Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:37 AM UTC

PDB ID	:	8IR6 / pdb_00008ir6
Title	:	XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 20-nanosecond delay
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.20 Å(reported)

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

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

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

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

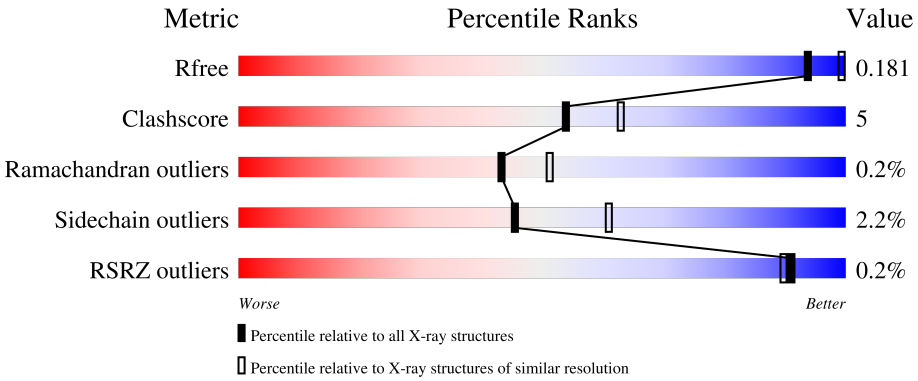
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



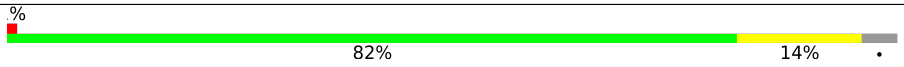
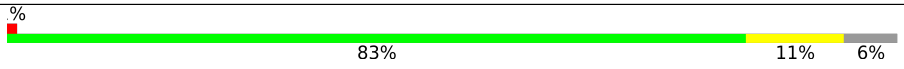
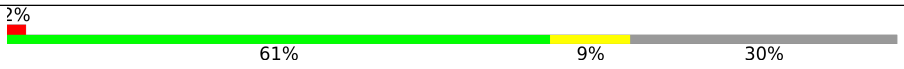
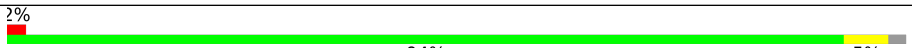
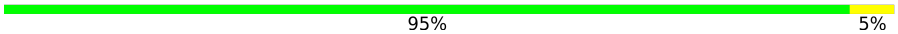
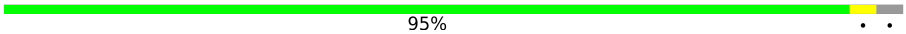
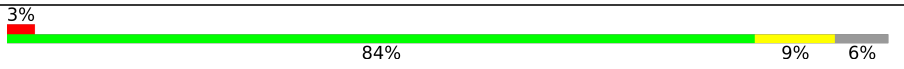
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 6% ·
1	a	344	89% 8% ·
2	B	505	93% 6%
2	b	505	91% 9%
3	C	455	91% 8% ·

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

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Mol	Chain	Length	Quality of chain
16	V	137	97%
16	v	137	91% 9%
17	X	40	90% 5% 5%
17	x	40	90% 5% 5%
18	Y	30	3% 83% 13%
18	y	30	60% 33%
19	Z	62	87% 11%
19	z	62	77% 21%
20	R	34	3% 68% 32%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	404[A]	X	-	-	-
23	CLA	A	404[B]	X	-	-	-
23	CLA	A	405[B]	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	601	X	-	-	-
23	CLA	B	602	X	-	-	-
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	402[A]	X	-	-	-
23	CLA	D	402[B]	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	a	404[A]	X	-	-	-
23	CLA	a	404[B]	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	b	601	X	-	-	-
23	CLA	b	602	X	-	-	-
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	c	501	X	-	-	-
23	CLA	c	502	X	-	-	-
23	CLA	c	503	X	-	-	-
23	CLA	c	504	X	-	-	-
23	CLA	c	505	X	-	-	-
23	CLA	c	506	X	-	-	-
23	CLA	c	507	X	-	-	-
23	CLA	c	508	X	-	-	-
23	CLA	c	509	X	-	-	-
23	CLA	c	510	X	-	-	-
23	CLA	c	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	c	512	X	-	-	-
23	CLA	c	513	X	-	-	-
23	CLA	d	402[A]	X	-	-	-
23	CLA	d	402[B]	X	-	-	-
23	CLA	d	404[A]	X	-	-	-
23	CLA	d	404[B]	X	-	-	-
23	CLA	d	405	X	-	-	-
27	GOL	A	418	-	-	X	-
27	GOL	a	418	-	-	X	-

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 62674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	222	0
			4338	2836	717	760	25			
1	a	334	Total	C	N	O	S	0	220	0
			4318	2821	715	757	25			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	22	0
			4166	2735	694	724	13			
2	b	504	Total	C	N	O	S	0	19	0
			4134	2718	687	716	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	99	0
			4272	2796	715	743	18			
3	c	455	Total	C	N	O	S	0	101	0
			4316	2827	720	751	18			

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	115	0
			3625	2390	597	623	15			
4	d	341	Total	C	N	O	S	0	119	0
			3658	2412	605	626	15			

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	96	Total	C	N	O	0	4	0
			800	508	133	159			
15	u	97	Total	C	N	O	0	5	0
			815	519	135	161			

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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

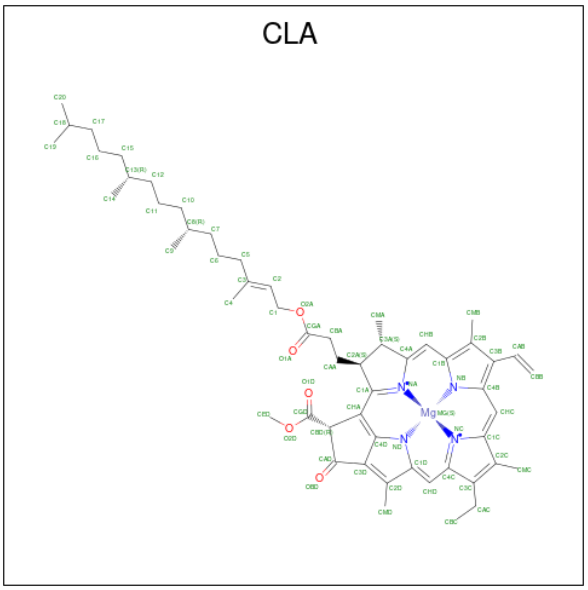
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 4	Cl 4	0	2

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

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



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

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

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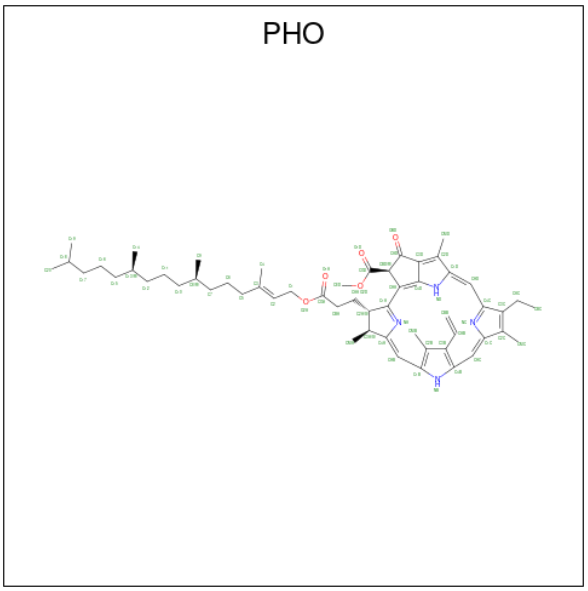
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110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

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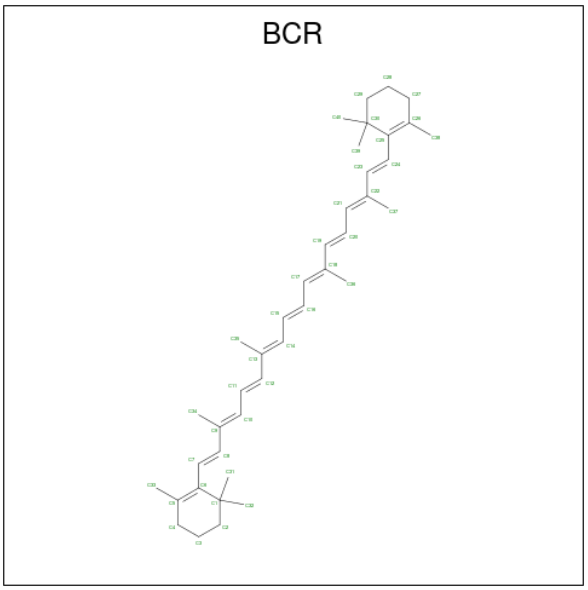
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



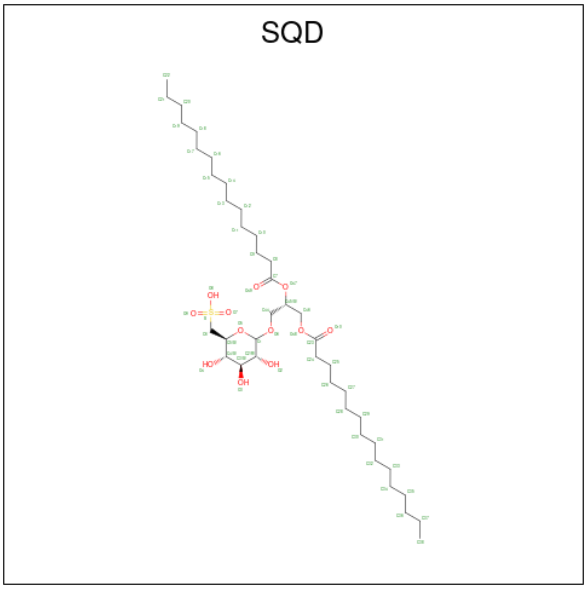
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	d	1	Total	C	N	O	0	1
			128	110	8	10		

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



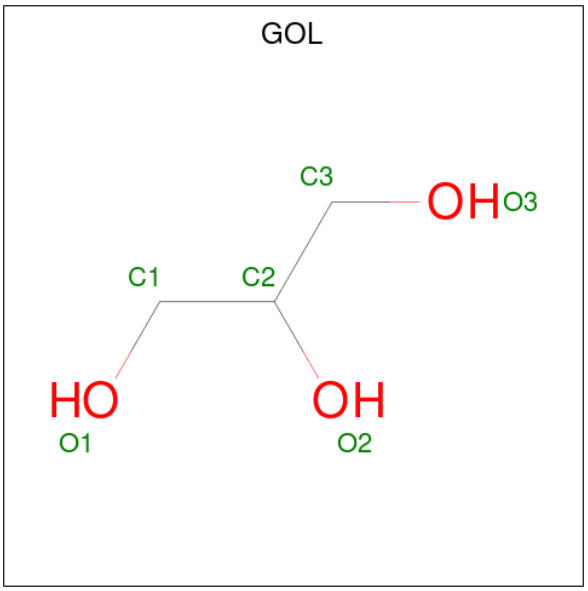
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



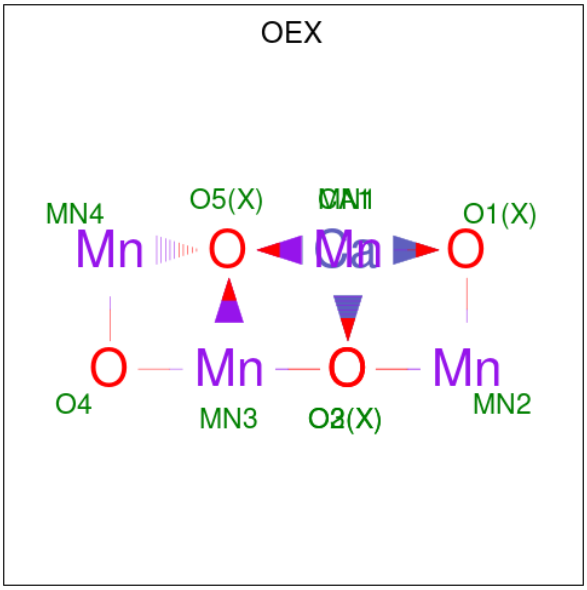
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

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

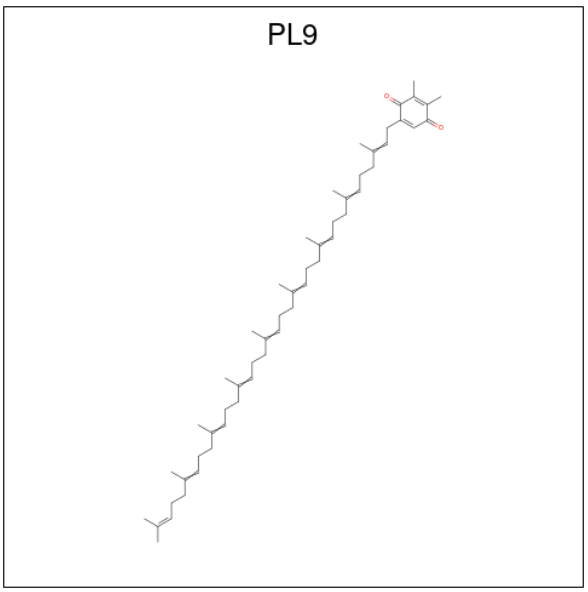
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

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

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



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

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

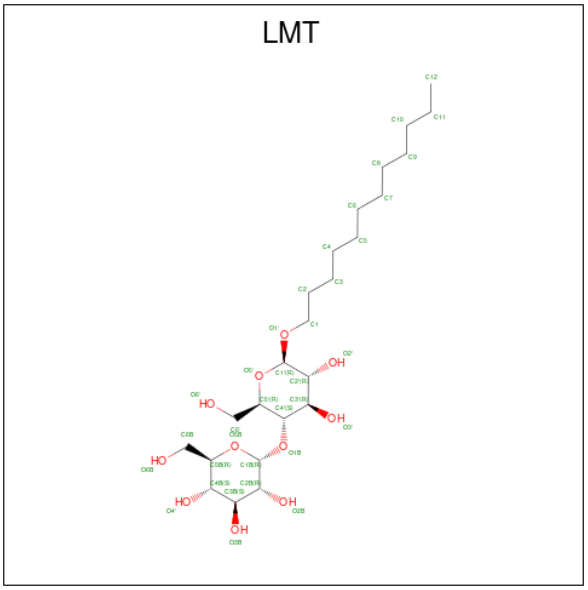
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 68 58 10	0	1
30	X	1	Total C O 18 16 2	0	0

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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 64 54 10	0	1
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: $C_{24}H_{46}O_{11}$).



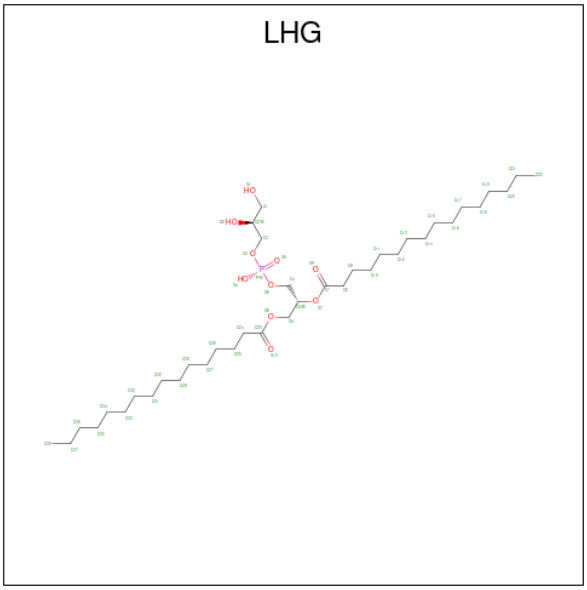
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0

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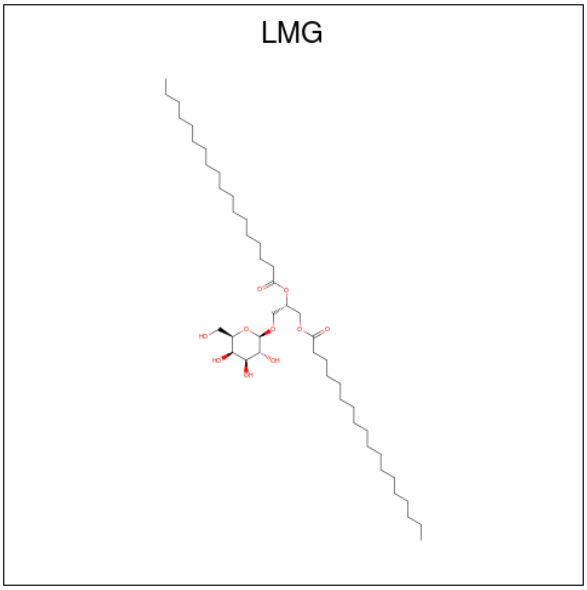
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 25 19 6	0	0
31	C	1	Total C O 35 24 11	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	T	1	Total C O 35 24 11	0	0
31	a	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 6	0	0
31	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-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

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



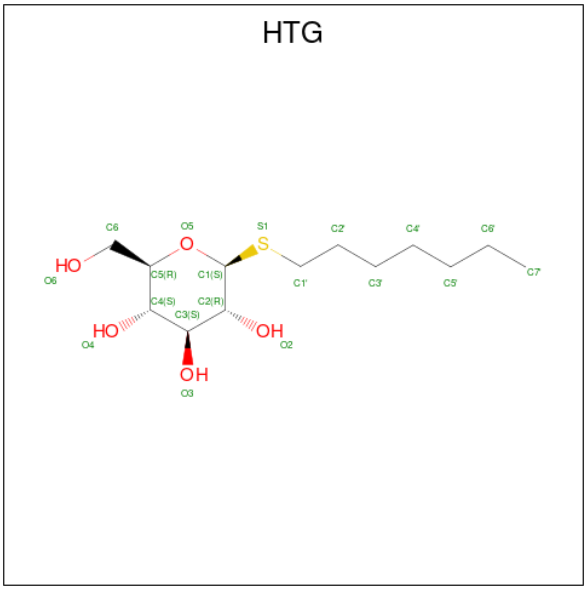
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	B	1	Total	C	O	0	0
			51	41	10		

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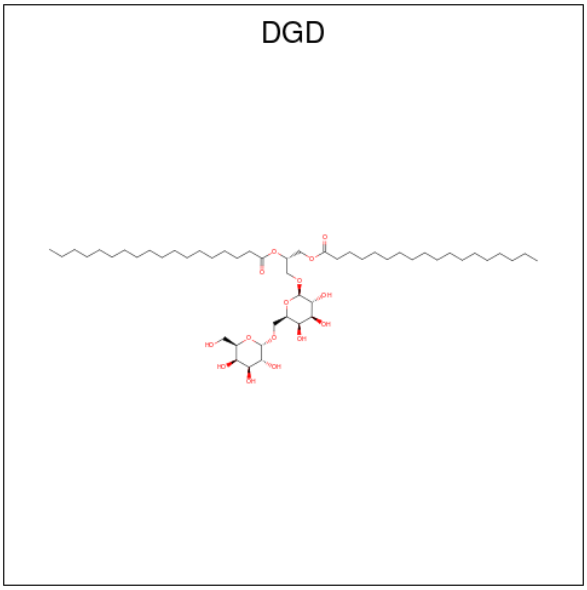
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	D	1	Total C O 51 41 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	m	1	Total C O 51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

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



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

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

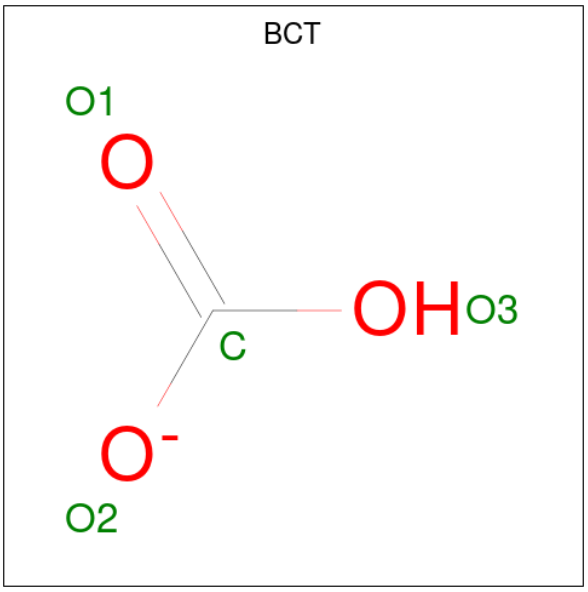


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

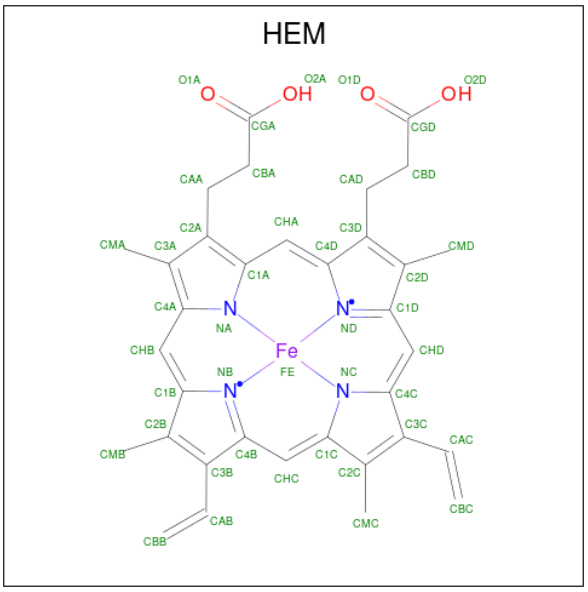
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- Molecule 37 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



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

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



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

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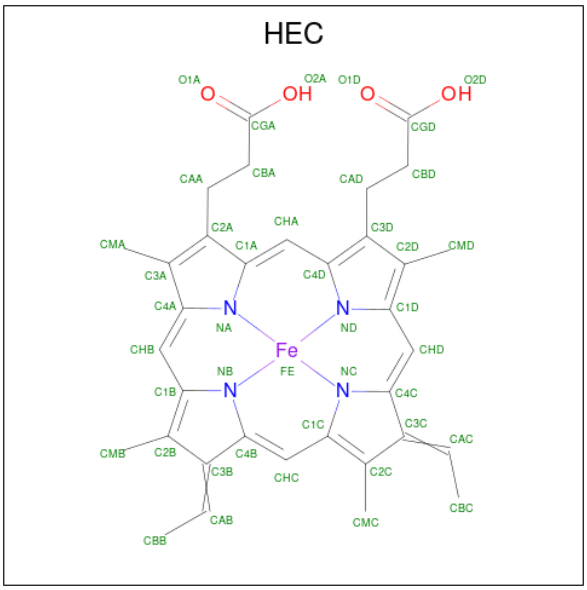
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	137	Total	O	0	85
			221	221		
41	B	187	Total	O	0	2
			189	189		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	169	Total O 206 206	0	38
41	D	122	Total O 157 157	0	35
41	E	16	Total O 16 16	0	0
41	F	5	Total O 5 5	0	0
41	H	21	Total O 21 21	0	0
41	I	5	Total O 5 5	0	0
41	J	5	Total O 5 5	0	0
41	K	6	Total O 6 6	0	0
41	L	8	Total O 9 9	0	1
41	M	5	Total O 5 5	0	0
41	O	106	Total O 110 110	0	4
41	T	11	Total O 14 14	0	3
41	U	45	Total O 48 48	0	3
41	V	81	Total O 82 82	0	1
41	X	8	Total O 8 8	0	0
41	a	133	Total O 213 213	0	81
41	b	199	Total O 202 202	0	3
41	c	157	Total O 190 190	0	34
41	d	121	Total O 153 153	0	32
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0

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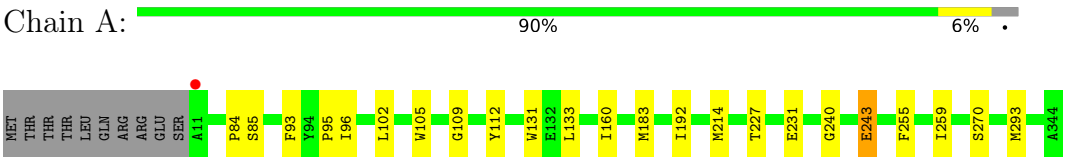
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	15	Total O 15 15	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	98	Total O 102 102	0	4
41	t	8	Total O 11 11	0	3
41	u	50	Total O 51 51	0	1
41	v	59	Total O 61 61	0	2
41	x	7	Total O 7 7	0	0
41	y	2	Total O 2 2	0	0

3 Residue-property plots (i)

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

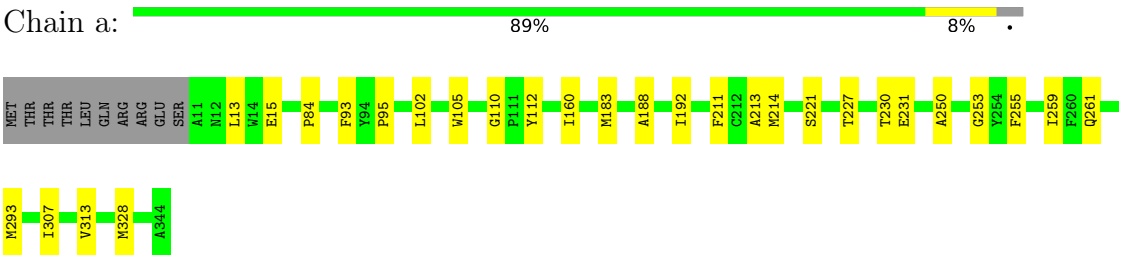
• Molecule 1: Photosystem II protein D1

Chain A:



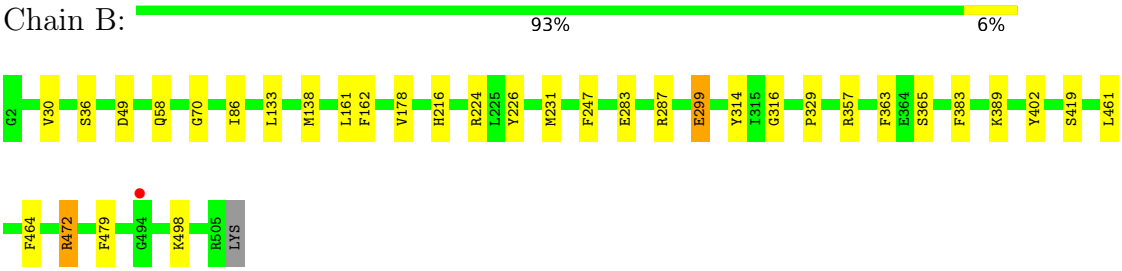
• Molecule 1: Photosystem II protein D1

Chain a:



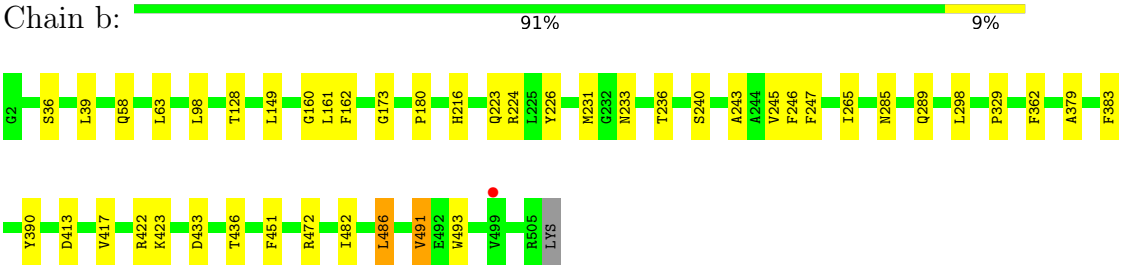
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



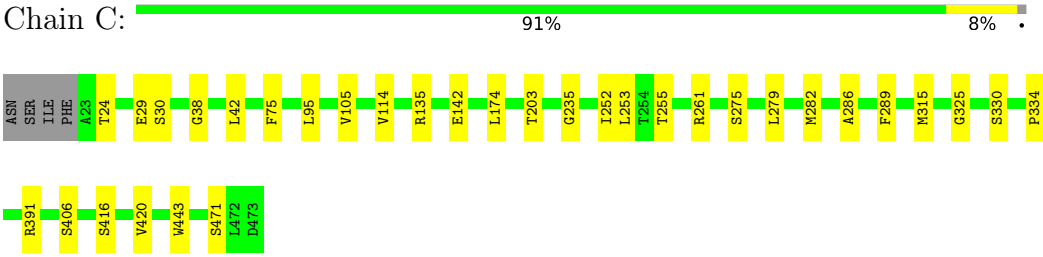
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



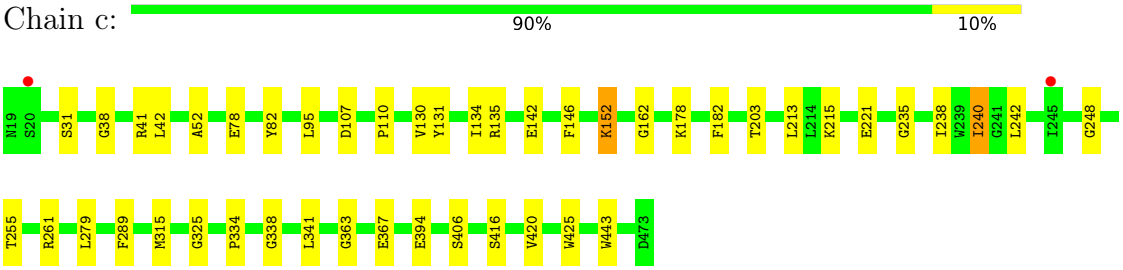
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



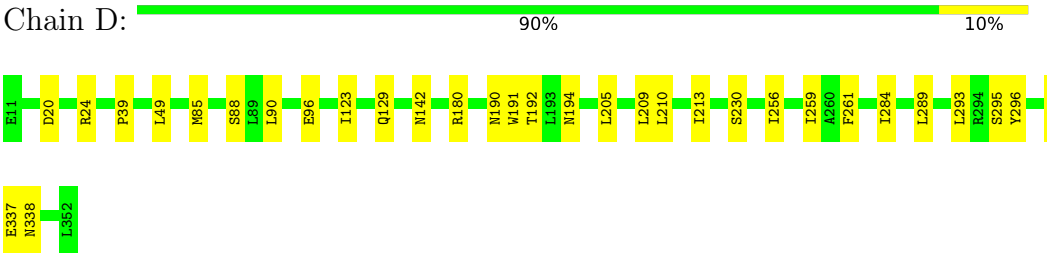
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



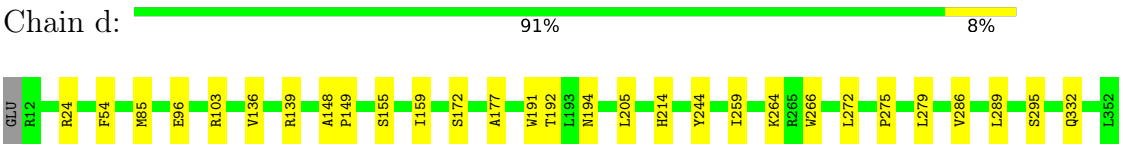
• Molecule 4: Photosystem II D2 protein

Chain D:



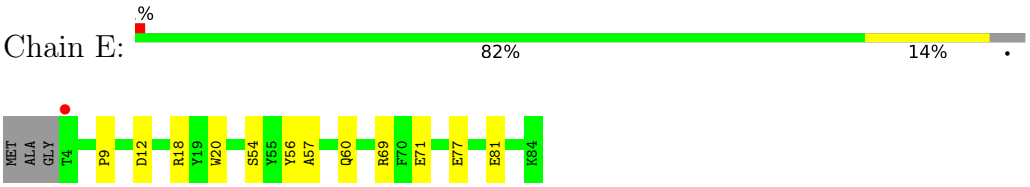
• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

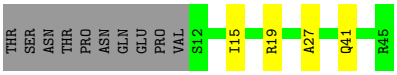




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

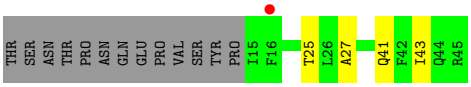




• Molecule 6: Cytochrome b559 subunit beta

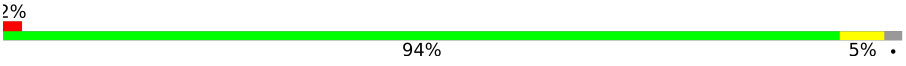
Chain f:

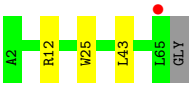




• Molecule 7: Photosystem II reaction center protein H

Chain H:

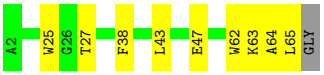




• Molecule 7: Photosystem II reaction center protein H

Chain h:

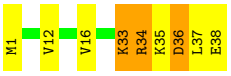




• Molecule 8: Photosystem II reaction center protein I

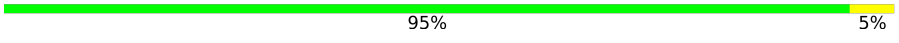
Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

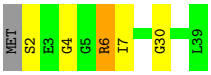




• Molecule 9: Photosystem II reaction center protein J

Chain J:

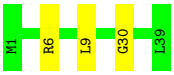




• Molecule 9: Photosystem II reaction center protein J

Chain j:

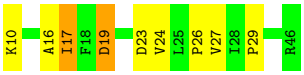




• Molecule 10: Photosystem II reaction center protein K

Chain K:

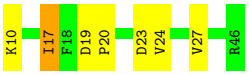




• Molecule 10: Photosystem II reaction center protein K

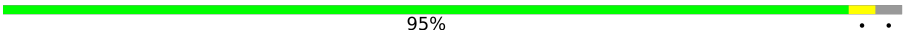
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

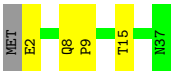




• Molecule 11: Photosystem II reaction center protein L

Chain l:





• Molecule 12: Photosystem II reaction center protein M

Chain M:

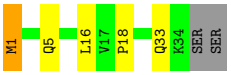




• Molecule 12: Photosystem II reaction center protein M

Chain m:

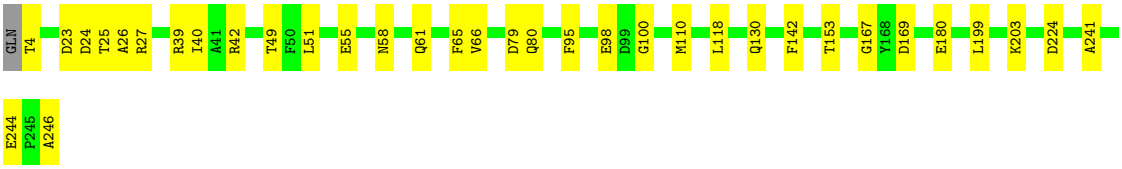




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

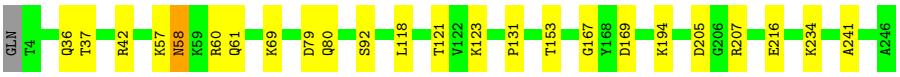




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

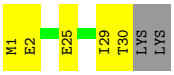




• Molecule 14: Photosystem II reaction center protein T

Chain T:

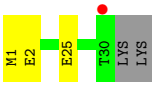




• Molecule 14: Photosystem II reaction center protein T

Chain t:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

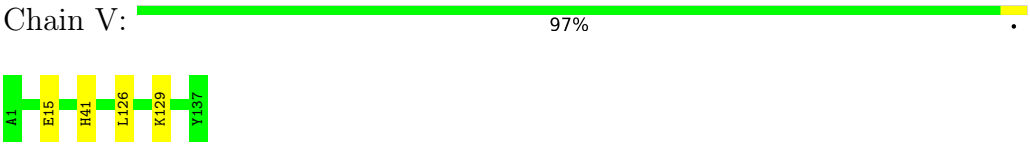
Chain u:





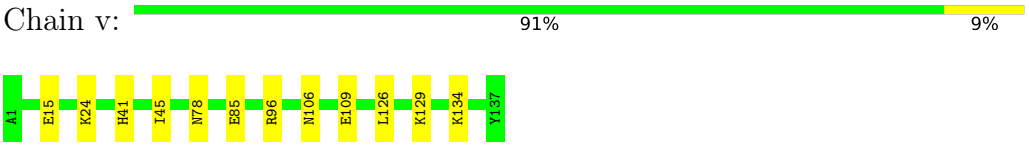
• Molecule 16: Cytochrome c-550

Chain V:



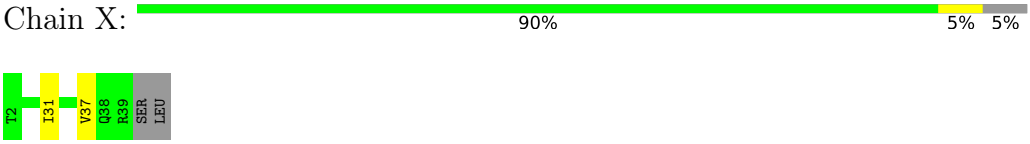
• Molecule 16: Cytochrome c-550

Chain v:



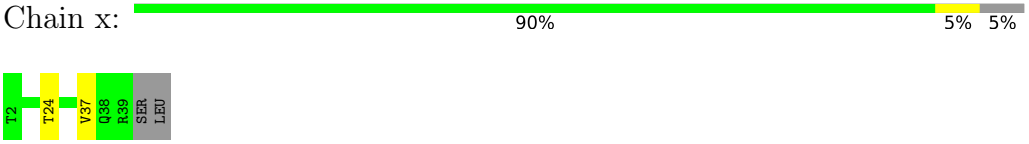
• Molecule 17: Photosystem II reaction center protein X

Chain X:



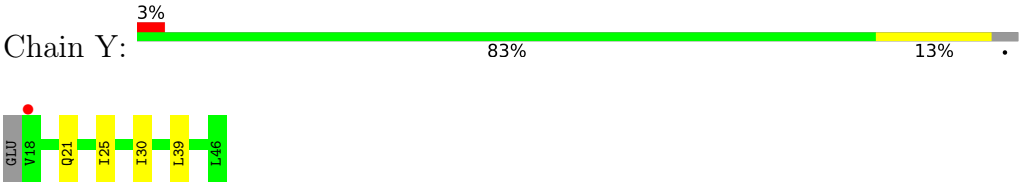
• Molecule 17: Photosystem II reaction center protein X

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



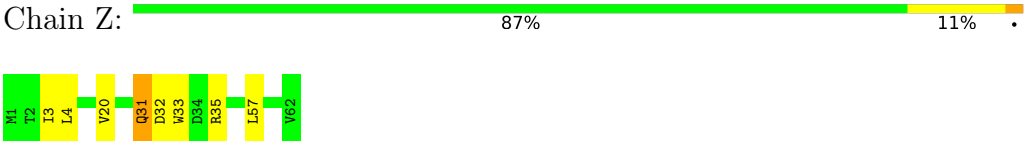
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



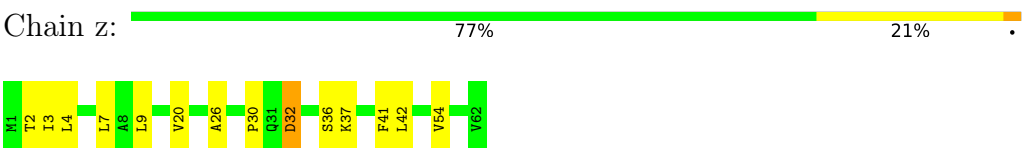
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



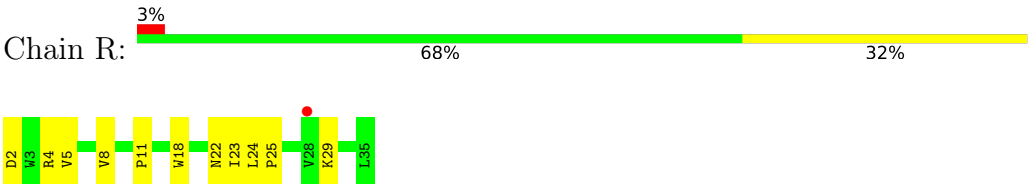
• Molecule 19: Photosystem II reaction center protein Z

Chain z:



• Molecule 20: Photosystem II protein Y

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.75Å 231.60Å 288.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.20) 99.7 (19.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 2.19Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.143 , 0.179 0.144 , 0.181	Depositor DCC
R_{free} test set	21187 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	62674	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

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

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCT, CL, FE2, PL9, MG, OEX, LHG, HEM, PHO, UNL, LMG, GOL, CA, HEC, DGD, CLA, HTG, LMT, SQD, FME, BCR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/4478	0.45	0/6098
1	a	0.25	0/4457	0.41	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.31	0/4285	0.48	0/5841
3	C	0.27	0/4416	0.42	0/6013
3	c	0.27	0/4467	0.42	0/6082
4	D	0.32	0/3746	0.47	0/5102
4	d	0.29	0/3780	0.44	0/5147
5	E	0.30	0/681	0.49	0/928
5	e	0.26	0/690	0.45	0/939
6	F	0.30	0/284	0.42	0/387
6	f	0.26	0/269	0.42	0/365
7	H	0.30	0/519	0.47	0/708
7	h	0.27	0/530	0.48	0/722
8	I	0.27	0/311	0.41	0/419
8	i	0.31	0/311	0.46	0/419
9	J	0.29	0/278	0.37	0/376
9	j	0.28	0/283	0.39	0/383
10	K	0.30	0/303	0.46	0/416
10	k	0.32	0/303	0.45	0/416
11	L	0.36	0/318	0.48	0/433
11	l	0.36	0/318	0.45	0/433
12	M	0.39	0/261	0.51	0/357
12	m	0.33	0/279	0.47	0/380
13	O	0.33	0/1991	0.50	0/2698
13	o	0.31	0/1966	0.48	0/2665
14	T	0.33	0/310	0.42	0/419
14	t	0.32	0/301	0.41	0/406
15	U	0.34	0/811	0.52	0/1095
15	u	0.34	0/826	0.51	0/1116
16	V	0.33	0/1142	0.48	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.29	0/1139	0.44	0/1542
17	X	0.22	0/292	0.34	0/395
17	x	0.23	0/284	0.34	0/384
18	Y	0.25	0/216	0.43	0/289
18	y	0.23	0/216	0.39	0/289
19	Z	0.21	0/490	0.36	0/669
19	z	0.20	0/490	0.32	0/669
20	R	0.23	0/279	0.33	0/383
All	All	0.29	0/50634	0.45	0/68876

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	23	0
1	a	4318	0	4124	33	0
2	B	4166	0	3999	28	0
2	b	4134	0	3976	41	0
3	C	4272	0	4138	24	0
3	c	4316	0	4184	35	0
4	D	3625	0	3489	33	0
4	d	3658	0	3522	25	0
5	E	662	0	648	8	0
5	e	670	0	655	7	0
6	F	275	0	282	4	0
6	f	261	0	269	5	0
7	H	506	0	529	2	0
7	h	517	0	541	6	0
8	I	314	0	328	6	0
8	i	314	0	328	1	0
9	J	272	0	279	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	2	0
10	K	293	0	305	5	0
10	k	293	0	305	5	0
11	L	311	0	320	1	0
11	l	311	0	320	5	0
12	M	268	0	285	4	0
12	m	286	0	305	7	0
13	O	1958	0	1920	23	0
13	o	1933	0	1900	15	0
14	T	311	0	318	3	0
14	t	302	0	311	2	0
15	U	800	0	796	4	0
15	u	815	0	817	5	0
16	V	1120	0	1122	2	0
16	v	1117	0	1131	7	0
17	X	289	0	322	2	0
17	x	281	0	312	3	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	4	0
20	R	273	0	305	5	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	18	0
23	B	1040	0	1152	32	0
23	C	845	0	936	31	0
23	D	195	0	216	6	0
23	a	325	0	360	15	0
23	b	1040	0	1152	22	0
23	c	845	0	936	41	0
23	d	325	0	360	12	0
24	A	256	0	296	5	0
24	a	128	0	148	1	0
24	d	128	0	148	4	0
25	A	40	0	56	1	0
25	B	120	0	168	6	0
25	C	80	0	112	3	0
25	D	40	0	56	2	0
25	H	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	K	40	0	56	2	0
25	T	40	0	56	7	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	10	0
25	c	80	0	112	3	0
25	d	40	0	56	1	0
25	h	40	0	56	4	0
25	k	40	0	56	2	0
25	t	40	0	56	4	0
25	y	40	0	56	2	0
26	A	162	0	233	3	0
26	X	43	0	53	2	0
26	a	162	0	232	12	0
26	b	54	0	78	3	0
26	f	43	0	53	0	0
26	l	54	0	78	1	0
27	A	12	0	15	4	0
27	B	12	0	16	3	0
27	C	12	0	16	0	0
27	D	6	0	7	2	0
27	O	12	0	16	3	0
27	V	12	0	16	0	0
27	a	18	0	24	5	0
27	b	12	0	16	1	0
27	c	18	0	24	0	0
27	d	6	0	8	0	0
27	l	12	0	16	1	0
27	o	12	0	16	0	0
27	v	12	0	16	2	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	18	0
29	D	110	0	160	0	0
29	a	110	0	160	11	0
29	d	110	0	160	1	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	l	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	35	0	46	1	0
31	B	95	0	127	1	0
31	C	35	0	46	1	0
31	F	35	0	46	0	0
31	M	35	0	46	1	0
31	T	35	0	46	0	0
31	a	35	0	46	1	0
31	b	50	0	70	2	0
31	e	35	0	46	1	0
31	m	35	0	46	0	0
31	t	26	0	35	1	0
32	A	98	0	148	3	0
32	D	196	0	296	10	0
32	E	84	0	114	7	0
32	L	98	0	148	0	0
32	a	84	0	114	8	0
32	b	98	0	148	0	0
32	d	294	0	444	26	0
33	B	51	0	72	1	0
33	C	153	0	216	3	0
33	D	51	0	72	0	0
33	Z	37	0	44	1	0
33	a	51	0	72	0	0
33	c	102	0	144	2	0
33	d	51	0	72	4	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	2	0
34	C	19	0	26	0	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	57	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	c	19	0	26	1	0
34	d	16	0	17	0	0
35	C	310	0	410	11	0
35	H	62	0	82	1	0
35	c	310	0	410	9	0
35	h	62	0	82	2	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	8	0	0	0	0
37	d	8	0	0	0	0
38	E	43	0	30	1	0
38	f	43	0	30	2	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	221	0	0	1	0
41	B	189	0	0	1	0
41	C	206	0	0	2	0
41	D	157	0	0	3	0
41	E	16	0	0	1	0
41	F	5	0	0	0	0
41	H	21	0	0	0	0
41	I	5	0	0	0	0
41	J	5	0	0	0	0
41	K	6	0	0	0	0
41	L	9	0	0	0	0
41	M	5	0	0	0	0
41	O	110	0	0	2	0
41	T	14	0	0	0	0
41	U	48	0	0	0	0
41	V	82	0	0	0	0
41	X	8	0	0	0	0
41	a	213	0	0	2	0
41	b	202	0	0	0	0
41	c	190	0	0	3	0
41	d	153	0	0	1	0
41	e	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	f	3	0	0	0	0
41	h	15	0	0	0	0
41	i	2	0	0	0	0
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	13	0	0	0	0
41	o	102	0	0	0	0
41	t	11	0	0	0	0
41	u	51	0	0	1	0
41	v	61	0	0	0	0
41	x	7	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61528	593	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (593) 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	1.42	1.02
23:B:604:CLA:H42	23:B:605:CLA:H2	1.49	0.94
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.55	0.89
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:c:503:CLA:HBB1	23:c:512:CLA:H41	1.60	0.83
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.61	0.81
4:d:192[B]:THR:HG23	23:d:404[B]:CLA:HBC2	1.63	0.81
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.62	0.80
4:d:192[A]:THR:HG23	23:d:404[A]:CLA:HBC2	1.64	0.80
23:B:601:CLA:H12	23:B:601:CLA:H71	1.63	0.78
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.66	0.77
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.69	0.74
27:a:418:GOL:O2	41:a:501:HOH:O	2.05	0.73
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.72	0.72
23:a:407:CLA:H192	23:c:505:CLA:H142	1.72	0.70
32:D:407[A]:LHG:H112	32:D:407[A]:LHG:H382	1.74	0.70
23:c:505:CLA:HHC	23:c:505:CLA:HBB1	1.73	0.70
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.73	0.69
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.73	0.69
35:C:517[B]:DGD:O1A	41:C:601[B]:HOH:O	2.09	0.69
2:B:226:TYR:HA	2:B:231:MET:HG3	1.73	0.69
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.75	0.67
27:a:417:GOL:H32	12:m:1:FME:HG3	1.77	0.67
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.27	0.67
3:c:213:LEU:HD13	23:c:506:CLA:H202	1.77	0.66
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.77	0.66
27:A:418:GOL:O2	41:A:501:HOH:O	2.12	0.65
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.30	0.65
10:K:17:ILE:H	10:K:17:ILE:HD13	1.61	0.65
23:c:505:CLA:CMD	23:c:507:CLA:HAB	2.27	0.65
23:A:408:CLA:H193	23:C:507:CLA:H101	1.79	0.64
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.28	0.64
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H112	1.80	0.64
29:A:414[B]:PL9:H262	32:E:101[B]:LHG:H223	1.79	0.64
29:A:414[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.64
34:B:621:HTG:H4'1	31:B:628:LMT:H52	1.80	0.63
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.80	0.63
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.79	0.63
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.81	0.62
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.82	0.62
23:b:601:CLA:H72	23:b:601:CLA:H2	1.81	0.62
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.82	0.61
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.01	0.60
23:c:502:CLA:H61	23:c:512:CLA:H42	1.83	0.60
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.82	0.60
23:C:507:CLA:H142	35:C:517[B]:DGD:HAF2	1.83	0.60
23:a:407:CLA:H152	23:c:506:CLA:H142	1.83	0.60
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.83	0.60
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.32	0.60
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.01	0.60
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.83	0.60
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.82	0.59
2:b:285:ASN:O	2:b:289:GLN:HG2	2.02	0.59
23:C:507:CLA:H142	35:C:517[A]:DGD:HAF2	1.85	0.59
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.85	0.59
23:C:514:CLA:H202	33:C:521:LMG:H402	1.83	0.59
10:k:17:ILE:HD13	10:k:17:ILE:H	1.68	0.59
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:HBB1	1.85	0.59
27:b:628:GOL:O3	27:b:628:GOL:O1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.30	0.58
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.85	0.58
23:d:402[A]:CLA:HHC	23:d:402[A]:CLA:HBB1	1.85	0.58
26:a:409[A]:SQD:H152	32:d:409[A]:LHG:H172	1.86	0.58
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.16	0.58
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.86	0.58
3:c:134[B]:ILE:HD13	23:c:511:CLA:H43	1.86	0.58
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.12	0.58
29:A:414[B]:PL9:H253	23:D:402[B]:CLA:H141	1.85	0.57
26:a:409[B]:SQD:H141	32:d:409[B]:LHG:H152	1.85	0.57
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.87	0.57
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.86	0.57
23:b:604:CLA:H42	23:b:605:CLA:H2	1.85	0.57
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.88	0.56
3:c:134[B]:ILE:HD11	23:c:511:CLA:H71	1.86	0.56
23:c:511:CLA:H191	33:z:101:LMG:H241	1.87	0.56
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.06	0.56
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.87	0.56
26:a:409[A]:SQD:H141	32:d:409[A]:LHG:H152	1.86	0.56
23:c:501:CLA:C4D	23:c:503:CLA:H2	2.36	0.56
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.39	0.56
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	1.88	0.56
20:R:18:TRP:O	20:R:22:ASN:ND2	2.38	0.56
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.88	0.55
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.88	0.55
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.36	0.55
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.70	0.55
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.88	0.55
26:a:409[A]:SQD:H321	23:c:508:CLA:H102	1.88	0.55
23:b:602:CLA:HHC	23:b:602:CLA:HBB1	1.88	0.55
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.04	0.55
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.87	0.55
25:C:515:BCR:H352	33:C:521:LMG:H352	1.89	0.55
23:a:404[B]:CLA:H201	32:d:408[B]:LHG:H161	1.89	0.55
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.88	0.55
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.41	0.54
23:a:405[A]:CLA:H191	32:a:419[A]:LHG:H111	1.88	0.54
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.89	0.54
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.89	0.54
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	1.88	0.54
23:b:613:CLA:H172	25:b:618:BCR:H312	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:416[B]:PHO:H3A	23:D:402[B]:CLA:H142	1.90	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.90	0.54
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.41	0.54
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.21	0.53
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.43	0.53
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.08	0.53
32:d:409[B]:LHG:H151	32:d:409[B]:LHG:H342	1.91	0.53
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.90	0.53
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.91	0.53
4:D:192[A]:THR:HG23	23:D:402[A]:CLA:HBC2	1.90	0.53
4:D:192[B]:THR:HG23	23:D:402[B]:CLA:HBC2	1.89	0.53
25:b:619:BCR:H331	25:b:619:BCR:C8	2.39	0.53
26:a:409[B]:SQD:H321	23:c:508:CLA:H102	1.90	0.53
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.43	0.53
4:D:85:MET:CE	4:D:96:GLU:HG2	2.39	0.53
38:E:102:HEM:HAC	6:F:27:ALA:HB1	1.91	0.53
32:d:415[B]:LHG:H211	12:m:18:PRO:HG3	1.91	0.53
4:D:323[A]:GLU:O	27:D:412:GOL:O2	2.27	0.52
26:a:409[B]:SQD:H152	32:d:409[B]:LHG:H172	1.92	0.52
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.91	0.52
4:D:230[B]:SER:HB2	41:D:557:HOH:O	2.10	0.52
17:X:31:ILE:HD11	26:X:101:SQD:H102	1.91	0.52
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.10	0.52
32:a:419[B]:LHG:HC31	5:e:9:PRO:HA	1.91	0.52
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.92	0.52
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.90	0.52
27:a:418:GOL:O3	14:t:2:GLU:OE1	2.28	0.52
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.92	0.52
32:a:419[A]:LHG:HC31	5:e:9:PRO:HA	1.91	0.52
3:c:42:LEU:HD21	23:c:511:CLA:H2A	1.92	0.52
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.92	0.52
23:a:405[A]:CLA:H203	33:d:413:LMG:H412	1.92	0.52
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.90	0.52
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.75	0.51
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.45	0.51
33:c:519:LMG:H181	10:k:27:VAL:HG11	1.92	0.51
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.45	0.51
4:d:85:MET:CE	4:d:96:GLU:HG2	2.38	0.51
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.93	0.51
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.09	0.51
33:z:101:LMG:H302	33:z:101:LMG:H141	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.45	0.51
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.92	0.51
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	1.91	0.51
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.93	0.51
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.46	0.51
29:a:413[A]:PL9:H28	32:a:419[A]:LHG:H222	1.92	0.51
1:a:15:GLU:HB2	31:a:416:LMT:H6'2	1.93	0.51
23:c:501:CLA:C3D	23:c:503:CLA:H2	2.40	0.51
23:A:408:CLA:H18	23:C:506:CLA:H142	1.93	0.50
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.92	0.50
27:l:103[A]:GOL:H32	14:t:25:GLU:HB2	1.92	0.50
23:a:405[B]:CLA:H191	32:a:419[B]:LHG:H111	1.91	0.50
29:a:413[A]:PL9:H351	6:f:25:THR:OG1	2.12	0.50
4:d:279:LEU:HD22	24:d:403[B]:PHO:HBC3	1.91	0.50
23:c:513:CLA:HBB1	25:c:514:BCR:H24C	1.92	0.50
29:A:414[A]:PL9:H253	23:D:402[A]:CLA:H141	1.92	0.50
5:E:77:GLU:O	5:E:81:GLU:HG2	2.12	0.50
2:b:422:ARG:NH2	13:o:169:ASP:OD2	2.40	0.50
32:d:408[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.94	0.50
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.94	0.50
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.42	0.50
27:a:418:GOL:H11	12:m:1:FME:HE3	1.94	0.50
35:c:516[B]:DGD:HG11	41:c:605[B]:HOH:O	2.12	0.50
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.13	0.49
1:a:214[B]:MET:HB3	29:a:413[B]:PL9:H103	1.94	0.49
35:c:518:DGD:HBH2	32:d:409[B]:LHG:H211	1.94	0.49
23:c:504:CLA:H62	35:c:518:DGD:HB62	1.95	0.49
13:O:224:ASP:OD2	41:O:401:HOH:O	2.20	0.49
23:a:407:CLA:H203	23:c:506:CLA:H101	1.95	0.49
23:B:606:CLA:H202	26:a:411:SQD:H302	1.95	0.49
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.48	0.49
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.94	0.49
32:A:419[A]:LHG:H361	23:B:613:CLA:H51	1.95	0.49
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.92	0.49
4:D:261[B]:PHE:CZ	32:D:406[B]:LHG:HC81	2.48	0.49
1:a:160[B]:ILE:HD11	35:c:516[B]:DGD:HBT1	1.94	0.49
23:a:404[A]:CLA:H201	32:d:408[A]:LHG:H161	1.95	0.49
25:T:102:BCR:H19C	25:b:618:BCR:H363	1.95	0.49
32:d:408[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.95	0.49
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.94	0.49
13:o:92:SER:HB3	13:o:131:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.95	0.48
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.43	0.48
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.48	0.48
23:b:605:CLA:H41	23:b:605:CLA:H62	1.53	0.48
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.46	0.48
27:a:418:GOL:H31	12:m:1:FME:HG2	1.96	0.48
32:d:409[A]:LHG:H331	32:d:409[A]:LHG:H361	1.55	0.48
29:A:414[A]:PL9:H503	26:X:101:SQD:H341	1.94	0.48
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.94	0.48
2:B:383[A]:PHE:CZ	13:O:167:GLY:HA2	2.49	0.48
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.48	0.48
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.13	0.48
23:B:614:CLA:H71	23:B:614:CLA:H112	1.60	0.48
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:H132	1.96	0.48
2:b:36:SER:OG	25:b:618:BCR:H362	2.13	0.48
23:C:511:CLA:H112	23:C:511:CLA:H152	1.51	0.48
23:c:508:CLA:H18	35:c:517[B]:DGD:HAT2	1.96	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.94	0.48
4:D:323[B]:GLU:O	27:D:412:GOL:O2	2.32	0.48
29:a:413[B]:PL9:H28	32:a:419[B]:LHG:H222	1.95	0.48
32:d:409[A]:LHG:H122	32:d:409[A]:LHG:C38	2.44	0.48
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.96	0.48
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H132	1.96	0.48
3:c:95:LEU:HD21	23:c:501:CLA:OBD	2.14	0.48
26:l:101:SQD:H462	26:l:101:SQD:H1	1.96	0.47
19:z:32:ASP:O	19:z:36:SER:OG	2.22	0.47
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.74	0.47
3:C:203:THR:O	3:C:235:GLY:HA3	2.14	0.47
13:O:42:ARG:O	13:O:241:ALA:HA	2.15	0.47
13:o:58:ASN:C	13:o:60:ARG:H	2.22	0.47
1:A:240[A]:GLY:HA3	14:T:29[A]:ILE:HG23	1.96	0.47
4:D:230[A]:SER:HB2	41:D:557:HOH:O	2.13	0.47
23:a:405[B]:CLA:H203	33:d:413:LMG:H412	1.95	0.47
2:b:98:LEU:HD13	34:b:622:HTG:H7'1	1.97	0.47
1:a:160[A]:ILE:HD11	35:c:516[A]:DGD:HBT1	1.96	0.47
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.95	0.47
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.80	0.47
23:B:613:CLA:H162	23:B:613:CLA:H121	1.59	0.47
13:O:25:THR:O	13:O:27:ARG:N	2.47	0.47
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.49	0.47
26:A:410[A]:SQD:H152	26:A:410[A]:SQD:H122	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414[B]:PL9:H171	29:A:414[B]:PL9:H151	1.51	0.47
23:C:502:CLA:H42	23:C:503:CLA:HMD3	1.96	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.40	0.47
41:E:202:HOH:O	9:J:6:ARG:HG3	2.13	0.47
23:c:508:CLA:H18	35:c:517[A]:DGD:HAT2	1.96	0.47
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.97	0.47
27:A:418:GOL:H31	12:M:1:FME:HE3	1.95	0.47
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.80	0.47
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	1.96	0.47
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.97	0.47
4:d:279:LEU:HD22	24:d:403[A]:PHO:HBC3	1.96	0.47
1:A:214[A]:MET:HE2	1:A:255[A]:PHE:CE1	2.49	0.47
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.96	0.47
27:A:418:GOL:H12	14:T:2:GLU:OE1	2.15	0.47
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.95	0.47
34:B:624:HTG:H61	1:a:102:LEU:HD12	1.96	0.47
23:C:507:CLA:H18	23:C:507:CLA:H152	1.40	0.47
8:I:35:LYS:O	8:I:37:LEU:N	2.48	0.47
31:A:417:LMT:H71	2:b:39:LEU:HD13	1.97	0.47
2:B:133:LEU:HB2	27:B:626:GOL:H31	1.97	0.47
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.50	0.47
32:d:409[A]:LHG:H332	32:d:409[A]:LHG:H302	1.77	0.47
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.54	0.46
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.79	0.46
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.97	0.46
2:b:226:TYR:HA	2:b:231:MET:HG3	1.96	0.46
23:b:614:CLA:H112	23:b:614:CLA:H72	1.64	0.46
25:h:101:BCR:H331	25:h:101:BCR:C8	2.45	0.46
29:a:413[A]:PL9:H171	29:a:413[A]:PL9:H151	1.57	0.46
23:c:512:CLA:HMB2	23:c:512:CLA:H192	1.97	0.46
1:A:160[B]:ILE:HD11	35:C:517[B]:DGD:HBT2	1.97	0.46
32:E:101[A]:LHG:O2	6:F:19:ARG:NH1	2.48	0.46
8:I:33:LYS:HB3	8:I:34:ARG:H	1.56	0.46
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.98	0.46
15:u:10[A]:VAL:HG12	41:u:247:HOH:O	2.15	0.46
1:A:183[B]:MET:HA	23:A:404[B]:CLA:HMD1	1.96	0.46
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.51	0.46
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.81	0.46
23:c:509:CLA:H142	23:c:509:CLA:H112	1.79	0.46
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.97	0.46
25:H:101:BCR:C8	25:H:101:BCR:H331	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414[B]:PL9:H472	4:D:39:PRO:HD3	1.98	0.46
23:C:505:CLA:H62	23:C:505:CLA:H41	1.70	0.46
3:c:425[A]:TRP:CD1	23:c:504:CLA:HMA3	2.50	0.46
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	1.98	0.46
23:B:614:CLA:H8	25:B:617:BCR:H362	1.98	0.46
4:D:49:LEU:HD13	25:D:404:BCR:C15	2.45	0.46
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.50	0.46
3:C:330:SER:HB3	13:O:100:GLY:O	2.16	0.46
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.16	0.46
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.98	0.46
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.98	0.46
33:c:520:LMG:H232	33:c:520:LMG:H391	1.98	0.46
18:y:20:ALA:O	18:y:24:MET:HG2	2.16	0.46
24:A:407[B]:PHO:HAB	4:D:205[B]:LEU:HD13	1.98	0.45
23:C:503:CLA:HBD	23:C:503:CLA:HAA1	1.98	0.45
23:d:402[A]:CLA:HBA1	23:d:402[A]:CLA:C4A	2.45	0.45
32:d:409[B]:LHG:H361	32:d:409[B]:LHG:H331	1.64	0.45
20:R:8:VAL:O	20:R:11:PRO:HD2	2.16	0.45
29:a:413[B]:PL9:H171	29:a:413[B]:PL9:H151	1.54	0.45
29:a:413[B]:PL9:H351	6:f:25:THR:OG1	2.15	0.45
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.74	0.45
3:c:279:LEU:HD22	23:c:509:CLA:HED2	1.98	0.45
3:c:363:GLY:O	3:c:367:GLU:HG2	2.16	0.45
23:A:408:CLA:H41	23:A:408:CLA:H61	1.56	0.45
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.98	0.45
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.98	0.45
35:C:518[A]:DGD:HAT1	35:C:519:DGD:HBE1	1.97	0.45
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.17	0.45
27:O:303:GOL:O1	41:O:402:HOH:O	2.20	0.45
25:T:102:BCR:H321	25:T:102:BCR:HC8	1.98	0.45
6:f:27:ALA:HB1	38:f:101:HEM:HAC	1.98	0.45
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.31	0.45
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.17	0.45
8:I:12:VAL:O	8:I:16:VAL:HG23	2.16	0.45
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.16	0.45
3:c:52:ALA:HB2	23:c:511:CLA:HMA1	1.99	0.45
4:d:332[A]:GLN:NE2	41:d:505:HOH:O	2.49	0.45
6:F:15:ILE:HD13	20:R:23:ILE:HD11	1.99	0.45
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.17	0.45
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.99	0.45
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:409[B]:LHG:H122	32:d:409[B]:LHG:C38	2.47	0.45
12:m:5[B]:GLN:H	12:m:5[B]:GLN:CD	2.22	0.45
26:a:409[A]:SQD:H271	32:d:409[A]:LHG:H141	1.98	0.45
32:d:409[A]:LHG:H342	32:d:409[A]:LHG:H151	1.99	0.45
18:y:31:ALA:O	18:y:35:ILE:HG13	2.16	0.45
2:B:58:GLN:C	2:B:329:PRO:HB3	2.42	0.45
3:C:443[B]:TRP:CE2	23:C:509:CLA:HMD2	2.52	0.45
3:c:146:PHE:HZ	23:c:512:CLA:HBB2	1.82	0.45
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.46	0.45
3:C:252:ILE:HG22	3:C:253:LEU:HD23	1.99	0.45
4:D:129[B]:GLN:HE21	4:D:142[B]:ASN:ND2	2.15	0.45
4:D:317[B]:LYS:NZ	41:D:512[B]:HOH:O	2.46	0.45
13:O:51:LEU:HB3	13:O:65:PHE:HB3	1.99	0.45
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.52	0.45
25:d:406:BCR:H383	33:d:413:LMG:H171	1.99	0.45
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	2.00	0.44
25:C:516:BCR:H11C	25:C:516:BCR:H341	1.88	0.44
3:c:443[A]:TRP:CE2	23:c:508:CLA:HMD2	2.53	0.44
23:c:509:CLA:H91	23:c:509:CLA:H111	1.83	0.44
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.82	0.44
2:b:233:ASN:O	2:b:236:THR:HG22	2.18	0.44
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.17	0.44
33:d:413:LMG:H221	33:d:413:LMG:H191	1.63	0.44
2:B:283:GLU:O	2:B:287:ARG:HG3	2.17	0.44
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.52	0.44
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	1.99	0.44
23:a:404[A]:CLA:H203	23:a:404[A]:CLA:H162	1.80	0.44
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	1.99	0.44
4:D:261[A]:PHE:CZ	32:D:406[A]:LHG:HC81	2.52	0.44
26:a:409[A]:SQD:H302	23:c:508:CLA:H71	2.00	0.44
3:c:203:THR:O	3:c:235:GLY:HA3	2.18	0.44
25:c:514:BCR:H11C	25:c:514:BCR:H341	1.75	0.44
4:d:266[A]:TRP:CD1	32:d:408[A]:LHG:HC31	2.52	0.44
1:A:214[B]:MET:HE2	1:A:255[B]:PHE:CE1	2.53	0.44
2:B:49:ASP:OD2	13:o:57:LYS:NZ	2.49	0.44
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.72	0.44
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.72	0.44
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.73	0.44
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.00	0.44
35:C:518[B]:DGD:HAT1	35:C:519:DGD:HBE1	1.99	0.44
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:T:102:BCR:H24C	25:T:102:BCR:H371	1.82	0.44
23:C:503:CLA:H141	23:C:503:CLA:H161	1.82	0.44
29:A:414[A]:PL9:H322	29:A:414[A]:PL9:H301	1.77	0.44
29:A:414[B]:PL9:H322	29:A:414[B]:PL9:H301	1.73	0.44
32:A:419[A]:LHG:H252	2:B:464:PHE:CZ	2.53	0.44
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CH2	2.53	0.44
2:b:379:ALA:HA	2:b:390:TYR:HB3	2.00	0.44
3:c:325:GLY:O	15:u:51:LYS:NZ	2.48	0.44
35:c:518:DGD:HBH2	32:d:409[A]:LHG:H211	2.00	0.44
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.76	0.44
23:A:408:CLA:H171	23:C:507:CLA:H121	1.98	0.44
29:A:414[B]:PL9:H121	29:A:414[B]:PL9:HC8	1.80	0.44
2:B:357[A]:ARG:HH12	27:B:623:GOL:H32	1.82	0.44
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.77	0.44
4:D:293:LEU:HD12	4:D:293:LEU:HA	1.90	0.44
23:b:615:CLA:H112	23:b:615:CLA:H91	1.77	0.44
23:d:404[A]:CLA:HBD	23:d:404[A]:CLA:HAA2	2.00	0.44
13:O:110:MET:HE2	13:O:110:MET:HB3	1.87	0.43
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.00	0.43
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.79	0.43
35:c:516[A]:DGD:HG11	41:c:605[A]:HOH:O	2.18	0.43
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.18	0.43
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:CBB	2.48	0.43
23:d:405:CLA:H41	23:d:405:CLA:H61	1.72	0.43
25:t:102:BCR:H11C	25:t:102:BCR:H341	1.89	0.43
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.54	0.43
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.43
10:K:26:PRO:O	10:K:29:PRO:HD2	2.18	0.43
23:d:402[B]:CLA:HBA1	23:d:402[B]:CLA:C4A	2.47	0.43
13:o:121:THR:OG1	13:o:123:LYS:HG3	2.19	0.43
1:A:93[B]:PHE:CD2	1:A:95:PRO:HD3	2.53	0.43
32:A:419[B]:LHG:H361	23:B:613:CLA:H51	2.00	0.43
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	2.00	0.43
25:T:102:BCR:HC7	25:T:102:BCR:H331	1.63	0.43
3:c:107:ASP:O	3:c:110:PRO:HD2	2.18	0.43
4:d:286:VAL:HG21	23:d:404[B]:CLA:HED2	2.01	0.43
13:o:42:ARG:O	13:o:241:ALA:HA	2.18	0.43
23:A:404[A]:CLA:H143	24:A:407[A]:PHO:H61	2.01	0.43
2:B:363:PHE:HB3	2:B:365:SER:O	2.17	0.43
3:C:279:LEU:HA	3:C:282:MET:HE3	2.00	0.43
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:31:SER:CB	3:c:41:ARG:HG2	2.48	0.43
32:d:409[A]:LHG:H242	32:d:409[A]:LHG:H272	1.86	0.43
29:A:414[B]:PL9:H221	29:A:414[B]:PL9:H201	1.84	0.43
3:C:42:LEU:HD21	23:C:512:CLA:H2A	2.00	0.43
32:D:406[A]:LHG:HC62	11:L:15[A]:THR:HG23	2.00	0.43
23:c:512:CLA:HBA2	23:c:512:CLA:H3A	1.76	0.43
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.89	0.43
35:C:517[A]:DGD:HG11	41:C:601[A]:HOH:O	2.18	0.43
25:b:618:BCR:H20C	25:b:618:BCR:H361	1.92	0.43
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	2.00	0.43
23:B:610:CLA:H122	23:B:615:CLA:HAA1	2.00	0.43
3:C:174:LEU:HB3	23:C:503:CLA:H152	2.00	0.43
8:I:36:ASP:OD1	8:I:36:ASP:N	2.52	0.43
2:b:58:GLN:C	2:b:329:PRO:HB3	2.43	0.43
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.53	0.43
2:b:245:VAL:HG22	23:b:612:CLA:H202	2.01	0.43
23:b:607:CLA:H112	23:b:607:CLA:H91	1.74	0.43
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.83	0.43
23:A:405[A]:CLA:HHC	23:A:405[A]:CLA:HBB1	2.01	0.43
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.76	0.43
24:A:416[A]:PHO:H3A	23:D:402[A]:CLA:H142	1.99	0.43
29:a:413[A]:PL9:H503	17:x:24:THR:OG1	2.18	0.43
13:o:79:ASP:OD1	13:o:80:GLN:N	2.47	0.43
25:a:408:BCR:H24C	25:a:408:BCR:H371	1.77	0.43
13:O:79:ASP:OD1	13:O:80:GLN:N	2.46	0.42
25:T:102:BCR:HC8	25:T:102:BCR:H311	2.00	0.42
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CZ3	2.54	0.42
1:a:307:ILE:HG22	1:a:313:VAL:HA	2.01	0.42
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.01	0.42
32:d:409[B]:LHG:H372	32:d:409[B]:LHG:H142	2.01	0.42
1:A:270[B]:SER:HB2	26:A:410[B]:SQD:O49	2.19	0.42
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.00	0.42
25:K:102:BCR:H15C	25:K:102:BCR:H351	1.88	0.42
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.41	0.42
13:O:130:GLN:H	13:O:130:GLN:CD	2.21	0.42
2:b:491[A]:VAL:HG13	4:d:136[A]:VAL:HG13	2.02	0.42
23:c:501:CLA:H42	23:c:502:CLA:HMD3	2.01	0.42
35:h:102:DGD:HB62	35:h:102:DGD:HB32	1.81	0.42
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.72	0.42
32:a:419[A]:LHG:H241	32:a:419[A]:LHG:HC61	1.89	0.42
3:c:215:LYS:HD3	3:c:221:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:c:505:CLA:HMD3	23:c:507:CLA:HAB	2.02	0.42
5:e:68:ASP:O	5:e:72:ALA:HB2	2.19	0.42
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.85	0.42
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.49	0.42
23:c:505:CLA:HMD2	23:c:507:CLA:HAB	2.01	0.42
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	2.01	0.42
29:A:414[A]:PL9:H171	29:A:414[A]:PL9:H151	1.53	0.42
2:B:162:PHE:O	23:B:606:CLA:HHD	2.20	0.42
4:d:214[B]:HIS:HA	29:d:407[B]:PL9:O2	2.20	0.42
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.83	0.42
16:v:41:HIS:HA	16:v:45[A]:ILE:O	2.20	0.42
20:R:2:ASP:HB3	20:R:5:VAL:HG23	2.02	0.42
3:C:334[A]:PRO:HA	13:O:153:THR:OG1	2.20	0.42
3:C:338[A]:GLY:HA3	3:C:341[A]:LEU:O	2.20	0.42
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.54	0.42
4:d:155:SER:HA	4:d:159:ILE:HB	2.01	0.42
25:k:101:BCR:H24C	25:k:101:BCR:H371	1.69	0.42
20:R:24:LEU:N	20:R:25:PRO:HD2	2.33	0.42
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.50	0.42
3:C:279:LEU:HD12	3:C:282:MET:HE3	2.02	0.42
32:D:407[A]:LHG:H332	32:D:407[A]:LHG:H302	1.85	0.42
26:b:620:SQD:H462	26:b:620:SQD:H1	2.01	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	2.01	0.42
25:D:404:BCR:H11C	25:D:404:BCR:H341	1.98	0.42
25:Y:101:BCR:HC7	25:Y:101:BCR:H331	1.80	0.42
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.54	0.42
2:B:461:LEU:HD21	4:D:284:ILE:HD11	2.01	0.42
2:B:472:ARG:HD2	2:B:479[A]:PHE:CE1	2.55	0.42
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.85	0.42
25:C:515:BCR:H371	25:C:515:BCR:H24C	1.77	0.42
35:C:519:DGD:HBE2	35:C:519:DGD:HB81	1.81	0.42
4:D:210[B]:LEU:HA	4:D:213[B]:ILE:HG22	2.02	0.42
23:a:404[B]:CLA:H203	23:a:404[B]:CLA:H162	1.74	0.42
32:a:419[B]:LHG:H241	32:a:419[B]:LHG:HC61	1.90	0.42
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.87	0.42
23:b:601:CLA:HHC	23:b:601:CLA:HBB1	2.02	0.42
23:c:505:CLA:HBD	23:c:505:CLA:HAA1	2.02	0.42
23:c:512:CLA:H121	23:c:513:CLA:H142	2.01	0.42
35:h:102:DGD:HB61	35:h:102:DGD:HB91	1.90	0.42
23:A:405[A]:CLA:HBA1	23:A:405[A]:CLA:C4A	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.49	0.42
26:A:410[B]:SQD:H122	26:A:410[B]:SQD:H152	1.65	0.42
2:B:86:ILE:H	2:B:86:ILE:HG13	1.74	0.42
3:C:114:VAL:HG22	33:C:521:LMG:H182	2.01	0.42
3:C:338[B]:GLY:HA3	3:C:341[B]:LEU:O	2.20	0.42
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:C11	2.45	0.42
25:T:102:BCR:H351	26:b:620:SQD:H211	2.02	0.42
23:c:512:CLA:H142	23:c:512:CLA:H111	1.92	0.42
25:h:101:BCR:H24C	25:h:101:BCR:H371	1.68	0.42
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	2.02	0.41
31:C:525:LMT:O3'	31:C:525:LMT:H6'2	2.20	0.41
23:a:407:CLA:H172	23:c:506:CLA:H91	2.02	0.41
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.02	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.90	0.41
23:A:404[A]:CLA:H192	23:A:404[A]:CLA:H161	1.80	0.41
23:B:615:CLA:H71	23:B:616:CLA:H172	2.01	0.41
35:C:518[B]:DGD:HB61	35:C:518[B]:DGD:HB32	1.81	0.41
32:D:407[A]:LHG:H362	32:D:407[A]:LHG:H331	1.86	0.41
16:V:41:HIS:CD2	40:V:201:HEC:NB	2.88	0.41
23:b:601:CLA:H92	25:h:101:BCR:H403	2.02	0.41
26:b:620:SQD:H311	26:b:620:SQD:H341	1.71	0.41
3:c:38:GLY:HA3	23:c:511:CLA:HMD2	2.01	0.41
24:d:403[B]:PHO:NC	24:d:403[B]:PHO:ND	2.68	0.41
2:B:216:HIS:CE1	23:B:609:CLA:NA	2.88	0.41
3:C:135:ARG:HA	3:C:135:ARG:HD2	1.96	0.41
3:C:325:GLY:O	15:U:51:LYS:NZ	2.36	0.41
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.56	0.41
32:d:409[B]:LHG:H242	32:d:409[B]:LHG:H272	1.91	0.41
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.41
15:u:92:VAL:HG12	15:u:97:ARG:HD2	2.02	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41
23:B:601:CLA:H72	23:B:601:CLA:C3D	2.50	0.41
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.03	0.41
1:a:214[A]:MET:HB3	29:a:413[A]:PL9:H103	2.01	0.41
1:a:230:THR:HG21	11:l:8:GLN:NE2	2.35	0.41
2:b:224:ARG:HH21	31:b:621:LMT:H11	1.84	0.41
3:c:443[B]:TRP:CE2	23:c:508:CLA:HMD2	2.54	0.41
24:d:403[A]:PHO:H42	24:d:403[A]:PHO:H11	1.92	0.41
23:d:404[B]:CLA:HAA2	23:d:404[B]:CLA:HBD	2.03	0.41
2:B:357[A]:ARG:HH12	27:B:623:GOL:C3	2.33	0.41
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:23:ASP:OD1	13:O:24:ASP:N	2.53	0.41
1:a:93[B]:PHE:CD2	1:a:95:PRO:HD3	2.54	0.41
1:a:211[B]:PHE:CD1	29:a:413[B]:PL9:H101	2.56	0.41
4:d:148[A]:ALA:HB3	4:d:149[A]:PRO:HD3	2.03	0.41
32:d:409[A]:LHG:H372	32:d:409[A]:LHG:H142	2.03	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.97	0.41
23:B:614:CLA:HAA1	23:B:614:CLA:HBD	2.02	0.41
13:O:142:PHE:HB2	13:O:199:LEU:HB2	2.03	0.41
24:a:406[B]:PHO:HAB	4:d:205[B]:LEU:HD13	2.02	0.41
26:a:411:SQD:H1	41:a:624:HOH:O	2.21	0.41
2:b:433:ASP:OD2	2:b:436:THR:OG1	2.33	0.41
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.36	0.41
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.41
1:A:85[A]:SER:HA	1:A:109[A]:GLY:HA3	2.03	0.41
1:A:231:GLU:HB3	41:B:871:HOH:O	2.21	0.41
2:B:247:PHE:CE2	23:B:602:CLA:H102	2.56	0.41
23:C:509:CLA:H142	23:C:509:CLA:H111	1.78	0.41
35:C:518[B]:DGD:HA62	35:C:518[B]:DGD:HA31	1.91	0.41
1:a:213[B]:ALA:HB2	4:d:275[B]:PRO:HG2	2.03	0.41
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.55	0.41
2:b:413:ASP:O	2:b:417:VAL:HG23	2.20	0.41
32:d:409[B]:LHG:H332	32:d:409[B]:LHG:H302	1.82	0.41
5:e:26:THR:HB	38:f:101:HEM:HAB	2.03	0.41
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.02	0.41
32:E:101[A]:LHG:H291	32:E:101[A]:LHG:H261	1.75	0.41
29:a:413[B]:PL9:H503	17:x:24:THR:OG1	2.20	0.41
3:c:182:PHE:HA	34:c:521:HTG:H61	2.03	0.41
7:h:43:LEU:O	7:h:47:GLU:HG3	2.21	0.41
31:t:101:LMT:H112	31:t:101:LMT:H81	1.74	0.41
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB1	2.03	0.41
2:B:383[B]:PHE:CZ	13:O:167:GLY:HA2	2.56	0.41
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.46	0.41
13:O:39[A]:ARG:HB2	13:O:246:ALA:HB2	2.03	0.41
26:a:409[B]:SQD:H302	23:c:508:CLA:H71	2.02	0.41
2:b:162:PHE:O	23:b:606:CLA:HHD	2.20	0.41
3:c:131:TYR:CD1	3:c:135:ARG:HB3	2.56	0.41
3:c:334[A]:PRO:HA	13:o:153:THR:OG1	2.21	0.41
25:c:514:BCR:H15C	25:c:514:BCR:H351	1.83	0.41
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.20	0.41
23:d:405:CLA:H3A	23:d:405:CLA:HBA1	1.83	0.41
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:451:PHE:CD1	2:b:451:PHE:C	2.99	0.41
3:c:334[B]:PRO:HA	13:o:153:THR:OG1	2.21	0.41
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.40
23:A:404[A]:CLA:CBD	23:A:405[A]:CLA:HAC2	2.51	0.40
25:B:618:BCR:C8	25:B:618:BCR:H331	2.50	0.40
32:E:101[B]:LHG:H291	32:E:101[B]:LHG:H261	1.76	0.40
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.85	0.40
25:T:102:BCR:H11C	25:T:102:BCR:H341	1.83	0.40
1:a:230:THR:HG21	11:l:8:GLN:HE22	1.86	0.40
3:c:82:TYR:OH	3:c:394[B]:GLU:OE2	2.32	0.40
3:c:152:LYS:HD2	41:c:739:HOH:O	2.20	0.40
29:A:414[A]:PL9:H121	29:A:414[A]:PL9:HC8	1.78	0.40
23:B:615:CLA:H91	23:B:615:CLA:H112	1.74	0.40
10:K:16:ALA:O	10:K:19:ASP:HB2	2.21	0.40
10:k:20:PRO:HB3	18:y:21:GLN:HG3	2.02	0.40
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	2.04	0.40
23:B:601:CLA:HAA1	23:B:601:CLA:HBD	2.03	0.40
23:B:605:CLA:H192	23:B:605:CLA:H162	1.93	0.40
10:K:23:ASP:OD2	18:Y:21:GLN:NE2	2.53	0.40
26:a:409[B]:SQD:H271	32:d:409[B]:LHG:H141	2.02	0.40
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.80	0.40
3:c:238:ILE:O	3:c:242:LEU:HG	2.21	0.40
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:HC2	1.71	0.40
23:B:602:CLA:H162	23:B:602:CLA:H203	1.63	0.40
33:B:620:LMG:H112	33:B:620:LMG:H141	1.84	0.40
5:E:18:ARG:H	9:J:2:SER:N	2.18	0.40
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.04	0.40
18:Y:39:LEU:HD23	18:Y:39:LEU:HA	1.92	0.40
2:b:247:PHE:CE2	23:b:602:CLA:H102	2.57	0.40
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.03	0.40
18:y:22:LEU:HA	18:y:25:ILE:HG22	2.02	0.40
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.86	0.40
23:B:613:CLA:H143	23:B:613:CLA:H111	1.89	0.40
3:C:275:SER:HB3	23:C:510:CLA:HED3	2.03	0.40
35:C:518[A]:DGD:HAE2	35:C:518[A]:DGD:HA81	1.86	0.40
4:D:209[B]:LEU:HD23	4:D:209[B]:LEU:C	2.46	0.40
5:E:9:PRO:HA	32:E:101[A]:LHG:HC31	2.03	0.40
23:a:407:CLA:H41	23:a:407:CLA:H61	1.90	0.40
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	553/344 (161%)	546 (99%)	5 (1%)	2 (0%)	30 34
1	a	551/344 (160%)	539 (98%)	10 (2%)	2 (0%)	30 34
2	B	524/505 (104%)	517 (99%)	7 (1%)	0	100 100
2	b	521/505 (103%)	511 (98%)	10 (2%)	0	100 100
3	C	548/455 (120%)	541 (99%)	6 (1%)	1 (0%)	43 51
3	c	554/455 (122%)	539 (97%)	14 (2%)	1 (0%)	43 51
4	D	454/342 (133%)	438 (96%)	16 (4%)	0	100 100
4	d	457/342 (134%)	444 (97%)	13 (3%)	0	100 100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100 100
5	e	79/84 (94%)	78 (99%)	1 (1%)	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%)	61 (98%)	1 (2%)	0	100 100
7	h	63/65 (97%)	61 (97%)	1 (2%)	1 (2%)	7 6
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4 2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
9	J	36/39 (92%)	36 (100%)	0	0	100 100
9	j	37/39 (95%)	36 (97%)	1 (3%)	0	100 100
10	K	35/37 (95%)	35 (100%)	0	0	100 100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
11	L	36/37 (97%)	36 (100%)	0	0	100 100
11	l	36/37 (97%)	36 (100%)	0	0	100 100
12	M	32/36 (89%)	32 (100%)	0	0	100 100
12	m	34/36 (94%)	33 (97%)	1 (3%)	0	100 100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	92 (95%)	5 (5%)	0	100	100
15	u	99/104 (95%)	95 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	137 (98%)	3 (2%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7	5
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7	5
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	6180/5384 (115%)	6038 (98%)	131 (2%)	11 (0%)	43	51

All (11) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	444/279 (159%)	442 (100%)	2 (0%)	81 90
1	a	442/279 (158%)	441 (100%)	1 (0%)	87 94
2	B	423/403 (105%)	418 (99%)	5 (1%)	63 78
2	b	420/403 (104%)	408 (97%)	12 (3%)	37 51
3	C	431/356 (121%)	422 (98%)	9 (2%)	47 63
3	c	437/356 (123%)	430 (98%)	7 (2%)	55 71
4	D	368/277 (133%)	365 (99%)	3 (1%)	73 85
4	d	372/277 (134%)	368 (99%)	4 (1%)	65 79
5	E	72/73 (99%)	70 (97%)	2 (3%)	38 52
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 75
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30 41
7	h	55/54 (102%)	54 (98%)	1 (2%)	51 68
8	I	34/34 (100%)	32 (94%)	2 (6%)	18 22
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 51
9	J	26/27 (96%)	25 (96%)	1 (4%)	29 40
9	j	26/27 (96%)	25 (96%)	1 (4%)	29 40
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 3
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 7
11	L	36/35 (103%)	36 (100%)	0	100 100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 52
12	M	30/32 (94%)	27 (90%)	3 (10%)	7 7
12	m	32/32 (100%)	30 (94%)	2 (6%)	16 19
13	O	216/207 (104%)	210 (97%)	6 (3%)	38 52
13	o	213/207 (103%)	207 (97%)	6 (3%)	38 52
14	T	32/28 (114%)	28 (88%)	4 (12%)	4 4
14	t	31/28 (111%)	31 (100%)	0	100 100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44 59
15	u	88/89 (99%)	86 (98%)	2 (2%)	44 59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	V	123/117 (105%)	122 (99%)	1 (1%)	73 85
16	v	123/117 (105%)	119 (97%)	4 (3%)	33 45
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24 33
18	y	22/23 (96%)	18 (82%)	4 (18%)	2 1
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 22
19	z	52/52 (100%)	45 (86%)	7 (14%)	4 3
20	R	29/29 (100%)	27 (93%)	2 (7%)	14 16
All	All	5110/4403 (116%)	5001 (98%)	109 (2%)	45 63

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
2	B	161	LEU
2	B	299	GLU
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	30	SER
3	C	142	GLU
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	54	SER
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG

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Mol	Chain	Res	Type
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
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
18	Y	30	ILE
1	a	13	LEU
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
2	b	240	SER
2	b	298	LEU
2	b	362	PHE
2	b	472	ARG
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	491[A]	VAL
2	b	491[B]	VAL
3	c	142	GLU
3	c	152	LYS
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET

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Mol	Chain	Res	Type
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	71	GLU
7	h	65	LEU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	109	GLU
18	y	18	VAL
18	y	19	ILE
18	y	30	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	20	VAL
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	32	ASP
19	z	42	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	322	GLN
5	E	60	GLN
11	L	8	GLN
13	O	231	HIS
15	U	78	ASN
2	b	14	ASN
2	b	331	ASN
3	c	19	ASN
3	c	201	ASN
3	c	415	ASN
10	k	40	GLN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN
18	y	45	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	0.63	0	8,9,11	1.16	1 (12%)
14	FME	T	1	14	8,9,10	0.69	0	8,9,11	1.59	3 (37%)
8	FME	I	1	8	8,9,10	0.65	0	8,9,11	1.17	1 (12%)
12	FME	m	1	12	8,9,10	0.61	0	8,9,11	1.40	2 (25%)
14	FME	t	1	14	8,9,10	0.77	0	8,9,11	1.62	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	FME	i	1	8	8,9,10	0.68	0	8,9,11	1.10	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	M	1	12	-	2/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
12	FME	m	1	12	-	1/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-2.96	118.27	122.82
14	T	1	FME	CB-CA-N	-2.74	105.53	110.52
14	t	1	FME	O-C-CA	-2.54	118.23	124.77
12	m	1	FME	O1-CN-N	-2.28	119.42	125.32
12	m	1	FME	CA-N-CN	-2.27	119.34	122.82
8	I	1	FME	O-C-CA	-2.23	119.03	124.77
14	T	1	FME	CA-N-CN	2.23	126.25	122.82
12	M	1	FME	O-C-CA	-2.16	119.22	124.77
14	T	1	FME	CG-CB-CA	2.10	119.29	112.87

