA	CHD-C4C-NC	2.57	128.25	124.20
23	B	602	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	a	405	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	B	601	CLA	CHC-C1C-C2C	-2.57	119.60	126.73
23	C	507	CLA	C4-C3-C5	2.57	119.59	115.27
31	m	103	LMT	C1'-O5'-C5'	-2.56	108.66	113.69
23	C	506	CLA	CHD-C4C-NC	2.56	128.24	124.20
23	D	402	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	C	502	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	D	402	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
35	c	517	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
31	M	101	LMT	C3'-C4'-C5'	-2.56	105.06	110.93
25	d	403	BCR	C21-C20-C19	-2.56	115.23	123.22
23	B	612	CLA	C1-C2-C3	-2.56	121.62	126.04
23	b	606	CLA	C1-C2-C3	-2.56	121.62	126.04
23	b	609	CLA	O2A-CGA-O1A	-2.55	117.14	123.59
25	T	102	BCR	C2-C1-C6	2.55	114.41	110.48
23	D	403	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
23	a	409	CLA	CMA-C3A-C2A	-2.55	103.53	113.83
23	b	608	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	b	606	CLA	CMC-C2C-C1C	2.55	128.92	125.04
23	c	511	CLA	C4-C3-C2	-2.55	117.14	123.68
23	b	614	CLA	O2A-CGA-CBA	2.55	119.90	111.91
23	C	508	CLA	C4-C3-C5	2.54	119.55	115.27
27	b	628	GOL	C3-C2-C1	-2.54	101.81	111.70
25	A	409	BCR	C15-C14-C13	-2.54	123.68	127.31
25	a	410	BCR	C24-C23-C22	-2.54	122.39	126.23
23	A	405	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	C	507	CLA	O2A-CGA-CBA	2.54	119.88	111.91
23	C	510	CLA	O2A-CGA-CBA	2.54	119.88	111.91
23	C	503	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	B	616	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
26	F	103	SQD	O47-C7-O49	-2.54	117.57	123.70
25	y	101	BCR	C21-C20-C19	-2.54	115.30	123.22
31	B	628	LMT	C2'-C3'-C4'	2.54	115.48	109.68
24	a	417	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	D	403	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
26	F	103	SQD	O48-C23-C24	2.53	119.86	111.91
26	b	620	SQD	O7-S-C6	2.53	109.95	106.94
29	A	414	PL9	C35-C34-C36	2.53	119.53	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	C3B-C4B-NB	2.53	112.86	110.52
23	A	405	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	B	613	CLA	CAC-C3C-C4C	2.53	128.09	124.81
40	V	201	HEC	C4B-NB-C1B	2.53	107.68	105.07
35	h	102	DGD	O3G-C1D-C2D	2.53	112.25	108.30
25	c	515	BCR	C33-C5-C6	-2.53	121.69	124.53
25	t	102	BCR	C20-C21-C22	-2.52	123.71	127.31
23	c	508	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	c	508	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
23	C	508	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	a	407	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	b	616	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	A	406	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
23	c	505	CLA	C2A-C1A-CHA	-2.52	119.46	123.86
23	c	506	CLA	C1-C2-C3	-2.52	121.69	126.04
25	B	618	BCR	C37-C22-C23	2.52	122.04	118.08
23	c	507	CLA	CBC-CAC-C3C	-2.51	105.50	112.43
23	b	615	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
31	B	630	LMT	O5'-C5'-C6'	2.51	112.69	106.44
29	a	415	PL9	C47-C48-C49	-2.51	119.16	127.75
23	b	609	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
23	c	509	CLA	CAA-C2A-C3A	-2.51	105.90	112.78
23	a	406	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
24	A	407	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407	PHO	CMB-C2B-C3B	2.51	129.37	124.68
23	B	611	CLA	C4-C3-C5	2.51	119.49	115.27
23	B	615	CLA	C6-C7-C8	-2.51	107.81	115.92
23	b	601	CLA	C1-O2A-CGA	2.51	123.03	116.44
23	B	612	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	a	407	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	B	602	CLA	C11-C12-C13	-2.51	107.82	115.92
23	C	504	CLA	C4-C3-C5	2.50	119.48	115.27
23	b	611	CLA	CMB-C2B-C1B	2.50	129.18	125.37
23	c	507	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	b	601	CLA	CAC-C3C-C4C	2.50	128.05	124.81
38	F	102	HEM	CBA-CAA-C2A	-2.50	105.69	112.63
23	a	405	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	B	611	CLA	CMB-C2B-C3B	2.49	132.63	126.59
25	k	101	BCR	C39-C30-C25	-2.49	106.25	110.30
23	A	408	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	Y	101	BCR	C36-C18-C17	-2.49	119.43	122.92
23	D	403	CLA	CMA-C3A-C4A	-2.49	105.08	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	CMC-C2C-C1C	2.49	128.83	125.04
23	a	407	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	B	604	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	c	514	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
23	b	604	CLA	CMB-C2B-C1B	2.49	129.16	125.37
23	b	602	CLA	C11-C12-C13	-2.49	107.88	115.92
23	C	502	CLA	CHD-C4C-NC	2.49	128.12	124.20
24	a	408	PHO	CMB-C2B-C3B	2.48	129.33	124.68
34	B	622	HTG	C1-O5-C5	2.48	117.16	112.58
35	C	515	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	404	PL9	C17-C18-C19	-2.48	121.69	127.66
25	t	102	BCR	C1-C6-C7	2.48	122.79	115.78
25	d	403	BCR	C24-C23-C22	-2.48	122.49	126.23
23	A	408	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	502	CLA	C4-C3-C5	2.48	119.44	115.27
23	C	507	CLA	C1-C2-C3	-2.48	121.76	126.04
24	A	407	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
23	C	512	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
23	A	404	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	c	509	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
23	a	409	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
23	c	506	CLA	C4-C3-C5	2.47	119.43	115.27
23	C	503	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	512	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	B	608	CLA	O2A-CGA-CBA	2.47	119.66	111.91
25	H	101	BCR	C7-C8-C9	-2.47	122.50	126.23
23	C	505	CLA	O2A-CGA-CBA	2.47	119.66	111.91
26	B	620	SQD	C44-O6-C1	-2.47	108.91	113.74
23	C	509	CLA	C11-C12-C13	-2.47	107.94	115.92
23	B	616	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
34	b	622	HTG	O5-C1-C2	2.47	113.42	110.31
25	d	403	BCR	C16-C17-C18	-2.47	123.79	127.31
23	C	508	CLA	CAC-C3C-C4C	2.47	128.01	124.81
23	b	612	CLA	CHB-C1B-NB	-2.46	121.65	124.26
23	B	612	CLA	C3B-C4B-NB	2.46	112.80	110.52
25	c	516	BCR	C33-C5-C6	-2.46	121.76	124.53
23	C	502	CLA	O2A-CGA-CBA	2.46	119.64	111.91
23	C	503	CLA	O2A-CGA-CBA	2.46	119.64	111.91
33	d	405	LHG	O8-C23-O10	-2.46	117.38	123.59
23	A	408	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	c	516	BCR	C21-C20-C19	-2.46	115.54	123.22
26	a	411	SQD	O7-S-C6	2.46	109.86	106.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	H	102	DGD	O1G-C1A-C2A	2.46	119.62	111.91
34	B	625	HTG	O5-C5-C4	2.46	114.16	109.69
25	h	101	BCR	C24-C23-C22	-2.46	122.52	126.23
25	B	619	BCR	C21-C20-C19	-2.46	115.56	123.22
23	C	505	CLA	CHD-C4C-NC	2.45	128.07	124.20
23	c	502	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
23	a	406	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	b	613	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
25	Y	101	BCR	C15-C16-C17	-2.45	118.45	123.47
23	A	405	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
26	a	413	SQD	O8-S-C6	2.45	109.64	105.74
23	c	506	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	a	415	PL9	C40-C39-C41	2.45	119.39	115.27
31	B	631	LMT	C3'-C4'-C5'	-2.45	105.32	110.93
23	c	507	CLA	C4-C3-C5	2.45	119.39	115.27
40	v	201	HEC	C4B-NB-C1B	2.45	107.60	105.07
29	D	405	PL9	C27-C28-C29	-2.44	121.77	127.66
29	a	415	PL9	C20-C19-C21	2.44	119.38	115.27
25	h	101	BCR	C36-C18-C17	-2.44	119.50	122.92
31	m	103	LMT	C3'-C4'-C5'	-2.44	105.33	110.93
25	T	102	BCR	C21-C20-C19	-2.44	115.59	123.22
23	b	607	CLA	CBC-CAC-C3C	-2.44	105.70	112.43
23	b	615	CLA	CAC-C3C-C4C	2.44	127.98	124.81
34	C	520	HTG	C1-O5-C5	2.44	117.08	112.58
23	c	509	CLA	CHD-C4C-NC	2.44	128.05	124.20
23	A	405	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	a	405	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	Y	101	BCR	C28-C27-C26	-2.44	109.73	114.08
34	b	625	HTG	C1'-S1-C1	2.43	104.64	100.09
25	Y	101	BCR	C37-C22-C23	2.43	121.91	118.08
25	K	103	BCR	C36-C18-C19	2.43	121.91	118.08
23	b	602	CLA	C1-C2-C3	-2.43	121.83	126.04
23	C	513	CLA	CAA-C2A-C3A	-2.43	106.12	112.78
25	c	515	BCR	C38-C26-C25	-2.43	121.80	124.53
24	a	408	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
23	A	408	CLA	CMA-C3A-C2A	-2.43	104.03	113.83
23	c	502	CLA	O2A-CGA-CBA	2.43	119.53	111.91
25	H	101	BCR	C37-C22-C21	-2.43	119.52	122.92
23	C	502	CLA	CAC-C3C-C4C	2.43	127.96	124.81
40	v	201	HEC	C4A-NA-C1A	2.43	107.72	105.35
23	c	504	CLA	CAC-C3C-C4C	2.43	127.96	124.81
29	d	404	PL9	C47-C48-C49	-2.42	119.47	127.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	c	504	CLA	CHC-C1C-C2C	-2.42	120.00	126.73
25	A	409	BCR	C16-C17-C18	-2.42	123.85	127.31
23	D	403	CLA	O2A-CGA-CBA	2.42	119.51	111.91
23	c	503	CLA	C1-C2-C3	-2.42	121.86	126.04
32	A	419	LMG	C6-C5-C4	2.42	118.67	113.00
23	B	606	CLA	CAC-C3C-C4C	2.42	127.95	124.81
23	B	601	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	C	510	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
26	B	620	SQD	O48-C23-O10	-2.42	117.49	123.59
23	D	403	CLA	C2A-C1A-CHA	-2.42	119.63	123.86
23	b	606	CLA	CMB-C2B-C1B	2.42	129.05	125.37
23	c	513	CLA	C3B-C4B-NB	2.42	112.76	110.52
26	a	411	SQD	O8-S-C6	2.41	109.59	105.74
29	A	414	PL9	C35-C34-C33	-2.41	117.49	123.68
31	A	421	LMT	O1'-C1'-C2'	2.41	112.07	108.30
34	c	522	HTG	O5-C1-C2	2.41	113.34	110.31
23	B	607	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
23	b	610	CLA	C3B-C4B-NB	2.41	112.75	110.52
23	B	613	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	b	602	CLA	CHB-C1B-C2B	-2.41	120.44	127.24
23	B	605	CLA	CHC-C1C-C2C	-2.41	120.05	126.73
29	A	414	PL9	C42-C43-C44	-2.41	121.87	127.66
23	C	501	CLA	C4-C3-C5	2.40	119.31	115.27
40	v	201	HEC	CBD-CAD-C3D	-2.40	105.95	112.63
23	B	602	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
23	b	601	CLA	O2A-CGA-CBA	2.40	119.44	111.91
25	B	618	BCR	C37-C22-C21	-2.40	119.56	122.92
23	B	604	CLA	C11-C12-C13	-2.40	108.16	115.92
23	c	503	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	C	512	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	B	605	CLA	C3B-C4B-NB	2.40	112.74	110.52
23	b	611	CLA	O2A-CGA-CBA	2.40	119.43	111.91
23	c	511	CLA	C11-C10-C8	-2.40	108.18	115.92
25	C	514	BCR	C32-C1-C6	-2.40	106.41	110.30
32	B	621	LMG	C12-C11-C10	-2.39	104.91	113.62
26	f	102	SQD	O47-C7-O49	-2.39	117.92	123.70
23	B	613	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	D	403	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
25	y	101	BCR	C40-C30-C25	-2.39	106.42	110.30
26	a	413	SQD	C1-O5-C5	2.39	118.37	113.69
23	C	505	CLA	CHB-C1B-NB	-2.38	121.73	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	CHB-C1B-NB	-2.38	121.74	124.26
23	B	601	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
25	T	102	BCR	C3-C4-C5	-2.38	109.83	114.08
35	H	102	DGD	O1G-C1A-O1A	-2.38	117.58	123.59
23	A	408	CLA	OBD-CAD-C3D	-2.38	122.79	128.52
33	L	101	LHG	O8-C23-O10	-2.38	117.59	123.59
23	B	601	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	b	613	CLA	CMB-C2B-C1B	2.38	128.99	125.37
25	b	617	BCR	C24-C23-C22	-2.38	122.64	126.23
23	C	506	CLA	C4C-C3C-C2C	-2.38	103.43	106.90
23	c	508	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
23	c	507	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
29	a	415	PL9	C10-C9-C8	-2.38	117.58	123.68
23	B	611	CLA	CAC-C3C-C4C	2.38	127.89	124.81
23	C	510	CLA	CMC-C2C-C1C	2.38	128.66	125.04
29	d	404	PL9	C7-C8-C9	-2.38	122.84	126.79
23	C	513	CLA	CHB-C1B-NB	-2.38	121.74	124.26
29	D	405	PL9	C45-C44-C46	2.38	119.27	115.27
25	D	404	BCR	C24-C23-C22	-2.37	122.65	126.23
25	H	101	BCR	C16-C15-C14	-2.37	118.62	123.47
38	F	102	HEM	O2A-CGA-CBA	2.37	121.65	114.03
38	F	102	HEM	C4A-NA-C1A	2.37	107.67	105.35
23	b	608	CLA	C11-C10-C8	-2.37	108.26	115.92
23	C	507	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
23	c	510	CLA	CMC-C2C-C1C	2.37	128.65	125.04
26	a	413	SQD	O5-C5-C4	2.37	113.99	109.69
23	C	506	CLA	O2A-CGA-CBA	2.37	119.33	111.91
25	A	409	BCR	C40-C30-C25	-2.37	106.46	110.30
32	C	518	LMG	O8-C28-O10	-2.36	117.62	123.59
23	C	512	CLA	CAC-C3C-C4C	2.36	127.88	124.81
23	b	601	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	c	504	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	B	603	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
25	D	404	BCR	C3-C4-C5	-2.36	109.86	114.08
29	D	405	PL9	C22-C23-C24	-2.36	121.98	127.66
23	B	609	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	b	612	CLA	CHD-C4C-NC	2.36	127.92	124.20
25	c	515	BCR	C36-C18-C17	-2.36	119.62	122.92
25	c	516	BCR	C38-C26-C25	-2.36	121.88	124.53
23	b	615	CLA	CBC-CAC-C3C	-2.36	105.94	112.43
23	B	601	CLA	C1-O2A-CGA	2.35	122.62	116.44
23	c	512	CLA	CHB-C1B-NB	-2.35	121.77	124.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	416	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
23	C	503	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	A	414	PL9	C45-C44-C46	2.35	119.22	115.27
35	C	516	DGD	O6E-C5E-C6E	2.35	112.28	106.44
29	a	415	PL9	C45-C44-C46	2.35	119.22	115.27
23	C	502	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
31	F	101	LMT	C1'-O5'-C5'	-2.35	109.08	113.69
23	B	609	CLA	C1-C2-C3	-2.35	121.98	126.04
23	a	406	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	C	512	CLA	CMA-C3A-C4A	-2.35	105.47	111.77
26	b	620	SQD	O48-C23-C24	2.34	119.27	111.91
23	C	512	CLA	C3B-C4B-NB	2.34	112.69	110.52
40	v	201	HEC	CHA-C4D-ND	2.34	126.96	124.42
23	b	610	CLA	CMB-C2B-C1B	2.34	128.94	125.37
23	B	611	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
23	B	612	CLA	C4-C3-C5	2.34	119.21	115.27
23	b	602	CLA	C4-C3-C5	2.34	119.21	115.27
23	c	514	CLA	C4-C3-C5	2.34	119.21	115.27
23	b	616	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	C	506	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	C	512	CLA	C2A-C1A-CHA	-2.34	119.77	123.86
23	c	507	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	d	402	CLA	O2A-CGA-CBA	2.34	119.24	111.91
23	b	609	CLA	CMA-C3A-C4A	-2.34	105.50	111.77
23	B	614	CLA	OBD-CAD-C3D	-2.34	122.90	128.52
25	d	403	BCR	C39-C30-C25	-2.33	106.51	110.30
23	c	507	CLA	CMC-C2C-C1C	2.33	128.59	125.04
23	D	402	CLA	CHD-C4C-NC	2.33	127.88	124.20
25	D	404	BCR	C15-C14-C13	-2.33	123.98	127.31
23	a	406	CLA	C1-O2A-CGA	2.33	122.56	116.44
25	b	618	BCR	C3-C4-C5	-2.33	109.92	114.08
25	T	102	BCR	C1-C6-C7	2.33	122.37	115.78
23	C	510	CLA	CMB-C2B-C1B	2.33	128.92	125.37
23	b	604	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	b	615	CLA	C6-C7-C8	-2.33	108.39	115.92
29	a	415	PL9	C35-C34-C33	-2.33	117.70	123.68
35	C	516	DGD	O1G-C1A-C2A	2.33	119.21	111.91
35	c	518	DGD	O1G-C1A-C2A	2.33	119.21	111.91
26	A	412	SQD	C4-C3-C2	-2.33	106.76	110.82
23	b	606	CLA	O2A-CGA-CBA	2.33	119.21	111.91
23	d	402	CLA	C1-O2A-CGA	2.33	122.55	116.44
26	b	620	SQD	C44-O6-C1	-2.33	109.19	113.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	405	LHG	O8-C23-C24	2.33	119.21	111.91
23	c	503	CLA	C4C-C3C-C2C	-2.33	103.51	106.90
23	b	610	CLA	CMC-C2C-C1C	2.32	128.58	125.04
35	c	519	DGD	O3G-C3G-C2G	-2.32	105.29	110.90
35	c	517	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
25	k	101	BCR	C36-C18-C19	2.32	121.74	118.08
23	b	614	CLA	CMC-C2C-C1C	2.32	128.57	125.04
40	V	201	HEC	CHA-C4D-ND	2.32	126.94	124.42
23	a	407	CLA	C4-C3-C5	2.32	119.17	115.27
23	B	602	CLA	CAA-CBA-CGA	-2.32	106.48	113.25
23	A	404	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	b	604	CLA	C4-C3-C5	2.32	119.17	115.27
31	B	630	LMT	O5'-C5'-C4'	2.32	114.64	109.75
38	F	102	HEM	O2D-CGD-CBD	2.32	121.47	114.03
23	C	504	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
26	a	411	SQD	O48-C23-C24	2.32	119.17	111.91
25	A	409	BCR	C11-C10-C9	-2.31	124.01	127.31
32	d	410	LMG	O8-C28-C29	2.31	119.17	111.91
25	k	101	BCR	C16-C17-C18	-2.31	124.01	127.31
25	d	403	BCR	C3-C4-C5	-2.31	109.95	114.08
23	c	509	CLA	CAC-C3C-C4C	2.31	127.81	124.81
23	B	613	CLA	CHB-C4A-NA	2.31	127.71	124.51
29	A	414	PL9	C37-C36-C34	-2.31	105.38	112.98
26	a	413	SQD	O48-C23-O10	-2.31	117.76	123.59
25	D	404	BCR	C15-C16-C17	-2.31	118.74	123.47
25	Y	101	BCR	C34-C9-C8	2.31	121.71	118.08
23	d	401	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	C	501	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
23	C	503	CLA	CHB-C1B-C2B	-2.30	120.73	127.24
23	d	402	CLA	CHB-C4A-NA	2.30	127.70	124.51
23	c	514	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
29	A	414	PL9	C2-C3-C4	2.30	121.97	118.80
25	b	617	BCR	C29-C30-C25	2.30	114.02	110.48
32	C	519	LMG	C9-C8-C7	-2.30	106.35	111.79
23	b	608	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
23	c	510	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
23	A	404	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	b	609	CLA	C7-C6-C5	-2.30	107.12	113.36
23	C	506	CLA	CGD-CBD-CAD	-2.30	103.30	110.73
26	F	103	SQD	O5-C1-O6	2.29	115.41	109.97
23	B	615	CLA	O2A-CGA-O1A	-2.29	117.80	123.59
23	b	604	CLA	C6-C5-C3	-2.29	107.44	113.45

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	-2.29	106.11	112.43
32	C	518	LMG	C8-O7-C10	-2.29	112.15	117.79
29	A	414	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	417	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
23	B	604	CLA	O2A-CGA-CBA	2.29	119.10	111.91
23	C	509	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
23	B	610	CLA	CMC-C2C-C1C	2.29	128.53	125.04
32	d	410	LMG	O7-C10-O9	-2.29	118.17	123.70
23	b	608	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
33	d	406	LHG	O8-C23-O10	-2.29	117.82	123.59
23	a	407	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	b	602	CLA	CHC-C1C-C2C	-2.29	120.38	126.73
23	c	507	CLA	CAA-C2A-C3A	-2.29	106.52	112.78
23	b	601	CLA	CMC-C2C-C1C	2.29	128.52	125.04
23	b	602	CLA	CAA-CBA-CGA	-2.29	106.57	113.25
23	c	512	CLA	C1-O2A-CGA	2.28	122.44	116.44
23	C	509	CLA	CHB-C1B-NB	-2.28	121.84	124.26
31	B	631	LMT	O5'-C5'-C4'	2.28	114.57	109.75
25	c	516	BCR	C37-C22-C23	2.28	121.67	118.08
26	A	412	SQD	O48-C23-O10	-2.28	117.83	123.59
23	b	608	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	b	607	CLA	C1-O2A-CGA	2.28	122.43	116.44
23	b	606	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	C	510	CLA	CAC-C3C-C4C	2.28	127.77	124.81
25	y	101	BCR	C16-C17-C18	-2.28	124.06	127.31
34	b	625	HTG	O5-C1-S1	-2.28	104.38	109.82
23	B	606	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
23	b	608	CLA	C11-C12-C13	-2.28	108.56	115.92
23	C	513	CLA	CMB-C2B-C1B	2.28	128.84	125.37
23	B	604	CLA	C4-C3-C5	2.28	119.10	115.27
25	a	410	BCR	C34-C9-C10	-2.28	119.74	122.92
23	B	610	CLA	CAC-C3C-C4C	2.27	127.76	124.81
23	c	507	CLA	CMB-C2B-C1B	2.27	128.83	125.37
23	a	405	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	c	512	CLA	CMA-C3A-C4A	2.27	117.88	111.77
29	d	404	PL9	C31-C32-C33	-2.27	104.42	111.88
23	c	513	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	A	408	CLA	CMB-C2B-C1B	2.27	128.82	125.37
26	b	620	SQD	O47-C7-O49	-2.27	118.22	123.70
23	c	511	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
24	A	416	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
23	B	613	CLA	CMA-C3A-C4A	-2.27	105.68	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	101	BCR	C36-C18-C19	2.26	121.64	118.08
23	b	616	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
25	a	410	BCR	C7-C8-C9	-2.26	122.82	126.23
25	y	101	BCR	C34-C9-C10	-2.26	119.75	122.92
23	B	616	CLA	CBC-CAC-C3C	-2.26	106.20	112.43
33	d	411	LHG	O7-C7-O9	-2.26	118.24	123.70
23	D	402	CLA	C4-C3-C5	2.26	119.07	115.27
23	C	508	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
33	d	405	LHG	C6-C5-C4	-2.26	106.44	111.79
23	C	501	CLA	O2A-CGA-CBA	2.26	119.00	111.91
23	b	603	CLA	CMB-C2B-C1B	2.26	128.81	125.37
35	C	517	DGD	O2G-C1B-C2B	2.26	116.37	111.50
23	B	614	CLA	CAA-C2A-C3A	-2.26	106.60	112.78
33	b	630	LHG	O8-C23-O10	-2.26	117.90	123.59
24	a	417	PHO	C4-C3-C2	-2.26	117.89	123.68
23	c	510	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	k	101	BCR	C10-C11-C12	-2.25	116.19	123.22
23	b	611	CLA	CMC-C2C-C1C	2.25	128.47	125.04
32	d	410	LMG	C7-O1-C1	-2.25	109.34	113.74
23	B	612	CLA	C6-C5-C3	-2.25	107.55	113.45
23	B	610	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
25	Y	101	BCR	C38-C26-C25	-2.25	122.00	124.53
25	H	101	BCR	C10-C11-C12	-2.25	116.20	123.22
25	h	101	BCR	C37-C22-C21	-2.25	119.77	122.92
29	D	405	PL9	C20-C19-C21	2.25	119.05	115.27
25	b	619	BCR	C39-C30-C25	-2.25	106.65	110.30
23	c	505	CLA	CMC-C2C-C1C	2.25	128.46	125.04
24	A	416	PHO	CMB-C2B-C3B	2.25	128.88	124.68
23	a	409	CLA	CHC-C1C-C2C	-2.25	120.49	126.73
23	C	508	CLA	O2A-CGA-CBA	2.25	118.96	111.91
40	v	201	HEC	CAD-CBD-CGD	-2.25	108.77	113.60
23	c	514	CLA	CBC-CAC-C3C	-2.24	106.24	112.43
23	C	507	CLA	CMC-C2C-C1C	2.24	128.46	125.04
23	B	604	CLA	C6-C5-C3	-2.24	107.57	113.45
23	c	509	CLA	CHB-C1B-NB	-2.24	121.88	124.26
25	b	618	BCR	C37-C22-C23	2.24	121.61	118.08
23	B	614	CLA	CMB-C2B-C1B	2.24	128.78	125.37
23	d	402	CLA	CMA-C3A-C2A	-2.24	104.78	113.83
25	t	102	BCR	C34-C9-C10	-2.24	119.78	122.92
24	a	417	PHO	CED-O2D-CGD	2.24	121.00	115.94
23	C	504	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	K	103	BCR	C37-C22-C21	-2.24	119.79	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	B	621	LMG	O8-C28-O10	-2.24	117.94	123.59
23	c	508	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
23	c	512	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
25	c	515	BCR	C34-C9-C10	-2.24	119.79	122.92
23	c	506	CLA	CHD-C4C-NC	2.24	127.73	124.20
32	c	521	LMG	O8-C28-O10	-2.23	117.95	123.59
23	c	506	CLA	CHB-C1B-NB	-2.23	121.89	124.26
23	a	409	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
29	D	405	PL9	C36-C37-C38	-2.23	104.54	111.88
23	b	609	CLA	O2A-CGA-CBA	2.23	118.91	111.91
23	b	607	CLA	CMB-C2B-C1B	2.23	128.77	125.37
31	B	631	LMT	O1'-C1'-C2'	2.23	111.79	108.30
23	b	616	CLA	CAC-C3C-C4C	2.23	127.70	124.81
31	A	421	LMT	O5'-C5'-C4'	2.23	114.45	109.75
23	B	608	CLA	C11-C10-C8	-2.23	108.72	115.92
23	a	405	CLA	C7-C6-C5	-2.22	107.32	113.36
23	B	608	CLA	CHD-C4C-NC	2.22	127.71	124.20
32	Z	101	LMG	C1-O6-C5	2.22	118.05	113.69
23	C	505	CLA	CHA-C1A-NA	-2.22	121.31	126.40
26	A	410	SQD	O8-S-C6	2.22	109.28	105.74
23	C	503	CLA	C3B-C4B-NB	2.22	112.58	110.52
35	h	102	DGD	C6D-C5D-C4D	2.22	116.73	112.09
25	c	516	BCR	C20-C21-C22	-2.22	124.14	127.31
25	D	404	BCR	C21-C20-C19	-2.22	116.29	123.22
26	b	620	SQD	C1-C2-C3	-2.22	105.37	110.00
25	h	101	BCR	C33-C5-C6	-2.22	122.03	124.53
23	c	502	CLA	CAC-C3C-C4C	2.22	127.69	124.81
23	C	502	CLA	CMC-C2C-C1C	2.22	128.42	125.04
23	B	608	CLA	CMA-C3A-C2A	-2.22	104.88	113.83
23	A	405	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	C	505	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
23	b	613	CLA	CHB-C1B-NB	-2.22	121.91	124.26
25	Y	101	BCR	C10-C11-C12	-2.22	116.30	123.22
23	b	613	CLA	CED-O2D-CGD	2.22	120.95	115.94
23	b	609	CLA	C16-C15-C13	-2.22	108.75	115.92
23	B	614	CLA	CBC-CAC-C3C	-2.22	106.32	112.43
35	C	515	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
35	c	518	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
23	b	605	CLA	O2A-C1-C2	-2.21	102.81	108.64
23	c	504	CLA	O2A-CGA-CBA	2.21	118.86	111.91
23	c	508	CLA	C3B-C4B-NB	2.21	112.57	110.52
25	c	516	BCR	C37-C22-C21	-2.21	119.82	122.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	CHB-C1B-NB	-2.21	121.92	124.26
23	c	511	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
26	f	102	SQD	O48-C23-O10	-2.21	118.01	123.59
23	b	614	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
25	c	516	BCR	C15-C16-C17	-2.21	118.95	123.47
38	f	101	HEM	CMD-C2D-C1D	2.21	128.40	125.04
23	c	514	CLA	CMB-C2B-C1B	2.21	128.73	125.37
23	C	512	CLA	O2A-CGA-O1A	-2.21	118.03	123.59
26	F	103	SQD	O8-S-O7	-2.20	105.89	111.27
23	C	503	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
23	b	601	CLA	CMB-C2B-C1B	2.20	128.72	125.37
23	b	614	CLA	CHB-C1B-NB	-2.20	121.93	124.26
24	A	407	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	407	CLA	CAC-C3C-C4C	2.20	127.67	124.81
23	a	409	CLA	CMB-C2B-C1B	2.20	128.72	125.37
23	b	601	CLA	CBC-CAC-C3C	-2.20	106.37	112.43
23	c	510	CLA	C4-C3-C2	-2.20	118.04	123.68
25	Y	101	BCR	C1-C6-C7	2.20	122.00	115.78
29	A	414	PL9	C51-C49-C50	2.20	119.46	114.60
25	C	514	BCR	C29-C30-C25	2.20	113.86	110.48
24	A	416	PHO	O2A-CGA-CBA	2.20	118.80	111.91
23	C	504	CLA	CMB-C2B-C1B	2.19	128.71	125.37
23	c	502	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
23	c	506	CLA	CMA-C3A-C4A	-2.19	105.88	111.77
23	B	602	CLA	C4-C3-C5	2.19	118.96	115.27
23	B	601	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
23	b	606	CLA	CAC-C3C-C4C	2.19	127.65	124.81
23	B	609	CLA	CHA-C1A-NA	-2.19	121.39	126.40
25	b	618	BCR	C8-C7-C6	-2.19	121.06	127.20
34	B	625	HTG	C3-C4-C5	2.19	114.14	110.24
23	D	402	CLA	CED-O2D-CGD	2.19	120.88	115.94
25	T	102	BCR	C35-C13-C12	2.18	121.52	118.08
26	a	411	SQD	O9-S-O7	-2.18	106.39	113.95
23	b	602	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	c	513	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	c	515	BCR	C28-C27-C26	-2.18	110.18	114.08
23	b	609	CLA	CHA-C1A-NA	-2.18	121.41	126.40
23	C	510	CLA	CHB-C4A-NA	2.18	127.53	124.51
29	d	404	PL9	C51-C49-C50	2.18	119.42	114.60
23	c	502	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
23	d	401	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	c	502	CLA	C4-C3-C5	2.18	118.93	115.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	101	BCR	C34-C9-C8	2.18	121.51	118.08
35	c	518	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
23	A	408	CLA	CHB-C1B-NB	-2.17	121.95	124.26
23	B	602	CLA	CMB-C2B-C1B	2.17	128.68	125.37
35	H	102	DGD	O2G-C1B-C2B	2.17	116.18	111.50
23	b	615	CLA	CHA-C1A-NA	-2.17	121.42	126.40
25	A	409	BCR	C8-C7-C6	-2.17	121.11	127.20
23	B	605	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
23	b	615	CLA	C11-C12-C13	-2.17	108.90	115.92
25	d	403	BCR	C38-C26-C27	2.17	117.78	113.62
24	a	408	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
23	c	505	CLA	CBC-CAC-C3C	-2.17	106.45	112.43
32	m	101	LMG	O8-C28-O10	-2.17	118.12	123.59
33	A	420	LHG	O4-P-O5	2.17	122.95	112.24
23	c	502	CLA	CBC-CAC-C3C	-2.17	106.46	112.43
31	e	101	LMT	O1'-C1'-C2'	2.17	111.69	108.30
23	B	612	CLA	CHC-C1C-C2C	-2.17	120.71	126.73
25	K	103	BCR	C11-C10-C9	-2.16	124.22	127.31
23	A	405	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
23	B	612	CLA	CMA-C3A-C2A	-2.16	105.11	113.83
23	B	606	CLA	CAA-C2A-C3A	-2.16	106.86	112.78
25	c	515	BCR	C36-C18-C19	2.16	121.48	118.08
35	c	519	DGD	O3G-C1D-C2D	-2.16	104.93	108.30
26	A	410	SQD	O9-S-O7	-2.16	106.48	113.95
26	B	620	SQD	O5-C1-C2	-2.16	105.79	110.35
34	B	622	HTG	O2-C2-C3	-2.15	105.37	110.35
23	B	608	CLA	CMB-C2B-C1B	2.15	128.65	125.37
23	b	606	CLA	CHB-C1B-C2B	-2.15	121.16	127.24
23	b	605	CLA	C1-O2A-CGA	2.15	122.09	116.44
25	d	403	BCR	C33-C5-C6	-2.15	122.11	124.53
23	A	408	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
35	C	516	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	b	602	CLA	C1-O2A-CGA	2.15	122.08	116.44
23	C	504	CLA	CAA-C2A-C3A	-2.15	106.89	112.78
35	c	517	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
29	d	404	PL9	C35-C34-C36	2.15	118.88	115.27
23	D	403	CLA	C1-C2-C3	-2.15	122.33	126.04
23	B	605	CLA	OBD-CAD-C3D	-2.15	123.36	128.52
23	C	504	CLA	CHB-C1B-NB	-2.15	121.98	124.26
23	C	510	CLA	CHB-C1B-NB	-2.15	121.99	124.26
23	a	409	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
25	B	617	BCR	C15-C14-C13	-2.14	124.25	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	CMA-C3A-C2A	-2.14	105.18	113.83
23	C	510	CLA	C4-C3-C2	-2.14	118.18	123.68
25	Y	101	BCR	C24-C23-C22	-2.14	123.00	126.23
23	b	607	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
23	B	610	CLA	C4-C3-C5	2.14	118.87	115.27
34	b	622	HTG	C6-C5-C4	-2.14	107.99	113.00
32	a	418	LMG	O8-C28-C29	2.14	118.62	111.91
29	A	414	PL9	C25-C24-C26	2.14	118.87	115.27
26	A	412	SQD	O7-S-C6	2.14	109.48	106.94
23	B	604	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
23	c	504	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
40	v	201	HEC	C2A-C1A-NA	-2.14	108.24	110.32
31	m	103	LMT	C3B-C4B-C5B	-2.14	106.43	110.24
38	F	102	HEM	C4D-ND-C1D	2.14	107.28	105.07
23	C	504	CLA	OBD-CAD-C3D	-2.14	123.38	128.52
23	c	513	CLA	CBA-CAA-C2A	-2.14	107.56	113.86
24	A	407	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
35	H	102	DGD	C3E-C4E-C5E	-2.13	106.43	110.24
23	b	603	CLA	CAC-C3C-C4C	2.13	127.58	124.81
23	b	608	CLA	C4-C3-C5	2.13	118.86	115.27
25	b	618	BCR	C33-C5-C6	-2.13	122.14	124.53
25	C	514	BCR	C21-C20-C19	-2.13	116.57	123.22
25	D	404	BCR	C38-C26-C27	2.13	117.70	113.62
35	C	515	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
35	c	518	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
25	D	404	BCR	C16-C17-C18	-2.12	124.28	127.31
31	F	101	LMT	C3B-C4B-C5B	-2.12	106.45	110.24
23	C	508	CLA	CMB-C2B-C1B	2.12	128.60	125.37
24	a	417	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
25	A	409	BCR	C31-C1-C6	-2.12	106.86	110.30
25	y	101	BCR	C1-C6-C7	2.12	121.78	115.78
32	c	521	LMG	C1-C2-C3	-2.12	105.58	110.00
23	A	408	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	b	606	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
35	C	515	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
25	k	101	BCR	C20-C21-C22	-2.12	124.28	127.31
32	m	101	LMG	C7-O1-C1	-2.12	109.59	113.74
23	A	405	CLA	O2A-CGA-CBA	2.12	118.56	111.91
23	C	509	CLA	C4-C3-C5	2.12	118.84	115.27
25	b	619	BCR	C16-C15-C14	-2.12	119.13	123.47
40	v	201	HEC	CBB-CAB-C3B	-2.12	106.59	112.43
25	K	103	BCR	C2-C1-C6	2.12	113.74	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414	PL9	C12-C13-C14	-2.12	122.56	127.66
27	A	418	GOL	C3-C2-C1	-2.12	103.47	111.70
23	b	613	CLA	CHA-C1A-NA	-2.12	121.55	126.40
25	K	101	BCR	C24-C23-C22	-2.12	123.04	126.23
23	B	611	CLA	OBD-CAD-C3D	-2.12	123.43	128.52
23	b	608	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	c	505	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
23	c	512	CLA	C11-C10-C8	-2.11	109.09	115.92
23	B	610	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
34	b	625	HTG	C1-C2-C3	-2.11	106.42	110.59
25	T	102	BCR	C7-C6-C5	-2.11	116.35	121.46
23	C	510	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
27	B	624	GOL	C3-C2-C1	-2.11	103.50	111.70
23	C	501	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
32	c	520	LMG	O7-C10-O9	-2.11	118.61	123.70
23	c	503	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
23	b	607	CLA	CMC-C2C-C1C	2.11	128.25	125.04
26	f	102	SQD	C44-O6-C1	-2.11	109.62	113.74
24	A	416	PHO	C6-C5-C3	-2.11	107.94	113.45
25	c	516	BCR	C11-C10-C9	-2.10	124.31	127.31
29	d	404	PL9	C12-C13-C14	-2.10	122.60	127.66
25	y	101	BCR	C35-C13-C14	-2.10	119.98	122.92
25	B	619	BCR	C10-C11-C12	-2.10	116.66	123.22
25	H	101	BCR	C36-C18-C17	-2.10	119.98	122.92
23	b	615	CLA	CMC-C2C-C1C	2.10	128.24	125.04
25	B	618	BCR	C7-C8-C9	-2.10	123.06	126.23
33	b	630	LHG	O7-C7-O9	-2.10	118.63	123.70
23	B	608	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
25	k	101	BCR	C3-C4-C5	-2.10	110.33	114.08
23	b	613	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
26	B	620	SQD	C9-C8-C7	-2.10	106.00	113.62
35	c	519	DGD	O2G-C1B-O1B	-2.10	118.64	123.70
23	c	506	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
25	t	102	BCR	C7-C6-C5	-2.10	116.39	121.46
23	c	503	CLA	C1-O2A-CGA	2.09	121.94	116.44
23	b	610	CLA	CHB-C4A-NA	2.09	127.41	124.51
23	c	513	CLA	CHA-C1A-NA	-2.09	121.60	126.40
33	E	101	LHG	O7-C7-O9	-2.09	118.64	123.70
23	B	608	CLA	C6-C7-C8	-2.09	109.15	115.92
23	D	402	CLA	CMB-C2B-C1B	2.09	128.56	125.37
25	B	619	BCR	C37-C22-C21	-2.09	119.99	122.92
25	d	403	BCR	C11-C10-C9	-2.09	124.33	127.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	SQD	O8-S-C6	2.09	109.07	105.74
23	b	602	CLA	O2A-CGA-CBA	2.09	118.46	111.91
23	B	606	CLA	CHB-C1B-C2B	-2.09	121.34	127.24
26	F	103	SQD	C3-C4-C5	2.09	113.96	110.24
23	A	404	CLA	C7-C6-C5	-2.09	107.69	113.36
23	c	506	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
23	c	513	CLA	CBC-CAC-C3C	-2.09	106.68	112.43
35	H	102	DGD	O6E-C5E-C6E	2.08	111.62	106.44
23	d	401	CLA	CHD-C4C-NC	2.08	127.49	124.20
25	Y	101	BCR	C3-C4-C5	-2.08	110.36	114.08
25	B	619	BCR	C7-C8-C9	-2.08	123.09	126.23
23	C	507	CLA	CHA-C1A-NA	-2.08	121.63	126.40
23	C	512	CLA	C4-C3-C2	-2.08	118.34	123.68
23	b	601	CLA	CHB-C1B-C2B	-2.08	121.37	127.24
23	c	505	CLA	CED-O2D-CGD	2.08	120.64	115.94
23	B	612	CLA	C7-C6-C5	-2.08	107.72	113.36
38	F	102	HEM	O2D-CGD-O1D	-2.08	118.12	123.30
23	b	616	CLA	C11-C12-C13	-2.08	109.21	115.92
25	a	410	BCR	C33-C5-C6	-2.08	122.20	124.53
23	C	506	CLA	CMB-C2B-C1B	2.08	128.53	125.37
31	M	101	LMT	C3B-C4B-C5B	-2.07	106.54	110.24
34	B	622	HTG	C2'-C1'-S1	-2.07	105.70	112.40
23	c	513	CLA	CHB-C1B-C2B	-2.07	121.38	127.24
38	F	102	HEM	CHA-C1A-NA	2.07	127.66	123.85
23	C	505	CLA	O1D-CGD-CBD	-2.07	120.24	124.48
40	V	201	HEC	CMD-C2D-C1D	2.07	128.20	125.04
35	H	102	DGD	C3B-C2B-C1B	-2.07	106.08	113.62
23	B	609	CLA	C7-C6-C5	-2.07	107.73	113.36
23	C	507	CLA	C3B-C4B-NB	2.07	112.44	110.52
23	A	404	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405	PL9	C12-C13-C14	-2.07	122.68	127.66
23	A	408	CLA	C1-O2A-CGA	2.07	121.87	116.44
32	d	410	LMG	O8-C28-O10	-2.07	118.37	123.59
32	A	419	LMG	O6-C1-O1	-2.07	105.07	109.97
23	C	512	CLA	CBA-CAA-C2A	-2.07	107.76	113.86
25	y	101	BCR	C37-C22-C23	2.07	121.34	118.08
29	D	405	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	415	PL9	C51-C49-C50	2.07	119.17	114.60
25	t	102	BCR	C28-C27-C26	-2.07	110.39	114.08
34	B	623	HTG	O5-C1-C2	2.07	112.91	110.31
29	D	405	PL9	C25-C24-C23	-2.06	118.38	123.68
23	B	613	CLA	CBC-CAC-C3C	-2.06	106.74	112.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	t	101	LMT	C1-O1'-C1'	2.06	117.26	113.84
26	B	620	SQD	O47-C7-O49	-2.06	118.72	123.70
23	b	614	CLA	C4-C3-C5	2.06	118.74	115.27
23	c	509	CLA	C2A-C1A-CHA	-2.06	120.25	123.86
25	C	514	BCR	C3-C4-C5	-2.06	110.40	114.08
32	z	101	LMG	C8-O7-C10	-2.06	112.72	117.79
25	b	619	BCR	C7-C8-C9	-2.06	123.12	126.23
35	h	102	DGD	C3B-C2B-C1B	-2.06	106.14	113.62
23	d	402	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
23	C	513	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
31	B	628	LMT	C1B-C2B-C3B	2.05	114.27	110.00
25	d	403	BCR	C16-C15-C14	-2.05	119.27	123.47
23	c	512	CLA	C2A-C1A-CHA	-2.05	120.27	123.86
38	f	101	HEM	C4A-NA-C1A	2.05	107.36	105.35
35	C	515	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	A	406	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	B	607	CLA	O2A-CGA-CBA	2.05	118.34	111.91
23	c	505	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
23	b	612	CLA	OBD-CAD-C3D	-2.05	123.59	128.52
32	A	419	LMG	O8-C28-C29	2.05	118.34	111.91
23	A	404	CLA	CHB-C4A-NA	2.05	127.34	124.51
25	b	617	BCR	C21-C20-C19	-2.05	116.83	123.22
23	B	613	CLA	C4-C3-C2	-2.05	118.43	123.68
25	h	101	BCR	C10-C11-C12	-2.04	116.84	123.22
33	D	407	LHG	O4-P-O5	2.04	122.34	112.24
23	b	611	CLA	CBC-CAC-C3C	-2.04	106.80	112.43
23	B	610	CLA	CHB-C4A-NA	2.04	127.33	124.51
24	A	407	PHO	C4-C3-C5	2.04	118.70	115.27
23	b	611	CLA	CHB-C1B-NB	-2.04	122.10	124.26
23	b	611	CLA	C7-C6-C5	-2.04	107.82	113.36
23	B	607	CLA	C11-C10-C8	-2.04	109.33	115.92
27	O	303	GOL	C3-C2-C1	-2.04	103.78	111.70
25	B	618	BCR	C28-C27-C26	-2.04	110.44	114.08
25	B	619	BCR	C34-C9-C8	2.04	121.29	118.08
25	t	102	BCR	C2-C1-C6	2.04	113.62	110.48
23	b	602	CLA	C11-C10-C8	-2.04	109.33	115.92
23	B	611	CLA	C2C-C1C-NC	2.04	111.88	109.97
23	b	608	CLA	CMA-C3A-C4A	-2.04	106.30	111.77
31	M	101	LMT	O5B-C5B-C6B	2.03	111.50	106.44
25	d	403	BCR	C37-C22-C23	2.03	121.28	118.08
23	B	611	CLA	O2A-CGA-CBA	2.03	118.29	111.91
32	c	520	LMG	O8-C28-O10	-2.03	118.46	123.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	t	102	BCR	C37-C22-C23	2.03	121.28	118.08
23	c	508	CLA	C2A-C1A-CHA	-2.03	120.31	123.86
23	a	405	CLA	CMB-C2B-C3B	2.03	131.51	126.59
23	b	601	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
23	C	508	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
23	a	406	CLA	CAC-C3C-C2C	2.03	131.00	127.53
23	B	614	CLA	CMA-C3A-C2A	-2.03	105.64	113.83
25	K	103	BCR	C15-C14-C13	-2.03	124.41	127.31
26	a	411	SQD	O48-C23-O10	-2.03	118.47	123.59
23	b	604	CLA	CHD-C4C-NC	2.03	127.40	124.20
23	B	606	CLA	C11-C10-C8	-2.03	109.36	115.92
23	b	602	CLA	CHB-C4A-NA	2.03	127.32	124.51
24	a	408	PHO	CBC-CAC-C3C	-2.03	109.91	112.88
23	A	408	CLA	C11-C12-C13	-2.03	109.37	115.92
25	d	403	BCR	C40-C30-C39	2.03	114.75	108.53
29	d	404	PL9	C45-C44-C46	2.03	118.68	115.27
25	a	410	BCR	C15-C16-C17	-2.03	119.33	123.47
23	C	512	CLA	OBD-CAD-C3D	-2.02	123.65	128.52
23	B	606	CLA	C7-C6-C5	-2.02	107.86	113.36
23	C	508	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	a	417	PHO	O2A-CGA-CBA	2.02	118.25	111.91
23	B	601	CLA	C1-C2-C3	-2.02	122.55	126.04
23	c	511	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
23	A	406	CLA	CHB-C4A-NA	2.02	127.30	124.51
23	C	507	CLA	C6-C7-C8	-2.02	109.39	115.92
23	c	502	CLA	CMC-C2C-C1C	2.02	128.11	125.04
23	b	609	CLA	C4-C3-C5	2.02	118.66	115.27
23	C	512	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	A	416	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	d	401	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	a	408	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
25	C	514	BCR	C2-C1-C6	2.01	113.58	110.48
40	V	201	HEC	C1D-C2D-C3D	-2.01	104.84	106.96
35	C	517	DGD	O3G-C3G-C2G	-2.01	106.04	110.90
25	h	101	BCR	C16-C15-C14	-2.01	119.35	123.47
40	v	201	HEC	CHA-C1A-NA	2.01	126.61	124.44
37	D	401	BCT	O2-C-O1	2.01	124.76	119.55
23	D	402	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
37	a	404	BCT	O2-C-O1	2.01	124.76	119.55
29	D	405	PL9	O2-C1-C6	-2.01	117.11	120.59
23	B	604	CLA	CHA-C1A-NA	-2.01	121.81	126.40
25	c	515	BCR	C31-C1-C6	-2.00	107.05	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	A	419	LMG	O7-C10-O9	-2.00	118.86	123.70
25	c	516	BCR	C2-C1-C6	2.00	113.56	110.48
23	C	501	CLA	C11-C12-C13	-2.00	109.45	115.92
25	D	404	BCR	C30-C25-C24	2.00	121.44	115.78
23	B	605	CLA	O2A-CGA-CBA	2.00	118.19	111.91

All (2) chirality outliers are listed below:

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

All (1309) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	510	CLA	C11-C10-C8-C9
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
23	d	402	CLA	C2-C3-C5-C6
23	d	402	CLA	C4-C3-C5-C6
25	B	617	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	b	617	BCR	C1-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410	SQD	O49-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O49-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	413	SQD	O6-C44-C45-O47
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
26	b	620	SQD	O49-C7-O47-C45
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	B	624	GOL	C1-C2-C3-O3
27	B	629	GOL	C1-C2-C3-O3
27	V	203	GOL	C1-C2-C3-O3
27	a	412	GOL	O1-C1-C2-C3
27	a	419	GOL	O1-C1-C2-C3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
27	o	302	GOL	C1-C2-C3-O3
27	o	303	GOL	O1-C1-C2-C3
27	o	303	GOL	C1-C2-C3-O3
29	A	414	PL9	C9-C11-C12-C13
29	A	414	PL9	C15-C14-C16-C17
29	A	414	PL9	C14-C16-C17-C18
29	a	415	PL9	C9-C11-C12-C13
29	a	415	PL9	C14-C16-C17-C18
29	a	415	PL9	C25-C24-C26-C27
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	421	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	F	101	LMT	O5'-C1'-O1'-C1
31	T	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
32	C	519	LMG	C11-C10-O7-C8
32	c	521	LMG	O9-C10-O7-C8
32	c	521	LMG	C11-C10-O7-C8
32	Z	101	LMG	O9-C10-O7-C8
32	Z	101	LMG	C11-C10-O7-C8
32	z	101	LMG	O6-C1-O1-C7
33	D	406	LHG	O2-C2-C3-O3
33	D	406	LHG	C3-O3-P-O4
33	D	406	LHG	C3-O3-P-O5
33	D	406	LHG	C3-O3-P-O6
33	D	406	LHG	C4-O6-P-O4
33	E	101	LHG	C3-O3-P-O4
33	E	101	LHG	C3-O3-P-O5
33	E	101	LHG	O10-C23-O8-C6
33	E	101	LHG	C24-C23-O8-C6
33	L	101	LHG	C4-O6-P-O4
33	L	101	LHG	C4-O6-P-O5
33	a	421	LHG	C3-O3-P-O4
33	a	421	LHG	C4-O6-P-O5
33	a	421	LHG	O10-C23-O8-C6
33	a	421	LHG	C24-C23-O8-C6
33	b	630	LHG	C4-O6-P-O3
33	b	630	LHG	C4-O6-P-O4
33	b	630	LHG	C4-O6-P-O5
33	d	405	LHG	C3-O3-P-O5
33	d	405	LHG	C4-O6-P-O4
33	d	411	LHG	C3-O3-P-O5
34	B	622	HTG	C2'-C1'-S1-C1
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
31	A	421	LMT	O5B-C1B-O1B-C4'
31	B	630	LMT	C4'-C5'-C6'-O6'
31	T	101	LMT	O5'-C5'-C6'-O6'
32	C	519	LMG	O9-C10-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	T	101	LMT	C4B-C5B-C6B-O6B
23	D	403	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	402	CLA	C3-C5-C6-C7
26	A	410	SQD	C8-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
31	m	103	LMT	C4B-C5B-C6B-O6B
31	m	103	LMT	O5B-C5B-C6B-O6B
23	C	504	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
23	D	403	CLA	C2-C3-C5-C6
29	A	414	PL9	C18-C19-C21-C22
23	B	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
31	c	501	LMT	O5B-C5B-C6B-O6B
32	c	521	LMG	O6-C5-C6-O5
34	b	625	HTG	S1-C1'-C2'-C3'
31	B	628	LMT	C4'-C5'-C6'-O6'
31	B	628	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	O5B-C5B-C6B-O6B
23	C	501	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CBD-CGD-O2D-CED
33	E	101	LHG	O2-C2-C3-O3
33	d	405	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
32	C	519	LMG	O6-C5-C6-O5
34	b	625	HTG	O5-C5-C6-O6
31	T	101	LMT	C4'-C5'-C6'-O6'
34	D	410	HTG	C4-C5-C6-O6
32	z	101	LMG	C11-C10-O7-C8
31	B	628	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	O5-C5-C6-O6
31	B	628	LMT	C6-C7-C8-C9
31	b	621	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	S1-C1'-C2'-C3'
34	d	409	HTG	S1-C1'-C2'-C3'
31	A	421	LMT	O5B-C5B-C6B-O6B
31	A	421	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	O5'-C5'-C6'-O6'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	B	631	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5B-C5B-C6B-O6B
31	e	101	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
29	A	414	PL9	C20-C19-C21-C22
29	a	415	PL9	C15-C14-C16-C17
29	a	415	PL9	C30-C29-C31-C32
31	c	501	LMT	C4B-C5B-C6B-O6B
23	B	605	CLA	C2-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414	PL9	C13-C14-C16-C17
29	a	415	PL9	C13-C14-C16-C17
29	a	415	PL9	C28-C29-C31-C32
23	b	606	CLA	C2A-CAA-CBA-CGA
31	b	627	LMT	O5'-C5'-C6'-O6'
31	t	101	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	C4B-C5B-C6B-O6B
31	F	101	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
29	D	405	PL9	C39-C41-C42-C43
34	B	625	HTG	O5-C5-C6-O6
31	A	421	LMT	C4B-C5B-C6B-O6B
40	V	201	HEC	C2C-C3C-CAC-CBC
23	C	513	CLA	CBD-CGD-O2D-CED
33	d	405	LHG	C1-C2-C3-O3
32	z	101	LMG	O9-C10-O7-C8
31	b	627	LMT	C4'-C5'-C6'-O6'
23	c	510	CLA	CBA-CGA-O2A-C1
32	c	521	LMG	C4-C5-C6-O5
25	T	102	BCR	C13-C14-C15-C16
26	F	103	SQD	C23-C24-C25-C26
23	b	614	CLA	C8-C10-C11-C12
31	e	101	LMT	O5B-C5B-C6B-O6B
32	B	621	LMG	C39-C40-C41-C42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	B	621	LMG	C15-C16-C17-C18
33	D	407	LHG	C33-C34-C35-C36
31	B	631	LMT	C4'-C5'-C6'-O6'
31	A	421	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
40	v	201	HEC	C2C-C3C-CAC-CBC
23	C	504	CLA	C2-C3-C5-C6
29	a	415	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
23	C	502	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
25	b	619	BCR	C7-C8-C9-C34
25	d	403	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
35	C	517	DGD	C6B-C7B-C8B-C9B
26	B	620	SQD	C7-C8-C9-C10
23	c	513	CLA	C15-C16-C17-C18
31	A	421	LMT	C5'-C4'-O1B-C1B
23	A	408	CLA	C5-C6-C7-C8
23	C	508	CLA	C10-C11-C12-C13
23	c	511	CLA	CBD-CGD-O2D-CED
34	b	623	HTG	C1'-C2'-C3'-C4'
31	B	628	LMT	C5'-C4'-O1B-C1B
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	C	507	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
31	A	421	LMT	C4'-C5'-C6'-O6'
40	V	201	HEC	C4C-C3C-CAC-CBC
27	O	302	GOL	O1-C1-C2-O2
27	V	203	GOL	O2-C2-C3-O3
27	a	412	GOL	O1-C1-C2-O2
27	a	419	GOL	O1-C1-C2-O2
31	e	101	LMT	O5'-C5'-C6'-O6'
23	B	606	CLA	C10-C11-C12-C13
23	B	608	CLA	C13-C15-C16-C17
34	b	622	HTG	S1-C1'-C2'-C3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
31	c	501	LMT	O1'-C1-C2-C3
23	B	603	CLA	C13-C15-C16-C17
23	b	604	CLA	C8-C10-C11-C12
32	Z	101	LMG	C10-C11-C12-C13
33	E	101	LHG	C23-C24-C25-C26
35	c	518	DGD	C1B-C2B-C3B-C4B
23	C	512	CLA	CBD-CGD-O2D-CED
23	B	602	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	B	606	CLA	C11-C10-C8-C7
23	C	510	CLA	C11-C12-C13-C15
23	D	403	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	B	610	CLA	C2A-CAA-CBA-CGA
23	c	514	CLA	C10-C11-C12-C13
35	h	102	DGD	C6B-C7B-C8B-C9B
23	c	510	CLA	O1A-CGA-O2A-C1
23	c	514	CLA	CBD-CGD-O2D-CED
31	b	621	LMT	C4'-C5'-C6'-O6'
26	F	103	SQD	O5-C1-O6-C44
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
23	C	512	CLA	C10-C11-C12-C13
29	A	414	PL9	C44-C46-C47-C48
29	d	404	PL9	C39-C41-C42-C43
31	A	421	LMT	O1'-C1-C2-C3
23	B	614	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C15-C16-C17-C18
23	a	409	CLA	CBA-CGA-O2A-C1
31	B	628	LMT	C4B-C5B-C6B-O6B
23	b	606	CLA	C10-C11-C12-C13
23	b	611	CLA	C8-C10-C11-C12
26	b	620	SQD	C18-C19-C20-C21
31	A	417	LMT	O1'-C1-C2-C3
34	b	625	HTG	C4-C5-C6-O6
23	a	405	CLA	C15-C16-C17-C18
23	b	604	CLA	C5-C6-C7-C8
33	E	101	LHG	C3-O3-P-O6
33	E	101	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
33	a	421	LHG	C3-O3-P-O6
33	a	421	LHG	C4-O6-P-O3
33	d	405	LHG	C3-O3-P-O6
40	V	201	HEC	C2B-C3B-CAB-CBB
26	A	410	SQD	C7-C8-C9-C10
33	D	406	LHG	C1-C2-C3-O3
32	B	621	LMG	O9-C10-O7-C8
23	B	615	CLA	C10-C11-C12-C13
23	D	403	CLA	C10-C11-C12-C13
26	A	410	SQD	C15-C16-C17-C18
26	F	103	SQD	C30-C31-C32-C33
33	L	101	LHG	C12-C13-C14-C15
32	B	621	LMG	C11-C10-O7-C8
23	c	507	CLA	C15-C16-C17-C18
34	B	622	HTG	C1'-C2'-C3'-C4'
26	F	103	SQD	C24-C25-C26-C27
31	A	421	LMT	C3-C4-C5-C6
31	b	627	LMT	C7-C8-C9-C10
32	B	621	LMG	C34-C35-C36-C37
32	D	411	LMG	C19-C20-C21-C22
32	a	418	LMG	C30-C31-C32-C33
33	L	101	LHG	C17-C18-C19-C20
33	d	411	LHG	C16-C17-C18-C19
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	518	DGD	CAA-CBA-CCA-CDA
31	t	101	LMT	C4'-C5'-C6'-O6'
23	c	510	CLA	C16-C17-C18-C20
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	518	DGD	C9A-CAA-CBA-CCA
23	C	503	CLA	CBD-CGD-O2D-CED
26	f	102	SQD	C32-C33-C34-C35
31	B	631	LMT	C3-C4-C5-C6
32	D	411	LMG	C35-C36-C37-C38
35	C	516	DGD	CCB-CDB-CEB-CFB
35	h	102	DGD	C7B-C8B-C9B-CAB
26	A	412	SQD	C17-C18-C19-C20
32	C	519	LMG	C18-C19-C20-C21
35	c	517	DGD	C2B-C3B-C4B-C5B
35	c	519	DGD	CBB-CCB-CDB-CEB
35	C	515	DGD	C4B-C5B-C6B-C7B
23	c	510	CLA	C3-C5-C6-C7
31	b	621	LMT	C2'-C1'-O1'-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	C	516	DGD	C2E-C1E-O5D-C6D
31	e	101	LMT	C4-C5-C6-C7
32	D	411	LMG	C12-C13-C14-C15
32	m	101	LMG	C35-C36-C37-C38
35	C	515	DGD	C5B-C6B-C7B-C8B
35	c	517	DGD	C9A-CAA-CBA-CCA
23	b	606	CLA	C15-C16-C17-C18
23	a	409	CLA	O1A-CGA-O2A-C1
23	B	603	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	d	402	CLA	C16-C17-C18-C20
29	A	414	PL9	C45-C44-C46-C47
33	D	406	LHG	C16-C17-C18-C19
33	a	421	LHG	C26-C27-C28-C29
33	b	630	LHG	C14-C15-C16-C17
35	h	102	DGD	C9A-CAA-CBA-CCA
29	d	404	PL9	C13-C14-C16-C17
23	B	613	CLA	C11-C12-C13-C14
23	a	407	CLA	C11-C12-C13-C14
32	C	519	LMG	C17-C18-C19-C20
33	D	407	LHG	C32-C33-C34-C35
33	L	101	LHG	C15-C16-C17-C18
32	A	419	LMG	C12-C13-C14-C15
33	d	411	LHG	C32-C33-C34-C35
35	c	518	DGD	CBA-CCA-CDA-CEA
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	O1-C1-C2-C3
27	B	629	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	412	GOL	C1-C2-C3-O3
31	c	501	LMT	C1-C2-C3-C4
32	Z	101	LMG	O6-C5-C6-O5
31	e	101	LMT	C5-C6-C7-C8
33	L	101	LHG	C25-C26-C27-C28
32	a	418	LMG	C10-C11-C12-C13
26	B	620	SQD	C11-C10-C9-C8
31	B	630	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	419	LMG	C17-C18-C19-C20
32	D	411	LMG	C30-C31-C32-C33
32	c	520	LMG	C34-C35-C36-C37
33	A	420	LHG	C34-C35-C36-C37
33	d	405	LHG	C11-C10-C9-C8
35	H	102	DGD	C5B-C6B-C7B-C8B
23	c	508	CLA	C4B-C3B-CAB-CBB
23	B	603	CLA	C16-C17-C18-C20
23	C	502	CLA	C15-C16-C17-C18
26	A	410	SQD	C12-C13-C14-C15
31	B	631	LMT	C11-C10-C9-C8
32	d	410	LMG	C29-C30-C31-C32
35	H	102	DGD	CCB-CDB-CEB-CFB
26	F	103	SQD	C29-C30-C31-C32
31	M	101	LMT	C3-C4-C5-C6
31	t	101	LMT	C4-C5-C6-C7
32	B	621	LMG	C17-C18-C19-C20
32	C	519	LMG	C13-C14-C15-C16
33	L	101	LHG	C13-C14-C15-C16
33	d	405	LHG	C34-C35-C36-C37
31	B	630	LMT	C2-C3-C4-C5
32	m	101	LMG	C39-C40-C41-C42
33	d	406	LHG	C27-C28-C29-C30
32	c	520	LMG	C33-C34-C35-C36
23	C	501	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C5-C6-C7-C8
23	C	502	CLA	C13-C15-C16-C17
31	A	421	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
31	T	101	LMT	C7-C8-C9-C10
32	a	418	LMG	C34-C35-C36-C37
34	b	622	HTG	C3'-C4'-C5'-C6'
23	b	602	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
26	a	413	SQD	C31-C32-C33-C34
32	C	518	LMG	C16-C17-C18-C19
33	A	420	LHG	C12-C13-C14-C15
33	b	630	LHG	C16-C17-C18-C19
32	C	519	LMG	C19-C20-C21-C22
33	E	101	LHG	C24-C25-C26-C27
35	c	517	DGD	O6D-C5D-C6D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	511	CLA	C3-C5-C6-C7
31	A	421	LMT	C1-C2-C3-C4
29	d	404	PL9	C15-C14-C16-C17
35	c	517	DGD	C2A-C1A-O1G-C1G
23	C	505	CLA	C2-C3-C5-C6
29	A	414	PL9	C12-C11-C9-C8
29	A	414	PL9	C43-C44-C46-C47
29	D	405	PL9	C13-C14-C16-C17
32	m	101	LMG	C11-C10-O7-C8
26	b	620	SQD	C13-C14-C15-C16
23	c	508	CLA	C2A-CAA-CBA-CGA
27	B	624	GOL	O2-C2-C3-O3
27	B	629	GOL	O1-C1-C2-O2
27	a	412	GOL	O2-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
26	b	620	SQD	C14-C15-C16-C17
26	f	102	SQD	C25-C26-C27-C28
31	B	631	LMT	C4-C5-C6-C7
32	C	518	LMG	C17-C18-C19-C20
35	c	518	DGD	CBB-CCB-CDB-CEB
31	m	103	LMT	O5'-C5'-C6'-O6'
23	a	409	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	d	402	CLA	C16-C17-C18-C19
23	a	407	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
33	D	407	LHG	C15-C16-C17-C18
35	c	517	DGD	C5A-C6A-C7A-C8A
31	e	101	LMT	C1-C2-C3-C4
32	c	520	LMG	C10-C11-C12-C13
31	b	627	LMT	C3-C4-C5-C6
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	517	DGD	CAA-CBA-CCA-CDA
32	m	101	LMG	O9-C10-O7-C8
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
32	D	411	LMG	C36-C37-C38-C39
33	d	411	LHG	C29-C30-C31-C32
23	C	510	CLA	C10-C11-C12-C13
31	b	627	LMT	C5-C6-C7-C8
32	c	520	LMG	C31-C32-C33-C34
35	c	517	DGD	C7A-C8A-C9A-CAA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C16-C17-C18-C19
32	A	419	LMG	C10-C11-C12-C13
25	D	404	BCR	C23-C24-C25-C26
25	D	404	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
26	a	413	SQD	C25-C26-C27-C28
26	b	620	SQD	C27-C28-C29-C30
35	h	102	DGD	CAA-CBA-CCA-CDA
23	b	614	CLA	C10-C11-C12-C13
35	c	518	DGD	C6A-C7A-C8A-C9A
35	h	102	DGD	C3B-C4B-C5B-C6B
23	C	505	CLA	C4-C3-C5-C6
23	C	510	CLA	C4-C3-C5-C6
23	c	506	CLA	C4-C3-C5-C6
29	A	414	PL9	C30-C29-C31-C32
29	D	405	PL9	C15-C14-C16-C17
23	A	408	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C7
23	C	510	CLA	C2-C3-C5-C6
23	a	407	CLA	C11-C12-C13-C15
23	c	505	CLA	C12-C13-C15-C16
23	c	506	CLA	C2-C3-C5-C6
31	A	421	LMT	C3'-C4'-O1B-C1B
31	B	628	LMT	C3'-C4'-O1B-C1B
40	v	201	HEC	C4C-C3C-CAC-CBC
31	b	621	LMT	C3'-C4'-O1B-C1B
23	C	506	CLA	C5-C6-C7-C8
23	C	502	CLA	C16-C17-C18-C19
23	C	512	CLA	CBA-CGA-O2A-C1
32	A	419	LMG	C13-C14-C15-C16
32	m	101	LMG	C38-C39-C40-C41
33	D	407	LHG	C29-C30-C31-C32
23	b	610	CLA	C2A-CAA-CBA-CGA
31	t	101	LMT	O1'-C1-C2-C3
33	D	406	LHG	C13-C14-C15-C16
35	h	102	DGD	C2B-C3B-C4B-C5B
32	A	419	LMG	C36-C37-C38-C39
35	C	515	DGD	C8A-C9A-CAA-CBA
35	c	517	DGD	O1A-C1A-O1G-C1G
23	c	513	CLA	CBA-CGA-O2A-C1
23	b	606	CLA	C16-C17-C18-C20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
35	C	516	DGD	O6E-C1E-O5D-C6D
23	D	403	CLA	O1D-CGD-O2D-CED
26	A	412	SQD	C26-C27-C28-C29
26	a	411	SQD	C9-C10-C11-C12
26	b	620	SQD	C26-C27-C28-C29
32	A	419	LMG	C19-C20-C21-C22
35	C	517	DGD	C2B-C3B-C4B-C5B
34	B	625	HTG	S1-C1'-C2'-C3'
23	B	601	CLA	C13-C15-C16-C17
23	B	614	CLA	C5-C6-C7-C8
26	B	620	SQD	C34-C35-C36-C37
31	e	101	LMT	C4B-C5B-C6B-O6B
26	A	410	SQD	O6-C44-C45-O47
34	B	622	HTG	C2'-C3'-C4'-C5'
23	c	509	CLA	C16-C17-C18-C20
31	B	630	LMT	C6-C7-C8-C9
35	C	515	DGD	C9A-CAA-CBA-CCA
35	c	518	DGD	C2B-C3B-C4B-C5B
34	b	623	HTG	O5-C5-C6-O6
23	c	514	CLA	C4-C3-C5-C6
32	A	419	LMG	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	505	CLA	C14-C13-C15-C16
35	C	515	DGD	O6E-C5E-C6E-O5E
33	b	630	LHG	C13-C14-C15-C16
32	m	101	LMG	C37-C38-C39-C40
32	z	101	LMG	C19-C20-C21-C22
35	c	519	DGD	CBA-CCA-CDA-CEA
25	d	403	BCR	C21-C22-C23-C24
23	A	405	CLA	C1A-C2A-CAA-CBA
32	d	410	LMG	O6-C5-C6-O5
23	B	610	CLA	C16-C17-C18-C20
23	C	502	CLA	C16-C17-C18-C20
31	b	621	LMT	C11-C10-C9-C8
33	D	407	LHG	C17-C18-C19-C20
23	A	406	CLA	C13-C15-C16-C17
26	b	620	SQD	C24-C23-O48-C46
32	a	418	LMG	C35-C36-C37-C38
32	c	520	LMG	C28-C29-C30-C31
31	B	628	LMT	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	A	419	LMG	C20-C21-C22-C23
23	A	404	CLA	C13-C15-C16-C17
23	B	610	CLA	C16-C17-C18-C19
23	d	401	CLA	C16-C17-C18-C20
33	d	406	LHG	C25-C26-C27-C28
31	B	631	LMT	O1'-C1-C2-C3
31	b	621	LMT	C3-C4-C5-C6
32	a	418	LMG	C29-C30-C31-C32
31	A	421	LMT	C4-C5-C6-C7
32	C	518	LMG	C34-C35-C36-C37
35	c	518	DGD	C4A-C5A-C6A-C7A
26	A	410	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
26	a	411	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
32	a	418	LMG	C7-C8-C9-O8
35	H	102	DGD	C7A-C8A-C9A-CAA
33	E	101	LHG	C25-C26-C27-C28
35	C	516	DGD	C2G-C3G-O3G-C1D
35	C	516	DGD	C5D-C6D-O5D-C1E
35	c	518	DGD	C2G-C3G-O3G-C1D
35	c	518	DGD	C5D-C6D-O5D-C1E
35	C	516	DGD	CDA-CEA-CFA-CGA
26	b	620	SQD	C11-C10-C9-C8
35	C	517	DGD	CAB-CBB-CCB-CDB
35	c	517	DGD	C4D-C5D-C6D-O5D
32	d	410	LMG	C10-C11-C12-C13
23	C	512	CLA	O1A-CGA-O2A-C1
35	C	515	DGD	C3B-C4B-C5B-C6B
34	c	522	HTG	C4'-C5'-C6'-C7'
27	A	411	GOL	O1-C1-C2-O2
27	B	629	GOL	O2-C2-C3-O3
27	O	303	GOL	O1-C1-C2-O2
27	o	302	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
23	A	405	CLA	C15-C16-C17-C18
35	c	517	DGD	O6E-C5E-C6E-O5E
29	a	415	PL9	C12-C11-C9-C10
23	B	615	CLA	C16-C17-C18-C19
35	h	102	DGD	CDB-CEB-CFB-CGB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C10-C11-C12-C13
31	B	628	LMT	C1-C2-C3-C4
34	b	623	HTG	S1-C1'-C2'-C3'
23	a	406	CLA	C2C-C3C-CAC-CBC
33	d	411	LHG	C33-C34-C35-C36
26	b	620	SQD	C46-C45-O47-C7
32	D	411	LMG	O6-C5-C6-O5
23	b	601	CLA	C8-C10-C11-C12
23	C	509	CLA	C2-C1-O2A-CGA
33	d	406	LHG	C34-C35-C36-C37
26	a	411	SQD	C12-C13-C14-C15
31	c	501	LMT	C3-C4-C5-C6
33	D	406	LHG	C12-C13-C14-C15
23	C	513	CLA	O1D-CGD-O2D-CED
26	B	620	SQD	C30-C31-C32-C33
31	c	501	LMT	C2-C3-C4-C5
23	B	615	CLA	C16-C17-C18-C20
23	B	613	CLA	C13-C15-C16-C17
23	B	610	CLA	C13-C15-C16-C17
23	b	601	CLA	C13-C15-C16-C17
35	h	102	DGD	C9B-CAB-CBB-CCB
35	C	515	DGD	O6D-C5D-C6D-O5D
23	c	513	CLA	C13-C15-C16-C17
23	d	401	CLA	C16-C17-C18-C19
33	d	406	LHG	C29-C30-C31-C32
23	a	409	CLA	C4-C3-C5-C6
23	b	604	CLA	C15-C16-C17-C18
23	A	406	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	510	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	606	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C12-C13-C15
23	B	602	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	C	510	CLA	C14-C13-C15-C16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C11-C10-C8-C9
23	D	403	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	c	506	CLA	C11-C12-C13-C14
23	d	402	CLA	C11-C12-C13-C14
32	A	419	LMG	C39-C40-C41-C42
33	d	406	LHG	C28-C29-C30-C31
23	B	601	CLA	CBA-CGA-O2A-C1
35	C	517	DGD	CAA-CBA-CCA-CDA
23	c	513	CLA	O1A-CGA-O2A-C1
26	a	413	SQD	C16-C17-C18-C19
31	c	501	LMT	C9-C10-C11-C12
31	e	101	LMT	C9-C10-C11-C12
32	B	621	LMG	C36-C37-C38-C39
33	b	630	LHG	C27-C28-C29-C30
26	b	620	SQD	O10-C23-O48-C46
23	c	512	CLA	CBA-CGA-O2A-C1
26	F	103	SQD	C7-C8-C9-C10
32	C	518	LMG	C36-C37-C38-C39
32	m	101	LMG	C14-C15-C16-C17
35	C	516	DGD	C5B-C6B-C7B-C8B
23	A	406	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C4B-C3B-CAB-CBB
23	a	407	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
33	E	101	LHG	O6-C4-C5-C6
33	b	630	LHG	O6-C4-C5-C6
33	D	406	LHG	C10-C11-C12-C13
33	D	407	LHG	C13-C14-C15-C16
33	d	406	LHG	C9-C10-C11-C12
35	H	102	DGD	CAB-CBB-CCB-CDB
32	C	518	LMG	C31-C32-C33-C34
31	A	417	LMT	O5B-C5B-C6B-O6B
23	c	511	CLA	C4-C3-C5-C6
29	d	404	PL9	C45-C44-C46-C47
23	c	511	CLA	C2-C3-C5-C6
32	z	101	LMG	C10-C11-C12-C13
32	C	518	LMG	C37-C38-C39-C40
33	A	420	LHG	C26-C27-C28-C29
33	d	405	LHG	C13-C14-C15-C16
26	b	620	SQD	C31-C32-C33-C34
35	C	515	DGD	C7A-C8A-C9A-CAA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	c	514	CLA	O1D-CGD-O2D-CED
23	c	507	CLA	C3A-C2A-CAA-CBA
35	h	102	DGD	CAB-CBB-CCB-CDB
31	e	101	LMT	C2-C1-O1'-C1'
23	B	612	CLA	C10-C11-C12-C13
35	c	518	DGD	CDA-CEA-CFA-CGA
26	a	413	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
33	a	421	LHG	C4-C5-C6-O8
33	L	101	LHG	C24-C25-C26-C27
33	a	421	LHG	C10-C11-C12-C13
31	M	101	LMT	O1'-C1-C2-C3
33	b	630	LHG	C12-C13-C14-C15
24	a	408	PHO	O2A-C1-C2-C3
23	B	602	CLA	C15-C16-C17-C18
31	e	101	LMT	C3-C4-C5-C6
32	A	419	LMG	C29-C30-C31-C32
26	A	412	SQD	C27-C28-C29-C30
35	c	518	DGD	C5A-C6A-C7A-C8A
24	a	408	PHO	C4-C3-C5-C6
29	D	405	PL9	C43-C44-C46-C47
32	B	621	LMG	C20-C21-C22-C23
33	L	101	LHG	C11-C12-C13-C14
33	a	421	LHG	C7-C8-C9-C10
34	B	625	HTG	C4'-C5'-C6'-C7'
23	C	512	CLA	O1D-CGD-O2D-CED
26	F	103	SQD	C32-C33-C34-C35
31	m	103	LMT	C7-C8-C9-C10
33	E	101	LHG	O6-C4-C5-O7
32	C	519	LMG	C12-C13-C14-C15
23	B	601	CLA	O1A-CGA-O2A-C1
23	A	406	CLA	C16-C17-C18-C20
33	b	630	LHG	C31-C32-C33-C34
23	b	606	CLA	C2B-C3B-CAB-CBB
26	a	411	SQD	C34-C35-C36-C37
26	a	411	SQD	O6-C44-C45-O47
26	f	102	SQD	O47-C45-C46-O48
26	F	103	SQD	C24-C23-O48-C46
23	C	503	CLA	O1D-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
23	b	601	CLA	CAA-CBA-CGA-O2A
35	C	516	DGD	C8B-C9B-CAB-CBB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	z	101	LMG	C14-C15-C16-C17
33	E	101	LHG	C17-C18-C19-C20
23	b	610	CLA	C15-C16-C17-C18
29	a	415	PL9	C24-C26-C27-C28
33	D	407	LHG	C10-C11-C12-C13
35	h	102	DGD	CBA-CCA-CDA-CEA
23	b	608	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
32	d	410	LMG	C11-C12-C13-C14
23	C	513	CLA	C6-C7-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	c	503	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
35	C	517	DGD	CDB-CEB-CFB-CGB
23	C	510	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	c	512	CLA	O1A-CGA-O2A-C1
26	F	103	SQD	C34-C35-C36-C37
35	C	516	DGD	C8A-C9A-CAA-CBA
23	B	601	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C5-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	d	403	BCR	C23-C24-C25-C26
25	d	403	BCR	C23-C24-C25-C30
23	B	601	CLA	C15-C16-C17-C18
32	C	519	LMG	C35-C36-C37-C38
25	D	404	BCR	C37-C22-C23-C24
33	d	411	LHG	C25-C26-C27-C28
25	D	404	BCR	C21-C22-C23-C24
23	c	508	CLA	C5-C6-C7-C8
26	b	620	SQD	C33-C34-C35-C36
23	C	511	CLA	C8-C10-C11-C12
32	z	101	LMG	C20-C21-C22-C23
35	H	102	DGD	CCA-CDA-CEA-CFA
31	t	101	LMT	C7-C8-C9-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	614	CLA	C12-C13-C15-C16
23	C	502	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C15
23	C	506	CLA	C6-C7-C8-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C15
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
24	a	408	PHO	C2-C3-C5-C6
31	F	101	LMT	C2-C3-C4-C5
23	c	510	CLA	C15-C16-C17-C18
23	b	606	CLA	C16-C17-C18-C19
33	L	101	LHG	C11-C10-C9-C8
33	d	411	LHG	C24-C25-C26-C27
33	b	630	LHG	C34-C35-C36-C37
26	b	620	SQD	C28-C29-C30-C31
35	C	515	DGD	CCA-CDA-CEA-CFA
33	b	630	LHG	C9-C10-C11-C12
34	c	522	HTG	C2'-C1'-S1-C1
23	C	510	CLA	CBA-CGA-O2A-C1
23	b	601	CLA	CBA-CGA-O2A-C1
31	b	627	LMT	C6-C7-C8-C9
32	a	418	LMG	C21-C22-C23-C24
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407	PHO	CAD-CBD-CGD-O2D
24	a	408	PHO	CAD-CBD-CGD-O2D
26	B	620	SQD	C46-C45-O47-C7
38	F	102	HEM	C2B-C3B-CAB-CBB
38	f	101	HEM	C2C-C3C-CAC-CBC
34	B	625	HTG	C4-C5-C6-O6
31	F	101	LMT	C4-C5-C6-C7
33	E	101	LHG	C13-C14-C15-C16
26	a	411	SQD	C27-C28-C29-C30
26	A	412	SQD	C24-C23-O48-C46
32	c	521	LMG	C29-C28-O8-C9
35	c	519	DGD	C2A-C1A-O1G-C1G
33	D	406	LHG	C34-C35-C36-C37
33	E	101	LHG	C4-C5-C6-O8
33	b	630	LHG	O6-C4-C5-O7
35	C	516	DGD	C7A-C8A-C9A-CAA
23	B	601	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	C	506	CLA	C15-C16-C17-C18
23	B	607	CLA	C3-C5-C6-C7
23	C	510	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	O47-C45-C46-O48
32	a	418	LMG	O7-C8-C9-O8
33	a	421	LHG	O7-C5-C6-O8
27	B	624	GOL	O1-C1-C2-O2
27	B	627	GOL	O1-C1-C2-O2
27	c	527	GOL	O1-C1-C2-O2
31	A	421	LMT	C5-C6-C7-C8
32	C	518	LMG	C29-C30-C31-C32
29	D	405	PL9	C45-C44-C46-C47
26	B	620	SQD	C24-C25-C26-C27
35	c	518	DGD	C1A-C2A-C3A-C4A
35	C	517	DGD	C8A-C9A-CAA-CBA
23	B	611	CLA	C11-C12-C13-C14
35	C	515	DGD	C4D-C5D-C6D-O5D
23	b	601	CLA	O1A-CGA-O2A-C1
26	F	103	SQD	O10-C23-O48-C46
35	c	519	DGD	O1A-C1A-O1G-C1G
23	b	612	CLA	C8-C10-C11-C12
32	B	621	LMG	C29-C30-C31-C32
23	a	405	CLA	C2C-C3C-CAC-CBC
25	Y	101	BCR	C21-C22-C23-C24
23	a	406	CLA	C1A-C2A-CAA-CBA
33	d	406	LHG	C24-C23-O8-C6
33	A	420	LHG	C32-C33-C34-C35
35	c	519	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	C6A-C7A-C8A-C9A
31	b	627	LMT	C1-C2-C3-C4
33	D	406	LHG	C4-O6-P-O3
33	d	411	LHG	C3-O3-P-O6
33	a	421	LHG	C23-C24-C25-C26
26	a	411	SQD	C35-C36-C37-C38
23	c	505	CLA	C4-C3-C5-C6
33	D	407	LHG	C2-C3-O3-P
33	d	406	LHG	C2-C3-O3-P
32	C	519	LMG	C4-C5-C6-O5
31	b	621	LMT	C7-C8-C9-C10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	c	521	LMG	O10-C28-O8-C9
23	C	512	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
33	D	406	LHG	C4-O6-P-O5
33	E	101	LHG	C4-O6-P-O5
33	a	421	LHG	C4-O6-P-O4
33	d	405	LHG	C3-O3-P-O4
35	C	517	DGD	C7B-C8B-C9B-CAB
31	c	501	LMT	O5'-C1'-O1'-C1
35	c	517	DGD	O6E-C1E-O5D-C6D
23	B	606	CLA	C15-C16-C17-C18
23	b	615	CLA	C10-C11-C12-C13
23	c	507	CLA	C10-C11-C12-C13
33	L	101	LHG	O6-C4-C5-C6
26	A	410	SQD	C18-C19-C20-C21
23	C	509	CLA	C3-C5-C6-C7
23	B	606	CLA	C16-C17-C18-C19
33	d	411	LHG	C27-C28-C29-C30
35	C	517	DGD	CDA-CEA-CFA-CGA
35	c	517	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
31	M	101	LMT	C2-C3-C4-C5
35	h	102	DGD	CDA-CEA-CFA-CGA
26	A	412	SQD	O10-C23-O48-C46
40	V	201	HEC	C4B-C3B-CAB-CBB
31	M	101	LMT	O5'-C5'-C6'-O6'
33	D	407	LHG	C24-C23-O8-C6
33	E	101	LHG	C1-C2-C3-O3
23	C	501	CLA	C16-C17-C18-C20
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	616	CLA	C6-C7-C8-C10
23	c	506	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C7
23	c	510	CLA	C6-C7-C8-C10
33	d	406	LHG	O10-C23-O8-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CAA-CBA-CGA-O2A
32	c	520	LMG	C29-C30-C31-C32
35	C	516	DGD	C1A-C2A-C3A-C4A
35	C	517	DGD	C6A-C7A-C8A-C9A
33	D	407	LHG	O10-C23-O8-C6
35	c	517	DGD	C8B-C9B-CAB-CBB
26	A	410	SQD	C34-C35-C36-C37
26	B	620	SQD	O47-C45-C46-O48
33	E	101	LHG	O7-C5-C6-O8
26	A	412	SQD	C30-C31-C32-C33
26	a	413	SQD	C26-C27-C28-C29
26	a	411	SQD	C11-C12-C13-C14
23	c	514	CLA	C2-C3-C5-C6
35	H	102	DGD	O2G-C1B-C2B-C3B
23	A	406	CLA	C14-C13-C15-C16
23	B	603	CLA	C11-C12-C13-C14
23	B	610	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C9
23	D	403	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	510	CLA	C8-C10-C11-C12
32	Z	101	LMG	C11-C12-C13-C14
23	d	402	CLA	O1A-CGA-O2A-C1
24	a	408	PHO	C8-C10-C11-C12
25	K	103	BCR	C7-C8-C9-C34
25	Y	101	BCR	C37-C22-C23-C24
23	C	506	CLA	C16-C17-C18-C20
23	A	406	CLA	C2B-C3B-CAB-CBB
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	505	CLA	C2B-C3B-CAB-CBB
34	b	622	HTG	C1'-C2'-C3'-C4'
29	a	415	PL9	C12-C11-C9-C8
23	c	507	CLA	C13-C15-C16-C17
33	d	411	LHG	C34-C35-C36-C37
23	B	611	CLA	C8-C10-C11-C12
26	B	620	SQD	C29-C30-C31-C32
33	d	406	LHG	C32-C33-C34-C35
23	b	601	CLA	C3-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	501	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
26	A	410	SQD	C16-C17-C18-C19
23	B	606	CLA	C8-C10-C11-C12
32	C	518	LMG	C30-C31-C32-C33
33	d	405	LHG	O10-C23-O8-C6
33	L	101	LHG	O6-C4-C5-O7
31	B	628	LMT	C9-C10-C11-C12
23	C	512	CLA	C3-C5-C6-C7
29	A	414	PL9	C28-C29-C31-C32
33	d	405	LHG	C24-C23-O8-C6
23	a	406	CLA	C4C-C3C-CAC-CBC
23	b	602	CLA	C10-C11-C12-C13
26	A	412	SQD	O5-C1-O6-C44
35	c	518	DGD	O6E-C1E-O5D-C6D
35	C	515	DGD	C6A-C7A-C8A-C9A
23	b	612	CLA	C10-C11-C12-C13
26	A	412	SQD	C2-C1-O6-C44
31	c	501	LMT	C2'-C1'-O1'-C1
35	c	517	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	C2E-C1E-O5D-C6D
33	L	101	LHG	C26-C27-C28-C29
23	c	510	CLA	C10-C11-C12-C13
33	L	101	LHG	C27-C28-C29-C30
23	a	409	CLA	C15-C16-C17-C18
23	B	603	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	a	409	CLA	C2-C3-C5-C6
23	b	608	CLA	C12-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	C	510	CLA	C11-C12-C13-C14
23	a	409	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	B	606	CLA	C16-C17-C18-C20
32	a	418	LMG	C31-C32-C33-C34
23	c	508	CLA	C8-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	a	405	CLA	C4C-C3C-CAC-CBC
32	a	418	LMG	O8-C28-C29-C30
33	D	407	LHG	C27-C28-C29-C30
23	B	613	CLA	C15-C16-C17-C18
35	c	517	DGD	C4B-C5B-C6B-C7B
33	d	411	LHG	C1-C2-C3-O3
34	b	622	HTG	O5-C5-C6-O6
23	B	603	CLA	C4-C3-C5-C6
32	d	410	LMG	C28-C29-C30-C31
27	o	303	GOL	O1-C1-C2-O2
35	H	102	DGD	CDB-CEB-CFB-CGB
23	d	402	CLA	CBA-CGA-O2A-C1
31	b	627	LMT	O1'-C1-C2-C3
31	c	501	LMT	C7-C8-C9-C10
33	d	406	LHG	C33-C34-C35-C36
23	C	504	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	505	CLA	C4B-C3B-CAB-CBB
23	C	507	CLA	C2A-CAA-CBA-CGA
35	c	519	DGD	CDA-CEA-CFA-CGA
38	F	102	HEM	CAD-CBD-CGD-O1D
32	d	410	LMG	C35-C36-C37-C38
23	b	609	CLA	C2-C3-C5-C6
26	A	410	SQD	C11-C10-C9-C8
32	z	101	LMG	C13-C14-C15-C16
33	b	630	LHG	C25-C26-C27-C28
23	B	608	CLA	C2-C1-O2A-CGA
23	C	513	CLA	C2-C1-O2A-CGA
23	c	504	CLA	C8-C10-C11-C12
23	c	503	CLA	C16-C17-C18-C19
33	D	406	LHG	C11-C10-C9-C8
32	Z	101	LMG	C2-C1-O1-C7
38	f	101	HEM	CAD-CBD-CGD-O1D
26	F	103	SQD	O47-C45-C46-O48
33	a	421	LHG	C24-C25-C26-C27
31	e	101	LMT	C2B-C1B-O1B-C4'
32	B	621	LMG	C32-C33-C34-C35
23	b	601	CLA	C4-C3-C5-C6
29	a	415	PL9	C4-C3-C7-C8
35	h	102	DGD	CCB-CDB-CEB-CFB
32	B	621	LMG	O8-C28-C29-C30
23	A	408	CLA	C11-C12-C13-C14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	C6-C7-C8-C9
23	C	512	CLA	C6-C7-C8-C9
23	a	407	CLA	C6-C7-C8-C9
23	b	616	CLA	C11-C10-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	B	605	CLA	C5-C6-C7-C8
35	c	518	DGD	C7B-C8B-C9B-CAB
32	A	419	LMG	C7-C8-C9-O8
32	B	621	LMG	C14-C15-C16-C17
32	Z	101	LMG	C19-C20-C21-C22
33	L	101	LHG	C23-C24-C25-C26
23	c	512	CLA	C8-C10-C11-C12
32	C	519	LMG	C20-C21-C22-C23
35	H	102	DGD	C8A-C9A-CAA-CBA
32	B	621	LMG	O6-C1-O1-C7
23	a	406	CLA	C15-C16-C17-C18
31	A	417	LMT	C7-C8-C9-C10
26	A	410	SQD	C13-C14-C15-C16
32	d	410	LMG	C18-C19-C20-C21
35	C	517	DGD	C7A-C8A-C9A-CAA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
35	c	519	DGD	CDB-CEB-CFB-CGB
23	C	513	CLA	C11-C12-C13-C15
23	b	601	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7
23	b	614	CLA	C11-C10-C8-C7
23	c	513	CLA	C12-C13-C15-C16
23	A	404	CLA	C2C-C3C-CAC-CBC
33	A	420	LHG	C18-C19-C20-C21
33	b	630	LHG	C17-C18-C19-C20
31	B	631	LMT	C6-C7-C8-C9
32	a	418	LMG	C13-C14-C15-C16
38	f	101	HEM	CAD-CBD-CGD-O2D
40	V	201	HEC	CAD-CBD-CGD-O1D
23	C	510	CLA	C8-C10-C11-C12
26	a	413	SQD	C24-C23-O48-C46
33	D	406	LHG	C26-C27-C28-C29
33	d	405	LHG	C16-C17-C18-C19
23	b	616	CLA	C4-C3-C5-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	d	404	PL9	C43-C44-C46-C47
23	c	502	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C2B-C3B-CAB-CBB
35	c	519	DGD	O6D-C5D-C6D-O5D
38	F	102	HEM	CAD-CBD-CGD-O2D
34	B	622	HTG	C3'-C4'-C5'-C6'
40	v	201	HEC	C2B-C3B-CAB-CBB
32	z	101	LMG	O7-C10-C11-C12
25	t	102	BCR	C13-C14-C15-C16
23	b	613	CLA	C5-C6-C7-C8
31	T	101	LMT	C3-C4-C5-C6
26	f	102	SQD	C7-C8-C9-C10
23	A	406	CLA	C16-C17-C18-C19
32	B	621	LMG	C21-C22-C23-C24
26	a	413	SQD	O10-C23-O48-C46
29	A	414	PL9	C39-C41-C42-C43
32	Z	101	LMG	C29-C28-O8-C9
29	a	415	PL9	C45-C44-C46-C47
23	b	613	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C3-C5-C6
31	A	417	LMT	C2B-C1B-O1B-C4'
40	V	201	HEC	CAD-CBD-CGD-O2D
32	A	419	LMG	C18-C19-C20-C21
33	A	420	LHG	C29-C30-C31-C32
35	c	517	DGD	CAB-CBB-CCB-CDB
23	b	608	CLA	C16-C17-C18-C20
35	C	517	DGD	C3B-C4B-C5B-C6B
25	c	515	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
35	C	517	DGD	C4A-C5A-C6A-C7A
27	A	418	GOL	O1-C1-C2-C3
27	l	102	GOL	O1-C1-C2-C3
27	v	202	GOL	O1-C1-C2-C3
32	d	410	LMG	C19-C20-C21-C22
29	D	405	PL9	C35-C34-C36-C37
25	K	103	BCR	C7-C8-C9-C10
25	y	101	BCR	C21-C22-C23-C24
23	b	605	CLA	C5-C6-C7-C8
23	b	616	CLA	C5-C6-C7-C8
29	a	415	PL9	C43-C44-C46-C47
35	h	102	DGD	O2G-C1B-C2B-C3B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
38	f	101	HEM	CAA-CBA-CGA-O2A
26	B	620	SQD	C31-C32-C33-C34
23	A	404	CLA	C16-C17-C18-C19
32	m	101	LMG	C32-C33-C34-C35
33	A	420	LHG	C35-C36-C37-C38
31	F	101	LMT	C9-C10-C11-C12
23	c	503	CLA	C4B-C3B-CAB-CBB
33	b	630	LHG	C10-C11-C12-C13
35	C	517	DGD	C9A-CAA-CBA-CCA
23	B	613	CLA	C11-C10-C8-C7
23	a	407	CLA	C6-C7-C8-C10
23	c	509	CLA	C12-C13-C15-C16
23	D	403	CLA	C8-C10-C11-C12
33	L	101	LHG	C16-C17-C18-C19
27	A	418	GOL	O1-C1-C2-O2
23	b	607	CLA	C3-C5-C6-C7
23	D	403	CLA	O1A-CGA-O2A-C1
31	T	101	LMT	C1-C2-C3-C4
23	C	512	CLA	CAA-CBA-CGA-O2A
32	B	621	LMG	C2-C1-O1-C7
32	m	101	LMG	C2-C1-O1-C7
26	a	413	SQD	C18-C19-C20-C21
31	e	101	LMT	C2-C3-C4-C5
32	d	410	LMG	C16-C17-C18-C19
23	b	611	CLA	C13-C15-C16-C17
31	B	630	LMT	C3-C4-C5-C6
33	A	420	LHG	O8-C23-C24-C25
23	c	512	CLA	CBD-CGD-O2D-CED
23	B	603	CLA	C2-C3-C5-C6
23	c	505	CLA	C2-C3-C5-C6
35	c	518	DGD	C9B-CAB-CBB-CCB
35	h	102	DGD	CCA-CDA-CEA-CFA
23	B	616	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	a	407	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C3A-C2A-CAA-CBA
23	B	613	CLA	CAA-CBA-CGA-O2A
32	a	418	LMG	C33-C34-C35-C36
40	v	201	HEC	CAD-CBD-CGD-O2D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
24	a	417	PHO	CAD-CBD-CGD-O2D
33	D	407	LHG	C28-C29-C30-C31
33	b	630	LHG	C30-C31-C32-C33
32	Z	101	LMG	O7-C10-C11-C12
33	L	101	LHG	O7-C7-C8-C9
33	a	421	LHG	O8-C23-C24-C25
23	b	609	CLA	C4-C3-C5-C6
29	A	414	PL9	C25-C24-C26-C27
23	b	605	CLA	C3-C5-C6-C7
32	B	621	LMG	C30-C31-C32-C33
32	c	520	LMG	C32-C33-C34-C35
23	b	616	CLA	C2-C3-C5-C6
32	c	520	LMG	C30-C31-C32-C33
32	B	621	LMG	O1-C7-C8-C9
23	b	610	CLA	C13-C15-C16-C17
33	b	630	LHG	O7-C7-C8-C9
26	b	620	SQD	C30-C31-C32-C33
31	F	101	LMT	C6-C7-C8-C9
38	f	101	HEM	CAA-CBA-CGA-O1A
23	A	404	CLA	C15-C16-C17-C18
23	B	602	CLA	O2A-C1-C2-C3
24	A	407	PHO	O2A-C1-C2-C3
23	A	404	CLA	C4C-C3C-CAC-CBC
38	F	102	HEM	C4B-C3B-CAB-CBB
40	v	201	HEC	CAD-CBD-CGD-O1D
35	C	517	DGD	CBA-CCA-CDA-CEA
23	C	506	CLA	C16-C17-C18-C19
26	f	102	SQD	C26-C27-C28-C29
23	A	405	CLA	CHA-CBD-CGD-O1D
23	A	405	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	a	406	CLA	CHA-CBD-CGD-O1D
23	a	406	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O2D
31	A	417	LMT	O5B-C1B-O1B-C4'
23	B	608	CLA	C16-C17-C18-C20
23	C	510	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
32	c	520	LMG	O7-C10-C11-C12
26	b	620	SQD	C10-C11-C12-C13
33	A	420	LHG	C17-C18-C19-C20
33	d	411	LHG	C13-C14-C15-C16
32	c	521	LMG	O1-C7-C8-O7
35	C	516	DGD	CAB-CBB-CCB-CDB
23	c	513	CLA	CAA-CBA-CGA-O2A
26	a	413	SQD	C15-C16-C17-C18
24	A	407	PHO	CHA-CBD-CGD-O1D
23	b	601	CLA	CAA-CBA-CGA-O1A
23	B	607	CLA	C12-C13-C15-C16
23	a	406	CLA	C11-C12-C13-C15
23	b	610	CLA	C16-C17-C18-C19
29	A	414	PL9	C4-C3-C7-C8
31	A	417	LMT	C9-C10-C11-C12
23	B	605	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	b	608	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	B	612	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	O1A-CGA-O2A-C1
33	d	411	LHG	C18-C19-C20-C21
23	B	602	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	C	503	CLA	C2A-CAA-CBA-CGA
33	b	630	LHG	C24-C25-C26-C27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
34	b	623	HTG	C4'-C5'-C6'-C7'
23	b	604	CLA	C13-C15-C16-C17
32	d	410	LMG	C40-C41-C42-C43
27	B	627	GOL	C1-C2-C3-O3
27	b	629	GOL	C1-C2-C3-O3
27	c	527	GOL	O1-C1-C2-C3
27	l	102	GOL	C1-C2-C3-O3
29	D	405	PL9	C28-C29-C31-C32
23	C	512	CLA	CAA-CBA-CGA-O1A
25	b	619	BCR	C21-C22-C23-C24
23	D	403	CLA	CBA-CGA-O2A-C1
23	b	616	CLA	CBA-CGA-O2A-C1
23	c	507	CLA	C1A-C2A-CAA-CBA
32	Z	101	LMG	O9-C10-C11-C12
33	A	420	LHG	O10-C23-C24-C25
23	b	616	CLA	O1A-CGA-O2A-C1
26	A	412	SQD	C31-C32-C33-C34
23	b	603	CLA	C5-C6-C7-C8
33	a	421	LHG	O10-C23-C24-C25
33	b	630	LHG	O9-C7-C8-C9
26	F	103	SQD	C44-C45-C46-O48
35	c	517	DGD	O2G-C1B-C2B-C3B
23	b	602	CLA	C2A-CAA-CBA-CGA
23	B	613	CLA	CAA-CBA-CGA-O1A
26	f	102	SQD	C34-C35-C36-C37
33	E	101	LHG	O7-C7-C8-C9
23	c	506	CLA	C4B-C3B-CAB-CBB
33	d	405	LHG	C4-O6-P-O5
23	A	408	CLA	C16-C17-C18-C19
23	b	610	CLA	C16-C17-C18-C20
23	c	511	CLA	O1A-CGA-O2A-C1
32	A	419	LMG	C15-C16-C17-C18
25	K	101	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C26
25	y	101	BCR	C23-C24-C25-C26
32	c	520	LMG	O9-C10-C11-C12
33	L	101	LHG	O9-C7-C8-C9
32	D	411	LMG	C34-C35-C36-C37
23	c	503	CLA	C16-C17-C18-C20
24	A	416	PHO	C2C-C3C-CAC-CBC
35	c	517	DGD	C1A-C2A-C3A-C4A
23	c	513	CLA	CAA-CBA-CGA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
25	a	410	BCR	C19-C20-C21-C22
31	c	501	LMT	C4-C5-C6-C7
32	a	418	LMG	C14-C15-C16-C17
29	d	404	PL9	C11-C12-C13-C14
32	c	520	LMG	C4-C5-C6-O5
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
26	a	411	SQD	C10-C11-C12-C13
23	b	613	CLA	CAA-CBA-CGA-O2A
23	b	608	CLA	C13-C15-C16-C17
23	B	607	CLA	C14-C13-C15-C16
23	B	615	CLA	C14-C13-C15-C16
23	C	512	CLA	C11-C10-C8-C9
23	a	406	CLA	C11-C12-C13-C14
23	B	612	CLA	C8-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
35	C	517	DGD	O1A-C1A-O1G-C1G
32	B	621	LMG	C37-C38-C39-C40
32	D	411	LMG	C16-C17-C18-C19
26	A	412	SQD	O48-C23-C24-C25
26	a	413	SQD	O48-C23-C24-C25
33	D	407	LHG	O8-C23-C24-C25
35	C	517	DGD	O1G-C1A-C2A-C3A
32	d	410	LMG	C38-C39-C40-C41
32	D	411	LMG	O7-C10-C11-C12
26	a	411	SQD	C19-C20-C21-C22
31	B	630	LMT	C7-C8-C9-C10
29	D	405	PL9	C40-C39-C41-C42
23	b	604	CLA	C10-C11-C12-C13
32	B	621	LMG	C18-C19-C20-C21
35	c	517	DGD	CBA-CCA-CDA-CEA
23	B	601	CLA	C11-C12-C13-C15
23	B	602	CLA	C6-C7-C8-C10
23	B	605	CLA	C11-C12-C13-C15
23	C	501	CLA	C11-C12-C13-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C12-C13-C15-C16
23	b	615	CLA	C11-C12-C13-C15
23	c	511	CLA	C12-C13-C15-C16
33	E	101	LHG	O8-C23-C24-C25
35	C	516	DGD	O2G-C1B-C2B-C3B
33	D	406	LHG	C28-C29-C30-C31
25	d	403	BCR	C7-C8-C9-C10
33	D	407	LHG	O10-C23-C24-C25
35	c	517	DGD	O1B-C1B-C2B-C3B
35	C	516	DGD	C3A-C4A-C5A-C6A
31	B	628	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
32	m	101	LMG	O6-C1-O1-C7
23	C	510	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
26	a	413	SQD	O10-C23-C24-C25
32	D	411	LMG	O9-C10-C11-C12
26	A	412	SQD	O10-C23-C24-C25
33	E	101	LHG	O9-C7-C8-C9
33	E	101	LHG	O10-C23-C24-C25
23	b	602	CLA	C8-C10-C11-C12
35	C	516	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

147 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	628	GOL	2	0
26	f	102	SQD	1	0
23	c	514	CLA	3	0
27	O	303	GOL	2	0
23	C	507	CLA	2	0
23	c	504	CLA	3	0
23	C	502	CLA	2	0
25	h	101	BCR	3	0
32	z	101	LMG	2	0
31	e	101	LMT	1	0
35	C	516	DGD	2	0
23	C	509	CLA	1	0
23	B	604	CLA	2	0
23	C	511	CLA	1	0
23	d	401	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	617	BCR	2	0
25	K	101	BCR	3	0
26	b	620	SQD	2	0
35	h	102	DGD	1	0
25	D	404	BCR	3	0
23	C	508	CLA	4	0
25	Y	101	BCR	2	0
31	t	101	LMT	2	0
23	a	406	CLA	2	0
23	A	404	CLA	5	0
31	B	631	LMT	1	0
23	c	512	CLA	5	0
34	c	522	HTG	1	0
26	B	620	SQD	1	0
25	b	619	BCR	3	0
23	C	512	CLA	1	0
23	b	616	CLA	1	0
25	t	102	BCR	5	0
23	b	601	CLA	3	0
23	C	505	CLA	5	0
33	A	420	LHG	2	0
23	b	609	CLA	3	0
23	C	506	CLA	4	0
23	B	605	CLA	5	0
24	A	407	PHO	2	0
25	B	619	BCR	1	0
25	T	102	BCR	7	0
25	b	617	BCR	1	0
27	a	419	GOL	1	0
23	B	616	CLA	4	0
23	B	614	CLA	1	0
40	V	201	HEC	1	0
23	B	610	CLA	2	0
23	b	615	CLA	2	0
32	Z	101	LMG	2	0
24	A	416	PHO	1	0
26	A	412	SQD	1	0
23	A	406	CLA	1	0
31	A	421	LMT	1	0
23	b	613	CLA	1	0
23	c	503	CLA	2	0
35	H	102	DGD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	D	406	LHG	2	0
25	d	403	BCR	2	0
23	b	607	CLA	2	0
33	d	406	LHG	9	0
23	C	513	CLA	2	0
23	C	504	CLA	1	0
26	A	410	SQD	2	0
27	A	418	GOL	3	0
34	b	625	HTG	1	0
32	c	520	LMG	1	0
26	a	411	SQD	4	0
27	b	629	GOL	1	0
23	c	513	CLA	5	0
23	c	506	CLA	6	0
23	c	505	CLA	3	0
23	C	501	CLA	5	0
23	A	405	CLA	4	0
35	c	517	DGD	2	0
23	c	510	CLA	2	0
31	M	101	LMT	1	0
31	b	621	LMT	1	0
35	C	515	DGD	2	0
33	E	101	LHG	4	0
32	c	521	LMG	1	0
23	C	503	CLA	3	0
27	B	627	GOL	1	0
32	B	621	LMG	1	0
25	c	515	BCR	4	0
31	c	501	LMT	2	0
31	B	630	LMT	1	0
23	B	602	CLA	1	0
23	B	612	CLA	4	0
26	a	413	SQD	1	0
23	B	613	CLA	3	0
31	A	417	LMT	1	0
23	c	502	CLA	3	0
23	B	606	CLA	4	0
25	y	101	BCR	2	0
35	c	519	DGD	2	0
31	B	628	LMT	1	0
23	b	602	CLA	1	0
23	c	509	CLA	4	0

Continued on next page...

Continued from previous page...

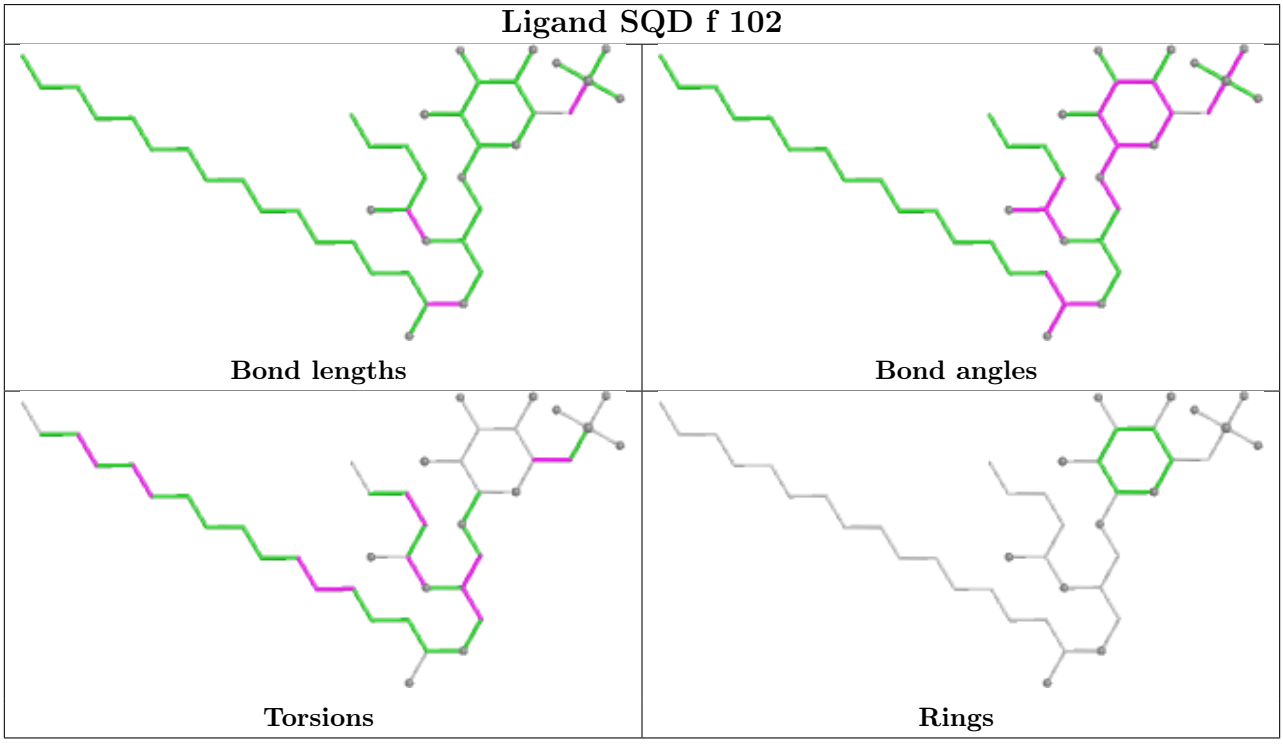
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	103	BCR	1	0
35	c	518	DGD	1	0
23	C	510	CLA	3	0
26	F	103	SQD	2	0
27	B	629	GOL	2	0
34	B	622	HTG	2	0
32	d	410	LMG	2	0
38	F	102	HEM	1	0
32	C	519	LMG	4	0
27	O	302	GOL	1	0
33	a	421	LHG	4	0
34	B	625	HTG	1	0
29	A	414	PL9	10	0
23	B	601	CLA	2	0
33	d	405	LHG	3	0
27	v	202	GOL	1	0
25	a	410	BCR	2	0
33	D	407	LHG	5	0
25	b	618	BCR	3	0
27	l	102	GOL	1	0
23	c	508	CLA	3	0
34	b	622	HTG	2	0
25	B	618	BCR	2	0
25	C	514	BCR	1	0
23	D	402	CLA	3	0
23	b	605	CLA	3	0
23	a	405	CLA	3	0
23	c	507	CLA	2	0
23	a	407	CLA	2	0
27	a	420	GOL	5	0
23	a	409	CLA	2	0
25	c	516	BCR	2	0
35	C	517	DGD	2	0
24	a	417	PHO	2	0
34	d	409	HTG	1	0
23	b	614	CLA	2	0
23	B	609	CLA	2	0
25	A	409	BCR	2	0
34	D	410	HTG	1	0
23	b	606	CLA	2	0
23	B	603	CLA	1	0
29	a	415	PL9	4	0

Continued on next page...

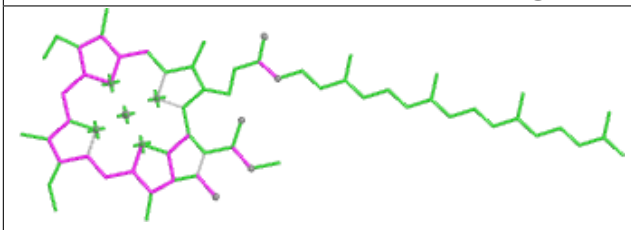
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	615	CLA	5	0
23	d	402	CLA	1	0
23	b	604	CLA	2	0
23	A	408	CLA	4	0
27	B	624	GOL	2	0
25	H	101	BCR	2	0

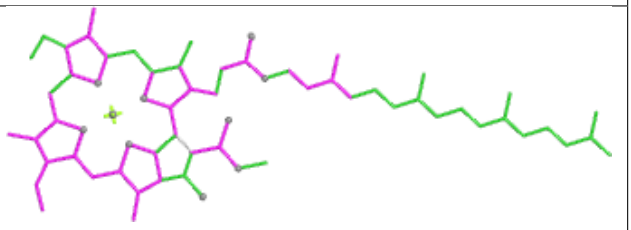
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