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 274 ligands modelled in this entry, 21 are monoatomic and 20 are unknown - leaving 233 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
27	GOL	D	412	-	5,5,5	1.51	1 (20%)	5,5,5	0.92	0
32	LHG	d	409[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	4 (7%)
26	SQD	f	102	-	41,43,54	1.13	2 (4%)	51,54,65	1.51	9 (17%)
31	LMT	b	627	-	25,25,36	0.89	1 (4%)	30,30,47	1.13	3 (10%)
23	CLA	a	405[B]	41	69,73,73	2.00	20 (28%)	82,113,113	2.71	31 (37%)
27	GOL	c	525[B]	-	5,5,5	0.83	0	5,5,5	1.07	0
34	HTG	V	202	-	11,11,19	0.31	0	15,15,24	1.07	1 (6%)
37	BCT	d	401[B]	21	3,3,3	0.47	0	2,3,3	1.21	0
31	LMT	t	101	-	26,26,36	0.89	1 (3%)	31,31,47	1.28	1 (3%)
35	DGD	C	517[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.15	8 (10%)
29	PL9	a	413[A]	-	55,55,55	0.67	2 (3%)	68,69,69	2.01	21 (30%)
23	CLA	B	607	41	69,73,73	1.92	19 (27%)	82,113,113	2.71	31 (37%)
33	LMG	a	415	-	51,51,55	0.92	2 (3%)	59,59,63	1.20	4 (6%)
25	BCR	B	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.38	8 (14%)
27	GOL	A	411	-	5,5,5	1.26	0	5,5,5	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	C	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	1.01	5 (6%)
23	CLA	B	602	-	69,73,73	2.00	20 (28%)	82,113,113	2.73	32 (39%)
32	LHG	D	406[B]	-	48,48,48	0.88	2 (4%)	51,54,54	0.99	3 (5%)
27	GOL	B	623	-	5,5,5	0.78	0	5,5,5	1.24	1 (20%)
23	CLA	b	614	-	69,73,73	1.98	20 (28%)	82,113,113	2.83	34 (41%)
33	LMG	c	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.36	8 (13%)
27	GOL	b	628	-	5,5,5	0.42	0	5,5,5	1.51	1 (20%)
25	BCR	A	409	-	41,41,41	1.01	1 (2%)	56,56,56	1.31	7 (12%)
23	CLA	b	601	41	69,73,73	2.07	20 (28%)	82,113,113	2.63	30 (36%)
23	CLA	A	405[B]	41	69,73,73	1.97	20 (28%)	82,113,113	2.68	35 (42%)
24	PHO	A	407[B]	-	58,69,69	2.70	10 (17%)	55,99,99	2.89	14 (25%)
28	OEX	a	412[A]	3,41,1	0,15,15	-	-	-		
27	GOL	a	418	-	5,5,5	1.49	1 (20%)	5,5,5	0.89	0
25	BCR	y	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.62	9 (16%)
23	CLA	A	404[B]	-	69,73,73	2.04	20 (28%)	82,113,113	2.71	31 (37%)
27	GOL	O	303	-	5,5,5	0.98	0	5,5,5	1.21	1 (20%)
32	LHG	d	409[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	3 (5%)
32	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.16	3 (5%)
27	GOL	c	525[A]	-	5,5,5	0.99	0	5,5,5	1.02	0
37	BCT	d	401[A]	21	3,3,3	0.46	0	2,3,3	1.59	0
34	HTG	b	622	-	19,19,19	1.05	2 (10%)	23,24,24	1.89	6 (26%)
25	BCR	h	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	14 (25%)
35	DGD	C	517[A]	-	63,63,67	0.82	2 (3%)	77,77,81	1.21	9 (11%)
23	CLA	d	405	-	69,73,73	2.02	20 (28%)	82,113,113	2.65	31 (37%)
27	GOL	o	303	-	5,5,5	1.09	1 (20%)	5,5,5	1.19	1 (20%)
23	CLA	d	402[B]	41	69,73,73	2.00	16 (23%)	82,113,113	2.69	32 (39%)
34	HTG	B	624	-	19,19,19	0.95	2 (10%)	23,24,24	1.16	3 (13%)
35	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.03	5 (6%)
23	CLA	B	609	-	69,73,73	1.97	17 (24%)	82,113,113	2.69	30 (36%)
27	GOL	v	202[B]	-	5,5,5	1.17	0	5,5,5	0.85	0
25	BCR	B	619	-	41,41,41	1.09	1 (2%)	56,56,56	1.31	6 (10%)
27	GOL	B	626	-	5,5,5	1.13	0	5,5,5	1.00	0
23	CLA	B	606	-	69,73,73	1.94	18 (26%)	82,113,113	2.84	31 (37%)
25	BCR	b	619	-	41,41,41	1.13	1 (2%)	56,56,56	1.39	6 (10%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.07	4 (8%)
23	CLA	C	502	-	69,73,73	1.94	19 (27%)	82,113,113	2.71	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LHG	d	415[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.09	5 (9%)
23	CLA	A	405[A]	41	69,73,73	1.91	18 (26%)	82,113,113	2.74	36 (43%)
23	CLA	B	615	-	69,73,73	2.03	17 (24%)	82,113,113	2.70	31 (37%)
24	PHO	A	407[A]	-	58,69,69	2.70	13 (22%)	55,99,99	2.89	15 (27%)
40	HEC	v	201	16	46,50,50	1.95	5 (10%)	58,82,82	1.86	4 (6%)
33	LMG	D	411	39	51,51,55	0.81	2 (3%)	59,59,63	1.07	4 (6%)
27	GOL	c	526	-	5,5,5	1.17	1 (20%)	5,5,5	1.07	0
33	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	1.15	7 (11%)
26	SQD	a	409[B]	-	52,54,54	0.91	2 (3%)	62,65,65	1.61	13 (20%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.53	12 (21%)
31	LMT	F	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.06	3 (6%)
23	CLA	A	404[A]	-	69,73,73	1.97	19 (27%)	82,113,113	2.69	33 (40%)
23	CLA	c	501	-	69,73,73	1.95	19 (27%)	82,113,113	2.75	31 (37%)
32	LHG	L	101[B]	-	48,48,48	0.93	3 (6%)	51,54,54	1.04	4 (7%)
34	HTG	B	622	-	19,19,19	0.71	1 (5%)	23,24,24	1.33	2 (8%)
31	LMT	T	101	-	36,36,36	1.07	4 (11%)	47,47,47	1.08	2 (4%)
23	CLA	B	613	-	69,73,73	1.96	19 (27%)	82,113,113	2.63	31 (37%)
23	CLA	c	502	-	69,73,73	1.97	17 (24%)	82,113,113	2.58	28 (34%)
25	BCR	Y	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.80	15 (26%)
35	DGD	c	516[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	6 (7%)
24	PHO	a	406[B]	-	58,69,69	2.76	13 (22%)	55,99,99	2.83	17 (30%)
23	CLA	d	402[A]	41	69,73,73	1.98	17 (24%)	82,113,113	2.66	30 (36%)
31	LMT	B	629	-	25,25,36	0.87	1 (4%)	30,30,47	1.21	3 (10%)
27	GOL	v	202[A]	-	5,5,5	1.35	1 (20%)	5,5,5	0.77	0
23	CLA	A	406[B]	41	69,73,73	2.02	19 (27%)	82,113,113	2.70	32 (39%)
23	CLA	B	603	-	69,73,73	1.98	19 (27%)	82,113,113	2.74	32 (39%)
23	CLA	c	511	3	69,73,73	2.05	19 (27%)	82,113,113	2.69	33 (40%)
25	BCR	a	408	-	41,41,41	1.02	1 (2%)	56,56,56	1.41	9 (16%)
29	PL9	A	414[A]	-	55,55,55	0.70	3 (5%)	68,69,69	2.11	27 (39%)
35	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.93	4 (5%)
23	CLA	B	616	-	69,73,73	1.95	19 (27%)	82,113,113	2.76	31 (37%)
31	LMT	C	525	-	36,36,36	1.04	2 (5%)	47,47,47	1.17	4 (8%)
32	LHG	d	415[A]	-	48,48,48	0.90	2 (4%)	51,54,54	1.14	5 (9%)
23	CLA	b	609	-	69,73,73	1.99	19 (27%)	82,113,113	2.67	32 (39%)
32	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.20	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	B	610	41	69,73,73	2.03	19 (27%)	82,113,113	2.78	31 (37%)
23	CLA	C	504	-	69,73,73	1.99	20 (28%)	82,113,113	2.66	31 (37%)
34	HTG	b	625	-	19,19,19	0.98	2 (10%)	23,24,24	1.45	3 (13%)
35	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	0.99	5 (6%)
35	DGD	c	518	-	63,63,67	0.88	4 (6%)	77,77,81	1.04	5 (6%)
26	SQD	a	411	-	52,54,54	1.01	2 (3%)	62,65,65	1.21	7 (11%)
23	CLA	C	508	41	69,73,73	1.98	19 (27%)	82,113,113	2.65	29 (35%)
31	LMT	B	627	-	36,36,36	1.16	3 (8%)	47,47,47	1.37	5 (10%)
26	SQD	a	409[A]	-	52,54,54	0.89	2 (3%)	62,65,65	1.74	12 (19%)
27	GOL	C	523[B]	-	5,5,5	1.09	0	5,5,5	0.94	0
23	CLA	B	604	-	69,73,73	1.98	22 (31%)	82,113,113	2.60	31 (37%)
25	BCR	K	102	-	41,41,41	1.09	1 (2%)	56,56,56	1.41	8 (14%)
27	GOL	A	418	-	5,5,5	1.60	2 (40%)	5,5,5	1.17	1 (20%)
31	LMT	a	416	-	36,36,36	0.98	2 (5%)	47,47,47	1.05	1 (2%)
28	OEX	A	413[A]	3,41,1	0,15,15	-	-	-		
23	CLA	A	408	-	69,73,73	1.93	19 (27%)	82,113,113	2.77	36 (43%)
23	CLA	D	403	-	69,73,73	2.07	19 (27%)	82,113,113	2.66	34 (41%)
23	CLA	b	608	-	69,73,73	1.98	20 (28%)	82,113,113	2.70	31 (37%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.45	7 (12%)
33	LMG	d	413	39	51,51,55	0.88	2 (3%)	59,59,63	1.14	5 (8%)
35	DGD	c	516[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
27	GOL	V	203[B]	-	5,5,5	1.08	0	5,5,5	0.99	0
23	CLA	a	407	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	31 (37%)
23	CLA	C	514	-	69,73,73	2.01	18 (26%)	82,113,113	2.68	31 (37%)
25	BCR	k	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.60	16 (28%)
25	BCR	C	516	-	41,41,41	1.06	1 (2%)	56,56,56	1.40	7 (12%)
24	PHO	a	406[A]	-	58,69,69	2.73	11 (18%)	55,99,99	2.83	15 (27%)
27	GOL	b	624	-	5,5,5	1.18	1 (20%)	5,5,5	0.87	0
29	PL9	A	414[B]	-	55,55,55	0.67	3 (5%)	68,69,69	2.04	25 (36%)
25	BCR	c	514	-	41,41,41	1.01	1 (2%)	56,56,56	1.69	14 (25%)
23	CLA	A	406[A]	41	69,73,73	1.97	18 (26%)	82,113,113	2.71	33 (40%)
37	BCT	D	401[B]	21	3,3,3	0.48	0	2,3,3	1.26	0
35	DGD	c	517[A]	-	63,63,67	0.84	3 (4%)	77,77,81	0.98	5 (6%)
23	CLA	C	509	-	69,73,73	2.05	21 (30%)	82,113,113	2.64	28 (34%)
26	SQD	b	620	-	52,54,54	0.99	2 (3%)	62,65,65	1.64	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	504	41	69,73,73	2.05	20 (28%)	82,113,113	2.69	33 (40%)
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.33	6 (11%)
27	GOL	a	417	-	5,5,5	1.20	0	5,5,5	1.10	0
25	BCR	d	406	-	41,41,41	1.16	2 (4%)	56,56,56	1.90	14 (25%)
33	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.13	6 (10%)
33	LMG	C	501	-	51,51,55	0.93	2 (3%)	59,59,63	1.47	9 (15%)
27	GOL	C	523[A]	-	5,5,5	1.24	0	5,5,5	0.89	0
28	OEX	A	413[B]	3,41,1	0,15,15	-	-	-		
27	GOL	O	302	-	5,5,5	0.97	0	5,5,5	0.92	0
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.12	4 (9%)
24	PHO	A	416[B]	-	58,69,69	2.76	14 (24%)	55,99,99	3.04	18 (32%)
29	PL9	D	405[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.62	16 (23%)
31	LMT	M	101	-	36,36,36	1.10	3 (8%)	47,47,47	1.19	5 (10%)
23	CLA	C	507	-	69,73,73	2.02	20 (28%)	82,113,113	2.69	34 (41%)
23	CLA	B	611	-	69,73,73	2.51	20 (28%)	82,113,113	3.62	33 (40%)
23	CLA	C	512	3	69,73,73	2.00	22 (31%)	82,113,113	2.60	29 (35%)
23	CLA	C	513	-	69,73,73	2.02	20 (28%)	82,113,113	2.71	36 (43%)
23	CLA	D	402[B]	-	69,73,73	2.00	19 (27%)	82,113,113	2.76	31 (37%)
23	CLA	b	605	-	69,73,73	1.92	20 (28%)	82,113,113	2.86	28 (34%)
23	CLA	c	510	-	69,73,73	2.00	20 (28%)	82,113,113	2.75	33 (40%)
27	GOL	V	203[A]	-	5,5,5	1.29	1 (20%)	5,5,5	0.97	0
29	PL9	d	407[B]	-	55,55,55	0.67	2 (3%)	68,69,69	1.59	15 (22%)
32	LHG	d	408[B]	-	48,48,48	0.89	3 (6%)	51,54,54	1.05	4 (7%)
27	GOL	l	103[B]	-	5,5,5	0.95	0	5,5,5	1.05	0
33	LMG	B	620	-	51,51,55	0.93	2 (3%)	59,59,63	1.32	4 (6%)
26	SQD	A	410[B]	-	52,54,54	0.86	2 (3%)	62,65,65	1.77	11 (17%)
23	CLA	c	506	-	69,73,73	1.99	19 (27%)	82,113,113	2.67	32 (39%)
37	BCT	D	401[A]	21	3,3,3	0.43	0	2,3,3	1.83	0
23	CLA	d	404[B]	-	69,73,73	1.96	19 (27%)	82,113,113	2.67	32 (39%)
40	HEC	V	201	16	46,50,50	1.91	6 (13%)	58,82,82	1.77	8 (13%)
34	HTG	d	412	-	16,16,19	0.89	1 (6%)	20,21,24	1.35	1 (5%)
23	CLA	c	507	41	69,73,73	2.00	18 (26%)	82,113,113	2.72	31 (37%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.30	7 (12%)
26	SQD	l	101	-	52,54,54	1.01	3 (5%)	62,65,65	1.72	11 (17%)
31	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.21	3 (10%)
35	DGD	H	102	-	63,63,67	0.90	4 (6%)	77,77,81	1.05	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HTG	b	623	-	19,19,19	0.97	1 (5%)	23,24,24	1.72	2 (8%)
23	CLA	B	614	-	69,73,73	2.03	20 (28%)	82,113,113	2.83	32 (39%)
23	CLA	B	612	-	69,73,73	1.95	19 (27%)	82,113,113	2.74	30 (36%)
33	LMG	m	101	-	51,51,55	0.88	2 (3%)	59,59,63	1.28	6 (10%)
38	HEM	f	101	6,5	50,50,50	1.50	6 (12%)	67,82,82	1.66	11 (16%)
32	LHG	D	407[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.96	3 (5%)
23	CLA	b	606	-	69,73,73	1.96	19 (27%)	82,113,113	2.73	32 (39%)
32	LHG	E	101[A]	-	41,41,48	1.07	2 (4%)	44,47,54	1.12	3 (6%)
24	PHO	A	416[A]	-	58,69,69	2.74	14 (24%)	55,99,99	2.91	17 (30%)
29	PL9	D	405[A]	-	55,55,55	0.64	2 (3%)	68,69,69	1.64	18 (26%)
31	LMT	B	628	-	36,36,36	0.94	1 (2%)	47,47,47	1.18	4 (8%)
31	LMT	e	101	-	36,36,36	0.99	1 (2%)	47,47,47	0.99	1 (2%)
29	PL9	d	407[A]	-	55,55,55	0.67	1 (1%)	68,69,69	1.62	15 (22%)
32	LHG	b	629[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.06	3 (5%)
32	LHG	d	408[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.09	4 (7%)
23	CLA	D	402[A]	-	69,73,73	1.96	18 (26%)	82,113,113	2.75	33 (40%)
23	CLA	B	605	-	69,73,73	1.97	18 (26%)	82,113,113	2.81	32 (39%)
32	LHG	a	419[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
27	GOL	l	103[A]	-	5,5,5	1.01	0	5,5,5	1.04	0
27	GOL	a	410	-	5,5,5	1.01	0	5,5,5	1.06	0
34	HTG	C	522	-	19,19,19	0.83	1 (5%)	23,24,24	1.25	2 (8%)
23	CLA	b	616	-	69,73,73	1.99	20 (28%)	82,113,113	2.86	33 (40%)
23	CLA	a	404[A]	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	34 (41%)
25	BCR	D	404	-	41,41,41	1.12	1 (2%)	56,56,56	1.85	16 (28%)
23	CLA	b	610	41	69,73,73	2.00	20 (28%)	82,113,113	2.69	31 (37%)
23	CLA	d	404[A]	-	69,73,73	1.92	19 (27%)	82,113,113	2.67	30 (36%)
26	SQD	A	412	-	52,54,54	0.97	2 (3%)	62,65,65	1.22	8 (12%)
31	LMT	m	103	-	36,36,36	1.06	2 (5%)	47,47,47	1.09	3 (6%)
24	PHO	d	403[A]	-	58,69,69	2.76	13 (22%)	55,99,99	3.06	17 (30%)
25	BCR	t	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.62	12 (21%)
23	CLA	C	503	-	69,73,73	2.01	20 (28%)	82,113,113	2.55	30 (36%)
23	CLA	C	510	-	69,73,73	2.03	21 (30%)	82,113,113	2.70	31 (37%)
23	CLA	b	611	-	69,73,73	1.95	19 (27%)	82,113,113	2.82	29 (35%)
23	CLA	b	604	-	69,73,73	1.97	18 (26%)	82,113,113	2.71	29 (35%)
23	CLA	c	508	-	69,73,73	2.08	21 (30%)	82,113,113	2.64	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	511	-	69,73,73	2.00	19 (27%)	82,113,113	2.76	33 (40%)
23	CLA	c	513	-	69,73,73	2.07	21 (30%)	82,113,113	2.69	31 (37%)
23	CLA	c	505	-	69,73,73	2.02	19 (27%)	82,113,113	2.69	30 (36%)
25	BCR	B	617	-	41,41,41	1.10	1 (2%)	56,56,56	1.33	10 (17%)
34	HTG	D	410	-	16,16,19	0.97	1 (6%)	20,21,24	1.28	1 (5%)
23	CLA	C	505	41	69,73,73	1.97	19 (27%)	82,113,113	2.63	29 (35%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	4 (7%)
32	LHG	b	629[A]	-	48,48,48	0.86	3 (6%)	51,54,54	1.05	4 (7%)
34	HTG	B	621	-	19,19,19	1.02	2 (10%)	23,24,24	1.54	4 (17%)
23	CLA	b	615	-	69,73,73	1.96	17 (24%)	82,113,113	2.70	31 (37%)
26	SQD	A	410[A]	-	52,54,54	0.86	2 (3%)	62,65,65	1.79	9 (14%)
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.94	2 (4%)
23	CLA	C	506	-	69,73,73	1.98	19 (27%)	82,113,113	2.68	30 (36%)
23	CLA	c	512	-	69,73,73	2.04	19 (27%)	82,113,113	2.68	33 (40%)
23	CLA	c	503	-	69,73,73	2.05	19 (27%)	82,113,113	2.74	30 (36%)
23	CLA	B	601	41	69,73,73	2.04	21 (30%)	82,113,113	2.70	31 (37%)
23	CLA	a	404[B]	-	69,73,73	1.97	19 (27%)	82,113,113	2.77	35 (42%)
23	CLA	a	405[A]	41	69,73,73	1.94	19 (27%)	82,113,113	2.70	33 (40%)
38	HEM	E	102	6,5	50,50,50	1.54	7 (14%)	67,82,82	1.78	14 (20%)
33	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.36	7 (11%)
29	PL9	a	413[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.98	23 (33%)
23	CLA	c	509	-	69,73,73	2.01	18 (26%)	82,113,113	2.70	31 (37%)
31	LMT	A	417	-	36,36,36	0.90	2 (5%)	47,47,47	1.06	2 (4%)
24	PHO	d	403[B]	-	58,69,69	2.78	14 (24%)	55,99,99	3.00	17 (30%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.09	5 (6%)
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.44	6 (13%)
23	CLA	b	612	-	69,73,73	1.97	20 (28%)	82,113,113	2.71	32 (39%)
26	SQD	X	101	-	41,43,54	1.17	3 (7%)	51,54,65	2.13	13 (25%)
27	GOL	o	302	-	5,5,5	1.03	0	5,5,5	1.05	0
25	BCR	T	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.59	12 (21%)
23	CLA	b	613	-	69,73,73	1.89	19 (27%)	82,113,113	2.62	30 (36%)
34	HTG	c	521	-	19,19,19	0.87	1 (5%)	23,24,24	1.36	2 (8%)
23	CLA	b	607	41	69,73,73	1.97	20 (28%)	82,113,113	2.59	30 (36%)
32	LHG	D	406[A]	-	48,48,48	0.86	3 (6%)	51,54,54	1.00	4 (7%)
27	GOL	d	414	-	5,5,5	1.09	0	5,5,5	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	C	515	-	41,41,41	1.07	1 (2%)	56,56,56	1.42	7 (12%)
23	CLA	B	608	-	69,73,73	1.94	21 (30%)	82,113,113	2.68	35 (42%)
23	CLA	b	602	-	69,73,73	2.06	19 (27%)	82,113,113	2.75	37 (45%)
28	OEX	a	412[B]	3,41,1	0,15,15	-	-	-		
23	CLA	b	603	-	69,73,73	1.95	20 (28%)	82,113,113	2.72	35 (42%)
25	BCR	c	515	-	41,41,41	1.01	1 (2%)	56,56,56	1.40	12 (21%)

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	D	412	-	-	4/4/4/4	-
32	LHG	d	409[B]	-	-	12/53/53/53	-
26	SQD	f	102	-	-	13/38/58/69	0/1/1/1
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	a	405[B]	41	-	3/39/115/115	-
27	GOL	c	525[B]	-	-	0/4/4/4	-
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
35	DGD	C	517[B]	-	-	15/51/91/95	0/2/2/2
29	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	607	41	1/1/15/20	1/39/115/115	-
33	LMG	a	415	-	-	12/46/66/70	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
27	GOL	A	411	-	-	2/4/4/4	-
35	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	B	602	-	1/1/15/20	10/39/115/115	-
32	LHG	D	406[B]	-	-	16/53/53/53	-
27	GOL	B	623	-	-	4/4/4/4	-
23	CLA	b	614	-	1/1/15/20	12/39/115/115	-
33	LMG	c	520	-	-	7/46/66/70	0/1/1/1
27	GOL	b	628	-	-	0/4/4/4	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	b	601	41	1/1/15/20	15/39/115/115	-
23	CLA	A	405[B]	41	1/1/15/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PHO	A	407[B]	-	-	0/37/103/103	0/5/6/6
27	GOL	a	418	-	-	0/4/4/4	-
25	BCR	y	101	-	-	2/29/63/63	0/2/2/2
23	CLA	A	404[B]	-	1/1/15/20	2/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
32	LHG	d	409[A]	-	-	11/53/53/53	-
32	LHG	L	101[A]	-	-	19/53/53/53	-
27	GOL	c	525[A]	-	-	0/4/4/4	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
35	DGD	C	517[A]	-	-	12/51/91/95	0/2/2/2
23	CLA	d	405	-	1/1/15/20	8/39/115/115	-
27	GOL	o	303	-	-	2/4/4/4	-
23	CLA	d	402[B]	41	1/1/15/20	4/39/115/115	-
34	HTG	B	624	-	-	3/10/30/30	0/1/1/1
35	DGD	C	518[A]	-	-	14/51/91/95	0/2/2/2
23	CLA	B	609	-	1/1/15/20	0/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	B	626	-	-	2/4/4/4	-
23	CLA	B	606	-	1/1/15/20	7/39/115/115	-
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	C	502	-	1/1/15/20	5/39/115/115	-
32	LHG	d	415[B]	-	-	10/53/53/53	-
23	CLA	A	405[A]	41	-	2/39/115/115	-
23	CLA	B	615	-	1/1/15/20	8/39/115/115	-
24	PHO	A	407[A]	-	-	1/37/103/103	0/5/6/6
40	HEC	v	201	16	-	6/14/54/54	-
33	LMG	D	411	39	-	9/46/66/70	0/1/1/1
27	GOL	c	526	-	-	3/4/4/4	-
33	LMG	C	520	-	-	10/46/66/70	0/1/1/1
26	SQD	a	409[B]	-	-	11/49/69/69	0/1/1/1
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	404[A]	-	1/1/15/20	5/39/115/115	-
23	CLA	c	501	-	1/1/15/20	4/39/115/115	-
32	LHG	L	101[B]	-	-	19/53/53/53	-
34	HTG	B	622	-	-	2/10/30/30	0/1/1/1
31	LMT	T	101	-	-	10/21/61/61	0/2/2/2
23	CLA	B	613	-	1/1/15/20	7/39/115/115	-
23	CLA	c	502	-	1/1/15/20	2/39/115/115	-
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
35	DGD	c	516[B]	-	-	18/51/91/95	0/2/2/2
24	PHO	a	406[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	d	402[A]	41	1/1/15/20	4/39/115/115	-
31	LMT	B	629	-	-	11/17/37/61	0/1/1/2
27	GOL	v	202[A]	-	-	1/4/4/4	-
23	CLA	A	406[B]	41	-	6/39/115/115	-
23	CLA	B	603	-	1/1/15/20	6/39/115/115	-
23	CLA	c	511	3	1/1/15/20	7/39/115/115	-
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
35	DGD	c	517[B]	-	-	16/51/91/95	0/2/2/2
23	CLA	B	616	-	1/1/15/20	5/39/115/115	-
31	LMT	C	525	-	-	15/21/61/61	0/2/2/2
32	LHG	d	415[A]	-	-	12/53/53/53	-
23	CLA	b	609	-	1/1/15/20	0/39/115/115	-
32	LHG	A	419[B]	-	-	12/53/53/53	-
23	CLA	B	610	41	1/1/15/20	8/39/115/115	-
23	CLA	C	504	-	1/1/15/20	2/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
35	DGD	C	519	-	-	17/51/91/95	0/2/2/2
35	DGD	c	518	-	-	12/51/91/95	0/2/2/2
26	SQD	a	411	-	-	13/49/69/69	0/1/1/1
23	CLA	C	508	41	1/1/15/20	8/39/115/115	-
31	LMT	B	627	-	-	11/21/61/61	0/2/2/2
26	SQD	a	409[A]	-	-	9/49/69/69	0/1/1/1
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	B	604	-	1/1/15/20	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	K	102	-	-	3/29/63/63	0/2/2/2
27	GOL	A	418	-	-	1/4/4/4	-
31	LMT	a	416	-	-	11/21/61/61	0/2/2/2
23	CLA	A	408	-	1/1/15/20	8/39/115/115	-
23	CLA	D	403	-	1/1/15/20	15/39/115/115	-
23	CLA	b	608	-	-	4/39/115/115	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
33	LMG	d	413	39	-	8/46/66/70	0/1/1/1
35	DGD	c	516[A]	-	-	20/51/91/95	0/2/2/2
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	a	407	-	1/1/15/20	9/39/115/115	-
23	CLA	C	514	-	1/1/15/20	6/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
27	GOL	b	624	-	-	2/4/4/4	-
29	PL9	A	414[B]	-	-	18/53/73/73	0/1/1/1
25	BCR	c	514	-	-	0/29/63/63	0/2/2/2
23	CLA	A	406[A]	41	-	7/39/115/115	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
23	CLA	C	509	-	1/1/15/20	4/39/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
23	CLA	c	504	41	1/1/15/20	6/39/115/115	-
32	LHG	A	419[A]	-	-	10/53/53/53	-
27	GOL	a	417	-	-	2/4/4/4	-
25	BCR	d	406	-	-	4/29/63/63	0/2/2/2
33	LMG	c	519	-	-	12/46/66/70	0/1/1/1
33	LMG	C	501	-	-	14/46/66/70	0/1/1/1
27	GOL	C	523[A]	-	-	0/4/4/4	-
27	GOL	O	302	-	-	2/4/4/4	-
32	LHG	E	101[B]	-	-	18/46/46/53	-
24	PHO	A	416[B]	-	-	1/37/103/103	0/5/6/6
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
23	CLA	C	507	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	611	-	1/1/15/20	2/39/115/115	-
23	CLA	C	512	3	1/1/15/20	3/39/115/115	-
23	CLA	C	513	-	1/1/15/20	9/39/115/115	-
23	CLA	D	402[B]	-	1/1/15/20	2/39/115/115	-
23	CLA	b	605	-	1/1/15/20	6/39/115/115	-
23	CLA	c	510	-	1/1/15/20	11/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
29	PL9	d	407[B]	-	-	6/53/73/73	0/1/1/1
32	LHG	d	408[B]	-	-	13/53/53/53	-
27	GOL	l	103[B]	-	-	2/4/4/4	-
33	LMG	B	620	-	-	16/46/66/70	0/1/1/1
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
23	CLA	c	506	-	1/1/15/20	8/39/115/115	-
23	CLA	d	404[B]	-	1/1/15/20	4/39/115/115	-
40	HEC	V	201	16	-	6/14/54/54	-
34	HTG	d	412	-	-	1/7/27/30	0/1/1/1
23	CLA	c	507	41	1/1/15/20	9/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	SQD	l	101	-	-	13/49/69/69	0/1/1/1
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
35	DGD	H	102	-	-	7/51/91/95	0/2/2/2
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
23	CLA	B	614	-	1/1/15/20	13/39/115/115	-
23	CLA	B	612	-	1/1/15/20	4/39/115/115	-
33	LMG	m	101	-	-	10/46/66/70	0/1/1/1
38	HEM	f	101	6,5	-	8/14/54/54	-
32	LHG	D	407[B]	-	-	12/53/53/53	-
23	CLA	b	606	-	1/1/15/20	11/39/115/115	-
32	LHG	E	101[A]	-	-	21/46/46/53	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
29	PL9	D	405[A]	-	-	7/53/73/73	0/1/1/1
31	LMT	B	628	-	-	11/21/61/61	0/2/2/2
31	LMT	e	101	-	-	13/21/61/61	0/2/2/2
29	PL9	d	407[A]	-	-	6/53/73/73	0/1/1/1
32	LHG	b	629[B]	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	d	408[A]	-	-	12/53/53/53	-
23	CLA	D	402[A]	-	1/1/15/20	0/39/115/115	-
23	CLA	B	605	-	1/1/15/20	7/39/115/115	-
32	LHG	a	419[B]	-	-	16/46/46/53	-
27	GOL	l	103[A]	-	-	1/4/4/4	-
27	GOL	a	410	-	-	4/4/4/4	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
23	CLA	b	616	-	1/1/15/20	10/39/115/115	-
23	CLA	a	404[A]	-	1/1/15/20	3/39/115/115	-
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
23	CLA	b	610	41	1/1/15/20	5/39/115/115	-
23	CLA	d	404[A]	-	1/1/15/20	2/39/115/115	-
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2
24	PHO	d	403[A]	-	-	0/37/103/103	0/5/6/6
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	C	503	-	1/1/15/20	7/39/115/115	-
23	CLA	C	510	-	1/1/15/20	6/39/115/115	-
23	CLA	b	611	-	1/1/15/20	3/39/115/115	-
23	CLA	b	604	-	1/1/15/20	10/39/115/115	-
23	CLA	c	508	-	1/1/15/20	2/39/115/115	-
23	CLA	C	511	-	1/1/15/20	13/39/115/115	-
23	CLA	c	513	-	1/1/15/20	8/39/115/115	-
23	CLA	c	505	-	1/1/15/20	6/39/115/115	-
25	BCR	B	617	-	-	0/29/63/63	0/2/2/2
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	C	505	41	1/1/15/20	9/39/115/115	-
32	LHG	D	407[A]	-	-	13/53/53/53	-
32	LHG	b	629[A]	-	-	20/53/53/53	-
34	HTG	B	621	-	-	3/10/30/30	0/1/1/1
23	CLA	b	615	-	1/1/15/20	8/39/115/115	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
32	LHG	a	419[A]	-	-	16/46/46/53	-
23	CLA	C	506	-	1/1/15/20	4/39/115/115	-
23	CLA	c	512	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	503	-	1/1/15/20	1/39/115/115	-
23	CLA	B	601	41	1/1/15/20	10/39/115/115	-
23	CLA	a	404[B]	-	1/1/15/20	2/39/115/115	-
23	CLA	a	405[A]	41	-	5/39/115/115	-
38	HEM	E	102	6,5	-	4/14/54/54	-
33	LMG	C	521	-	-	15/46/66/70	0/1/1/1
29	PL9	a	413[B]	-	-	14/53/73/73	0/1/1/1
23	CLA	c	509	-	1/1/15/20	15/39/115/115	-
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
24	PHO	d	403[B]	-	-	3/37/103/103	0/5/6/6
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
33	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
23	CLA	b	612	-	1/1/15/20	3/39/115/115	-
26	SQD	X	101	-	-	15/38/58/69	0/1/1/1
27	GOL	o	302	-	-	2/4/4/4	-
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	613	-	1/1/15/20	4/39/115/115	-
34	HTG	c	521	-	-	1/10/30/30	0/1/1/1
23	CLA	b	607	41	1/1/15/20	3/39/115/115	-
32	LHG	D	406[A]	-	-	16/53/53/53	-
27	GOL	d	414	-	-	3/4/4/4	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	b	602	-	1/1/15/20	4/39/115/115	-
23	CLA	B	608	-	-	3/39/115/115	-
23	CLA	b	603	-	1/1/15/20	4/39/115/115	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2

All (1837) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[A]	PHO	C1D-C2D	9.27	1.49	1.39
24	a	406[B]	PHO	C1B-C2B	9.25	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	9.20	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	9.11	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	9.03	1.49	1.39
24	d	403[B]	PHO	C1D-C2D	8.95	1.49	1.39
24	d	403[A]	PHO	C1B-C2B	8.92	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403[B]	PHO	C1B-C2B	8.86	1.49	1.39
24	A	416[A]	PHO	C1D-C2D	8.86	1.49	1.39
24	d	403[A]	PHO	C1D-C2D	8.73	1.49	1.39
24	A	416[B]	PHO	C1D-C2D	8.66	1.49	1.39
24	a	406[A]	PHO	C1D-C2D	8.59	1.48	1.39
24	a	406[B]	PHO	C1D-C2D	8.58	1.48	1.39
24	A	407[A]	PHO	C1B-C2B	8.44	1.48	1.39
24	A	416[A]	PHO	C1B-C2B	8.41	1.48	1.39
24	A	416[B]	PHO	C1B-C2B	8.26	1.48	1.39
24	d	403[A]	PHO	C3B-C4B	8.05	1.49	1.41
24	A	416[B]	PHO	C3B-C4B	7.79	1.49	1.41
24	d	403[B]	PHO	C3B-C4B	7.77	1.49	1.41
24	A	416[A]	PHO	C3B-C4B	7.47	1.49	1.41
24	a	406[B]	PHO	C3B-C4B	7.46	1.49	1.41
24	a	406[A]	PHO	C3B-C4B	7.36	1.49	1.41
24	A	407[A]	PHO	C3B-C4B	7.26	1.48	1.41
23	B	611	CLA	CMB-C2B	7.25	1.65	1.50
40	V	201	HEC	CAC-C3C	7.03	1.57	1.35
40	v	201	HEC	CAC-C3C	6.95	1.57	1.35
24	A	416[B]	PHO	C4D-CHA	6.88	1.49	1.39
24	A	407[B]	PHO	C4D-CHA	6.85	1.49	1.39
24	a	406[B]	PHO	C4D-CHA	6.84	1.49	1.39
24	A	416[A]	PHO	C4D-CHA	6.82	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.81	1.49	1.39
24	a	406[A]	PHO	C4D-CHA	6.79	1.49	1.39
24	A	407[B]	PHO	C3B-C4B	6.78	1.48	1.41
24	d	403[B]	PHO	C4D-CHA	6.66	1.49	1.39
23	B	611	CLA	C1B-C2B	6.65	1.58	1.43
40	v	201	HEC	CAB-C3B	6.60	1.56	1.35
24	d	403[A]	PHO	C4D-CHA	6.52	1.49	1.39
24	a	406[A]	PHO	C3B-C2B	6.52	1.49	1.40
24	d	403[B]	PHO	C3B-C2B	6.48	1.49	1.40
24	a	406[B]	PHO	C3B-C2B	6.40	1.49	1.40
24	A	416[B]	PHO	C3B-C2B	6.37	1.49	1.40
23	B	611	CLA	C1D-ND	6.37	1.46	1.37
24	A	407[A]	PHO	C3B-C2B	6.34	1.49	1.40
24	A	407[B]	PHO	C3B-C2B	6.27	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	6.26	1.48	1.40
40	V	201	HEC	CAB-C3B	6.19	1.55	1.35
24	d	403[A]	PHO	C3B-C2B	6.05	1.48	1.40
24	a	406[B]	PHO	C3D-C2D	5.82	1.49	1.39
23	B	611	CLA	CHC-C1C	5.74	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	C3D-C2D	5.72	1.53	1.38
23	c	508	CLA	C3C-C2C	5.59	1.48	1.36
24	a	406[A]	PHO	C3D-C2D	5.56	1.49	1.39
23	d	402[B]	CLA	C3C-C2C	5.54	1.48	1.36
23	C	504	CLA	C3C-C2C	5.50	1.48	1.36
23	B	610	CLA	C3C-C2C	5.50	1.48	1.36
23	d	405	CLA	C3C-C2C	5.48	1.48	1.36
23	c	505	CLA	C3C-C2C	5.45	1.48	1.36
24	d	403[A]	PHO	C3D-C2D	5.42	1.48	1.39
23	b	605	CLA	C3C-C2C	5.40	1.48	1.36
24	A	416[A]	PHO	C3D-C2D	5.39	1.48	1.39
23	D	403	CLA	C3C-C2C	5.39	1.48	1.36
23	C	513	CLA	C3C-C2C	5.39	1.48	1.36
23	C	509	CLA	C3C-C2C	5.38	1.48	1.36
23	b	610	CLA	C3C-C2C	5.37	1.48	1.36
23	c	509	CLA	C3C-C2C	5.37	1.48	1.36
23	c	512	CLA	C3C-C2C	5.36	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.35	1.48	1.36
24	A	416[B]	PHO	OBD-CAD	5.31	1.29	1.22
23	b	609	CLA	O2D-CGD	5.30	1.46	1.33
23	c	503	CLA	C3C-C2C	5.29	1.48	1.36
23	b	612	CLA	C3C-C2C	5.29	1.48	1.36
23	c	509	CLA	O2D-CGD	5.29	1.46	1.33
24	A	416[B]	PHO	C3D-C2D	5.29	1.48	1.39
24	d	403[B]	PHO	C3D-C2D	5.29	1.48	1.39
23	B	605	CLA	C3C-C2C	5.27	1.48	1.36
23	C	511	CLA	C1D-ND	5.26	1.44	1.37
23	B	611	CLA	C3C-C2C	5.26	1.48	1.36
23	d	402[A]	CLA	C3C-C2C	5.26	1.48	1.36
23	c	504	CLA	O2D-CGD	5.25	1.46	1.33
23	a	405[A]	CLA	C3C-C2C	5.24	1.48	1.36
23	b	601	CLA	C3C-C2C	5.22	1.48	1.36
23	b	615	CLA	C3C-C2C	5.22	1.48	1.36
23	a	404[B]	CLA	C3C-C2C	5.22	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.21	1.48	1.36
23	b	614	CLA	C3C-C2C	5.21	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.21	1.48	1.36
25	C	515	BCR	C23-C22	-5.20	1.34	1.46
23	b	603	CLA	C3C-C2C	5.19	1.48	1.36
25	d	406	BCR	C23-C22	-5.18	1.34	1.46
23	D	402[B]	CLA	O2D-CGD	5.17	1.45	1.33
23	c	508	CLA	O2D-CGD	5.17	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	C3C-C2C	5.17	1.47	1.36
23	a	405[B]	CLA	C3C-C2C	5.16	1.47	1.36
23	B	604	CLA	C3C-C2C	5.16	1.47	1.36
24	d	403[A]	PHO	OBD-CAD	5.16	1.29	1.22
23	A	404[B]	CLA	C1D-ND	5.15	1.44	1.37
23	C	505	CLA	C3C-C2C	5.14	1.47	1.36
23	B	608	CLA	C3C-C2C	5.14	1.47	1.36
23	a	407	CLA	CHC-C1C	5.14	1.48	1.38
23	B	603	CLA	C3C-C2C	5.14	1.47	1.36
23	d	404[A]	CLA	C3C-C2C	5.14	1.47	1.36
23	c	510	CLA	O2D-CGD	5.13	1.45	1.33
23	C	503	CLA	C3C-C2C	5.13	1.47	1.36
25	k	101	BCR	C23-C22	-5.13	1.35	1.46
23	d	402[B]	CLA	O2D-CGD	5.13	1.45	1.33
23	C	508	CLA	C3C-C2C	5.13	1.47	1.36
23	D	402[A]	CLA	C3C-C2C	5.13	1.47	1.36
23	B	601	CLA	C3C-C2C	5.12	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	5.12	1.47	1.36
23	c	505	CLA	CHC-C1C	5.12	1.48	1.38
23	B	601	CLA	O2A-CGA	5.12	1.48	1.33
23	C	513	CLA	CHC-C1C	5.11	1.48	1.38
23	b	602	CLA	C3C-C2C	5.11	1.47	1.36
23	B	606	CLA	C3C-C2C	5.11	1.47	1.36
23	C	509	CLA	O2D-CGD	5.11	1.45	1.33
24	d	403[B]	PHO	OBD-CAD	5.10	1.29	1.22
23	c	511	CLA	C1D-ND	5.10	1.44	1.37
23	B	616	CLA	C3C-C2C	5.10	1.47	1.36
23	d	404[B]	CLA	C3C-C2C	5.10	1.47	1.36
40	V	201	HEC	C3D-C2D	5.10	1.52	1.38
23	b	602	CLA	O2D-CGD	5.09	1.45	1.33
23	c	513	CLA	C3C-C2C	5.09	1.47	1.36
23	b	605	CLA	O2D-CGD	5.08	1.45	1.33
23	b	601	CLA	C1D-ND	5.08	1.44	1.37
23	C	510	CLA	C3C-C2C	5.08	1.47	1.36
24	A	407[B]	PHO	C3D-C2D	5.08	1.48	1.39
23	C	511	CLA	C3C-C2C	5.07	1.47	1.36
23	D	402[B]	CLA	C3C-C2C	5.07	1.47	1.36
23	B	613	CLA	O2D-CGD	5.07	1.45	1.33
23	b	602	CLA	CHC-C1C	5.07	1.48	1.38
23	c	507	CLA	C3C-C2C	5.06	1.47	1.36
23	C	512	CLA	O2D-CGD	5.06	1.45	1.33
24	d	403[B]	PHO	O2D-CGD	5.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C3C-C2C	5.05	1.47	1.36
23	c	501	CLA	C3C-C2C	5.04	1.47	1.36
24	a	406[B]	PHO	O2D-CGD	5.04	1.45	1.33
23	b	606	CLA	C3C-C2C	5.04	1.47	1.36
23	d	402[B]	CLA	C1D-ND	5.03	1.44	1.37
23	A	406[B]	CLA	O2D-CGD	5.03	1.45	1.33
23	c	513	CLA	C1D-ND	5.03	1.44	1.37
23	C	502	CLA	CHC-C1C	5.03	1.48	1.38
23	C	507	CLA	O2D-CGD	5.03	1.45	1.33
23	B	602	CLA	C3C-C2C	5.02	1.47	1.36
23	B	614	CLA	C3C-C2C	5.02	1.47	1.36
23	b	613	CLA	CHC-C1C	5.02	1.48	1.38
24	A	416[B]	PHO	O2D-CGD	5.01	1.45	1.33
23	c	510	CLA	C3C-C2C	5.01	1.47	1.36
23	B	601	CLA	O2D-CGD	5.01	1.45	1.33
24	A	407[A]	PHO	C3D-C2D	5.00	1.48	1.39
23	b	603	CLA	O2D-CGD	5.00	1.45	1.33
25	B	617	BCR	C23-C22	-5.00	1.35	1.46
23	B	615	CLA	C3C-C2C	4.99	1.47	1.36
23	C	506	CLA	CHC-C1C	4.99	1.48	1.38
23	C	509	CLA	C1D-ND	4.98	1.44	1.37
23	B	616	CLA	CHC-C1C	4.98	1.48	1.38
38	f	101	HEM	FE-NB	4.98	2.10	1.94
23	D	403	CLA	C1D-ND	4.98	1.44	1.37
24	a	406[A]	PHO	O2D-CGD	4.98	1.45	1.33
23	b	610	CLA	CHC-C1C	4.98	1.48	1.38
23	c	511	CLA	C3C-C2C	4.97	1.47	1.36
23	C	503	CLA	O2D-CGD	4.97	1.45	1.33
25	B	619	BCR	C23-C22	-4.97	1.35	1.46
23	c	502	CLA	C3C-C2C	4.97	1.47	1.36
23	B	609	CLA	C3C-C2C	4.96	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	4.96	1.47	1.36
24	A	407[B]	PHO	OBD-CAD	4.96	1.28	1.22
23	B	613	CLA	CHC-C1C	4.96	1.48	1.38
23	c	504	CLA	C1D-ND	4.96	1.44	1.37
23	c	503	CLA	CHC-C1C	4.96	1.48	1.38
23	B	615	CLA	O2D-CGD	4.94	1.45	1.33
23	C	504	CLA	CHC-C1C	4.94	1.48	1.38
23	b	616	CLA	C3C-C2C	4.94	1.47	1.36
23	a	407	CLA	C3C-C2C	4.93	1.47	1.36
23	c	513	CLA	O2D-CGD	4.93	1.45	1.33
23	C	503	CLA	C1D-ND	4.93	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	O2D-CGD	4.93	1.45	1.33
23	b	614	CLA	CHC-C1C	4.93	1.48	1.38
23	C	514	CLA	C1D-ND	4.93	1.44	1.37
23	b	616	CLA	CHC-C1C	4.92	1.48	1.38
23	C	514	CLA	C3C-C2C	4.91	1.47	1.36
23	C	508	CLA	CHC-C1C	4.90	1.48	1.38
24	d	403[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	c	512	CLA	O2D-CGD	4.90	1.45	1.33
23	C	502	CLA	C3C-C2C	4.90	1.47	1.36
38	E	102	HEM	FE-NB	4.90	2.10	1.94
25	K	102	BCR	C23-C22	-4.90	1.35	1.46
23	C	506	CLA	C3C-C2C	4.90	1.47	1.36
23	A	405[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	c	503	CLA	C1D-ND	4.89	1.44	1.37
23	c	506	CLA	O2D-CGD	4.89	1.45	1.33
23	a	405[B]	CLA	CHC-C1C	4.88	1.48	1.38
23	c	512	CLA	CHC-C1C	4.88	1.48	1.38
23	B	609	CLA	O2D-CGD	4.88	1.45	1.33
23	c	508	CLA	C1D-ND	4.87	1.44	1.37
23	B	612	CLA	C3C-C2C	4.87	1.47	1.36
23	c	504	CLA	C3C-C2C	4.87	1.47	1.36
25	D	404	BCR	C23-C22	-4.86	1.35	1.46
24	A	416[A]	PHO	O2D-CGD	4.86	1.45	1.33
23	C	507	CLA	C3C-C2C	4.86	1.47	1.36
23	b	601	CLA	O2A-CGA	4.85	1.47	1.33
24	A	407[A]	PHO	O2D-CGD	4.85	1.45	1.33
23	A	406[A]	CLA	O2D-CGD	4.85	1.45	1.33
23	B	604	CLA	CHC-C1C	4.85	1.48	1.38
23	B	614	CLA	C1D-ND	4.85	1.44	1.37
23	b	609	CLA	CHC-C1C	4.85	1.48	1.38
26	X	101	SQD	O47-C7	4.85	1.48	1.34
23	C	510	CLA	O2D-CGD	4.84	1.45	1.33
23	B	602	CLA	CHC-C1C	4.84	1.48	1.38
25	T	102	BCR	C23-C22	-4.84	1.35	1.46
23	a	407	CLA	O2D-CGD	4.84	1.45	1.33
23	c	506	CLA	C3C-C2C	4.83	1.47	1.36
23	B	609	CLA	CHC-C1C	4.83	1.48	1.38
23	B	611	CLA	CHC-C4B	4.83	1.50	1.39
23	c	511	CLA	O2D-CGD	4.83	1.45	1.33
23	B	606	CLA	CHC-C1C	4.82	1.48	1.38
23	B	601	CLA	C1D-ND	4.82	1.44	1.37
23	C	511	CLA	O2D-CGD	4.82	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3C-C2C	4.81	1.47	1.36
23	C	514	CLA	O2D-CGD	4.81	1.45	1.33
23	b	601	CLA	O2D-CGD	4.81	1.45	1.33
23	B	607	CLA	C3C-C2C	4.81	1.47	1.36
24	A	407[B]	PHO	O2D-CGD	4.80	1.45	1.33
23	A	406[A]	CLA	CHC-C1C	4.80	1.48	1.38
25	b	619	BCR	C23-C22	-4.80	1.35	1.46
23	B	604	CLA	O2D-CGD	4.80	1.45	1.33
23	b	608	CLA	C3C-C2C	4.79	1.47	1.36
23	c	501	CLA	C1D-ND	4.79	1.44	1.37
25	c	514	BCR	C23-C22	-4.79	1.35	1.46
23	C	512	CLA	C3C-C2C	4.79	1.47	1.36
23	d	405	CLA	CHC-C1C	4.79	1.48	1.38
23	a	405[B]	CLA	O2D-CGD	4.78	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	4.78	1.45	1.33
23	A	405[B]	CLA	C1D-ND	4.78	1.44	1.37
23	b	606	CLA	CHC-C1C	4.78	1.48	1.38
23	A	405[A]	CLA	C3C-C2C	4.78	1.47	1.36
23	d	405	CLA	C1D-ND	4.77	1.44	1.37
23	c	507	CLA	O2D-CGD	4.77	1.45	1.33
23	d	402[A]	CLA	C1D-ND	4.77	1.44	1.37
23	B	603	CLA	C1D-ND	4.77	1.44	1.37
24	a	406[B]	PHO	OBD-CAD	4.76	1.28	1.22
23	b	616	CLA	C1D-ND	4.76	1.44	1.37
23	D	402[A]	CLA	O2D-CGD	4.75	1.44	1.33
23	b	613	CLA	C3C-C2C	4.74	1.47	1.36
25	b	617	BCR	C23-C22	-4.74	1.35	1.46
23	D	403	CLA	CHC-C1C	4.74	1.48	1.38
23	A	405[B]	CLA	C3C-C2C	4.73	1.47	1.36
23	b	616	CLA	O2D-CGD	4.73	1.44	1.33
23	B	615	CLA	CHC-C1C	4.73	1.48	1.38
23	C	513	CLA	C1D-ND	4.73	1.44	1.37
23	A	406[B]	CLA	CHC-C1C	4.73	1.48	1.38
23	d	404[B]	CLA	O2D-CGD	4.73	1.44	1.33
23	A	406[B]	CLA	C1D-ND	4.72	1.44	1.37
25	A	409	BCR	C23-C22	-4.72	1.35	1.46
23	c	507	CLA	CHC-C1C	4.72	1.47	1.38
23	b	615	CLA	O2D-CGD	4.71	1.44	1.33
23	c	506	CLA	C1D-ND	4.71	1.44	1.37
23	b	614	CLA	O2D-CGD	4.71	1.44	1.33
23	c	508	CLA	CHC-C1C	4.70	1.47	1.38
23	b	604	CLA	C3C-C2C	4.70	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	O2D-CGD	4.70	1.44	1.33
25	C	516	BCR	C23-C22	-4.70	1.35	1.46
23	C	510	CLA	C1D-ND	4.70	1.44	1.37
23	B	601	CLA	CHC-C1C	4.69	1.47	1.38
33	c	520	LMG	O7-C10	4.69	1.47	1.34
23	B	605	CLA	O2D-CGD	4.69	1.44	1.33
23	b	604	CLA	CHC-C1C	4.69	1.47	1.38
23	A	404[A]	CLA	O2D-CGD	4.68	1.44	1.33
23	c	509	CLA	C1D-ND	4.68	1.44	1.37
23	c	502	CLA	O2D-CGD	4.68	1.44	1.33
23	b	601	CLA	CHC-C1C	4.67	1.47	1.38
23	B	605	CLA	C1D-ND	4.67	1.44	1.37
23	b	615	CLA	CHC-C1C	4.66	1.47	1.38
23	B	613	CLA	C1D-ND	4.66	1.44	1.37
23	D	403	CLA	O2D-CGD	4.66	1.44	1.33
23	a	405[A]	CLA	CHC-C1C	4.66	1.47	1.38
23	D	403	CLA	CHD-C1D	4.66	1.47	1.38
23	c	511	CLA	CHC-C1C	4.66	1.47	1.38
23	B	615	CLA	C1D-ND	4.65	1.44	1.37
23	b	611	CLA	O2D-CGD	4.65	1.44	1.33
25	t	102	BCR	C23-C22	-4.65	1.36	1.46
24	a	406[A]	PHO	OBD-CAD	4.64	1.28	1.22
23	D	402[B]	CLA	CHC-C1C	4.64	1.47	1.38
23	A	405[A]	CLA	CHC-C1C	4.63	1.47	1.38
23	C	505	CLA	O2D-CGD	4.63	1.44	1.33
23	b	609	CLA	C3C-C2C	4.63	1.46	1.36
23	C	506	CLA	O2D-CGD	4.63	1.44	1.33
23	c	513	CLA	CHC-C1C	4.63	1.47	1.38
23	B	612	CLA	CHC-C1C	4.62	1.47	1.38
23	B	605	CLA	CHC-C1C	4.62	1.47	1.38
23	d	404[A]	CLA	O2D-CGD	4.62	1.44	1.33
23	B	610	CLA	CHC-C1C	4.61	1.47	1.38
23	C	513	CLA	O2D-CGD	4.61	1.44	1.33
23	B	602	CLA	O2D-CGD	4.61	1.44	1.33
23	C	511	CLA	CHC-C1C	4.61	1.47	1.38
25	c	515	BCR	C23-C22	-4.61	1.36	1.46
23	A	408	CLA	CHC-C1C	4.61	1.47	1.38
23	C	512	CLA	CHC-C1C	4.60	1.47	1.38
23	b	612	CLA	CHC-C1C	4.60	1.47	1.38
24	A	416[A]	PHO	OBD-CAD	4.60	1.28	1.22
23	c	505	CLA	O2D-CGD	4.60	1.44	1.33
23	B	614	CLA	CHC-C1C	4.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CHC-C1C	4.60	1.47	1.38
23	b	602	CLA	C1D-ND	4.59	1.43	1.37
25	y	101	BCR	C23-C22	-4.59	1.36	1.46
23	c	501	CLA	CHC-C1C	4.58	1.47	1.38
23	C	502	CLA	C1D-ND	4.58	1.43	1.37
23	b	604	CLA	C1D-ND	4.58	1.43	1.37
23	b	606	CLA	O2D-CGD	4.58	1.44	1.33
26	a	411	SQD	O48-C23	4.58	1.46	1.33
23	b	612	CLA	O2D-CGD	4.58	1.44	1.33
23	B	611	CLA	O2D-CGD	4.57	1.44	1.33
23	c	512	CLA	C1D-ND	4.57	1.43	1.37
33	C	521	LMG	O7-C10	4.57	1.47	1.34
23	c	510	CLA	C1D-ND	4.56	1.43	1.37
23	a	405[B]	CLA	C1D-ND	4.56	1.43	1.37
23	b	613	CLA	O2D-CGD	4.55	1.44	1.33
25	h	101	BCR	C23-C22	-4.55	1.36	1.46
33	C	521	LMG	O8-C28	4.55	1.46	1.33
23	b	608	CLA	O2D-CGD	4.55	1.44	1.33
23	A	404[B]	CLA	CHC-C1C	4.53	1.47	1.38
23	A	408	CLA	O2D-CGD	4.53	1.44	1.33
23	c	503	CLA	CHD-C1D	4.53	1.47	1.38
23	a	407	CLA	O2A-CGA	4.53	1.46	1.33
23	C	514	CLA	CHC-C1C	4.53	1.47	1.38
23	B	606	CLA	O2D-CGD	4.52	1.44	1.33
23	b	611	CLA	CHC-C1C	4.52	1.47	1.38
23	c	502	CLA	C1D-ND	4.52	1.43	1.37
23	c	512	CLA	O2A-CGA	4.51	1.46	1.33
23	b	603	CLA	CHC-C1C	4.51	1.47	1.38
23	B	602	CLA	C1D-ND	4.51	1.43	1.37
26	l	101	SQD	O47-C7	4.51	1.47	1.34
23	b	607	CLA	O2D-CGD	4.50	1.44	1.33
23	d	405	CLA	O2D-CGD	4.50	1.44	1.33
23	B	614	CLA	O2D-CGD	4.50	1.44	1.33
23	a	404[A]	CLA	O2D-CGD	4.49	1.44	1.33
23	b	602	CLA	CHD-C1D	4.49	1.47	1.38
23	C	505	CLA	CHC-C1C	4.49	1.47	1.38
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
23	A	405[B]	CLA	CHC-C1C	4.48	1.47	1.38
23	d	402[A]	CLA	CHC-C1C	4.48	1.47	1.38
23	B	604	CLA	CHD-C1D	4.48	1.47	1.38
23	B	603	CLA	O2D-CGD	4.48	1.44	1.33
23	c	513	CLA	CHD-C1D	4.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	z	101	LMG	O8-C28	4.48	1.46	1.33
23	C	504	CLA	C1D-ND	4.48	1.43	1.37
23	d	405	CLA	CHD-C1D	4.48	1.47	1.38
23	a	404[B]	CLA	O2D-CGD	4.47	1.44	1.33
26	f	102	SQD	O47-C7	4.47	1.46	1.34
23	b	605	CLA	C1D-ND	4.47	1.43	1.37
23	B	608	CLA	O2D-CGD	4.47	1.44	1.33
23	b	601	CLA	CHD-C1D	4.46	1.47	1.38
23	B	616	CLA	O2D-CGD	4.46	1.44	1.33
26	A	412	SQD	O48-C23	4.46	1.46	1.33
23	C	507	CLA	CHD-C1D	4.46	1.47	1.38
23	B	610	CLA	C1D-ND	4.46	1.43	1.37
23	a	405[A]	CLA	O2D-CGD	4.45	1.44	1.33
23	b	605	CLA	CHC-C1C	4.44	1.47	1.38
23	C	509	CLA	CHC-C1C	4.44	1.47	1.38
23	C	508	CLA	O2D-CGD	4.44	1.44	1.33
23	a	404[A]	CLA	CHC-C1C	4.44	1.47	1.38
23	B	606	CLA	C1D-ND	4.44	1.43	1.37
23	B	610	CLA	O2D-CGD	4.44	1.44	1.33
23	d	402[A]	CLA	C3D-C2D	4.43	1.51	1.39
23	B	613	CLA	C3C-C2C	4.43	1.46	1.36
23	B	607	CLA	CHC-C1C	4.42	1.47	1.38
23	d	404[B]	CLA	CHC-C1C	4.42	1.47	1.38
24	A	407[A]	PHO	OBD-CAD	4.41	1.28	1.22
32	E	101[B]	LHG	O8-C23	4.41	1.46	1.33
23	B	612	CLA	CHB-C1B	4.41	1.49	1.39
32	a	419[A]	LHG	O8-C23	4.40	1.46	1.33
23	A	408	CLA	O2A-CGA	4.40	1.46	1.33
23	C	508	CLA	C1D-ND	4.40	1.43	1.37
23	B	612	CLA	C1B-NB	-4.40	1.32	1.37
23	c	510	CLA	CHC-C1C	4.40	1.47	1.38
33	B	620	LMG	O8-C28	4.39	1.46	1.33
23	A	404[A]	CLA	CHC-C1C	4.39	1.47	1.38
23	C	506	CLA	C1D-ND	4.39	1.43	1.37
25	a	408	BCR	C23-C22	-4.39	1.36	1.46
23	a	404[B]	CLA	CHC-C1C	4.39	1.47	1.38
23	C	510	CLA	CHD-C1D	4.38	1.47	1.38
23	C	504	CLA	O2D-CGD	4.38	1.44	1.33
23	b	607	CLA	CHC-C1C	4.37	1.47	1.38
23	c	513	CLA	O2A-CGA	4.37	1.46	1.33
25	H	101	BCR	C23-C22	-4.37	1.36	1.46
23	b	604	CLA	O2D-CGD	4.37	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	CHD-C1D	4.36	1.46	1.38
23	b	615	CLA	C1D-ND	4.36	1.43	1.37
32	a	419[B]	LHG	O8-C23	4.36	1.46	1.33
23	b	607	CLA	CHD-C1D	4.36	1.46	1.38
23	b	606	CLA	C1D-ND	4.35	1.43	1.37
38	E	102	HEM	FE-NC	4.35	2.09	1.95
23	d	405	CLA	O2A-CGA	4.35	1.46	1.33
23	c	506	CLA	CHC-C1C	4.35	1.47	1.38
23	a	404[B]	CLA	C1D-ND	4.35	1.43	1.37
26	b	620	SQD	O47-C7	4.35	1.46	1.34
25	Y	101	BCR	C23-C22	-4.34	1.36	1.46
23	B	615	CLA	CHD-C1D	4.34	1.46	1.38
23	A	404[B]	CLA	CHD-C1D	4.34	1.46	1.38
23	b	609	CLA	C1D-ND	4.33	1.43	1.37
23	C	507	CLA	C1D-ND	4.33	1.43	1.37
23	c	502	CLA	O2A-CGA	4.32	1.46	1.33
23	D	402[A]	CLA	CHC-C1C	4.32	1.47	1.38
23	d	402[B]	CLA	C3D-C2D	4.32	1.50	1.39
26	f	102	SQD	O48-C23	4.32	1.45	1.33
23	A	404[B]	CLA	CHD-C4C	4.32	1.49	1.39
32	d	409[A]	LHG	O8-C23	4.32	1.45	1.33
23	b	608	CLA	CHC-C1C	4.31	1.47	1.38
23	C	509	CLA	C3D-C2D	4.30	1.50	1.39
23	A	405[A]	CLA	O2D-CGD	4.30	1.43	1.33
23	c	510	CLA	CHB-C1B	4.30	1.49	1.39
23	b	611	CLA	C1D-ND	4.30	1.43	1.37
23	B	615	CLA	O2A-CGA	4.30	1.45	1.33
23	d	402[B]	CLA	CHC-C1C	4.30	1.47	1.38
23	b	611	CLA	O2A-CGA	4.30	1.45	1.33
23	B	607	CLA	O2D-CGD	4.29	1.43	1.33
23	b	614	CLA	C1D-ND	4.28	1.43	1.37
33	C	520	LMG	O8-C28	4.28	1.45	1.33
23	c	507	CLA	C1D-ND	4.28	1.43	1.37
26	b	620	SQD	O48-C23	4.28	1.45	1.33
23	c	507	CLA	O2A-CGA	4.27	1.45	1.33
23	c	511	CLA	CHD-C1D	4.27	1.46	1.38
23	D	402[B]	CLA	O2A-CGA	4.27	1.45	1.33
23	C	511	CLA	CHD-C4C	4.27	1.48	1.39
23	a	404[A]	CLA	C1D-ND	4.26	1.43	1.37
23	C	514	CLA	O2A-CGA	4.26	1.45	1.33
23	A	406[B]	CLA	CHD-C1D	4.26	1.46	1.38
25	b	618	BCR	C23-C22	-4.26	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C1D-ND	4.26	1.43	1.37
23	B	607	CLA	C1B-NB	-4.25	1.32	1.37
23	c	502	CLA	CHC-C1C	4.25	1.47	1.38
33	c	520	LMG	O8-C28	4.25	1.45	1.33
23	C	503	CLA	CHD-C1D	4.24	1.46	1.38
23	c	507	CLA	CHD-C1D	4.24	1.46	1.38
23	B	614	CLA	CHD-C4C	4.23	1.48	1.39
23	C	503	CLA	CHC-C1C	4.23	1.47	1.38
32	d	409[B]	LHG	O8-C23	4.23	1.45	1.33
23	D	402[A]	CLA	O2A-CGA	4.23	1.45	1.33
26	a	409[B]	SQD	O47-C7	4.22	1.46	1.34
23	C	514	CLA	CHD-C1D	4.22	1.46	1.38
23	B	610	CLA	OBD-CAD	4.22	1.29	1.22
33	m	101	LMG	O8-C28	4.22	1.45	1.33
23	d	402[B]	CLA	O2A-CGA	4.21	1.45	1.33
23	c	505	CLA	CHC-C4B	4.21	1.48	1.39
38	f	101	HEM	FE-NC	4.21	2.09	1.95
23	A	405[B]	CLA	O2A-CGA	4.21	1.45	1.33
23	d	404[A]	CLA	CHC-C1C	4.21	1.46	1.38
23	C	509	CLA	O2A-CGA	4.21	1.45	1.33
23	B	609	CLA	CHD-C1D	4.20	1.46	1.38
33	Z	101	LMG	O7-C10	4.20	1.46	1.34
23	c	505	CLA	CHD-C1D	4.20	1.46	1.38
23	B	615	CLA	OBD-CAD	4.20	1.29	1.22
35	c	518	DGD	O1G-C1A	4.20	1.45	1.33
23	b	608	CLA	C3D-C2D	4.20	1.50	1.39
23	c	511	CLA	CHB-C1B	4.20	1.48	1.39
23	b	602	CLA	CHD-C4C	4.20	1.48	1.39
35	c	517[B]	DGD	O1G-C1A	4.20	1.45	1.33
23	c	512	CLA	CHD-C1D	4.20	1.46	1.38
23	C	513	CLA	CHD-C1D	4.20	1.46	1.38
23	c	503	CLA	O2A-CGA	4.19	1.45	1.33
23	c	509	CLA	CHC-C1C	4.19	1.46	1.38
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	c	511	CLA	O2A-CGA	4.19	1.45	1.33
23	B	609	CLA	O2A-CGA	4.19	1.45	1.33
23	C	506	CLA	CHD-C1D	4.18	1.46	1.38
23	b	610	CLA	CHD-C1D	4.18	1.46	1.38
23	c	506	CLA	O2A-CGA	4.18	1.45	1.33
23	B	611	CLA	C4B-NB	-4.18	1.32	1.37
23	c	503	CLA	CHD-C4C	4.18	1.48	1.39
23	b	601	CLA	C3D-C2D	4.18	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404[B]	CLA	O2A-CGA	4.16	1.45	1.33
26	A	412	SQD	O47-C7	4.16	1.46	1.34
23	B	603	CLA	CHC-C1C	4.16	1.46	1.38
23	B	615	CLA	C3D-C2D	4.16	1.50	1.39
26	l	101	SQD	O48-C23	4.16	1.45	1.33
23	C	508	CLA	O2A-CGA	4.16	1.45	1.33
23	b	607	CLA	CHB-C1B	4.16	1.48	1.39
23	b	609	CLA	CHB-C1B	4.16	1.48	1.39
23	D	402[B]	CLA	C1D-ND	4.16	1.43	1.37
25	B	618	BCR	C23-C22	-4.15	1.37	1.46
23	d	405	CLA	C3D-C2D	4.15	1.50	1.39
32	a	419[B]	LHG	O7-C7	4.15	1.46	1.34
23	b	602	CLA	CHC-C4B	4.15	1.48	1.39
23	A	406[A]	CLA	CHD-C1D	4.15	1.46	1.38
23	C	506	CLA	CHB-C1B	4.15	1.48	1.39
23	C	503	CLA	C3D-C2D	4.15	1.50	1.39
33	c	519	LMG	O7-C10	4.15	1.46	1.34
23	b	604	CLA	CHD-C1D	4.15	1.46	1.38
23	C	512	CLA	CHD-C1D	4.14	1.46	1.38
23	B	611	CLA	C3B-C2B	4.14	1.55	1.41
23	B	614	CLA	C4B-NB	-4.14	1.32	1.37
32	E	101[B]	LHG	O7-C7	4.14	1.46	1.34
35	C	517[B]	DGD	O2G-C1B	4.14	1.46	1.34
32	a	419[A]	LHG	O7-C7	4.13	1.46	1.34
26	X	101	SQD	O48-C23	4.13	1.45	1.33
23	D	403	CLA	C3D-C2D	4.13	1.50	1.39
23	B	605	CLA	CHC-C4B	4.13	1.48	1.39
23	b	612	CLA	CHB-C1B	4.13	1.48	1.39
23	a	405[A]	CLA	O2A-CGA	4.13	1.45	1.33
23	B	614	CLA	CHB-C1B	4.12	1.48	1.39
23	C	507	CLA	CHC-C1C	4.12	1.46	1.38
23	c	508	CLA	CHD-C1D	4.12	1.46	1.38
23	c	502	CLA	CHD-C1D	4.12	1.46	1.38
23	b	616	CLA	O2A-CGA	4.11	1.45	1.33
23	B	616	CLA	CHB-C1B	4.11	1.48	1.39
32	L	101[B]	LHG	O8-C23	4.11	1.45	1.33
23	d	404[A]	CLA	CHB-C1B	4.11	1.48	1.39
23	A	405[B]	CLA	C3D-C2D	4.11	1.50	1.39
23	b	609	CLA	CHD-C1D	4.11	1.46	1.38
23	C	505	CLA	C1D-ND	4.11	1.43	1.37
23	b	601	CLA	CHD-C4C	4.10	1.48	1.39
23	b	611	CLA	CHB-C1B	4.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[A]	CLA	C3D-C2D	4.10	1.50	1.39
23	C	513	CLA	O2A-CGA	4.10	1.45	1.33
33	z	101	LMG	O7-C10	4.10	1.45	1.34
23	b	612	CLA	CHD-C1D	4.10	1.46	1.38
23	C	508	CLA	CHD-C1D	4.10	1.46	1.38
33	C	501	LMG	O8-C28	4.10	1.45	1.33
23	d	402[A]	CLA	O2A-CGA	4.09	1.45	1.33
35	c	516[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	c	505	CLA	C1D-ND	4.09	1.43	1.37
23	C	502	CLA	O2D-CGD	4.09	1.43	1.33
23	c	501	CLA	O2D-CGD	4.09	1.43	1.33
23	C	510	CLA	O2A-CGA	4.09	1.45	1.33
23	c	513	CLA	CHD-C4C	4.08	1.48	1.39
23	C	510	CLA	CHC-C1C	4.08	1.46	1.38
23	b	608	CLA	O2A-CGA	4.08	1.45	1.33
33	a	415	LMG	O8-C28	4.08	1.45	1.33
23	C	509	CLA	OBD-CAD	4.08	1.29	1.22
23	B	612	CLA	O2D-CGD	4.08	1.43	1.33
23	B	608	CLA	C3D-C2D	4.07	1.50	1.39
23	c	512	CLA	C3D-C2D	4.07	1.50	1.39
26	a	409[A]	SQD	O47-C7	4.07	1.45	1.34
23	C	504	CLA	CHD-C4C	4.07	1.48	1.39
32	d	415[B]	LHG	O8-C23	4.07	1.45	1.33
23	B	614	CLA	O2A-CGA	4.07	1.45	1.33
23	C	504	CLA	CHD-C1D	4.07	1.46	1.38
23	c	502	CLA	CHD-C4C	4.06	1.48	1.39
35	C	518[B]	DGD	O1G-C1A	4.06	1.45	1.33
23	B	608	CLA	C1D-ND	4.06	1.43	1.37
35	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
23	b	616	CLA	CHD-C1D	4.06	1.46	1.38
23	d	404[A]	CLA	O2A-CGA	4.06	1.45	1.33
23	C	507	CLA	O2A-CGA	4.06	1.45	1.33
33	a	415	LMG	O7-C10	4.06	1.45	1.34
23	c	502	CLA	C3D-C2D	4.05	1.50	1.39
33	c	519	LMG	O8-C28	4.05	1.45	1.33
23	D	402[A]	CLA	CHB-C1B	4.05	1.48	1.39
23	c	504	CLA	C3D-C2D	4.05	1.50	1.39
23	C	506	CLA	CHD-C4C	4.05	1.48	1.39
23	B	602	CLA	CHD-C1D	4.04	1.46	1.38
23	c	501	CLA	CHD-C1D	4.04	1.46	1.38
23	B	610	CLA	C3D-C2D	4.04	1.50	1.39
35	c	516[B]	DGD	O2G-C1B	4.04	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	CHD-C1D	4.04	1.46	1.38
23	C	512	CLA	O2A-CGA	4.04	1.45	1.33
33	C	520	LMG	O7-C10	4.04	1.45	1.34
23	d	404[B]	CLA	CHB-C1B	4.03	1.48	1.39
23	b	615	CLA	CHD-C1D	4.03	1.46	1.38
32	D	407[B]	LHG	O7-C7	4.03	1.45	1.34
23	c	506	CLA	CHD-C1D	4.03	1.46	1.38
23	b	604	CLA	CHC-C4B	4.03	1.48	1.39
23	c	508	CLA	O2A-CGA	4.03	1.45	1.33
23	b	607	CLA	C1D-ND	4.02	1.43	1.37
23	B	611	CLA	CHB-C1B	4.02	1.48	1.39
33	d	413	LMG	O8-C28	4.02	1.45	1.33
23	C	505	CLA	CHD-C1D	4.02	1.46	1.38
23	B	616	CLA	C1D-ND	4.02	1.43	1.37
23	c	503	CLA	O2D-CGD	4.02	1.43	1.33
23	a	405[B]	CLA	O2A-CGA	4.02	1.45	1.33
23	C	513	CLA	CHC-C4B	4.02	1.48	1.39
23	b	610	CLA	CHB-C1B	4.02	1.48	1.39
23	B	613	CLA	C3D-C2D	4.01	1.49	1.39
23	C	505	CLA	O2A-CGA	4.01	1.45	1.33
33	C	501	LMG	O7-C10	4.01	1.45	1.34
23	b	603	CLA	CHD-C1D	4.01	1.46	1.38
26	a	409[B]	SQD	O48-C23	4.01	1.45	1.33
23	B	603	CLA	CHB-C1B	4.01	1.48	1.39
23	C	502	CLA	O2A-CGA	4.01	1.45	1.33
23	B	608	CLA	CHD-C1D	4.01	1.46	1.38
23	c	508	CLA	C3D-C2D	4.00	1.49	1.39
23	c	501	CLA	CHD-C4C	4.00	1.48	1.39
26	a	411	SQD	O47-C7	4.00	1.45	1.34
23	A	404[A]	CLA	CHD-C1D	4.00	1.46	1.38
23	c	509	CLA	O2A-CGA	4.00	1.45	1.33
23	D	403	CLA	CHC-C4B	4.00	1.48	1.39
23	B	610	CLA	C1B-NB	-4.00	1.32	1.37
23	b	613	CLA	C1D-ND	3.99	1.43	1.37
23	c	507	CLA	CHD-C4C	3.99	1.48	1.39
26	a	409[A]	SQD	O48-C23	3.99	1.45	1.33
23	c	503	CLA	CHC-C4B	3.99	1.48	1.39
23	a	404[B]	CLA	CHD-C1D	3.98	1.46	1.38
23	B	607	CLA	CHB-C1B	3.98	1.48	1.39
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
23	c	505	CLA	CHD-C4C	3.98	1.48	1.39
23	C	512	CLA	CHB-C1B	3.98	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404[A]	CLA	CHD-C4C	3.98	1.48	1.39
23	C	514	CLA	C3D-C2D	3.97	1.49	1.39
23	b	608	CLA	CHD-C1D	3.97	1.46	1.38
23	b	613	CLA	C3D-C2D	3.97	1.49	1.39
23	c	512	CLA	CHD-C4C	3.97	1.48	1.39
35	h	102	DGD	O1G-C1A	3.97	1.44	1.33
23	A	406[B]	CLA	O2A-CGA	3.97	1.44	1.33
23	D	403	CLA	CHD-C4C	3.97	1.48	1.39
23	b	614	CLA	C3D-C2D	3.97	1.49	1.39
23	B	616	CLA	O2A-CGA	3.97	1.44	1.33
24	A	416[B]	PHO	O2A-CGA	3.97	1.44	1.33
23	B	609	CLA	C3D-C2D	3.96	1.49	1.39
23	b	616	CLA	CHC-C4B	3.96	1.48	1.39
23	a	404[A]	CLA	CHD-C1D	3.96	1.46	1.38
35	H	102	DGD	O1G-C1A	3.95	1.44	1.33
23	B	601	CLA	CHD-C1D	3.95	1.46	1.38
23	B	604	CLA	CHD-C4C	3.95	1.48	1.39
23	B	610	CLA	CHB-C1B	3.95	1.48	1.39
23	B	602	CLA	CHD-C4C	3.95	1.48	1.39
23	a	405[A]	CLA	C3D-C2D	3.95	1.49	1.39
23	C	504	CLA	CHC-C4B	3.95	1.48	1.39
23	c	501	CLA	CHB-C1B	3.95	1.48	1.39
23	A	404[B]	CLA	C3D-C2D	3.95	1.49	1.39
23	d	405	CLA	CHC-C4B	3.95	1.48	1.39
23	b	603	CLA	C1D-ND	3.95	1.43	1.37
23	a	404[B]	CLA	CHD-C4C	3.94	1.48	1.39
23	B	616	CLA	C3D-C2D	3.94	1.49	1.39
23	b	615	CLA	O2A-CGA	3.94	1.44	1.33
23	C	514	CLA	CHD-C4C	3.94	1.48	1.39
23	B	602	CLA	C3D-C2D	3.94	1.49	1.39
23	C	503	CLA	CHB-C1B	3.94	1.48	1.39
23	B	601	CLA	CHC-C4B	3.94	1.48	1.39
33	B	620	LMG	O7-C10	3.94	1.45	1.34
23	D	402[A]	CLA	C1D-ND	3.94	1.43	1.37
23	c	509	CLA	CHD-C1D	3.93	1.46	1.38
23	C	507	CLA	CHD-C4C	3.93	1.48	1.39
23	B	614	CLA	CHC-C4B	3.93	1.48	1.39
23	A	406[B]	CLA	OBD-CAD	3.93	1.29	1.22
23	b	614	CLA	CHD-C4C	3.92	1.48	1.39
23	D	402[A]	CLA	CHD-C4C	3.92	1.48	1.39
23	c	503	CLA	CHB-C1B	3.92	1.48	1.39
23	C	511	CLA	O2A-CGA	3.92	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	C3D-C2D	3.92	1.49	1.39
23	b	616	CLA	CHD-C4C	3.91	1.48	1.39
32	D	407[A]	LHG	O8-C23	3.91	1.44	1.33
23	B	613	CLA	CHB-C1B	3.91	1.48	1.39
23	c	502	CLA	CHB-C1B	3.91	1.48	1.39
23	A	408	CLA	C1D-ND	3.91	1.43	1.37
35	C	519	DGD	O1G-C1A	3.90	1.44	1.33
23	B	615	CLA	CHB-C1B	3.90	1.48	1.39
23	c	504	CLA	CHD-C1D	3.90	1.46	1.38
23	B	609	CLA	C1D-ND	3.90	1.43	1.37
23	c	506	CLA	C3D-C2D	3.90	1.49	1.39
23	c	513	CLA	C3D-C2D	3.90	1.49	1.39
23	C	503	CLA	O2A-CGA	3.89	1.44	1.33
23	A	404[A]	CLA	C1D-ND	3.89	1.43	1.37
23	b	611	CLA	CHD-C4C	3.89	1.48	1.39
23	C	503	CLA	CHC-C4B	3.89	1.48	1.39
23	b	612	CLA	CHC-C4B	3.89	1.48	1.39
32	L	101[B]	LHG	O7-C7	3.89	1.45	1.34
23	b	615	CLA	CHD-C4C	3.89	1.48	1.39
23	a	404[B]	CLA	O2A-CGA	3.89	1.44	1.33
23	D	402[A]	CLA	CHD-C1D	3.89	1.46	1.38
23	C	513	CLA	C3D-C2D	3.89	1.49	1.39
23	b	604	CLA	C3D-C2D	3.89	1.49	1.39
23	A	406[A]	CLA	C3D-C2D	3.89	1.49	1.39
23	D	403	CLA	CHB-C1B	3.89	1.48	1.39
26	A	410[B]	SQD	O48-C23	3.89	1.44	1.33
23	B	604	CLA	OBD-CAD	3.88	1.29	1.22
23	B	602	CLA	O2A-CGA	3.88	1.44	1.33
24	d	403[B]	PHO	O2A-CGA	3.88	1.44	1.33
23	b	606	CLA	CHD-C1D	3.88	1.46	1.38
23	B	608	CLA	CHC-C1C	3.88	1.46	1.38
24	A	407[B]	PHO	O2A-CGA	3.88	1.44	1.33
23	B	605	CLA	C3D-C2D	3.88	1.49	1.39
23	C	505	CLA	CHB-C1B	3.88	1.48	1.39
23	c	505	CLA	CHB-C1B	3.88	1.48	1.39
23	C	508	CLA	CHC-C4B	3.88	1.48	1.39
23	c	508	CLA	OBD-CAD	3.88	1.29	1.22
23	a	405[B]	CLA	CHD-C1D	3.87	1.46	1.38
23	c	507	CLA	C3D-C2D	3.87	1.49	1.39
23	D	402[B]	CLA	CHD-C1D	3.87	1.46	1.38
23	D	402[B]	CLA	CHD-C4C	3.87	1.48	1.39
23	B	603	CLA	C3D-C2D	3.87	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404[B]	CLA	C3D-C2D	3.87	1.49	1.39
32	b	629[B]	LHG	O7-C7	3.86	1.45	1.34
24	A	416[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	D	402[B]	CLA	CHB-C1B	3.86	1.48	1.39
23	b	602	CLA	C3D-C2D	3.86	1.49	1.39
23	C	510	CLA	CHD-C4C	3.86	1.48	1.39
23	b	613	CLA	O2A-CGA	3.86	1.44	1.33
23	C	510	CLA	C3D-C2D	3.86	1.49	1.39
23	B	611	CLA	O2A-CGA	3.86	1.44	1.33
23	b	603	CLA	C3D-C2D	3.86	1.49	1.39
23	B	606	CLA	O2A-CGA	3.86	1.44	1.33
23	b	604	CLA	CHD-C4C	3.86	1.48	1.39
32	D	406[B]	LHG	O7-C7	3.85	1.45	1.34
32	d	408[B]	LHG	O7-C7	3.85	1.45	1.34
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	a	405[B]	CLA	C3D-C2D	3.85	1.49	1.39
23	a	405[B]	CLA	OBD-CAD	3.85	1.29	1.22
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	B	606	CLA	CHB-C1B	3.85	1.48	1.39
32	D	407[B]	LHG	O8-C23	3.85	1.44	1.33
23	c	510	CLA	CHD-C4C	3.85	1.48	1.39
32	L	101[A]	LHG	O8-C23	3.85	1.44	1.33
23	b	612	CLA	C3D-C2D	3.85	1.49	1.39
23	C	509	CLA	CHB-C1B	3.84	1.48	1.39
23	b	609	CLA	C3D-C2D	3.84	1.49	1.39
35	c	517[A]	DGD	O1G-C1A	3.84	1.44	1.33
32	d	409[B]	LHG	O7-C7	3.84	1.45	1.34
23	A	405[A]	CLA	O2A-CGA	3.84	1.44	1.33
35	C	518[B]	DGD	O2G-C1B	3.84	1.45	1.34
23	b	610	CLA	C1D-ND	3.84	1.42	1.37
23	B	609	CLA	CHC-C4B	3.84	1.48	1.39
23	d	402[B]	CLA	CHD-C1D	3.84	1.45	1.38
23	b	605	CLA	CHD-C1D	3.84	1.45	1.38
23	C	509	CLA	CHD-C1D	3.84	1.45	1.38
24	d	403[A]	PHO	O2A-CGA	3.84	1.44	1.33
23	c	506	CLA	CHD-C4C	3.83	1.47	1.39
23	A	406[B]	CLA	CHD-C4C	3.83	1.47	1.39
23	C	510	CLA	OBD-CAD	3.83	1.29	1.22
23	c	509	CLA	CHB-C1B	3.83	1.48	1.39
23	b	607	CLA	C1B-NB	-3.83	1.32	1.37
23	a	405[A]	CLA	C1D-ND	3.83	1.42	1.37
23	C	514	CLA	CHB-C1B	3.83	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CHB-C1B	3.83	1.48	1.39
23	c	510	CLA	O2A-CGA	3.83	1.44	1.33
32	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
23	b	615	CLA	C3D-C2D	3.82	1.49	1.39
23	B	610	CLA	CHD-C1D	3.82	1.45	1.38
23	b	612	CLA	C1D-ND	3.82	1.42	1.37
23	B	603	CLA	O2A-CGA	3.82	1.44	1.33
23	b	610	CLA	CHC-C4B	3.82	1.48	1.39
23	A	408	CLA	CHD-C4C	3.82	1.47	1.39
23	B	613	CLA	CHD-C1D	3.82	1.45	1.38
23	c	501	CLA	C3D-C2D	3.82	1.49	1.39
23	C	502	CLA	CHC-C4B	3.81	1.48	1.39
23	C	505	CLA	C3D-C2D	3.81	1.49	1.39
35	c	516[B]	DGD	O1G-C1A	3.81	1.44	1.33
23	B	604	CLA	CHB-C1B	3.81	1.48	1.39
23	C	513	CLA	CHD-C4C	3.81	1.47	1.39
23	c	506	CLA	CHB-C1B	3.81	1.48	1.39
23	C	512	CLA	CHD-C4C	3.81	1.47	1.39
23	b	616	CLA	C3D-C2D	3.81	1.49	1.39
23	b	609	CLA	OBD-CAD	3.81	1.29	1.22
23	a	407	CLA	CHC-C4B	3.81	1.48	1.39
23	A	406[A]	CLA	O2A-CGA	3.81	1.44	1.33
23	B	602	CLA	CHC-C4B	3.80	1.47	1.39
23	D	402[B]	CLA	C3D-C2D	3.80	1.49	1.39
23	A	408	CLA	CHD-C1D	3.80	1.45	1.38
23	c	512	CLA	CHC-C4B	3.80	1.47	1.39
35	c	517[B]	DGD	O2G-C1B	3.80	1.45	1.34
23	B	611	CLA	CHD-C4C	3.80	1.47	1.39
23	A	406[A]	CLA	CHC-C4B	3.79	1.47	1.39
23	b	610	CLA	CHD-C4C	3.79	1.47	1.39
23	C	507	CLA	C3D-C2D	3.79	1.49	1.39
23	a	405[B]	CLA	CHD-C4C	3.78	1.47	1.39
23	b	611	CLA	CHC-C4B	3.78	1.47	1.39
35	C	517[B]	DGD	O1G-C1A	3.78	1.44	1.33
23	c	507	CLA	OBD-CAD	3.78	1.29	1.22
23	c	501	CLA	O2A-CGA	3.78	1.44	1.33
23	c	511	CLA	CHD-C4C	3.78	1.47	1.39
23	b	610	CLA	OBD-CAD	3.78	1.29	1.22
23	A	405[A]	CLA	CHB-C1B	3.78	1.47	1.39
23	B	610	CLA	CHD-C4C	3.78	1.47	1.39
23	d	404[A]	CLA	CHD-C1D	3.78	1.45	1.38
23	b	614	CLA	CHD-C1D	3.77	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	OBD-CAD	3.77	1.29	1.22
23	b	608	CLA	CHB-C1B	3.77	1.47	1.39
23	b	603	CLA	CHD-C4C	3.77	1.47	1.39
23	C	512	CLA	C3D-C2D	3.77	1.49	1.39
23	B	605	CLA	CHB-C1B	3.77	1.47	1.39
23	B	601	CLA	C3D-C2D	3.77	1.49	1.39
23	c	504	CLA	O2A-CGA	3.77	1.44	1.33
23	d	402[A]	CLA	CHD-C1D	3.77	1.45	1.38
23	c	513	CLA	CHB-C1B	3.76	1.47	1.39
23	B	611	CLA	OBD-CAD	3.76	1.29	1.22
23	B	606	CLA	CHC-C4B	3.76	1.47	1.39
23	c	509	CLA	C3D-C2D	3.76	1.49	1.39
23	A	404[A]	CLA	CHD-C4C	3.76	1.47	1.39
23	B	603	CLA	CHD-C1D	3.75	1.45	1.38
23	B	605	CLA	CHD-C1D	3.75	1.45	1.38
23	d	405	CLA	CHB-C1B	3.75	1.47	1.39
23	B	602	CLA	CHB-C1B	3.75	1.47	1.39
32	d	415[A]	LHG	O8-C23	3.75	1.44	1.33
35	h	102	DGD	O2G-C1B	3.75	1.44	1.34
23	c	508	CLA	CHD-C4C	3.75	1.47	1.39
23	B	609	CLA	CHD-C4C	3.75	1.47	1.39
23	C	511	CLA	CHD-C1D	3.75	1.45	1.38
23	a	405[A]	CLA	CHB-C1B	3.75	1.47	1.39
23	d	404[B]	CLA	CHD-C1D	3.75	1.45	1.38
33	m	101	LMG	O7-C10	3.75	1.44	1.34
23	b	612	CLA	OBD-CAD	3.74	1.28	1.22
23	C	508	CLA	C3D-C2D	3.74	1.49	1.39
23	a	405[B]	CLA	CHB-C1B	3.74	1.47	1.39
23	c	512	CLA	CHB-C1B	3.74	1.47	1.39
32	A	419[B]	LHG	O8-C23	3.74	1.44	1.33
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	b	611	CLA	CHD-C1D	3.74	1.45	1.38
23	A	405[B]	CLA	CHB-C1B	3.73	1.47	1.39
23	d	404[B]	CLA	CHD-C4C	3.73	1.47	1.39
23	b	606	CLA	O2A-CGA	3.73	1.44	1.33
23	B	612	CLA	CHD-C1D	3.73	1.45	1.38
23	C	510	CLA	CHB-C1B	3.73	1.47	1.39
33	d	413	LMG	O7-C10	3.73	1.44	1.34
23	d	402[B]	CLA	CHD-C4C	3.73	1.47	1.39
32	d	408[A]	LHG	O7-C7	3.72	1.44	1.34
23	D	403	CLA	O2A-CGA	3.72	1.44	1.33
23	B	607	CLA	CHD-C1D	3.72	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	518[A]	DGD	O1G-C1A	3.72	1.44	1.33
23	C	503	CLA	CHD-C4C	3.72	1.47	1.39
23	c	507	CLA	CHC-C4B	3.72	1.47	1.39
23	c	510	CLA	C3D-C2D	3.71	1.49	1.39
23	c	504	CLA	CHD-C4C	3.71	1.47	1.39
23	a	404[B]	CLA	CHB-C1B	3.71	1.47	1.39
23	a	404[A]	CLA	C3D-C2D	3.71	1.49	1.39
23	b	602	CLA	O2A-CGA	3.71	1.44	1.33
23	B	605	CLA	O2A-CGA	3.71	1.44	1.33
32	d	415[B]	LHG	O7-C7	3.71	1.44	1.34
23	c	505	CLA	O2A-CGA	3.71	1.44	1.33
23	C	504	CLA	C3D-C2D	3.71	1.49	1.39
23	A	406[A]	CLA	C1D-ND	3.71	1.42	1.37
23	A	405[B]	CLA	CHD-C1D	3.70	1.45	1.38
23	C	511	CLA	CHB-C1B	3.70	1.47	1.39
23	d	404[B]	CLA	C1D-ND	3.70	1.42	1.37
23	c	509	CLA	CHD-C4C	3.70	1.47	1.39
23	b	606	CLA	C3D-C2D	3.69	1.49	1.39
23	A	406[A]	CLA	CHD-C4C	3.69	1.47	1.39
23	A	405[A]	CLA	CHD-C1D	3.69	1.45	1.38
23	a	404[A]	CLA	CHB-C1B	3.69	1.47	1.39
23	c	511	CLA	C3D-C2D	3.69	1.49	1.39
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	A	404[A]	CLA	C3D-C2D	3.68	1.49	1.39
23	C	502	CLA	CHD-C4C	3.68	1.47	1.39
23	b	610	CLA	C3D-C2D	3.68	1.49	1.39
23	b	605	CLA	CHD-C4C	3.68	1.47	1.39
23	a	405[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	d	404[A]	CLA	C1B-NB	-3.68	1.33	1.37
23	C	504	CLA	CHB-C1B	3.68	1.47	1.39
23	A	405[B]	CLA	CHD-C4C	3.68	1.47	1.39
23	B	607	CLA	CHD-C4C	3.68	1.47	1.39
23	b	606	CLA	CHB-C1B	3.68	1.47	1.39
23	a	407	CLA	C1D-ND	3.67	1.42	1.37
23	B	606	CLA	CHD-C1D	3.67	1.45	1.38
23	a	407	CLA	CHD-C1D	3.67	1.45	1.38
23	c	510	CLA	CHD-C1D	3.67	1.45	1.38
23	B	613	CLA	C1B-NB	-3.67	1.33	1.37
23	b	615	CLA	CHB-C1B	3.67	1.47	1.39
23	c	510	CLA	CHC-C4B	3.67	1.47	1.39
23	a	404[B]	CLA	OBD-CAD	3.67	1.28	1.22
23	C	507	CLA	CHB-C1B	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	CHB-C1B	3.67	1.47	1.39
23	b	606	CLA	CHD-C4C	3.67	1.47	1.39
23	a	407	CLA	CHD-C4C	3.66	1.47	1.39
23	c	501	CLA	CHC-C4B	3.66	1.47	1.39
23	b	608	CLA	OBD-CAD	3.66	1.28	1.22
32	d	409[A]	LHG	O7-C7	3.66	1.44	1.34
23	d	405	CLA	CHD-C4C	3.66	1.47	1.39
23	a	407	CLA	CHB-C1B	3.66	1.47	1.39
23	b	615	CLA	CHC-C4B	3.65	1.47	1.39
23	B	615	CLA	CHD-C4C	3.65	1.47	1.39
23	C	506	CLA	O2A-CGA	3.65	1.44	1.33
23	b	609	CLA	O2A-CGA	3.65	1.44	1.33
23	c	507	CLA	CHB-C1B	3.65	1.47	1.39
23	C	505	CLA	CHD-C4C	3.65	1.47	1.39
23	B	601	CLA	CHD-C4C	3.65	1.47	1.39
24	A	407[A]	PHO	O2A-CGA	3.65	1.44	1.33
23	B	611	CLA	C1C-C2C	3.65	1.51	1.44
23	D	402[B]	CLA	OBD-CAD	3.64	1.28	1.22
23	b	614	CLA	CHC-C4B	3.64	1.47	1.39
23	d	402[A]	CLA	CHD-C4C	3.64	1.47	1.39
23	b	602	CLA	OBD-CAD	3.64	1.28	1.22
23	b	611	CLA	C3D-C2D	3.64	1.48	1.39
23	c	502	CLA	OBD-CAD	3.64	1.28	1.22
23	B	608	CLA	CHD-C4C	3.64	1.47	1.39
23	c	505	CLA	C3D-C2D	3.64	1.48	1.39
23	b	606	CLA	OBD-CAD	3.64	1.28	1.22
23	B	610	CLA	CHC-C4B	3.63	1.47	1.39
23	B	609	CLA	CHB-C1B	3.63	1.47	1.39
23	b	601	CLA	OBD-CAD	3.63	1.28	1.22
23	C	511	CLA	C3D-C2D	3.63	1.48	1.39
35	c	516[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	b	608	CLA	CHD-C4C	3.62	1.47	1.39
23	b	614	CLA	CHB-C1B	3.62	1.47	1.39
32	d	408[B]	LHG	O8-C23	3.62	1.43	1.33
23	b	603	CLA	CHC-C4B	3.62	1.47	1.39
32	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	C	502	CLA	C3D-C2D	3.62	1.48	1.39
23	B	612	CLA	C4B-NB	-3.62	1.33	1.37
23	a	404[A]	CLA	OBD-CAD	3.62	1.28	1.22
35	H	102	DGD	O2G-C1B	3.61	1.44	1.34
23	A	404[B]	CLA	O2A-CGA	3.61	1.43	1.33
23	B	604	CLA	CHC-C4B	3.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	CHC-C4B	3.61	1.47	1.39
32	b	629[B]	LHG	O8-C23	3.61	1.43	1.33
23	B	607	CLA	CHC-C4B	3.61	1.47	1.39
23	a	405[A]	CLA	CHD-C4C	3.61	1.47	1.39
23	B	613	CLA	CHD-C4C	3.60	1.47	1.39
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	d	404[A]	CLA	C3D-C2D	3.60	1.48	1.39
35	c	518	DGD	O2G-C1B	3.60	1.44	1.34
23	b	607	CLA	C3D-C2D	3.60	1.48	1.39
32	D	406[B]	LHG	O8-C23	3.59	1.43	1.33
23	B	603	CLA	CHC-C4B	3.59	1.47	1.39
23	d	404[A]	CLA	CHD-C4C	3.59	1.47	1.39
23	D	402[B]	CLA	CHC-C4B	3.59	1.47	1.39
23	b	609	CLA	CHC-C4B	3.59	1.47	1.39
23	C	508	CLA	CHB-C1B	3.59	1.47	1.39
23	B	616	CLA	CHC-C4B	3.59	1.47	1.39
23	B	608	CLA	O2A-CGA	3.59	1.43	1.33
23	C	507	CLA	OBD-CAD	3.59	1.28	1.22
26	A	410[B]	SQD	O47-C7	3.59	1.44	1.34
23	B	610	CLA	O2A-CGA	3.58	1.43	1.33
23	C	504	CLA	O2A-CGA	3.58	1.43	1.33
23	b	605	CLA	C3D-C2D	3.58	1.48	1.39
23	C	514	CLA	OBD-CAD	3.58	1.28	1.22
23	b	605	CLA	CHC-C4B	3.58	1.47	1.39
23	A	405[A]	CLA	C1D-ND	3.58	1.42	1.37
23	A	405[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	b	613	CLA	CHD-C1D	3.58	1.45	1.38
23	b	613	CLA	CHC-C4B	3.58	1.47	1.39
23	C	505	CLA	CHC-C4B	3.58	1.47	1.39
23	d	404[B]	CLA	C3D-C2D	3.58	1.48	1.39
23	B	605	CLA	CHD-C4C	3.57	1.47	1.39
32	A	419[B]	LHG	O7-C7	3.57	1.44	1.34
23	B	608	CLA	CHB-C1B	3.57	1.47	1.39
23	b	614	CLA	O2A-CGA	3.57	1.43	1.33
23	B	603	CLA	CHD-C4C	3.57	1.47	1.39
23	A	404[B]	CLA	C1B-NB	-3.57	1.33	1.37
23	D	403	CLA	OBD-CAD	3.57	1.28	1.22
23	B	607	CLA	O2A-CGA	3.57	1.43	1.33
23	c	512	CLA	OBD-CAD	3.57	1.28	1.22
24	a	406[B]	PHO	O2A-CGA	3.56	1.43	1.33
23	C	503	CLA	OBD-CAD	3.56	1.28	1.22
23	B	601	CLA	CHB-C1B	3.56	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	517[A]	DGD	O1G-C1A	3.56	1.43	1.33
23	A	405[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	C	512	CLA	C1D-ND	3.55	1.42	1.37
23	A	404[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	C	502	CLA	CHB-C1B	3.55	1.47	1.39
23	C	506	CLA	CHC-C4B	3.55	1.47	1.39
23	d	404[B]	CLA	OBD-CAD	3.55	1.28	1.22
23	d	402[B]	CLA	OBD-CAD	3.55	1.28	1.22
23	c	503	CLA	C3D-C2D	3.55	1.48	1.39
23	B	604	CLA	C1D-ND	3.54	1.42	1.37
23	D	402[A]	CLA	C1B-NB	-3.54	1.33	1.37
23	c	511	CLA	OBD-CAD	3.54	1.28	1.22
35	c	517[A]	DGD	O2G-C1B	3.54	1.44	1.34
33	D	411	LMG	O8-C28	3.54	1.43	1.33
32	d	408[A]	LHG	O8-C23	3.54	1.43	1.33
23	C	507	CLA	C4B-NB	-3.53	1.33	1.37
23	C	513	CLA	OBD-CAD	3.53	1.28	1.22
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	c	508	CLA	CHC-C4B	3.53	1.47	1.39
23	C	512	CLA	C4B-NB	-3.53	1.33	1.37
32	A	419[A]	LHG	O8-C23	3.53	1.43	1.33
23	B	603	CLA	OBD-CAD	3.52	1.28	1.22
23	c	506	CLA	OBD-CAD	3.52	1.28	1.22
23	b	601	CLA	CHC-C4B	3.52	1.47	1.39
23	b	603	CLA	O2A-CGA	3.52	1.43	1.33
23	C	508	CLA	CHD-C4C	3.52	1.47	1.39
23	A	406[B]	CLA	CHB-C1B	3.52	1.47	1.39
23	C	509	CLA	CHD-C4C	3.52	1.47	1.39
23	B	606	CLA	C3D-C2D	3.51	1.48	1.39
23	a	405[A]	CLA	CHD-C1D	3.51	1.45	1.38
23	b	608	CLA	C1B-NB	-3.51	1.33	1.37
23	b	615	CLA	OBD-CAD	3.51	1.28	1.22
23	b	601	CLA	CHB-C1B	3.51	1.47	1.39
32	d	415[A]	LHG	O7-C7	3.50	1.44	1.34
23	B	612	CLA	CHC-C4B	3.50	1.47	1.39
23	B	612	CLA	O2A-CGA	3.50	1.43	1.33
23	A	404[A]	CLA	C4B-NB	-3.50	1.33	1.37
23	B	611	CLA	C3D-C2D	3.50	1.48	1.39
23	A	406[B]	CLA	CHC-C4B	3.50	1.47	1.39
32	A	419[A]	LHG	O7-C7	3.50	1.44	1.34
23	B	612	CLA	C1D-ND	3.50	1.42	1.37
32	b	629[A]	LHG	O8-C23	3.50	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	CHC-C4B	3.49	1.47	1.39
23	b	609	CLA	CHD-C4C	3.49	1.47	1.39
23	A	406[A]	CLA	C1B-NB	-3.49	1.33	1.37
23	A	404[B]	CLA	CHB-C1B	3.49	1.47	1.39
23	a	405[B]	CLA	CHC-C4B	3.49	1.47	1.39
23	A	405[B]	CLA	C1B-NB	-3.49	1.33	1.37
23	B	614	CLA	CHD-C1D	3.49	1.45	1.38
23	d	404[B]	CLA	CHC-C4B	3.48	1.47	1.39
23	c	509	CLA	C4B-NB	-3.48	1.33	1.37
23	D	402[A]	CLA	C3D-C2D	3.48	1.48	1.39
23	a	407	CLA	C3D-C2D	3.48	1.48	1.39
23	A	405[A]	CLA	C1B-NB	-3.48	1.33	1.37
23	c	504	CLA	CHB-C1B	3.48	1.47	1.39
23	c	513	CLA	OBD-CAD	3.48	1.28	1.22
23	d	402[A]	CLA	CHB-C1B	3.47	1.47	1.39
23	c	504	CLA	OBD-CAD	3.47	1.28	1.22
23	b	603	CLA	OBD-CAD	3.47	1.28	1.22
23	b	604	CLA	OBD-CAD	3.47	1.28	1.22
35	C	519	DGD	O2G-C1B	3.46	1.44	1.34
23	d	402[A]	CLA	CHC-C4B	3.46	1.47	1.39
23	A	408	CLA	C3D-C2D	3.46	1.48	1.39
23	b	607	CLA	CHD-C4C	3.46	1.47	1.39
23	d	402[B]	CLA	C1B-NB	-3.46	1.33	1.37
23	B	601	CLA	OBD-CAD	3.46	1.28	1.22
23	B	612	CLA	C3D-C2D	3.45	1.48	1.39
23	A	405[B]	CLA	CHC-C4B	3.45	1.47	1.39
23	C	510	CLA	C4B-NB	-3.45	1.33	1.37
23	C	512	CLA	CHC-C4B	3.44	1.47	1.39
23	B	616	CLA	CHD-C1D	3.44	1.45	1.38
23	b	605	CLA	CHB-C1B	3.44	1.47	1.39
23	b	603	CLA	CHB-C1B	3.44	1.47	1.39
23	A	406[A]	CLA	CHB-C1B	3.42	1.47	1.39
23	B	607	CLA	OBD-CAD	3.42	1.28	1.22
23	C	503	CLA	C4B-NB	-3.42	1.33	1.37
23	b	604	CLA	O2A-CGA	3.42	1.43	1.33
23	d	404[A]	CLA	CHC-C4B	3.42	1.47	1.39
23	B	613	CLA	OBD-CAD	3.42	1.28	1.22
23	d	404[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	d	402[B]	CLA	CHB-C1B	3.41	1.47	1.39
23	b	616	CLA	OBD-CAD	3.40	1.28	1.22
23	c	513	CLA	CHC-C4B	3.40	1.47	1.39
34	b	623	HTG	C1'-S1	-3.40	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	CHC-C4B	3.40	1.47	1.39
23	c	504	CLA	CHC-C4B	3.40	1.47	1.39
23	b	613	CLA	CHB-C1B	3.40	1.47	1.39
23	b	614	CLA	C1B-NB	-3.40	1.33	1.37
23	C	506	CLA	C3D-C2D	3.40	1.48	1.39
23	c	509	CLA	C1B-NB	-3.40	1.33	1.37
24	a	406[A]	PHO	O2A-CGA	3.40	1.43	1.33
23	c	511	CLA	CHC-C4B	3.39	1.47	1.39
23	b	612	CLA	CHD-C4C	3.39	1.46	1.39
23	C	502	CLA	C1B-NB	-3.39	1.33	1.37
23	c	509	CLA	OBD-CAD	3.38	1.28	1.22
23	C	507	CLA	C1B-NB	-3.37	1.33	1.37
23	B	607	CLA	C3D-C2D	3.37	1.48	1.39
34	B	621	HTG	C1'-S1	-3.37	1.76	1.81
23	C	511	CLA	C4B-NB	-3.36	1.33	1.37
23	B	604	CLA	O2A-CGA	3.36	1.43	1.33
23	C	504	CLA	OBD-CAD	3.36	1.28	1.22
23	b	605	CLA	O2A-CGA	3.36	1.43	1.33
23	a	404[A]	CLA	CHC-C4B	3.36	1.46	1.39
23	b	615	CLA	C1B-NB	-3.36	1.33	1.37
23	c	511	CLA	C1B-C2B	3.36	1.51	1.43
38	E	102	HEM	C1B-NB	-3.35	1.34	1.40
23	B	614	CLA	C3D-C2D	3.34	1.48	1.39
23	b	602	CLA	C1B-NB	-3.34	1.33	1.37
23	C	512	CLA	OBD-CAD	3.34	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	A	408	CLA	CHC-C4B	3.34	1.46	1.39
23	B	606	CLA	CHD-C4C	3.34	1.46	1.39
23	c	504	CLA	C1B-NB	-3.33	1.33	1.37
23	C	511	CLA	C1B-NB	-3.33	1.33	1.37
23	a	407	CLA	C1B-NB	-3.33	1.33	1.37
23	c	505	CLA	OBD-CAD	3.33	1.28	1.22
23	D	402[A]	CLA	CHC-C4B	3.33	1.46	1.39
23	C	506	CLA	OBD-CAD	3.33	1.28	1.22
23	c	510	CLA	OBD-CAD	3.32	1.28	1.22
23	C	514	CLA	CHC-C4B	3.32	1.46	1.39
23	b	608	CLA	C4B-NB	-3.32	1.33	1.37
23	c	513	CLA	C1B-NB	-3.32	1.33	1.37
23	d	405	CLA	OBD-CAD	3.31	1.28	1.22
23	b	605	CLA	OBD-CAD	3.31	1.28	1.22
38	f	101	HEM	C4D-ND	-3.31	1.34	1.40
23	B	615	CLA	CHC-C4B	3.30	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B	624	HTG	C1'-S1	-3.30	1.76	1.81
23	C	509	CLA	CHC-C4B	3.30	1.46	1.39
23	A	405[B]	CLA	OBD-CAD	3.29	1.28	1.22
23	B	603	CLA	C1B-NB	-3.29	1.33	1.37
23	b	612	CLA	O2A-CGA	3.28	1.42	1.33
23	C	510	CLA	CHC-C4B	3.28	1.46	1.39
23	b	610	CLA	O2A-CGA	3.28	1.42	1.33
23	C	510	CLA	C1B-NB	-3.28	1.33	1.37
38	f	101	HEM	C1B-NB	-3.27	1.34	1.40
34	b	622	HTG	C1'-S1	-3.27	1.76	1.81
23	c	502	CLA	CHC-C4B	3.27	1.46	1.39
23	B	602	CLA	OBD-CAD	3.27	1.28	1.22
23	c	506	CLA	CHC-C4B	3.27	1.46	1.39
23	B	608	CLA	CHC-C4B	3.27	1.46	1.39
23	D	402[A]	CLA	OBD-CAD	3.26	1.28	1.22
23	B	612	CLA	CHD-C4C	3.26	1.46	1.39
33	D	411	LMG	O7-C10	3.25	1.43	1.34
23	b	610	CLA	C1B-NB	-3.25	1.33	1.37
23	B	602	CLA	C1B-NB	-3.25	1.33	1.37
23	a	404[B]	CLA	C1B-NB	-3.25	1.33	1.37
23	A	408	CLA	OBD-CAD	3.24	1.28	1.22
23	C	506	CLA	C1B-C2B	3.24	1.50	1.43
23	B	607	CLA	C1D-ND	3.24	1.42	1.37
23	B	612	CLA	OBD-CAD	3.24	1.28	1.22
23	b	614	CLA	OBD-CAD	3.24	1.28	1.22
23	B	606	CLA	C4B-NB	-3.23	1.33	1.37
23	c	507	CLA	C1B-NB	-3.23	1.33	1.37
23	C	513	CLA	CHB-C1B	3.23	1.46	1.39
23	a	405[A]	CLA	CHC-C4B	3.23	1.46	1.39
24	A	416[A]	PHO	CHA-CBD	-3.23	1.47	1.51
23	B	616	CLA	CHD-C4C	3.22	1.46	1.39
23	b	602	CLA	C1C-C2C	3.22	1.51	1.44
23	b	616	CLA	CHB-C1B	3.22	1.46	1.39
23	b	613	CLA	CHD-C4C	3.22	1.46	1.39
24	A	416[B]	PHO	CHA-CBD	-3.22	1.47	1.51
23	B	608	CLA	C4B-NB	-3.22	1.33	1.37
23	B	604	CLA	C3D-C2D	3.21	1.47	1.39
23	C	511	CLA	OBD-CAD	3.21	1.28	1.22
23	B	613	CLA	CHC-C4B	3.21	1.46	1.39
23	d	402[A]	CLA	C1B-NB	-3.20	1.33	1.37
23	B	605	CLA	C4B-NB	-3.20	1.33	1.37
23	b	604	CLA	C1B-NB	-3.20	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404[B]	CLA	CHC-C4B	3.20	1.46	1.39
23	A	404[A]	CLA	O2A-CGA	3.20	1.42	1.33
23	c	513	CLA	C4B-NB	-3.19	1.33	1.37
23	B	609	CLA	C1B-NB	-3.19	1.33	1.37
23	d	402[B]	CLA	CHC-C4B	3.19	1.46	1.39
23	D	402[B]	CLA	C1B-NB	-3.19	1.33	1.37
23	C	514	CLA	C4B-NB	-3.18	1.33	1.37
23	c	505	CLA	C1B-NB	-3.17	1.33	1.37
23	b	613	CLA	C1B-NB	-3.16	1.33	1.37
23	C	505	CLA	C1B-NB	-3.15	1.33	1.37
23	a	404[B]	CLA	C4B-NB	-3.15	1.33	1.37
23	A	404[A]	CLA	CHC-C4B	3.15	1.46	1.39
23	b	604	CLA	C1B-C2B	3.15	1.50	1.43
23	a	404[A]	CLA	C1B-NB	-3.15	1.33	1.37
23	b	602	CLA	CHB-C1B	3.14	1.46	1.39
23	c	506	CLA	C1B-NB	-3.14	1.33	1.37
23	d	404[B]	CLA	C4B-NB	-3.13	1.33	1.37
23	b	612	CLA	C4B-NB	-3.12	1.33	1.37
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
23	c	504	CLA	C4B-NB	-3.11	1.33	1.37
38	E	102	HEM	C4D-ND	-3.11	1.34	1.40
23	B	609	CLA	OBD-CAD	3.10	1.27	1.22
23	d	404[B]	CLA	C1B-NB	-3.10	1.33	1.37
23	A	404[B]	CLA	CHC-C4B	3.10	1.46	1.39
23	B	613	CLA	O2A-CGA	3.09	1.42	1.33
23	c	504	CLA	C1B-C2B	3.09	1.50	1.43
23	C	514	CLA	C1B-NB	-3.09	1.33	1.37
23	A	408	CLA	CHB-C1B	3.08	1.46	1.39
23	a	404[A]	CLA	O2A-CGA	3.08	1.42	1.33
23	b	607	CLA	C1B-C2B	3.07	1.50	1.43
23	C	512	CLA	C4D-CHA	3.07	1.48	1.38
23	A	404[B]	CLA	OBD-CAD	3.07	1.27	1.22
23	C	508	CLA	OBD-CAD	3.07	1.27	1.22
23	C	506	CLA	C1B-NB	-3.07	1.33	1.37
23	C	505	CLA	OBD-CAD	3.07	1.27	1.22
24	A	407[A]	PHO	CBD-CGD	-3.06	1.48	1.52
23	b	607	CLA	O2A-CGA	3.06	1.42	1.33
23	C	508	CLA	C4B-NB	-3.06	1.33	1.37
23	c	510	CLA	C1C-C2C	3.05	1.50	1.44
23	B	604	CLA	C1B-C2B	3.04	1.50	1.43
23	B	612	CLA	C1C-C2C	3.04	1.50	1.44
23	D	403	CLA	C1C-C2C	3.03	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	CHC-C4B	3.03	1.46	1.39
23	B	608	CLA	C1B-NB	-3.03	1.33	1.37
23	D	402[A]	CLA	C4B-NB	-3.03	1.33	1.37
23	b	606	CLA	C1B-NB	-3.02	1.33	1.37
23	c	510	CLA	C1B-NB	-3.02	1.33	1.37
23	B	604	CLA	C1B-NB	-3.02	1.33	1.37
23	a	404[A]	CLA	C4B-NB	-3.02	1.33	1.37
23	b	613	CLA	C4B-NB	-3.02	1.33	1.37
23	B	607	CLA	C4D-CHA	3.02	1.48	1.38
23	b	611	CLA	C1B-C2B	3.02	1.50	1.43
23	b	601	CLA	C1B-NB	-3.01	1.33	1.37
23	B	611	CLA	C3B-C4B	3.01	1.51	1.42
23	A	406[B]	CLA	C4B-NB	-3.01	1.33	1.37
23	d	404[A]	CLA	C1D-ND	3.01	1.41	1.37
23	a	407	CLA	C1B-C2B	3.00	1.50	1.43
23	A	404[A]	CLA	C4C-C3C	3.00	1.50	1.45
23	C	505	CLA	C4D-CHA	3.00	1.48	1.38
23	c	509	CLA	CHC-C4B	3.00	1.46	1.39
23	B	610	CLA	C4D-CHA	3.00	1.48	1.38
23	D	403	CLA	C4C-C3C	3.00	1.50	1.45
23	c	506	CLA	C1B-C2B	3.00	1.50	1.43
23	C	507	CLA	C4C-C3C	2.99	1.50	1.45
23	b	612	CLA	C1B-C2B	2.99	1.50	1.43
23	B	616	CLA	C1B-NB	-2.99	1.33	1.37
23	B	615	CLA	C1B-C2B	2.98	1.50	1.43
23	A	404[B]	CLA	C4B-NB	-2.98	1.33	1.37
23	b	604	CLA	C4D-CHA	2.97	1.48	1.38
23	c	503	CLA	OBD-CAD	2.96	1.27	1.22
23	B	602	CLA	C1C-C2C	2.96	1.50	1.44
24	d	403[B]	PHO	C3A-C2A	-2.96	1.52	1.54
23	a	407	CLA	OBD-CAD	2.96	1.27	1.22
23	c	509	CLA	C1B-C2B	2.96	1.50	1.43
23	A	404[B]	CLA	C4C-C3C	2.96	1.50	1.45
23	A	404[A]	CLA	C1B-NB	-2.95	1.34	1.37
23	a	405[A]	CLA	C1B-NB	-2.95	1.34	1.37
23	C	511	CLA	CHC-C4B	2.95	1.46	1.39
23	b	611	CLA	OBD-CAD	2.95	1.27	1.22
29	A	414[A]	PL9	C6-C5	2.94	1.49	1.35
23	B	606	CLA	OBD-CAD	2.94	1.27	1.22
29	a	413[A]	PL9	C6-C5	2.93	1.49	1.35
23	B	608	CLA	C4D-CHA	2.93	1.48	1.38
23	a	407	CLA	C1C-C2C	2.93	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	OBD-CAD	2.93	1.27	1.22
34	b	625	HTG	C1'-S1	-2.92	1.77	1.81
23	B	616	CLA	C4B-NB	-2.92	1.34	1.37
29	A	414[B]	PL9	C6-C5	2.92	1.49	1.35
23	c	511	CLA	C4B-NB	-2.91	1.34	1.37
23	B	616	CLA	OBD-CAD	2.91	1.27	1.22
23	b	613	CLA	C4D-CHA	2.91	1.48	1.38
23	c	510	CLA	C1B-C2B	2.91	1.50	1.43
23	b	605	CLA	C1B-NB	-2.91	1.34	1.37
34	D	410	HTG	C1'-S1	-2.91	1.77	1.81
23	c	507	CLA	C4B-NB	-2.90	1.34	1.37
23	D	402[A]	CLA	C1B-C2B	2.90	1.49	1.43
23	B	608	CLA	OBD-CAD	2.89	1.27	1.22
23	B	605	CLA	OBD-CAD	2.89	1.27	1.22
23	B	611	CLA	MG-NB	2.89	2.11	2.05
23	c	508	CLA	C4B-NB	-2.89	1.34	1.37
29	a	413[B]	PL9	C6-C5	2.89	1.49	1.35
23	c	508	CLA	C4C-C3C	2.89	1.49	1.45
23	b	613	CLA	C1B-C2B	2.89	1.49	1.43
23	c	502	CLA	C4B-NB	-2.88	1.34	1.37
23	B	609	CLA	C3B-C4B	2.88	1.51	1.42
23	c	501	CLA	OBD-CAD	2.88	1.27	1.22
23	A	406[B]	CLA	C1B-NB	-2.88	1.34	1.37
23	b	612	CLA	C1C-C2C	2.87	1.50	1.44
23	C	508	CLA	C4D-CHA	2.87	1.48	1.38
23	b	609	CLA	C1B-NB	-2.87	1.34	1.37
23	b	607	CLA	OBD-CAD	2.87	1.27	1.22
23	D	402[B]	CLA	C4B-NB	-2.87	1.34	1.37
23	C	508	CLA	C1B-NB	-2.87	1.34	1.37
23	c	512	CLA	C1B-NB	-2.87	1.34	1.37
23	C	505	CLA	C1B-C2B	2.87	1.49	1.43
35	H	102	DGD	O5D-C1E	2.87	1.45	1.40
23	C	510	CLA	C1B-C2B	2.87	1.49	1.43
23	b	603	CLA	C1B-C2B	2.86	1.49	1.43
23	c	504	CLA	C1C-C2C	2.86	1.50	1.44
23	B	605	CLA	C1B-NB	-2.86	1.34	1.37
23	B	614	CLA	C4D-CHA	2.86	1.48	1.38
23	d	404[A]	CLA	C4B-NB	-2.86	1.34	1.37
23	B	616	CLA	C1B-C2B	2.85	1.49	1.43
23	c	502	CLA	C1B-C2B	2.85	1.49	1.43
23	D	403	CLA	C1B-C2B	2.85	1.49	1.43
23	b	614	CLA	C1B-C2B	2.85	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	c	521	HTG	C1'-S1	-2.85	1.77	1.81
23	a	405[B]	CLA	C1B-C2B	2.84	1.49	1.43
23	A	408	CLA	C1B-NB	-2.84	1.34	1.37
23	c	513	CLA	C1B-C2B	2.83	1.49	1.43
23	C	507	CLA	C1B-C2B	2.83	1.49	1.43
23	A	408	CLA	C1B-C2B	2.83	1.49	1.43
34	d	412	HTG	C1'-S1	-2.83	1.77	1.81
23	d	402[B]	CLA	C1B-C2B	2.83	1.49	1.43
23	C	513	CLA	C1B-NB	-2.83	1.34	1.37
23	A	406[A]	CLA	C4D-CHA	2.83	1.48	1.38
23	B	612	CLA	C4D-CHA	2.82	1.48	1.38
23	B	615	CLA	C4D-CHA	2.82	1.48	1.38
23	b	606	CLA	C4B-NB	-2.82	1.34	1.37
23	c	506	CLA	C4B-NB	-2.82	1.34	1.37
23	C	502	CLA	C4D-CHA	2.82	1.48	1.38
23	A	404[A]	CLA	C1B-C2B	2.82	1.49	1.43
23	D	402[A]	CLA	C4D-CHA	2.81	1.48	1.38
23	c	503	CLA	C1B-NB	-2.81	1.34	1.37
23	B	612	CLA	C1B-C2B	2.81	1.49	1.43
23	B	603	CLA	C4B-NB	-2.81	1.34	1.37
23	B	613	CLA	C4D-CHA	2.81	1.48	1.38
23	b	611	CLA	C1B-NB	-2.80	1.34	1.37
23	b	609	CLA	C4D-CHA	2.80	1.48	1.38
23	A	404[B]	CLA	C4D-CHA	2.80	1.48	1.38
23	C	509	CLA	C1B-C2B	2.80	1.49	1.43
33	Z	101	LMG	O8-C28	2.80	1.46	1.33
23	B	614	CLA	C1B-NB	-2.80	1.34	1.37
23	c	501	CLA	C4C-C3C	2.80	1.49	1.45
23	c	505	CLA	C3B-C4B	2.80	1.50	1.42
23	c	507	CLA	C1B-C2B	2.80	1.49	1.43
34	b	625	HTG	C1-S1	-2.79	1.76	1.80
23	c	503	CLA	C4B-NB	-2.79	1.34	1.37
27	a	418	GOL	C1-C2	2.79	1.62	1.51
23	d	402[A]	CLA	C1B-C2B	2.79	1.49	1.43
23	B	607	CLA	C1B-C2B	2.78	1.49	1.43
23	A	405[A]	CLA	C4D-CHA	2.78	1.47	1.38
23	B	601	CLA	C1B-NB	-2.78	1.34	1.37
23	b	607	CLA	C4D-CHA	2.78	1.47	1.38
23	c	512	CLA	C4D-CHA	2.78	1.47	1.38
23	c	511	CLA	C4D-CHA	2.78	1.47	1.38
23	b	607	CLA	C4C-C3C	2.77	1.49	1.45
23	B	615	CLA	C1C-C2C	2.77	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C1B-C2B	2.77	1.49	1.43
23	B	616	CLA	C4D-CHA	2.77	1.47	1.38
23	D	403	CLA	C1B-NB	-2.77	1.34	1.37
23	c	507	CLA	C4D-CHA	2.77	1.47	1.38
34	C	522	HTG	C1'-S1	-2.77	1.77	1.81
23	C	511	CLA	C4C-C3C	2.77	1.49	1.45
23	c	501	CLA	C4D-CHA	2.76	1.47	1.38
23	C	505	CLA	C4B-NB	-2.76	1.34	1.37
23	A	406[B]	CLA	C1B-C2B	2.76	1.49	1.43
23	a	405[B]	CLA	C4B-NB	-2.76	1.34	1.37
23	B	605	CLA	C4D-CHA	2.76	1.47	1.38
23	C	514	CLA	C1B-C2B	2.75	1.49	1.43
23	c	501	CLA	C1B-C2B	2.75	1.49	1.43
23	c	510	CLA	C4D-CHA	2.75	1.47	1.38
23	B	610	CLA	C1B-C2B	2.75	1.49	1.43
23	c	505	CLA	C1B-C2B	2.75	1.49	1.43
23	b	616	CLA	C1B-C2B	2.75	1.49	1.43
24	A	416[B]	PHO	C3A-C2A	-2.74	1.52	1.54
23	A	406[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	b	614	CLA	C4B-NB	-2.74	1.34	1.37
23	c	503	CLA	C1B-C2B	2.74	1.49	1.43
23	C	513	CLA	C4D-CHA	2.74	1.47	1.38
23	B	604	CLA	C4D-CHA	2.74	1.47	1.38
23	a	405[A]	CLA	C1B-C2B	2.74	1.49	1.43
23	A	404[B]	CLA	C1B-C2B	2.74	1.49	1.43
23	b	609	CLA	C1B-C2B	2.74	1.49	1.43
23	B	605	CLA	C1B-C2B	2.73	1.49	1.43
23	C	506	CLA	C4C-C3C	2.73	1.49	1.45
23	B	606	CLA	C1C-C2C	2.73	1.50	1.44
23	a	404[B]	CLA	C1B-C2B	2.73	1.49	1.43
23	b	602	CLA	C4C-C3C	2.73	1.49	1.45
23	b	611	CLA	C4B-NB	-2.72	1.34	1.37
23	D	403	CLA	C3B-C4B	2.72	1.50	1.42
23	c	503	CLA	C3B-C4B	2.72	1.50	1.42
23	C	513	CLA	C1C-C2C	2.72	1.50	1.44
23	a	404[A]	CLA	C1B-C2B	2.72	1.49	1.43
23	b	610	CLA	C4D-CHA	2.72	1.47	1.38
23	a	405[A]	CLA	C4D-CHA	2.72	1.47	1.38
23	b	602	CLA	C3B-C4B	2.72	1.50	1.42
23	b	603	CLA	C4B-NB	-2.72	1.34	1.37
23	d	404[A]	CLA	C1B-C2B	2.71	1.49	1.43
23	c	502	CLA	C1B-NB	-2.71	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	C4D-CHA	2.71	1.47	1.38
23	c	511	CLA	C1B-NB	-2.71	1.34	1.37
23	c	503	CLA	C1C-C2C	2.71	1.50	1.44
23	A	408	CLA	C3D-C4D	-2.70	1.38	1.44
23	A	408	CLA	C4D-CHA	2.70	1.47	1.38
24	d	403[A]	PHO	C3A-C2A	-2.70	1.52	1.54
23	b	607	CLA	C4B-NB	-2.70	1.34	1.37
23	a	405[B]	CLA	C1B-NB	-2.70	1.34	1.37
23	C	507	CLA	C4D-CHA	2.70	1.47	1.38
23	B	601	CLA	C4B-NB	-2.69	1.34	1.37
23	A	405[B]	CLA	C1B-C2B	2.69	1.49	1.43
23	c	508	CLA	C1B-C2B	2.69	1.49	1.43
23	C	504	CLA	C1B-NB	-2.69	1.34	1.37
23	B	614	CLA	C1B-C2B	2.68	1.49	1.43
23	C	509	CLA	C1B-NB	-2.68	1.34	1.37
23	A	405[A]	CLA	C1B-C2B	2.68	1.49	1.43
23	d	404[B]	CLA	C4D-CHA	2.68	1.47	1.38
23	b	611	CLA	C4C-C3C	2.68	1.49	1.45
23	B	606	CLA	C1B-NB	-2.68	1.34	1.37
23	C	503	CLA	C1B-C2B	2.68	1.49	1.43
23	a	405[B]	CLA	C1C-C2C	2.67	1.49	1.44
23	d	405	CLA	C4D-CHA	2.67	1.47	1.38
23	c	504	CLA	C1C-NC	-2.67	1.33	1.37
23	C	514	CLA	C4D-CHA	2.67	1.47	1.38
23	A	404[A]	CLA	C4D-CHA	2.66	1.47	1.38
23	D	402[B]	CLA	C1B-C2B	2.66	1.49	1.43
23	b	607	CLA	C1C-C2C	2.66	1.49	1.44
23	B	603	CLA	C1B-C2B	2.66	1.49	1.43
23	b	615	CLA	C4D-CHA	2.66	1.47	1.38
23	C	509	CLA	C4D-CHA	2.66	1.47	1.38
23	C	511	CLA	C1B-C2B	2.66	1.49	1.43
23	B	613	CLA	C1B-C2B	2.65	1.49	1.43
23	c	505	CLA	C4C-C3C	2.65	1.49	1.45
23	b	612	CLA	C1B-NB	-2.65	1.34	1.37
23	B	614	CLA	C3D-C4D	-2.65	1.38	1.44
23	C	512	CLA	C1B-C2B	2.65	1.49	1.43
23	c	509	CLA	C4D-CHA	2.65	1.47	1.38
23	b	605	CLA	C4D-CHA	2.65	1.47	1.38
23	b	616	CLA	C1C-C2C	2.65	1.49	1.44
23	c	504	CLA	C4D-CHA	2.64	1.47	1.38
23	A	405[B]	CLA	C4D-CHA	2.64	1.47	1.38
23	b	616	CLA	C1B-NB	-2.64	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C4D-CHA	2.64	1.47	1.38
23	b	601	CLA	C4D-CHA	2.64	1.47	1.38
23	B	609	CLA	C4D-CHA	2.64	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.64	1.47	1.38
23	C	508	CLA	C1B-C2B	2.64	1.49	1.43
23	C	510	CLA	C4D-CHA	2.63	1.47	1.38
23	B	607	CLA	C3D-C4D	-2.63	1.38	1.44
29	D	405[B]	PL9	C6-C5	2.63	1.48	1.35
23	B	606	CLA	C4D-CHA	2.63	1.47	1.38
23	b	616	CLA	C3B-C4B	2.63	1.50	1.42
23	B	610	CLA	C4C-C3C	2.63	1.49	1.45
23	c	508	CLA	C1C-C2C	2.63	1.49	1.44
23	b	601	CLA	C4B-NB	-2.63	1.34	1.37
23	B	609	CLA	C1B-C2B	2.63	1.49	1.43
23	B	615	CLA	C1B-NB	-2.62	1.34	1.37
23	C	509	CLA	C4C-C3C	2.62	1.49	1.45
23	C	511	CLA	C4D-CHA	2.62	1.47	1.38
23	b	612	CLA	C4D-CHA	2.62	1.47	1.38
23	a	405[A]	CLA	C1C-C2C	2.62	1.49	1.44
23	A	405[A]	CLA	C4B-NB	-2.62	1.34	1.37
23	b	609	CLA	C4B-NB	-2.62	1.34	1.37
23	b	615	CLA	C1B-C2B	2.61	1.49	1.43
23	C	502	CLA	C1C-C2C	2.61	1.49	1.44
23	c	512	CLA	C1B-C2B	2.61	1.49	1.43
23	A	406[B]	CLA	C4D-CHA	2.61	1.47	1.38
23	C	509	CLA	C4B-NB	-2.61	1.34	1.37
23	C	512	CLA	C1B-NB	-2.60	1.34	1.37
23	c	503	CLA	C4D-CHA	2.60	1.47	1.38
23	C	506	CLA	C4D-CHA	2.60	1.47	1.38
23	C	502	CLA	C1B-C2B	2.60	1.49	1.43
23	d	404[A]	CLA	C4C-C3C	2.59	1.49	1.45
23	C	504	CLA	C4D-CHA	2.59	1.47	1.38
23	C	512	CLA	C1C-C2C	2.59	1.49	1.44
23	B	608	CLA	C1B-C2B	2.59	1.49	1.43
38	E	102	HEM	C1C-C2C	-2.59	1.40	1.45
23	d	402[B]	CLA	C4D-CHA	2.59	1.47	1.38
23	c	506	CLA	C4D-CHA	2.58	1.47	1.38
23	B	602	CLA	C4D-CHA	2.58	1.47	1.38
23	c	505	CLA	C4D-CHA	2.58	1.47	1.38
23	C	510	CLA	C1C-C2C	2.58	1.49	1.44
23	c	512	CLA	C4B-NB	-2.58	1.34	1.37
23	A	405[A]	CLA	C3B-C4B	2.58	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C4D-CHA	2.58	1.47	1.38
23	d	404[B]	CLA	C1B-C2B	2.58	1.49	1.43
23	B	613	CLA	C1C-C2C	2.57	1.49	1.44
23	b	610	CLA	C1B-C2B	2.57	1.49	1.43
23	a	404[B]	CLA	C4D-CHA	2.57	1.47	1.38
23	a	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	C	502	CLA	OBD-CAD	2.57	1.26	1.22
29	d	407[B]	PL9	C6-C5	2.57	1.47	1.35
23	d	402[A]	CLA	C4D-CHA	2.57	1.47	1.38
35	C	519	DGD	O2G-C2G	-2.57	1.40	1.46
23	B	611	CLA	C4D-CHA	2.56	1.47	1.38
23	C	504	CLA	C4B-NB	-2.56	1.34	1.37
23	B	607	CLA	C1C-C2C	2.56	1.49	1.44
23	b	612	CLA	C4C-C3C	2.56	1.49	1.45
23	b	605	CLA	C1B-C2B	2.56	1.49	1.43
23	b	610	CLA	C1C-C2C	2.56	1.49	1.44
23	c	502	CLA	C4D-CHA	2.56	1.47	1.38
23	B	605	CLA	C3B-C4B	2.55	1.50	1.42
23	c	509	CLA	C4C-C3C	2.55	1.49	1.45
27	A	418	GOL	C3-C2	2.55	1.61	1.51
23	C	508	CLA	C1C-C2C	2.55	1.49	1.44
23	A	408	CLA	C4B-NB	-2.55	1.34	1.37
23	c	513	CLA	C4D-CHA	2.55	1.47	1.38
23	b	608	CLA	C4D-CHA	2.55	1.47	1.38
23	B	616	CLA	C3B-C2B	2.54	1.49	1.41
23	c	513	CLA	C1C-C2C	2.54	1.49	1.44
23	c	503	CLA	C3D-C4D	-2.54	1.38	1.44
23	a	407	CLA	C4B-NB	-2.54	1.34	1.37
23	C	503	CLA	C1C-C2C	2.54	1.49	1.44
23	C	505	CLA	C1C-C2C	2.54	1.49	1.44
23	b	616	CLA	C4D-CHA	2.54	1.47	1.38
23	C	509	CLA	C3B-C2B	2.53	1.49	1.41
23	C	507	CLA	C3D-C4D	-2.53	1.38	1.44
23	a	404[A]	CLA	C4C-C3C	2.53	1.49	1.45
23	C	502	CLA	C3B-C4B	2.53	1.50	1.42
23	b	614	CLA	C4D-CHA	2.53	1.47	1.38
23	B	606	CLA	C1B-C2B	2.53	1.49	1.43
23	b	606	CLA	C1B-C2B	2.53	1.49	1.43
23	D	402[B]	CLA	C4D-CHA	2.53	1.47	1.38
23	B	604	CLA	C4B-NB	-2.53	1.34	1.37
23	b	614	CLA	C3D-C4D	-2.52	1.38	1.44
24	a	406[A]	PHO	CBD-CGD	-2.52	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[A]	CLA	C3B-C4B	2.52	1.50	1.42
23	d	404[B]	CLA	C4C-C3C	2.52	1.49	1.45
23	c	511	CLA	C1C-C2C	2.52	1.49	1.44
23	a	405[A]	CLA	C4B-NB	-2.52	1.34	1.37
23	C	506	CLA	C3B-C4B	2.52	1.50	1.42
23	B	601	CLA	C1B-C2B	2.51	1.49	1.43
23	C	513	CLA	C4B-NB	-2.51	1.34	1.37
23	B	608	CLA	C4C-C3C	2.51	1.49	1.45
23	B	616	CLA	C1C-C2C	2.51	1.49	1.44
29	d	407[A]	PL9	C6-C5	2.51	1.47	1.35
23	b	608	CLA	C1B-C2B	2.50	1.49	1.43
23	A	406[A]	CLA	C1B-C2B	2.50	1.49	1.43
23	B	610	CLA	C1C-C2C	2.50	1.49	1.44
23	B	601	CLA	C4D-CHA	2.50	1.47	1.38
23	b	611	CLA	C1C-C2C	2.50	1.49	1.44
23	b	608	CLA	C3D-C4D	-2.50	1.38	1.44
23	c	507	CLA	C1C-C2C	2.49	1.49	1.44
23	b	606	CLA	C3D-C4D	-2.49	1.38	1.44
29	D	405[A]	PL9	C6-C5	2.49	1.47	1.35
23	B	602	CLA	C4B-NB	-2.49	1.34	1.37
24	A	416[A]	PHO	C3A-C2A	-2.49	1.52	1.54
23	d	405	CLA	C4B-NB	-2.49	1.34	1.37
23	d	405	CLA	C3B-C4B	2.49	1.50	1.42
23	D	402[B]	CLA	C4C-C3C	2.48	1.49	1.45
33	C	521	LMG	O1-C1	2.48	1.44	1.40
23	c	502	CLA	C3B-C2B	2.48	1.49	1.41
23	b	615	CLA	C4B-NB	-2.48	1.34	1.37
23	a	407	CLA	C4D-CHA	2.48	1.46	1.38
23	b	602	CLA	C4D-CHA	2.48	1.46	1.38
23	C	504	CLA	C1C-C2C	2.48	1.49	1.44
23	C	513	CLA	C3D-C4D	-2.47	1.38	1.44
23	a	404[B]	CLA	C4C-C3C	2.47	1.49	1.45
23	B	603	CLA	C4C-C3C	2.47	1.49	1.45
23	D	403	CLA	C4D-CHA	2.47	1.46	1.38
23	C	512	CLA	C3B-C2B	2.47	1.49	1.41
23	A	406[B]	CLA	C3B-C4B	2.47	1.49	1.42
40	v	201	HEC	CMC-C2C	2.47	1.55	1.50
23	a	407	CLA	C3B-C4B	2.47	1.49	1.42
38	f	101	HEM	C1C-C2C	-2.47	1.40	1.45
23	d	405	CLA	C1C-C2C	2.47	1.49	1.44
23	d	404[A]	CLA	C4D-CHA	2.47	1.46	1.38
23	B	601	CLA	C1C-C2C	2.47	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	101	LMT	O2'-C2'	-2.46	1.36	1.43
23	C	513	CLA	C3B-C4B	2.46	1.49	1.42
24	A	416[A]	PHO	C3D-C4D	-2.46	1.37	1.41
23	a	405[B]	CLA	C3B-C4B	2.46	1.49	1.42
23	C	505	CLA	C4C-C3C	2.46	1.49	1.45
23	c	504	CLA	C4C-C3C	2.46	1.49	1.45
23	a	405[A]	CLA	C3B-C4B	2.46	1.49	1.42
23	a	405[A]	CLA	C3D-C4D	-2.46	1.38	1.44
23	B	610	CLA	C3B-C4B	2.45	1.49	1.42
23	B	613	CLA	C4B-NB	-2.45	1.34	1.37
23	C	503	CLA	C1B-NB	-2.45	1.34	1.37
23	c	505	CLA	C1C-C2C	2.45	1.49	1.44
38	f	101	HEM	C1D-ND	-2.45	1.34	1.38
31	t	101	LMT	O3'-C3'	-2.44	1.36	1.43
23	B	608	CLA	C3B-C2B	2.44	1.49	1.41
23	B	606	CLA	C3D-C4D	-2.44	1.38	1.44
23	B	601	CLA	C3B-C4B	2.44	1.49	1.42
23	b	601	CLA	C3B-C4B	2.44	1.49	1.42
23	c	501	CLA	C4B-NB	-2.44	1.34	1.37
31	C	525	LMT	O3'-C3'	-2.44	1.36	1.43
23	C	512	CLA	C3D-C4D	-2.43	1.38	1.44
24	d	403[B]	PHO	C4B-NB	-2.43	1.34	1.38
23	A	405[B]	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	507	CLA	C1C-C2C	2.43	1.49	1.44
23	b	610	CLA	C4C-C3C	2.43	1.49	1.45
23	B	602	CLA	C3D-C4D	-2.43	1.38	1.44
23	c	512	CLA	C3B-C4B	2.42	1.49	1.42
23	c	508	CLA	C1B-NB	-2.42	1.34	1.37
31	B	627	LMT	C3'-C2'	2.42	1.58	1.52
23	b	606	CLA	C3B-C4B	2.42	1.49	1.42
23	B	605	CLA	C3D-C4D	-2.42	1.38	1.44
23	C	504	CLA	C1B-C2B	2.42	1.48	1.43
23	c	508	CLA	C3B-C2B	2.42	1.49	1.41
23	C	504	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	602	CLA	C3D-C4D	-2.42	1.38	1.44
23	B	609	CLA	C1C-C2C	2.41	1.49	1.44
23	C	514	CLA	C3B-C2B	2.41	1.49	1.41
23	b	615	CLA	C4C-C3C	2.41	1.49	1.45
23	b	603	CLA	C3B-C4B	2.41	1.49	1.42
23	b	610	CLA	C3D-C4D	-2.41	1.38	1.44
23	D	402[A]	CLA	C3D-C4D	-2.41	1.38	1.44
23	D	402[B]	CLA	C1C-C2C	2.41	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	201	HEC	CMC-C2C	2.41	1.55	1.50
23	b	611	CLA	C4D-CHA	2.41	1.46	1.38
23	B	612	CLA	C3B-C2B	2.40	1.49	1.41
23	b	612	CLA	C3B-C2B	2.40	1.49	1.41
23	b	601	CLA	C3B-C2B	2.40	1.49	1.41
27	A	418	GOL	O2-C2	-2.40	1.36	1.43
23	B	605	CLA	C1C-C2C	2.40	1.49	1.44
23	C	512	CLA	C4C-C3C	2.40	1.49	1.45
23	A	404[A]	CLA	C1C-C2C	2.40	1.49	1.44
23	b	616	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	513	CLA	C1B-C2B	2.40	1.48	1.43
23	C	511	CLA	C3D-C4D	-2.39	1.38	1.44
23	A	405[B]	CLA	C4B-NB	-2.39	1.34	1.37
23	b	609	CLA	C3B-C4B	2.39	1.49	1.42
23	c	510	CLA	C4C-C3C	2.39	1.49	1.45
23	c	510	CLA	C4B-NB	-2.39	1.34	1.37
23	b	615	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	504	CLA	C3B-C4B	2.39	1.49	1.42
23	C	510	CLA	C3B-C2B	2.39	1.49	1.41
23	a	405[B]	CLA	C3D-C4D	-2.39	1.38	1.44
35	c	518	DGD	O2G-C2G	-2.39	1.41	1.46
23	B	603	CLA	C4D-CHA	2.39	1.46	1.38
26	X	101	SQD	O6-C1	2.39	1.44	1.40
23	b	601	CLA	C1C-C2C	2.38	1.49	1.44
23	c	506	CLA	C4C-C3C	2.38	1.49	1.45
23	d	402[A]	CLA	C3B-C4B	2.38	1.49	1.42
23	B	603	CLA	C3B-C2B	2.38	1.49	1.41
31	M	101	LMT	O2B-C2B	-2.38	1.37	1.43
23	b	609	CLA	C1C-C2C	2.38	1.49	1.44
23	C	510	CLA	C4C-C3C	2.38	1.49	1.45
29	D	405[B]	PL9	C2-C3	2.38	1.40	1.34
23	B	613	CLA	C3B-C2B	2.38	1.49	1.41
23	B	614	CLA	C1C-C2C	2.37	1.49	1.44
23	b	613	CLA	C3B-C2B	2.37	1.49	1.41
23	c	505	CLA	C4B-NB	-2.37	1.34	1.37
23	d	405	CLA	C1B-C2B	2.37	1.48	1.43
24	A	416[B]	PHO	C4B-NB	-2.37	1.34	1.38
24	A	407[B]	PHO	CBD-CGD	-2.37	1.49	1.52
23	A	408	CLA	C3B-C2B	2.37	1.49	1.41
23	c	504	CLA	C3B-C2B	2.37	1.49	1.41
23	B	610	CLA	C3D-C4D	-2.37	1.38	1.44
23	C	508	CLA	C4C-C3C	2.37	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	616	CLA	C4B-NB	-2.36	1.34	1.37
31	B	627	LMT	O3'-C3'	-2.36	1.37	1.43
23	C	506	CLA	C1C-C2C	2.36	1.49	1.44
23	b	606	CLA	C1C-C2C	2.36	1.49	1.44
23	d	404[B]	CLA	C3D-C4D	-2.36	1.38	1.44
31	T	101	LMT	O3'-C3'	-2.36	1.37	1.43
31	b	621	LMT	C3'-C2'	2.36	1.58	1.52
23	A	405[A]	CLA	C3D-C4D	-2.36	1.38	1.44
23	C	509	CLA	C1C-C2C	2.36	1.49	1.44
23	b	603	CLA	C3D-C4D	-2.36	1.38	1.44
23	b	608	CLA	C3B-C2B	2.35	1.49	1.41
23	c	513	CLA	C4C-C3C	2.35	1.49	1.45
23	C	511	CLA	C1C-C2C	2.35	1.49	1.44
23	D	402[B]	CLA	C3D-C4D	-2.35	1.38	1.44
23	c	506	CLA	C3D-C4D	-2.35	1.38	1.44
24	A	416[A]	PHO	C4B-NB	-2.35	1.34	1.38
23	c	511	CLA	C3B-C2B	2.35	1.49	1.41
35	h	102	DGD	O5D-C1E	2.35	1.44	1.40
31	m	103	LMT	O2B-C2B	-2.35	1.37	1.43
23	a	404[B]	CLA	C3B-C2B	2.35	1.49	1.41
23	b	612	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	602	CLA	C4B-NB	-2.34	1.34	1.37
23	b	603	CLA	C3B-C2B	2.34	1.49	1.41
23	c	510	CLA	C3B-C2B	2.34	1.49	1.41
23	b	605	CLA	C4B-NB	-2.34	1.34	1.37
23	A	406[B]	CLA	C1C-C2C	2.34	1.49	1.44
23	A	405[B]	CLA	C3B-C4B	2.34	1.49	1.42
23	c	501	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	613	CLA	OBD-CAD	2.34	1.26	1.22
23	a	404[A]	CLA	C3B-C2B	2.34	1.49	1.41
23	A	404[A]	CLA	C3B-C2B	2.34	1.49	1.41
24	a	406[B]	PHO	C4B-NB	-2.34	1.34	1.38
23	B	613	CLA	C4C-C3C	2.33	1.49	1.45
23	b	614	CLA	C3B-C2B	2.33	1.49	1.41
23	c	513	CLA	C3D-C4D	-2.33	1.38	1.44
23	B	609	CLA	C3D-C4D	-2.33	1.38	1.44
31	B	629	LMT	O3'-C3'	-2.33	1.37	1.43
23	b	609	CLA	C3D-C4D	-2.33	1.38	1.44
25	d	406	BCR	C30-C25	-2.33	1.50	1.53
23	A	406[B]	CLA	C3D-C4D	-2.32	1.39	1.44
23	b	604	CLA	C4B-NB	-2.32	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[A]	CLA	C1C-C2C	2.32	1.49	1.44
23	A	406[A]	CLA	C1C-C2C	2.32	1.49	1.44
23	d	404[A]	CLA	C3D-C4D	-2.32	1.39	1.44
35	H	102	DGD	O2G-C2G	-2.32	1.41	1.46
31	C	525	LMT	O2'-C2'	-2.31	1.37	1.43
23	c	503	CLA	C4C-C3C	2.31	1.49	1.45
23	c	501	CLA	C1B-NB	-2.31	1.34	1.37
23	A	405[B]	CLA	C1C-C2C	2.31	1.49	1.44
23	b	608	CLA	C1C-C2C	2.30	1.49	1.44
23	B	615	CLA	C3B-C4B	2.30	1.49	1.42
23	b	611	CLA	C3B-C2B	2.30	1.48	1.41
29	a	413[A]	PL9	C2-C3	2.30	1.40	1.34
23	b	603	CLA	C1C-C2C	2.30	1.49	1.44
23	A	404[B]	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	514	CLA	C1C-C2C	2.30	1.49	1.44
23	C	503	CLA	C3B-C2B	2.30	1.48	1.41
23	C	505	CLA	C3B-C2B	2.30	1.48	1.41
23	d	402[B]	CLA	C4B-NB	-2.29	1.34	1.37
31	e	101	LMT	O3'-C3'	-2.29	1.37	1.43
23	C	502	CLA	C3D-C4D	-2.29	1.39	1.44
23	c	511	CLA	C4C-C3C	2.29	1.48	1.45
23	c	513	CLA	C3B-C4B	2.29	1.49	1.42
23	c	512	CLA	C3D-C4D	-2.29	1.39	1.44
23	a	404[B]	CLA	C1C-C2C	2.28	1.49	1.44
23	b	601	CLA	C4C-C3C	2.28	1.48	1.45
24	A	416[A]	PHO	C1D-ND	-2.28	1.34	1.38
23	d	405	CLA	C4C-C3C	2.28	1.48	1.45
23	B	602	CLA	C3B-C2B	2.28	1.48	1.41
23	B	606	CLA	C3B-C4B	2.28	1.49	1.42
34	B	624	HTG	C1-S1	-2.28	1.76	1.80
23	C	506	CLA	C3D-C4D	-2.28	1.39	1.44
23	c	501	CLA	C3B-C4B	2.28	1.49	1.42
23	b	605	CLA	C3B-C4B	2.28	1.49	1.42
24	A	416[B]	PHO	C3D-C4D	-2.28	1.38	1.41
23	b	614	CLA	C3B-C4B	2.27	1.49	1.42
23	c	510	CLA	C3B-C4B	2.27	1.49	1.42
23	B	602	CLA	C4C-C3C	2.27	1.48	1.45
23	C	503	CLA	C4D-CHA	2.27	1.46	1.38
23	B	615	CLA	MG-NA	2.27	2.11	2.06
23	C	505	CLA	C3D-C4D	-2.27	1.39	1.44
23	b	614	CLA	C1C-C2C	2.27	1.49	1.44
34	B	621	HTG	O5-C1	2.26	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1C-NC	-2.26	1.34	1.37
24	a	406[B]	PHO	C1D-ND	-2.26	1.34	1.38
23	b	610	CLA	C4B-NB	-2.26	1.34	1.37
23	C	508	CLA	C3D-C4D	-2.26	1.39	1.44
40	V	201	HEC	CMB-C2B	2.26	1.55	1.50
23	A	406[A]	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	604	CLA	C3B-C2B	2.26	1.48	1.41
27	D	412	GOL	O2-C2	-2.26	1.36	1.43
35	C	518[A]	DGD	O5D-C1E	2.26	1.44	1.40
23	b	604	CLA	C1C-C2C	2.25	1.49	1.44
34	b	622	HTG	O5-C1	2.25	1.46	1.42
23	d	402[B]	CLA	C3B-C4B	2.25	1.49	1.42
23	a	405[B]	CLA	C4C-C3C	2.25	1.48	1.45
29	a	413[B]	PL9	C2-C3	2.25	1.40	1.34
23	B	601	CLA	C3B-C2B	2.25	1.48	1.41
23	B	601	CLA	C4C-C3C	2.25	1.48	1.45
23	d	404[B]	CLA	C3B-C2B	2.25	1.48	1.41
23	B	607	CLA	C4B-NB	-2.25	1.34	1.37
29	d	407[B]	PL9	C2-C3	2.24	1.40	1.34
23	D	402[A]	CLA	C4C-C3C	2.24	1.48	1.45
23	C	514	CLA	C3D-C4D	-2.24	1.39	1.44
23	c	501	CLA	C1C-C2C	2.23	1.49	1.44
23	C	512	CLA	C3B-C4B	2.23	1.49	1.42
23	C	513	CLA	C3B-C2B	2.23	1.48	1.41
24	a	406[A]	PHO	C4B-NB	-2.22	1.34	1.38
23	D	402[B]	CLA	C3B-C2B	2.22	1.48	1.41
23	b	607	CLA	C3D-C4D	-2.22	1.39	1.44
23	c	508	CLA	C3D-C4D	-2.22	1.39	1.44
23	d	404[A]	CLA	C1C-C2C	2.22	1.49	1.44
23	c	506	CLA	C3B-C2B	2.22	1.48	1.41
23	b	610	CLA	C3B-C4B	2.22	1.49	1.42
23	D	403	CLA	C4B-NB	-2.22	1.35	1.37
23	b	608	CLA	C4C-C3C	2.21	1.48	1.45
24	d	403[A]	PHO	C4B-NB	-2.21	1.34	1.38
23	C	510	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.21	1.39	1.44
23	B	613	CLA	C3D-C4D	-2.21	1.39	1.44
23	C	507	CLA	C1D-C2D	2.21	1.49	1.45
23	D	402[A]	CLA	C3B-C2B	2.21	1.48	1.41
38	E	102	HEM	C3B-C4B	2.21	1.49	1.44
24	A	407[A]	PHO	C4B-NB	-2.21	1.34	1.38
23	c	505	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	A	414[A]	PL9	C2-C1	-2.21	1.39	1.44
23	c	509	CLA	C3B-C2B	2.20	1.48	1.41
23	B	614	CLA	C4C-C3C	2.20	1.48	1.45
23	d	405	CLA	C1B-NB	-2.20	1.35	1.37
24	a	406[B]	PHO	C3A-C2A	-2.20	1.52	1.54
31	a	416	LMT	O3'-C3'	-2.20	1.37	1.43
23	b	604	CLA	C3B-C4B	2.20	1.49	1.42
38	E	102	HEM	C1D-ND	-2.20	1.34	1.38
31	M	101	LMT	O3'-C3'	-2.20	1.37	1.43
23	c	508	CLA	C3B-C4B	2.19	1.49	1.42
23	b	612	CLA	C3B-C4B	2.19	1.49	1.42
23	C	509	CLA	C1C-NC	-2.19	1.34	1.37
40	V	201	HEC	CMA-C3A	2.19	1.55	1.50
31	F	101	LMT	O3'-C3'	-2.19	1.37	1.43
23	b	601	CLA	C1B-C2B	2.19	1.48	1.43
23	c	507	CLA	C3D-C4D	-2.18	1.39	1.44
27	o	303	GOL	C1-C2	2.18	1.60	1.51
23	b	613	CLA	C1C-C2C	2.18	1.48	1.44
23	c	504	CLA	C3D-C4D	-2.18	1.39	1.44
23	b	610	CLA	C3B-C2B	2.18	1.48	1.41
23	A	404[B]	CLA	C3B-C2B	2.18	1.48	1.41
23	B	608	CLA	C3D-C4D	-2.18	1.39	1.44
23	A	408	CLA	C3B-C4B	2.18	1.49	1.42
24	A	407[A]	PHO	C1B-NB	-2.18	1.34	1.38
23	b	614	CLA	C4C-C3C	2.17	1.48	1.45
23	C	510	CLA	C3B-C4B	2.17	1.49	1.42
24	d	403[A]	PHO	CBD-CGD	-2.17	1.49	1.52
23	C	513	CLA	C4C-C3C	2.17	1.48	1.45
23	c	512	CLA	C1C-C2C	2.17	1.48	1.44
23	C	512	CLA	C1C-NC	-2.17	1.34	1.37
23	a	404[A]	CLA	C1C-C2C	2.17	1.48	1.44
27	b	624	GOL	C3-C2	2.16	1.60	1.51
24	d	403[B]	PHO	C1B-NB	-2.16	1.34	1.38
31	m	103	LMT	C3'-C2'	2.16	1.57	1.52
23	b	605	CLA	C1C-C2C	2.16	1.48	1.44
32	L	101[B]	LHG	O7-C5	-2.16	1.41	1.46
32	b	629[A]	LHG	O7-C5	-2.16	1.41	1.46
23	B	614	CLA	C3B-C4B	2.15	1.49	1.42
23	B	604	CLA	C3B-C4B	2.15	1.49	1.42
23	B	603	CLA	C1C-C2C	2.15	1.48	1.44
23	B	608	CLA	C1C-C2C	2.15	1.48	1.44
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	C3B-C2B	2.15	1.48	1.41
23	c	513	CLA	C3B-C2B	2.15	1.48	1.41
35	c	518	DGD	O5D-C1E	2.15	1.43	1.40
23	c	512	CLA	C4C-C3C	2.15	1.48	1.45
23	c	502	CLA	C3D-C4D	-2.15	1.39	1.44
23	B	601	CLA	C1C-NC	-2.15	1.34	1.37
24	A	407[A]	PHO	C1D-ND	-2.14	1.34	1.38
31	T	101	LMT	O1'-C1'	-2.14	1.36	1.40
34	B	622	HTG	C1'-S1	-2.14	1.78	1.81
23	c	510	CLA	C3D-C4D	-2.14	1.39	1.44
27	V	203[A]	GOL	C1-C2	2.14	1.59	1.51
23	C	502	CLA	C4C-C3C	2.14	1.48	1.45
40	v	201	HEC	CMD-C2D	2.14	1.55	1.50
26	l	101	SQD	O6-C1	2.14	1.43	1.40
23	C	503	CLA	C4C-C3C	2.14	1.48	1.45
23	B	602	CLA	C3B-C4B	2.14	1.49	1.42
29	D	405[A]	PL9	C2-C3	2.14	1.40	1.34
31	A	417	LMT	O2'-C2'	-2.14	1.37	1.43
23	C	511	CLA	C3B-C2B	2.14	1.48	1.41
23	B	611	CLA	C3D-C4D	-2.14	1.39	1.44
23	B	604	CLA	C1A-CHA	2.13	1.51	1.43
23	c	509	CLA	C3D-C4D	-2.13	1.39	1.44
23	C	504	CLA	C4C-C3C	2.13	1.48	1.45
31	B	628	LMT	O2'-C2'	-2.13	1.37	1.43
23	b	613	CLA	C3D-C4D	-2.12	1.39	1.44
23	C	503	CLA	C3B-C4B	2.12	1.48	1.42
23	B	612	CLA	C1C-NC	-2.12	1.34	1.37
23	A	404[B]	CLA	C1D-C2D	2.12	1.49	1.45
23	d	402[A]	CLA	C4B-NB	-2.12	1.35	1.37
23	b	613	CLA	C4C-C3C	2.12	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.12	1.39	1.44
23	b	608	CLA	C3B-C4B	2.12	1.48	1.42
23	a	405[A]	CLA	C4C-C3C	2.12	1.48	1.45
31	B	627	LMT	O5'-C5'	-2.12	1.39	1.44
23	B	604	CLA	C1C-C2C	2.11	1.48	1.44
23	B	604	CLA	MG-NA	2.11	2.11	2.06
23	B	616	CLA	C1C-NC	-2.11	1.34	1.37
24	d	403[A]	PHO	C1B-NB	-2.11	1.34	1.38
23	B	610	CLA	C4B-NB	-2.11	1.35	1.37
23	A	405[B]	CLA	C4C-C3C	2.11	1.48	1.45
23	C	509	CLA	C3D-C4D	-2.11	1.39	1.44
23	B	604	CLA	C4C-C3C	2.11	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C4C-C3C	2.11	1.48	1.45
23	C	504	CLA	C3B-C2B	2.10	1.48	1.41
23	A	405[B]	CLA	C3B-C2B	2.10	1.48	1.41
23	B	603	CLA	C3D-C4D	-2.10	1.39	1.44
23	A	408	CLA	C1C-NC	-2.10	1.34	1.37
23	d	404[B]	CLA	C1C-C2C	2.10	1.48	1.44
35	c	517[A]	DGD	O2G-C2G	-2.10	1.41	1.46
23	c	507	CLA	C1D-C2D	2.09	1.49	1.45
29	A	414[B]	PL9	C2-C1	-2.09	1.39	1.44
23	C	502	CLA	C3B-C2B	2.09	1.48	1.41
23	B	612	CLA	C4C-C3C	2.09	1.48	1.45
27	v	202[A]	GOL	C3-C2	2.09	1.59	1.51
23	d	404[A]	CLA	C3B-C2B	2.09	1.48	1.41
23	B	604	CLA	C3B-C2B	2.09	1.48	1.41
29	A	414[B]	PL9	C2-C3	2.08	1.39	1.34
23	b	607	CLA	C3B-C2B	2.08	1.48	1.41
24	d	403[B]	PHO	C1D-ND	-2.08	1.34	1.38
23	b	605	CLA	C3B-C2B	2.08	1.48	1.41
23	a	407	CLA	C4C-C3C	2.08	1.48	1.45
23	b	602	CLA	C1B-C2B	2.08	1.48	1.43
23	C	507	CLA	C3B-C2B	2.08	1.48	1.41
23	C	510	CLA	C1C-NC	-2.07	1.34	1.37
23	a	404[B]	CLA	C3D-C4D	-2.07	1.39	1.44
31	T	101	LMT	O2'-C2'	-2.07	1.37	1.43
23	b	603	CLA	C1B-NB	-2.07	1.35	1.37
23	a	404[A]	CLA	C3B-C4B	2.07	1.48	1.42
23	A	404[B]	CLA	C1C-C2C	2.07	1.48	1.44
24	A	416[B]	PHO	C1D-ND	-2.07	1.34	1.38
23	b	616	CLA	C3B-C2B	2.07	1.48	1.41
23	a	407	CLA	C3B-C2B	2.07	1.48	1.41
31	T	101	LMT	O3B-C3B	-2.07	1.37	1.43
23	d	405	CLA	C3D-C4D	-2.07	1.39	1.44
23	b	607	CLA	C1A-CHA	2.07	1.51	1.43
23	b	605	CLA	C1D-C2D	2.06	1.49	1.45
23	b	616	CLA	C4C-C3C	2.06	1.48	1.45
24	d	403[B]	PHO	CHA-CBD	-2.05	1.49	1.51
23	b	603	CLA	C4C-C3C	2.05	1.48	1.45
23	C	512	CLA	C1A-CHA	2.05	1.51	1.43
23	c	513	CLA	C1D-C2D	2.05	1.49	1.45
23	D	403	CLA	C3D-C4D	-2.05	1.39	1.44
23	C	503	CLA	C3D-C4D	-2.05	1.39	1.44
31	A	417	LMT	O3'-C3'	-2.05	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3B-C4B	2.04	1.48	1.42
23	d	402[A]	CLA	C1C-C2C	2.04	1.48	1.44
23	C	509	CLA	C1A-CHA	2.04	1.51	1.43
24	a	406[B]	PHO	CHA-CBD	-2.03	1.49	1.51
23	B	607	CLA	C3B-C2B	2.03	1.48	1.41
23	B	608	CLA	C3B-C4B	2.03	1.48	1.42
23	A	404[A]	CLA	C3D-C4D	-2.03	1.39	1.44
32	D	406[A]	LHG	O7-C5	-2.03	1.41	1.46
23	b	609	CLA	C1C-NC	-2.03	1.34	1.37
29	A	414[A]	PL9	C2-C3	2.02	1.39	1.34
23	b	601	CLA	C3D-C4D	-2.02	1.39	1.44
23	c	506	CLA	C1C-C2C	2.01	1.48	1.44
23	c	508	CLA	C1C-NC	-2.01	1.34	1.37
23	a	405[B]	CLA	C3B-C2B	2.01	1.48	1.41
23	C	506	CLA	C4B-NB	-2.01	1.35	1.37
31	a	416	LMT	O2'-C2'	-2.01	1.38	1.43
23	C	508	CLA	C3B-C2B	2.01	1.47	1.41
31	b	627	LMT	O3'-C3'	-2.01	1.38	1.43
23	d	405	CLA	C3B-C2B	2.01	1.47	1.41
23	c	511	CLA	C1C-NC	-2.00	1.34	1.37
23	B	614	CLA	C3B-C2B	2.00	1.47	1.41
23	A	406[B]	CLA	C3B-C2B	2.00	1.47	1.41
32	d	408[B]	LHG	O7-C5	-2.00	1.41	1.46
27	c	526	GOL	C3-C2	2.00	1.59	1.51