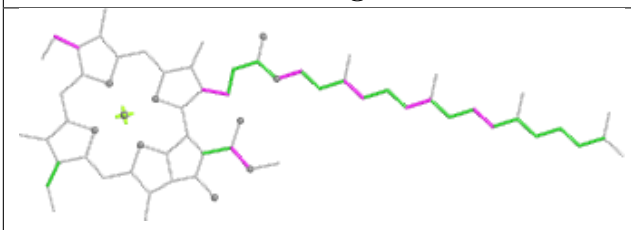
Ligand CLA c 514



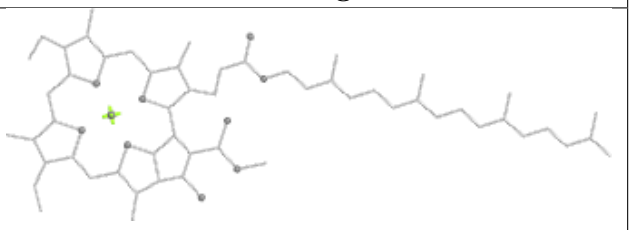
Bond lengths



Bond angles

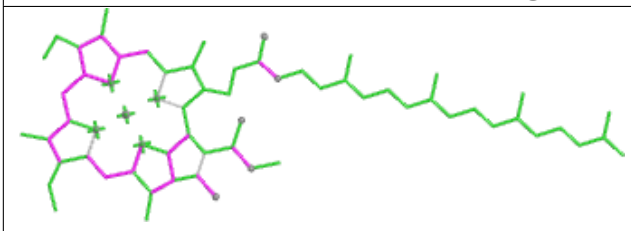


Torsions

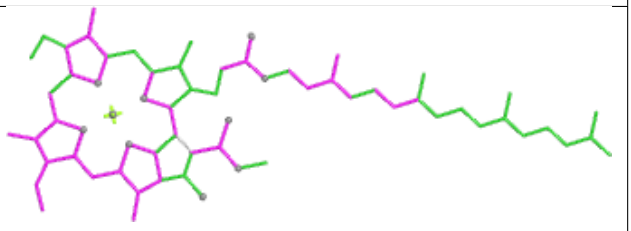


Rings

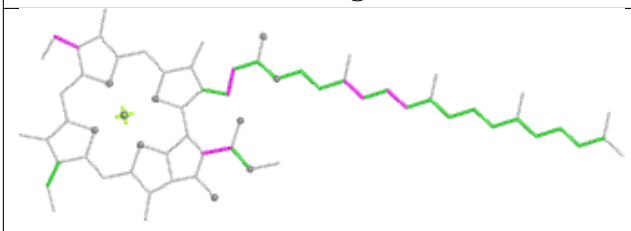
Ligand CLA C 507



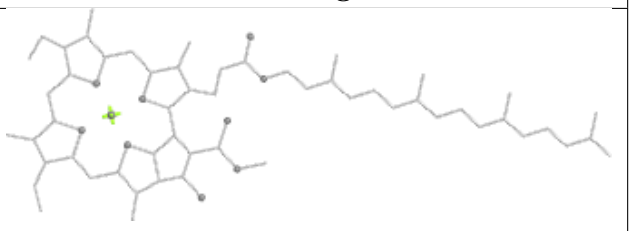
Bond lengths



Bond angles

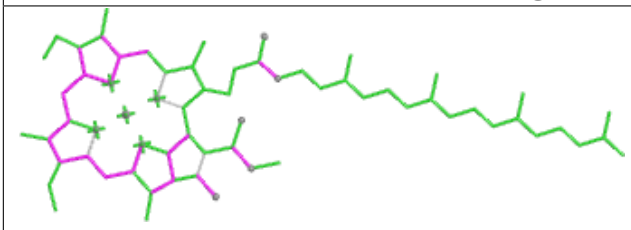


Torsions

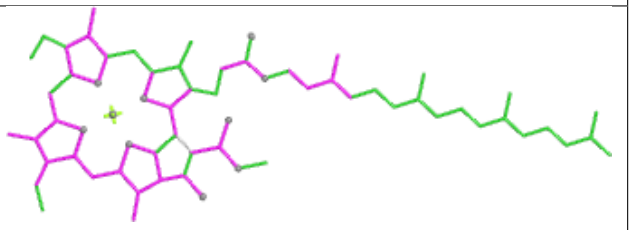


Rings

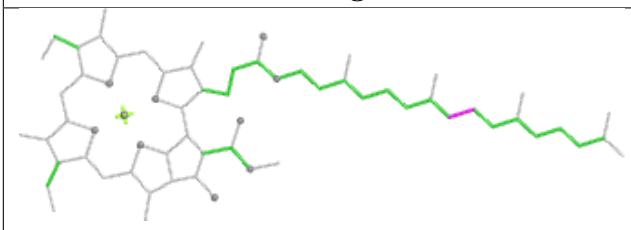
Ligand CLA c 504



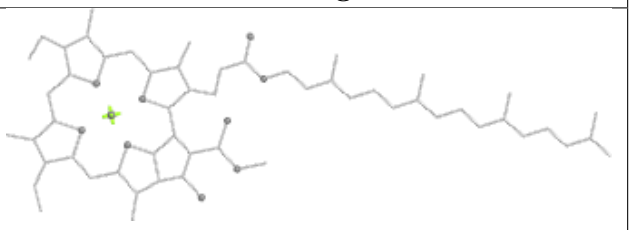
Bond lengths



Bond angles

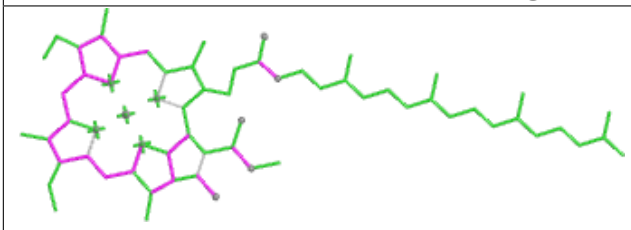


Torsions

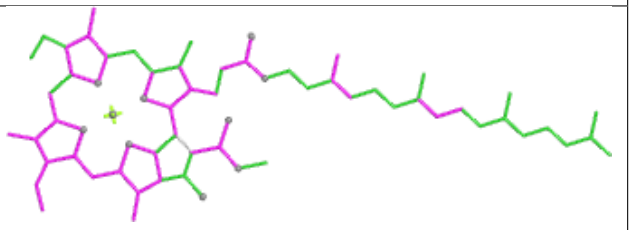


Rings

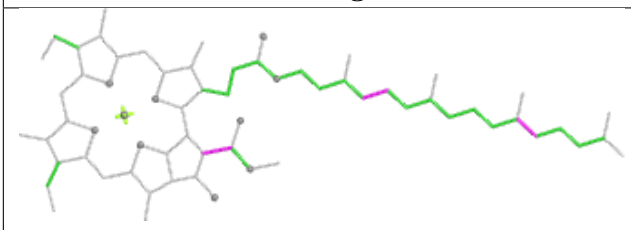
Ligand CLA B 607



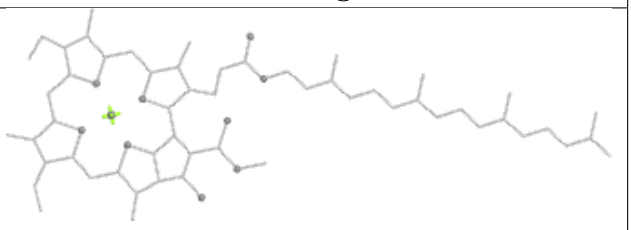
Bond lengths



Bond angles

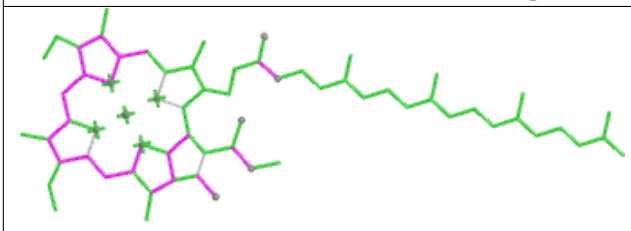


Torsions

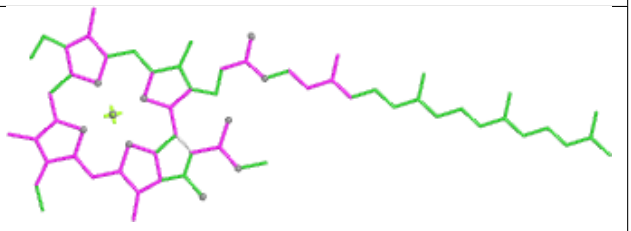


Rings

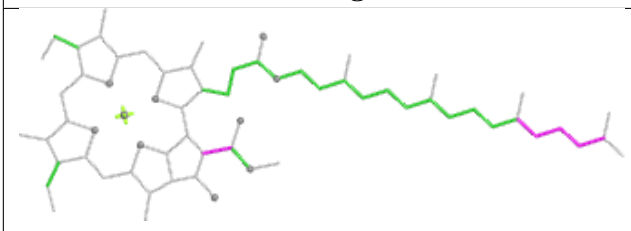
Ligand CLA C 502



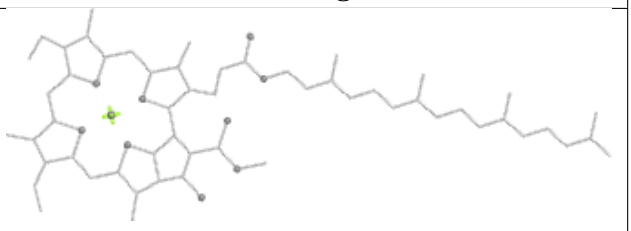
Bond lengths



Bond angles

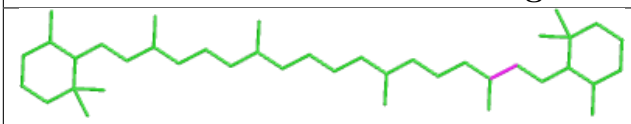


Torsions

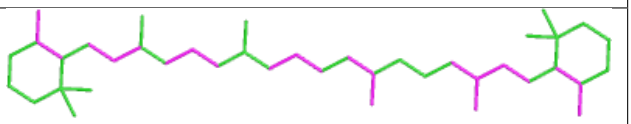


Rings

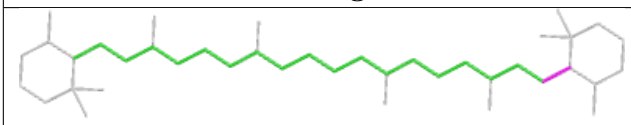
Ligand BCR h 101



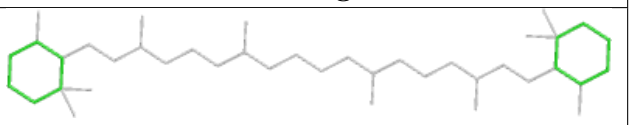
Bond lengths



Bond angles

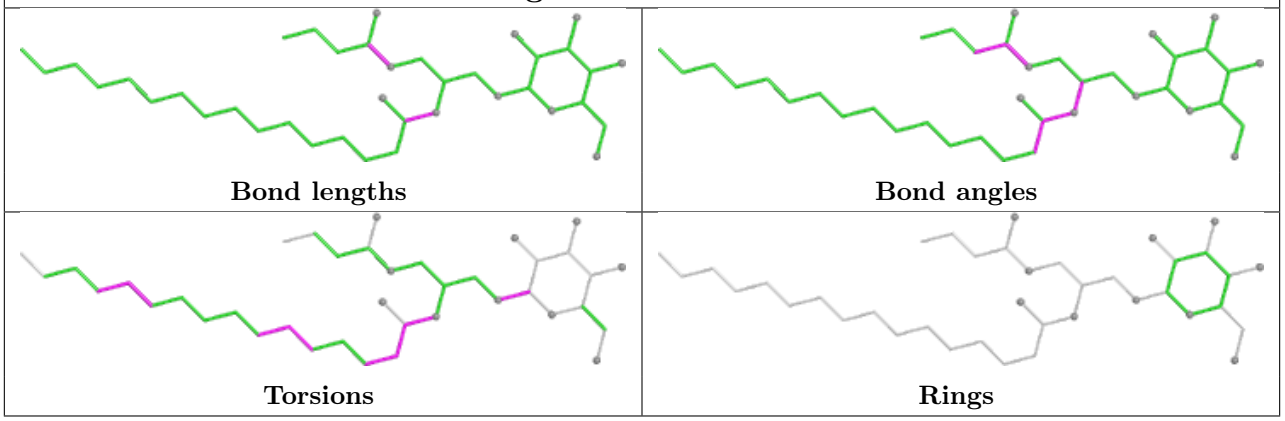


Torsions

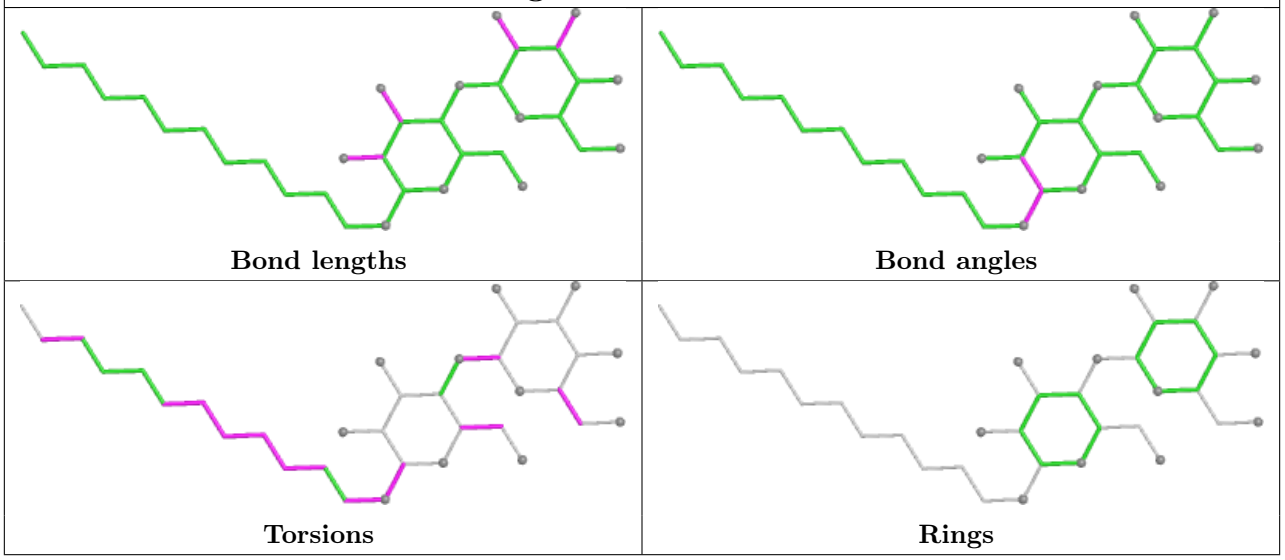


Rings

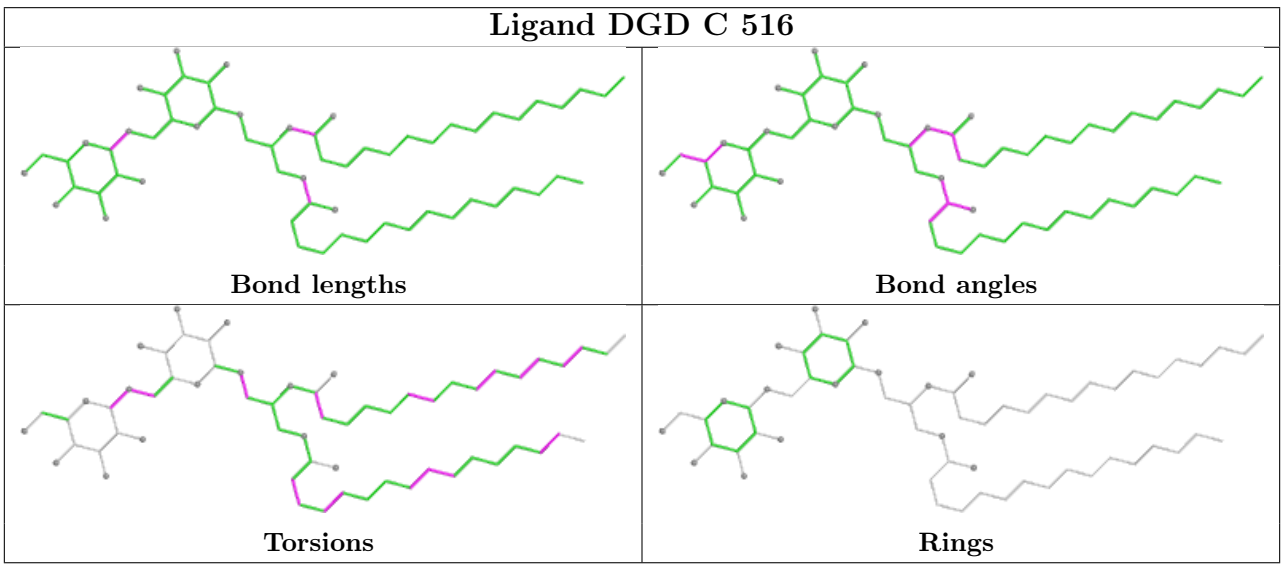
Ligand LMG z 101



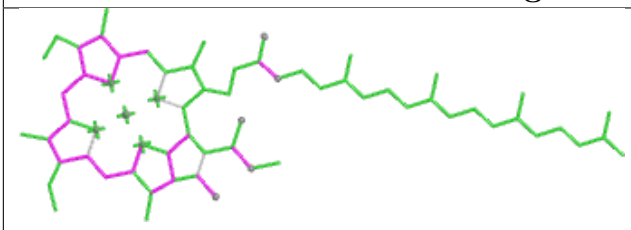
Ligand LMT e 101



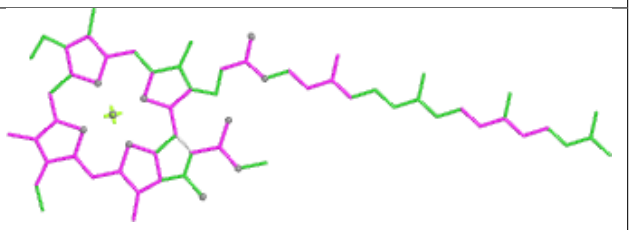
Ligand DGD C 516



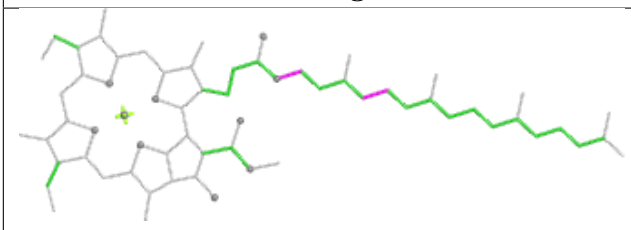
Ligand CLA C 509



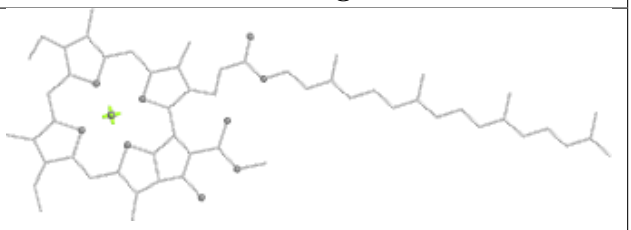
Bond lengths



Bond angles

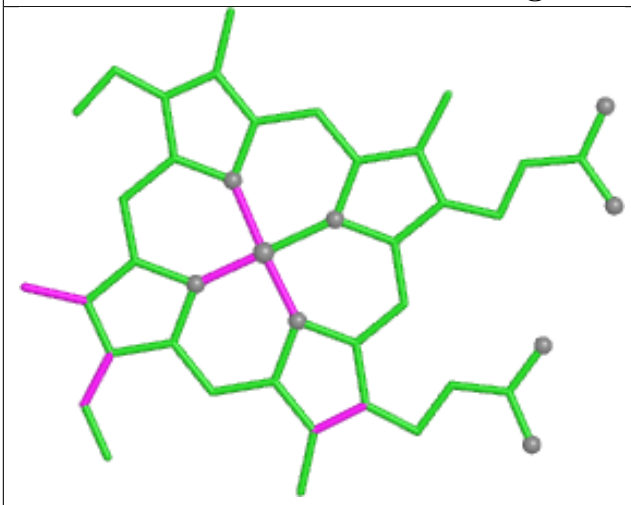


Torsions

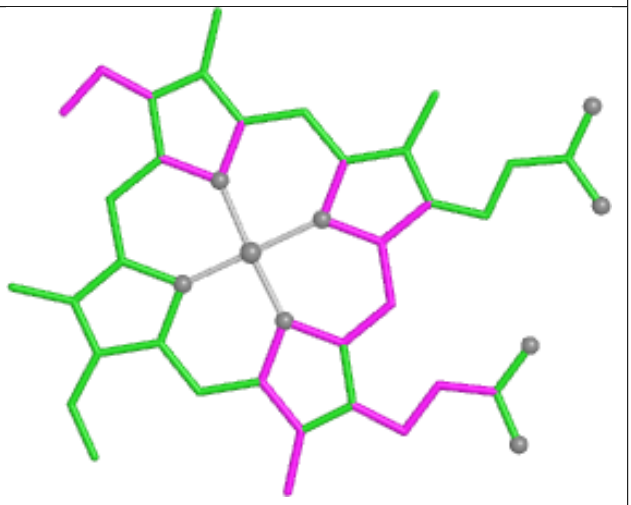


Rings

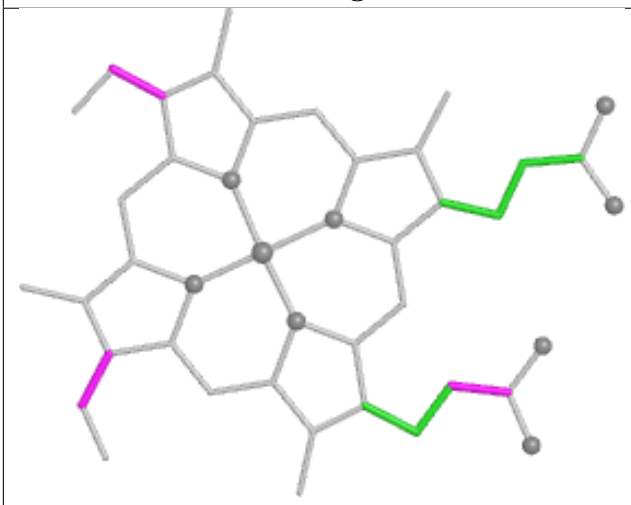
Ligand HEC v 201



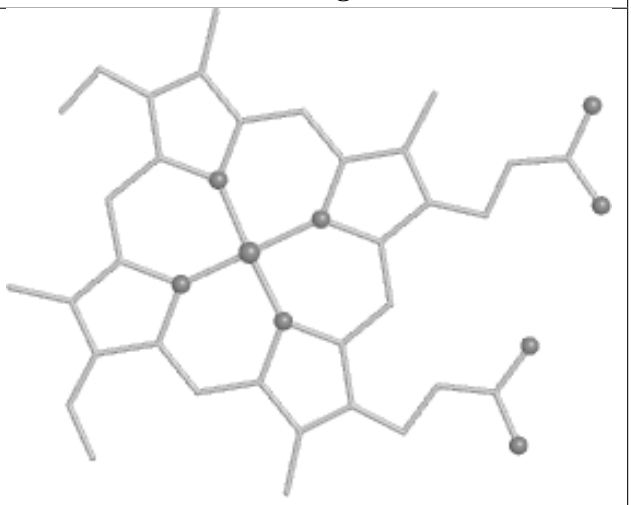
Bond lengths



Bond angles

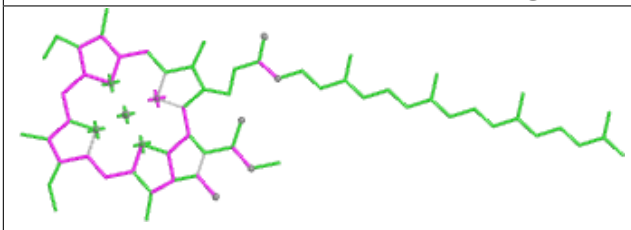


Torsions

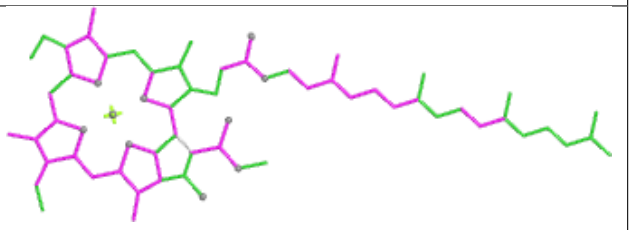


Rings

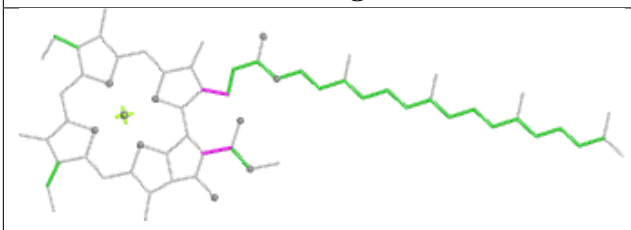
Ligand CLA B 604



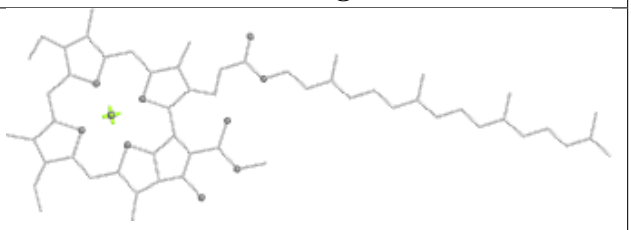
Bond lengths



Bond angles

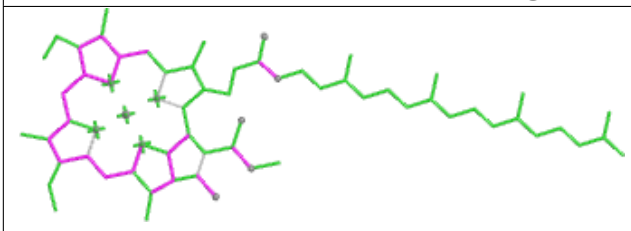


Torsions

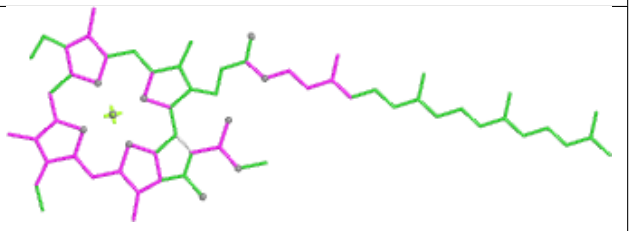


Rings

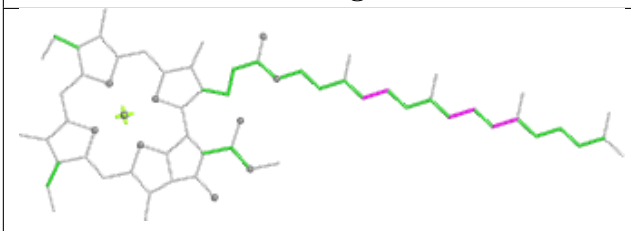
Ligand CLA C 511



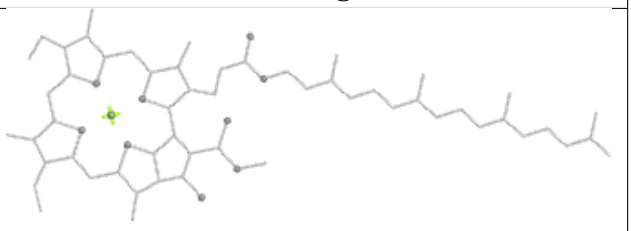
Bond lengths



Bond angles

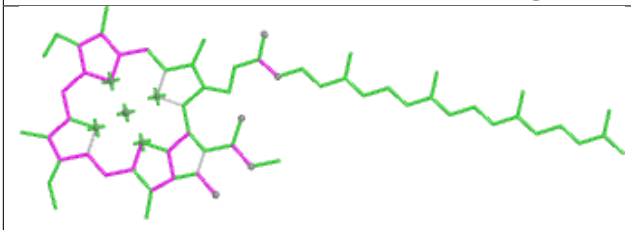


Torsions

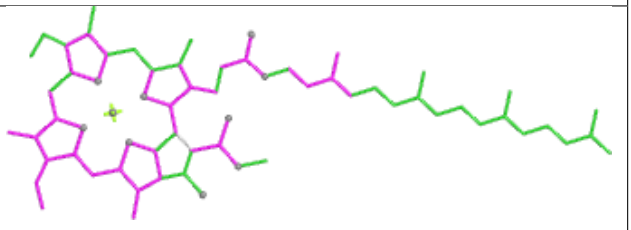


Rings

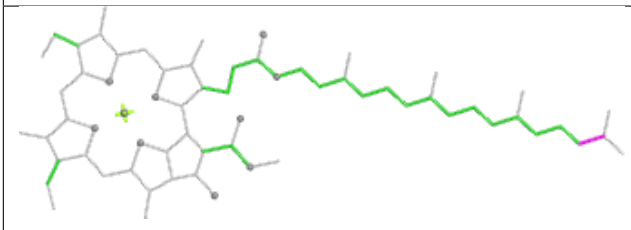
Ligand CLA d 401



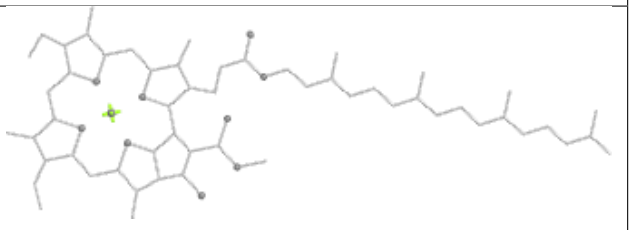
Bond lengths



Bond angles

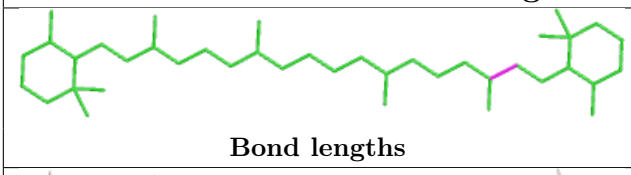


Torsions

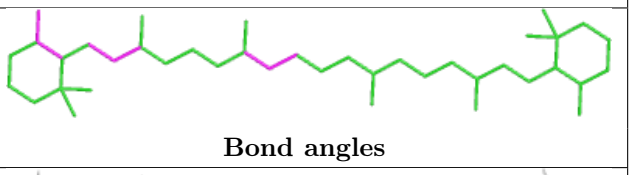


Rings

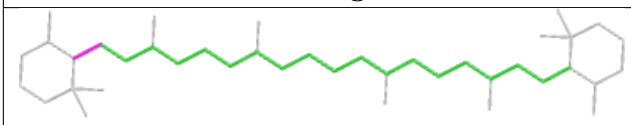
Ligand BCR B 617



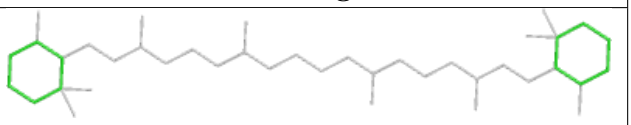
Bond lengths



Bond angles



Torsions

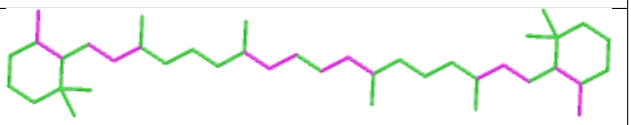


Rings

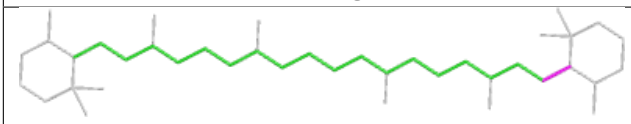
Ligand BCR K 101



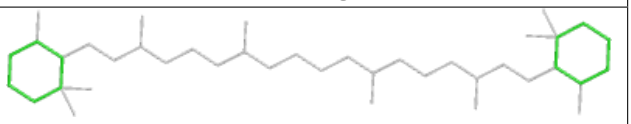
Bond lengths



Bond angles

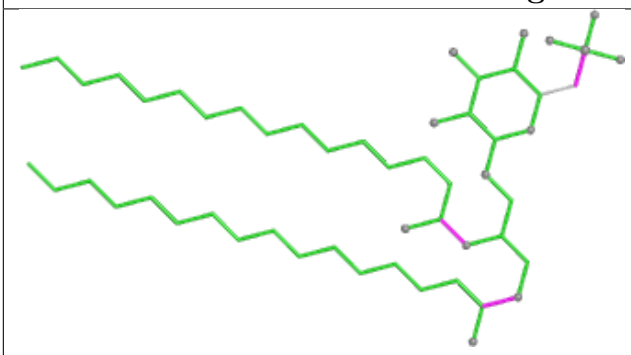


Torsions

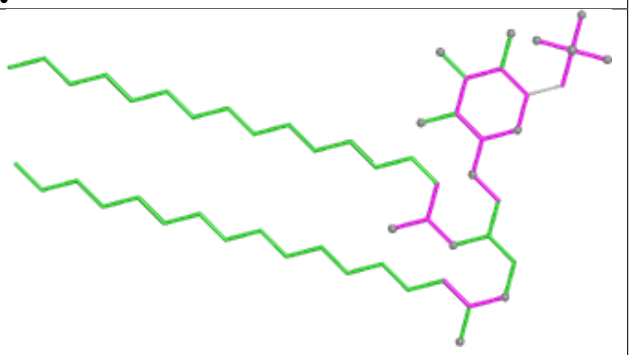


Rings

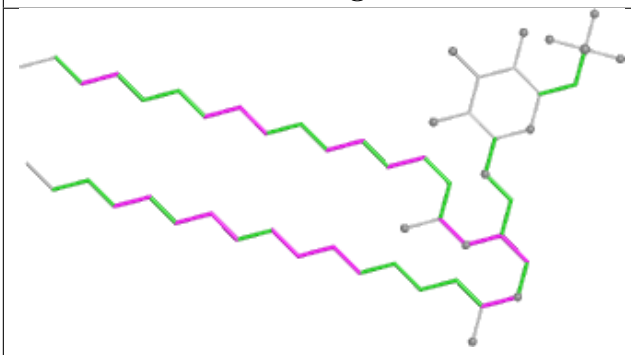
Ligand SQD b 620



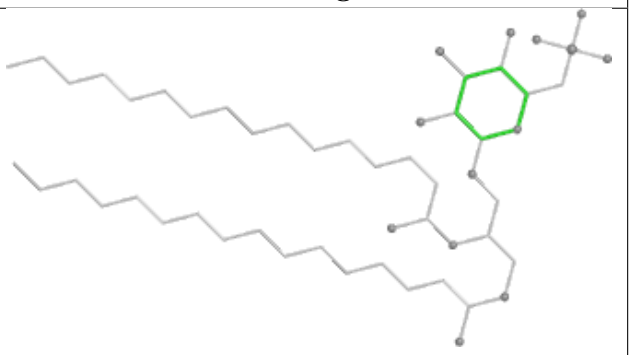
Bond lengths



Bond angles

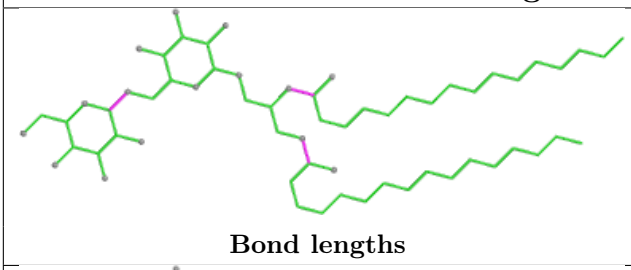


Torsions

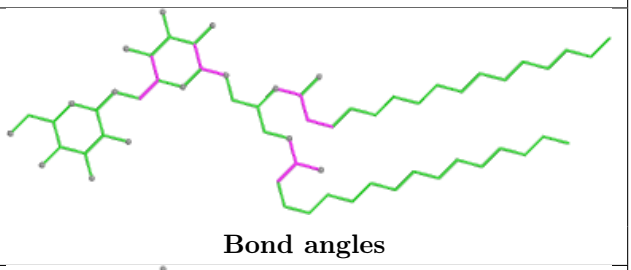


Rings

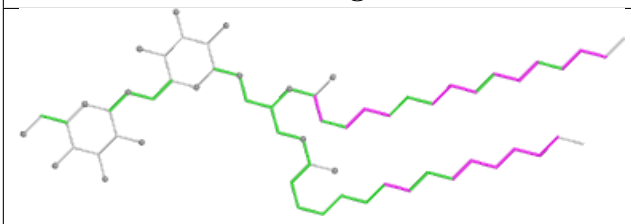
Ligand DGD h 102



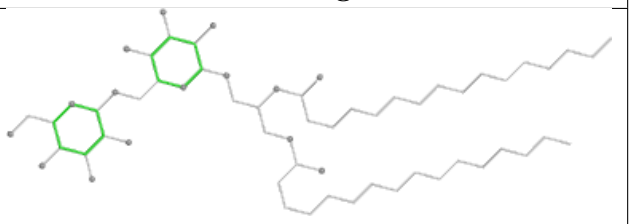
Bond lengths



Bond angles

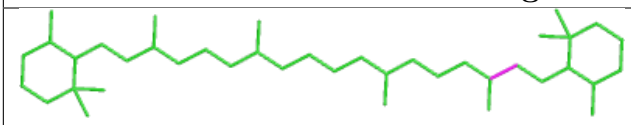


Torsions

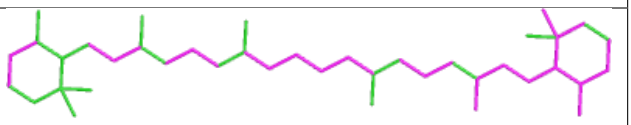


Rings

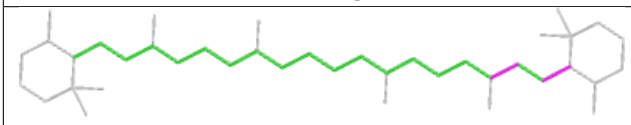
Ligand BCR D 404



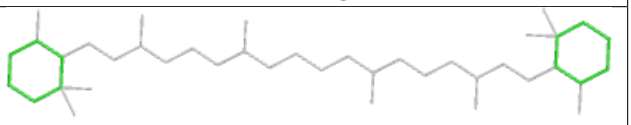
Bond lengths



Bond angles

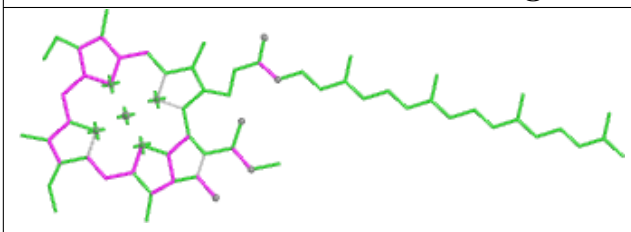


Torsions

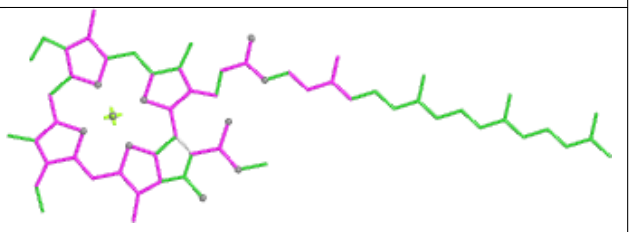


Rings

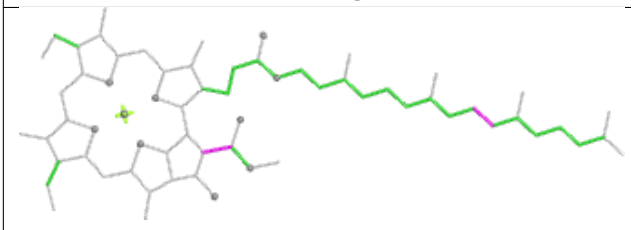
Ligand CLA C 508



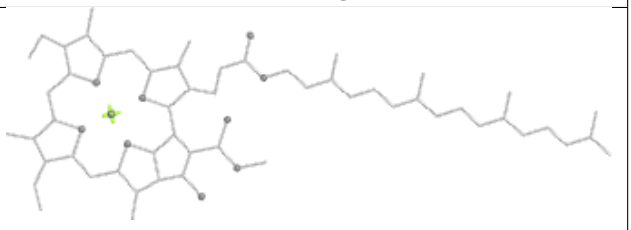
Bond lengths



Bond angles

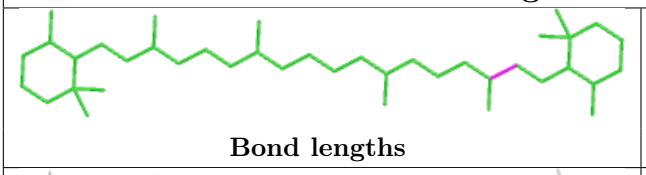


Torsions

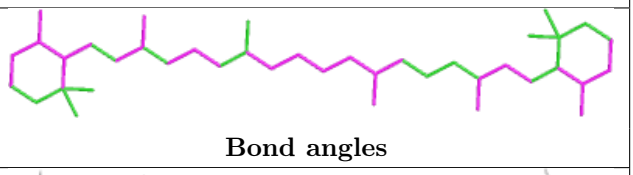


Rings

Ligand BCR Y 101



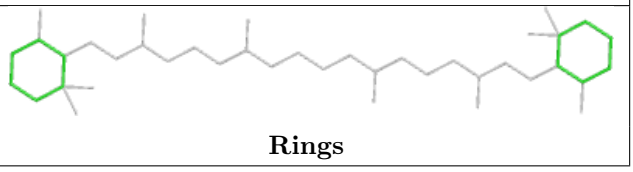
Bond lengths



Bond angles

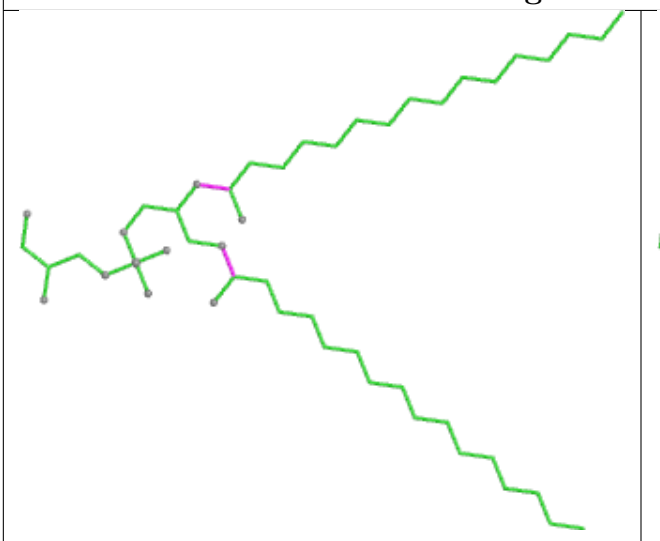


Torsions

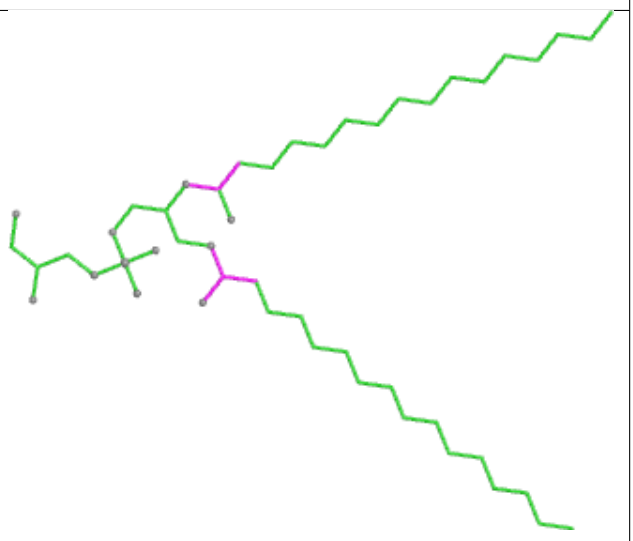


Rings

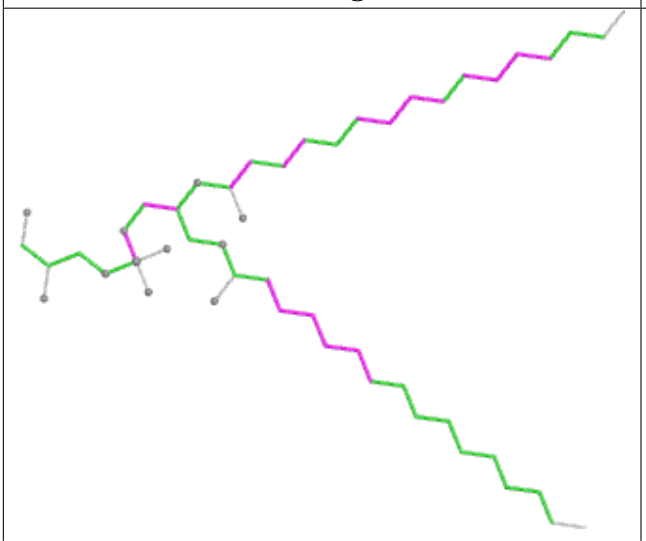
Ligand LHG L 101



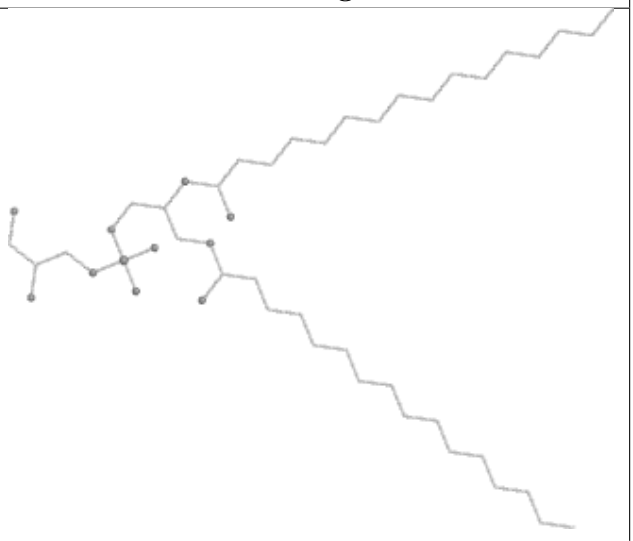
Bond lengths



Bond angles

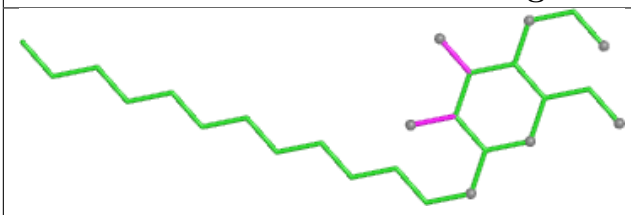


Torsions

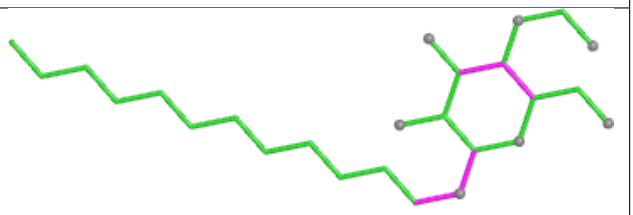


Rings

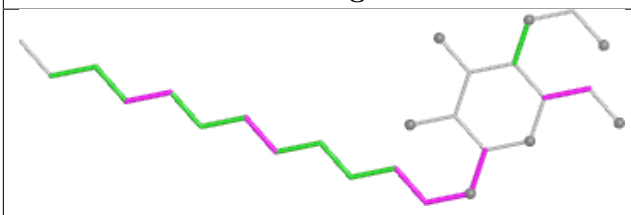
Ligand LMT t 101



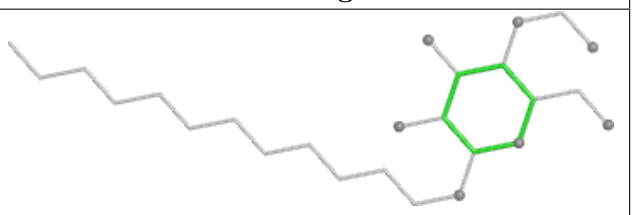
Bond lengths



Bond angles

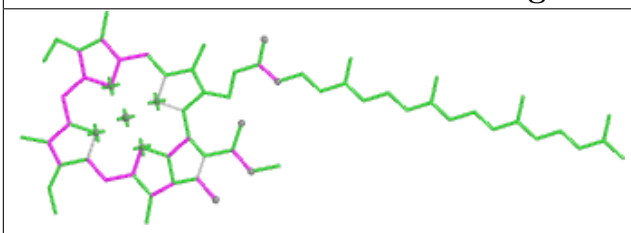


Torsions

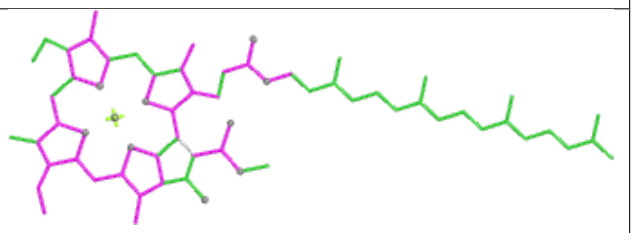


Rings

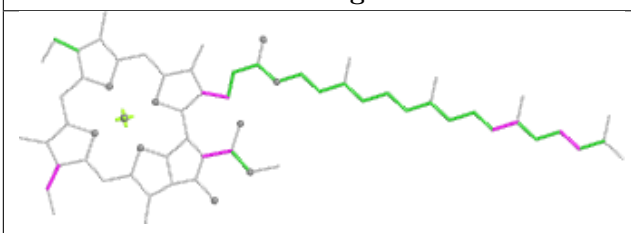
Ligand CLA a 406



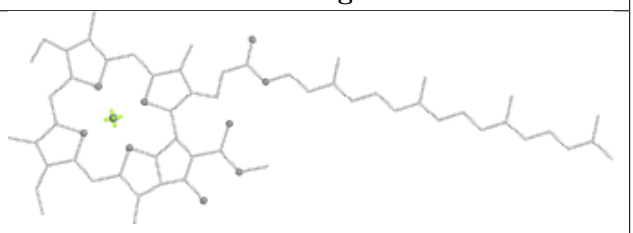
Bond lengths



Bond angles

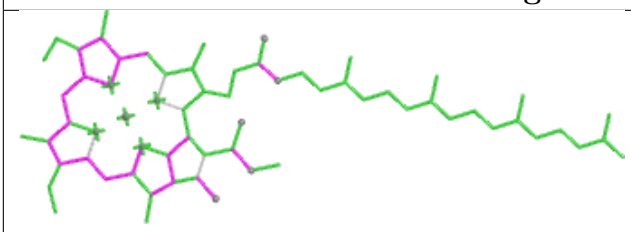


Torsions

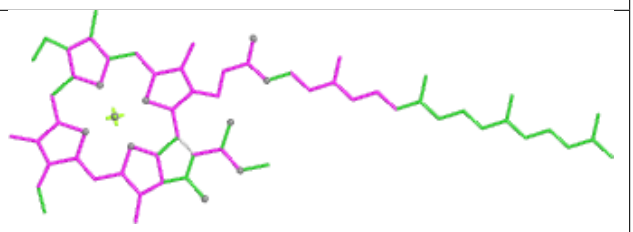


Rings

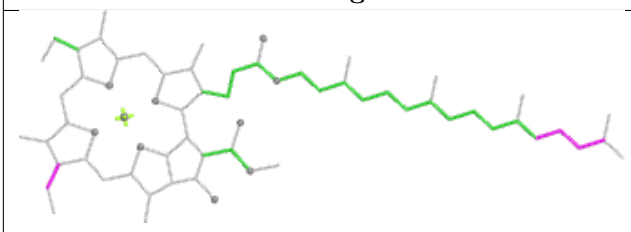
Ligand CLA A 404



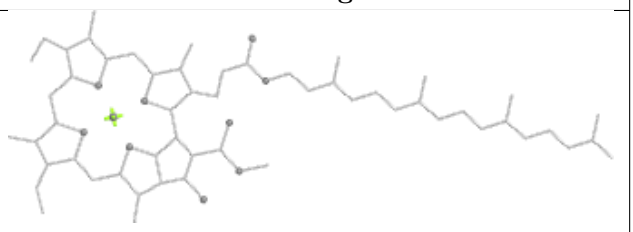
Bond lengths



Bond angles

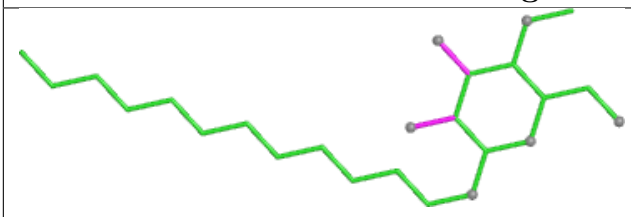


Torsions

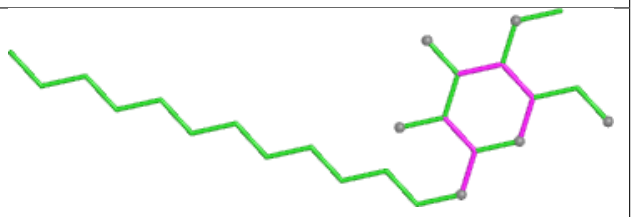


Rings

Ligand LMT B 631



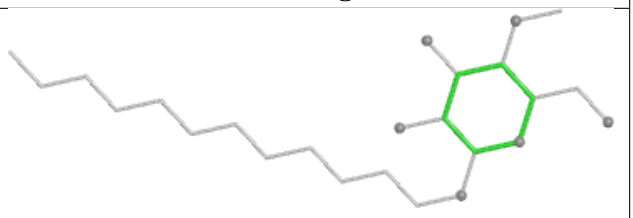
Bond lengths



Bond angles

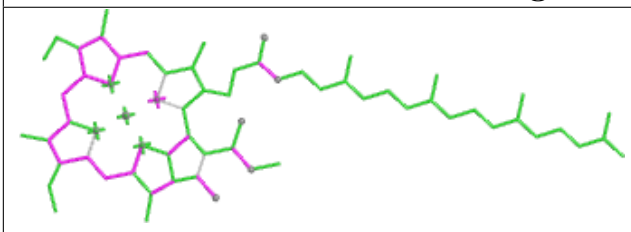


Torsions

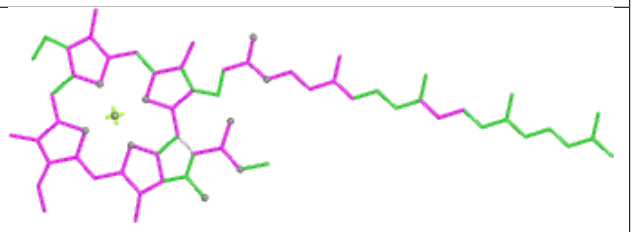


Rings

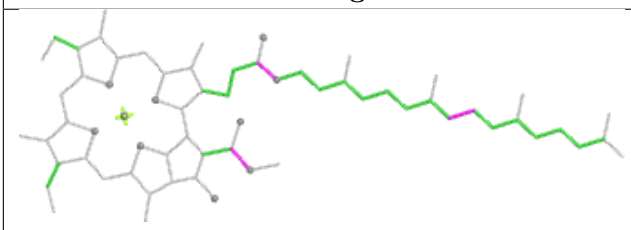
Ligand CLA c 512



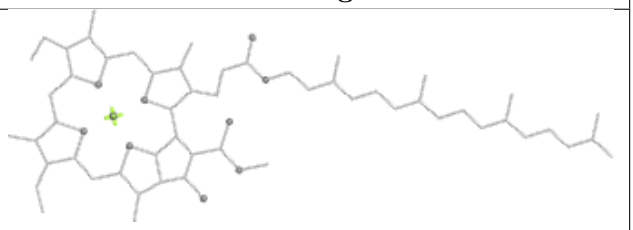
Bond lengths



Bond angles

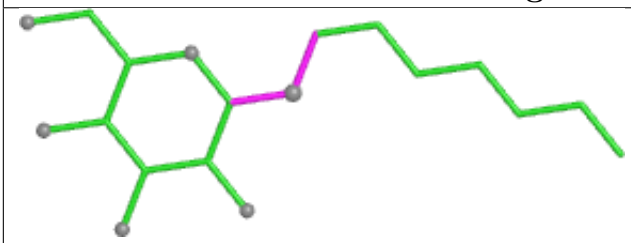


Torsions

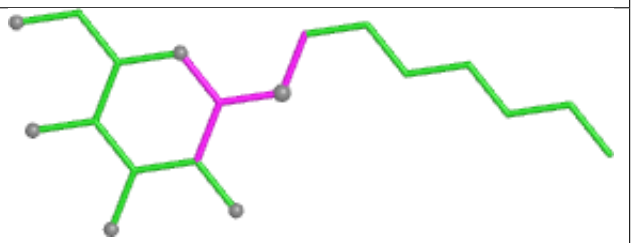


Rings

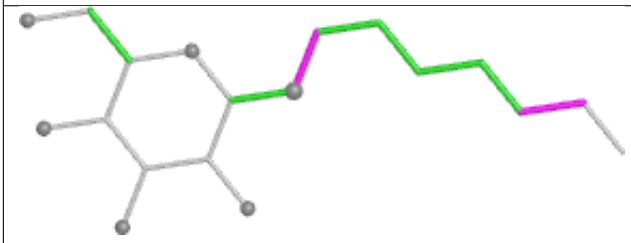
Ligand HTG c 522



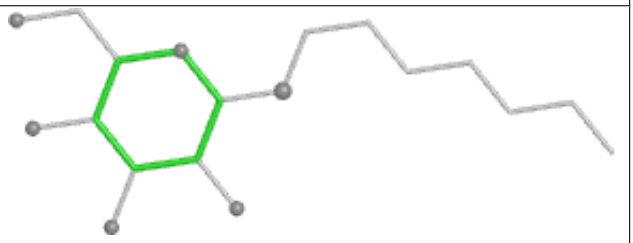
Bond lengths



Bond angles

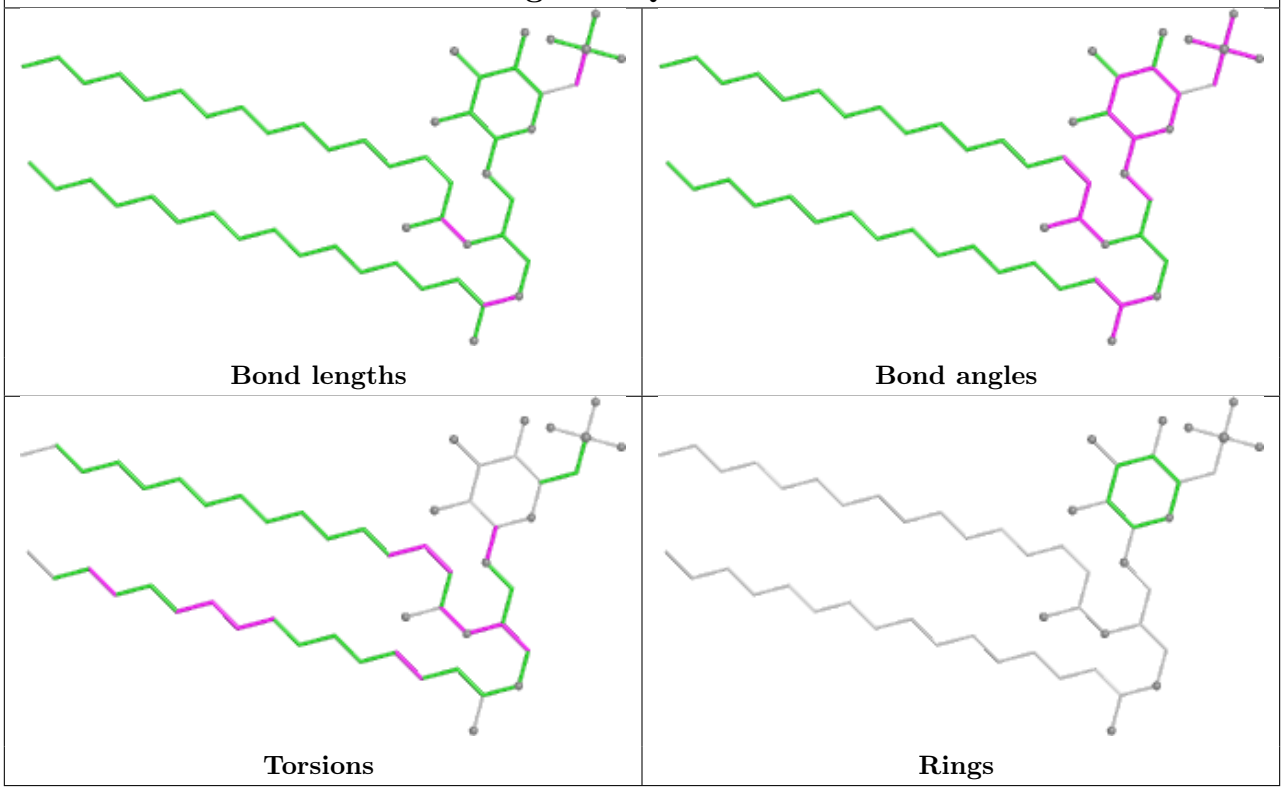


Torsions

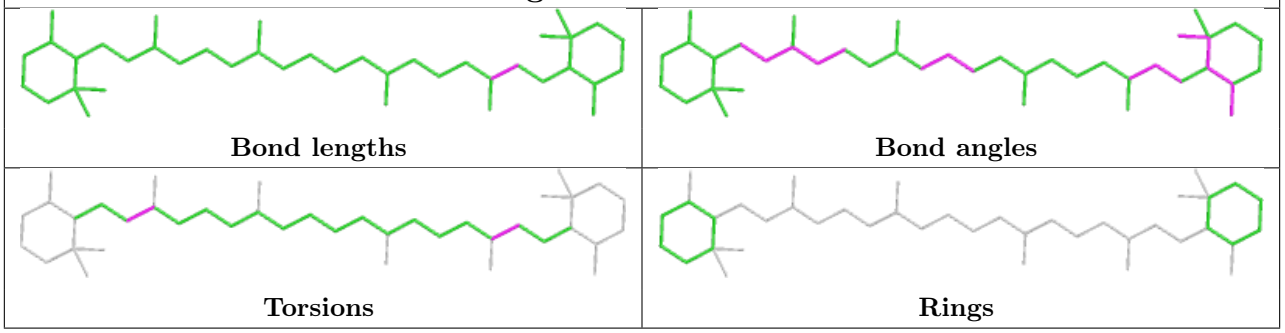


Rings

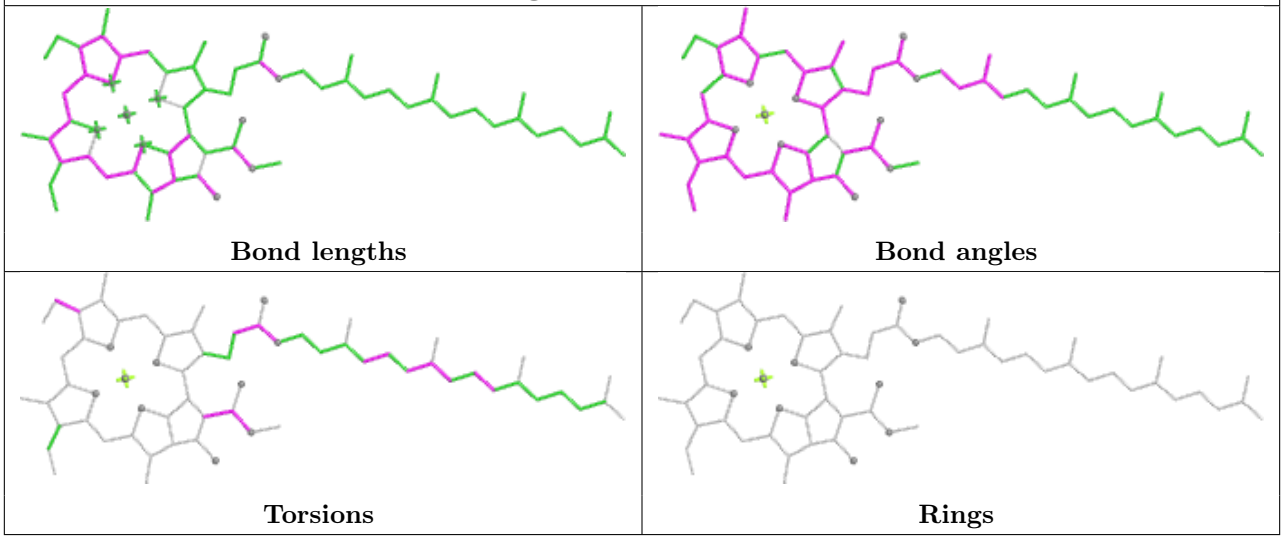
Ligand SQD B 620



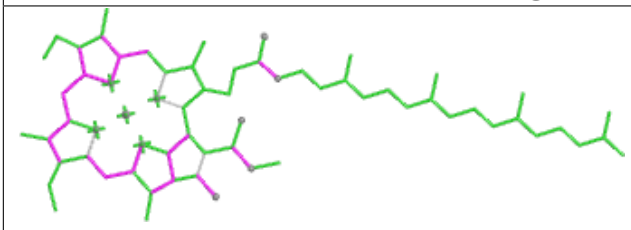
Ligand BCR b 619



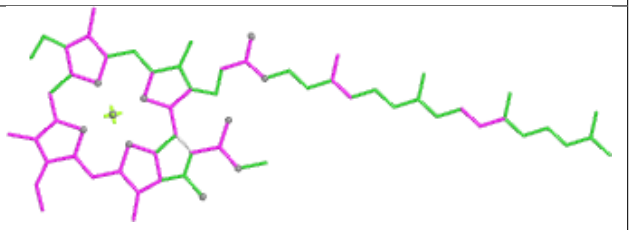
Ligand CLA C 512



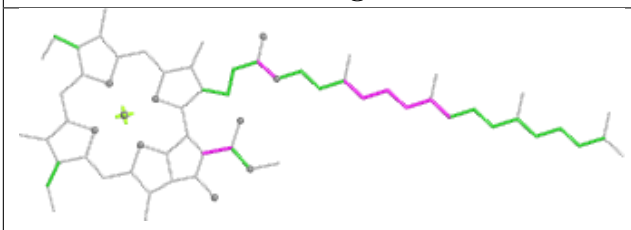
Ligand CLA b 616



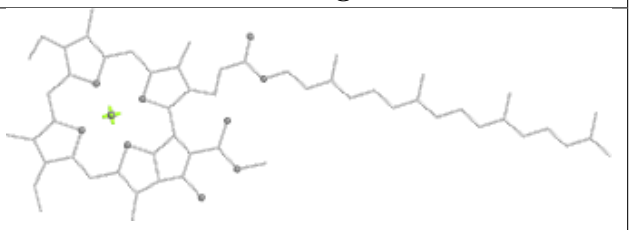
Bond lengths



Bond angles



Torsions

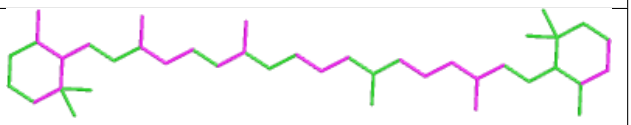


Rings

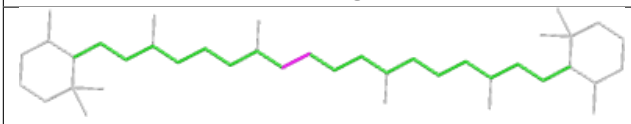
Ligand BCR t 102



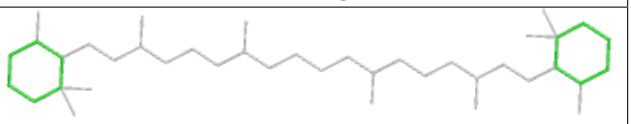
Bond lengths



Bond angles

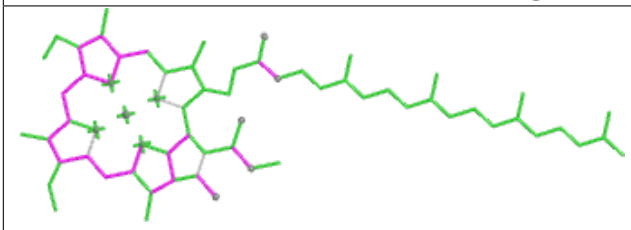


Torsions

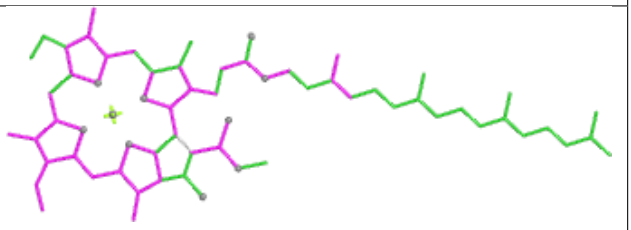


Rings

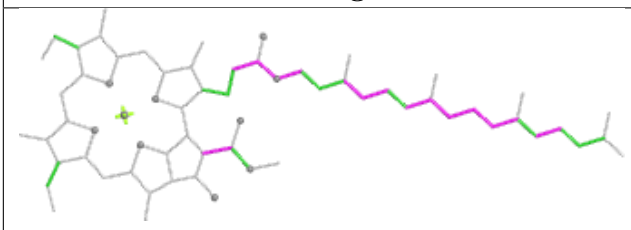
Ligand CLA b 601



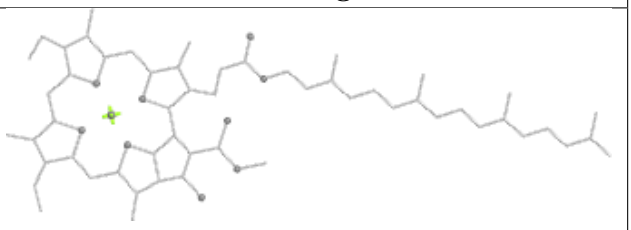
Bond lengths



Bond angles

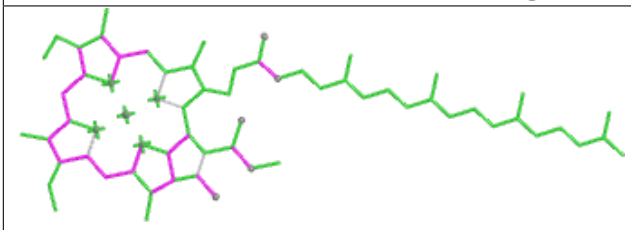


Torsions

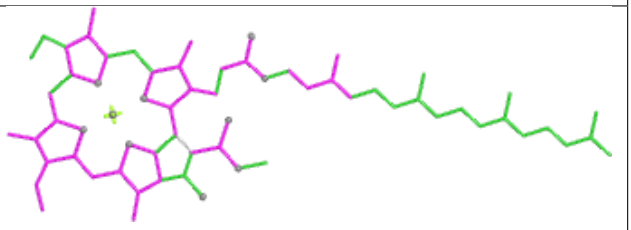


Rings

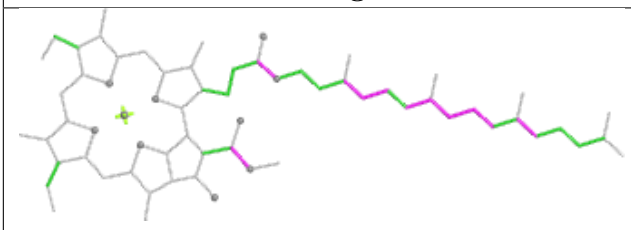
Ligand CLA D 403



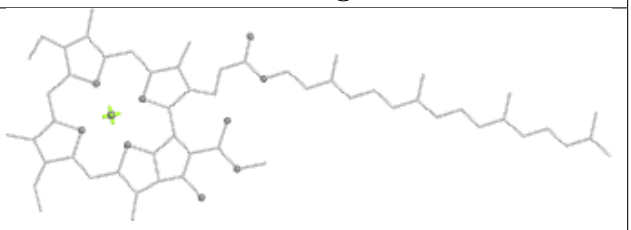
Bond lengths



Bond angles

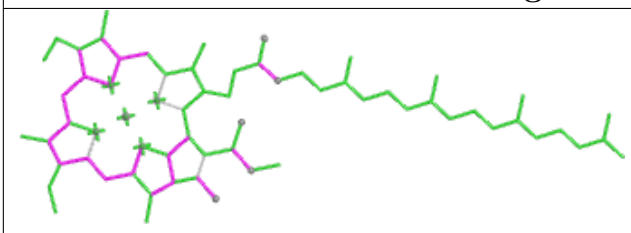


Torsions

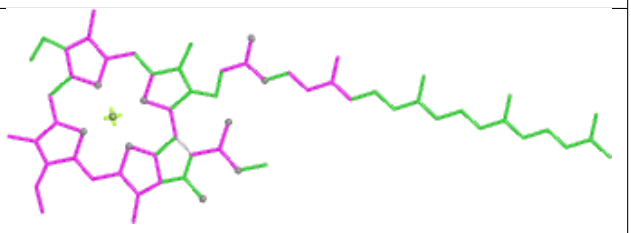


Rings

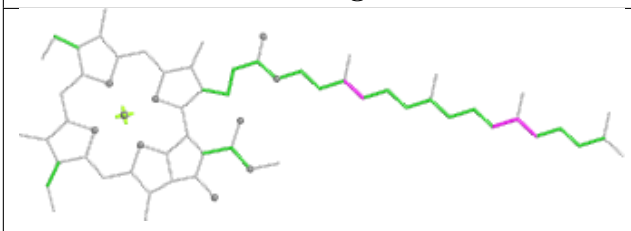
Ligand CLA C 505



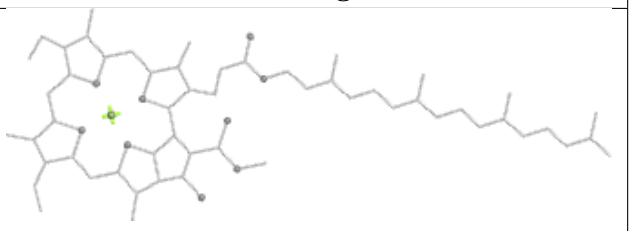
Bond lengths



Bond angles

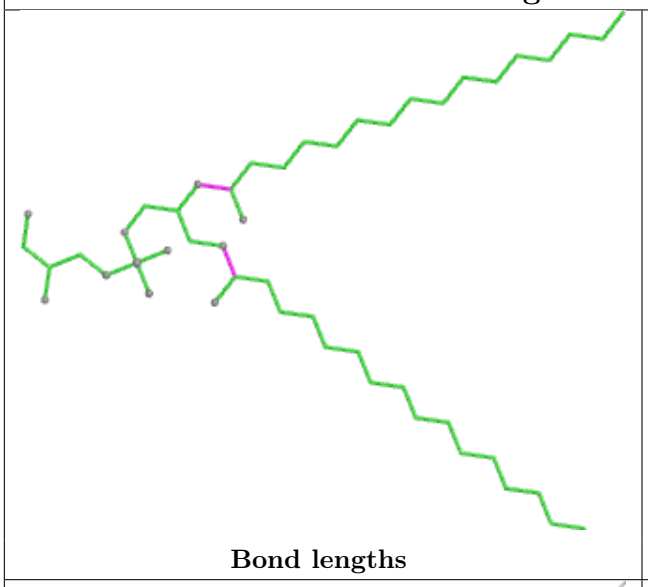


Torsions

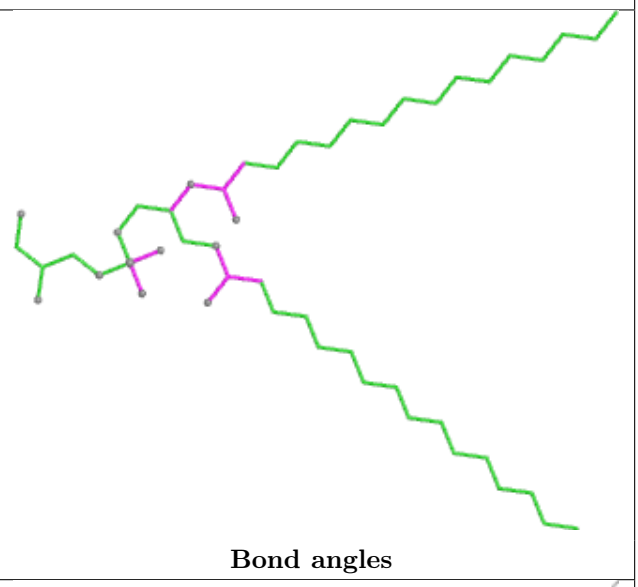


Rings

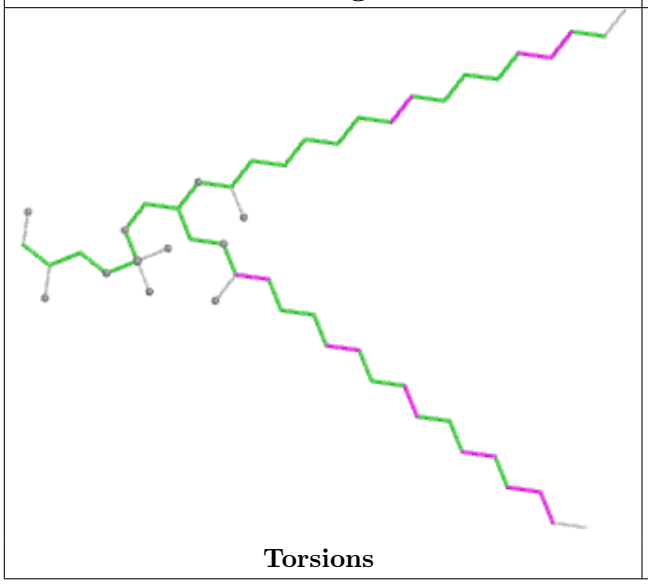
Ligand LHG A 420



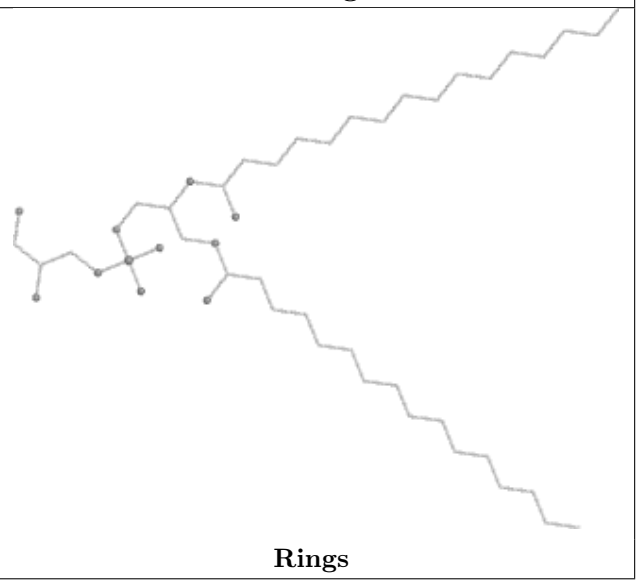
Bond lengths



Bond angles

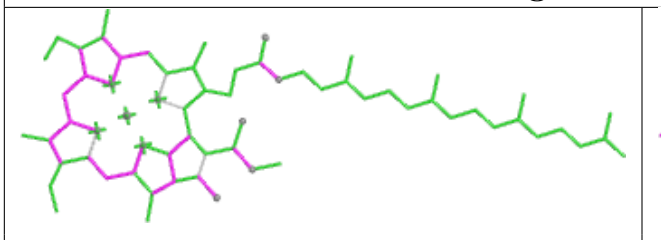


Torsions

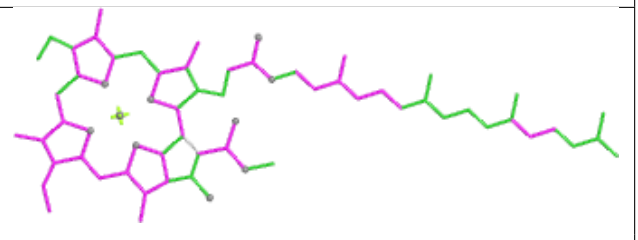


Rings

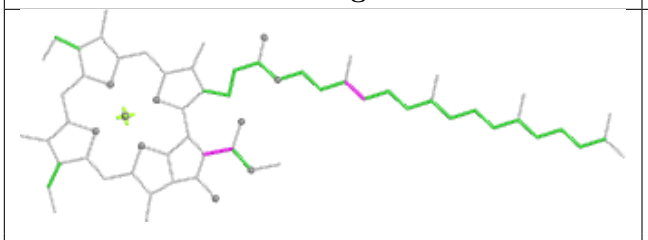
Ligand CLA b 609



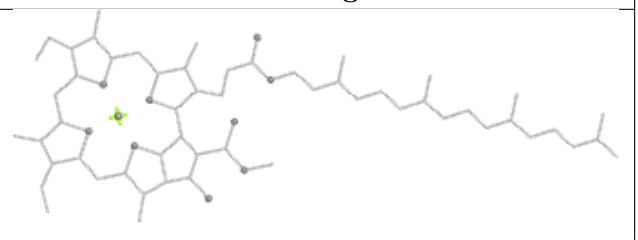
Bond lengths



Bond angles

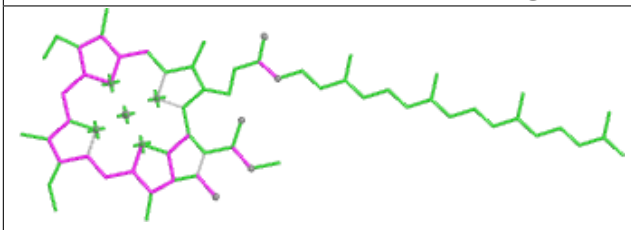


Torsions

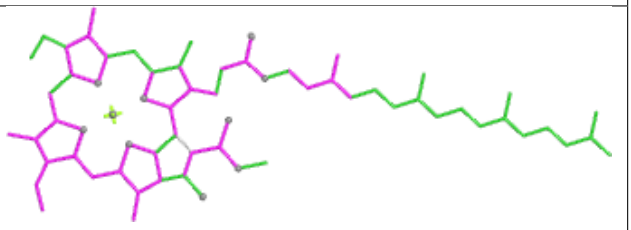


Rings

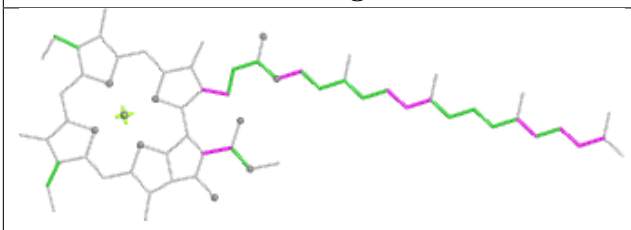
Ligand CLA C 506



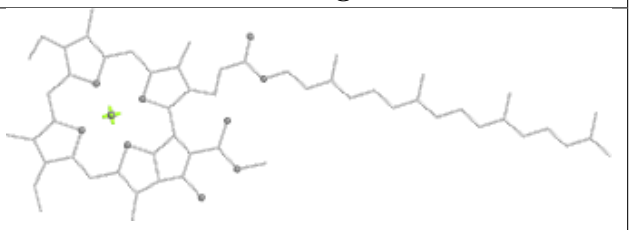
Bond lengths



Bond angles

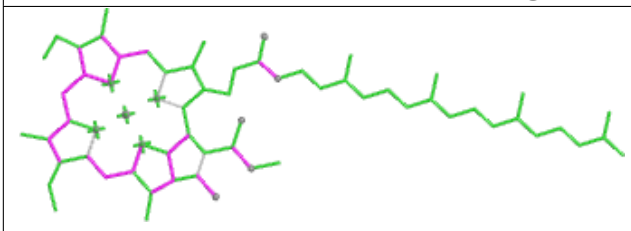


Torsions

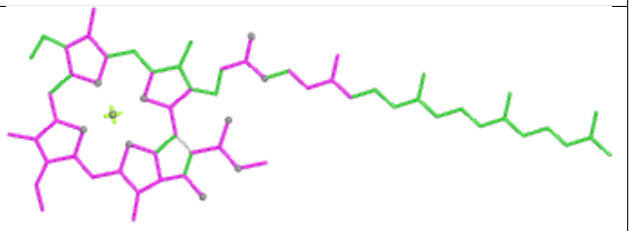


Rings

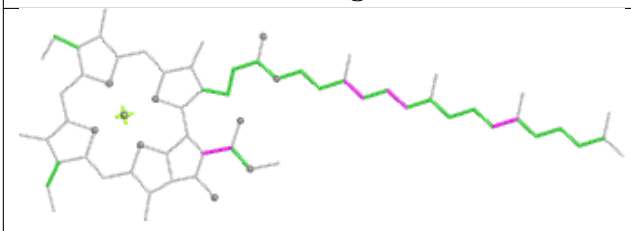
Ligand CLA B 605



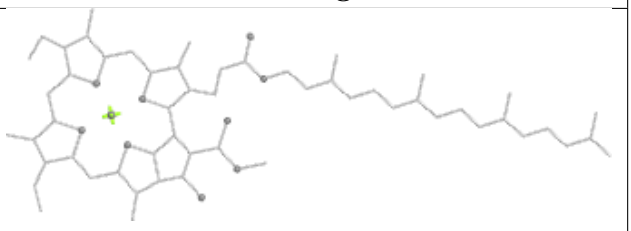
Bond lengths



Bond angles

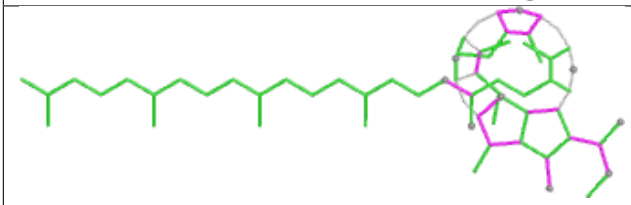


Torsions

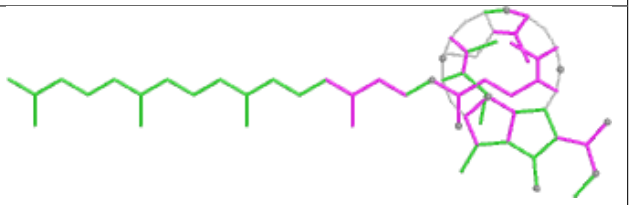


Rings

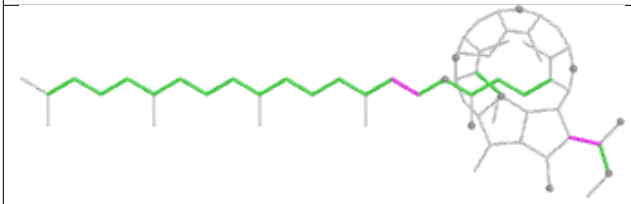
Ligand PHO A 407



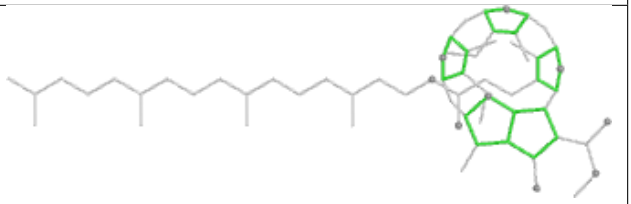
Bond lengths



Bond angles

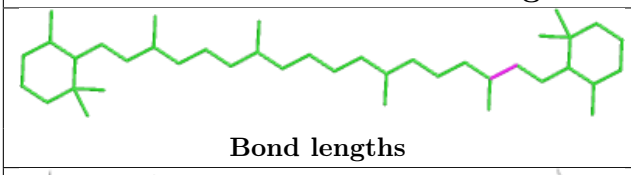


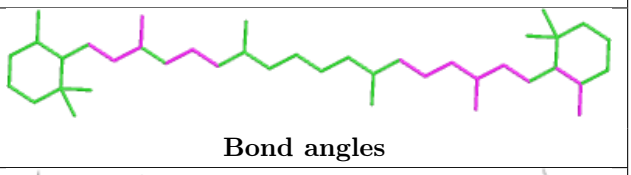
Torsions

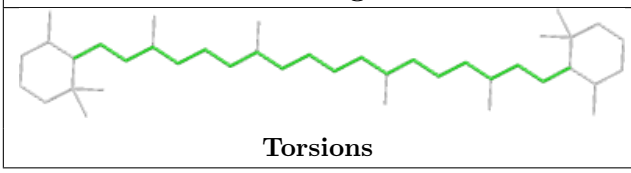


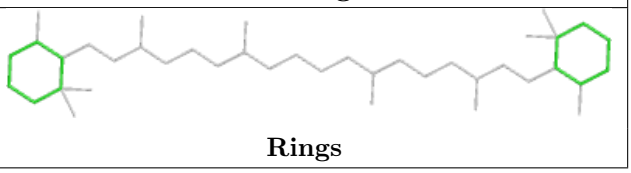
Rings

Ligand BCR B 619

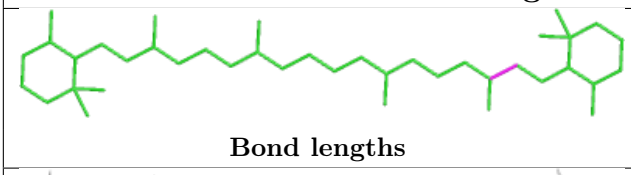

Bond lengths

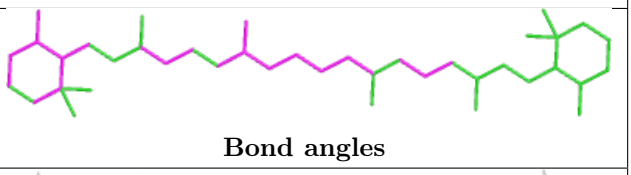

Bond angles

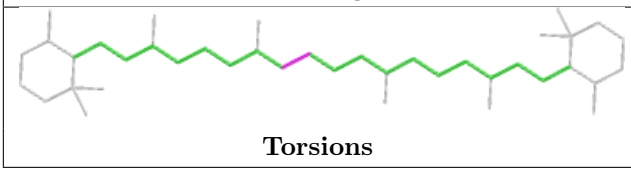

Torsions

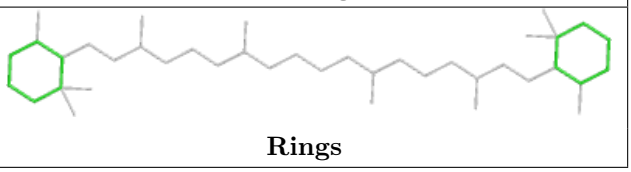

Rings

Ligand BCR T 102

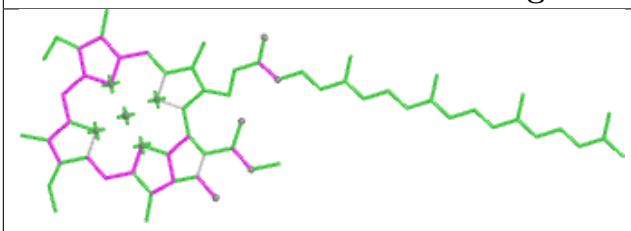

Bond lengths

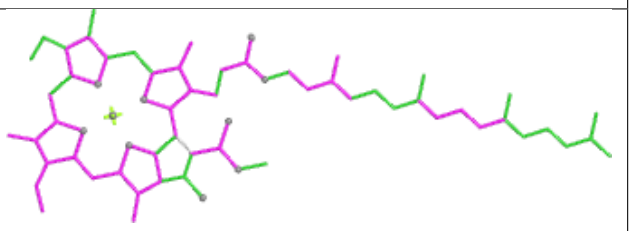

Bond angles

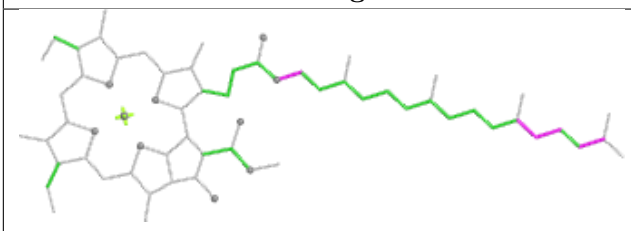

Torsions

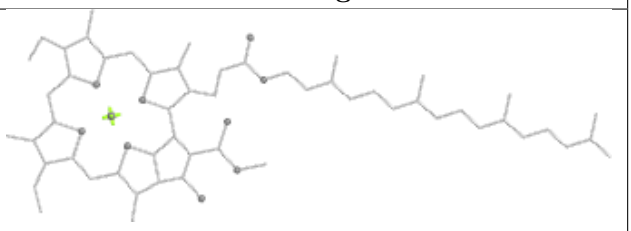

Rings

Ligand CLA b 608

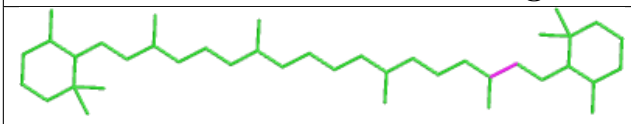

Bond lengths

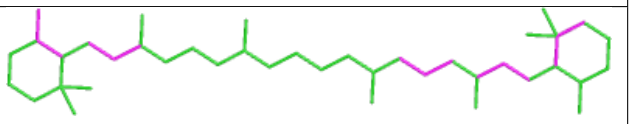

Bond angles


Torsions

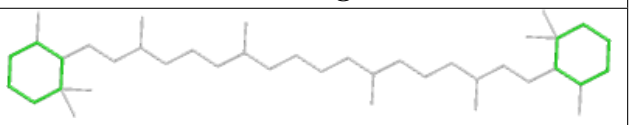

Rings

Ligand BCR b 617

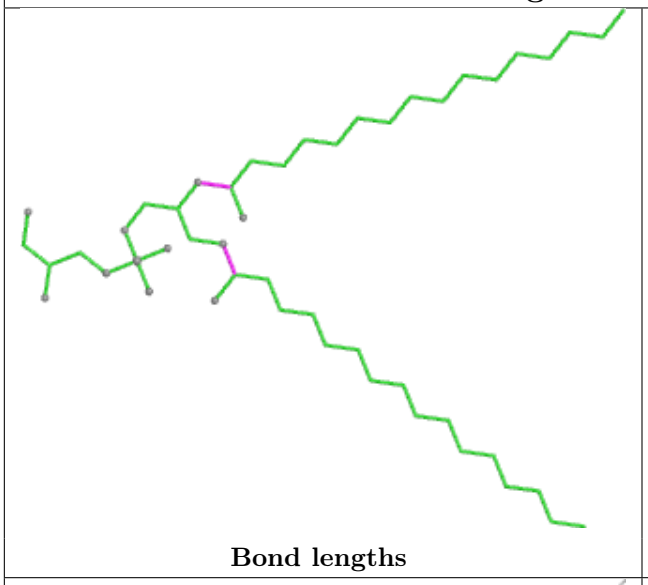

Bond lengths


Bond angles

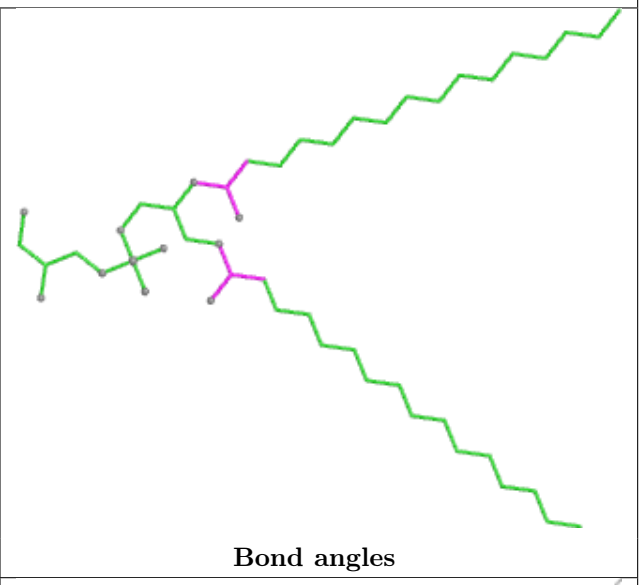

Torsions


Rings

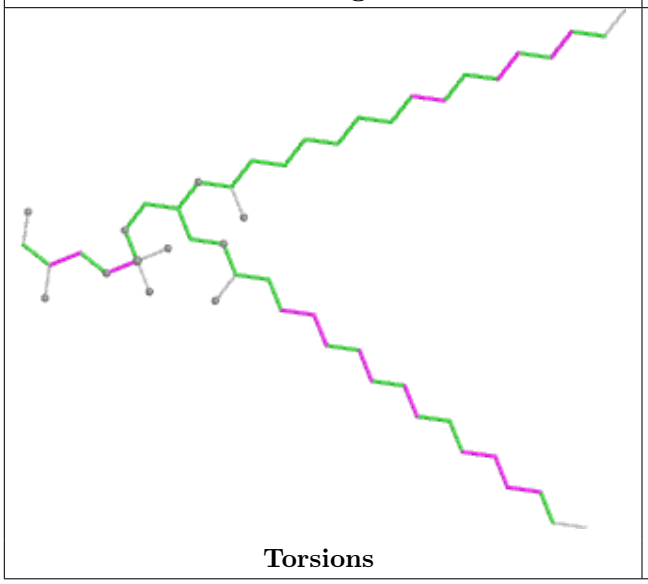
Ligand LHG d 411



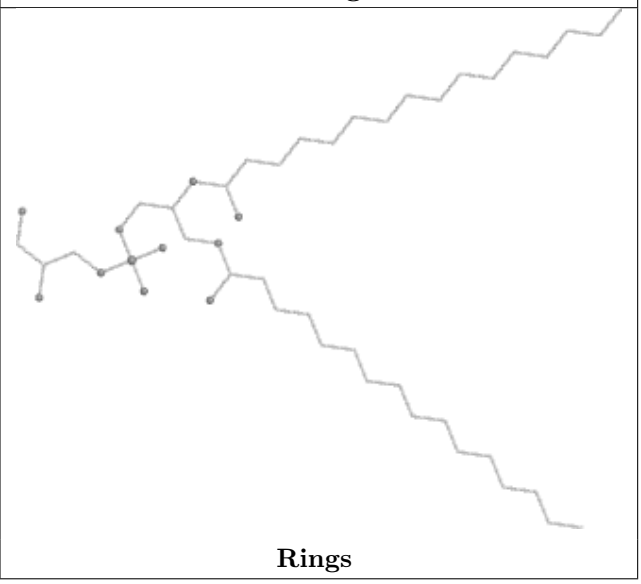
Bond lengths



Bond angles

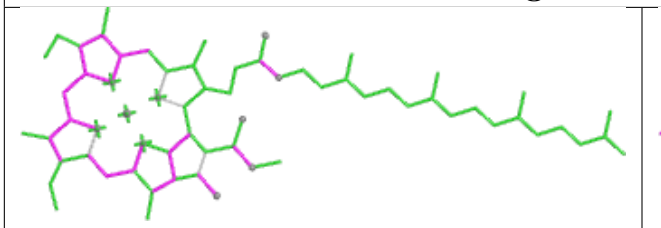


Torsions

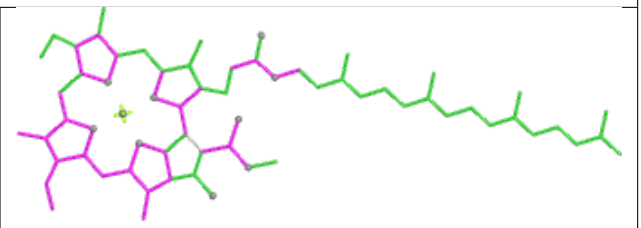


Rings

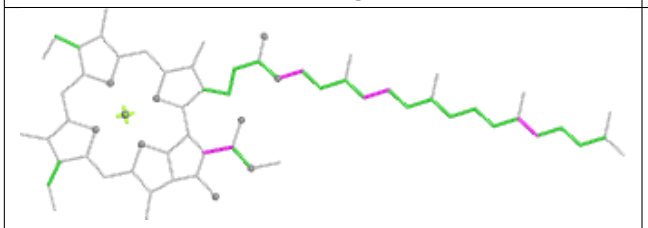
Ligand CLA B 616



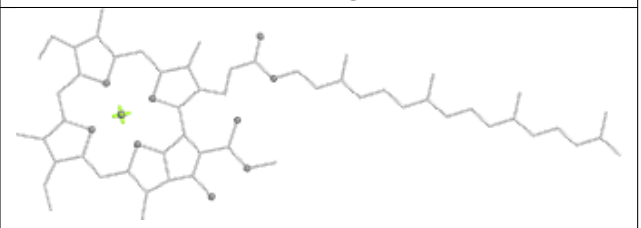
Bond lengths



Bond angles

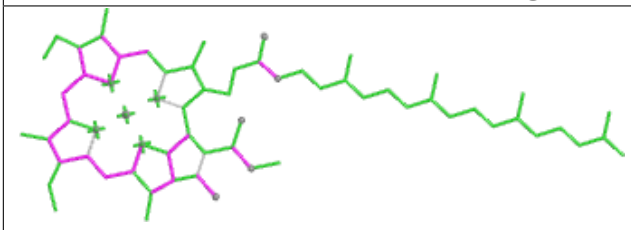


Torsions

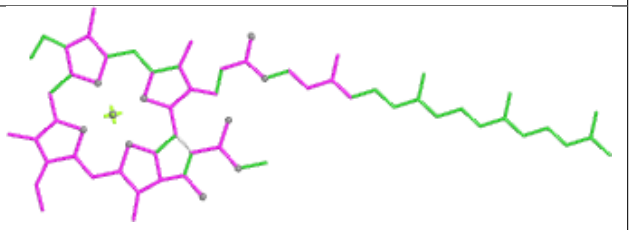


Rings

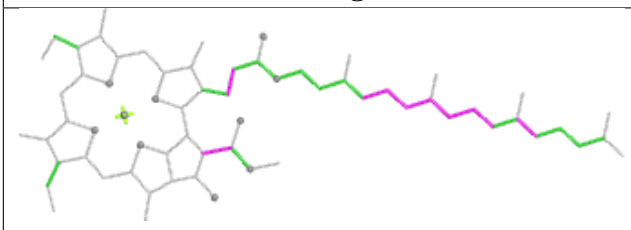
Ligand CLA B 614



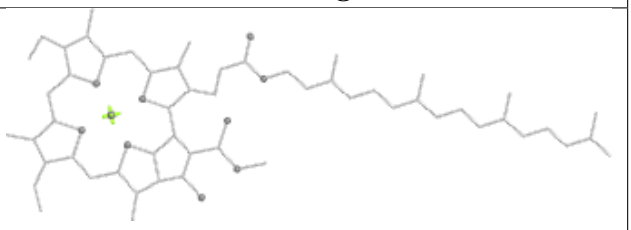
Bond lengths



Bond angles

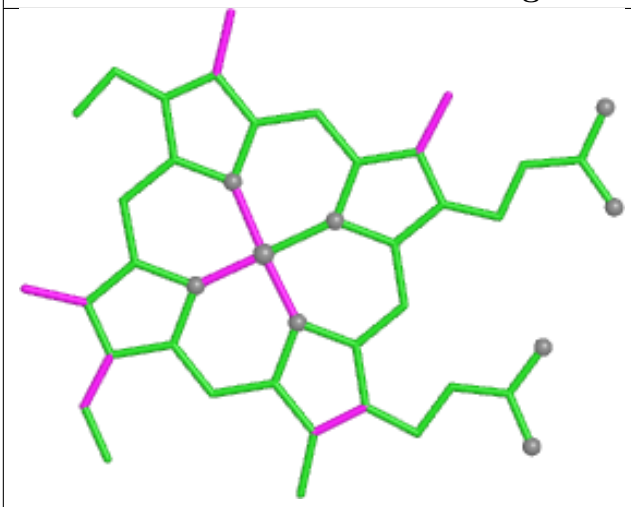


Torsions

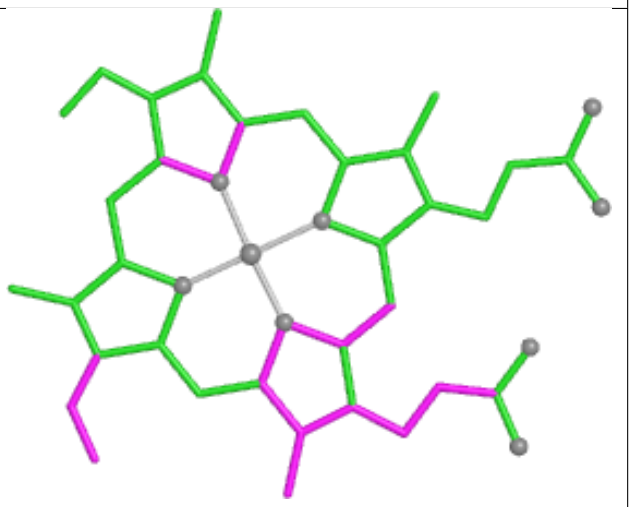


Rings

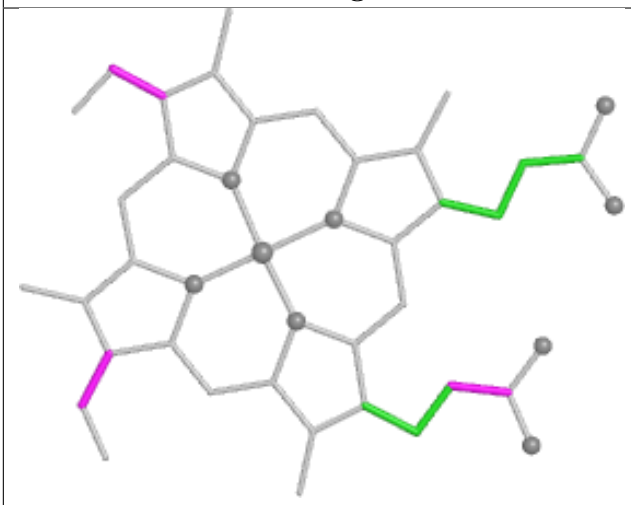
Ligand HEC V 201



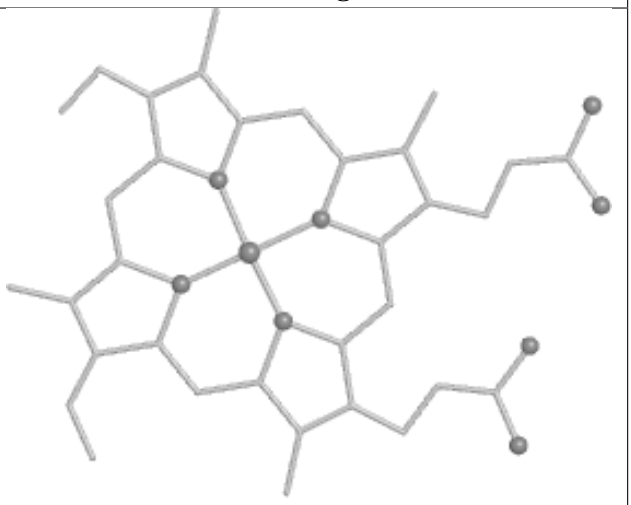
Bond lengths



Bond angles

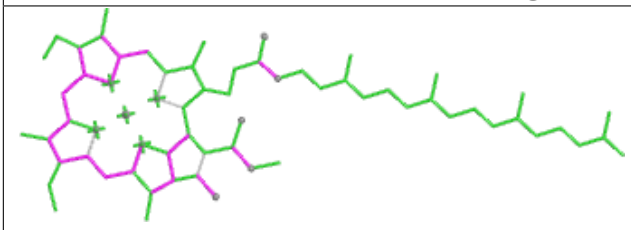


Torsions

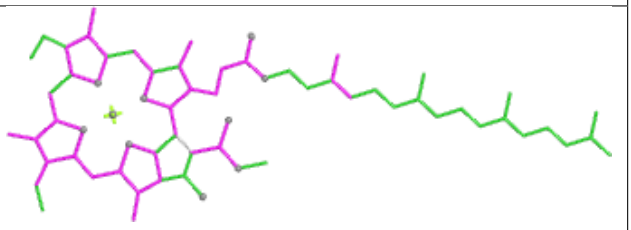


Rings

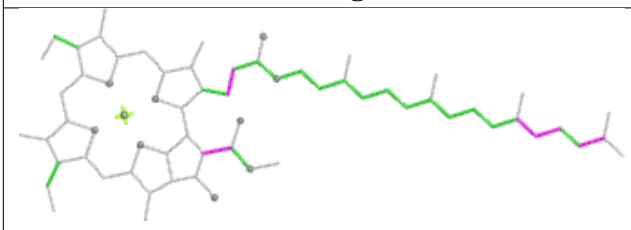
Ligand CLA B 610



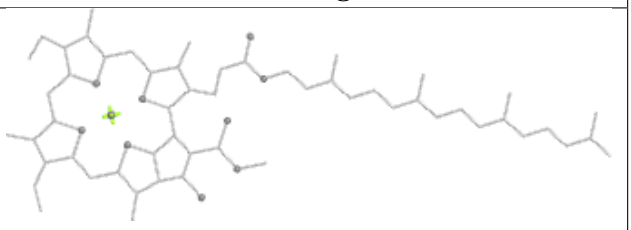
Bond lengths



Bond angles

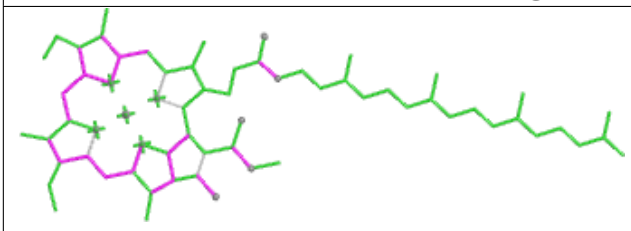


Torsions

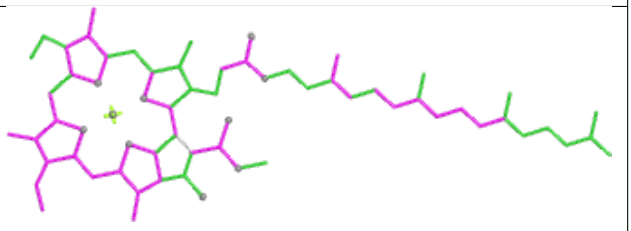


Rings

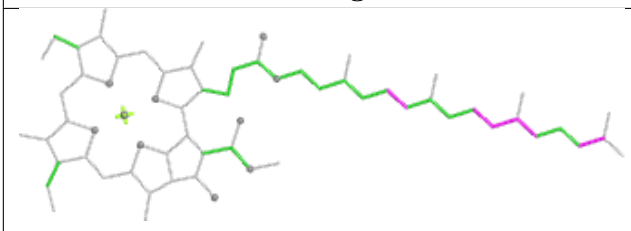
Ligand CLA b 615



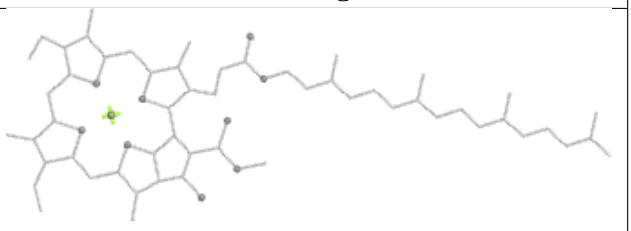
Bond lengths



Bond angles

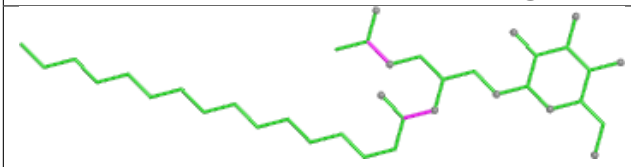


Torsions

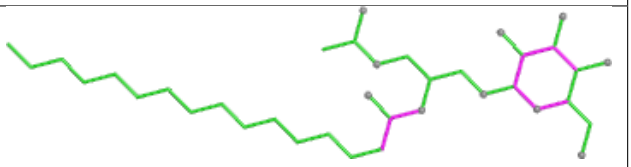


Rings

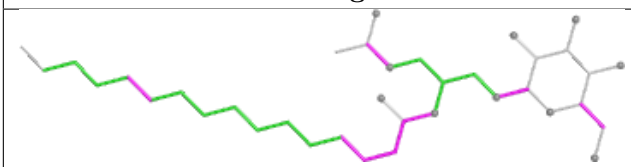
Ligand LMG Z 101



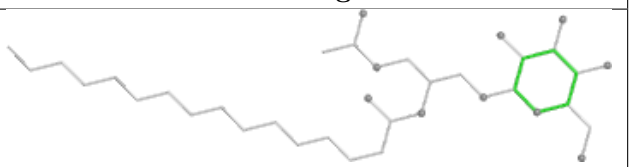
Bond lengths



Bond angles

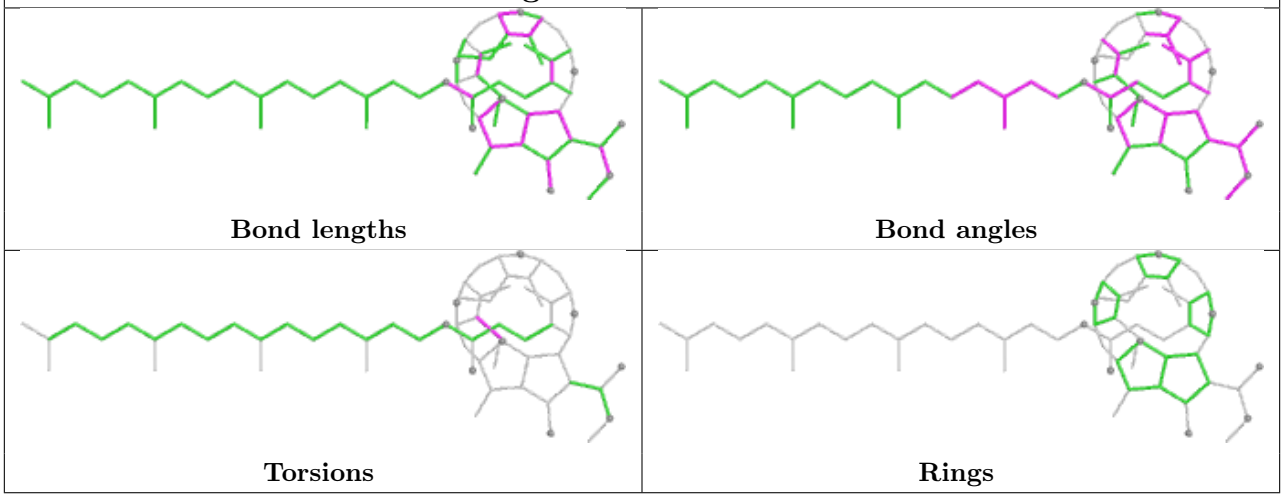


Torsions

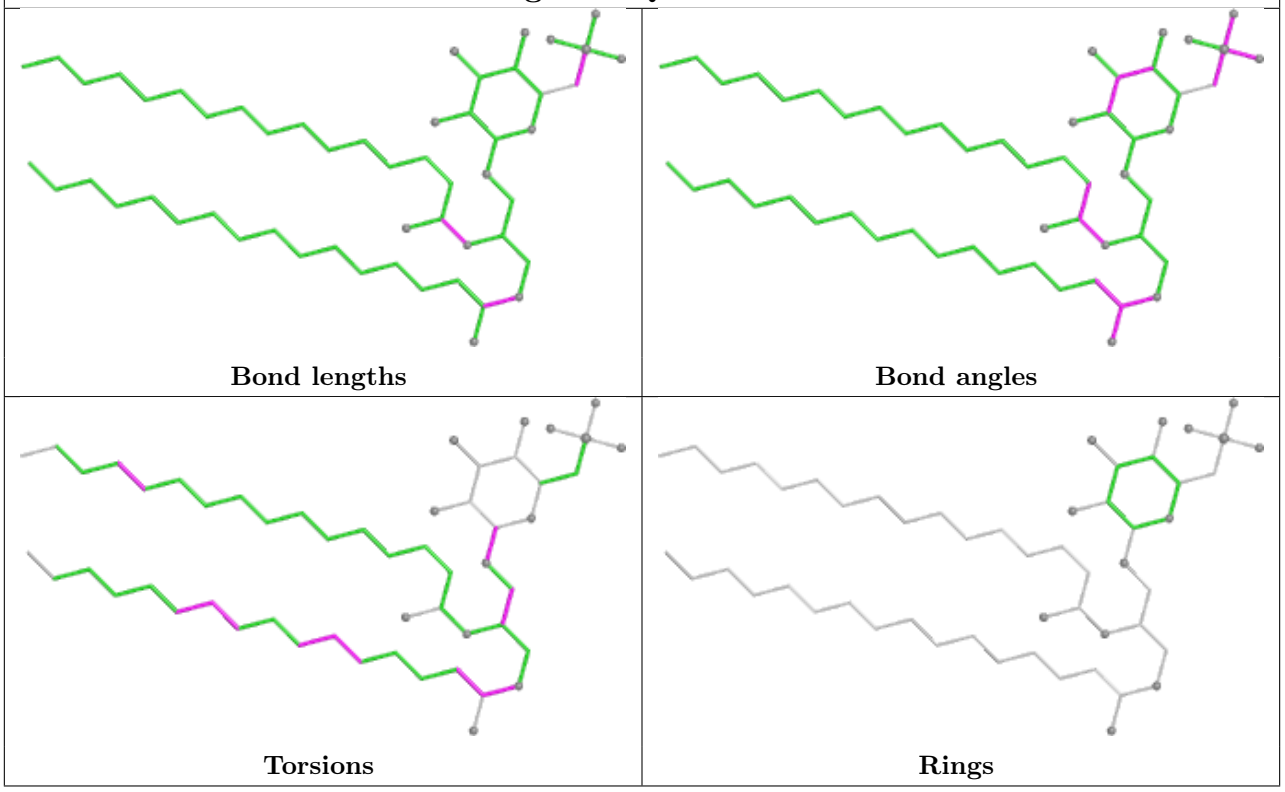


Rings

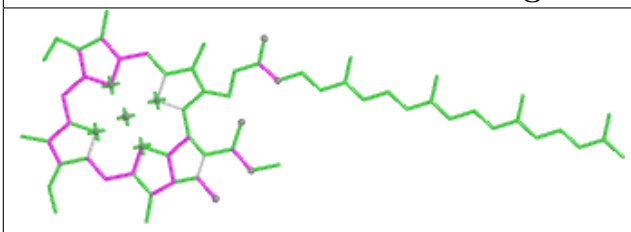
Ligand PHO A 416



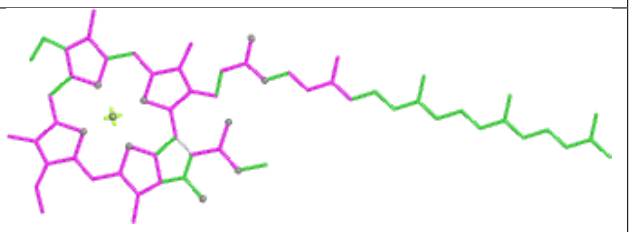
Ligand SQD A 412



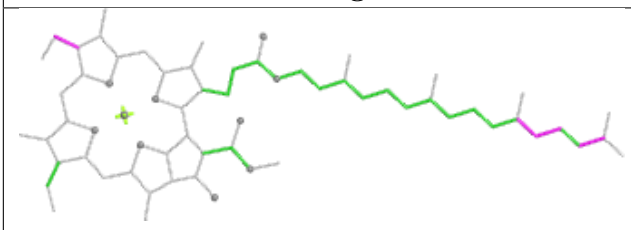
Ligand CLA A 406



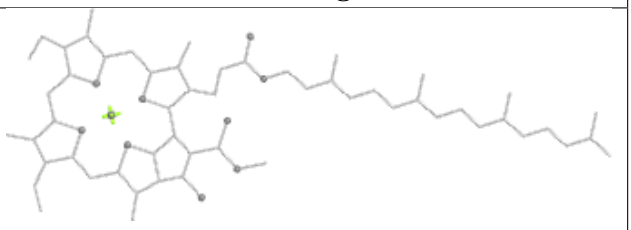
Bond lengths



Bond angles

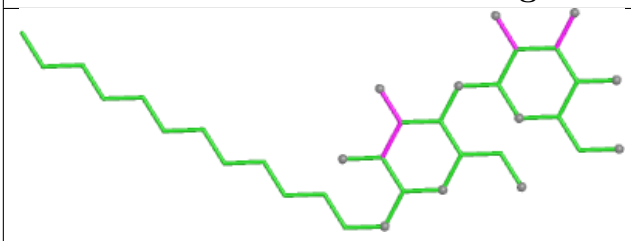


Torsions

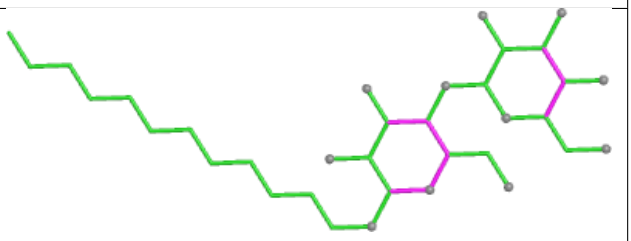


Rings

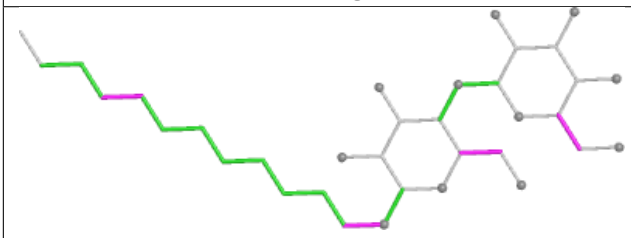
Ligand LMT m 103



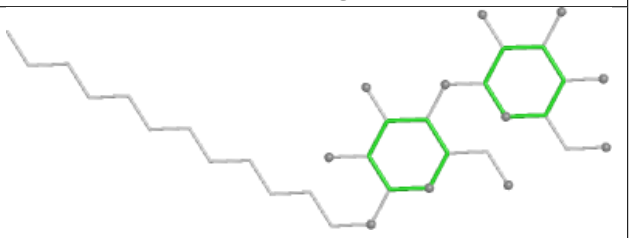
Bond lengths



Bond angles

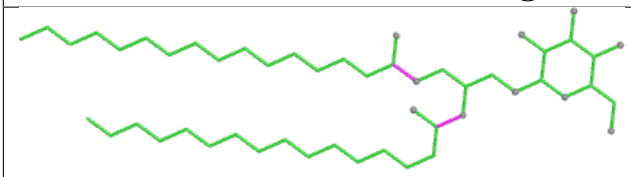


Torsions

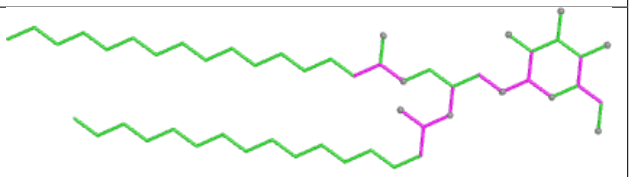


Rings

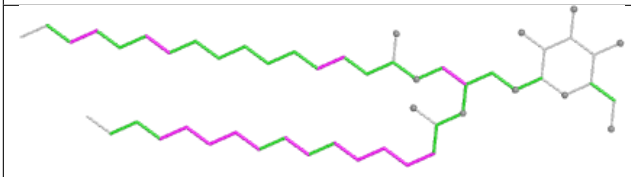
Ligand LMG A 419



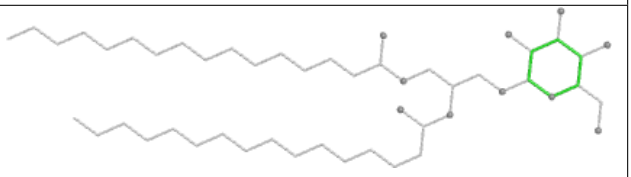
Bond lengths



Bond angles

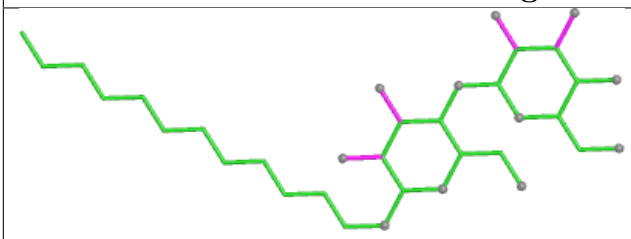


Torsions

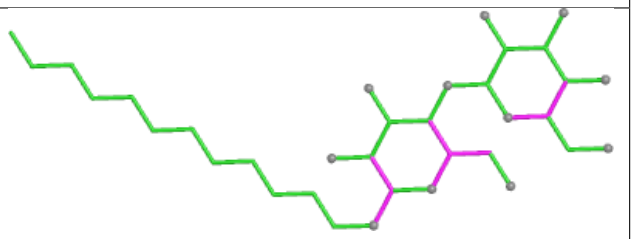


Rings

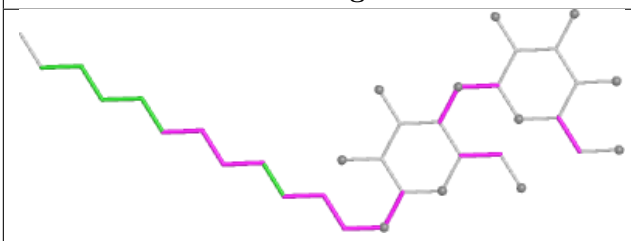
Ligand LMT A 421



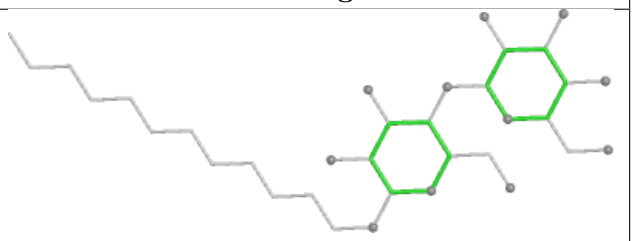
Bond lengths



Bond angles

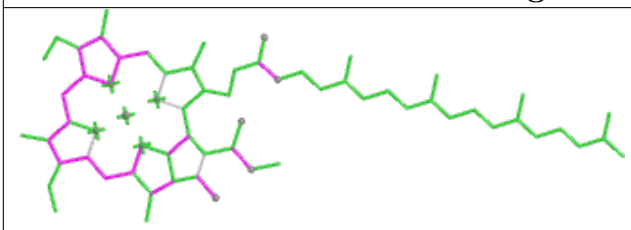


Torsions

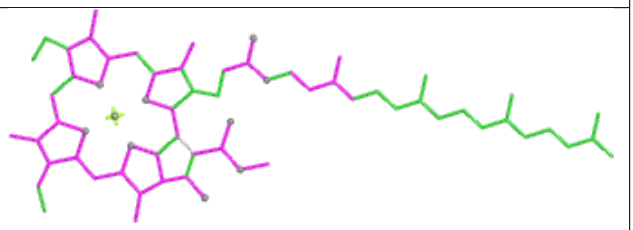


Rings

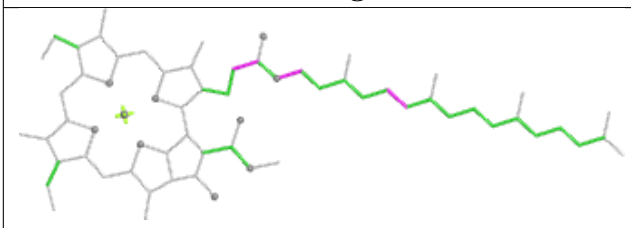
Ligand CLA b 613



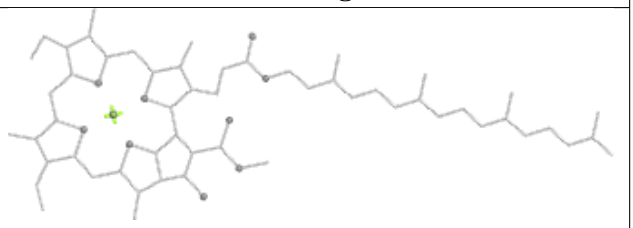
Bond lengths



Bond angles

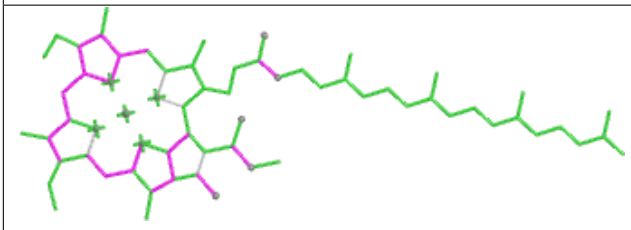


Torsions

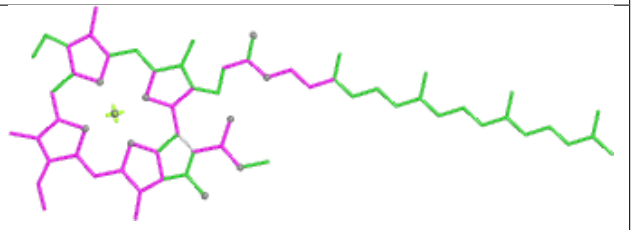


Rings

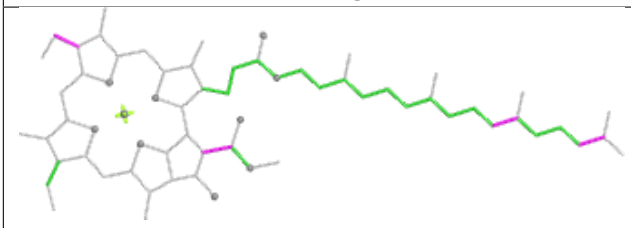
Ligand CLA c 503



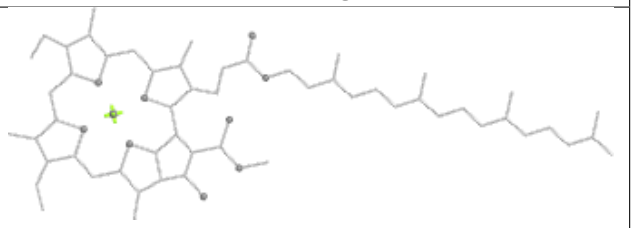
Bond lengths



Bond angles

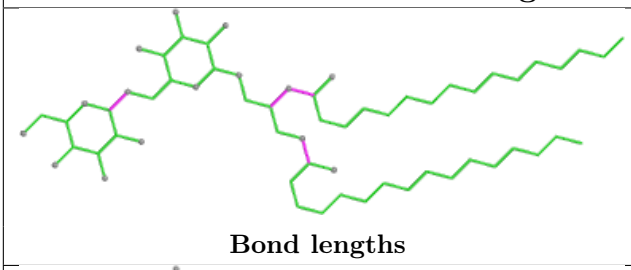


Torsions

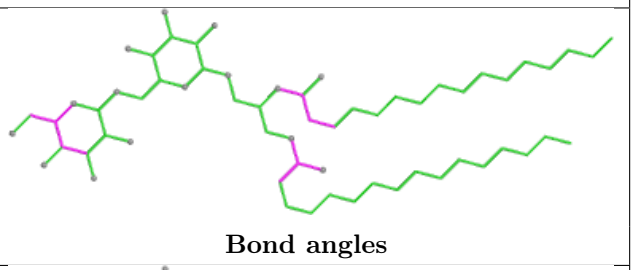


Rings

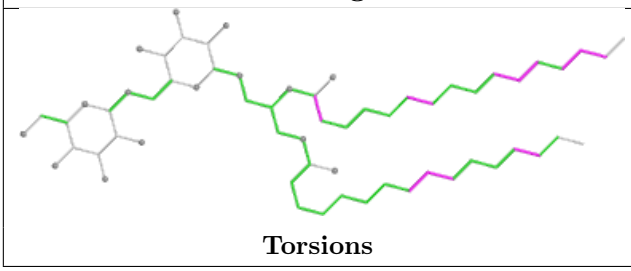
Ligand DGD H 102



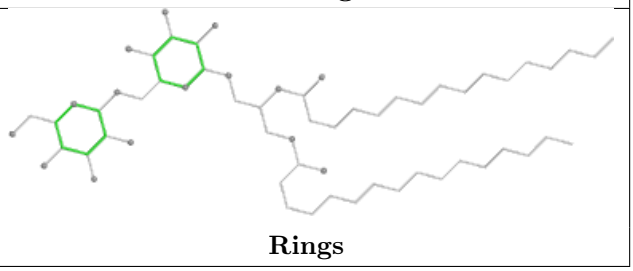
Bond lengths



Bond angles

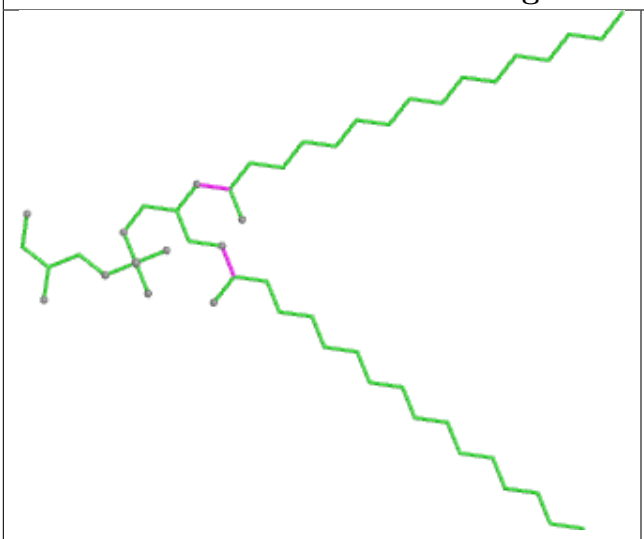


Torsions

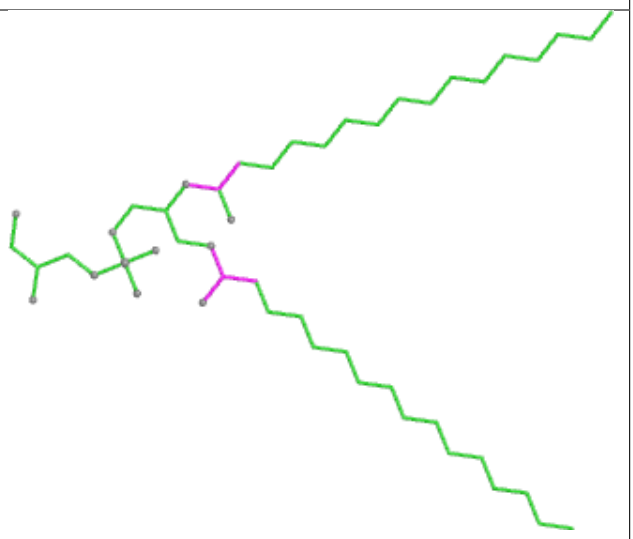


Rings

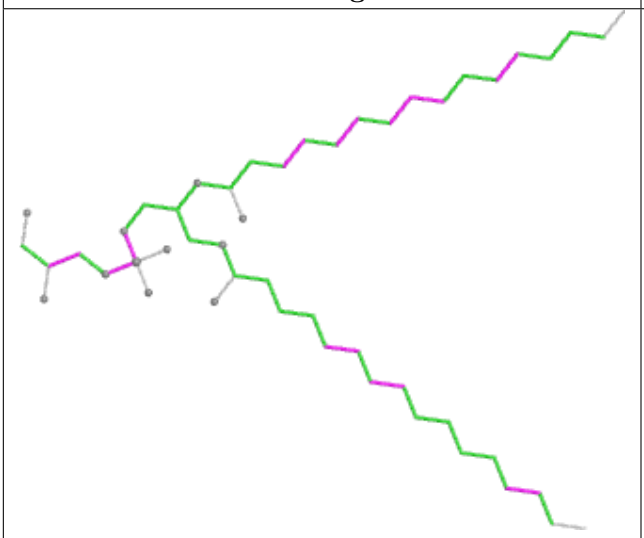
Ligand LHG D 406



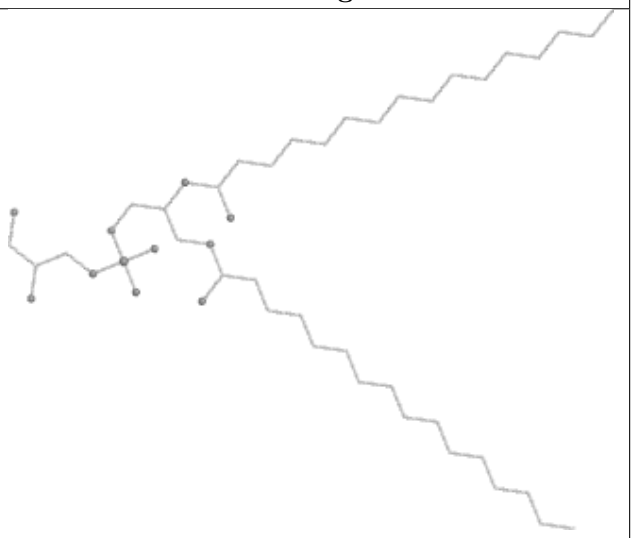
Bond lengths



Bond angles

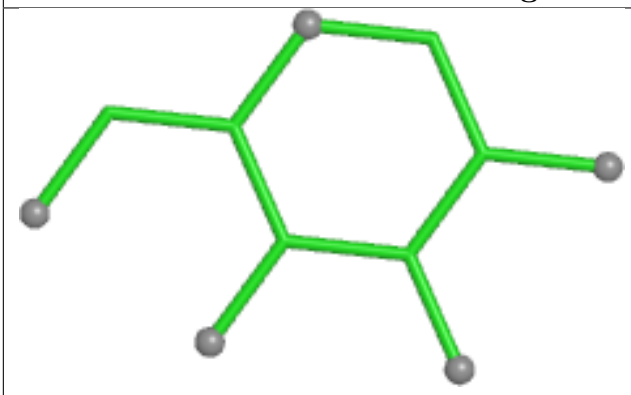


Torsions

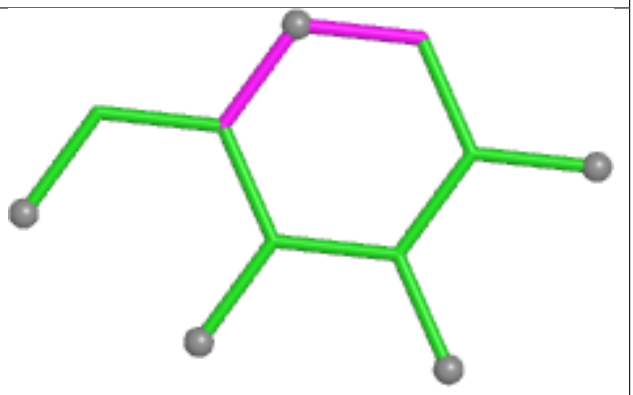


Rings

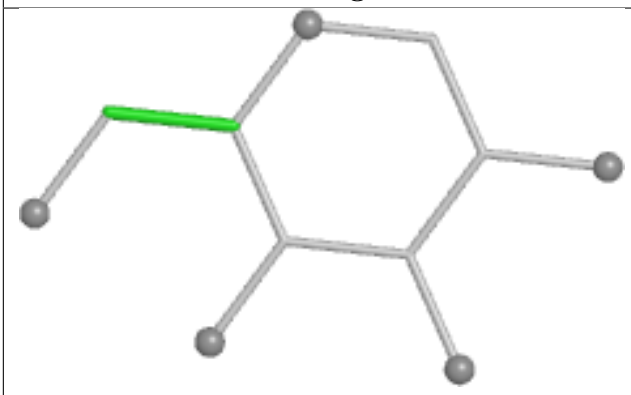
Ligand HTG V 202



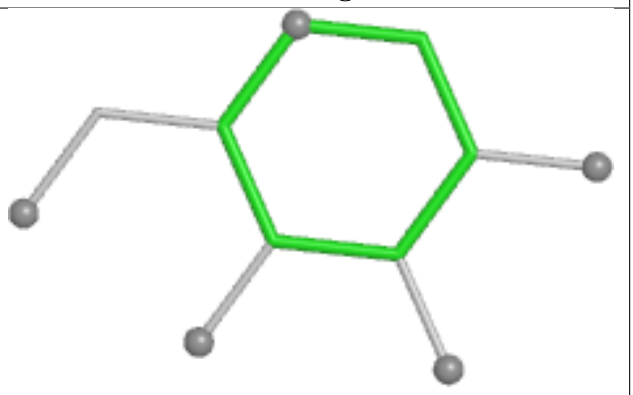
Bond lengths



Bond angles

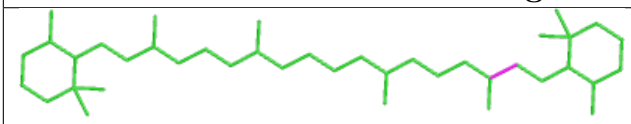


Torsions

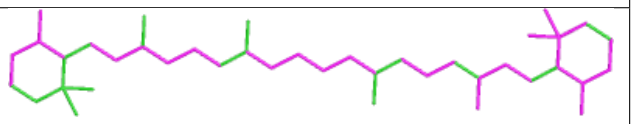


Rings

Ligand BCR d 403



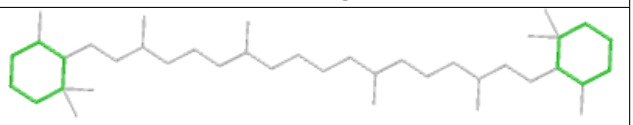
Bond lengths



Bond angles

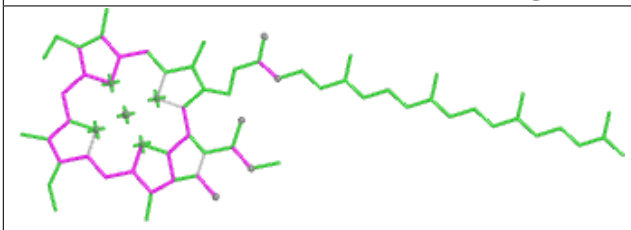


Torsions

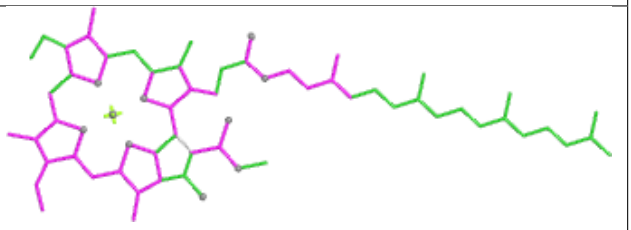


Rings

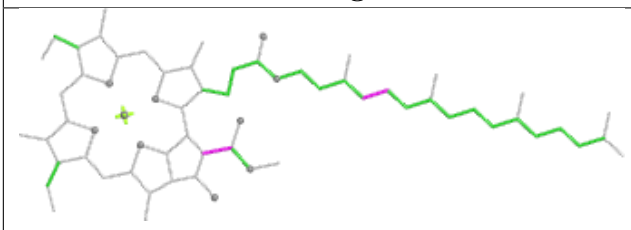
Ligand CLA b 607



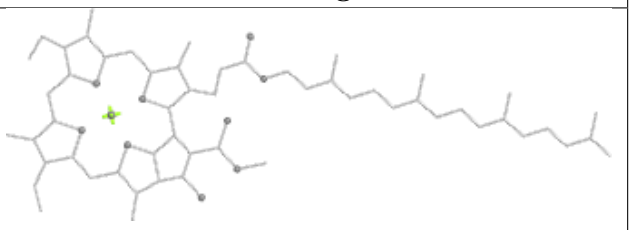
Bond lengths



Bond angles

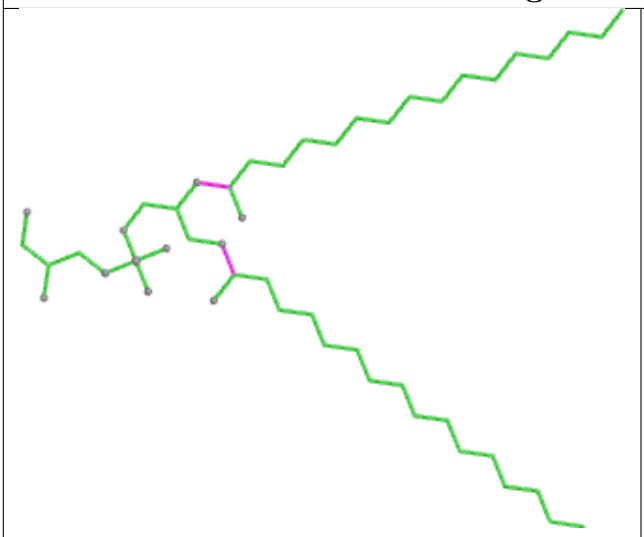


Torsions

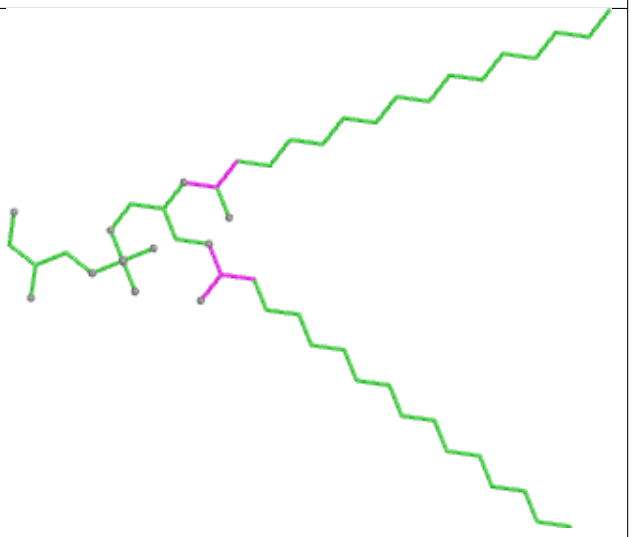


Rings

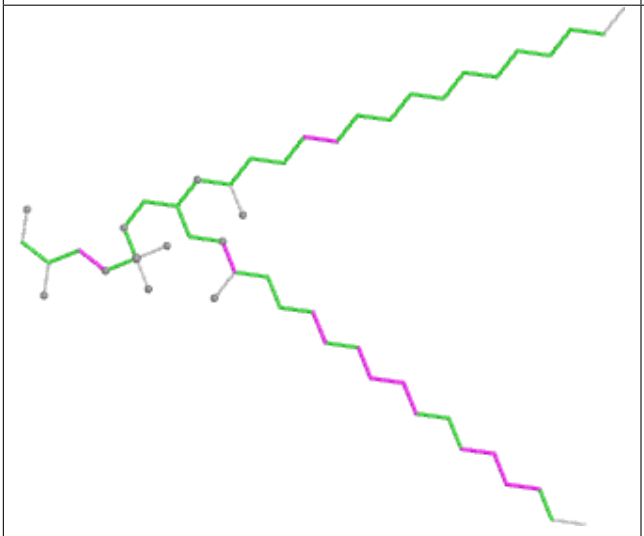
Ligand LHG d 406



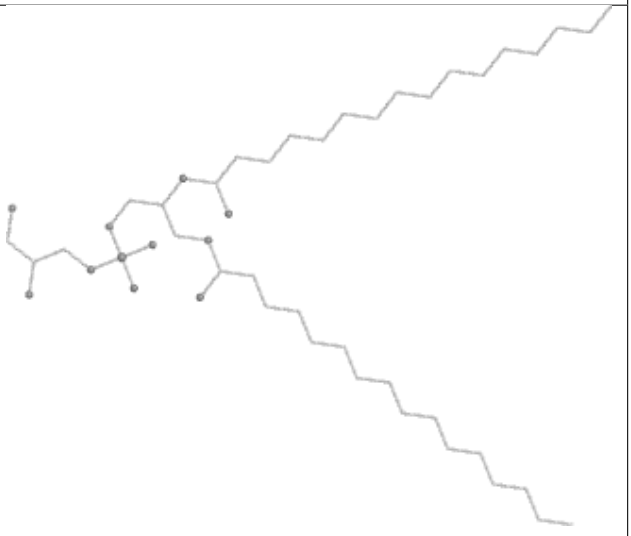
Bond lengths



Bond angles

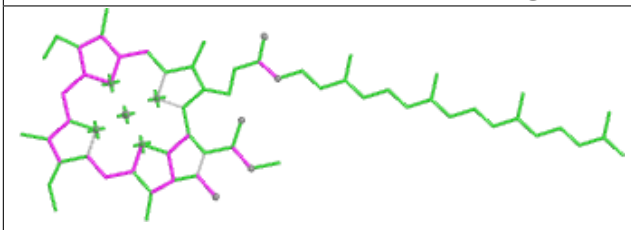


Torsions

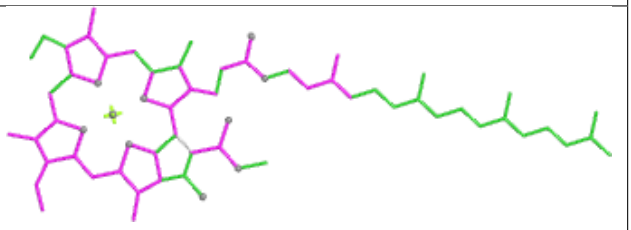


Rings

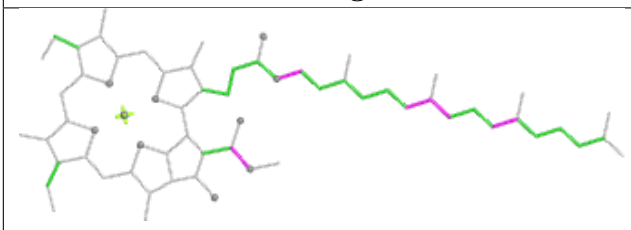
Ligand CLA C 513



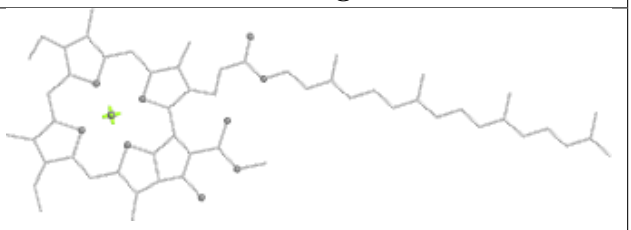
Bond lengths



Bond angles

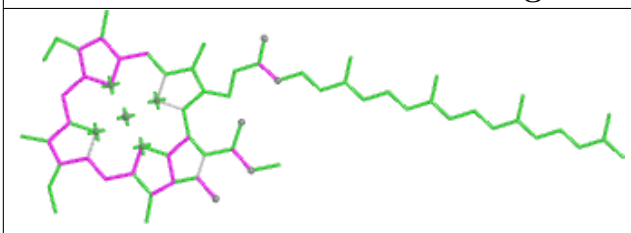


Torsions

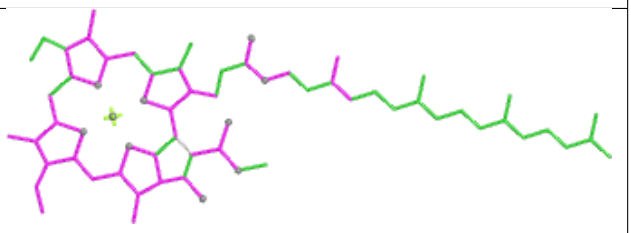


Rings

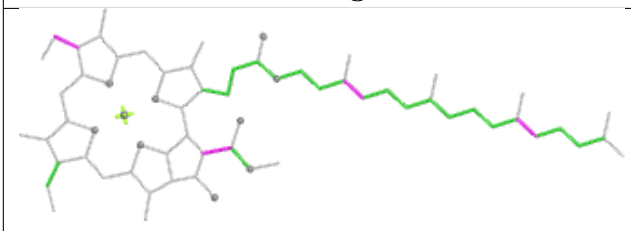
Ligand CLA C 504



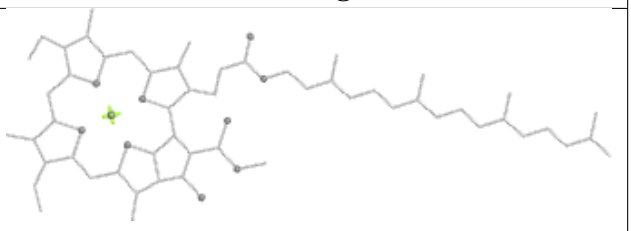
Bond lengths



Bond angles

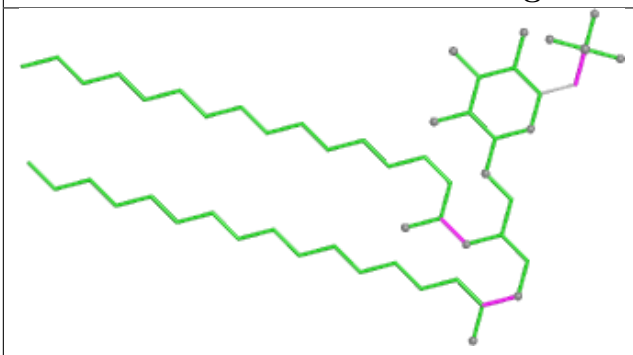


Torsions

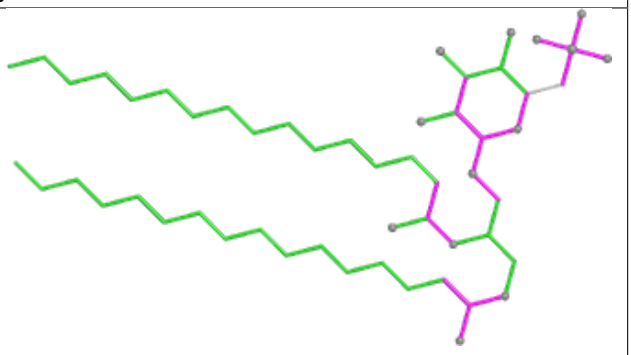


Rings

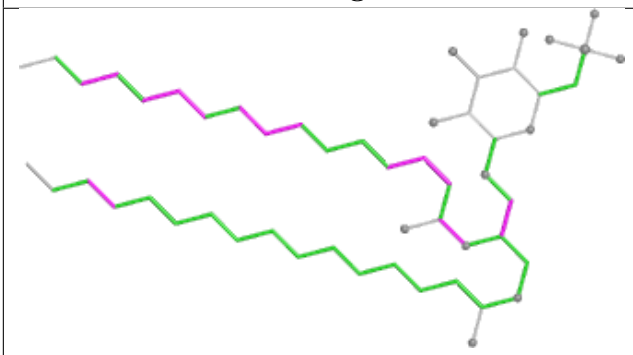
Ligand SQD A 410



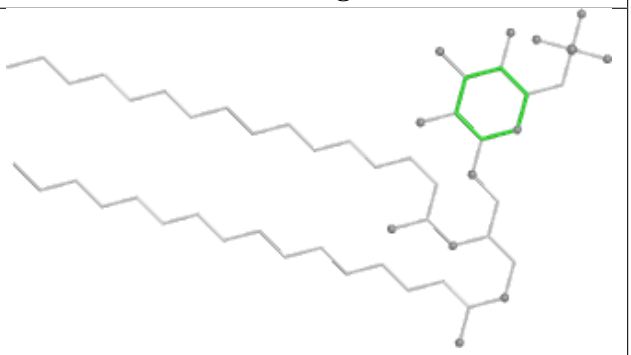
Bond lengths



Bond angles

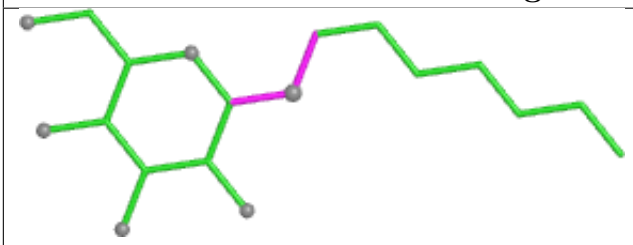


Torsions

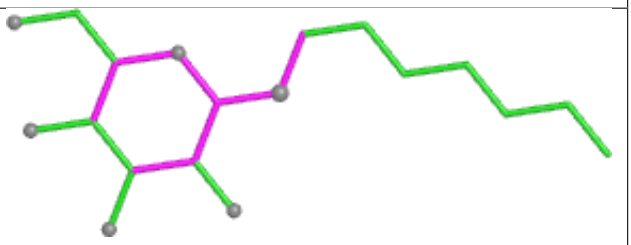


Rings

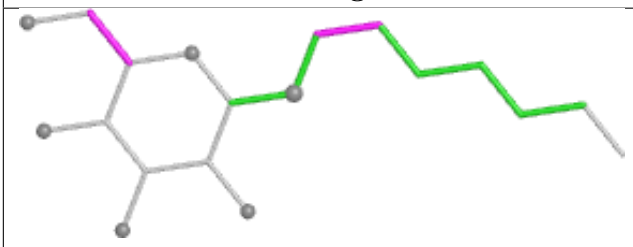
Ligand HTG b 625



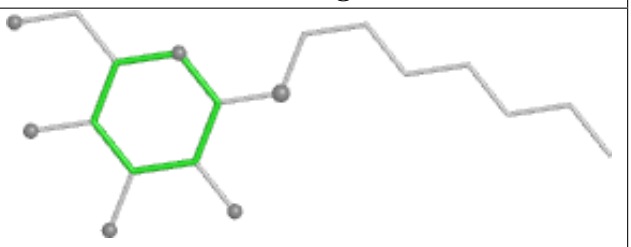
Bond lengths



Bond angles

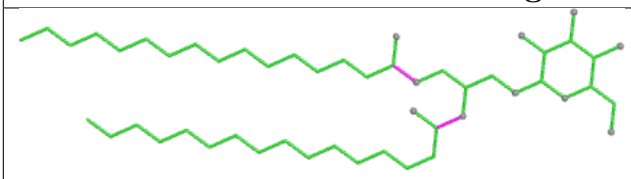


Torsions

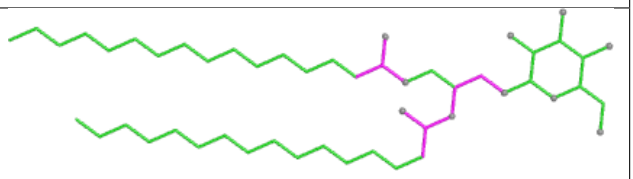


Rings

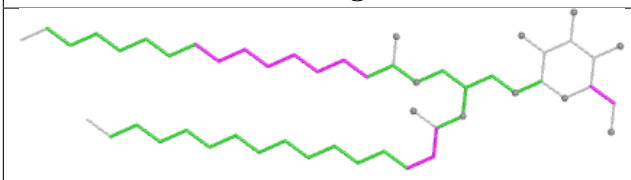
Ligand LMG c 520



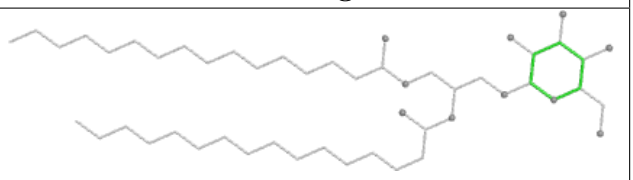
Bond lengths



Bond angles

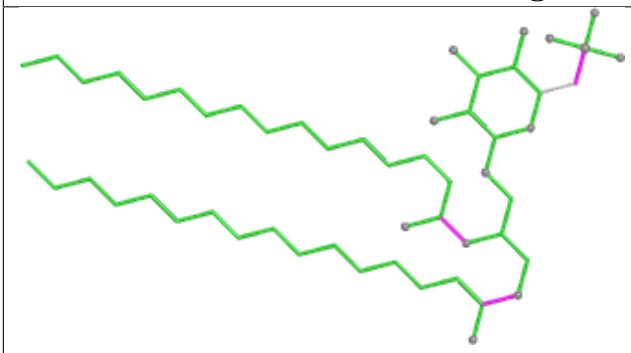


Torsions

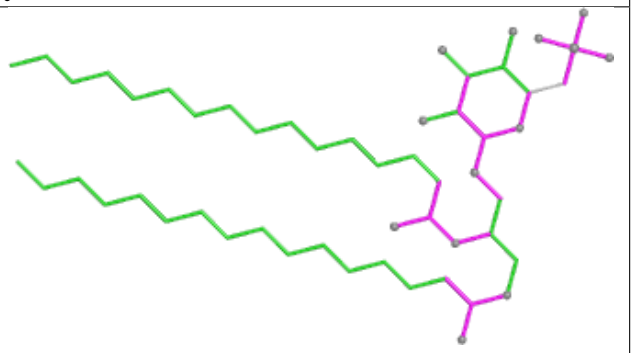


Rings

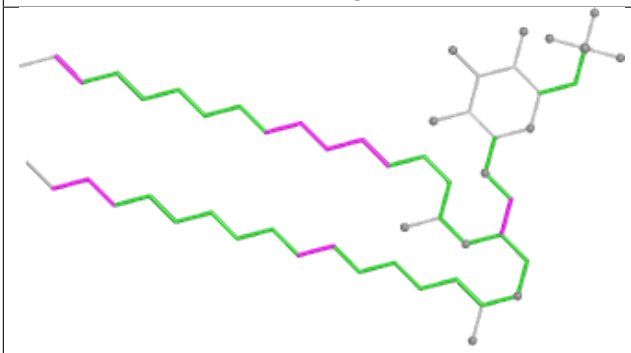
Ligand SQD a 411



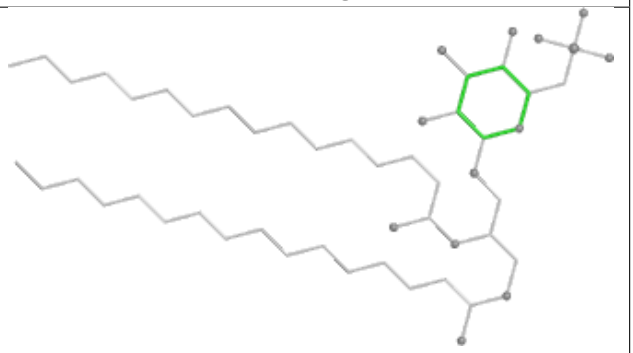
Bond lengths



Bond angles

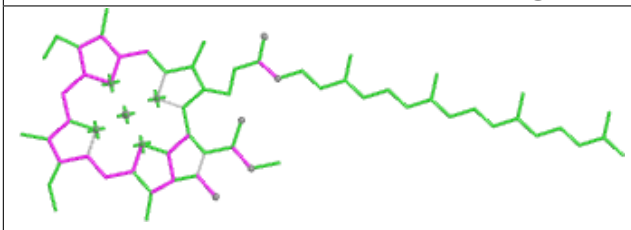


Torsions

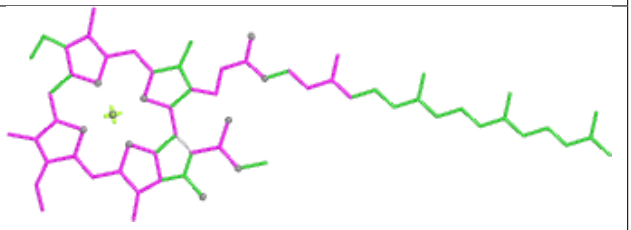


Rings

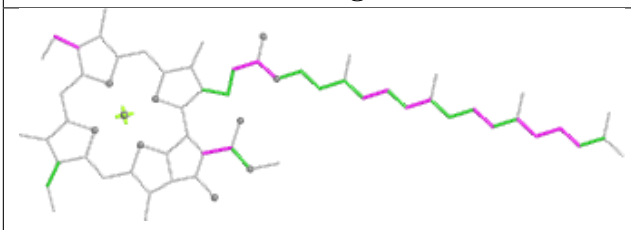
Ligand CLA c 513



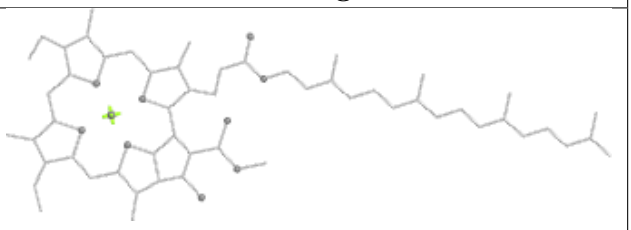
Bond lengths



Bond angles

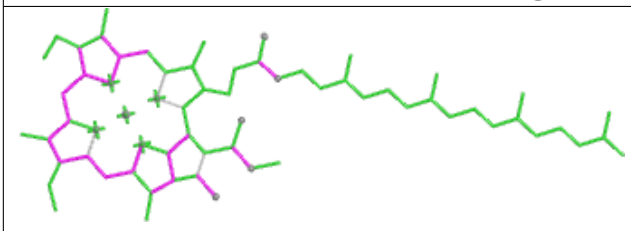


Torsions

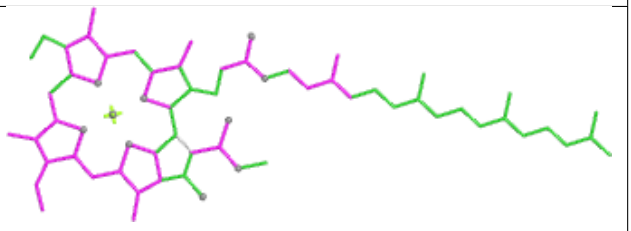


Rings

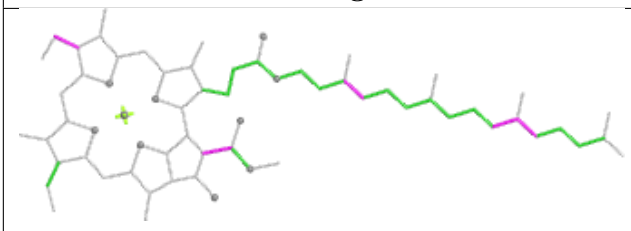
Ligand CLA c 506



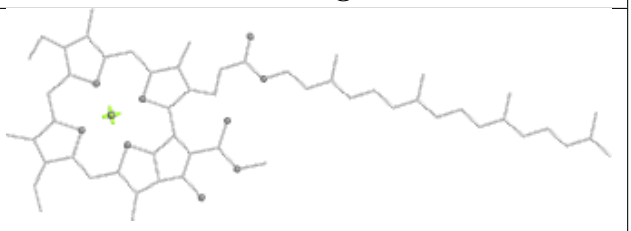
Bond lengths



Bond angles

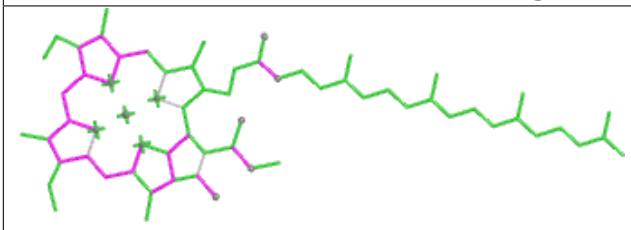


Torsions

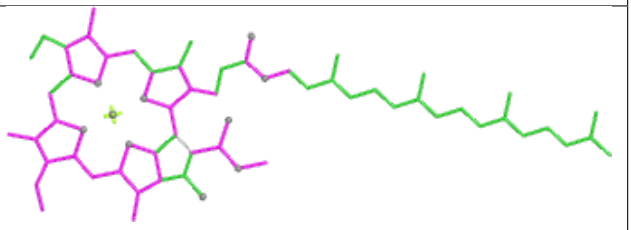


Rings

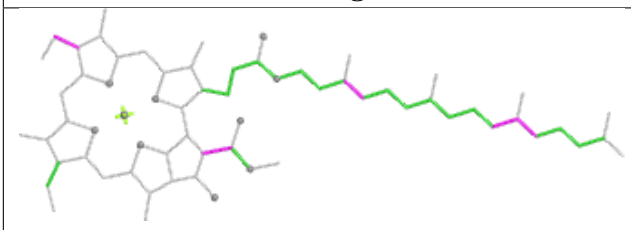
Ligand CLA c 505



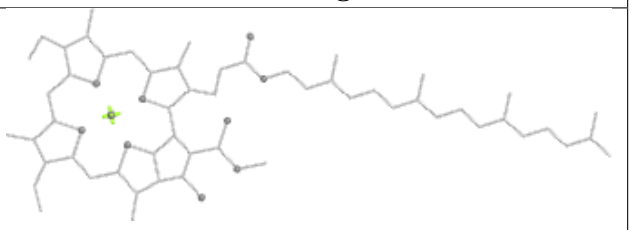
Bond lengths



Bond angles

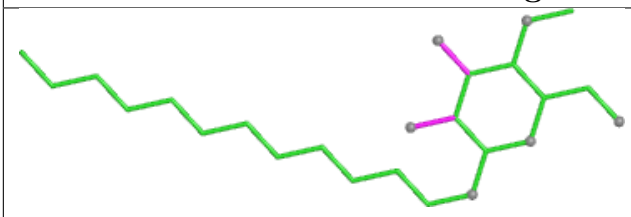


Torsions

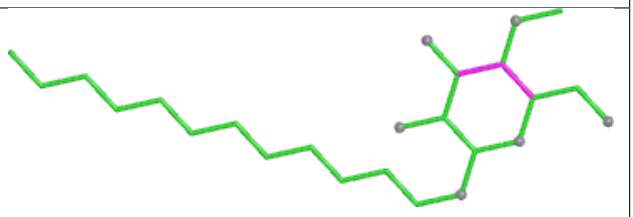


Rings

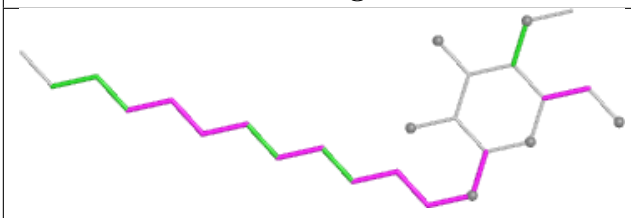
Ligand LMT b 627



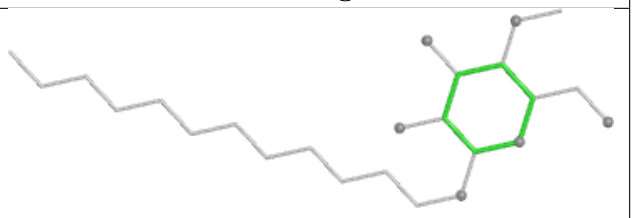
Bond lengths



Bond angles

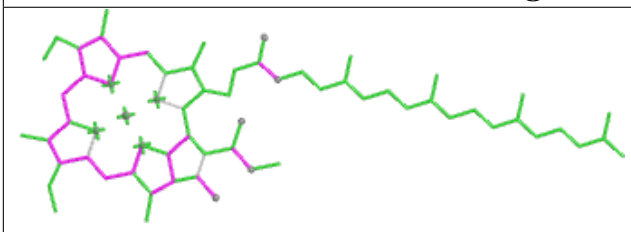


Torsions

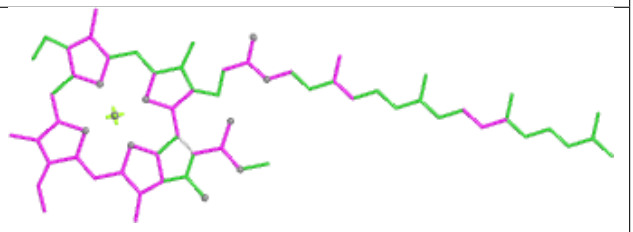


Rings

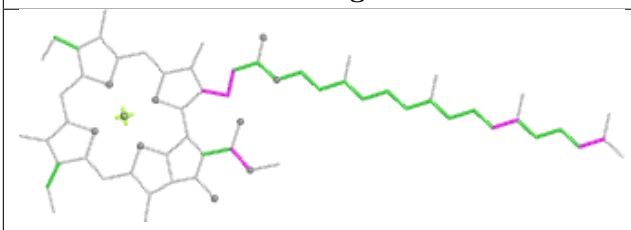
Ligand CLA C 501



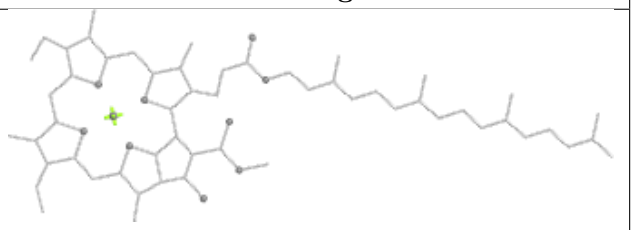
Bond lengths



Bond angles

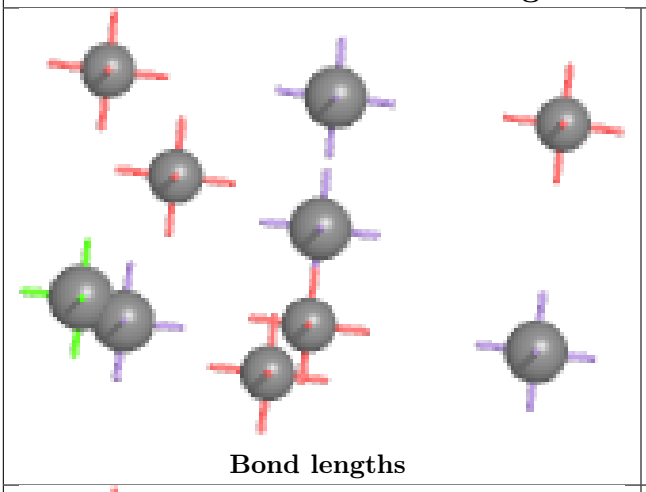


Torsions

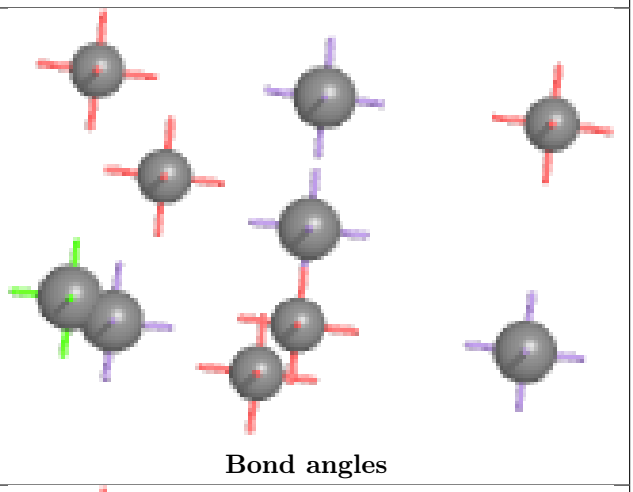


Rings

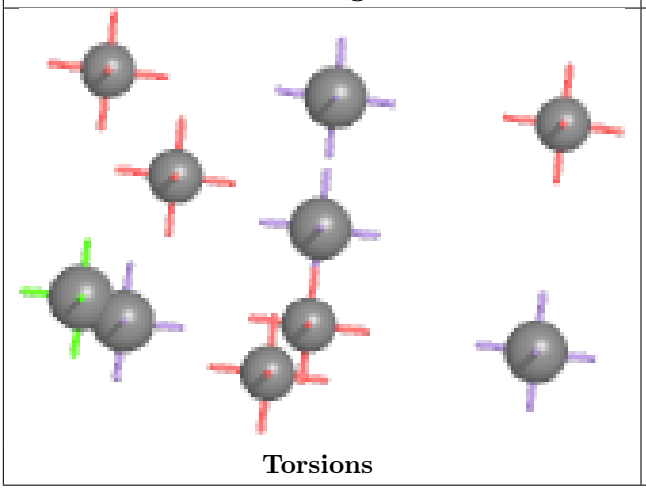
Ligand OEX A 413



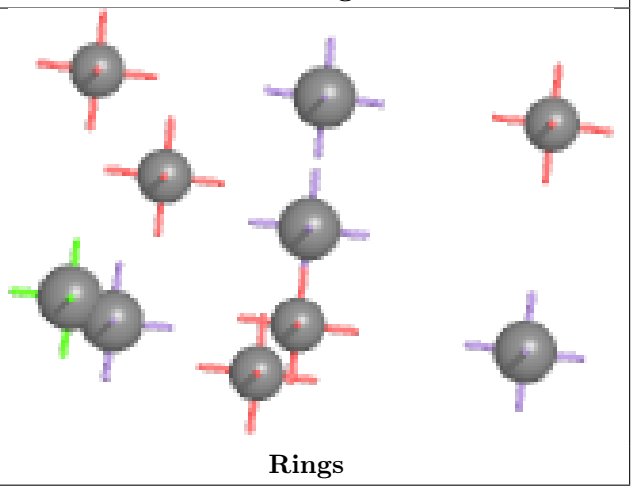
Bond lengths



Bond angles

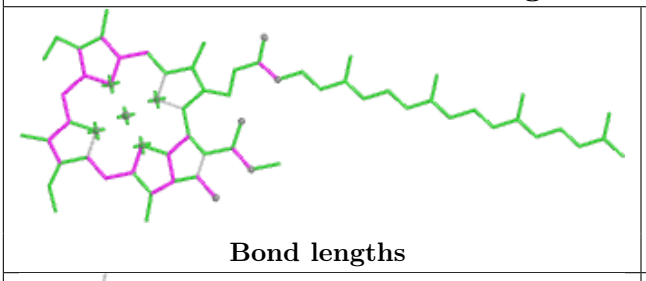


Torsions

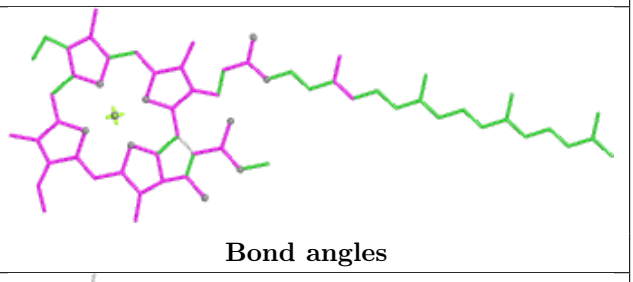


Rings

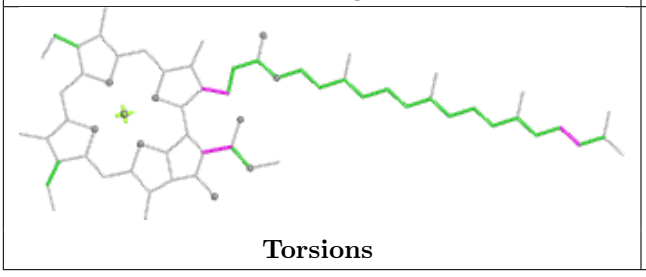
Ligand CLA A 405



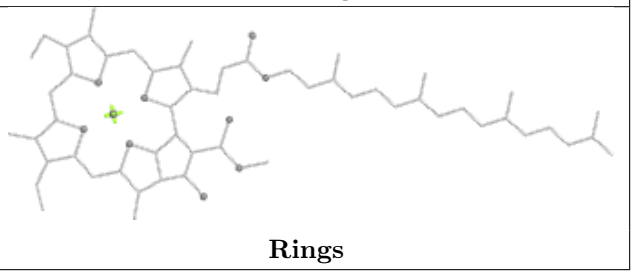
Bond lengths



Bond angles

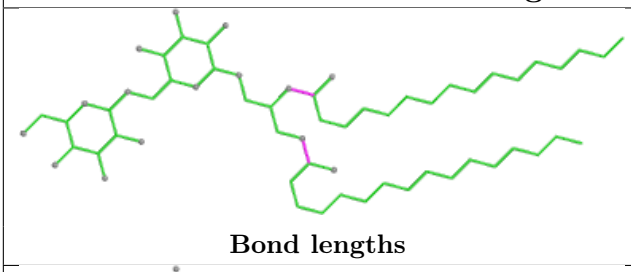


Torsions

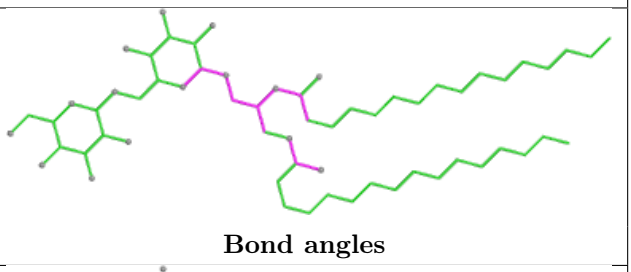


Rings

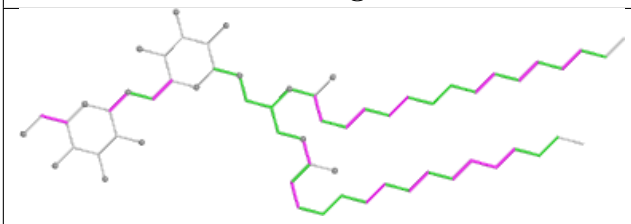
Ligand DGD c 517



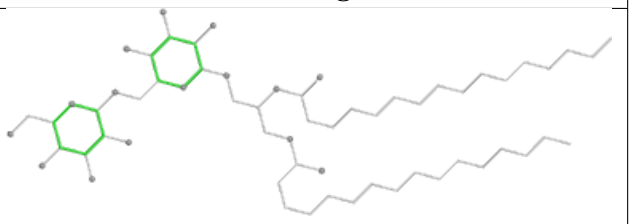
Bond lengths



Bond angles

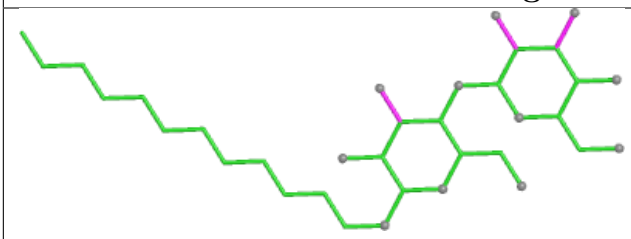


Torsions

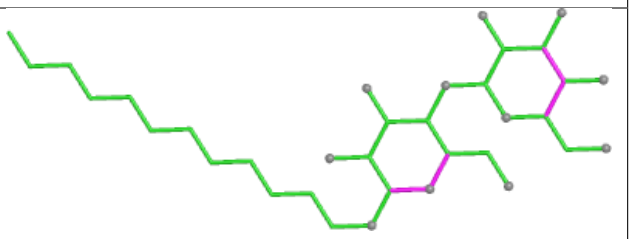


Rings

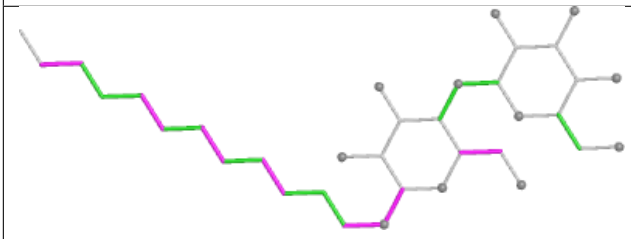
Ligand LMT F 101



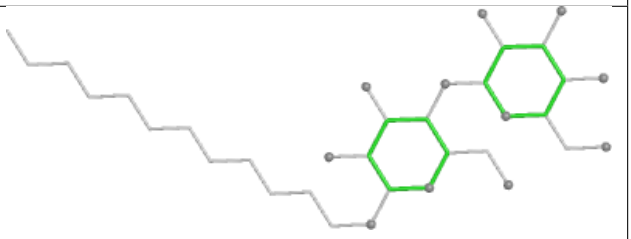
Bond lengths



Bond angles

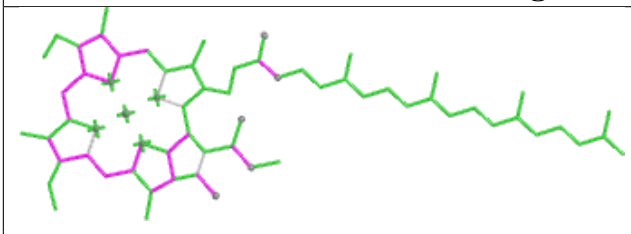


Torsions

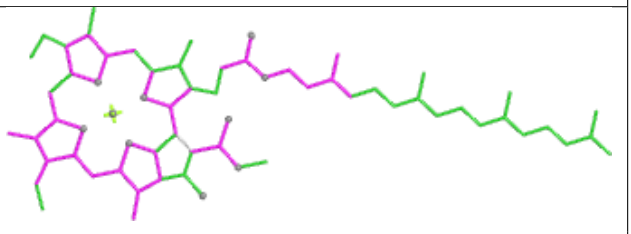


Rings

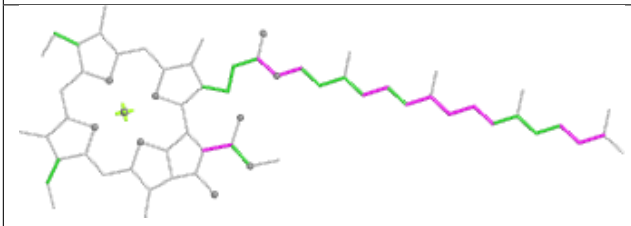
Ligand CLA c 510



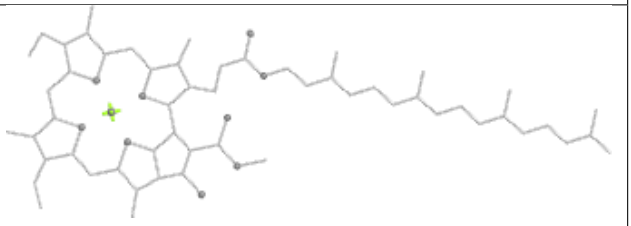
Bond lengths



Bond angles

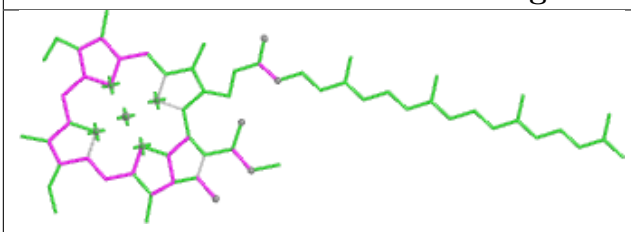


Torsions

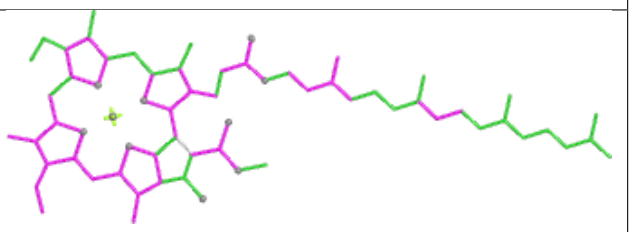


Rings

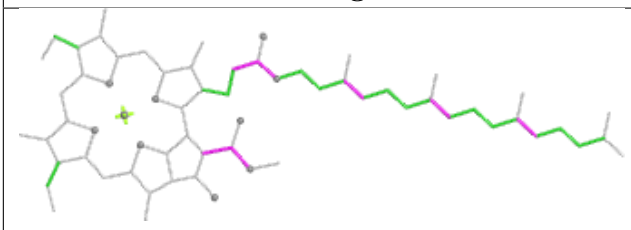
Ligand CLA c 511



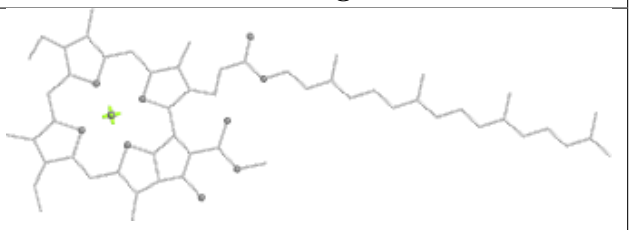
Bond lengths



Bond angles

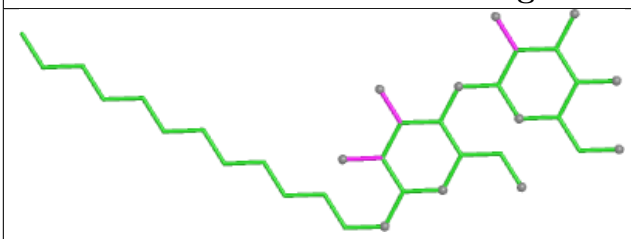


Torsions

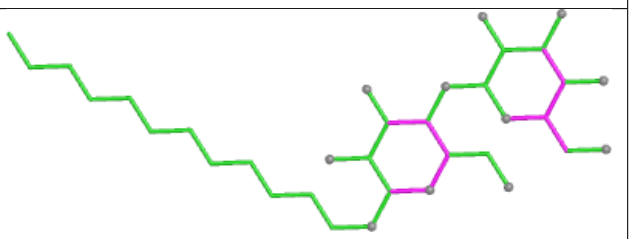


Rings

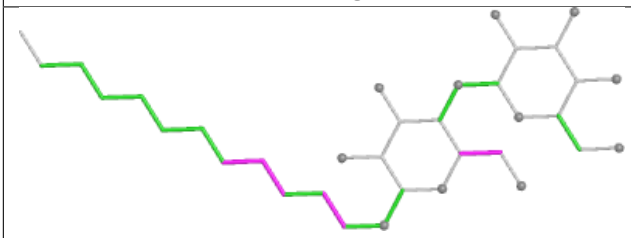
Ligand LMT M 101



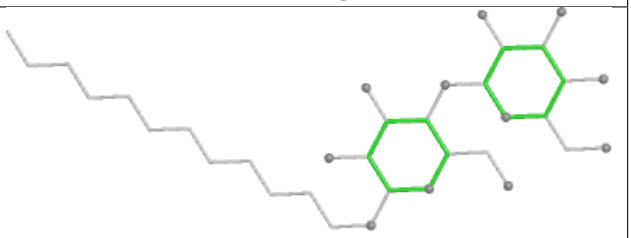
Bond lengths



Bond angles



Torsions

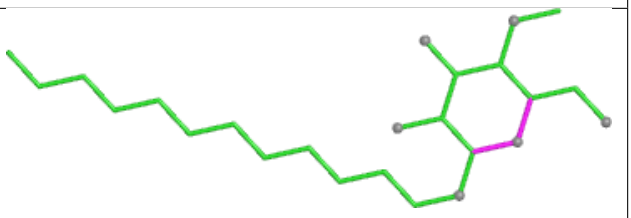


Rings

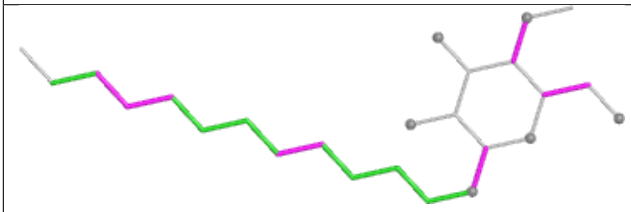
Ligand LMT b 621



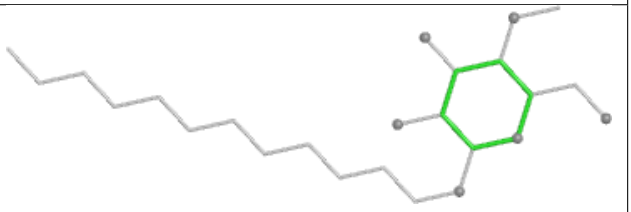
Bond lengths



Bond angles

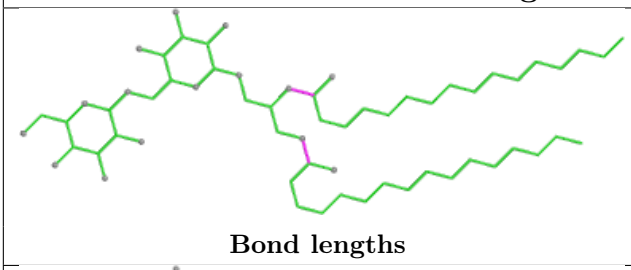


Torsions

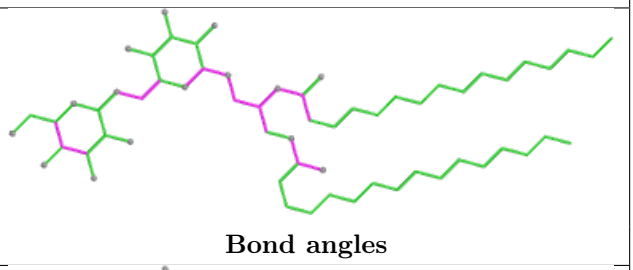


Rings

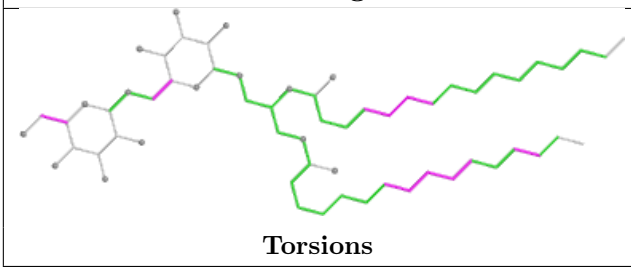
Ligand DGD C 515



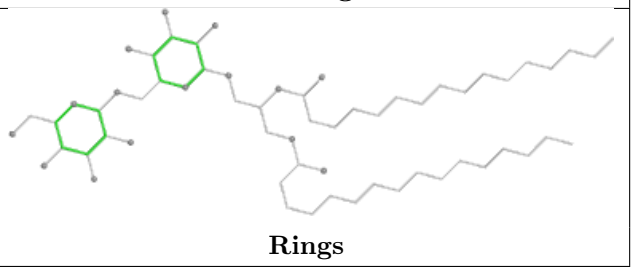
Bond lengths



Bond angles

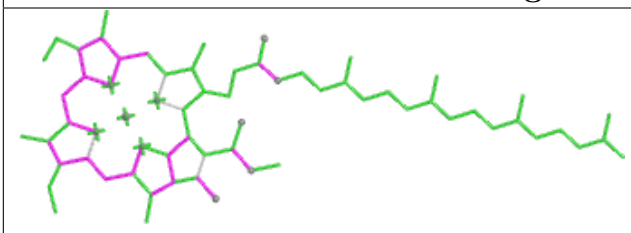


Torsions

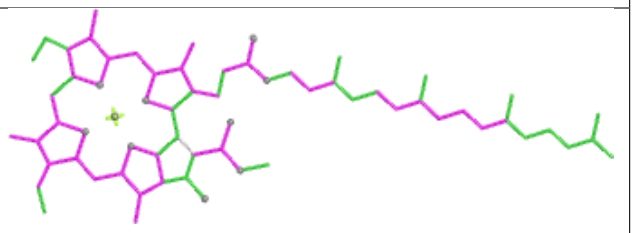


Rings

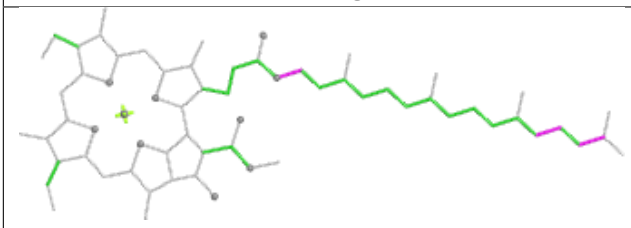
Ligand CLA B 608



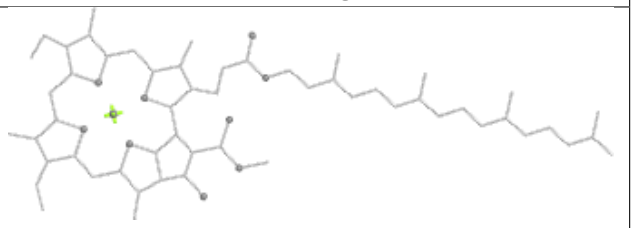
Bond lengths



Bond angles

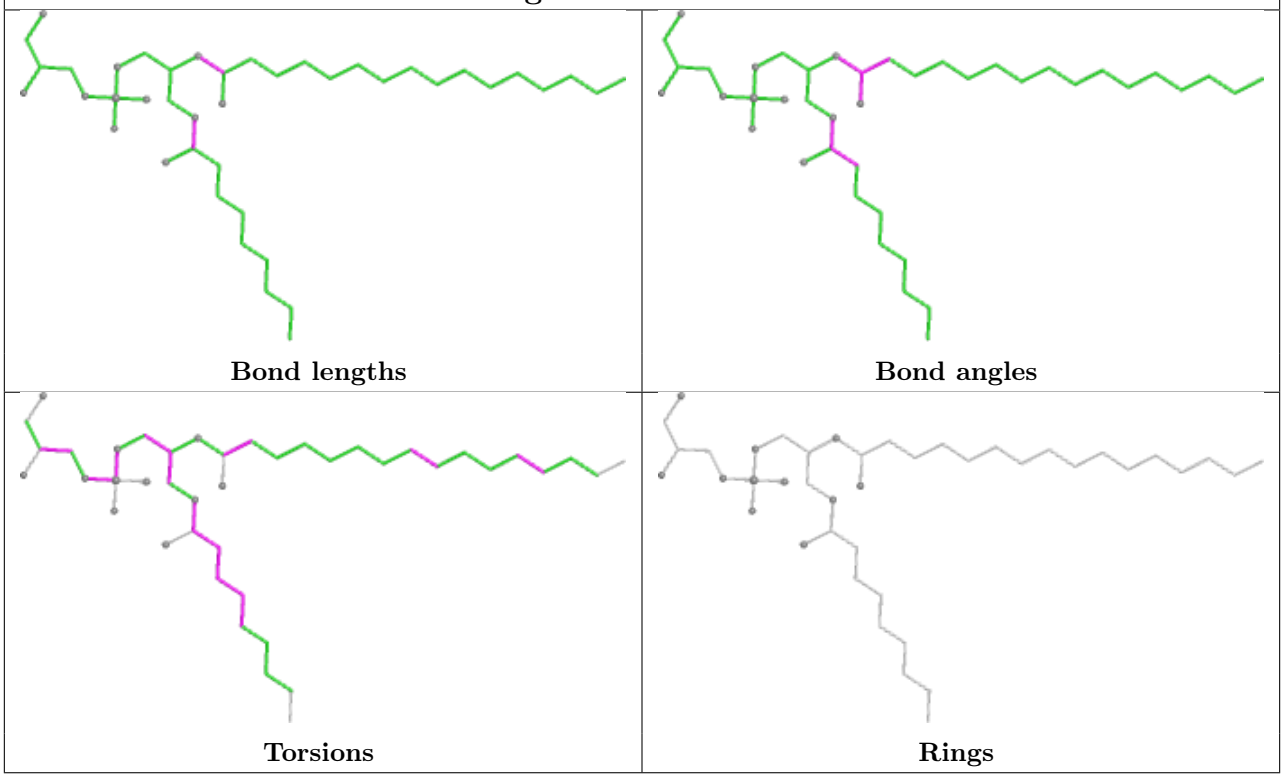


Torsions

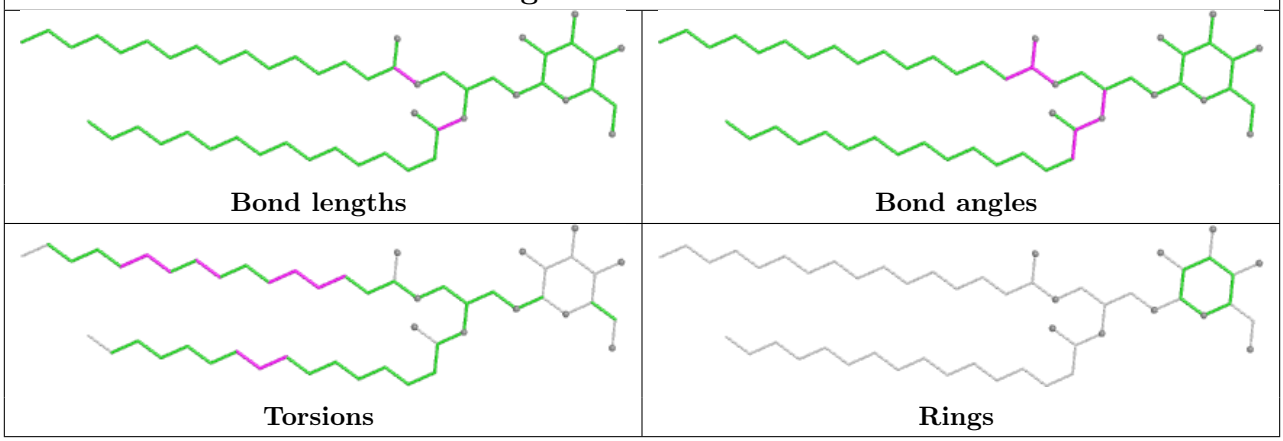


Rings

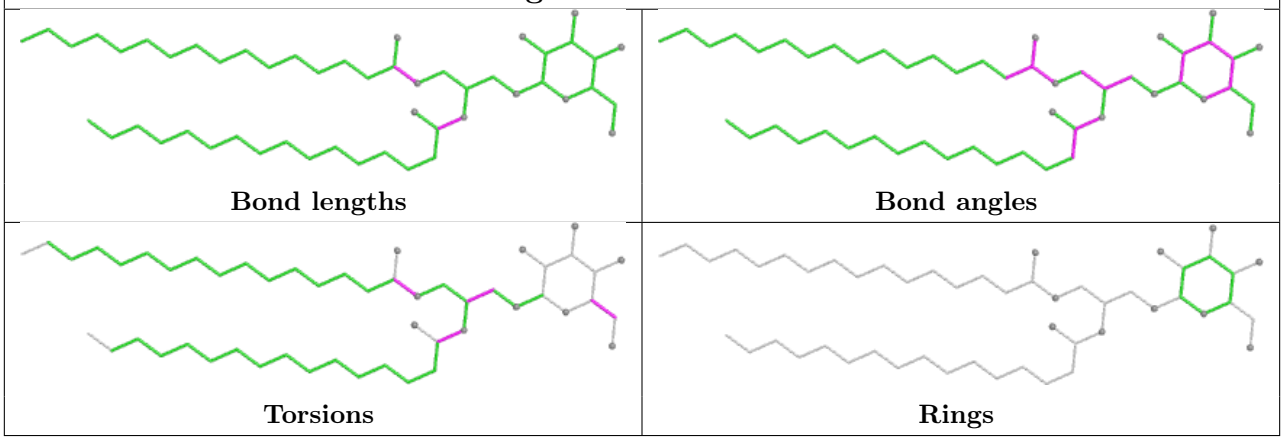
Ligand LHG E 101



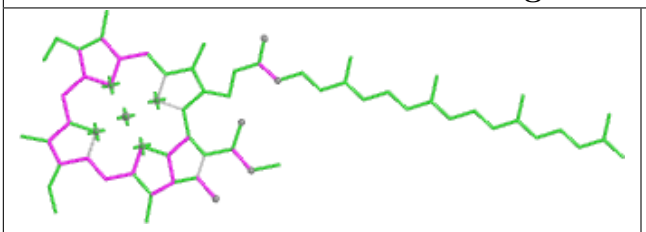
Ligand LMG C 518



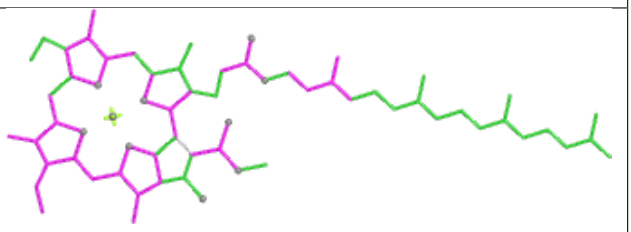
Ligand LMG c 521



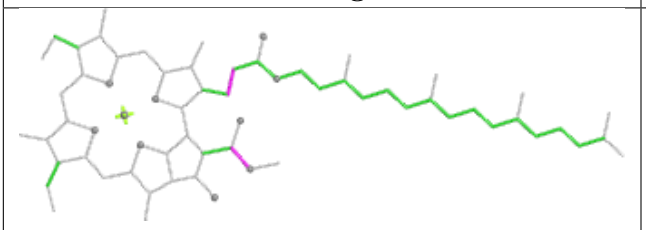
Ligand CLA C 503



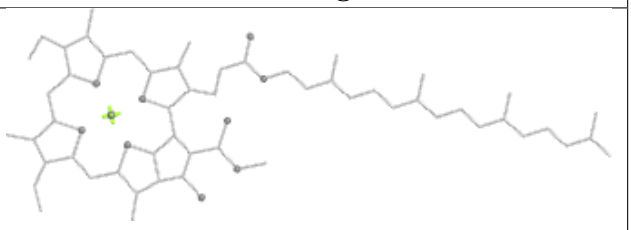
Bond lengths



Bond angles

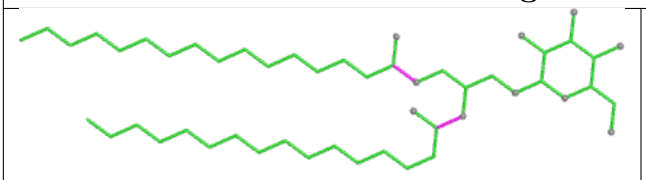


Torsions

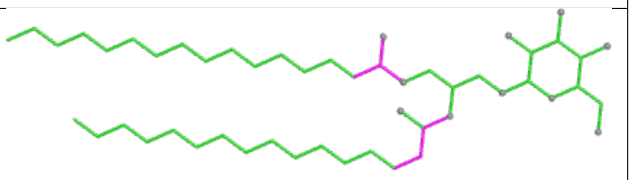


Rings

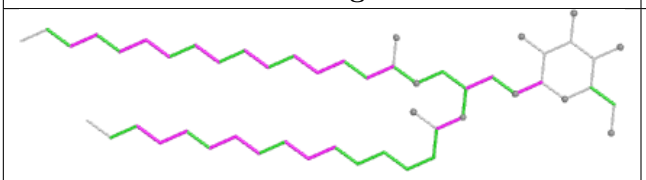
Ligand LMG B 621



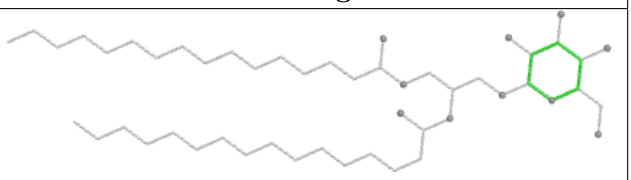
Bond lengths



Bond angles

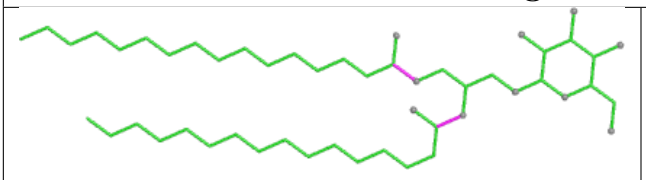


Torsions

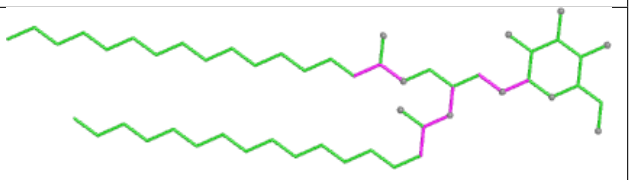


Rings

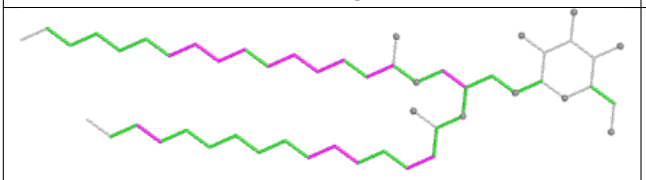
Ligand LMG a 418



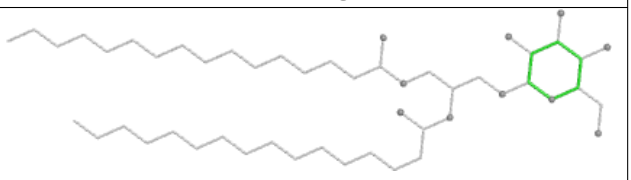
Bond lengths



Bond angles

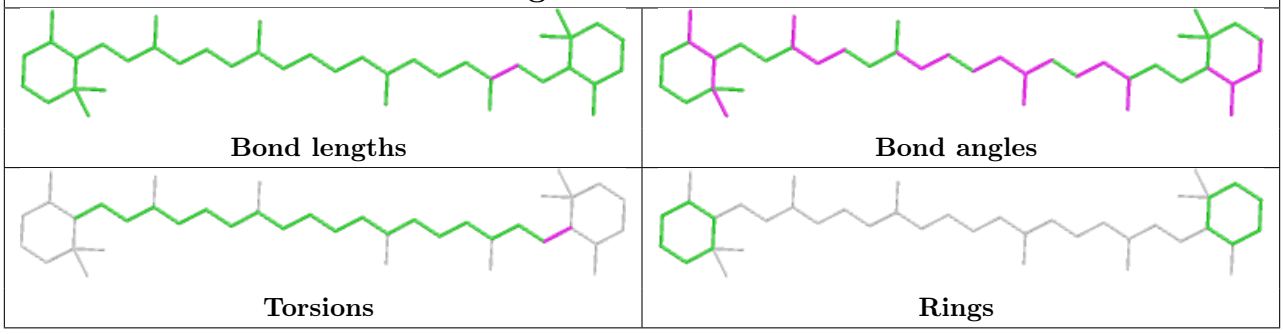


Torsions

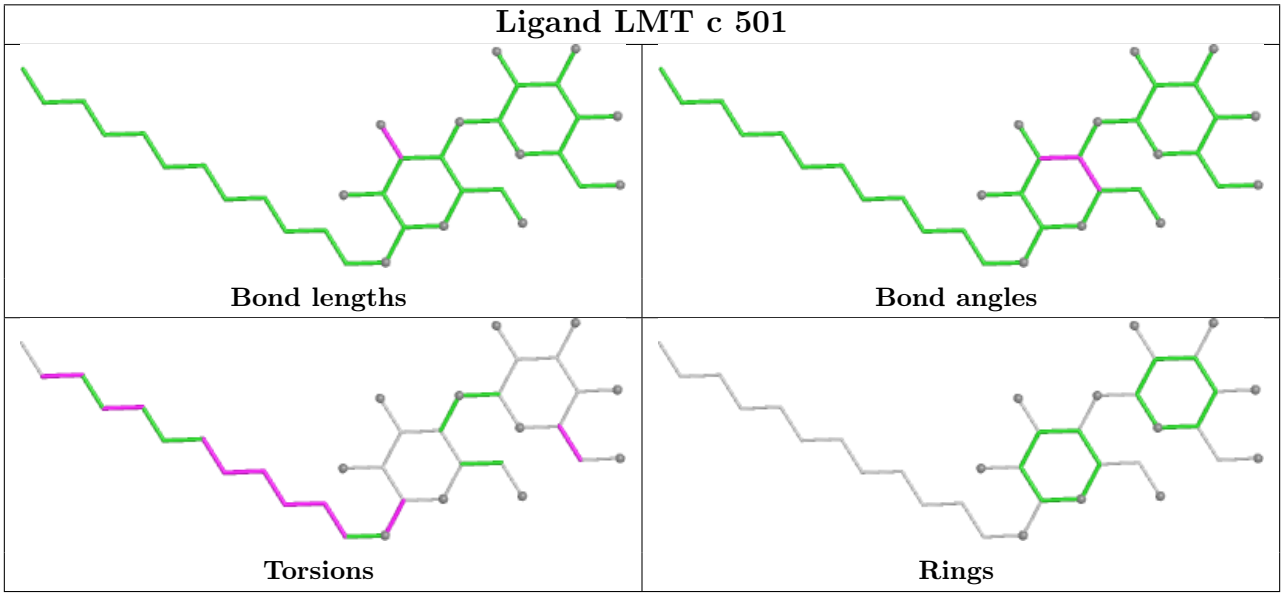


Rings

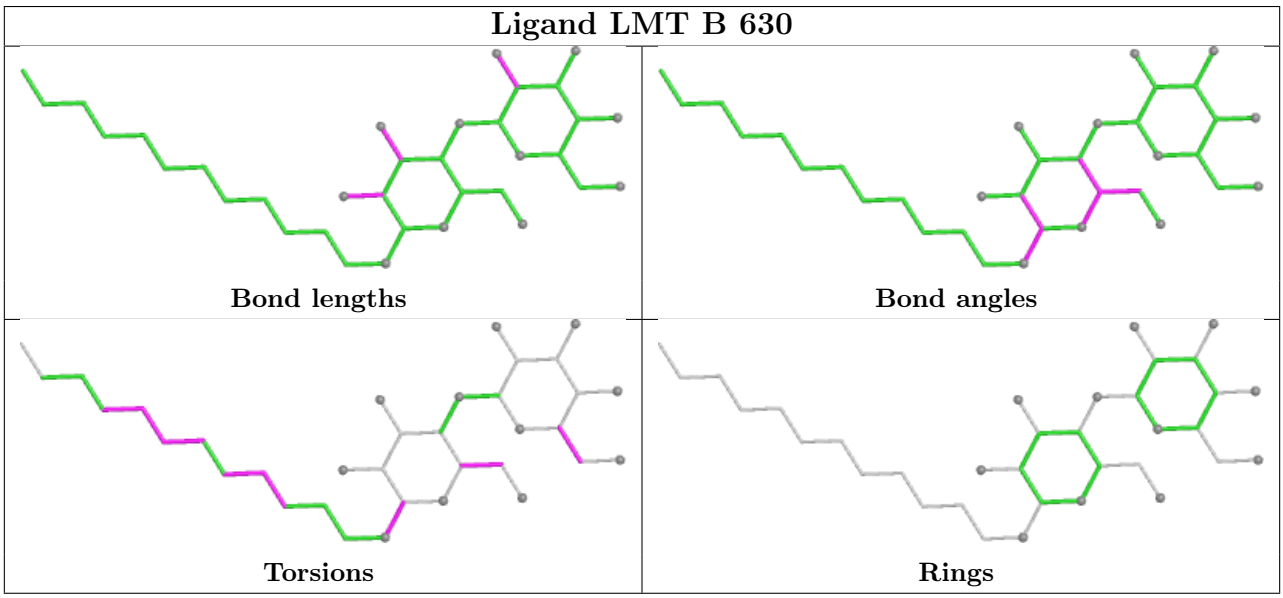
Ligand BCR c 515



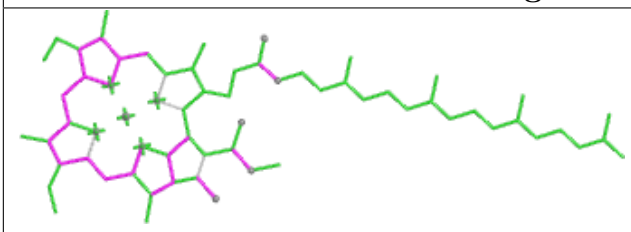
Ligand LMT c 501



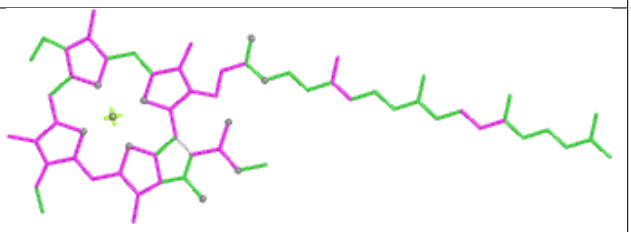
Ligand LMT B 630



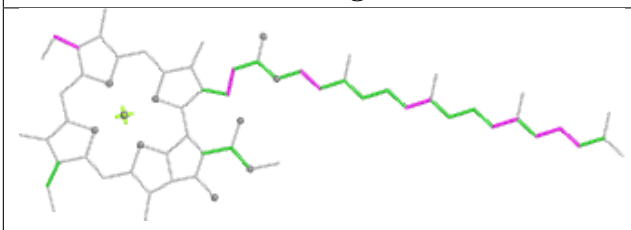
Ligand CLA B 602



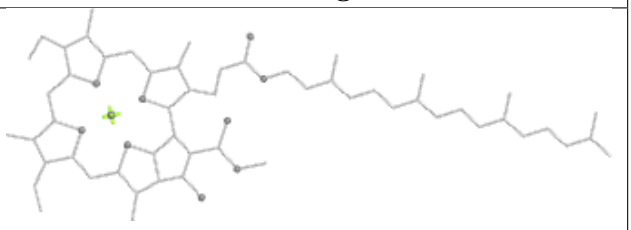
Bond lengths



Bond angles

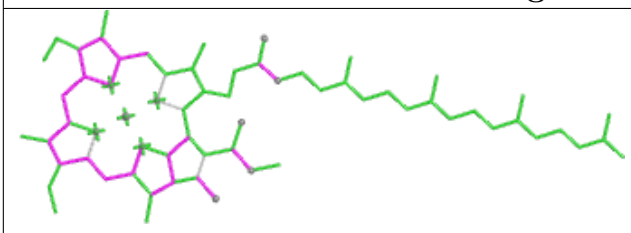


Torsions

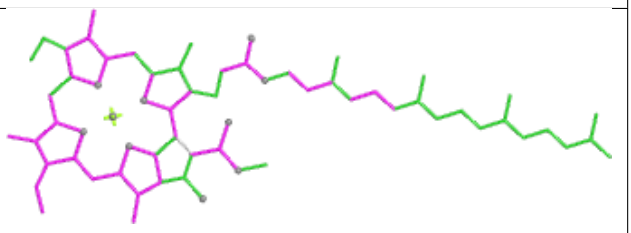


Rings

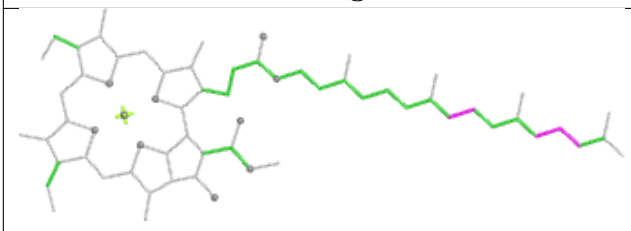
Ligand CLA b 611



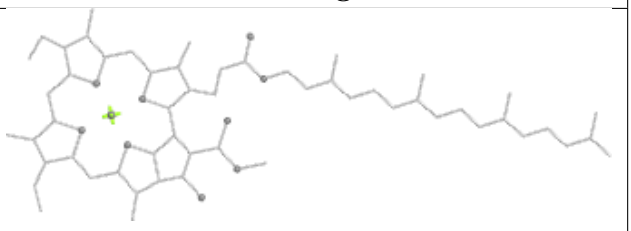
Bond lengths



Bond angles

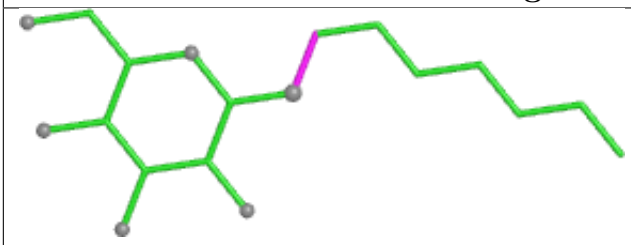


Torsions

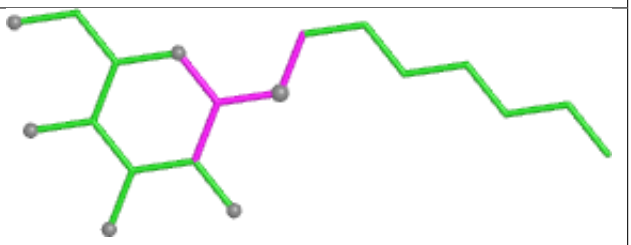


Rings

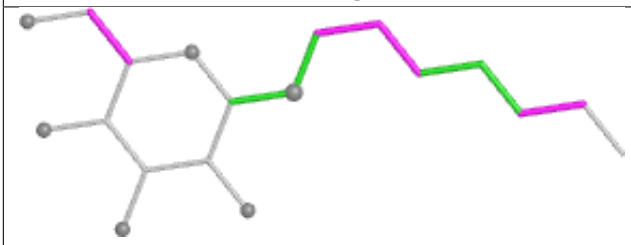
Ligand HTG b 623



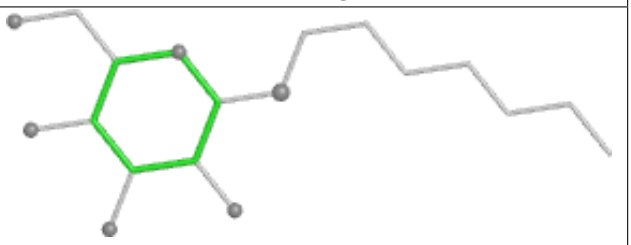
Bond lengths



Bond angles

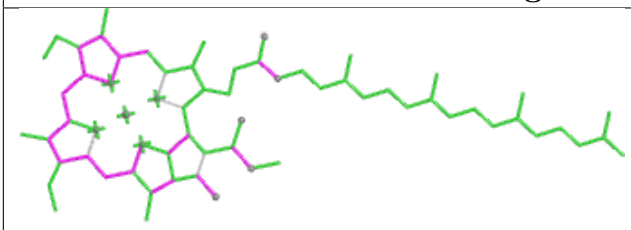


Torsions

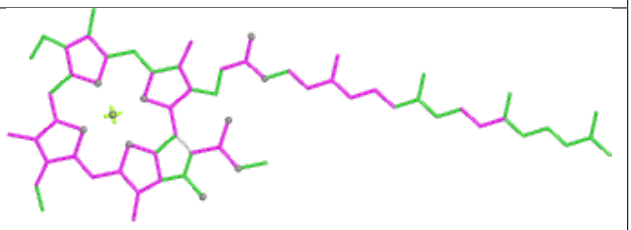


Rings

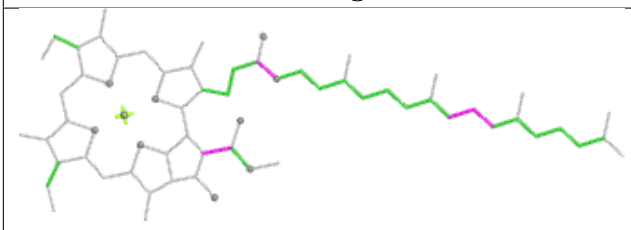
Ligand CLA B 612



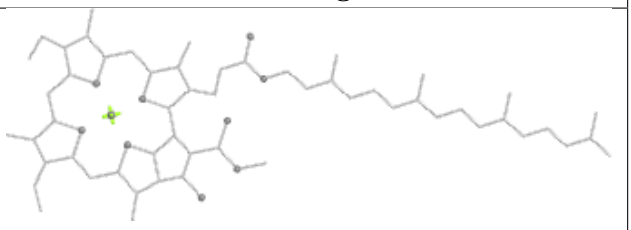
Bond lengths



Bond angles

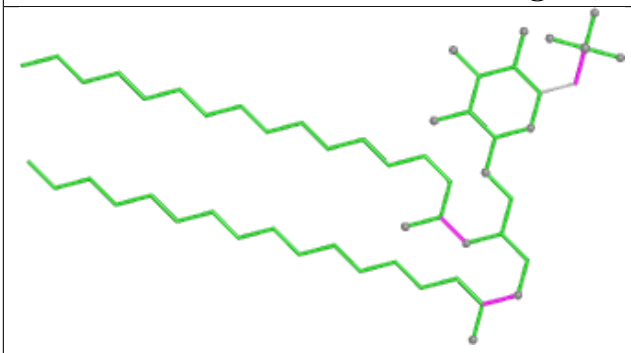


Torsions

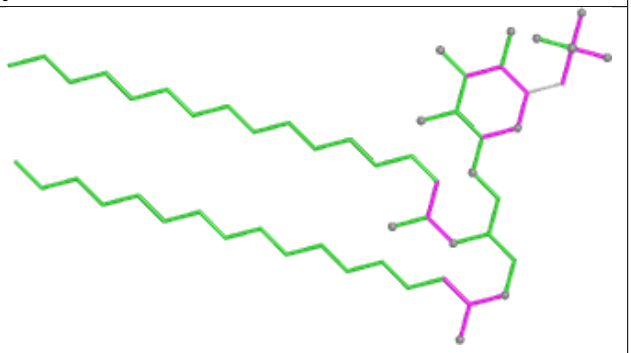


Rings

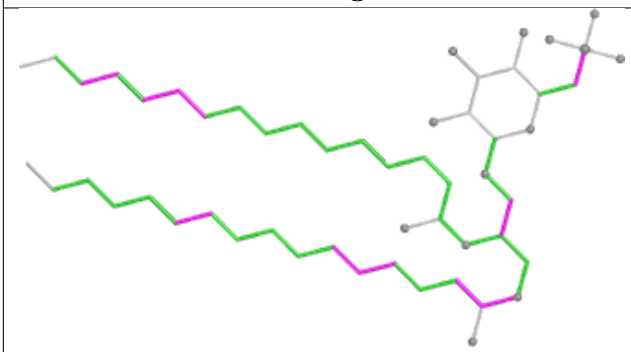
Ligand SQD a 413



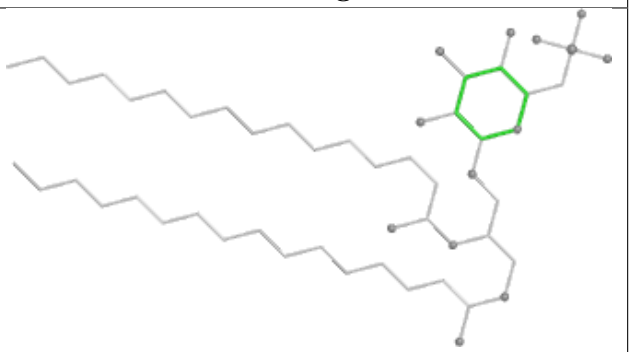
Bond lengths



Bond angles

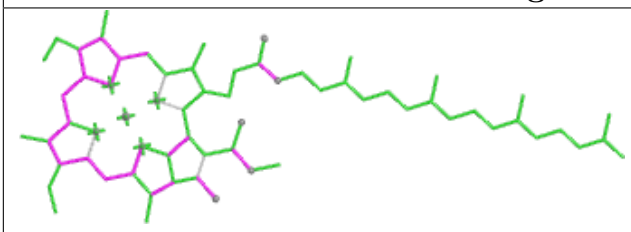


Torsions

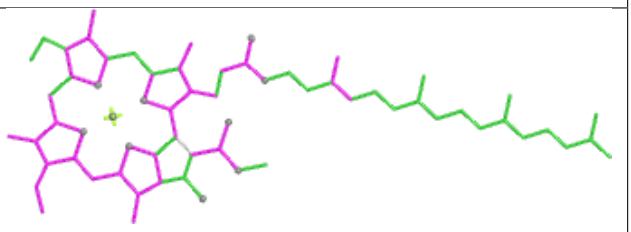


Rings

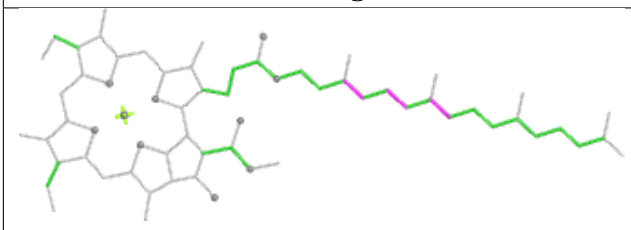
Ligand CLA b 603



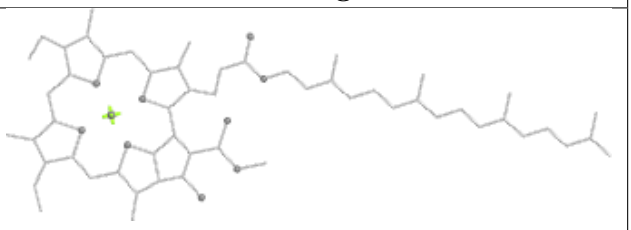
Bond lengths



Bond angles

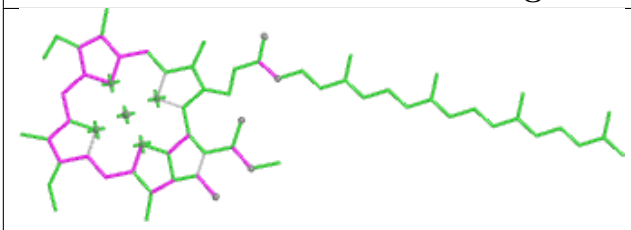


Torsions

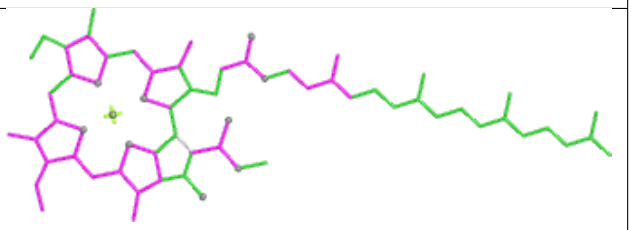


Rings

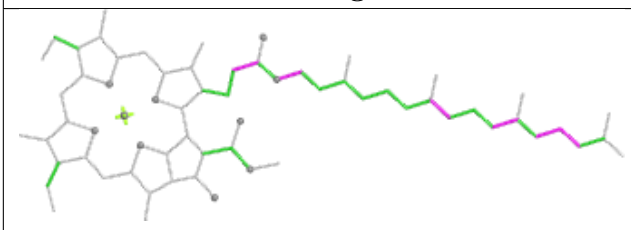
Ligand CLA B 613



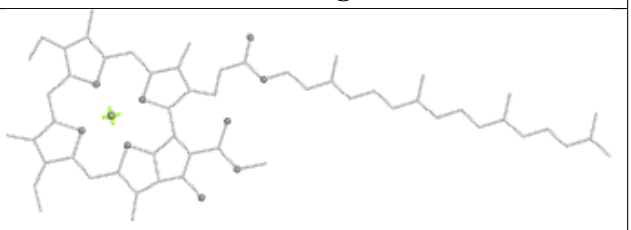
Bond lengths



Bond angles

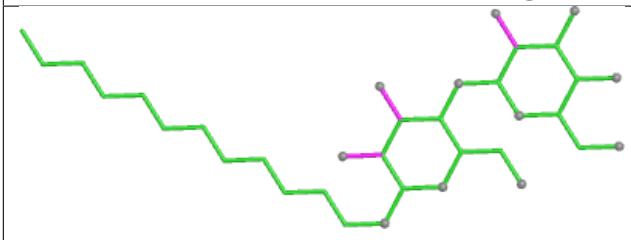


Torsions

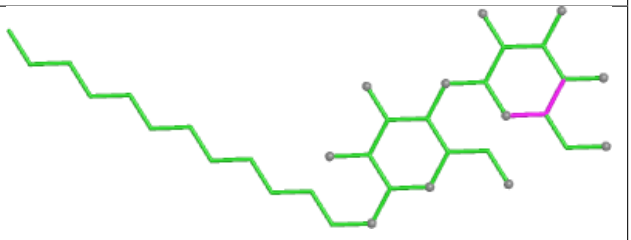


Rings

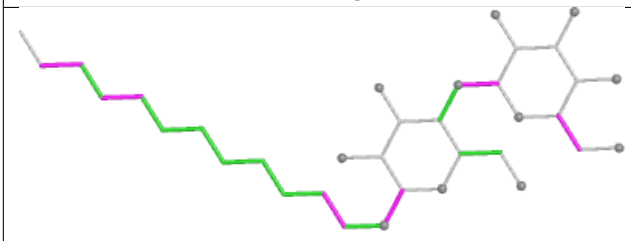
Ligand LMT A 417



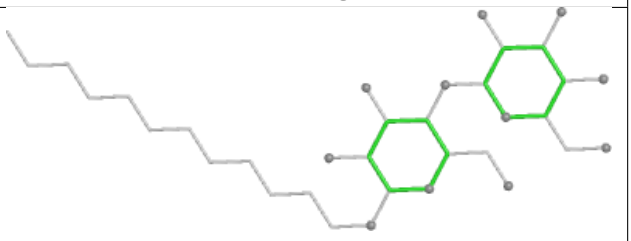
Bond lengths



Bond angles

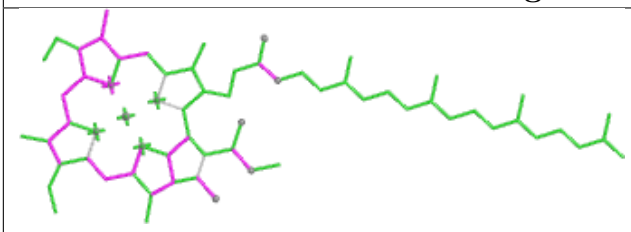


Torsions

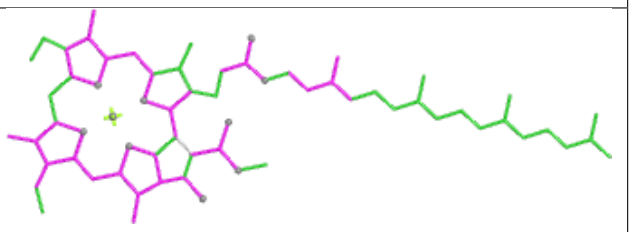


Rings

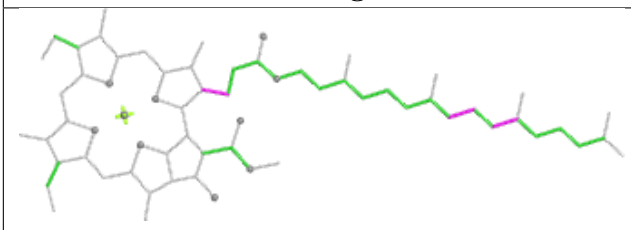
Ligand CLA B 611



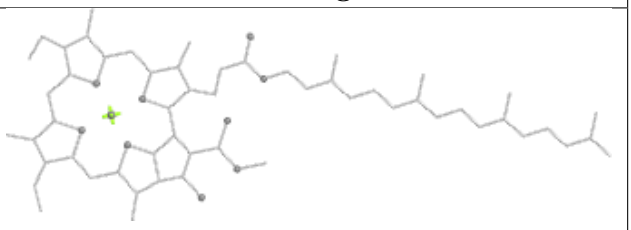
Bond lengths



Bond angles

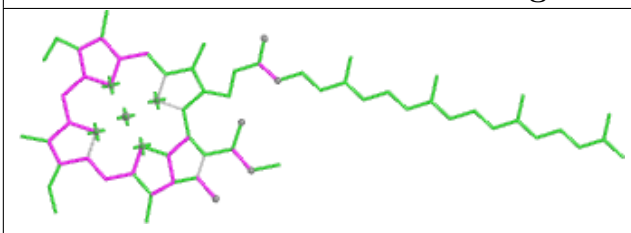


Torsions

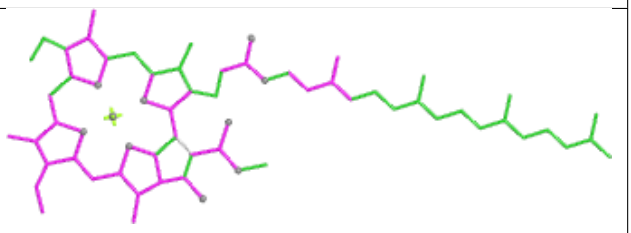


Rings

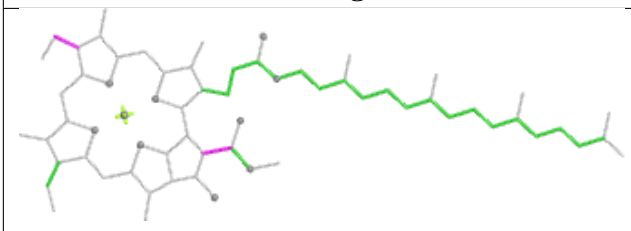
Ligand CLA c 502



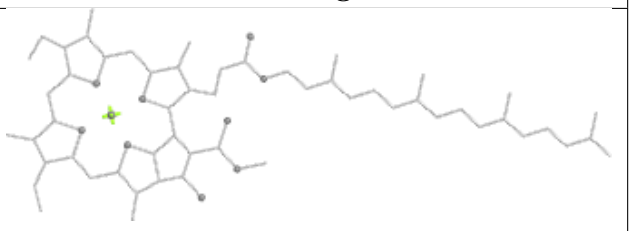
Bond lengths



Bond angles

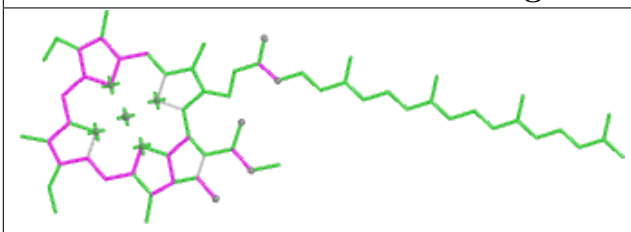


Torsions

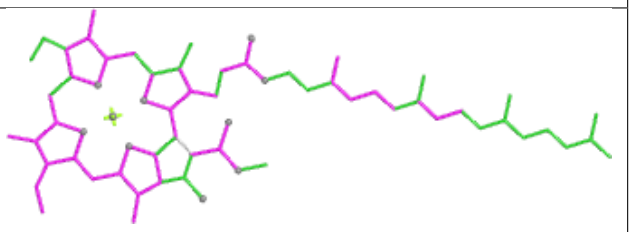


Rings

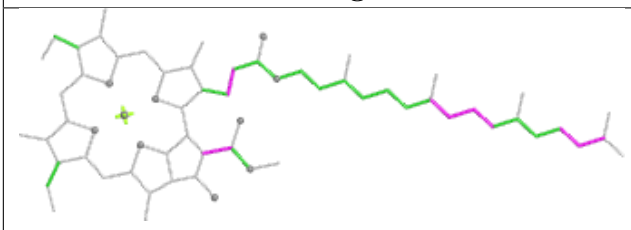
Ligand CLA B 606



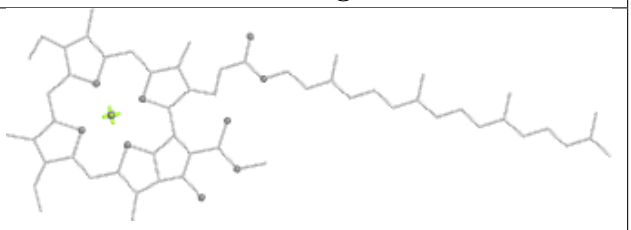
Bond lengths



Bond angles

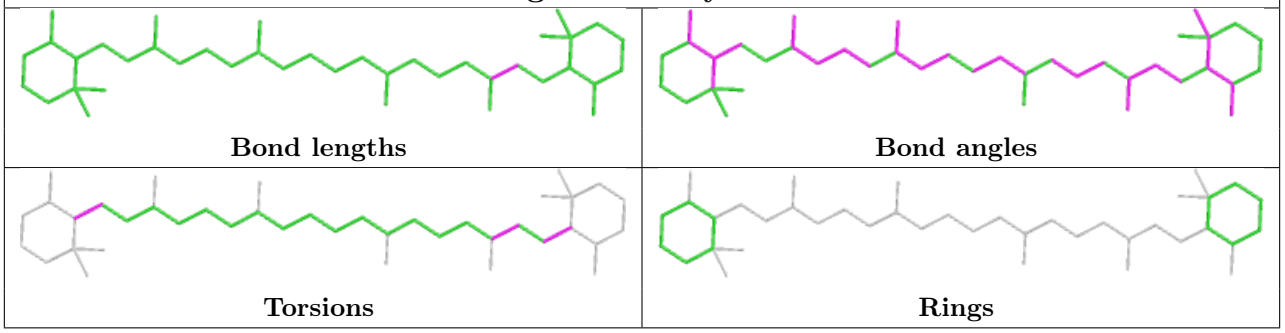


Torsions

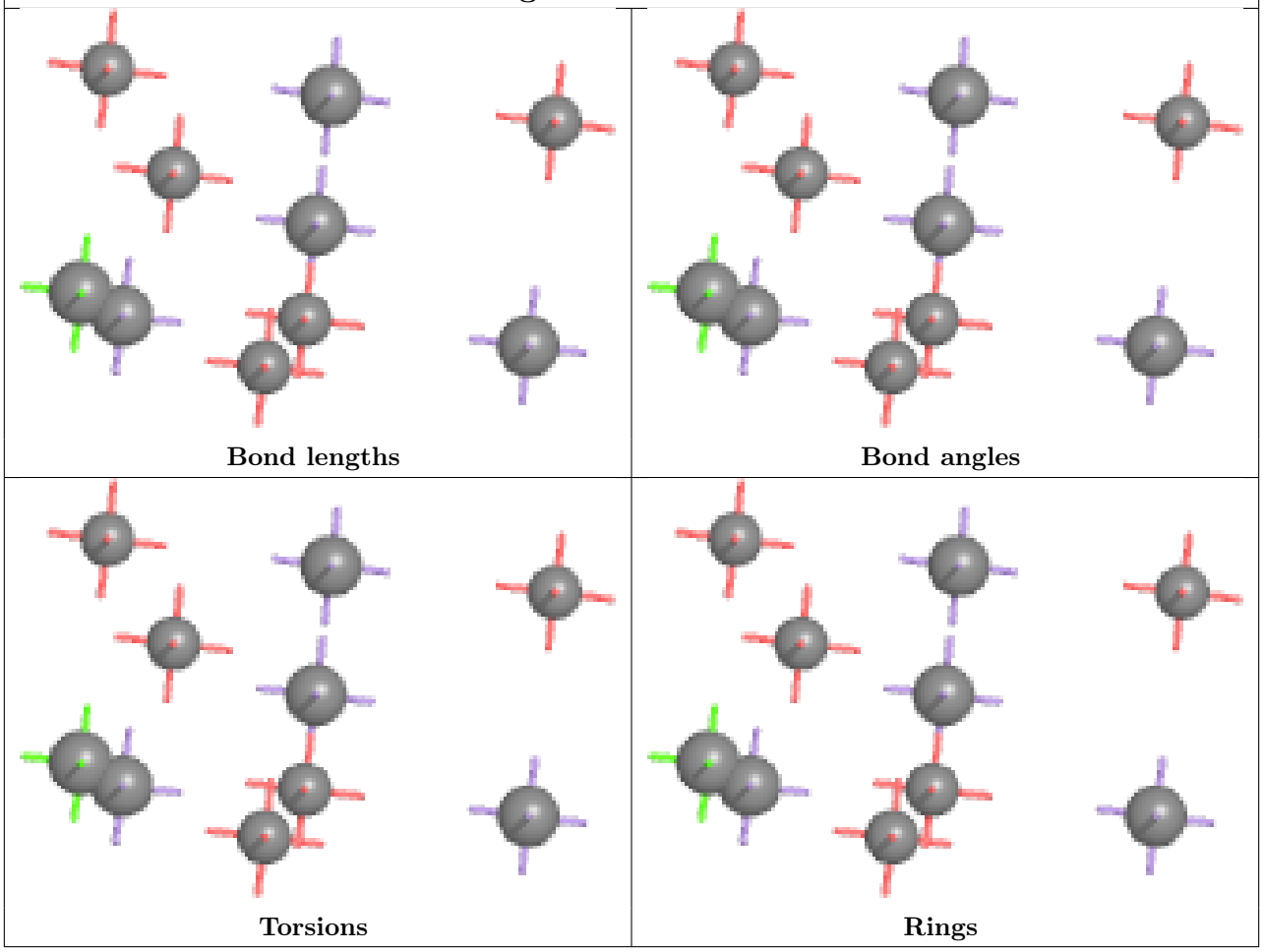


Rings

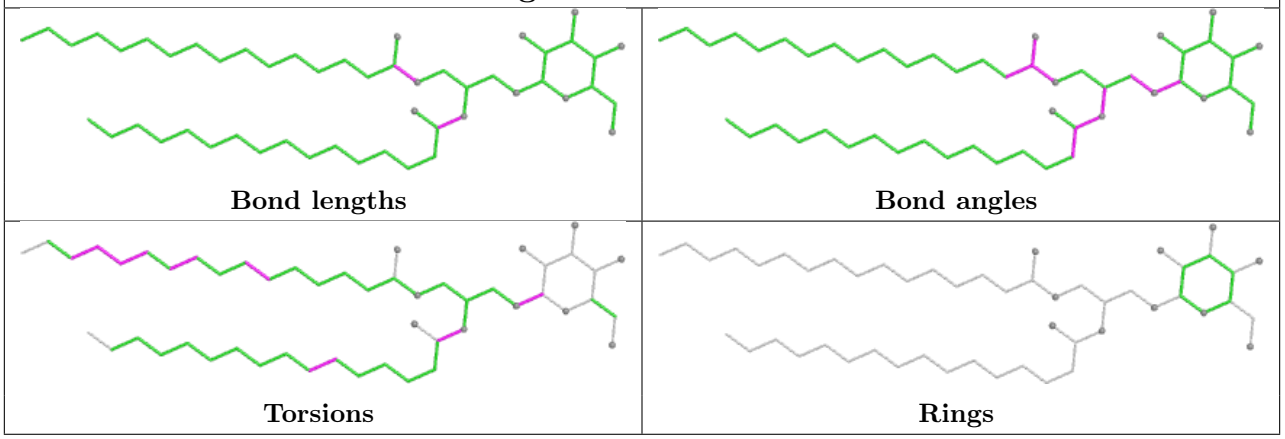
Ligand BCR y 101



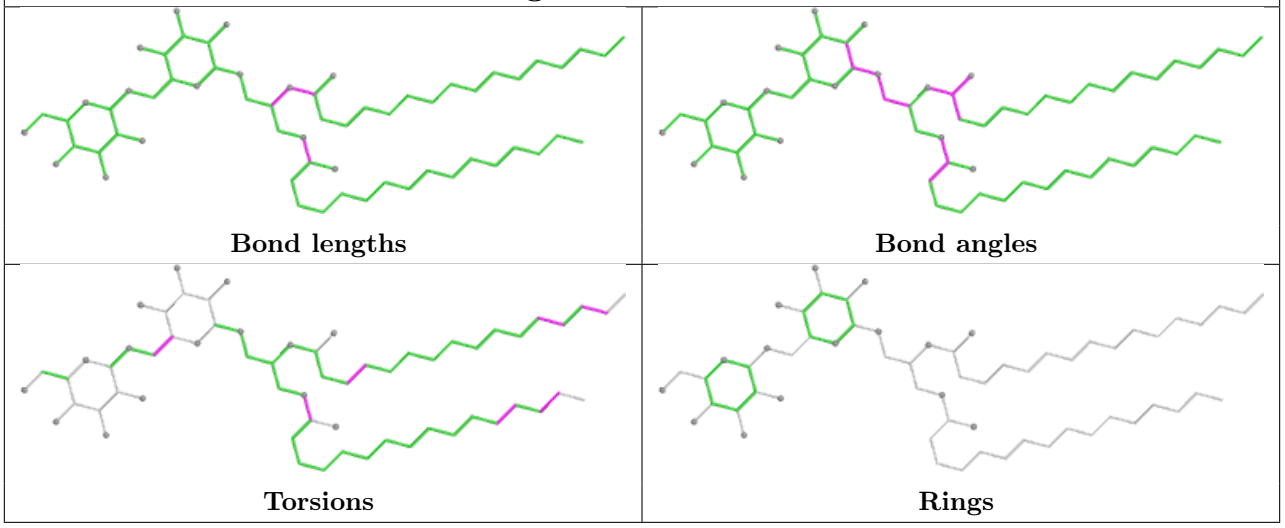
Ligand OEX a 414



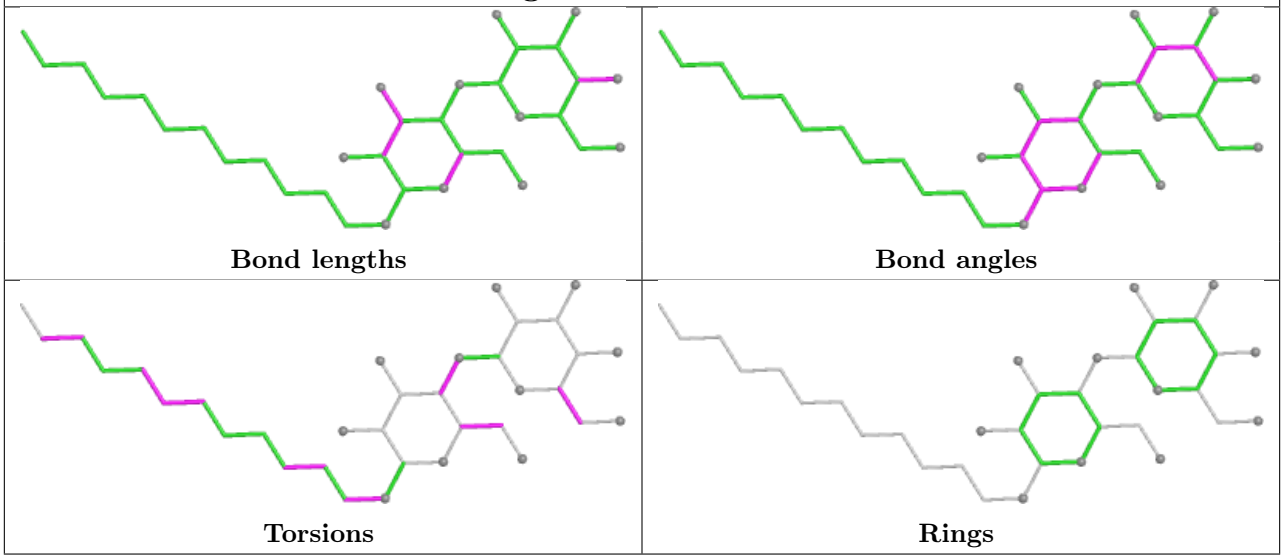
Ligand LMG m 101



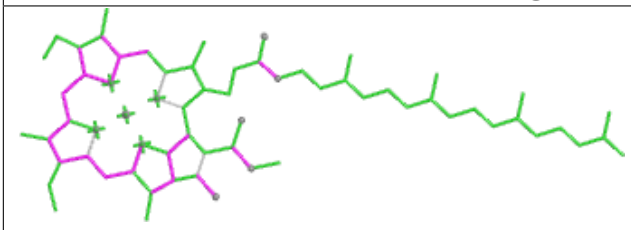
Ligand DGD c 519



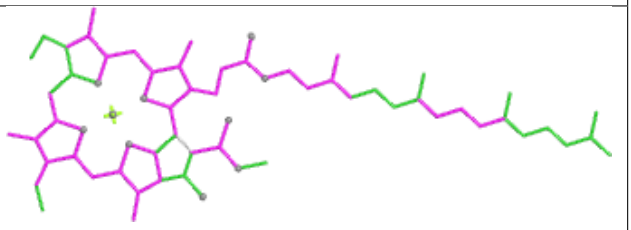
Ligand LMT B 628



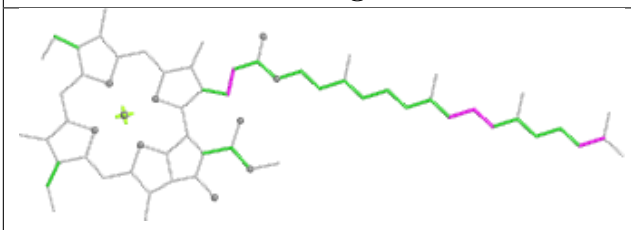
Ligand CLA b 602



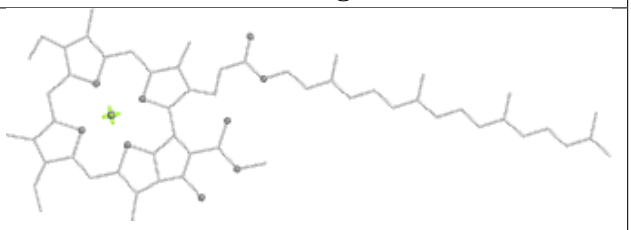
Bond lengths



Bond angles

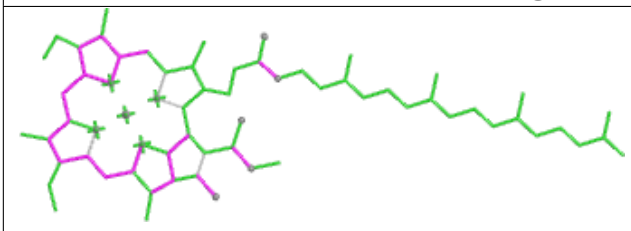


Torsions

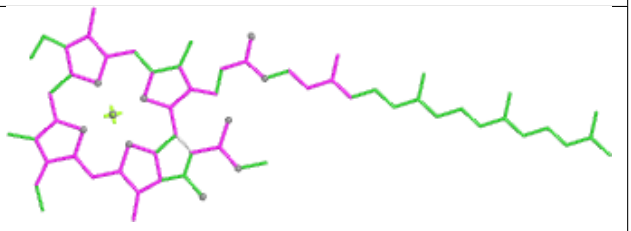


Rings

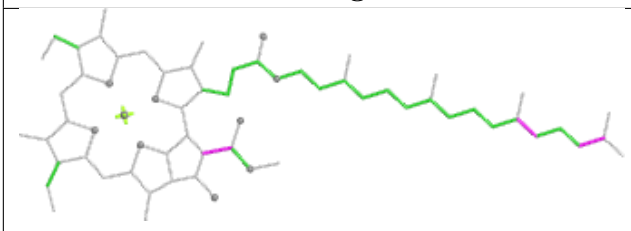
Ligand CLA c 509



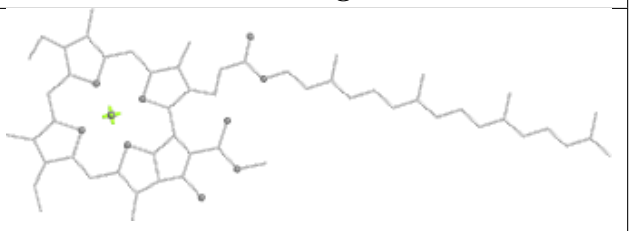
Bond lengths



Bond angles

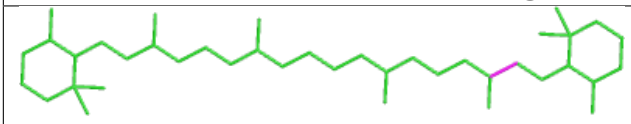


Torsions

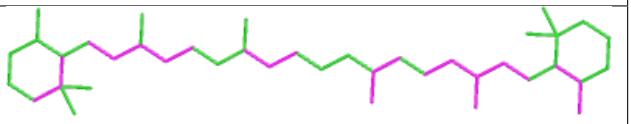


Rings

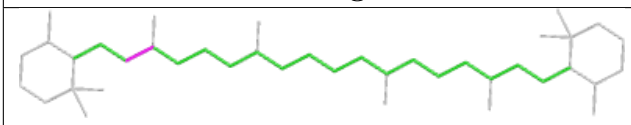
Ligand BCR K 103



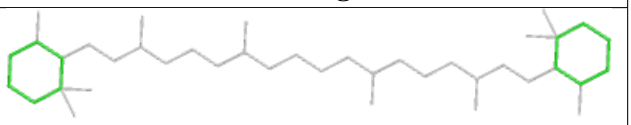
Bond lengths



Bond angles

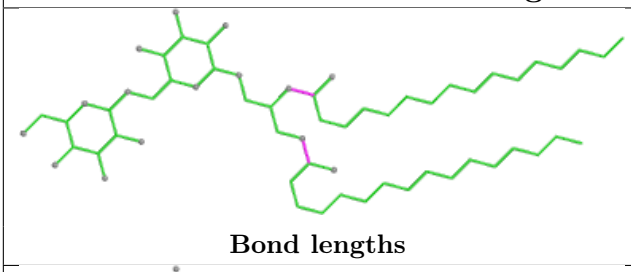


Torsions

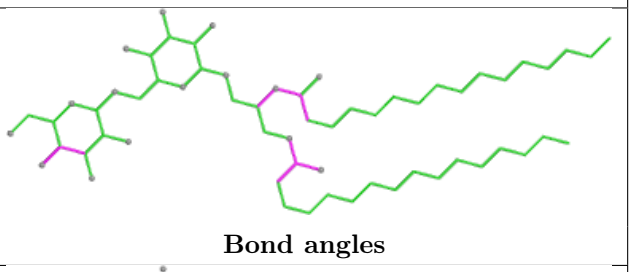


Rings

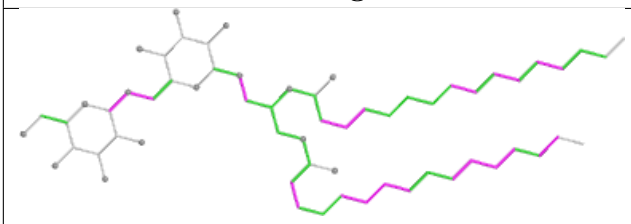
Ligand DGD c 518



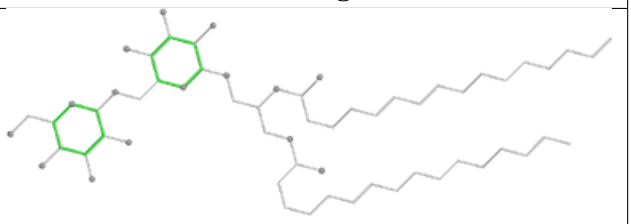
Bond lengths



Bond angles

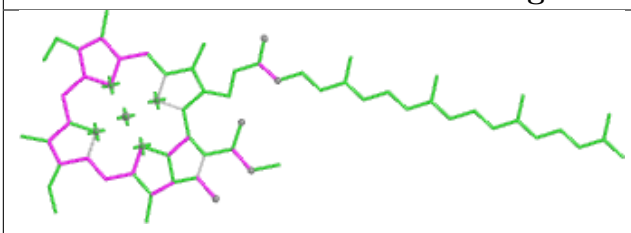


Torsions

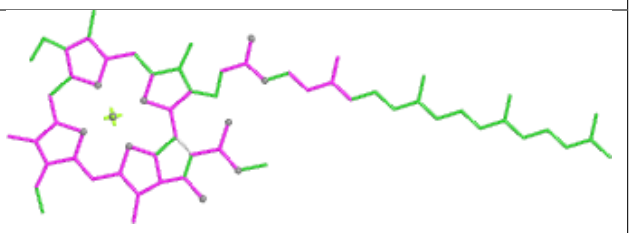


Rings

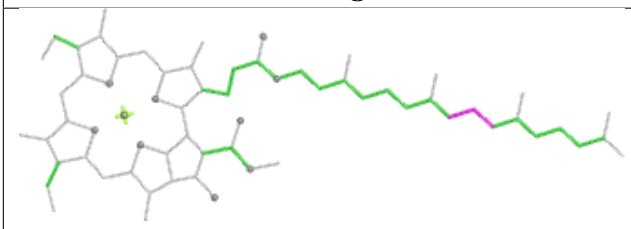
Ligand CLA b 612



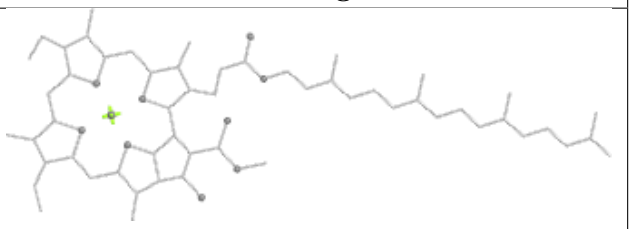
Bond lengths



Bond angles

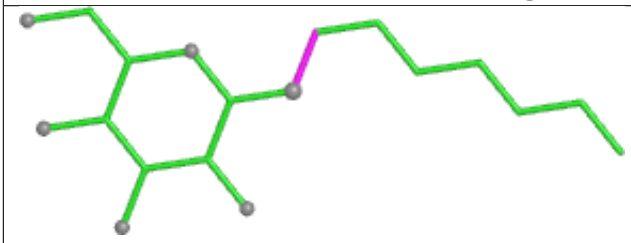


Torsions

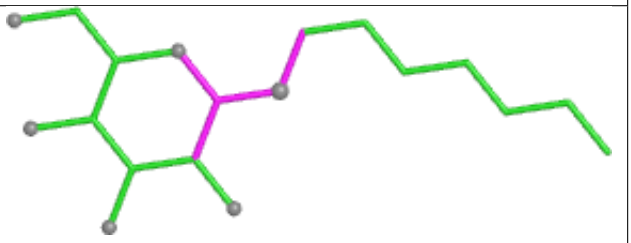


Rings

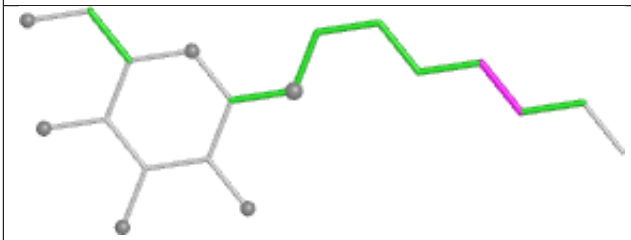
Ligand HTG B 623



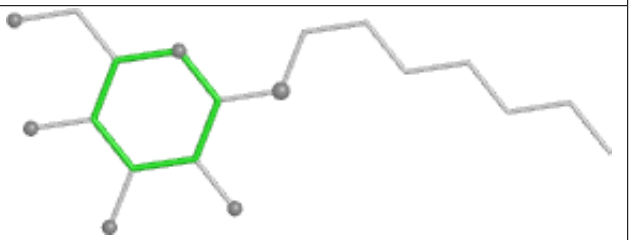
Bond lengths



Bond angles

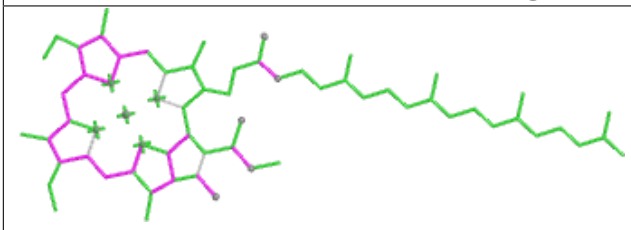


Torsions

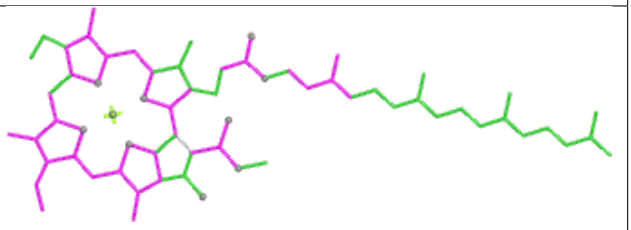


Rings

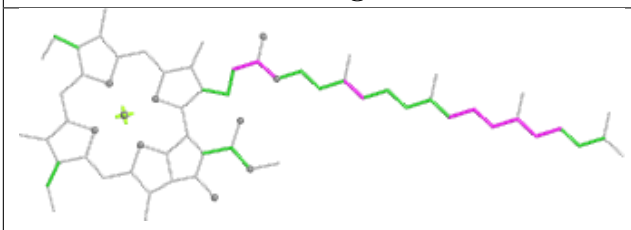
Ligand CLA C 510



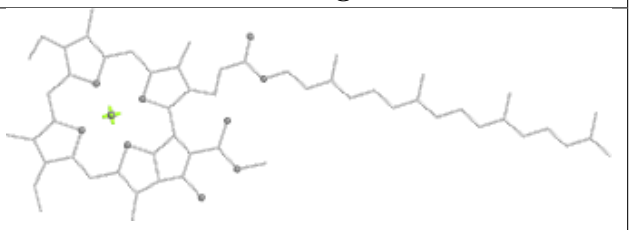
Bond lengths



Bond angles

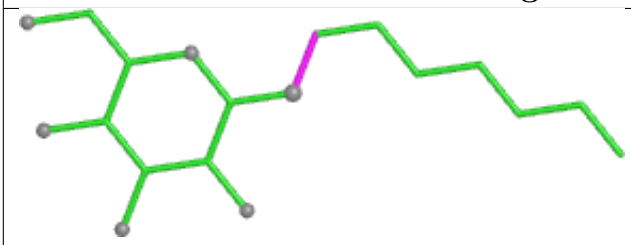


Torsions

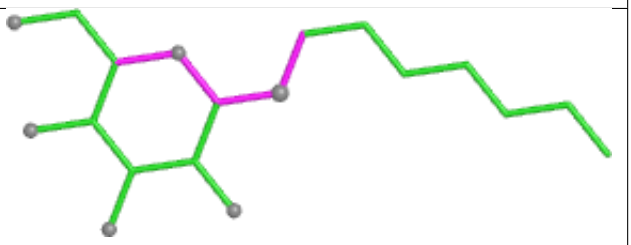


Rings

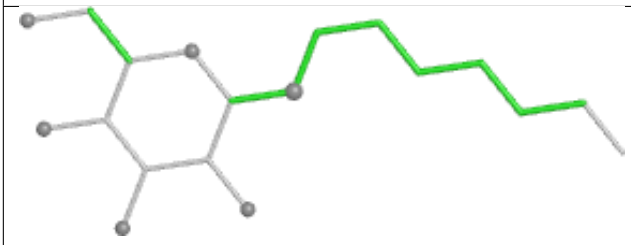
Ligand HTG C 520



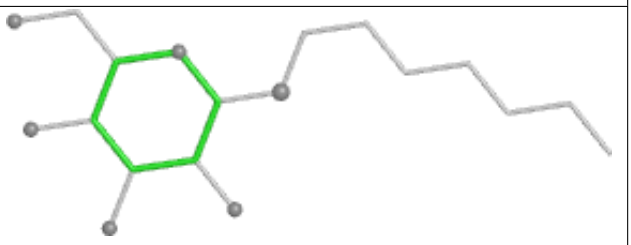
Bond lengths



Bond angles

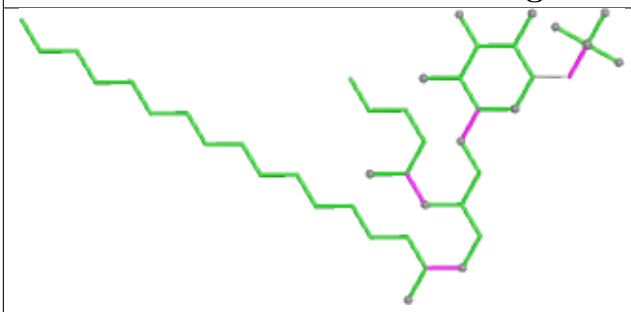


Torsions

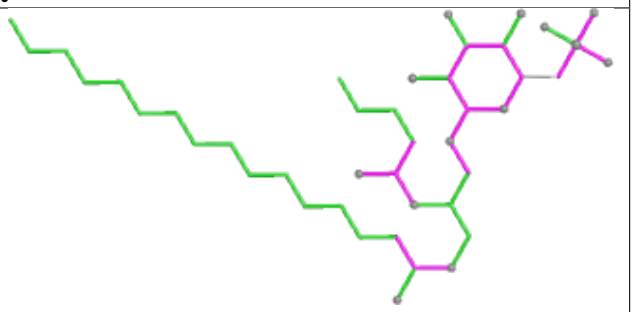


Rings

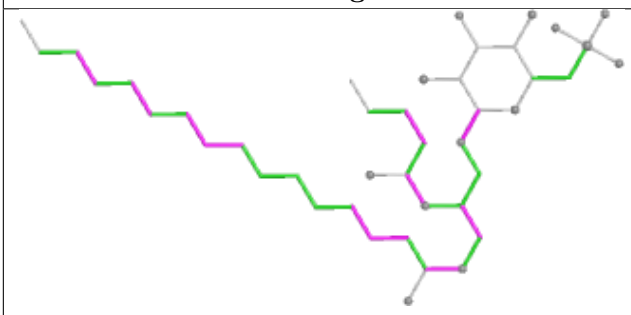
Ligand SQD F 103



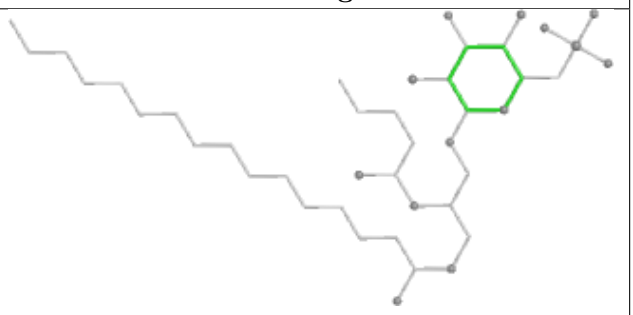
Bond lengths



Bond angles

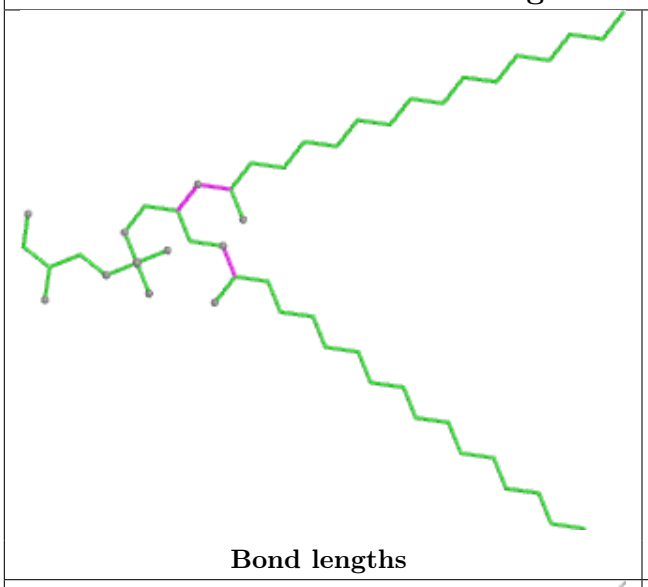


Torsions

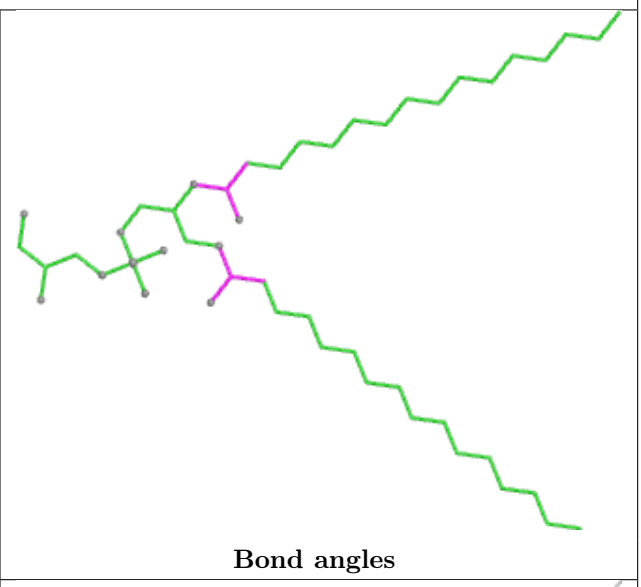


Rings

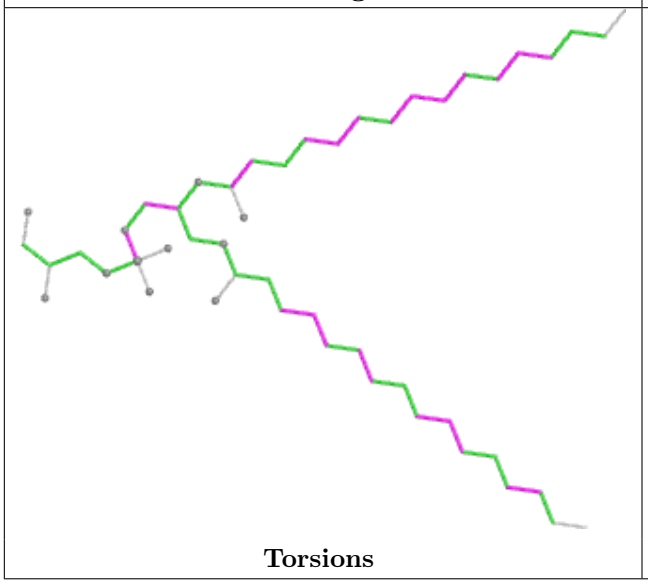
Ligand LHG b 630



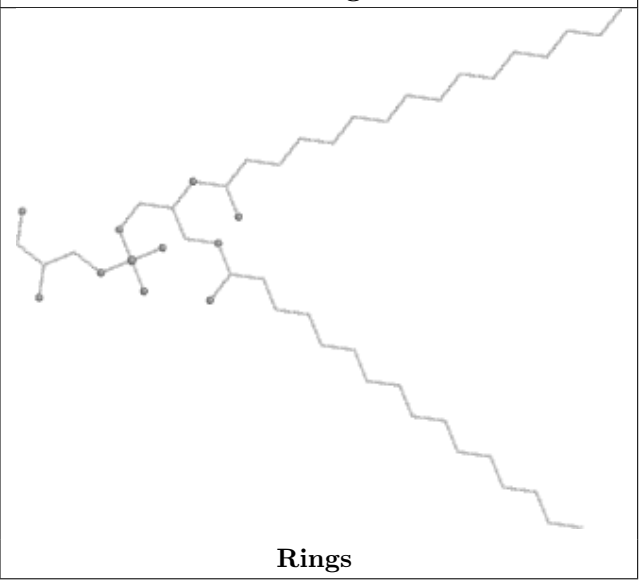
Bond lengths



Bond angles

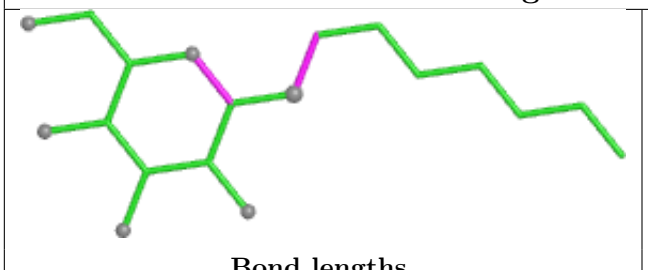


Torsions

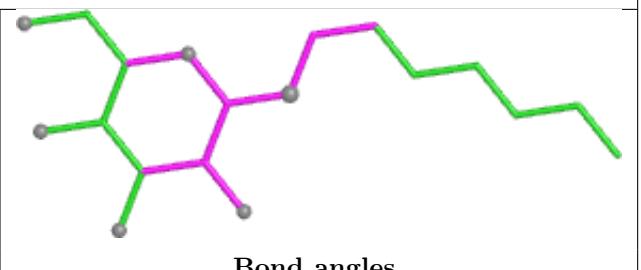


Rings

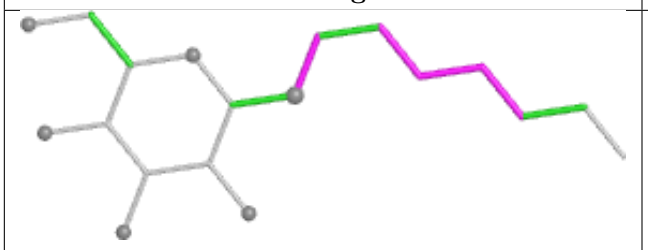
Ligand HTG B 622



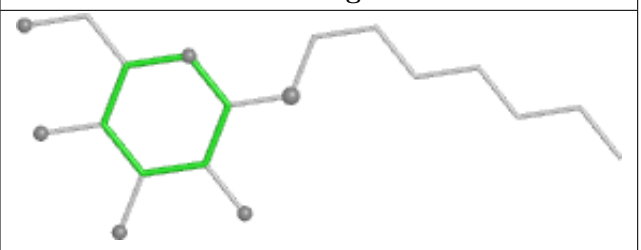
Bond lengths



Bond angles

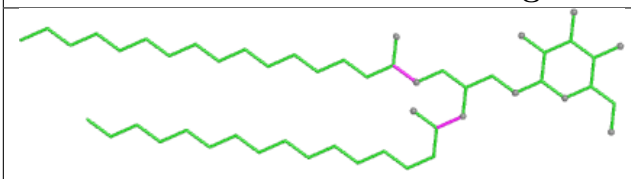


Torsions

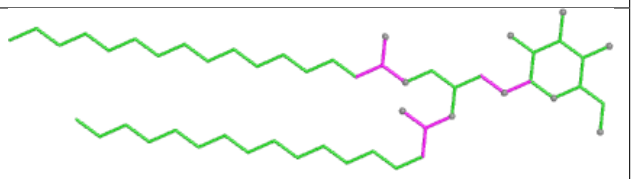


Rings

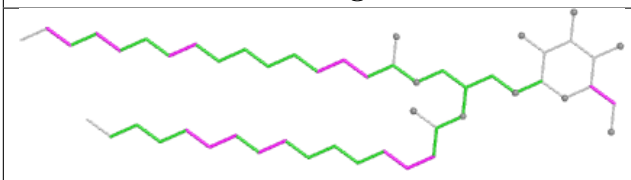
Ligand LMG d 410



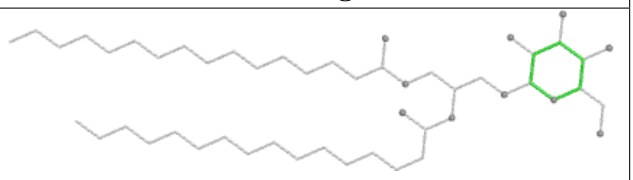
Bond lengths



Bond angles

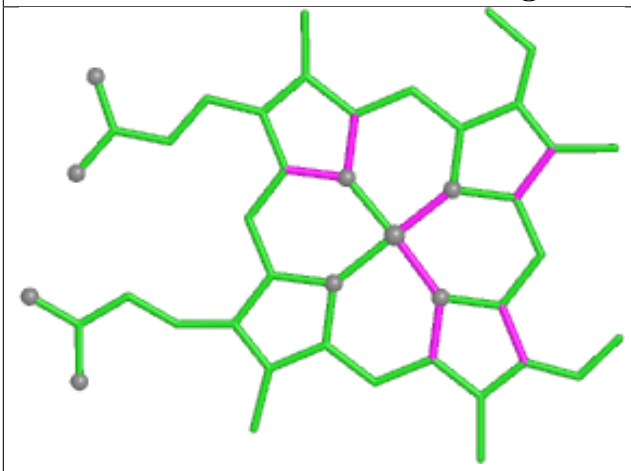


Torsions

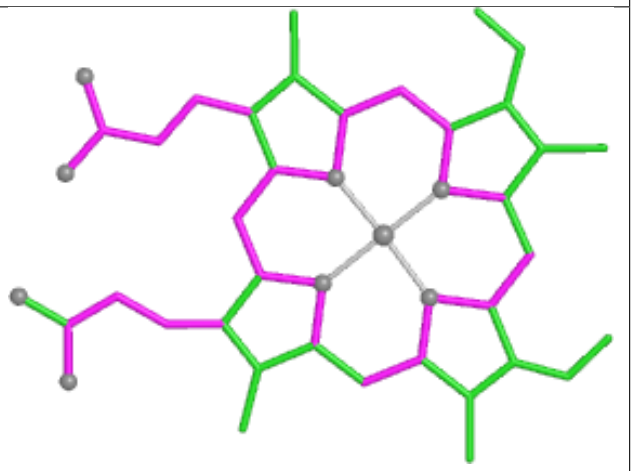


Rings

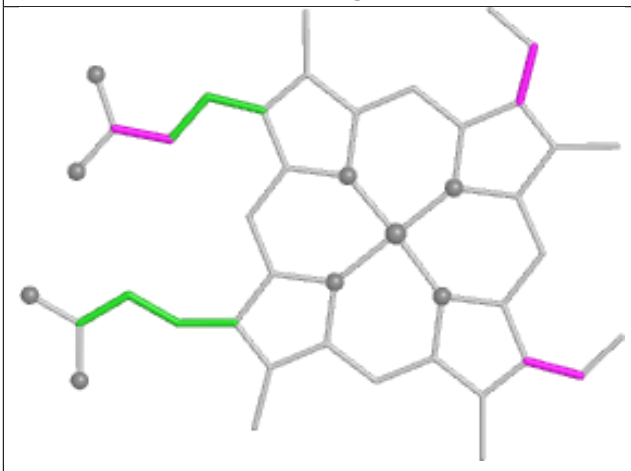
Ligand HEM F 102



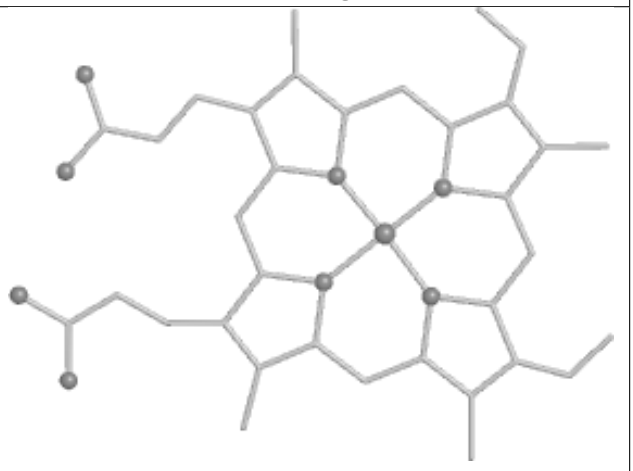
Bond lengths



Bond angles

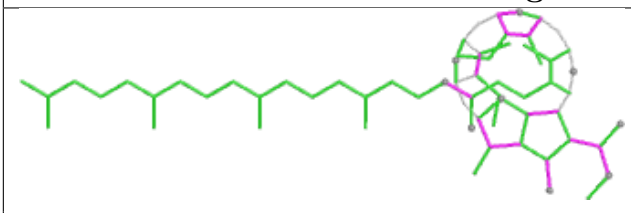


Torsions

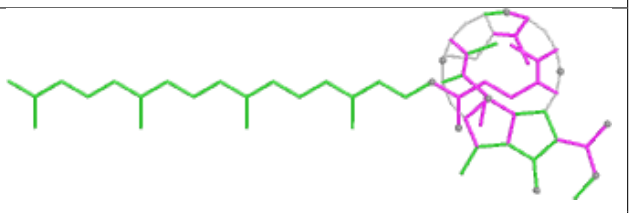


Rings

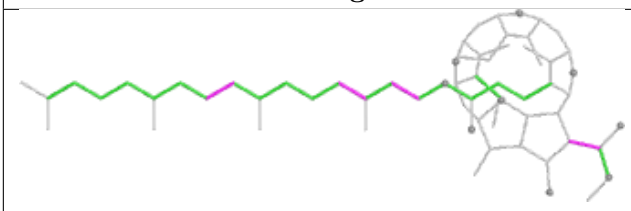
Ligand PHO a 408



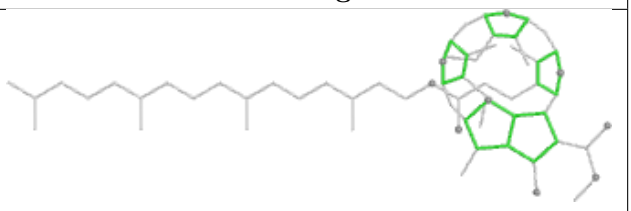
Bond lengths



Bond angles



Torsions

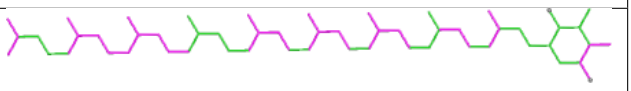


Rings

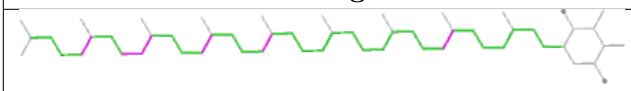
Ligand PL9 D 405



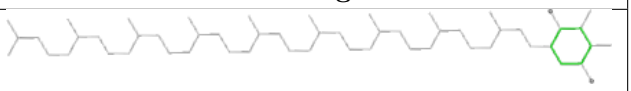
Bond lengths



Bond angles

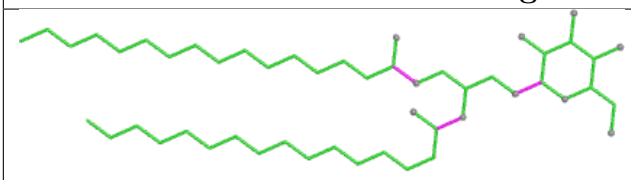


Torsions

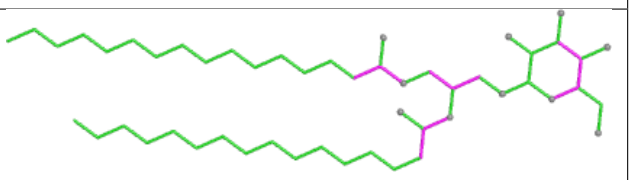


Rings

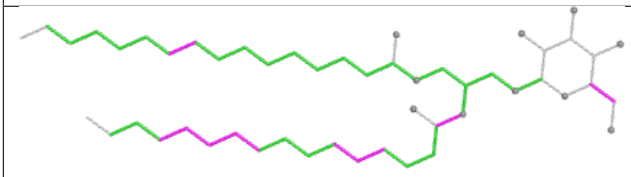
Ligand LMG C 519



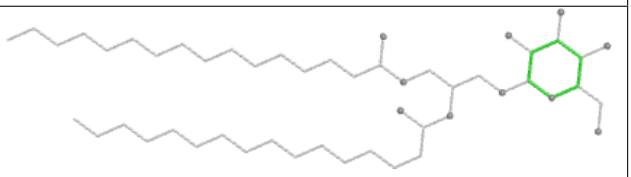
Bond lengths



Bond angles

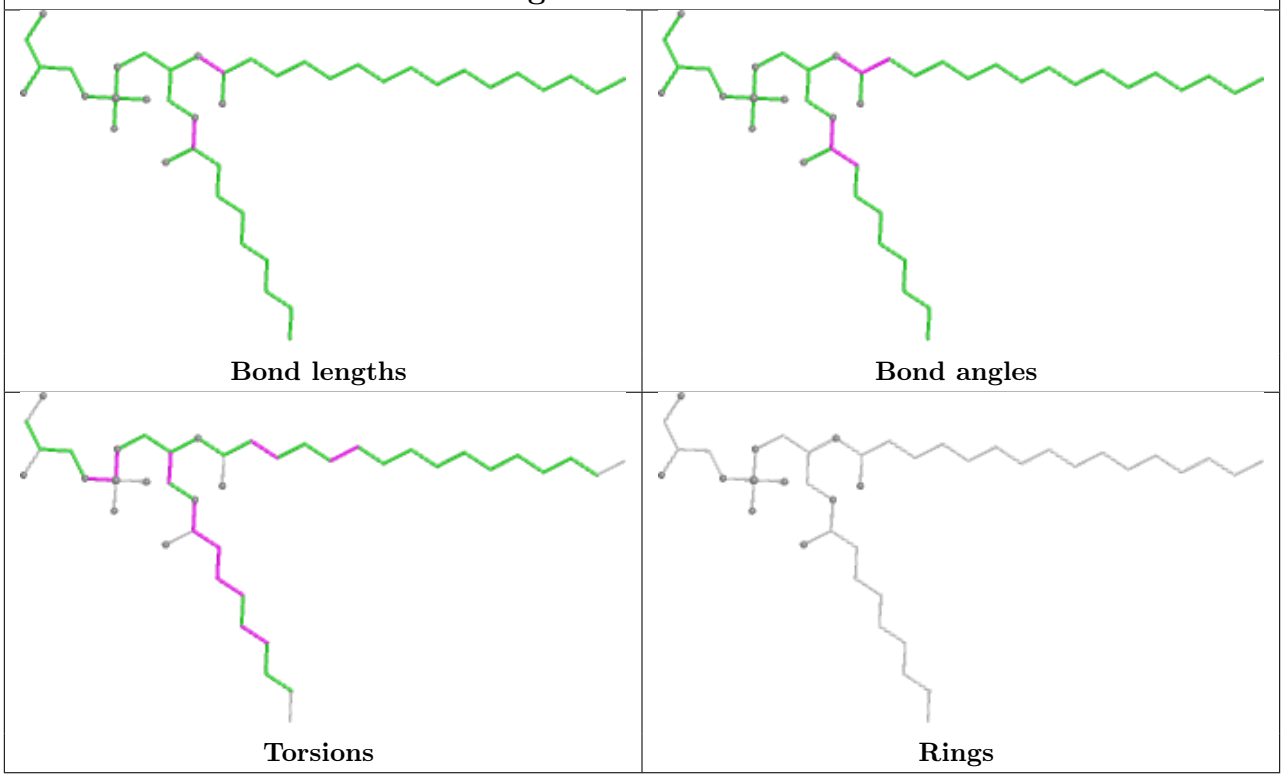


Torsions

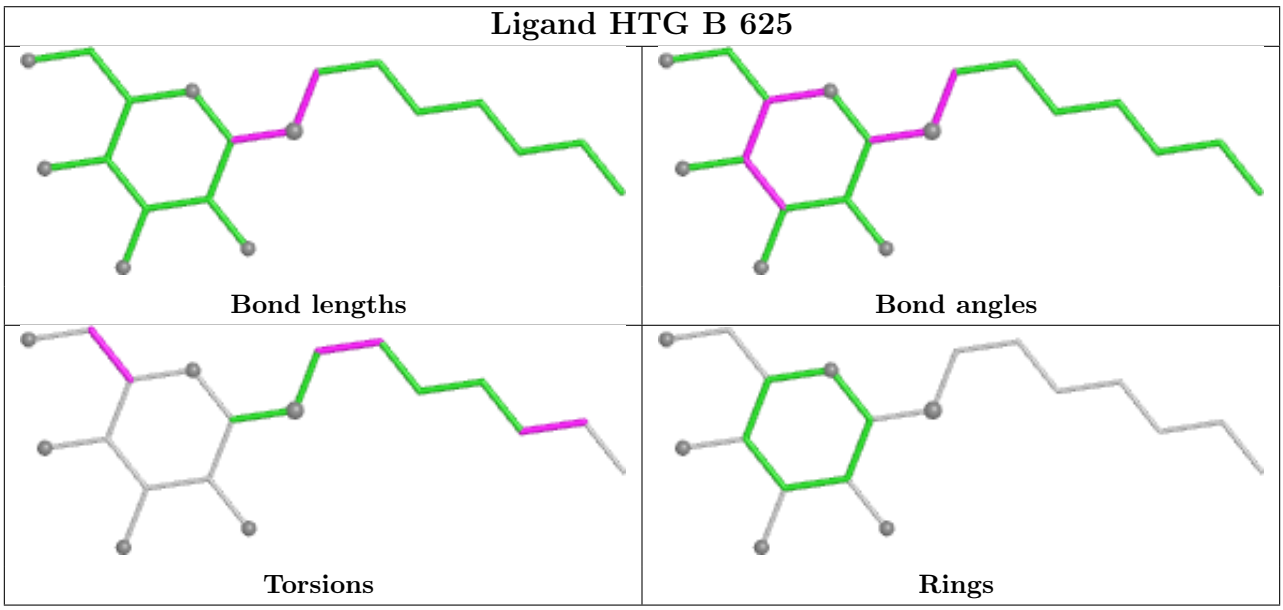


Rings

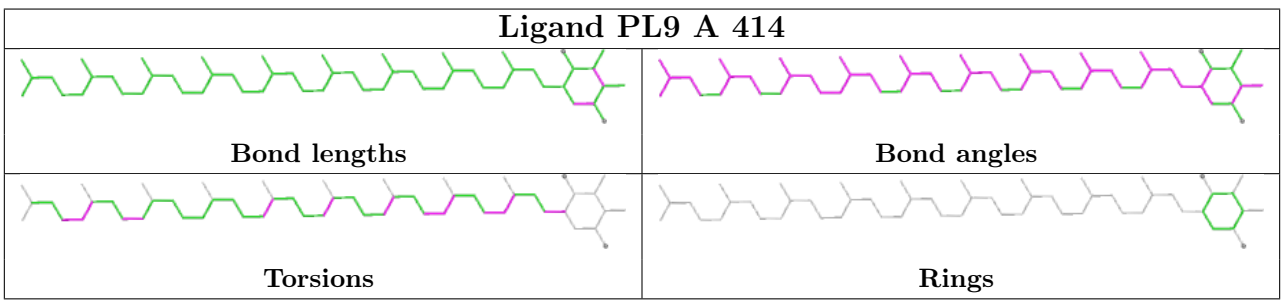
Ligand LHG a 421



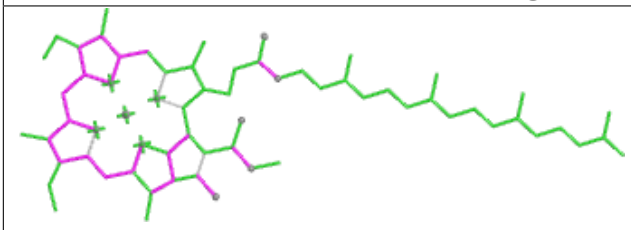
Ligand HTG B 625



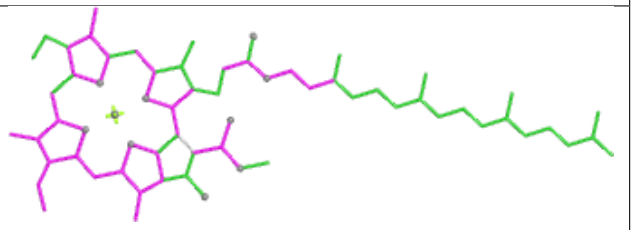
Ligand PL9 A 414



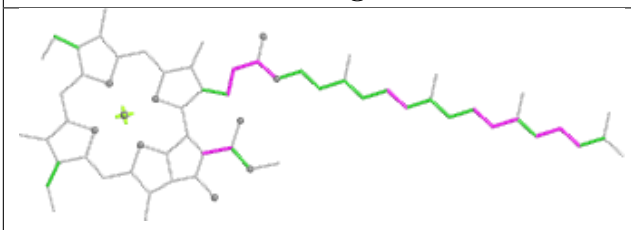
Ligand CLA B 601



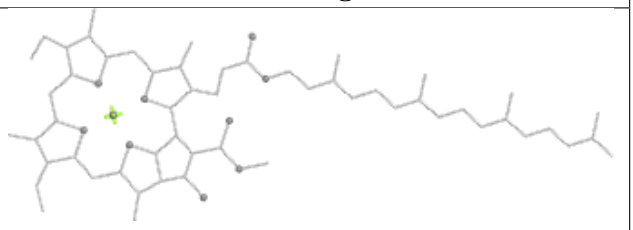
Bond lengths



Bond angles

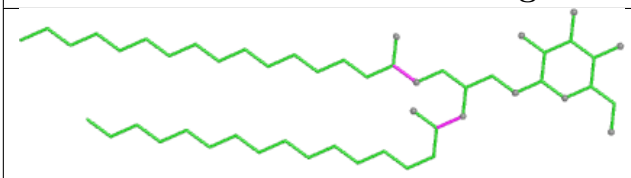


Torsions

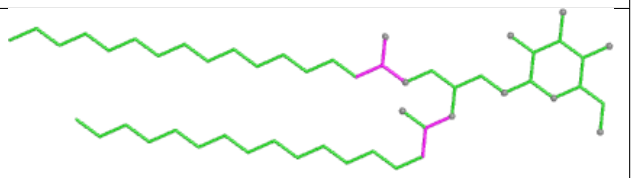


Rings

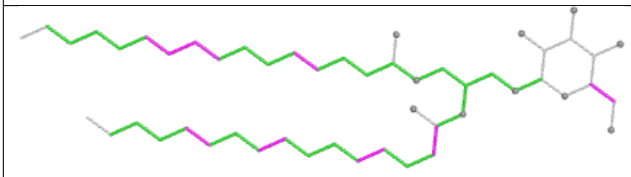
Ligand LMG D 411



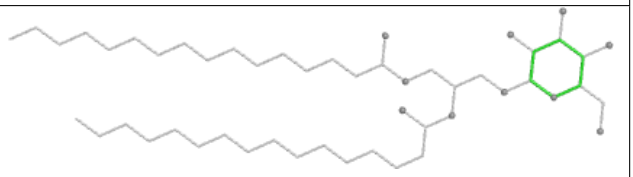
Bond lengths



Bond angles

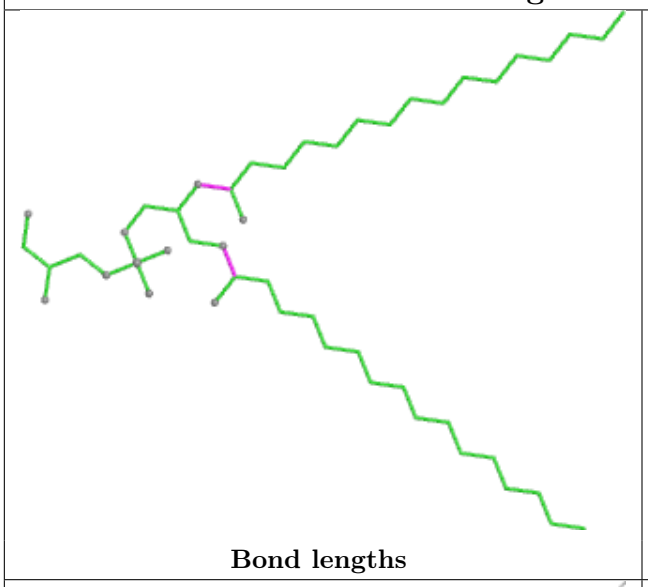


Torsions

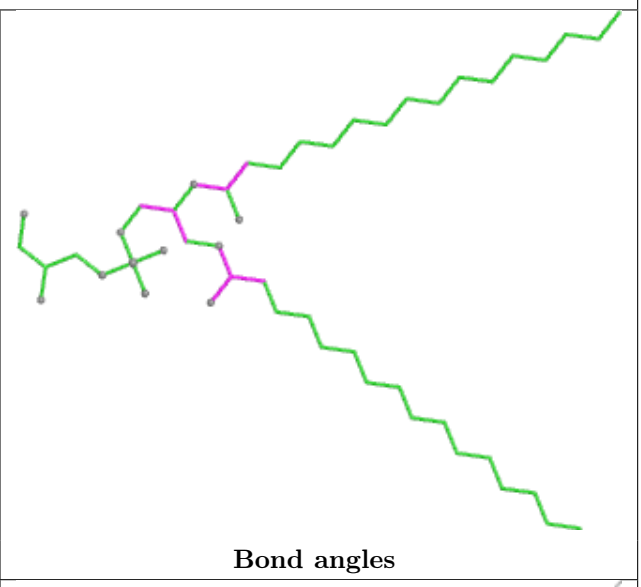


Rings

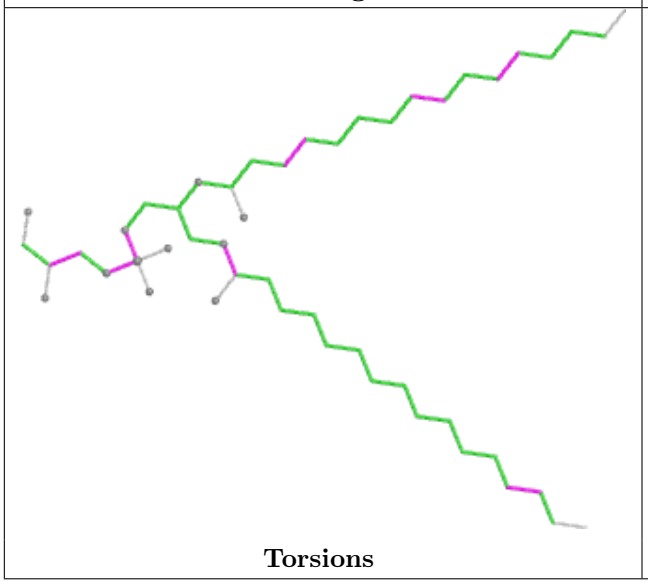
Ligand LHG d 405



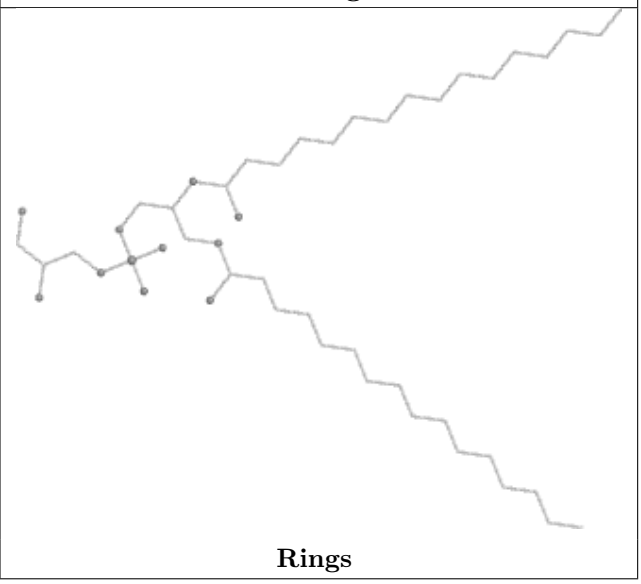
Bond lengths



Bond angles



Torsions

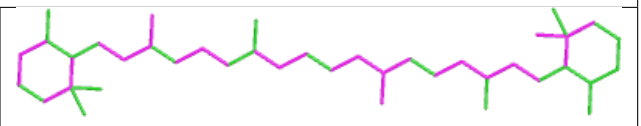


Rings

Ligand BCR k 101



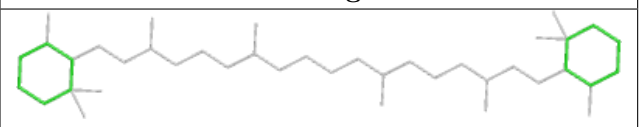
Bond lengths



Bond angles

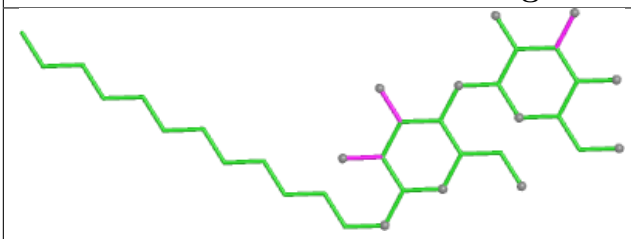


Torsions

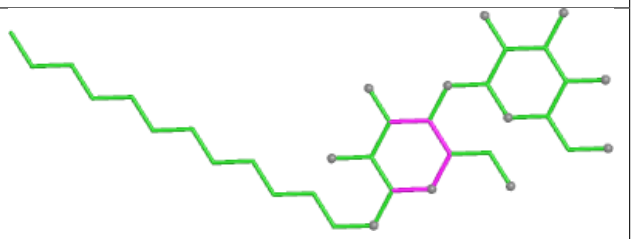


Rings

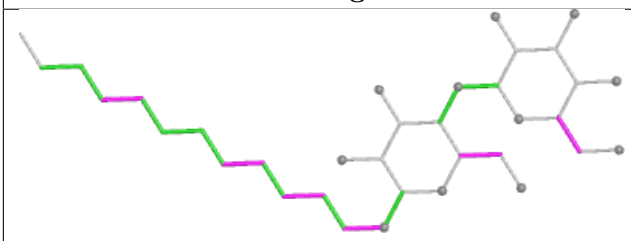
Ligand LMT T 101



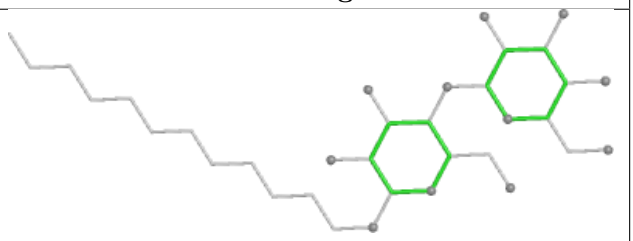
Bond lengths



Bond angles

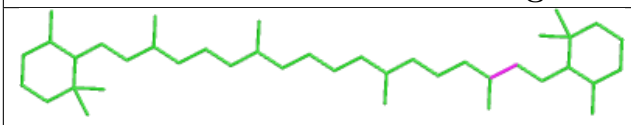


Torsions

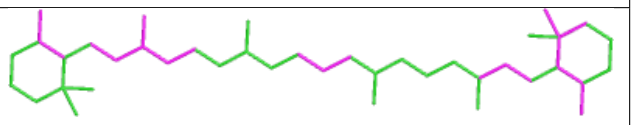


Rings

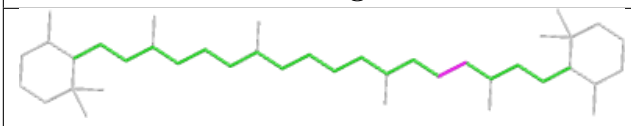
Ligand BCR a 410



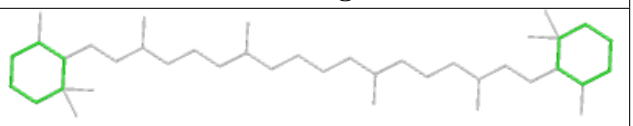
Bond lengths



Bond angles

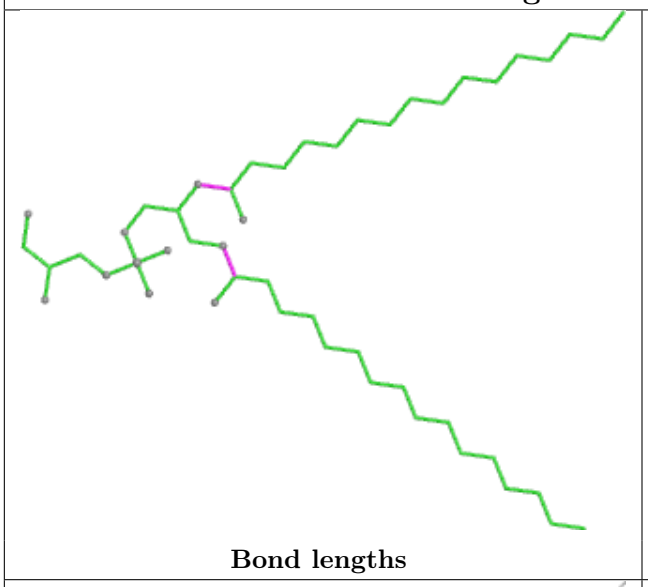


Torsions

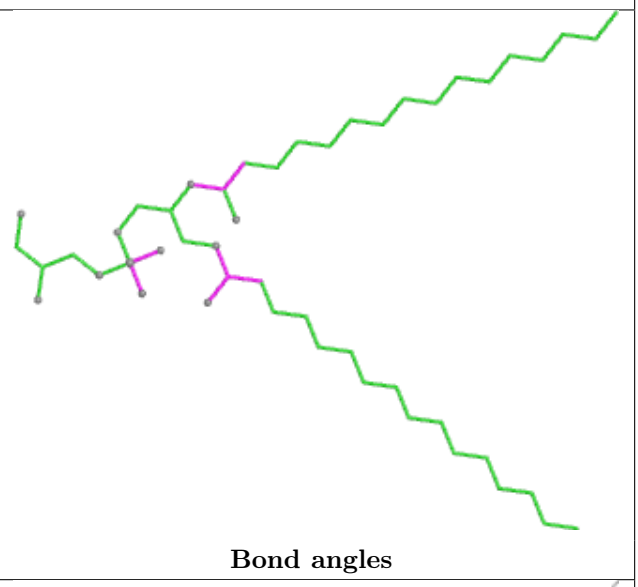


Rings

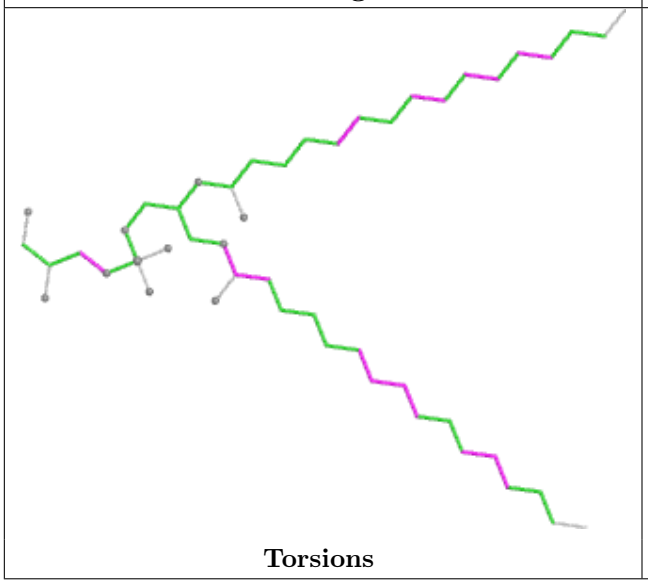
Ligand LHG D 407



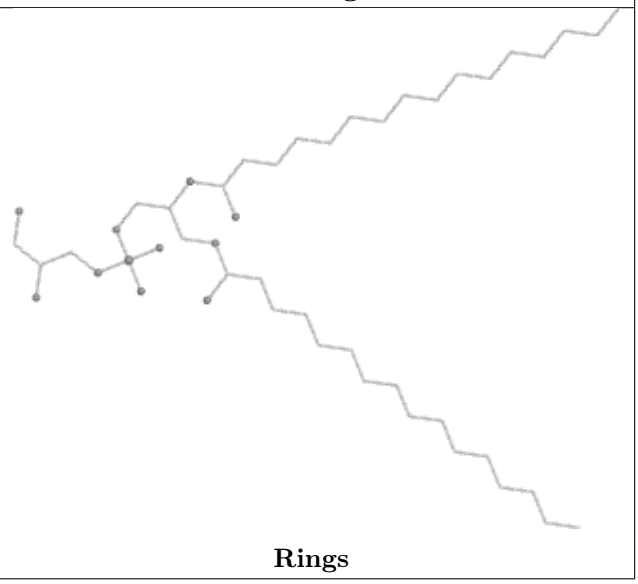
Bond lengths



Bond angles



Torsions

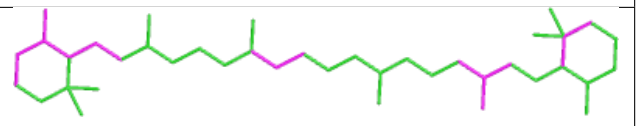


Rings

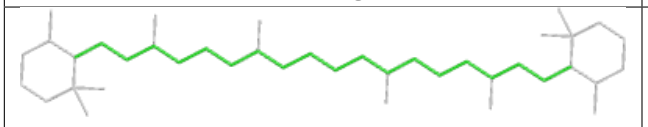
Ligand BCR b 618



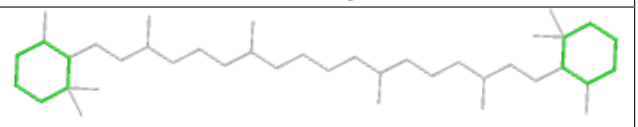
Bond lengths



Bond angles

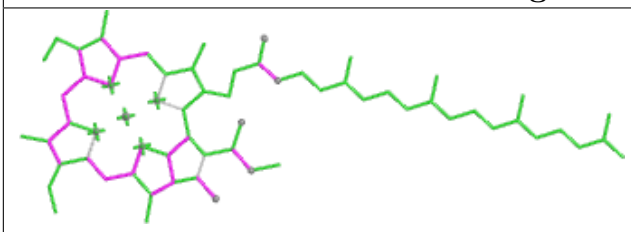


Torsions

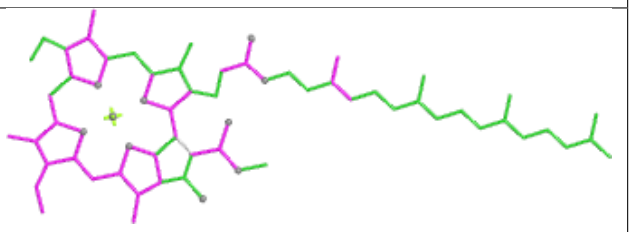


Rings

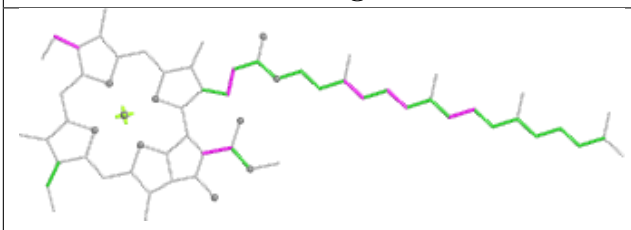
Ligand CLA c 508



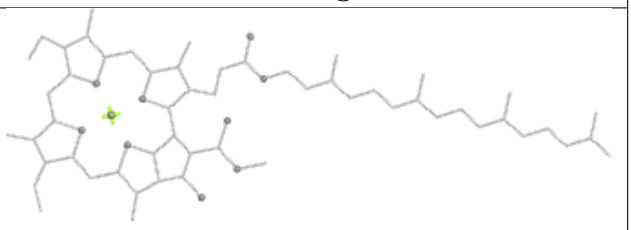
Bond lengths



Bond angles



Torsions



Rings

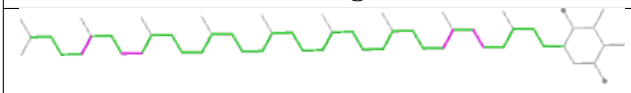
Ligand PL9 d 404



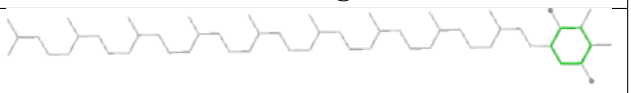
Bond lengths



Bond angles

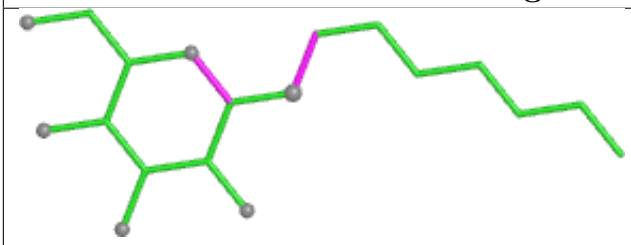


Torsions

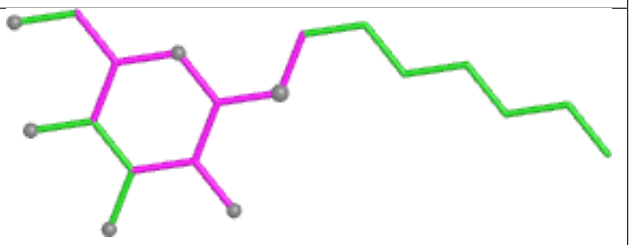


Rings

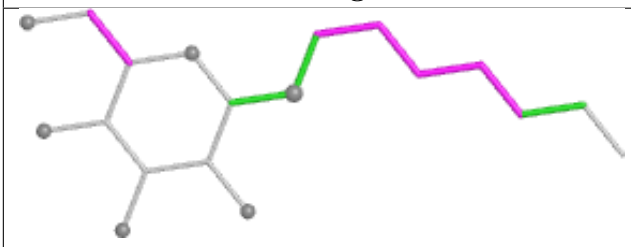
Ligand HTG b 622



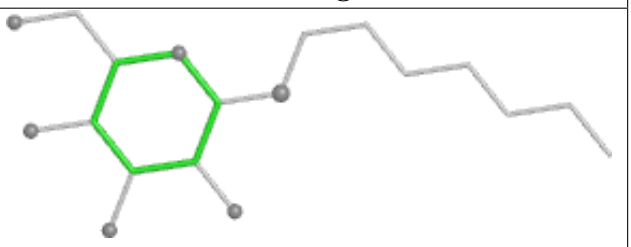
Bond lengths



Bond angles

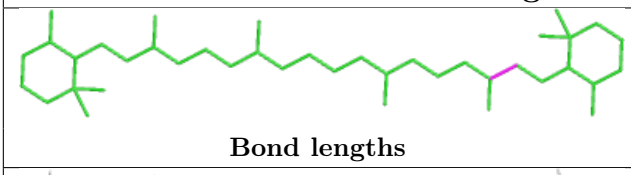


Torsions

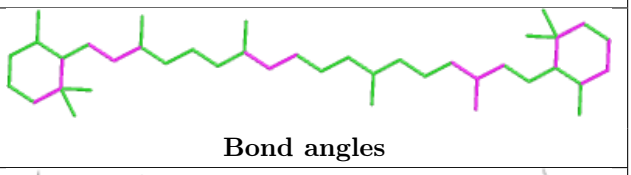


Rings

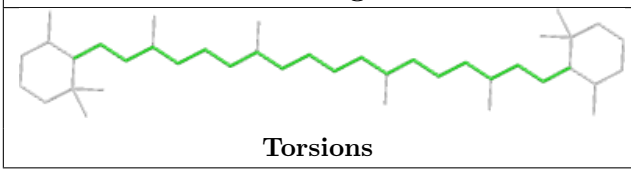
Ligand BCR B 618



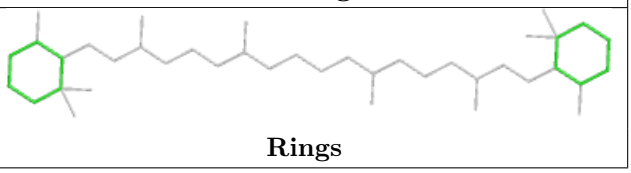
Bond lengths



Bond angles

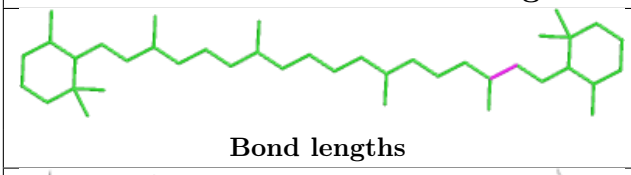


Torsions

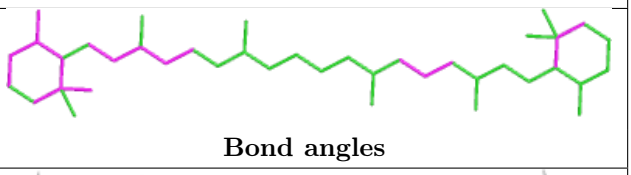


Rings

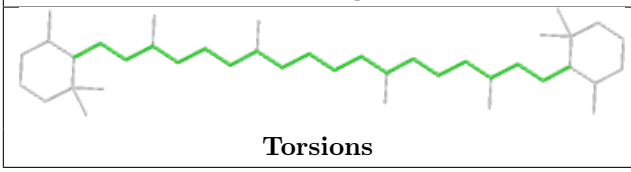
Ligand BCR C 514



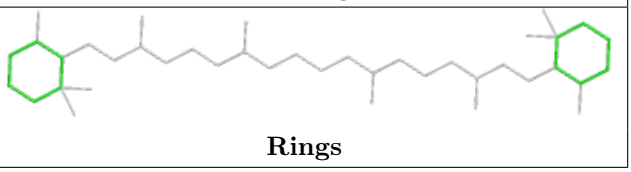
Bond lengths



Bond angles

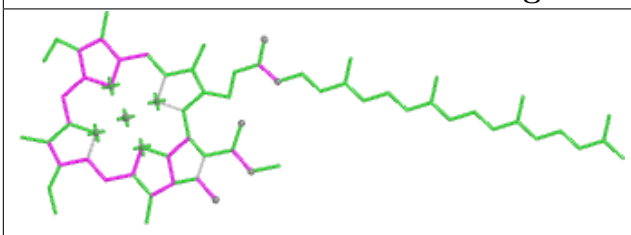


Torsions

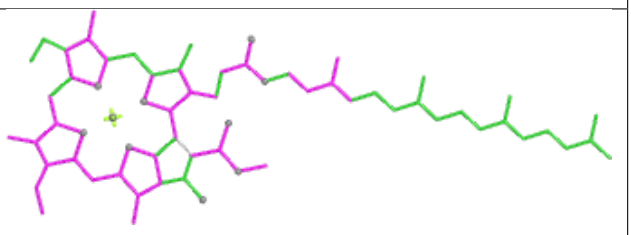


Rings

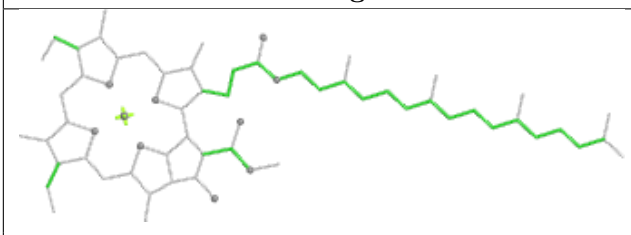
Ligand CLA D 402



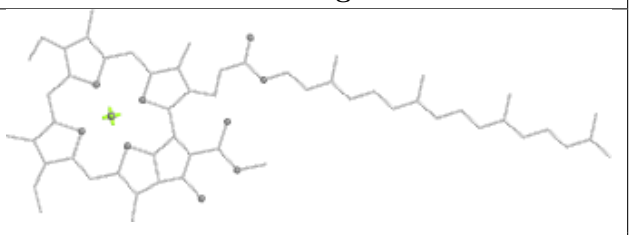
Bond lengths



Bond angles

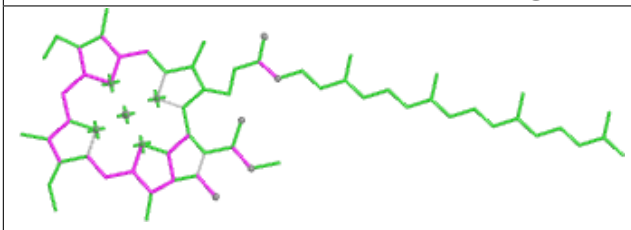


Torsions

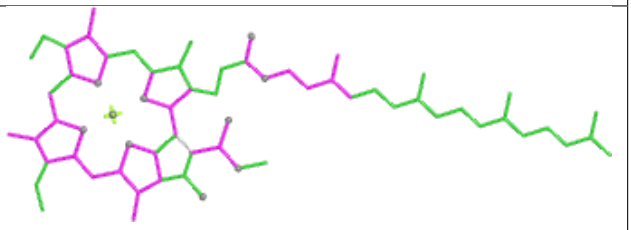


Rings

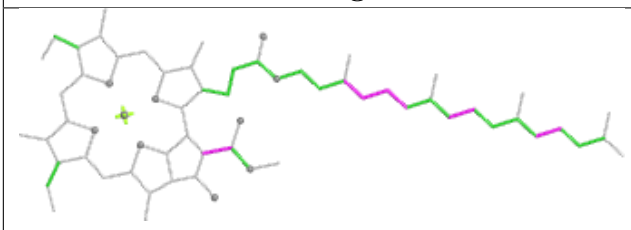
Ligand CLA b 605



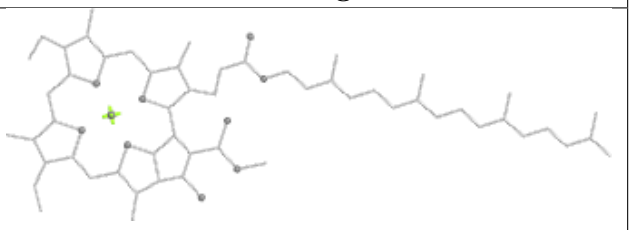
Bond lengths



Bond angles

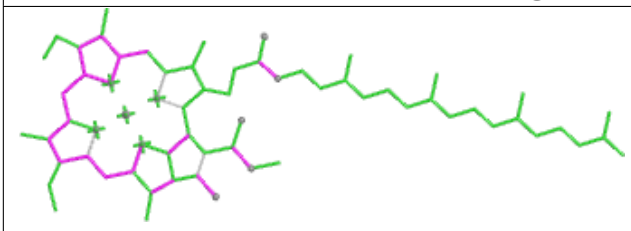


Torsions

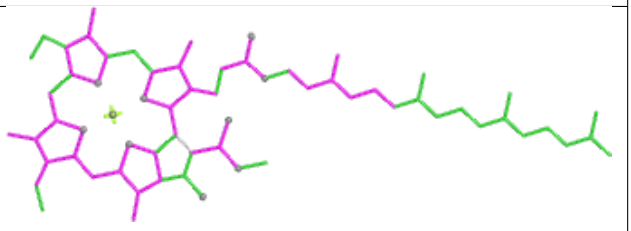


Rings

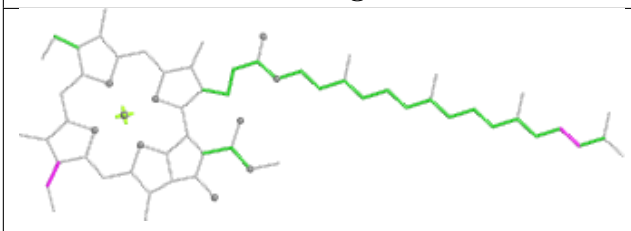
Ligand CLA a 405



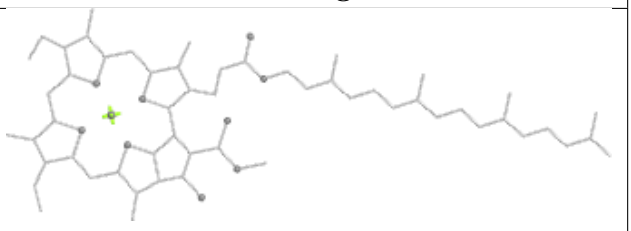
Bond lengths



Bond angles

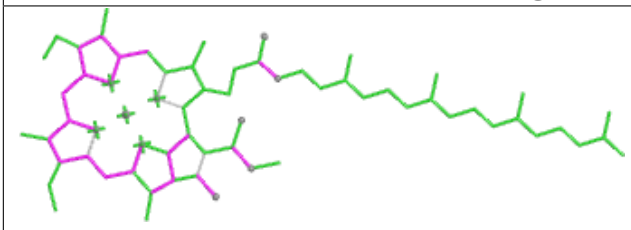


Torsions

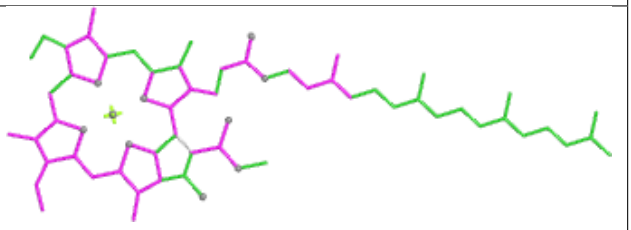


Rings

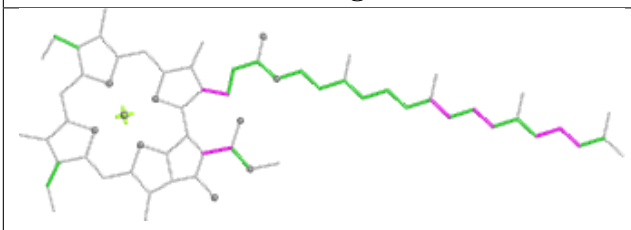
Ligand CLA c 507



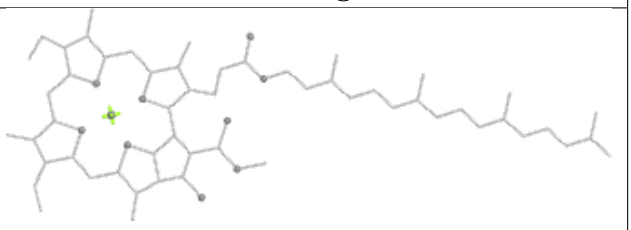
Bond lengths



Bond angles

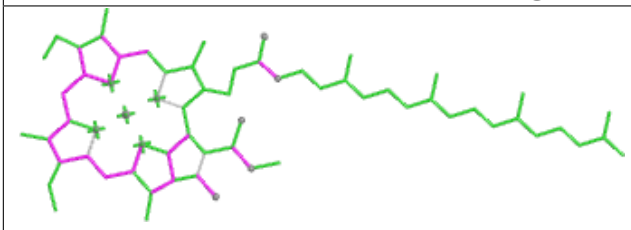


Torsions

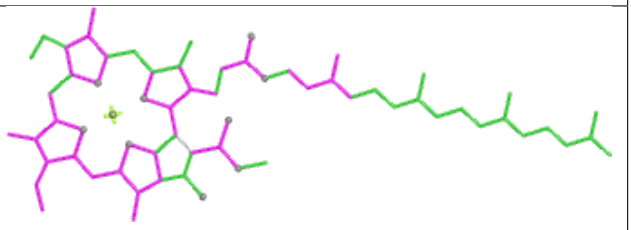


Rings

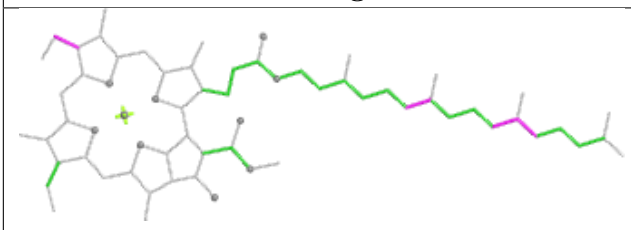
Ligand CLA a 407



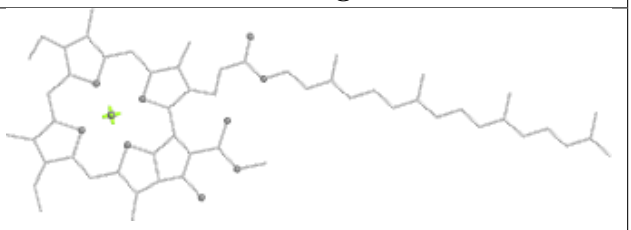
Bond lengths



Bond angles

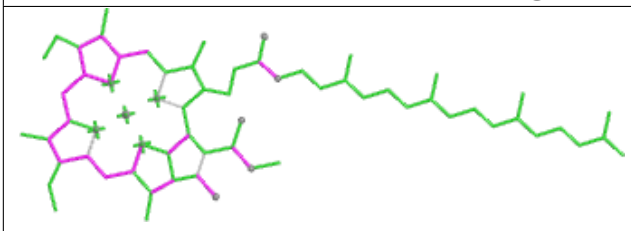


Torsions

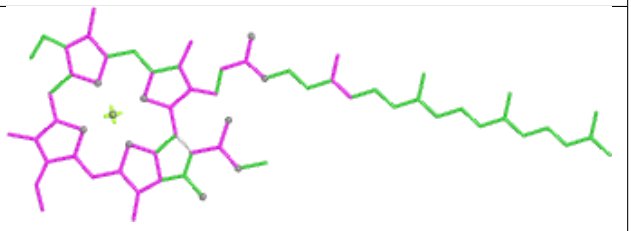


Rings

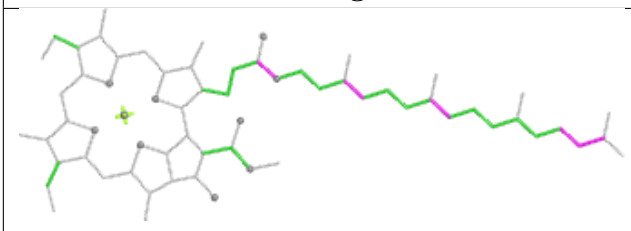
Ligand CLA a 409



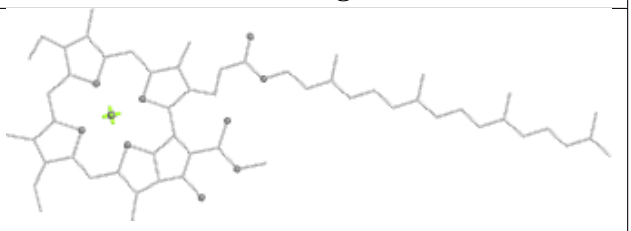
Bond lengths



Bond angles

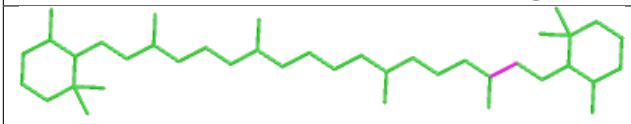


Torsions

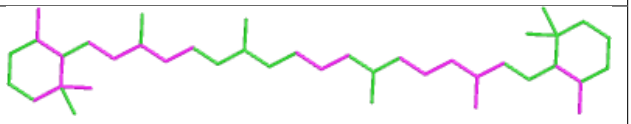


Rings

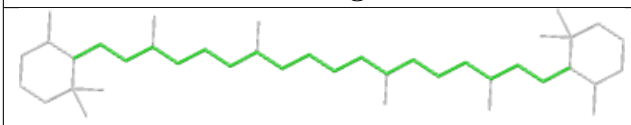
Ligand BCR c 516



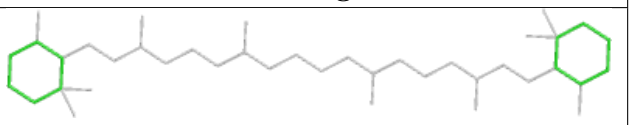
Bond lengths



Bond angles

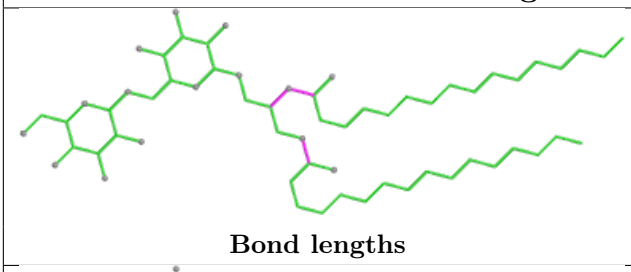


Torsions

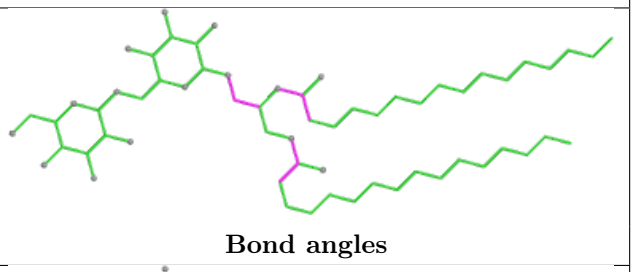


Rings

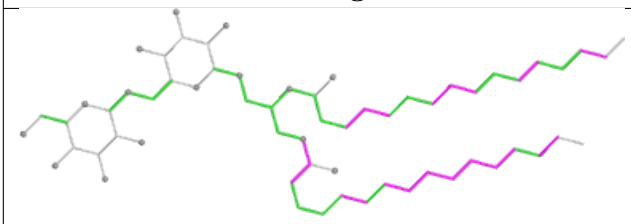
Ligand DGD C 517



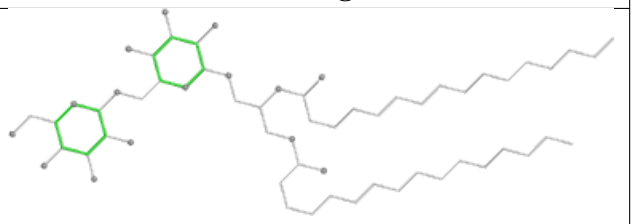
Bond lengths



Bond angles

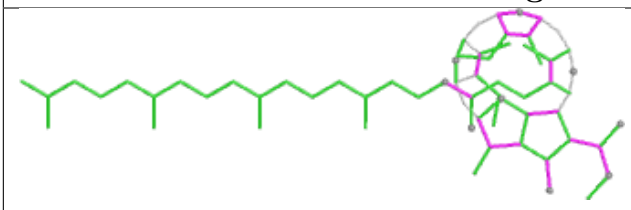


Torsions

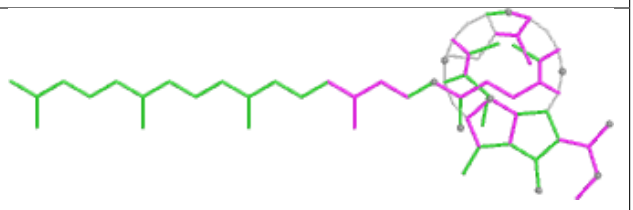


Rings