All (3415) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C3B-C2B-C1B	-13.95	90.73	107.17
24	d	403[A]	PHO	C2D-C1D-ND	11.51	117.75	109.43
23	B	611	CLA	C1D-ND-C4D	-11.36	98.34	106.31
24	d	403[B]	PHO	C2D-C1D-ND	11.36	117.64	109.43
24	A	416[B]	PHO	C2D-C1D-ND	11.25	117.56	109.43
23	B	611	CLA	C2B-C1B-NB	11.11	121.85	110.33
24	A	407[B]	PHO	C2D-C1D-ND	11.07	117.43	109.43
24	A	407[A]	PHO	C2D-C1D-ND	11.05	117.42	109.43
23	B	612	CLA	C1D-ND-C4D	-11.05	98.56	106.31
24	a	406[A]	PHO	C2D-C1D-ND	10.84	117.26	109.43
24	a	406[B]	PHO	C2D-C1D-ND	10.62	117.11	109.43
23	b	605	CLA	C1D-ND-C4D	-10.57	98.90	106.31
23	a	407	CLA	C1D-ND-C4D	-10.44	98.99	106.31
24	A	416[A]	PHO	C2D-C1D-ND	10.38	116.93	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[B]	CLA	C1D-ND-C4D	-10.21	99.15	106.31
23	b	611	CLA	C1D-ND-C4D	-10.07	99.25	106.31
40	v	201	HEC	CBB-CAB-C3B	-10.03	107.40	127.43
23	B	614	CLA	C1D-ND-C4D	-9.96	99.33	106.31
23	B	601	CLA	C1D-ND-C4D	-9.87	99.39	106.31
23	a	405[A]	CLA	C1D-ND-C4D	-9.78	99.45	106.31
23	c	503	CLA	C1D-ND-C4D	-9.75	99.47	106.31
23	c	511	CLA	C1D-ND-C4D	-9.71	99.50	106.31
23	B	606	CLA	C1D-ND-C4D	-9.69	99.51	106.31
23	c	501	CLA	C1D-ND-C4D	-9.68	99.52	106.31
23	B	615	CLA	C1D-ND-C4D	-9.68	99.52	106.31
23	A	408	CLA	C1D-ND-C4D	-9.64	99.55	106.31
23	c	505	CLA	C1D-ND-C4D	-9.58	99.59	106.31
23	B	602	CLA	C1D-ND-C4D	-9.56	99.60	106.31
23	C	502	CLA	C1D-ND-C4D	-9.50	99.65	106.31
23	B	607	CLA	C1D-ND-C4D	-9.50	99.65	106.31
23	C	504	CLA	C1D-ND-C4D	-9.49	99.65	106.31
23	A	406[A]	CLA	C1D-ND-C4D	-9.49	99.65	106.31
23	C	506	CLA	C1D-ND-C4D	-9.42	99.70	106.31
23	b	616	CLA	C1D-ND-C4D	-9.36	99.75	106.31
23	B	605	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	A	406[B]	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	c	506	CLA	C1D-ND-C4D	-9.35	99.75	106.31
23	C	514	CLA	C1D-ND-C4D	-9.33	99.76	106.31
23	b	615	CLA	C1D-ND-C4D	-9.33	99.77	106.31
23	d	405	CLA	C1D-ND-C4D	-9.31	99.78	106.31
23	B	609	CLA	C1D-ND-C4D	-9.27	99.81	106.31
23	b	614	CLA	C1D-ND-C4D	-9.24	99.83	106.31
23	c	513	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	D	402[A]	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	b	606	CLA	C1D-ND-C4D	-9.22	99.84	106.31
23	b	609	CLA	C1D-ND-C4D	-9.20	99.85	106.31
23	b	610	CLA	C1D-ND-C4D	-9.16	99.88	106.31
23	C	511	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	a	404[B]	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	b	612	CLA	C1D-ND-C4D	-9.16	99.89	106.31
23	d	404[B]	CLA	C1D-ND-C4D	-9.15	99.89	106.31
23	A	405[A]	CLA	C1D-ND-C4D	-9.14	99.90	106.31
23	d	404[A]	CLA	C1D-ND-C4D	-9.11	99.92	106.31
23	B	616	CLA	C1D-ND-C4D	-9.11	99.92	106.31
23	b	603	CLA	C1D-ND-C4D	-9.06	99.95	106.31
23	a	404[A]	CLA	C1D-ND-C4D	-9.05	99.96	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	601	CLA	C1D-ND-C4D	-9.01	99.99	106.31
23	D	402[B]	CLA	C1D-ND-C4D	-9.00	99.99	106.31
23	d	402[B]	CLA	C1D-ND-C4D	-8.97	100.02	106.31
23	c	504	CLA	C1D-ND-C4D	-8.93	100.05	106.31
23	C	510	CLA	C1D-ND-C4D	-8.92	100.06	106.31
23	c	510	CLA	C1D-ND-C4D	-8.90	100.07	106.31
23	C	505	CLA	C1D-ND-C4D	-8.90	100.07	106.31
23	c	509	CLA	C1D-ND-C4D	-8.89	100.07	106.31
23	B	610	CLA	C1D-ND-C4D	-8.89	100.08	106.31
23	b	602	CLA	C1D-ND-C4D	-8.87	100.09	106.31
23	C	512	CLA	C1D-ND-C4D	-8.78	100.15	106.31
23	b	607	CLA	C1D-ND-C4D	-8.75	100.17	106.31
23	d	402[A]	CLA	C1D-ND-C4D	-8.74	100.18	106.31
23	C	508	CLA	C1D-ND-C4D	-8.73	100.18	106.31
23	C	509	CLA	C1D-ND-C4D	-8.72	100.19	106.31
23	B	613	CLA	C1D-ND-C4D	-8.70	100.21	106.31
23	B	603	CLA	C1D-ND-C4D	-8.67	100.23	106.31
23	C	503	CLA	C1D-ND-C4D	-8.67	100.23	106.31
23	A	405[B]	CLA	C1D-ND-C4D	-8.65	100.24	106.31
40	V	201	HEC	CBB-CAB-C3B	-8.64	110.17	127.43
24	A	407[B]	PHO	O2D-CGD-CBD	8.64	120.44	110.95
23	c	502	CLA	C1D-ND-C4D	-8.63	100.26	106.31
23	c	512	CLA	C1D-ND-C4D	-8.61	100.27	106.31
23	B	608	CLA	C1D-ND-C4D	-8.59	100.28	106.31
23	b	608	CLA	C1D-ND-C4D	-8.59	100.28	106.31
23	D	403	CLA	C1D-ND-C4D	-8.59	100.29	106.31
24	A	416[A]	PHO	O2D-CGD-CBD	8.55	120.34	110.95
23	C	507	CLA	C1D-ND-C4D	-8.54	100.32	106.31
24	A	416[B]	PHO	O2D-CGD-CBD	8.48	120.27	110.95
23	c	507	CLA	C1D-ND-C4D	-8.45	100.38	106.31
23	A	404[B]	CLA	C1D-ND-C4D	-8.36	100.45	106.31
24	d	403[A]	PHO	O2D-CGD-CBD	8.36	120.13	110.95
23	b	613	CLA	C1D-ND-C4D	-8.34	100.46	106.31
23	c	508	CLA	C1D-ND-C4D	-8.33	100.47	106.31
24	a	406[B]	PHO	O2D-CGD-CBD	8.33	120.10	110.95
23	b	604	CLA	C1D-ND-C4D	-8.32	100.47	106.31
24	a	406[A]	PHO	O2D-CGD-CBD	8.30	120.07	110.95
24	d	403[B]	PHO	O2D-CGD-CBD	8.28	120.04	110.95
23	C	513	CLA	C1D-ND-C4D	-8.23	100.54	106.31
24	A	407[A]	PHO	C3B-C4B-NB	8.22	112.82	107.46
23	B	604	CLA	C1D-ND-C4D	-8.21	100.55	106.31
24	A	407[B]	PHO	C3B-C4B-NB	8.19	112.80	107.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406[B]	PHO	C3B-C4B-NB	8.12	112.76	107.46
24	A	407[A]	PHO	O2D-CGD-CBD	8.01	119.75	110.95
24	a	406[A]	PHO	C3B-C4B-NB	8.00	112.68	107.46
23	A	404[A]	CLA	C1D-ND-C4D	-7.76	100.87	106.31
24	d	403[A]	PHO	C3B-C4B-NB	7.69	112.47	107.46
24	d	403[B]	PHO	C3B-C4B-NB	7.56	112.39	107.46
24	A	416[B]	PHO	C3B-C4B-NB	7.50	112.35	107.46
23	B	611	CLA	CMB-C2B-C1B	7.44	136.75	125.42
23	B	606	CLA	CMD-C2D-C1D	7.43	137.80	124.73
23	B	610	CLA	O2D-CGD-CBD	7.40	124.17	111.23
26	X	101	SQD	O6-C1-C2	7.38	119.48	108.27
23	B	611	CLA	CHD-C4C-C3C	-7.36	114.03	124.77
23	c	501	CLA	CMD-C2D-C1D	7.35	137.67	124.73
23	B	616	CLA	O2D-CGD-CBD	7.33	124.04	111.23
23	C	511	CLA	CMD-C2D-C1D	7.31	137.59	124.73
23	c	507	CLA	O2D-CGD-CBD	7.27	123.93	111.23
23	B	611	CLA	CHB-C1B-NB	-7.26	113.15	124.05
23	B	616	CLA	CHD-C4C-C3C	-7.26	114.19	124.77
23	B	611	CLA	C2D-C1D-ND	7.25	117.31	110.13
23	c	503	CLA	C4A-NA-C1A	-7.23	103.38	106.68
23	b	602	CLA	C4A-NA-C1A	-7.22	103.39	106.68
23	B	612	CLA	C2D-C1D-ND	7.17	117.23	110.13
23	D	402[B]	CLA	C4A-NA-C1A	-7.16	103.41	106.68
23	B	605	CLA	CHD-C4C-C3C	-7.15	114.34	124.77
23	a	407	CLA	C2D-C1D-ND	7.14	117.19	110.13
23	b	605	CLA	CHD-C4C-C3C	-7.09	114.43	124.77
23	b	616	CLA	C4A-NA-C1A	-7.04	103.47	106.68
23	b	605	CLA	C2D-C1D-ND	7.02	117.08	110.13
23	C	513	CLA	C4A-NA-C1A	-7.02	103.48	106.68
23	B	606	CLA	C2D-C1D-ND	7.01	117.06	110.13
23	b	616	CLA	O2D-CGD-CBD	7.00	123.46	111.23
23	C	504	CLA	C4A-NA-C1A	-6.99	103.49	106.68
23	B	611	CLA	CMD-C2D-C1D	6.96	136.98	124.73
24	A	416[A]	PHO	C2B-C1B-NB	6.94	114.44	109.43
24	d	403[A]	PHO	C2B-C1B-NB	6.93	114.44	109.43
23	b	611	CLA	C2D-C1D-ND	6.92	116.98	110.13
23	B	614	CLA	CMD-C2D-C1D	6.90	136.89	124.73
24	A	416[B]	PHO	C2B-C1B-NB	6.90	114.42	109.43
23	b	616	CLA	CHD-C4C-C3C	-6.84	114.80	124.77
23	A	404[B]	CLA	CMD-C2D-C1D	6.82	136.75	124.73
23	B	603	CLA	O2D-CGD-CBD	6.81	123.14	111.23
24	A	416[A]	PHO	C3B-C4B-NB	6.78	111.89	107.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CMD-C2D-C1D	6.78	136.66	124.73
23	a	407	CLA	CHD-C4C-C3C	-6.75	114.92	124.77
23	B	612	CLA	CHD-C4C-C3C	-6.75	114.94	124.77
23	c	503	CLA	CMD-C2D-C1D	6.74	136.59	124.73
23	A	405[A]	CLA	C2D-C1D-ND	6.74	116.79	110.13
23	C	508	CLA	CMD-C2D-C1D	6.72	136.56	124.73
23	b	611	CLA	CMD-C2D-C1D	6.71	136.54	124.73
24	d	403[B]	PHO	C2B-C1B-NB	6.68	114.26	109.43
23	c	513	CLA	CMD-C2D-C1D	6.68	136.50	124.73
23	C	506	CLA	CMD-C2D-C1D	6.68	136.49	124.73
23	B	615	CLA	C4A-NA-C1A	-6.66	103.64	106.68
23	b	613	CLA	C2D-C1D-ND	6.64	116.69	110.13
23	B	607	CLA	C2D-C1D-ND	6.62	116.68	110.13
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.73
23	b	605	CLA	CMD-C2D-C1D	6.60	136.35	124.73
23	b	614	CLA	C2D-C1D-ND	6.59	116.65	110.13
23	c	507	CLA	CMD-C2D-C1D	6.59	136.33	124.73
23	C	502	CLA	C4A-NA-C1A	-6.58	103.68	106.68
23	B	610	CLA	C2D-C1D-ND	6.58	116.64	110.13
23	C	504	CLA	CMD-C2D-C1D	6.58	136.31	124.73
23	b	614	CLA	O2D-CGD-CBD	6.57	122.72	111.23
23	b	615	CLA	C4A-NA-C1A	-6.57	103.68	106.68
23	B	615	CLA	C2D-C1D-ND	6.55	116.61	110.13
23	B	616	CLA	C2D-C1D-ND	6.55	116.61	110.13
23	a	405[A]	CLA	C2D-C1D-ND	6.54	116.60	110.13
23	a	405[B]	CLA	C2D-C1D-ND	6.53	116.59	110.13
23	b	609	CLA	CHD-C4C-C3C	-6.53	115.26	124.77
23	b	606	CLA	CHD-C4C-C3C	-6.51	115.29	124.77
23	B	606	CLA	CHD-C4C-C3C	-6.50	115.30	124.77
23	b	601	CLA	O2D-CGD-CBD	6.50	122.59	111.23
23	c	501	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	B	605	CLA	C2D-C1D-ND	6.49	116.55	110.13
23	c	511	CLA	CHD-C4C-C3C	-6.49	115.31	124.77
23	B	606	CLA	C4A-NA-C1A	-6.49	103.72	106.68
23	B	615	CLA	CHD-C4C-C3C	-6.48	115.32	124.77
23	B	609	CLA	C4A-NA-C1A	-6.48	103.72	106.68
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.73
23	A	408	CLA	CMD-C2D-C1D	6.44	136.07	124.73
26	X	101	SQD	O47-C7-C8	6.44	125.41	111.48
23	b	613	CLA	CHD-C4C-C3C	-6.43	115.39	124.77
23	B	614	CLA	C2D-C1D-ND	6.43	116.49	110.13
34	b	623	HTG	C1'-S1-C1	6.43	114.34	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	CMD-C2D-C1D	6.42	136.04	124.73
23	B	609	CLA	CMD-C2D-C1D	6.42	136.03	124.73
23	B	605	CLA	CMD-C2D-C1D	6.39	135.98	124.73
23	A	406[A]	CLA	C2D-C1D-ND	6.39	116.45	110.13
23	B	602	CLA	CHD-C4C-C3C	-6.38	115.47	124.77
23	B	613	CLA	C2D-C1D-ND	6.37	116.43	110.13
23	D	402[A]	CLA	C4A-NA-C1A	-6.37	103.77	106.68
23	b	604	CLA	O2D-CGD-CBD	6.37	122.36	111.23
23	C	508	CLA	CHD-C4C-C3C	-6.36	115.50	124.77
23	b	615	CLA	CMD-C2D-C1D	6.35	135.92	124.73
23	C	513	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
23	C	509	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
23	a	405[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.77
23	c	505	CLA	O2D-CGD-CBD	6.33	122.30	111.23
23	C	505	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	d	402[A]	CLA	C2D-C1D-ND	6.33	116.39	110.13
23	A	408	CLA	C2D-C1D-ND	6.32	116.38	110.13
23	b	610	CLA	CHD-C4C-C3C	-6.32	115.56	124.77
23	D	402[B]	CLA	CMD-C2D-C1D	6.31	135.84	124.73
23	b	616	CLA	C2D-C1D-ND	6.29	116.36	110.13
23	b	611	CLA	CHD-C4C-C3C	-6.29	115.60	124.77
23	D	402[A]	CLA	C2D-C1D-ND	6.29	116.35	110.13
23	C	512	CLA	CHD-C4C-C3C	-6.29	115.61	124.77
23	B	601	CLA	C2D-C1D-ND	6.27	116.33	110.13
24	a	406[B]	PHO	C2B-C1B-NB	6.27	113.96	109.43
23	c	510	CLA	CHD-C4C-C3C	-6.26	115.64	124.77
24	a	406[A]	PHO	C2B-C1B-NB	6.26	113.95	109.43
23	c	511	CLA	C2D-C1D-ND	6.26	116.32	110.13
23	b	612	CLA	CHD-C4C-C3C	-6.24	115.67	124.77
23	c	503	CLA	CHD-C4C-C3C	-6.24	115.68	124.77
23	B	601	CLA	CHD-C4C-C3C	-6.24	115.68	124.77
23	B	601	CLA	O2D-CGD-CBD	6.23	122.13	111.23
23	C	504	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
23	B	602	CLA	C2D-C1D-ND	6.23	116.29	110.13
23	A	404[B]	CLA	C4A-NA-C1A	-6.23	103.84	106.68
26	A	410[A]	SQD	O6-C1-C2	6.22	117.72	108.27
23	d	402[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	b	614	CLA	CHD-C4C-C3C	-6.22	115.70	124.77
23	B	601	CLA	CMD-C2D-C1D	6.22	135.68	124.73
23	c	505	CLA	CMD-C2D-C1D	6.21	135.66	124.73
23	d	402[B]	CLA	C2D-C1D-ND	6.20	116.26	110.13
23	C	511	CLA	O2D-CGD-CBD	6.20	122.06	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404[B]	CLA	CMD-C2D-C1D	6.19	135.62	124.73
23	C	510	CLA	CMD-C2D-C1D	6.19	135.62	124.73
23	c	504	CLA	CMD-C2D-C1D	6.17	135.59	124.73
23	c	508	CLA	C2D-C1D-ND	6.16	116.23	110.13
23	c	506	CLA	CMD-C2D-C1D	6.16	135.58	124.73
23	b	615	CLA	C2D-C1D-ND	6.16	116.23	110.13
23	B	609	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
23	c	510	CLA	CMD-C2D-C1D	6.16	135.57	124.73
23	d	405	CLA	C2D-C1D-ND	6.16	116.22	110.13
24	A	416[B]	PHO	C4D-ND-C1D	-6.15	101.50	108.87
23	A	405[B]	CLA	CMD-C2D-C1D	6.14	135.53	124.73
23	B	609	CLA	C2D-C1D-ND	6.12	116.18	110.13
25	Y	101	BCR	C33-C5-C6	-6.12	117.81	124.48
23	b	601	CLA	CMD-C2D-C1D	6.12	135.50	124.73
23	b	616	CLA	CMD-C2D-C1D	6.12	135.50	124.73
23	c	509	CLA	C1-C2-C3	-6.12	116.18	126.20
23	d	402[B]	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	B	614	CLA	CHD-C4C-C3C	-6.11	115.86	124.77
23	B	607	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
23	C	502	CLA	C2D-C1D-ND	6.10	116.17	110.13
24	A	407[A]	PHO	C2B-C1B-NB	6.10	113.84	109.43
23	a	405[B]	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
23	d	405	CLA	CMD-C2D-C1D	6.09	135.46	124.73
23	b	607	CLA	CMD-C2D-C1D	6.09	135.46	124.73
23	b	605	CLA	O2D-CGD-CBD	6.07	121.84	111.23
23	C	512	CLA	C2D-C1D-ND	6.07	116.13	110.13
23	b	606	CLA	C4A-NA-C1A	-6.06	103.92	106.68
23	A	405[B]	CLA	C2D-C1D-ND	6.06	116.12	110.13
23	C	514	CLA	C2D-C1D-ND	6.05	116.12	110.13
23	c	509	CLA	CMD-C2D-C1D	6.05	135.39	124.73
26	A	410[B]	SQD	O6-C1-C2	6.05	117.46	108.27
23	c	507	CLA	CHD-C4C-C3C	-6.05	115.95	124.77
23	b	607	CLA	C2D-C1D-ND	6.05	116.11	110.13
24	d	403[A]	PHO	C4D-ND-C1D	-6.05	101.62	108.87
23	a	404[A]	CLA	C4A-NA-C1A	-6.04	103.92	106.68
23	c	505	CLA	C4A-NA-C1A	-6.03	103.93	106.68
23	B	612	CLA	O2D-CGD-CBD	6.03	121.77	111.23
23	c	510	CLA	C2D-C1D-ND	6.02	116.08	110.13
23	A	406[B]	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	b	603	CLA	C4A-NA-C1A	-6.01	103.94	106.68
23	c	503	CLA	C2D-C1D-ND	6.01	116.08	110.13
23	c	504	CLA	CHD-C4C-C3C	-6.01	116.01	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	601	CLA	C4A-NA-C1A	-6.01	103.94	106.68
23	B	610	CLA	CHD-C4C-C3C	-6.01	116.01	124.77
23	C	514	CLA	CHD-C4C-C3C	-6.01	116.01	124.77
23	c	506	CLA	C2D-C1D-ND	6.01	116.07	110.13
23	c	512	CLA	C4A-NA-C1A	-6.00	103.94	106.68
23	C	502	CLA	CMD-C2D-C1D	6.00	135.29	124.73
23	C	502	CLA	CHD-C4C-C3C	-6.00	116.03	124.77
23	b	609	CLA	C2D-C1D-ND	6.00	116.06	110.13
26	l	101	SQD	O6-C1-C2	5.99	117.38	108.27
23	b	602	CLA	O2D-CGD-CBD	5.99	121.71	111.23
23	c	502	CLA	C2D-C1D-ND	5.99	116.06	110.13
23	A	406[A]	CLA	CHD-C4C-C3C	-5.99	116.05	124.77
23	C	513	CLA	CMD-C2D-C1D	5.99	135.27	124.73
23	C	504	CLA	C2D-C1D-ND	5.98	116.05	110.13
23	a	405[B]	CLA	CMD-C2D-C1D	5.98	135.25	124.73
23	C	508	CLA	O2D-CGD-CBD	5.97	121.67	111.23
23	c	502	CLA	CHD-C4C-C3C	-5.97	116.06	124.77
23	c	505	CLA	CHD-C4C-C3C	-5.97	116.07	124.77
23	c	502	CLA	C2C-C1C-NC	5.97	116.25	109.98
23	B	603	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	a	404[A]	CLA	C2D-C1D-ND	5.96	116.02	110.13
23	c	511	CLA	CMD-C2D-C1D	5.95	135.21	124.73
23	A	406[B]	CLA	CMD-C2D-C1D	5.94	135.19	124.73
24	d	403[B]	PHO	C4D-ND-C1D	-5.94	101.75	108.87
23	C	502	CLA	O2D-CGD-CBD	5.94	121.61	111.23
24	A	407[B]	PHO	C4D-ND-C1D	-5.94	101.76	108.87
23	B	610	CLA	CMD-C2D-C1D	5.93	135.18	124.73
23	C	507	CLA	C2C-C1C-NC	5.93	116.21	109.98
23	C	509	CLA	C2C-C1C-NC	5.93	116.21	109.98
23	B	615	CLA	CMD-C2D-C1D	5.91	135.13	124.73
23	C	508	CLA	C2D-C1D-ND	5.91	115.97	110.13
23	b	608	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
23	b	610	CLA	CMD-C2D-C1D	5.90	135.11	124.73
23	A	405[B]	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
23	d	404[A]	CLA	C4A-NA-C1A	-5.88	104.00	106.68
23	C	509	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	d	404[A]	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	b	604	CLA	C2D-C1D-ND	5.88	115.94	110.13
23	b	615	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
23	B	611	CLA	C3D-C2D-C1D	-5.87	97.82	105.83
23	C	510	CLA	C2D-C1D-ND	5.87	115.93	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C2C-C1C-NC	5.86	116.14	109.98
23	B	603	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
24	A	407[A]	PHO	C4D-ND-C1D	-5.85	101.86	108.87
23	b	608	CLA	C4A-NA-C1A	-5.85	104.01	106.68
23	c	504	CLA	C2D-C1D-ND	5.84	115.91	110.13
23	a	404[B]	CLA	CMD-C2D-C1D	5.84	135.01	124.73
23	c	509	CLA	C2D-C1D-ND	5.84	115.90	110.13
23	a	404[B]	CLA	C2D-C1D-ND	5.83	115.90	110.13
23	b	604	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
23	b	610	CLA	C2D-C1D-ND	5.83	115.90	110.13
23	c	505	CLA	C2D-C1D-ND	5.83	115.89	110.13
23	B	613	CLA	CHD-C4C-C3C	-5.83	116.28	124.77
23	B	608	CLA	C2D-C1D-ND	5.82	115.89	110.13
23	A	406[B]	CLA	CHD-C4C-C3C	-5.82	116.29	124.77
23	a	404[B]	CLA	C4A-NA-C1A	-5.81	104.03	106.68
23	C	510	CLA	CHD-C4C-C3C	-5.81	116.31	124.77
23	D	402[B]	CLA	C2D-C1D-ND	5.80	115.87	110.13
23	B	614	CLA	O2D-CGD-CBD	5.80	121.37	111.23
23	c	506	CLA	CHD-C4C-C3C	-5.80	116.31	124.77
23	b	601	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
23	d	404[A]	CLA	C2C-C1C-NC	5.80	116.07	109.98
23	b	602	CLA	CMD-C2D-C1D	5.80	134.93	124.73
23	b	606	CLA	C2D-C1D-ND	5.79	115.86	110.13
23	b	611	CLA	O2D-CGD-CBD	5.79	121.35	111.23
23	b	602	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
23	B	606	CLA	O2D-CGD-CBD	5.79	121.35	111.23
23	C	512	CLA	CMD-C2D-C1D	5.79	134.92	124.73
23	C	503	CLA	CHD-C4C-C3C	-5.77	116.36	124.77
23	b	614	CLA	CMD-C2D-C1D	5.77	134.89	124.73
23	c	508	CLA	CMD-C2D-C1D	5.76	134.87	124.73
23	B	605	CLA	C4A-NA-C1A	-5.76	104.05	106.68
23	c	512	CLA	O2D-CGD-CBD	5.76	121.30	111.23
24	d	403[A]	PHO	C1-C2-C3	-5.76	116.76	126.20
26	a	409[A]	SQD	O6-C1-C2	5.76	117.02	108.27
23	c	512	CLA	C2D-C1D-ND	5.76	115.82	110.13
23	d	405	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
23	B	608	CLA	CHD-C4C-C3C	-5.75	116.40	124.77
23	a	404[A]	CLA	CMD-C2D-C1D	5.74	134.84	124.73
23	A	404[A]	CLA	C4A-NA-C1A	-5.74	104.06	106.68
23	c	512	CLA	CHD-C4C-C3C	-5.74	116.40	124.77
23	b	601	CLA	C2D-C1D-ND	5.74	115.81	110.13
23	B	606	CLA	C3D-C2D-C1D	-5.74	98.00	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
29	A	414[A]	PL9	C7-C8-C9	-5.71	116.99	126.83
23	B	604	CLA	C2C-C1C-NC	5.71	115.98	109.98
23	b	612	CLA	C2D-C1D-ND	5.71	115.77	110.13
23	c	508	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
23	D	403	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
23	a	404[B]	CLA	C2C-C1C-NC	5.70	115.97	109.98
23	C	503	CLA	C2D-C1D-ND	5.69	115.76	110.13
23	D	402[B]	CLA	CHD-C4C-C3C	-5.68	116.49	124.77
23	b	610	CLA	O2D-CGD-CBD	5.68	121.15	111.23
23	d	404[B]	CLA	C2C-C1C-NC	5.68	115.94	109.98
23	C	514	CLA	CMD-C2D-C1D	5.67	134.72	124.73
23	d	402[B]	CLA	CMD-C2D-C1D	5.67	134.72	124.73
23	b	607	CLA	C2C-C1C-NC	5.66	115.93	109.98
23	b	603	CLA	C2D-C1D-ND	5.66	115.73	110.13
25	t	102	BCR	C33-C5-C6	-5.66	118.31	124.48
23	d	404[B]	CLA	C2D-C1D-ND	5.66	115.73	110.13
23	b	608	CLA	C2D-C1D-ND	5.66	115.73	110.13
23	A	408	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
23	c	507	CLA	C2D-C1D-ND	5.65	115.71	110.13
23	b	609	CLA	CMD-C2D-C1D	5.64	134.66	124.73
23	c	513	CLA	C2D-C1D-ND	5.63	115.70	110.13
23	d	404[A]	CLA	CMD-C2D-C1D	5.63	134.65	124.73
23	c	509	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
23	B	604	CLA	CMD-C2D-C1D	5.62	134.63	124.73
23	C	506	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
23	B	604	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
26	A	410[A]	SQD	C1-O5-C5	-5.61	102.77	113.72
23	d	402[A]	CLA	C4A-NA-C1A	-5.60	104.12	106.68
23	b	604	CLA	C2C-C1C-NC	5.60	115.87	109.98
23	B	602	CLA	O2D-CGD-CBD	5.60	121.02	111.23
23	B	613	CLA	CMD-C2D-C1D	5.60	134.58	124.73
23	D	403	CLA	CMD-C2D-C1D	5.59	134.57	124.73
23	C	505	CLA	CMD-C2D-C1D	5.59	134.57	124.73
23	A	404[A]	CLA	C2D-C1D-ND	5.59	115.66	110.13
23	B	608	CLA	O2D-CGD-CBD	5.58	120.99	111.23
23	A	406[A]	CLA	C4A-NA-C1A	-5.58	104.13	106.68
23	D	402[A]	CLA	C2C-C1C-NC	5.57	115.84	109.98
23	a	404[A]	CLA	C2C-C1C-NC	5.57	115.83	109.98
23	a	404[B]	CLA	CHD-C4C-C3C	-5.56	116.66	124.77
23	c	507	CLA	C4A-NA-C1A	-5.56	104.14	106.68
23	b	608	CLA	O2D-CGD-CBD	5.56	120.95	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	620	SQD	O6-C1-C2	5.56	116.72	108.27
23	b	607	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
23	c	504	CLA	O2D-CGD-CBD	5.55	120.93	111.23
23	d	404[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.77
23	b	605	CLA	C3D-C2D-C1D	-5.54	98.26	105.83
24	A	416[B]	PHO	C3D-C4D-ND	5.54	114.81	107.71
23	c	513	CLA	CHD-C4C-C3C	-5.54	116.70	124.77
23	C	506	CLA	C2D-C1D-ND	5.54	115.61	110.13
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.77
23	D	403	CLA	C2D-C1D-ND	5.53	115.60	110.13
23	c	508	CLA	C2C-C1C-NC	5.52	115.78	109.98
23	C	511	CLA	C2D-C1D-ND	5.52	115.58	110.13
23	B	603	CLA	CMD-C2D-C1D	5.51	134.44	124.73
23	c	510	CLA	C4A-NA-C1A	-5.51	104.16	106.68
24	A	407[A]	PHO	C3D-C4D-ND	5.51	114.77	107.71
25	b	617	BCR	C7-C8-C9	-5.51	118.09	126.23
23	c	513	CLA	C4A-NA-C1A	-5.50	104.17	106.68
23	d	405	CLA	O2D-CGD-CBD	5.50	120.84	111.23
24	A	416[A]	PHO	C4D-ND-C1D	-5.48	102.30	108.87
24	A	407[B]	PHO	C2B-C1B-NB	5.48	113.39	109.43
23	B	604	CLA	O2D-CGD-CBD	5.48	120.81	111.23
25	D	404	BCR	C7-C8-C9	-5.47	118.14	126.23
23	A	405[A]	CLA	O2D-CGD-CBD	5.46	120.78	111.23
24	A	407[B]	PHO	C3D-C4D-ND	5.46	114.70	107.71
23	C	513	CLA	O2D-CGD-CBD	5.45	120.76	111.23
23	c	512	CLA	CMD-C2D-C1D	5.45	134.32	124.73
23	A	404[B]	CLA	C2C-C1C-NC	5.45	115.70	109.98
23	C	505	CLA	CHD-C4C-C3C	-5.44	116.83	124.77
23	d	404[B]	CLA	C4A-NA-C1A	-5.43	104.20	106.68
23	C	506	CLA	O2D-CGD-CBD	5.43	120.72	111.23
24	a	406[A]	PHO	C4D-ND-C1D	-5.42	102.38	108.87
24	d	403[A]	PHO	C3D-C4D-ND	5.42	114.66	107.71
23	A	404[A]	CLA	C2C-C1C-NC	5.41	115.67	109.98
23	a	405[A]	CLA	C4A-NA-C1A	-5.41	104.21	106.68
23	C	511	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
23	d	404[B]	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
23	C	506	CLA	C4A-NA-C1A	-5.40	104.22	106.68
24	d	403[B]	PHO	C1-C2-C3	-5.40	117.35	126.20
23	b	604	CLA	C1-C2-C3	-5.40	117.36	126.20
23	D	403	CLA	O2D-CGD-CBD	5.39	120.65	111.23
23	b	612	CLA	C4A-NA-C1A	-5.39	104.22	106.68
23	a	404[A]	CLA	CHD-C4C-C3C	-5.38	116.92	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	C2B-C1B-NB	5.38	115.90	110.33
23	c	512	CLA	C3B-C2B-C1B	-5.36	100.86	107.17
23	c	508	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
23	b	614	CLA	C3D-C2D-C1D	-5.35	98.53	105.83
23	B	607	CLA	O2D-CGD-CBD	5.35	120.58	111.23
23	B	614	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
23	D	402[B]	CLA	C2C-C1C-NC	5.33	115.58	109.98
24	d	403[B]	PHO	C3D-C4D-ND	5.33	114.55	107.71
23	a	405[A]	CLA	CMD-C2D-C1D	5.33	134.12	124.73
23	b	613	CLA	C2C-C1C-NC	5.33	115.58	109.98
23	B	605	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
23	C	507	CLA	CHD-C4C-C3C	-5.32	117.02	124.77
23	b	611	CLA	C3D-C2D-C1D	-5.32	98.58	105.83
23	b	603	CLA	CMD-C2D-C1D	5.31	134.08	124.73
26	X	101	SQD	C1-O5-C5	-5.31	103.35	113.72
23	a	405[B]	CLA	C4A-NA-C1A	-5.31	104.26	106.68
23	A	405[B]	CLA	C2C-C1C-NC	5.30	115.55	109.98
23	C	513	CLA	C2D-C1D-ND	5.29	115.36	110.13
23	c	506	CLA	C2C-C1C-NC	5.29	115.54	109.98
23	c	509	CLA	C2C-C1C-NC	5.29	115.54	109.98
23	b	602	CLA	C2B-C1B-NB	5.29	115.81	110.33
23	C	507	CLA	C2D-C1D-ND	5.29	115.36	110.13
23	B	602	CLA	CMD-C2D-C1D	5.28	134.03	124.73
26	a	409[B]	SQD	O6-C1-C2	5.28	116.30	108.27
23	c	501	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
23	B	602	CLA	C4A-NA-C1A	-5.27	104.28	106.68
23	b	613	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	C	509	CLA	O2D-CGD-CBD	5.26	120.43	111.23
23	b	604	CLA	C4A-NA-C1A	-5.26	104.28	106.68
23	C	513	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
23	C	511	CLA	C2C-C1C-NC	5.26	115.50	109.98
23	b	612	CLA	C2C-C1C-NC	5.26	115.50	109.98
23	B	610	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
23	C	514	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
24	A	416[A]	PHO	C3D-C4D-ND	5.23	114.42	107.71
23	b	604	CLA	CMD-C2D-C1D	5.22	133.92	124.73
23	B	608	CLA	C4A-NA-C1A	-5.21	104.30	106.68
23	C	513	CLA	C2B-C1B-NB	5.21	115.73	110.33
23	C	509	CLA	CMD-C2D-C1D	5.20	133.89	124.73
26	a	409[A]	SQD	O47-C7-C8	5.20	122.73	111.48
26	A	410[A]	SQD	C1-C2-C3	-5.20	99.07	110.01
23	B	603	CLA	C2C-C1C-NC	5.20	115.44	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	CMD-C2D-C1D	5.20	133.88	124.73
23	b	602	CLA	C2D-C1D-ND	5.19	115.26	110.13
26	l	101	SQD	O47-C7-C8	5.19	122.70	111.48
23	b	612	CLA	C1-C2-C3	-5.19	117.70	126.20
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	d	402[A]	CLA	CMD-C2D-C1D	5.18	133.85	124.73
23	c	508	CLA	C4A-NA-C1A	-5.18	104.32	106.68
23	c	509	CLA	O2D-CGD-CBD	5.18	120.28	111.23
23	B	611	CLA	O2D-CGD-CBD	5.18	120.28	111.23
23	d	402[B]	CLA	C2C-C1C-NC	5.17	115.42	109.98
23	b	612	CLA	O2D-CGD-CBD	5.17	120.27	111.23
23	B	616	CLA	C4A-NA-C1A	-5.17	104.32	106.68
23	C	503	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
23	B	616	CLA	C3C-C4C-NC	5.17	117.05	110.43
23	A	408	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	c	502	CLA	O2D-CGD-CBD	5.16	120.25	111.23
23	b	609	CLA	C1-C2-C3	-5.16	117.75	126.20
23	B	614	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
26	A	410[B]	SQD	C1-O5-C5	-5.15	103.66	113.72
24	a	406[B]	PHO	C4D-ND-C1D	-5.15	102.70	108.87
23	D	403	CLA	C4A-NA-C1A	-5.15	104.33	106.68
23	b	614	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
23	b	611	CLA	C2C-C1C-NC	5.15	115.39	109.98
23	b	603	CLA	O2D-CGD-CBD	5.14	120.22	111.23
23	c	504	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
23	B	611	CLA	CMC-C2C-C1C	5.14	133.07	125.03
23	c	501	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
23	B	614	CLA	C4A-NA-C1A	-5.14	104.33	106.68
34	D	410	HTG	C1'-S1-C1	5.12	111.51	100.45
23	A	408	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
23	c	501	CLA	CHD-C1D-ND	-5.12	117.59	124.80
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	c	502	CLA	C1C-C2C-C3C	-5.12	101.60	106.98
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.73
23	A	408	CLA	C2B-C1B-NB	5.11	115.63	110.33
23	A	405[B]	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	b	606	CLA	O2D-CGD-CBD	5.11	120.16	111.23
23	b	610	CLA	C1-C2-C3	-5.11	117.83	126.20
23	b	614	CLA	C2B-C1B-NB	5.11	115.62	110.33
24	a	406[B]	PHO	C3D-C4D-ND	5.10	114.25	107.71
34	c	521	HTG	C1'-S1-C1	5.10	111.47	100.45
23	A	408	CLA	C4A-NA-C1A	-5.10	104.35	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CMD-C2D-C1D	5.10	133.71	124.73
23	B	612	CLA	CMD-C2D-C1D	5.10	133.71	124.73
23	b	615	CLA	C2C-C1C-NC	5.10	115.33	109.98
23	B	607	CLA	C2C-C1C-NC	5.10	115.33	109.98
23	C	508	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
23	C	512	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
23	b	616	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	B	616	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
23	B	604	CLA	C2D-C1D-ND	5.06	115.14	110.13
23	C	505	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	B	608	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
23	a	407	CLA	O2D-CGD-CBD	5.05	120.07	111.23
24	A	416[B]	PHO	C1-C2-C3	-5.05	117.92	126.20
23	b	607	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
29	A	414[B]	PL9	C7-C8-C9	-5.05	118.14	126.83
23	B	607	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	B	608	CLA	C2C-C1C-NC	5.04	115.28	109.98
23	B	607	CLA	C4A-NA-C1A	-5.03	104.38	106.68
33	B	620	LMG	O7-C10-C11	5.02	122.34	111.48
23	b	608	CLA	C2C-C1C-NC	5.02	115.25	109.98
23	B	603	CLA	C4A-NA-C1A	-5.01	104.39	106.68
23	A	404[A]	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
23	B	613	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
23	a	407	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
23	C	512	CLA	O2D-CGD-CBD	5.00	119.97	111.23
26	a	409[B]	SQD	O47-C7-C8	5.00	122.30	111.48
38	f	101	HEM	CHC-C4B-NB	4.99	129.79	124.42
23	b	605	CLA	C4A-NA-C1A	-4.99	104.40	106.68
23	d	402[A]	CLA	C2C-C1C-NC	4.99	115.22	109.98
23	D	402[B]	CLA	C1-C2-C3	-4.99	118.03	126.20
34	b	622	HTG	C1-O5-C5	4.98	121.50	112.56
23	d	405	CLA	C2B-C1B-NB	4.98	115.49	110.33
23	C	510	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
23	A	404[B]	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
23	C	514	CLA	O2D-CGD-CBD	4.98	119.93	111.23
24	a	406[A]	PHO	C3D-C4D-ND	4.97	114.08	107.71
23	C	506	CLA	C2C-C1C-NC	4.97	115.20	109.98
23	c	511	CLA	O2D-CGD-CBD	4.97	119.92	111.23
23	B	605	CLA	O2D-CGD-CBD	4.97	119.92	111.23
23	c	504	CLA	C4A-NA-C1A	-4.97	104.41	106.68
23	C	510	CLA	O2D-CGD-CBD	4.97	119.92	111.23
23	a	405[B]	CLA	O2D-CGD-CBD	4.97	119.91	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[B]	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
23	A	405[A]	CLA	C2C-C1C-NC	4.96	115.19	109.98
23	C	505	CLA	O2D-CGD-CBD	4.96	119.90	111.23
23	C	510	CLA	C4A-NA-C1A	-4.96	104.42	106.68
23	B	601	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
23	c	503	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	b	613	CLA	CMD-C2D-C1D	4.94	133.44	124.73
23	c	501	CLA	O2D-CGD-CBD	4.94	119.87	111.23
23	a	407	CLA	CMD-C2D-C1D	4.94	133.43	124.73
23	C	503	CLA	C2C-C1C-NC	4.94	115.17	109.98
23	d	405	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
23	c	507	CLA	C2C-C1C-NC	4.92	115.15	109.98
38	E	102	HEM	CHC-C4B-NB	4.92	129.72	124.42
40	v	201	HEC	CBC-CAC-C3C	-4.92	117.61	127.43
23	a	405[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	A	404[B]	CLA	C2B-C1B-NB	4.91	115.42	110.33
23	C	514	CLA	C2C-C1C-NC	4.91	115.13	109.98
23	b	603	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
23	C	510	CLA	C2C-C1C-NC	4.90	115.13	109.98
26	b	620	SQD	O47-C7-C8	4.90	122.08	111.48
23	c	501	CLA	C2C-C1C-NC	4.89	115.12	109.98
23	d	402[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
25	y	101	BCR	C33-C5-C6	-4.89	119.15	124.48
23	B	601	CLA	C2B-C1B-NB	4.89	115.39	110.33
23	A	406[B]	CLA	O2D-CGD-CBD	4.88	119.77	111.23
23	b	606	CLA	C2B-C1B-NB	4.88	115.39	110.33
23	a	405[B]	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	b	613	CLA	C3C-C4C-NC	4.88	116.68	110.43
23	c	513	CLA	C2C-C1C-NC	4.87	115.10	109.98
24	A	416[A]	PHO	C1-C2-C3	-4.87	118.22	126.20
23	b	605	CLA	C3D-C4D-ND	4.87	117.90	109.99
23	D	402[B]	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
23	c	513	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
23	b	602	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
23	A	405[B]	CLA	C1C-C2C-C3C	-4.86	101.86	106.98
23	C	508	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	c	508	CLA	C1-C2-C3	-4.86	118.24	126.20
23	C	503	CLA	CMD-C2D-C1D	4.86	133.28	124.73
23	A	404[B]	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
23	C	508	CLA	C2C-C1C-NC	4.85	115.08	109.98
23	A	406[B]	CLA	C4A-NA-C1A	-4.85	104.47	106.68
23	B	608	CLA	CMD-C2D-C1D	4.85	133.26	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
25	d	406	BCR	C7-C8-C9	-4.84	119.07	126.23
23	A	406[A]	CLA	O2D-CGD-CBD	4.84	119.69	111.23
23	d	402[B]	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	b	613	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
23	c	506	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
23	A	408	CLA	C2C-C1C-NC	4.83	115.06	109.98
23	A	404[A]	CLA	CHD-C4C-C3C	-4.83	117.73	124.77
33	C	501	LMG	O1-C1-C2	4.83	115.61	108.27
23	c	507	CLA	C3B-C2B-C1B	-4.83	101.48	107.17
23	B	604	CLA	C4A-NA-C1A	-4.83	104.48	106.68
23	B	612	CLA	C3D-C4D-ND	4.83	117.83	109.99
23	C	507	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
23	b	606	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
23	A	404[B]	CLA	C2D-C1D-ND	4.82	114.90	110.13
23	b	610	CLA	C4A-NA-C1A	-4.82	104.48	106.68
23	c	504	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	d	404[B]	CLA	O2D-CGD-CBD	4.82	119.65	111.23
23	a	405[A]	CLA	C3D-C4D-ND	4.81	117.81	109.99
23	B	616	CLA	CMD-C2D-C1D	4.81	133.21	124.73
23	B	615	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	B	612	CLA	C3C-C4C-NC	4.81	116.59	110.43
23	b	605	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
23	B	616	CLA	O2D-CGD-O1D	-4.79	114.52	123.85
23	C	504	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	c	510	CLA	C2C-C1C-NC	4.79	115.02	109.98
23	b	615	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	b	611	CLA	C3B-C2B-C1B	-4.79	101.52	107.17
23	B	613	CLA	C2C-C1C-NC	4.79	115.01	109.98
23	B	613	CLA	O2D-CGD-CBD	4.78	119.59	111.23
23	c	510	CLA	C1-C2-C3	-4.78	118.37	126.20
23	D	403	CLA	C2B-C1B-NB	4.78	115.28	110.33
23	C	512	CLA	C2C-C1C-NC	4.78	115.00	109.98
23	A	406[B]	CLA	C2C-C1C-NC	4.77	115.00	109.98
23	B	603	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
34	d	412	HTG	C1'-S1-C1	4.77	110.76	100.45
23	B	616	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
23	B	602	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
23	C	502	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	c	513	CLA	C2B-C1B-NB	4.77	115.27	110.33
23	a	405[B]	CLA	C3D-C4D-ND	4.76	117.72	109.99
34	B	622	HTG	C1'-S1-C1	4.76	110.72	100.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	C2B-C1B-NB	4.76	115.26	110.33
23	b	616	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	b	603	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	B	609	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	C	514	CLA	C2B-C1B-NB	4.75	115.25	110.33
29	A	414[B]	PL9	C32-C33-C34	-4.75	116.75	127.62
23	A	406[B]	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	C	504	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	b	601	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	c	503	CLA	C2B-C1B-NB	4.75	115.25	110.33
23	b	603	CLA	C2C-C1C-NC	4.75	114.97	109.98
23	c	511	CLA	C3B-C2B-C1B	-4.75	101.58	107.17
23	B	613	CLA	C1-C2-C3	-4.75	118.42	126.20
23	A	406[A]	CLA	C2C-C1C-NC	4.74	114.97	109.98
23	A	406[B]	CLA	C2B-C1B-NB	4.74	115.24	110.33
23	C	509	CLA	C3C-C4C-NC	4.74	116.50	110.43
23	B	614	CLA	C2C-C1C-NC	4.74	114.96	109.98
23	c	502	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
23	A	405[A]	CLA	C1C-C2C-C3C	-4.73	102.00	106.98
25	H	101	BCR	C38-C26-C25	-4.73	119.33	124.48
23	A	405[A]	CLA	C4A-NA-C1A	-4.72	104.53	106.68
23	b	612	CLA	C3C-C4C-NC	4.72	116.47	110.43
23	C	514	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	d	405	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
23	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	a	404[B]	CLA	C2B-C1B-NB	4.70	115.20	110.33
23	B	605	CLA	C2C-C1C-NC	4.70	114.92	109.98
23	C	510	CLA	C1-C2-C3	-4.70	118.49	126.20
23	A	406[B]	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
23	C	511	CLA	C1-C2-C3	-4.69	118.51	126.20
25	c	514	BCR	C11-C10-C9	-4.69	120.70	127.28
23	B	601	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
26	f	102	SQD	O47-C7-C8	4.69	121.62	111.48
23	c	509	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
23	A	406[A]	CLA	C3D-C4D-ND	4.69	117.61	109.99
23	b	608	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
23	B	602	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	b	609	CLA	C4A-NA-C1A	-4.68	104.54	106.68
23	B	606	CLA	CHD-C1D-ND	-4.68	118.22	124.80
23	c	506	CLA	C4A-NA-C1A	-4.68	104.55	106.68
23	a	405[A]	CLA	O2D-CGD-CBD	4.67	119.40	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C2C-C1C-NC	4.67	114.89	109.98
29	A	414[A]	PL9	C7-C3-C2	-4.67	117.89	123.39
23	d	402[B]	CLA	O2D-CGD-CBD	4.67	119.39	111.23
23	c	508	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
23	b	609	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	C	503	CLA	O2D-CGD-CBD	4.66	119.38	111.23
23	b	612	CLA	CMD-C2D-C1D	4.66	132.94	124.73
23	C	509	CLA	C1-C2-C3	-4.66	118.56	126.20
23	b	614	CLA	O2D-CGD-O1D	-4.66	114.79	123.85
23	c	512	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	C	511	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	D	402[A]	CLA	O2D-CGD-CBD	4.65	119.36	111.23
33	d	413	LMG	O7-C10-C11	4.65	121.54	111.48
23	c	505	CLA	C3D-C4D-ND	4.65	117.54	109.99
26	b	620	SQD	C1-O5-C5	-4.64	104.66	113.72
23	c	505	CLA	C2B-C1B-NB	4.64	115.14	110.33
23	C	507	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	c	507	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	C	505	CLA	C1C-C2C-C3C	-4.63	102.11	106.98
23	C	510	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	c	510	CLA	O2D-CGD-CBD	4.63	119.32	111.23
23	c	508	CLA	O2D-CGD-CBD	4.63	119.32	111.23
23	c	513	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	c	510	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	c	502	CLA	CMD-C2D-C1D	4.62	132.86	124.73
23	C	512	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
26	A	410[B]	SQD	C1-C2-C3	-4.61	100.31	110.01
23	D	403	CLA	CMB-C2B-C1B	4.61	132.44	125.42
23	b	602	CLA	C3D-C4D-ND	4.61	117.48	109.99
23	B	604	CLA	C1-C2-C3	-4.61	118.64	126.20
23	B	606	CLA	C2C-C1C-NC	4.61	114.82	109.98
23	b	614	CLA	C2C-C1C-NC	4.60	114.81	109.98
23	a	404[A]	CLA	C3B-C2B-C1B	-4.60	101.75	107.17
23	b	605	CLA	CHD-C1D-ND	-4.60	118.33	124.80
23	A	406[B]	CLA	C3D-C4D-ND	4.59	117.45	109.99
23	c	507	CLA	CHD-C1D-ND	-4.59	118.34	124.80
23	B	603	CLA	O2D-CGD-O1D	-4.59	114.92	123.85
23	b	605	CLA	C2C-C1C-NC	4.59	114.80	109.98
23	B	609	CLA	C3D-C4D-ND	4.59	117.44	109.99
23	B	602	CLA	C3D-C4D-ND	4.59	117.44	109.99
23	C	511	CLA	C2B-C1B-NB	4.58	115.08	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	C3D-C4D-ND	4.58	117.44	109.99
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	407	CLA	C3D-C4D-ND	4.58	117.43	109.99
23	c	502	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
29	a	413[B]	PL9	C7-C3-C4	4.57	120.68	116.91
23	a	405[B]	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
23	c	509	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	d	404[A]	CLA	C3D-C4D-ND	4.57	117.42	109.99
23	b	608	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	B	608	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	507	CLA	O2D-CGD-CBD	4.57	119.22	111.23
23	b	601	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
23	A	404[A]	CLA	C2B-C1B-NB	4.56	115.06	110.33
23	c	511	CLA	C2C-C1C-NC	4.56	114.77	109.98
23	d	402[B]	CLA	C1C-C2C-C3C	-4.56	102.19	106.98
23	b	606	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	d	402[B]	CLA	C4A-NA-C1A	-4.56	104.60	106.68
23	c	503	CLA	O2D-CGD-CBD	4.56	119.19	111.23
23	b	608	CLA	C1C-C2C-C3C	-4.55	102.19	106.98
23	B	605	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
23	a	407	CLA	C3B-C2B-C1B	-4.55	101.80	107.17
23	B	609	CLA	C2C-C1C-NC	4.55	114.76	109.98
23	b	611	CLA	C3D-C4D-ND	4.55	117.38	109.99
23	c	506	CLA	C3D-C4D-ND	4.55	117.38	109.99
23	C	504	CLA	O2D-CGD-CBD	4.55	119.18	111.23
23	A	405[A]	CLA	CMD-C2D-C1D	4.54	132.73	124.73
23	d	404[B]	CLA	C3D-C4D-ND	4.54	117.37	109.99
23	b	601	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	b	608	CLA	C2B-C1B-NB	4.54	115.03	110.33
26	f	102	SQD	C1-O5-C5	4.54	122.58	113.72
23	c	503	CLA	C3B-C2B-C1B	-4.54	101.82	107.17
23	b	616	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	b	609	CLA	C2C-C1C-NC	4.53	114.74	109.98
23	c	505	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
23	c	504	CLA	C2B-C1B-NB	4.52	115.02	110.33
23	A	405[B]	CLA	C4A-NA-C1A	-4.52	104.61	106.68
23	C	506	CLA	C3D-C4D-ND	4.52	117.33	109.99
23	B	611	CLA	C3D-C4D-ND	4.51	117.32	109.99
23	A	408	CLA	CHD-C1D-ND	-4.51	118.45	124.80
23	C	512	CLA	C2B-C1B-NB	4.51	115.00	110.33
23	d	402[A]	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
23	c	504	CLA	C2C-C1C-NC	4.51	114.72	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402[A]	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
23	B	610	CLA	C2C-C1C-NC	4.51	114.71	109.98
23	d	405	CLA	C3D-C4D-ND	4.50	117.31	109.99
29	A	414[A]	PL9	C32-C33-C34	-4.50	117.31	127.62
23	b	612	CLA	C3D-C4D-ND	4.50	117.31	109.99
23	B	602	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	B	604	CLA	C3C-C4C-NC	4.50	116.19	110.43
23	A	406[A]	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	C	510	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	A	404[B]	CLA	CHD-C1D-ND	-4.50	118.47	124.80
23	d	402[B]	CLA	C2B-C1B-NB	4.50	114.99	110.33
23	D	402[B]	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	b	612	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
29	a	413[B]	PL9	C7-C3-C2	-4.50	118.09	123.39
23	b	601	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	C	504	CLA	C2B-C1B-NB	4.49	114.99	110.33
23	d	404[B]	CLA	C3B-C2B-C1B	-4.49	101.87	107.17
23	C	507	CLA	C1C-C2C-C3C	-4.49	102.25	106.98
23	B	615	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	B	601	CLA	C3D-C4D-ND	4.49	117.29	109.99
23	d	402[A]	CLA	O2D-CGD-CBD	4.48	119.07	111.23
23	b	615	CLA	C3B-C2B-C1B	-4.48	101.88	107.17
23	c	501	CLA	CMB-C2B-C1B	4.48	132.25	125.42
23	c	501	CLA	O2D-CGD-O1D	-4.48	115.13	123.85
23	C	509	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	B	611	CLA	C4A-NA-C1A	-4.48	104.64	106.68
23	B	611	CLA	C1D-CHD-C4C	-4.48	116.50	126.02
23	B	607	CLA	C1C-C2C-C3C	-4.48	102.27	106.98
29	a	413[A]	PL9	C7-C8-C9	-4.47	119.13	126.83
23	c	510	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
23	c	513	CLA	C3D-C4D-ND	4.47	117.25	109.99
23	A	404[A]	CLA	C3B-C4B-NB	4.47	114.52	110.53
23	d	404[A]	CLA	C1C-C2C-C3C	-4.47	102.28	106.98
23	b	611	CLA	C2B-C1B-NB	4.47	114.96	110.33
23	b	607	CLA	C3C-C4C-NC	4.46	116.15	110.43
23	B	610	CLA	C4A-NA-C1A	-4.46	104.64	106.68
23	a	404[B]	CLA	C3D-C4D-ND	4.46	117.24	109.99
23	D	403	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	A	408	CLA	C3D-C4D-ND	4.45	117.22	109.99
23	B	614	CLA	C2B-C1B-NB	4.45	114.94	110.33
23	b	604	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	c	503	CLA	C1D-CHD-C4C	-4.44	116.58	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	C1D-CHD-C4C	-4.44	116.58	126.02
23	B	612	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	A	404[B]	CLA	C3B-C4B-NB	4.44	114.49	110.53
23	B	613	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
23	B	613	CLA	C3C-C4C-NC	4.43	116.11	110.43
23	A	404[B]	CLA	C3D-C4D-ND	4.43	117.19	109.99
23	C	504	CLA	C3D-C4D-ND	4.43	117.19	109.99
23	C	513	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	a	404[A]	CLA	C2B-C1B-NB	4.43	114.92	110.33
23	B	610	CLA	O2A-CGA-CBA	4.43	125.34	111.83
23	b	610	CLA	C3D-C4D-ND	4.43	117.19	109.99
23	c	507	CLA	C1C-C2C-C3C	-4.43	102.32	106.98
23	c	503	CLA	C3D-C4D-ND	4.43	117.18	109.99
23	B	614	CLA	C1-C2-C3	-4.43	118.95	126.20
33	c	520	LMG	O6-C5-C4	4.42	117.67	109.70
23	a	404[B]	CLA	C3B-C4B-NB	4.42	114.47	110.53
23	C	503	CLA	C2B-C1B-NB	4.41	114.90	110.33
38	E	102	HEM	CAD-CBD-CGD	4.41	125.37	113.67
23	b	610	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	a	407	CLA	C2C-C1C-NC	4.41	114.61	109.98
23	b	603	CLA	C1D-CHD-C4C	-4.41	116.65	126.02
23	b	611	CLA	C4A-NA-C1A	-4.41	104.67	106.68
23	c	501	CLA	C4A-NA-C1A	-4.40	104.67	106.68
23	B	604	CLA	C1C-C2C-C3C	-4.40	102.35	106.98
23	a	405[A]	CLA	C2C-C1C-NC	4.39	114.60	109.98
23	B	606	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
23	B	601	CLA	C2C-C1C-NC	4.39	114.59	109.98
23	C	506	CLA	CMB-C2B-C1B	4.39	132.10	125.42
23	D	403	CLA	C2C-C1C-NC	4.39	114.59	109.98
25	H	101	BCR	C16-C17-C18	-4.38	121.13	127.28
23	d	404[B]	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
23	C	507	CLA	C4A-NA-C1A	-4.38	104.68	106.68
23	c	513	CLA	O2D-CGD-CBD	4.38	118.89	111.23
23	a	407	CLA	C2B-C1B-NB	4.37	114.86	110.33
23	C	511	CLA	C3D-C4D-ND	4.37	117.10	109.99
23	c	504	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	C	503	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	C	502	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	D	402[B]	CLA	C3D-C4D-ND	4.37	117.09	109.99
23	c	505	CLA	C2C-C1C-NC	4.37	114.57	109.98
23	C	514	CLA	C3D-C4D-ND	4.37	117.08	109.99
23	C	507	CLA	C2B-C1B-NB	4.37	114.85	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[A]	CLA	CHD-C1D-ND	-4.37	118.66	124.80
23	C	507	CLA	C3D-C4D-ND	4.36	117.08	109.99
23	a	405[B]	CLA	CHD-C1D-ND	-4.36	118.67	124.80
23	c	505	CLA	C3C-C4C-NC	4.36	116.01	110.43
29	a	413[A]	PL9	C7-C3-C2	-4.36	118.25	123.39
23	c	501	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
23	c	511	CLA	C3B-C4B-NB	4.36	114.42	110.53
23	d	402[B]	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	a	404[A]	CLA	C3D-C4D-ND	4.35	117.06	109.99
23	A	404[B]	CLA	C1C-C2C-C3C	-4.35	102.41	106.98
23	D	403	CLA	O2D-CGD-O1D	-4.35	115.39	123.85
23	b	615	CLA	C2B-C1B-NB	4.35	114.83	110.33
23	B	609	CLA	C2B-C1B-NB	4.35	114.83	110.33
23	b	609	CLA	C3D-C4D-ND	4.34	117.05	109.99
23	B	612	CLA	O2D-CGD-O1D	-4.34	115.39	123.85
23	B	616	CLA	C2C-C1C-NC	4.34	114.55	109.98
23	A	404[A]	CLA	C1C-C2C-C3C	-4.34	102.41	106.98
23	a	405[A]	CLA	C2B-C1B-NB	4.34	114.83	110.33
23	b	608	CLA	C3D-C4D-ND	4.34	117.04	109.99
23	a	404[B]	CLA	C1C-C2C-C3C	-4.34	102.42	106.98
23	D	403	CLA	C3D-C4D-ND	4.34	117.04	109.99
23	a	407	CLA	C4A-NA-C1A	-4.34	104.70	106.68
23	b	606	CLA	C2C-C1C-NC	4.34	114.54	109.98
23	D	402[B]	CLA	C2B-C1B-NB	4.33	114.82	110.33
33	a	415	LMG	O7-C10-C11	4.33	120.85	111.48
23	D	402[B]	CLA	O2D-CGD-CBD	4.33	118.80	111.23
23	c	504	CLA	CHD-C1D-ND	-4.33	118.71	124.80
23	C	503	CLA	C4A-NA-C1A	-4.33	104.70	106.68
23	b	610	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
23	c	501	CLA	C3D-C4D-ND	4.33	117.02	109.99
23	C	503	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
23	C	509	CLA	C3B-C4B-NB	4.33	114.39	110.53
23	c	513	CLA	CHD-C1D-ND	-4.32	118.72	124.80
29	A	414[B]	PL9	C7-C3-C2	-4.32	118.29	123.39
23	d	405	CLA	CHD-C1D-ND	-4.32	118.72	124.80
31	t	101	LMT	C3'-C4'-C5'	-4.32	101.35	110.93
23	a	405[A]	CLA	C3B-C2B-C1B	-4.32	102.07	107.17
23	b	604	CLA	C1C-C2C-C3C	-4.32	102.43	106.98
25	Y	101	BCR	C16-C17-C18	-4.32	121.22	127.28
23	b	606	CLA	C3D-C4D-ND	4.32	117.01	109.99
23	B	615	CLA	CHD-C1D-ND	-4.32	118.72	124.80
23	b	605	CLA	C2B-C1B-NB	4.32	114.81	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.48
23	c	510	CLA	C2B-C1B-NB	4.32	114.80	110.33
23	c	513	CLA	C1D-CHD-C4C	-4.31	116.85	126.02
23	a	404[A]	CLA	CAA-C2A-C3A	-4.31	101.34	113.00
23	a	404[A]	CLA	C1C-C2C-C3C	-4.31	102.45	106.98
23	a	404[B]	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	B	608	CLA	C3D-C4D-ND	4.31	116.99	109.99
34	C	522	HTG	C1'-S1-C1	4.31	109.75	100.45
23	C	508	CLA	C3C-C4C-NC	4.30	115.94	110.43
23	B	612	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	b	615	CLA	C3D-C4D-ND	4.30	116.98	109.99
23	b	604	CLA	C3C-C4C-NC	4.30	115.94	110.43
23	B	609	CLA	O2D-CGD-CBD	4.30	118.75	111.23
23	c	503	CLA	C2C-C1C-NC	4.30	114.50	109.98
23	c	509	CLA	C1D-CHD-C4C	-4.29	116.89	126.02
23	C	511	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
23	B	607	CLA	C3D-C4D-ND	4.29	116.96	109.99
23	b	609	CLA	C3C-C4C-NC	4.29	115.93	110.43
23	B	610	CLA	C2B-C1B-NB	4.29	114.77	110.33
32	E	101[B]	LHG	O7-C7-C8	4.29	120.76	111.48
23	B	615	CLA	CMB-C2B-C1B	4.29	131.94	125.42
29	a	413[A]	PL9	C7-C3-C4	4.28	120.44	116.91
23	a	404[B]	CLA	CAA-C2A-C3A	-4.28	101.43	113.00
23	A	405[B]	CLA	O2D-CGD-CBD	4.28	118.70	111.23
23	d	402[B]	CLA	C3B-C2B-C1B	-4.27	102.13	107.17
23	D	402[A]	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	B	609	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	c	503	CLA	CHD-C1D-ND	-4.27	118.79	124.80
23	c	511	CLA	C3D-C4D-ND	4.27	116.93	109.99
23	D	403	CLA	C3B-C2B-C1B	-4.27	102.14	107.17
23	c	508	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	a	405[B]	CLA	C2B-C1B-NB	4.27	114.75	110.33
23	b	606	CLA	CHD-C1D-ND	-4.26	118.80	124.80
23	b	607	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	C	505	CLA	C3C-C4C-NC	4.26	115.89	110.43
23	B	604	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	b	611	CLA	C3C-C4C-NC	4.26	115.89	110.43
23	b	613	CLA	C4A-NA-C1A	-4.26	104.74	106.68
23	B	605	CLA	C3D-C4D-ND	4.26	116.91	109.99
23	B	612	CLA	C3B-C2B-C1B	-4.26	102.15	107.17
23	b	614	CLA	C3D-C4D-ND	4.26	116.90	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[A]	CLA	C3D-C4D-ND	4.25	116.90	109.99
23	c	511	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
23	b	610	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	b	604	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	A	404[B]	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	a	404[A]	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
23	C	505	CLA	C3B-C2B-C1B	-4.25	102.16	107.17
23	b	613	CLA	C2B-C1B-NB	4.25	114.73	110.33
23	C	508	CLA	C4A-NA-C1A	-4.25	104.74	106.68
23	b	611	CLA	CHD-C1D-ND	-4.24	118.83	124.80
23	D	402[A]	CLA	C1-C2-C3	-4.24	119.25	126.20
23	B	605	CLA	C1D-CHD-C4C	-4.24	117.01	126.02
23	A	405[A]	CLA	C2B-C1B-NB	4.24	114.72	110.33
23	C	511	CLA	C3B-C4B-NB	4.24	114.31	110.53
23	a	404[A]	CLA	C3B-C4B-NB	4.24	114.31	110.53
23	b	607	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
23	B	603	CLA	C3C-C4C-NC	4.24	115.86	110.43
23	b	608	CLA	CMC-C2C-C1C	4.24	131.65	125.03
23	b	616	CLA	C3D-C4D-ND	4.23	116.87	109.99
23	b	615	CLA	C1D-CHD-C4C	-4.23	117.02	126.02
23	A	405[A]	CLA	C3D-C4D-ND	4.23	116.87	109.99
33	C	521	LMG	O6-C5-C4	4.23	117.31	109.70
23	a	407	CLA	C3C-C4C-NC	4.22	115.84	110.43
23	d	402[A]	CLA	C2B-C1B-NB	4.22	114.71	110.33
23	B	616	CLA	C3D-C4D-ND	4.22	116.84	109.99
23	C	513	CLA	C1D-CHD-C4C	-4.22	117.06	126.02
23	c	509	CLA	C3B-C4B-NB	4.22	114.29	110.53
23	A	404[A]	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
23	A	405[A]	CLA	CAA-C2A-C3A	-4.21	101.61	113.00
23	b	611	CLA	C3B-C4B-NB	4.21	114.29	110.53
23	B	606	CLA	C3C-C4C-NC	4.21	115.83	110.43
23	A	406[B]	CLA	C1C-C2C-C3C	-4.21	102.55	106.98
23	A	404[B]	CLA	CAA-C2A-C3A	-4.21	101.62	113.00
23	A	404[B]	CLA	O2D-CGD-CBD	4.21	118.59	111.23
23	C	502	CLA	C2B-C1B-NB	4.21	114.69	110.33
23	d	404[A]	CLA	O2D-CGD-CBD	4.20	118.58	111.23
23	C	502	CLA	C1D-CHD-C4C	-4.20	117.08	126.02
23	c	506	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
23	D	402[A]	CLA	C3D-C4D-ND	4.20	116.82	109.99
23	c	505	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
23	C	504	CLA	C1D-CHD-C4C	-4.20	117.09	126.02
23	c	506	CLA	C3B-C4B-NB	4.20	114.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	C4A-NA-C1A	-4.20	104.76	106.68
23	C	507	CLA	CHD-C1D-ND	-4.20	118.89	124.80
23	C	509	CLA	C3D-C4D-ND	4.20	116.81	109.99
23	B	615	CLA	C2C-C1C-NC	4.20	114.39	109.98
23	b	614	CLA	C1D-CHD-C4C	-4.20	117.10	126.02
23	d	404[A]	CLA	C3C-C4C-NC	4.19	115.80	110.43
23	b	610	CLA	C3C-C4C-NC	4.19	115.80	110.43
23	C	512	CLA	C3D-C4D-ND	4.19	116.80	109.99
23	c	505	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	d	405	CLA	C2C-C1C-NC	4.19	114.39	109.98
23	C	511	CLA	CHD-C1D-ND	-4.19	118.91	124.80
23	c	512	CLA	C3D-C4D-ND	4.19	116.79	109.99
33	C	501	LMG	O7-C10-C11	4.18	120.53	111.48
23	A	406[B]	CLA	CHD-C1D-ND	-4.18	118.91	124.80
23	C	513	CLA	C1-C2-C3	-4.18	119.34	126.20
23	C	506	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
23	B	615	CLA	C3B-C2B-C1B	-4.18	102.24	107.17
33	C	501	LMG	C7-O1-C1	-4.18	104.83	113.80
23	b	601	CLA	C2C-C1C-NC	4.18	114.37	109.98
23	A	406[A]	CLA	C1C-C2C-C3C	-4.18	102.59	106.98
23	D	402[B]	CLA	CHD-C1D-ND	-4.18	118.92	124.80
23	a	404[B]	CLA	C1D-CHD-C4C	-4.18	117.14	126.02
23	c	502	CLA	C3D-C4D-ND	4.17	116.77	109.99
23	B	603	CLA	C1D-CHD-C4C	-4.17	117.15	126.02
23	C	509	CLA	C3B-C2B-C1B	-4.17	102.25	107.17
23	C	502	CLA	C2C-C1C-NC	4.17	114.36	109.98
23	B	608	CLA	O2D-CGD-O1D	-4.17	115.73	123.85
23	D	402[B]	CLA	C3C-C4C-NC	4.17	115.77	110.43
29	a	413[B]	PL9	C32-C33-C34	-4.17	118.09	127.62
23	D	402[A]	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
23	c	501	CLA	C1C-C2C-C3C	-4.16	102.61	106.98
23	c	502	CLA	C1D-CHD-C4C	-4.16	117.19	126.02
26	a	409[A]	SQD	C1-C2-C3	-4.15	101.27	110.01
23	b	603	CLA	CAA-C2A-C3A	-4.15	101.78	113.00
23	c	506	CLA	O2D-CGD-CBD	4.15	118.49	111.23
23	d	402[B]	CLA	CAA-C2A-C3A	-4.15	101.78	113.00
23	c	501	CLA	C2B-C1B-NB	4.15	114.63	110.33
23	C	514	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
23	B	608	CLA	C3C-C4C-NC	4.15	115.75	110.43
23	c	508	CLA	C1C-C2C-C3C	-4.15	102.62	106.98
23	B	610	CLA	CAA-C2A-C3A	-4.15	101.79	113.00
23	d	404[B]	CLA	C3D-C2D-C1D	-4.15	100.17	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Z	101	LMG	O7-C10-C11	4.15	120.45	111.48
23	b	603	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	B	614	CLA	C1D-CHD-C4C	-4.14	117.22	126.02
23	B	614	CLA	C3D-C4D-ND	4.14	116.72	109.99
23	C	506	CLA	C3C-C4C-NC	4.14	115.73	110.43
23	b	605	CLA	O2D-CGD-O1D	-4.14	115.80	123.85
23	C	505	CLA	C3D-C4D-ND	4.13	116.71	109.99
25	d	406	BCR	C15-C14-C13	-4.13	121.49	127.28
23	C	511	CLA	C4A-NA-C1A	-4.13	104.80	106.68
29	d	407[A]	PL9	C42-C43-C44	-4.12	118.19	127.62
31	B	627	LMT	C1'-O5'-C5'	-4.12	105.67	113.72
23	C	508	CLA	CMB-C2B-C1B	4.12	131.70	125.42
23	b	611	CLA	C1-C2-C3	-4.12	119.44	126.20
23	d	405	CLA	C4A-NA-C1A	-4.12	104.80	106.68
23	B	610	CLA	C3D-C4D-ND	4.12	116.68	109.99
23	B	609	CLA	C3C-C4C-NC	4.12	115.70	110.43
23	B	613	CLA	C2B-C1B-NB	4.11	114.59	110.33
23	c	509	CLA	C3D-C4D-ND	4.11	116.67	109.99
23	d	404[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
26	a	409[A]	SQD	C1-O5-C5	-4.11	105.69	113.72
23	C	510	CLA	C3D-C4D-ND	4.11	116.67	109.99
23	b	606	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
23	b	609	CLA	O2D-CGD-CBD	4.11	118.41	111.23
23	C	505	CLA	C4A-NA-C1A	-4.11	104.81	106.68
23	d	404[A]	CLA	C3B-C2B-C1B	-4.10	102.34	107.17
23	c	506	CLA	C1-C2-C3	-4.10	119.48	126.20
23	b	602	CLA	O2D-CGD-O1D	-4.10	115.88	123.85
23	b	614	CLA	C1-C2-C3	-4.09	119.49	126.20
23	C	507	CLA	C3B-C4B-NB	4.09	114.18	110.53
23	b	604	CLA	C3B-C4B-NB	4.09	114.18	110.53
23	d	402[A]	CLA	C3B-C2B-C1B	-4.09	102.34	107.17
23	b	602	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
23	A	406[A]	CLA	CHD-C1D-ND	-4.09	119.05	124.80
23	b	605	CLA	C3C-C4C-NC	4.09	115.67	110.43
23	c	512	CLA	C1-C2-C3	-4.09	119.50	126.20
23	c	508	CLA	C3C-C4C-NC	4.09	115.66	110.43
23	c	510	CLA	C3C-C4C-NC	4.09	115.66	110.43
29	a	413[A]	PL9	C32-C33-C34	-4.08	118.28	127.62
23	d	402[B]	CLA	C1D-CHD-C4C	-4.08	117.35	126.02
23	B	602	CLA	C1D-CHD-C4C	-4.08	117.35	126.02
23	c	509	CLA	C2B-C1B-NB	4.08	114.56	110.33
23	C	512	CLA	C3C-C4C-NC	4.08	115.65	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404[B]	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
23	c	501	CLA	C1-C2-C3	-4.07	119.52	126.20
35	C	517[A]	DGD	O2G-C1B-C2B	4.07	120.29	111.48
23	B	605	CLA	C2B-C1B-NB	4.07	114.55	110.33
23	B	613	CLA	CAC-C3C-C4C	4.07	130.09	124.79
23	C	506	CLA	C2B-C1B-NB	4.07	114.54	110.33
23	a	404[B]	CLA	CHD-C1D-ND	-4.06	119.08	124.80
23	C	503	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
23	B	603	CLA	C3B-C2B-C1B	-4.06	102.38	107.17
23	B	603	CLA	CAC-C3C-C4C	4.06	130.07	124.79
23	c	504	CLA	C3B-C4B-NB	4.05	114.15	110.53
25	B	618	BCR	C29-C30-C25	4.05	116.33	110.44
23	D	403	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
23	d	402[A]	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
23	A	406[A]	CLA	C3B-C2B-C1B	-4.05	102.39	107.17
23	b	613	CLA	C1-C2-C3	-4.05	119.56	126.20
29	a	413[B]	PL9	C7-C8-C9	-4.05	119.86	126.83
23	b	601	CLA	C1D-CHD-C4C	-4.05	117.42	126.02
23	c	512	CLA	C2C-C1C-NC	4.05	114.23	109.98
33	m	101	LMG	O7-C10-C11	4.04	120.23	111.48
23	A	404[A]	CLA	CHD-C1D-ND	-4.04	119.11	124.80
23	A	405[B]	CLA	C3D-C4D-ND	4.04	116.56	109.99
23	b	603	CLA	O2D-CGD-O1D	-4.04	115.98	123.85
23	d	402[B]	CLA	CHD-C1D-ND	-4.04	119.12	124.80
23	C	508	CLA	C3D-C4D-ND	4.04	116.55	109.99
23	b	601	CLA	CHD-C1D-ND	-4.04	119.12	124.80
23	b	607	CLA	C3B-C2B-C1B	-4.04	102.41	107.17
23	A	408	CLA	C1-C2-C3	-4.04	119.58	126.20
23	c	510	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
23	C	513	CLA	C3C-C4C-NC	4.03	115.60	110.43
23	b	604	CLA	C2B-C1B-NB	4.03	114.51	110.33
23	b	607	CLA	C3B-C4B-NB	4.03	114.13	110.53
23	B	603	CLA	C3D-C4D-ND	4.03	116.54	109.99
33	c	520	LMG	O7-C10-C11	4.03	120.20	111.48
23	C	504	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	c	506	CLA	CHD-C1D-ND	-4.03	119.13	124.80
23	C	508	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
23	B	601	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
23	C	513	CLA	C3D-C4D-ND	4.03	116.53	109.99
33	C	520	LMG	O7-C10-C11	4.02	120.19	111.48
23	b	607	CLA	O2D-CGD-CBD	4.02	118.27	111.23
23	B	605	CLA	C4-C3-C5	4.02	122.21	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[B]	CLA	C3B-C2B-C1B	-4.02	102.43	107.17
23	C	505	CLA	C3B-C4B-NB	4.02	114.12	110.53
23	b	616	CLA	O2D-CGD-O1D	-4.02	116.03	123.85
38	E	102	HEM	CHD-C4C-NC	4.02	128.83	124.45
23	c	507	CLA	C3D-C4D-ND	4.02	116.52	109.99
23	B	605	CLA	CHD-C1D-ND	-4.02	119.15	124.80
23	B	616	CLA	C2B-C1B-NB	4.01	114.49	110.33
23	a	405[B]	CLA	C2C-C1C-NC	4.01	114.20	109.98
23	C	512	CLA	C4A-NA-C1A	-4.01	104.85	106.68
23	B	605	CLA	C3C-C4C-NC	4.01	115.57	110.43
23	B	606	CLA	C1C-C2C-C3C	-4.01	102.76	106.98
23	c	510	CLA	C3D-C4D-ND	4.01	116.51	109.99
23	A	405[A]	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
23	A	405[B]	CLA	CHD-C1D-ND	-4.01	119.16	124.80
23	b	614	CLA	C4A-NA-C1A	-4.00	104.85	106.68
23	b	602	CLA	C2C-C1C-NC	4.00	114.19	109.98
23	d	402[A]	CLA	CAA-C2A-C3A	-4.00	102.19	113.00
23	B	611	CLA	C3C-C4C-NC	4.00	115.55	110.43
23	B	612	CLA	C1D-CHD-C4C	-4.00	117.53	126.02
23	b	616	CLA	O2A-CGA-CBA	4.00	124.02	111.83
23	B	602	CLA	C3C-C4C-NC	3.99	115.55	110.43
23	B	606	CLA	C1D-CHD-C4C	-3.99	117.53	126.02
23	b	606	CLA	C4-C3-C5	3.99	122.16	115.23
23	C	511	CLA	C1D-CHD-C4C	-3.99	117.54	126.02
23	D	402[B]	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
33	C	521	LMG	O7-C10-C11	3.99	120.11	111.48
23	A	405[B]	CLA	CAA-C2A-C3A	-3.99	102.22	113.00
23	c	502	CLA	C2B-C1B-NB	3.99	114.46	110.33
23	B	607	CLA	C3C-C4C-NC	3.99	115.54	110.43
23	B	604	CLA	C3D-C4D-ND	3.99	116.47	109.99
23	B	604	CLA	C1D-CHD-C4C	-3.99	117.55	126.02
25	d	406	BCR	C29-C30-C25	3.98	116.23	110.44
23	b	616	CLA	CMB-C2B-C1B	3.98	131.49	125.42
23	B	611	CLA	CHD-C4C-NC	3.98	130.41	124.23
23	B	607	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
23	B	601	CLA	CHD-C1D-ND	-3.98	119.20	124.80
23	A	405[B]	CLA	C2B-C1B-NB	3.98	114.45	110.33
23	C	512	CLA	C1D-CHD-C4C	-3.97	117.58	126.02
23	b	615	CLA	O2D-CGD-CBD	3.97	118.17	111.23
25	k	101	BCR	C29-C30-C25	3.97	116.20	110.44
23	B	606	CLA	C3D-C4D-ND	3.97	116.44	109.99
23	C	513	CLA	C2C-C1C-NC	3.97	114.15	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	l	101	SQD	C3-C4-C5	3.97	117.43	110.23
23	b	610	CLA	O2A-CGA-CBA	3.96	123.92	111.83
23	C	506	CLA	CHD-C1D-ND	-3.96	119.23	124.80
23	c	512	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
23	C	504	CLA	C2C-C1C-NC	3.96	114.14	109.98
23	C	514	CLA	CHD-C1D-ND	-3.96	119.23	124.80
23	B	614	CLA	CHD-C1D-ND	-3.95	119.24	124.80
23	b	602	CLA	CHD-C1D-ND	-3.95	119.24	124.80
23	b	606	CLA	O2D-CGD-O1D	-3.95	116.16	123.85
23	a	405[A]	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
23	b	612	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
23	b	602	CLA	C3C-C4C-NC	3.95	115.48	110.43
23	c	508	CLA	C3D-C4D-ND	3.94	116.40	109.99
23	c	505	CLA	CHD-C1D-ND	-3.94	119.25	124.80
23	B	605	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
32	d	409[B]	LHG	O7-C7-C8	3.94	120.00	111.48
23	B	601	CLA	C3C-C4C-NC	3.94	115.47	110.43
23	d	404[B]	CLA	CHD-C1D-ND	-3.94	119.26	124.80
23	C	507	CLA	C1-C2-C3	-3.93	119.75	126.20
32	A	419[A]	LHG	O8-C23-O10	-3.93	113.79	123.63
23	B	616	CLA	C4C-C3C-C2C	-3.93	101.17	106.89
23	b	612	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
23	B	610	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
23	B	615	CLA	C2B-C1B-NB	3.92	114.39	110.33
23	c	502	CLA	C3B-C4B-NB	3.92	114.03	110.53
23	b	610	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
25	b	617	BCR	C33-C5-C6	-3.92	120.21	124.48
23	b	604	CLA	C3D-C4D-ND	3.91	116.35	109.99
23	b	613	CLA	C1C-C2C-C3C	-3.91	102.86	106.98
23	B	615	CLA	C3C-C4C-NC	3.91	115.44	110.43
23	A	408	CLA	C3B-C4B-NB	3.91	114.02	110.53
23	b	605	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
33	c	519	LMG	O7-C10-C11	3.91	119.93	111.48
23	a	404[B]	CLA	O2D-CGD-CBD	3.91	118.06	111.23
23	C	502	CLA	CHD-C1D-ND	-3.90	119.31	124.80
23	b	609	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
23	B	616	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
25	T	102	BCR	C15-C16-C17	-3.90	115.55	123.52
25	d	406	BCR	C40-C30-C25	-3.89	104.14	110.24
23	C	505	CLA	CHD-C1D-ND	-3.89	119.33	124.80
40	V	201	HEC	C4D-ND-C1D	3.89	112.16	105.82
23	D	402[A]	CLA	C3C-C4C-NC	3.89	115.41	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	C3B-C2B-C1B	-3.89	102.59	107.17
25	C	515	BCR	C7-C8-C9	-3.88	120.49	126.23
23	B	615	CLA	C1C-C2C-C3C	-3.88	102.89	106.98
23	b	609	CLA	C3B-C2B-C1B	-3.88	102.59	107.17
23	c	511	CLA	C2B-C1B-NB	3.88	114.35	110.33
23	C	510	CLA	CHD-C1D-ND	-3.88	119.34	124.80
23	b	608	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
35	c	516[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.48
23	b	603	CLA	C3C-C4C-NC	3.88	115.40	110.43
23	c	502	CLA	O2D-CGD-O1D	-3.88	116.30	123.85
23	d	404[A]	CLA	CHD-C1D-ND	-3.88	119.35	124.80
23	C	502	CLA	C3B-C2B-C1B	-3.87	102.61	107.17
23	C	514	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
23	B	610	CLA	CMB-C2B-C1B	3.87	131.31	125.42
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	C	504	CLA	C3C-C4C-NC	3.86	115.38	110.43
23	C	506	CLA	C1-C2-C3	-3.86	119.87	126.20
23	C	509	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	b	616	CLA	C3C-C4C-NC	3.86	115.38	110.43
23	C	510	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
23	A	405[A]	CLA	CHD-C1D-ND	-3.86	119.37	124.80
23	d	404[B]	CLA	C2B-C1B-NB	3.86	114.33	110.33
23	b	615	CLA	C3C-C4C-NC	3.86	115.37	110.43
29	D	405[B]	PL9	C42-C43-C44	-3.86	118.80	127.62
23	A	404[A]	CLA	C3D-C4D-ND	3.85	116.25	109.99
23	d	402[B]	CLA	C3B-C4B-NB	3.85	113.97	110.53
23	B	610	CLA	C3C-C4C-NC	3.85	115.37	110.43
23	C	502	CLA	O2D-CGD-O1D	-3.85	116.35	123.85
23	b	616	CLA	CHD-C1D-ND	-3.85	119.38	124.80
35	C	518[B]	DGD	O2G-C1B-C2B	3.85	119.81	111.48
23	d	404[A]	CLA	C1-C2-C3	-3.85	119.89	126.20
23	A	408	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
23	c	506	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
26	A	412	SQD	O47-C7-C8	3.85	119.80	111.48
29	A	414[A]	PL9	C37-C38-C39	-3.84	118.82	127.62
23	c	513	CLA	C3B-C4B-NB	3.84	113.96	110.53
24	A	407[B]	PHO	C1A-C2A-C3A	-3.84	99.18	102.84
23	c	511	CLA	C4A-NA-C1A	-3.83	104.93	106.68
23	a	405[A]	CLA	C3C-C4C-NC	3.83	115.34	110.43
23	A	405[A]	CLA	CBC-CAC-C3C	-3.83	102.04	112.42
23	a	407	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
23	c	507	CLA	CMB-C2B-C1B	3.83	131.25	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	CHD-C1D-ND	-3.83	119.42	124.80
23	A	408	CLA	O2D-CGD-CBD	3.83	117.92	111.23
23	C	510	CLA	C1D-CHD-C4C	-3.82	117.90	126.02
23	C	510	CLA	C3B-C4B-NB	3.82	113.94	110.53
23	c	507	CLA	C2B-C1B-NB	3.82	114.29	110.33
23	C	506	CLA	CAC-C3C-C4C	3.82	129.76	124.79
29	A	414[A]	PL9	C7-C3-C4	3.82	120.05	116.91
23	a	404[B]	CLA	C3C-C4C-NC	3.82	115.32	110.43
23	C	503	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	b	613	CLA	C3B-C4B-NB	3.81	113.93	110.53
23	c	507	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	c	511	CLA	C3C-C4C-NC	3.81	115.31	110.43
23	B	615	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
23	b	604	CLA	CMC-C2C-C1C	3.81	130.98	125.03
23	A	405[B]	CLA	C1D-CHD-C4C	-3.80	117.94	126.02
24	A	416[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
23	b	609	CLA	C2B-C1B-NB	3.80	114.27	110.33
23	d	402[A]	CLA	CHD-C1D-ND	-3.80	119.46	124.80
34	b	625	HTG	C1-O5-C5	3.80	119.38	112.56
23	b	606	CLA	C3C-C4C-NC	3.80	115.30	110.43
23	b	608	CLA	C3B-C4B-NB	3.80	113.92	110.53
32	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.48
23	C	508	CLA	CHD-C1D-ND	-3.79	119.46	124.80
23	B	608	CLA	C3B-C4B-NB	3.79	113.92	110.53
23	b	610	CLA	C2B-C1B-NB	3.79	114.26	110.33
23	c	510	CLA	CMC-C2C-C1C	3.79	130.96	125.03
25	K	102	BCR	C7-C8-C9	-3.79	120.63	126.23
23	A	405[A]	CLA	CMC-C2C-C1C	3.79	130.95	125.03
23	B	602	CLA	CMC-C2C-C1C	3.79	130.95	125.03
23	a	407	CLA	CHD-C1D-ND	-3.78	119.48	124.80
23	d	404[B]	CLA	C3C-C4C-NC	3.78	115.28	110.43
23	B	613	CLA	C3D-C4D-ND	3.78	116.13	109.99
23	c	510	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
23	B	605	CLA	CHD-C4C-NC	3.78	130.09	124.23
23	B	607	CLA	CHD-C1D-ND	-3.78	119.49	124.80
23	B	610	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
29	A	414[B]	PL9	C7-C3-C4	3.78	120.02	116.91
23	C	503	CLA	CHD-C1D-ND	-3.78	119.49	124.80
25	k	101	BCR	C7-C8-C9	-3.77	120.65	126.23
23	C	514	CLA	C3B-C4B-NB	3.77	113.90	110.53
23	d	402[A]	CLA	CMB-C2B-C1B	3.77	131.16	125.42
33	c	520	LMG	C3-C4-C5	3.77	117.06	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	C1D-CHD-C4C	-3.77	118.01	126.02
23	D	402[A]	CLA	C3B-C4B-NB	3.76	113.89	110.53
23	C	514	CLA	C4A-NA-C1A	-3.76	104.96	106.68
23	b	615	CLA	CHD-C1D-ND	-3.76	119.51	124.80
23	B	605	CLA	CMB-C2B-C1B	3.76	131.14	125.42
26	a	411	SQD	O47-C7-C8	3.76	119.61	111.48
29	A	414[B]	PL9	C37-C38-C39	-3.75	119.03	127.62
23	c	505	CLA	C4C-C3C-C2C	-3.75	101.43	106.89
23	B	602	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
23	D	403	CLA	CHD-C1D-ND	-3.75	119.53	124.80
23	b	603	CLA	CHD-C1D-ND	-3.75	119.53	124.80
23	B	606	CLA	C2B-C1B-NB	3.75	114.21	110.33
23	b	603	CLA	C3B-C4B-NB	3.75	113.87	110.53
26	X	101	SQD	O8-S-C6	3.75	113.20	105.97
23	A	406[B]	CLA	C1D-CHD-C4C	-3.74	118.06	126.02
23	c	510	CLA	CHD-C1D-ND	-3.74	119.53	124.80
23	C	514	CLA	C3C-C4C-NC	3.74	115.23	110.43
23	b	609	CLA	CAC-C3C-C4C	3.74	129.66	124.79
23	c	511	CLA	O2D-CGD-O1D	-3.74	116.56	123.85
33	Z	101	LMG	C1-C2-C3	3.74	117.88	110.01
23	b	612	CLA	C2B-C1B-NB	3.74	114.20	110.33
26	A	410[B]	SQD	C44-O6-C1	-3.74	105.78	113.80
23	B	611	CLA	CHD-C1D-ND	-3.74	119.54	124.80
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.48
23	c	513	CLA	C1C-C2C-C3C	-3.73	103.05	106.98
23	B	614	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
23	b	612	CLA	CAC-C3C-C4C	3.73	129.64	124.79
23	c	506	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
23	B	604	CLA	C2B-C1B-NB	3.73	114.19	110.33
23	A	406[B]	CLA	CMB-C2B-C1B	3.73	131.09	125.42
23	C	505	CLA	C2B-C1B-NB	3.73	114.19	110.33
23	B	609	CLA	C3B-C2B-C1B	-3.73	102.78	107.17
23	b	614	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
23	c	509	CLA	C1C-C2C-C3C	-3.73	103.06	106.98
23	a	407	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
23	b	612	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
23	C	509	CLA	C2B-C1B-NB	3.72	114.19	110.33
23	c	513	CLA	C3C-C4C-NC	3.72	115.20	110.43
23	d	405	CLA	CMB-C2B-C1B	3.72	131.09	125.42
23	c	503	CLA	C3C-C4C-NC	3.72	115.20	110.43
23	b	602	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
23	c	512	CLA	CHD-C1D-ND	-3.72	119.57	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	C3C-C4C-NC	3.72	115.19	110.43
23	b	609	CLA	CHD-C1D-ND	-3.72	119.57	124.80
23	c	507	CLA	CMC-C2C-C1C	3.72	130.84	125.03
23	B	613	CLA	C3B-C4B-NB	3.72	113.85	110.53
23	a	404[A]	CLA	O2A-CGA-O1A	-3.71	114.34	123.63
29	a	413[A]	PL9	C27-C28-C29	-3.71	119.13	127.62
23	b	602	CLA	CAA-C2A-C3A	-3.71	102.98	113.00
23	d	404[A]	CLA	C3B-C4B-NB	3.71	113.84	110.53
23	C	513	CLA	C4-C3-C5	3.70	121.66	115.23
23	a	404[A]	CLA	CHD-C1D-ND	-3.70	119.59	124.80
23	D	402[A]	CLA	C2B-C1B-NB	3.70	114.17	110.33
23	c	504	CLA	C1-O2A-CGA	3.70	125.61	116.65
23	C	509	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
23	C	509	CLA	C4C-C3C-C2C	-3.70	101.51	106.89
23	b	603	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
23	b	613	CLA	C3D-C4D-ND	3.70	116.00	109.99
23	b	614	CLA	C3C-C4C-NC	3.69	115.16	110.43
35	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.48
23	B	604	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
23	b	611	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
40	V	201	HEC	CBC-CAC-C3C	-3.68	120.07	127.43
29	A	414[A]	PL9	C22-C23-C24	-3.68	119.19	127.62
23	D	403	CLA	C3C-C4C-NC	3.68	115.14	110.43
25	T	102	BCR	C16-C17-C18	-3.68	122.12	127.28
23	B	616	CLA	C3B-C4B-NB	3.68	113.81	110.53
23	c	504	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
32	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.48
23	b	608	CLA	CHD-C1D-ND	-3.68	119.63	124.80
23	b	612	CLA	C1C-C2C-C3C	-3.67	103.11	106.98
25	D	404	BCR	C38-C26-C25	-3.67	120.47	124.48
25	C	515	BCR	C33-C5-C6	-3.67	120.48	124.48
23	a	405[B]	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
23	b	612	CLA	C3B-C4B-NB	3.67	113.81	110.53
23	c	510	CLA	C3B-C4B-NB	3.67	113.81	110.53
25	C	516	BCR	C7-C8-C9	-3.67	120.81	126.23
24	d	403[A]	PHO	C4-C3-C5	3.67	121.59	115.23
25	D	404	BCR	C10-C11-C12	-3.67	112.58	123.20
23	A	406[A]	CLA	C3C-C4C-NC	3.67	115.13	110.43
23	B	612	CLA	C4C-C3C-C2C	-3.66	101.56	106.89
23	d	402[A]	CLA	C3C-C4C-NC	3.66	115.12	110.43
23	d	405	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
23	b	605	CLA	CHD-C4C-NC	3.66	129.90	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	C1D-CHD-C4C	-3.65	118.25	126.02
26	a	409[B]	SQD	C1-C2-C3	-3.65	102.33	110.01
32	b	629[B]	LHG	O7-C7-C8	3.65	119.38	111.48
23	b	616	CLA	C2C-C1C-NC	3.65	113.81	109.98
34	B	621	HTG	O5-C1-C2	3.65	115.35	110.32
29	a	413[A]	PL9	C15-C14-C16	3.65	121.56	115.23
23	b	614	CLA	C3B-C4B-NB	3.65	113.78	110.53
29	a	413[B]	PL9	C27-C28-C29	-3.65	119.28	127.62
25	B	617	BCR	C33-C5-C6	-3.64	120.51	124.48
23	A	406[A]	CLA	CMB-C2B-C1B	3.64	130.97	125.42
23	a	405[B]	CLA	C3C-C4C-NC	3.64	115.10	110.43
23	a	407	CLA	CMC-C2C-C1C	3.64	130.73	125.03
23	A	408	CLA	CAA-C2A-C3A	-3.64	103.16	113.00
40	V	201	HEC	CBD-CAD-C3D	-3.64	102.47	112.53
23	C	512	CLA	CHD-C1D-ND	-3.64	119.68	124.80
29	D	405[A]	PL9	C42-C43-C44	-3.64	119.29	127.62
23	C	507	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
23	C	508	CLA	C2B-C1B-NB	3.64	114.10	110.33
23	B	610	CLA	CHD-C1D-ND	-3.64	119.69	124.80
23	c	507	CLA	O2D-CGD-O1D	-3.64	116.77	123.85
23	b	606	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
26	X	101	SQD	C44-O6-C1	-3.63	106.02	113.80
23	c	506	CLA	C2B-C1B-NB	3.62	114.08	110.33
23	c	505	CLA	CMB-C2B-C1B	3.62	130.93	125.42
23	B	603	CLA	CHD-C1D-ND	-3.62	119.71	124.80
23	c	508	CLA	C1D-CHD-C4C	-3.62	118.34	126.02
38	E	102	HEM	C1B-NB-C4B	3.61	109.48	105.21
23	A	404[A]	CLA	O2D-CGD-CBD	3.61	117.54	111.23
32	A	419[B]	LHG	O7-C7-C8	3.61	119.29	111.48
23	C	506	CLA	C1D-CHD-C4C	-3.61	118.35	126.02
29	A	414[B]	PL9	C22-C23-C24	-3.61	119.36	127.62
23	B	603	CLA	CAA-C2A-C3A	-3.61	103.25	113.00
25	b	619	BCR	C24-C23-C22	-3.61	120.90	126.23
23	c	506	CLA	C3C-C4C-NC	3.61	115.05	110.43
23	A	404[A]	CLA	O2A-CGA-CBA	3.61	122.83	111.83
23	A	405[A]	CLA	O2D-CGD-O1D	-3.61	116.83	123.85
23	b	616	CLA	CHD-C4C-NC	3.60	129.82	124.23
23	B	607	CLA	C3B-C4B-NB	3.60	113.75	110.53
23	b	604	CLA	O2D-CGD-O1D	-3.60	116.84	123.85
25	y	101	BCR	C15-C14-C13	-3.60	122.23	127.28
23	b	608	CLA	C1-C2-C3	-3.60	120.30	126.20
32	d	415[B]	LHG	O7-C7-C8	3.60	119.26	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	102	BCR	C38-C26-C25	-3.60	120.56	124.48
23	C	510	CLA	C3C-C4C-NC	3.60	115.04	110.43
23	B	610	CLA	C1D-CHD-C4C	-3.60	118.38	126.02
23	B	603	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
23	c	509	CLA	C4A-NA-C1A	-3.59	105.04	106.68
26	a	409[A]	SQD	C44-O6-C1	-3.59	106.09	113.80
23	d	404[A]	CLA	O2A-CGA-CBA	3.59	122.77	111.83
23	B	612	CLA	CAC-C3C-C4C	3.59	129.46	124.79
23	B	608	CLA	C1D-CHD-C4C	-3.58	118.40	126.02
23	B	613	CLA	C4A-NA-C1A	-3.58	105.04	106.68
23	b	614	CLA	CHD-C1D-ND	-3.58	119.76	124.80
23	D	403	CLA	C1C-C2C-C3C	-3.58	103.21	106.98
23	c	508	CLA	C3B-C4B-NB	3.58	113.73	110.53
23	c	502	CLA	C4A-NA-C1A	-3.58	105.05	106.68
23	B	603	CLA	C3B-C4B-NB	3.58	113.73	110.53
23	d	404[B]	CLA	O2A-CGA-CBA	3.58	122.74	111.83
23	B	608	CLA	C4C-C3C-C2C	-3.58	101.69	106.89
23	B	607	CLA	CMC-C2C-C1C	3.58	130.62	125.03
23	b	605	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
23	D	402[B]	CLA	C3B-C4B-NB	3.57	113.72	110.53
35	c	516[B]	DGD	O2G-C1B-C2B	3.57	119.21	111.48
23	d	404[A]	CLA	C2B-C1B-NB	3.57	114.03	110.33
23	c	504	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
23	a	404[A]	CLA	C3C-C4C-NC	3.57	115.00	110.43
23	C	512	CLA	O2D-CGD-O1D	-3.57	116.90	123.85
23	B	602	CLA	CAA-C2A-C3A	-3.57	103.36	113.00
23	A	405[B]	CLA	CBC-CAC-C3C	-3.57	102.75	112.42
23	A	404[A]	CLA	C3C-C4C-NC	3.57	115.00	110.43
23	b	604	CLA	CHD-C1D-ND	-3.56	119.79	124.80
23	A	406[B]	CLA	C3B-C4B-NB	3.56	113.71	110.53
23	B	611	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
38	f	101	HEM	CHA-C4D-ND	3.56	128.77	124.37
23	B	609	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
23	d	404[B]	CLA	C1-C2-C3	-3.56	120.37	126.20
23	B	608	CLA	CHD-C1D-ND	-3.56	119.80	124.80
23	B	615	CLA	CED-O2D-CGD	3.55	123.98	115.92
23	d	404[B]	CLA	C3B-C4B-NB	3.55	113.70	110.53
23	a	404[A]	CLA	O2D-CGD-CBD	3.55	117.43	111.23
23	b	612	CLA	C4-C3-C5	3.55	121.38	115.23
23	A	404[A]	CLA	C1D-CHD-C4C	-3.54	118.49	126.02
23	C	509	CLA	C4A-NA-C1A	-3.54	105.06	106.68
23	B	613	CLA	O2A-CGA-O1A	-3.54	114.77	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	C3C-C4C-NC	3.54	114.97	110.43
23	b	604	CLA	C1D-CHD-C4C	-3.54	118.50	126.02
23	a	404[A]	CLA	O2A-CGA-CBA	3.54	122.61	111.83
23	b	615	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
23	b	612	CLA	CMC-C2C-C1C	3.53	130.55	125.03
23	b	610	CLA	C4C-C3C-C2C	-3.53	101.76	106.89
23	C	502	CLA	C3C-C4C-NC	3.53	114.95	110.43
23	c	506	CLA	CAC-C3C-C4C	3.53	129.38	124.79
23	b	615	CLA	CMB-C2B-C1B	3.53	130.79	125.42
33	Z	101	LMG	O6-C1-C2	3.53	117.61	110.37
23	a	405[A]	CLA	C1D-CHD-C4C	-3.53	118.53	126.02
23	c	502	CLA	C3C-C4C-NC	3.52	114.94	110.43
23	b	607	CLA	CHD-C1D-ND	-3.52	119.85	124.80
24	A	416[A]	PHO	C4D-CHA-CBD	3.52	110.14	108.45
23	b	613	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
25	d	406	BCR	C38-C26-C25	-3.51	120.65	124.48
23	C	503	CLA	C1-C2-C3	-3.51	120.44	126.20
23	d	402[B]	CLA	C3C-C4C-NC	3.51	114.93	110.43
23	b	610	CLA	CAA-C2A-C3A	-3.51	103.51	113.00
23	d	405	CLA	C3C-C4C-NC	3.51	114.92	110.43
23	B	609	CLA	CMB-C2B-C1B	3.51	130.76	125.42
23	A	406[A]	CLA	O2A-CGA-O1A	-3.51	114.85	123.63
35	c	517[B]	DGD	O2G-C1B-C2B	3.51	119.07	111.48
23	B	603	CLA	C2B-C1B-NB	3.51	113.96	110.33
23	B	607	CLA	C1D-CHD-C4C	-3.51	118.57	126.02
23	B	606	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
31	A	417	LMT	O5B-C5B-C4B	3.50	116.01	109.70
23	d	404[B]	CLA	C1D-CHD-C4C	-3.50	118.58	126.02
23	B	602	CLA	CHD-C1D-ND	-3.50	119.88	124.80
33	B	620	LMG	O8-C28-C29	3.50	122.50	111.83
23	C	507	CLA	C3C-C4C-NC	3.50	114.91	110.43
23	A	406[B]	CLA	C3C-C4C-NC	3.49	114.91	110.43
29	a	413[B]	PL9	C15-C14-C16	3.49	121.29	115.23
23	C	502	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
23	B	613	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
25	a	408	BCR	C38-C26-C25	-3.49	120.68	124.48
32	A	419[B]	LHG	C5-O7-C7	-3.48	109.46	117.80
34	V	202	HTG	C1-O5-C5	3.48	116.86	112.19
23	A	405[A]	CLA	C3C-C4C-NC	3.48	114.89	110.43
23	B	604	CLA	C3B-C4B-NB	3.48	113.64	110.53
23	C	510	CLA	CMC-C2C-C1C	3.48	130.48	125.03
23	B	614	CLA	O2D-CGD-O1D	-3.48	117.08	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407[A]	PHO	CMA-C3A-C4A	-3.48	107.11	114.61
26	A	410[B]	SQD	O9-S-C6	3.48	111.95	106.76
23	B	602	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
23	c	503	CLA	CMB-C2B-C1B	3.47	130.71	125.42
24	d	403[B]	PHO	C4-C3-C5	3.47	121.26	115.23
23	C	509	CLA	C4B-C3B-C2B	-3.47	102.99	107.30
26	A	410[A]	SQD	C44-O6-C1	-3.47	106.36	113.80
25	A	409	BCR	C24-C23-C22	-3.47	121.10	126.23
23	b	607	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
23	B	615	CLA	CMC-C2C-C1C	3.47	130.45	125.03
23	c	512	CLA	CMB-C2B-C1B	3.47	130.70	125.42
23	a	405[B]	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
23	b	604	CLA	CAC-C3C-C4C	3.47	129.30	124.79
23	C	503	CLA	C1D-CHD-C4C	-3.47	118.65	126.02
25	C	515	BCR	C15-C14-C13	-3.46	122.42	127.28
29	d	407[A]	PL9	C40-C39-C41	3.46	121.23	115.23
23	b	612	CLA	C4C-C3C-C2C	-3.46	101.86	106.89
23	C	513	CLA	CHD-C1D-ND	-3.45	119.94	124.80
23	B	614	CLA	C3B-C4B-NB	3.45	113.61	110.53
40	v	201	HEC	C4D-ND-C1D	3.45	111.44	105.82
23	b	609	CLA	C3B-C4B-NB	3.45	113.61	110.53
23	B	606	CLA	O2A-CGA-O1A	-3.44	115.02	123.63
23	B	613	CLA	C1D-CHD-C4C	-3.44	118.71	126.02
23	B	614	CLA	C3C-C4C-NC	3.44	114.84	110.43
23	B	607	CLA	CAA-C2A-C3A	-3.43	103.72	113.00
23	C	512	CLA	C3B-C4B-NB	3.43	113.59	110.53
23	C	508	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
23	A	406[A]	CLA	C3B-C4B-NB	3.43	113.59	110.53
23	C	507	CLA	O2D-CGD-O1D	-3.43	117.17	123.85
23	C	512	CLA	C1C-C2C-C3C	-3.43	103.37	106.98
26	l	101	SQD	C1-O5-C5	-3.43	107.03	113.72
29	A	414[A]	PL9	C15-C14-C16	3.43	121.18	115.23
23	b	610	CLA	CHD-C1D-ND	-3.43	119.98	124.80
32	L	101[B]	LHG	O7-C7-C8	3.43	118.89	111.48
23	B	609	CLA	C4B-C3B-C2B	-3.43	103.04	107.30
26	a	411	SQD	O48-C23-C24	3.42	122.27	111.83
23	C	509	CLA	O2D-CGD-O1D	-3.42	117.19	123.85
23	B	605	CLA	O2A-CGA-O1A	-3.42	115.08	123.63
23	C	508	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
23	c	503	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
25	d	406	BCR	C10-C11-C12	-3.41	113.31	123.20
23	b	601	CLA	C3C-C4C-NC	3.41	114.80	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	O2A-CGA-O1A	-3.41	115.10	123.63
23	b	611	CLA	C1D-CHD-C4C	-3.41	118.77	126.02
25	D	404	BCR	C29-C30-C25	3.41	115.39	110.44
25	b	619	BCR	C11-C10-C9	-3.41	122.50	127.28
23	d	405	CLA	C1D-CHD-C4C	-3.40	118.78	126.02
29	D	405[B]	PL9	C10-C9-C11	3.40	121.13	115.23
23	b	607	CLA	C4B-C3B-C2B	-3.40	103.07	107.30
23	A	405[B]	CLA	CMB-C2B-C1B	3.40	130.60	125.42
29	a	413[A]	PL9	C30-C29-C31	3.40	121.13	115.23
23	C	506	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
23	B	603	CLA	C4B-C3B-C2B	-3.40	103.08	107.30
23	a	405[A]	CLA	C1-C2-C3	-3.39	120.64	126.20
23	A	408	CLA	C3C-C4C-NC	3.39	114.78	110.43
23	B	612	CLA	CHD-C1D-ND	-3.39	120.03	124.80
23	A	405[B]	CLA	CMC-C2C-C1C	3.39	130.33	125.03
23	c	512	CLA	C3C-C4C-NC	3.39	114.77	110.43
23	b	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
23	C	508	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
23	B	607	CLA	C2B-C1B-NB	3.38	113.83	110.33
23	C	510	CLA	CAC-C3C-C4C	3.38	129.19	124.79
23	b	612	CLA	C2A-C1A-CHA	-3.38	118.00	123.87
23	A	405[A]	CLA	C4B-C3B-C2B	-3.38	103.10	107.30
23	B	614	CLA	O2A-CGA-CBA	3.37	122.12	111.83
29	D	405[B]	PL9	C25-C24-C26	3.37	121.08	115.23
23	B	601	CLA	C4C-C3C-C2C	-3.37	101.98	106.89
23	B	608	CLA	C1C-C2C-C3C	-3.37	103.44	106.98
35	c	517[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.48
23	a	404[A]	CLA	C4B-C3B-C2B	-3.37	103.11	107.30
25	B	618	BCR	C15-C14-C13	-3.37	122.56	127.28
33	z	101	LMG	O7-C10-C11	3.36	118.76	111.48
23	d	404[A]	CLA	C1D-CHD-C4C	-3.36	118.87	126.02
23	b	602	CLA	CMC-C2C-C1C	3.36	130.28	125.03
23	B	609	CLA	C1D-CHD-C4C	-3.36	118.88	126.02
23	b	604	CLA	C4B-C3B-C2B	-3.36	103.13	107.30
25	h	101	BCR	C38-C26-C25	-3.36	120.82	124.48
23	C	511	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
23	d	405	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
33	C	521	LMG	C3-C4-C5	3.36	116.32	110.23
29	D	405[A]	PL9	C53-C6-C1	3.35	122.15	115.28
23	B	607	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
32	d	415[B]	LHG	O8-C23-C24	3.35	122.05	111.83
25	c	514	BCR	C15-C14-C13	-3.35	122.58	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C3B-C4B-NB	3.35	113.52	110.53
23	B	614	CLA	CMC-C2C-C1C	3.34	130.26	125.03
23	b	616	CLA	C4C-C3C-C2C	-3.34	102.02	106.89
32	d	415[A]	LHG	O8-C23-O10	-3.34	115.27	123.63
23	b	606	CLA	CHD-C4C-NC	3.34	129.41	124.23
23	c	507	CLA	C1D-CHD-C4C	-3.34	118.92	126.02
35	C	517[B]	DGD	O2G-C1B-C2B	3.34	118.70	111.48
23	A	405[A]	CLA	C3B-C4B-NB	3.34	113.51	110.53
23	a	404[A]	CLA	C1-C2-C3	-3.34	120.73	126.20
23	a	407	CLA	CAA-C2A-C3A	-3.34	103.98	113.00
23	b	602	CLA	CAC-C3C-C4C	3.34	129.13	124.79
29	A	414[B]	PL9	C27-C28-C29	-3.34	119.99	127.62
29	a	413[A]	PL9	C17-C18-C19	-3.34	119.99	127.62
23	A	405[B]	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
23	D	403	CLA	C3B-C4B-NB	3.33	113.51	110.53
32	d	415[A]	LHG	O8-C23-C24	3.33	122.00	111.83
23	B	610	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
23	A	406[A]	CLA	C4B-C3B-C2B	-3.33	103.16	107.30
25	b	618	BCR	C29-C30-C25	3.33	115.28	110.44
29	a	413[A]	PL9	C35-C34-C36	3.33	121.01	115.23
23	b	609	CLA	CBC-CAC-C3C	-3.33	103.39	112.42
25	T	102	BCR	C11-C10-C9	-3.33	122.61	127.28
29	A	414[A]	PL9	C27-C28-C29	-3.33	120.01	127.62
23	c	506	CLA	C4B-C3B-C2B	-3.33	103.17	107.30
23	b	608	CLA	CBC-CAC-C3C	-3.33	103.41	112.42
23	b	601	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
29	a	413[B]	PL9	C37-C38-C39	-3.32	120.02	127.62
26	a	409[B]	SQD	C1-O5-C5	-3.32	107.23	113.72
23	c	511	CLA	CHD-C4C-NC	3.32	129.38	124.23
29	d	407[B]	PL9	C40-C39-C41	3.32	120.99	115.23
23	C	505	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
25	Y	101	BCR	C15-C14-C13	-3.32	122.63	127.28
23	c	512	CLA	C4-C3-C5	3.32	120.98	115.23
23	c	509	CLA	CHC-C1C-C2C	-3.32	117.53	126.95
23	b	608	CLA	CHD-C4C-NC	3.31	129.37	124.23
23	c	502	CLA	CHC-C1C-C2C	-3.31	117.53	126.95
23	b	613	CLA	O2D-CGD-CBD	3.31	117.02	111.23
23	C	505	CLA	C4B-C3B-C2B	-3.31	103.19	107.30
23	B	612	CLA	CMC-C2C-C1C	3.31	130.21	125.03
29	D	405[A]	PL9	C25-C24-C26	3.31	120.97	115.23
23	B	601	CLA	O2D-CGD-O1D	-3.31	117.41	123.85
23	A	405[B]	CLA	C3C-C4C-NC	3.30	114.66	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
23	B	603	CLA	C4C-C3C-C2C	-3.30	102.08	106.89
23	b	607	CLA	C2B-C1B-NB	3.30	113.75	110.33
23	B	609	CLA	CBC-CAC-C3C	-3.30	103.47	112.42
23	C	504	CLA	O2A-CGA-O1A	-3.30	115.38	123.63
23	C	507	CLA	CAC-C3C-C4C	3.30	129.08	124.79
24	A	416[B]	PHO	C1A-C2A-C3A	-3.30	99.70	102.84
38	f	101	HEM	CHD-C4C-NC	3.30	128.04	124.45
23	C	504	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
26	l	101	SQD	O48-C23-C24	3.30	121.88	111.83
29	D	405[A]	PL9	C17-C18-C19	-3.30	120.08	127.62
23	b	608	CLA	C4B-C3B-C2B	-3.29	103.20	107.30
38	E	102	HEM	CHB-C1B-NB	3.29	128.44	124.37
23	c	507	CLA	C4-C3-C5	3.29	120.94	115.23
23	A	404[A]	CLA	C1-C2-C3	-3.29	120.81	126.20
23	c	503	CLA	C1-C2-C3	-3.29	120.81	126.20
32	d	409[A]	LHG	O7-C7-C8	3.29	118.59	111.48
23	c	501	CLA	C3C-C4C-NC	3.29	114.64	110.43
23	A	405[B]	CLA	C3B-C4B-NB	3.29	113.46	110.53
23	c	512	CLA	O2A-CGA-CBA	3.28	121.85	111.83
33	c	520	LMG	C9-C8-C7	-3.28	104.13	111.78
23	c	508	CLA	C4C-C3C-C2C	-3.28	102.11	106.89
25	d	406	BCR	C16-C17-C18	-3.28	122.68	127.28
23	C	512	CLA	C4C-C3C-C2C	-3.28	102.11	106.89
23	b	608	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
23	B	602	CLA	C3B-C4B-NB	3.28	113.46	110.53
23	B	607	CLA	CBC-CAC-C3C	-3.28	103.53	112.42
23	C	507	CLA	CHC-C1C-C2C	-3.28	117.64	126.95
29	d	407[B]	PL9	C42-C43-C44	-3.27	120.13	127.62
23	B	609	CLA	CMC-C2C-C1C	3.27	130.15	125.03
32	A	419[B]	LHG	O8-C23-O10	-3.27	115.44	123.63
23	B	608	CLA	CAC-C3C-C4C	3.27	129.05	124.79
23	d	404[A]	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
23	a	404[B]	CLA	C1-C2-C3	-3.27	120.84	126.20
23	c	509	CLA	CHD-C1D-ND	-3.27	120.20	124.80
23	c	505	CLA	CAC-C3C-C4C	3.27	129.04	124.79
23	B	611	CLA	CAC-C3C-C4C	3.26	129.04	124.79
32	A	419[A]	LHG	O8-C23-C24	3.26	121.79	111.83
23	c	512	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
38	f	101	HEM	CHD-C1D-ND	3.26	127.93	124.42
29	A	414[B]	PL9	C15-C14-C16	3.26	120.89	115.23
23	c	505	CLA	C1D-CHD-C4C	-3.26	119.09	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	C4-C3-C5	3.26	120.89	115.23
25	c	514	BCR	C16-C17-C18	-3.26	122.71	127.28
23	B	607	CLA	C4B-C3B-C2B	-3.26	103.25	107.30
23	A	408	CLA	C1D-CHD-C4C	-3.25	119.10	126.02
23	B	610	CLA	CAA-CBA-CGA	-3.25	103.97	113.21
23	b	609	CLA	CMC-C2C-C1C	3.25	130.12	125.03
23	A	404[B]	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
23	B	610	CLA	C3B-C4B-NB	3.25	113.43	110.53
31	B	627	LMT	O1'-C1'-C2'	3.25	113.21	108.27
23	C	514	CLA	C1-C2-C3	-3.25	120.87	126.20
23	C	502	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
25	B	619	BCR	C24-C23-C22	-3.25	121.43	126.23
23	B	614	CLA	O2A-CGA-O1A	-3.25	115.50	123.63
34	b	622	HTG	O2-C2-C1	3.25	116.07	110.30
23	A	404[B]	CLA	CHC-C1C-C2C	-3.25	117.72	126.95
23	B	614	CLA	CHD-C4C-NC	3.25	129.26	124.23
38	E	102	HEM	CBD-CAD-C3D	-3.25	103.56	112.53
23	B	613	CLA	C4-C3-C5	3.24	120.86	115.23
32	d	415[A]	LHG	O7-C7-C8	3.24	118.50	111.48
23	d	402[B]	CLA	C4B-C3B-C2B	-3.24	103.27	107.30
23	b	602	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
32	A	419[A]	LHG	C5-O7-C7	-3.24	110.03	117.80
23	b	611	CLA	O2D-CGD-O1D	-3.24	117.54	123.85
23	B	615	CLA	O2D-CGD-CBD	3.24	116.89	111.23
25	D	404	BCR	C16-C17-C18	-3.24	122.74	127.28
33	a	415	LMG	C7-O1-C1	-3.24	106.85	113.80
23	b	609	CLA	C4B-C3B-C2B	-3.24	103.28	107.30
26	A	410[B]	SQD	O47-C7-C8	3.24	118.48	111.48
24	A	407[A]	PHO	O1D-CGD-CBD	-3.24	119.81	124.72
23	C	505	CLA	C1D-CHD-C4C	-3.24	119.14	126.02
23	d	402[A]	CLA	C3B-C4B-NB	3.24	113.42	110.53
23	c	509	CLA	CAC-C3C-C4C	3.23	129.00	124.79
23	B	613	CLA	C4B-C3B-C2B	-3.23	103.28	107.30
23	c	508	CLA	CHD-C1D-ND	-3.23	120.25	124.80
23	C	502	CLA	CBC-CAC-C3C	-3.23	103.65	112.42
23	a	404[B]	CLA	C4-C3-C5	3.23	120.84	115.23
23	B	604	CLA	CMB-C2B-C1B	3.23	130.34	125.42
23	b	614	CLA	O2A-CGA-O1A	-3.23	115.55	123.63
25	D	404	BCR	C28-C27-C26	-3.23	108.30	114.06
23	B	611	CLA	CHB-C4A-NA	3.23	129.06	124.40
23	B	603	CLA	CMC-C2C-C1C	3.23	130.08	125.03
23	B	615	CLA	CHD-C4C-NC	3.23	129.24	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[B]	CLA	CHC-C1C-C2C	-3.23	117.78	126.95
23	c	501	CLA	C3B-C4B-NB	3.23	113.41	110.53
29	a	413[B]	PL9	C30-C29-C31	3.23	120.83	115.23
23	a	407	CLA	CHD-C4C-NC	3.23	129.23	124.23
34	b	625	HTG	O5-C5-C4	3.22	115.51	109.70
23	b	609	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
23	c	511	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
23	D	402[B]	CLA	C1D-CHD-C4C	-3.22	119.17	126.02
23	b	603	CLA	C2A-C1A-CHA	-3.22	118.27	123.87
24	d	403[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
25	T	102	BCR	C2-C1-C6	3.22	115.12	110.44
23	C	506	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
29	A	414[B]	PL9	C17-C18-C19	-3.22	120.26	127.62
26	a	409[B]	SQD	C44-O6-C1	-3.22	106.90	113.80
23	a	405[B]	CLA	C1-C2-C3	-3.22	120.93	126.20
23	b	609	CLA	C4C-C3C-C2C	-3.21	102.21	106.89
33	C	521	LMG	O8-C28-C29	3.21	121.63	111.83
23	B	601	CLA	C1C-C2C-C3C	-3.21	103.60	106.98
23	c	510	CLA	C4-C3-C5	3.21	120.81	115.23
23	A	404[A]	CLA	O2A-CGA-O1A	-3.21	115.59	123.63
23	b	609	CLA	CMB-C2B-C1B	3.21	130.31	125.42
23	B	605	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
23	c	509	CLA	C1-O2A-CGA	3.21	124.42	116.65
23	d	402[B]	CLA	CHD-C4C-NC	3.21	129.21	124.23
23	C	514	CLA	CBC-CAC-C3C	-3.21	103.73	112.42
23	B	611	CLA	C2A-C1A-CHA	-3.20	118.31	123.87
23	b	608	CLA	CAC-C3C-C4C	3.20	128.96	124.79
23	B	610	CLA	O2A-CGA-O1A	-3.20	115.61	123.63
23	c	509	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
23	b	616	CLA	C3B-C4B-NB	3.20	113.39	110.53
23	b	604	CLA	CMB-C2B-C1B	3.20	130.29	125.42
23	D	402[A]	CLA	C1D-CHD-C4C	-3.20	119.22	126.02
23	A	406[A]	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
23	a	404[A]	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
23	C	509	CLA	CHD-C1D-ND	-3.20	120.30	124.80
23	b	613	CLA	CHD-C1D-ND	-3.20	120.30	124.80
23	C	511	CLA	CHC-C1C-C2C	-3.20	117.86	126.95
23	C	509	CLA	CHC-C1C-C2C	-3.19	117.88	126.95
23	c	511	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
24	a	406[B]	PHO	O2A-CGA-CBA	3.19	121.57	111.83
23	b	614	CLA	CMB-C2B-C1B	3.19	130.27	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
23	C	505	CLA	C1-O2A-CGA	3.19	124.36	116.65
23	C	511	CLA	C4-C3-C5	3.19	120.76	115.23
23	b	607	CLA	C4A-NA-C1A	-3.18	105.23	106.68
23	d	402[A]	CLA	CHD-C4C-NC	3.18	129.17	124.23
23	D	402[B]	CLA	CAC-C3C-C4C	3.18	128.93	124.79
23	B	613	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
23	b	610	CLA	C1C-C2C-C3C	-3.18	103.63	106.98
31	b	627	LMT	C3'-C4'-C5'	-3.18	103.88	110.93
23	c	504	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
23	A	405[B]	CLA	CHD-C4C-NC	3.18	129.16	124.23
23	B	606	CLA	CMC-C2C-C1C	3.18	130.00	125.03
23	B	604	CLA	O2A-CGA-O1A	-3.18	115.68	123.63
31	C	525	LMT	O5B-C5B-C4B	3.18	115.43	109.70
23	B	606	CLA	O2A-CGA-CBA	3.18	121.52	111.83
23	c	502	CLA	CHD-C1D-ND	-3.18	120.33	124.80
23	B	611	CLA	C4C-C3C-C2C	-3.17	102.27	106.89
23	a	407	CLA	C3B-C4B-NB	3.17	113.36	110.53
23	b	612	CLA	O2A-CGA-O1A	-3.17	115.69	123.63
23	b	605	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	b	603	CLA	C4-C3-C5	3.17	120.73	115.23
23	b	616	CLA	CBC-CAC-C3C	-3.17	103.83	112.42
23	B	613	CLA	CHD-C1D-ND	-3.17	120.35	124.80
23	b	615	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
23	B	613	CLA	O2A-CGA-CBA	3.16	121.48	111.83
23	D	402[A]	CLA	O2A-CGA-CBA	3.16	121.48	111.83
29	a	413[B]	PL9	C22-C23-C24	-3.16	120.38	127.62
29	d	407[A]	PL9	C37-C38-C39	-3.16	120.38	127.62
34	b	622	HTG	C1'-S1-C1	3.16	107.28	100.45
23	a	405[A]	CLA	CHD-C4C-NC	3.16	129.13	124.23
23	a	404[B]	CLA	CAA-C2A-C1A	-3.16	101.62	111.97
23	B	610	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
23	b	614	CLA	CHD-C4C-NC	3.16	129.13	124.23
23	b	601	CLA	C1C-C2C-C3C	-3.16	103.66	106.98
23	D	403	CLA	CAC-C3C-C4C	3.16	128.90	124.79
23	b	611	CLA	C4C-C3C-C2C	-3.15	102.30	106.89
23	b	610	CLA	O2A-CGA-O1A	-3.15	115.74	123.63
23	a	405[A]	CLA	C3B-C4B-NB	3.15	113.34	110.53
29	a	413[A]	PL9	C42-C43-C44	-3.15	120.41	127.62
23	b	608	CLA	C3C-C4C-NC	3.15	114.47	110.43
23	A	408	CLA	CBC-CAC-C3C	-3.15	103.87	112.42
23	B	616	CLA	CAC-C3C-C4C	3.15	128.89	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	C4B-C3B-C2B	-3.15	103.39	107.30
29	a	413[B]	PL9	C17-C18-C19	-3.15	120.42	127.62
23	d	404[A]	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
23	c	503	CLA	CHD-C4C-NC	3.14	129.11	124.23
23	b	612	CLA	CHD-C1D-ND	-3.14	120.38	124.80
23	C	513	CLA	C1C-C2C-C3C	-3.14	103.67	106.98
26	X	101	SQD	C1-C2-C3	-3.14	103.40	110.01
23	A	406[A]	CLA	O2A-CGA-CBA	3.14	121.42	111.83
29	d	407[B]	PL9	C37-C38-C39	-3.14	120.44	127.62
26	A	412	SQD	O48-C23-C24	3.14	121.41	111.83
23	B	608	CLA	CMA-C3A-C4A	-3.14	103.34	111.77
23	c	509	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
23	B	603	CLA	C4-C3-C5	3.13	120.67	115.23
23	d	402[B]	CLA	CMB-C2B-C1B	3.13	130.19	125.42
23	a	404[B]	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	B	612	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
25	D	404	BCR	C37-C22-C23	3.13	122.87	118.09
23	A	404[A]	CLA	C4B-C3B-C2B	-3.13	103.41	107.30
23	D	402[B]	CLA	O2A-CGA-CBA	3.13	121.38	111.83
23	b	611	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
23	B	615	CLA	C3B-C4B-NB	3.13	113.32	110.53
25	h	101	BCR	C7-C8-C9	-3.13	121.61	126.23
23	A	406[B]	CLA	O2A-CGA-O1A	-3.12	115.82	123.63
23	c	506	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
23	A	405[A]	CLA	CMB-C2B-C1B	3.12	130.17	125.42
23	b	613	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
29	D	405[B]	PL9	C17-C18-C19	-3.12	120.49	127.62
23	b	601	CLA	C1-O2A-CGA	3.12	124.19	116.65
23	C	503	CLA	C3B-C4B-NB	3.12	113.31	110.53
23	b	607	CLA	CAC-C3C-C4C	3.12	128.84	124.79
23	b	607	CLA	CBC-CAC-C3C	-3.11	103.98	112.42
24	a	406[A]	PHO	O1D-CGD-CBD	-3.11	120.01	124.72
33	C	520	LMG	O8-C28-C29	3.11	121.31	111.83
26	f	102	SQD	O5-C1-C2	3.11	116.76	110.37
23	c	501	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
25	b	619	BCR	C38-C26-C25	-3.10	121.10	124.48
23	B	614	CLA	CAC-C3C-C4C	3.10	128.82	124.79
23	b	614	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
23	b	613	CLA	O2A-CGA-O1A	-3.10	115.88	123.63
29	a	413[A]	PL9	C25-C24-C26	3.10	120.61	115.23
23	b	615	CLA	CHC-C1C-C2C	-3.10	118.15	126.95
32	D	407[A]	LHG	O8-C23-C24	3.09	121.27	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	C3B-C4B-NB	3.09	113.29	110.53
32	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.48
23	a	405[B]	CLA	CHD-C4C-NC	3.09	129.02	124.23
26	a	409[B]	SQD	C45-O47-C7	-3.09	110.41	117.80
23	C	502	CLA	CHD-C4C-NC	3.09	129.02	124.23
23	B	607	CLA	C4-C3-C5	3.09	120.58	115.23
23	A	408	CLA	O2A-CGA-CBA	3.09	121.24	111.83
26	a	409[A]	SQD	C45-O47-C7	-3.08	110.42	117.80
23	c	509	CLA	O2A-CGA-CBA	3.08	121.23	111.83
23	B	601	CLA	CAC-C3C-C4C	3.08	128.80	124.79
32	E	101[A]	LHG	O8-C23-C24	3.08	121.23	111.83
24	A	416[A]	PHO	C4-C3-C5	3.08	120.58	115.23
23	C	511	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
23	d	402[B]	CLA	CHC-C1C-C2C	-3.08	118.19	126.95
23	b	615	CLA	C4-C3-C5	3.08	120.58	115.23
23	A	404[B]	CLA	O2A-CGA-CBA	3.08	121.22	111.83
33	m	101	LMG	O8-C28-C29	3.08	121.21	111.83
23	d	404[A]	CLA	C2A-C1A-CHA	-3.07	118.53	123.87
23	a	407	CLA	C4-C3-C5	3.07	120.56	115.23
23	d	404[B]	CLA	C4-C3-C5	3.07	120.56	115.23
23	b	612	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
23	C	511	CLA	O2A-CGA-CBA	3.07	121.20	111.83
29	d	407[B]	PL9	C7-C8-C9	-3.07	121.54	126.83
23	d	404[A]	CLA	O2A-CGA-O1A	-3.07	115.94	123.63
29	A	414[A]	PL9	C17-C18-C19	-3.07	120.59	127.62
23	c	501	CLA	CAC-C3C-C4C	3.07	128.78	124.79
23	c	502	CLA	CHD-C4C-NC	3.07	128.99	124.23
29	d	407[A]	PL9	C22-C23-C24	-3.07	120.60	127.62
23	b	602	CLA	C1-C2-C3	-3.07	121.17	126.20
23	A	404[B]	CLA	C3C-C4C-NC	3.07	114.36	110.43
32	a	419[B]	LHG	O7-C7-C8	3.07	118.11	111.48
35	h	102	DGD	O1G-C1A-C2A	3.06	121.17	111.83
23	d	402[A]	CLA	CMA-C3A-C2A	-3.06	102.14	113.98
38	f	101	HEM	C1B-NB-C4B	3.06	108.83	105.21
29	d	407[A]	PL9	C27-C28-C29	-3.06	120.61	127.62
23	B	602	CLA	CHD-C4C-NC	3.06	128.98	124.23
23	c	503	CLA	C3B-C4B-NB	3.06	113.26	110.53
23	B	603	CLA	CHC-C1C-C2C	-3.06	118.25	126.95
23	b	601	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
33	z	101	LMG	O8-C28-C29	3.06	121.16	111.83
23	b	610	CLA	CMB-C2B-C1B	3.06	130.07	125.42
29	a	413[B]	PL9	C25-C24-C26	3.06	120.53	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	CAC-C3C-C4C	3.06	128.77	124.79
23	C	510	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
23	A	405[B]	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
32	d	408[B]	LHG	O7-C7-C8	3.05	118.08	111.48
23	C	503	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
29	a	413[A]	PL9	C22-C23-C24	-3.05	120.64	127.62
23	b	613	CLA	O2A-CGA-CBA	3.05	121.13	111.83
23	B	616	CLA	CHD-C1D-ND	-3.05	120.51	124.80
23	c	513	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
23	C	503	CLA	CMB-C2B-C1B	3.05	130.06	125.42
23	C	513	CLA	O2A-CGA-CBA	3.05	121.12	111.83
35	C	519	DGD	O1G-C1A-C2A	3.05	121.12	111.83
23	B	609	CLA	C1-C2-C3	-3.05	121.21	126.20
24	A	416[B]	PHO	C4-C3-C5	3.04	120.51	115.23
23	d	404[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
23	A	406[A]	CLA	CAA-C2A-C3A	-3.04	104.78	113.00
23	D	402[A]	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
23	d	402[B]	CLA	CBC-CAC-C3C	-3.04	104.19	112.42
29	A	414[B]	PL9	C20-C19-C21	3.04	120.50	115.23
23	C	506	CLA	C3B-C4B-NB	3.04	113.24	110.53
29	D	405[A]	PL9	C10-C9-C11	3.03	120.50	115.23
23	C	504	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	B	611	CLA	C1-C2-C3	-3.03	121.23	126.20
25	b	619	BCR	C39-C30-C25	-3.03	105.49	110.24
23	D	402[B]	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
23	A	405[A]	CLA	CHD-C4C-NC	3.03	128.93	124.23
23	A	406[B]	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
23	B	611	CLA	C4B-C3B-C2B	3.03	111.07	107.30
29	A	414[A]	PL9	C10-C9-C11	3.03	120.48	115.23
23	C	507	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
23	C	511	CLA	C3C-C4C-NC	3.02	114.30	110.43
25	y	101	BCR	C10-C11-C12	-3.02	114.45	123.20
23	d	404[B]	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
35	c	518	DGD	O2G-C1B-C2B	3.02	118.01	111.48
23	B	612	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
23	B	616	CLA	C1-O2A-CGA	3.02	123.96	116.65
26	A	410[A]	SQD	O48-C23-C24	3.02	121.04	111.83
23	b	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
23	b	607	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
23	b	605	CLA	CMB-C2B-C1B	3.02	130.01	125.42
23	D	402[A]	CLA	CAC-C3C-C4C	3.02	128.71	124.79
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402[B]	CLA	CMC-C2C-C1C	3.01	129.74	125.03
26	a	409[A]	SQD	O9-S-C6	3.01	111.25	106.76
25	k	101	BCR	C24-C23-C22	-3.01	121.78	126.23
29	a	413[A]	PL9	C10-C9-C11	3.01	120.45	115.23
33	c	519	LMG	O1-C7-C8	-3.01	103.50	110.82
33	a	415	LMG	C8-O7-C10	-3.01	110.59	117.80
32	d	408[A]	LHG	O7-C7-C8	3.01	117.99	111.48
26	A	410[B]	SQD	O48-C23-C24	3.01	121.01	111.83
25	B	619	BCR	C38-C26-C25	-3.01	121.20	124.48
23	d	402[A]	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
23	c	513	CLA	CAA-C2A-C3A	-3.01	104.88	113.00
23	B	613	CLA	CMC-C2C-C1C	3.01	129.73	125.03
23	C	513	CLA	CHD-C4C-NC	3.00	128.89	124.23
26	b	620	SQD	C3-C4-C5	3.00	115.68	110.23
23	B	609	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
33	c	519	LMG	O8-C28-C29	3.00	120.99	111.83
31	B	628	LMT	O1'-C1'-C2'	3.00	112.83	108.27
23	C	506	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
23	b	601	CLA	CHD-C4C-NC	3.00	128.88	124.23
23	c	513	CLA	CAC-C3C-C4C	3.00	128.69	124.79
23	b	601	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
23	b	611	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
25	C	516	BCR	C11-C10-C9	-3.00	123.07	127.28
23	a	405[B]	CLA	CMC-C2C-C1C	3.00	129.72	125.03
23	A	404[A]	CLA	CHC-C1C-C2C	-3.00	118.43	126.95
29	D	405[A]	PL9	C51-C49-C50	3.00	121.49	114.59
29	a	413[A]	PL9	C37-C38-C39	-3.00	120.77	127.62
29	A	414[B]	PL9	C10-C9-C11	2.99	120.43	115.23
38	f	101	HEM	CHB-C1B-NB	2.99	128.07	124.37
34	b	622	HTG	O5-C5-C4	2.99	115.09	109.70
25	Y	101	BCR	C38-C26-C25	-2.99	121.22	124.48
23	c	510	CLA	O2A-CGA-CBA	2.99	120.96	111.83
23	B	606	CLA	CHD-C4C-NC	2.99	128.87	124.23
25	C	516	BCR	C33-C5-C6	-2.99	121.22	124.48
29	d	407[B]	PL9	C10-C9-C11	2.99	120.41	115.23
23	B	604	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
23	a	405[B]	CLA	C3B-C4B-NB	2.99	113.20	110.53
23	C	510	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
29	d	407[A]	PL9	C10-C9-C11	2.98	120.41	115.23
23	a	407	CLA	O2A-CGA-CBA	2.98	120.94	111.83
23	b	602	CLA	C1C-C2C-C3C	-2.98	103.84	106.98
23	d	404[B]	CLA	O2A-CGA-O1A	-2.98	116.17	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[A]	CLA	C4-C3-C5	2.98	120.41	115.23
23	a	407	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
25	y	101	BCR	C38-C26-C25	-2.98	121.23	124.48
23	B	604	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
24	a	406[A]	PHO	O2A-CGA-CBA	2.98	120.92	111.83
23	c	511	CLA	C4B-C3B-C2B	-2.98	103.60	107.30
29	a	413[B]	PL9	C42-C43-C44	-2.98	120.81	127.62
23	b	607	CLA	C4C-C3C-C2C	-2.98	102.56	106.89
23	a	405[A]	CLA	CMC-C2C-C1C	2.98	129.68	125.03
23	c	513	CLA	O2A-CGA-CBA	2.98	120.91	111.83
23	B	601	CLA	CHD-C4C-NC	2.97	128.84	124.23
32	D	406[A]	LHG	O8-C23-O10	-2.97	116.19	123.63
23	d	404[B]	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
32	d	415[B]	LHG	O8-C23-O10	-2.97	116.19	123.63
24	A	407[B]	PHO	O1D-CGD-CBD	-2.97	120.22	124.72
23	a	407	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
29	a	413[B]	PL9	C35-C34-C36	2.97	120.38	115.23
23	b	610	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
29	A	414[A]	PL9	C20-C19-C21	2.97	120.38	115.23
23	B	605	CLA	CMC-C2C-C1C	2.97	129.67	125.03
23	d	402[A]	CLA	CBC-CAC-C3C	-2.97	104.38	112.42
23	c	503	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	B	605	CLA	C1-C2-C3	-2.96	121.34	126.20
23	A	406[A]	CLA	CHD-C4C-NC	2.96	128.83	124.23
23	c	512	CLA	CHD-C4C-NC	2.96	128.82	124.23
23	d	402[A]	CLA	CHC-C1C-C2C	-2.96	118.53	126.95
23	B	616	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
23	B	605	CLA	CBC-CAC-C3C	-2.96	104.39	112.42
23	B	612	CLA	C11-C12-C13	-2.96	106.13	115.97
23	c	513	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
23	b	614	CLA	C4C-C3C-C2C	-2.96	102.59	106.89
23	C	511	CLA	CHD-C4C-NC	2.96	128.81	124.23
23	B	609	CLA	C3B-C4B-NB	2.96	113.17	110.53
32	b	629[A]	LHG	O8-C23-C24	2.96	120.84	111.83
23	d	404[A]	CLA	C4-C3-C5	2.95	120.36	115.23
23	c	508	CLA	CMB-C2B-C1B	2.95	129.92	125.42
23	C	511	CLA	O2A-CGA-O1A	-2.95	116.24	123.63
23	C	503	CLA	C2A-C1A-CHA	-2.95	118.74	123.87
23	A	406[B]	CLA	CHC-C1C-C2C	-2.95	118.55	126.95
23	b	609	CLA	CHD-C4C-NC	2.95	128.81	124.23
32	E	101[B]	LHG	O8-C23-C24	2.95	120.84	111.83
23	C	505	CLA	CHC-C1C-C2C	-2.95	118.56	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	C4C-C3C-C2C	-2.95	102.59	106.89
23	C	502	CLA	CAC-C3C-C4C	2.95	128.63	124.79
23	b	613	CLA	C4B-C3B-C2B	-2.95	103.63	107.30
32	D	406[B]	LHG	O7-C7-C8	2.95	117.86	111.48
23	D	403	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
25	k	101	BCR	C39-C30-C25	-2.95	105.62	110.24
34	B	624	HTG	C1'-S1-C1	2.95	106.82	100.45
32	D	407[A]	LHG	O8-C23-O10	-2.95	116.25	123.63
23	A	406[B]	CLA	CHD-C4C-NC	2.95	128.80	124.23
23	B	607	CLA	CMB-C2B-C1B	2.95	129.91	125.42
23	C	504	CLA	C4-C3-C5	2.95	120.34	115.23
23	B	604	CLA	CHD-C1D-ND	-2.95	120.66	124.80
23	C	510	CLA	O2A-CGA-CBA	2.95	120.82	111.83
23	A	406[B]	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
23	c	504	CLA	CHD-C4C-NC	2.95	128.80	124.23
23	B	604	CLA	CHC-C1C-C2C	-2.94	118.58	126.95
23	D	403	CLA	CHC-C1C-C2C	-2.94	118.58	126.95
23	c	513	CLA	C1-C2-C3	-2.94	121.38	126.20
23	a	405[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
23	a	405[B]	CLA	CMB-C2B-C1B	2.94	129.89	125.42
23	B	616	CLA	CMC-C2C-C1C	2.94	129.62	125.03
32	D	407[B]	LHG	O7-C7-C8	2.94	117.83	111.48
32	a	419[A]	LHG	O7-C7-C8	2.93	117.83	111.48
23	c	502	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
23	c	508	CLA	CAA-C2A-C3A	-2.93	105.07	113.00
23	c	504	CLA	CBC-CAC-C3C	-2.93	104.47	112.42
23	C	507	CLA	O2A-CGA-CBA	2.93	120.78	111.83
23	B	608	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
23	B	616	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
23	C	505	CLA	CBC-CAC-C3C	-2.93	104.48	112.42
35	h	102	DGD	O2G-C1B-C2B	2.93	117.81	111.48
23	c	512	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
24	A	416[B]	PHO	C4D-CHA-CBD	2.92	109.86	108.45
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.63	106.89
23	C	514	CLA	CHD-C4C-NC	2.92	128.76	124.23
23	a	404[A]	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
23	c	508	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
23	C	512	CLA	C4-C3-C5	2.92	120.30	115.23
23	c	502	CLA	CMB-C2B-C1B	2.92	129.87	125.42
23	c	512	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
23	A	404[B]	CLA	C1-C2-C3	-2.92	121.41	126.20
33	D	411	LMG	O7-C10-C11	2.92	117.80	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	C1-C2-C3	-2.92	121.42	126.20
23	b	604	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
23	B	606	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
38	f	101	HEM	CAD-CBD-CGD	2.91	121.39	113.67
23	A	408	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
23	D	402[A]	CLA	O2A-CGA-O1A	-2.91	116.35	123.63
23	B	612	CLA	O2A-CGA-CBA	2.91	120.71	111.83
23	B	616	CLA	CHD-C4C-NC	2.91	128.74	124.23
23	A	406[B]	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
23	C	512	CLA	CHD-C4C-NC	2.91	128.74	124.23
25	d	406	BCR	C21-C20-C19	-2.91	114.78	123.20
23	a	407	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
26	f	102	SQD	C4-C3-C2	-2.90	105.73	110.83
23	c	508	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
23	c	507	CLA	CHD-C4C-NC	2.90	128.73	124.23
23	b	606	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
23	c	505	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
23	b	615	CLA	C11-C10-C8	-2.90	106.32	115.97
23	a	405[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	c	508	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
23	c	506	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
23	A	405[B]	CLA	C4-C3-C5	2.90	120.26	115.23
23	c	503	CLA	CMC-C2C-C1C	2.90	129.56	125.03
32	b	629[B]	LHG	O8-C23-C24	2.90	120.67	111.83
23	b	614	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
25	t	102	BCR	C15-C16-C17	-2.89	117.60	123.52
23	c	506	CLA	O2D-CGD-O1D	-2.89	118.21	123.85
23	A	404[B]	CLA	C2A-C1A-CHA	-2.89	118.84	123.87
23	A	405[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
24	d	403[B]	PHO	CMB-C2B-C3B	2.89	130.47	124.68
23	D	402[A]	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
23	B	606	CLA	CMB-C2B-C1B	2.89	129.82	125.42
23	C	503	CLA	CHC-C1C-C2C	-2.89	118.73	126.95
23	c	504	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
23	B	615	CLA	C4-C3-C5	2.89	120.25	115.23
23	C	510	CLA	C4C-C3C-C2C	-2.89	102.68	106.89
23	c	502	CLA	CBC-CAC-C3C	-2.89	104.59	112.42
34	B	621	HTG	C1-O5-C5	2.89	117.74	112.56
23	D	403	CLA	C4-C3-C5	2.89	120.24	115.23
23	b	601	CLA	C4-C3-C5	2.89	120.24	115.23
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
23	b	614	CLA	CBC-CAC-C3C	-2.89	104.59	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[A]	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
24	d	403[A]	PHO	CMB-C2B-C3B	2.88	130.44	124.68
23	b	607	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
23	c	510	CLA	CHD-C4C-NC	2.88	128.69	124.23
23	d	404[B]	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
26	a	409[A]	SQD	O47-C7-O49	-2.88	116.98	123.70
23	A	408	CLA	CHD-C4C-NC	2.88	128.69	124.23
29	A	414[A]	PL9	C30-C29-C31	2.88	120.22	115.23
23	B	608	CLA	CHC-C1C-C2C	-2.87	118.78	126.95
23	b	607	CLA	O2A-CGA-O1A	-2.87	116.44	123.63
23	c	507	CLA	O2A-CGA-CBA	2.87	120.59	111.83
23	d	405	CLA	CHD-C4C-NC	2.87	128.68	124.23
23	C	502	CLA	C3B-C4B-NB	2.87	113.09	110.53
23	b	614	CLA	CAC-C3C-C4C	2.87	128.52	124.79
23	a	404[B]	CLA	O2A-CGA-CBA	2.87	120.57	111.83
35	H	102	DGD	O1G-C1A-C2A	2.87	120.57	111.83
29	d	407[B]	PL9	C27-C28-C29	-2.86	121.07	127.62
23	a	405[A]	CLA	CMB-C2B-C1B	2.86	129.78	125.42
23	C	507	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
25	t	102	BCR	C21-C20-C19	-2.86	114.91	123.20
23	b	616	CLA	C4B-C3B-C2B	-2.86	103.75	107.30
24	a	406[A]	PHO	CMA-C3A-C4A	-2.86	108.45	114.61
23	D	402[B]	CLA	C4-C3-C5	2.86	120.19	115.23
23	C	513	CLA	CMA-C3A-C4A	-2.86	104.09	111.77
26	l	101	SQD	O7-S-C6	2.86	111.02	106.76
23	d	405	CLA	C4-C3-C5	2.86	120.19	115.23
23	A	408	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
23	D	403	CLA	C4B-C3B-C2B	-2.85	103.75	107.30
23	b	602	CLA	C11-C12-C13	-2.85	106.48	115.97
23	C	506	CLA	CMC-C2C-C1C	2.85	129.49	125.03
26	l	101	SQD	O48-C23-O10	-2.85	116.49	123.63
23	C	510	CLA	CHD-C4C-NC	2.85	128.66	124.23
23	C	514	CLA	CMC-C2C-C1C	2.85	129.49	125.03
29	A	414[B]	PL9	C30-C29-C31	2.85	120.18	115.23
23	d	404[B]	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
23	a	404[B]	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	a	406[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	B	609	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
23	C	508	CLA	C1-C2-C3	-2.85	121.53	126.20
25	D	404	BCR	C40-C30-C25	-2.85	105.78	110.24
23	b	610	CLA	C4-C3-C5	2.85	120.17	115.23
23	C	511	CLA	CAC-C3C-C4C	2.85	128.49	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	CHC-C1C-C2C	-2.84	118.87	126.95
23	A	404[A]	CLA	CAA-CBA-CGA	-2.84	105.14	113.21
32	A	419[B]	LHG	O8-C23-C24	2.84	120.50	111.83
23	b	610	CLA	CHD-C4C-NC	2.84	128.64	124.23
23	A	405[A]	CLA	C4-C3-C5	2.84	120.16	115.23
25	b	618	BCR	C37-C22-C21	-2.84	118.22	122.82
23	D	402[A]	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
23	B	605	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
29	a	413[B]	PL9	C10-C9-C11	2.84	120.15	115.23
29	A	414[B]	PL9	C40-C39-C41	2.84	120.15	115.23
23	c	506	CLA	CHD-C4C-NC	2.84	128.63	124.23
23	B	607	CLA	O2A-CGA-O1A	-2.84	116.53	123.63
23	b	614	CLA	O2A-CGA-CBA	2.84	120.48	111.83
23	B	610	CLA	CHD-C4C-NC	2.83	128.62	124.23
23	C	502	CLA	C1-O2A-CGA	2.83	123.51	116.65
23	b	606	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
23	C	503	CLA	O2A-CGA-O1A	-2.83	116.54	123.63
23	C	505	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
25	h	101	BCR	C24-C23-C22	-2.83	122.05	126.23
32	d	409[A]	LHG	O8-C23-C24	2.83	120.46	111.83
35	c	516[B]	DGD	C3G-C2G-C1G	-2.83	105.19	111.78
23	C	514	CLA	O2A-CGA-CBA	2.83	120.46	111.83
23	b	603	CLA	CMA-C3A-C2A	-2.83	103.05	113.98
23	C	514	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
23	A	408	CLA	C4B-C3B-C2B	-2.82	103.79	107.30
25	t	102	BCR	C1-C6-C7	2.82	123.31	115.65
23	d	405	CLA	CMC-C2C-C1C	2.82	129.44	125.03
23	b	603	CLA	O2A-CGA-CBA	2.82	120.43	111.83
23	A	405[B]	CLA	CMA-C3A-C2A	-2.82	103.08	113.98
25	k	101	BCR	C2-C1-C6	2.82	114.53	110.44
23	C	503	CLA	O2A-CGA-CBA	2.82	120.42	111.83
38	E	102	HEM	CHD-C1D-ND	2.82	127.45	124.42
23	B	602	CLA	C4B-C3B-C2B	-2.82	103.80	107.30
29	D	405[B]	PL9	C40-C39-C41	2.82	120.11	115.23
23	b	608	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
31	B	629	LMT	O1'-C1'-C2'	2.81	112.55	108.27
32	D	407[B]	LHG	O8-C23-C24	2.81	120.42	111.83
23	B	604	CLA	O2A-CGA-CBA	2.81	120.41	111.83
23	B	607	CLA	CHD-C4C-NC	2.81	128.59	124.23
25	B	617	BCR	C11-C10-C9	-2.81	123.33	127.28
23	b	605	CLA	C1-C2-C3	-2.81	121.59	126.20
32	A	419[A]	LHG	O7-C7-O9	-2.81	117.13	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	406[B]	LHG	O8-C23-O10	-2.81	116.60	123.63
23	d	404[A]	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
35	C	517[A]	DGD	C2G-O2G-C1B	-2.81	111.07	117.80
33	D	411	LMG	O8-C28-O10	-2.81	116.60	123.63
23	B	606	CLA	C4C-C3C-C2C	-2.81	102.80	106.89
23	b	605	CLA	O2A-CGA-O1A	-2.81	116.61	123.63
23	B	615	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
23	c	511	CLA	CMB-C2B-C1B	2.80	129.69	125.42
23	B	609	CLA	O2A-CGA-CBA	2.80	120.39	111.83
23	C	502	CLA	CMC-C2C-C1C	2.80	129.42	125.03
25	D	404	BCR	C3-C4-C5	-2.80	109.06	114.06
23	c	509	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
23	C	505	CLA	CAC-C3C-C4C	2.80	128.44	124.79
27	b	628	GOL	C3-C2-C1	-2.80	101.52	111.80
23	C	504	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
23	A	406[A]	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
23	b	603	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
29	D	405[A]	PL9	C37-C38-C39	-2.80	121.22	127.62
23	B	602	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
31	a	416	LMT	C3'-C4'-C5'	-2.80	104.73	110.93
25	b	618	BCR	C37-C22-C23	2.79	122.36	118.09
23	B	608	CLA	CHB-C4A-NA	2.79	128.43	124.40
23	b	601	CLA	C3B-C4B-NB	2.79	113.02	110.53
31	B	627	LMT	C2'-C3'-C4'	2.79	116.02	109.68
23	B	616	CLA	O2A-CGA-CBA	2.79	120.35	111.83
23	B	614	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
23	c	510	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
23	C	505	CLA	CMC-C2C-C1C	2.79	129.39	125.03
23	b	614	CLA	CMC-C2C-C1C	2.79	129.39	125.03
31	M	101	LMT	C1'-O5'-C5'	-2.79	108.27	113.72
23	C	507	CLA	CBC-CAC-C3C	-2.79	104.86	112.42
23	D	402[B]	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
23	b	615	CLA	O2A-CGA-O1A	-2.79	116.65	123.63
23	A	406[B]	CLA	O2A-CGA-CBA	2.79	120.34	111.83
23	a	404[B]	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
38	E	102	HEM	CHA-C4D-ND	2.79	127.81	124.37
23	C	510	CLA	O2A-CGA-O1A	-2.78	116.66	123.63
32	D	407[A]	LHG	O7-C7-C8	2.78	117.50	111.48
23	C	506	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
23	b	615	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
23	b	606	CLA	O2A-CGA-O1A	-2.78	116.67	123.63
23	b	605	CLA	CHC-C1C-C2C	-2.78	119.04	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[B]	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
23	d	405	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
23	d	402[B]	CLA	O2A-CGA-CBA	2.78	120.31	111.83
26	a	411	SQD	O7-S-C6	2.78	110.91	106.76
25	c	515	BCR	C11-C10-C9	-2.78	123.38	127.28
24	A	407[B]	PHO	CMA-C3A-C4A	-2.78	108.62	114.61
24	A	416[B]	PHO	O2D-CGD-O1D	-2.78	118.44	123.85
23	b	606	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
32	d	409[B]	LHG	O8-C23-C24	2.78	120.31	111.83
23	C	507	CLA	O2A-CGA-O1A	-2.78	116.68	123.63
23	b	601	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
32	a	419[A]	LHG	O8-C23-C24	2.78	120.30	111.83
23	C	508	CLA	CHD-C4C-NC	2.78	128.54	124.23
35	H	102	DGD	O1G-C1A-O1A	-2.78	116.68	123.63
23	b	605	CLA	C2A-C1A-CHA	-2.78	119.05	123.87
24	d	403[A]	PHO	O1D-CGD-CBD	-2.78	120.51	124.72
23	b	603	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
23	a	405[A]	CLA	CAA-C2A-C3A	-2.78	105.50	113.00
23	c	511	CLA	C1-C2-C3	-2.77	121.65	126.20
23	A	406[A]	CLA	CBC-CAC-C3C	-2.77	104.90	112.42
31	b	621	LMT	C1'-O5'-C5'	-2.77	108.31	113.72
23	C	502	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
23	C	512	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
23	c	503	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
23	c	501	CLA	C1D-CHD-C4C	-2.77	120.13	126.02
23	d	404[B]	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
29	d	407[A]	PL9	C53-C6-C1	2.77	120.95	115.28
23	b	615	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	B	601	CLA	C3B-C4B-NB	2.77	113.00	110.53
23	A	404[B]	CLA	CAA-C2A-C1A	-2.77	102.90	111.97
23	b	611	CLA	C2A-C1A-CHA	-2.77	119.06	123.87
23	C	503	CLA	CAC-C3C-C4C	2.77	128.39	124.79
23	c	512	CLA	CAC-C3C-C4C	2.77	128.39	124.79
23	B	613	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
23	D	402[B]	CLA	O2A-CGA-O1A	-2.77	116.71	123.63
26	l	101	SQD	C4-C3-C2	2.77	115.69	110.83
23	d	405	CLA	CAA-C2A-C3A	-2.77	105.53	113.00
23	C	504	CLA	C1-C2-C3	-2.76	121.67	126.20
29	D	405[A]	PL9	C42-C41-C39	-2.76	104.03	113.19
29	D	405[B]	PL9	C37-C38-C39	-2.76	121.30	127.62
23	b	611	CLA	CHD-C4C-NC	2.76	128.51	124.23
23	B	610	CLA	CHC-C1C-C2C	-2.76	119.10	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	514	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
23	B	604	CLA	C6-C7-C8	-2.76	106.79	115.97
35	c	516[A]	DGD	O3G-C3G-C2G	-2.76	104.11	110.82
25	Y	101	BCR	C10-C11-C12	-2.76	115.20	123.20
23	B	614	CLA	C2A-C1A-CHA	-2.76	119.08	123.87
29	D	405[B]	PL9	C51-C49-C50	2.76	120.94	114.59
23	a	407	CLA	CBC-CAC-C3C	-2.76	104.95	112.42
23	b	606	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
23	B	609	CLA	CHD-C4C-NC	2.75	128.50	124.23
26	A	412	SQD	C4-C3-C2	-2.75	106.00	110.83
40	v	201	HEC	CBD-CAD-C3D	-2.75	104.93	112.53
23	c	506	CLA	CMC-C2C-C1C	2.75	129.33	125.03
23	b	609	CLA	CHC-C1C-C2C	-2.75	119.14	126.95
23	B	603	CLA	C2A-C1A-CHA	-2.75	119.10	123.87
23	B	601	CLA	C1-O2A-CGA	2.74	123.29	116.65
29	A	414[B]	PL9	C12-C13-C14	-2.74	121.34	127.62
23	C	514	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
23	C	508	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
23	A	404[A]	CLA	CAC-C3C-C4C	2.74	128.36	124.79
23	b	602	CLA	CMB-C2B-C1B	2.74	129.59	125.42
25	c	514	BCR	C20-C21-C22	-2.74	123.44	127.28
26	f	102	SQD	O48-C23-C24	2.74	120.19	111.83
23	b	616	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
23	b	604	CLA	O2A-CGA-CBA	2.74	120.19	111.83
23	b	611	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
23	d	402[A]	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
23	A	408	CLA	CMB-C2B-C1B	2.74	129.59	125.42
23	B	615	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
35	C	517[A]	DGD	O3G-C3G-C2G	-2.74	104.16	110.82
23	C	507	CLA	C4-C3-C5	2.74	119.98	115.23
23	c	501	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
25	y	101	BCR	C24-C23-C22	-2.74	122.19	126.23
23	B	606	CLA	C4-C3-C5	2.74	119.98	115.23
23	c	509	CLA	C4-C3-C5	2.74	119.98	115.23
35	C	518[A]	DGD	O1G-C1A-O1A	-2.74	116.78	123.63
23	d	404[A]	CLA	CAA-C2A-C3A	-2.74	105.61	113.00
23	C	514	CLA	CAA-C2A-C3A	-2.74	105.61	113.00
26	X	101	SQD	O47-C7-O49	-2.73	117.31	123.70
26	l	101	SQD	O9-S-C6	2.73	110.84	106.76
23	b	606	CLA	CBC-CAC-C3C	-2.73	105.01	112.42
23	C	510	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
23	B	612	CLA	CHD-C4C-NC	2.73	128.47	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	CMB-C2B-C1B	2.73	129.58	125.42
23	a	405[B]	CLA	C4-C3-C5	2.73	119.97	115.23
23	A	406[A]	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
23	A	404[A]	CLA	C2A-C1A-CHA	-2.73	119.13	123.87
23	d	405	CLA	CHC-C1C-C2C	-2.73	119.19	126.95
38	f	101	HEM	CBD-CAD-C3D	-2.73	104.99	112.53
23	B	603	CLA	O2A-CGA-O1A	-2.73	116.81	123.63
23	b	605	CLA	C1-O2A-CGA	2.73	123.25	116.65
23	a	405[A]	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
23	C	503	CLA	C4C-C3C-C2C	-2.72	102.92	106.89
23	c	509	CLA	CHD-C4C-NC	2.72	128.46	124.23
33	m	101	LMG	C8-O7-C10	-2.72	111.28	117.80
33	c	520	LMG	O8-C28-C29	2.72	120.14	111.83
26	X	101	SQD	O48-C23-C24	2.72	120.14	111.83
23	c	505	CLA	CHC-C1C-C2C	-2.72	119.21	126.95
23	B	615	CLA	C11-C10-C8	-2.72	106.92	115.97
24	a	406[B]	PHO	O2A-CGA-O1A	-2.72	116.82	123.63
23	b	610	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
26	X	101	SQD	O5-C1-O6	2.72	116.47	110.04
31	T	101	LMT	C1'-O5'-C5'	-2.72	108.41	113.72
23	C	504	CLA	CMB-C2B-C1B	2.72	129.56	125.42
32	a	419[B]	LHG	O8-C23-C24	2.72	120.12	111.83
23	c	513	CLA	CHC-C1C-C2C	-2.71	119.23	126.95
29	A	414[A]	PL9	C10-C9-C8	-2.71	116.66	123.63
23	B	614	CLA	CBC-CAC-C3C	-2.71	105.07	112.42
35	c	516[A]	DGD	C3G-C2G-C1G	-2.71	105.46	111.78
25	B	618	BCR	C37-C22-C23	2.71	122.23	118.09
25	b	617	BCR	C24-C23-C22	-2.71	122.22	126.23
23	D	402[B]	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
23	c	501	CLA	C4-C3-C5	2.71	119.93	115.23
32	D	406[A]	LHG	O8-C23-C24	2.71	120.09	111.83
26	f	102	SQD	O5-C5-C4	2.71	114.58	109.70
23	c	510	CLA	O2A-CGA-O1A	-2.70	116.86	123.63
23	B	612	CLA	C2A-C1A-CHA	-2.70	119.17	123.87
23	b	607	CLA	CAA-C2A-C3A	-2.70	105.69	113.00
23	C	507	CLA	CMC-C2C-C1C	2.70	129.26	125.03
23	C	508	CLA	C4-C3-C5	2.70	119.92	115.23
23	B	615	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
25	k	101	BCR	C15-C14-C13	-2.70	123.49	127.28
23	B	601	CLA	CMB-C2B-C1B	2.70	129.53	125.42
23	d	405	CLA	C2A-C1A-CHA	-2.70	119.18	123.87
23	b	615	CLA	CHD-C4C-NC	2.70	128.42	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	504	CLA	O2A-CGA-O1A	-2.70	116.87	123.63
29	D	405[A]	PL9	C2-C1-C6	2.70	122.21	119.00
25	t	102	BCR	C11-C10-C9	-2.70	123.49	127.28
23	b	612	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
32	L	101[A]	LHG	O8-C23-C24	2.70	120.06	111.83
25	H	101	BCR	C7-C8-C9	-2.70	122.24	126.23
23	b	612	CLA	O2A-CGA-CBA	2.70	120.06	111.83
34	B	621	HTG	C1'-S1-C1	2.70	106.27	100.45
23	C	510	CLA	C16-C15-C13	-2.70	107.00	115.97
23	a	405[A]	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
23	B	601	CLA	O2A-CGA-CBA	2.69	120.05	111.83
23	d	402[A]	CLA	O2A-CGA-CBA	2.69	120.05	111.83
26	A	410[A]	SQD	O48-C23-O10	-2.69	116.89	123.63
23	A	405[A]	CLA	CMA-C3A-C2A	-2.69	103.58	113.98
35	c	518	DGD	O1G-C1A-C2A	2.69	120.04	111.83
23	b	604	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
23	c	513	CLA	CMC-C2C-C1C	2.69	129.24	125.03
29	A	414[A]	PL9	C40-C39-C41	2.69	119.90	115.23
23	d	402[B]	CLA	C1-C2-C3	-2.69	121.79	126.20
23	D	402[B]	CLA	C2A-C1A-CHA	-2.69	119.20	123.87
23	A	405[A]	CLA	CAC-C3C-C4C	2.69	128.29	124.79
23	c	511	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
23	B	601	CLA	CHC-C1C-C2C	-2.69	119.32	126.95
25	B	617	BCR	C15-C14-C13	-2.69	123.51	127.28
23	D	402[B]	CLA	CAA-C2A-C3A	-2.69	105.74	113.00
23	b	604	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
23	D	403	CLA	CHD-C4C-NC	2.68	128.39	124.23
25	k	101	BCR	C38-C26-C25	-2.68	121.56	124.48
23	c	503	CLA	C2A-C1A-CHA	-2.68	119.21	123.87
33	C	501	LMG	C1-O6-C5	-2.68	108.48	113.72
23	b	615	CLA	CAC-C3C-C4C	2.68	128.28	124.79
23	B	607	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
35	C	517[B]	DGD	O3G-C3G-C2G	-2.68	104.30	110.82
33	D	411	LMG	O8-C28-C29	2.68	120.00	111.83
38	E	102	HEM	CBA-CAA-C2A	-2.68	105.13	112.53
23	B	604	CLA	CMC-C2C-C1C	2.68	129.22	125.03
25	a	408	BCR	C29-C30-C25	2.68	114.33	110.44
23	D	403	CLA	CAA-C2A-C3A	-2.68	105.77	113.00
23	a	407	CLA	CMA-C3A-C2A	-2.67	103.64	113.98
23	c	506	CLA	CMB-C2B-C1B	2.67	129.49	125.42
33	Z	101	LMG	C4-C3-C2	2.67	115.52	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	CMA-C3A-C2A	-2.67	103.66	113.98
23	b	601	CLA	CAC-C3C-C4C	2.67	128.26	124.79
23	c	510	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
23	A	406[B]	CLA	CBC-CAC-C3C	-2.67	105.19	112.42
23	c	507	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
23	B	605	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
25	H	101	BCR	C10-C11-C12	-2.67	115.48	123.20
23	D	403	CLA	O2A-CGA-CBA	2.66	119.96	111.83
26	a	411	SQD	C3-C4-C5	2.66	115.06	110.23
23	C	502	CLA	C4C-C3C-C2C	-2.66	103.02	106.89
23	B	602	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
23	a	404[A]	CLA	CAC-C3C-C4C	2.66	128.25	124.79
23	b	603	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
23	a	405[B]	CLA	C4B-C3B-C2B	-2.66	104.00	107.30
23	B	613	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
31	T	101	LMT	C3'-C4'-C5'	-2.66	105.04	110.93
23	C	504	CLA	O2A-CGA-CBA	2.66	119.93	111.83
25	b	618	BCR	C15-C14-C13	-2.66	123.55	127.28
23	b	607	CLA	CMC-C2C-C1C	2.66	129.18	125.03
23	a	405[B]	CLA	CAC-C3C-C4C	2.65	128.24	124.79
23	A	406[B]	CLA	C4C-C3C-C2C	-2.65	103.03	106.89
23	b	611	CLA	O2A-CGA-CBA	2.65	119.92	111.83
23	c	511	CLA	O2A-CGA-CBA	2.65	119.92	111.83
23	b	602	CLA	CMA-C3A-C4A	-2.65	104.64	111.77
31	M	101	LMT	C3'-C4'-C5'	-2.65	105.05	110.93
25	c	515	BCR	C37-C22-C23	2.65	122.14	118.09
24	A	416[A]	PHO	O2D-CGD-O1D	-2.65	118.69	123.85
23	b	613	CLA	CAC-C3C-C4C	2.65	128.24	124.79
23	b	605	CLA	CMC-C2C-C1C	2.65	129.17	125.03
23	C	513	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
29	D	405[B]	PL9	C53-C6-C1	2.65	120.70	115.28
38	f	101	HEM	C4D-ND-C1D	2.65	108.34	105.21
23	c	504	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
26	b	620	SQD	O7-S-C6	2.64	110.70	106.76
34	b	623	HTG	O5-C1-C2	2.64	113.96	110.32
24	d	403[A]	PHO	CBA-CAA-C2A	-2.64	105.99	113.78
23	C	509	CLA	O2A-CGA-CBA	2.64	119.89	111.83
23	C	503	CLA	CHD-C4C-NC	2.64	128.33	124.23
31	C	525	LMT	O5'-C5'-C6'	2.64	112.98	106.44
32	d	408[B]	LHG	O8-C23-O10	-2.64	117.02	123.63
23	B	615	CLA	C6-C7-C8	-2.64	107.19	115.97
23	c	511	CLA	CAC-C3C-C4C	2.64	128.22	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	CMA-C3A-C4A	-2.64	104.68	111.77
31	B	627	LMT	C4B-C3B-C2B	2.64	115.46	110.83
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
23	c	504	CLA	CMB-C2B-C1B	2.64	129.43	125.42
23	B	615	CLA	C1-O2A-CGA	2.64	123.03	116.65
31	B	629	LMT	C3'-C4'-C5'	-2.64	105.09	110.93
23	C	514	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	C	513	CLA	O2A-CGA-O1A	-2.63	117.04	123.63
23	B	602	CLA	CAC-C3C-C4C	2.63	128.21	124.79
23	D	402[A]	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	b	606	CLA	CMC-C2C-C1C	2.63	129.15	125.03
23	B	606	CLA	C3B-C4B-NB	2.63	112.88	110.53
29	d	407[B]	PL9	C53-C6-C1	2.63	120.67	115.28
23	b	616	CLA	CHC-C1C-C2C	-2.63	119.47	126.95
23	a	404[B]	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
23	C	506	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
23	C	514	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
23	C	512	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
40	V	201	HEC	CAD-CBD-CGD	-2.63	106.69	113.67
23	B	609	CLA	CHC-C1C-C2C	-2.63	119.48	126.95
23	C	504	CLA	CHC-C1C-C2C	-2.63	119.49	126.95
23	A	405[A]	CLA	OBD-CAD-C3D	-2.63	122.28	128.42
23	B	614	CLA	C4C-C3C-C2C	-2.62	103.07	106.89
23	A	404[A]	CLA	CMA-C3A-C2A	-2.62	103.85	113.98
23	c	506	CLA	O2A-CGA-O1A	-2.62	117.07	123.63
25	c	514	BCR	C33-C5-C6	-2.62	121.62	124.48
35	C	518[B]	DGD	C2G-O2G-C1B	-2.62	111.53	117.80
25	t	102	BCR	C37-C22-C23	2.62	122.09	118.09
29	d	407[B]	PL9	C17-C18-C19	-2.62	121.63	127.62
33	C	501	LMG	C6-C5-C4	2.62	119.45	113.02
25	d	406	BCR	C28-C27-C26	-2.62	109.39	114.06
23	A	406[A]	CLA	CMC-C2C-C1C	2.62	129.12	125.03
23	b	616	CLA	CAC-C3C-C4C	2.62	128.19	124.79
29	a	413[A]	PL9	C53-C6-C1	2.62	120.64	115.28
23	B	616	CLA	C2A-C1A-CHA	-2.61	119.33	123.87
23	c	505	CLA	O2A-CGA-CBA	2.61	119.80	111.83
23	c	501	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
23	c	507	CLA	C3B-C4B-NB	2.61	112.86	110.53
23	a	404[A]	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
23	B	606	CLA	C4B-C3B-C2B	-2.61	104.06	107.30
29	D	405[B]	PL9	C27-C28-C29	-2.61	121.65	127.62
23	A	406[B]	CLA	C4-C3-C5	2.61	119.76	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[B]	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
24	A	407[A]	PHO	O2A-CGA-CBA	2.61	119.78	111.83
23	b	616	CLA	CMC-C2C-C1C	2.61	129.11	125.03
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.48
25	c	515	BCR	C2-C1-C6	2.60	114.22	110.44
23	B	603	CLA	O2A-CGA-CBA	2.60	119.77	111.83
23	a	405[B]	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
23	C	512	CLA	C1-O2A-CGA	2.60	122.95	116.65
29	d	407[B]	PL9	C22-C23-C24	-2.60	121.67	127.62
23	B	605	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
23	c	507	CLA	CHC-C1C-C2C	-2.60	119.56	126.95
35	c	516[A]	DGD	O1G-C1A-O1A	-2.60	117.13	123.63
25	A	409	BCR	C40-C30-C25	-2.60	106.17	110.24
23	A	406[B]	CLA	C2A-C1A-CHA	-2.60	119.36	123.87
23	c	513	CLA	C2A-C1A-CHA	-2.60	119.36	123.87
29	D	405[B]	PL9	C20-C19-C21	2.60	119.73	115.23
23	A	404[B]	CLA	CAC-C3C-C4C	2.60	128.17	124.79
29	d	407[A]	PL9	C17-C18-C19	-2.59	121.69	127.62
23	d	405	CLA	O2A-CGA-CBA	2.59	119.74	111.83
23	b	602	CLA	C2A-C1A-CHA	-2.59	119.37	123.87
38	E	102	HEM	C3B-C4B-NB	-2.59	107.61	109.47
29	D	405[A]	PL9	C40-C39-C41	2.59	119.72	115.23
23	B	611	CLA	O2A-CGA-O1A	-2.59	117.15	123.63
24	a	406[B]	PHO	O2D-CGD-O1D	-2.59	118.81	123.85
23	C	512	CLA	CMC-C2C-C1C	2.59	129.08	125.03
23	D	402[A]	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
29	A	414[B]	PL9	C42-C43-C44	-2.59	121.70	127.62
29	A	414[B]	PL9	C35-C34-C36	2.59	119.72	115.23
23	a	405[A]	CLA	O2A-CGA-CBA	2.59	119.72	111.83
23	B	603	CLA	CMA-C3A-C2A	-2.58	103.99	113.98
31	B	628	LMT	O5'-C5'-C4'	2.58	115.07	109.72
23	b	608	CLA	C2A-C1A-CHA	-2.58	119.38	123.87
23	b	603	CLA	CBC-CAC-C3C	-2.58	105.42	112.42
23	d	405	CLA	CBC-CAC-C3C	-2.58	105.42	112.42
23	d	405	CLA	CAC-C3C-C4C	2.58	128.15	124.79
23	D	403	CLA	CMC-C2C-C1C	2.58	129.07	125.03
23	c	507	CLA	C1-C2-C3	-2.58	121.97	126.20
23	D	402[A]	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
23	c	502	CLA	O2A-CGA-CBA	2.58	119.70	111.83
33	C	501	LMG	C8-O7-C10	-2.58	111.62	117.80
23	A	406[A]	CLA	C4-C3-C5	2.58	119.70	115.23
23	A	408	CLA	CMC-C2C-C1C	2.58	129.06	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	F	101	LMT	C1'-O5'-C5'	-2.58	108.69	113.72
23	c	504	CLA	CAC-C3C-C4C	2.57	128.14	124.79
23	C	507	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
23	a	405[B]	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
23	C	504	CLA	CAC-C3C-C4C	2.57	128.13	124.79
23	d	402[B]	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
23	c	511	CLA	CMC-C2C-C1C	2.57	129.05	125.03
23	c	504	CLA	CMC-C2C-C1C	2.57	129.05	125.03
25	B	617	BCR	C29-C30-C25	2.57	114.17	110.44
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	A	408	CLA	CHB-C4A-NA	2.57	128.11	124.40
23	C	513	CLA	CAC-C3C-C4C	2.57	128.13	124.79
23	C	513	CLA	CMC-C2C-C1C	2.56	129.04	125.03
23	B	609	CLA	CAC-C3C-C4C	2.56	128.12	124.79
38	E	102	HEM	O2A-CGA-CBA	2.56	122.10	114.00
25	C	516	BCR	C32-C1-C6	-2.56	106.23	110.24
29	a	413[B]	PL9	C53-C6-C1	2.56	120.52	115.28
25	b	618	BCR	C2-C1-C6	2.56	114.16	110.44
23	B	613	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
23	B	601	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
23	c	507	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
25	T	102	BCR	C12-C13-C14	-2.56	114.99	119.01
25	B	617	BCR	C7-C8-C9	-2.56	122.45	126.23
24	A	407[B]	PHO	C1-C2-C3	-2.56	122.01	126.20
29	D	405[A]	PL9	C27-C28-C29	-2.56	121.77	127.62
23	C	513	CLA	CMB-C2B-C1B	2.56	129.31	125.42
35	h	102	DGD	O1G-C1A-O1A	-2.55	117.24	123.63
23	A	405[A]	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
23	b	603	CLA	CHD-C4C-NC	2.55	128.19	124.23
23	A	405[B]	CLA	CAC-C3C-C4C	2.55	128.11	124.79
23	c	505	CLA	C4B-C3B-C2B	-2.55	104.13	107.30
23	c	506	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
23	b	602	CLA	CHD-C4C-NC	2.55	128.18	124.23
23	A	408	CLA	CMA-C3A-C2A	-2.55	104.13	113.98
25	C	516	BCR	C29-C30-C25	2.55	114.14	110.44
24	a	406[B]	PHO	C1A-C2A-C3A	-2.55	100.42	102.84
23	b	611	CLA	CAC-C3C-C4C	2.55	128.10	124.79
23	a	405[A]	CLA	C2A-C1A-CHA	-2.55	119.45	123.87
23	a	405[A]	CLA	O2A-CGA-O1A	-2.54	117.26	123.63
23	C	506	CLA	O2A-CGA-CBA	2.54	119.59	111.83
29	a	413[A]	PL9	C47-C48-C49	-2.54	119.16	127.64
23	c	512	CLA	C3B-C4B-NB	2.54	112.80	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	516[B]	DGD	O3G-C3G-C2G	-2.54	104.63	110.82
26	a	411	SQD	C1-O5-C5	2.54	118.69	113.72
25	a	408	BCR	C7-C8-C9	-2.54	122.47	126.23
23	a	405[B]	CLA	O2A-CGA-CBA	2.54	119.58	111.83
23	C	513	CLA	CHC-C1C-C2C	-2.54	119.73	126.95
29	a	413[B]	PL9	C40-C39-C41	2.54	119.64	115.23
25	c	515	BCR	C21-C20-C19	-2.54	115.84	123.20
23	D	403	CLA	C1-C2-C3	-2.54	122.04	126.20
23	C	514	CLA	C4-C3-C5	2.54	119.63	115.23
23	B	614	CLA	C4B-C3B-C2B	-2.54	104.15	107.30
23	d	402[A]	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
29	a	413[B]	PL9	C47-C48-C49	-2.53	119.19	127.64
23	A	404[B]	CLA	O2A-CGA-O1A	-2.53	117.29	123.63
25	d	406	BCR	C33-C5-C6	-2.53	121.72	124.48
23	B	611	CLA	CMB-C2B-C3B	2.53	132.51	126.55
23	C	507	CLA	C2A-C1A-CHA	-2.53	119.47	123.87
35	C	517[B]	DGD	C2G-O2G-C1B	-2.53	111.73	117.80
25	T	102	BCR	C33-C5-C6	-2.53	121.72	124.48
23	C	503	CLA	C4-C3-C5	2.53	119.62	115.23
23	b	610	CLA	CAA-CBA-CGA	-2.53	106.02	113.21
26	f	102	SQD	O47-C7-O49	-2.53	117.79	123.70
24	d	403[B]	PHO	O2D-CGD-O1D	-2.53	118.92	123.85
23	c	504	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
25	t	102	BCR	C20-C21-C22	-2.53	123.73	127.28
23	C	512	CLA	CAC-C3C-C4C	2.53	128.08	124.79
35	c	517[B]	DGD	O1G-C1A-C2A	2.53	119.54	111.83
23	A	406[B]	CLA	C1-C2-C3	-2.53	122.06	126.20
23	B	612	CLA	C1-C2-C3	-2.52	122.06	126.20
23	a	405[B]	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
25	H	101	BCR	C37-C22-C21	-2.52	118.73	122.82
23	d	402[B]	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
23	C	508	CLA	O2A-CGA-CBA	2.52	119.52	111.83
29	a	413[B]	PL9	C20-C19-C21	2.52	119.60	115.23
25	B	619	BCR	C29-C30-C25	2.52	114.10	110.44
23	C	510	CLA	C2A-C1A-CHA	-2.52	119.50	123.87
24	A	407[B]	PHO	O2A-CGA-CBA	2.52	119.51	111.83
23	A	404[B]	CLA	C4C-C3C-C2C	-2.52	103.23	106.89
29	A	414[A]	PL9	C42-C43-C44	-2.51	121.87	127.62
24	A	407[A]	PHO	O2A-CGA-O1A	-2.51	117.34	123.63
23	A	408	CLA	C4-C3-C5	2.51	119.59	115.23
23	b	607	CLA	C1-O2A-CGA	2.51	122.73	116.65
25	T	102	BCR	C21-C20-C19	-2.51	115.93	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	D	407[B]	LHG	O8-C23-O10	-2.51	117.35	123.63
23	A	405[B]	CLA	OBD-CAD-C3D	-2.51	122.55	128.42
25	t	102	BCR	C7-C6-C5	-2.51	115.78	121.56
23	b	610	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
23	A	404[B]	CLA	CHD-C4C-NC	2.51	128.12	124.23
38	E	102	HEM	O2D-CGD-CBD	2.51	121.92	114.00
23	B	608	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
31	m	103	LMT	C3'-C4'-C5'	-2.51	105.38	110.93
23	c	508	CLA	C4-C3-C5	2.50	119.58	115.23
23	B	615	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
23	C	512	CLA	C1-C2-C3	-2.50	122.10	126.20
31	C	525	LMT	O1'-C1'-C2'	2.50	112.07	108.27
23	B	608	CLA	C11-C12-C13	-2.50	107.65	115.97
25	K	102	BCR	C36-C18-C19	2.50	121.91	118.09
23	C	503	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
26	A	412	SQD	C1-C2-C3	-2.50	104.75	110.01
23	A	405[B]	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
25	D	404	BCR	C15-C14-C13	-2.50	123.77	127.28
23	B	612	CLA	C2B-C1B-NB	2.50	112.92	110.33
23	c	506	CLA	O2A-CGA-CBA	2.50	119.46	111.83
26	a	409[B]	SQD	O47-C7-O49	-2.50	117.86	123.70
24	A	416[A]	PHO	CMA-C3A-C4A	-2.50	109.23	114.61
23	c	503	CLA	C4-C3-C5	2.50	119.57	115.23
25	Y	101	BCR	C15-C16-C17	-2.50	118.41	123.52
23	B	608	CLA	C1-C2-C3	-2.50	122.10	126.20
32	d	408[A]	LHG	O8-C23-O10	-2.50	117.38	123.63
25	b	617	BCR	C29-C30-C25	2.50	114.07	110.44
25	Y	101	BCR	C36-C18-C19	2.50	121.90	118.09
23	c	502	CLA	CMC-C2C-C1C	2.50	128.94	125.03
25	K	102	BCR	C24-C23-C22	-2.50	122.54	126.23
23	B	601	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	C	503	CLA	CMC-C2C-C1C	2.49	128.93	125.03
23	c	504	CLA	C2A-C1A-CHA	-2.49	119.54	123.87
23	B	607	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
23	c	513	CLA	CHD-C4C-NC	2.49	128.10	124.23
23	b	602	CLA	C4-C3-C5	2.49	119.55	115.23
23	C	511	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
23	A	405[B]	CLA	C1-C2-C3	-2.49	122.11	126.20
25	T	102	BCR	C35-C13-C12	2.49	121.89	118.09
23	B	611	CLA	C3B-C4B-NB	2.49	112.75	110.53
23	A	404[B]	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
23	B	604	CLA	CAC-C3C-C4C	2.49	128.03	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	101	BCR	C1-C6-C7	2.49	122.40	115.65
23	c	510	CLA	C11-C10-C8	-2.49	107.70	115.97
23	d	405	CLA	C3B-C4B-NB	2.49	112.75	110.53
23	b	613	CLA	C4-C3-C5	2.48	119.54	115.23
23	B	610	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
25	B	618	BCR	C37-C22-C21	-2.48	118.79	122.82
32	D	406[B]	LHG	O8-C23-C24	2.48	119.41	111.83
24	d	403[B]	PHO	C4A-C3A-C2A	-2.48	100.48	102.84
23	b	614	CLA	CMA-C3A-C4A	-2.48	105.10	111.77
23	c	501	CLA	CHD-C4C-NC	2.48	128.08	124.23
23	B	604	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
23	c	501	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
29	D	405[B]	PL9	C45-C44-C46	2.48	119.53	115.23
24	A	416[A]	PHO	O1D-CGD-CBD	-2.48	120.96	124.72
23	c	503	CLA	CAC-C3C-C4C	2.48	128.01	124.79
29	A	414[A]	PL9	C35-C34-C36	2.48	119.53	115.23
23	c	501	CLA	CBC-CAC-C3C	-2.48	105.71	112.42
23	C	507	CLA	CHD-C4C-NC	2.48	128.07	124.23
24	A	416[B]	PHO	CMA-C3A-C4A	-2.48	109.28	114.61
23	A	405[A]	CLA	O2A-CGA-O1A	-2.48	117.44	123.63
23	d	402[B]	CLA	CMA-C3A-C2A	-2.47	104.42	113.98
25	y	101	BCR	C21-C20-C19	-2.47	116.03	123.20
25	A	409	BCR	C8-C7-C6	-2.47	120.40	127.00
23	B	602	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
29	A	414[A]	PL9	C53-C6-C1	2.47	120.33	115.28
26	A	410[A]	SQD	O9-S-C6	2.47	110.44	106.76
25	a	408	BCR	C20-C21-C22	-2.47	123.82	127.28
29	d	407[A]	PL9	C36-C34-C33	-2.47	115.63	121.17
23	b	613	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
23	c	503	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
24	a	406[A]	PHO	O2A-CGA-O1A	-2.47	117.46	123.63
29	D	405[A]	PL9	C22-C23-C24	-2.47	121.98	127.62
23	b	604	CLA	C4-C3-C5	2.47	119.51	115.23
31	B	629	LMT	O5'-C5'-C4'	2.46	114.82	109.72
23	B	606	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
23	b	602	CLA	CHB-C1B-C2B	-2.46	120.28	127.43
23	c	506	CLA	C4-C3-C5	2.46	119.50	115.23
24	A	416[B]	PHO	CED-O2D-CGD	2.46	121.50	115.92
23	C	513	CLA	CHB-C4A-NA	2.46	127.95	124.40
23	a	404[A]	CLA	CHD-C4C-NC	2.46	128.05	124.23
23	d	404[B]	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
35	h	102	DGD	O4D-C4D-C3D	-2.45	104.59	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	H	101	BCR	C33-C5-C6	-2.45	121.81	124.48
23	C	502	CLA	C4-C3-C5	2.45	119.48	115.23
29	d	407[A]	PL9	C47-C48-C49	-2.45	119.47	127.64
23	d	402[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.89
33	c	519	LMG	C8-O7-C10	-2.45	111.93	117.80
23	b	611	CLA	CMC-C2C-C1C	2.45	128.86	125.03
23	B	608	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
23	b	607	CLA	C4-C3-C5	2.45	119.48	115.23
23	b	615	CLA	O2A-CGA-CBA	2.45	119.30	111.83
23	C	502	CLA	C2A-C1A-CHA	-2.45	119.62	123.87
32	A	419[B]	LHG	O7-C7-O9	-2.45	117.98	123.70
25	h	101	BCR	C10-C11-C12	-2.45	116.11	123.20
23	b	606	CLA	C1-O2A-CGA	2.44	122.57	116.65
23	c	506	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
23	D	402[B]	CLA	CBC-CAC-C3C	-2.44	105.80	112.42
29	d	407[B]	PL9	C20-C19-C21	2.44	119.47	115.23
23	c	507	CLA	CBC-CAC-C3C	-2.44	105.80	112.42
23	D	403	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
33	C	520	LMG	O8-C28-O10	-2.44	117.52	123.63
23	b	606	CLA	C1-C2-C3	-2.44	122.20	126.20
23	d	402[A]	CLA	C1-O2A-CGA	2.44	122.56	116.65
23	a	407	CLA	CMB-C2B-C1B	2.44	129.13	125.42
23	C	510	CLA	C11-C12-C13	-2.44	107.86	115.97
23	c	510	CLA	CAA-C2A-C3A	-2.44	106.41	113.00
35	C	517[B]	DGD	C3G-C2G-C1G	-2.44	106.10	111.78
23	b	614	CLA	C2A-C1A-CHA	-2.44	119.64	123.87
23	a	404[A]	CLA	CMC-C2C-C1C	2.44	128.84	125.03
32	d	408[B]	LHG	O8-C23-C24	2.44	119.26	111.83
26	a	409[B]	SQD	O48-C23-C24	2.43	119.26	111.83
26	a	411	SQD	O48-C23-O10	-2.43	117.54	123.63
23	c	503	CLA	O2A-CGA-CBA	2.43	119.25	111.83
23	b	614	CLA	C4-C3-C5	2.43	119.45	115.23
23	B	615	CLA	C2A-C1A-CHA	-2.43	119.64	123.87
24	A	416[B]	PHO	O2A-CGA-CBA	2.43	119.25	111.83
32	d	415[B]	LHG	C5-O7-C7	-2.43	111.97	117.80
23	a	405[B]	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
35	C	518[B]	DGD	O1G-C1A-C2A	2.43	119.25	111.83
24	d	403[B]	PHO	O1D-CGD-CBD	-2.43	121.04	124.72
23	B	604	CLA	C6-C5-C3	-2.43	107.55	113.47
23	B	611	CLA	OBD-CAD-C3D	-2.43	122.73	128.42
23	A	406[B]	CLA	CMA-C3A-C2A	-2.43	104.58	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CHC-C1C-C2C	-2.43	120.05	126.95
23	a	404[B]	CLA	CHD-C4C-NC	2.43	128.00	124.23
23	C	504	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
23	b	606	CLA	O2A-CGA-CBA	2.43	119.23	111.83
33	C	520	LMG	C8-O7-C10	-2.43	111.99	117.80
25	B	619	BCR	C21-C20-C19	-2.42	116.17	123.20
24	a	406[B]	PHO	CMA-C3A-C4A	-2.42	109.39	114.61
38	f	101	HEM	CMD-C2D-C1D	2.42	128.82	125.03
23	c	508	CLA	O2A-CGA-CBA	2.42	119.22	111.83
25	d	406	BCR	C39-C30-C25	-2.42	106.44	110.24
26	b	620	SQD	O8-S-C6	2.42	110.65	105.97
25	B	618	BCR	C2-C1-C6	2.42	113.95	110.44
35	C	518[A]	DGD	O1G-C1A-C2A	2.42	119.21	111.83
35	c	517[A]	DGD	O1G-C1A-C2A	2.42	119.21	111.83
23	C	509	CLA	CHD-C4C-NC	2.42	127.98	124.23
32	d	408[A]	LHG	O8-C23-C24	2.42	119.21	111.83
24	a	406[B]	PHO	O1D-CGD-CBD	-2.42	121.06	124.72
23	b	609	CLA	C16-C15-C13	-2.42	107.93	115.97
24	A	407[A]	PHO	C1-C2-C3	-2.42	122.24	126.20
23	D	403	CLA	C2A-C1A-CHA	-2.42	119.67	123.87
23	B	606	CLA	C7-C6-C5	-2.42	106.82	113.26
27	A	418	GOL	C3-C2-C1	-2.42	102.93	111.80
25	k	101	BCR	C10-C11-C12	-2.42	116.20	123.20
35	H	102	DGD	O2G-C1B-C2B	2.42	116.71	111.48
23	B	612	CLA	O2A-CGA-O1A	-2.42	117.59	123.63
32	L	101[A]	LHG	O8-C23-O10	-2.42	117.59	123.63
24	a	406[B]	PHO	CMC-C2C-C1C	2.41	129.08	124.73
25	k	101	BCR	C11-C10-C9	-2.41	123.89	127.28
23	B	608	CLA	CBC-CAC-C3C	-2.41	105.88	112.42
26	A	410[B]	SQD	O48-C23-O10	-2.41	117.60	123.63
23	a	404[A]	CLA	CMA-C3A-C2A	-2.41	104.66	113.98
25	Y	101	BCR	C34-C9-C8	2.41	121.77	118.09
23	A	408	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
23	c	512	CLA	CMC-C2C-C1C	2.41	128.80	125.03
26	a	409[A]	SQD	O48-C23-C24	2.41	119.17	111.83
23	d	402[B]	CLA	C2A-C1A-CHA	-2.41	119.69	123.87
23	b	602	CLA	O2A-CGA-CBA	2.41	119.17	111.83
26	X	101	SQD	C46-C45-C44	-2.40	106.18	111.78
23	b	603	CLA	C7-C6-C5	-2.40	106.86	113.26
23	B	612	CLA	C3B-C4B-NB	2.40	112.68	110.53
23	b	609	CLA	C7-C6-C5	-2.40	106.86	113.26
23	b	607	CLA	C2A-C1A-CHA	-2.40	119.70	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	516[B]	DGD	O6D-C1D-O3G	-2.40	104.37	110.04
23	b	616	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
23	C	514	CLA	CMB-C2B-C1B	2.40	129.07	125.42
29	a	413[A]	PL9	C40-C39-C41	2.40	119.39	115.23
23	c	513	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
25	c	515	BCR	C7-C8-C9	-2.40	122.69	126.23
23	b	611	CLA	CMB-C2B-C1B	2.39	129.06	125.42
29	a	413[A]	PL9	C20-C19-C21	2.39	119.38	115.23
23	B	609	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
35	c	516[A]	DGD	C2G-O2G-C1B	-2.39	112.07	117.80
25	h	101	BCR	C16-C15-C14	-2.39	118.63	123.52
29	A	414[A]	PL9	C35-C34-C33	-2.39	117.49	123.63
26	b	620	SQD	C1-C2-C3	-2.39	104.98	110.01
23	C	503	CLA	C4B-C3B-C2B	-2.39	104.33	107.30
25	c	514	BCR	C29-C30-C25	2.39	113.91	110.44
25	Y	101	BCR	C37-C22-C23	2.39	121.73	118.09
23	b	613	CLA	CHD-C4C-NC	2.39	127.93	124.23
26	b	620	SQD	O48-C23-C24	2.39	119.11	111.83
23	c	504	CLA	O2A-CGA-CBA	2.38	119.11	111.83
23	C	513	CLA	C2A-C1A-CHA	-2.38	119.73	123.87
23	d	402[A]	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
23	C	504	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
23	b	613	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
33	d	413	LMG	O7-C10-O9	-2.38	118.14	123.70
23	c	505	CLA	CHD-C4C-NC	2.38	127.92	124.23
23	B	616	CLA	CBC-CAC-C3C	-2.38	105.97	112.42
25	C	515	BCR	C16-C17-C18	-2.38	123.94	127.28
25	D	404	BCR	C21-C20-C19	-2.38	116.31	123.20
23	a	404[B]	CLA	C7-C6-C5	-2.38	106.93	113.26
24	a	406[B]	PHO	CMB-C2B-C3B	2.38	129.43	124.68
23	d	402[B]	CLA	C1-O2A-CGA	2.38	122.40	116.65
29	A	414[A]	PL9	C2-C3-C4	2.38	121.97	118.78
25	c	515	BCR	C32-C1-C6	-2.37	106.52	110.24
25	h	101	BCR	C34-C9-C8	2.37	121.71	118.09
23	c	510	CLA	CBC-CAC-C3C	-2.37	105.99	112.42
25	h	101	BCR	C16-C17-C18	-2.37	123.95	127.28
23	c	502	CLA	C1-O2A-CGA	2.37	122.39	116.65
25	a	408	BCR	C15-C16-C17	-2.37	118.67	123.52
35	C	517[B]	DGD	O1G-C1A-O1A	-2.37	117.70	123.63
25	c	514	BCR	C36-C18-C19	2.37	121.71	118.09
23	c	501	CLA	CMC-C2C-C1C	2.37	128.74	125.03
31	B	628	LMT	O5'-C5'-C6'	2.37	112.31	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	406	BCR	C40-C30-C39	2.37	115.42	108.63
23	C	506	CLA	C4-C3-C5	2.37	119.34	115.23
23	B	612	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
23	A	408	CLA	CAC-C3C-C4C	2.37	127.87	124.79
25	c	514	BCR	C28-C27-C26	-2.36	109.84	114.06
23	c	502	CLA	C1-C2-C3	-2.36	122.33	126.20
29	A	414[B]	PL9	C45-C44-C46	2.36	119.33	115.23
23	d	404[B]	CLA	CAC-C3C-C4C	2.36	127.86	124.79
23	C	506	CLA	O2A-CGA-O1A	-2.36	117.72	123.63
23	c	512	CLA	CHB-C4A-NA	2.36	127.81	124.40
23	C	509	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
23	B	602	CLA	CMA-C3A-C2A	-2.36	104.86	113.98
25	c	514	BCR	C38-C26-C25	-2.36	121.91	124.48
23	b	605	CLA	C4-C3-C5	2.36	119.32	115.23
23	c	510	CLA	C4-C3-C2	-2.36	117.58	123.63
35	C	518[A]	DGD	O6E-C5E-C6E	2.36	112.28	106.44
29	A	414[A]	PL9	C37-C36-C34	-2.36	105.38	113.19
23	c	503	CLA	CBC-CAC-C3C	-2.35	106.04	112.42
23	B	613	CLA	CHB-C4A-NA	2.35	127.80	124.40
29	a	413[A]	PL9	C10-C9-C8	-2.35	117.58	123.63
23	B	603	CLA	CHD-C4C-NC	2.35	127.88	124.23
24	A	416[B]	PHO	CMB-C2B-C3B	2.35	129.38	124.68
23	c	504	CLA	CED-O2D-CGD	2.35	121.25	115.92
23	D	402[A]	CLA	CHD-C4C-NC	2.35	127.88	124.23
23	c	510	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
23	c	508	CLA	CHD-C4C-NC	2.35	127.88	124.23
24	A	407[A]	PHO	CMB-C2B-C3B	2.35	129.37	124.68
23	B	605	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
23	c	507	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
23	d	402[B]	CLA	CHB-C4A-NA	2.34	127.78	124.40
35	c	516[B]	DGD	C2G-O2G-C1B	-2.34	112.19	117.80
23	c	504	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
23	B	605	CLA	CED-O2D-CGD	2.34	121.23	115.92
23	c	511	CLA	CMA-C3A-C4A	2.34	118.07	111.77
25	B	618	BCR	C38-C26-C25	-2.34	121.93	124.48
23	D	403	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
23	b	612	CLA	CHD-C4C-NC	2.34	127.86	124.23
25	Y	101	BCR	C7-C6-C5	-2.34	116.17	121.56
23	B	601	CLA	CHB-C4A-NA	2.34	127.78	124.40
23	C	507	CLA	CMB-C2B-C1B	2.34	128.98	125.42
23	B	605	CLA	C3B-C4B-NB	2.34	112.62	110.53
23	B	608	CLA	CHD-C4C-NC	2.34	127.86	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	V	201	HEC	CHA-C1A-NA	2.34	127.00	124.45
32	d	415[A]	LHG	O7-C7-O9	-2.34	118.24	123.70
23	A	405[B]	CLA	O2A-CGA-O1A	-2.34	117.78	123.63
23	b	610	CLA	C3B-C4B-NB	2.34	112.62	110.53
23	d	404[B]	CLA	CBC-CAC-C3C	-2.34	106.08	112.42
29	A	414[B]	PL9	C10-C9-C8	-2.34	117.63	123.63
23	B	604	CLA	C11-C12-C13	-2.33	108.20	115.97
23	C	512	CLA	CMB-C2B-C1B	2.33	128.97	125.42
25	y	101	BCR	C16-C17-C18	-2.33	124.00	127.28
32	L	101[B]	LHG	O8-C23-C24	2.33	118.95	111.83
23	b	602	CLA	CHC-C1C-C2C	-2.33	120.31	126.95
23	C	512	CLA	O2A-CGA-CBA	2.33	118.95	111.83
26	A	410[B]	SQD	O9-S-O7	-2.33	106.24	113.82
26	a	411	SQD	O5-C5-C4	2.33	113.90	109.70
25	K	102	BCR	C20-C21-C22	-2.33	124.01	127.28
29	D	405[B]	PL9	C22-C23-C24	-2.33	122.29	127.62
25	h	101	BCR	C20-C21-C22	-2.33	124.01	127.28
29	D	405[A]	PL9	C45-C44-C46	2.33	119.27	115.23
35	C	517[B]	DGD	O6D-C1D-O3G	-2.32	104.55	110.04
23	c	509	CLA	CMB-C2B-C1B	2.32	128.96	125.42
23	B	614	CLA	OBD-CAD-C3D	-2.32	122.98	128.42
24	a	406[A]	PHO	CMB-C2B-C3B	2.32	129.33	124.68
24	A	407[B]	PHO	O2D-CGD-O1D	-2.32	119.33	123.85
32	d	409[A]	LHG	O8-C23-O10	-2.32	117.82	123.63
24	d	403[B]	PHO	C1A-C2A-C3A	-2.32	100.63	102.84
23	a	405[A]	CLA	CBC-CAC-C3C	-2.32	106.12	112.42
33	d	413	LMG	C7-O1-C1	-2.32	108.82	113.80
29	A	414[A]	PL9	C2-C1-C6	2.32	121.76	119.00
23	B	605	CLA	OBD-CAD-C3D	-2.32	122.99	128.42
27	O	303	GOL	C3-C2-C1	-2.32	103.28	111.80
23	d	404[B]	CLA	CHD-C4C-NC	2.32	127.83	124.23
34	B	624	HTG	C3-C4-C5	2.32	114.44	110.23
24	a	406[B]	PHO	CBA-CAA-C2A	-2.32	106.94	113.78
23	B	608	CLA	C11-C10-C8	-2.32	108.25	115.97
23	b	616	CLA	C4-C3-C5	2.32	119.25	115.23
33	C	521	LMG	O1-C1-C2	2.32	111.80	108.27
29	d	407[A]	PL9	C7-C8-C9	-2.32	122.84	126.83
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	B	608	CLA	CMC-C2C-C1C	2.32	128.66	125.03
34	b	622	HTG	O5-C1-C2	2.32	113.51	110.32
32	E	101[B]	LHG	O7-C7-O9	-2.32	118.29	123.70
26	A	412	SQD	O48-C23-O10	-2.32	117.83	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414[A]	PL9	C47-C48-C49	-2.32	119.92	127.64
23	A	405[B]	CLA	O2D-CGD-O1D	-2.32	119.34	123.85
23	B	612	CLA	C1-O2A-CGA	2.31	122.25	116.65
25	B	619	BCR	C10-C11-C12	-2.31	116.50	123.20
23	b	606	CLA	CMB-C2B-C1B	2.31	128.94	125.42
25	c	515	BCR	C20-C21-C22	-2.31	124.03	127.28
23	d	402[B]	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
23	B	608	CLA	CMA-C3A-C2A	-2.31	105.04	113.98
25	k	101	BCR	C32-C1-C6	-2.31	106.62	110.24
29	A	414[B]	PL9	C53-C6-C1	2.31	120.01	115.28
33	B	620	LMG	C12-C11-C10	-2.31	105.24	113.69
25	k	101	BCR	C34-C9-C8	2.31	121.61	118.09
23	b	602	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
25	B	617	BCR	C21-C20-C19	-2.31	116.52	123.20
24	d	403[A]	PHO	O2D-CGD-O1D	-2.31	119.36	123.85
25	c	514	BCR	C8-C7-C6	-2.31	120.84	127.00
29	a	413[A]	PL9	C35-C34-C33	-2.31	117.70	123.63
27	B	623	GOL	C3-C2-C1	-2.31	103.34	111.80
32	b	629[B]	LHG	O8-C23-O10	-2.31	117.86	123.63
33	d	413	LMG	O8-C28-C29	2.30	118.86	111.83
38	E	102	HEM	C4C-NC-C1C	2.30	109.58	105.82
29	D	405[B]	PL9	C30-C29-C31	2.30	119.23	115.23
23	b	606	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
23	b	601	CLA	O2A-CGA-CBA	2.30	118.86	111.83
29	a	413[B]	PL9	C45-C44-C46	2.30	119.23	115.23
29	A	414[A]	PL9	C45-C44-C46	2.30	119.22	115.23
29	a	413[A]	PL9	C45-C44-C46	2.30	119.22	115.23
23	C	511	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
23	c	513	CLA	CMB-C2B-C1B	2.30	128.92	125.42
23	d	405	CLA	CHB-C4A-NA	2.30	127.72	124.40
23	b	608	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
23	C	514	CLA	CAC-C3C-C4C	2.30	127.78	124.79
23	C	511	CLA	CMB-C2B-C1B	2.30	128.92	125.42
25	k	101	BCR	C3-C4-C5	-2.30	109.96	114.06
23	B	602	CLA	CMB-C2B-C1B	2.30	128.91	125.42
23	c	513	CLA	O2A-CGA-O1A	-2.30	117.89	123.63
31	B	628	LMT	O5B-C5B-C6B	2.29	112.13	106.44
23	b	603	CLA	CMC-C2C-C1C	2.29	128.62	125.03
32	d	408[B]	LHG	C6-C5-C4	-2.29	106.44	111.78
29	A	414[B]	PL9	C47-C48-C49	-2.29	120.00	127.64
23	c	511	CLA	C1-O2A-CGA	2.29	122.20	116.65
23	b	604	CLA	CHD-C4C-NC	2.29	127.78	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	b	629[A]	LHG	O8-C23-O10	-2.29	117.90	123.63
23	a	405[B]	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
32	d	408[A]	LHG	C6-C5-C4	-2.29	106.44	111.78
23	c	504	CLA	C1-C2-C3	-2.29	122.44	126.20
25	B	618	BCR	C10-C11-C12	-2.29	116.56	123.20
33	C	521	LMG	C9-C8-C7	-2.29	106.45	111.78
23	b	608	CLA	O2A-CGA-CBA	2.29	118.81	111.83
35	C	517[B]	DGD	O5D-C6D-C5D	-2.29	104.27	109.42
26	A	412	SQD	O8-S-C6	2.29	110.39	105.97
25	T	102	BCR	C1-C6-C7	2.29	121.85	115.65
26	a	409[A]	SQD	O9-S-O7	-2.29	106.39	113.82
23	c	513	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
23	b	602	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
24	d	403[B]	PHO	CBA-CAA-C2A	-2.28	107.05	113.78
24	A	416[A]	PHO	O2A-CGA-CBA	2.28	118.80	111.83
23	C	509	CLA	C4-C3-C5	2.28	119.19	115.23
25	c	515	BCR	C33-C5-C6	-2.28	121.99	124.48
23	c	501	CLA	O2A-CGA-CBA	2.28	118.79	111.83
23	B	601	CLA	CMC-C2C-C1C	2.28	128.60	125.03
23	b	601	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
23	b	602	CLA	CAA-CBA-CGA	-2.28	106.74	113.21
23	B	602	CLA	CHB-C4A-NA	2.28	127.69	124.40
25	A	409	BCR	C16-C17-C18	-2.28	124.09	127.28
23	B	605	CLA	O2A-CGA-CBA	2.28	118.77	111.83
34	B	624	HTG	O5-C5-C4	2.27	113.80	109.70
25	c	515	BCR	C37-C22-C21	-2.27	119.13	122.82
23	c	505	CLA	O2A-CGA-O1A	-2.27	117.94	123.63
23	A	404[B]	CLA	CMA-C3A-C2A	-2.27	105.19	113.98
35	C	519	DGD	O2G-C1B-C2B	2.27	116.40	111.48
24	a	406[B]	PHO	OBD-CAD-C3D	-2.27	124.35	127.89
23	a	405[A]	CLA	C4-C3-C5	2.27	119.17	115.23
24	A	416[A]	PHO	C6-C5-C3	-2.27	107.94	113.47
34	C	522	HTG	C1-O5-C5	2.27	116.64	112.56
23	C	514	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
24	A	407[B]	PHO	O2A-CGA-O1A	-2.27	117.95	123.63
33	c	520	LMG	O8-C28-O10	-2.27	117.95	123.63
23	A	406[B]	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
23	c	505	CLA	C3B-C4B-NB	2.27	112.55	110.53
23	a	404[B]	CLA	CAC-C3C-C4C	2.27	127.74	124.79
23	b	601	CLA	C2A-C1A-CHA	-2.27	119.94	123.87
23	a	404[B]	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
25	k	101	BCR	C16-C17-C18	-2.26	124.11	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B	621	HTG	O2-C2-C3	-2.26	105.04	110.38
23	D	402[B]	CLA	CHD-C4C-NC	2.26	127.74	124.23
24	A	416[B]	PHO	O1D-CGD-CBD	-2.26	121.30	124.72
32	A	419[A]	LHG	O4-P-O5	2.26	122.95	112.44
23	C	504	CLA	C4B-C3B-C2B	-2.26	104.49	107.30
23	b	602	CLA	C11-C10-C8	-2.26	108.46	115.97
29	d	407[B]	PL9	C45-C44-C46	2.26	119.15	115.23
26	b	620	SQD	O47-C7-O49	-2.26	118.43	123.70
26	A	410[A]	SQD	O9-S-O7	-2.26	106.48	113.82
23	b	603	CLA	CAC-C3C-C4C	2.26	127.72	124.79
23	C	505	CLA	C1-C2-C3	-2.26	122.50	126.20
23	c	505	CLA	C4-C3-C5	2.25	119.14	115.23
25	C	516	BCR	C39-C30-C25	-2.25	106.71	110.24
23	A	404[B]	CLA	CMC-C2C-C1C	2.25	128.55	125.03
23	d	405	CLA	C1-O2A-CGA	2.25	122.10	116.65
23	b	609	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
25	C	515	BCR	C24-C23-C22	-2.25	122.90	126.23
25	b	619	BCR	C21-C20-C19	-2.25	116.67	123.20
23	C	512	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
23	b	615	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
23	C	506	CLA	CHA-C1A-NA	-2.25	121.30	126.39
29	D	405[B]	PL9	C7-C8-C9	-2.25	122.96	126.83
23	d	404[A]	CLA	CMC-C2C-C1C	2.25	128.55	125.03
40	V	201	HEC	C2A-C1A-NA	-2.25	108.16	110.32
35	C	517[A]	DGD	C3G-C2G-C1G	-2.25	106.55	111.78
26	b	620	SQD	O5-C1-C2	-2.25	105.76	110.37
23	c	513	CLA	C4-C3-C5	2.25	119.13	115.23
25	a	408	BCR	C11-C10-C9	-2.25	124.13	127.28
23	B	610	CLA	CHB-C4A-NA	2.25	127.64	124.40
40	V	201	HEC	CBA-CAA-C2A	-2.25	106.33	112.53
23	C	507	CLA	CGD-CBD-CAD	-2.24	103.58	110.85
24	d	403[A]	PHO	CED-O2D-CGD	2.24	121.00	115.92
23	A	404[A]	CLA	CMC-C2C-C1C	2.24	128.54	125.03
23	C	508	CLA	CBC-CAC-C3C	-2.24	106.34	112.42
23	c	511	CLA	C2A-C1A-CHA	-2.24	119.97	123.87
25	D	404	BCR	C30-C25-C24	2.24	121.73	115.65
23	b	610	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
35	c	517[A]	DGD	C2G-O2G-C1B	-2.24	112.43	117.80
23	B	610	CLA	CMC-C2C-C1C	2.24	128.53	125.03
25	a	408	BCR	C3-C4-C5	-2.24	110.06	114.06
23	B	602	CLA	C1-C2-C3	-2.24	122.53	126.20
23	B	603	CLA	C7-C6-C5	-2.24	107.30	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	601	CLA	CAA-C2A-C3A	-2.24	106.96	113.00
23	B	602	CLA	C11-C12-C13	-2.24	108.53	115.97
33	a	415	LMG	O8-C28-C29	2.23	118.65	111.83
23	C	505	CLA	C4-C3-C5	2.23	119.11	115.23
25	h	101	BCR	C11-C10-C9	-2.23	124.14	127.28
23	B	608	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
26	a	409[B]	SQD	O8-S-C6	2.23	110.28	105.97
24	d	403[A]	PHO	C4-C3-C2	-2.23	117.89	123.63
25	b	617	BCR	C20-C21-C22	-2.23	124.15	127.28
25	c	514	BCR	C36-C18-C17	-2.23	119.20	122.82
23	C	506	CLA	CHD-C4C-NC	2.23	127.69	124.23
35	H	102	DGD	O3G-C3G-C2G	-2.23	105.39	110.82
23	C	502	CLA	C1-C2-C3	-2.23	122.54	126.20
23	a	404[A]	CLA	C7-C6-C5	-2.23	107.32	113.26
25	b	617	BCR	C21-C20-C19	-2.23	116.74	123.20
23	D	403	CLA	CBC-CAC-C3C	-2.23	106.38	112.42
23	a	407	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
34	b	625	HTG	C1-C2-C3	-2.23	106.19	110.55
31	e	101	LMT	O1'-C1'-C2'	2.23	111.66	108.27
23	c	504	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
23	c	512	CLA	CBA-CAA-C2A	-2.23	107.17	113.79
35	c	518	DGD	O2G-C1B-O1B	-2.23	118.50	123.70
25	K	102	BCR	C29-C30-C25	2.22	113.67	110.44
26	X	101	SQD	O48-C23-O10	-2.22	118.07	123.63
25	t	102	BCR	C35-C13-C12	2.22	121.48	118.09
25	k	101	BCR	C36-C18-C19	2.22	121.48	118.09
31	C	525	LMT	O5'-C5'-C4'	2.22	114.31	109.72
23	C	511	CLA	CMC-C2C-C1C	2.22	128.50	125.03
35	C	518[B]	DGD	O1G-C1A-O1A	-2.22	118.08	123.63
31	m	103	LMT	C3B-C4B-C5B	-2.22	106.21	110.23
23	b	609	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
23	B	611	CLA	C1C-C2C-C3C	-2.22	104.65	106.98
23	B	606	CLA	OBD-CAD-C3D	-2.22	123.24	128.42
23	b	608	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
23	D	402[A]	CLA	C4-C3-C5	2.22	119.07	115.23
23	C	504	CLA	C2A-C1A-CHA	-2.22	120.02	123.87
23	c	509	CLA	C2A-C1A-CHA	-2.21	120.02	123.87
23	a	404[B]	CLA	CMA-C3A-C2A	-2.21	105.42	113.98
23	C	505	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
35	C	518[A]	DGD	C2G-O2G-C1B	-2.21	112.50	117.80
29	A	414[A]	PL9	C12-C13-C14	-2.21	122.56	127.62
23	D	402[B]	CLA	O2D-CGD-O1D	-2.21	119.54	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	CHB-C4A-NA	2.21	127.59	124.40
23	B	608	CLA	O2A-CGA-CBA	2.21	118.58	111.83
23	b	615	CLA	C1-C2-C3	-2.21	122.57	126.20
33	B	620	LMG	O8-C28-O10	-2.21	118.10	123.63
35	c	518	DGD	O3G-C3G-C2G	-2.21	105.44	110.82
23	a	405[A]	CLA	CAC-C3C-C4C	2.21	127.67	124.79
23	A	408	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
29	A	414[B]	PL9	C35-C34-C33	-2.21	117.95	123.63
23	B	611	CLA	CMA-C3A-C2A	-2.21	105.44	113.98
23	C	509	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
23	A	405[A]	CLA	O2A-CGA-CBA	2.21	118.56	111.83
23	c	512	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
23	d	405	CLA	C4B-C3B-C2B	-2.21	104.56	107.30
29	D	405[A]	PL9	C20-C19-C21	2.20	119.05	115.23
23	B	604	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
23	A	405[A]	CLA	CHB-C4A-NA	2.20	127.58	124.40
23	B	601	CLA	C1-C2-C3	-2.20	122.59	126.20
29	d	407[A]	PL9	C2-C1-C6	2.20	121.62	119.00
35	C	517[A]	DGD	O5D-C6D-C5D	-2.20	104.46	109.42
23	c	510	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
25	B	619	BCR	C34-C9-C8	2.20	121.45	118.09
38	f	101	HEM	C4C-NC-C1C	2.20	109.41	105.82
25	T	102	BCR	C3-C4-C5	-2.20	110.13	114.06
23	A	406[B]	CLA	CHB-C4A-NA	2.20	127.57	124.40
29	A	414[B]	PL9	C25-C24-C26	2.20	119.04	115.23
33	c	519	LMG	O8-C28-O10	-2.20	118.13	123.63
31	m	103	LMT	C1'-O5'-C5'	-2.20	109.43	113.72
25	y	101	BCR	C40-C30-C25	-2.20	106.80	110.24
23	D	403	CLA	CHB-C4A-NA	2.20	127.57	124.40
29	d	407[A]	PL9	C12-C13-C14	-2.19	122.60	127.62
25	Y	101	BCR	C36-C18-C17	-2.19	119.26	122.82
23	C	509	CLA	CAC-C3C-C4C	2.19	127.64	124.79
23	C	513	CLA	C3B-C4B-NB	2.19	112.49	110.53
23	B	612	CLA	CMA-C3A-C2A	-2.19	105.51	113.98
25	h	101	BCR	C29-C30-C25	2.19	113.62	110.44
23	c	506	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
25	h	101	BCR	C36-C18-C19	2.19	121.43	118.09
23	C	505	CLA	CMB-C2B-C1B	2.19	128.75	125.42
23	b	608	CLA	C11-C12-C13	-2.19	108.69	115.97
26	A	412	SQD	O6-C1-C2	2.19	111.60	108.27
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.92
23	B	608	CLA	CMB-C2B-C1B	2.19	128.75	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404[A]	CLA	CAC-C3C-C4C	2.19	127.64	124.79
25	D	404	BCR	C24-C23-C22	-2.19	123.00	126.23
26	l	101	SQD	O5-C1-C2	-2.19	105.88	110.37
23	b	601	CLA	CHB-C1B-C2B	-2.18	121.08	127.43
35	c	517[A]	DGD	O4E-C4E-C3E	-2.18	105.23	110.38
23	B	614	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
29	d	407[B]	PL9	C35-C34-C36	2.18	119.02	115.23
35	c	516[A]	DGD	O6D-C1D-O3G	-2.18	104.89	110.04
23	A	405[B]	CLA	O2A-CGA-CBA	2.18	118.48	111.83
23	c	502	CLA	C4C-C3C-C2C	-2.18	103.72	106.89
23	b	613	CLA	CMB-C2B-C1B	2.18	128.74	125.42
23	C	513	CLA	C4B-C3B-C2B	-2.18	104.59	107.30
25	C	516	BCR	C2-C1-C6	2.18	113.60	110.44
23	b	609	CLA	CAA-C2A-C3A	-2.18	107.12	113.00
29	d	407[B]	PL9	C15-C14-C16	2.18	119.01	115.23
25	t	102	BCR	C2-C1-C6	2.18	113.60	110.44
23	B	611	CLA	C4-C3-C5	2.18	119.00	115.23
33	C	521	LMG	C1-C2-C3	-2.18	105.43	110.01
24	d	403[B]	PHO	CED-O2D-CGD	2.17	120.85	115.92
35	C	517[B]	DGD	O1G-C1A-C2A	2.17	118.47	111.83
23	B	613	CLA	CHD-C4C-NC	2.17	127.60	124.23
23	D	403	CLA	CMA-C3A-C2A	-2.17	105.58	113.98
29	D	405[B]	PL9	C42-C41-C39	-2.17	105.98	113.19
25	h	101	BCR	C37-C22-C21	-2.17	119.30	122.82
32	b	629[A]	LHG	O7-C7-O9	-2.17	118.63	123.70
31	b	621	LMT	C1-O1'-C1'	2.17	117.39	113.68
25	a	408	BCR	C24-C23-C22	-2.17	123.03	126.23
31	b	627	LMT	O1'-C1'-C2'	2.17	111.57	108.27
25	D	404	BCR	C15-C16-C17	-2.17	119.08	123.52
26	X	101	SQD	O8-S-O7	-2.17	105.98	111.40
25	C	515	BCR	C38-C26-C25	-2.17	122.12	124.48
23	b	607	CLA	CMB-C2B-C1B	2.17	128.72	125.42
23	a	407	CLA	CHC-C1C-C2C	-2.17	120.79	126.95
32	E	101[A]	LHG	O7-C7-O9	-2.17	118.64	123.70
23	c	501	CLA	C2A-C1A-CHA	-2.16	120.11	123.87
25	b	618	BCR	C8-C7-C6	-2.16	121.22	127.00
25	H	101	BCR	C37-C22-C23	2.16	121.39	118.09
23	b	608	CLA	C4C-C3C-C2C	-2.16	103.74	106.89
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.89
29	D	405[A]	PL9	C12-C13-C14	-2.16	122.68	127.62
23	c	507	CLA	C4B-C3B-C2B	-2.16	104.61	107.30
23	B	607	CLA	C2A-C1A-CHA	-2.16	120.12	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	501	LMG	C12-C11-C10	-2.16	105.78	113.69
35	C	517[A]	DGD	O1G-C1A-O1A	-2.16	118.22	123.63
29	A	414[B]	PL9	C2-C3-C4	2.16	121.68	118.78
23	B	609	CLA	C16-C15-C13	-2.16	108.78	115.97
35	c	517[A]	DGD	O1G-C1A-O1A	-2.16	118.23	123.63
23	C	502	CLA	O2A-CGA-CBA	2.16	118.42	111.83
23	B	612	CLA	C4A-NA-C1A	-2.16	105.69	106.68
23	c	505	CLA	CMC-C2C-C1C	2.16	128.41	125.03
29	d	407[B]	PL9	C51-C49-C50	2.16	119.56	114.59
29	a	413[B]	PL9	C35-C34-C33	-2.16	118.08	123.63
31	M	101	LMT	O5B-C5B-C6B	2.16	111.79	106.44
23	C	511	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
23	c	503	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
23	C	508	CLA	CAC-C3C-C4C	2.16	127.60	124.79
35	C	517[A]	DGD	O6D-C1D-O3G	-2.16	104.95	110.04
23	C	511	CLA	CHB-C4A-NA	2.16	127.51	124.40
23	A	405[B]	CLA	CAA-CBA-CGA	2.16	119.33	113.21
23	B	606	CLA	C2A-C1A-CHA	-2.16	120.13	123.87
25	K	102	BCR	C15-C14-C13	-2.15	124.26	127.28
23	C	508	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
25	c	514	BCR	C37-C22-C21	-2.15	119.33	122.82
25	B	617	BCR	C16-C17-C18	-2.15	124.26	127.28
23	c	509	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
33	m	101	LMG	O8-C28-O10	-2.15	118.24	123.63
23	B	616	CLA	CMB-C2B-C3B	2.15	131.61	126.55
23	C	502	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
23	b	605	CLA	C4B-C3B-C2B	-2.15	104.63	107.30
34	b	622	HTG	O2-C2-C3	-2.15	105.31	110.38
26	a	409[B]	SQD	O9-S-C6	2.15	109.96	106.76
23	b	606	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
29	A	414[B]	PL9	C51-C49-C50	2.15	119.53	114.59
24	A	416[B]	PHO	OBD-CAD-C3D	-2.15	124.54	127.89
31	M	101	LMT	C1-O1'-C1'	2.15	117.35	113.68
23	C	509	CLA	CAA-C2A-C3A	-2.15	107.20	113.00
25	d	406	BCR	C37-C22-C23	2.15	121.37	118.09
29	d	407[B]	PL9	C12-C13-C14	-2.15	122.71	127.62
23	B	616	CLA	C4-C3-C2	-2.14	118.12	123.63
23	C	502	CLA	CAA-C2A-C3A	-2.14	107.20	113.00
23	c	509	CLA	C4-C3-C2	-2.14	118.12	123.63
23	A	408	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
23	C	513	CLA	OBD-CAD-C3D	-2.14	123.41	128.42
35	C	518[B]	DGD	O2G-C1B-O1B	-2.14	118.70	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404[B]	CLA	CMC-C2C-C1C	2.14	128.38	125.03
23	B	609	CLA	C2A-C1A-CHA	-2.14	120.15	123.87
23	b	609	CLA	O2A-CGA-CBA	2.14	118.36	111.83
24	a	406[A]	PHO	CBA-CAA-C2A	-2.14	107.47	113.78
23	B	616	CLA	OBD-CAD-C3D	-2.14	123.42	128.42
23	c	505	CLA	C1-C2-C3	-2.14	122.70	126.20
23	B	606	CLA	CHB-C1B-C2B	-2.13	121.24	127.43
26	A	410[B]	SQD	O8-S-C6	2.13	110.09	105.97
25	y	101	BCR	C1-C6-C7	2.13	121.43	115.65
23	C	504	CLA	CHB-C1B-C2B	-2.13	121.25	127.43
23	b	607	CLA	C1-C2-C3	-2.13	122.71	126.20
33	C	501	LMG	O8-C28-C29	2.13	118.32	111.83
25	b	619	BCR	C16-C15-C14	-2.13	119.17	123.52
25	a	408	BCR	C37-C22-C21	-2.13	119.37	122.82
23	a	407	CLA	C2A-C1A-CHA	-2.13	120.17	123.87
32	D	407[A]	LHG	O4-P-O5	2.13	122.34	112.44
23	B	615	CLA	CHA-C1A-NA	-2.13	121.57	126.39
34	c	521	HTG	O5-C1-C2	2.13	113.25	110.32
23	C	513	CLA	C4-C3-C2	-2.12	118.17	123.63
23	b	605	CLA	CED-O2D-CGD	2.12	120.73	115.92
23	c	512	CLA	CHA-C1A-NA	-2.12	121.58	126.39
25	Y	101	BCR	C28-C27-C26	-2.12	110.27	114.06
24	d	403[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
23	a	404[B]	CLA	CHB-C4A-NA	2.12	127.46	124.40
23	B	602	CLA	C1-O2A-CGA	2.12	121.79	116.65
25	T	102	BCR	C15-C14-C13	2.12	130.25	127.28
31	B	627	LMT	C1B-C2B-C3B	2.12	114.47	110.01
23	b	613	CLA	C2A-C1A-CHA	-2.12	120.19	123.87
33	C	520	LMG	O7-C10-O9	-2.12	118.75	123.70
23	C	504	CLA	C3B-C4B-NB	2.12	112.42	110.53
38	E	102	HEM	CHA-C1A-NA	2.12	127.70	123.86
23	C	502	CLA	OBD-CAD-C3D	-2.12	123.47	128.42
25	B	617	BCR	C37-C22-C23	2.12	121.32	118.09
29	D	405[A]	PL9	O2-C1-C6	-2.12	117.11	120.48
33	Z	101	LMG	C9-C8-C7	-2.12	106.85	111.78
25	d	406	BCR	C29-C28-C27	-2.12	106.63	111.28
29	A	414[A]	PL9	C51-C49-C50	2.11	119.46	114.59
23	d	402[B]	CLA	C4-C3-C5	2.11	118.90	115.23
23	B	611	CLA	O2A-CGA-CBA	2.11	118.28	111.83
29	A	414[B]	PL9	C37-C36-C34	-2.11	106.18	113.19
35	C	519	DGD	O3G-C3G-C2G	-2.11	105.68	110.82
23	b	604	CLA	C6-C5-C3	-2.11	108.33	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	CAA-C2A-C3A	-2.11	107.30	113.00
23	C	513	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
23	a	404[A]	CLA	CMB-C2B-C3B	2.11	131.51	126.55
25	K	102	BCR	C39-C30-C25	-2.11	106.94	110.24
24	A	407[A]	PHO	CBA-CAA-C2A	-2.11	107.57	113.78
23	B	613	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	c	505	CLA	C2A-C1A-CHA	-2.11	120.21	123.87
23	C	508	CLA	C3B-C4B-NB	2.11	112.41	110.53
23	c	511	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
29	d	407[A]	PL9	C35-C34-C36	2.11	118.88	115.23
24	d	403[A]	PHO	O2A-CGA-CBA	2.10	118.25	111.83
23	b	602	CLA	C1-O2A-CGA	2.10	121.74	116.65
26	f	102	SQD	O48-C23-O10	-2.10	118.37	123.63
23	C	513	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
33	d	413	LMG	C8-O7-C10	-2.10	112.76	117.80
31	b	627	LMT	C1'-O5'-C5'	-2.10	109.61	113.72
24	A	416[A]	PHO	CMB-C2B-C3B	2.10	128.88	124.68
23	A	404[B]	CLA	CAA-CBA-CGA	-2.10	107.24	113.21
23	b	610	CLA	CMC-C2C-C1C	2.10	128.32	125.03
23	d	404[A]	CLA	CHD-C4C-NC	2.10	127.49	124.23
29	A	414[A]	PL9	C25-C24-C26	2.10	118.87	115.23
26	b	620	SQD	O9-S-C6	2.10	109.89	106.76
29	d	407[A]	PL9	C51-C49-C50	2.10	119.42	114.59
23	C	511	CLA	C4-C3-C2	-2.10	118.24	123.63
23	b	603	CLA	C5-C3-C2	-2.10	116.46	121.17
26	l	101	SQD	C44-O6-C1	-2.09	109.31	113.80
23	c	508	CLA	C2A-C1A-CHA	-2.09	120.23	123.87
32	d	409[B]	LHG	O8-C23-O10	-2.09	118.39	123.63
23	C	508	CLA	C6-C7-C8	-2.09	109.00	115.97
35	c	517[B]	DGD	C2G-O2G-C1B	-2.09	112.78	117.80
32	d	415[B]	LHG	O7-C7-O9	-2.09	118.81	123.70
23	b	615	CLA	CHA-C1A-NA	-2.09	121.65	126.39
29	A	414[A]	PL9	O1-C4-C3	-2.09	118.52	120.73
23	d	404[B]	CLA	CMB-C2B-C1B	2.09	128.60	125.42
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.26
25	c	515	BCR	C15-C16-C17	-2.09	119.24	123.52
23	A	405[A]	CLA	C1-C2-C3	-2.09	122.77	126.20
23	B	607	CLA	C1-C2-C3	-2.09	122.77	126.20
24	A	407[B]	PHO	C4-C3-C5	2.09	118.85	115.23
23	c	510	CLA	CED-O2D-CGD	2.09	120.65	115.92
25	c	514	BCR	C21-C20-C19	-2.09	117.15	123.20
23	b	614	CLA	CMA-C3A-C2A	-2.09	105.92	113.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	BCR	C33-C5-C6	-2.09	122.21	124.48
32	d	409[B]	LHG	C5-O7-C7	-2.09	112.81	117.80
23	b	602	CLA	CMA-C3A-C2A	-2.08	105.92	113.98
23	b	616	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
25	c	514	BCR	C15-C16-C17	-2.08	119.25	123.52
23	A	405[B]	CLA	C4C-C3C-C2C	-2.08	103.86	106.89
25	H	101	BCR	C31-C1-C6	-2.08	106.97	110.24
23	c	509	CLA	O2A-C1-C2	2.08	116.12	108.11
23	A	408	CLA	OBD-CAD-C3D	-2.08	123.55	128.42
25	Y	101	BCR	C3-C4-C5	-2.08	110.34	114.06
25	A	409	BCR	C11-C10-C9	-2.08	124.36	127.28
26	a	409[A]	SQD	O7-S-C6	2.08	109.86	106.76
23	B	614	CLA	CMA-C3A-C2A	-2.08	105.94	113.98
23	b	609	CLA	CHA-C1A-NA	-2.08	121.68	126.39
29	a	413[B]	PL9	C10-C9-C8	-2.08	118.29	123.63
23	C	511	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
31	M	101	LMT	O1B-C1B-C2B	2.08	113.20	108.09
34	B	622	HTG	C1-C2-C3	2.08	114.61	110.55
26	f	102	SQD	O8-S-C6	2.08	109.98	105.97
24	a	406[B]	PHO	CAC-C3C-C4C	2.07	129.36	124.03
23	C	502	CLA	C11-C12-C13	-2.07	109.07	115.97
23	B	616	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
33	m	101	LMG	C3-C4-C5	2.07	113.99	110.23
24	d	403[B]	PHO	O2A-CGA-CBA	2.07	118.15	111.83
23	c	506	CLA	CGD-CBD-CAD	-2.07	104.14	110.85
23	B	604	CLA	CED-O2D-CGD	2.07	120.61	115.92
23	b	608	CLA	CMA-C3A-C2A	-2.07	105.98	113.98
24	a	406[A]	PHO	CBC-CAC-C3C	-2.07	109.91	112.87
23	C	505	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
23	D	402[B]	CLA	CED-O2D-CGD	2.07	120.60	115.92
26	a	409[B]	SQD	O48-C23-O10	-2.06	118.46	123.63
35	C	517[A]	DGD	O1G-C1A-C2A	2.06	118.13	111.83
25	H	101	BCR	C29-C30-C25	2.06	113.44	110.44
23	B	611	CLA	CED-O2D-CGD	2.06	120.59	115.92
25	H	101	BCR	C16-C15-C14	-2.06	119.30	123.52
26	A	412	SQD	O6-C44-C45	-2.06	105.80	110.82
26	a	409[A]	SQD	O48-C23-O10	-2.06	118.47	123.63
35	h	102	DGD	O3G-C1D-C2D	2.06	111.40	108.27
25	D	404	BCR	C29-C28-C27	-2.06	106.75	111.28
35	H	102	DGD	C3E-C4E-C5E	-2.06	106.50	110.23
23	D	402[A]	CLA	CMB-C2B-C1B	2.06	128.56	125.42
31	F	101	LMT	C3B-C4B-C5B	-2.06	106.50	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	520	LMG	O1-C1-C2	-2.06	105.15	108.27
23	b	615	CLA	C6-C7-C8	-2.06	109.12	115.97
23	C	504	CLA	CMC-C2C-C1C	2.06	128.25	125.03
33	c	520	LMG	C1-O6-C5	2.06	117.74	113.72
23	B	601	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
29	D	405[B]	PL9	O2-C1-C6	-2.06	117.21	120.48
23	B	610	CLA	C1-C2-C3	-2.06	122.83	126.20
25	t	102	BCR	C28-C27-C26	-2.05	110.39	114.06
25	A	409	BCR	C15-C14-C13	-2.05	124.40	127.28
23	b	614	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
23	c	508	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
23	a	404[B]	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
33	c	519	LMG	O7-C10-O9	-2.05	118.91	123.70
33	C	501	LMG	O6-C1-O1	-2.05	105.19	110.04
23	b	612	CLA	OBD-CAD-C3D	-2.05	123.62	128.42
26	X	101	SQD	O5-C1-C2	-2.05	106.16	110.37
29	a	413[B]	PL9	C51-C49-C50	2.05	119.31	114.59
25	h	101	BCR	C36-C18-C17	-2.05	119.49	122.82
26	a	409[B]	SQD	C3-C4-C5	2.05	113.95	110.23
25	b	618	BCR	C21-C20-C19	-2.05	117.26	123.20
23	C	510	CLA	C4-C3-C5	2.05	118.79	115.23
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
23	c	507	CLA	CAC-C3C-C4C	2.05	127.46	124.79
33	D	411	LMG	C9-C8-C7	-2.05	107.00	111.78
23	a	404[B]	CLA	CMC-C2C-C1C	2.05	128.24	125.03
23	B	613	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
23	D	402[A]	CLA	CMA-C3A-C2A	-2.05	106.06	113.98
31	b	621	LMT	C2'-C3'-C4'	2.05	114.33	109.68
25	k	101	BCR	C21-C20-C19	-2.05	117.27	123.20
25	C	515	BCR	C10-C11-C12	-2.05	117.27	123.20
25	B	618	BCR	C28-C27-C26	-2.05	110.41	114.06
23	d	402[A]	CLA	CAA-CBA-CGA	2.04	119.01	113.21
32	E	101[B]	LHG	C5-O7-C7	-2.04	112.90	117.80
33	z	101	LMG	C8-O7-C10	-2.04	112.90	117.80
23	d	404[A]	CLA	CBC-CAC-C3C	-2.04	106.88	112.42
23	C	507	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
32	D	406[A]	LHG	O4-P-O5	2.04	121.95	112.44
25	h	101	BCR	C33-C5-C6	-2.04	122.25	124.48
29	D	405[A]	PL9	C25-C24-C23	-2.04	118.38	123.63
23	b	611	CLA	CHB-C4A-NA	2.04	127.35	124.40
23	A	404[A]	CLA	CHB-C4A-NA	2.04	127.34	124.40
23	D	402[A]	CLA	CBC-CAC-C3C	-2.04	106.89	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	407	CLA	CAC-C3C-C4C	2.04	127.44	124.79
29	a	413[B]	PL9	C12-C13-C14	-2.04	122.95	127.62
35	C	519	DGD	O1G-C1A-O1A	-2.04	118.53	123.63
24	d	403[B]	PHO	C4-C3-C2	-2.04	118.39	123.63
35	c	518	DGD	O3G-C1D-C2D	-2.04	105.18	108.27
35	c	517[B]	DGD	O6E-C1E-O5D	-2.04	105.23	110.04
32	d	415[A]	LHG	C5-O7-C7	-2.04	112.92	117.80
25	t	102	BCR	C36-C18-C19	2.04	121.20	118.09
23	B	607	CLA	C1-O2A-CGA	2.04	121.58	116.65
23	d	404[B]	CLA	CED-O2D-CGD	2.04	120.53	115.92
23	B	610	CLA	CAC-C3C-C4C	2.04	127.44	124.79
23	b	601	CLA	CMC-C2C-C1C	2.03	128.21	125.03
23	B	607	CLA	CAC-C3C-C4C	2.03	127.44	124.79
23	B	615	CLA	CAC-C3C-C4C	2.03	127.44	124.79
23	c	512	CLA	C4B-C3B-C2B	-2.03	104.77	107.30
23	C	510	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
23	b	612	CLA	CMB-C2B-C1B	2.03	128.52	125.42
23	c	505	CLA	C1-O2A-CGA	2.03	121.57	116.65
23	B	601	CLA	CBC-CAC-C3C	-2.03	106.91	112.42
23	B	614	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
25	k	101	BCR	C20-C21-C22	-2.03	124.43	127.28
23	b	616	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
33	m	101	LMG	O7-C10-O9	-2.03	118.95	123.70
32	L	101[B]	LHG	C5-O7-C7	-2.03	112.93	117.80
25	b	617	BCR	C15-C16-C17	-2.03	119.36	123.52
35	c	516[B]	DGD	O1G-C1A-C2A	2.03	118.03	111.83
26	b	620	SQD	C44-O6-C1	-2.03	109.44	113.80
23	b	616	CLA	C11-C12-C13	-2.03	109.22	115.97
23	A	404[A]	CLA	C4-C3-C5	2.03	118.75	115.23
23	C	507	CLA	CHB-C4A-NA	2.03	127.33	124.40
23	b	614	CLA	CED-O2D-CGD	2.03	120.52	115.92
25	D	404	BCR	C31-C1-C6	-2.03	107.06	110.24
23	A	405[B]	CLA	CED-O2D-CGD	2.03	120.52	115.92
23	C	508	CLA	CBB-CAB-C3B	-2.03	117.39	127.53
29	D	405[A]	PL9	C30-C29-C31	2.03	118.75	115.23
24	a	406[A]	PHO	O2D-CGD-O1D	-2.03	119.90	123.85
23	A	408	CLA	C11-C12-C13	-2.03	109.23	115.97
33	C	520	LMG	O1-C7-C8	-2.03	105.89	110.82
23	B	603	CLA	C2A-C3A-C4A	-2.03	98.59	101.87
23	b	610	CLA	C4-C3-C2	-2.03	118.42	123.63
25	B	617	BCR	C34-C9-C8	2.03	121.18	118.09
23	a	405[A]	CLA	CAA-CBA-CGA	2.02	118.96	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	H	101	BCR	C20-C21-C22	-2.02	124.44	127.28
24	A	416[B]	PHO	C4A-C3A-C2A	-2.02	100.91	102.84
23	c	501	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
23	a	405[A]	CLA	CMA-C3A-C2A	-2.02	106.16	113.98
35	C	517[A]	DGD	C3E-C4E-C5E	2.02	113.90	110.23
27	o	303	GOL	C3-C2-C1	-2.02	104.38	111.80
23	C	513	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
23	b	616	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
23	c	511	CLA	C11-C10-C8	-2.02	109.25	115.97
23	b	612	CLA	C4D-CHA-C1A	-2.02	118.83	121.24
26	a	409[B]	SQD	O9-S-O7	-2.02	107.25	113.82
33	z	101	LMG	O8-C28-O10	-2.02	118.58	123.63
33	Z	101	LMG	C1-O6-C5	2.02	117.66	113.72
24	A	416[A]	PHO	CED-O2D-CGD	2.02	120.49	115.92
23	c	511	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
25	c	515	BCR	C29-C30-C25	2.02	113.37	110.44
32	L	101[B]	LHG	O8-C23-O10	-2.02	118.59	123.63
31	F	101	LMT	C2'-C3'-C4'	2.01	114.25	109.68
23	C	506	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
25	Y	101	BCR	C21-C20-C19	-2.01	117.36	123.20
25	T	102	BCR	C7-C8-C9	-2.01	123.26	126.23
23	c	512	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
23	A	405[A]	CLA	C4D-C3D-CAD	-2.01	105.92	108.11
25	c	515	BCR	C38-C26-C25	-2.01	122.29	124.48
23	A	406[A]	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	c	502	CLA	C2A-C1A-CHA	-2.01	120.38	123.87
23	b	603	CLA	CHB-C1B-C2B	-2.01	121.59	127.43
33	c	520	LMG	C1-C2-C3	-2.01	105.78	110.01
23	B	603	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
23	b	603	CLA	CHB-C4A-NA	2.01	127.30	124.40
23	c	508	CLA	CAC-C3C-C4C	2.01	127.40	124.79
25	B	617	BCR	C31-C1-C6	-2.01	107.09	110.24
26	A	410[B]	SQD	C45-O47-C7	-2.01	112.99	117.80
31	A	417	LMT	O1'-C1'-C2'	2.01	111.32	108.27
23	c	512	CLA	CBC-CAC-C3C	-2.00	106.99	112.42
23	c	507	CLA	CHA-C1A-NA	-2.00	121.85	126.39
23	b	602	CLA	CHB-C4A-NA	2.00	127.29	124.40
35	C	519	DGD	O6E-C5E-C6E	2.00	111.40	106.44
24	A	407[A]	PHO	C4-C3-C5	2.00	118.70	115.23
25	H	101	BCR	C11-C10-C9	-2.00	124.47	127.28
23	b	612	CLA	CMA-C3A-C2A	-2.00	106.24	113.98