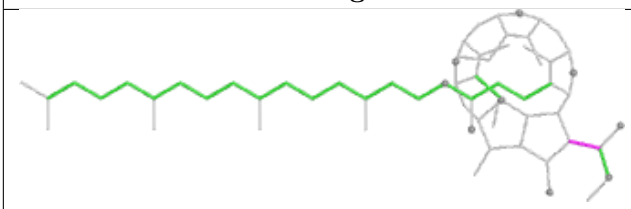
Ligand PHO a 417



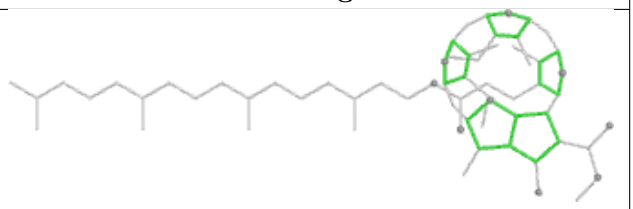
Bond lengths



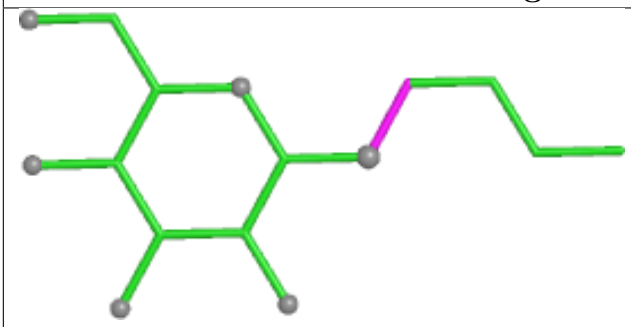
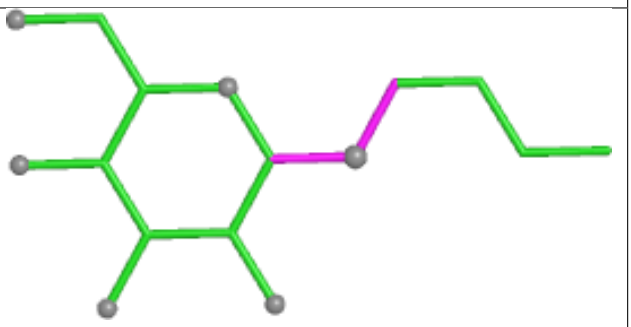
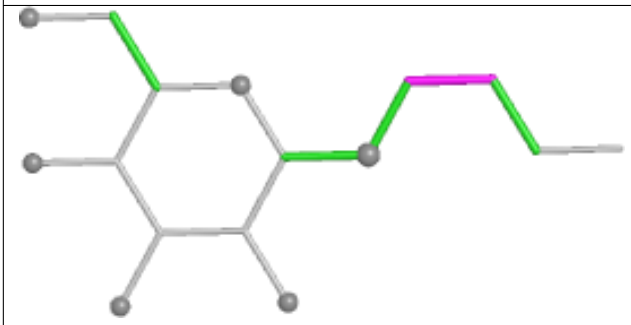
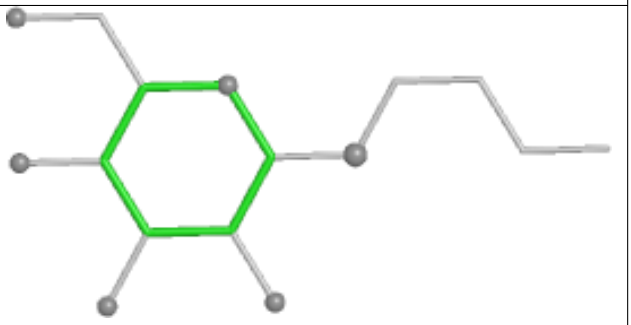
Bond angles

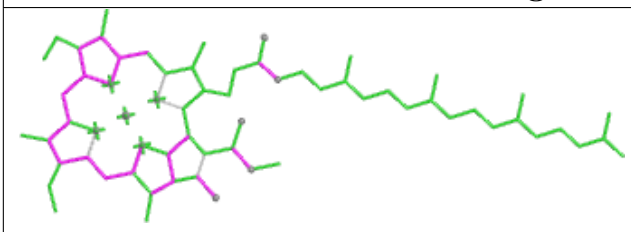
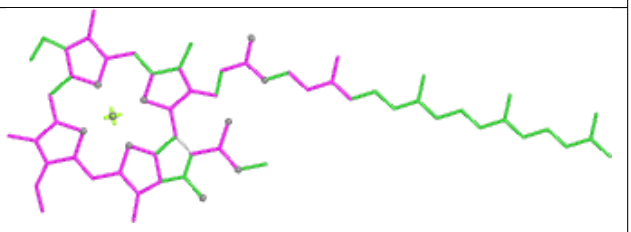
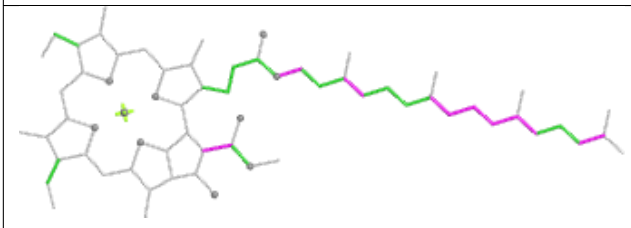
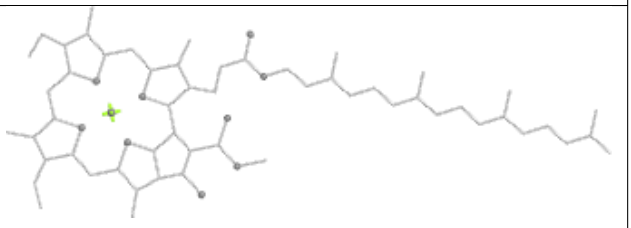


Torsions

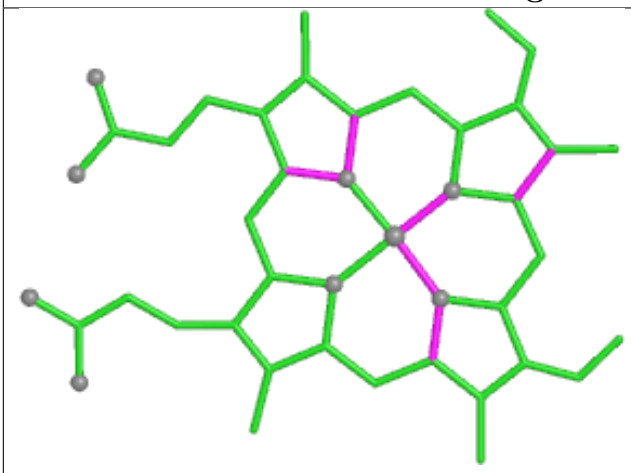


Rings

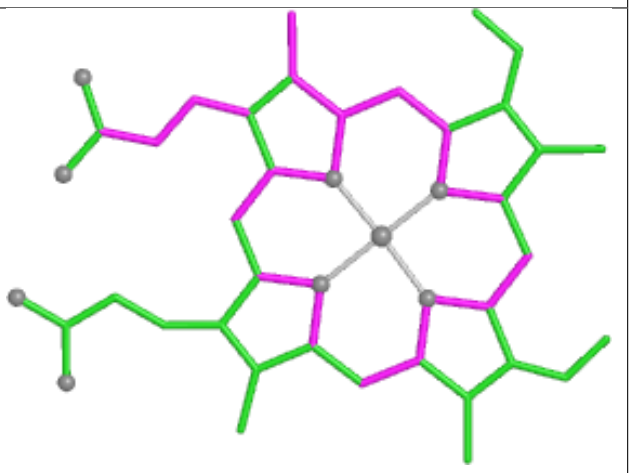
Ligand HTG d 409	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

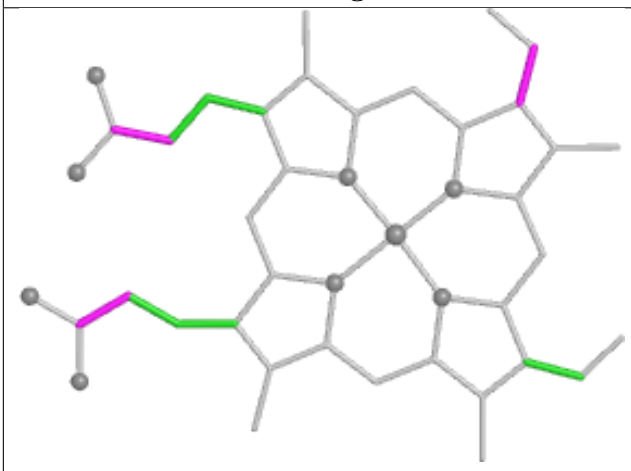
Ligand HEM f 101



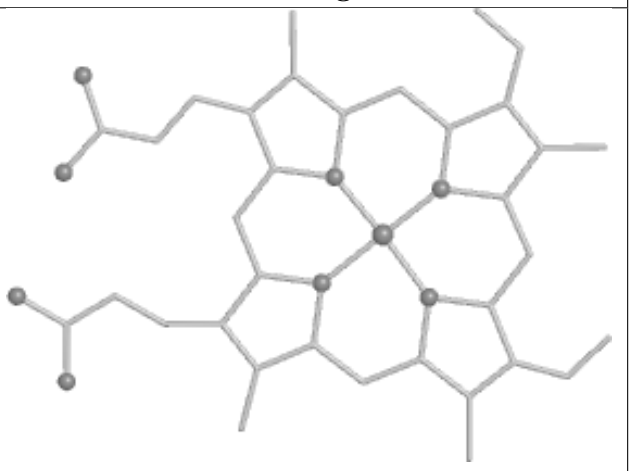
Bond lengths



Bond angles

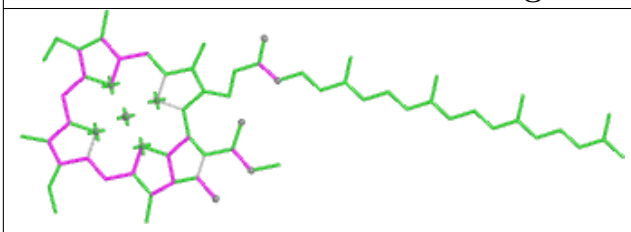


Torsions

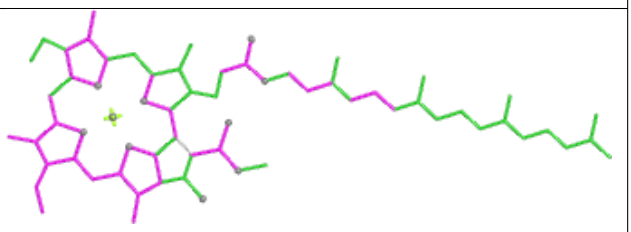


Rings

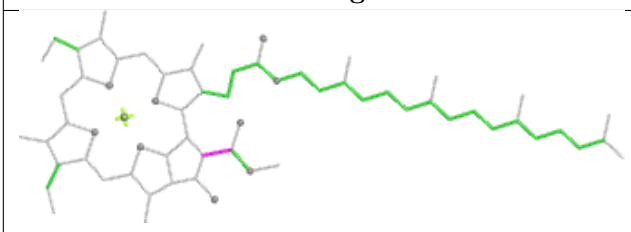
Ligand CLA B 609



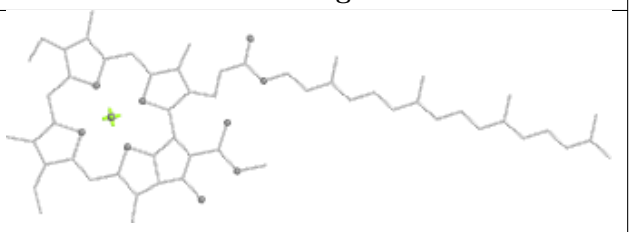
Bond lengths



Bond angles

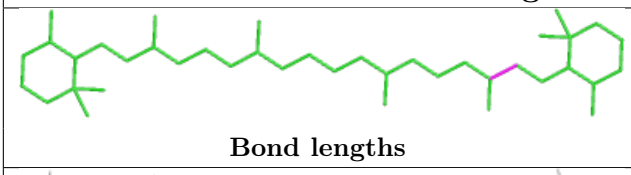


Torsions

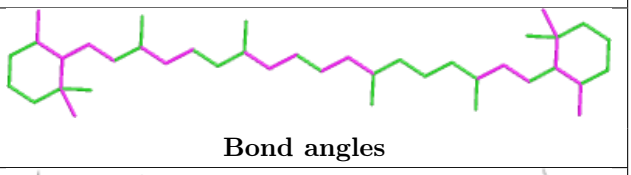


Rings

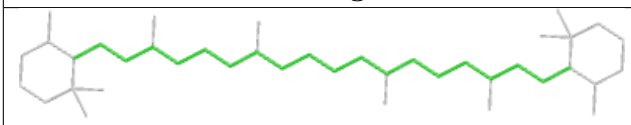
Ligand BCR A 409



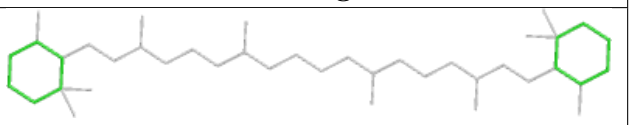
Bond lengths



Bond angles

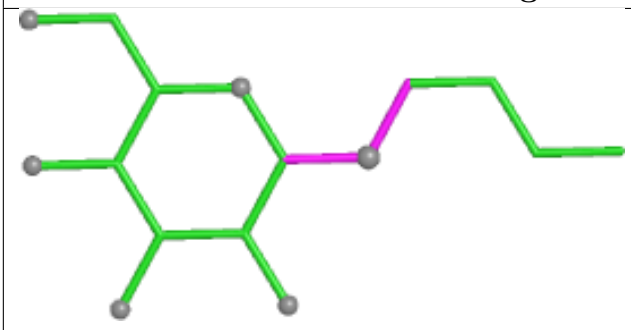


Torsions

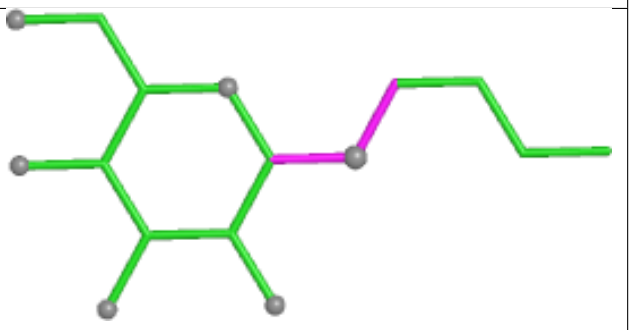


Rings

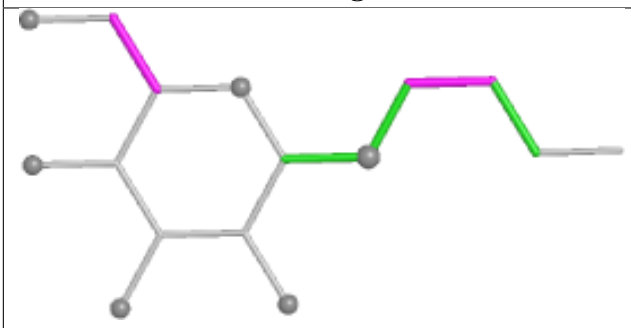
Ligand HTG D 410



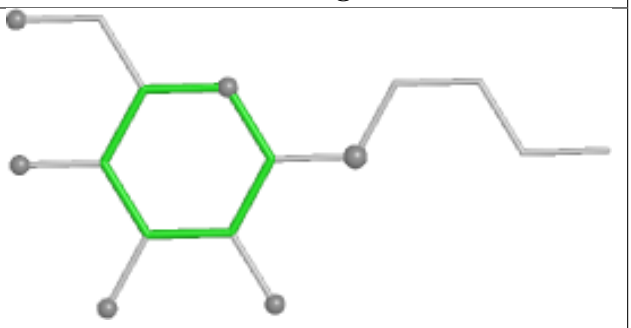
Bond lengths



Bond angles

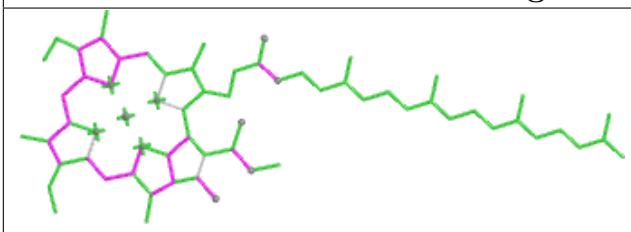


Torsions

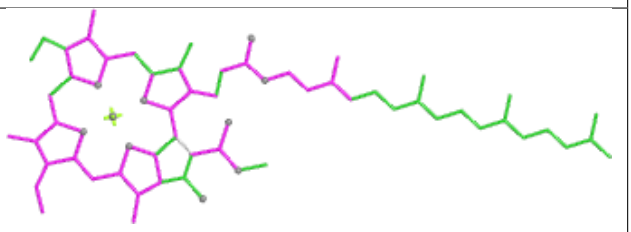


Rings

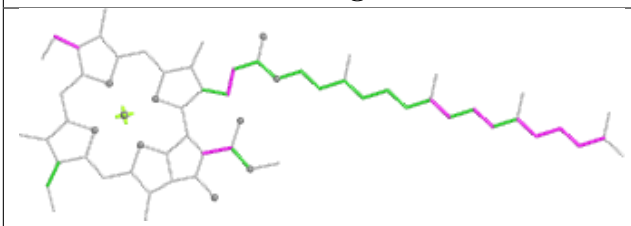
Ligand CLA b 606



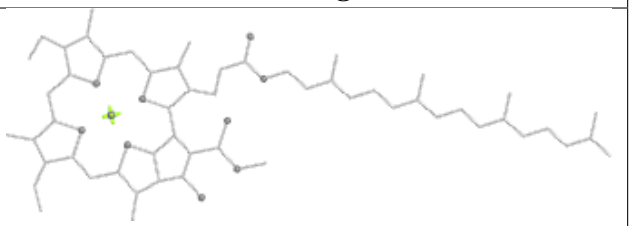
Bond lengths



Bond angles

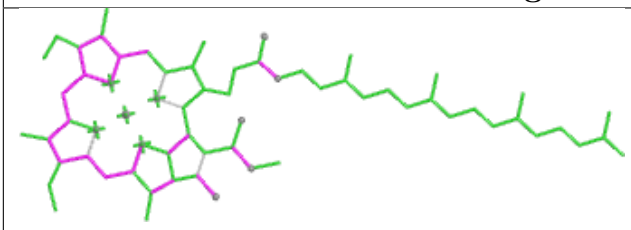


Torsions

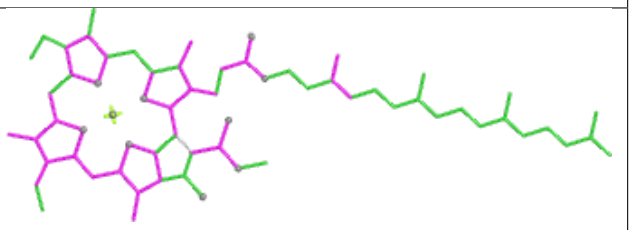


Rings

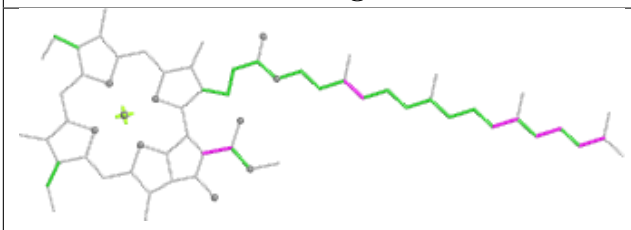
Ligand CLA B 603



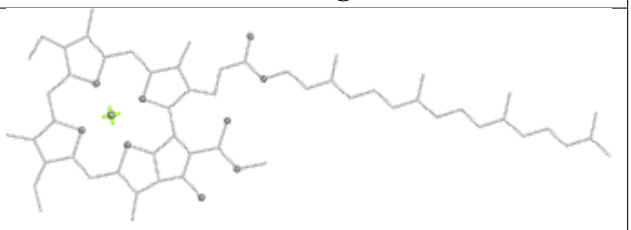
Bond lengths



Bond angles

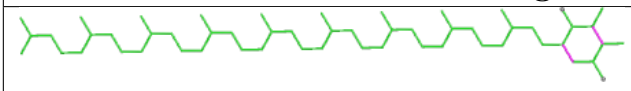


Torsions

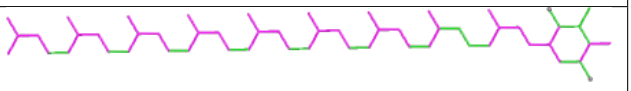


Rings

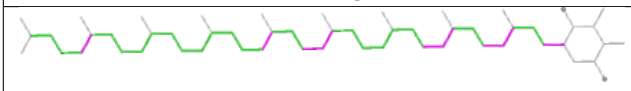
Ligand PL9 a 415



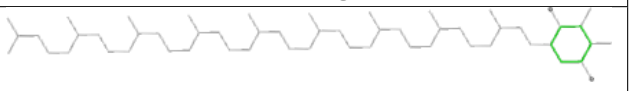
Bond lengths



Bond angles

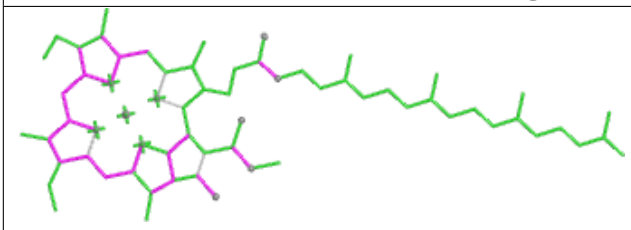


Torsions

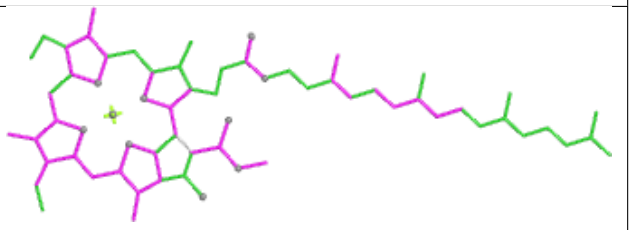


Rings

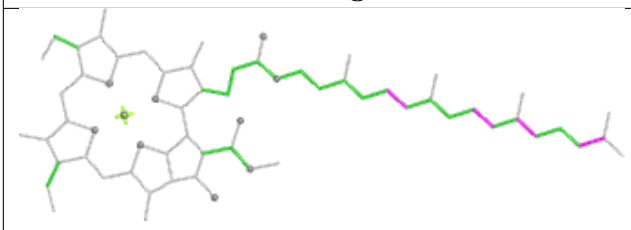
Ligand CLA B 615



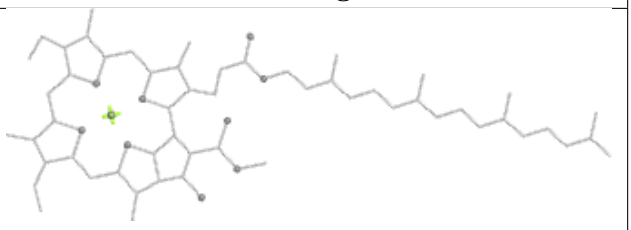
Bond lengths



Bond angles

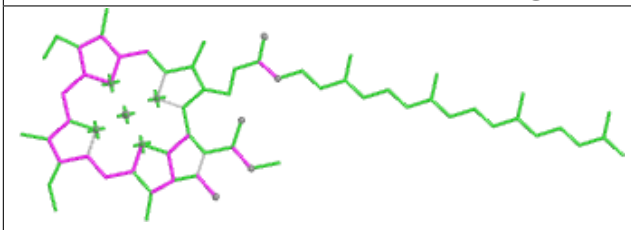


Torsions

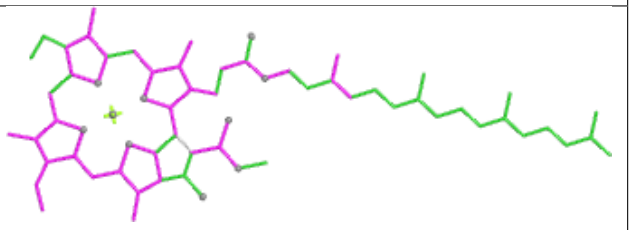


Rings

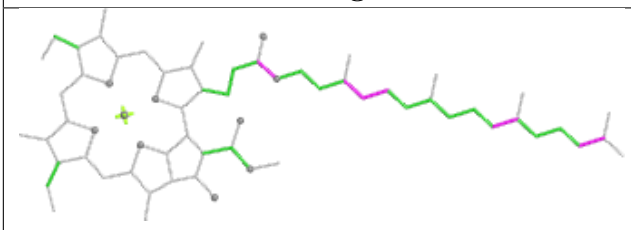
Ligand CLA d 402



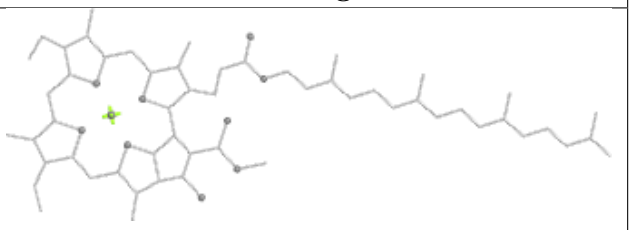
Bond lengths



Bond angles

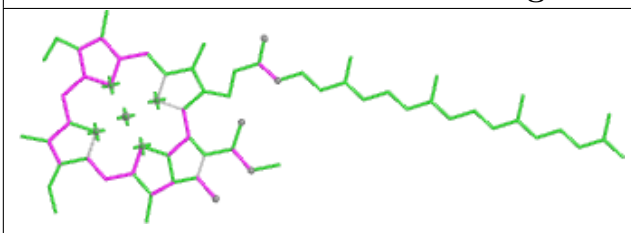


Torsions

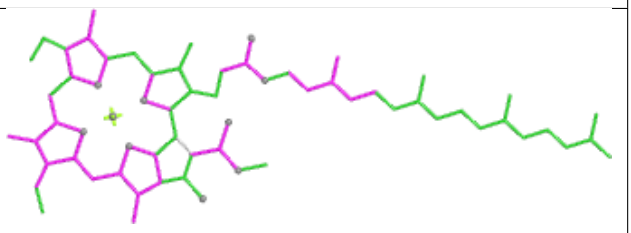


Rings

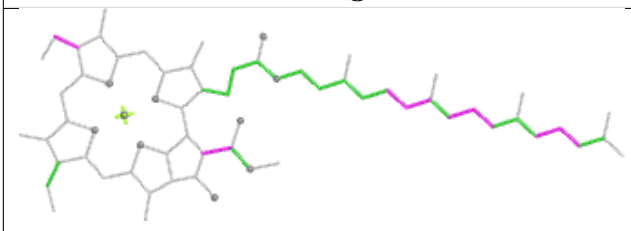
Ligand CLA b 604



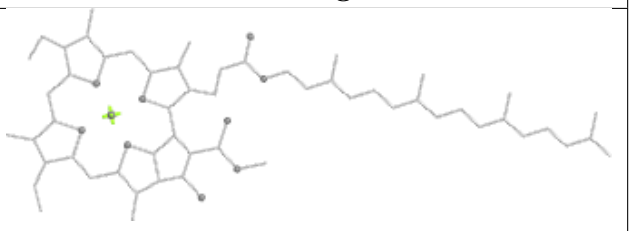
Bond lengths



Bond angles

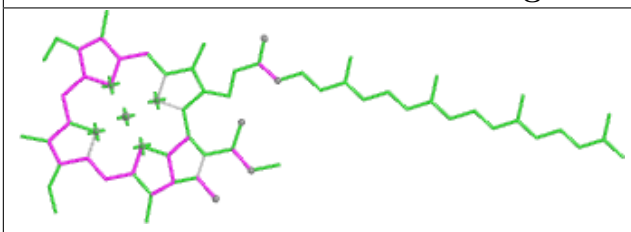


Torsions

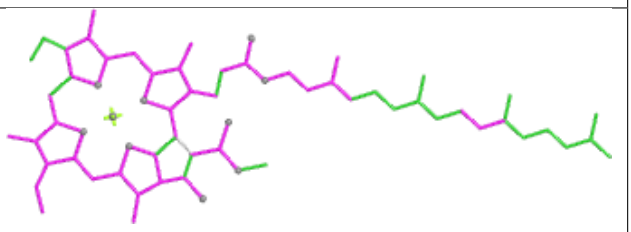


Rings

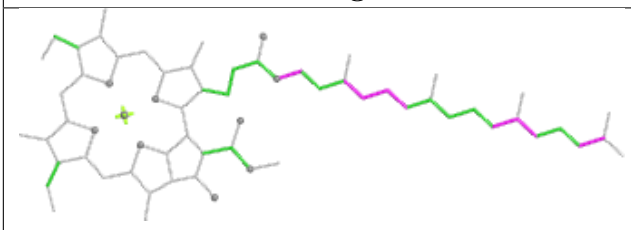
Ligand CLA A 408



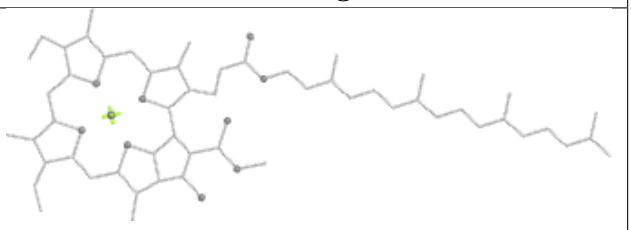
Bond lengths



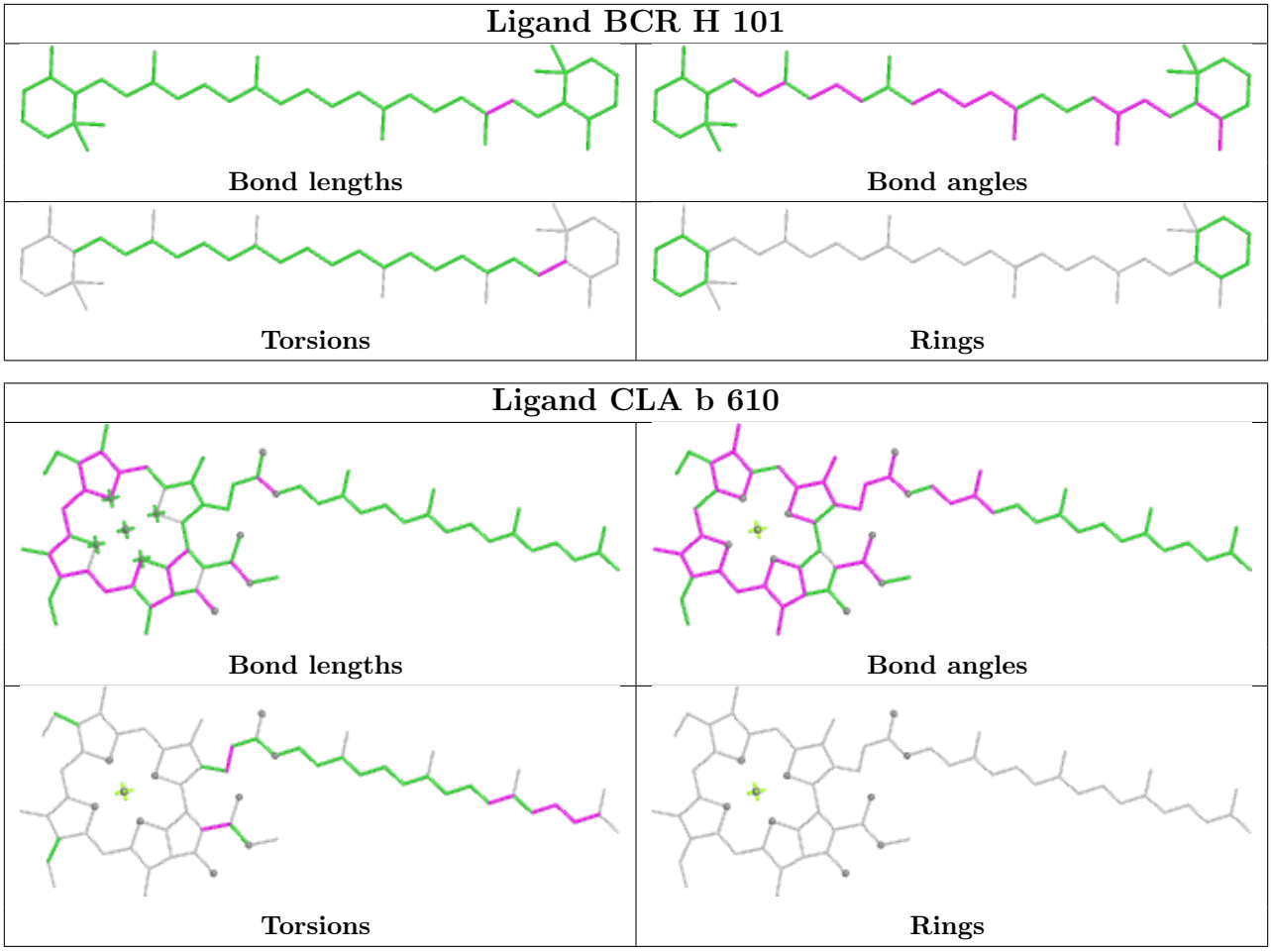
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.43	1 (0%) 90 91	24, 48, 69, 119	1 (0%)
1	a	334/344 (97%)	-0.43	2 (0%) 85 87	26, 52, 79, 125	2 (0%)
2	B	504/505 (99%)	-0.32	2 (0%) 88 90	22, 54, 79, 111	7 (1%)
2	b	504/505 (99%)	-0.25	8 (1%) 70 74	24, 58, 95, 164	6 (1%)
3	C	451/455 (99%)	-0.39	2 (0%) 88 90	30, 59, 79, 159	1 (0%)
3	c	455/455 (100%)	-0.38	1 (0%) 91 92	29, 66, 85, 128	5 (1%)
4	D	342/342 (100%)	-0.46	0 100 100	23, 50, 67, 137	1 (0%)
4	d	341/342 (99%)	-0.49	0 100 100	24, 54, 75, 131	2 (0%)
5	E	81/84 (96%)	-0.18	2 (2%) 58 62	53, 68, 94, 167	0
5	e	79/84 (94%)	-0.15	1 (1%) 75 78	33, 75, 110, 146	2 (2%)
6	F	34/44 (77%)	-0.43	0 100 100	54, 62, 83, 114	0
6	f	31/44 (70%)	-0.17	2 (6%) 25 28	55, 66, 89, 155	1 (3%)
7	H	64/65 (98%)	-0.10	2 (3%) 51 55	52, 61, 78, 106	0
7	h	64/65 (98%)	-0.21	1 (1%) 70 74	37, 69, 88, 110	1 (1%)
8	I	37/38 (97%)	0.05	1 (2%) 56 60	55, 63, 122, 168	0
8	i	37/38 (97%)	-0.09	1 (2%) 56 60	56, 64, 116, 142	0
9	J	38/39 (97%)	-0.17	0 100 100	52, 70, 117, 179	0
9	j	39/39 (100%)	-0.13	1 (2%) 57 61	59, 77, 125, 170	0
10	K	37/37 (100%)	-0.55	0 100 100	60, 68, 88, 102	0
10	k	37/37 (100%)	-0.41	0 100 100	65, 74, 95, 105	0
11	L	36/37 (97%)	-0.37	0 100 100	42, 47, 90, 145	0
11	l	36/37 (97%)	-0.36	2 (5%) 30 34	43, 49, 99, 122	0
12	M	32/36 (88%)	-0.36	0 100 100	26, 50, 70, 139	1 (3%)
12	m	33/36 (91%)	-0.28	0 100 100	24, 50, 70, 151	2 (6%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.36	0 100 100	35, 64, 113, 181	3 (1%)
13	o	243/244 (99%)	-0.29	0 100 100	45, 66, 117, 166	0
14	T	29/32 (90%)	-0.40	0 100 100	30, 48, 75, 116	1 (3%)
14	t	29/32 (90%)	-0.42	1 (3%) 48 52	45, 51, 77, 126	0
15	U	96/104 (92%)	-0.41	0 100 100	34, 59, 85, 91	1 (1%)
15	u	97/104 (93%)	-0.45	0 100 100	31, 63, 79, 135	1 (1%)
16	V	137/137 (100%)	-0.51	0 100 100	32, 57, 77, 101	2 (1%)
16	v	137/137 (100%)	-0.47	0 100 100	54, 71, 98, 133	0
17	X	38/40 (95%)	-0.10	0 100 100	35, 71, 89, 113	1 (2%)
17	x	38/40 (95%)	0.17	1 (2%) 57 61	63, 77, 117, 164	0
18	Y	29/30 (96%)	0.21	1 (3%) 48 52	68, 84, 120, 129	0
18	y	29/30 (96%)	-0.08	0 100 100	74, 90, 107, 113	0
19	Z	62/62 (100%)	-0.20	0 100 100	67, 80, 136, 162	0
19	z	62/62 (100%)	0.29	0 100 100	80, 92, 140, 192	0
20	R	34/34 (100%)	0.78	3 (8%) 15 17	79, 101, 126, 136	0
All	All	5283/5384 (98%)	-0.33	35 (0%) 84 85	22, 59, 97, 192	41 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.8
5	e	79[A]	PHE	4.7
2	b	479[A]	PHE	4.6
6	f	16[A]	PHE	4.2
8	i	37	LEU	3.5
2	B	494	GLY	3.4
2	b	499	VAL	3.4
3	c	245[A]	ILE	3.3
1	A	11	ALA	3.1
20	R	35	LEU	3.1
14	t	30	THR	3.0
17	x	37	VAL	2.8
18	Y	18	VAL	2.7
7	h	65	LEU	2.6
6	f	15	ILE	2.6
1	a	221[A]	SER	2.6
7	H	64	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	a	11	ALA	2.4
20	R	28	VAL	2.4
5	E	4	THR	2.4
2	b	486	LEU	2.4
20	R	24	LEU	2.3
2	b	491	VAL	2.3
3	C	246	ALA	2.3
2	b	502	VAL	2.2
11	l	3	PRO	2.2
2	b	210	ILE	2.2
9	j	2	SER	2.2
8	I	37	LEU	2.1
2	b	76[A]	SER	2.1
2	B	481	GLY	2.1
5	E	79	PHE	2.1
3	C	23	ALA	2.1
11	l	2	GLU	2.0
2	b	504	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.08	47,54,66,71	0
8	FME	I	1	10/11	0.95	0.07	61,69,78,79	0
14	FME	t	1	10/11	0.95	0.07	47,51,60,72	0
12	FME	m	1	10/11	0.96	0.07	54,64,82,94	0
12	FME	M	1	10/11	0.97	0.07	48,62,84,86	0
8	FME	i	1	10/11	0.97	0.07	59,69,77,78	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	a	419	6/6	0.50	0.18	80,92,94,96	0
31	LMT	B	630	35/35	0.61	0.17	82,106,122,128	0
31	LMT	A	417	35/35	0.64	0.16	86,110,122,126	0
30	UNL	j	101	10/-	0.64	0.22	86,95,100,102	0
30	UNL	A	415	28/-	0.66	0.16	103,117,125,134	0
30	UNL	J	101	10/-	0.68	0.27	80,86,89,96	0
30	UNL	m	102	10/-	0.68	0.22	80,83,89,95	0
31	LMT	F	101	35/35	0.68	0.17	115,135,160,163	0
30	UNL	a	416	30/-	0.69	0.14	107,122,136,137	0
31	LMT	e	101	35/35	0.69	0.16	124,145,169,174	0
30	UNL	I	101	40/-	0.70	0.17	85,110,133,135	0
31	LMT	c	501	35/35	0.72	0.15	122,132,145,151	0
31	LMT	A	421	35/35	0.72	0.14	121,134,154,156	0
34	HTG	B	623	19/19	0.72	0.17	71,85,102,104	0
34	HTG	C	520	19/19	0.73	0.14	121,127,141,144	0
30	UNL	K	102	34/-	0.74	0.14	94,112,126,126	0
26	SQD	f	102	43/54	0.74	0.14	115,129,152,155	0
30	UNL	i	101	40/-	0.75	0.15	82,104,130,136	0
27	GOL	o	302	6/6	0.75	0.18	88,101,106,109	0
30	UNL	l	101	10/-	0.75	0.17	73,79,91,91	0
32	LMG	C	519	51/55	0.76	0.13	69,116,136,139	0
30	UNL	D	409	40/-	0.76	0.14	74,93,114,120	0
31	LMT	b	621	25/35	0.76	0.14	94,115,138,141	0
36	CA	F	104	1/1	0.76	0.25	126,126,126,126	0
30	UNL	d	408	36/-	0.77	0.13	73,97,115,119	0
27	GOL	b	629	6/6	0.77	0.14	58,69,75,76	0
27	GOL	B	627	6/6	0.77	0.13	73,76,85,102	0
34	HTG	D	410	16/19	0.77	0.13	94,109,119,129	0
27	GOL	o	303	6/6	0.77	0.16	86,90,93,96	0
33	LHG	a	421	42/49	0.78	0.12	99,144,155,158	0
27	GOL	l	102	6/6	0.78	0.18	71,97,99,101	0
31	LMT	B	628	35/35	0.78	0.13	79,103,120,123	0
30	UNL	b	626	33/-	0.78	0.14	72,99,138,140	0
30	UNL	c	525	32/-	0.78	0.15	100,115,126,133	0
30	UNL	B	626	33/-	0.79	0.16	67,102,124,131	0
27	GOL	a	420	6/6	0.80	0.16	64,71,78,79	0
31	LMT	T	101	35/35	0.80	0.12	85,118,145,149	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	b	624	6/6	0.80	0.17	93,95,96,107	0
31	LMT	b	627	25/35	0.80	0.15	69,89,123,125	0
27	GOL	O	302	6/6	0.80	0.10	86,95,97,100	0
27	GOL	A	411	6/6	0.80	0.14	69,77,81,82	0
27	GOL	A	418	6/6	0.81	0.17	57,75,75,77	0
27	GOL	O	303	6/6	0.81	0.13	86,95,97,100	0
26	SQD	A	412	54/54	0.81	0.12	73,92,117,124	0
26	SQD	a	413	54/54	0.82	0.10	76,95,120,124	0
31	LMT	M	101	35/35	0.82	0.12	67,90,98,103	0
32	LMG	Z	101	37/55	0.82	0.15	77,118,134,143	0
34	HTG	c	522	19/19	0.82	0.10	123,132,138,140	0
29	PL9	A	414	55/55	0.82	0.15	76,100,113,116	0
36	CA	f	103	1/1	0.82	0.13	125,125,125,125	0
34	HTG	V	202	11/19	0.83	0.10	92,107,115,116	0
34	HTG	b	622	19/19	0.83	0.13	70,80,87,96	0
34	HTG	b	623	19/19	0.83	0.12	93,129,136,139	0
31	LMT	B	631	25/35	0.83	0.14	70,91,121,130	0
31	LMT	m	103	35/35	0.83	0.12	69,89,99,104	0
31	LMT	t	101	26/35	0.83	0.14	89,110,127,136	0
27	GOL	a	412	6/6	0.84	0.14	75,79,87,88	0
34	HTG	d	409	16/19	0.84	0.11	99,117,124,135	0
32	LMG	c	521	51/55	0.84	0.11	80,125,148,151	0
34	HTG	B	622	19/19	0.84	0.13	66,83,92,93	0
29	PL9	a	415	55/55	0.85	0.15	88,111,123,129	0
26	SQD	B	620	54/54	0.85	0.12	75,96,117,127	0
27	GOL	v	202	6/6	0.86	0.11	66,78,83,85	0
27	GOL	c	527	6/6	0.86	0.18	107,114,117,121	0
32	LMG	z	101	39/55	0.87	0.12	81,123,136,146	0
33	LHG	E	101	42/49	0.87	0.12	79,104,117,122	0
30	UNL	D	408	17/-	0.87	0.12	66,75,99,104	0
26	SQD	b	620	54/54	0.87	0.10	69,92,107,117	0
27	GOL	V	203	6/6	0.87	0.13	60,68,74,76	0
26	SQD	F	103	43/54	0.87	0.11	70,95,116,122	0
23	CLA	b	601	65/65	0.87	0.10	66,85,114,125	0
34	HTG	B	625	19/19	0.89	0.09	77,81,92,95	0
32	LMG	A	419	51/55	0.89	0.10	79,91,102,109	0
23	CLA	B	601	65/65	0.90	0.09	57,77,100,115	0
32	LMG	B	621	51/55	0.90	0.10	61,74,87,95	0
32	LMG	C	518	51/55	0.90	0.10	58,84,102,108	0
30	UNL	d	407	17/-	0.90	0.10	74,83,97,98	0
32	LMG	a	418	51/55	0.90	0.09	74,92,100,113	0
32	LMG	c	520	51/55	0.90	0.09	63,91,116,123	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	B	629	6/6	0.90	0.16	53,63,68,74	0
32	LMG	m	101	51/55	0.90	0.10	62,77,90,99	0
36	CA	o	301	1/1	0.90	0.07	102,102,102,102	0
27	GOL	C	521	6/6	0.91	0.14	57,60,65,66	0
25	BCR	T	102	40/40	0.91	0.07	47,58,68,69	0
32	LMG	D	411	51/55	0.91	0.10	51,67,103,106	0
23	CLA	b	616	65/65	0.92	0.09	54,62,117,125	0
34	HTG	b	625	19/19	0.92	0.08	71,82,88,96	0
23	CLA	c	514	65/65	0.92	0.09	71,89,112,120	0
33	LHG	A	420	49/49	0.92	0.10	52,65,81,84	0
27	GOL	B	624	6/6	0.92	0.08	73,77,85,86	0
32	LMG	d	410	51/55	0.92	0.09	58,71,102,107	0
23	CLA	C	513	65/65	0.92	0.08	65,83,103,109	0
23	CLA	C	506	65/65	0.93	0.09	59,69,103,104	0
25	BCR	d	403	40/40	0.93	0.08	53,67,92,95	0
33	LHG	d	411	49/49	0.93	0.09	57,68,77,81	0
25	BCR	t	102	40/40	0.93	0.07	48,57,75,79	0
26	SQD	A	410	54/54	0.93	0.09	59,81,104,109	0
23	CLA	A	408	65/65	0.93	0.09	45,53,110,114	0
23	CLA	B	614	65/65	0.93	0.08	43,51,85,92	0
23	CLA	b	614	65/65	0.93	0.07	45,52,84,88	0
26	SQD	a	411	54/54	0.93	0.09	64,84,111,117	0
23	CLA	B	616	65/65	0.93	0.10	49,59,106,115	0
23	CLA	c	507	65/65	0.93	0.08	58,69,100,105	0
23	CLA	c	513	65/65	0.93	0.09	66,80,114,117	0
23	CLA	C	504	65/65	0.93	0.08	47,56,89,99	0
23	CLA	d	402	65/65	0.93	0.09	55,65,113,123	0
35	DGD	C	516	62/66	0.93	0.08	51,64,102,106	0
25	BCR	D	404	40/40	0.93	0.09	50,60,92,98	0
25	BCR	K	101	40/40	0.93	0.08	62,76,85,89	0
33	LHG	D	407	49/49	0.93	0.09	52,61,99,105	0
27	GOL	c	526	6/6	0.94	0.07	65,65,71,74	0
25	BCR	h	101	40/40	0.94	0.09	57,68,87,93	0
30	UNL	X	101	18/-	0.94	0.12	66,74,99,102	0
23	CLA	b	606	65/65	0.94	0.08	48,60,97,106	0
23	CLA	C	512	65/65	0.94	0.08	63,72,101,106	0
23	CLA	B	606	65/65	0.94	0.08	44,57,97,104	0
25	BCR	H	101	40/40	0.94	0.08	53,65,85,87	0
23	CLA	c	505	65/65	0.94	0.07	56,63,97,100	0
25	BCR	K	103	40/40	0.94	0.09	57,64,72,74	0
23	CLA	a	409	65/65	0.94	0.10	47,55,113,119	0
25	BCR	Y	101	40/40	0.94	0.08	57,65,78,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	b	618	40/40	0.94	0.07	49,59,74,77	0
25	BCR	c	515	40/40	0.94	0.08	73,83,89,90	0
35	DGD	C	517	62/66	0.94	0.07	48,61,89,100	0
35	DGD	H	102	62/66	0.94	0.09	51,62,72,74	0
35	DGD	c	517	62/66	0.94	0.07	48,62,97,101	0
35	DGD	c	518	62/66	0.94	0.07	54,68,111,123	0
35	DGD	c	519	62/66	0.94	0.07	53,67,100,116	0
23	CLA	C	508	65/65	0.94	0.07	48,56,105,113	0
33	LHG	b	630	49/49	0.94	0.08	54,59,69,83	0
33	LHG	d	406	49/49	0.94	0.09	55,65,109,123	0
23	CLA	C	501	65/65	0.95	0.06	52,61,70,76	0
29	PL9	D	405	55/55	0.95	0.07	39,51,57,66	0
23	CLA	A	406	65/65	0.95	0.06	40,49,109,115	0
29	PL9	d	404	55/55	0.95	0.07	43,52,60,65	0
23	CLA	b	607	65/65	0.95	0.07	40,49,72,77	0
23	CLA	b	609	65/65	0.95	0.07	51,64,72,80	0
23	CLA	b	612	65/65	0.95	0.08	43,52,61,66	0
23	CLA	B	609	65/65	0.95	0.07	49,59,69,74	0
25	BCR	a	410	40/40	0.95	0.07	46,55,62,64	0
23	CLA	B	610	65/65	0.95	0.09	46,56,61,75	0
25	BCR	b	619	40/40	0.95	0.07	52,62,82,86	0
23	CLA	B	611	65/65	0.95	0.07	41,47,64,67	0
23	CLA	B	602	65/65	0.95	0.07	48,56,67,77	0
23	CLA	c	508	65/65	0.95	0.08	56,68,79,83	0
23	CLA	c	509	65/65	0.95	0.07	51,62,115,121	0
25	BCR	y	101	40/40	0.95	0.07	62,71,80,86	0
27	GOL	b	628	6/6	0.95	0.07	79,84,94,95	0
23	CLA	D	403	65/65	0.95	0.08	51,59,104,108	0
23	CLA	a	407	65/65	0.95	0.07	43,54,120,125	0
23	CLA	B	603	65/65	0.95	0.08	44,52,70,74	0
25	BCR	A	409	40/40	0.95	0.07	42,53,65,66	0
30	UNL	x	101	18/-	0.95	0.11	75,83,119,121	0
35	DGD	h	102	62/66	0.95	0.08	57,65,74,79	0
25	BCR	B	618	40/40	0.95	0.06	47,56,69,74	0
36	CA	O	301	1/1	0.95	0.04	100,100,100,100	0
25	BCR	B	619	40/40	0.95	0.07	51,60,83,88	0
25	BCR	C	514	40/40	0.95	0.06	55,64,71,80	0
37	BCT	a	404	4/4	0.95	0.07	58,60,68,77	0
24	PHO	A	416	64/64	0.96	0.06	39,51,58,64	0
24	PHO	a	417	64/64	0.96	0.06	46,54,62,68	0
33	LHG	d	405	49/49	0.96	0.07	49,58,72,76	0
23	CLA	b	604	65/65	0.96	0.07	42,52,87,99	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	B	617	40/40	0.96	0.06	45,53,61,64	0
23	CLA	b	605	65/65	0.96	0.07	43,51,71,77	0
23	CLA	B	612	65/65	0.96	0.06	39,49,59,63	0
23	CLA	C	507	65/65	0.96	0.07	52,62,78,87	0
23	CLA	B	613	65/65	0.96	0.06	41,47,84,90	0
23	CLA	b	611	65/65	0.96	0.06	43,51,66,70	0
23	CLA	C	509	65/65	0.96	0.07	52,58,77,80	0
23	CLA	b	613	65/65	0.96	0.06	43,50,81,87	0
23	CLA	C	510	65/65	0.96	0.06	52,60,75,76	0
23	CLA	B	607	65/65	0.96	0.07	40,47,68,73	0
23	CLA	c	502	65/65	0.96	0.07	59,66,75,78	0
25	BCR	b	617	40/40	0.96	0.05	48,54,61,61	0
35	DGD	C	515	62/66	0.96	0.07	48,56,95,100	0
23	CLA	c	504	65/65	0.96	0.06	53,69,78,88	0
23	CLA	A	404	65/65	0.96	0.06	38,45,62,66	0
23	CLA	c	506	65/65	0.96	0.07	52,63,84,92	0
25	BCR	c	516	40/40	0.96	0.06	60,66,73,78	0
23	CLA	B	605	65/65	0.96	0.07	43,49,66,73	0
23	CLA	C	503	65/65	0.96	0.06	49,61,68,77	0
25	BCR	k	101	40/40	0.96	0.08	60,74,81,82	0
23	CLA	A	405	65/65	0.96	0.06	37,44,58,70	0
23	CLA	C	505	65/65	0.96	0.07	51,59,83,90	0
36	CA	c	523	1/1	0.96	0.08	75,75,75,75	0
33	LHG	D	406	49/49	0.96	0.07	48,56,68,73	0
23	CLA	b	602	65/65	0.96	0.07	52,60,72,76	0
23	CLA	b	603	65/65	0.96	0.07	47,58,78,84	0
23	CLA	B	604	65/65	0.97	0.06	41,47,97,103	0
23	CLA	c	510	65/65	0.97	0.07	49,64,83,85	0
23	CLA	c	511	65/65	0.97	0.06	53,63,74,89	0
23	CLA	c	512	65/65	0.97	0.07	59,67,83,93	0
23	CLA	D	402	65/65	0.97	0.06	36,44,69,76	0
23	CLA	B	608	65/65	0.97	0.06	44,51,69,77	0
23	CLA	d	401	65/65	0.97	0.06	41,47,77,91	0
33	LHG	L	101	49/49	0.97	0.06	52,58,70,87	0
23	CLA	b	615	65/65	0.97	0.06	51,59,77,78	0
24	PHO	A	407	64/64	0.97	0.05	37,46,54,59	0
23	CLA	a	405	65/65	0.97	0.06	42,48,63,74	0
24	PHO	a	408	64/64	0.97	0.05	43,49,54,56	0
23	CLA	a	406	65/65	0.97	0.05	41,46,63,69	0
36	CA	C	522	1/1	0.97	0.05	73,73,73,73	0
23	CLA	c	503	65/65	0.97	0.07	49,60,89,107	0
23	CLA	C	502	65/65	0.97	0.06	48,56,78,85	0

Continued on next page...

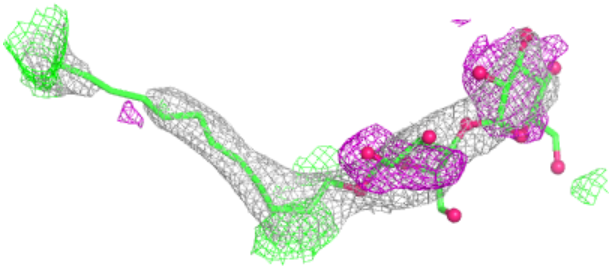
Continued from previous page...