All (71) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	A	404[A]	CLA	ND
23	A	404[B]	CLA	ND
23	A	405[B]	CLA	ND
23	A	408	CLA	ND
23	B	601	CLA	ND
23	B	602	CLA	ND
23	B	603	CLA	ND
23	B	604	CLA	ND
23	B	605	CLA	ND
23	B	606	CLA	ND
23	B	607	CLA	ND
23	B	609	CLA	ND
23	B	610	CLA	ND
23	B	611	CLA	ND
23	B	612	CLA	ND
23	B	613	CLA	ND
23	B	614	CLA	ND
23	B	615	CLA	ND
23	B	616	CLA	ND
23	C	502	CLA	ND
23	C	503	CLA	ND
23	C	504	CLA	ND
23	C	505	CLA	ND
23	C	506	CLA	ND
23	C	507	CLA	ND
23	C	508	CLA	ND
23	C	509	CLA	ND
23	C	510	CLA	ND
23	C	511	CLA	ND
23	C	512	CLA	ND
23	C	513	CLA	ND
23	C	514	CLA	ND
23	D	402[A]	CLA	ND
23	D	402[B]	CLA	ND
23	D	403	CLA	ND
23	a	404[A]	CLA	ND
23	a	404[B]	CLA	ND
23	a	407	CLA	ND
23	b	601	CLA	ND
23	b	602	CLA	ND
23	b	603	CLA	ND
23	b	604	CLA	ND
23	b	605	CLA	ND

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Mol	Chain	Res	Type	Atom
23	b	606	CLA	ND
23	b	607	CLA	ND
23	b	609	CLA	ND
23	b	610	CLA	ND
23	b	611	CLA	ND
23	b	612	CLA	ND
23	b	613	CLA	ND
23	b	614	CLA	ND
23	b	615	CLA	ND
23	b	616	CLA	ND
23	c	501	CLA	ND
23	c	502	CLA	ND
23	c	503	CLA	ND
23	c	504	CLA	ND
23	c	505	CLA	ND
23	c	506	CLA	ND
23	c	507	CLA	ND
23	c	508	CLA	ND
23	c	509	CLA	ND
23	c	510	CLA	ND
23	c	511	CLA	ND
23	c	512	CLA	ND
23	c	513	CLA	ND
23	d	402[A]	CLA	ND
23	d	402[B]	CLA	ND
23	d	404[A]	CLA	ND
23	d	404[B]	CLA	ND
23	d	405	CLA	ND

All (1555) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C14-C13-C15-C16
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C4B-C3B-CAB-CBB
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	X	101	SQD	O49-C7-O47-C45
26	X	101	SQD	C8-C7-O47-C45
26	a	411	SQD	O6-C44-C45-O47
26	a	411	SQD	C5-C6-S-O7
26	a	411	SQD	C5-C6-S-O8
26	a	411	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
26	l	101	SQD	O49-C7-O47-C45
27	A	411	GOL	O1-C1-C2-O2
27	A	411	GOL	O1-C1-C2-C3
27	B	623	GOL	C1-C2-C3-O3
27	D	412	GOL	C1-C2-C3-O3
27	O	302	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	C1-C2-C3-O3
27	a	410	GOL	O1-C1-C2-C3
27	b	624	GOL	C1-C2-C3-O3
27	c	526	GOL	C1-C2-C3-O3
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	413[A]	PL9	C25-C24-C26-C27
31	B	629	LMT	O5'-C1'-O1'-C1
31	B	629	LMT	C2-C1-O1'-C1'
31	C	525	LMT	O5'-C1'-O1'-C1
31	F	101	LMT	C2'-C1'-O1'-C1
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	t	101	LMT	O5'-C1'-O1'-C1
32	D	406[A]	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5
32	D	406[A]	LHG	C3-O3-P-O6
32	D	406[A]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	O2-C2-C3-O3
32	D	406[B]	LHG	C3-O3-P-O4
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O3
32	D	406[B]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O3
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C3-O3-P-O4
32	a	419[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	O10-C23-O8-C6
32	a	419[A]	LHG	C24-C23-O8-C6
32	a	419[B]	LHG	C3-O3-P-O4
32	a	419[B]	LHG	C3-O3-P-O6
32	a	419[B]	LHG	C4-O6-P-O3
32	a	419[B]	LHG	C4-O6-P-O5
32	a	419[B]	LHG	O10-C23-O8-C6
32	a	419[B]	LHG	C24-C23-O8-C6
32	b	629[A]	LHG	C4-O6-P-O3
32	b	629[A]	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
32	b	629[A]	LHG	C4-O6-P-O5
32	b	629[B]	LHG	C4-O6-P-O3
32	b	629[B]	LHG	C4-O6-P-O4
32	b	629[B]	LHG	C4-O6-P-O5
32	d	408[A]	LHG	C3-O3-P-O5
32	d	408[A]	LHG	C3-O3-P-O6
32	d	408[A]	LHG	C4-O6-P-O4
32	d	408[B]	LHG	C3-O3-P-O4
32	d	408[B]	LHG	C3-O3-P-O5
32	d	408[B]	LHG	C3-O3-P-O6
32	d	408[B]	LHG	C4-O6-P-O3
32	d	408[B]	LHG	C4-O6-P-O4
32	d	415[A]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	520	LMG	O9-C10-O7-C8
33	c	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
38	E	102	HEM	C2C-C3C-CAC-CBC
38	E	102	HEM	C4C-C3C-CAC-CBC
40	V	201	HEC	C2B-C3B-CAB-CBB
40	V	201	HEC	C4B-C3B-CAB-CBB
40	V	201	HEC	C2C-C3C-CAC-CBC
40	V	201	HEC	C4C-C3C-CAC-CBC
40	v	201	HEC	C2B-C3B-CAB-CBB
40	v	201	HEC	C4B-C3B-CAB-CBB
40	v	201	HEC	C2C-C3C-CAC-CBC
40	v	201	HEC	C4C-C3C-CAC-CBC
31	C	525	LMT	O5B-C1B-O1B-C4'
31	B	628	LMT	C4'-C5'-C6'-O6'
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
33	z	101	LMG	O9-C10-O7-C8
23	B	614	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	D	403	CLA	C3-C5-C6-C7
23	d	405	CLA	C3-C5-C6-C7
31	B	628	LMT	O5B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	l	101	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	d	405	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C25-C24-C26-C27
23	a	407	CLA	C2-C3-C5-C6
23	d	405	CLA	C2-C3-C5-C6
31	T	101	LMT	O5'-C5'-C6'-O6'
31	a	416	LMT	O5B-C5B-C6B-O6B
23	b	616	CLA	C3-C5-C6-C7
23	c	512	CLA	C3-C5-C6-C7
31	T	101	LMT	C4B-C5B-C6B-O6B
31	F	101	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	O5-C5-C6-O6
33	C	521	LMG	O9-C10-O7-C8
23	A	408	CLA	C3-C5-C6-C7
32	E	101[A]	LHG	O2-C2-C3-O3
32	E	101[B]	LHG	O2-C2-C3-O3
32	d	408[A]	LHG	O2-C2-C3-O3
32	d	408[B]	LHG	O2-C2-C3-O3
31	b	621	LMT	O5'-C5'-C6'-O6'
31	B	627	LMT	C4'-C5'-C6'-O6'
31	m	103	LMT	C4B-C5B-C6B-O6B
26	A	410[B]	SQD	C8-C7-O47-C45
33	C	521	LMG	O6-C5-C6-O5
33	c	520	LMG	C4-C5-C6-O5
34	D	410	HTG	C4-C5-C6-O6
34	b	625	HTG	S1-C1'-C2'-C3'
23	C	508	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	a	413[A]	PL9	C30-C29-C31-C32
29	a	413[B]	PL9	C30-C29-C31-C32
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
29	a	413[A]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C28-C29-C31-C32
29	a	413[B]	PL9	C13-C14-C16-C17
29	a	413[B]	PL9	C28-C29-C31-C32
31	b	627	LMT	O5'-C5'-C6'-O6'
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C14-C16-C17-C18
29	D	405[A]	PL9	C39-C41-C42-C43
29	a	413[A]	PL9	C9-C11-C12-C13
29	a	413[A]	PL9	C14-C16-C17-C18
29	a	413[B]	PL9	C9-C11-C12-C13
29	a	413[B]	PL9	C14-C16-C17-C18
31	B	628	LMT	C4B-C5B-C6B-O6B
31	T	101	LMT	C4'-C5'-C6'-O6'
31	a	416	LMT	C4B-C5B-C6B-O6B
34	b	625	HTG	O5-C5-C6-O6
31	F	101	LMT	C4'-C5'-C6'-O6'
26	l	101	SQD	O5-C1-O6-C44
31	A	417	LMT	O5'-C1'-O1'-C1
31	C	525	LMT	O5'-C5'-C6'-O6'
33	c	520	LMG	O6-C5-C6-O5
23	a	407	CLA	CBA-CGA-O2A-C1
23	C	504	CLA	CBD-CGD-O2D-CED
31	C	525	LMT	O5B-C5B-C6B-O6B
31	t	101	LMT	O5'-C5'-C6'-O6'
31	B	627	LMT	O5B-C5B-C6B-O6B
31	B	627	LMT	O5'-C5'-C6'-O6'
31	B	628	LMT	O5'-C5'-C6'-O6'
31	B	629	LMT	O5'-C5'-C6'-O6'
31	T	101	LMT	O5B-C5B-C6B-O6B
31	e	101	LMT	C4'-C5'-C6'-O6'
23	c	511	CLA	CBD-CGD-O2D-CED
31	B	627	LMT	C6-C7-C8-C9
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	408[A]	LHG	C1-C2-C3-O3
23	C	514	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CBD-CGD-O2D-CED
31	b	621	LMT	C4'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	c	507	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	413[A]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C15-C14-C16-C17
23	A	408	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	C	505	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
29	A	414[B]	PL9	C28-C29-C31-C32
29	a	413[A]	PL9	C23-C24-C26-C27
29	a	413[B]	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
23	C	503	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	b	616	CLA	C6-C7-C8-C9
23	c	504	CLA	C11-C12-C13-C14
23	c	509	CLA	C11-C10-C8-C9
31	C	525	LMT	C4B-C5B-C6B-O6B
26	X	101	SQD	C2-C1-O6-C44
31	A	417	LMT	C2'-C1'-O1'-C1
31	B	628	LMT	C2'-C1'-O1'-C1
31	C	525	LMT	C2'-C1'-O1'-C1
35	c	517[B]	DGD	C1B-C2B-C3B-C4B
31	B	627	LMT	C4B-C5B-C6B-O6B
31	b	627	LMT	C4'-C5'-C6'-O6'
25	b	619	BCR	C7-C8-C9-C34
34	D	410	HTG	S1-C1'-C2'-C3'
31	m	103	LMT	O5B-C5B-C6B-O6B
25	b	619	BCR	C7-C8-C9-C10
26	X	101	SQD	C23-C24-C25-C26
27	O	303	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	A	408	CLA	C12-C13-C15-C16
34	d	412	HTG	S1-C1'-C2'-C3'
33	B	620	LMG	C39-C40-C41-C42
31	a	416	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	C10-C11-C12-C13
26	l	101	SQD	C7-C8-C9-C10
25	T	102	BCR	C13-C14-C15-C16
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[B]	PL9	C39-C41-C42-C43
29	d	407[A]	PL9	C39-C41-C42-C43
29	d	407[B]	PL9	C39-C41-C42-C43
23	b	611	CLA	C15-C16-C17-C18
32	D	407[A]	LHG	C33-C34-C35-C36
23	B	601	CLA	C5-C6-C7-C8
23	c	512	CLA	C15-C16-C17-C18
31	C	525	LMT	O1'-C1-C2-C3
31	C	525	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C5-C6-C7-C8
23	C	508	CLA	C5-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
34	B	624	HTG	O5-C5-C6-O6
35	c	517[A]	DGD	C1B-C2B-C3B-C4B
23	a	407	CLA	O1A-CGA-O2A-C1
33	B	620	LMG	C15-C16-C17-C18
26	X	101	SQD	O5-C1-O6-C44
31	B	628	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
23	B	606	CLA	C10-C11-C12-C13
23	B	614	CLA	C8-C10-C11-C12
23	b	601	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
31	e	101	LMT	O5'-C5'-C6'-O6'
33	d	413	LMG	C10-C11-C12-C13
33	Z	101	LMG	C10-C11-C12-C13
31	e	101	LMT	O5B-C5B-C6B-O6B
31	C	525	LMT	C5'-C4'-O1B-C1B
23	b	605	CLA	C8-C10-C11-C12
23	c	513	CLA	C10-C11-C12-C13
32	E	101[A]	LHG	C23-C24-C25-C26
23	C	503	CLA	C13-C15-C16-C17
23	c	509	CLA	O1A-CGA-O2A-C1
33	B	620	LMG	O9-C10-O7-C8
32	D	406[A]	LHG	C1-C2-C3-O3
32	d	408[B]	LHG	C1-C2-C3-O3
23	B	606	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	CBA-CGA-O2A-C1
35	C	519	DGD	C6B-C7B-C8B-C9B
23	C	509	CLA	C10-C11-C12-C13
23	D	403	CLA	C10-C11-C12-C13
31	B	627	LMT	C5'-C4'-O1B-C1B
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
23	B	614	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
32	D	407[B]	LHG	C33-C34-C35-C36
31	M	101	LMT	O5'-C5'-C6'-O6'
31	m	103	LMT	O5'-C5'-C6'-O6'
31	B	629	LMT	C4'-C5'-C6'-O6'
34	b	622	HTG	S1-C1'-C2'-C3'
23	a	404[A]	CLA	C15-C16-C17-C18
23	a	404[B]	CLA	C15-C16-C17-C18
23	b	606	CLA	C10-C11-C12-C13
23	b	611	CLA	C8-C10-C11-C12
23	D	403	CLA	C4-C3-C5-C6
23	c	504	CLA	C4-C3-C5-C6
23	B	602	CLA	C13-C15-C16-C17
33	B	620	LMG	C11-C10-O7-C8
23	B	613	CLA	C11-C12-C13-C14
26	A	412	SQD	C2-C1-O6-C44
31	B	629	LMT	C2'-C1'-O1'-C1
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
34	b	623	HTG	C1'-C2'-C3'-C4'
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
26	l	101	SQD	C30-C31-C32-C33
23	B	603	CLA	C13-C15-C16-C17
25	D	404	BCR	C37-C22-C23-C24
25	K	102	BCR	C7-C8-C9-C34
34	B	624	HTG	S1-C1'-C2'-C3'
25	D	404	BCR	C21-C22-C23-C24
23	B	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C15-C16-C17-C18
23	c	506	CLA	C15-C16-C17-C18
27	B	623	GOL	O1-C1-C2-C3
27	B	626	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	V	203[B]	GOL	C1-C2-C3-O3
27	a	410	GOL	C1-C2-C3-O3
27	a	417	GOL	O1-C1-C2-C3
27	d	414	GOL	O1-C1-C2-C3
27	l	103[B]	GOL	O1-C1-C2-C3
27	o	303	GOL	C1-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-C3
32	A	419[B]	LHG	O1-C1-C2-C3
26	A	410[A]	SQD	C7-C8-C9-C10
23	B	603	CLA	C16-C17-C18-C20
23	a	407	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
35	C	519	DGD	CAB-CBB-CCB-CDB
31	A	417	LMT	O1'-C1-C2-C3
31	b	621	LMT	O5'-C1'-O1'-C1
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
34	B	621	HTG	C1'-C2'-C3'-C4'
35	c	516[B]	DGD	C2A-C1A-O1G-C1G
35	c	516[B]	DGD	O6D-C5D-C6D-O5D
23	B	616	CLA	C2-C1-O2A-CGA
23	B	615	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
23	b	614	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
23	d	405	CLA	C16-C17-C18-C20
31	C	525	LMT	C1-C2-C3-C4
35	h	102	DGD	C6B-C7B-C8B-C9B
26	A	410[A]	SQD	C15-C16-C17-C18
26	X	101	SQD	C30-C31-C32-C33
31	t	101	LMT	C4-C5-C6-C7
32	L	101[A]	LHG	C12-C13-C14-C15
32	d	415[A]	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	C	521	LMG	C18-C19-C20-C21
33	a	415	LMG	C30-C31-C32-C33
34	B	622	HTG	C3'-C4'-C5'-C6'
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
35	c	516[B]	DGD	C2B-C3B-C4B-C5B
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
33	Z	101	LMG	O6-C5-C6-O5
23	B	602	CLA	C15-C16-C17-C18
26	A	410[B]	SQD	C15-C16-C17-C18
31	e	101	LMT	C4-C5-C6-C7
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	516[A]	DGD	C2A-C1A-O1G-C1G
35	c	516[A]	DGD	O6D-C5D-C6D-O5D
26	f	102	SQD	C32-C33-C34-C35
32	D	406[B]	LHG	C16-C17-C18-C19
32	D	407[B]	LHG	C32-C33-C34-C35
32	L	101[A]	LHG	C17-C18-C19-C20
33	m	101	LMG	C35-C36-C37-C38
35	c	516[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
27	B	623	GOL	O2-C2-C3-O3
27	D	412	GOL	O1-C1-C2-O2
27	V	203[B]	GOL	O2-C2-C3-O3
27	a	410	GOL	O1-C1-C2-O2
27	b	624	GOL	O2-C2-C3-O3
27	c	526	GOL	O2-C2-C3-O3
31	t	101	LMT	C2-C1-O1'-C1'
33	B	620	LMG	C17-C18-C19-C20
33	B	620	LMG	C34-C35-C36-C37
34	b	622	HTG	C3'-C4'-C5'-C6'
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
23	B	602	CLA	C4B-C3B-CAB-CBB
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C20
31	C	525	LMT	C3-C4-C5-C6
23	A	406[B]	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C15
23	b	606	CLA	C12-C13-C15-C16
26	X	101	SQD	C24-C25-C26-C27
26	A	410[B]	SQD	C7-C8-C9-C10
31	a	416	LMT	C1-C2-C3-C4
31	B	629	LMT	C3-C4-C5-C6
33	C	521	LMG	C17-C18-C19-C20
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
33	a	415	LMG	C34-C35-C36-C37
31	e	101	LMT	C1-C2-C3-C4
35	c	516[A]	DGD	C2B-C3B-C4B-C5B
23	B	608	CLA	C13-C15-C16-C17
23	C	513	CLA	C10-C11-C12-C13
32	E	101[B]	LHG	C23-C24-C25-C26
32	D	407[A]	LHG	C32-C33-C34-C35
23	B	610	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C19
23	d	405	CLA	C16-C17-C18-C19
31	B	629	LMT	C4-C5-C6-C7
32	L	101[A]	LHG	C25-C26-C27-C28
33	C	520	LMG	C16-C17-C18-C19
32	d	415[A]	LHG	C32-C33-C34-C35
31	t	101	LMT	C4'-C5'-C6'-O6'
33	D	411	LMG	C19-C20-C21-C22
35	H	102	DGD	C5B-C6B-C7B-C8B
33	C	501	LMG	C10-C11-C12-C13
33	a	415	LMG	C10-C11-C12-C13
26	a	411	SQD	C25-C26-C27-C28
32	L	101[B]	LHG	C12-C13-C14-C15
32	L	101[B]	LHG	C25-C26-C27-C28
32	a	419[A]	LHG	C26-C27-C28-C29
32	d	408[A]	LHG	C11-C10-C9-C8
33	C	501	LMG	C36-C37-C38-C39
33	D	411	LMG	C35-C36-C37-C38
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	c	516[A]	DGD	C9A-CAA-CBA-CCA
33	a	415	LMG	C21-C22-C23-C24
35	h	102	DGD	C2B-C3B-C4B-C5B
32	b	629[A]	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
32	b	629[B]	LHG	C14-C15-C16-C17
34	b	622	HTG	C2'-C3'-C4'-C5'
31	b	621	LMT	C3'-C4'-O1B-C1B
32	d	415[B]	LHG	C16-C17-C18-C19
33	C	501	LMG	C17-C18-C19-C20
23	C	508	CLA	C2B-C3B-CAB-CBB
23	a	405[A]	CLA	C2B-C3B-CAB-CBB
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
32	b	629[B]	LHG	C16-C17-C18-C19
32	d	408[B]	LHG	C34-C35-C36-C37
23	C	509	CLA	CBD-CGD-O2D-CED
26	A	410[A]	SQD	C12-C13-C14-C15
31	b	627	LMT	C7-C8-C9-C10
32	E	101[B]	LHG	C24-C25-C26-C27
32	a	419[B]	LHG	C26-C27-C28-C29
32	b	629[A]	LHG	C16-C17-C18-C19
31	e	101	LMT	C5-C6-C7-C8
32	A	419[A]	LHG	C12-C13-C14-C15
32	L	101[A]	LHG	C15-C16-C17-C18
33	D	411	LMG	C30-C31-C32-C33
35	c	516[B]	DGD	O1A-C1A-O1G-C1G
29	D	405[B]	PL9	C4-C3-C7-C8
31	B	629	LMT	C11-C10-C9-C8
33	m	101	LMG	C38-C39-C40-C41
29	A	414[A]	PL9	C30-C29-C31-C32
32	D	406[A]	LHG	C16-C17-C18-C19
32	D	407[B]	LHG	C15-C16-C17-C18
32	E	101[A]	LHG	C24-C25-C26-C27
23	C	507	CLA	C5-C6-C7-C8
23	D	403	CLA	C2-C3-C5-C6
32	A	419[B]	LHG	C12-C13-C14-C15
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
35	c	518	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	C3B-C4B-C5B-C6B
35	h	102	DGD	C7B-C8B-C9B-CAB
23	C	504	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
23	C	512	CLA	C3-C5-C6-C7
26	b	620	SQD	C31-C32-C33-C34
32	A	419[A]	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	D	407[A]	LHG	C15-C16-C17-C18
35	c	516[A]	DGD	C5A-C6A-C7A-C8A
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	c	516[B]	DGD	C4D-C5D-C6D-O5D
32	A	419[B]	LHG	C34-C35-C36-C37
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	c	516[A]	DGD	O1A-C1A-O1G-C1G
26	A	412	SQD	C17-C18-C19-C20
31	B	628	LMT	C2-C3-C4-C5
35	c	517[A]	DGD	CBB-CCB-CDB-CEB
33	C	501	LMG	C12-C13-C14-C15
31	B	627	LMT	C5-C6-C7-C8
31	T	101	LMT	C7-C8-C9-C10
23	c	508	CLA	C16-C17-C18-C20
33	m	101	LMG	C11-C10-O7-C8
33	c	519	LMG	C33-C34-C35-C36
35	h	102	DGD	C9A-CAA-CBA-CCA
33	m	101	LMG	O9-C10-O7-C8
31	b	627	LMT	C3-C4-C5-C6
32	d	415[A]	LHG	C29-C30-C31-C32
35	c	516[A]	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	CAA-CBA-CCA-CDA
23	C	503	CLA	C15-C16-C17-C18
31	b	627	LMT	C5-C6-C7-C8
33	m	101	LMG	C39-C40-C41-C42
33	D	411	LMG	C12-C13-C14-C15
23	c	509	CLA	C3-C5-C6-C7
32	L	101[B]	LHG	C17-C18-C19-C20
23	B	610	CLA	C16-C17-C18-C20
33	d	413	LMG	C29-C30-C31-C32
29	A	414[A]	PL9	C45-C44-C46-C47
23	c	504	CLA	C2-C3-C5-C6
29	d	407[A]	PL9	C13-C14-C16-C17
38	f	101	HEM	C2C-C3C-CAC-CBC
32	L	101[A]	LHG	C13-C14-C15-C16
32	d	408[A]	LHG	C34-C35-C36-C37
33	c	519	LMG	C34-C35-C36-C37
31	B	628	LMT	C6-C7-C8-C9
35	c	516[B]	DGD	C5A-C6A-C7A-C8A
23	B	605	CLA	C5-C6-C7-C8
23	B	615	CLA	C5-C6-C7-C8
26	X	101	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
31	C	525	LMT	C3'-C4'-O1B-C1B
26	b	620	SQD	C14-C15-C16-C17
32	D	407[A]	LHG	C29-C30-C31-C32
32	d	409[A]	LHG	C27-C28-C29-C30
23	c	501	CLA	CBD-CGD-O2D-CED
23	c	507	CLA	C5-C6-C7-C8
33	c	519	LMG	C31-C32-C33-C34
35	c	516[B]	DGD	C7A-C8A-C9A-CAA
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
26	a	411	SQD	C31-C32-C33-C34
32	d	415[B]	LHG	C29-C30-C31-C32
32	d	415[B]	LHG	C32-C33-C34-C35
35	h	102	DGD	CAB-CBB-CCB-CDB
33	c	519	LMG	C28-C29-C30-C31
23	b	604	CLA	C15-C16-C17-C18
23	b	614	CLA	C10-C11-C12-C13
23	c	511	CLA	C8-C10-C11-C12
34	b	623	HTG	O5-C5-C6-O6
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
31	B	628	LMT	C5-C6-C7-C8
31	m	103	LMT	C7-C8-C9-C10
32	d	409[B]	LHG	C27-C28-C29-C30
26	l	101	SQD	C11-C10-C9-C8
29	D	405[B]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[B]	PL9	C12-C11-C9-C8
29	D	405[A]	PL9	C13-C14-C16-C17
33	C	501	LMG	C19-C20-C21-C22
35	c	516[A]	DGD	CAA-CBA-CCA-CDA
23	c	510	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	O1D-CGD-O2D-CED
31	B	627	LMT	C3'-C4'-O1B-C1B
35	c	516[B]	DGD	O6E-C5E-C6E-O5E
33	D	411	LMG	C36-C37-C38-C39
34	B	621	HTG	C2'-C3'-C4'-C5'
23	d	404[A]	CLA	C16-C17-C18-C20
27	D	412	GOL	O2-C2-C3-O3
27	a	410	GOL	O2-C2-C3-O3
27	a	417	GOL	O1-C1-C2-O2
27	o	303	GOL	O2-C2-C3-O3
35	c	516[A]	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C17-C18-C19-C20
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C1A-C2A-CAA-CBA
26	A	412	SQD	O5-C1-O6-C44
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
26	b	620	SQD	C28-C29-C30-C31
35	c	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
33	d	413	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
33	C	501	LMG	C11-C12-C13-C14
31	t	101	LMT	O1'-C1-C2-C3
23	B	602	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C10-C8-C7
23	B	614	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
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	c	504	CLA	C11-C12-C13-C15
23	c	505	CLA	C11-C12-C13-C15
23	c	512	CLA	C12-C13-C15-C16
23	A	406[A]	CLA	C13-C15-C16-C17
35	H	102	DGD	C7A-C8A-C9A-CAA
23	c	505	CLA	C2-C3-C5-C6
26	f	102	SQD	C25-C26-C27-C28
32	D	406[A]	LHG	C13-C14-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	511	CLA	C14-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
26	A	412	SQD	C26-C27-C28-C29
26	a	411	SQD	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C20
23	C	513	CLA	CBA-CGA-O2A-C1
23	A	404[A]	CLA	C13-C15-C16-C17
23	B	614	CLA	C5-C6-C7-C8
32	d	409[A]	LHG	C25-C26-C27-C28
23	b	601	CLA	C8-C10-C11-C12
26	A	410[A]	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	O6-C44-C45-C46
26	a	409[A]	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
26	l	101	SQD	C44-C45-C46-O48
32	E	101[B]	LHG	C4-C5-C6-O8
32	d	409[B]	LHG	C25-C26-C27-C28
34	b	625	HTG	C4-C5-C6-O6
35	c	516[B]	DGD	CAA-CBA-CCA-CDA
35	c	516[A]	DGD	O6E-C5E-C6E-O5E
26	a	409[A]	SQD	C9-C10-C11-C12
32	d	409[B]	LHG	C34-C35-C36-C37
23	c	512	CLA	O1A-CGA-O2A-C1
26	b	620	SQD	C13-C14-C15-C16
33	D	411	LMG	O6-C5-C6-O5
26	A	410[B]	SQD	C11-C10-C9-C8
32	E	101[A]	LHG	C25-C26-C27-C28
23	B	615	CLA	C10-C11-C12-C13
33	C	521	LMG	C19-C20-C21-C22
26	b	620	SQD	O10-C23-O48-C46
26	a	409[B]	SQD	C9-C10-C11-C12
35	c	517[B]	DGD	C4A-C5A-C6A-C7A
23	c	505	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C45-C44-C46-C47
31	M	101	LMT	C3-C4-C5-C6
23	A	404[B]	CLA	C13-C15-C16-C17
23	A	405[A]	CLA	C15-C16-C17-C18
23	C	507	CLA	C15-C16-C17-C18
23	C	511	CLA	C10-C11-C12-C13
23	b	610	CLA	C15-C16-C17-C18
32	D	406[B]	LHG	C12-C13-C14-C15
23	d	404[A]	CLA	C16-C17-C18-C19
32	D	407[B]	LHG	C29-C30-C31-C32
33	C	521	LMG	C13-C14-C15-C16
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
26	l	101	SQD	C34-C35-C36-C37
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
32	b	629[A]	LHG	C13-C14-C15-C16
32	D	407[B]	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	C46-C45-O47-C7
26	l	101	SQD	C46-C45-O47-C7
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
32	D	407[A]	LHG	C17-C18-C19-C20
33	C	501	LMG	C13-C14-C15-C16
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
23	B	613	CLA	C13-C15-C16-C17
35	c	517[B]	DGD	C6A-C7A-C8A-C9A
32	L	101[B]	LHG	C13-C14-C15-C16
35	c	518	DGD	CBA-CCA-CDA-CEA
31	C	525	LMT	C4-C5-C6-C7
31	a	416	LMT	C2-C3-C4-C5
32	b	629[B]	LHG	C27-C28-C29-C30
33	m	101	LMG	C14-C15-C16-C17
35	H	102	DGD	CCB-CDB-CEB-CFB
29	D	405[B]	PL9	C13-C14-C16-C17
29	d	407[B]	PL9	C13-C14-C16-C17
32	d	409[B]	LHG	C28-C29-C30-C31
23	C	514	CLA	O1D-CGD-O2D-CED
26	a	409[A]	SQD	C12-C13-C14-C15
26	b	620	SQD	C26-C27-C28-C29
32	d	409[B]	LHG	C29-C30-C31-C32
26	A	412	SQD	C27-C28-C29-C30
31	b	621	LMT	C11-C10-C9-C8
32	d	409[A]	LHG	C34-C35-C36-C37
35	c	517[A]	DGD	C4A-C5A-C6A-C7A
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
31	F	101	LMT	C4-C5-C6-C7
31	t	101	LMT	C7-C8-C9-C10
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
31	a	416	LMT	C3-C4-C5-C6
26	b	620	SQD	C11-C10-C9-C8
33	C	520	LMG	C36-C37-C38-C39
33	a	415	LMG	C35-C36-C37-C38
26	b	620	SQD	C27-C28-C29-C30
32	d	415[B]	LHG	C24-C25-C26-C27
33	C	501	LMG	C20-C21-C22-C23
23	B	612	CLA	C10-C11-C12-C13
23	b	601	CLA	C2-C1-O2A-CGA
33	m	101	LMG	C37-C38-C39-C40
35	h	102	DGD	CDB-CEB-CFB-CGB
33	C	520	LMG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	511	CLA	CBA-CGA-O2A-C1
32	d	408[B]	LHG	C24-C23-O8-C6
32	d	409[A]	LHG	C29-C30-C31-C32
23	D	403	CLA	O1D-CGD-O2D-CED
31	a	416	LMT	C9-C10-C11-C12
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
23	B	601	CLA	C13-C15-C16-C17
23	c	512	CLA	C10-C11-C12-C13
33	C	521	LMG	C35-C36-C37-C38
23	C	511	CLA	C4-C3-C5-C6
29	d	407[A]	PL9	C45-C44-C46-C47
33	c	520	LMG	C29-C28-O8-C9
34	c	521	HTG	C4'-C5'-C6'-C7'
26	b	620	SQD	C18-C19-C20-C21
32	d	415[A]	LHG	C33-C34-C35-C36
27	B	626	GOL	O1-C1-C2-O2
27	o	302	GOL	O2-C2-C3-O3
31	F	101	LMT	C2-C1-O1'-C1'
32	A	419[B]	LHG	O1-C1-C2-O2
23	B	602	CLA	C11-C12-C13-C14
23	B	614	CLA	C14-C13-C15-C16
23	D	403	CLA	C14-C13-C15-C16
23	c	505	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
23	b	605	CLA	C5-C6-C7-C8
23	A	406[A]	CLA	C4B-C3B-CAB-CBB
23	A	406[B]	CLA	C4B-C3B-CAB-CBB
23	a	405[A]	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
31	e	101	LMT	C3-C4-C5-C6
32	b	629[B]	LHG	C13-C14-C15-C16
32	D	406[A]	LHG	C12-C13-C14-C15
26	a	409[B]	SQD	C12-C13-C14-C15
32	D	407[B]	LHG	C17-C18-C19-C20
23	C	502	CLA	O1D-CGD-O2D-CED
33	d	413	LMG	C11-C12-C13-C14
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
32	L	101[B]	LHG	O6-C4-C5-C6
32	b	629[A]	LHG	O6-C4-C5-C6
32	b	629[B]	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
31	B	629	LMT	O1'-C1-C2-C3
23	A	406[A]	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	C	503	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	514	CLA	C11-C10-C8-C7
23	a	407	CLA	C11-C10-C8-C7
23	C	513	CLA	O1A-CGA-O2A-C1
23	d	404[B]	CLA	C16-C17-C18-C20
23	c	506	CLA	C3A-C2A-CAA-CBA
29	a	413[A]	PL9	C12-C11-C9-C10
31	M	101	LMT	O1'-C1-C2-C3
32	D	407[B]	LHG	O10-C23-O8-C6
31	e	101	LMT	C9-C10-C11-C12
26	X	101	SQD	C24-C23-O48-C46
32	d	409[A]	LHG	C28-C29-C30-C31
25	d	406	BCR	C7-C8-C9-C34
23	B	605	CLA	CBD-CGD-O2D-CED
33	a	415	LMG	C29-C30-C31-C32
35	c	517[A]	DGD	CDA-CEA-CFA-CGA
32	b	629[A]	LHG	C27-C28-C29-C30
23	B	601	CLA	C2A-CAA-CBA-CGA
23	d	405	CLA	CBA-CGA-O2A-C1
26	A	410[B]	SQD	O6-C44-C45-C46
26	a	411	SQD	O6-C44-C45-C46
32	a	419[A]	LHG	C4-C5-C6-O8
32	a	419[B]	LHG	C4-C5-C6-O8
33	a	415	LMG	C7-C8-C9-O8
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
32	D	407[A]	LHG	C13-C14-C15-C16
32	d	409[A]	LHG	C9-C10-C11-C12
32	D	406[A]	LHG	C10-C11-C12-C13
32	d	415[B]	LHG	C33-C34-C35-C36
23	B	610	CLA	C13-C15-C16-C17
32	d	408[A]	LHG	C13-C14-C15-C16
24	a	406[B]	PHO	C4-C3-C5-C6
29	a	413[B]	PL9	C12-C11-C9-C10
29	d	407[B]	PL9	C15-C14-C16-C17
31	b	621	LMT	C3-C4-C5-C6
23	C	511	CLA	C2-C3-C5-C6
24	a	406[B]	PHO	C2-C3-C5-C6
29	D	405[A]	PL9	C43-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C3-C5-C6-C7
32	E	101[B]	LHG	C25-C26-C27-C28
32	A	419[A]	LHG	C26-C27-C28-C29
32	E	101[A]	LHG	O6-C4-C5-O7
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
34	B	624	HTG	C4'-C5'-C6'-C7'
23	A	406[B]	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
25	b	617	BCR	C1-C6-C7-C8
23	B	607	CLA	C3-C5-C6-C7
31	C	525	LMT	C5-C6-C7-C8
32	A	419[B]	LHG	C26-C27-C28-C29
32	d	408[B]	LHG	C11-C10-C9-C8
23	c	509	CLA	C15-C16-C17-C18
32	D	406[B]	LHG	C26-C27-C28-C29
23	b	606	CLA	C16-C17-C18-C19
23	C	510	CLA	O1D-CGD-O2D-CED
26	a	409[A]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
34	b	623	HTG	O5-C1-S1-C1'
32	D	406[B]	LHG	C11-C10-C9-C8
29	d	407[A]	PL9	C15-C14-C16-C17
32	D	407[B]	LHG	C13-C14-C15-C16
32	a	419[A]	LHG	C10-C11-C12-C13
32	b	629[A]	LHG	C12-C13-C14-C15
33	C	520	LMG	C31-C32-C33-C34
23	A	405[B]	CLA	C15-C16-C17-C18
29	A	414[A]	PL9	C43-C44-C46-C47
32	L	101[A]	LHG	C24-C25-C26-C27
23	d	404[B]	CLA	C16-C17-C18-C19
32	D	407[B]	LHG	C10-C11-C12-C13
32	L	101[A]	LHG	C11-C12-C13-C14
33	z	101	LMG	C19-C20-C21-C22
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
35	c	517[B]	DGD	C9B-CAB-CBB-CCB
23	B	610	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	c	510	CLA	C11-C10-C8-C9
26	A	410[B]	SQD	C12-C13-C14-C15
34	b	623	HTG	S1-C1'-C2'-C3'
23	C	511	CLA	O1A-CGA-O2A-C1
26	a	409[A]	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
32	b	629[A]	LHG	C31-C32-C33-C34
33	C	520	LMG	C37-C38-C39-C40
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
33	Z	101	LMG	C11-C12-C13-C14
29	a	413[A]	PL9	C24-C26-C27-C28
26	X	101	SQD	C32-C33-C34-C35
33	z	101	LMG	C14-C15-C16-C17
32	E	101[A]	LHG	C17-C18-C19-C20
27	c	526	GOL	O1-C1-C2-O2
23	A	406[A]	CLA	C16-C17-C18-C20
23	C	509	CLA	O1D-CGD-O2D-CED
23	c	512	CLA	C13-C15-C16-C17
23	c	511	CLA	O1A-CGA-O2A-C1
32	L	101[B]	LHG	C15-C16-C17-C18
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
26	l	101	SQD	C24-C25-C26-C27
23	c	509	CLA	C10-C11-C12-C13
32	D	407[A]	LHG	C10-C11-C12-C13
23	B	601	CLA	O1A-CGA-O2A-C1
35	c	518	DGD	C2A-C1A-O1G-C1G
32	b	629[B]	LHG	C12-C13-C14-C15
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
32	E	101[A]	LHG	O6-C4-C5-C6
23	C	507	CLA	C16-C17-C18-C20
31	M	101	LMT	C2-C3-C4-C5
32	D	406[B]	LHG	C10-C11-C12-C13
32	a	419[B]	LHG	C10-C11-C12-C13
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C10-C8-C7
23	B	610	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	b	604	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C10-C8-C7
23	c	509	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
32	a	419[A]	LHG	C7-C8-C9-C10
31	A	417	LMT	C7-C8-C9-C10
33	z	101	LMG	C20-C21-C22-C23
23	C	510	CLA	C3-C5-C6-C7
23	b	607	CLA	C3-C5-C6-C7
25	K	102	BCR	C7-C8-C9-C10
25	d	406	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	C24-C23-O48-C46
23	d	405	CLA	O1A-CGA-O2A-C1
33	c	520	LMG	O10-C28-O8-C9
35	C	519	DGD	CDB-CEB-CFB-CGB
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	c	517[A]	DGD	C2G-C3G-O3G-C1D
35	c	517[A]	DGD	C5D-C6D-O5D-C1E
35	c	517[B]	DGD	C2G-C3G-O3G-C1D
33	z	101	LMG	C10-C11-C12-C13
23	b	601	CLA	C13-C15-C16-C17
32	d	415[A]	LHG	C25-C26-C27-C28
29	D	405[A]	PL9	C15-C14-C16-C17
29	D	405[A]	PL9	C45-C44-C46-C47
35	h	102	DGD	CDA-CEA-CFA-CGA
23	b	601	CLA	CAA-CBA-CGA-O2A
38	f	101	HEM	C2B-C3B-CAB-CBB
23	c	511	CLA	C3-C5-C6-C7
24	a	406[A]	PHO	O2A-C1-C2-C3
32	d	408[B]	LHG	O10-C23-O8-C6
32	d	415[B]	LHG	C25-C26-C27-C28
32	L	101[B]	LHG	O6-C4-C5-O7
32	b	629[A]	LHG	O6-C4-C5-O7
33	C	521	LMG	C4-C5-C6-O5
32	L	101[A]	LHG	C11-C10-C9-C8
32	d	415[A]	LHG	C24-C25-C26-C27
35	c	516[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[A]	LHG	C4-C5-C6-O8
32	b	629[A]	LHG	C34-C35-C36-C37
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
23	c	510	CLA	C4-C3-C5-C6
23	c	507	CLA	C2A-CAA-CBA-CGA
33	d	413	LMG	C35-C36-C37-C38
26	l	101	SQD	C29-C30-C31-C32
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	b	629[A]	LHG	C9-C10-C11-C12
26	a	409[B]	SQD	O6-C44-C45-O47
26	f	102	SQD	O47-C45-C46-O48
32	a	419[A]	LHG	O7-C5-C6-O8
23	C	512	CLA	C8-C10-C11-C12
23	C	507	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
32	E	101[A]	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
31	T	101	LMT	C1-C2-C3-C4
26	a	409[A]	SQD	C27-C28-C29-C30
31	B	628	LMT	C3-C4-C5-C6
32	d	409[B]	LHG	C9-C10-C11-C12
32	d	415[B]	LHG	C27-C28-C29-C30
33	c	519	LMG	C29-C30-C31-C32
35	c	518	DGD	O1A-C1A-O1G-C1G
26	a	409[B]	SQD	C27-C28-C29-C30
33	B	620	LMG	C36-C37-C38-C39
35	C	519	DGD	C7B-C8B-C9B-CAB
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
23	b	604	CLA	C10-C11-C12-C13
23	b	612	CLA	C8-C10-C11-C12
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
26	X	101	SQD	O10-C23-O48-C46
32	D	406[A]	LHG	C34-C35-C36-C37
35	h	102	DGD	C9B-CAB-CBB-CCB
32	E	101[B]	LHG	C17-C18-C19-C20
23	C	510	CLA	C2-C1-O2A-CGA
32	d	409[B]	LHG	C2-C3-O3-P
33	c	519	LMG	C10-C11-C12-C13
32	E	101[B]	LHG	C13-C14-C15-C16
35	C	519	DGD	CBA-CCA-CDA-CEA
31	b	627	LMT	C1-C2-C3-C4
31	b	627	LMT	C6-C7-C8-C9
23	B	603	CLA	C4-C3-C5-C6
33	a	415	LMG	O8-C28-C29-C30
35	c	518	DGD	C2B-C3B-C4B-C5B
32	d	409[A]	LHG	C24-C23-O8-C6
23	B	606	CLA	C8-C10-C11-C12
33	C	501	LMG	C39-C40-C41-C42
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
31	F	101	LMT	C6-C7-C8-C9
32	D	407[B]	LHG	C27-C28-C29-C30
23	C	513	CLA	C3-C5-C6-C7
23	b	605	CLA	C3-C5-C6-C7
23	b	601	CLA	CBA-CGA-O2A-C1
35	H	102	DGD	CCA-CDA-CEA-CFA
31	b	627	LMT	O1'-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-O2
31	C	525	LMT	C2-C1-O1'-C1'
33	C	501	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	C	513	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
23	c	513	CLA	C1A-C2A-CAA-CBA
23	d	402[A]	CLA	C1A-C2A-CAA-CBA
23	d	402[B]	CLA	C1A-C2A-CAA-CBA
26	A	412	SQD	C7-C8-C9-C10
23	b	602	CLA	C10-C11-C12-C13
26	a	409[A]	SQD	C35-C36-C37-C38
32	L	101[B]	LHG	C24-C25-C26-C27
32	L	101[B]	LHG	C27-C28-C29-C30
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
26	A	412	SQD	O10-C23-O48-C46
23	b	605	CLA	C13-C15-C16-C17
32	A	419[A]	LHG	C32-C33-C34-C35
23	B	616	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	c	509	CLA	C6-C7-C8-C10
23	d	404[B]	CLA	C11-C12-C13-C15
23	A	406[B]	CLA	C16-C17-C18-C20
32	d	409[A]	LHG	O10-C23-O8-C6
32	D	407[A]	LHG	C24-C23-O8-C6
32	b	629[B]	LHG	C25-C26-C27-C28
32	D	407[A]	LHG	O10-C23-O8-C6
35	c	517[A]	DGD	C1A-C2A-C3A-C4A
26	X	101	SQD	C34-C35-C36-C37
23	C	507	CLA	C3A-C2A-CAA-CBA
29	A	414[B]	PL9	C12-C11-C9-C10
23	b	601	CLA	O1A-CGA-O2A-C1
32	b	629[B]	LHG	O6-C4-C5-O7
26	A	410[A]	SQD	C18-C19-C20-C21
23	B	605	CLA	O1D-CGD-O2D-CED
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
32	A	419[B]	LHG	C18-C19-C20-C21
32	d	415[A]	LHG	C27-C28-C29-C30
33	D	411	LMG	C18-C19-C20-C21
35	c	516[A]	DGD	CCB-CDB-CEB-CFB
32	d	415[B]	LHG	C13-C14-C15-C16
26	l	101	SQD	O47-C45-C46-O48

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Mol	Chain	Res	Type	Atoms
32	E	101[A]	LHG	O7-C5-C6-O8
32	E	101[B]	LHG	O7-C5-C6-O8
32	a	419[B]	LHG	O7-C5-C6-O8
33	a	415	LMG	O7-C8-C9-O8
33	C	520	LMG	C29-C30-C31-C32
32	E	101[B]	LHG	C1-C2-C3-O3
26	a	409[B]	SQD	C35-C36-C37-C38
26	a	409[B]	SQD	O6-C44-C45-C46
23	B	611	CLA	C8-C10-C11-C12
23	c	510	CLA	C2-C3-C5-C6
29	a	413[A]	PL9	C12-C11-C9-C8
29	a	413[B]	PL9	C12-C11-C9-C8
26	a	409[B]	SQD	C34-C35-C36-C37
32	a	419[A]	LHG	C23-C24-C25-C26
23	B	601	CLA	CAD-CBD-CGD-O2D
23	B	605	CLA	CAD-CBD-CGD-O2D
23	C	503	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	D	403	CLA	C8-C10-C11-C12
23	b	616	CLA	C5-C6-C7-C8
23	d	402[B]	CLA	C15-C16-C17-C18
24	a	406[B]	PHO	C8-C10-C11-C12
31	B	627	LMT	C9-C10-C11-C12
31	B	629	LMT	C6-C7-C8-C9
26	A	410[A]	SQD	C34-C35-C36-C37
35	c	516[A]	DGD	C8B-C9B-CAB-CBB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O1D
23	c	502	CLA	CAD-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
25	t	102	BCR	C13-C14-C15-C16
32	D	406[A]	LHG	C4-O6-P-O3
32	D	406[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
32	a	419[B]	LHG	C4-O6-P-O4
32	d	408[A]	LHG	C3-O3-P-O4
32	d	408[B]	LHG	C4-O6-P-O5
32	d	415[B]	LHG	C3-O3-P-O5
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
24	a	406[A]	PHO	C8-C10-C11-C12
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
23	b	601	CLA	C4-C3-C5-C6
29	D	405[B]	PL9	C45-C44-C46-C47
29	d	407[B]	PL9	C45-C44-C46-C47
23	A	406[A]	CLA	C2B-C3B-CAB-CBB
23	B	602	CLA	C2B-C3B-CAB-CBB
29	A	414[A]	PL9	C28-C29-C31-C32
35	C	518[B]	DGD	C3B-C4B-C5B-C6B
23	c	501	CLA	O1D-CGD-O2D-CED
31	A	417	LMT	O5B-C5B-C6B-O6B
32	D	407[A]	LHG	C2-C3-O3-P
32	d	409[A]	LHG	C2-C3-O3-P
23	c	507	CLA	C8-C10-C11-C12
26	f	102	SQD	C23-C24-C25-C26
32	d	409[B]	LHG	O10-C23-O8-C6
31	a	416	LMT	O5'-C5'-C6'-O6'
26	a	409[A]	SQD	C11-C12-C13-C14
27	B	623	GOL	O1-C1-C2-O2
27	d	414	GOL	O1-C1-C2-O2
27	l	103[B]	GOL	O1-C1-C2-O2
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
29	A	414[B]	PL9	C4-C3-C7-C8
29	a	413[A]	PL9	C4-C3-C7-C8
29	a	413[B]	PL9	C4-C3-C7-C8
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
35	C	518[A]	DGD	C1A-C2A-C3A-C4A
23	B	601	CLA	C15-C16-C17-C18
31	B	629	LMT	C2-C3-C4-C5
32	L	101[B]	LHG	C11-C12-C13-C14
23	B	601	CLA	CAA-CBA-CGA-O2A
29	A	414[B]	PL9	C43-C44-C46-C47
32	L	101[A]	LHG	O6-C4-C5-C6
23	B	606	CLA	C11-C10-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	a	407	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	514	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
32	E	101[A]	LHG	C1-C2-C3-O3
32	L	101[A]	LHG	O6-C4-C5-O7
35	c	516[A]	DGD	O6E-C1E-O5D-C6D
32	b	629[B]	LHG	C34-C35-C36-C37
33	C	520	LMG	C30-C31-C32-C33
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
24	a	406[A]	PHO	C4-C3-C5-C6
23	B	603	CLA	C2-C3-C5-C6
29	a	413[B]	PL9	C43-C44-C46-C47
31	A	417	LMT	C9-C10-C11-C12
26	A	410[A]	SQD	C16-C17-C18-C19
32	d	408[A]	LHG	O10-C23-O8-C6
32	d	415[A]	LHG	C34-C35-C36-C37
32	D	407[B]	LHG	C2-C3-O3-P
35	H	102	DGD	O2G-C1B-C2B-C3B
32	d	409[A]	LHG	C32-C33-C34-C35
32	d	408[A]	LHG	C24-C23-O8-C6
32	a	419[B]	LHG	C23-C24-C25-C26
32	d	408[B]	LHG	C13-C14-C15-C16
35	C	518[B]	DGD	C4E-C5E-C6E-O5E
26	A	412	SQD	C15-C16-C17-C18
23	B	608	CLA	C16-C17-C18-C20
33	B	620	LMG	C37-C38-C39-C40
35	C	519	DGD	C2B-C3B-C4B-C5B
34	b	622	HTG	C1'-C2'-C3'-C4'
33	B	620	LMG	C29-C30-C31-C32
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
35	c	518	DGD	CDA-CEA-CFA-CGA
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
35	c	516[B]	DGD	C5D-C6D-O5D-C1E
23	c	506	CLA	C13-C15-C16-C17
23	C	502	CLA	C2A-CAA-CBA-CGA
25	K	102	BCR	C19-C20-C21-C22
35	h	102	DGD	CBA-CCA-CDA-CEA
35	c	517[B]	DGD	C1A-C2A-C3A-C4A
29	a	413[B]	PL9	C45-C44-C46-C47
24	a	406[A]	PHO	C2-C3-C5-C6
23	d	402[A]	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
32	L	101[A]	LHG	C26-C27-C28-C29
31	b	627	LMT	C2-C1-O1'-C1'
32	d	415[A]	LHG	C1-C2-C3-O3
23	c	509	CLA	C6-C7-C8-C9
26	a	409[B]	SQD	C11-C12-C13-C14
35	h	102	DGD	C6A-C7A-C8A-C9A
23	C	505	CLA	C4B-C3B-CAB-CBB
23	D	402[B]	CLA	C4B-C3B-CAB-CBB
32	L	101[A]	LHG	C27-C28-C29-C30
32	d	409[B]	LHG	C24-C23-O8-C6
23	C	511	CLA	C8-C10-C11-C12
29	d	407[A]	PL9	C43-C44-C46-C47
33	Z	101	LMG	C2-C1-O1-C7
35	c	516[B]	DGD	C1A-C2A-C3A-C4A
31	T	101	LMT	O1'-C1-C2-C3
38	f	101	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4C-C3C-CAC-CBC
23	C	507	CLA	C16-C17-C18-C19
32	d	409[B]	LHG	C32-C33-C34-C35
35	c	516[B]	DGD	C4B-C5B-C6B-C7B
23	D	403	CLA	C11-C10-C8-C7
23	b	615	CLA	C11-C12-C13-C15
23	C	511	CLA	C13-C15-C16-C17
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
32	D	406[B]	LHG	C13-C14-C15-C16
32	D	407[A]	LHG	C27-C28-C29-C30
32	d	409[A]	LHG	C33-C34-C35-C36
26	X	101	SQD	O47-C45-C46-O48
29	a	413[A]	PL9	C45-C44-C46-C47
32	b	629[B]	LHG	C31-C32-C33-C34
33	B	620	LMG	C32-C33-C34-C35
35	c	516[A]	DGD	C4B-C5B-C6B-C7B
23	d	402[A]	CLA	C15-C16-C17-C18
24	d	403[B]	PHO	C2C-C3C-CAC-CBC
23	b	614	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C3-C5-C6-C7
26	A	410[A]	SQD	C11-C10-C9-C8
32	L	101[B]	LHG	C23-C24-C25-C26
23	b	612	CLA	C10-C11-C12-C13
23	b	616	CLA	C4-C3-C5-C6
23	c	513	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	D	405[A]	PL9	C35-C34-C36-C37
29	D	405[B]	PL9	C35-C34-C36-C37
23	C	503	CLA	C3-C5-C6-C7
23	b	601	CLA	C2-C3-C5-C6
29	D	405[B]	PL9	C43-C44-C46-C47
29	a	413[A]	PL9	C43-C44-C46-C47
23	B	606	CLA	C16-C17-C18-C19
34	b	622	HTG	O5-C5-C6-O6
32	a	419[A]	LHG	C24-C25-C26-C27
29	a	413[B]	PL9	C24-C26-C27-C28
26	A	410[B]	SQD	C16-C17-C18-C19
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
23	D	403	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C11-C12-C13-C14
23	B	614	CLA	C6-C7-C8-C9
23	C	514	CLA	C6-C7-C8-C9
23	D	403	CLA	C11-C10-C8-C9
23	a	405[A]	CLA	C11-C12-C13-C14
23	c	504	CLA	C14-C13-C15-C16
23	c	506	CLA	C6-C7-C8-C9
27	l	103[A]	GOL	O1-C1-C2-C3
27	o	302	GOL	C1-C2-C3-O3
27	v	202[A]	GOL	O1-C1-C2-C3
26	a	409[B]	SQD	C7-C8-C9-C10
23	C	502	CLA	C16-C17-C18-C20
32	b	629[A]	LHG	C25-C26-C27-C28
35	C	519	DGD	C8A-C9A-CAA-CBA
32	D	406[A]	LHG	C11-C10-C9-C8
34	b	623	HTG	C4'-C5'-C6'-C7'
23	b	614	CLA	CBD-CGD-O2D-CED
23	b	616	CLA	CBA-CGA-O2A-C1
23	b	615	CLA	C5-C6-C7-C8
40	V	201	HEC	CAD-CBD-CGD-O1D
23	C	502	CLA	C1A-C2A-CAA-CBA
23	d	402[B]	CLA	C4C-C3C-CAC-CBC
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
35	c	518	DGD	O6D-C5D-C6D-O5D
32	a	419[B]	LHG	C24-C25-C26-C27
31	b	621	LMT	C7-C8-C9-C10
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	402[B]	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	D	403	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C2B-C3B-CAB-CBB
25	D	404	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C30
25	b	617	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	C13-C14-C15-C16
32	A	419[A]	LHG	C18-C19-C20-C21
23	A	406[A]	CLA	C16-C17-C18-C19
35	c	518	DGD	C6B-C7B-C8B-C9B
35	c	517[A]	DGD	C7B-C8B-C9B-CAB
40	V	201	HEC	CAD-CBD-CGD-O2D
32	b	629[A]	LHG	C17-C18-C19-C20
23	B	613	CLA	C11-C10-C8-C7
23	c	510	CLA	C12-C13-C15-C16
23	b	613	CLA	CBD-CGD-O2D-CED
33	m	101	LMG	C32-C33-C34-C35
31	B	627	LMT	C1-C2-C3-C4
32	a	419[B]	LHG	C7-C8-C9-C10
35	h	102	DGD	O1G-C1G-C2G-O2G
38	E	102	HEM	CAD-CBD-CGD-O1D
33	z	101	LMG	C13-C14-C15-C16
32	L	101[B]	LHG	C11-C10-C9-C8
29	A	414[A]	PL9	C4-C3-C7-C8
33	a	415	LMG	C13-C14-C15-C16
26	A	412	SQD	C30-C31-C32-C33
32	D	406[A]	LHG	C26-C27-C28-C29
23	b	610	CLA	C13-C15-C16-C17
25	Y	101	BCR	C37-C22-C23-C24
35	C	519	DGD	C4A-C5A-C6A-C7A
29	A	414[B]	PL9	C25-C24-C26-C27
32	d	408[A]	LHG	C16-C17-C18-C19
33	C	501	LMG	C29-C30-C31-C32
33	B	620	LMG	O8-C28-C29-C30
23	b	615	CLA	C13-C15-C16-C17
23	c	503	CLA	C8-C10-C11-C12
23	C	506	CLA	C2-C3-C5-C6
23	b	616	CLA	C2-C3-C5-C6
29	d	407[B]	PL9	C43-C44-C46-C47
33	B	620	LMG	C18-C19-C20-C21
31	e	101	LMT	O1'-C1-C2-C3
35	C	519	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
35	C	519	DGD	CAA-CBA-CCA-CDA
35	C	519	DGD	C7A-C8A-C9A-CAA
23	c	509	CLA	C8-C10-C11-C12
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
32	A	419[B]	LHG	C32-C33-C34-C35
35	c	516[B]	DGD	CBA-CCA-CDA-CEA
29	D	405[B]	PL9	C18-C19-C21-C22
23	c	506	CLA	C10-C11-C12-C13
35	c	516[A]	DGD	C2E-C1E-O5D-C6D
35	c	516[B]	DGD	C2E-C1E-O5D-C6D
32	D	406[B]	LHG	C28-C29-C30-C31
38	E	102	HEM	CAD-CBD-CGD-O2D
23	c	510	CLA	O1A-CGA-O2A-C1
32	L	101[A]	LHG	C23-C24-C25-C26
38	f	101	HEM	CAA-CBA-CGA-O2A
27	A	418	GOL	O1-C1-C2-O2
32	A	419[A]	LHG	C29-C30-C31-C32
33	z	101	LMG	O7-C10-C11-C12
35	C	519	DGD	C9A-CAA-CBA-CCA
23	c	510	CLA	O1D-CGD-O2D-CED
23	B	608	CLA	C16-C17-C18-C19
23	B	613	CLA	C15-C16-C17-C18
33	C	521	LMG	C12-C13-C14-C15
26	b	620	SQD	C10-C11-C12-C13
23	C	512	CLA	O1A-CGA-O2A-C1
31	e	101	LMT	C4B-C5B-C6B-O6B
40	v	201	HEC	CAD-CBD-CGD-O2D
23	A	404[A]	CLA	C16-C17-C18-C19
32	b	629[B]	LHG	C9-C10-C11-C12
32	A	419[B]	LHG	C1-C2-C3-O3
35	c	518	DGD	CDB-CEB-CFB-CGB
23	a	407	CLA	C15-C16-C17-C18
29	A	414[A]	PL9	C25-C24-C26-C27
23	b	615	CLA	C10-C11-C12-C13
32	L	101[B]	LHG	C26-C27-C28-C29
35	c	516[A]	DGD	CAB-CBB-CCB-CDB
31	a	416	LMT	O5'-C1'-O1'-C1
32	d	409[B]	LHG	C10-C11-C12-C13
35	H	102	DGD	CAB-CBB-CCB-CDB
40	v	201	HEC	CAD-CBD-CGD-O1D
23	A	408	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	a	405[B]	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
23	d	404[B]	CLA	C11-C12-C13-C14
23	d	405	CLA	C11-C12-C13-C14
31	F	101	LMT	C2-C3-C4-C5
32	d	415[B]	LHG	C18-C19-C20-C21
33	C	521	LMG	C8-C7-O1-C1
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	516[A]	DGD	C5D-C6D-O5D-C1E
23	B	614	CLA	C2A-CAA-CBA-CGA
23	a	404[B]	CLA	C2-C1-O2A-CGA
31	B	627	LMT	C7-C8-C9-C10
32	A	419[A]	LHG	C35-C36-C37-C38
32	b	629[A]	LHG	C10-C11-C12-C13
35	h	102	DGD	O2G-C1B-C2B-C3B
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
35	c	518	DGD	CAA-CBA-CCA-CDA
26	A	410[B]	SQD	C18-C19-C20-C21
32	L	101[A]	LHG	C16-C17-C18-C19
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
32	b	629[B]	LHG	C10-C11-C12-C13
23	C	508	CLA	C13-C15-C16-C17
33	C	521	LMG	C11-C12-C13-C14
23	C	506	CLA	C4-C3-C5-C6
35	c	517[B]	DGD	C5B-C6B-C7B-C8B
23	A	404[A]	CLA	C15-C16-C17-C18
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
35	c	517[A]	DGD	C9B-CAB-CBB-CCB
29	A	414[A]	PL9	C39-C41-C42-C43
29	A	414[B]	PL9	C39-C41-C42-C43
35	C	519	DGD	O1A-C1A-O1G-C1G
27	d	414	GOL	O2-C2-C3-O3
32	A	419[B]	LHG	C30-C31-C32-C33
38	f	101	HEM	CAA-CBA-CGA-O1A
32	D	407[A]	LHG	C28-C29-C30-C31
23	B	606	CLA	C16-C17-C18-C20
32	b	629[A]	LHG	C30-C31-C32-C33
32	b	629[B]	LHG	C28-C29-C30-C31
26	l	101	SQD	C33-C34-C35-C36
34	B	622	HTG	C4'-C5'-C6'-C7'
31	A	417	LMT	C2B-C1B-O1B-C4'
33	C	520	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	B	611	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C14
23	a	405[A]	CLA	C14-C13-C15-C16
23	C	511	CLA	CAA-CBA-CGA-O2A
32	b	629[B]	LHG	O7-C7-C8-C9
23	B	612	CLA	O1A-CGA-O2A-C1
38	f	101	HEM	CAD-CBD-CGD-O1D
25	Y	101	BCR	C21-C22-C23-C24
23	b	604	CLA	C13-C15-C16-C17
33	C	501	LMG	C15-C16-C17-C18
32	A	419[A]	LHG	O8-C23-C24-C25
33	c	519	LMG	C32-C33-C34-C35
23	C	507	CLA	C12-C13-C15-C16
23	a	405[A]	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C7
23	c	504	CLA	C12-C13-C15-C16
35	c	518	DGD	O6E-C5E-C6E-O5E
23	C	505	CLA	C2B-C3B-CAB-CBB
25	D	404	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C26
25	d	406	BCR	C23-C24-C25-C30
32	L	101[B]	LHG	O7-C7-C8-C9
31	T	101	LMT	C4-C5-C6-C7
23	B	613	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
35	C	519	DGD	CDA-CEA-CFA-CGA
26	A	410[B]	SQD	C34-C35-C36-C37
33	d	413	LMG	C16-C17-C18-C19
33	m	101	LMG	C11-C12-C13-C14
32	A	419[B]	LHG	O8-C23-C24-C25
23	B	612	CLA	CBA-CGA-O2A-C1
23	D	403	CLA	CBA-CGA-O2A-C1
33	c	519	LMG	C30-C31-C32-C33
33	Z	101	LMG	O7-C10-C11-C12
34	B	621	HTG	C2'-C1'-S1-C1
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
32	d	415[A]	LHG	C13-C14-C15-C16
32	L	101[A]	LHG	O7-C7-C8-C9
26	a	411	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
32	A	419[A]	LHG	C17-C18-C19-C20
35	C	518[A]	DGD	CAB-CBB-CCB-CDB
35	c	518	DGD	C9B-CAB-CBB-CCB
32	a	419[A]	LHG	O8-C23-C24-C25
32	b	629[A]	LHG	O7-C7-C8-C9
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
26	b	620	SQD	C30-C31-C32-C33
35	c	517[B]	DGD	CBB-CCB-CDB-CEB
26	f	102	SQD	C34-C35-C36-C37
32	d	409[B]	LHG	C33-C34-C35-C36
35	C	518[B]	DGD	C5A-C6A-C7A-C8A
33	Z	101	LMG	C29-C28-O8-C9
31	e	101	LMT	C2-C1-O1'-C1'
23	a	405[B]	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
26	X	101	SQD	C44-C45-C46-O48
33	B	620	LMG	O1-C7-C8-C9
33	C	501	LMG	O1-C7-C8-C9
35	h	102	DGD	C1G-C2G-C3G-O3G
23	C	509	CLA	C13-C15-C16-C17
23	B	610	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	501	CLA	C4B-C3B-CAB-CBB
23	c	506	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
32	D	406[B]	LHG	C32-C33-C34-C35
32	d	415[A]	LHG	C18-C19-C20-C21
32	b	629[A]	LHG	C24-C25-C26-C27
23	B	614	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C40-C39-C41-C42
33	B	620	LMG	O6-C1-O1-C7
23	B	613	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
33	c	519	LMG	O7-C10-C11-C12
26	X	101	SQD	C33-C34-C35-C36
33	c	520	LMG	O1-C7-C8-O7
25	d	406	BCR	C21-C22-C23-C24
35	c	516[B]	DGD	C8B-C9B-CAB-CBB
26	b	620	SQD	C25-C26-C27-C28
32	A	419[B]	LHG	C17-C18-C19-C20
33	d	413	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
26	a	411	SQD	O48-C23-C24-C25
32	E	101[B]	LHG	O7-C7-C8-C9
33	B	620	LMG	C21-C22-C23-C24
23	B	603	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
23	b	608	CLA	C13-C15-C16-C17
26	a	411	SQD	C15-C16-C17-C18
33	C	521	LMG	C38-C39-C40-C41
32	D	406[B]	LHG	C34-C35-C36-C37
23	C	513	CLA	CAA-CBA-CGA-O2A
23	b	611	CLA	C13-C15-C16-C17
26	A	412	SQD	C31-C32-C33-C34
23	A	408	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	512	CLA	C2-C1-O2A-CGA
32	a	419[B]	LHG	O8-C23-C24-C25
23	B	615	CLA	C12-C13-C15-C16
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	608	CLA	C12-C13-C15-C16
23	c	510	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C8-C10-C11-C12
24	a	406[B]	PHO	O2A-C1-C2-C3
23	b	613	CLA	O1D-CGD-O2D-CED
26	a	409[B]	SQD	C18-C19-C20-C21
26	f	102	SQD	C28-C29-C30-C31
33	c	519	LMG	C39-C40-C41-C42
23	b	601	CLA	CAA-CBA-CGA-O1A
23	B	602	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C16-C17-C18-C19
23	B	616	CLA	C16-C17-C18-C20
33	a	415	LMG	C14-C15-C16-C17
32	A	419[B]	LHG	O10-C23-C24-C25
23	b	603	CLA	C5-C6-C7-C8
38	f	101	HEM	CAD-CBD-CGD-O2D
33	B	620	LMG	C30-C31-C32-C33
32	L	101[B]	LHG	O9-C7-C8-C9
23	B	612	CLA	C13-C15-C16-C17
32	E	101[A]	LHG	O7-C7-C8-C9
33	D	411	LMG	O7-C10-C11-C12
35	c	516[A]	DGD	O2G-C1B-C2B-C3B
23	c	513	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	A	414[B]	PL9	C23-C24-C26-C27
26	a	409[A]	SQD	C10-C11-C12-C13
33	d	413	LMG	C38-C39-C40-C41
33	a	415	LMG	O10-C28-C29-C30
33	Z	101	LMG	O9-C10-C11-C12
33	c	519	LMG	O10-C28-O8-C9
31	a	416	LMT	C4'-C5'-C6'-O6'
23	b	613	CLA	CAA-CBA-CGA-O2A
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
29	A	414[B]	PL9	C46-C47-C48-C49
32	b	629[A]	LHG	O9-C7-C8-C9
23	A	405[B]	CLA	C13-C15-C16-C17
23	B	615	CLA	C13-C15-C16-C17
23	B	614	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	b	608	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
35	C	519	DGD	C2A-C1A-O1G-C1G
26	f	102	SQD	O5-C5-C6-S
23	c	510	CLA	CAA-CBA-CGA-O1A
32	A	419[A]	LHG	O10-C23-C24-C25
32	a	419[A]	LHG	O10-C23-C24-C25
32	b	629[B]	LHG	O9-C7-C8-C9
33	D	411	LMG	C34-C35-C36-C37
32	D	406[A]	LHG	C28-C29-C30-C31
33	C	521	LMG	C33-C34-C35-C36
32	E	101[B]	LHG	O9-C7-C8-C9
32	a	419[B]	LHG	O10-C23-C24-C25
26	a	411	SQD	C45-C44-O6-C1
35	C	517[A]	DGD	C5D-C6D-O5D-C1E
35	C	517[B]	DGD	C5D-C6D-O5D-C1E
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
32	L	101[B]	LHG	O9-C7-O7-C5
35	C	519	DGD	O6D-C5D-C6D-O5D
33	C	501	LMG	O1-C7-C8-O7
31	a	416	LMT	C2'-C1'-O1'-C1
23	C	511	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A
23	b	612	CLA	CAA-CBA-CGA-O2A
32	E	101[A]	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	O1-C7-C8-C9
23	B	613	CLA	CAA-CBA-CGA-O1A
33	c	519	LMG	O9-C10-C11-C12
29	d	407[A]	PL9	C11-C12-C13-C14
26	A	412	SQD	O48-C23-C24-C25
24	d	403[B]	PHO	C8-C10-C11-C12
26	a	411	SQD	O10-C23-C24-C25
32	L	101[A]	LHG	O9-C7-C8-C9
23	A	404[B]	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	406[A]	PHO	CAD-CBD-CGD-O2D
24	d	403[B]	PHO	CAD-CBD-CGD-O2D
23	c	512	CLA	CAA-CBA-CGA-O2A
26	a	409[B]	SQD	O47-C7-C8-C9
31	m	103	LMT	C4'-C5'-C6'-O6'
35	c	516[A]	DGD	C1A-C2A-C3A-C4A
23	b	610	CLA	C16-C17-C18-C19
29	d	407[B]	PL9	C11-C12-C13-C14
35	c	516[A]	DGD	CBA-CCA-CDA-CEA
31	T	101	LMT	C5'-C4'-O1B-C1B
26	f	102	SQD	C26-C27-C28-C29
35	C	519	DGD	C8B-C9B-CAB-CBB
33	C	521	LMG	C10-C11-C12-C13
32	D	407[A]	LHG	O8-C23-C24-C25
35	c	516[B]	DGD	O2G-C1B-C2B-C3B
31	B	628	LMT	C7-C8-C9-C10
32	D	407[B]	LHG	O8-C23-C24-C25
32	E	101[A]	LHG	O8-C23-C24-C25
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
33	m	101	LMG	C30-C31-C32-C33
23	b	604	CLA	C2C-C3C-CAC-CBC

There are no ring outliers.

171 monomers are involved in 360 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	412	GOL	2	0
32	d	409[B]	LHG	10	0
23	a	405[B]	CLA	2	0
31	t	101	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	517[B]	DGD	3	0
29	a	413[A]	PL9	5	0
25	B	618	BCR	4	0
35	C	518[B]	DGD	3	0
23	B	602	CLA	2	0
32	D	406[B]	LHG	1	0
27	B	623	GOL	2	0
23	b	614	CLA	1	0
33	c	520	LMG	1	0
27	b	628	GOL	1	0
25	A	409	BCR	1	0
23	b	601	CLA	3	0
23	A	405[B]	CLA	3	0
24	A	407[B]	PHO	1	0
27	a	418	GOL	4	0
25	y	101	BCR	2	0
23	A	404[B]	CLA	2	0
27	O	303	GOL	2	0
32	d	409[A]	LHG	10	0
34	b	622	HTG	1	0
25	h	101	BCR	4	0
35	C	517[A]	DGD	2	0
23	d	405	CLA	2	0
23	d	402[B]	CLA	3	0
34	B	624	HTG	1	0
35	C	518[A]	DGD	2	0
23	B	609	CLA	3	0
27	v	202[B]	GOL	1	0
25	B	619	BCR	1	0
27	B	626	GOL	1	0
23	B	606	CLA	2	0
25	b	619	BCR	5	0
33	z	101	LMG	2	0
23	C	502	CLA	6	0
32	d	415[B]	LHG	1	0
23	A	405[A]	CLA	4	0
23	B	615	CLA	7	0
24	A	407[A]	PHO	2	0
26	a	409[B]	SQD	5	0
25	H	101	BCR	1	0
23	A	404[A]	CLA	5	0
23	c	501	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	613	CLA	5	0
23	c	502	CLA	2	0
25	Y	101	BCR	2	0
35	c	516[B]	DGD	2	0
24	a	406[B]	PHO	1	0
23	d	402[A]	CLA	2	0
27	v	202[A]	GOL	1	0
23	A	406[B]	CLA	1	0
23	c	511	CLA	6	0
25	a	408	BCR	1	0
29	A	414[A]	PL9	9	0
35	c	517[B]	DGD	1	0
23	B	616	CLA	4	0
31	C	525	LMT	1	0
23	b	609	CLA	4	0
32	A	419[B]	LHG	1	0
23	B	610	CLA	1	0
23	C	504	CLA	3	0
34	b	625	HTG	1	0
35	C	519	DGD	3	0
35	c	518	DGD	3	0
26	a	411	SQD	2	0
23	C	508	CLA	2	0
26	a	409[A]	SQD	5	0
23	B	604	CLA	1	0
25	K	102	BCR	2	0
27	A	418	GOL	4	0
31	a	416	LMT	1	0
23	A	408	CLA	4	0
25	b	617	BCR	1	0
33	d	413	LMG	4	0
35	c	516[A]	DGD	2	0
23	a	407	CLA	5	0
23	C	514	CLA	1	0
25	k	101	BCR	2	0
25	C	516	BCR	1	0
29	A	414[B]	PL9	9	0
25	c	514	BCR	3	0
23	A	406[A]	CLA	1	0
35	c	517[A]	DGD	1	0
23	C	509	CLA	3	0
26	b	620	SQD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	504	CLA	2	0
32	A	419[A]	LHG	2	0
27	a	417	GOL	1	0
25	d	406	BCR	1	0
33	c	519	LMG	1	0
27	O	302	GOL	1	0
32	E	101[B]	LHG	2	0
24	A	416[B]	PHO	1	0
31	M	101	LMT	1	0
23	C	507	CLA	5	0
23	C	512	CLA	2	0
23	C	513	CLA	1	0
23	D	402[B]	CLA	3	0
23	b	605	CLA	3	0
29	d	407[B]	PL9	1	0
32	d	408[B]	LHG	2	0
33	B	620	LMG	1	0
26	A	410[B]	SQD	2	0
23	c	506	CLA	4	0
23	d	404[B]	CLA	3	0
40	V	201	HEC	1	0
23	c	507	CLA	3	0
25	b	618	BCR	4	0
26	l	101	SQD	1	0
31	b	621	LMT	2	0
35	H	102	DGD	1	0
23	B	614	CLA	3	0
23	B	612	CLA	1	0
38	f	101	HEM	2	0
32	D	407[B]	LHG	2	0
23	b	606	CLA	2	0
32	E	101[A]	LHG	5	0
24	A	416[A]	PHO	1	0
31	B	628	LMT	1	0
31	e	101	LMT	1	0
32	d	408[A]	LHG	3	0
23	D	402[A]	CLA	3	0
23	B	605	CLA	4	0
32	a	419[B]	LHG	4	0
27	l	103[A]	GOL	1	0
23	b	616	CLA	1	0
23	a	404[A]	CLA	3	0

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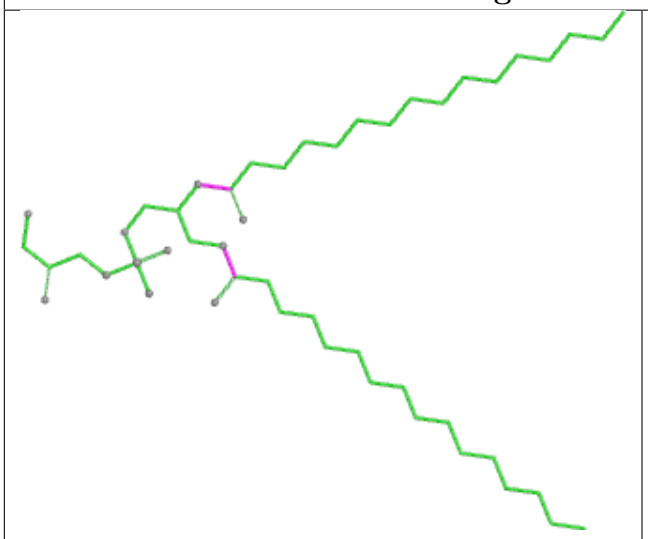
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	404	BCR	2	0
23	d	404[A]	CLA	2	0
24	d	403[A]	PHO	2	0
25	t	102	BCR	4	0
23	C	503	CLA	5	0
23	C	510	CLA	2	0
23	b	604	CLA	2	0
23	c	508	CLA	8	0
23	C	511	CLA	3	0
23	c	513	CLA	2	0
23	c	505	CLA	6	0
25	B	617	BCR	1	0
23	C	505	CLA	1	0
32	D	407[A]	LHG	5	0
34	B	621	HTG	1	0
23	b	615	CLA	1	0
26	A	410[A]	SQD	1	0
32	a	419[A]	LHG	4	0
23	C	506	CLA	4	0
23	c	512	CLA	7	0
23	c	503	CLA	3	0
23	B	601	CLA	4	0
23	a	404[B]	CLA	3	0
23	a	405[A]	CLA	2	0
38	E	102	HEM	1	0
33	C	521	LMG	3	0
29	a	413[B]	PL9	6	0
23	c	509	CLA	3	0
31	A	417	LMT	1	0
24	d	403[B]	PHO	2	0
35	h	102	DGD	2	0
33	Z	101	LMG	1	0
23	b	612	CLA	1	0
26	X	101	SQD	2	0
25	T	102	BCR	7	0
23	b	613	CLA	2	0
34	c	521	HTG	1	0
23	b	607	CLA	1	0
32	D	406[A]	LHG	2	0
25	C	515	BCR	2	0
23	b	602	CLA	2	0

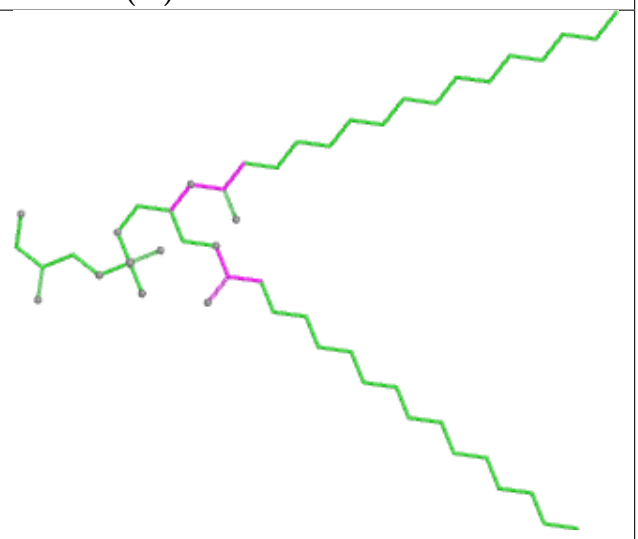
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

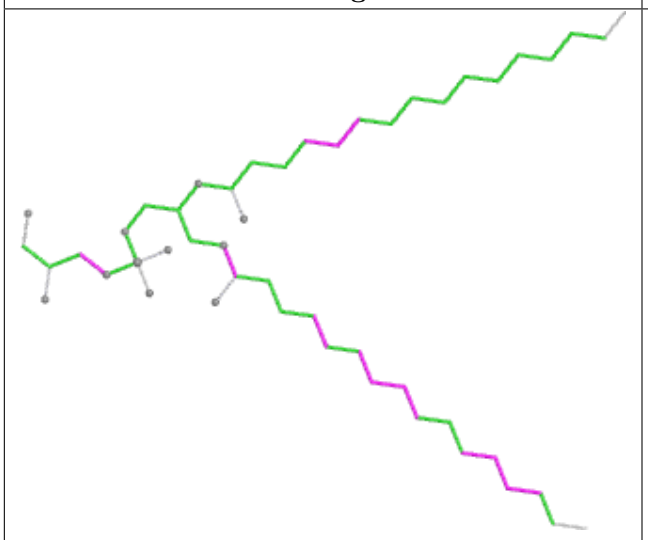
Ligand LHG d 409 (B)



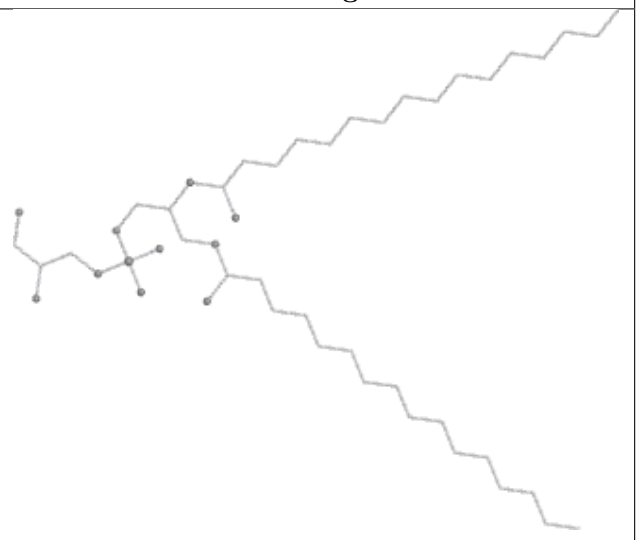
Bond lengths



Bond angles

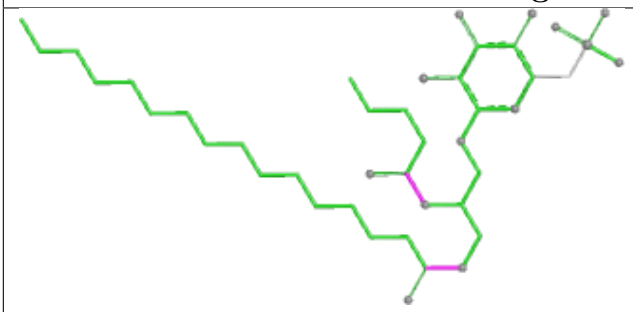


Torsions

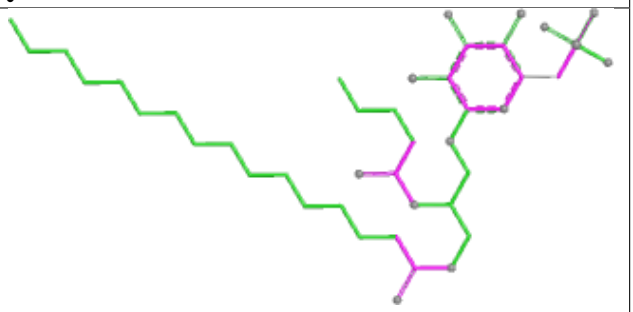


Rings

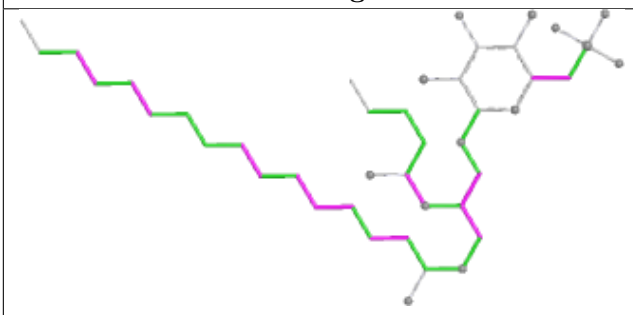
Ligand SQD f 102



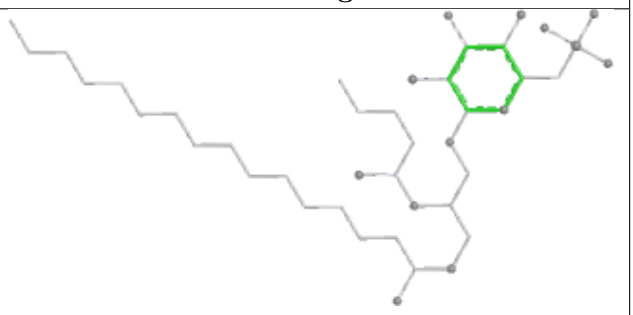
Bond lengths



Bond angles

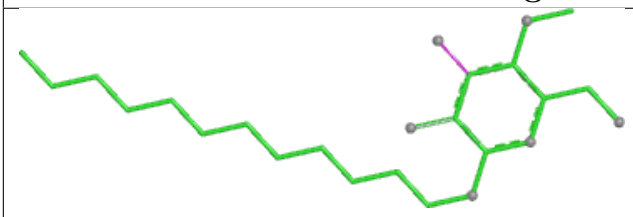


Torsions

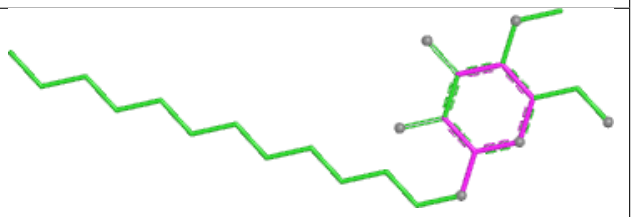


Rings

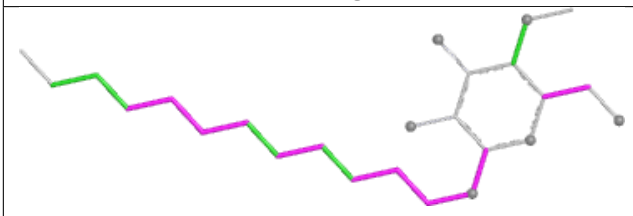
Ligand LMT b 627



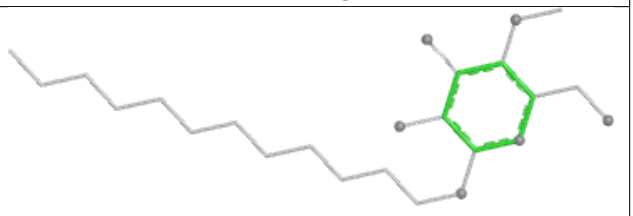
Bond lengths



Bond angles

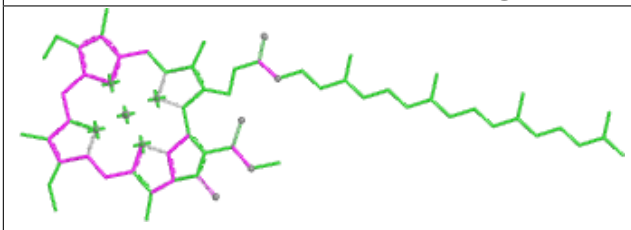


Torsions

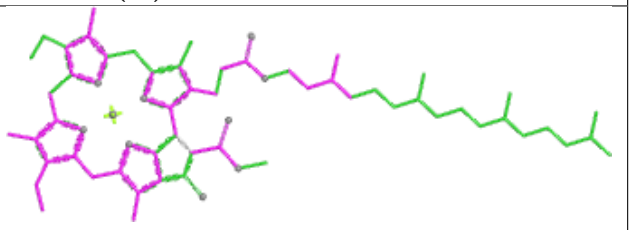


Rings

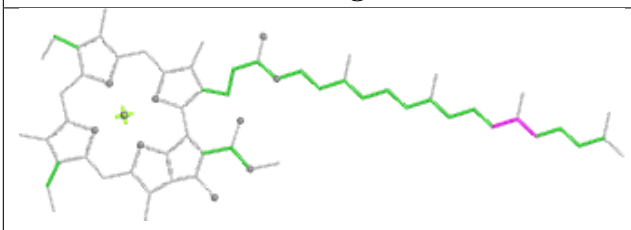
Ligand CLA a 405 (B)



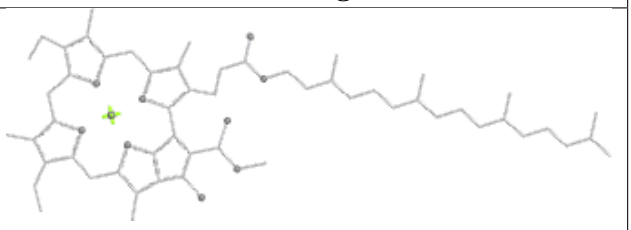
Bond lengths



Bond angles

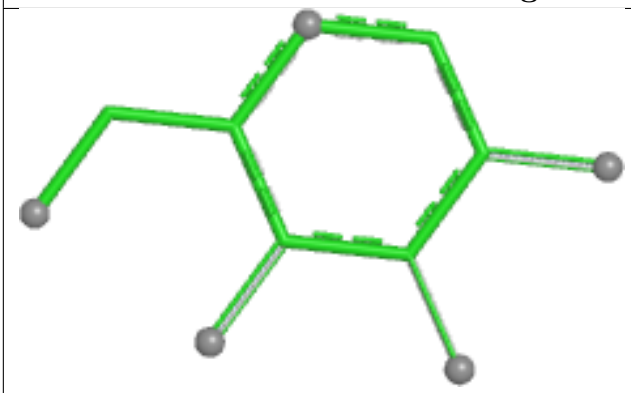


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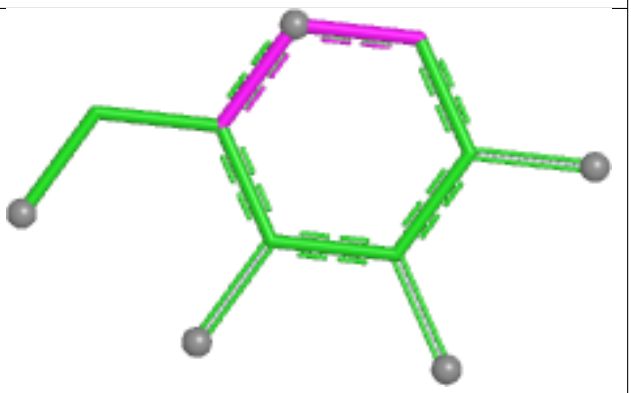


Rings

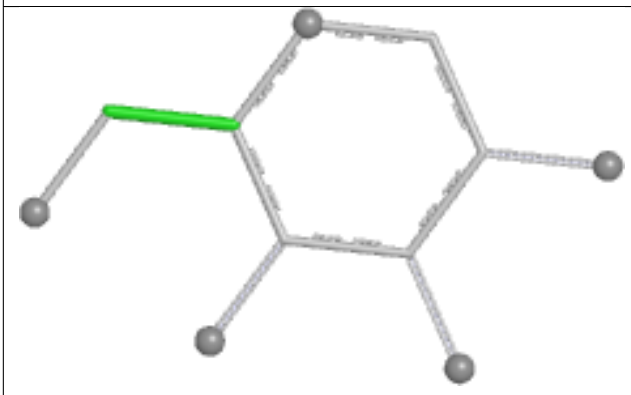
Ligand HTG V 202



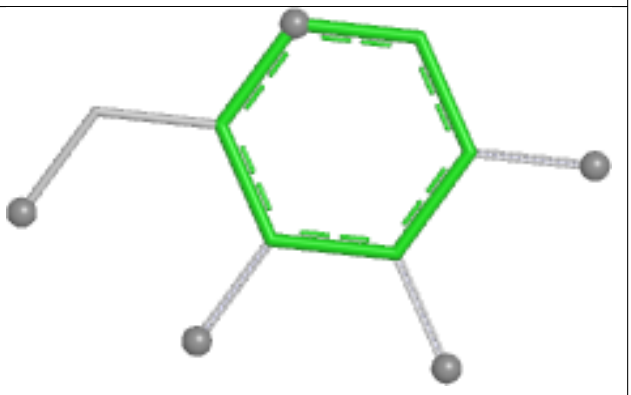
Bond lengths



Bond angles

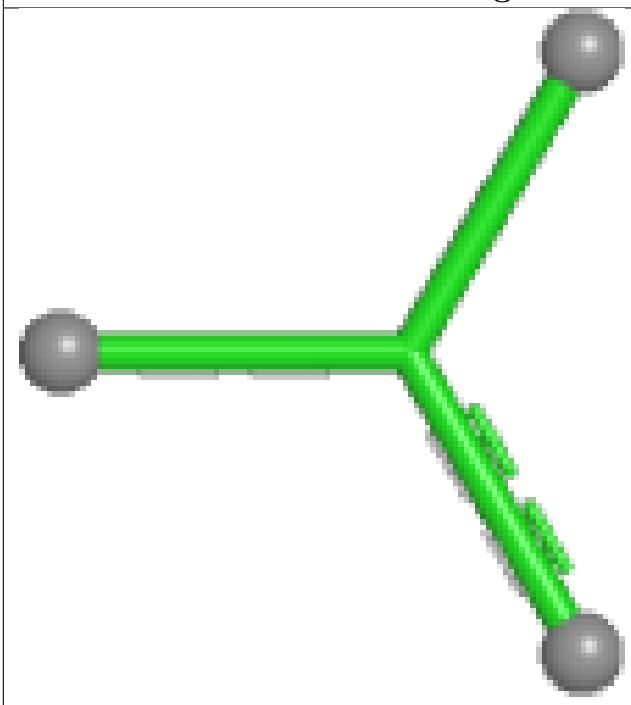


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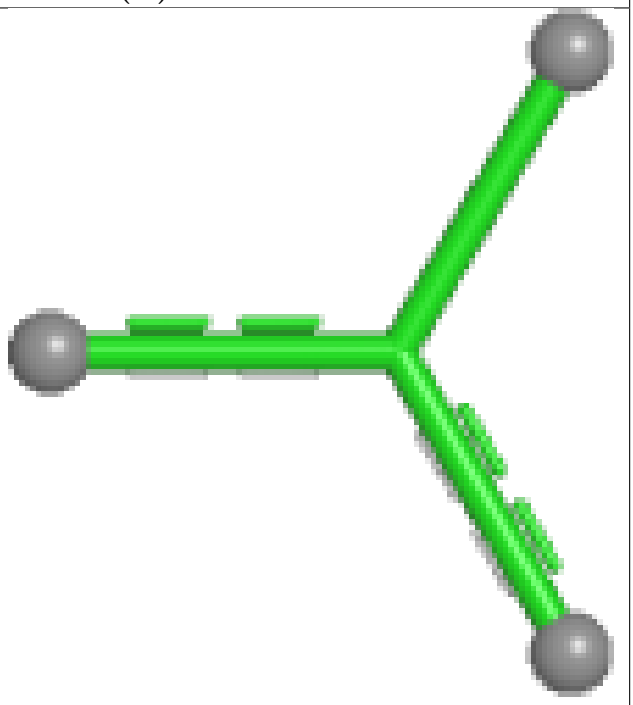