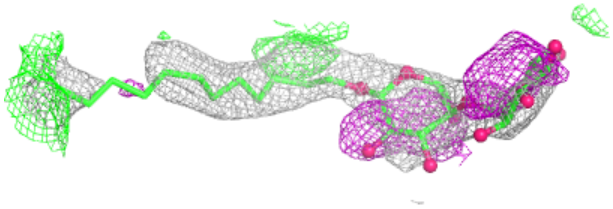
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	608	65/65	0.97	0.05	46,56,78,86	0
23	CLA	C	511	65/65	0.97	0.07	52,64,77,80	0
23	CLA	b	610	65/65	0.97	0.07	51,58,64,69	0
37	BCT	D	401	4/4	0.97	0.06	54,58,61,66	0
23	CLA	B	615	65/65	0.97	0.06	46,54,74,80	0
38	HEM	f	101	43/43	0.97	0.09	67,81,101,109	0
22	CL	A	403	1/1	0.98	0.04	47,47,47,47	0
22	CL	a	403	1/1	0.98	0.08	52,52,52,52	0
38	HEM	F	102	43/43	0.98	0.06	60,68,75,85	0
22	CL	A	402	1/1	0.98	0.07	43,43,43,43	0
39	MG	J	102	1/1	0.98	0.03	59,59,59,59	0
40	HEC	V	201	43/43	0.98	0.06	44,51,56,57	0
40	HEC	v	201	43/43	0.98	0.07	55,61,67,69	0
36	CA	c	524	1/1	0.99	0.04	76,76,76,76	0
22	CL	a	402	1/1	0.99	0.05	50,50,50,50	0
28	OEX	A	413	10/10	0.99	0.03	41,44,48,50	0
39	MG	j	102	1/1	0.99	0.06	63,63,63,63	0
28	OEX	a	414	10/10	0.99	0.03	47,50,51,55	0
21	FE2	a	401	1/1	0.99	0.02	55,55,55,55	0
21	FE2	A	401	1/1	1.00	0.02	52,52,52,52	0

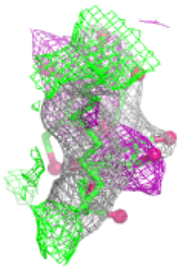
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 630:

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

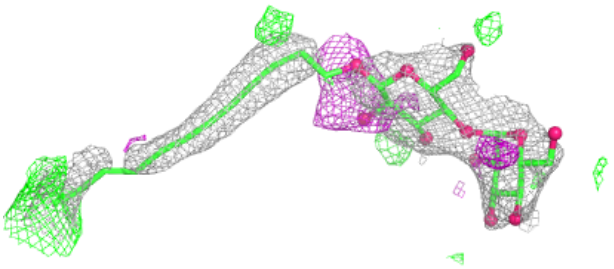


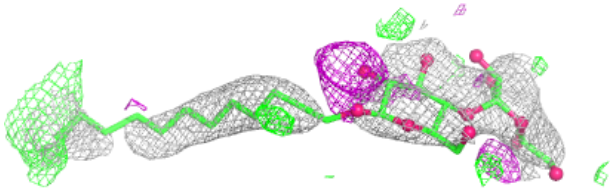


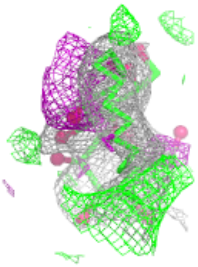


Electron density around LMT A 417:

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

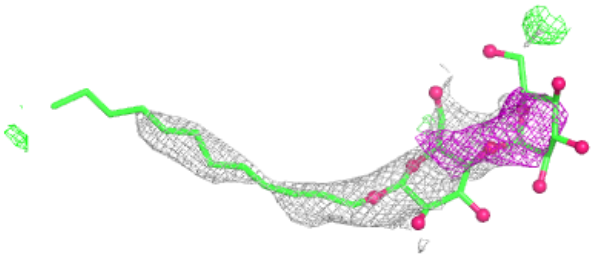


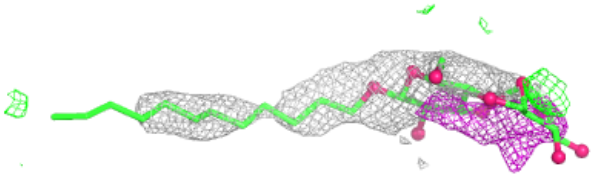


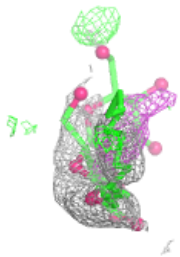


Electron density around LMT F 101:

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

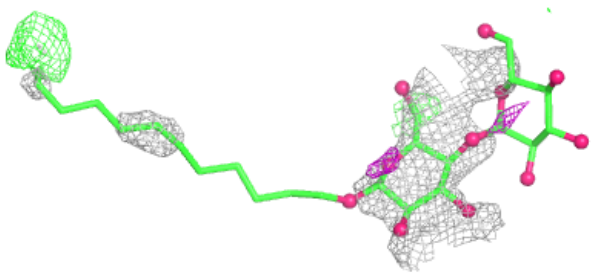


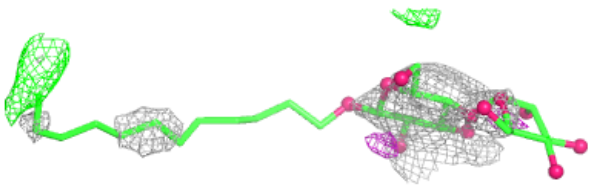


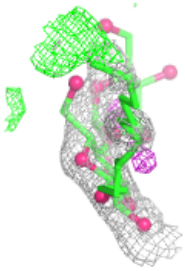


Electron density around LMT e 101:

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

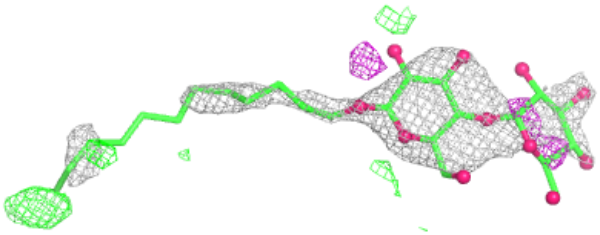


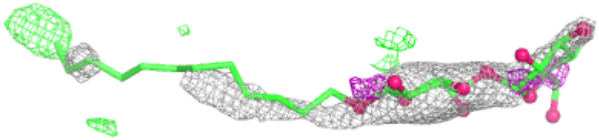


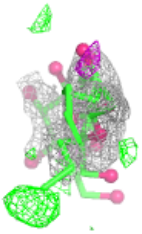


Electron density around LMT c 501:

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

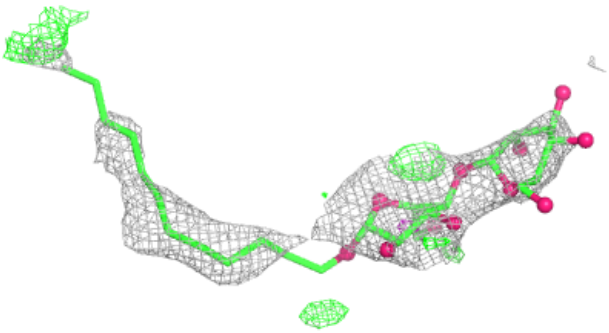


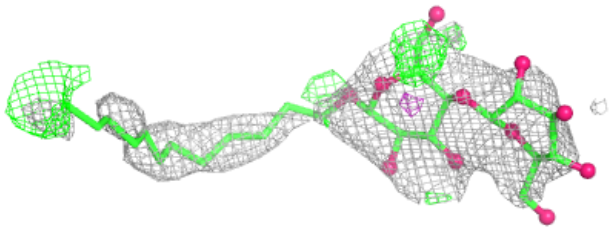


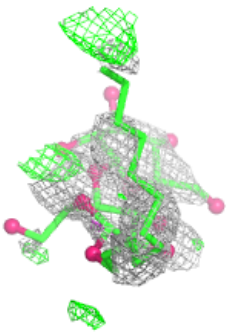


Electron density around LMT A 421:

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

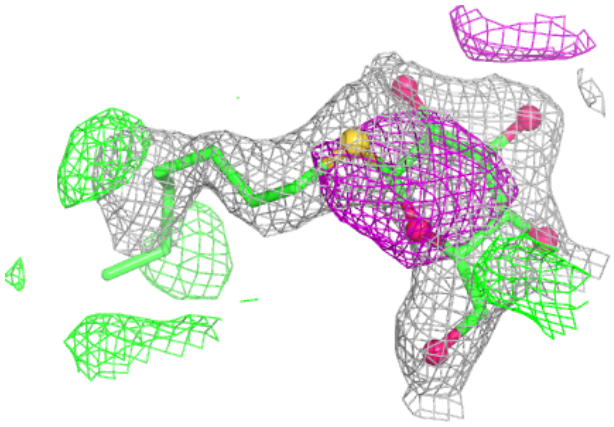


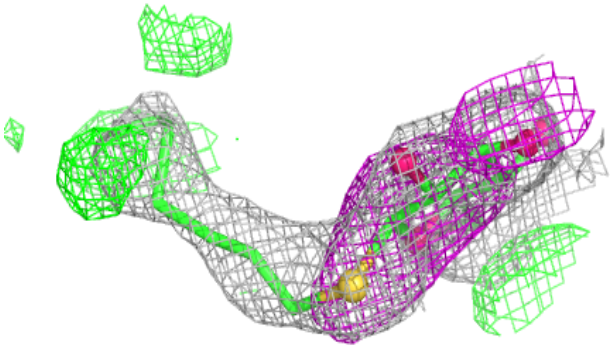


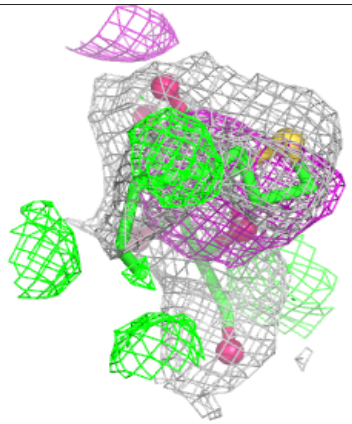


Electron density around HTG B 623:

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

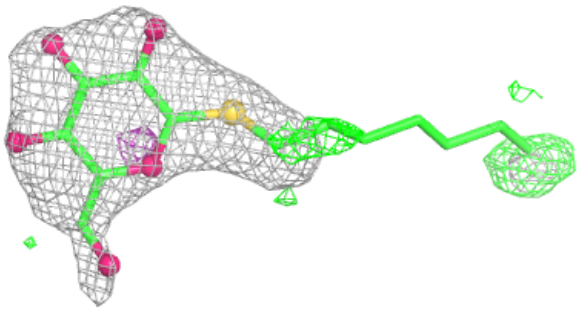


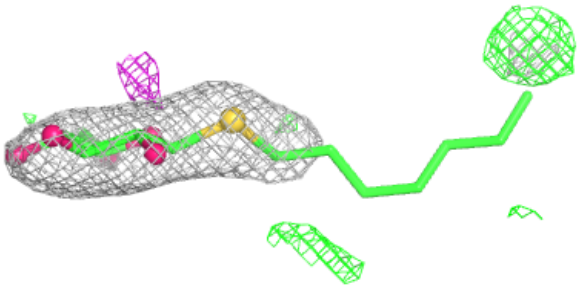


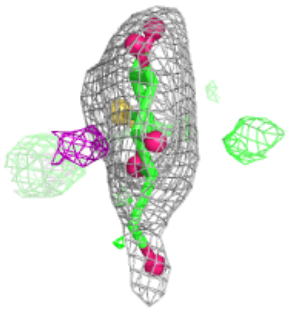


Electron density around HTG C 520:

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

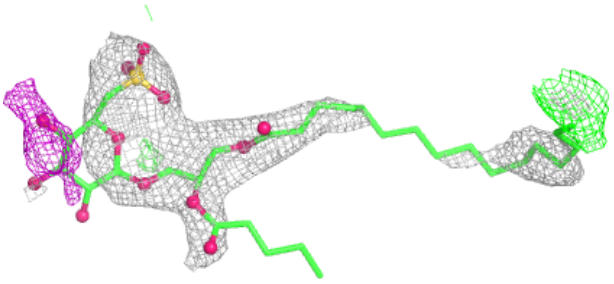


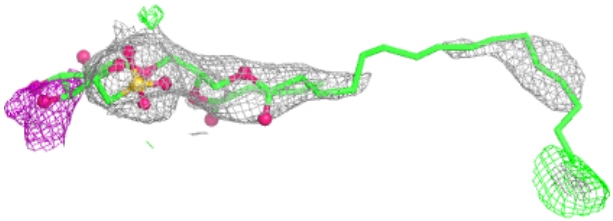


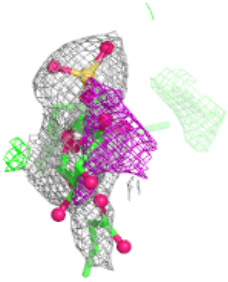


Electron density around SQD f 102:

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

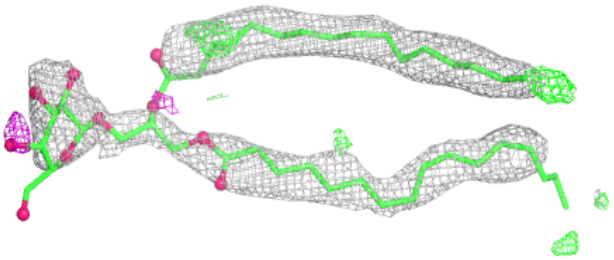


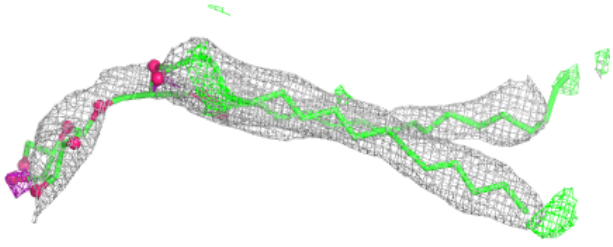


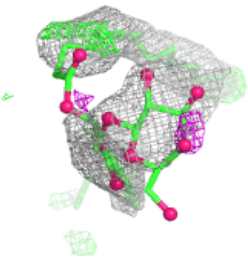


Electron density around LMG C 519:

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

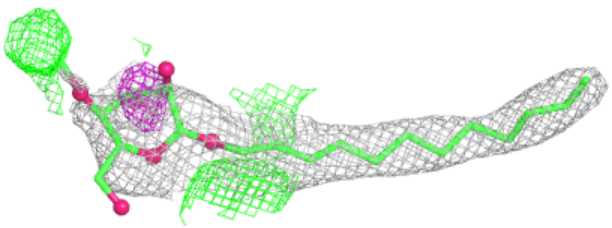


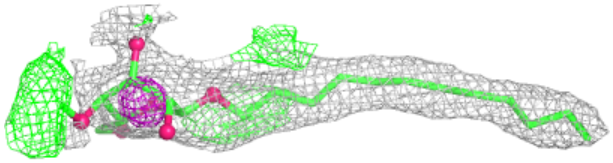


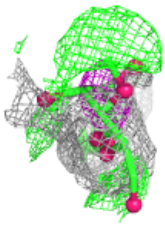


Electron density around LMT b 621:

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

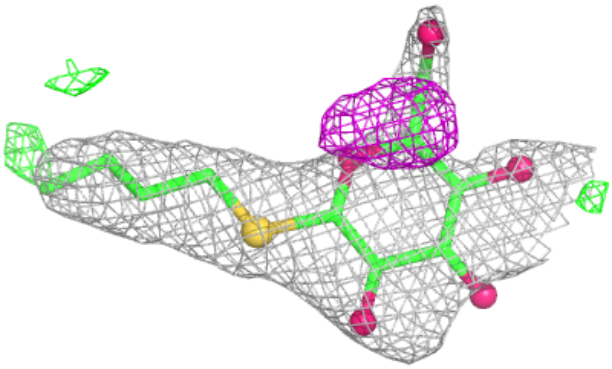


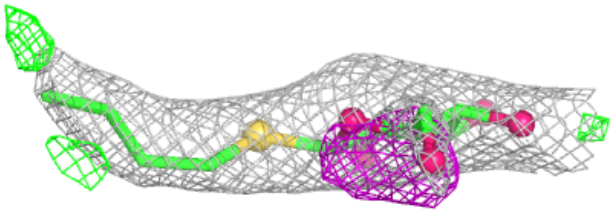


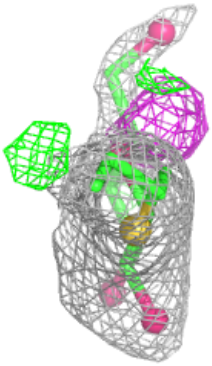


Electron density around HTG D 410:

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

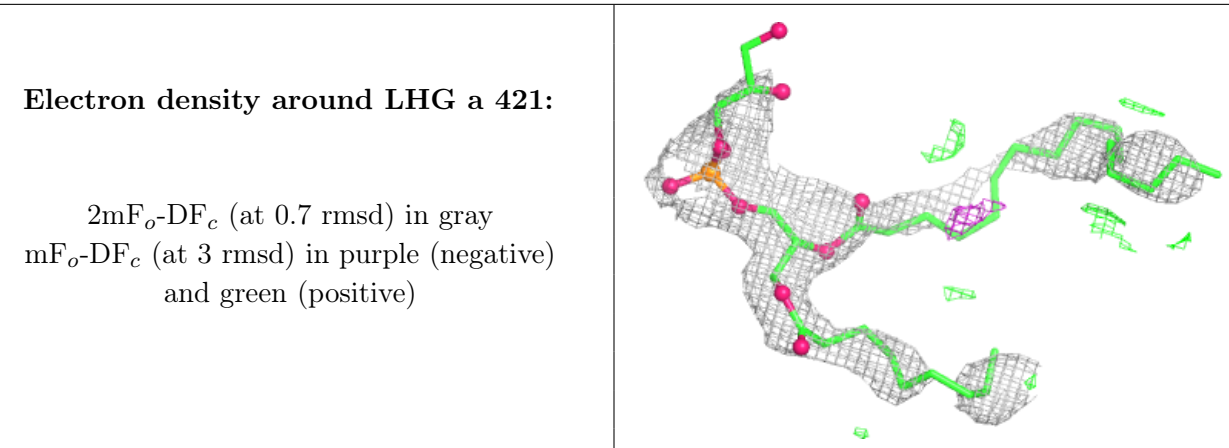






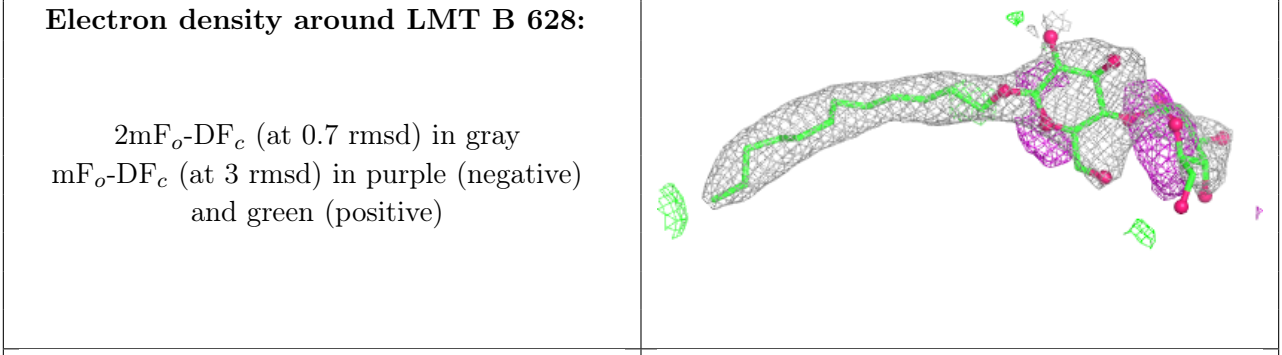
Electron density around LHG a 421:

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



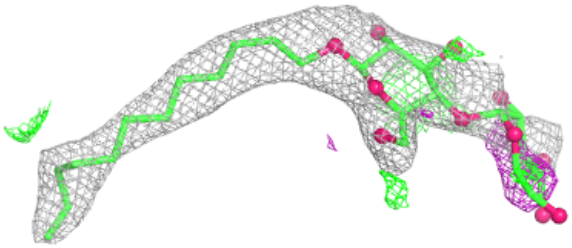
Electron density around LMT B 628:

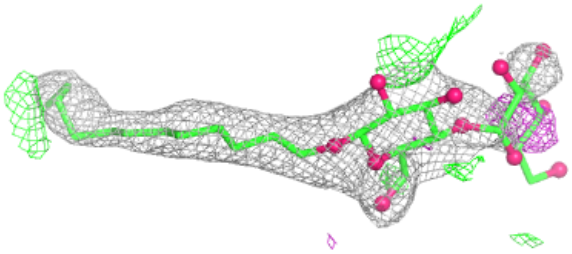
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

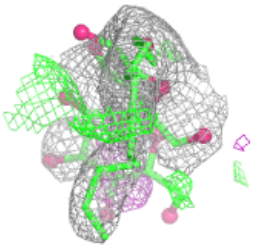


Electron density around LMT T 101:

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

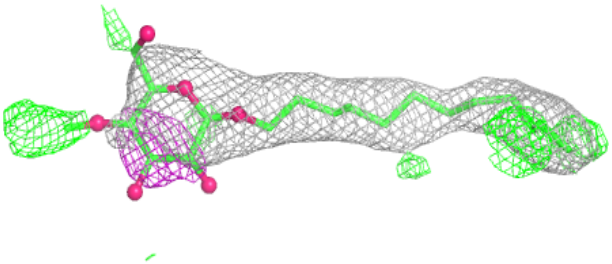


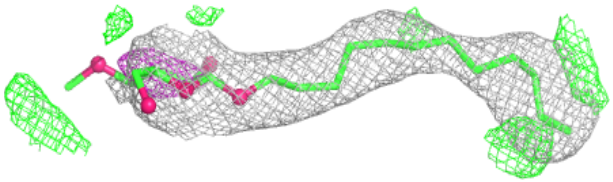


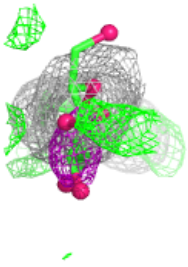


Electron density around LMT b 627:

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

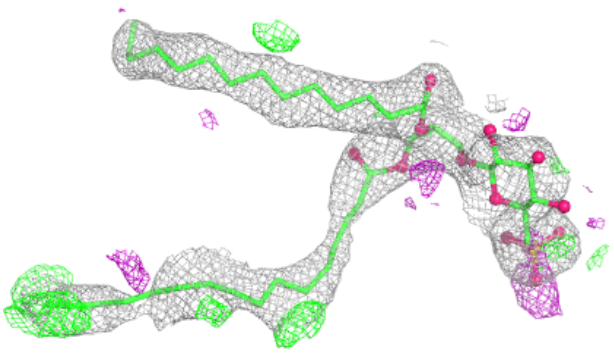


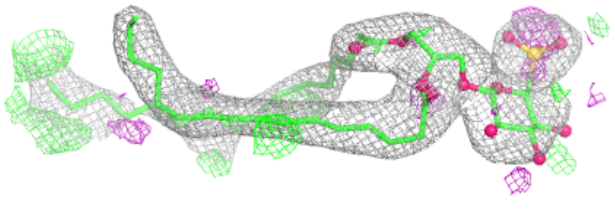


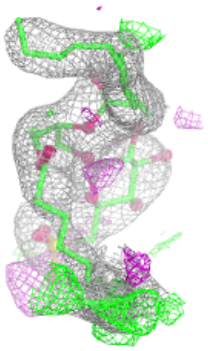


Electron density around SQD A 412:

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

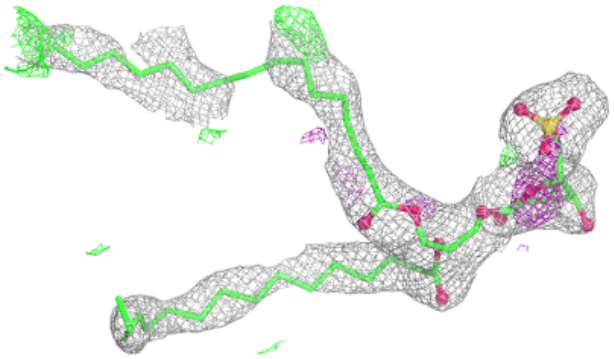


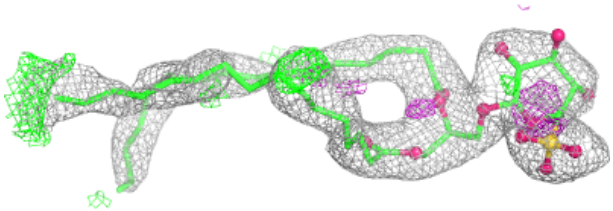


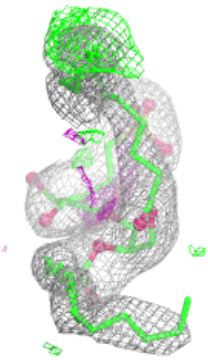


Electron density around SQD a 413:

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

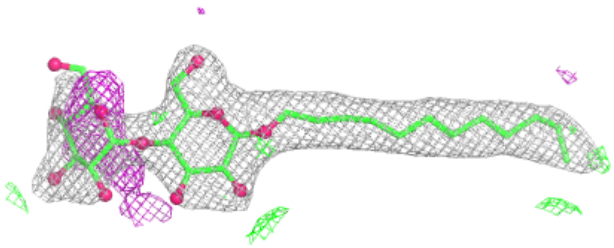


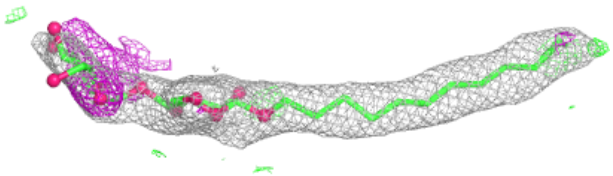




Electron density around LMT M 101:

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

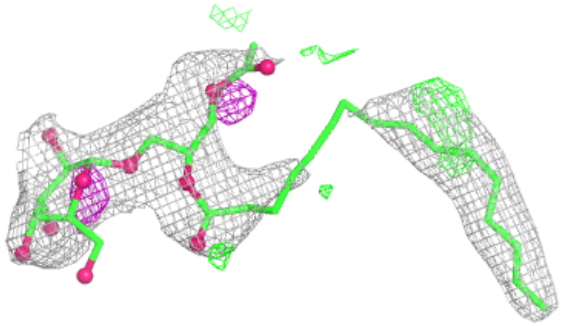


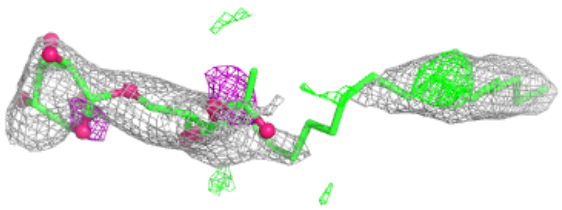


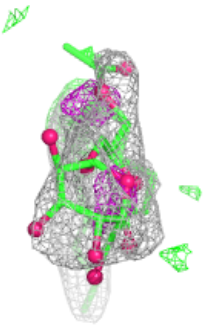


Electron density around LMG Z 101:

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

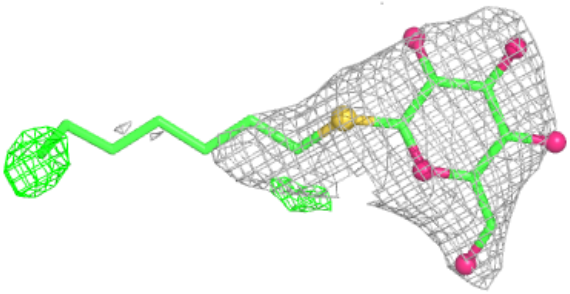


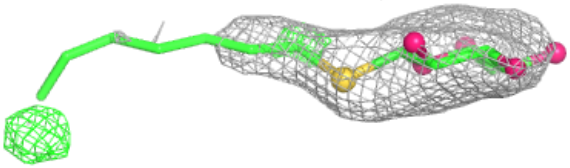


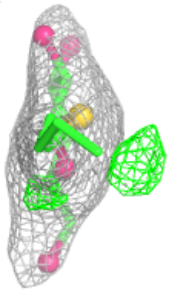


Electron density around HTG c 522:

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

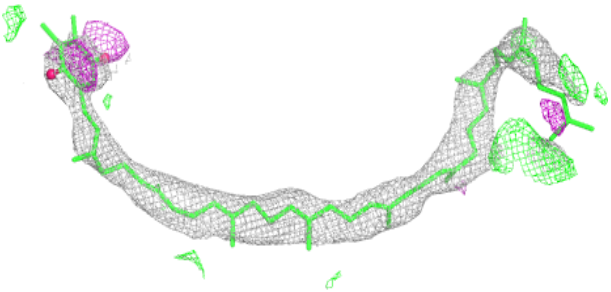


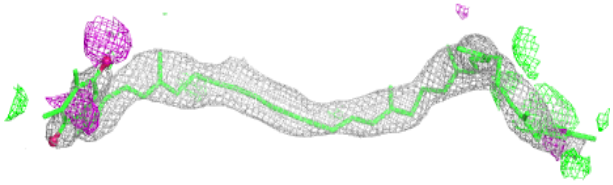


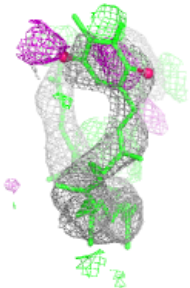


Electron density around PL9 A 414:

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

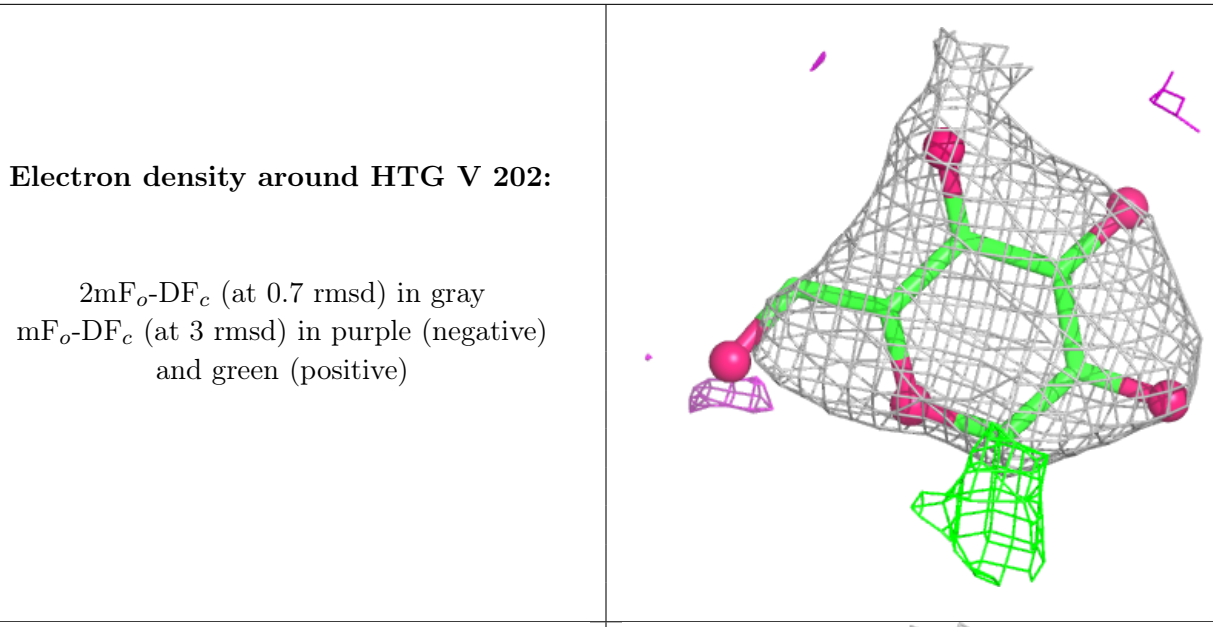


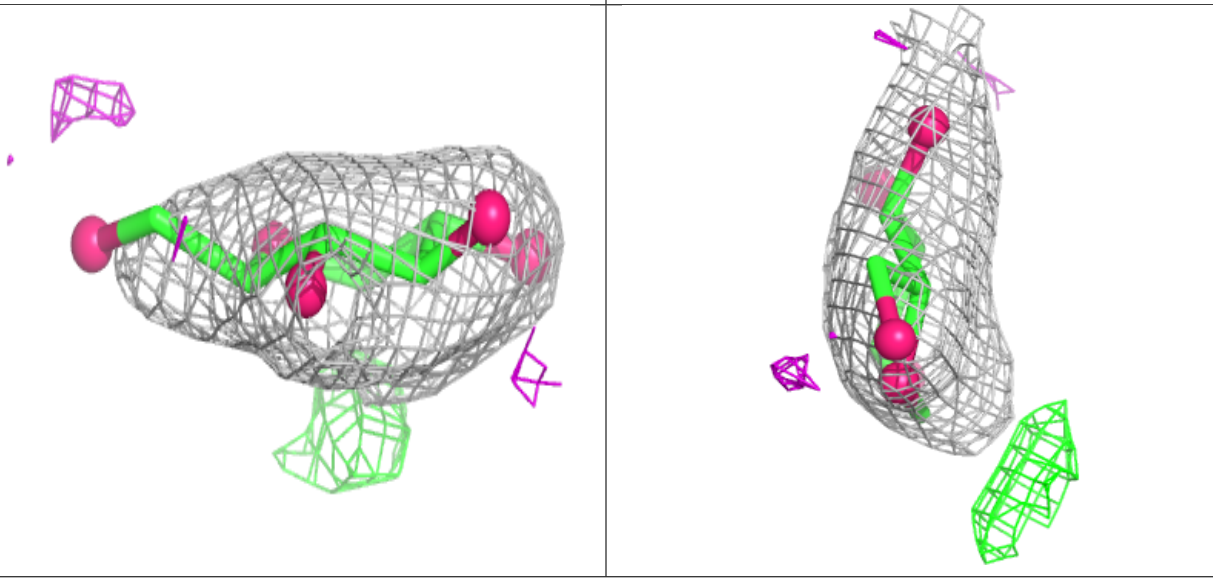




Electron density around HTG V 202:

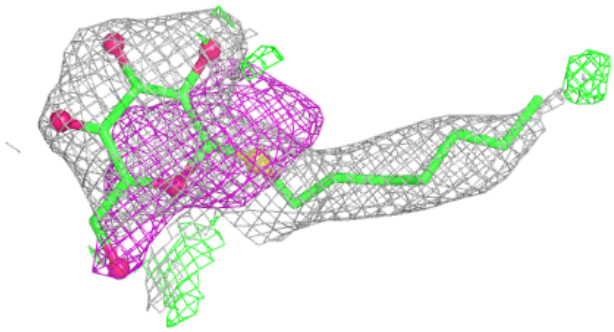
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

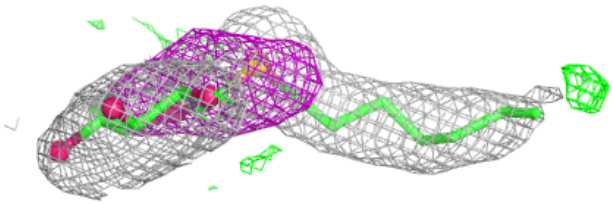


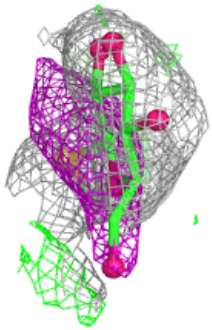


Electron density around HTG b 622:

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

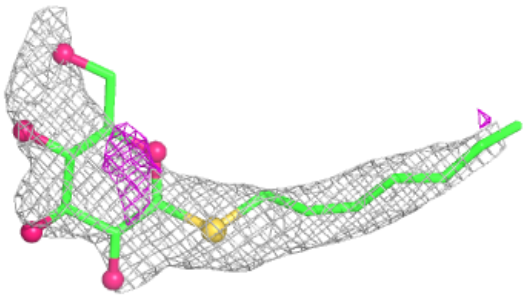


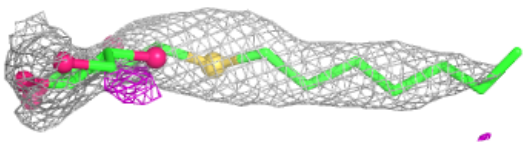


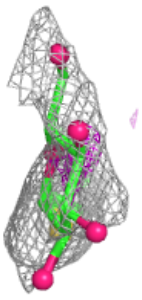


Electron density around HTG b 623:

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

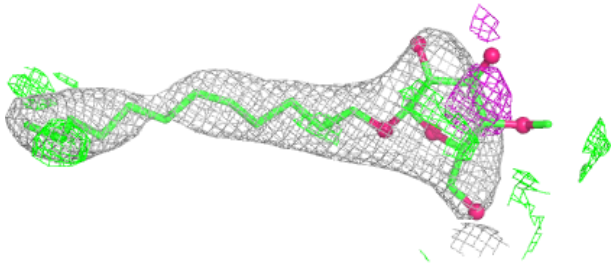


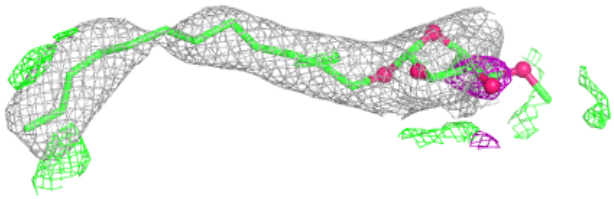


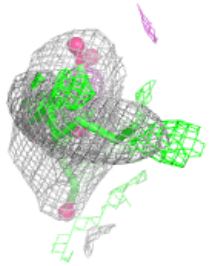


Electron density around LMT B 631:

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

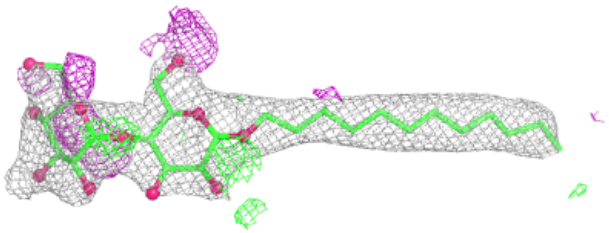


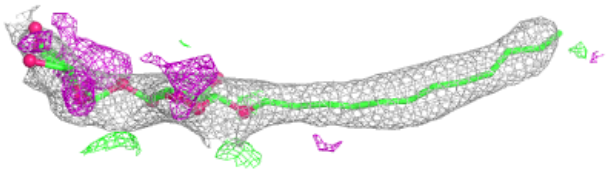


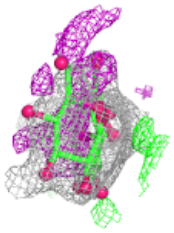


Electron density around LMT m 103:

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

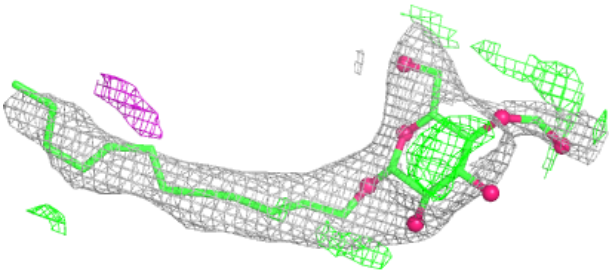


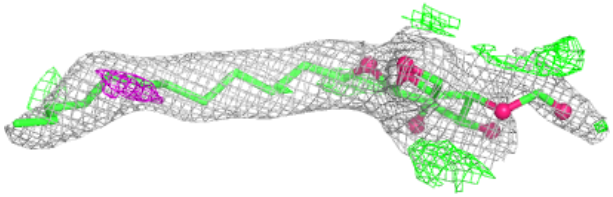


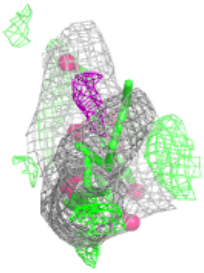


Electron density around LMT t 101:

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

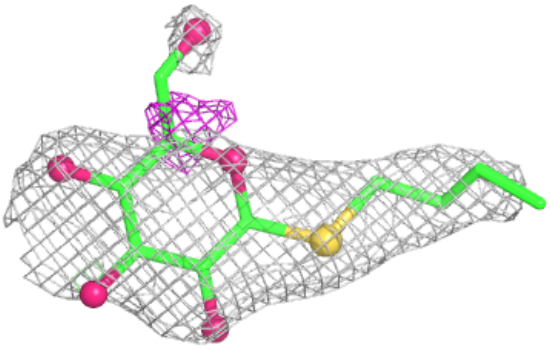


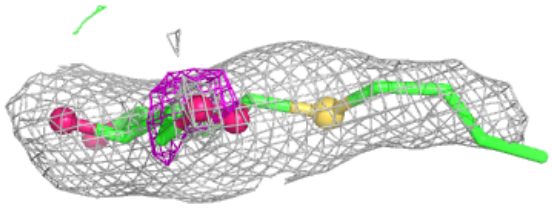


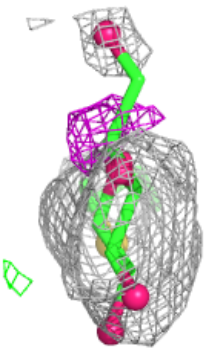


Electron density around HTG d 409:

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

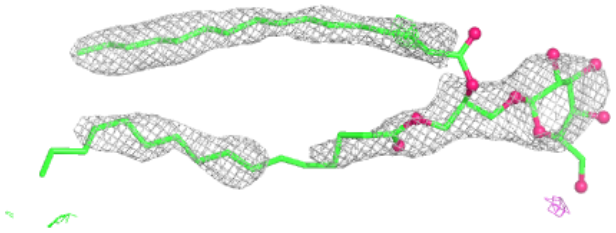


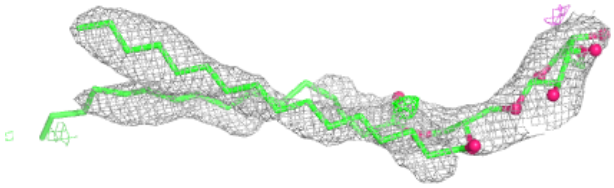


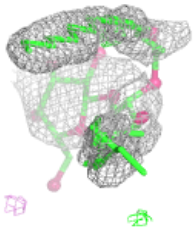


Electron density around LMG c 521:

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

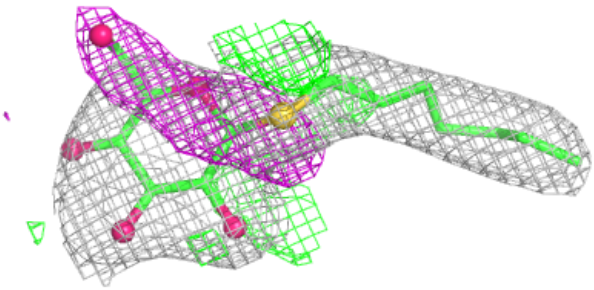


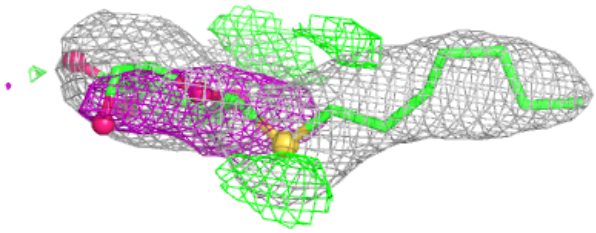


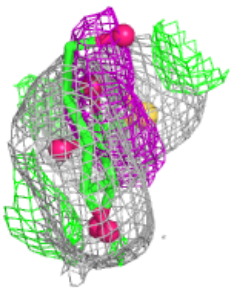


Electron density around HTG B 622:

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

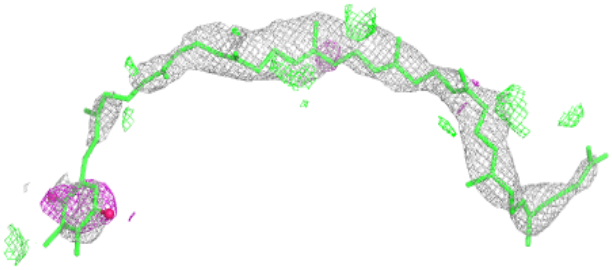


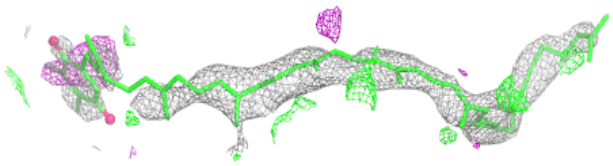


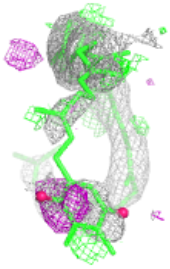


Electron density around PL9 a 415:

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

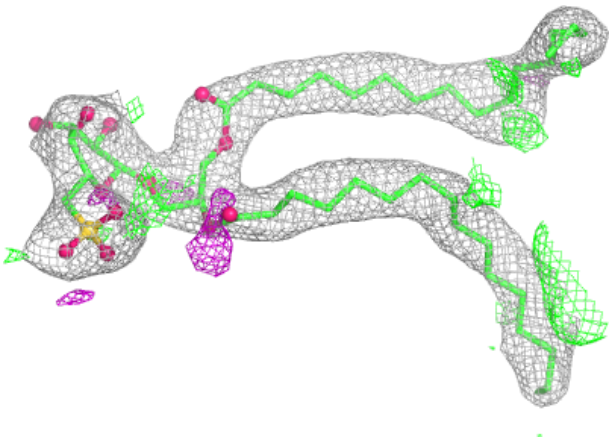


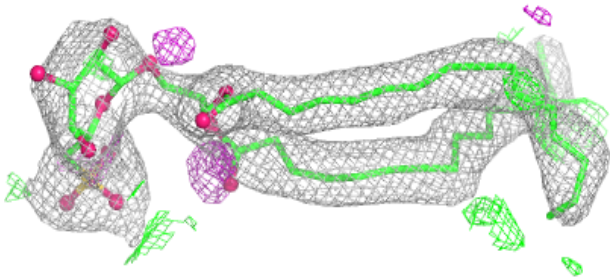


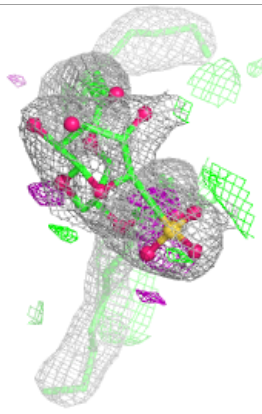


Electron density around SQD B 620:

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

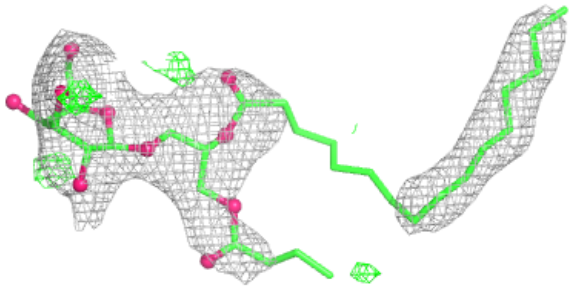


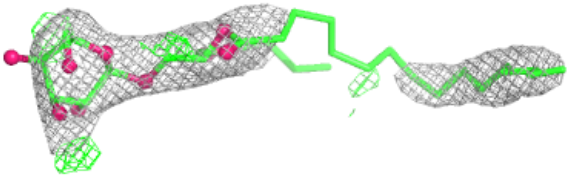




Electron density around LMG z 101:

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

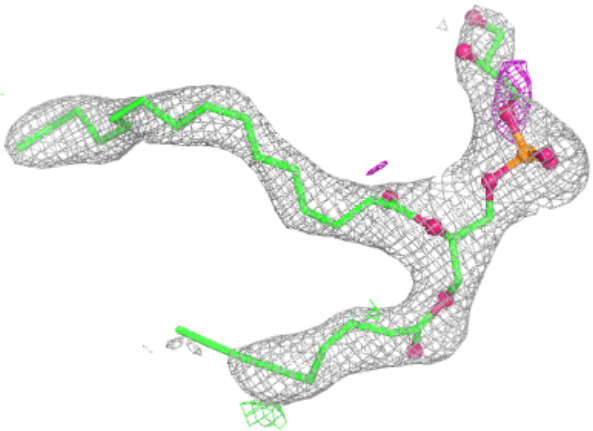


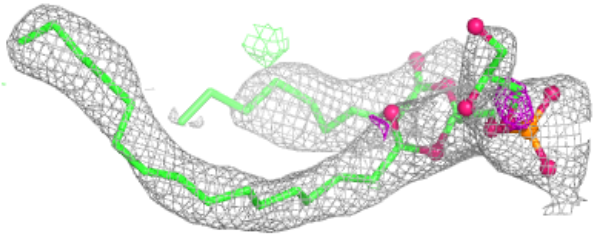


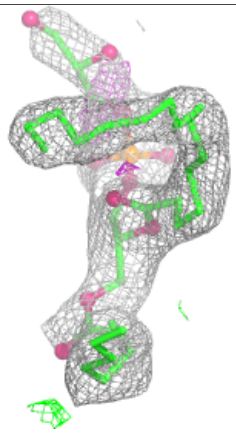


Electron density around LHG E 101:

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

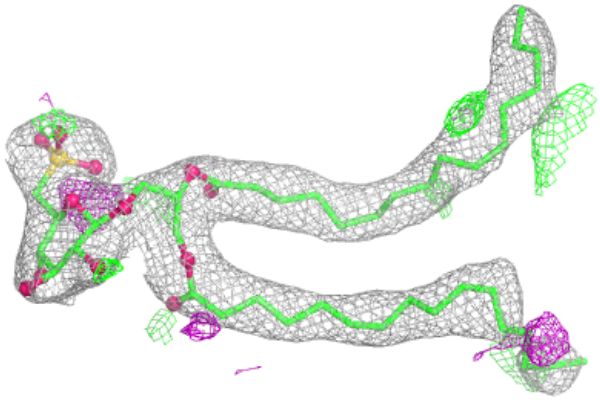


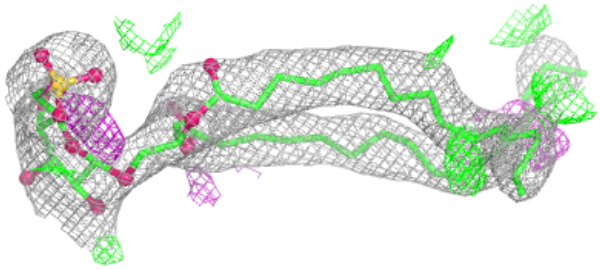


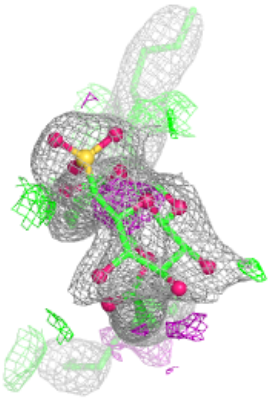


Electron density around SQD b 620:

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

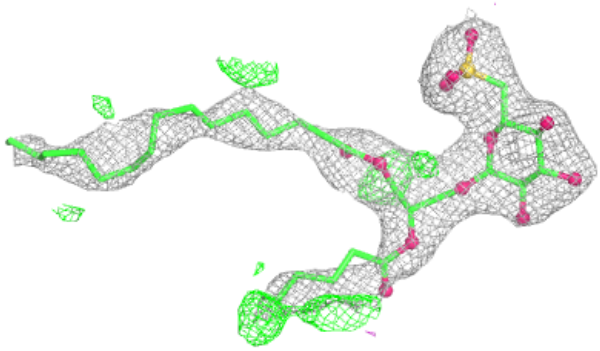


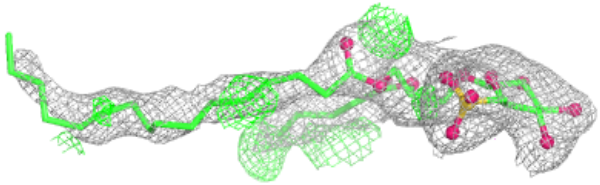


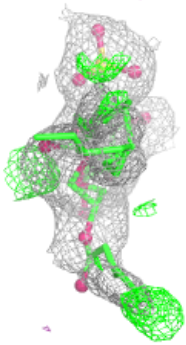


Electron density around SQD F 103:

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

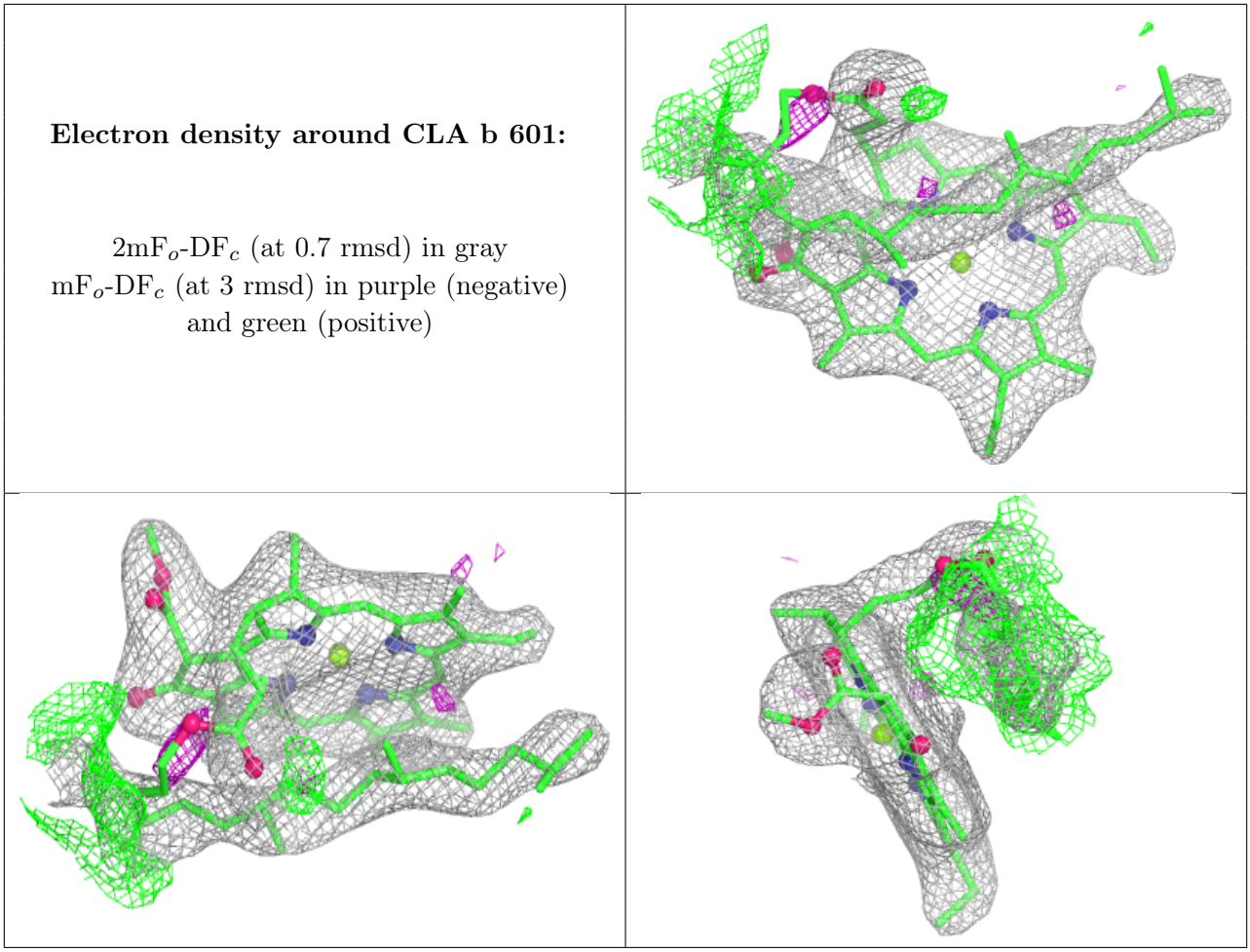






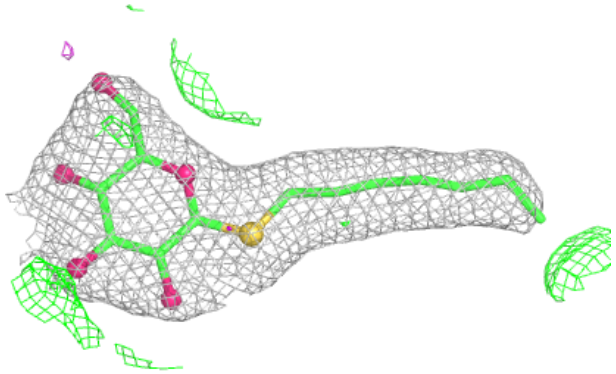
Electron density around CLA b 601:

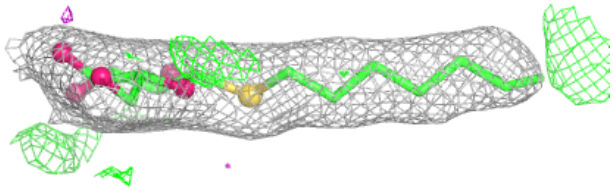
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

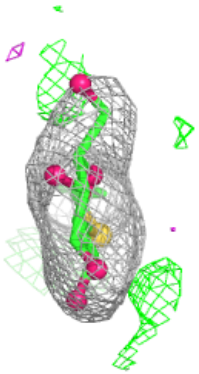


Electron density around HTG B 625:

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

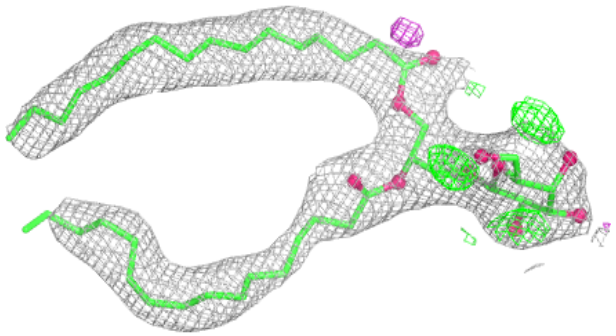


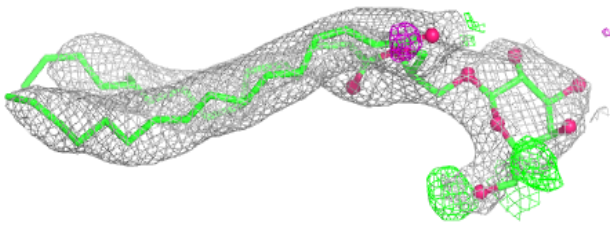


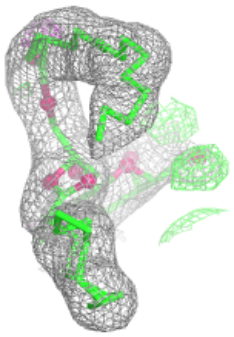


Electron density around LMG A 419:

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

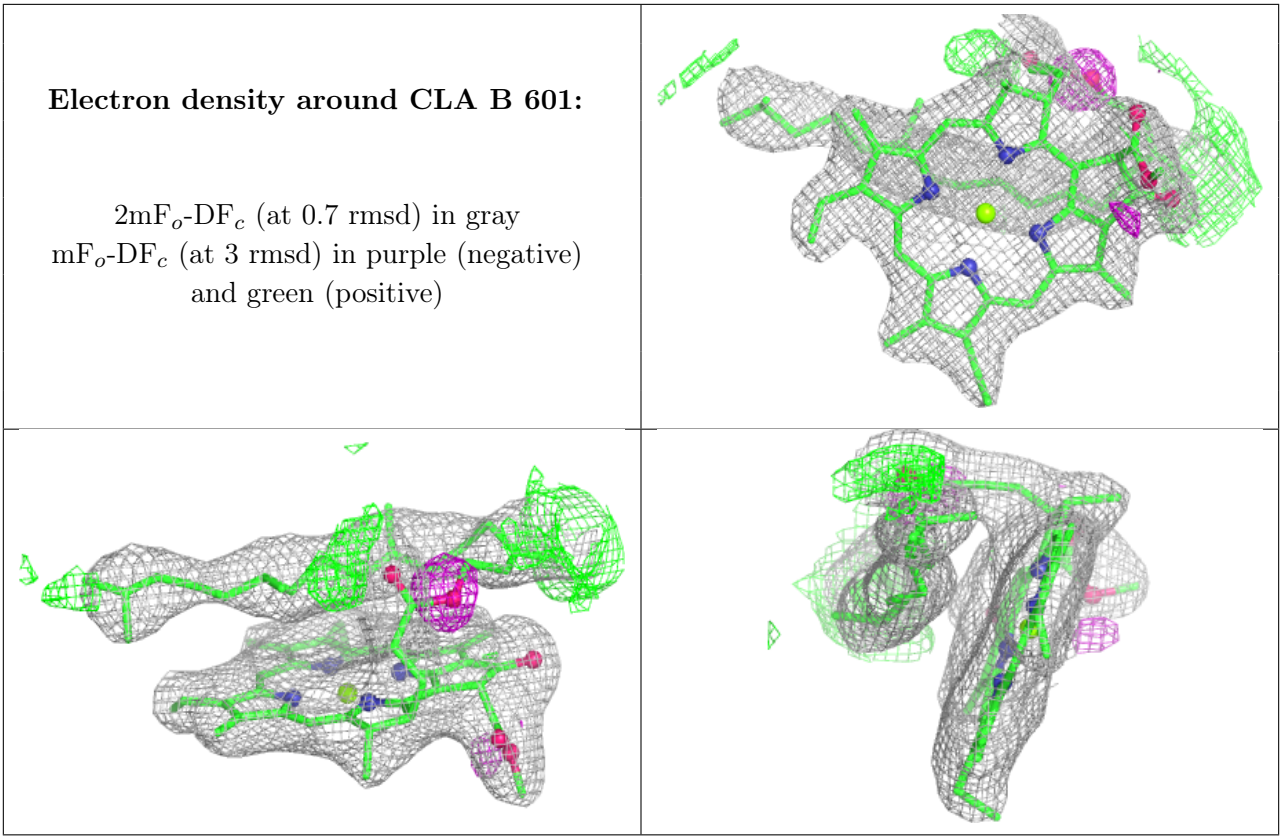






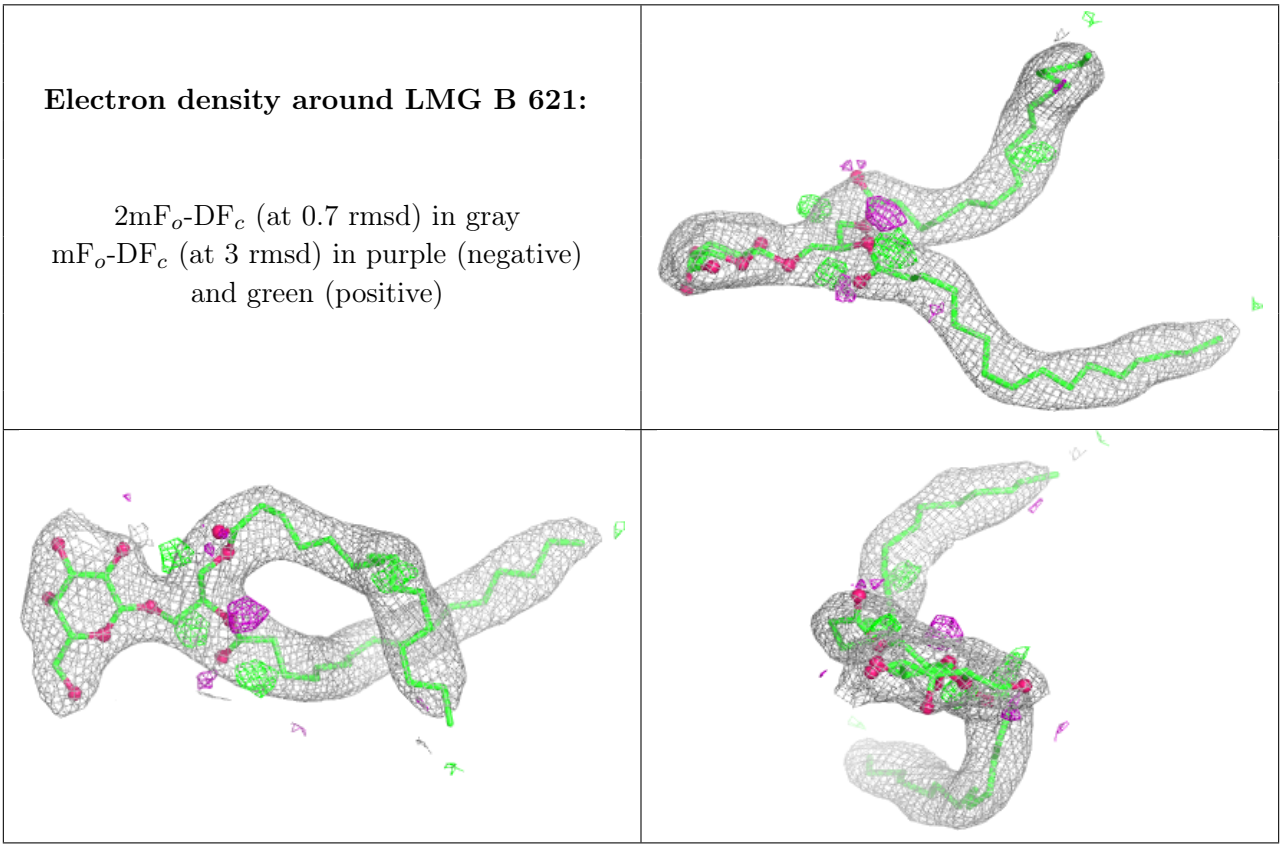
Electron density around CLA B 601:

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



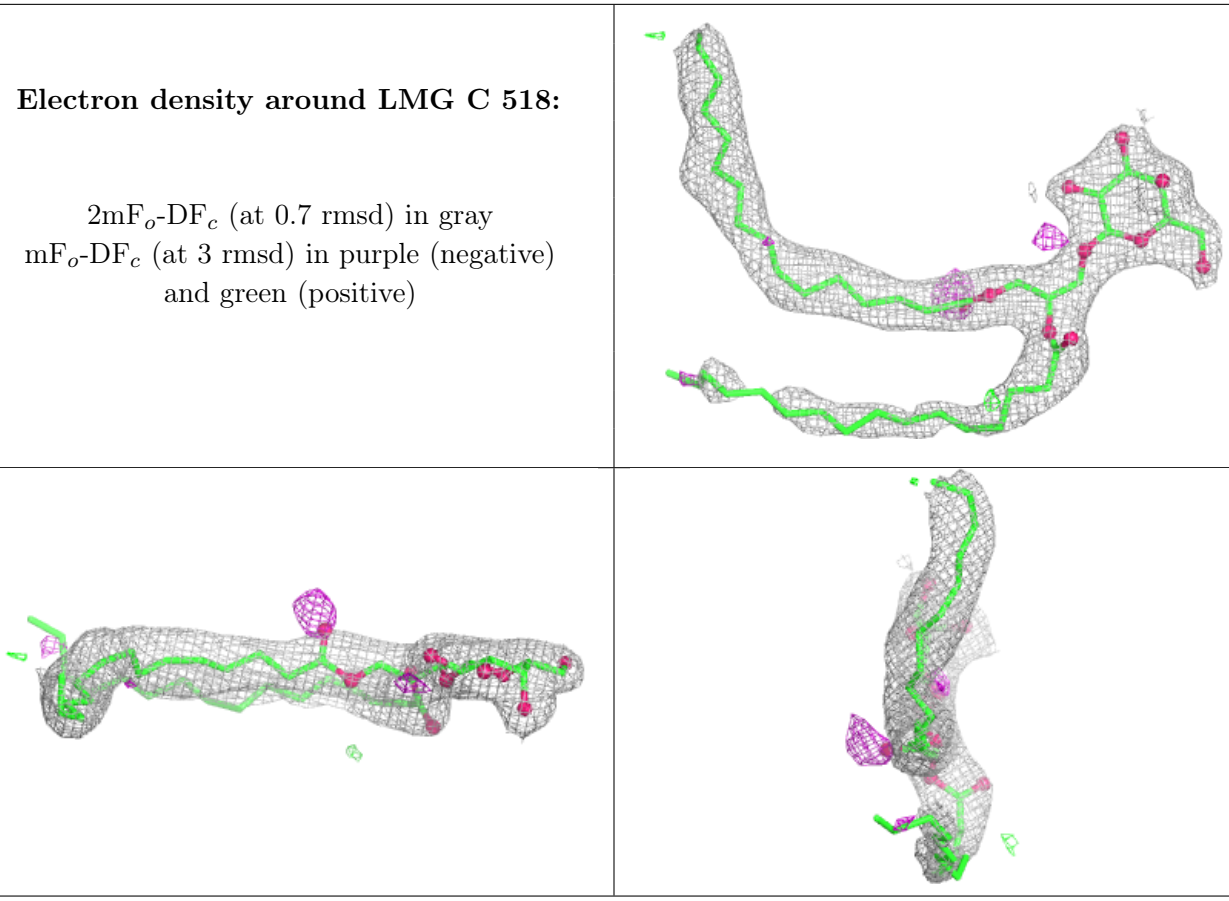
Electron density around LMG B 621:

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



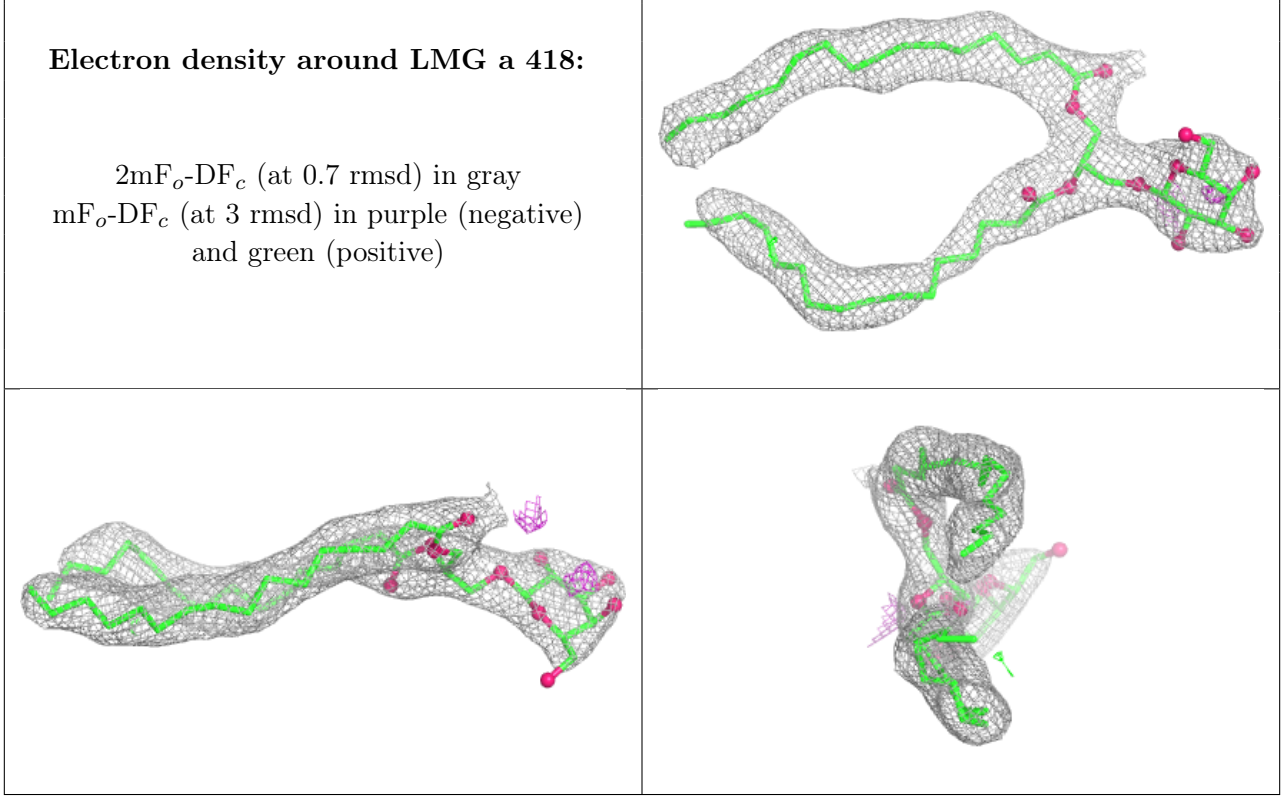
Electron density around LMG C 518:

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



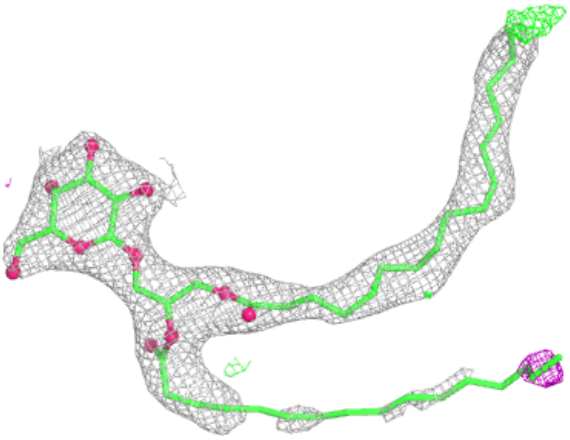
Electron density around LMG a 418:

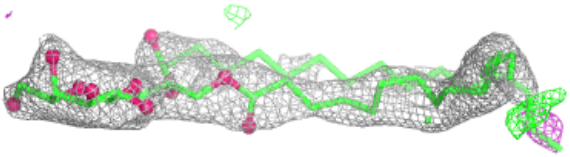
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

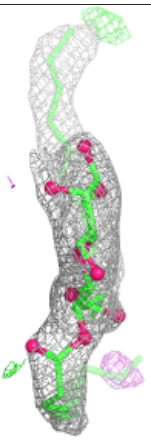


Electron density around LMG c 520:

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

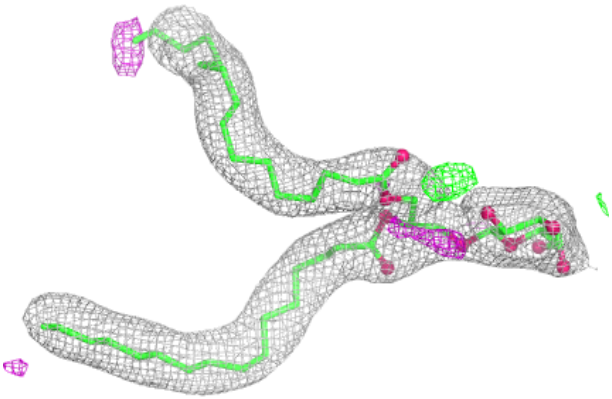


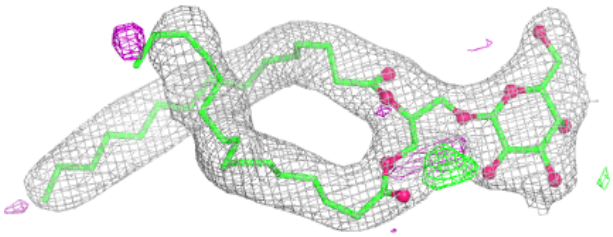


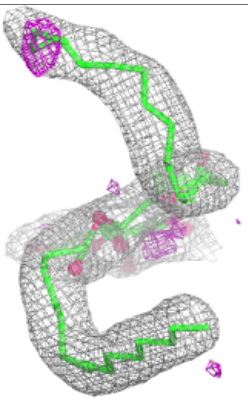


Electron density around LMG m 101:

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

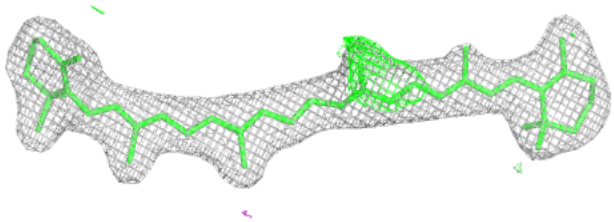


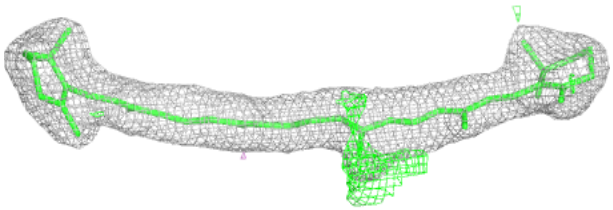


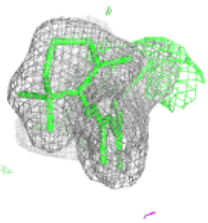


Electron density around BCR T 102:

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

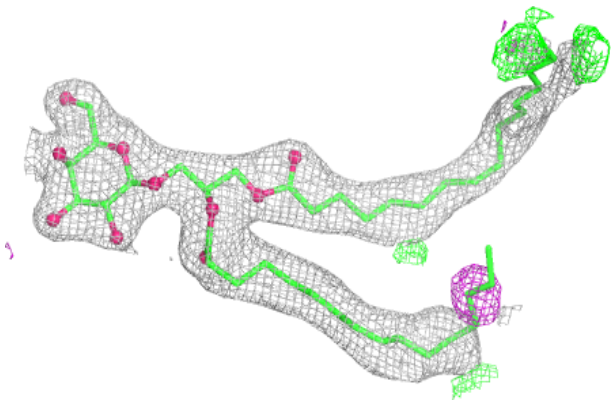


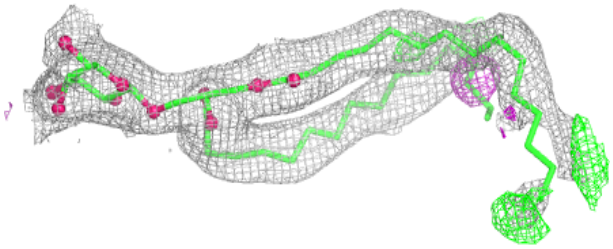


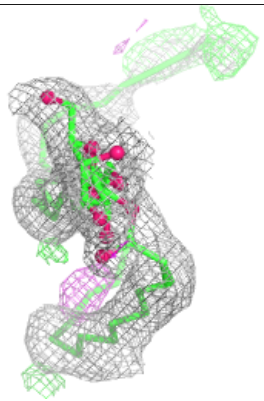


Electron density around LMG D 411:

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

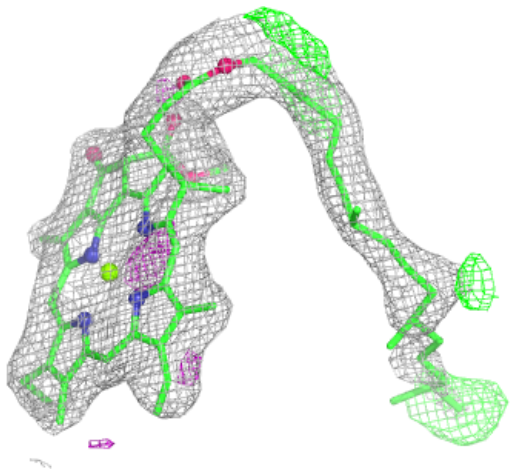


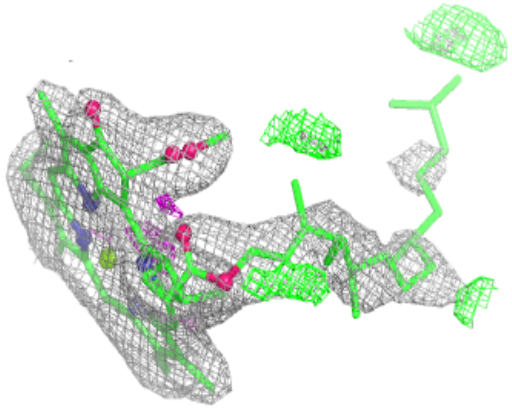


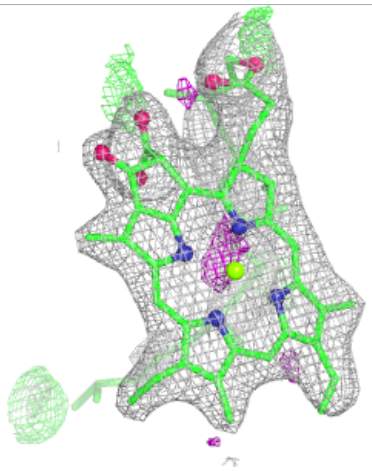


Electron density around CLA b 616:

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

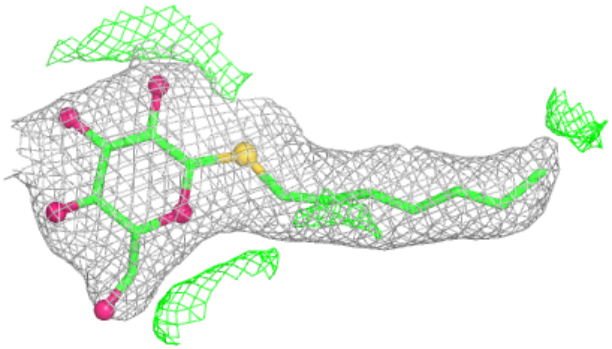


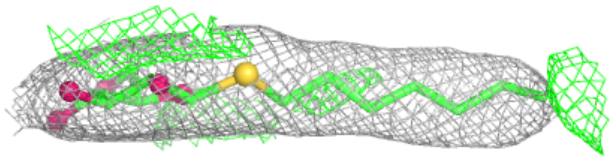


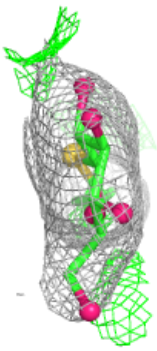


Electron density around HTG b 625:

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

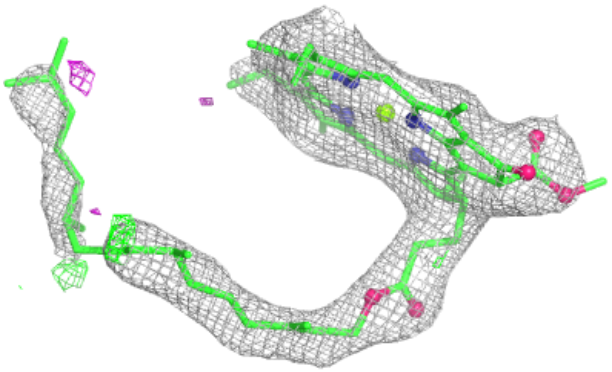


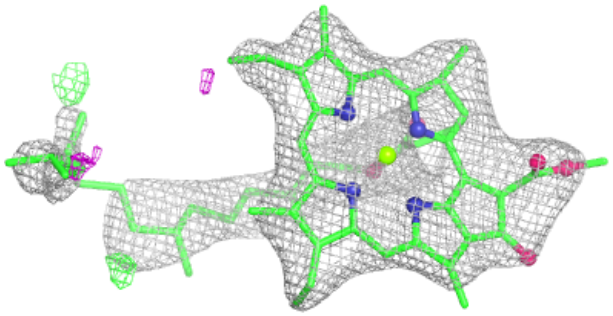


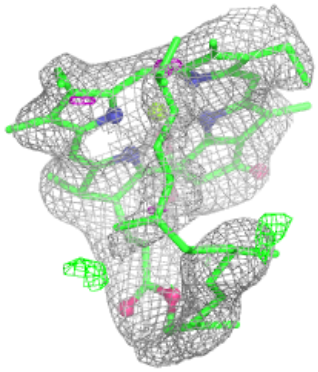


Electron density around CLA c 514:

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

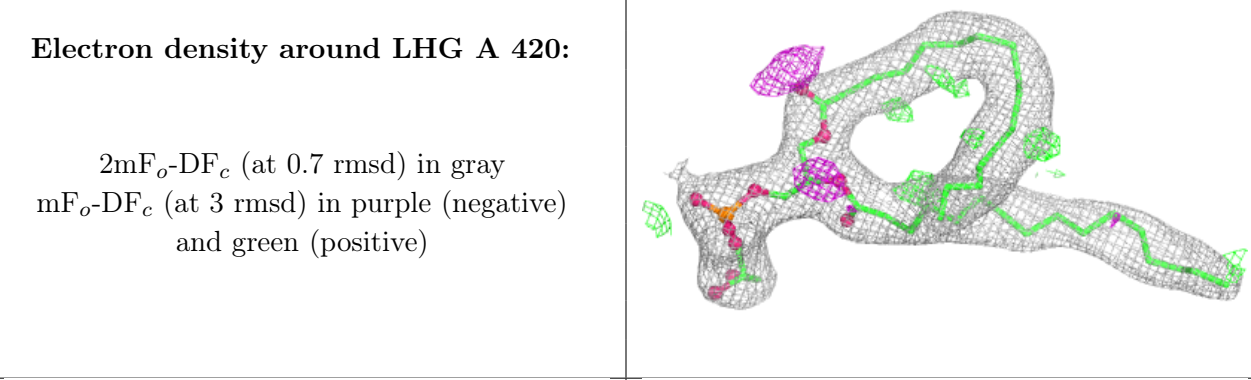






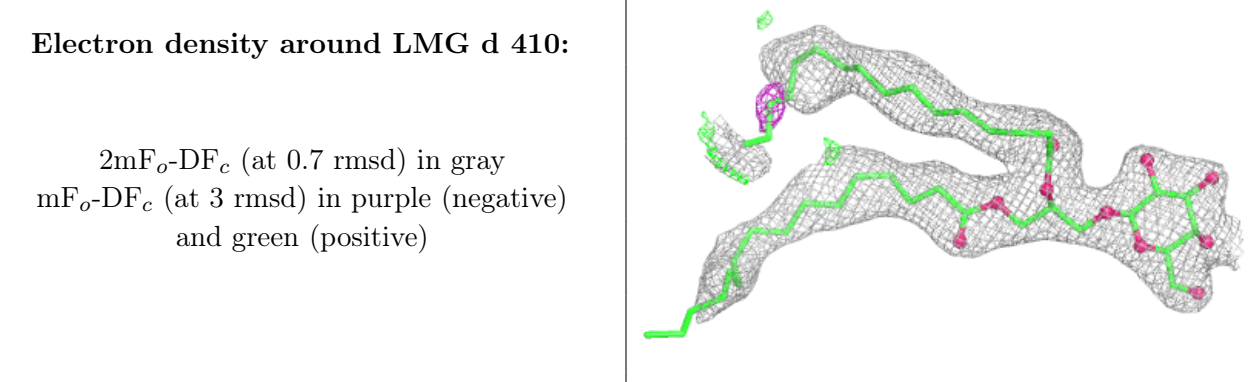
Electron density around LHG A 420:

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



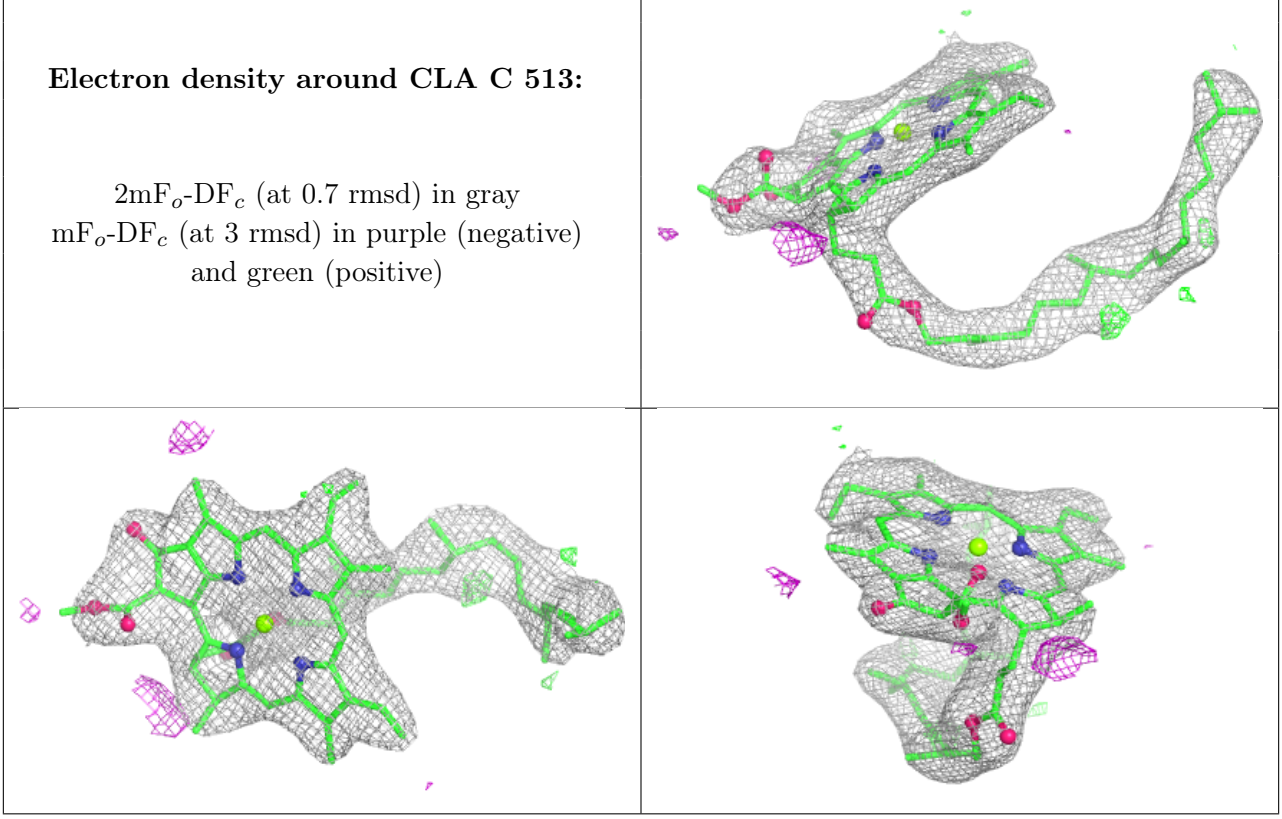
Electron density around LMG d 410:

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



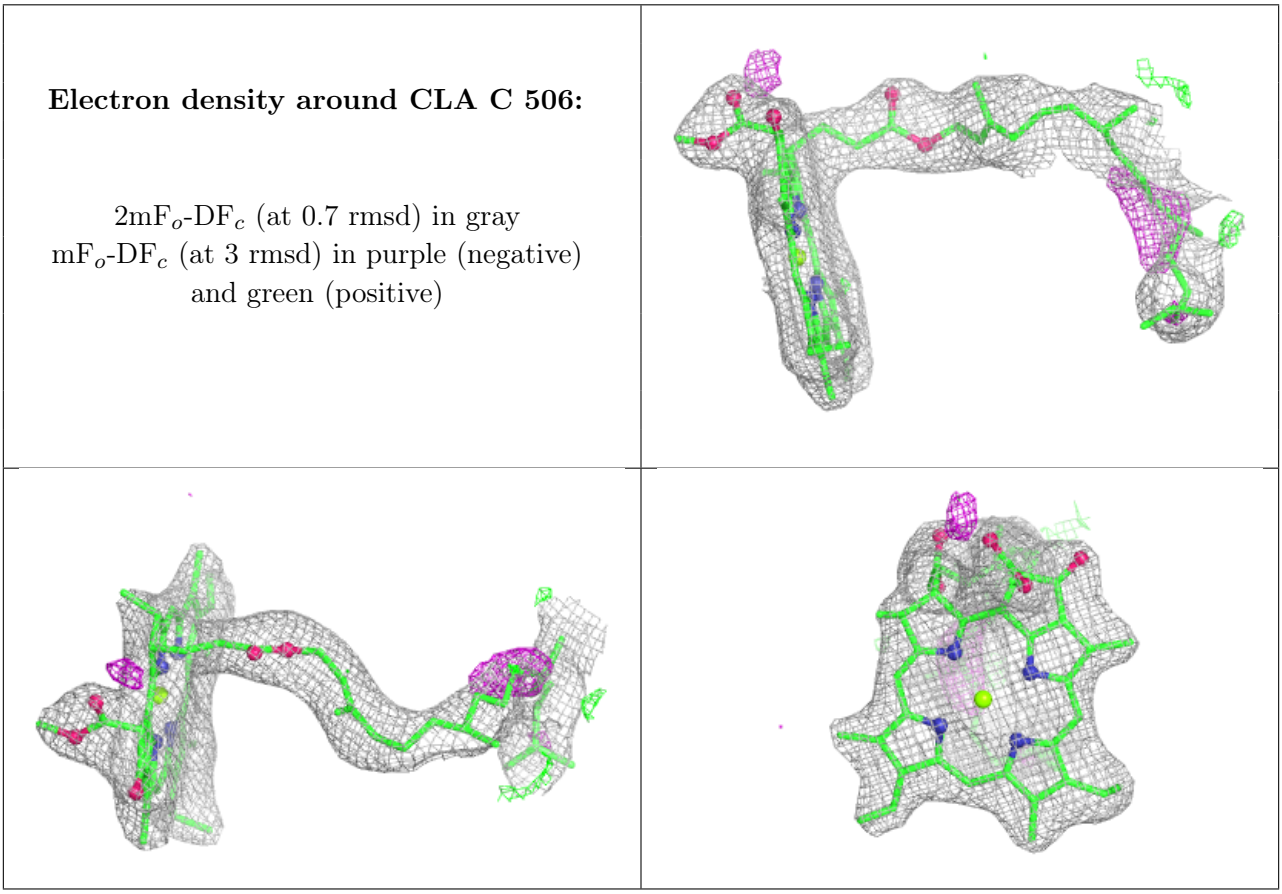
Electron density around CLA C 513:

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



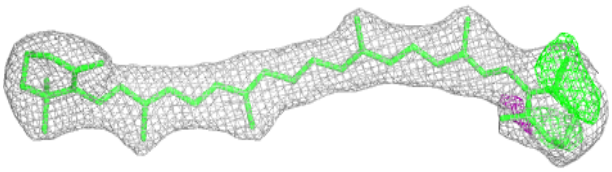
Electron density around CLA C 506:

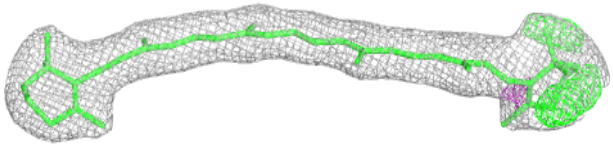
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

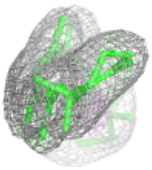


Electron density around BCR d 403:

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

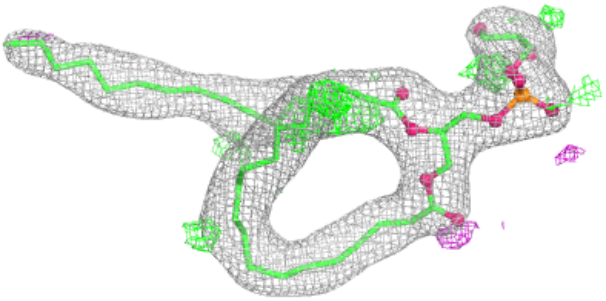


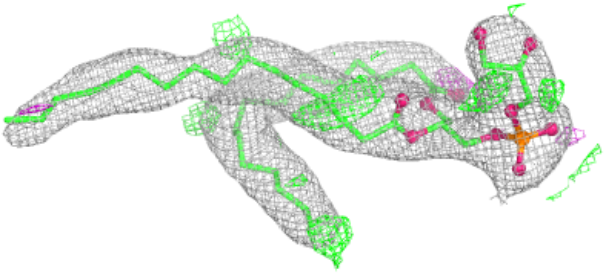


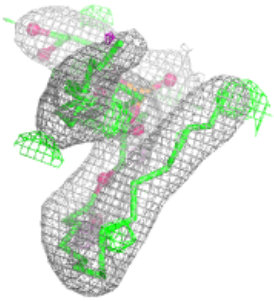


Electron density around LHG d 411:

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

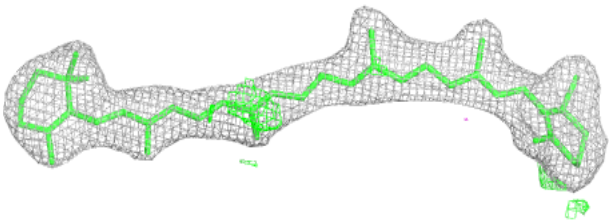


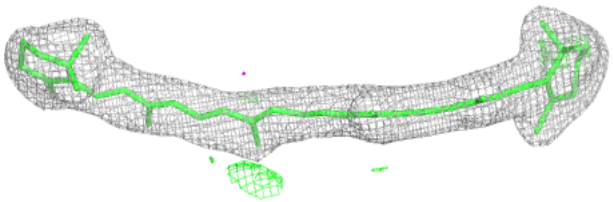


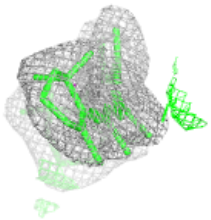


Electron density around BCR t 102:

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

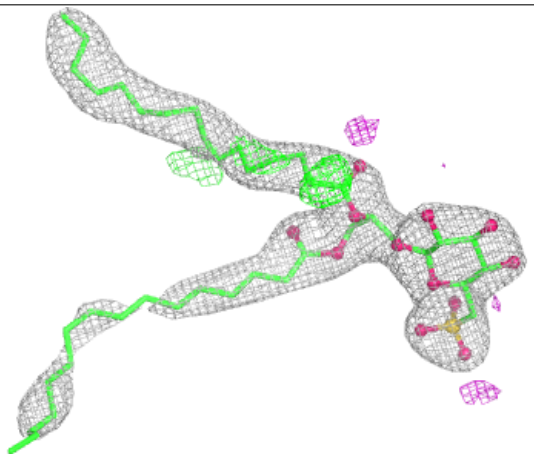


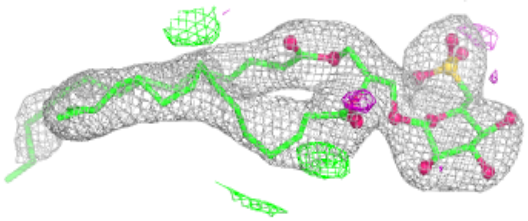


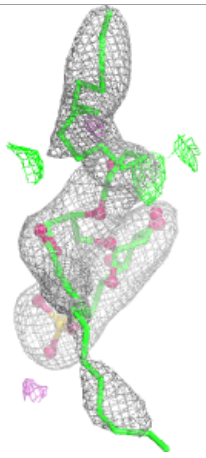


Electron density around SQD A 410:

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

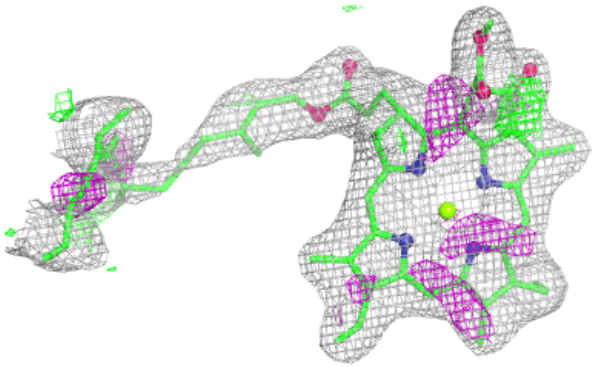


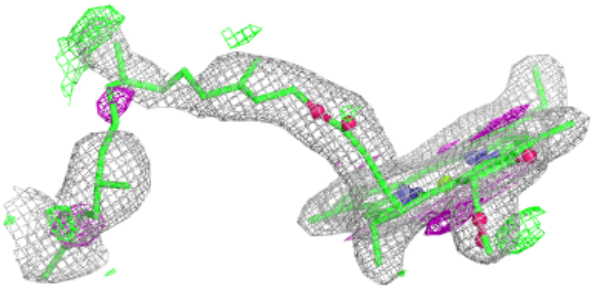


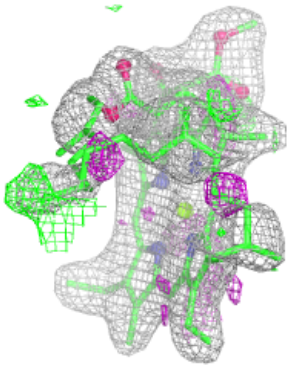


Electron density around CLA A 408:

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

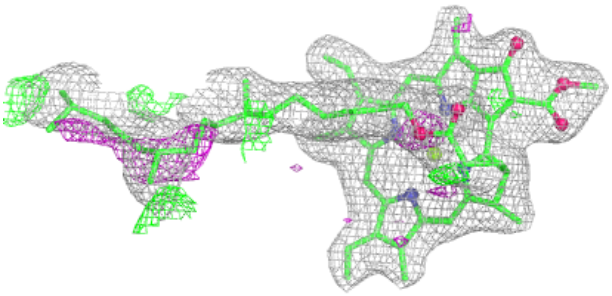


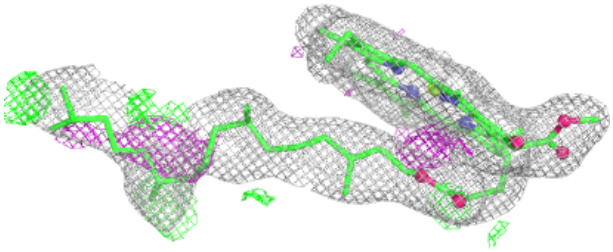




Electron density around CLA B 614:

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

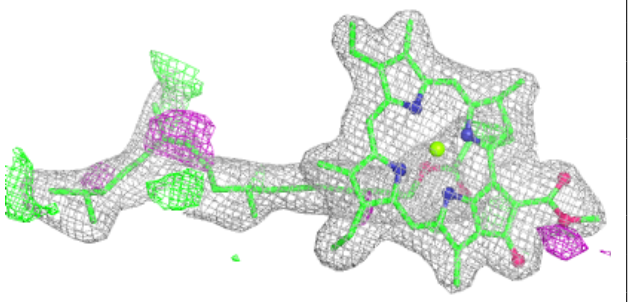


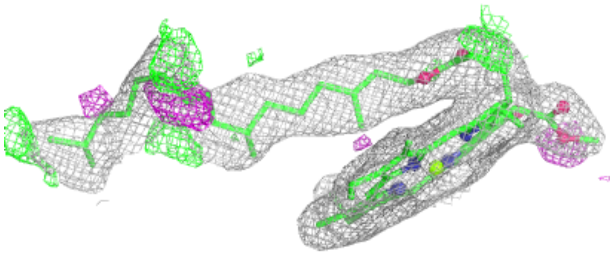


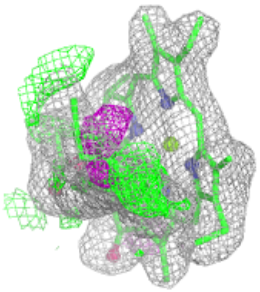


Electron density around CLA b 614:

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

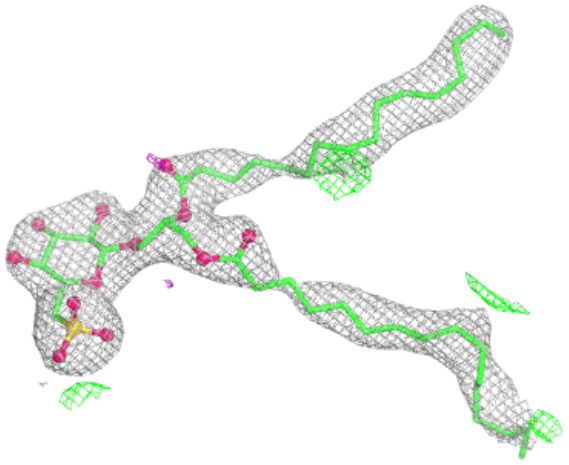


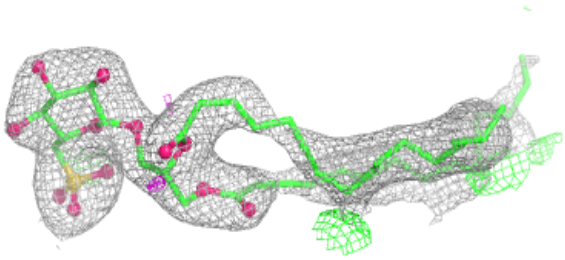


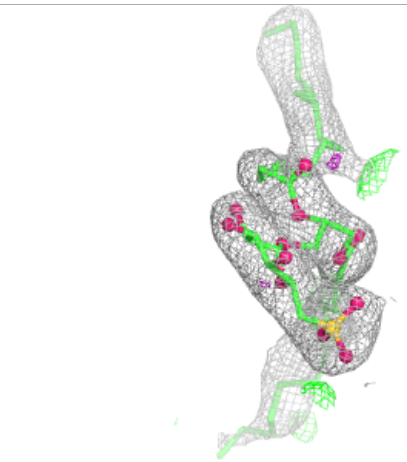


Electron density around SQD a 411:

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

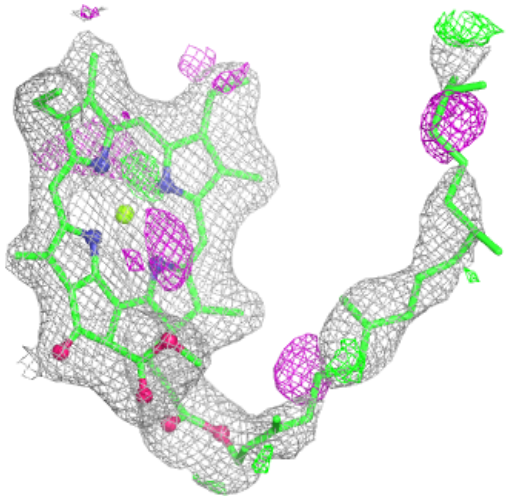


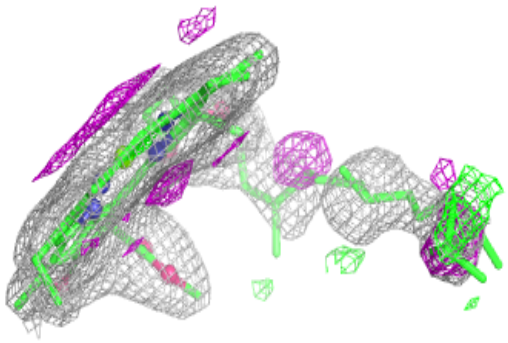


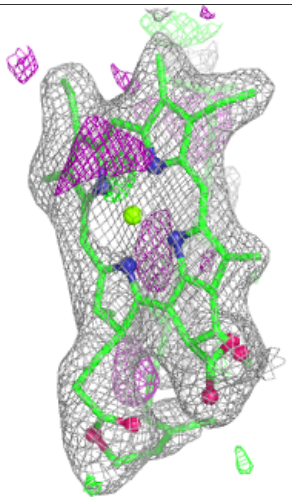


Electron density around CLA B 616:

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

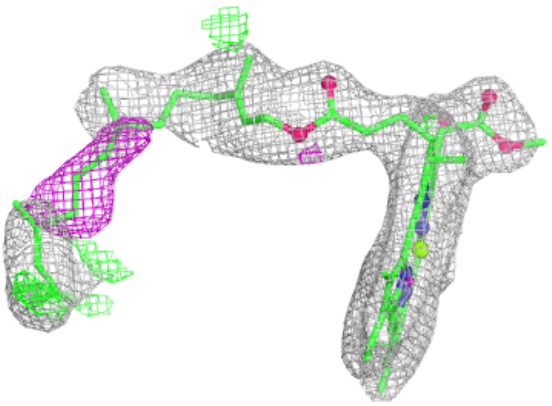


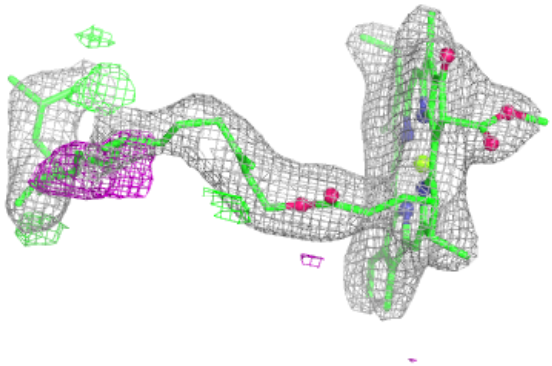


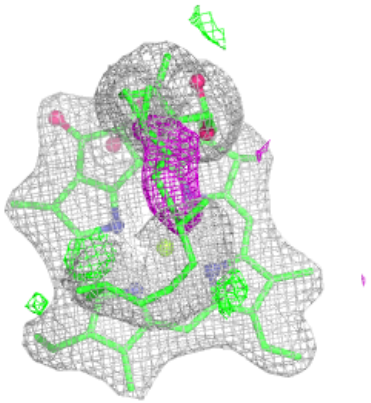


Electron density around CLA c 507:

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

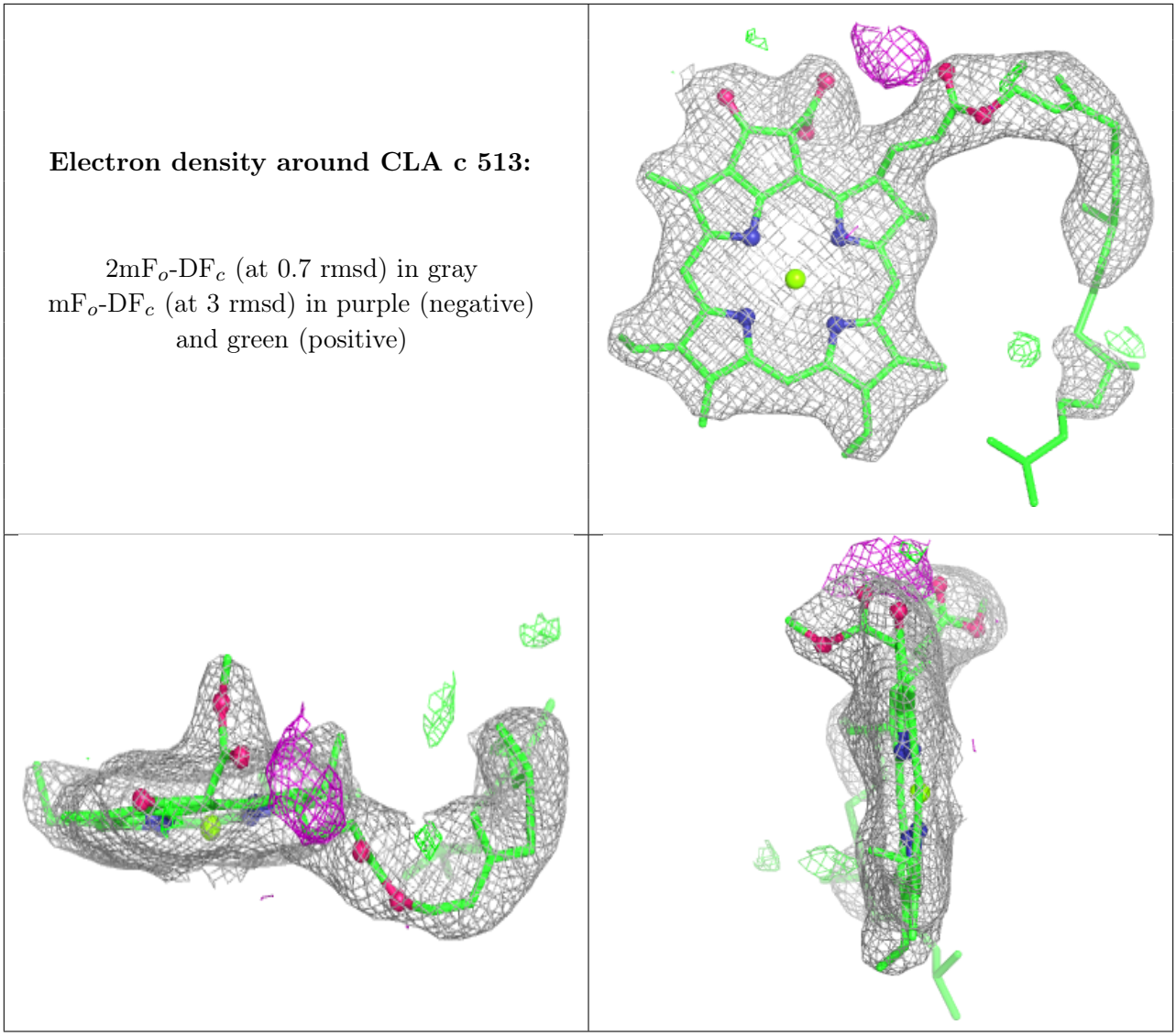






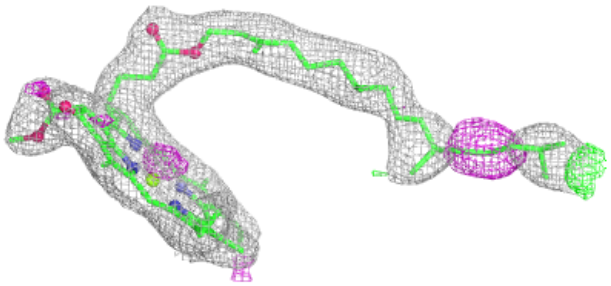
Electron density around CLA c 513:

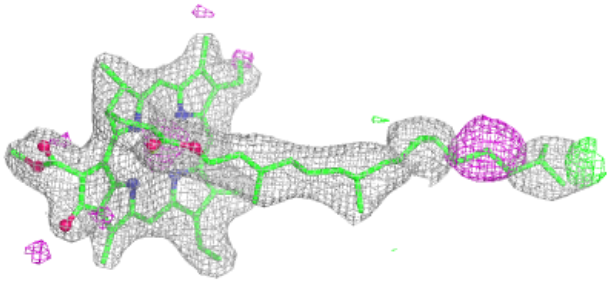
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

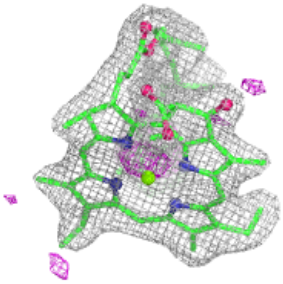


Electron density around CLA C 504:

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

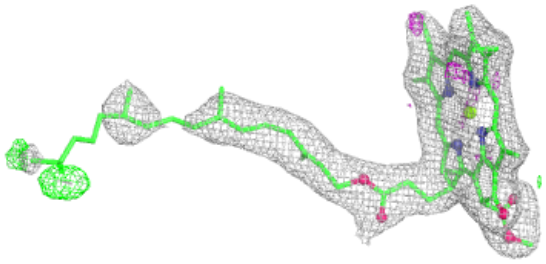


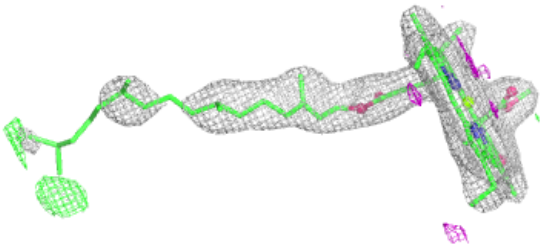


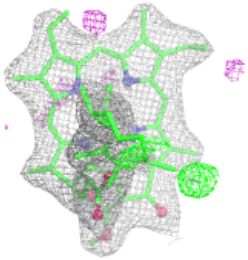


Electron density around CLA d 402:

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

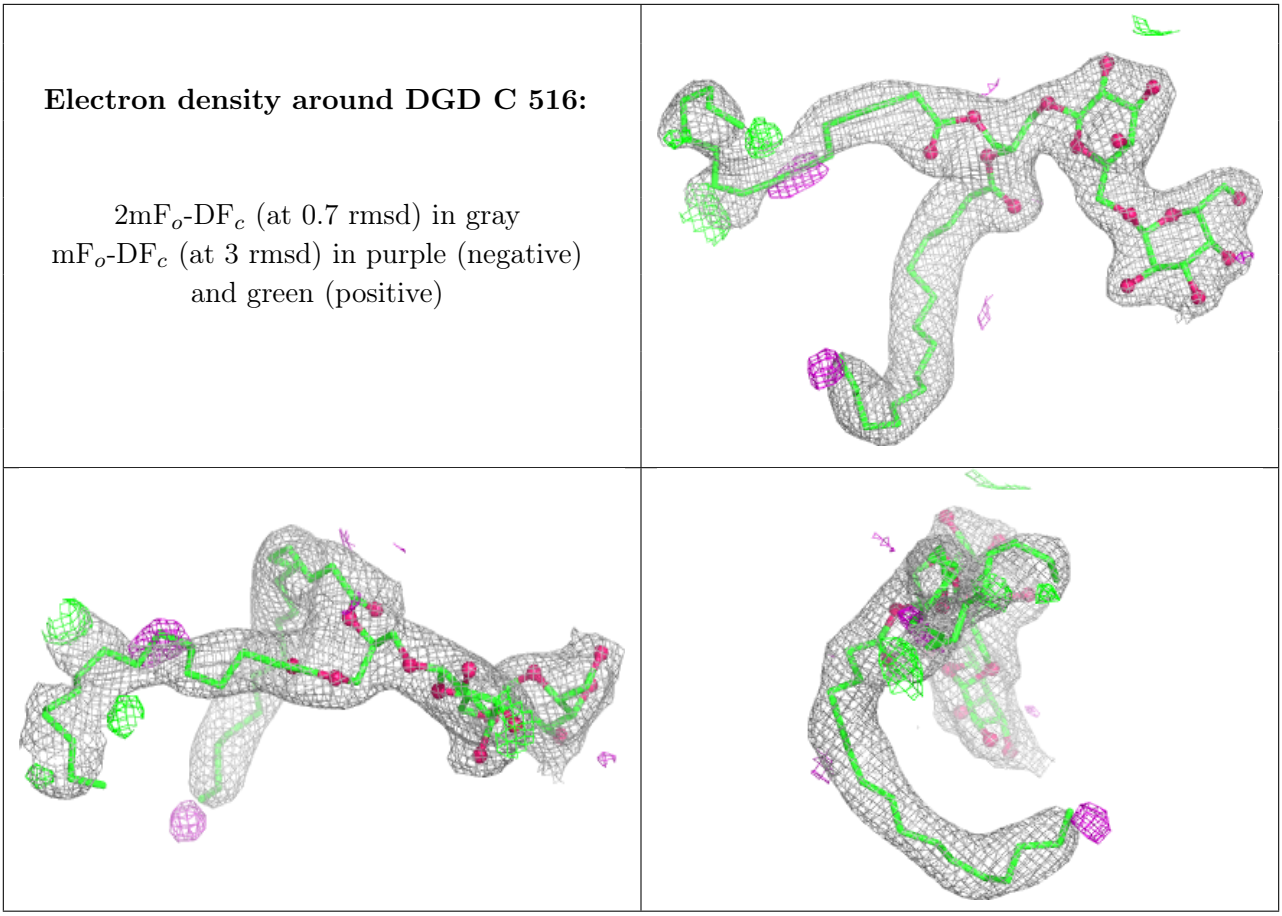






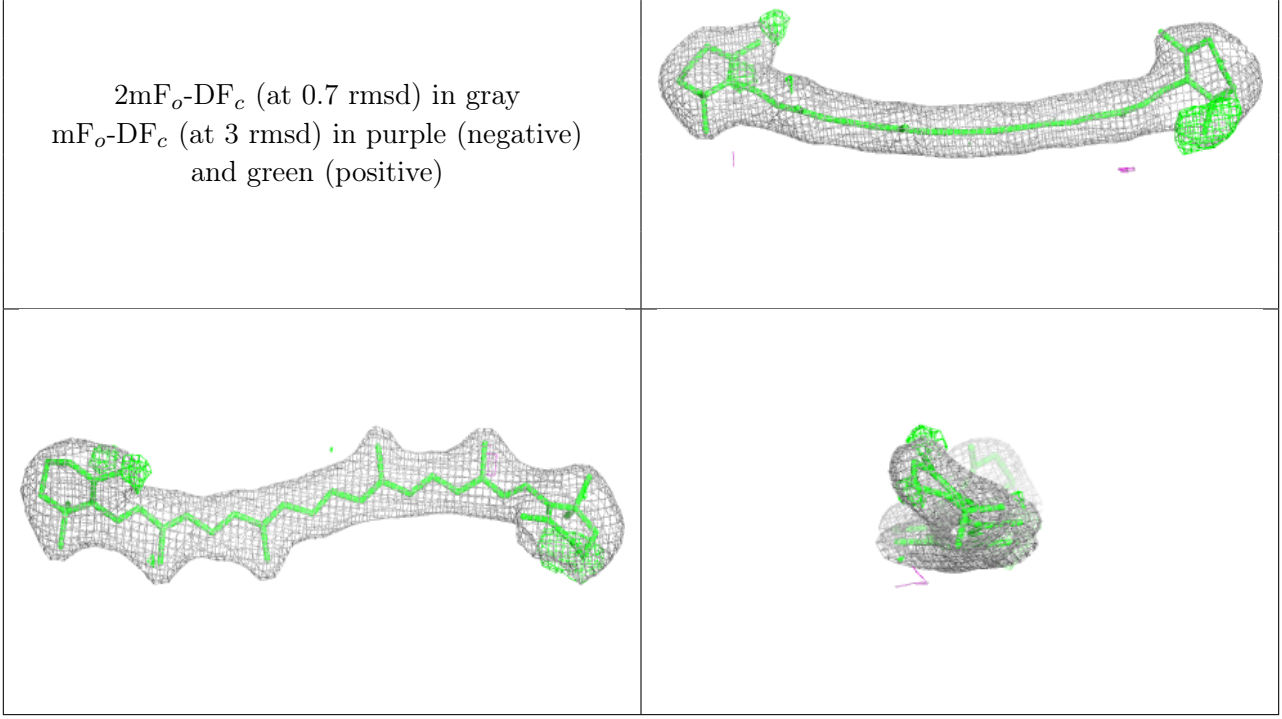
Electron density around DGD C 516:

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



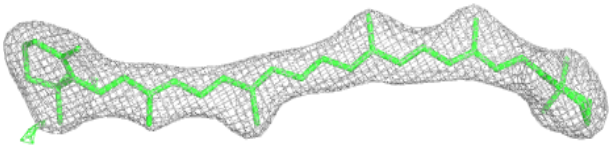
Electron density around BCR D 404:

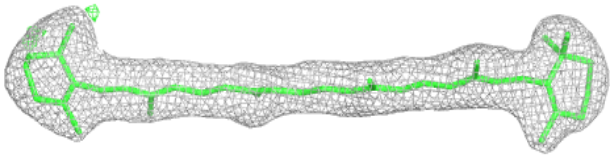
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

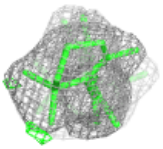


Electron density around BCR K 101:

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

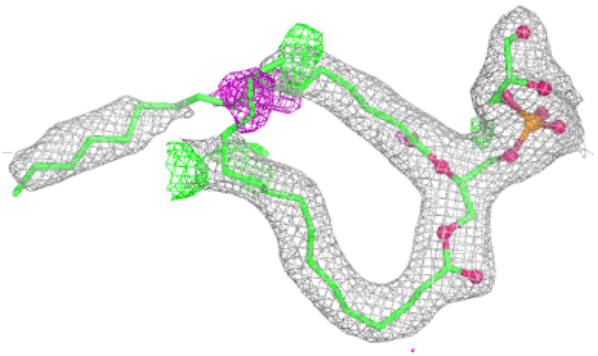


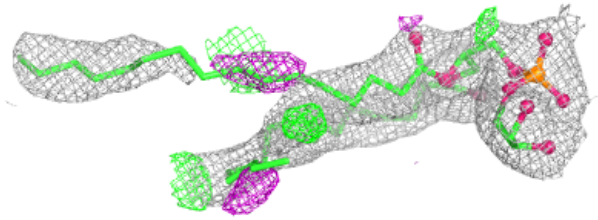


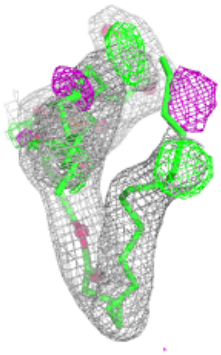


Electron density around LHG D 407:

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

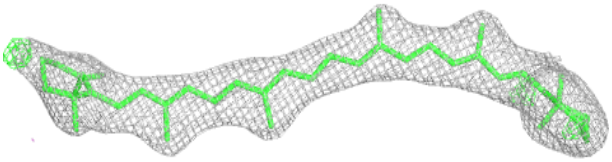


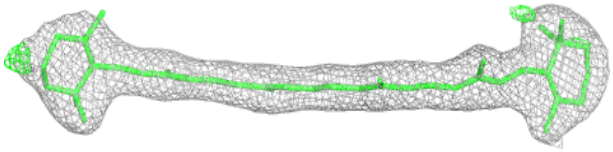


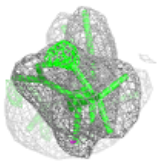


Electron density around BCR h 101:

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

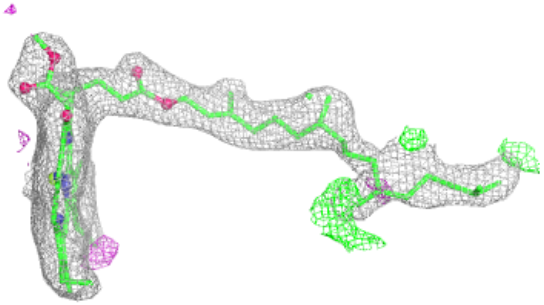


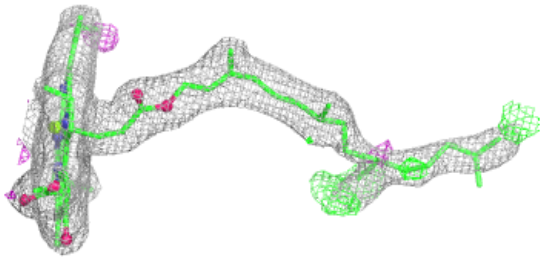


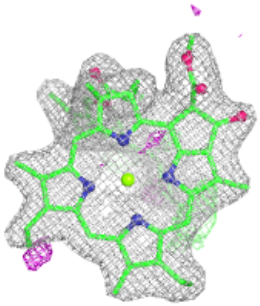


Electron density around CLA b 606:

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

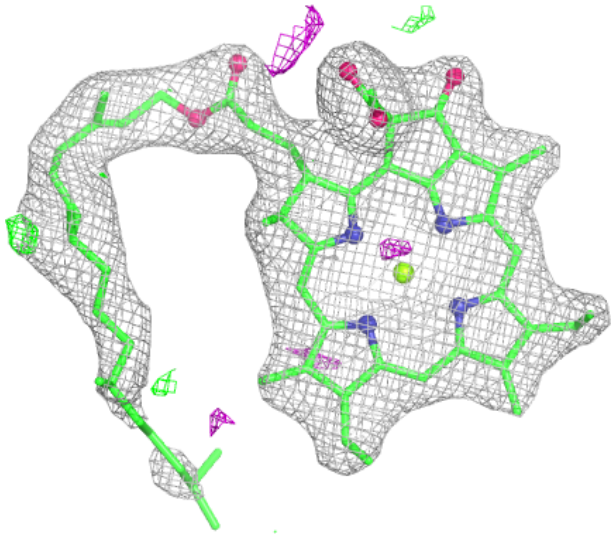


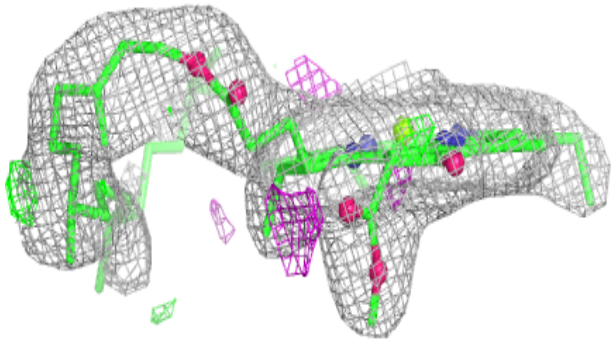


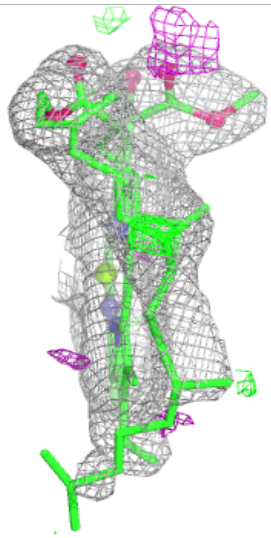


Electron density around CLA C 512:

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

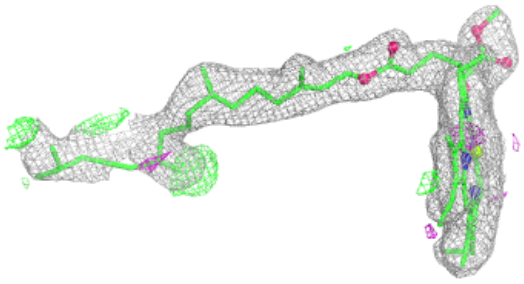


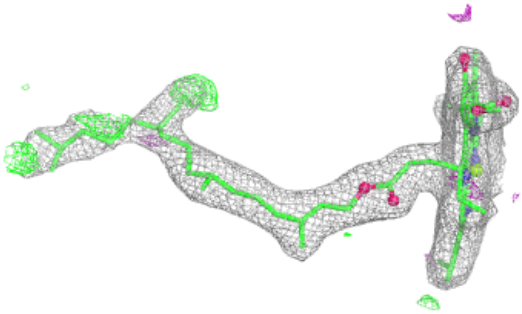


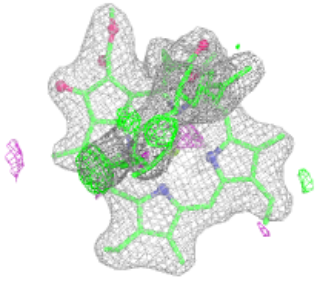


Electron density around CLA B 606:

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

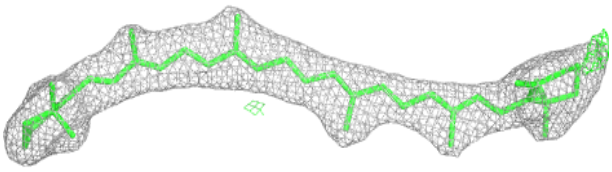


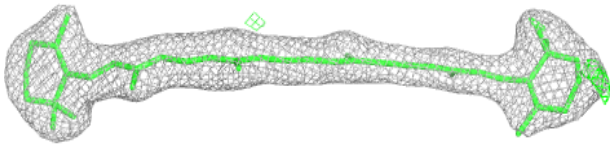


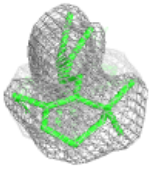


Electron density around BCR H 101:

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

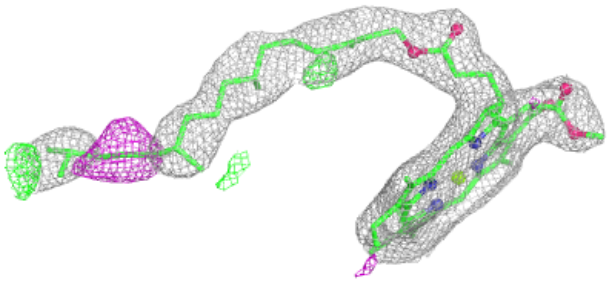


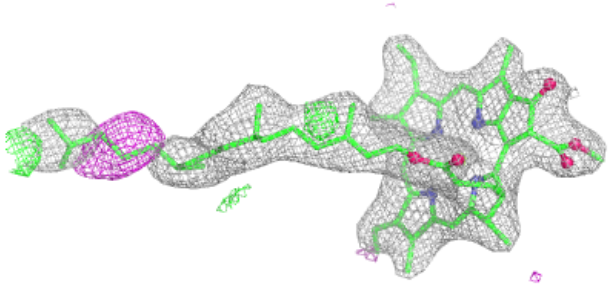


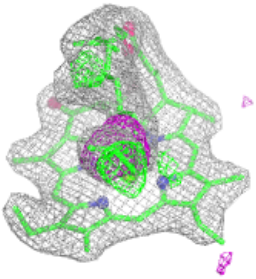


Electron density around CLA c 505:

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

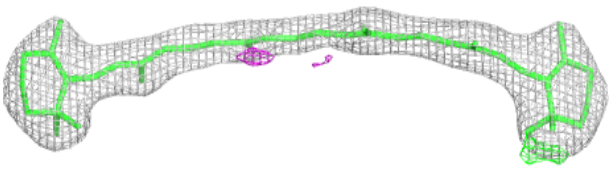


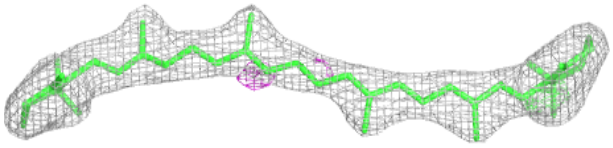


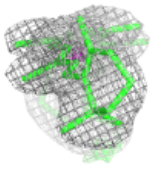


Electron density around BCR K 103:

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

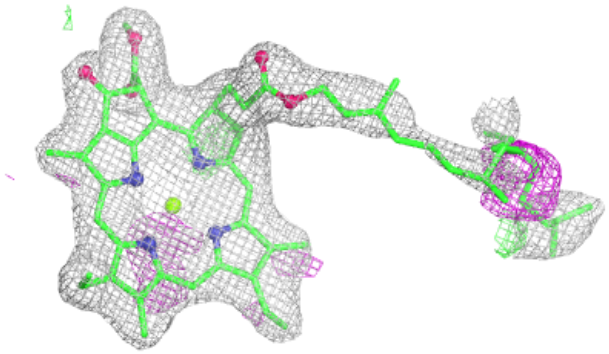


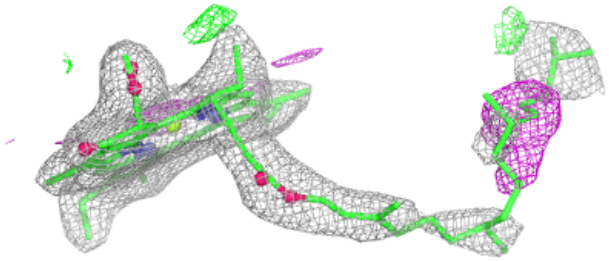


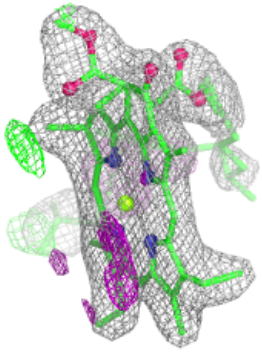


Electron density around CLA a 409:

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

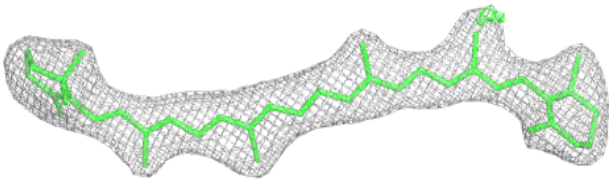


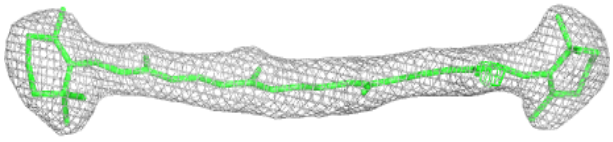


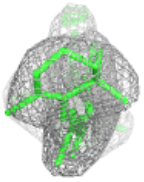


Electron density around BCR Y 101:

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

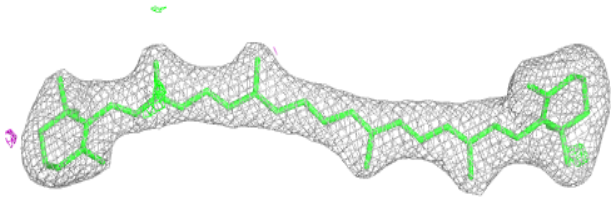


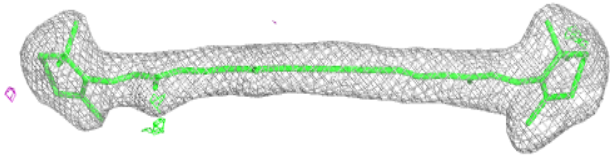


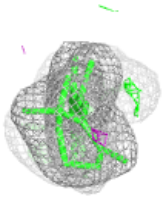


Electron density around BCR b 618:

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

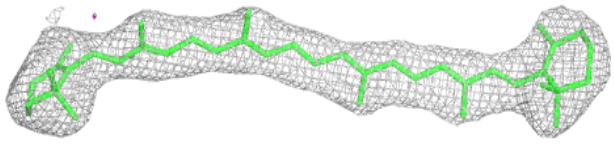


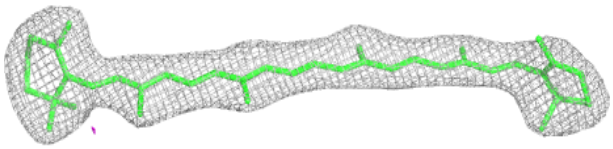


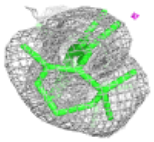


Electron density around BCR c 515:

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

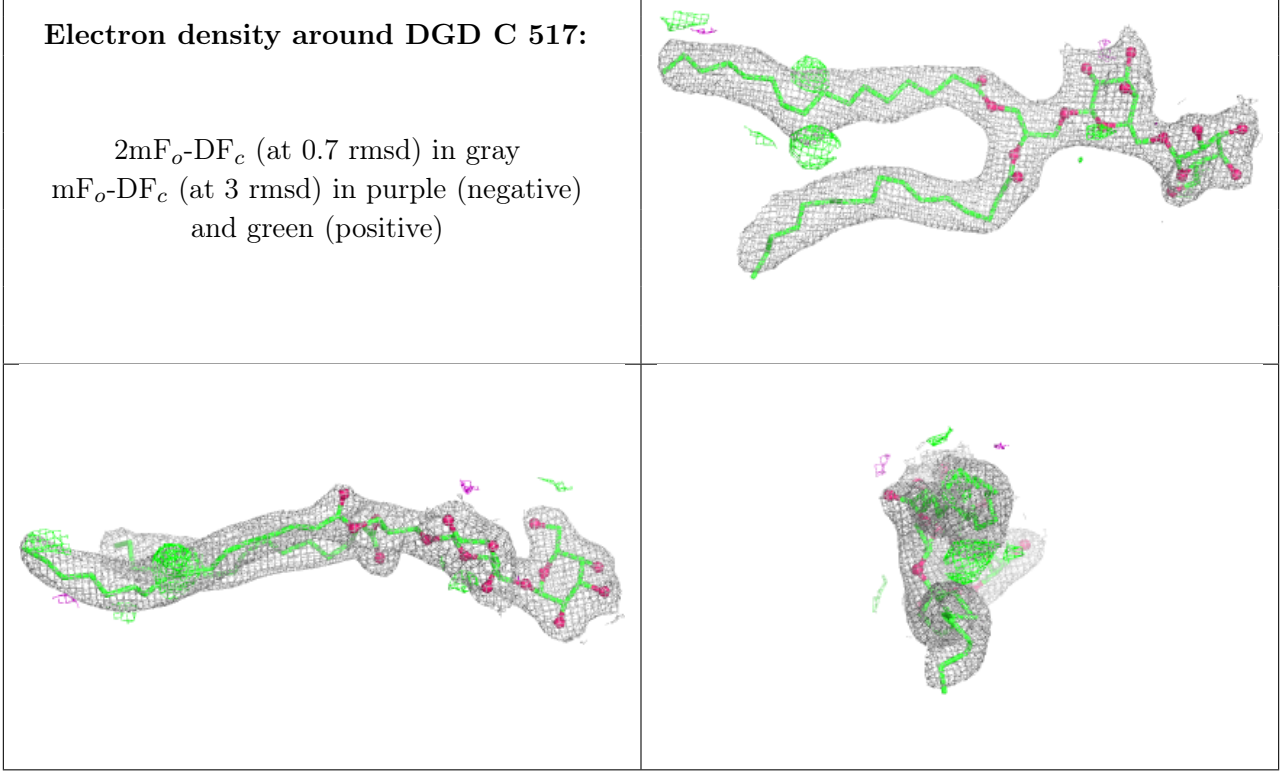






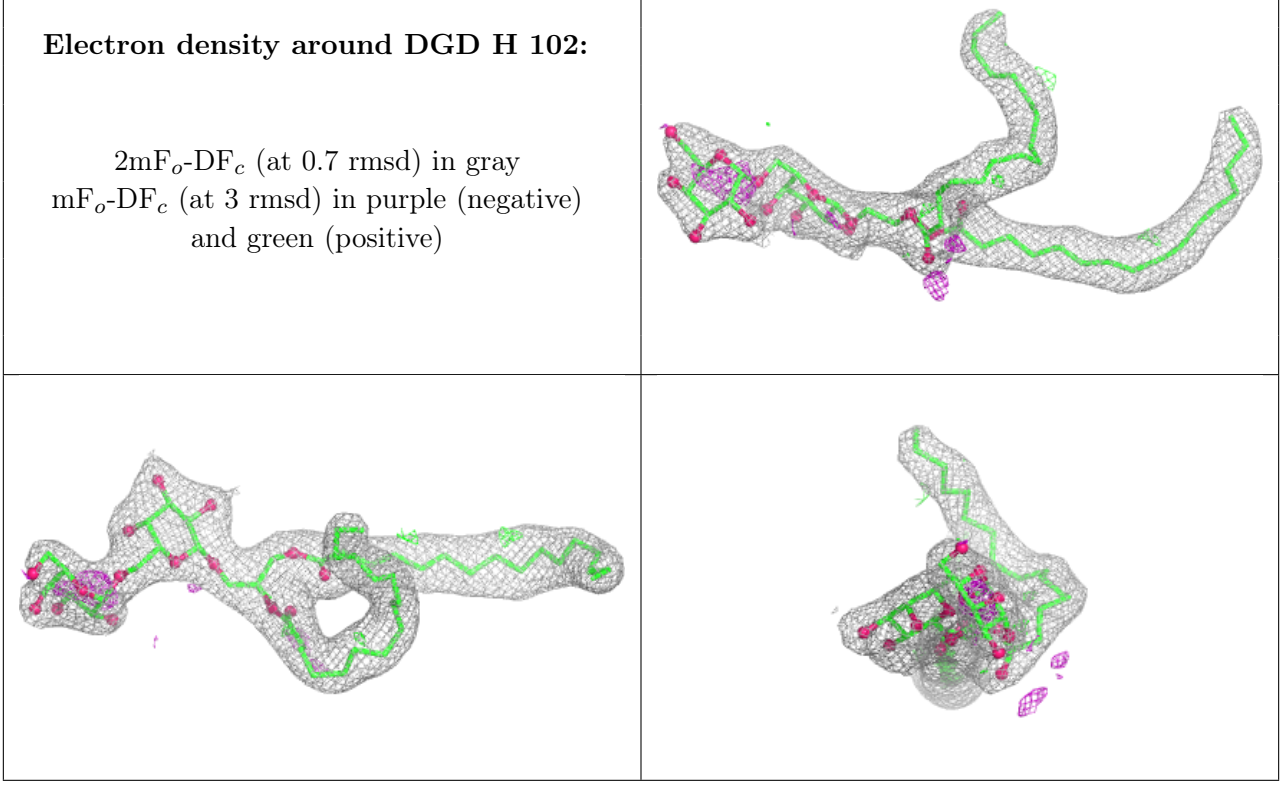
Electron density around DGD C 517:

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



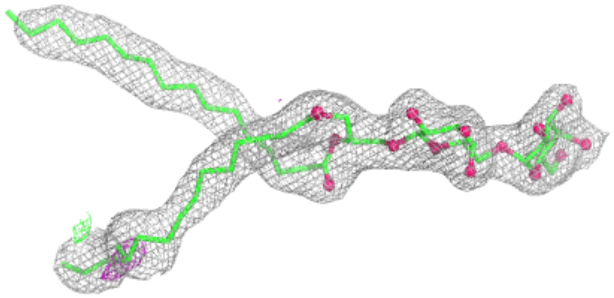
Electron density around DGD H 102:

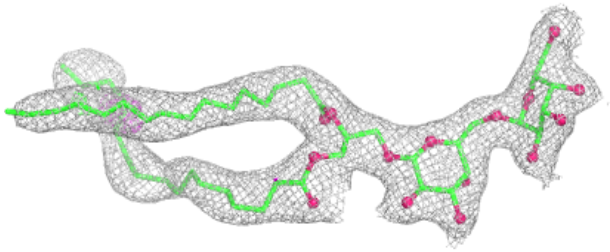
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

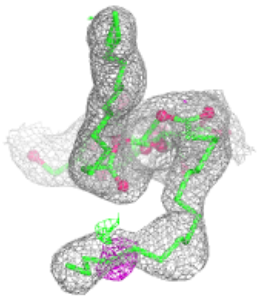


Electron density around DGD c 517:

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

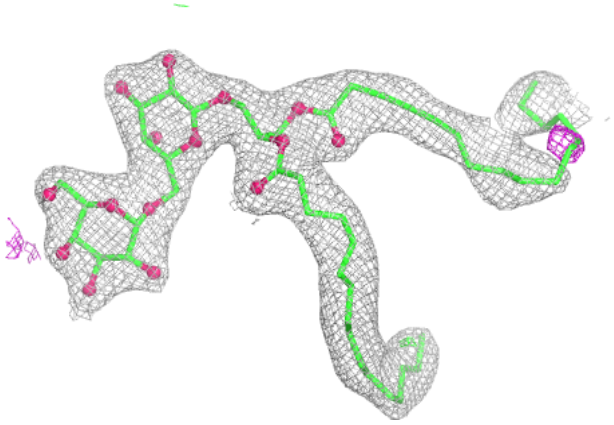


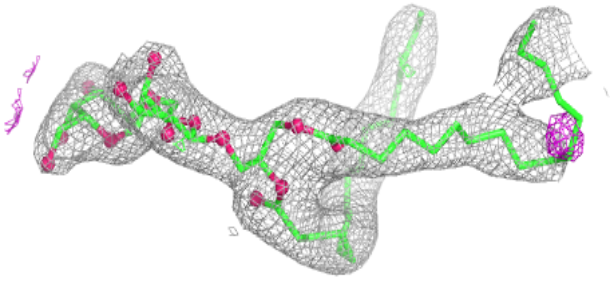


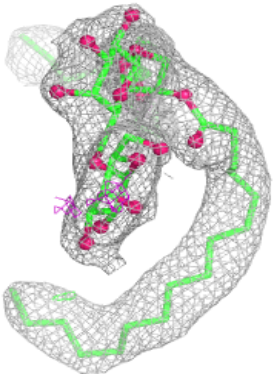


Electron density around DGD c 518:

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

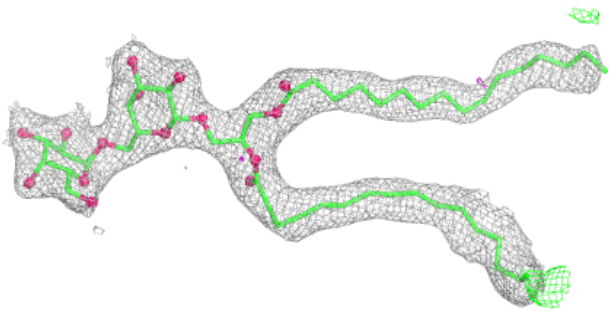


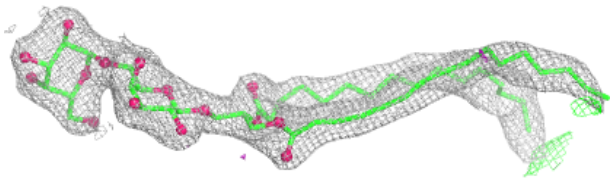


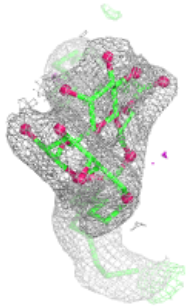


Electron density around DGD c 519:

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

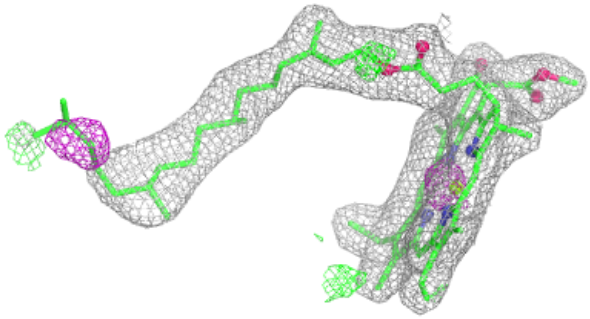


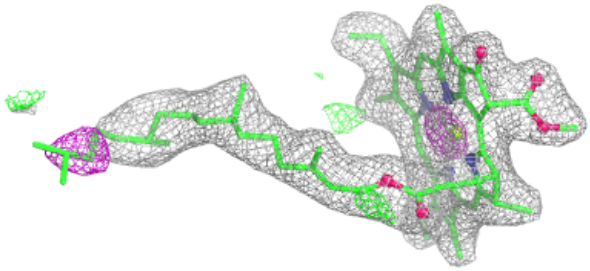


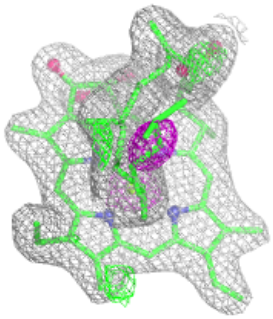


Electron density around CLA C 508:

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

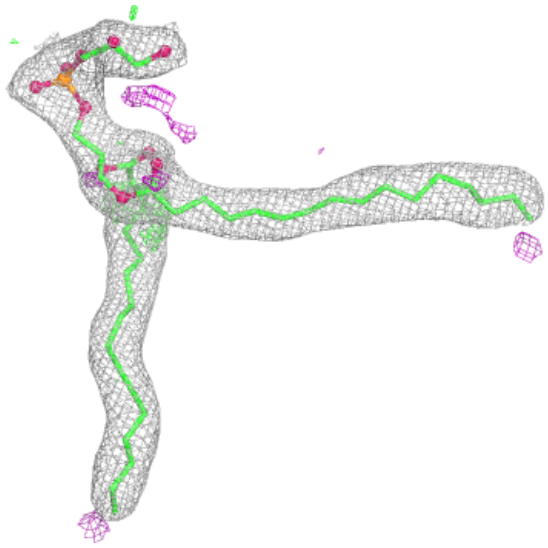


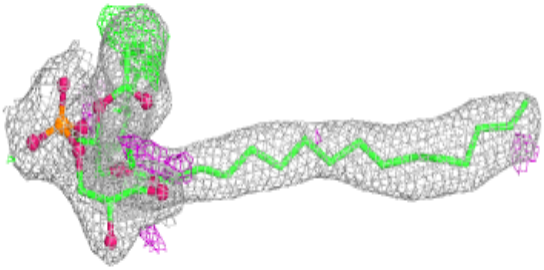


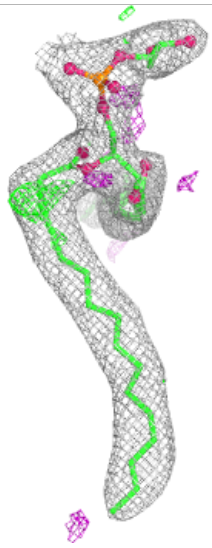


Electron density around LHG b 630:

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

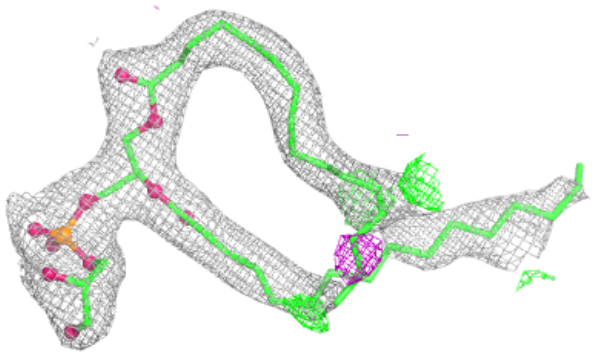


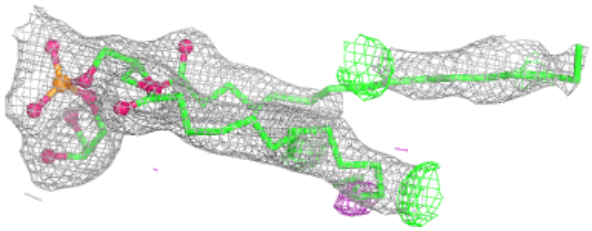


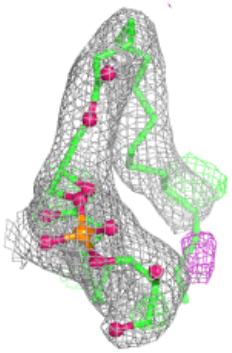


Electron density around LHG d 406:

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

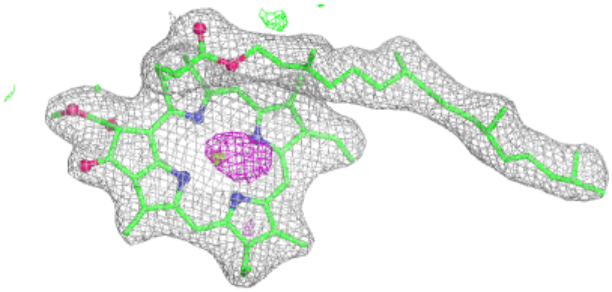


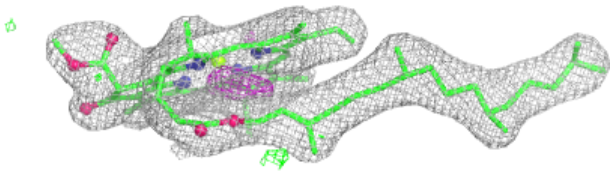


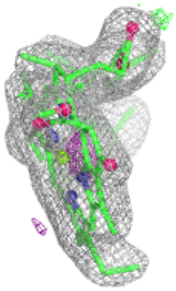


Electron density around CLA C 501:

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

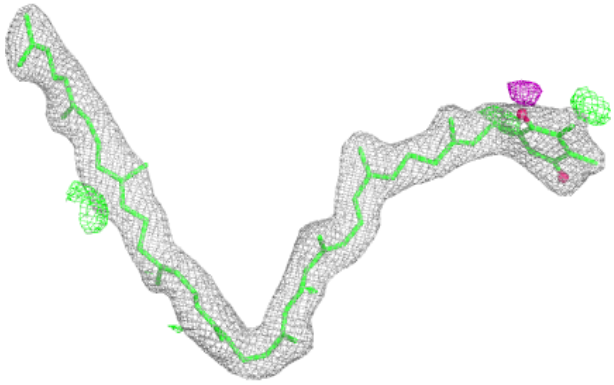


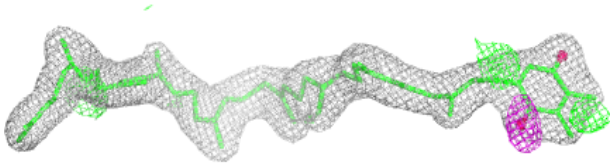


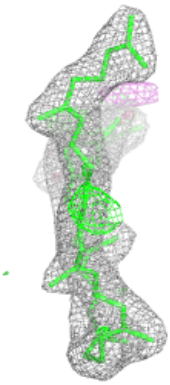


Electron density around PL9 D 405:

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

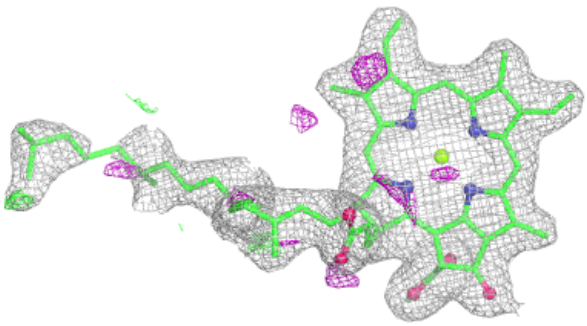


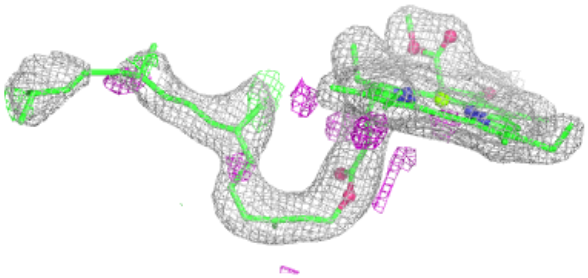


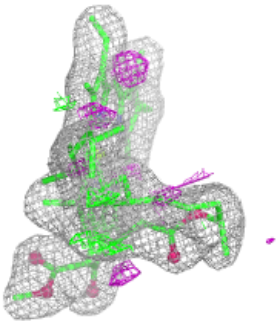


Electron density around CLA A 406:

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

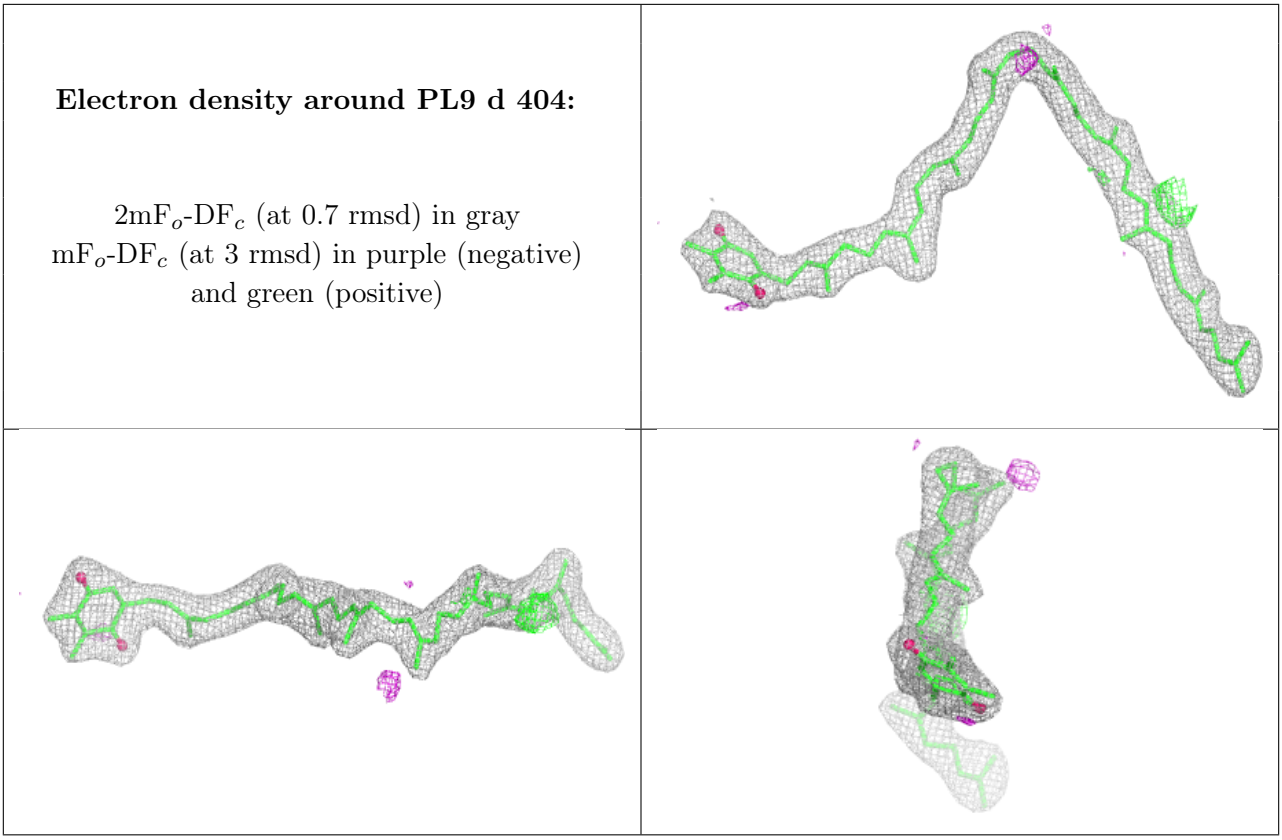






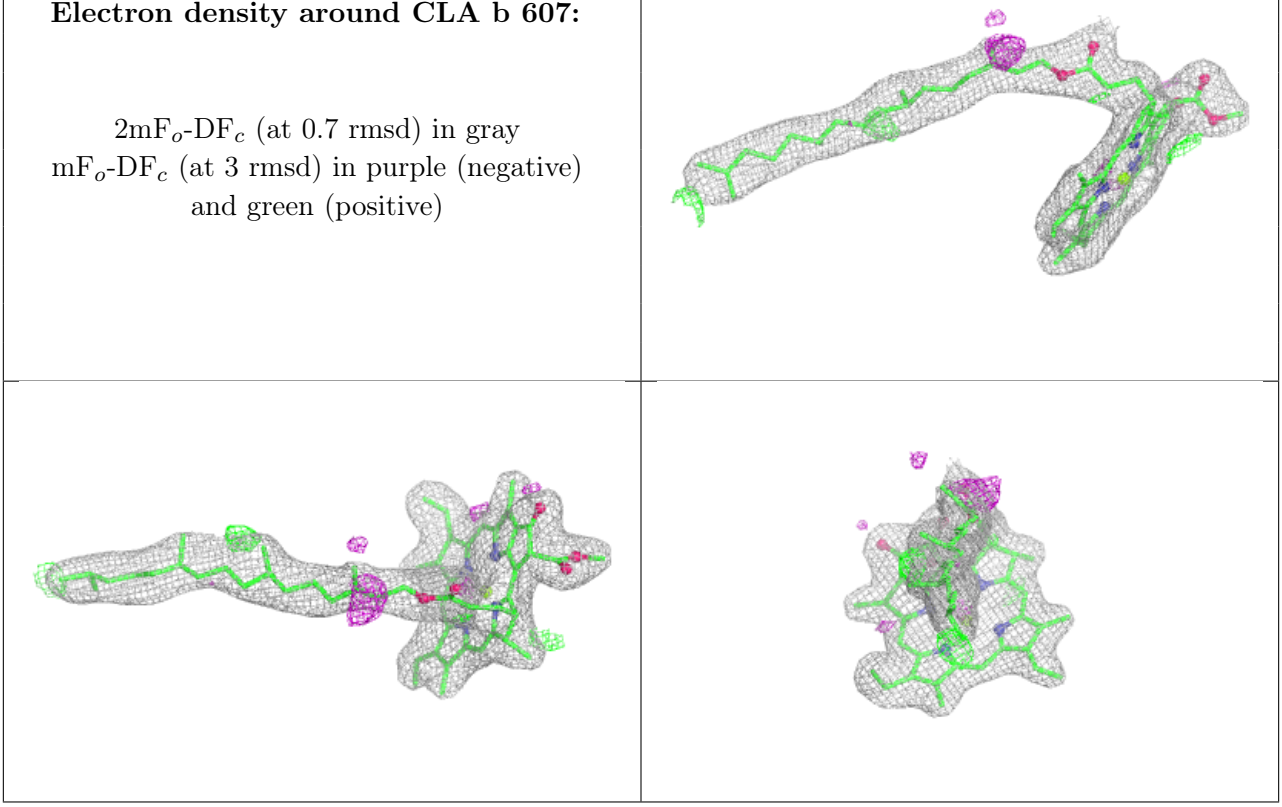
Electron density around PL9 d 404:

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



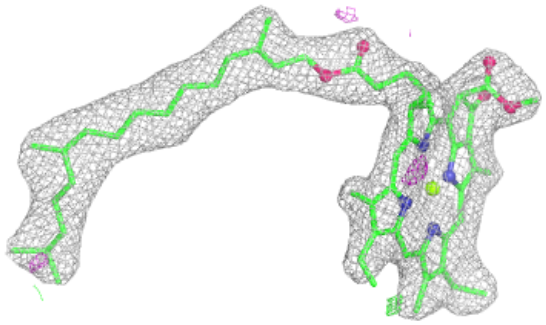
Electron density around CLA b 607:

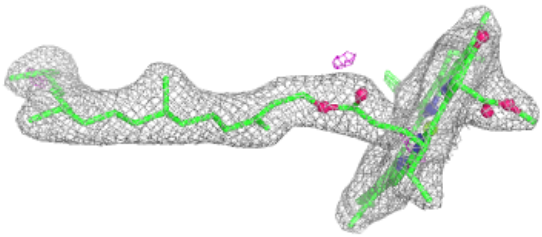
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

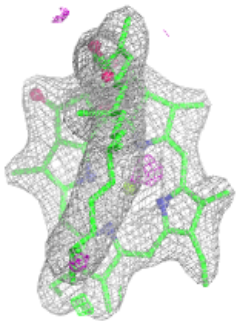


Electron density around CLA b 609:

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

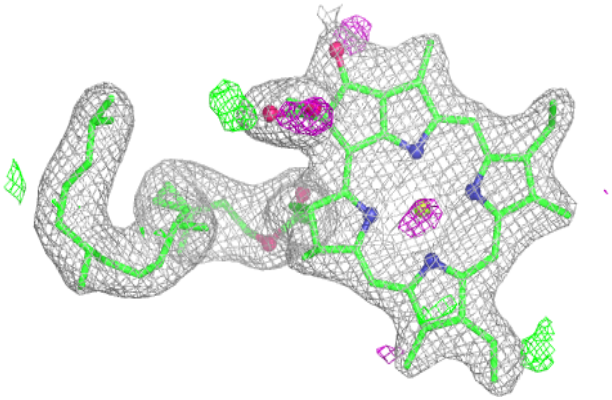


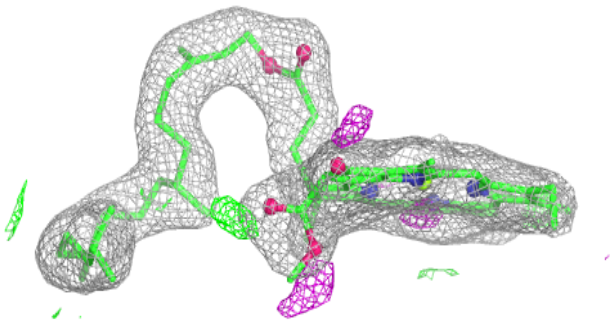




Electron density around CLA b 612:

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

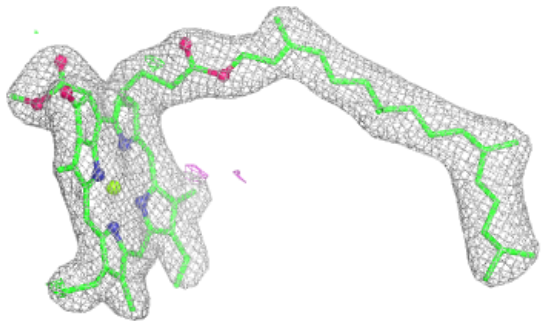


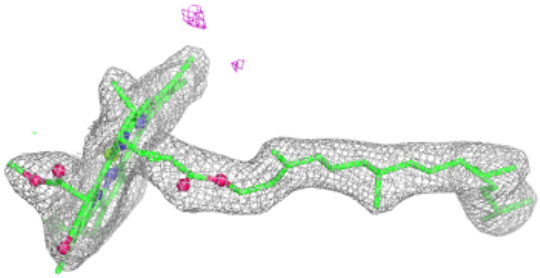


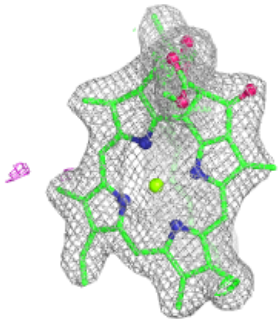


Electron density around CLA B 609:

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

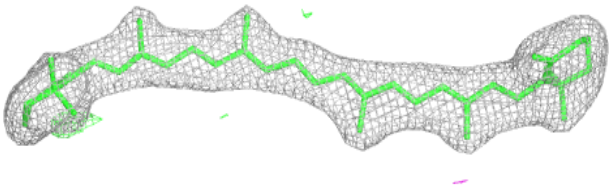


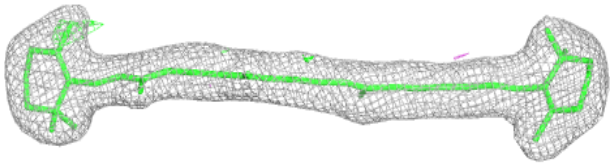


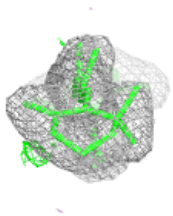


Electron density around BCR a 410:

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

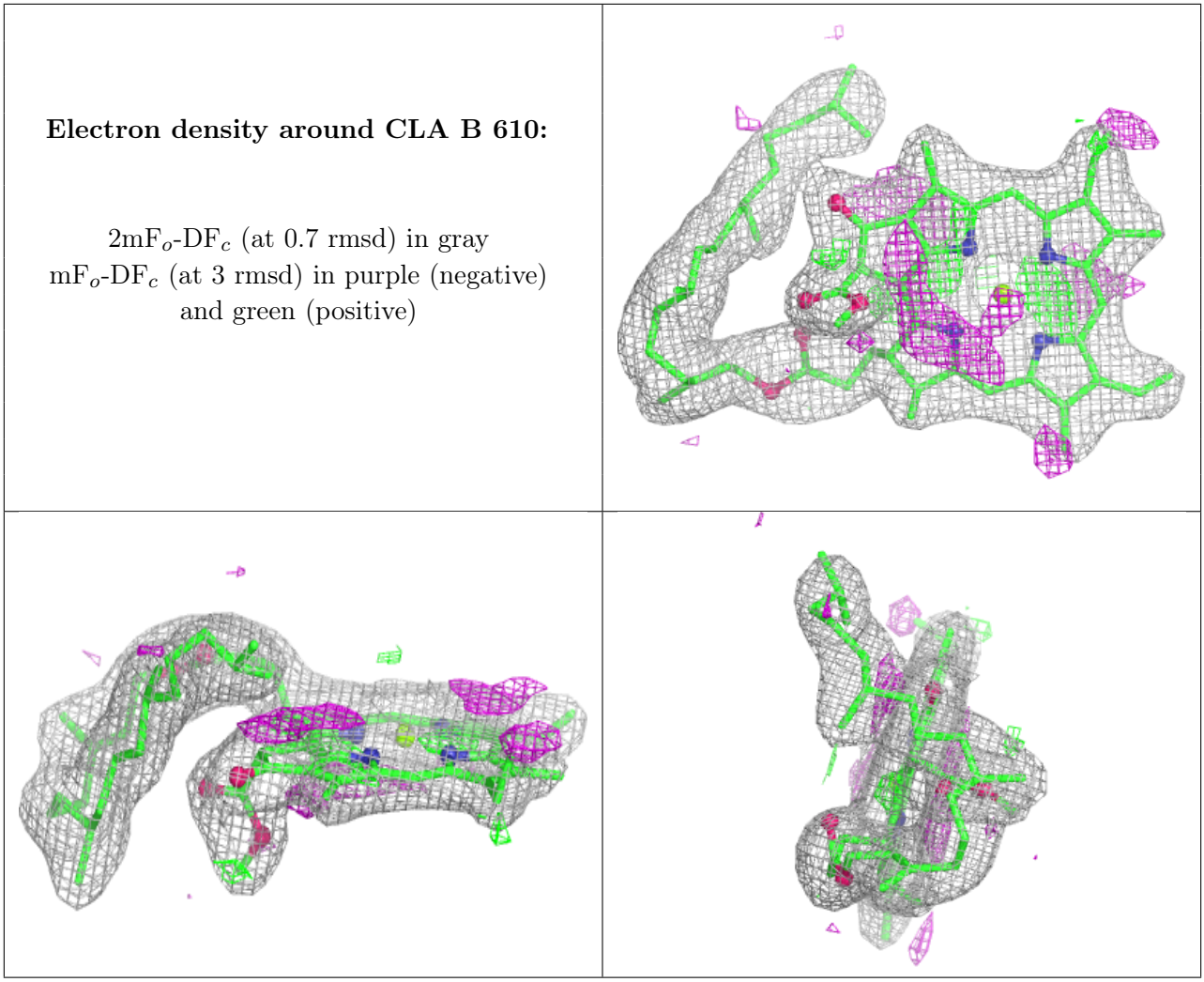






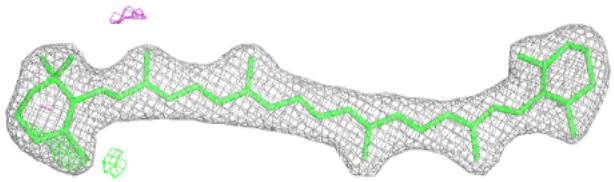
Electron density around CLA B 610:

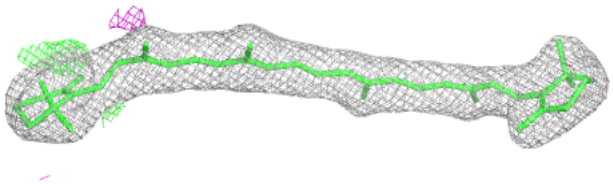
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

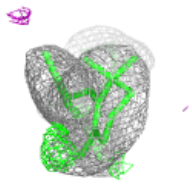


Electron density around BCR b 619:

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

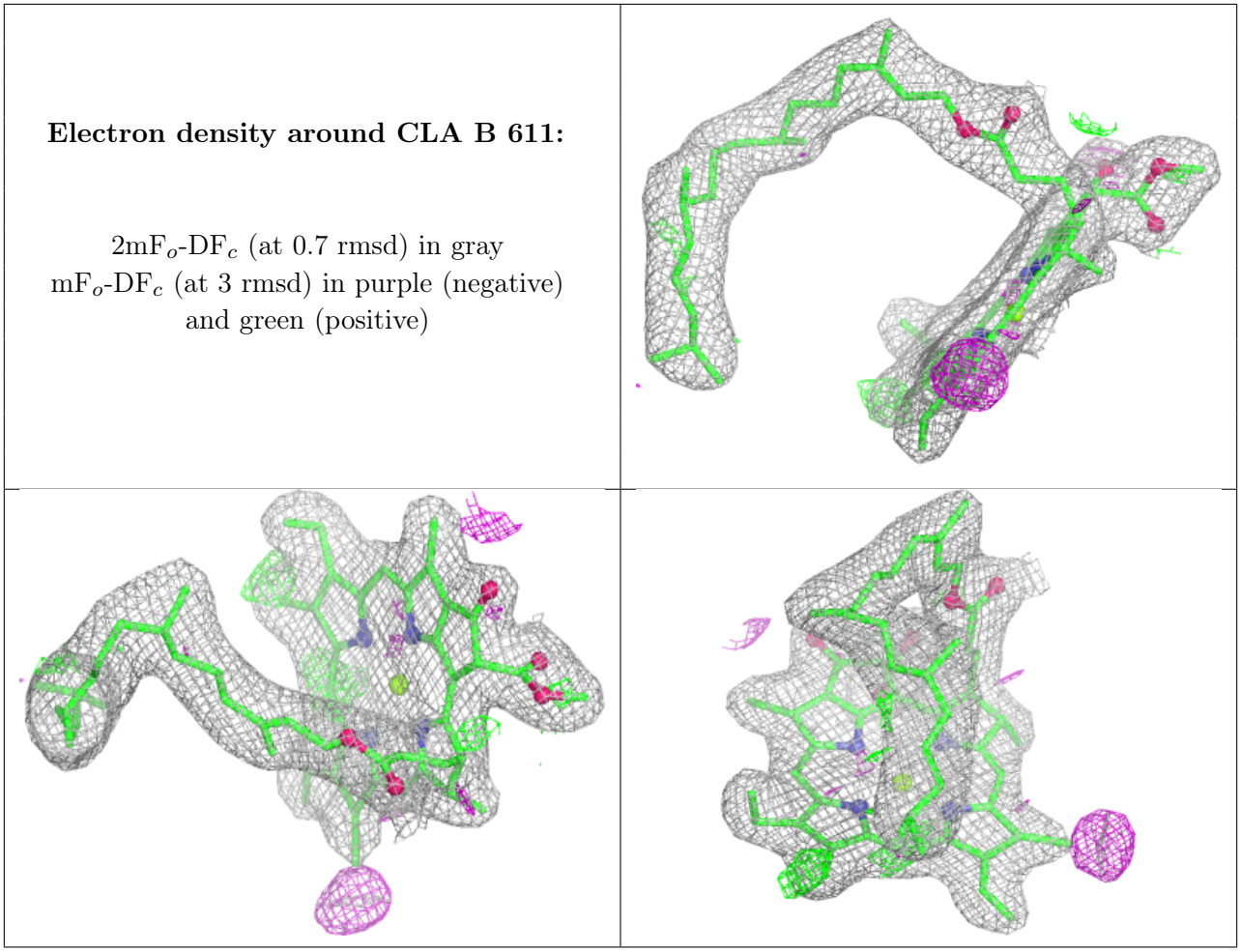






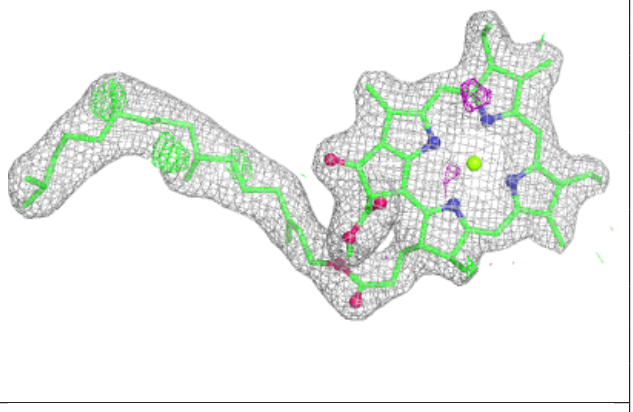
Electron density around CLA B 611:

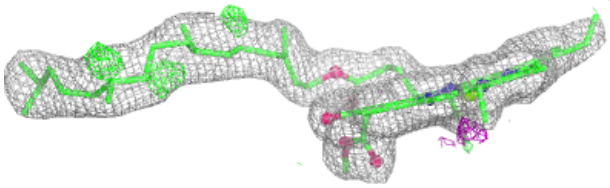
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

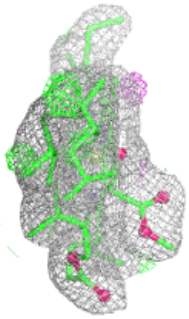


Electron density around CLA B 602:

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

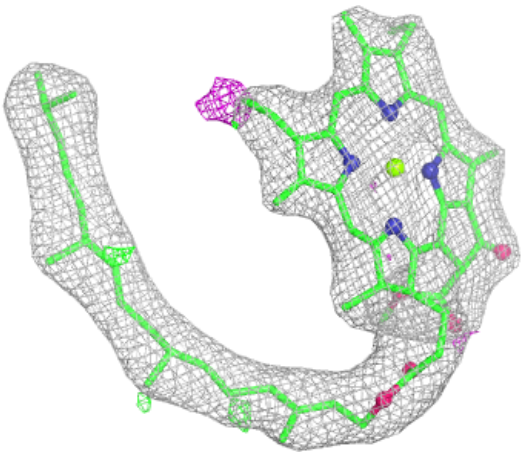


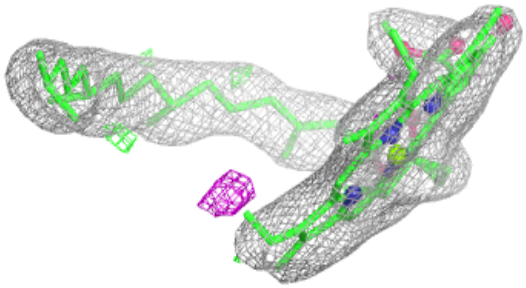


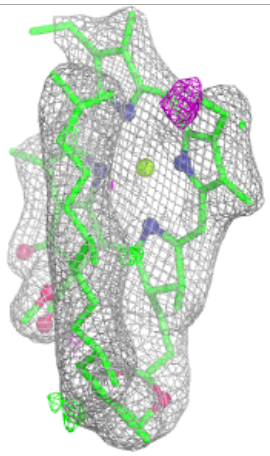


Electron density around CLA c 508:

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

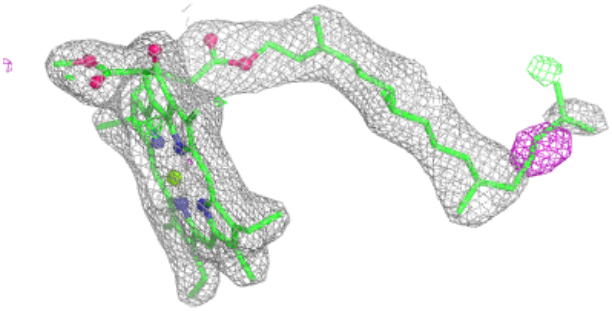


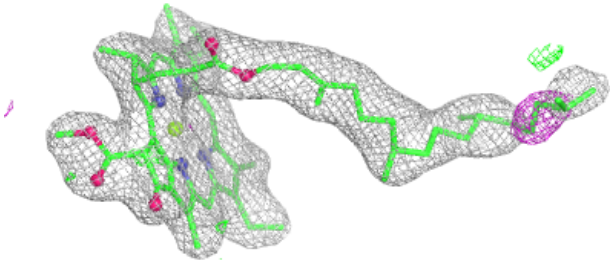


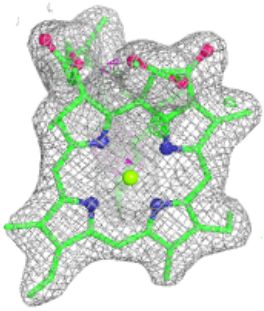


Electron density around CLA c 509:

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

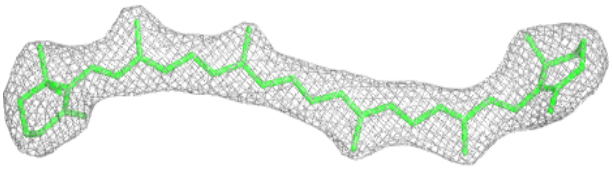


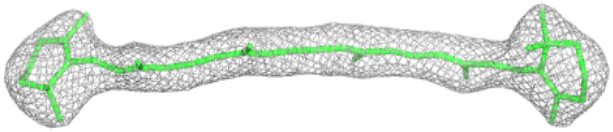


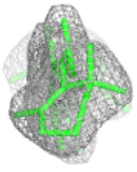


Electron density around BCR y 101:

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

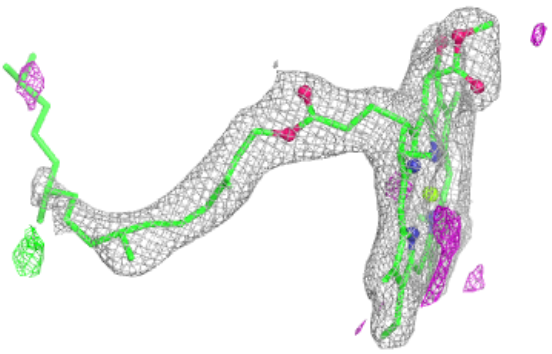


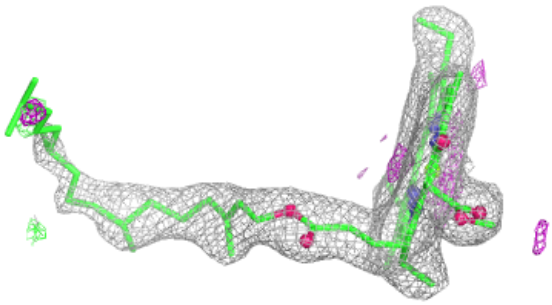


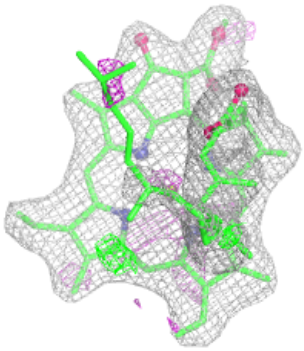


Electron density around CLA D 403:

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

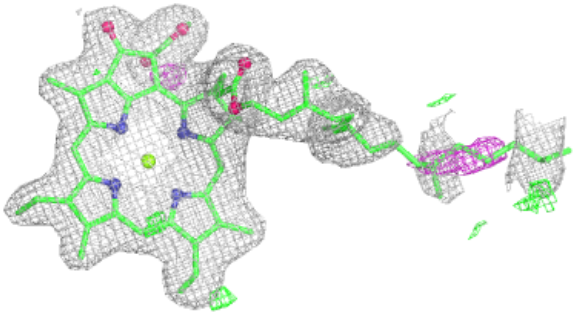


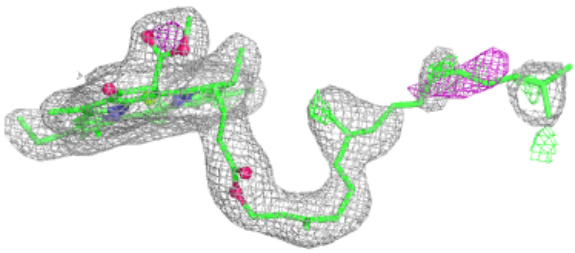


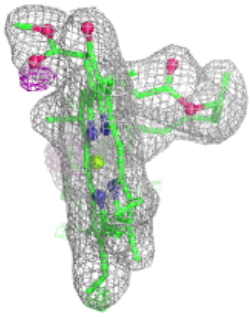


Electron density around CLA a 407:

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

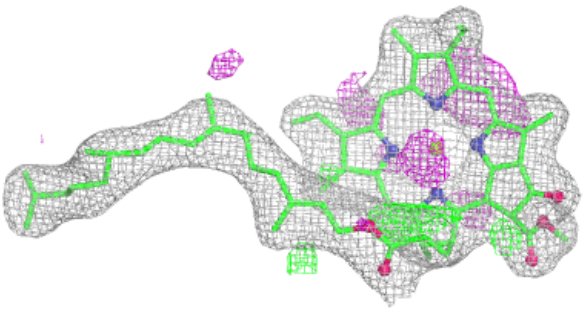


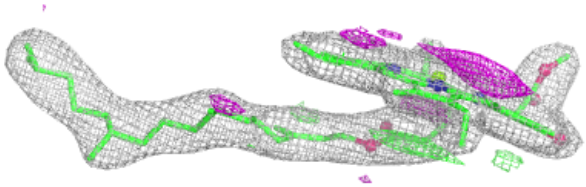


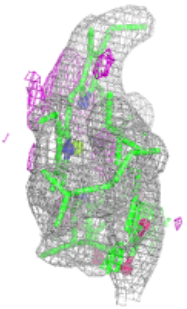


Electron density around CLA B 603:

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

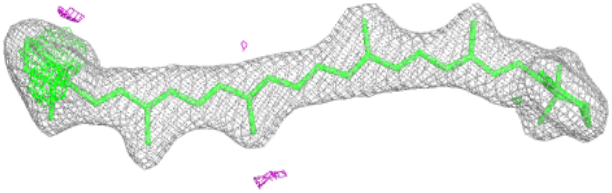


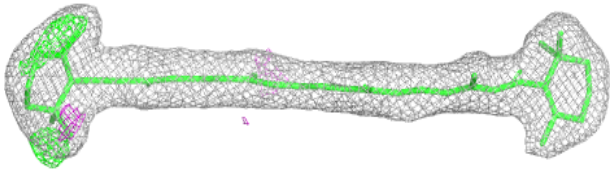


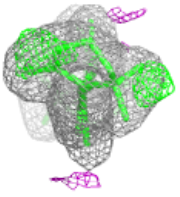


Electron density around BCR A 409:

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

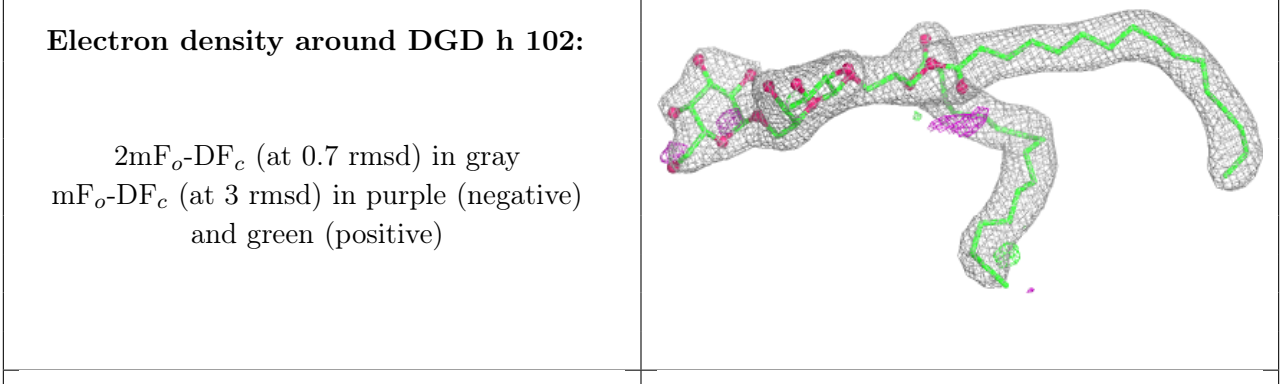






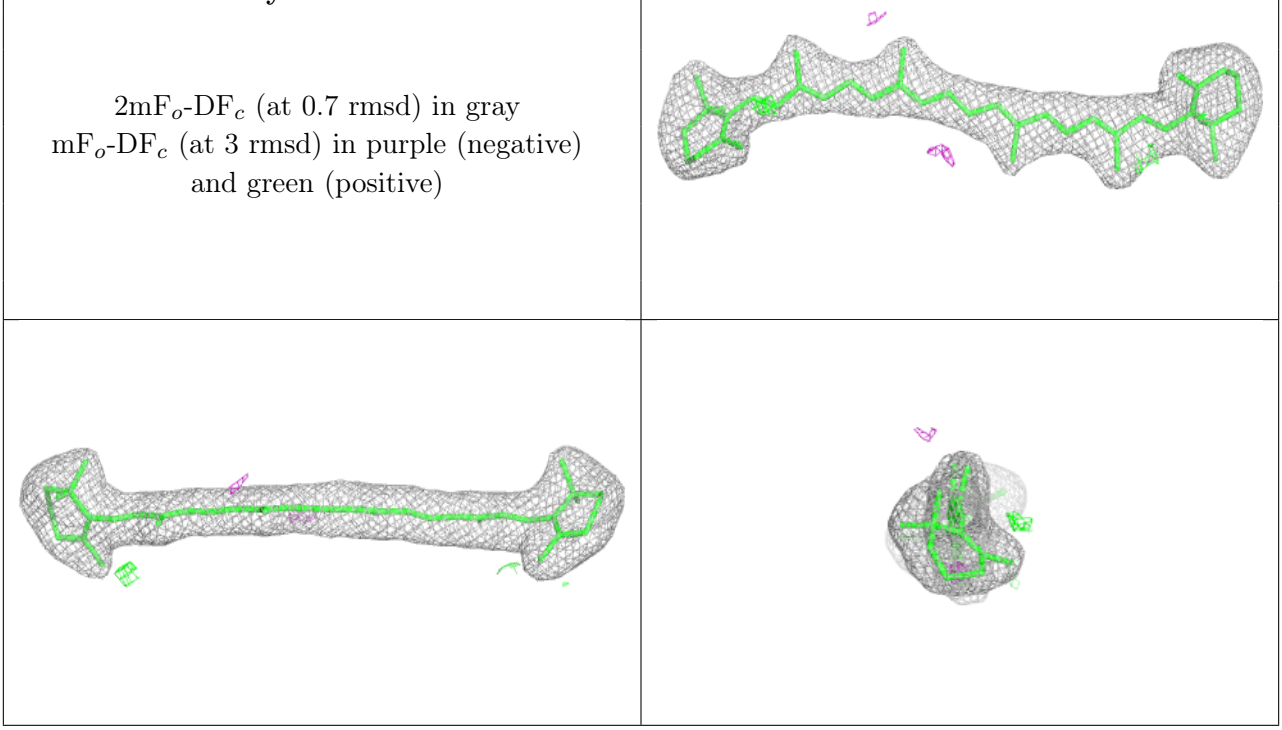
Electron density around DGD h 102:

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



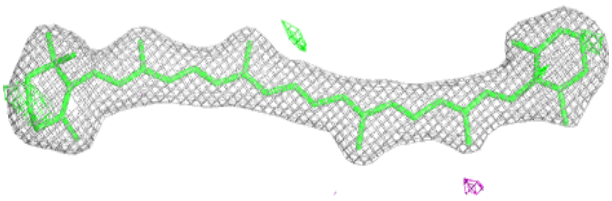
Electron density around BCR B 618:

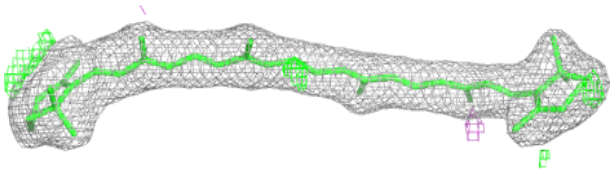
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

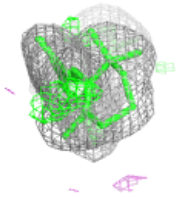


Electron density around BCR B 619:

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

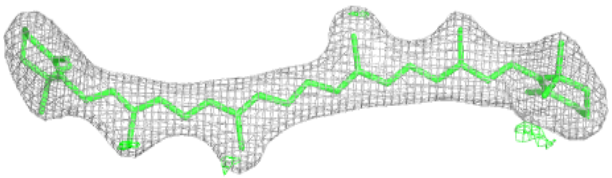


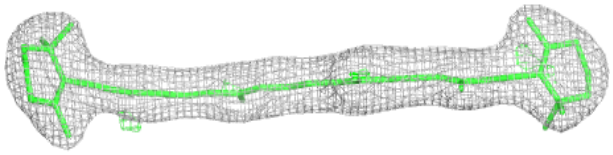


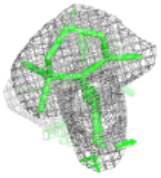


Electron density around BCR C 514:

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

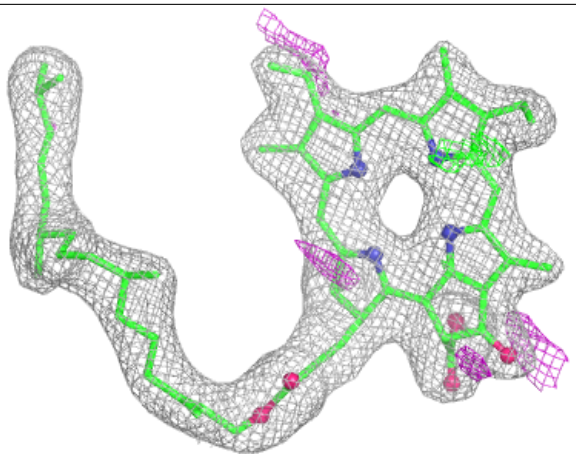


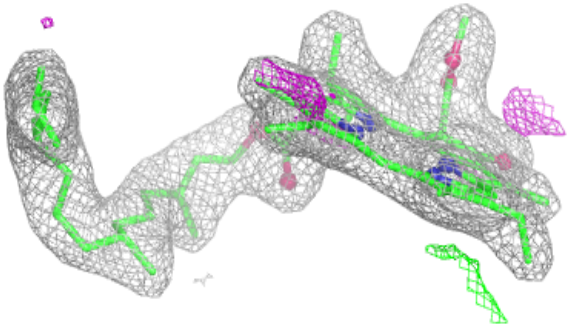


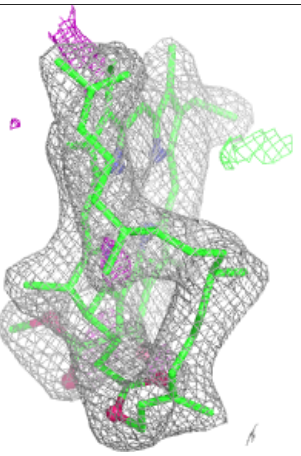


Electron density around PHO A 416:

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

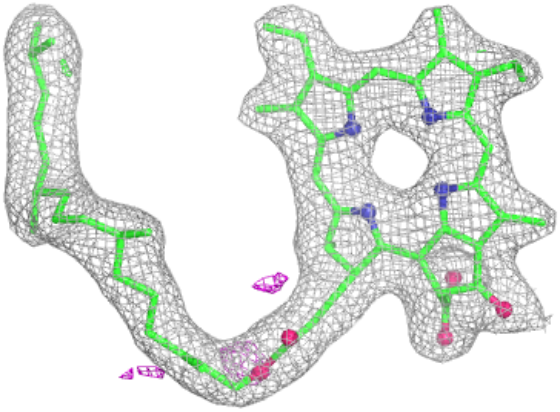


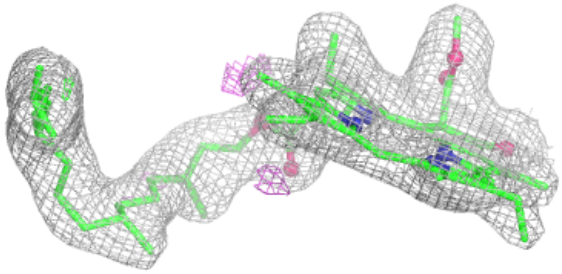


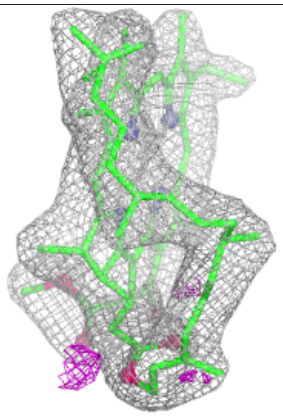


Electron density around PHO a 417:

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

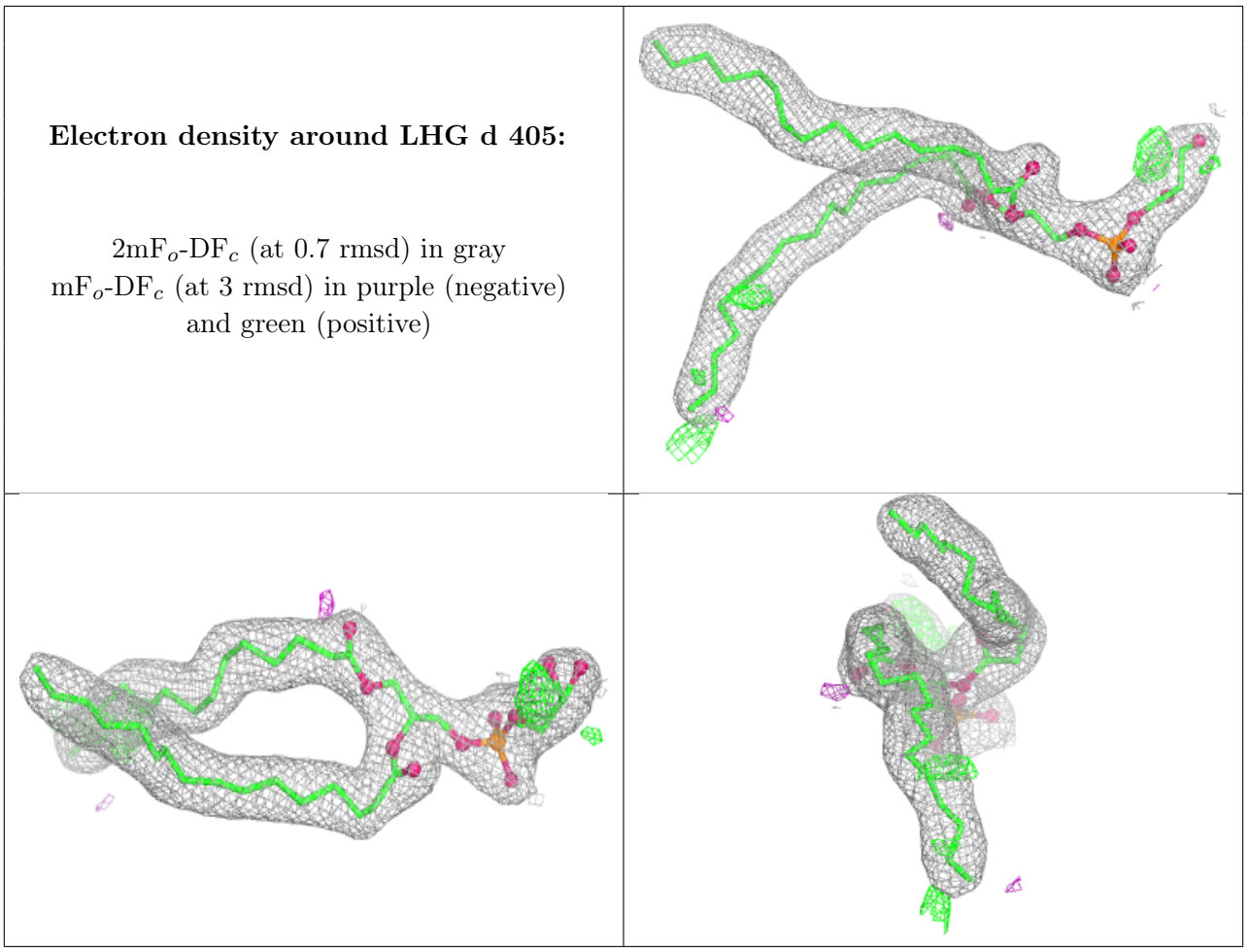






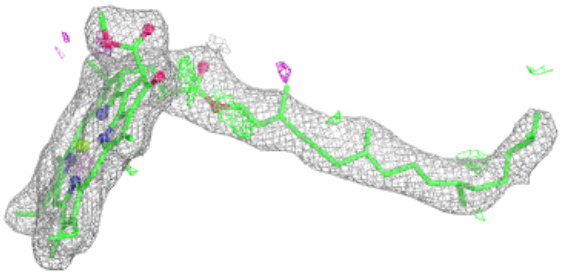
Electron density around LHG d 405:

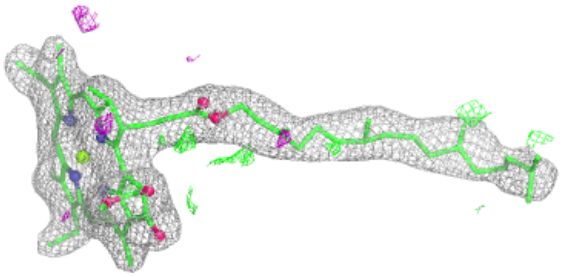
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

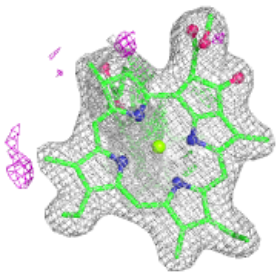


Electron density around CLA b 604:

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

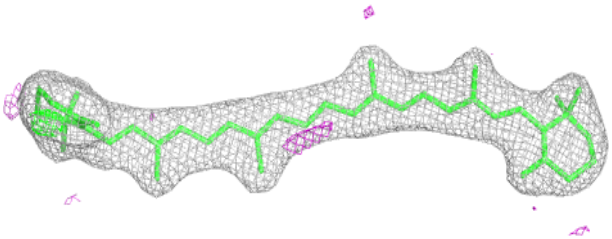


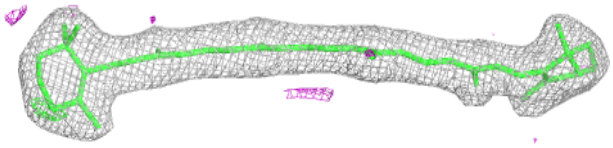


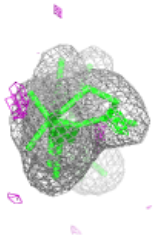


Electron density around BCR B 617:

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

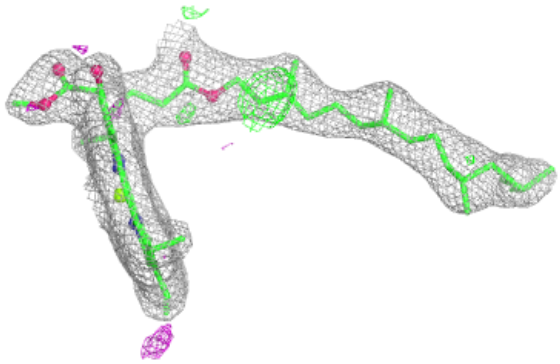


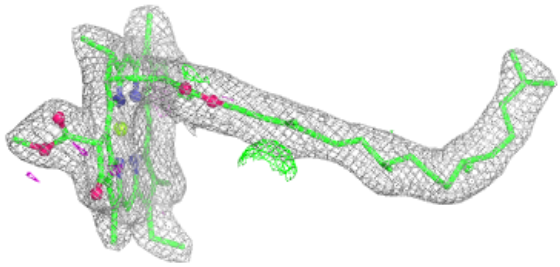


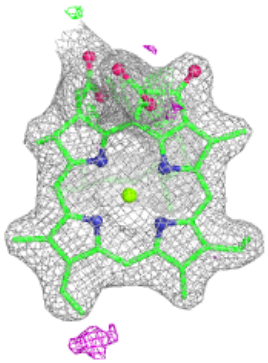


Electron density around CLA b 605:

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

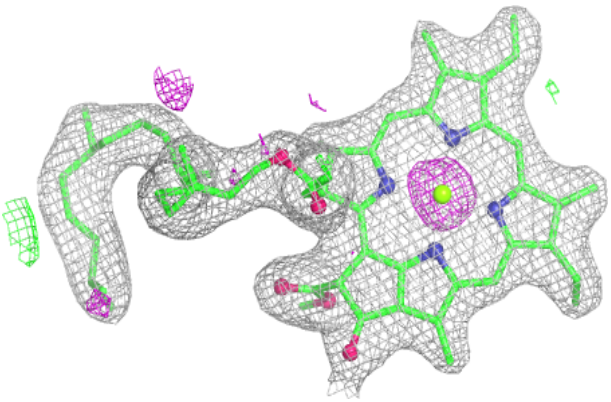


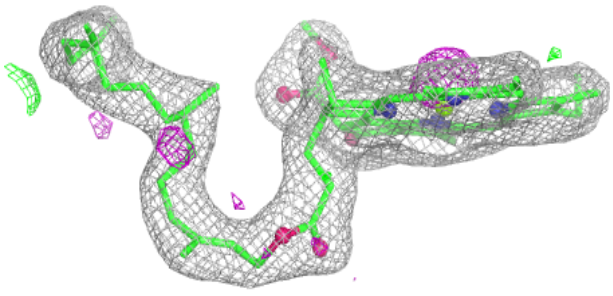


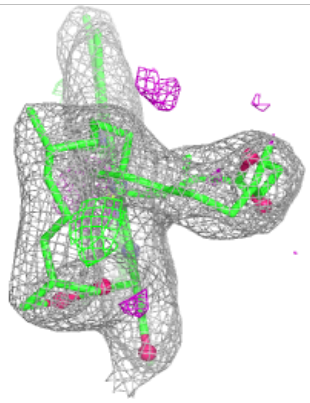


Electron density around CLA B 612:

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

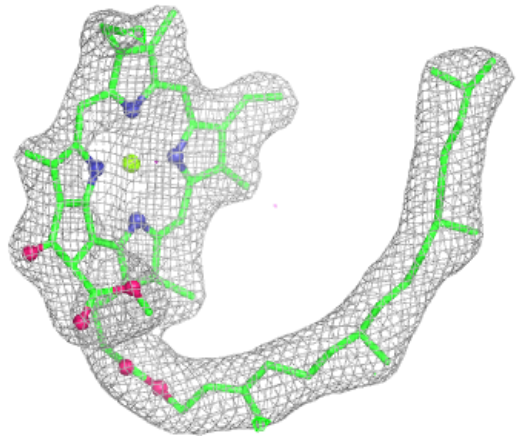


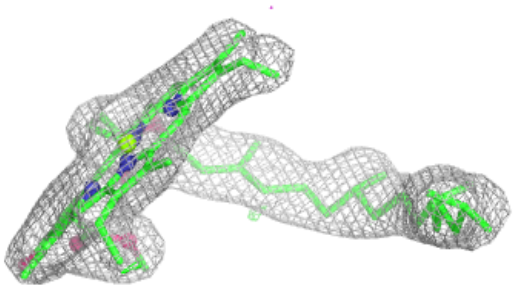


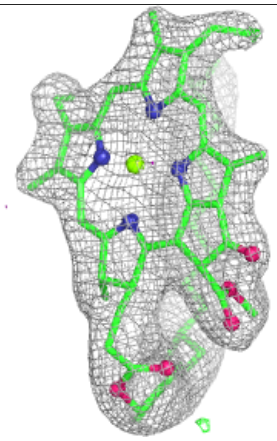


Electron density around CLA C 507:

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

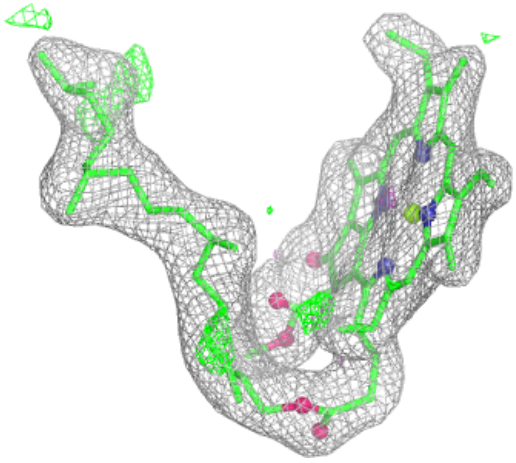


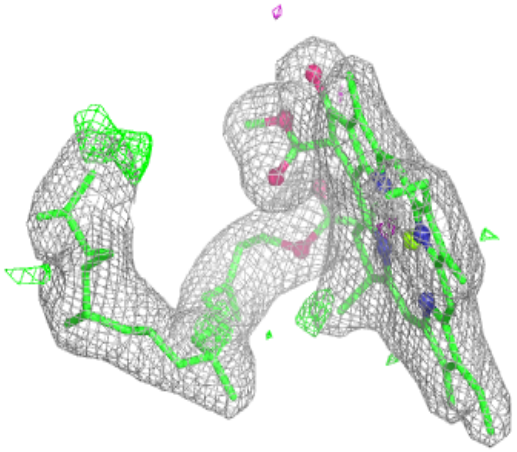


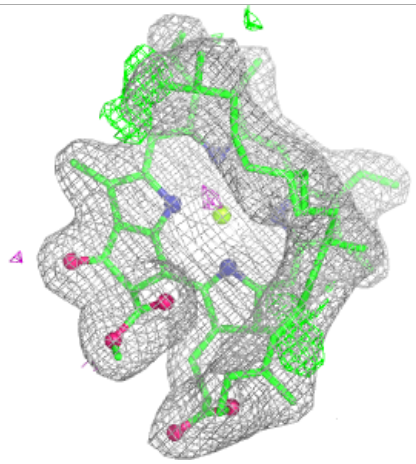


Electron density around CLA B 613:

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

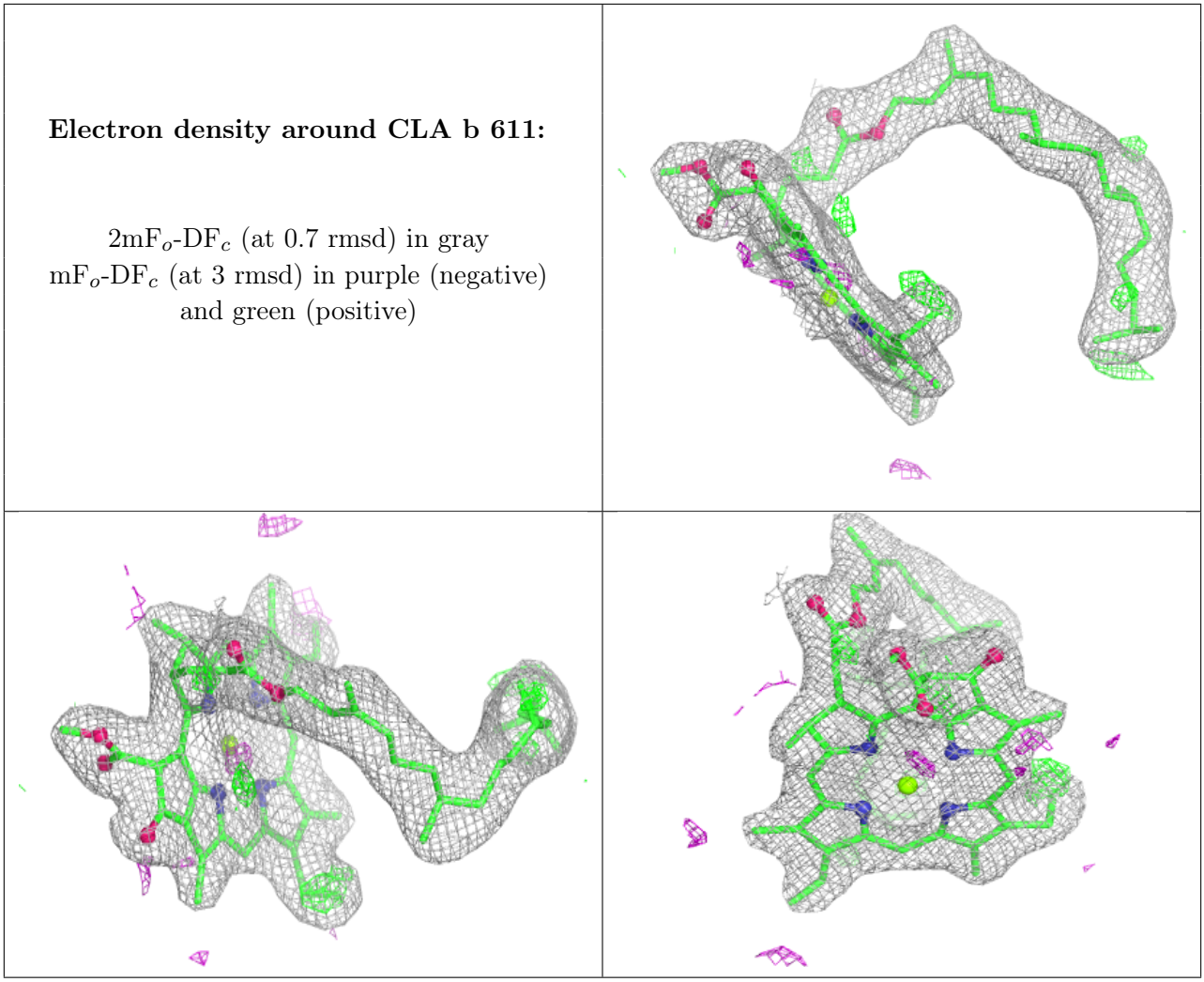






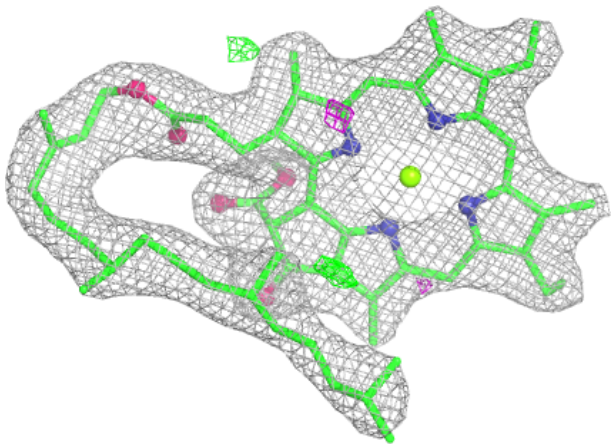
Electron density around CLA b 611:

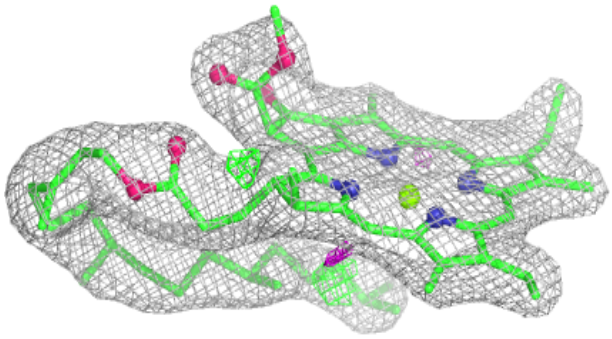
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

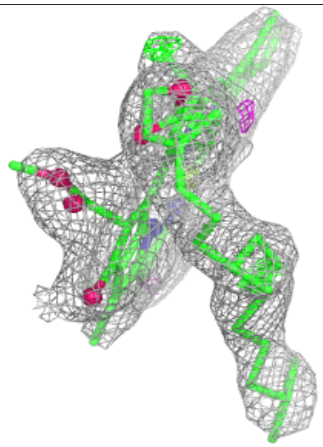


Electron density around CLA C 509:

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

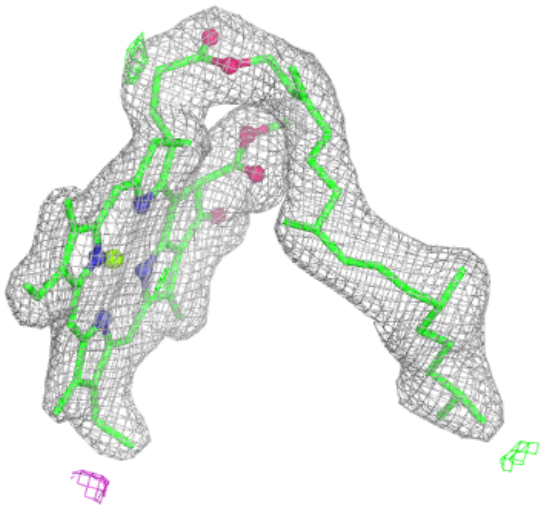


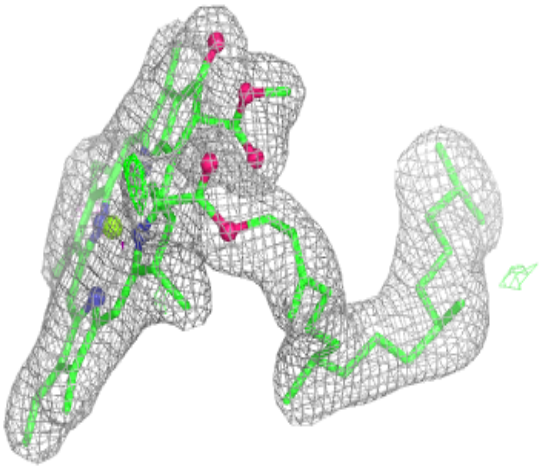


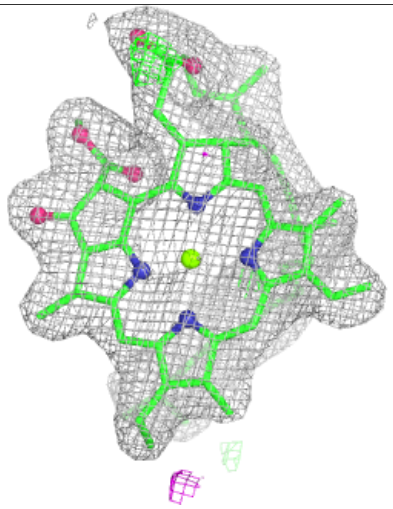


Electron density around CLA b 613:

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

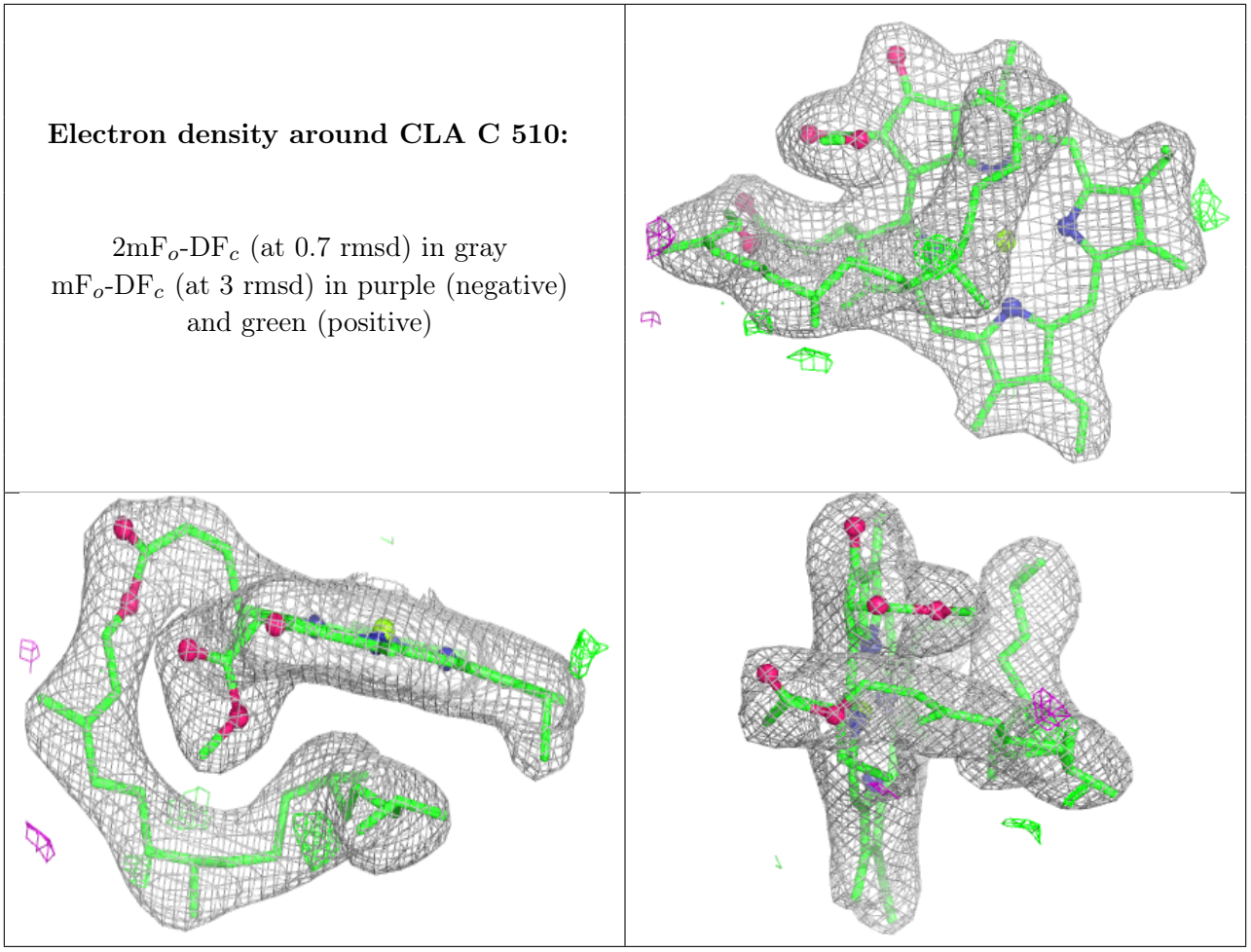






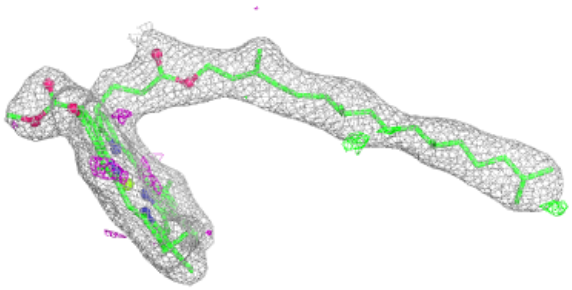
Electron density around CLA C 510:

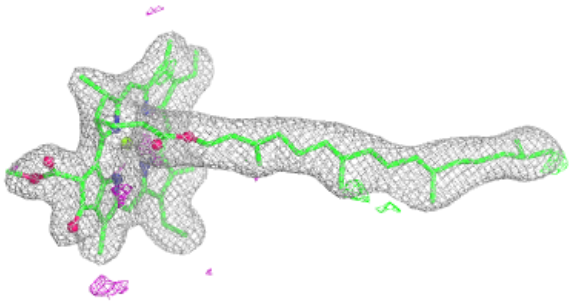
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

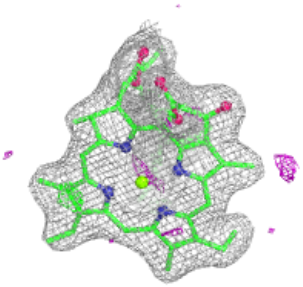


Electron density around CLA B 607:

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

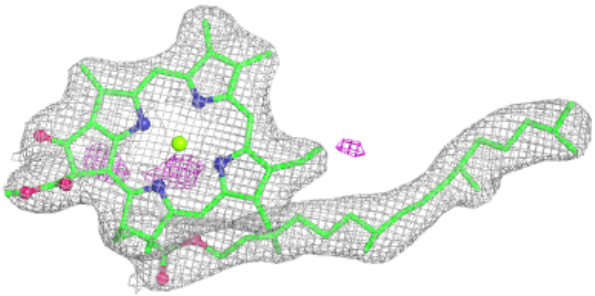


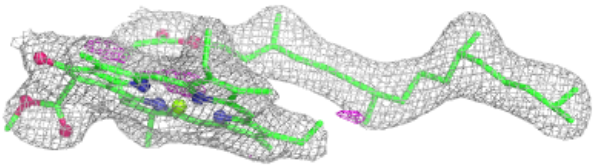


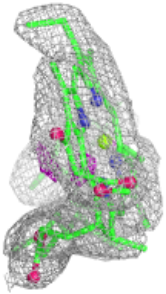


Electron density around CLA c 502:

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

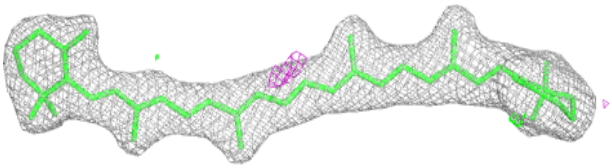


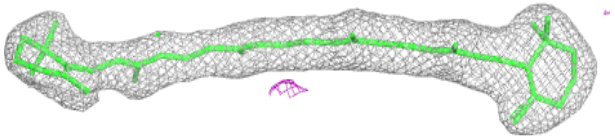


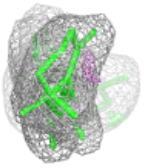


Electron density around BCR b 617:

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

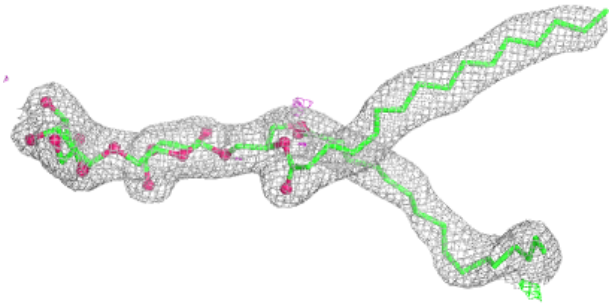


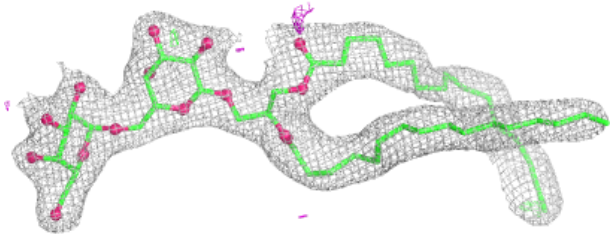


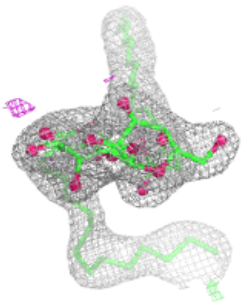


Electron density around DGD C 515:

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

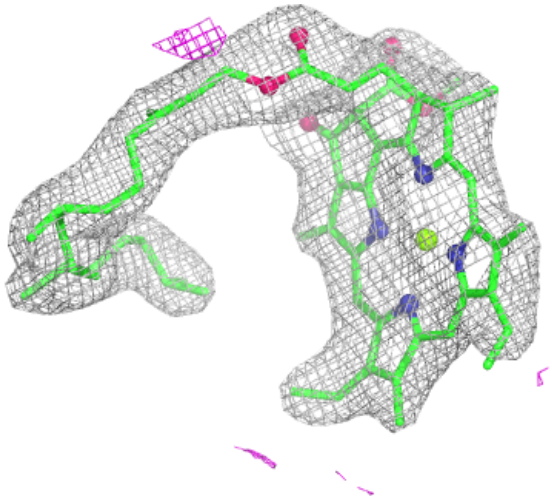


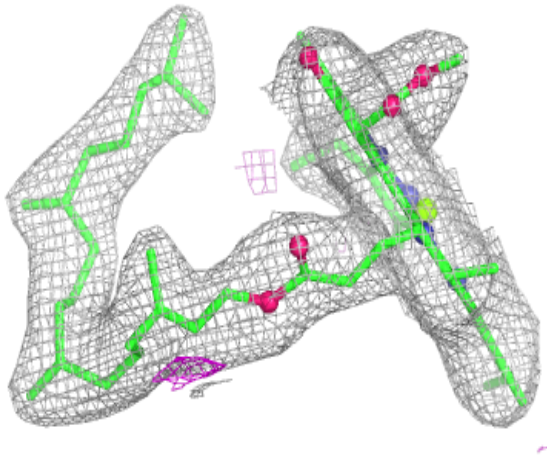


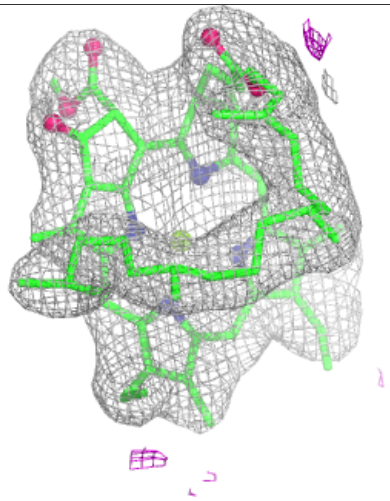


Electron density around CLA c 504:

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

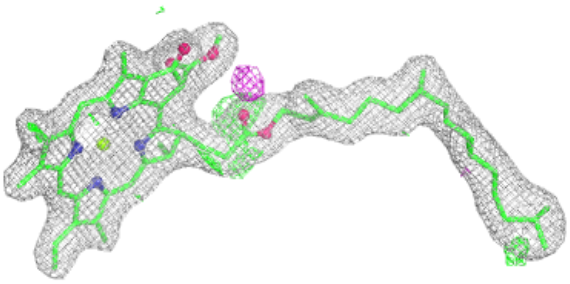


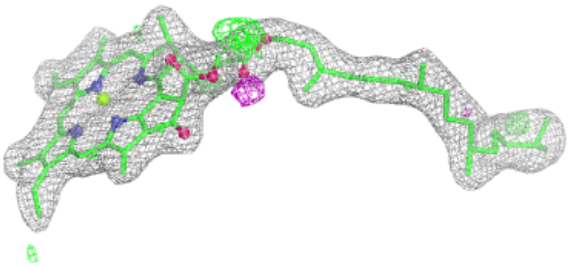


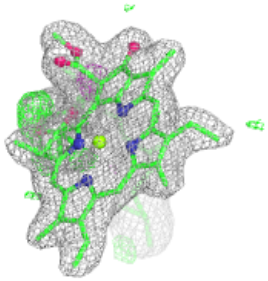


Electron density around CLA A 404:

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

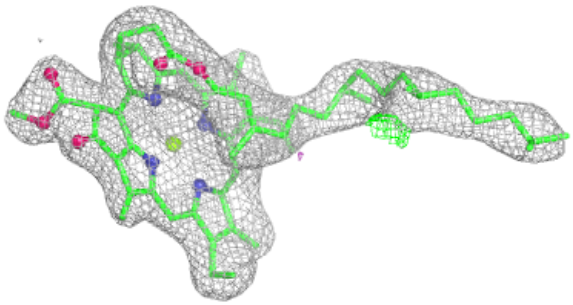


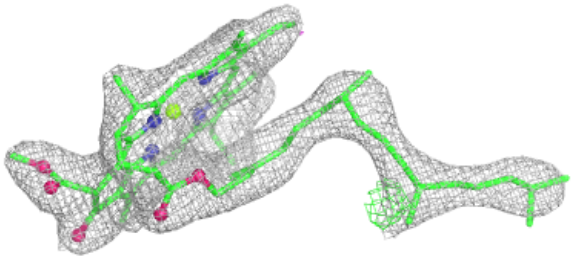


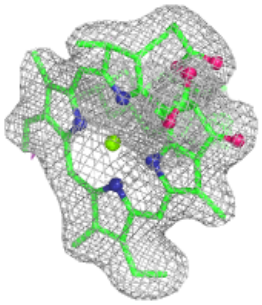


Electron density around CLA c 506:

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

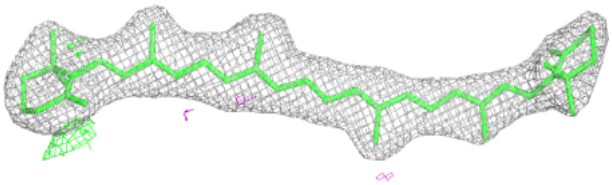


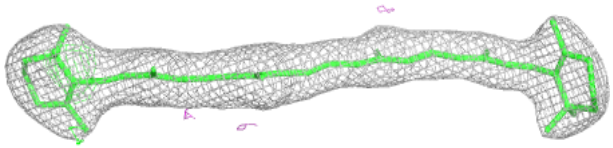


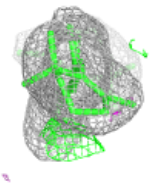


Electron density around BCR c 516:

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

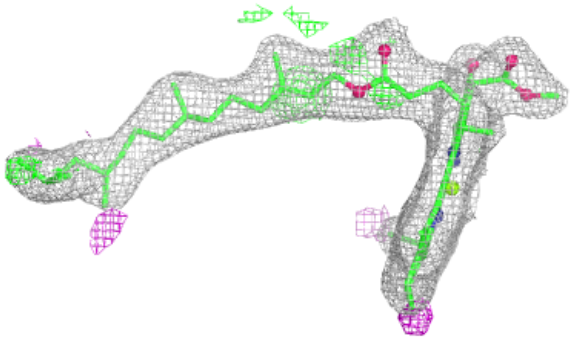


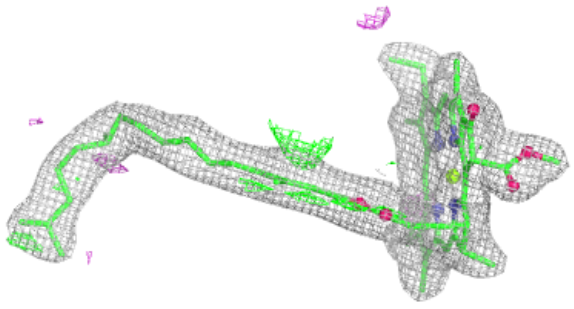


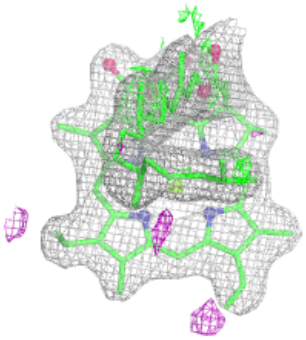


Electron density around CLA B 605:

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

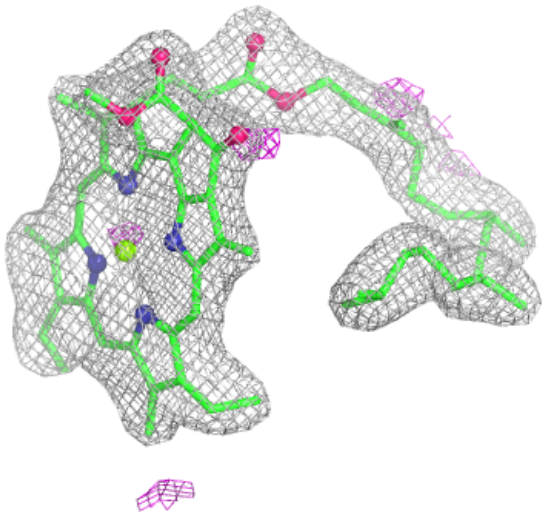


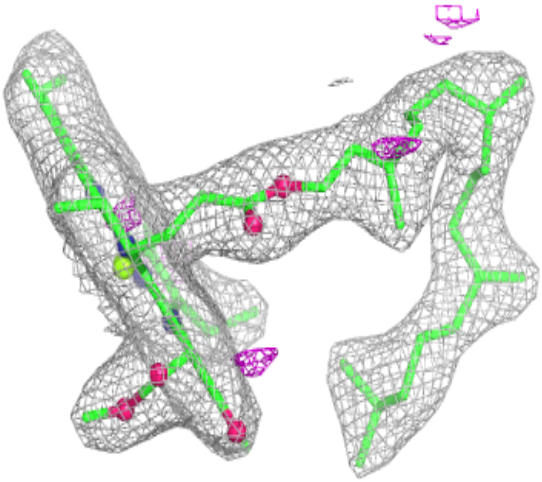


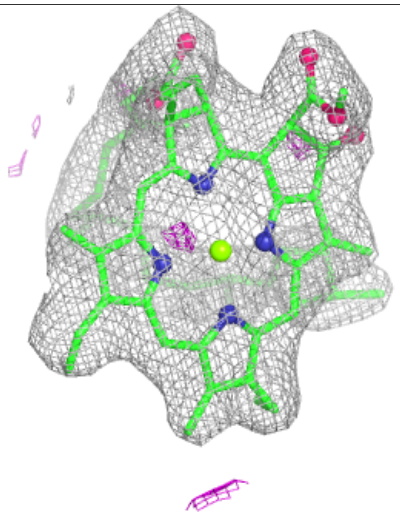


Electron density around CLA C 503:

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

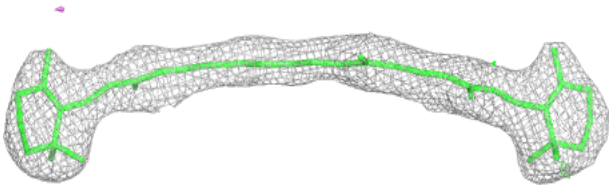


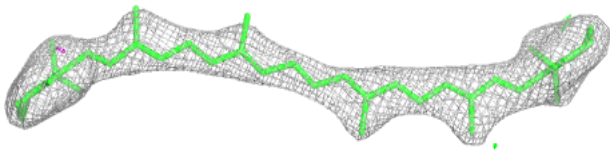


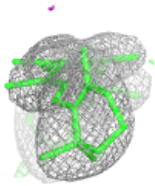


Electron density around BCR k 101:

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

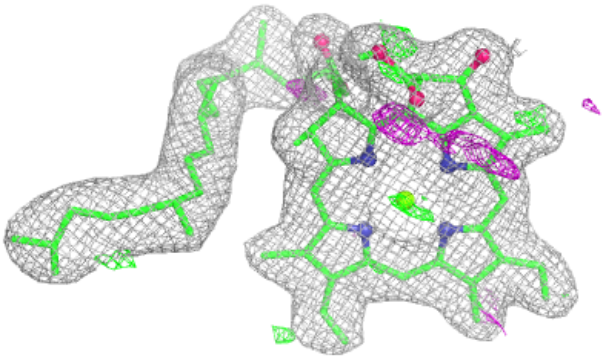


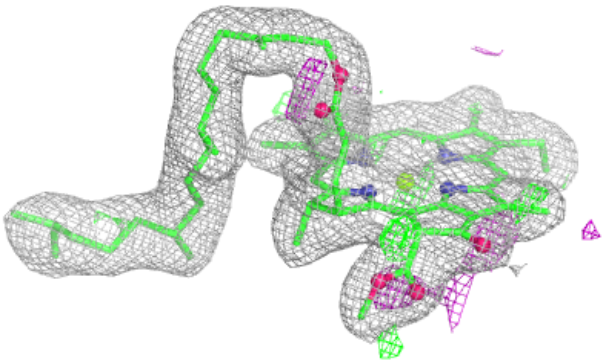


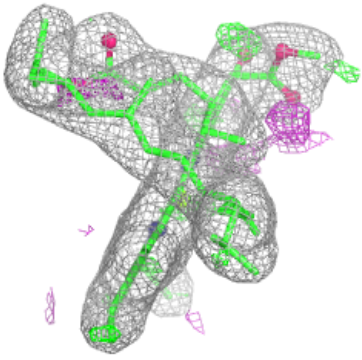


Electron density around CLA A 405:

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

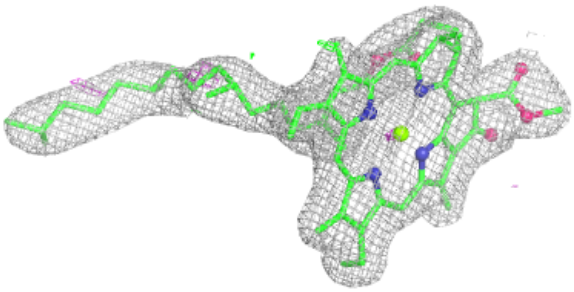


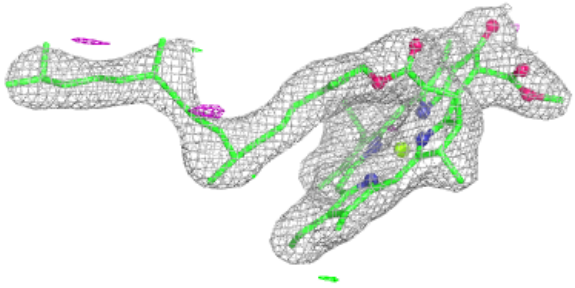


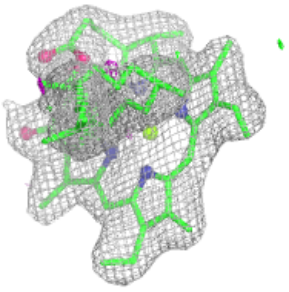


Electron density around CLA C 505:

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

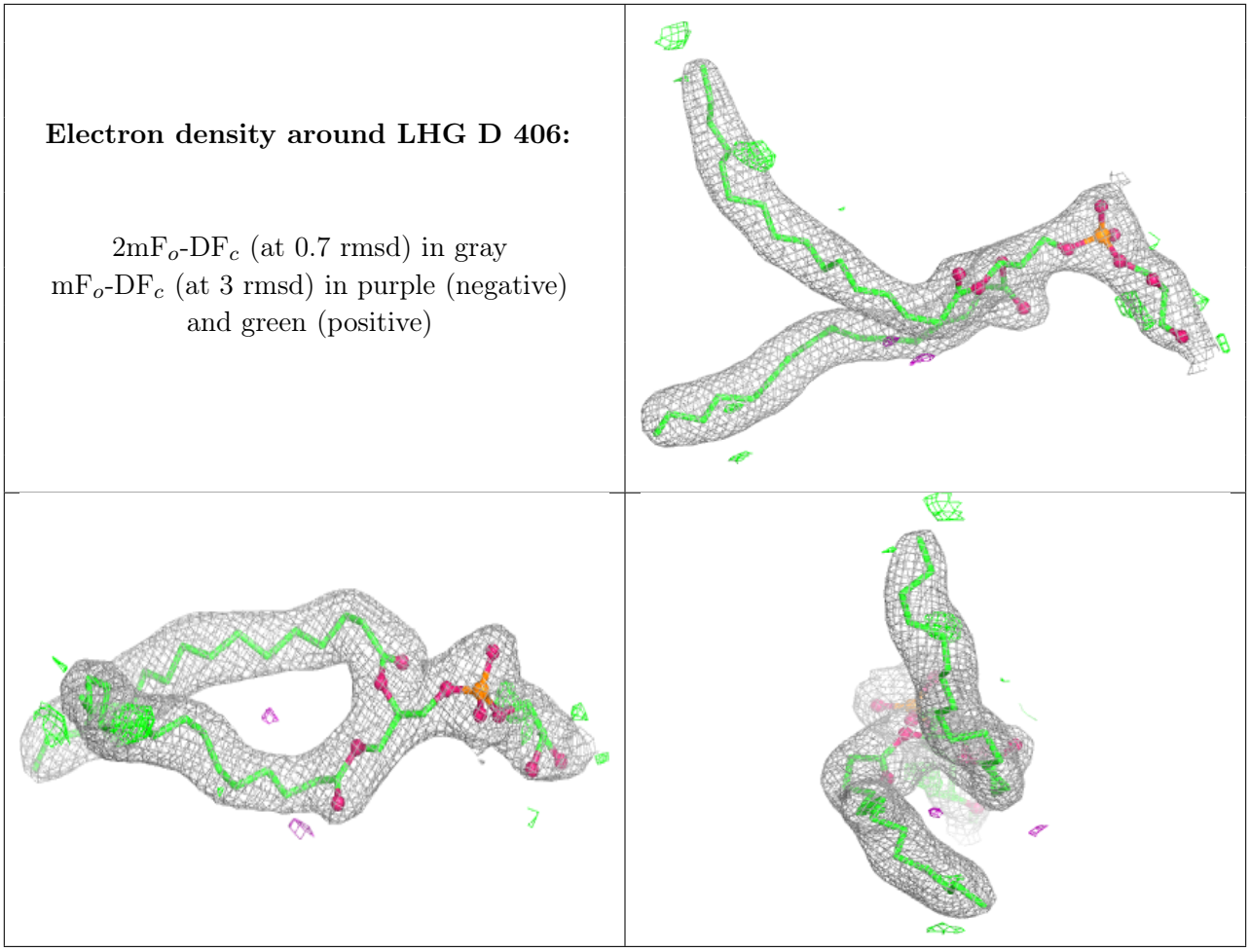






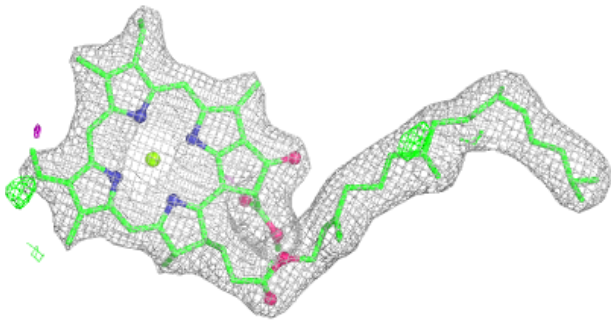
Electron density around LHG D 406:

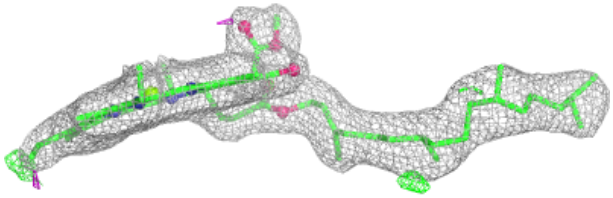
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

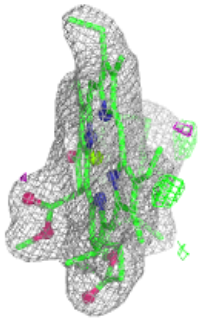


Electron density around CLA b 602:

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

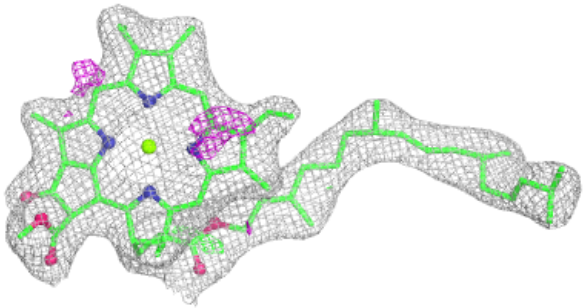


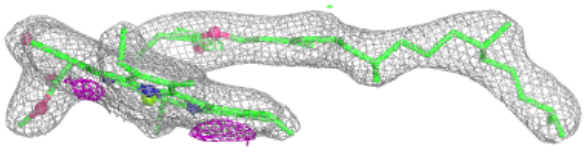


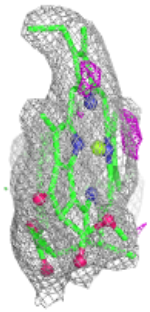


Electron density around CLA b 603:

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

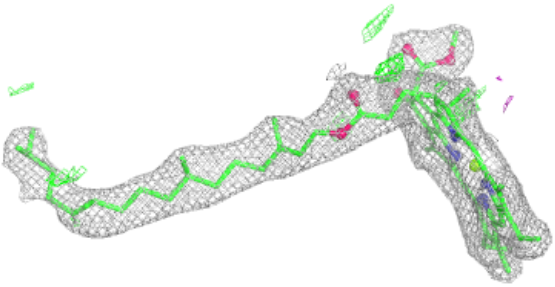


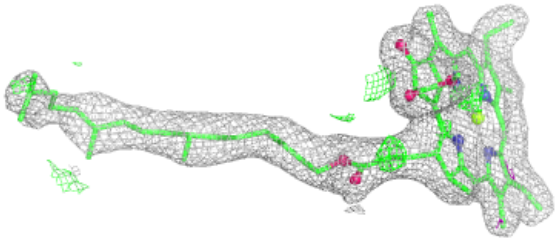


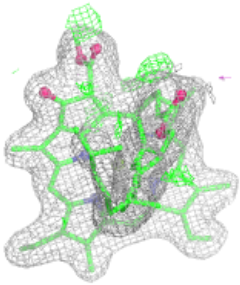


Electron density around CLA B 604:

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

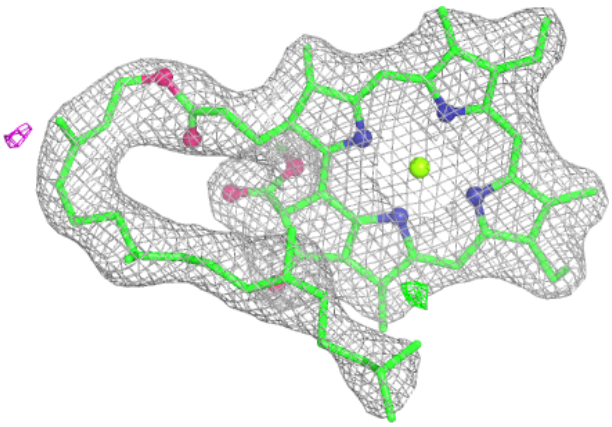


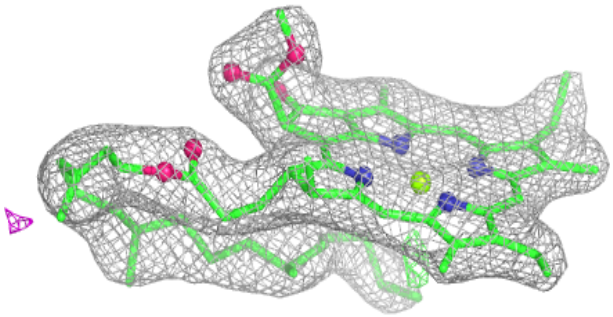


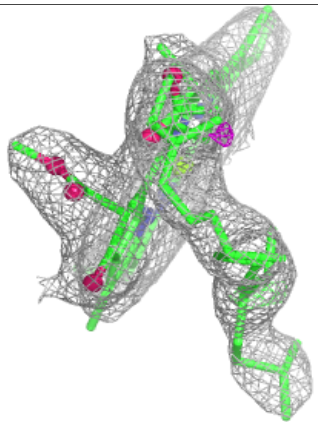


Electron density around CLA c 510:

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

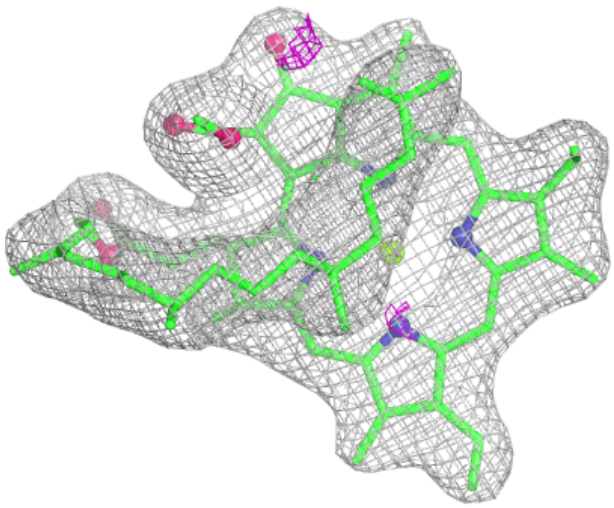


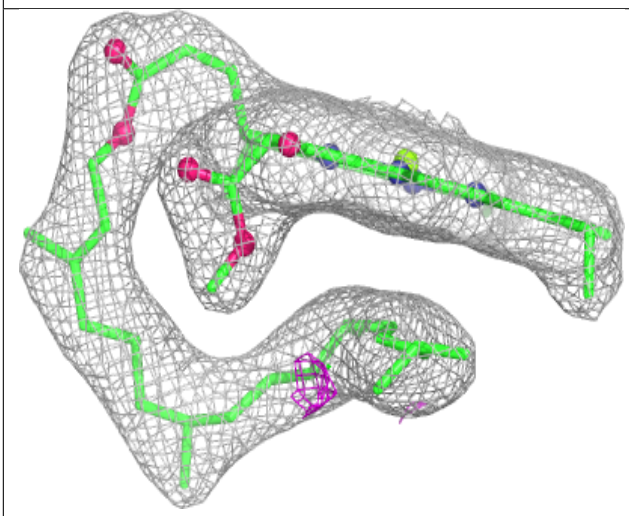


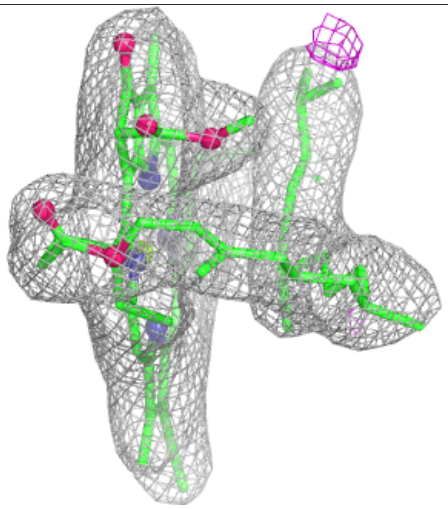


Electron density around CLA c 511:

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

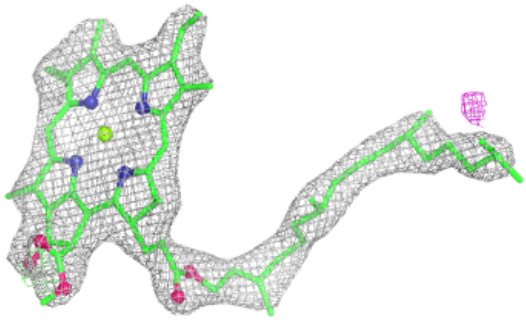


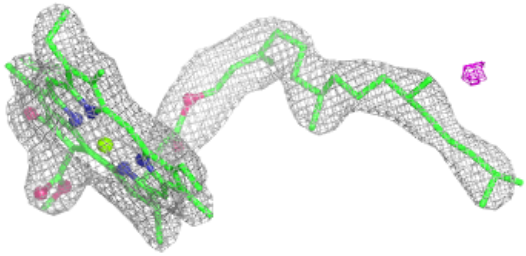


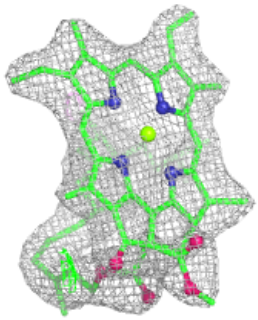


Electron density around CLA c 512:

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

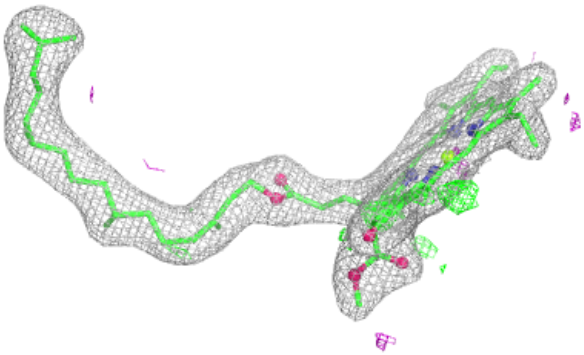


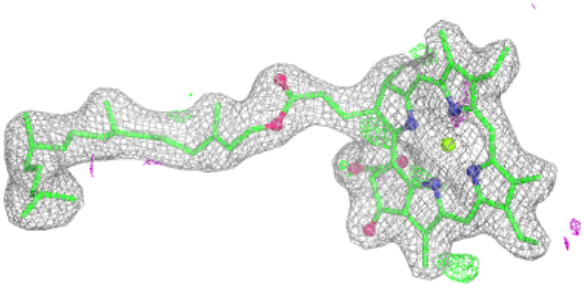


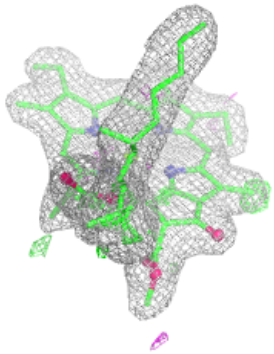


Electron density around CLA D 402:

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

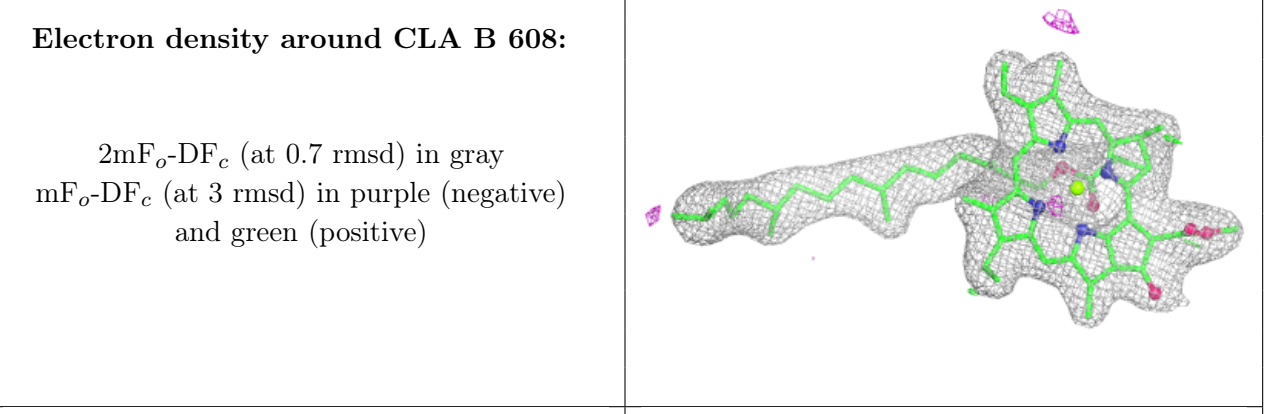






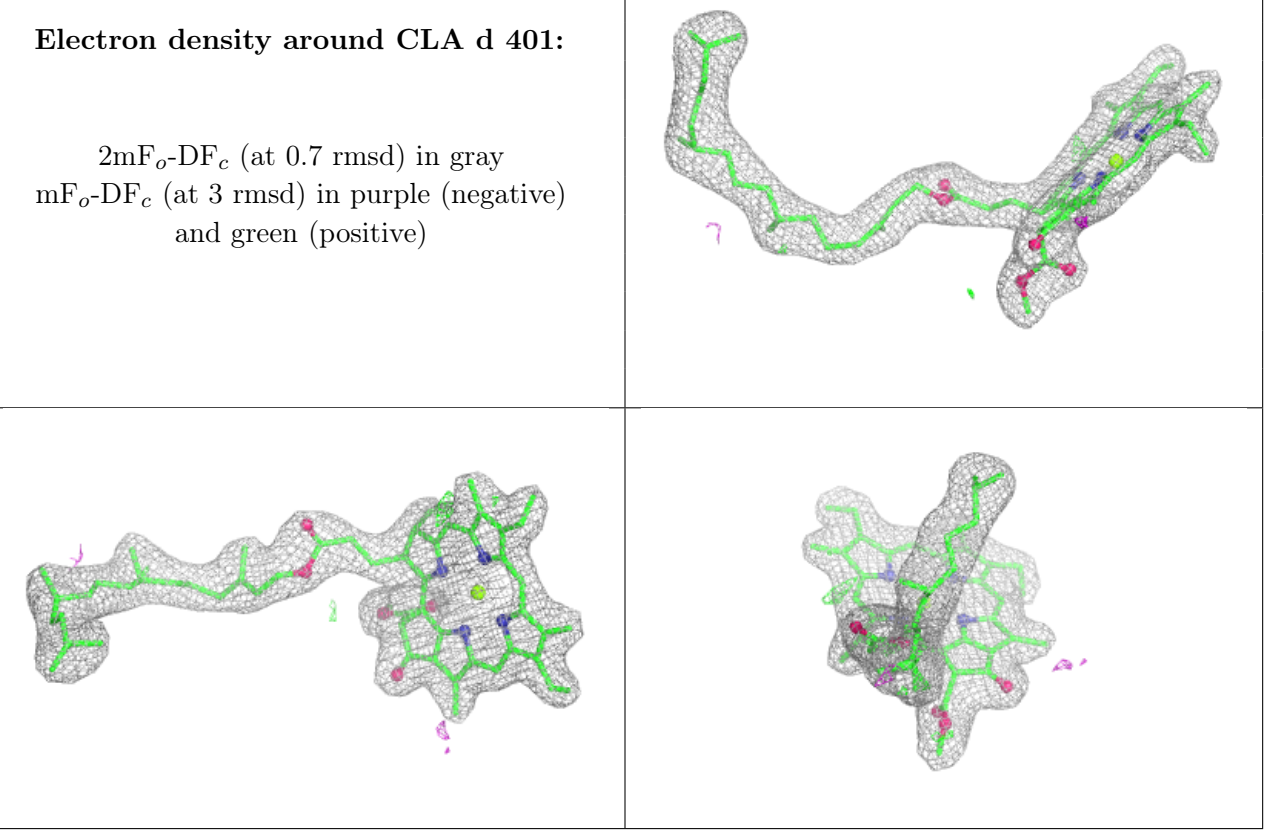
Electron density around CLA B 608:

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



Electron density around CLA d 401:

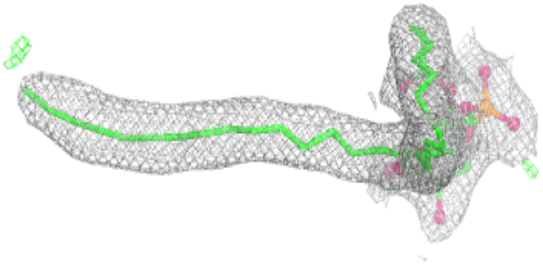
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

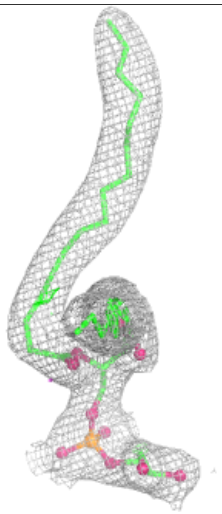


Electron density around LHG L 101:

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

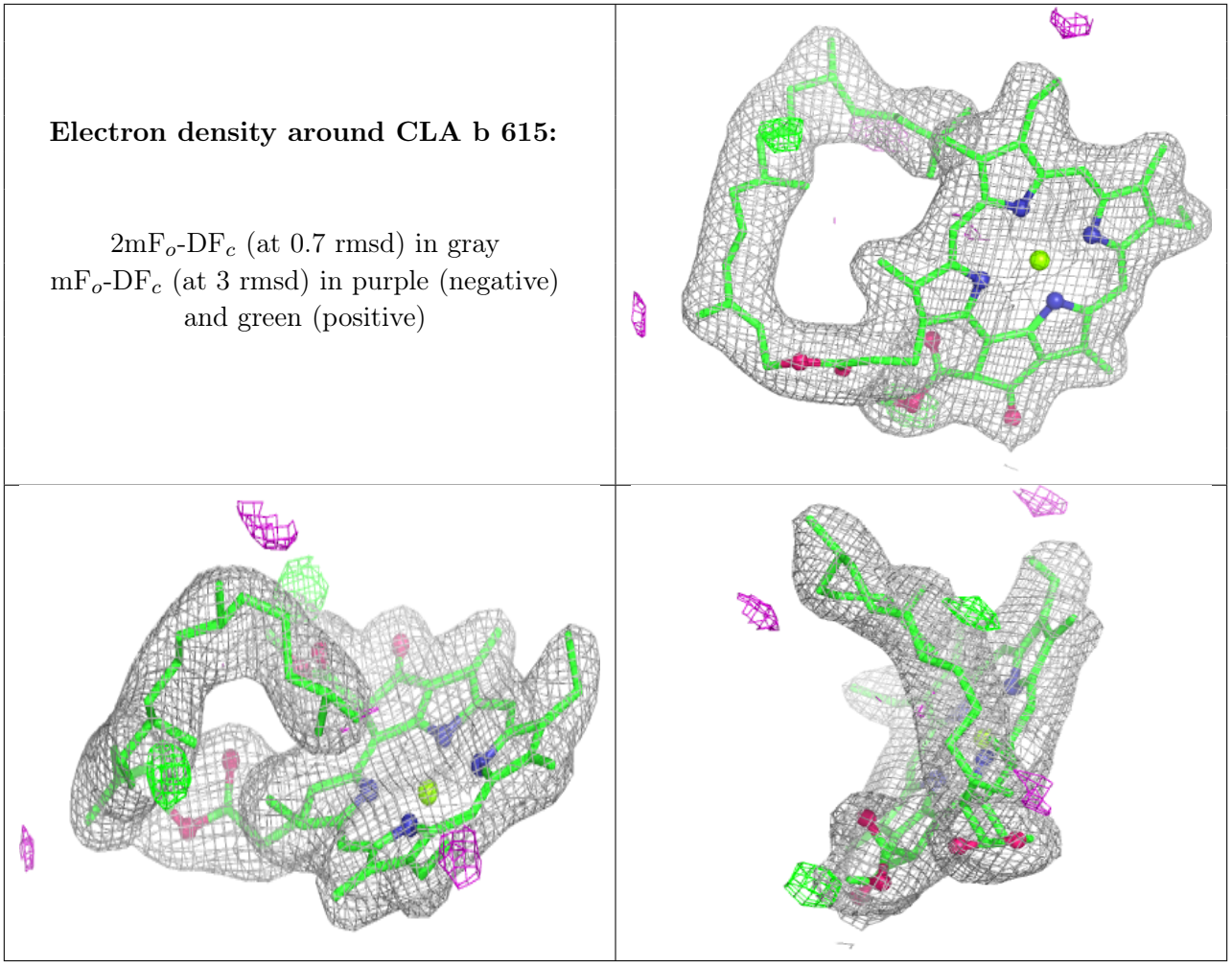






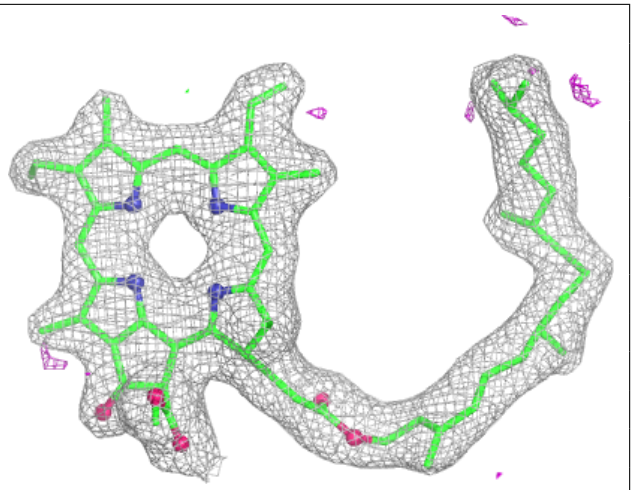
Electron density around CLA b 615:

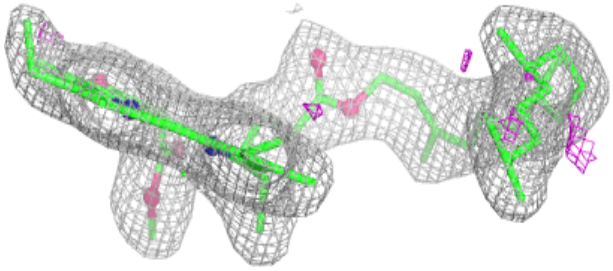
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

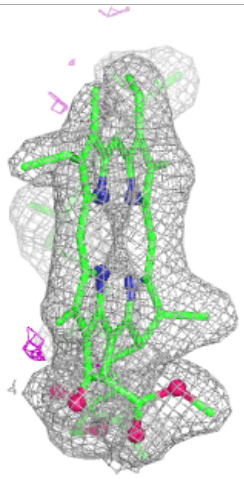


Electron density around PHO A 407:

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

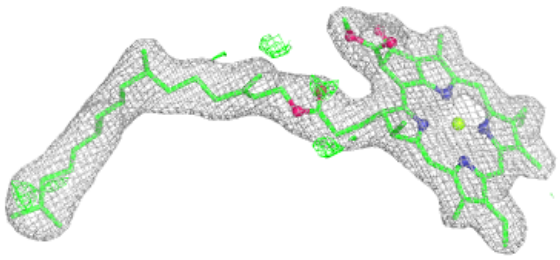


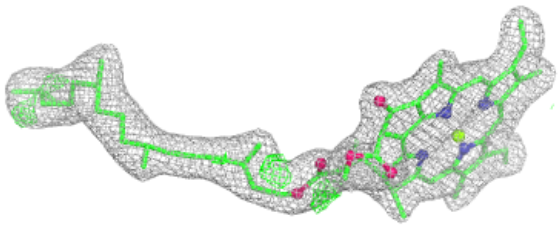


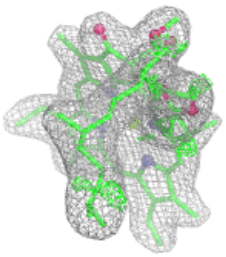


Electron density around CLA a 405:

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

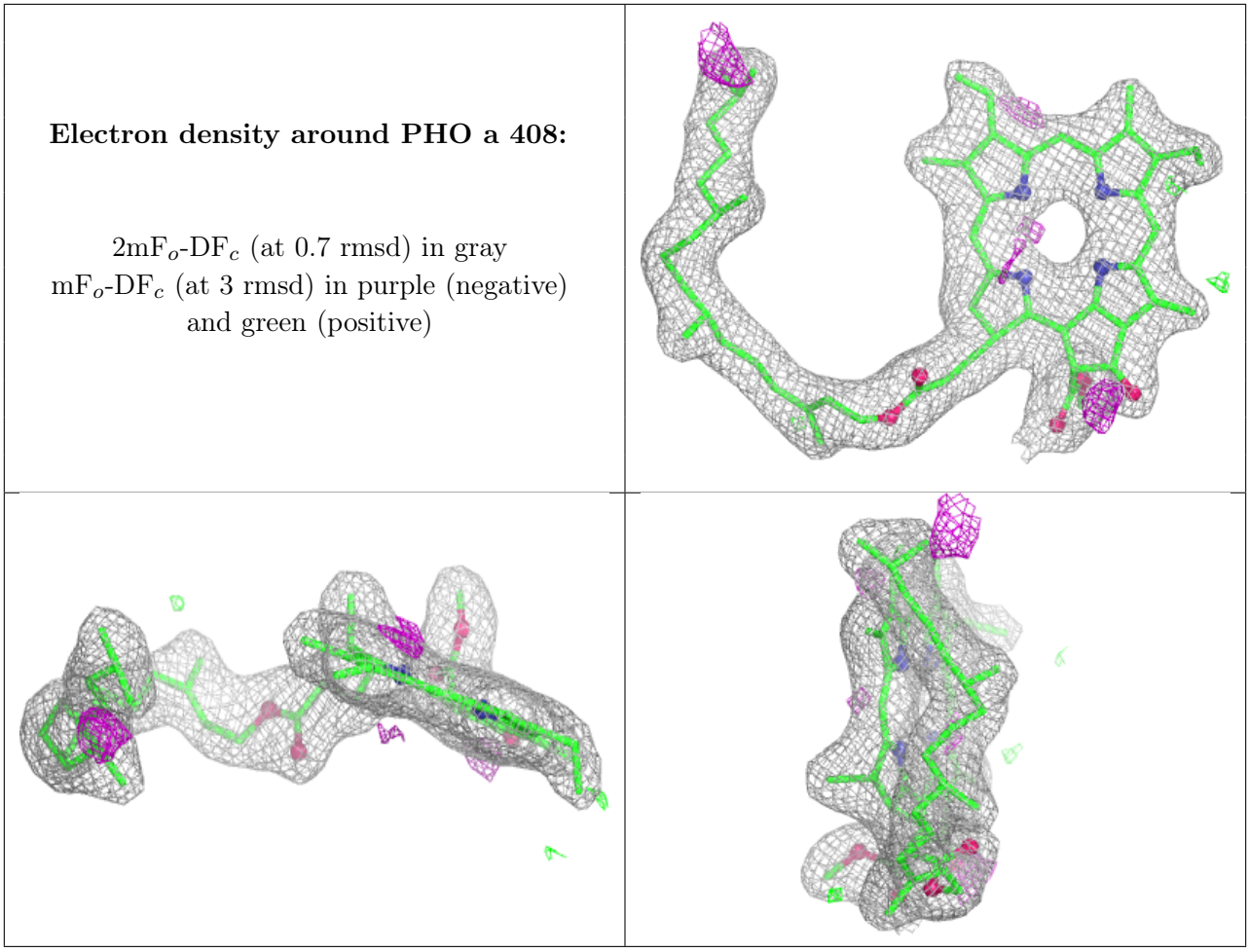






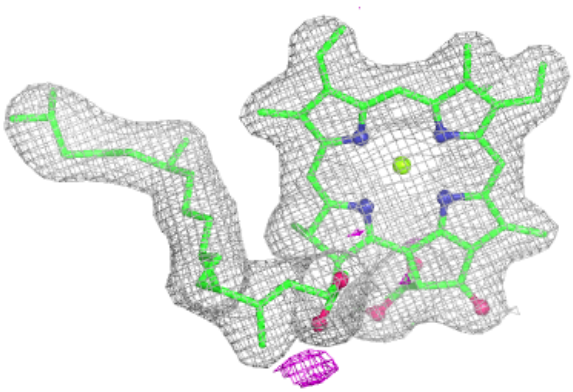
Electron density around PHO a 408:

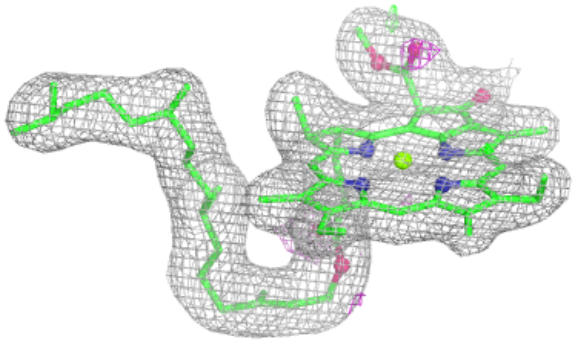
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

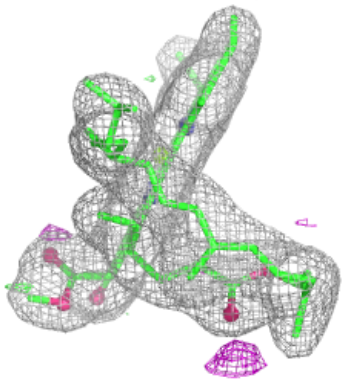


Electron density around CLA a 406:

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

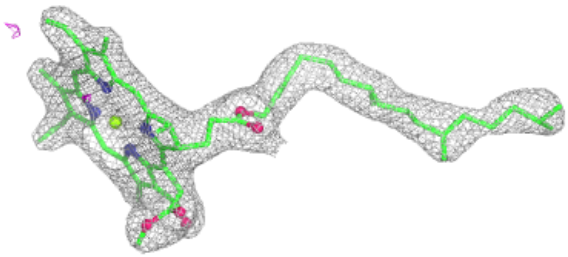


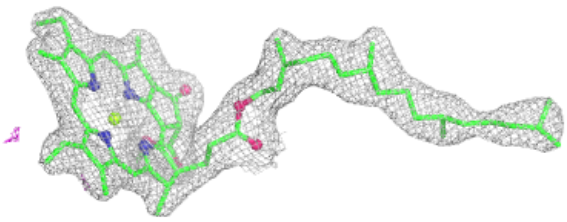


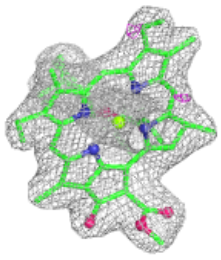


Electron density around CLA c 503:

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

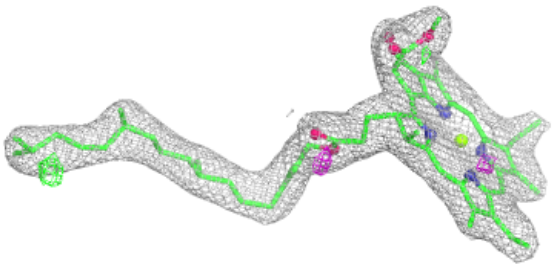


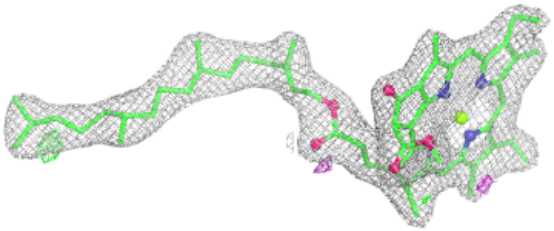


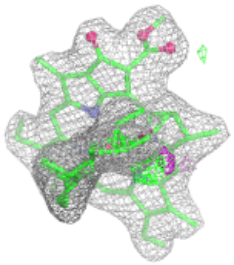


Electron density around CLA C 502:

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

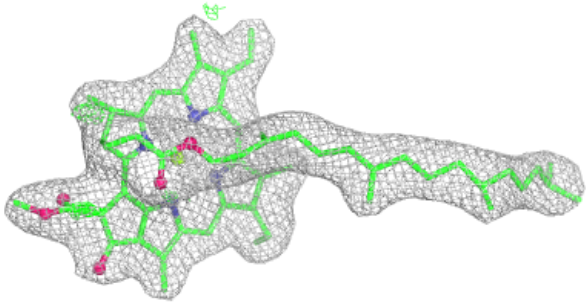


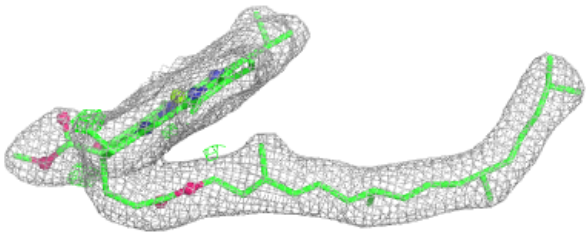


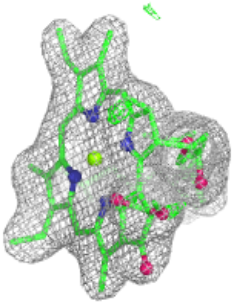


Electron density around CLA b 608:

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

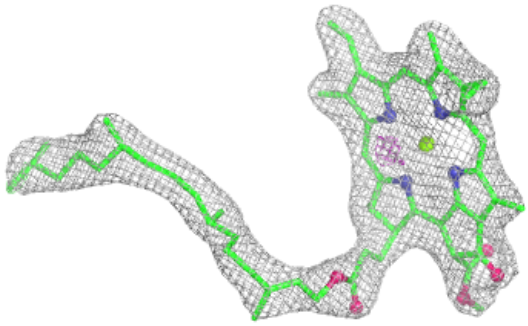


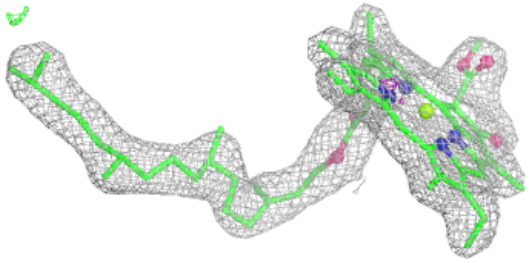


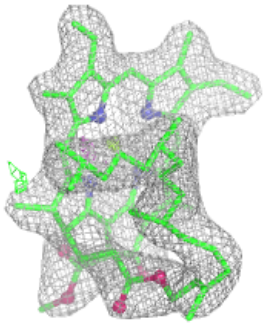


Electron density around CLA C 511:

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

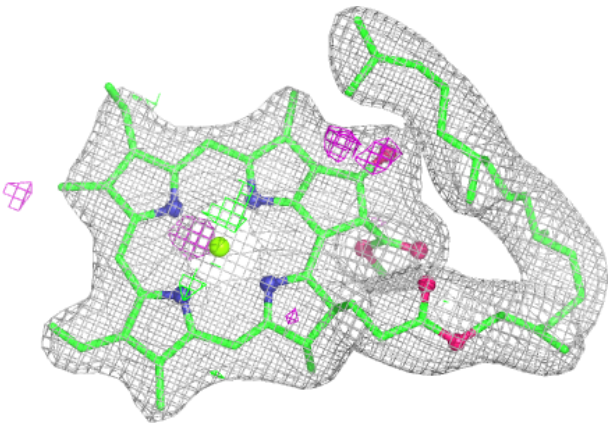


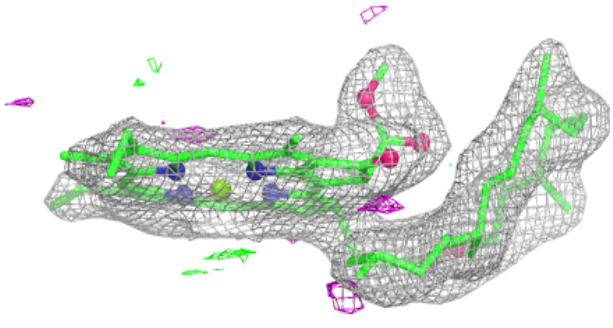


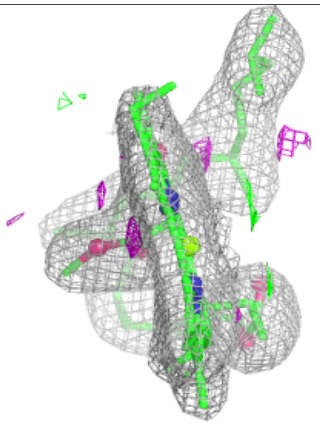


Electron density around CLA b 610:

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

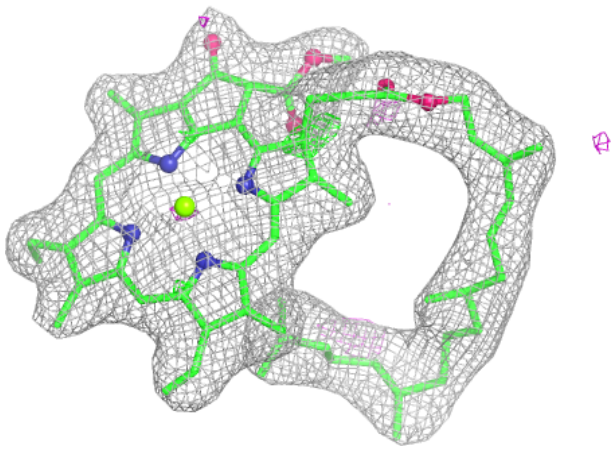


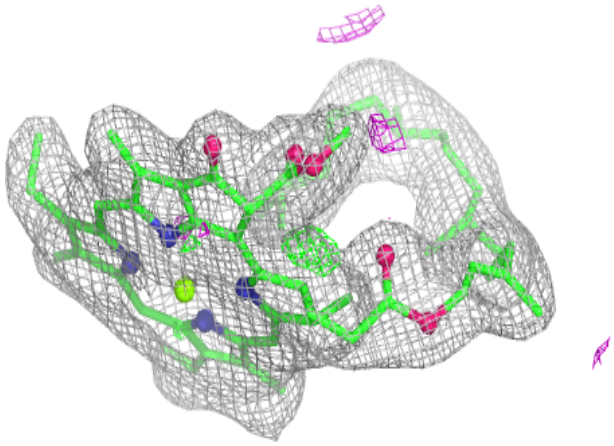


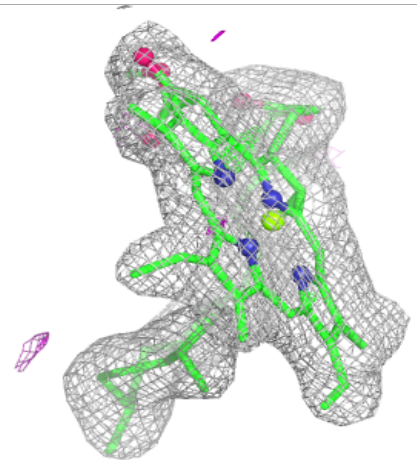


Electron density around CLA B 615:

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

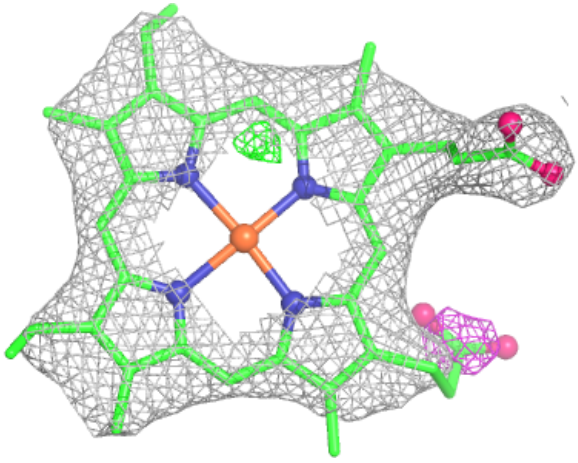


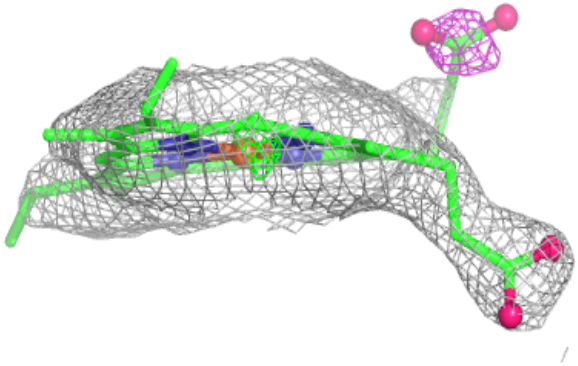


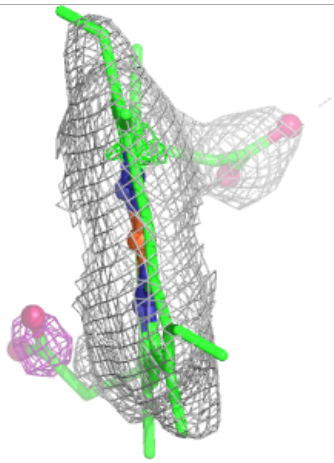


Electron density around HEM f 101:

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

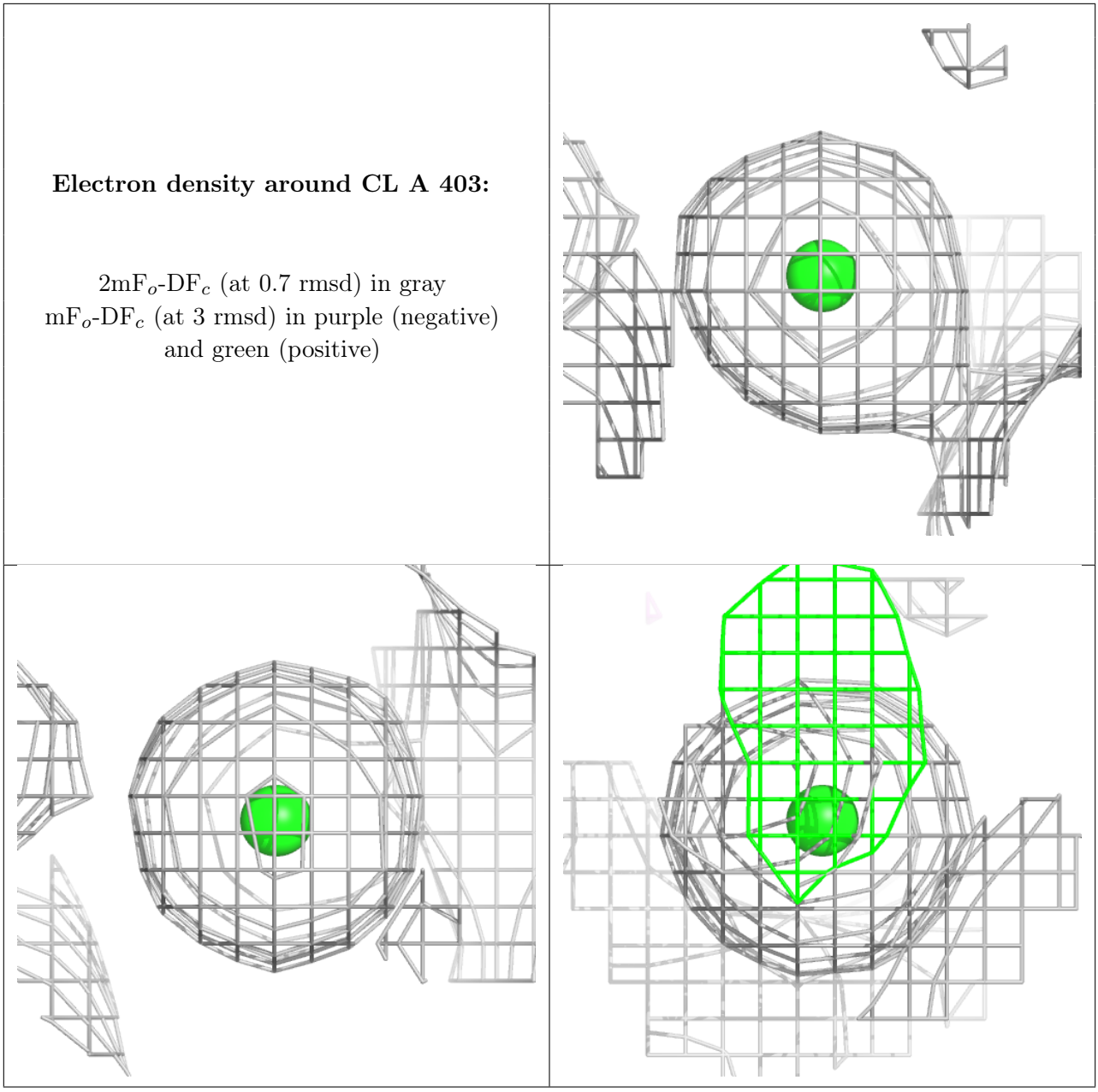






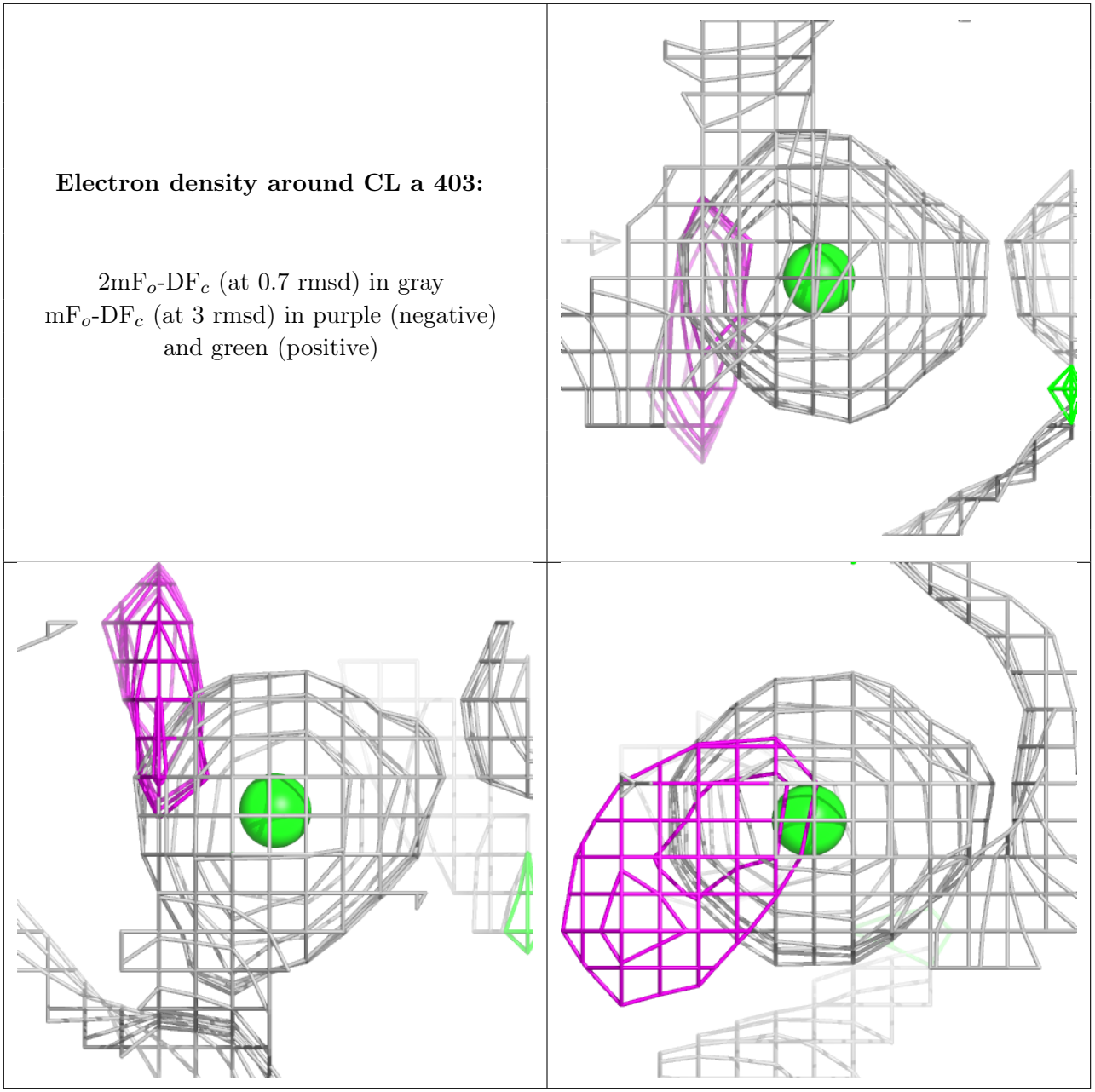
Electron density around CL A 403:

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



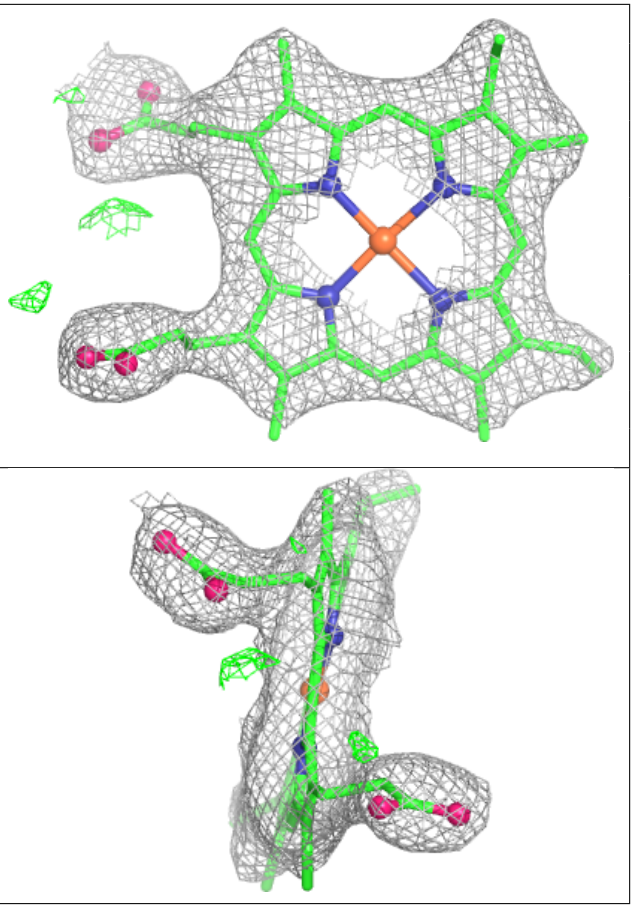
Electron density around CL a 403:

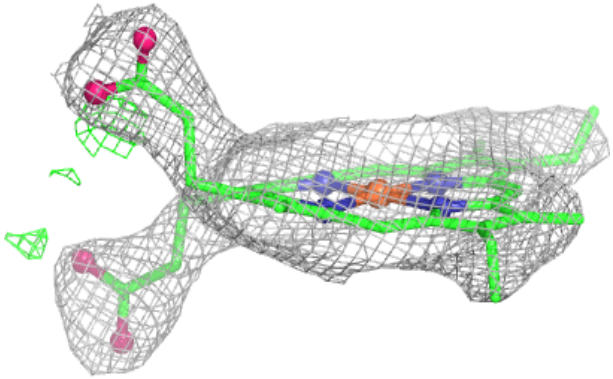
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around HEM F 102:

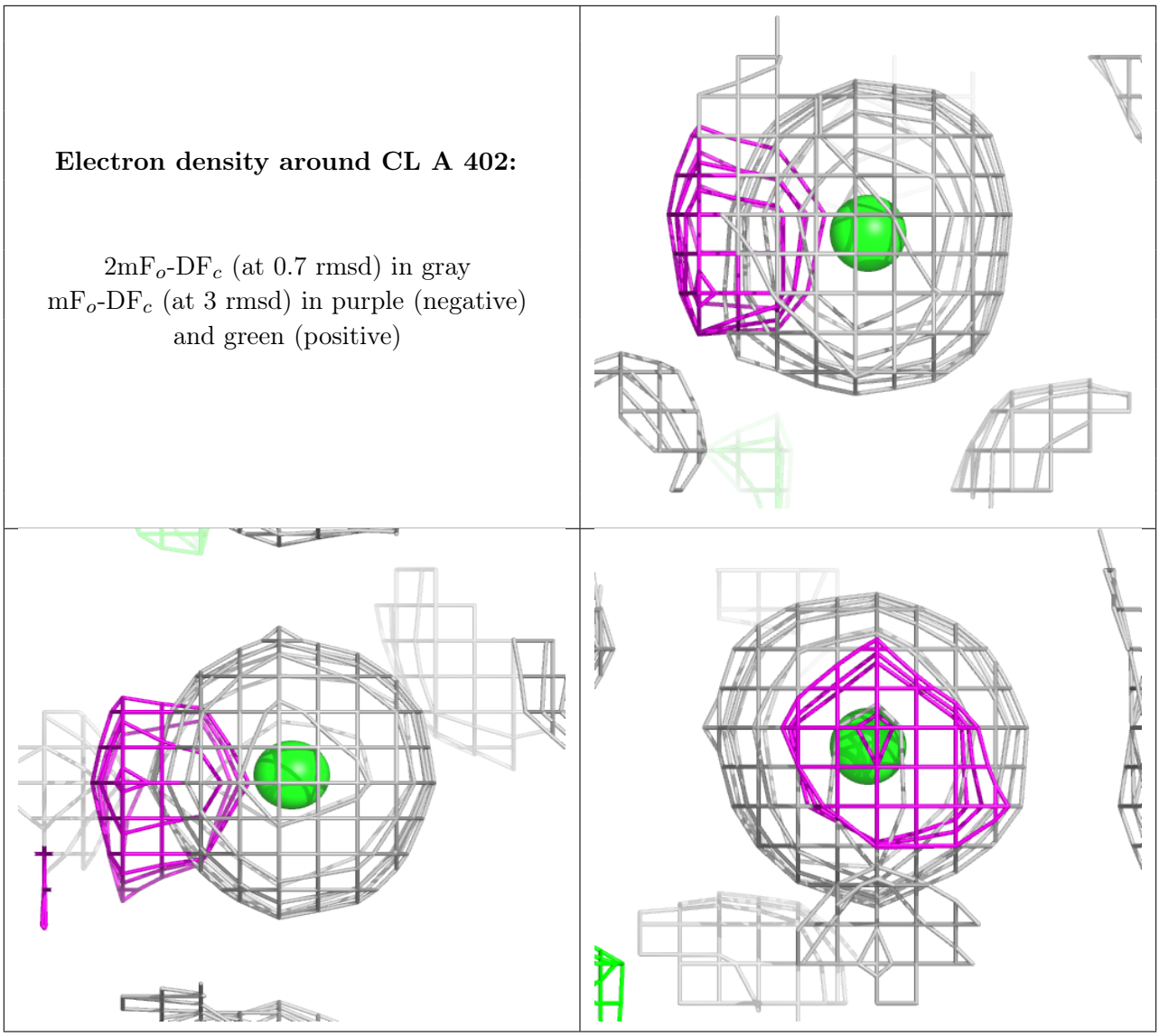
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





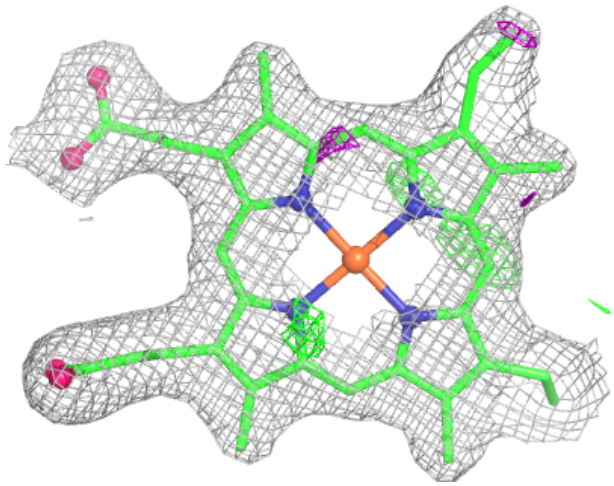
Electron density around CL A 402:

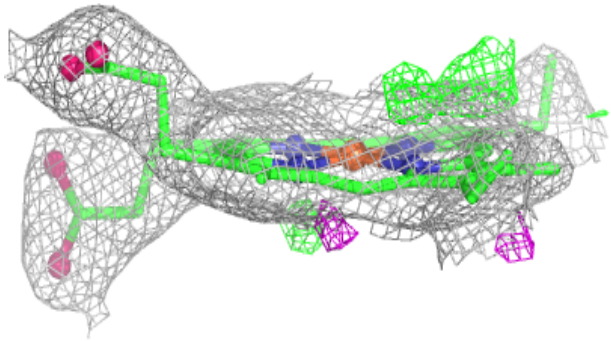
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

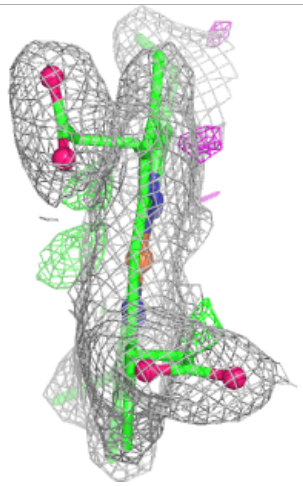


Electron density around HEC V 201:

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

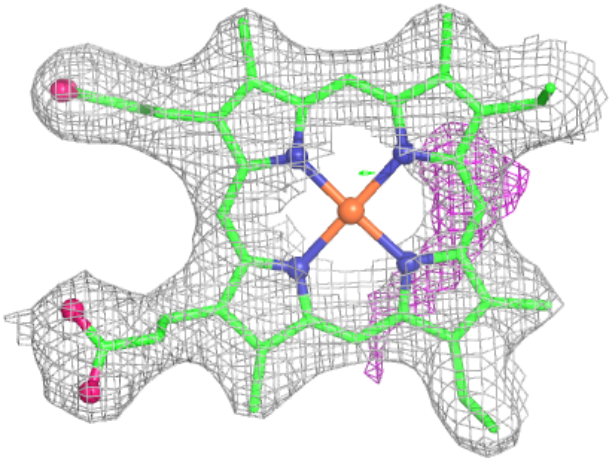


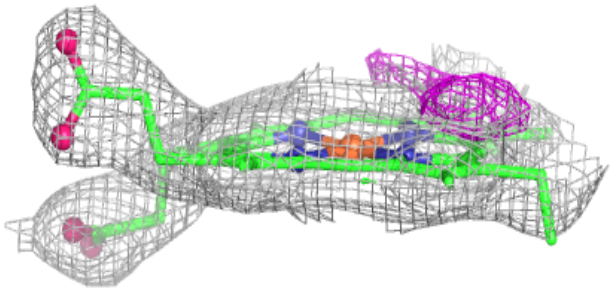




Electron density around HEC v 201:

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

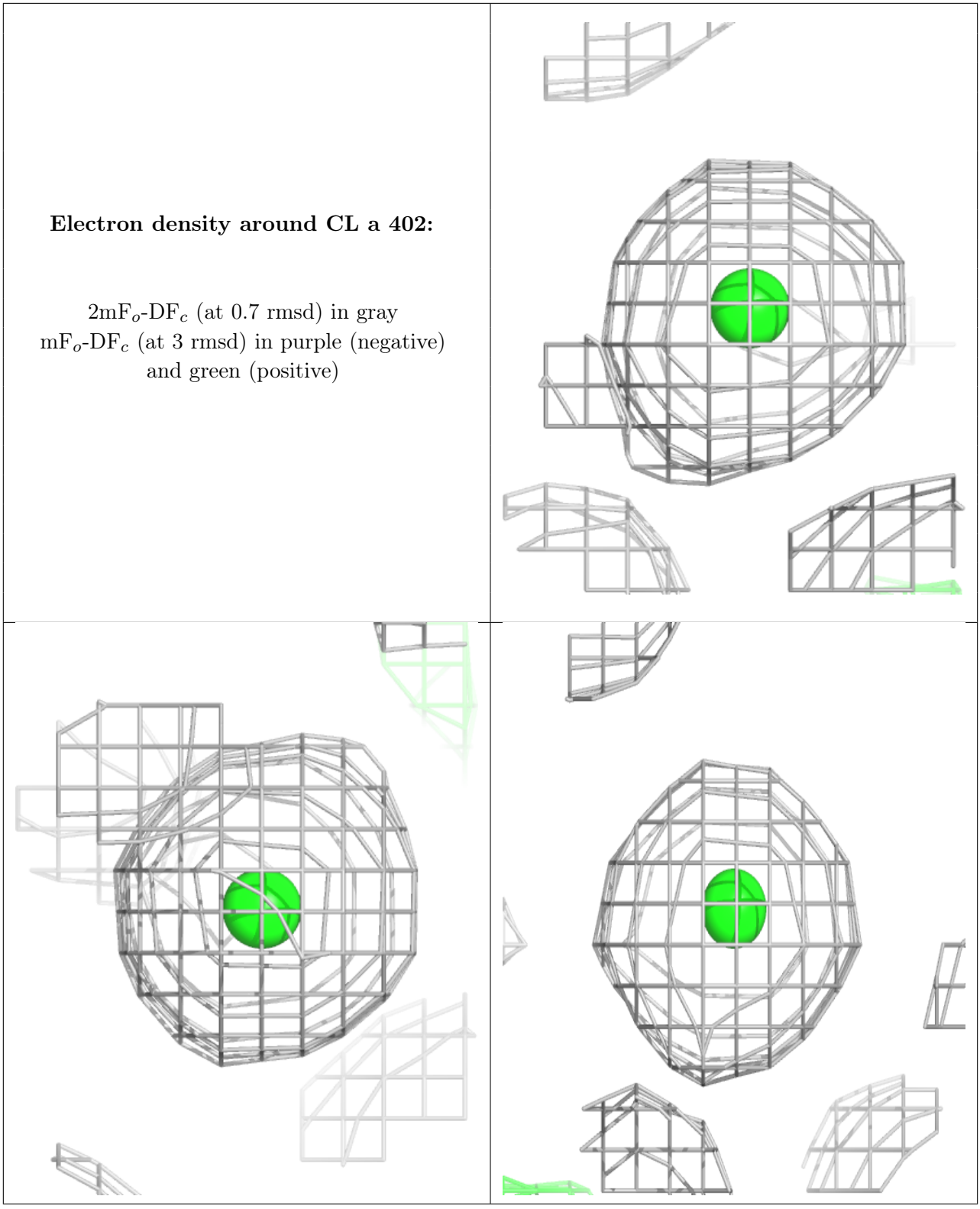






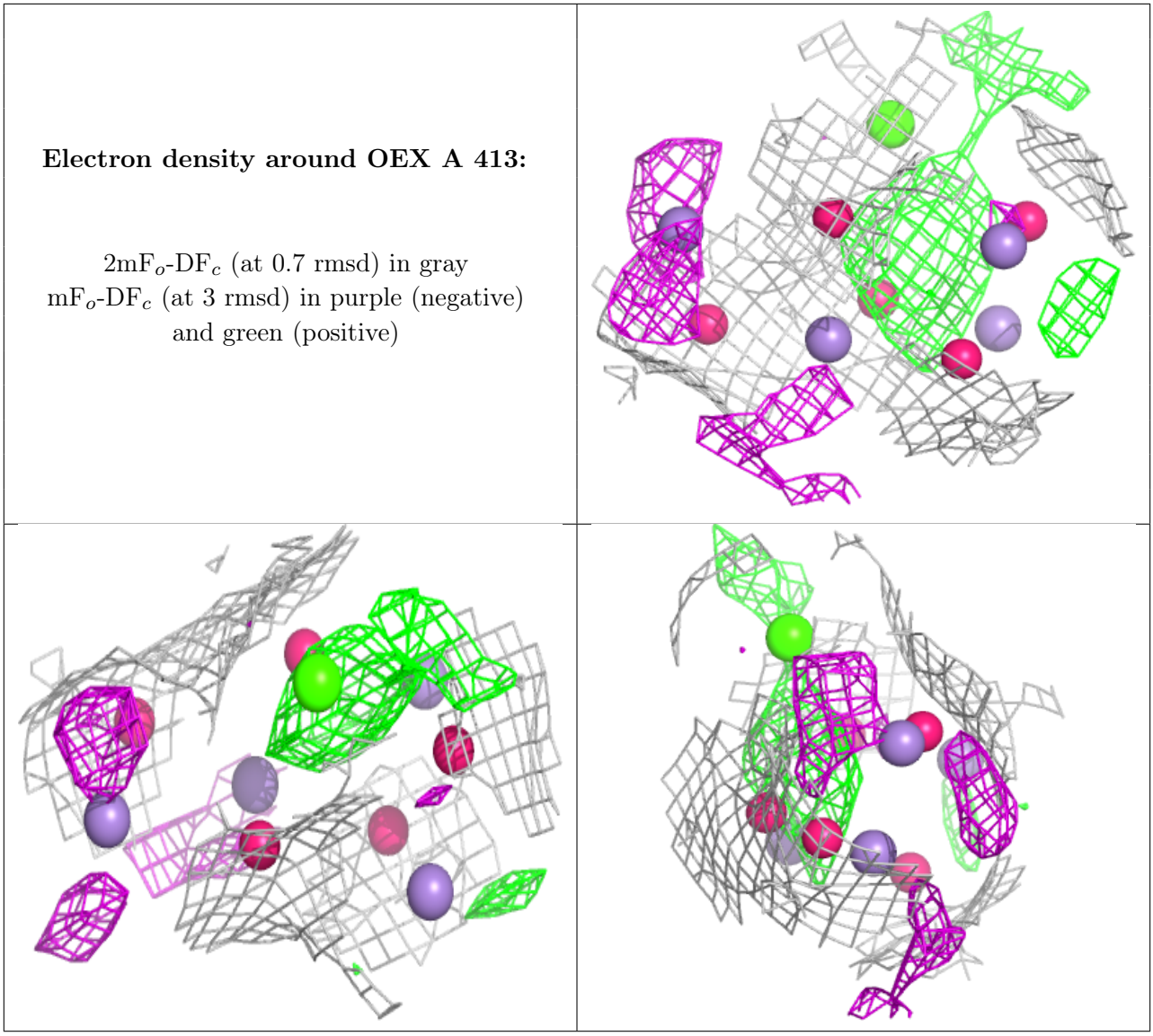
Electron density around CL a 402:

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



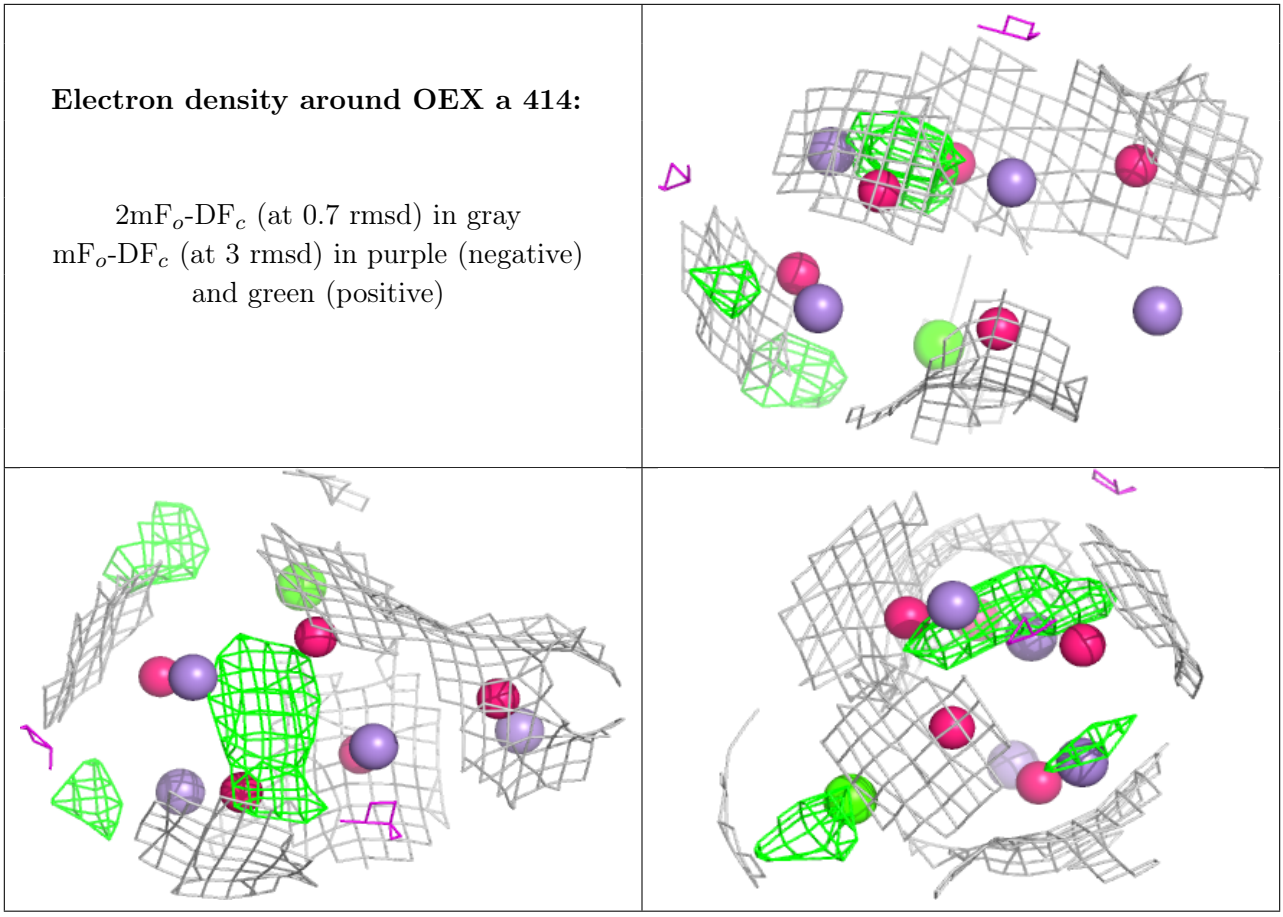
Electron density around OEX A 413:

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



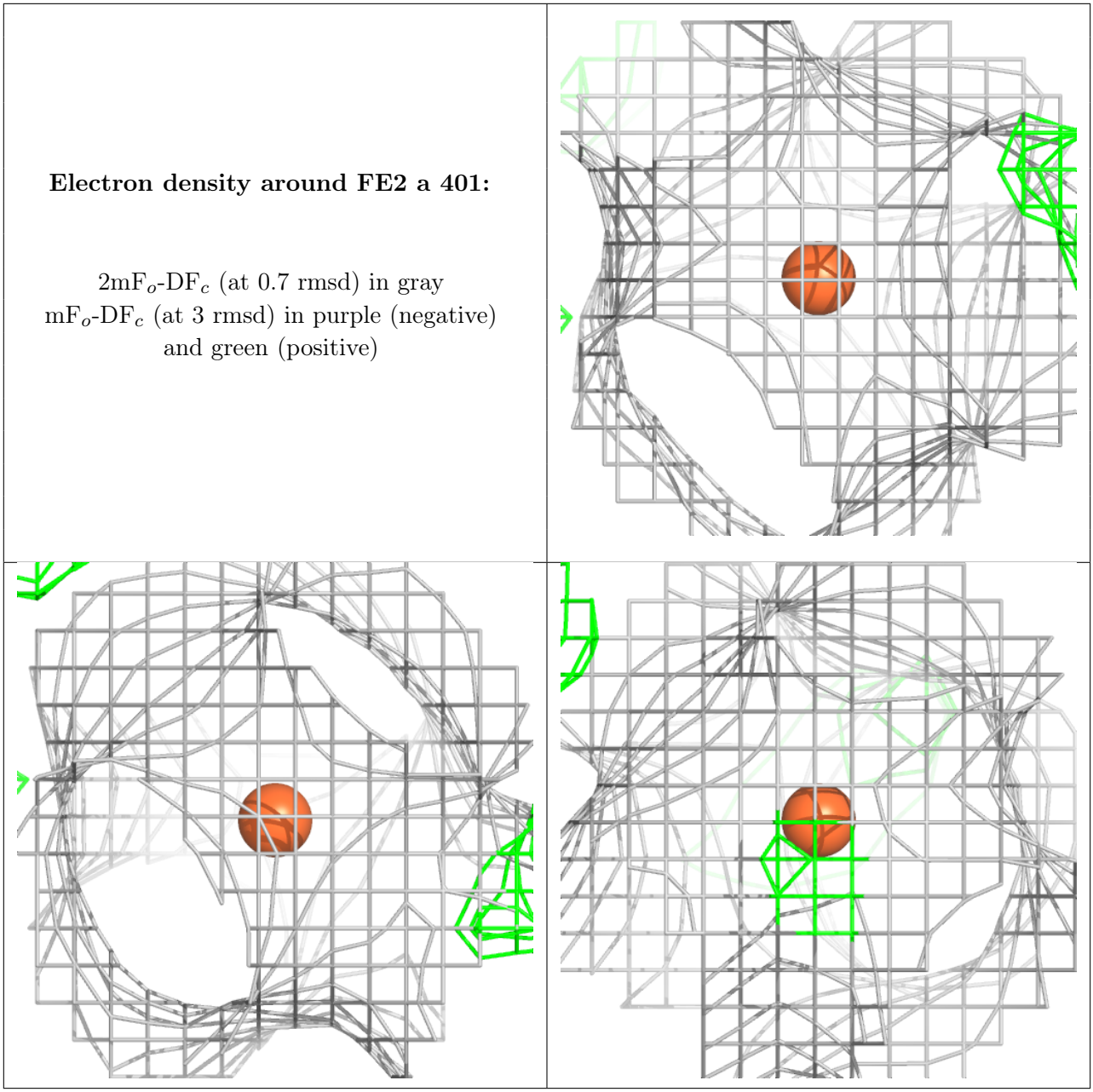
Electron density around OEX a 414:

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



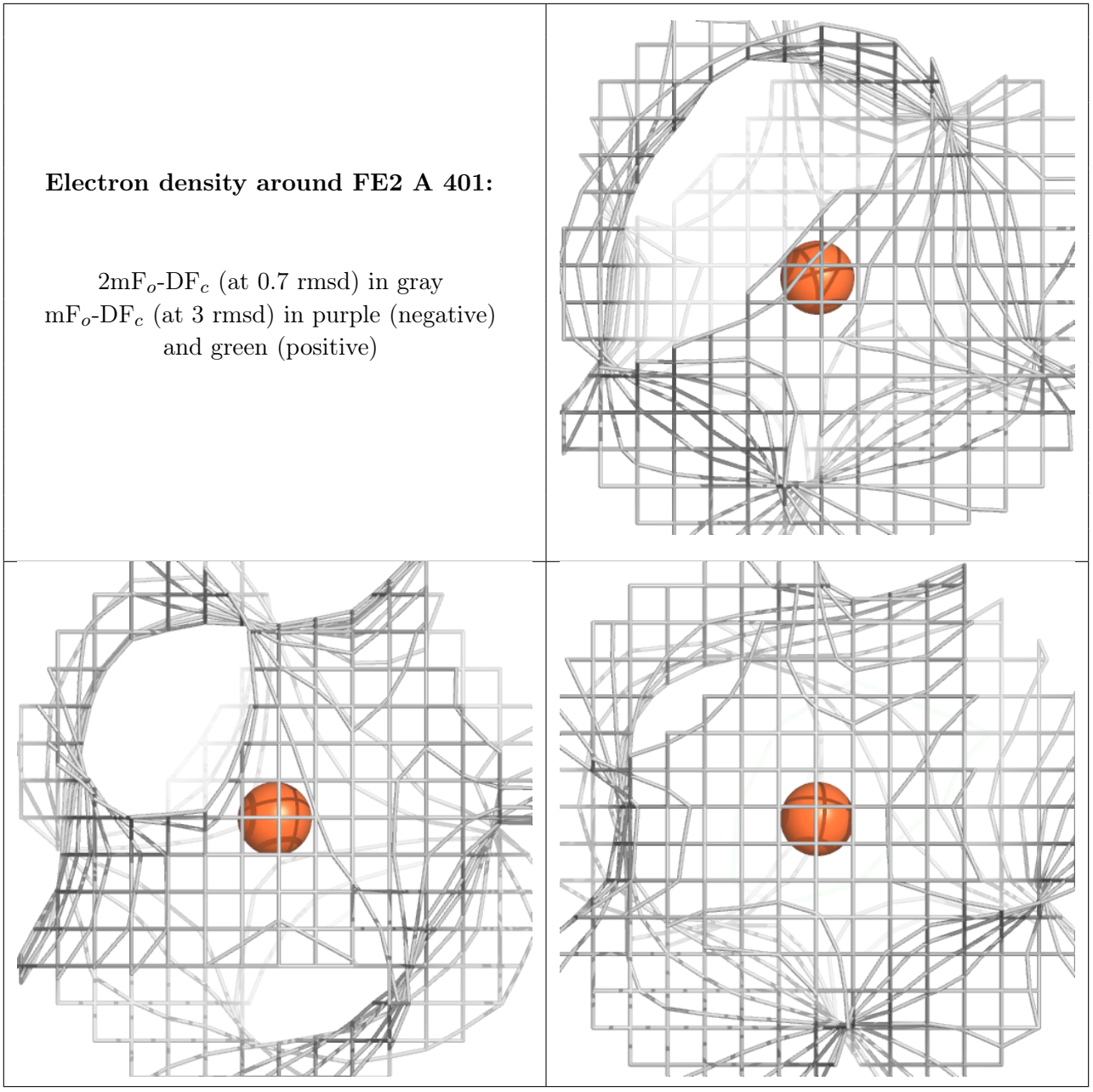
Electron density around FE2 a 401:

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



Electron density around FE2 A 401:

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



6.5 Other polymers (i)

There are no such residues in this entry.