Rings

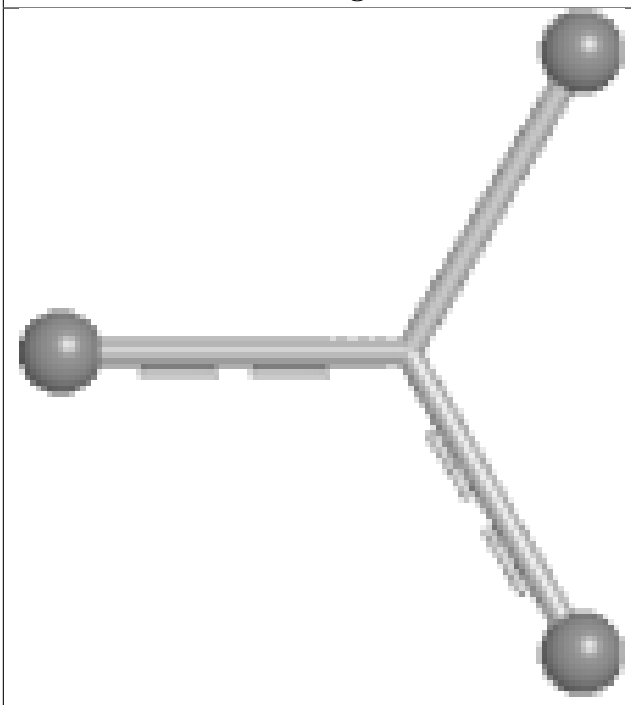
Ligand BCT d 401 (B)



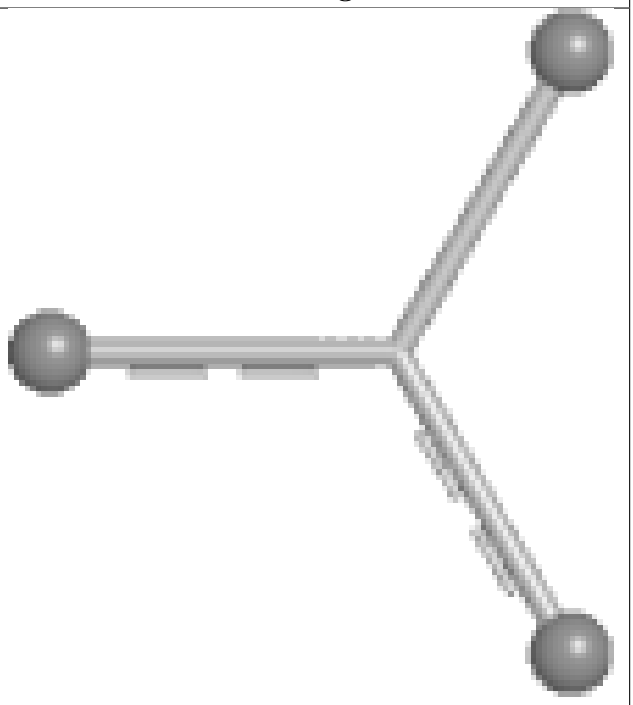
Bond lengths



Bond angles

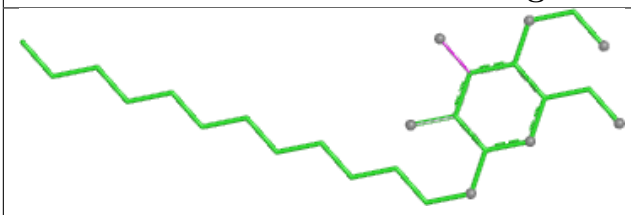


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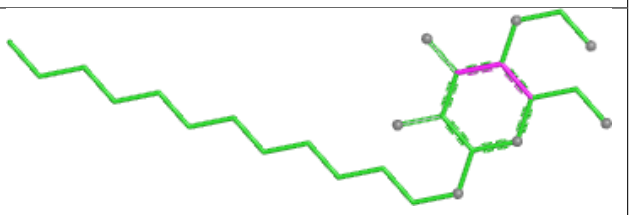


Rings

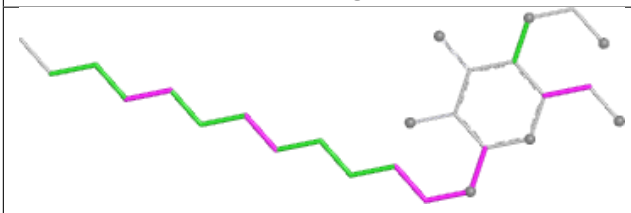
Ligand LMT t 101



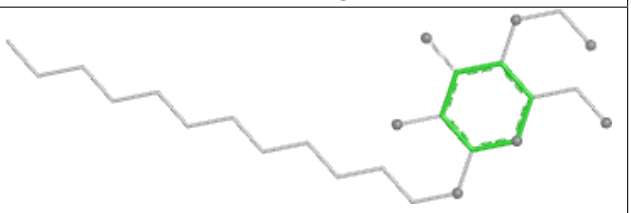
Bond lengths



Bond angles

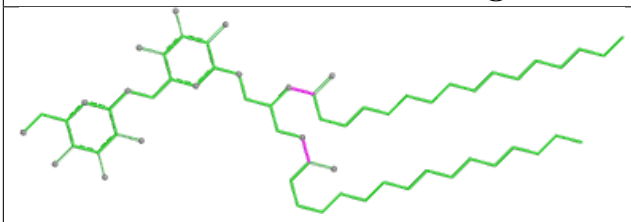


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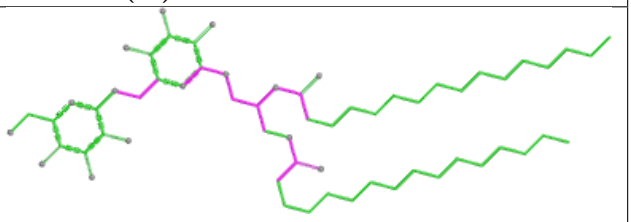


Rings

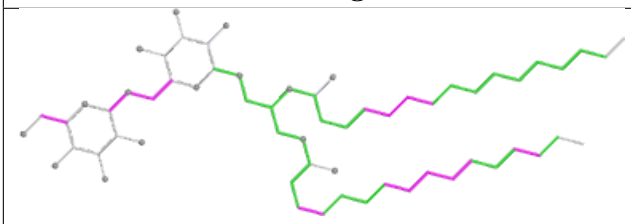
Ligand DGD C 517 (B)



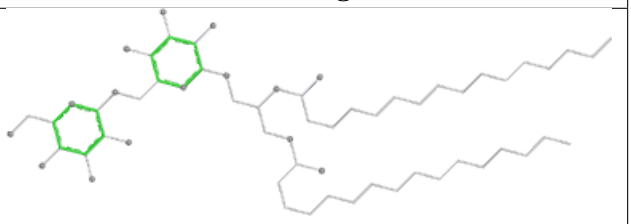
Bond lengths



Bond angles

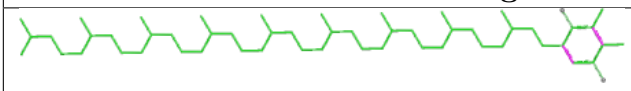


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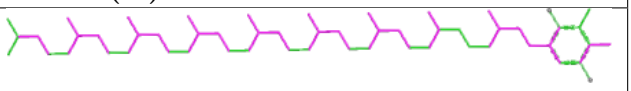


Rings

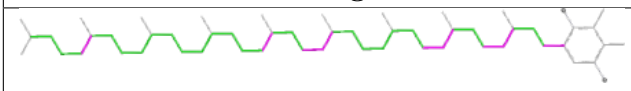
Ligand PL9 a 413 (A)



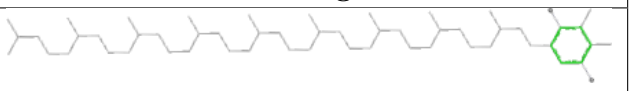
Bond lengths



Bond angles

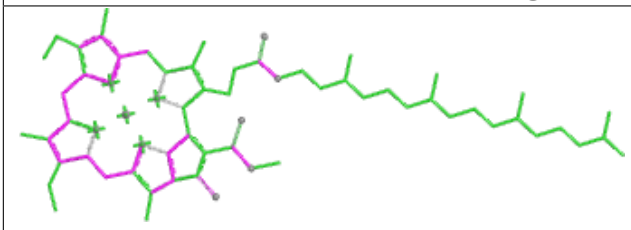


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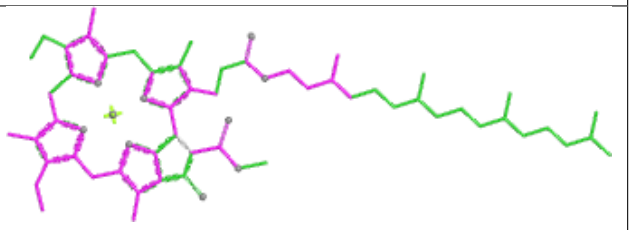


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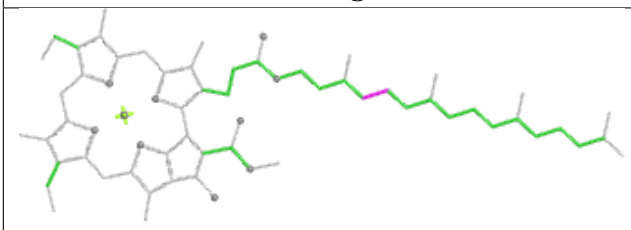
Ligand CLA B 607



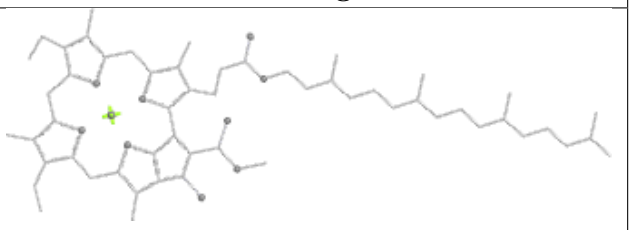
Bond lengths



Bond angles

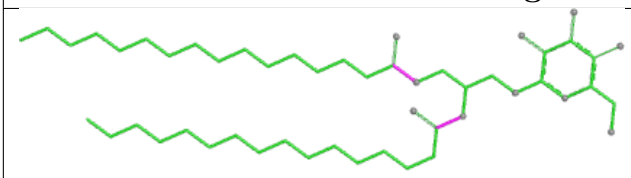


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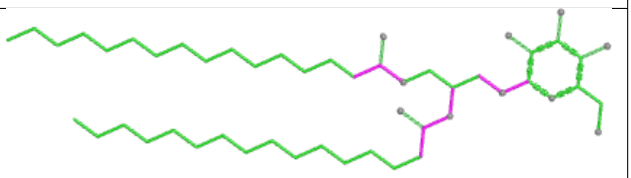


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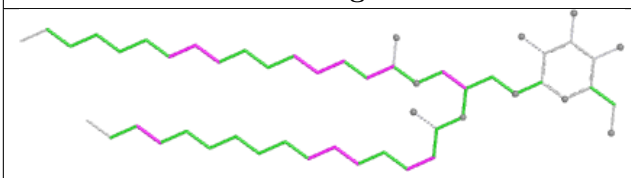
Ligand LMG a 415



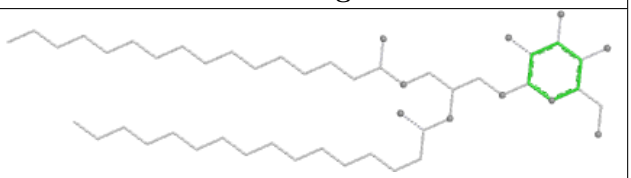
Bond lengths



Bond angles



Torsions

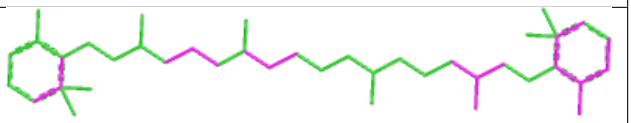


Rings

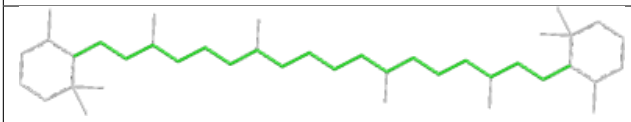
Ligand BCR B 618



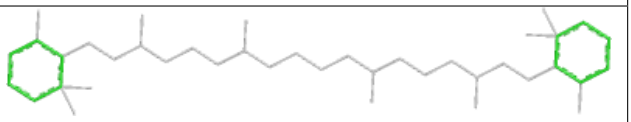
Bond lengths



Bond angles

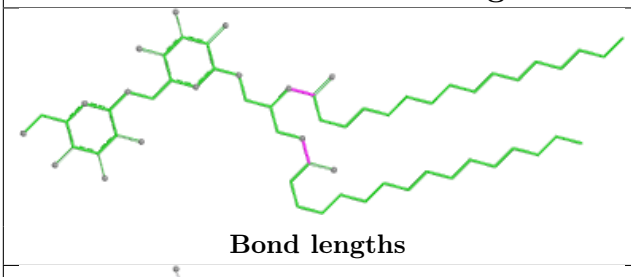


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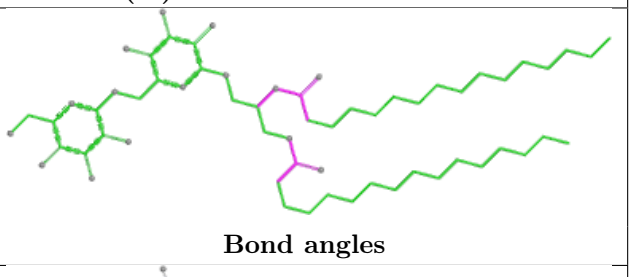


Rings

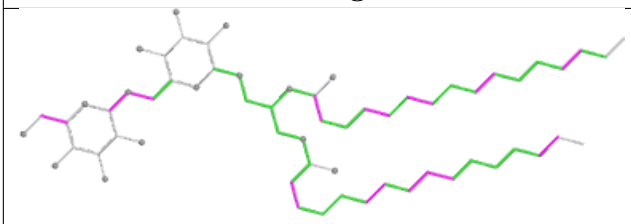
Ligand DGD C 518 (B)



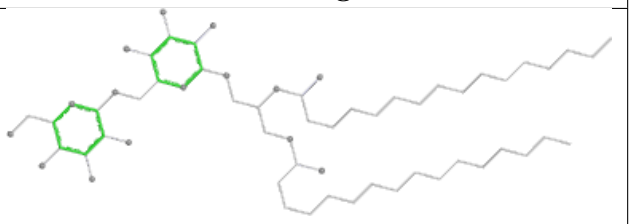
Bond lengths



Bond angles

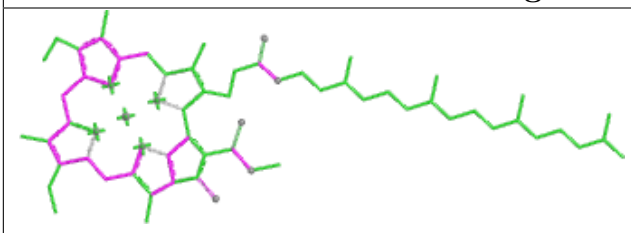


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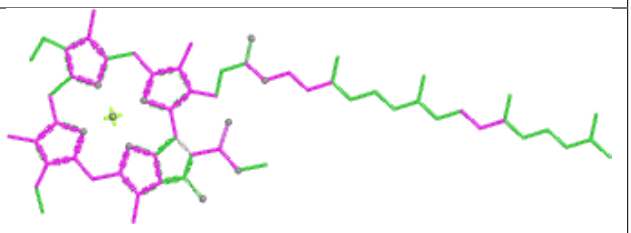


Rings

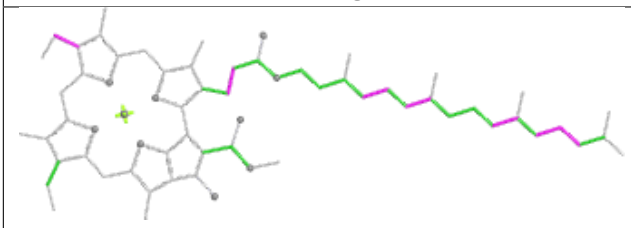
Ligand CLA B 602



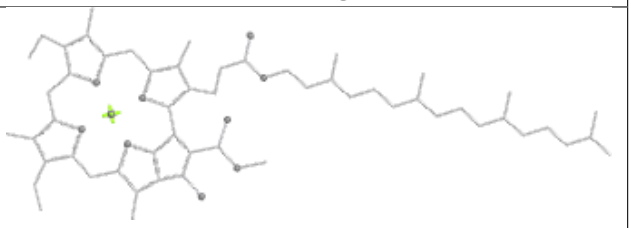
Bond lengths



Bond angles

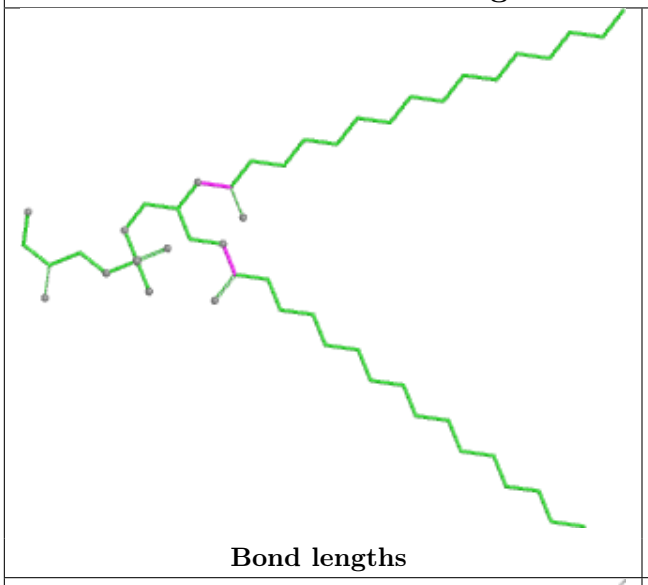


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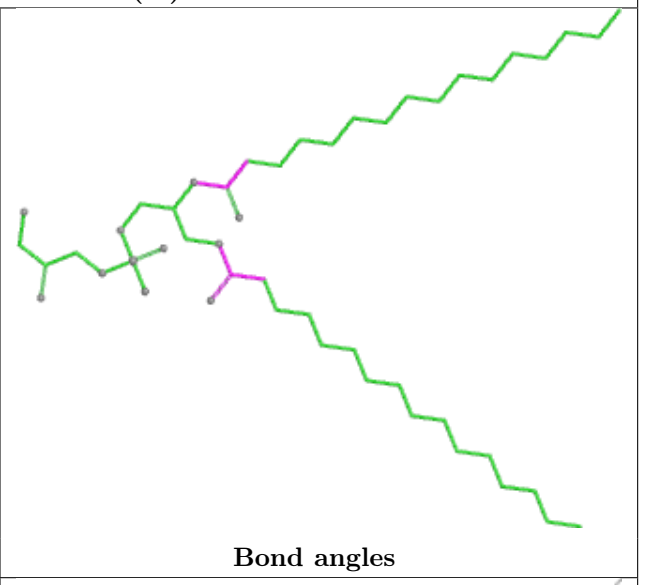


Rings

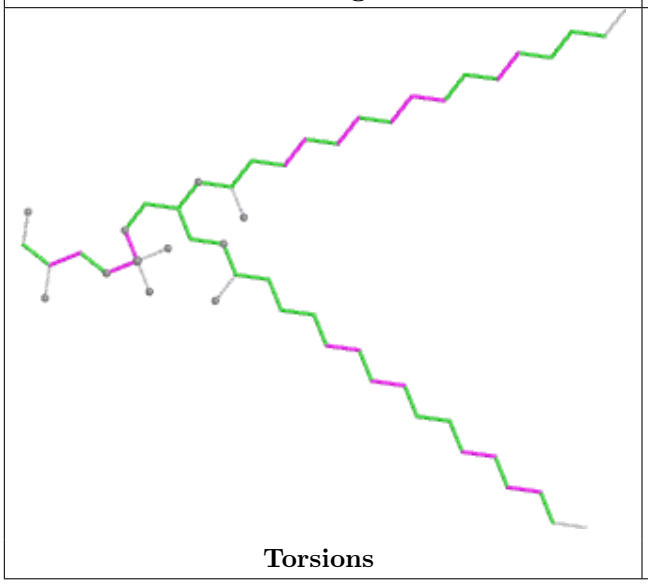
Ligand LHG D 406 (B)



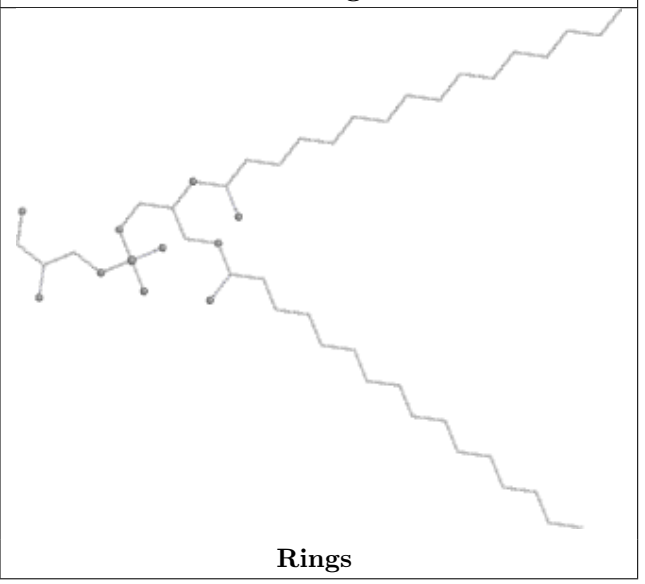
Bond lengths



Bond angles

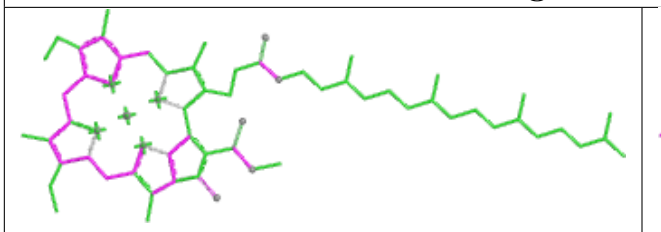


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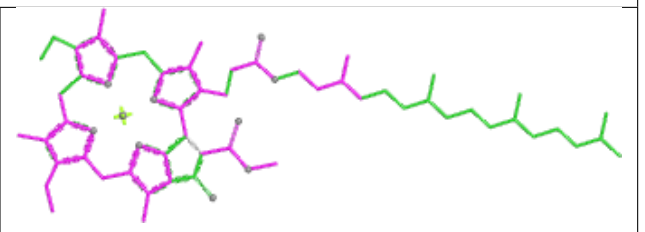


Rings

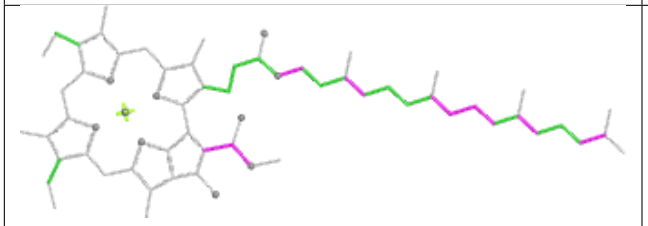
Ligand CLA b 614



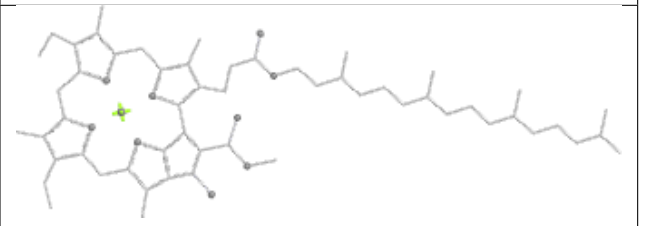
Bond lengths



Bond angles

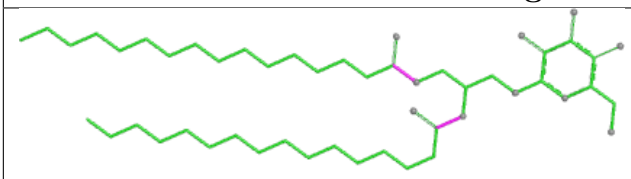


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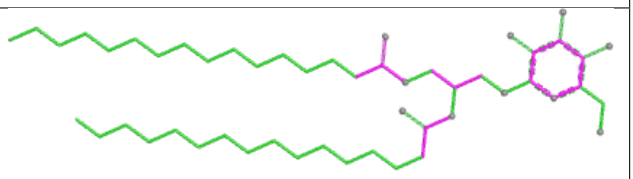


Rings

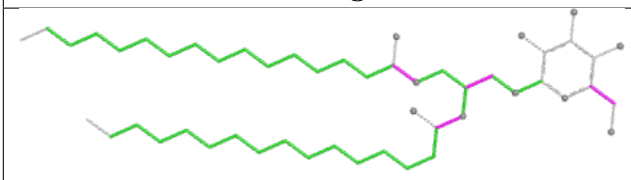
Ligand LMG c 520



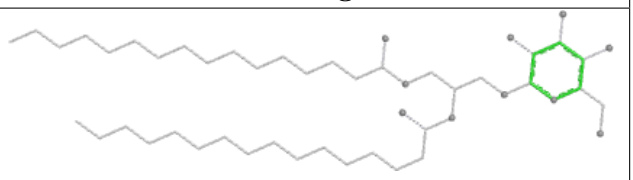
Bond lengths



Bond angles

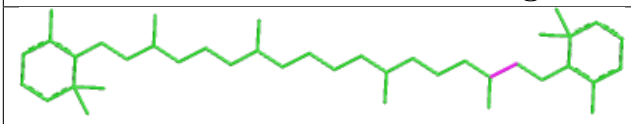


Torsions

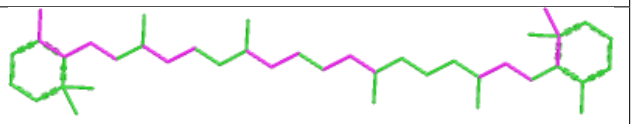


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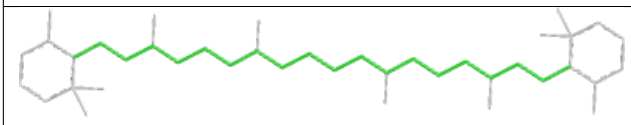
Ligand BCR A 409



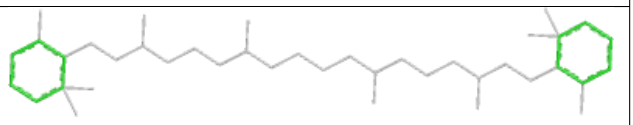
Bond lengths



Bond angles

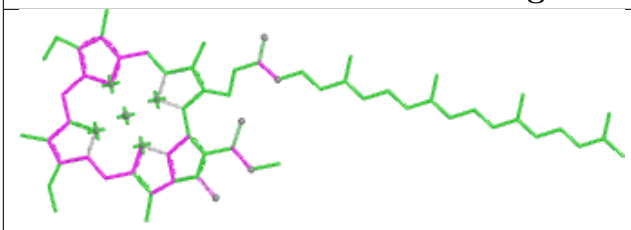


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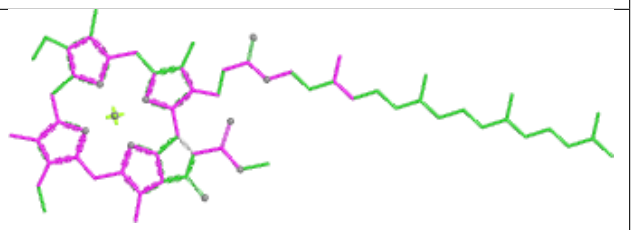


Rings

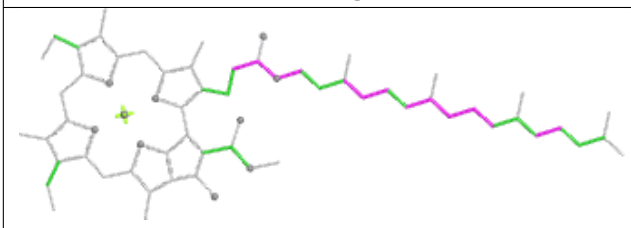
Ligand CLA b 601



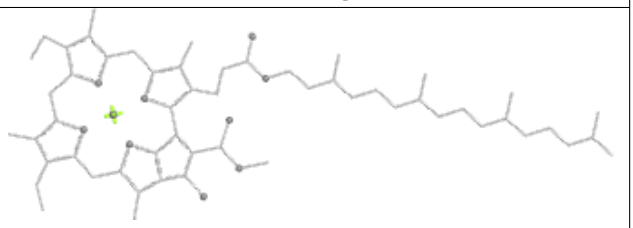
Bond lengths



Bond angles

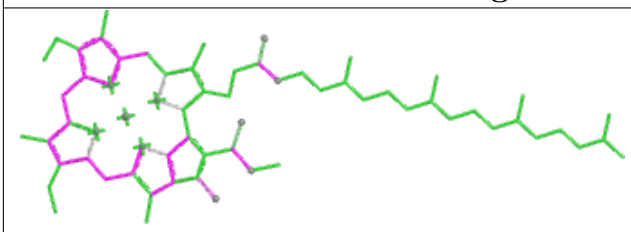


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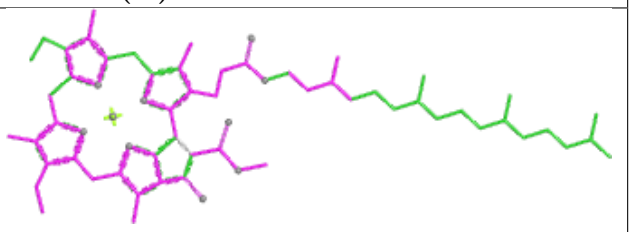


Rings

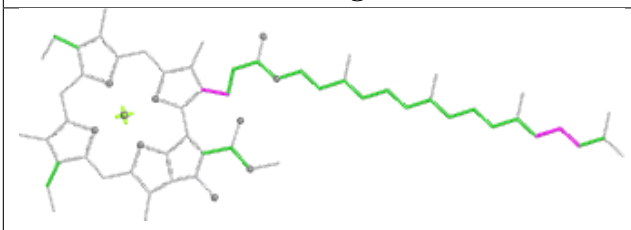
Ligand CLA A 405 (B)



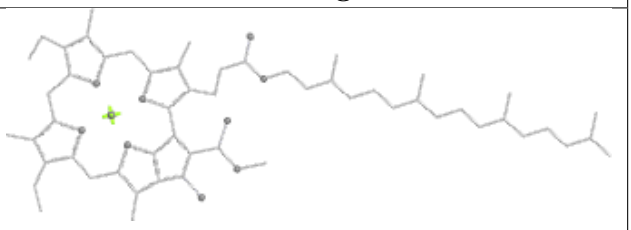
Bond lengths



Bond angles



Torsions

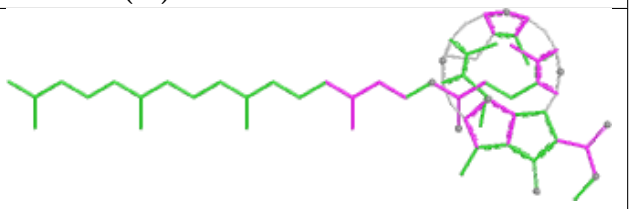


Rings

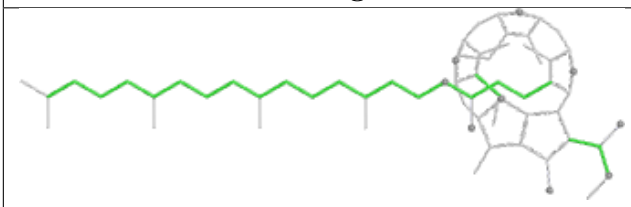
Ligand PHO A 407 (B)



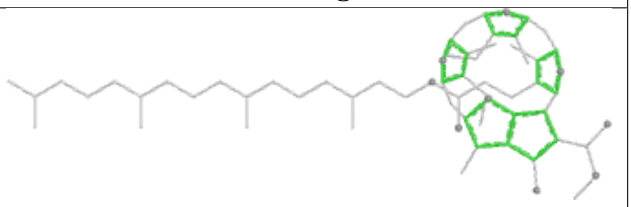
Bond lengths



Bond angles

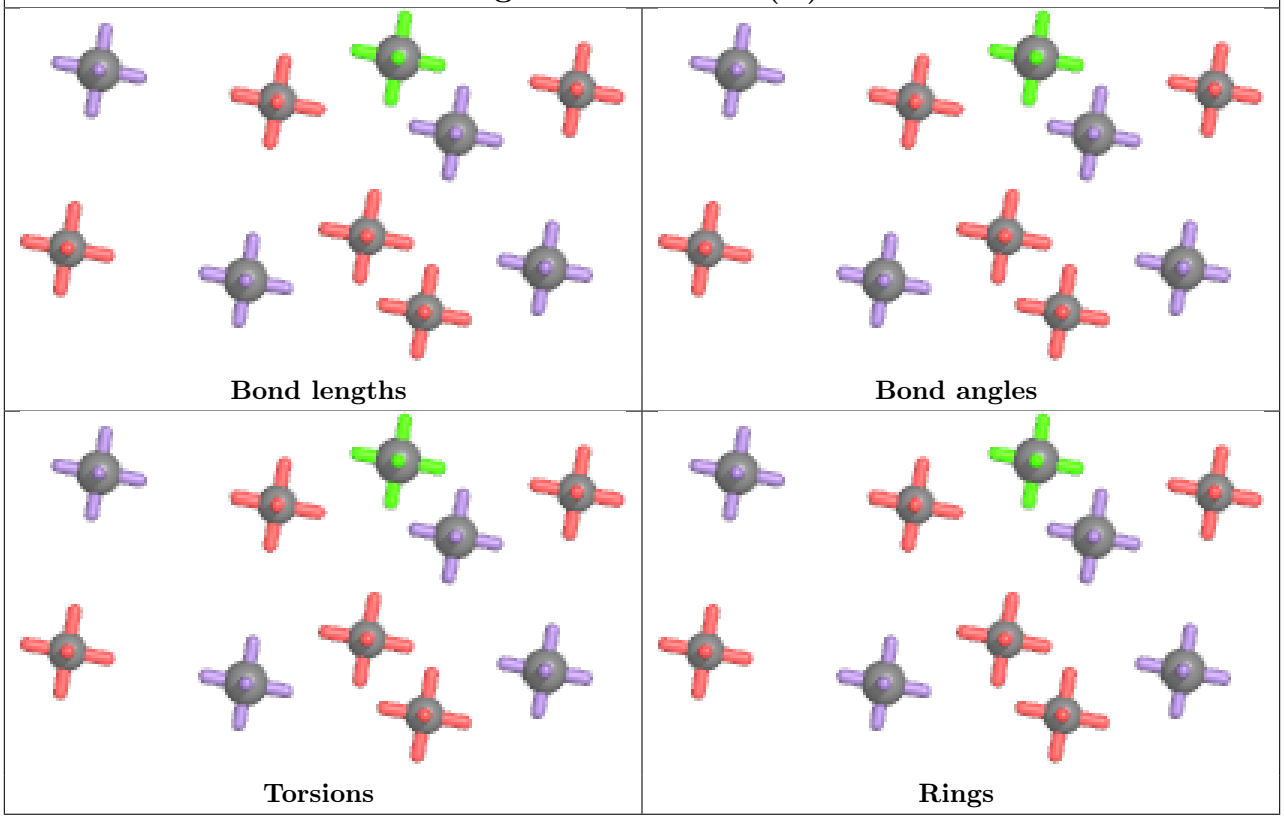


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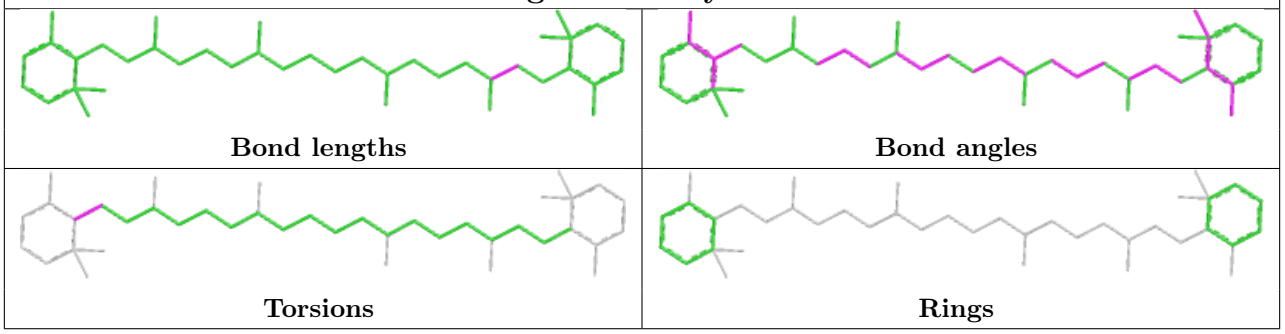


Rings

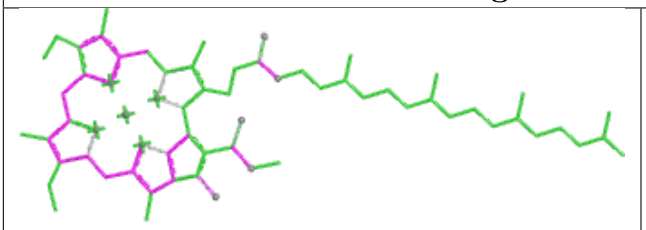
Ligand OEX a 412 (A)



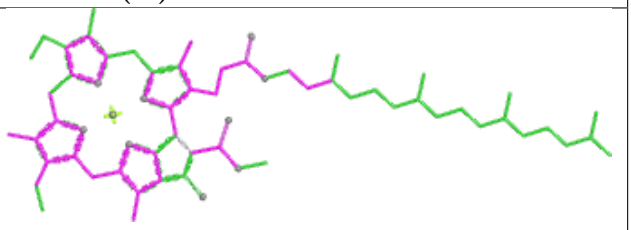
Ligand BCR y 101



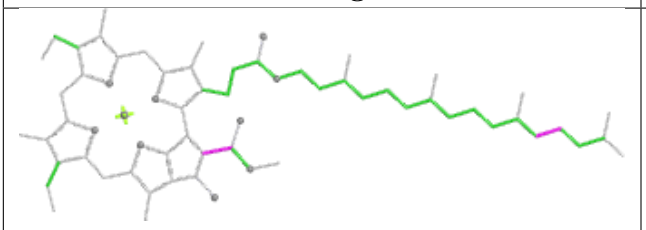
Ligand CLA A 404 (B)



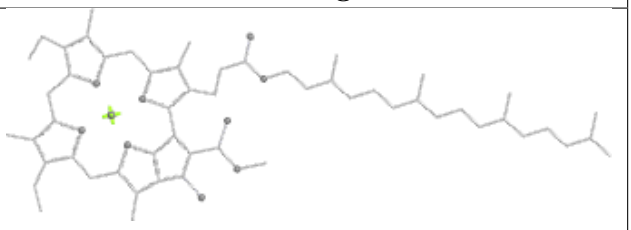
Bond lengths



Bond angles

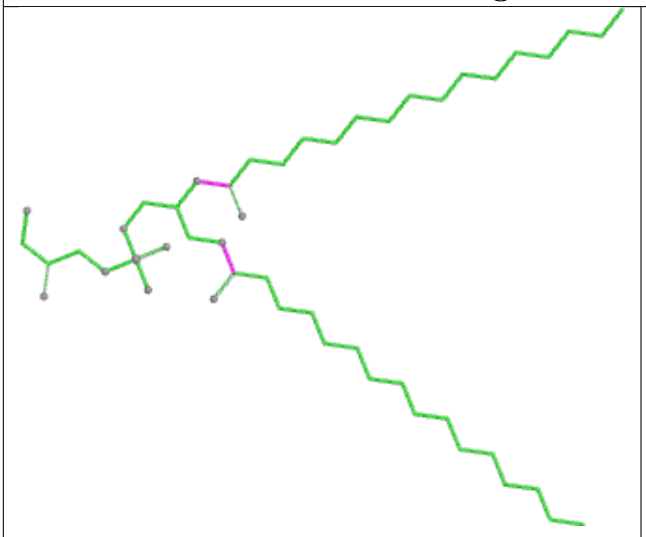


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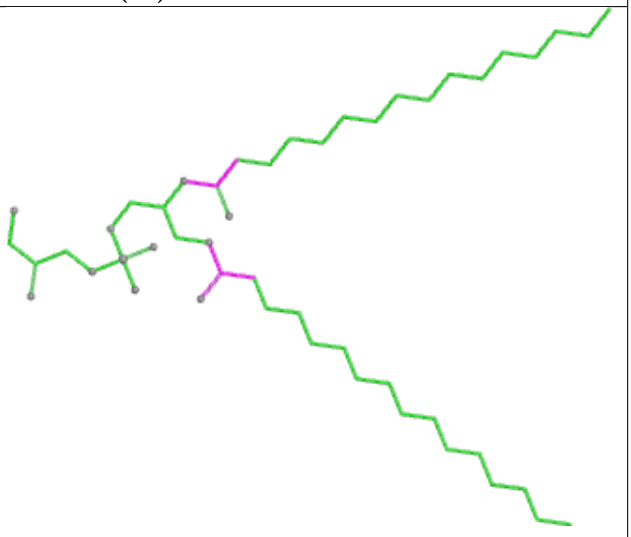


Rings

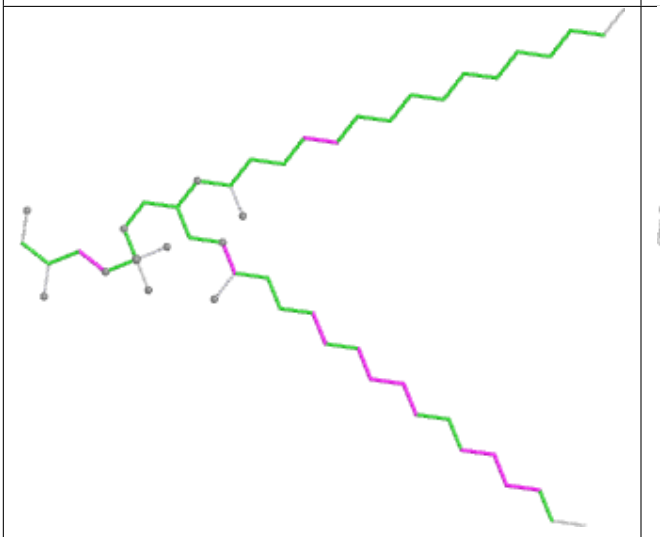
Ligand LHG d 409 (A)



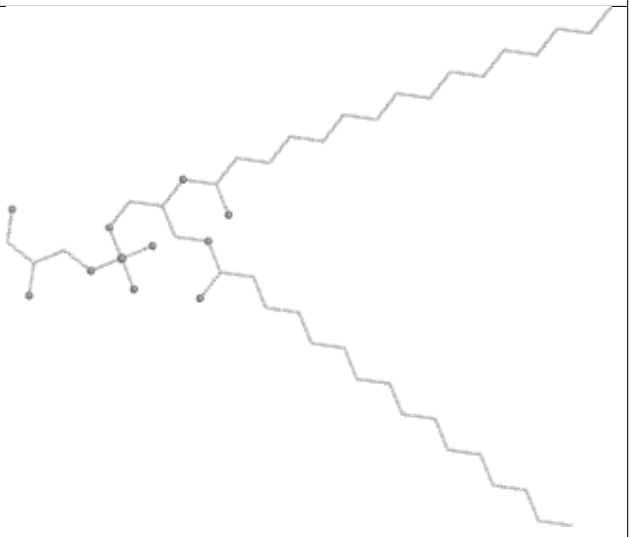
Bond lengths



Bond angles

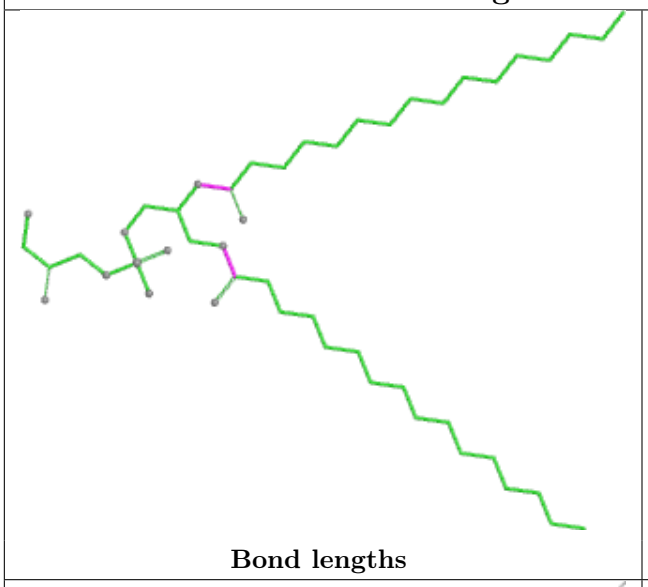


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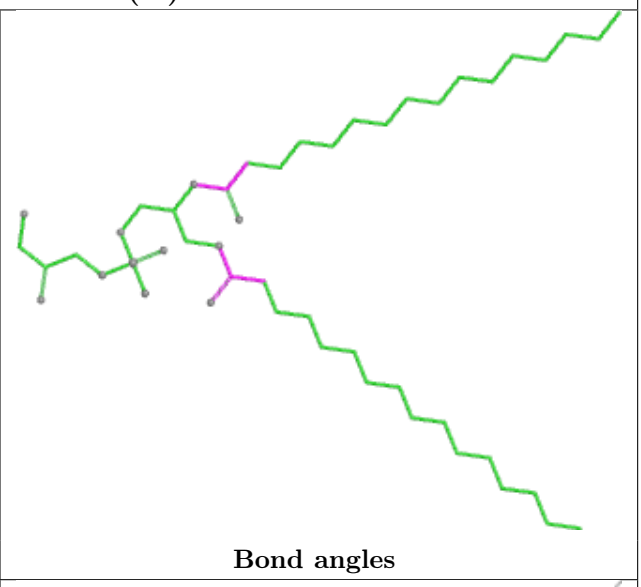


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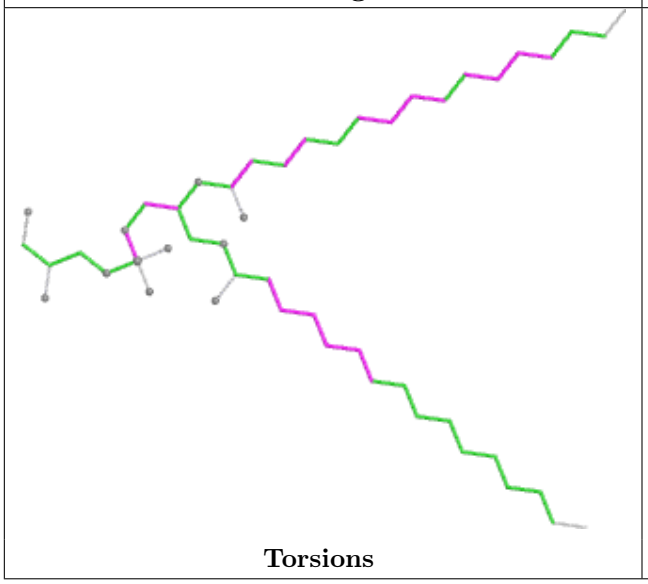
Ligand LHG L 101 (A)



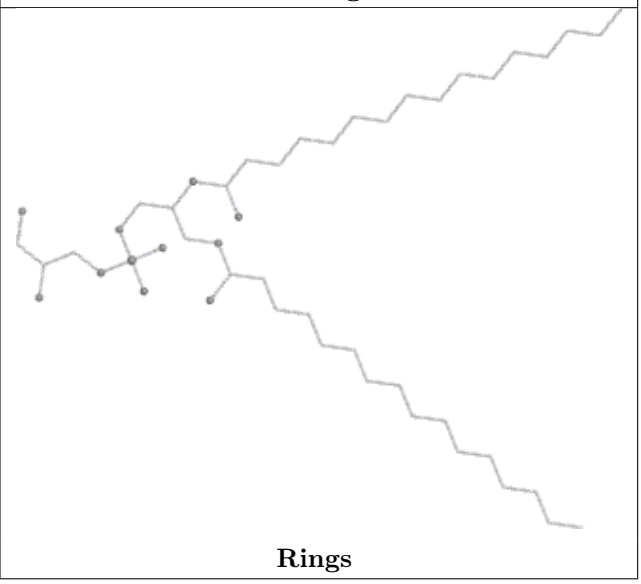
Bond lengths



Bond angles

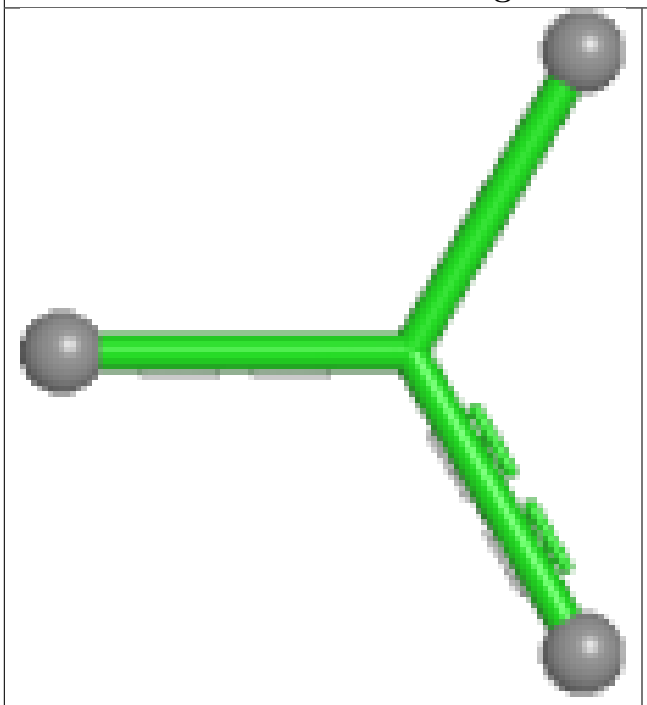


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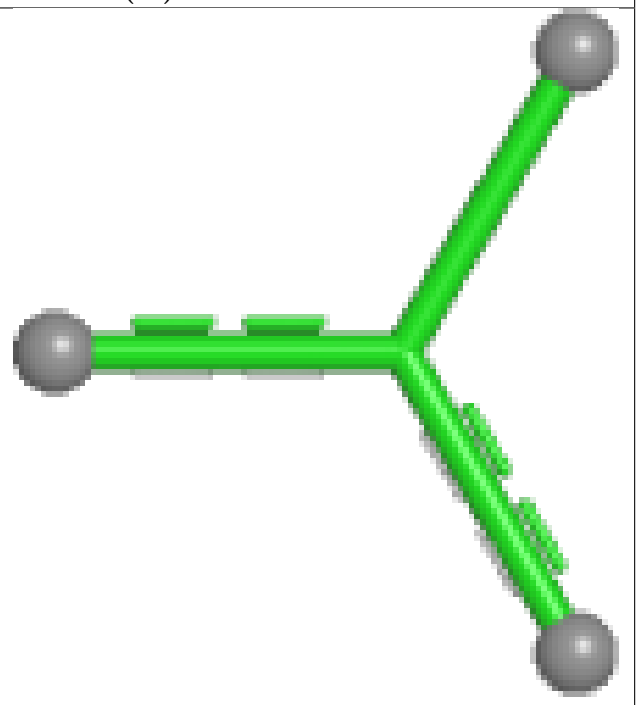


Rings

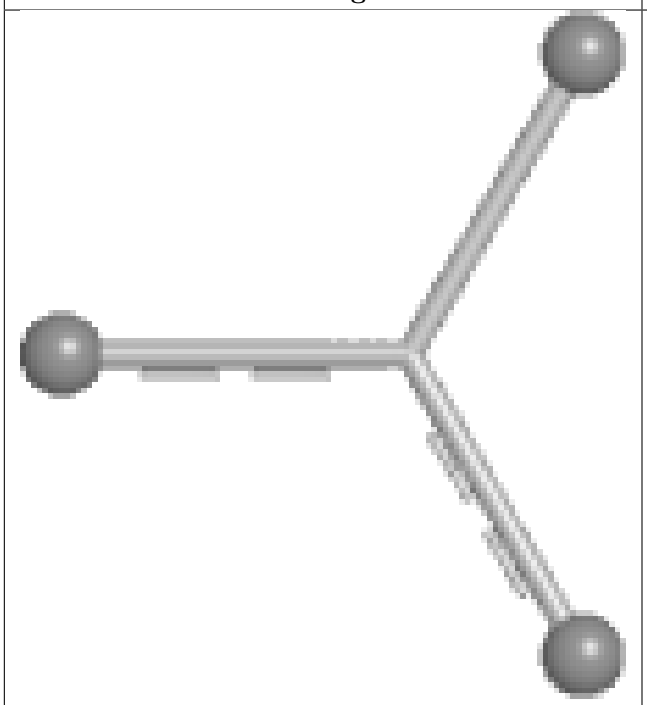
Ligand BCT d 401 (A)



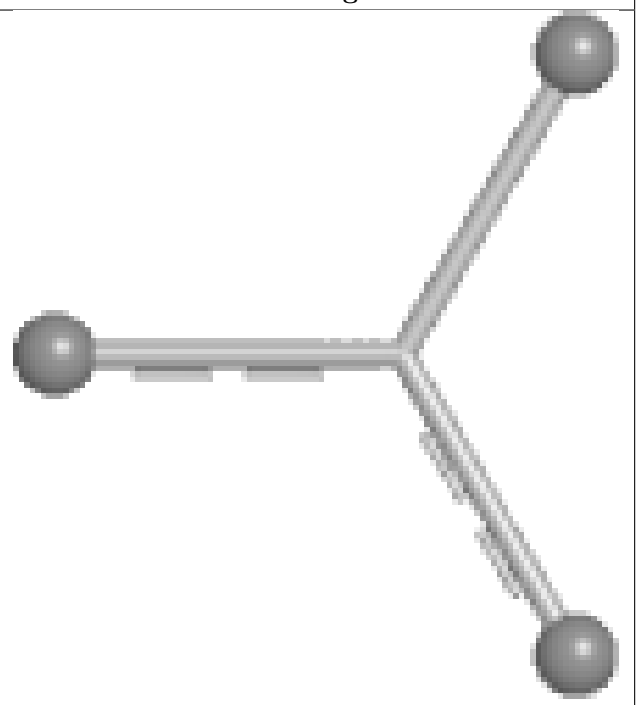
Bond lengths



Bond angles

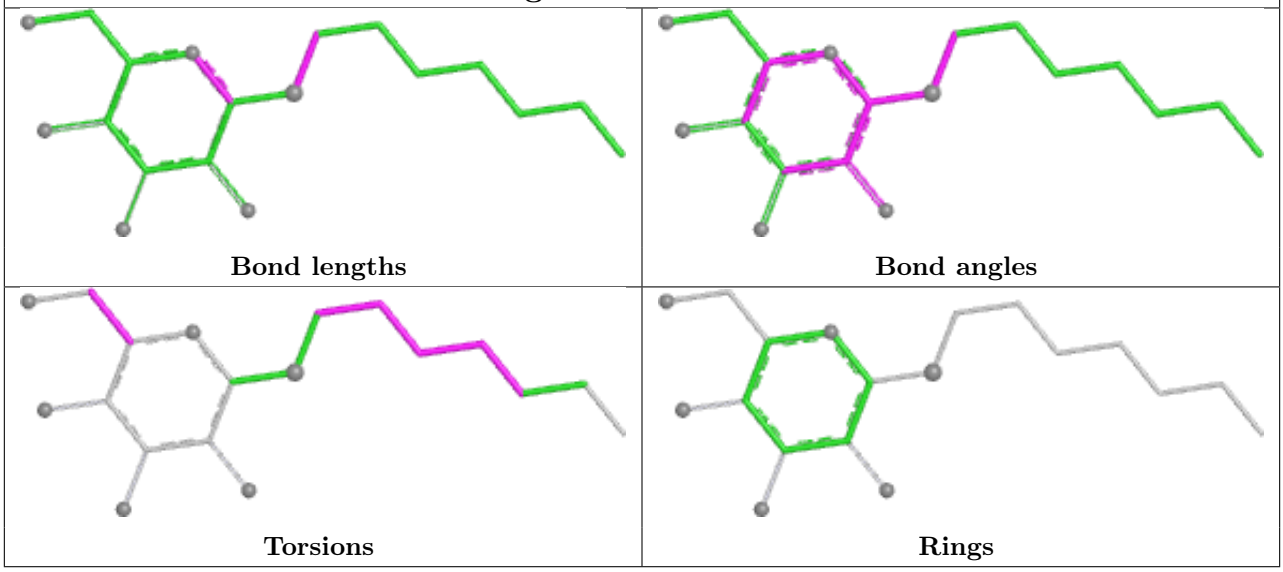


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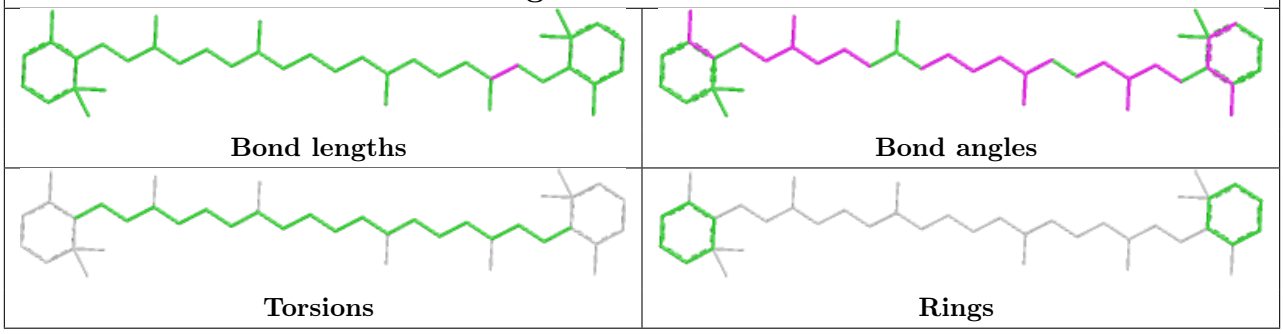


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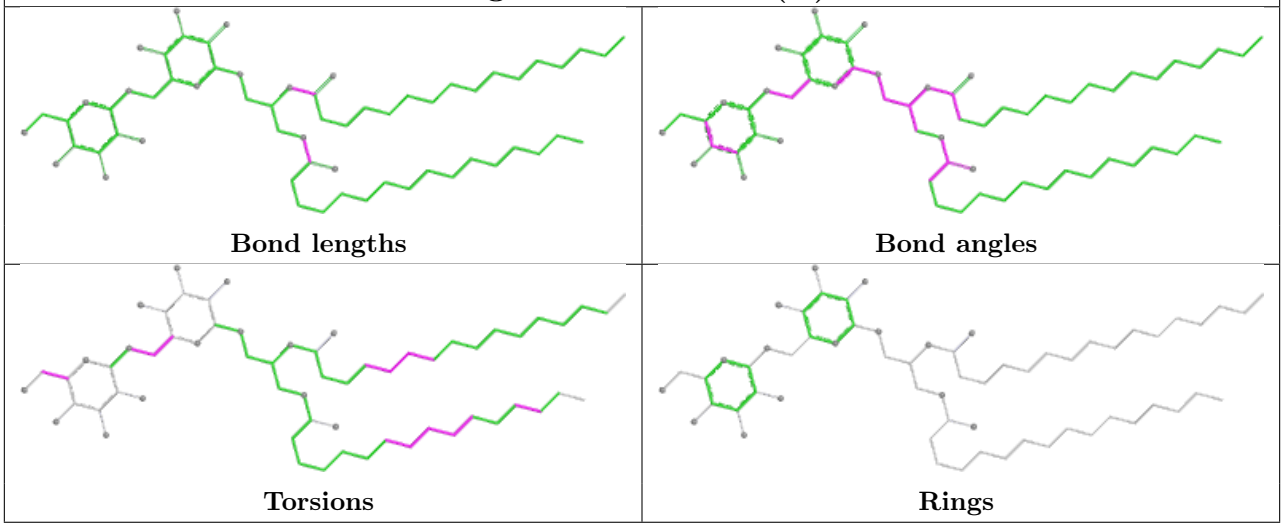
Ligand HTG b 622



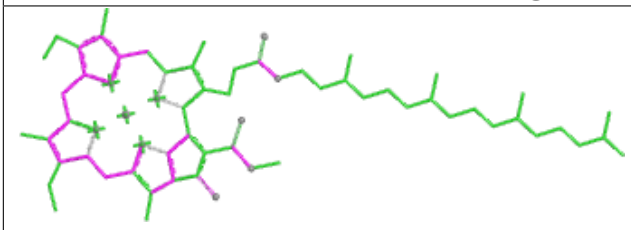
Ligand BCR h 101



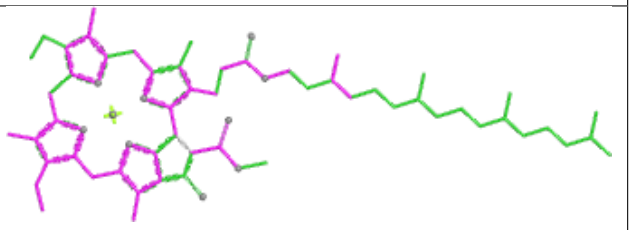
Ligand DGD C 517 (A)



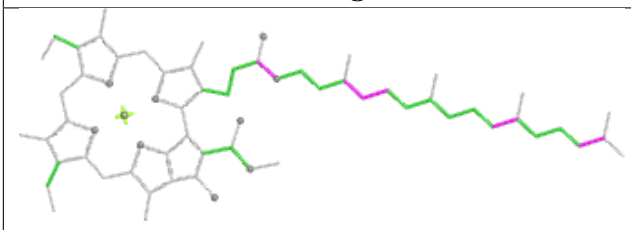
Ligand CLA d 405



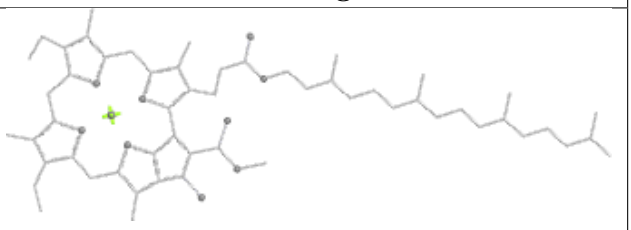
Bond lengths



Bond angles

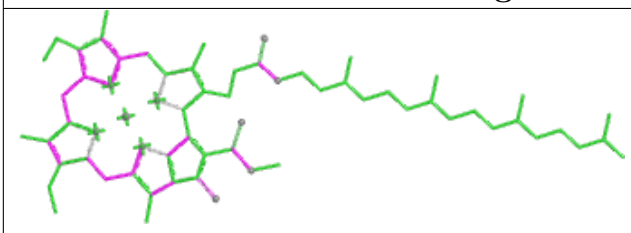


Torsions

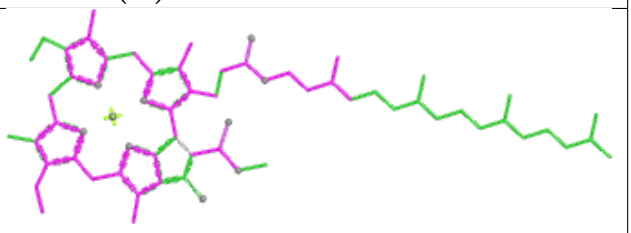


Rings

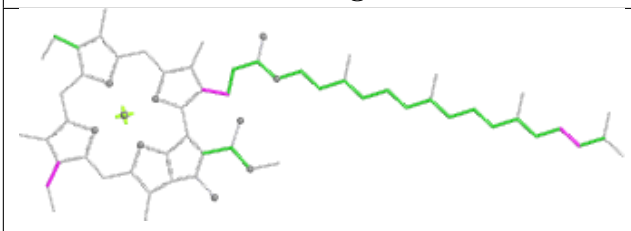
Ligand CLA d 402 (B)



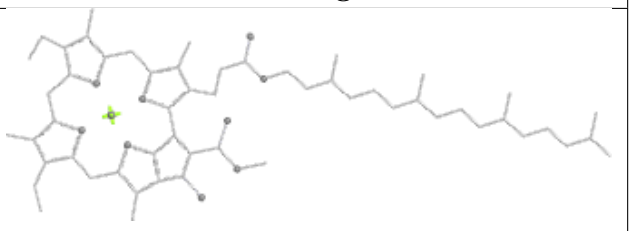
Bond lengths



Bond angles

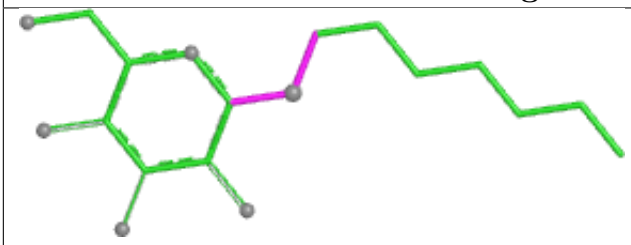


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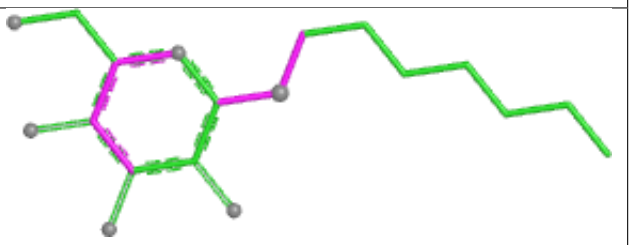


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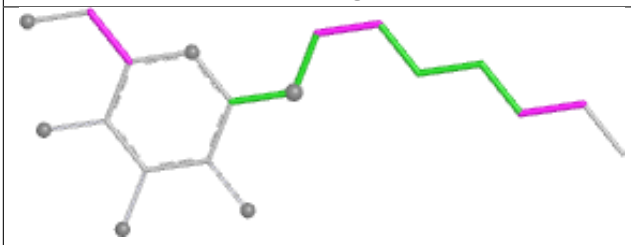
Ligand HTG B 624



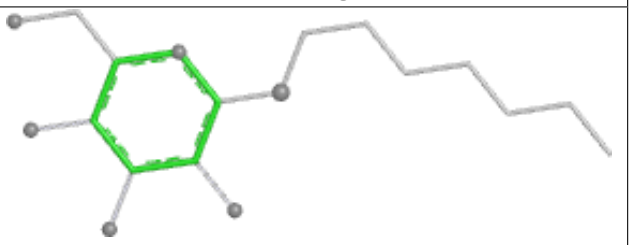
Bond lengths



Bond angles

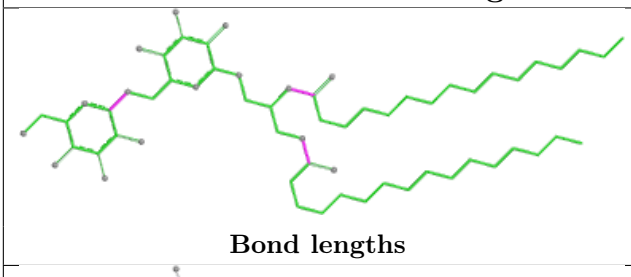


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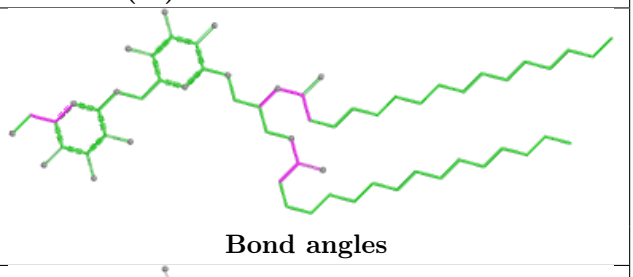


Rings

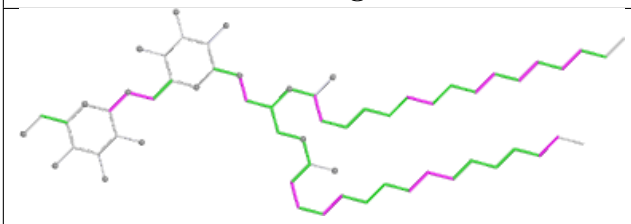
Ligand DGD C 518 (A)



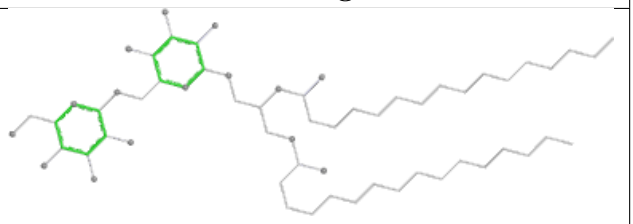
Bond lengths



Bond angles

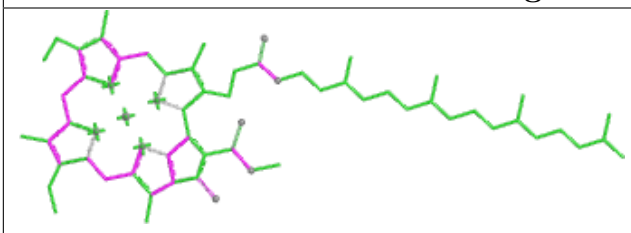


Torsions

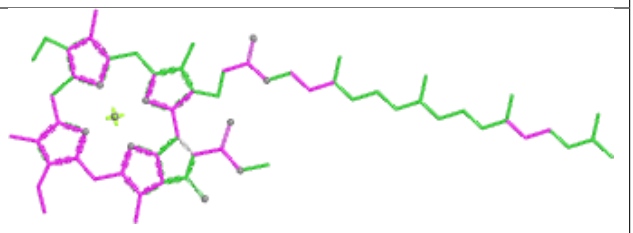


Rings

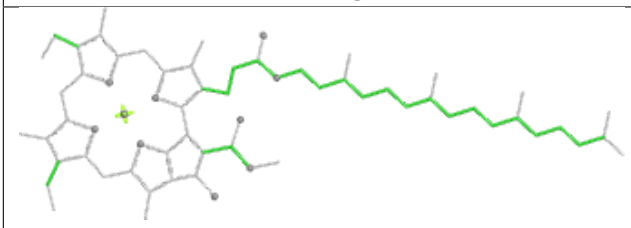
Ligand CLA B 609



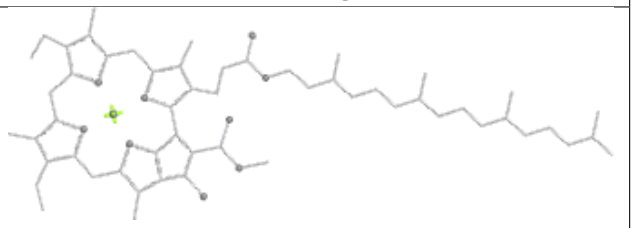
Bond lengths



Bond angles

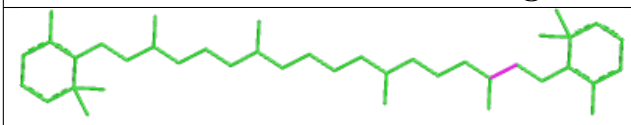


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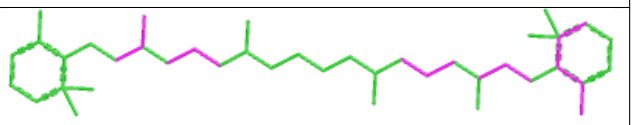


Rings

Ligand BCR B 619



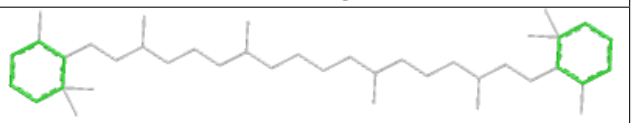
Bond lengths



Bond angles

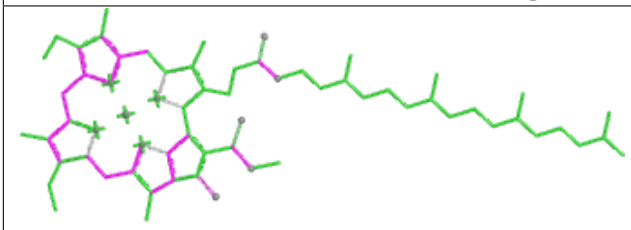


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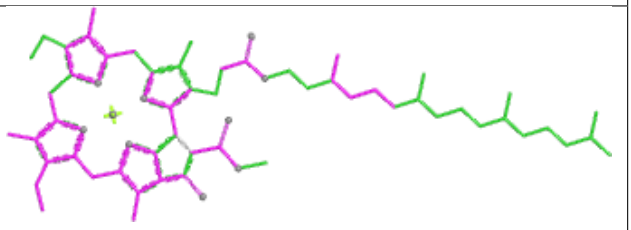


Rings

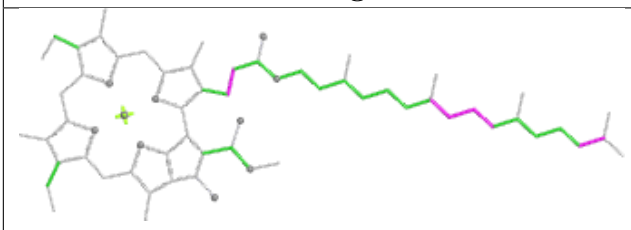
Ligand CLA B 606



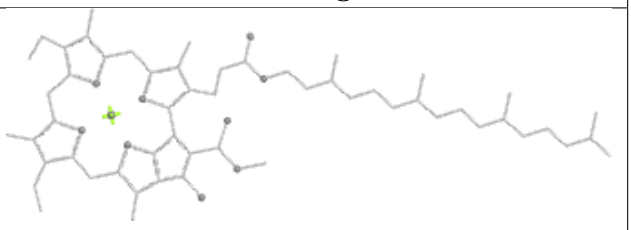
Bond lengths



Bond angles



Torsions

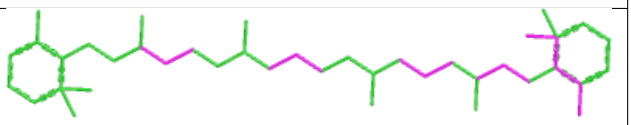


Rings

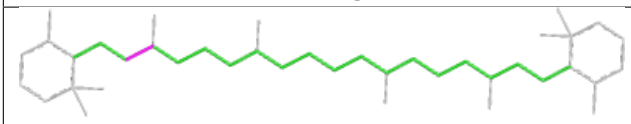
Ligand BCR b 619



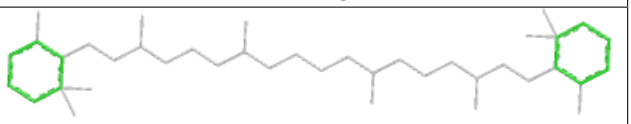
Bond lengths



Bond angles

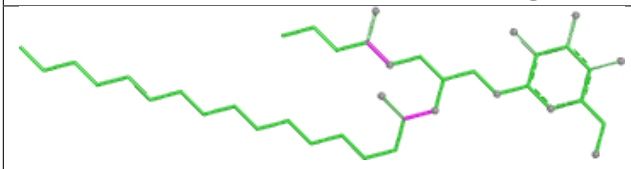


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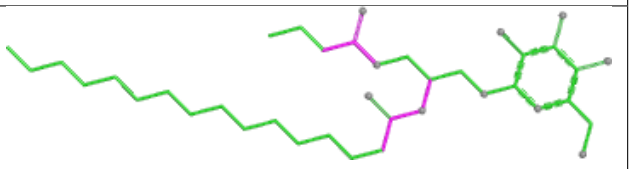


Rings

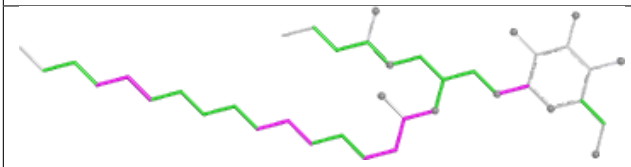
Ligand LMG z 101



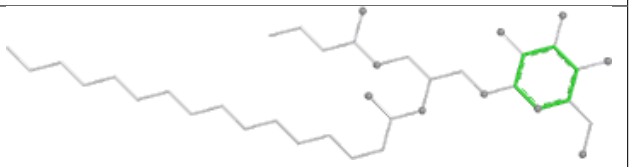
Bond lengths



Bond angles

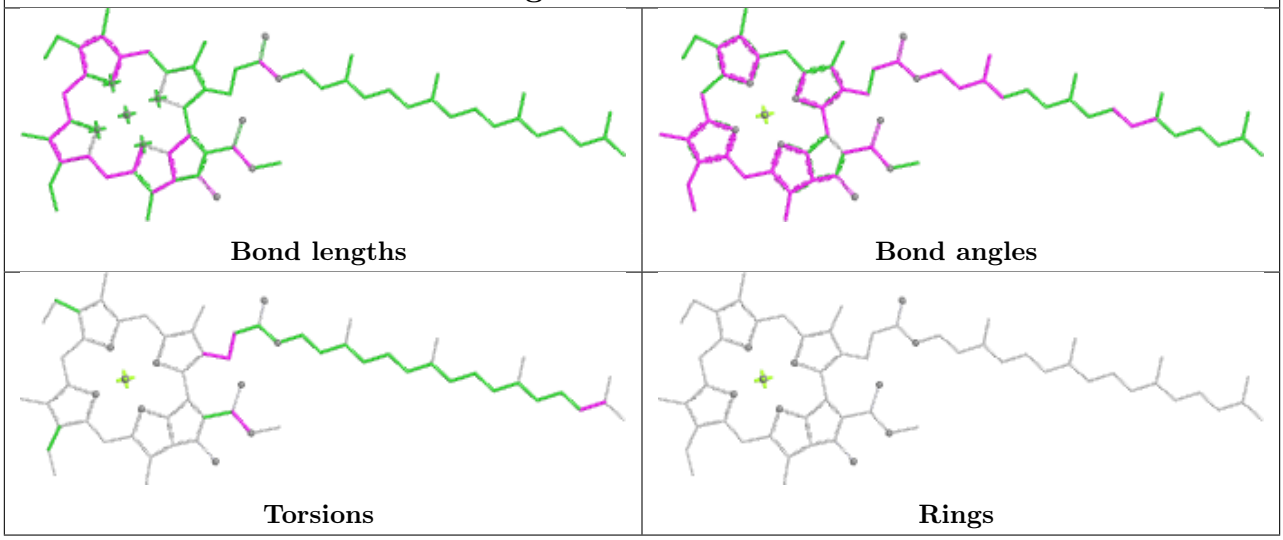


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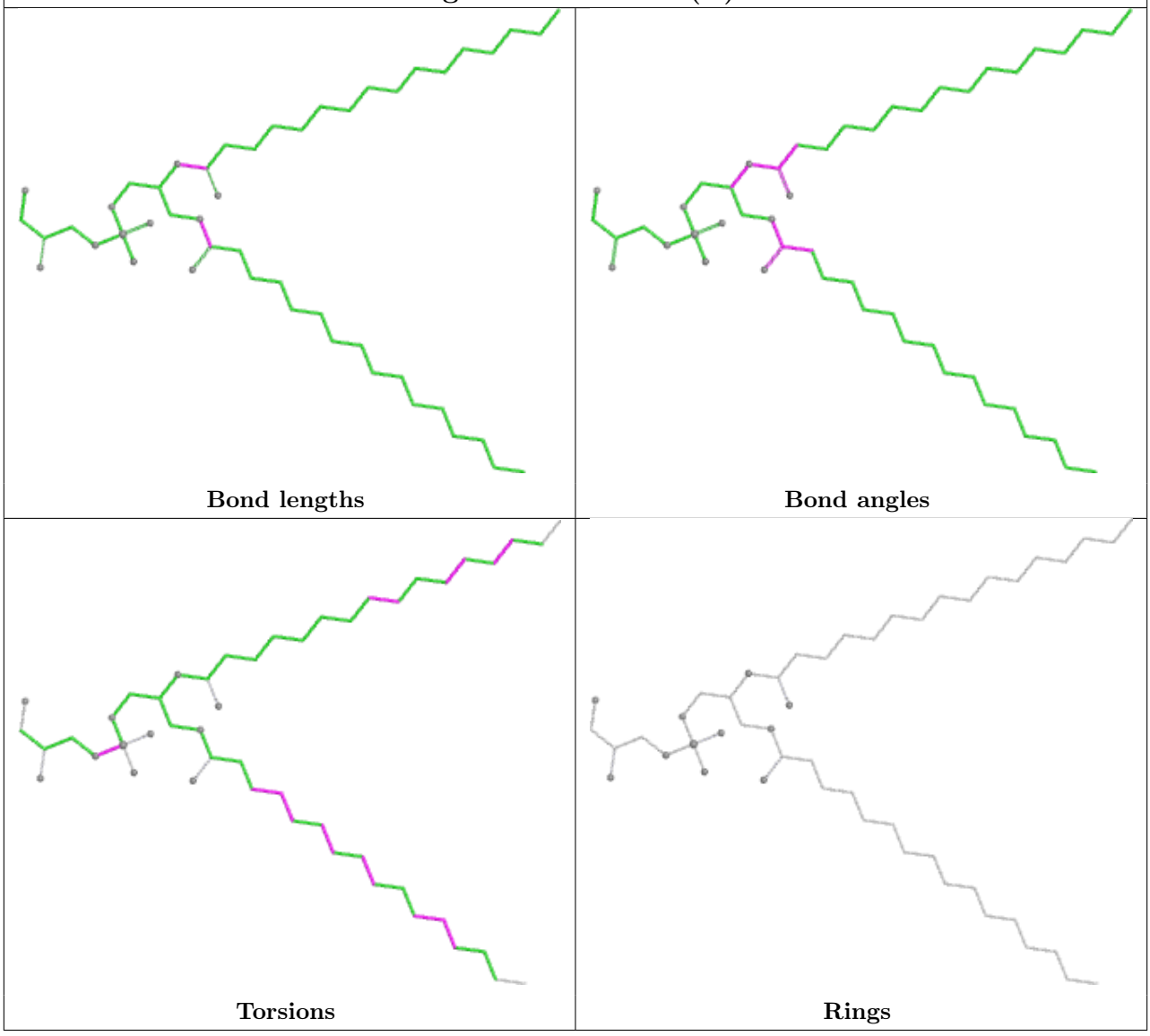


Rings

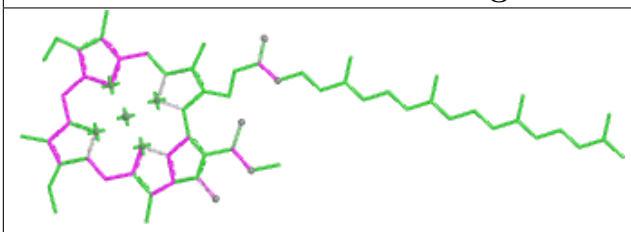
Ligand CLA C 502



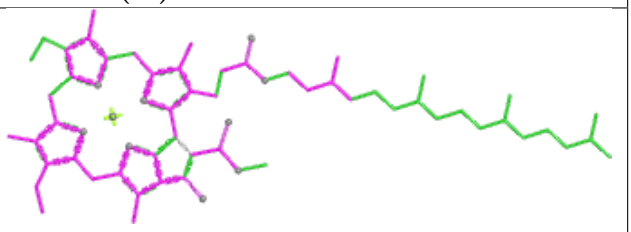
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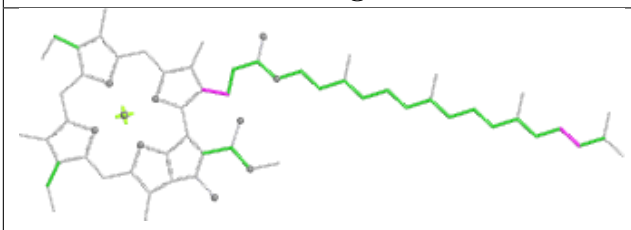
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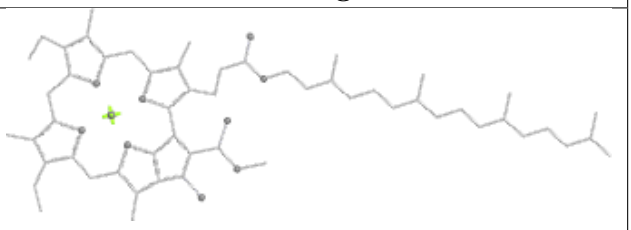
Bond lengths



Bond angles

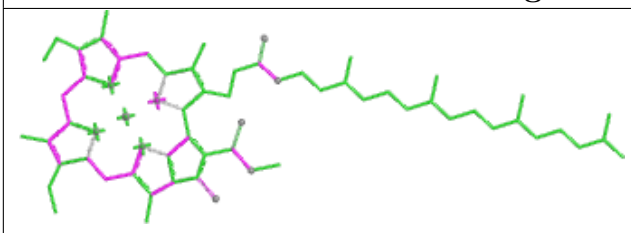


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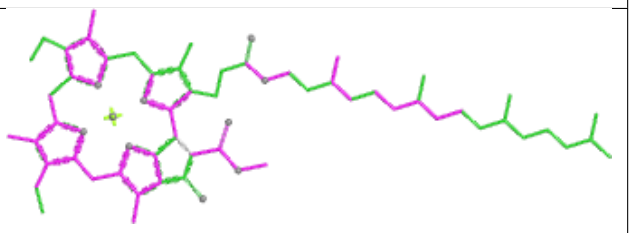


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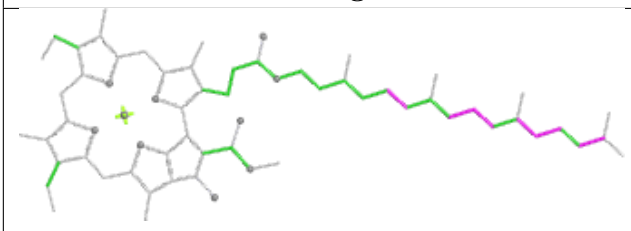
Ligand CLA B 615



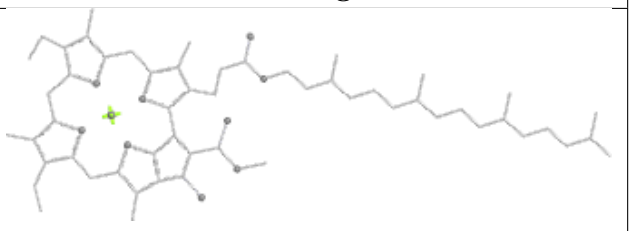
Bond lengths



Bond angles

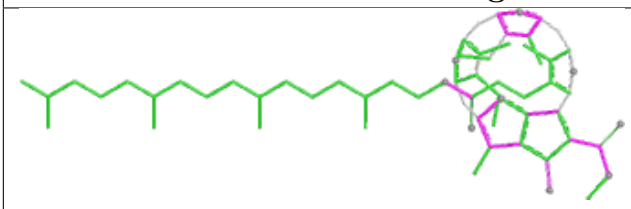


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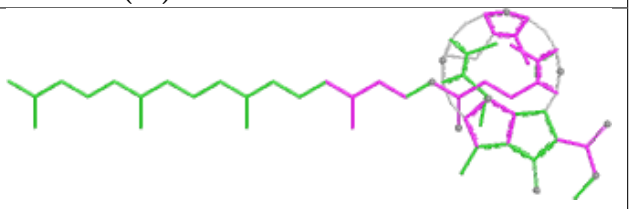


Rings

Ligand PHO A 407 (A)



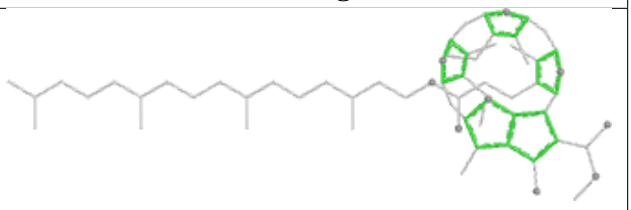
Bond lengths



Bond angles

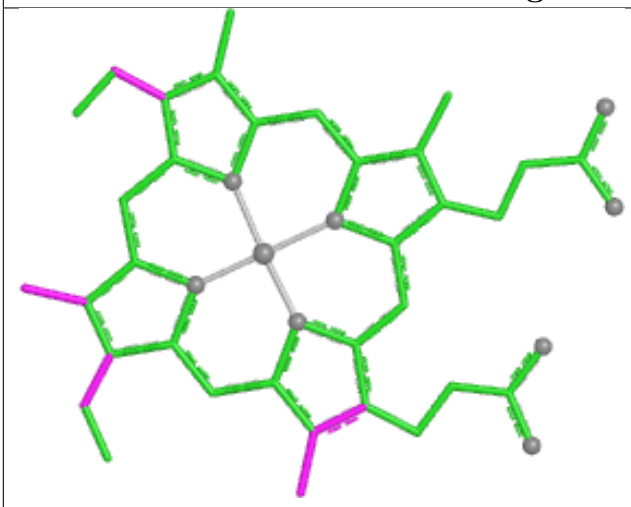


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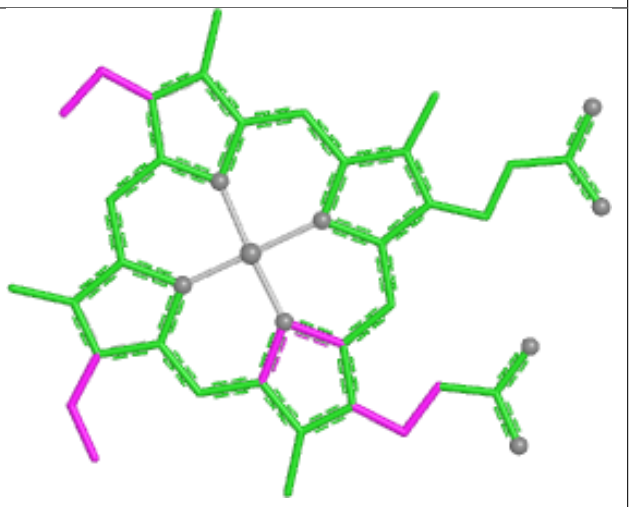


Rings

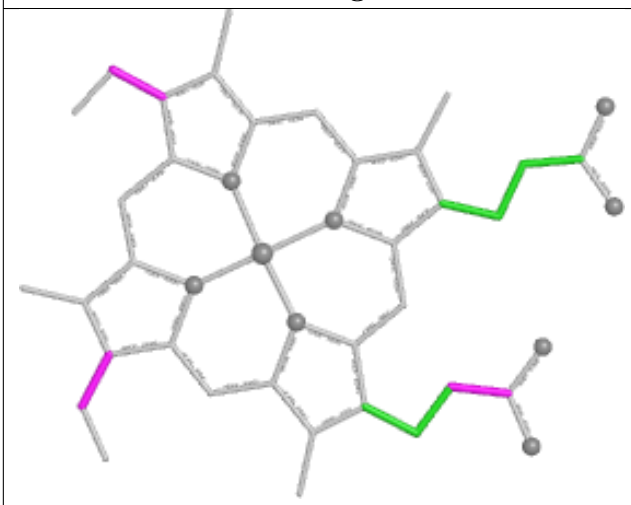
Ligand HEC v 201



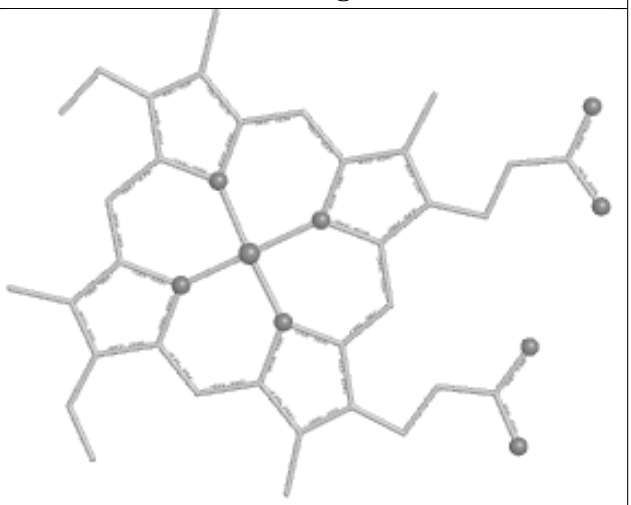
Bond lengths



Bond angles

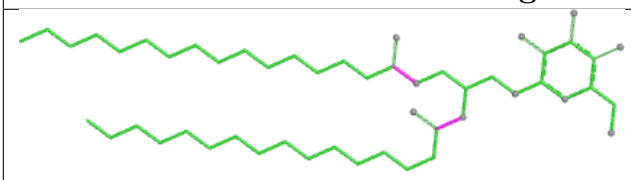


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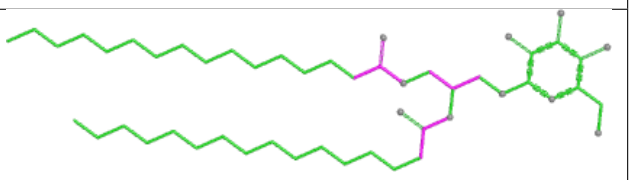


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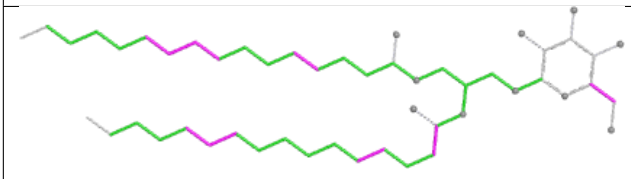
Ligand LMG D 411



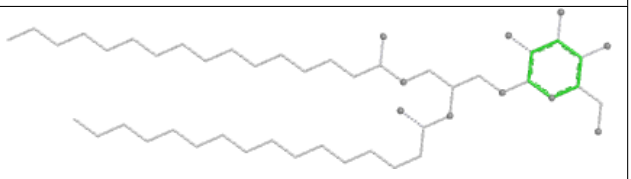
Bond lengths



Bond angles

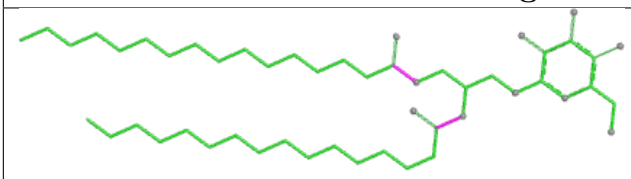


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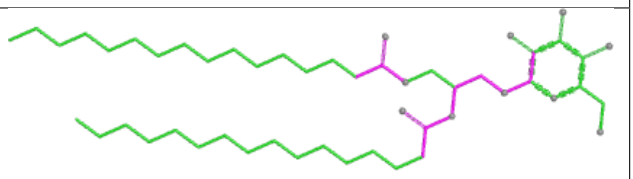


Rings

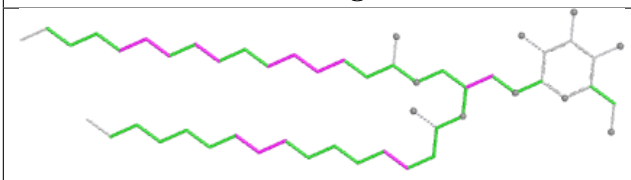
Ligand LMG C 520



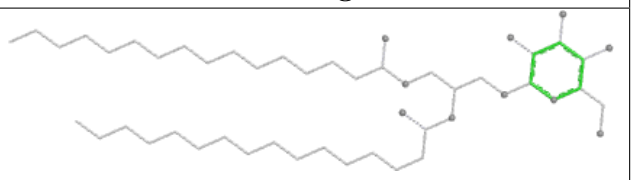
Bond lengths



Bond angles

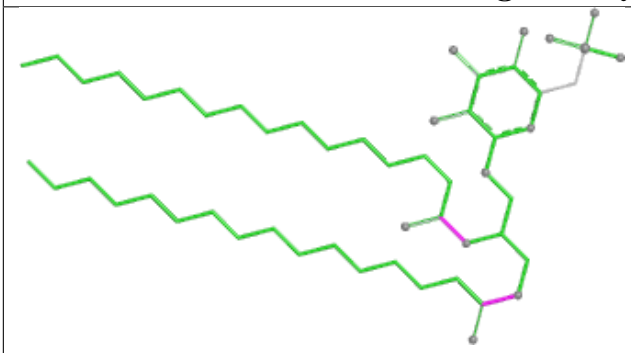


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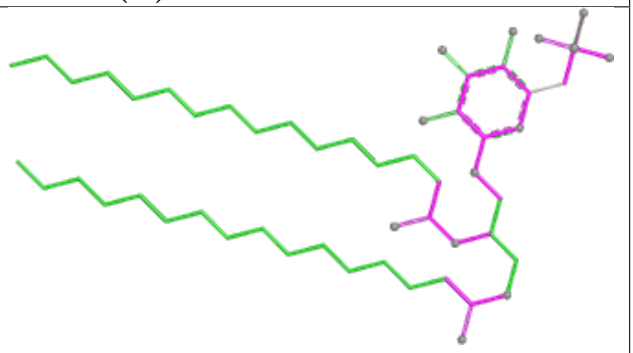


Rings

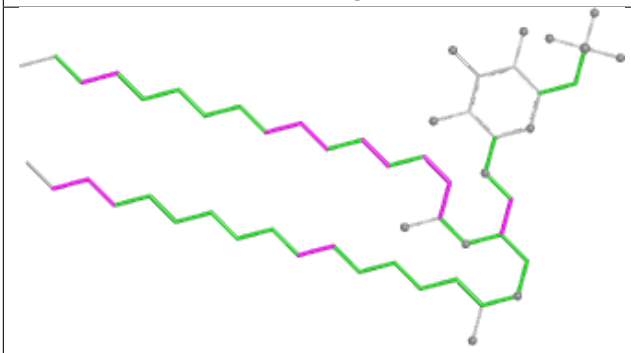
Ligand SQD a 409 (B)



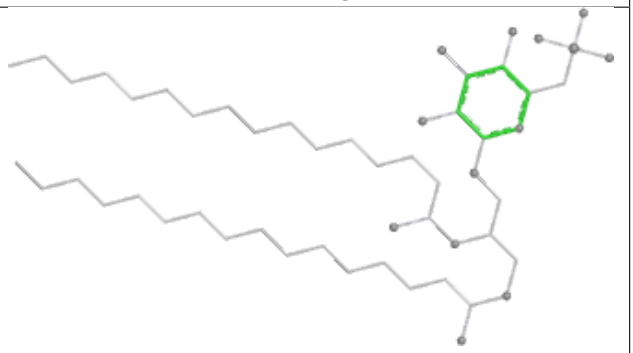
Bond lengths



Bond angles

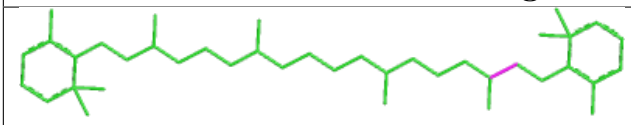


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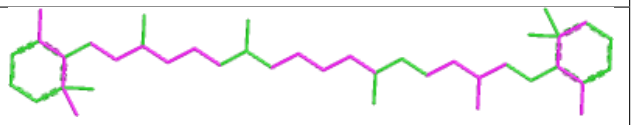


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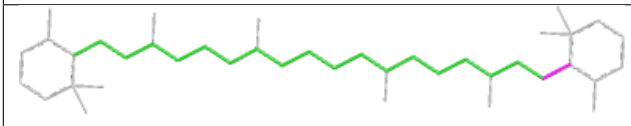
Ligand BCR H 101



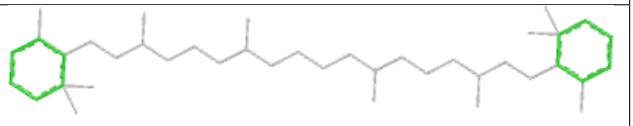
Bond lengths



Bond angles

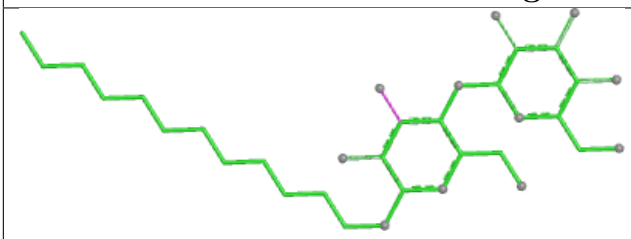


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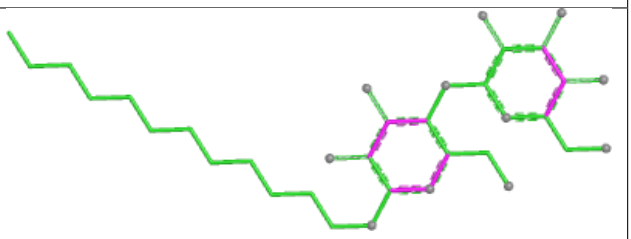


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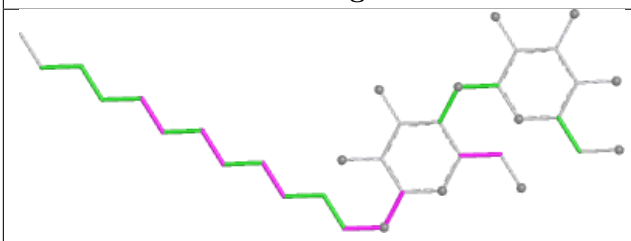
Ligand LMT F 101



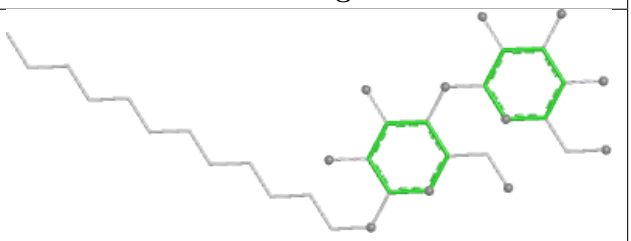
Bond lengths



Bond angles

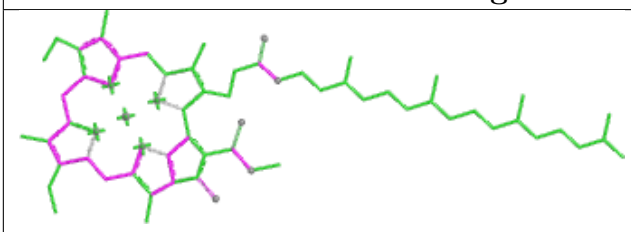


Torsions

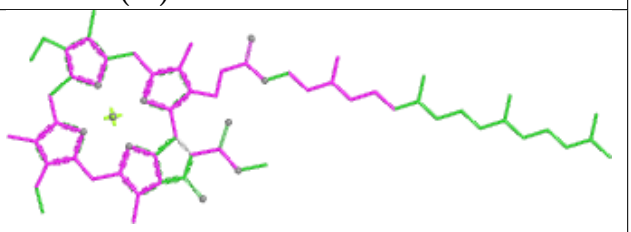


Rings

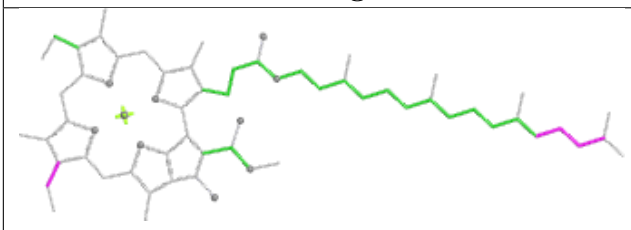
Ligand CLA A 404 (A)



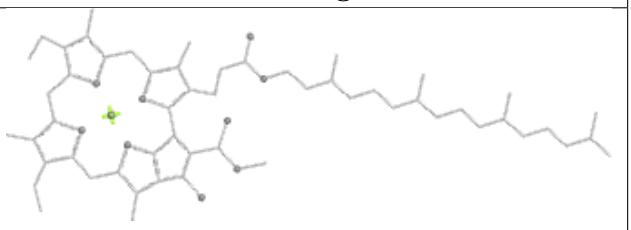
Bond lengths



Bond angles

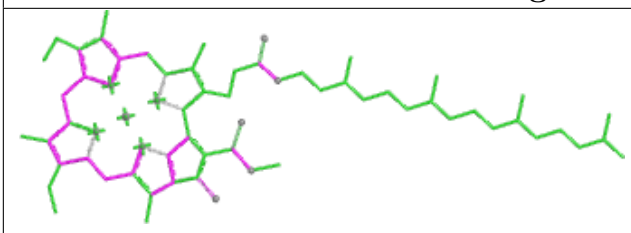


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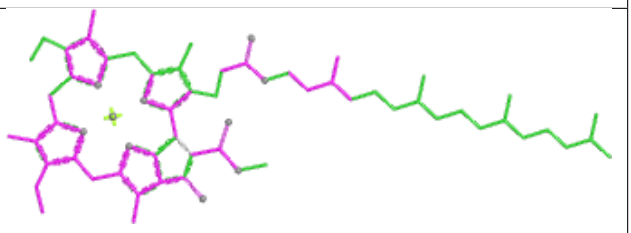


Rings

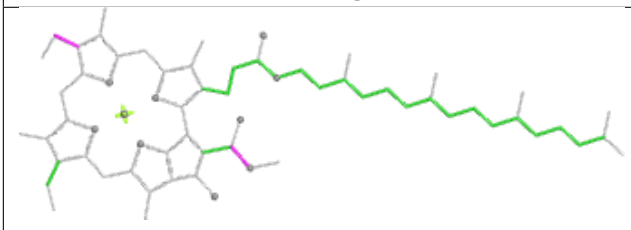
Ligand CLA c 501



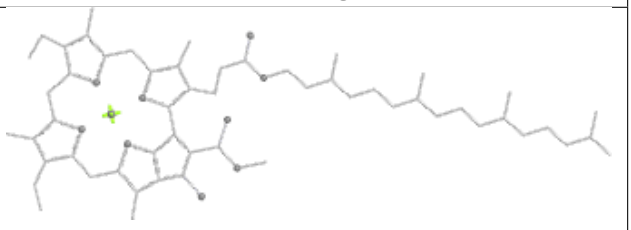
Bond lengths



Bond angles

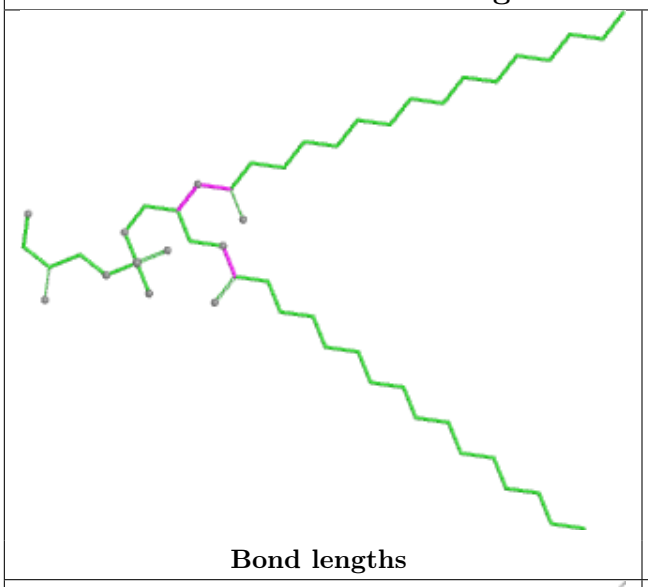


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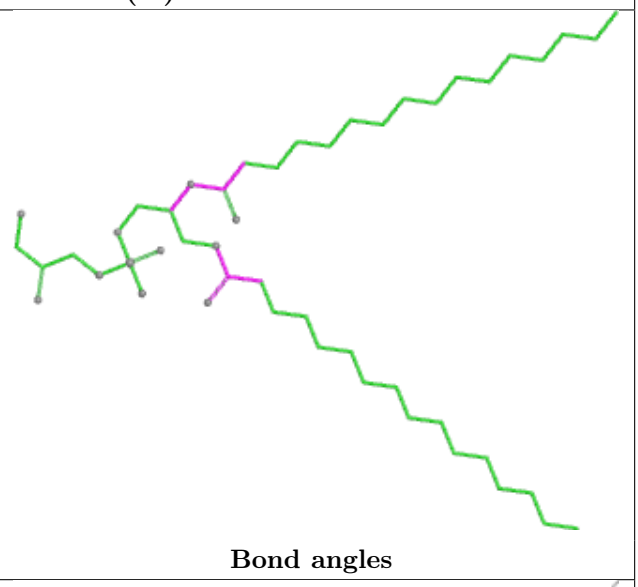


Rings

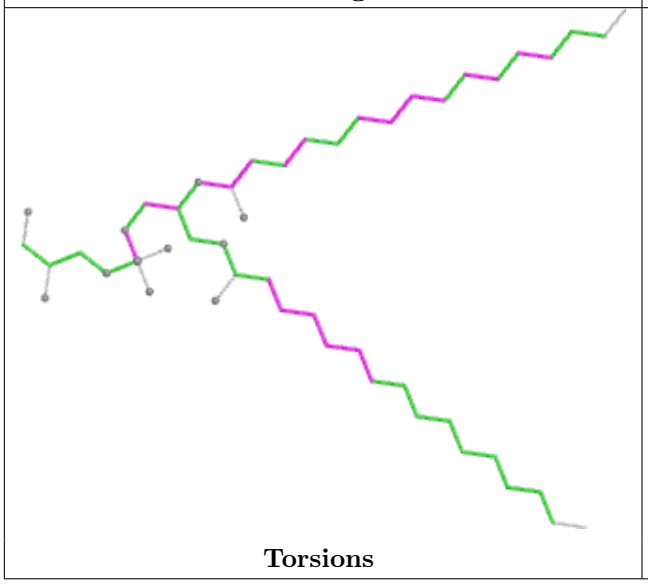
Ligand LHG L 101 (B)



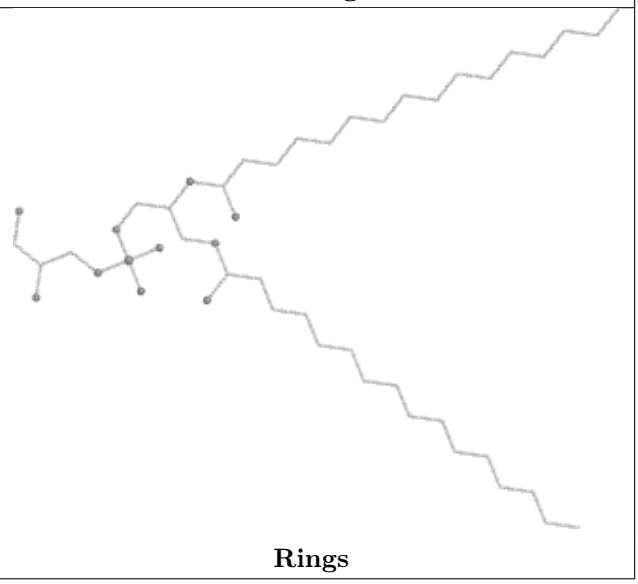
Bond lengths



Bond angles

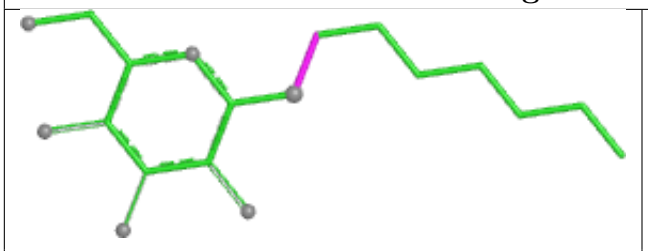


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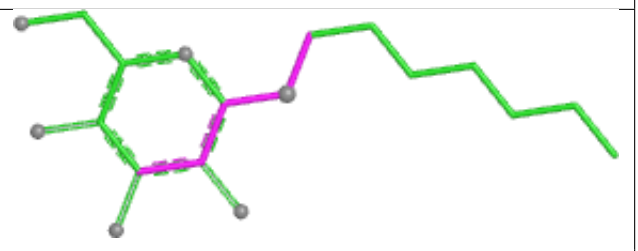


Rings

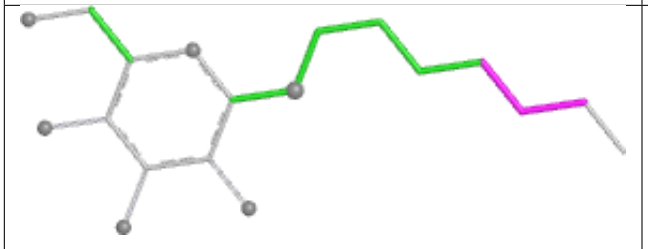
Ligand HTG B 622



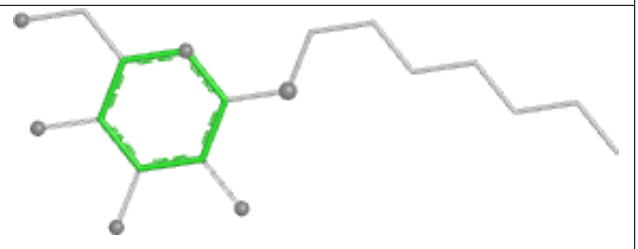
Bond lengths



Bond angles

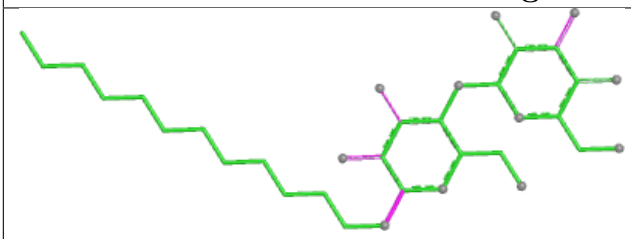


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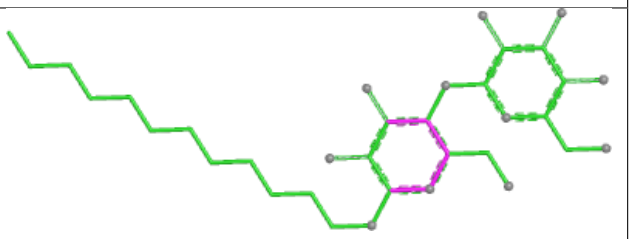


Rings

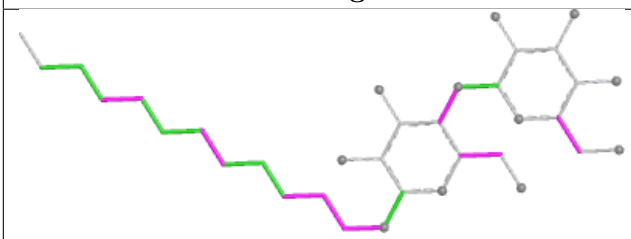
Ligand LMT T 101



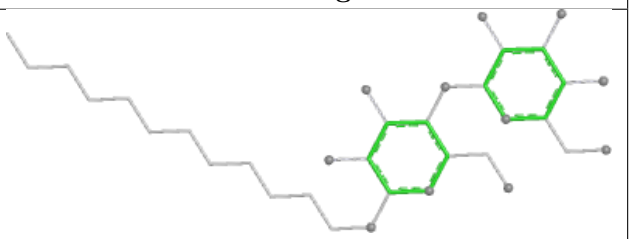
Bond lengths



Bond angles

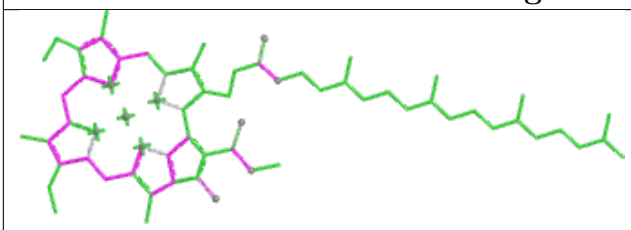


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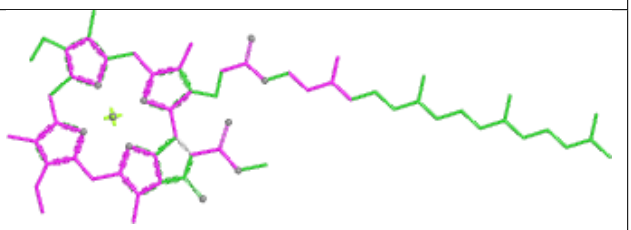


Rings

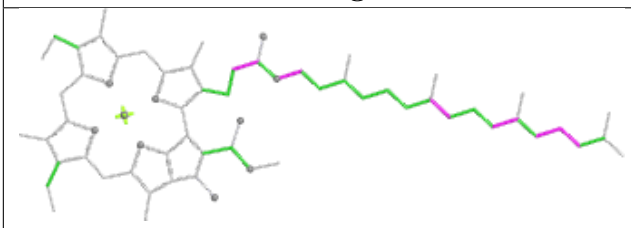
Ligand CLA B 613



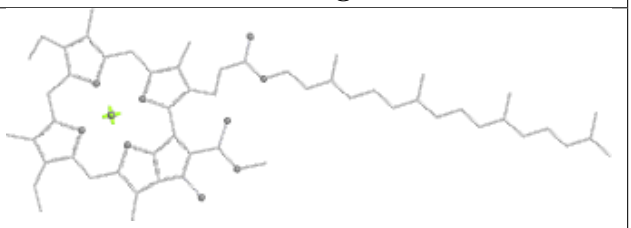
Bond lengths



Bond angles

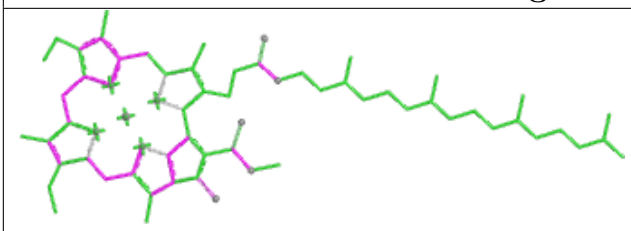


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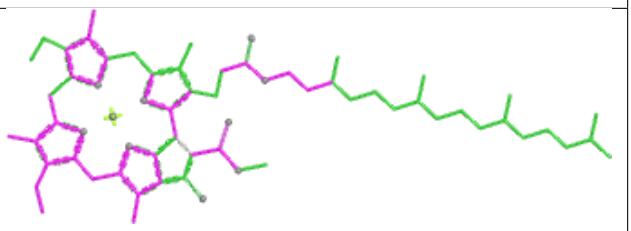


Rings

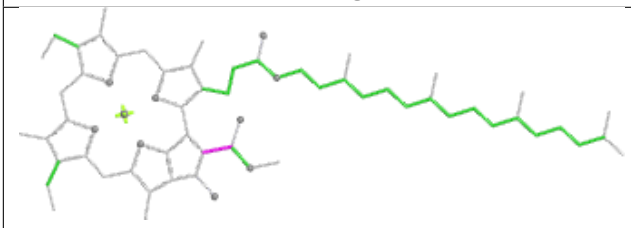
Ligand CLA c 502



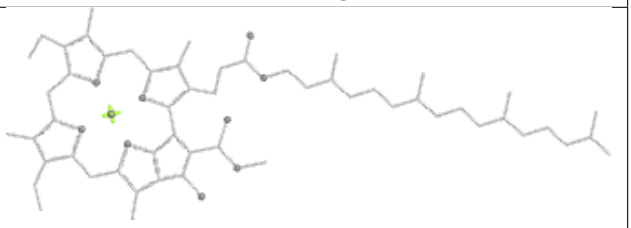
Bond lengths



Bond angles

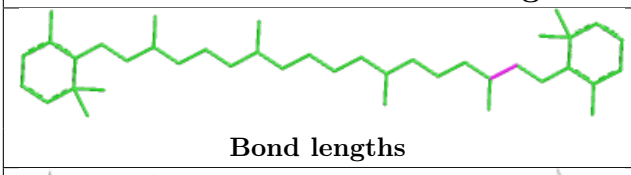


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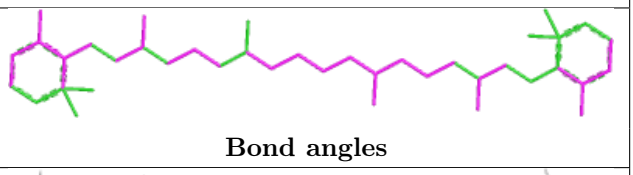


Rings

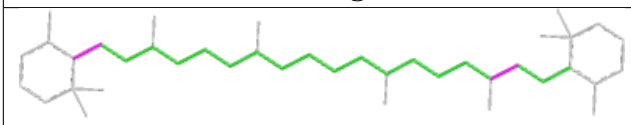
Ligand BCR Y 101



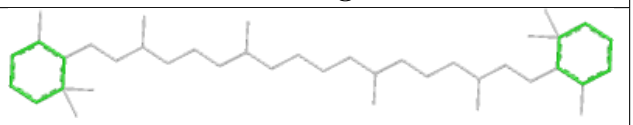
Bond lengths



Bond angles

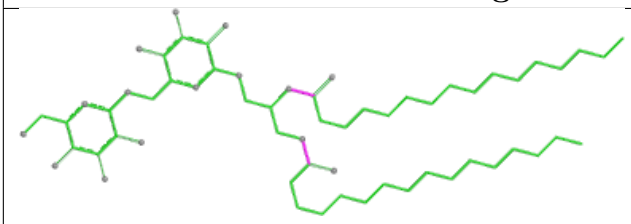


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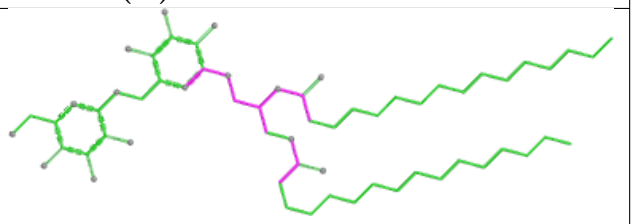


Rings

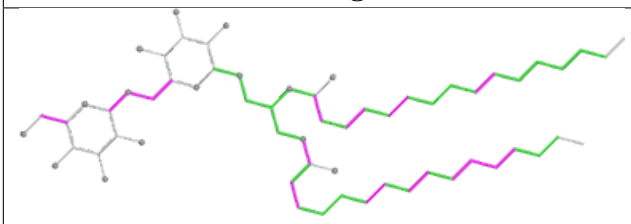
Ligand DGD c 516 (B)



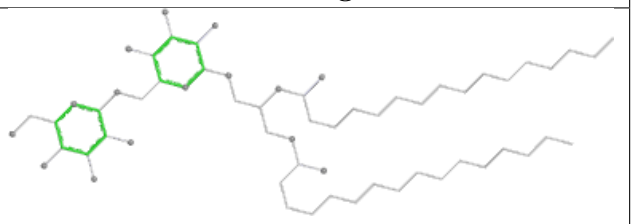
Bond lengths



Bond angles

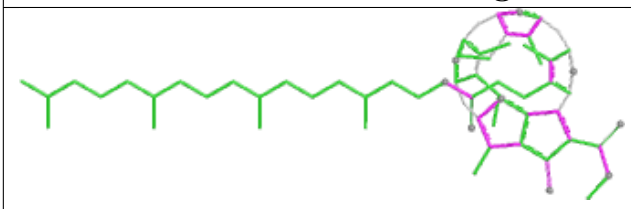


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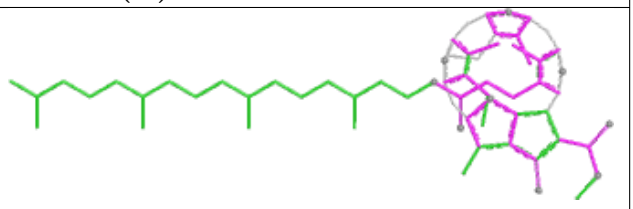


Rings

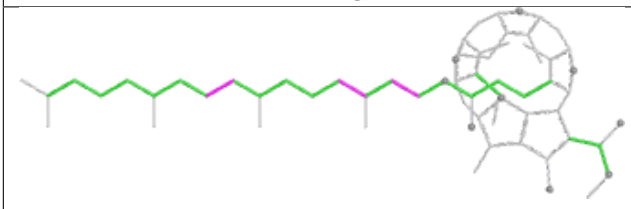
Ligand PHO a 406 (B)



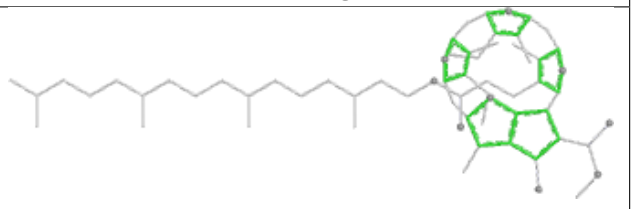
Bond lengths



Bond angles

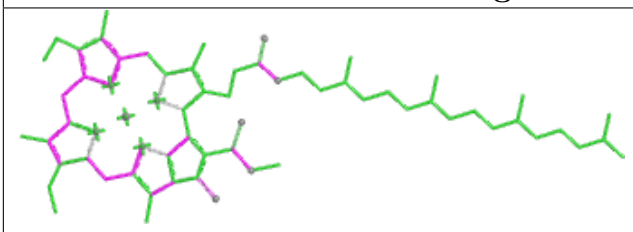


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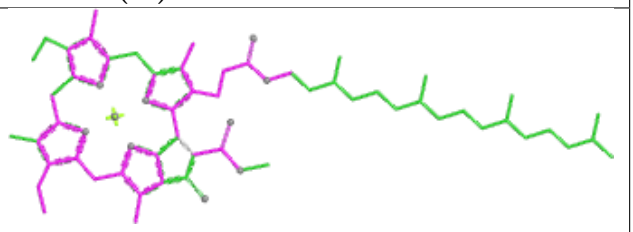


Rings

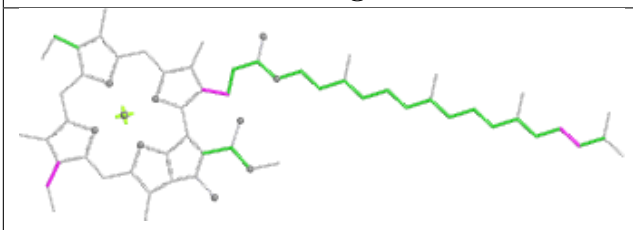
Ligand CLA d 402 (A)



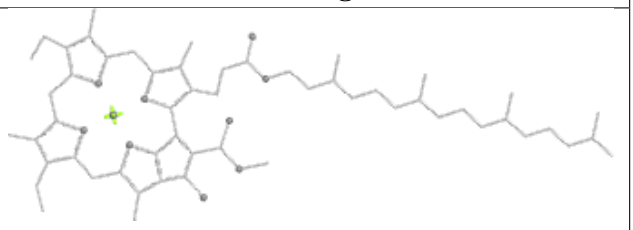
Bond lengths



Bond angles



Torsions



Rings

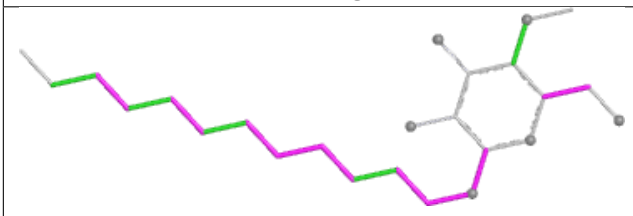
Ligand LMT B 629



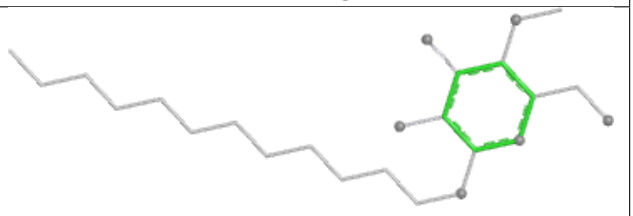
Bond lengths



Bond angles

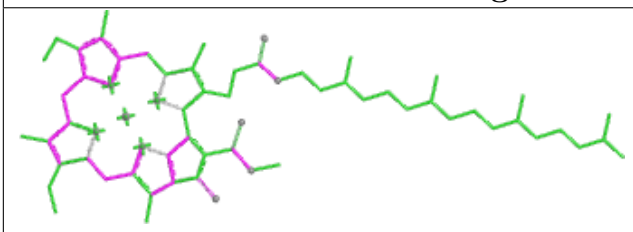


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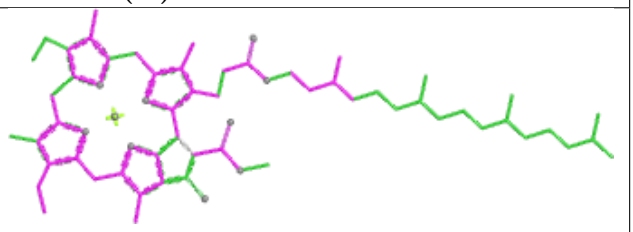


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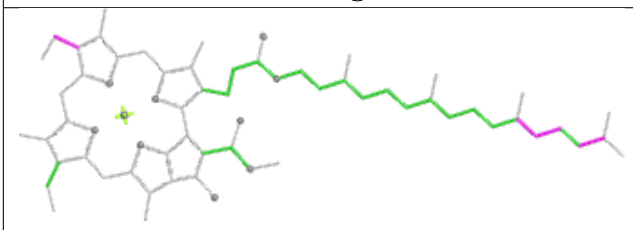
Ligand CLA A 406 (B)



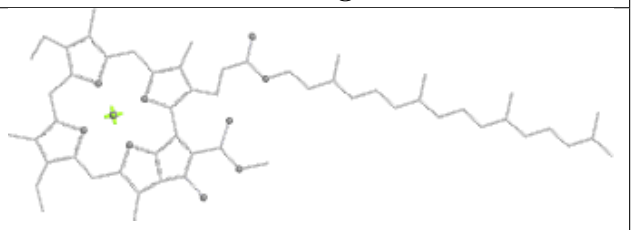
Bond lengths



Bond angles

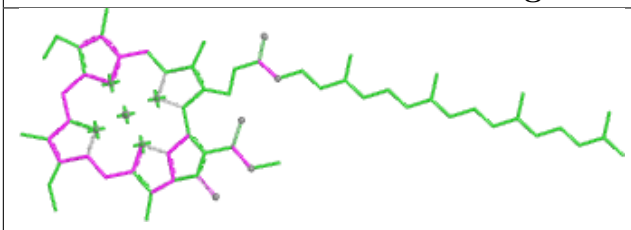


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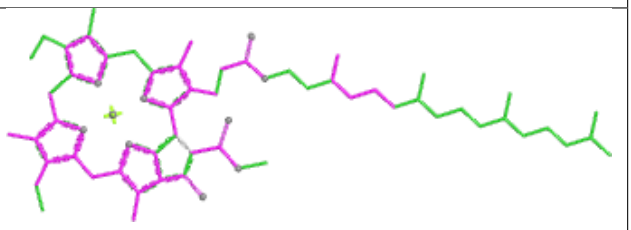


Rings

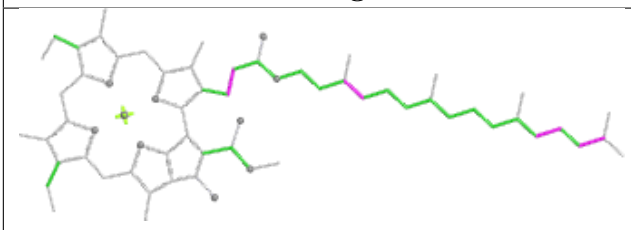
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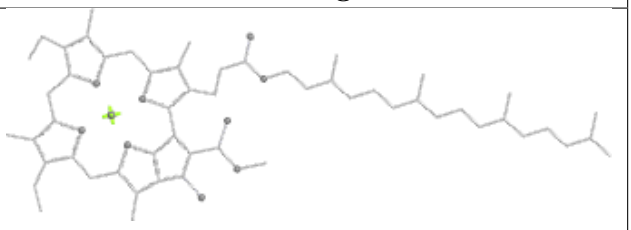
Bond lengths



Bond angles

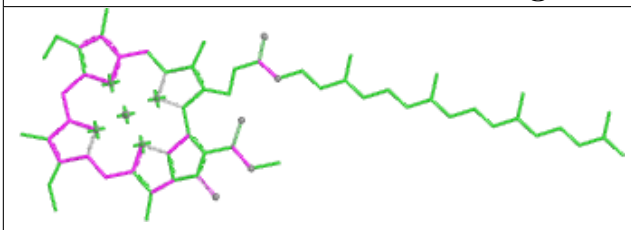


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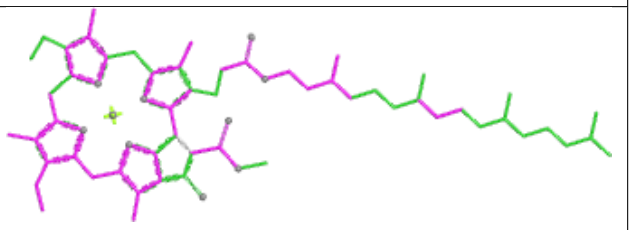


Rings

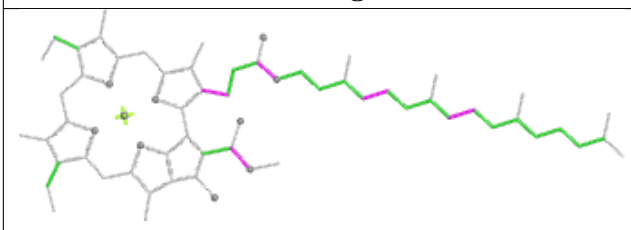
Ligand CLA c 511



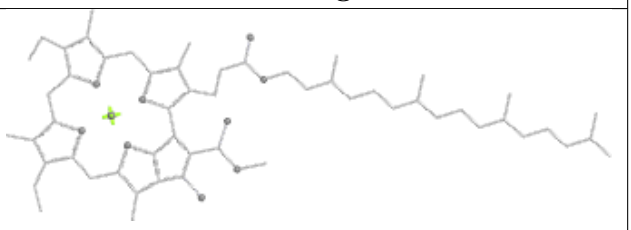
Bond lengths



Bond angles

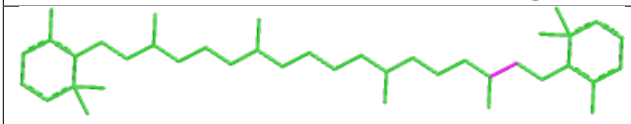


Torsions

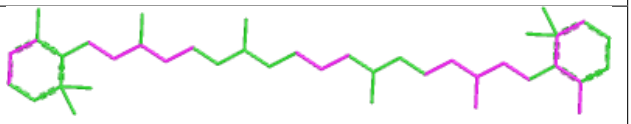


Rings

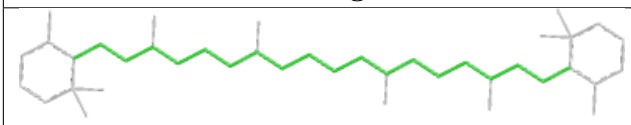
Ligand BCR a 408



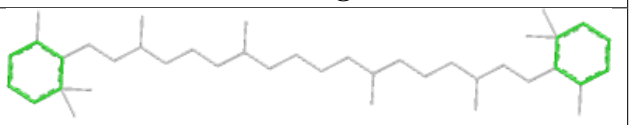
Bond lengths



Bond angles

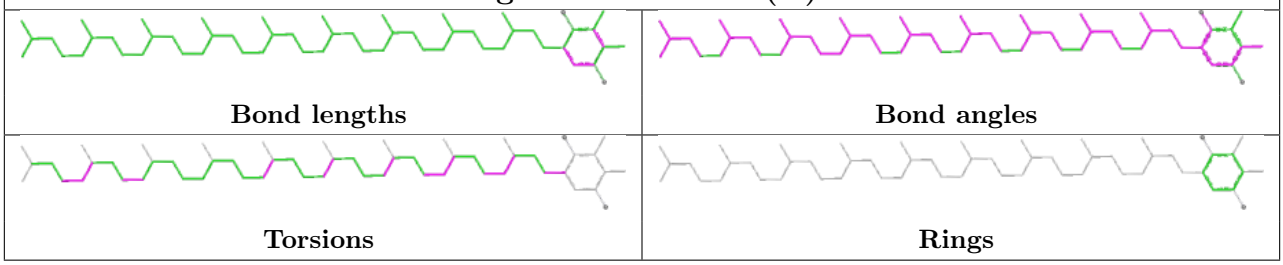


Torsions

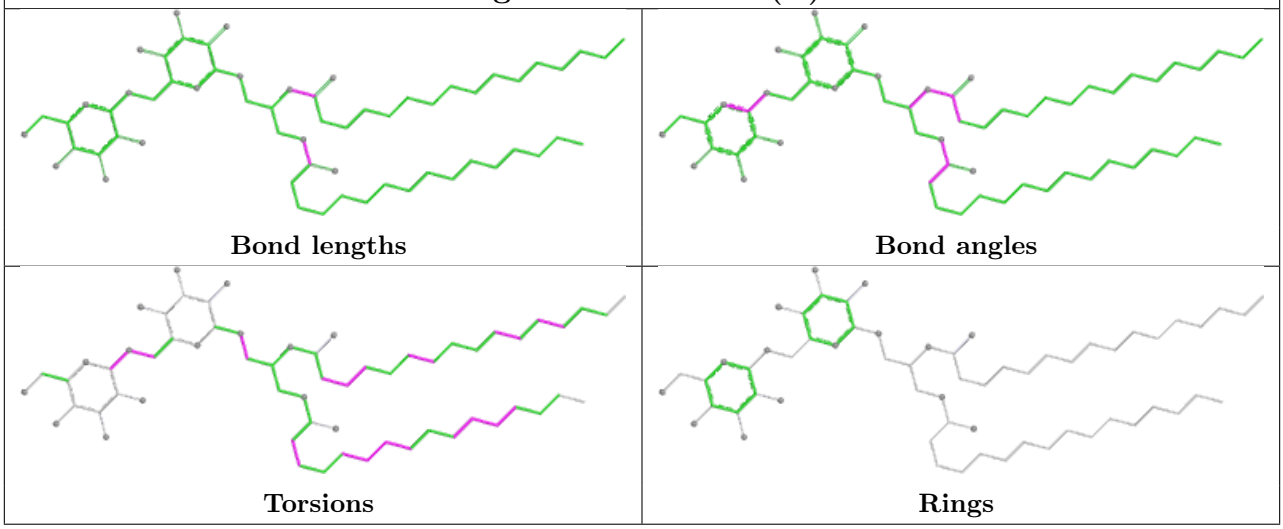


Rings

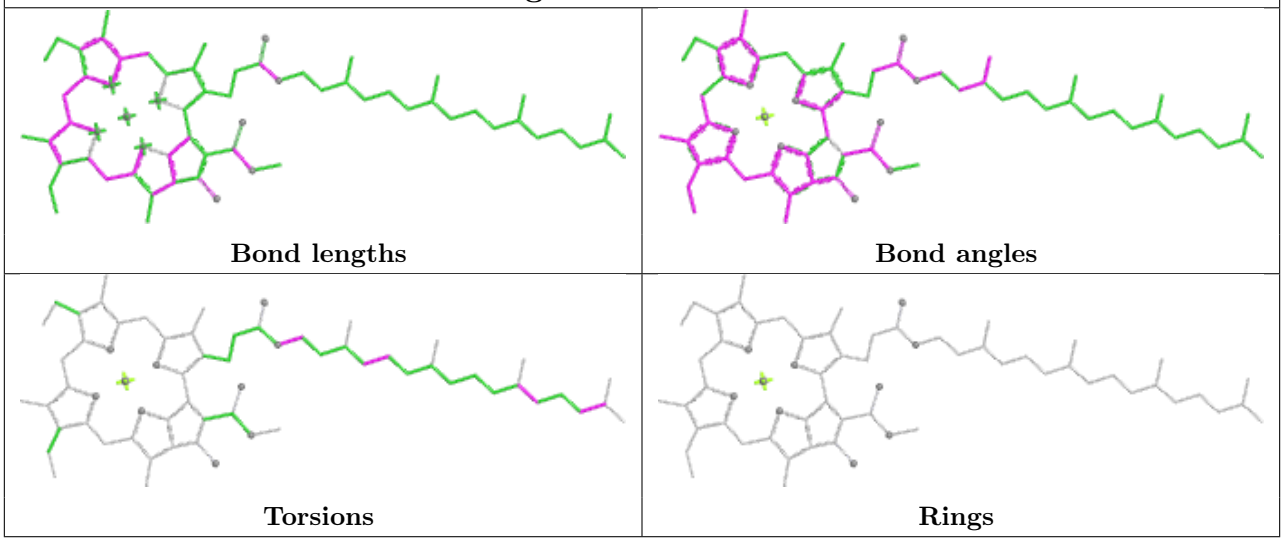
Ligand PL9 A 414 (A)



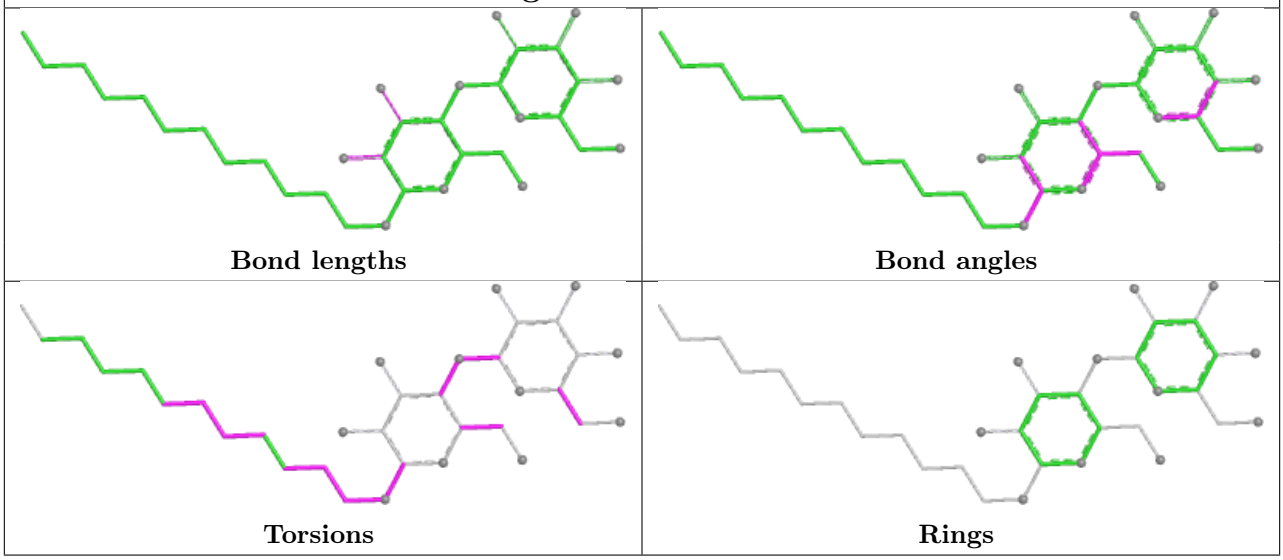
Ligand DGD c 517 (B)



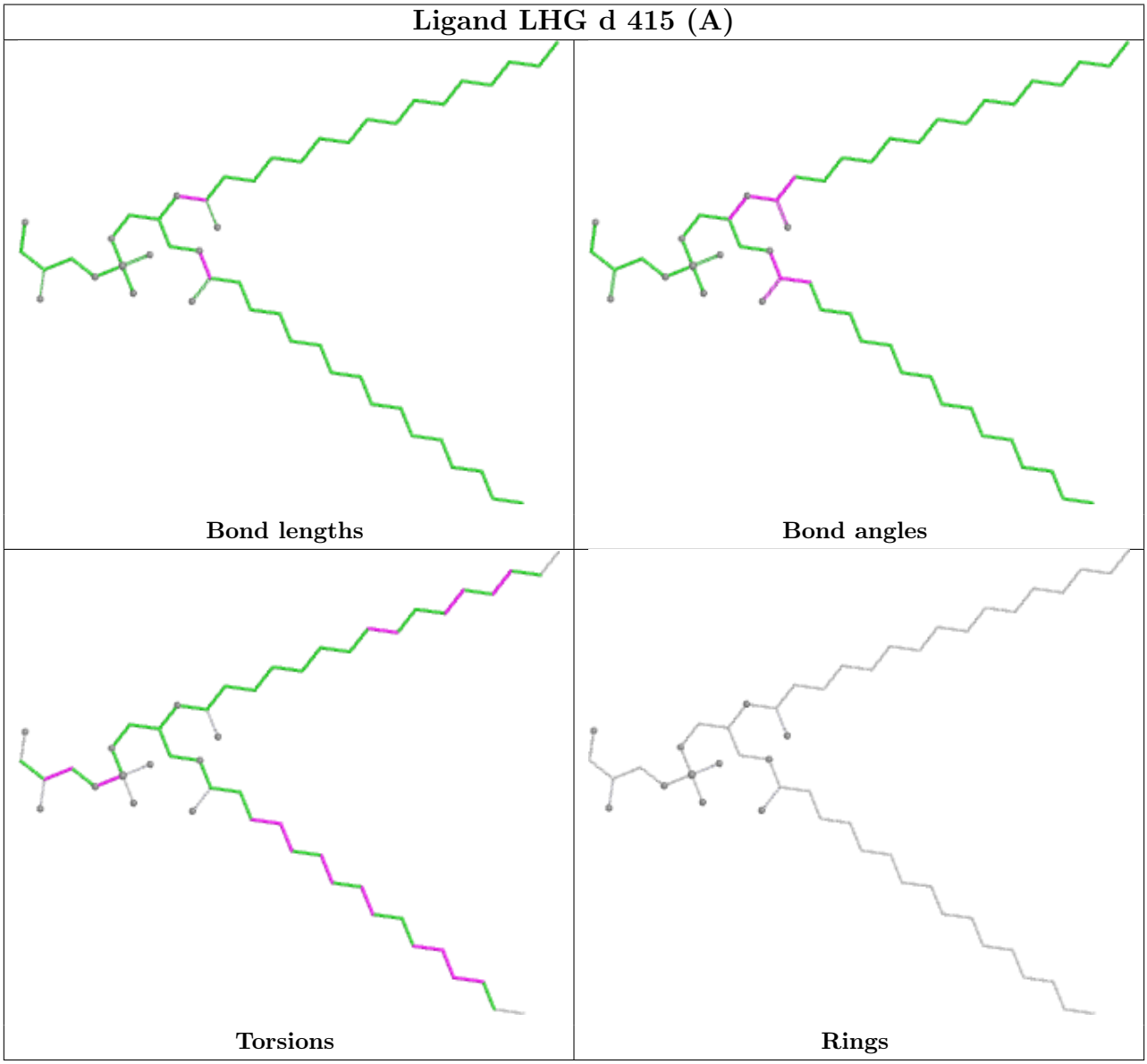
Ligand CLA B 616



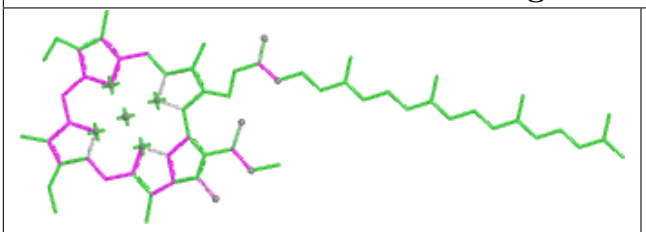
Ligand LMT C 525



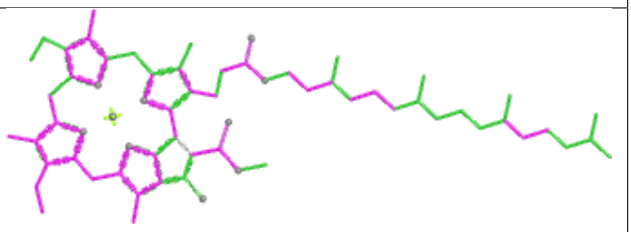
Ligand LHG d 415 (A)



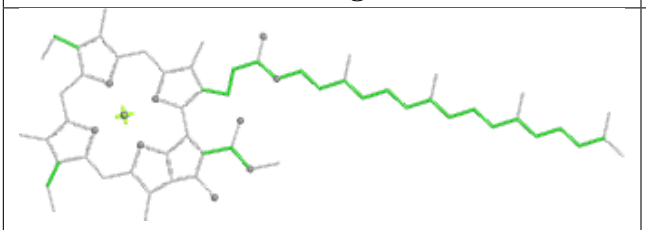
Ligand CLA b 609



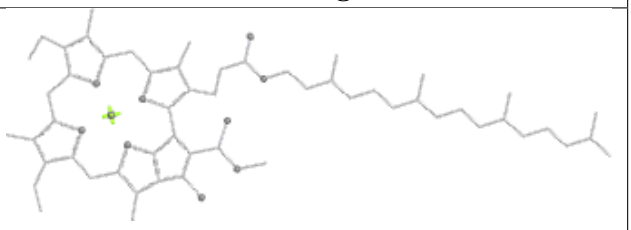
Bond lengths



Bond angles

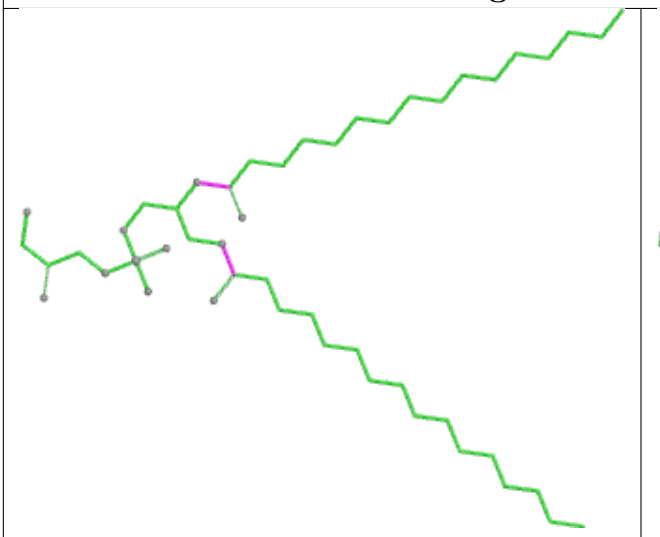


Torsions

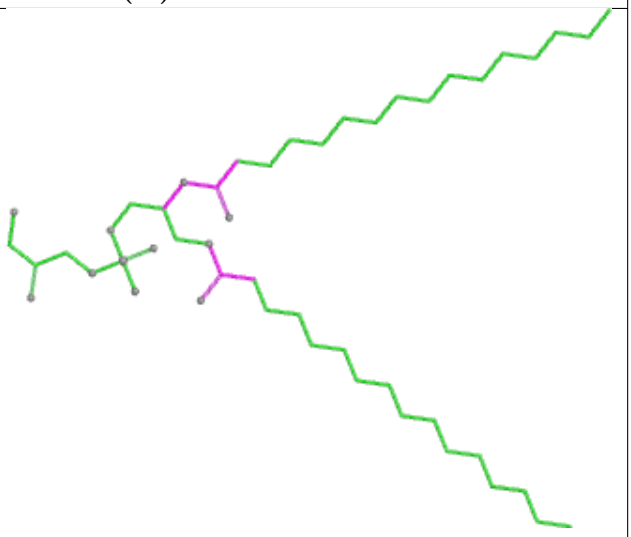


Rings

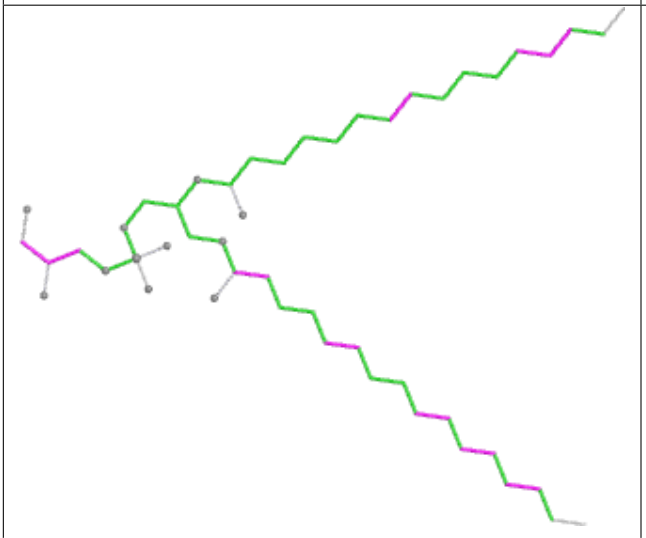
Ligand LHG A 419 (B)



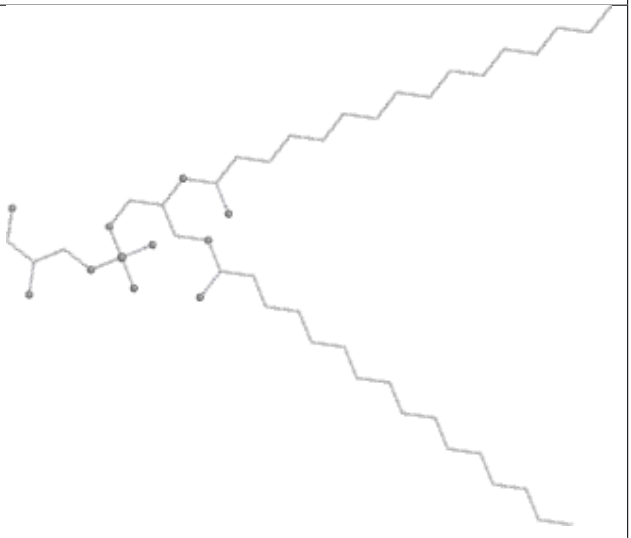
Bond lengths



Bond angles

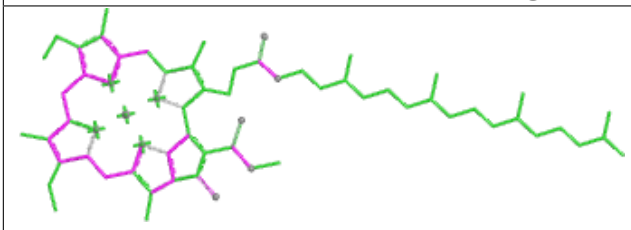


Torsions

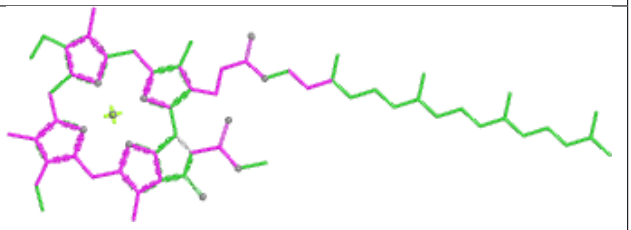


Rings

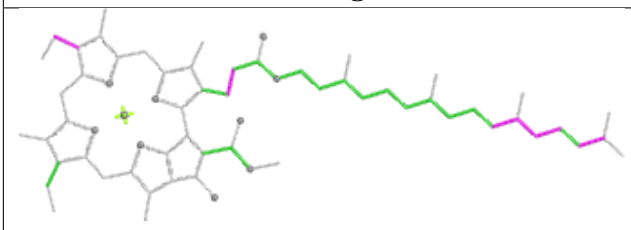
Ligand CLA B 610



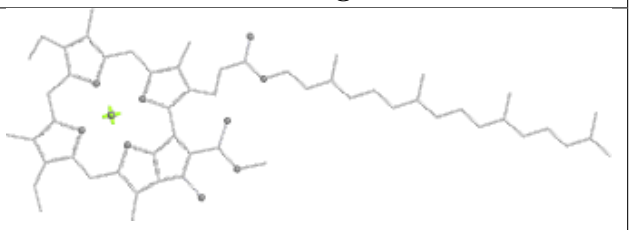
Bond lengths



Bond angles

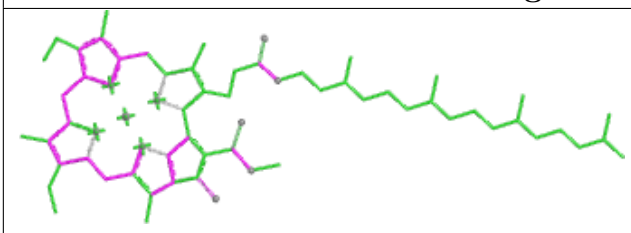


Torsions

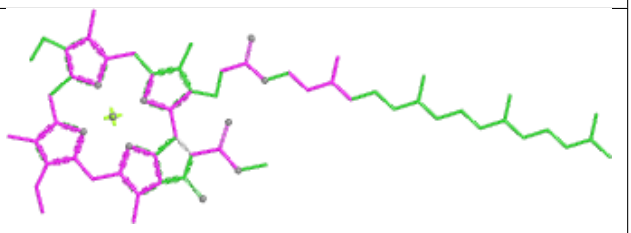


Rings

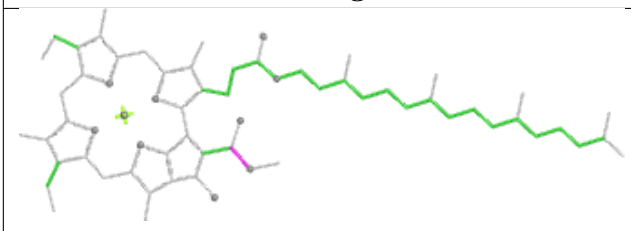
Ligand CLA C 504



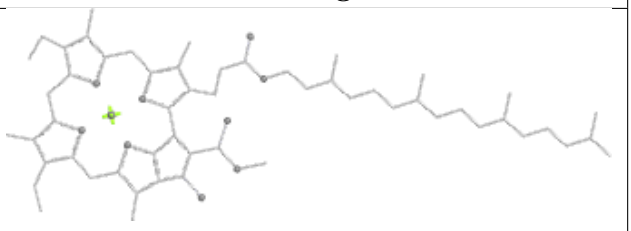
Bond lengths



Bond angles

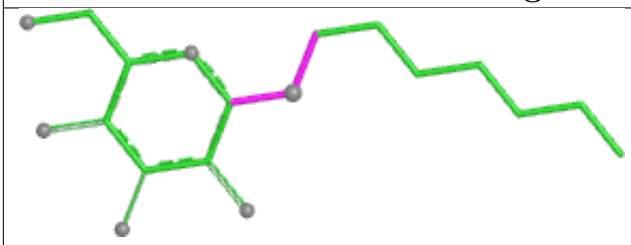


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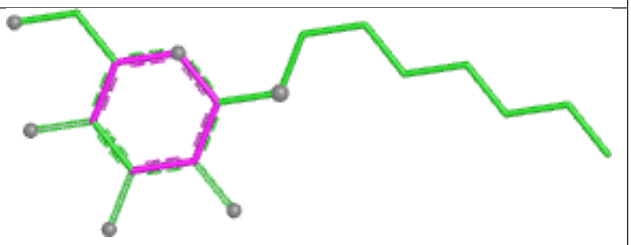


Rings

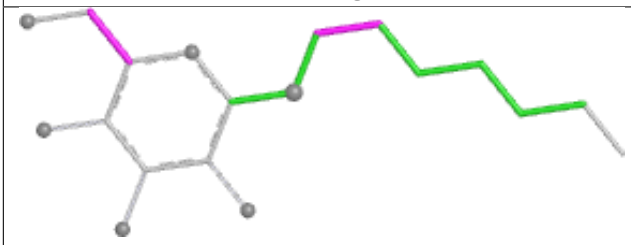
Ligand HTG b 625



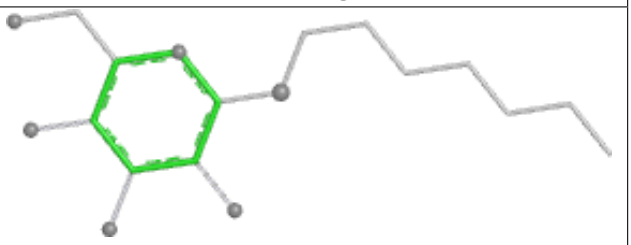
Bond lengths



Bond angles

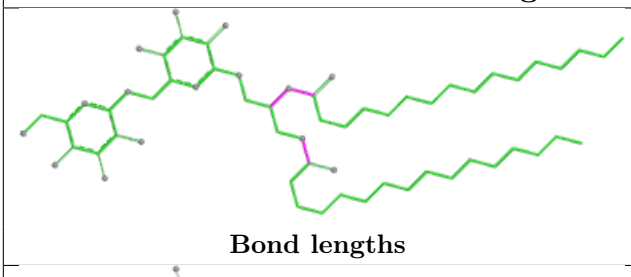


Torsions

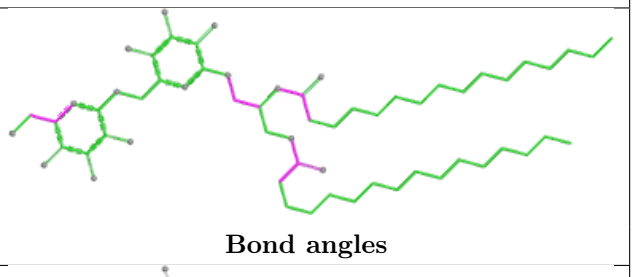


Rings

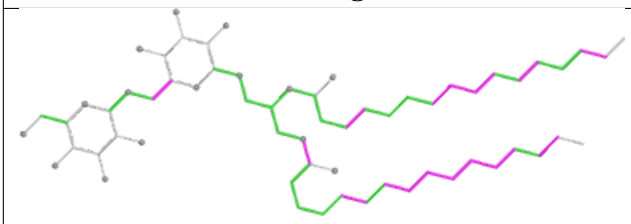
Ligand DGD C 519



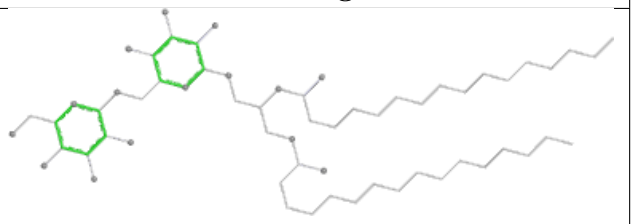
Bond lengths



Bond angles

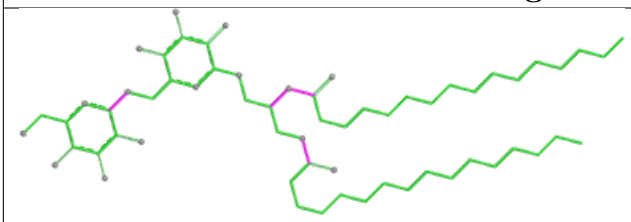


Torsions

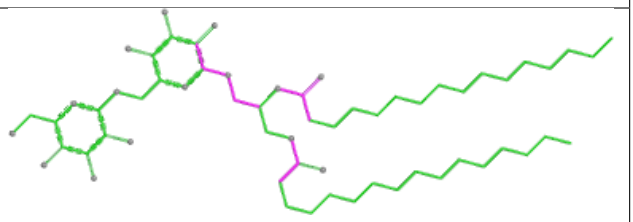


Rings

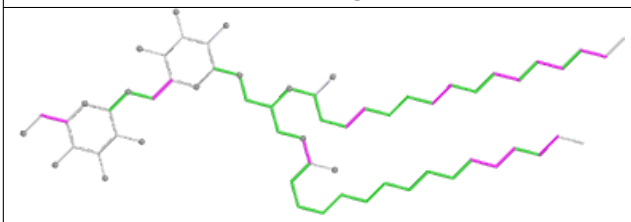
Ligand DGD c 518



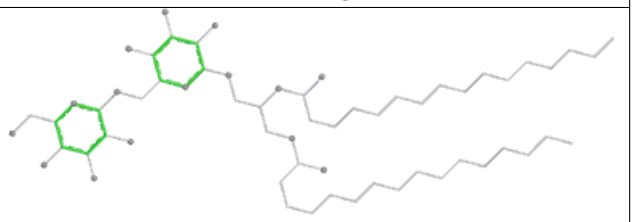
Bond lengths



Bond angles

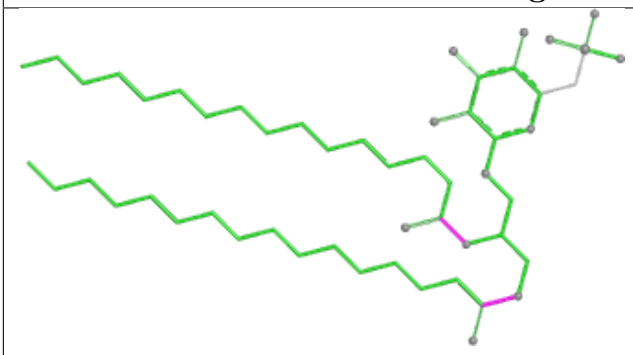


Torsions

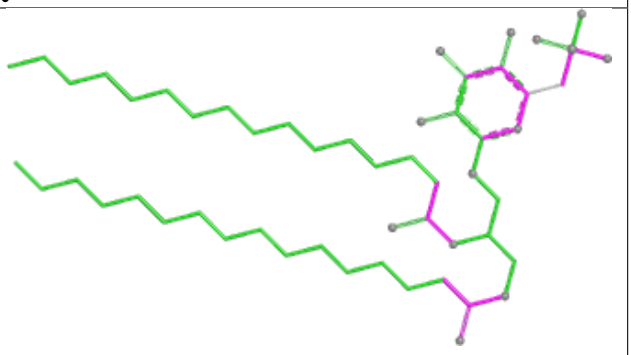


Rings

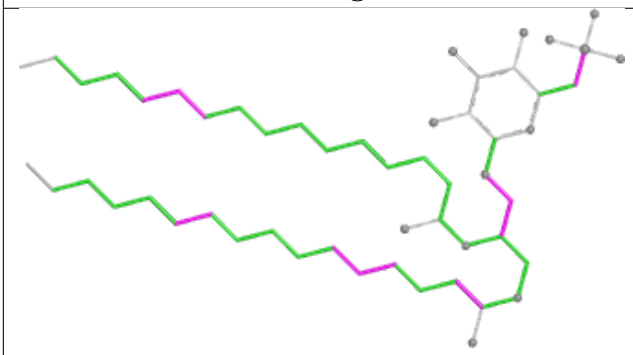
Ligand SQD a 411



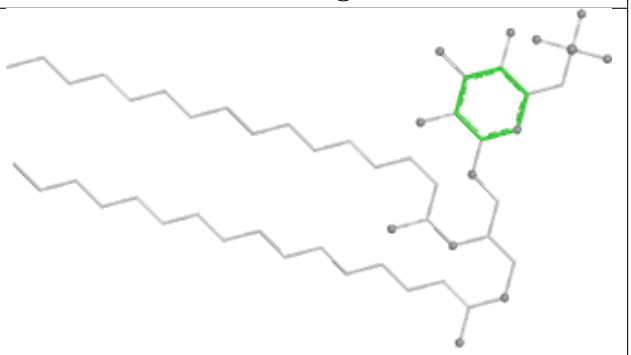
Bond lengths



Bond angles

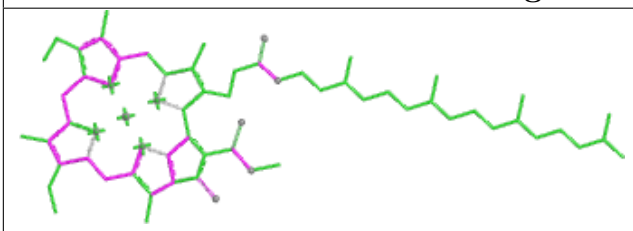


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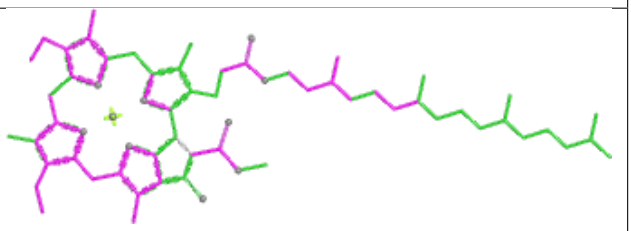


Rings

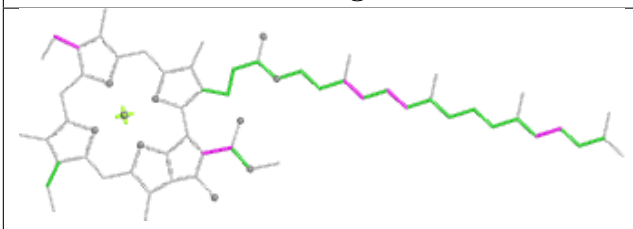
Ligand CLA C 508



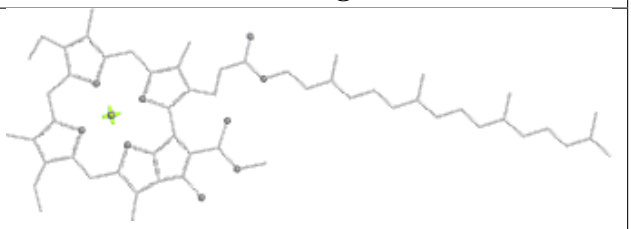
Bond lengths



Bond angles

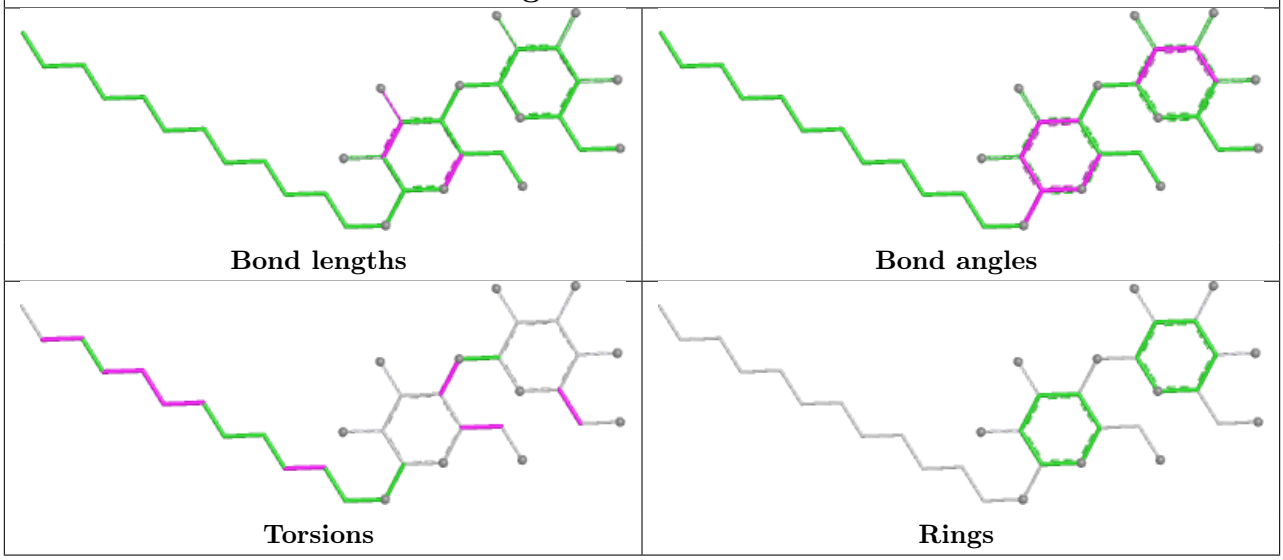


Torsions

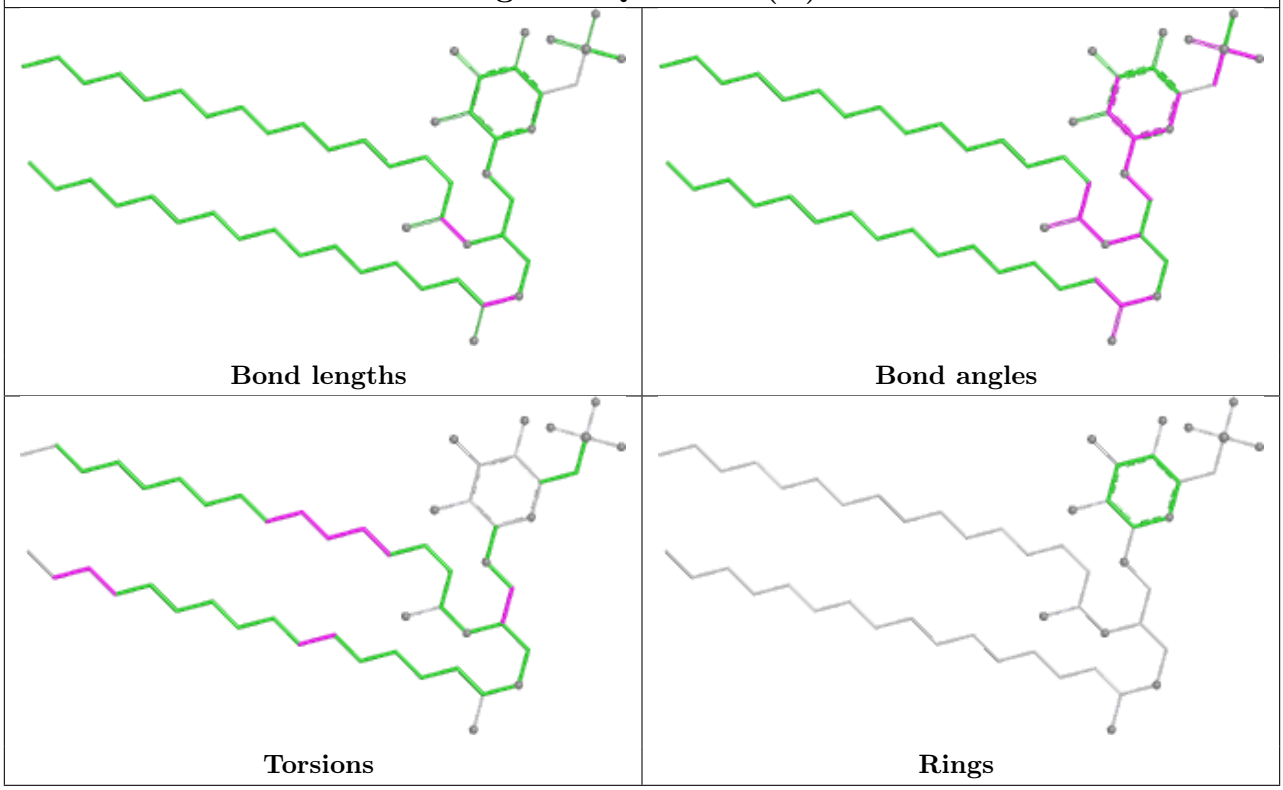


Rings

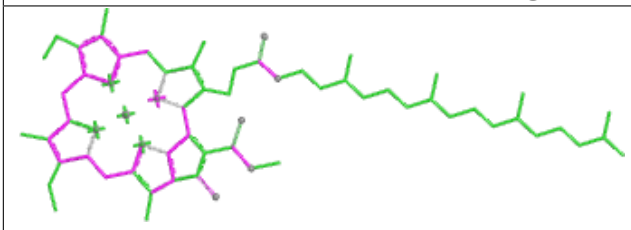
Ligand LMT B 627



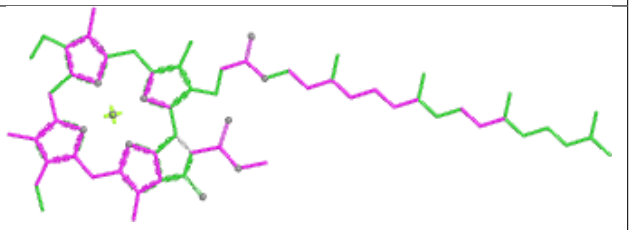
Ligand SQD a 409 (A)



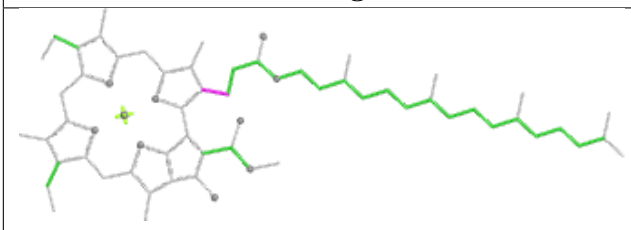
Ligand CLA B 604



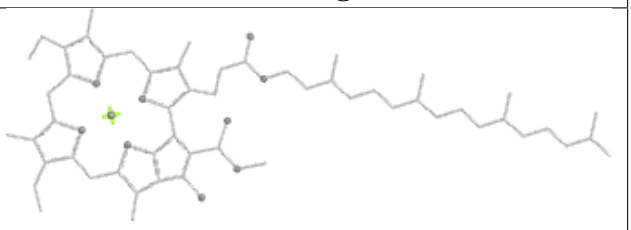
Bond lengths



Bond angles



Torsions



Rings

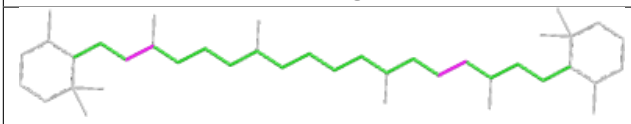
Ligand BCR K 102



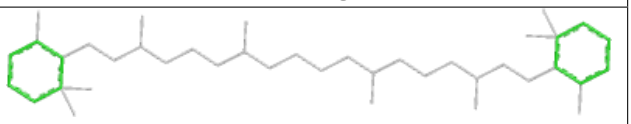
Bond lengths



Bond angles

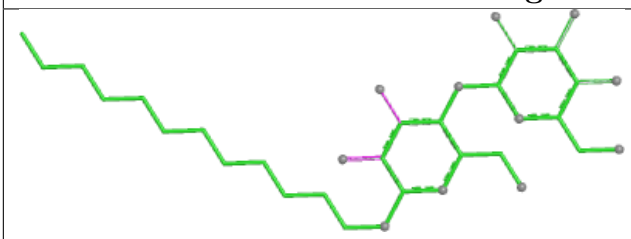


Torsions

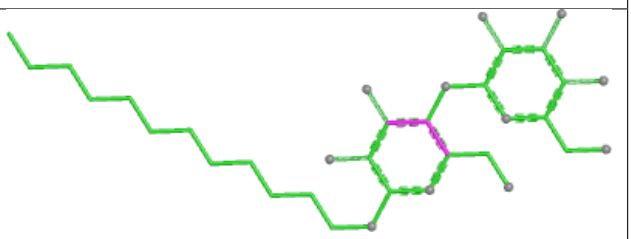


Rings

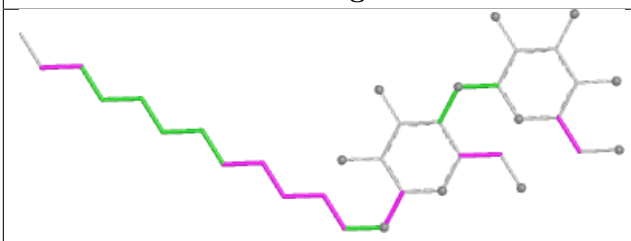
Ligand LMT a 416



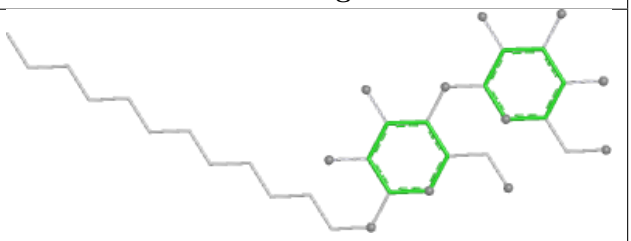
Bond lengths



Bond angles

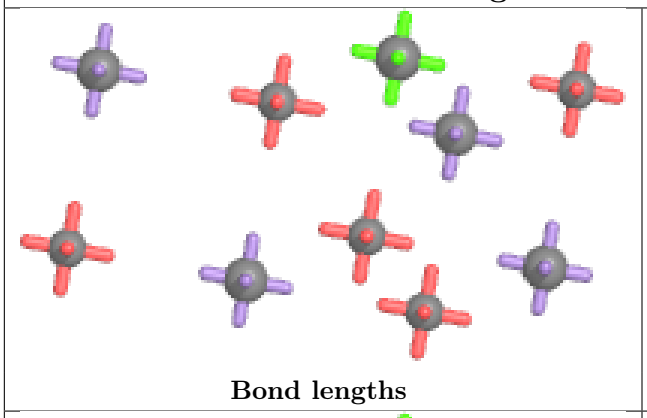


Torsions

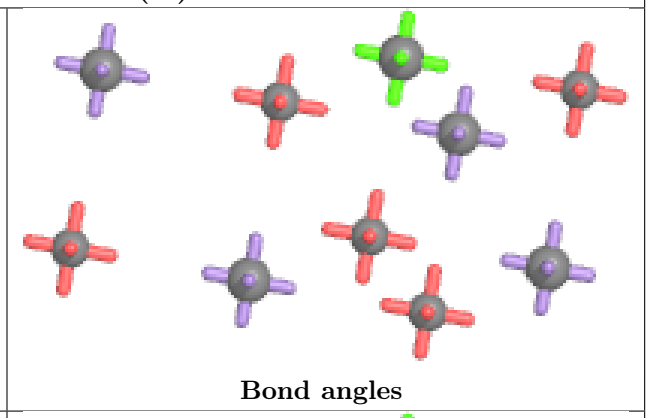


Rings

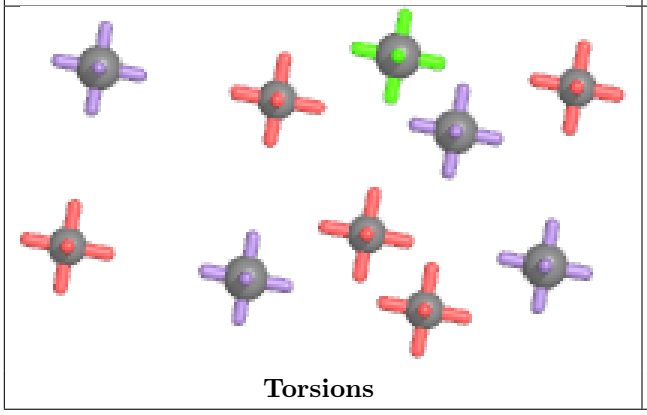
Ligand OEX A 413 (A)



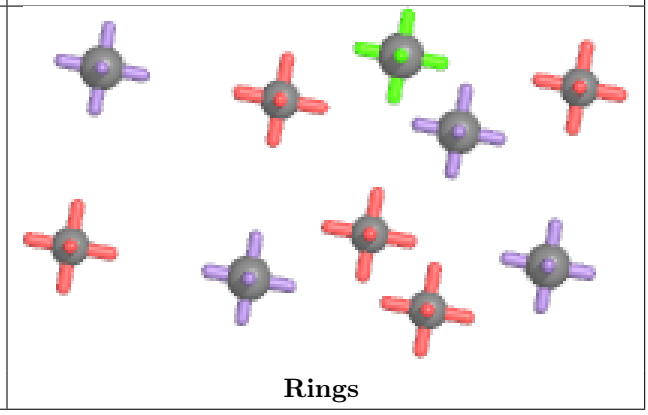
Bond lengths



Bond angles

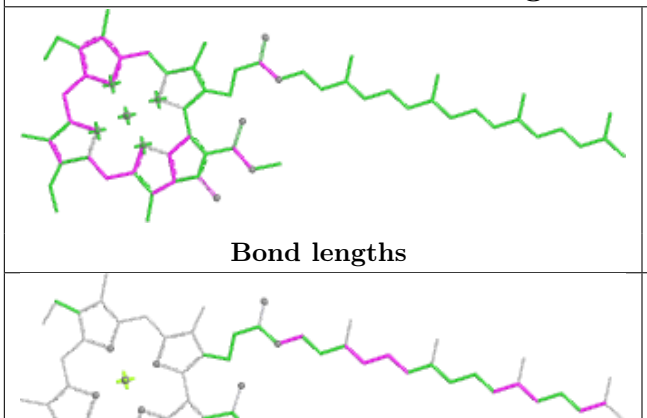


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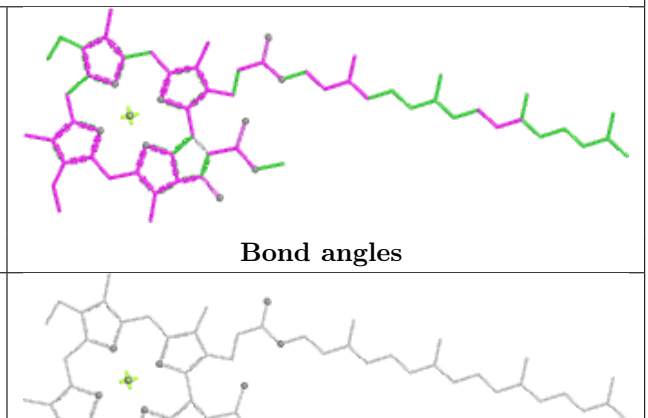


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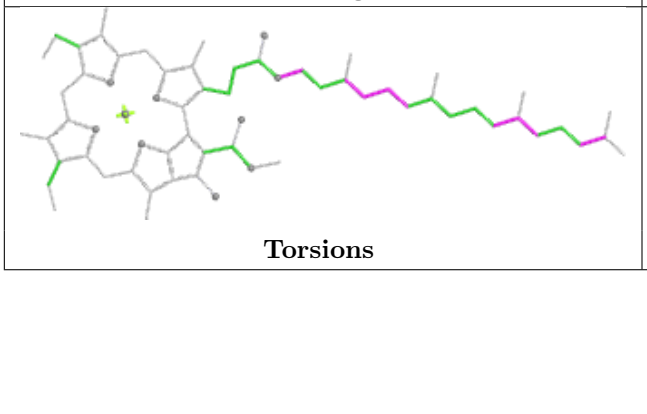
Ligand CLA A 408



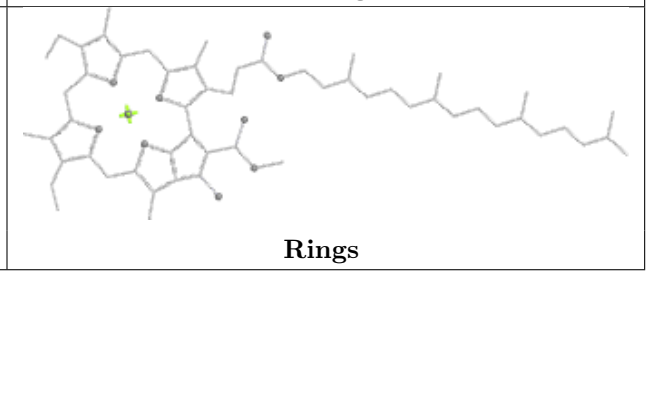
Bond lengths



Bond angles

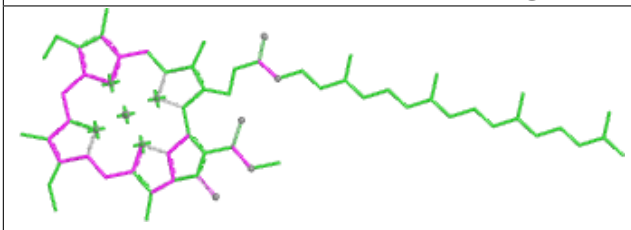


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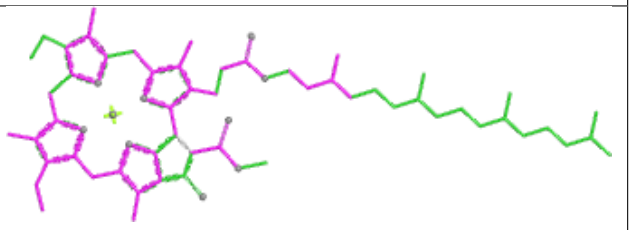


Rings

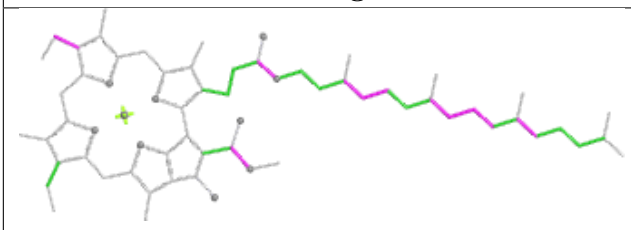
Ligand CLA D 403



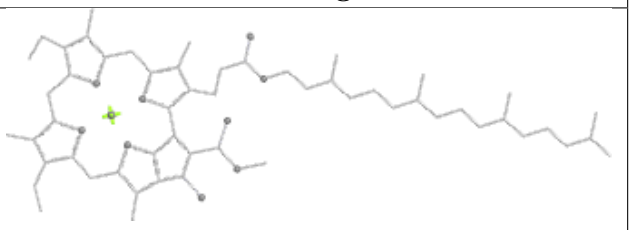
Bond lengths



Bond angles

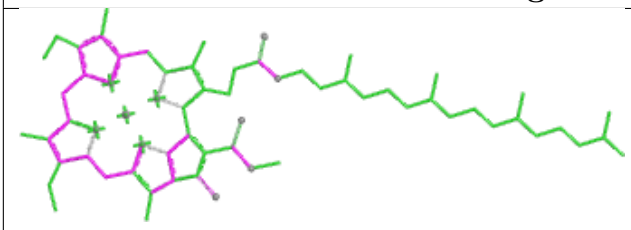


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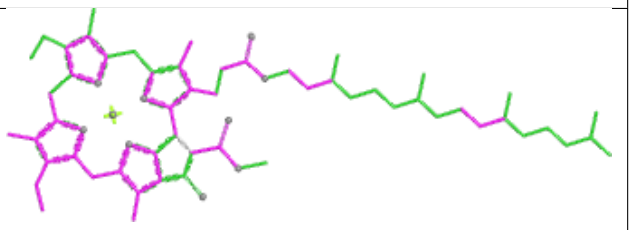


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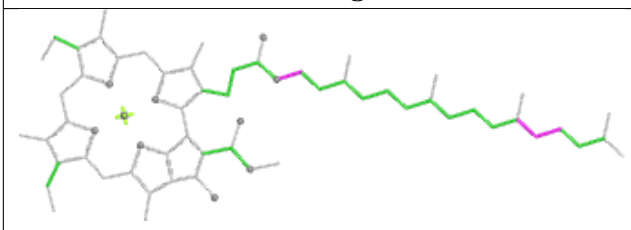
Ligand CLA b 608



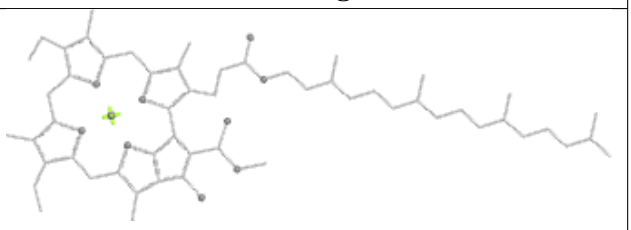
Bond lengths



Bond angles

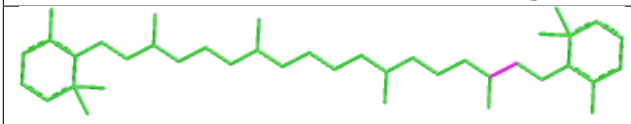


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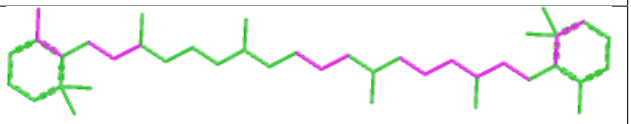


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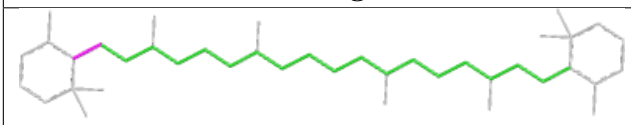
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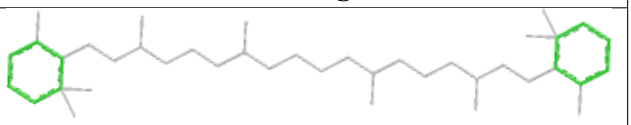
Bond lengths



Bond angles

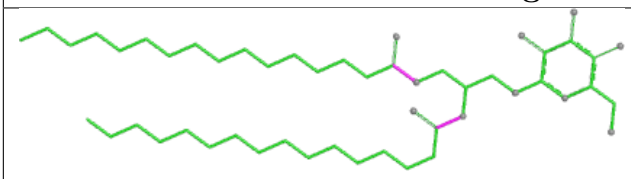


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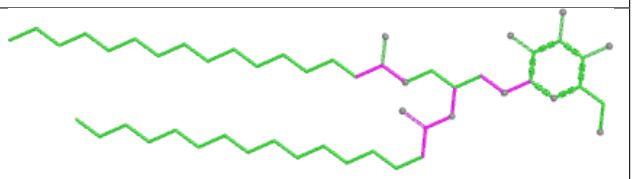


Rings

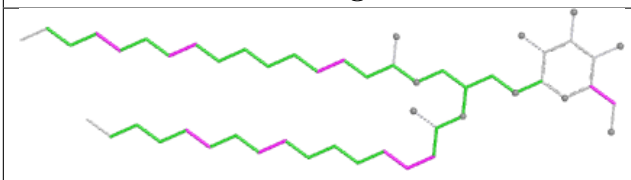
Ligand LMG d 413



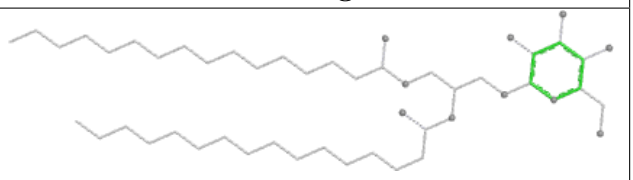
Bond lengths



Bond angles

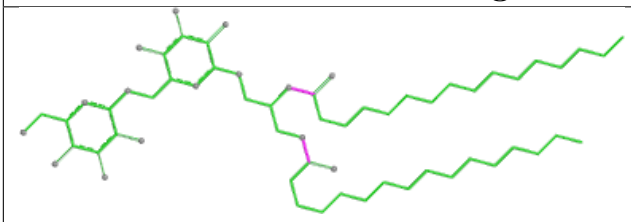


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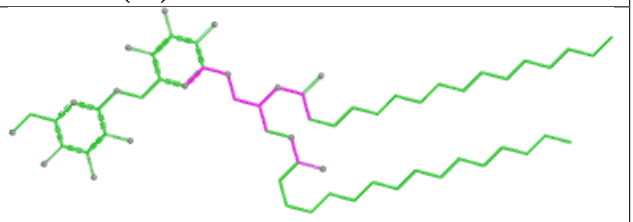


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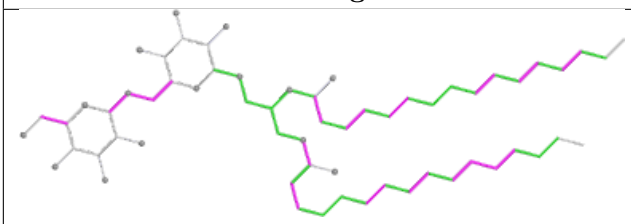
Ligand DGD c 516 (A)



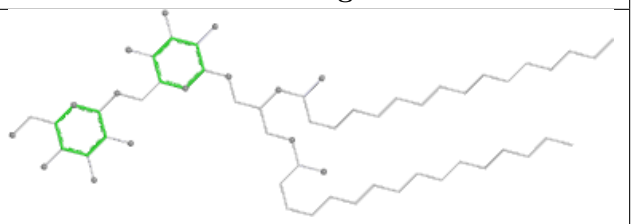
Bond lengths



Bond angles

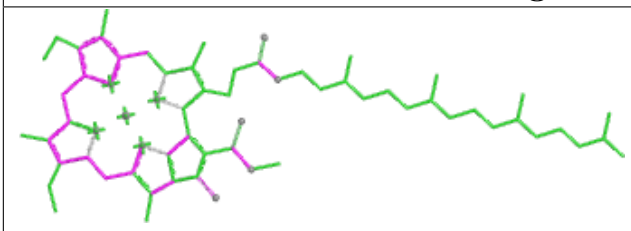


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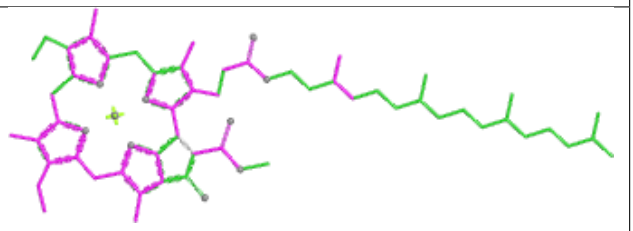


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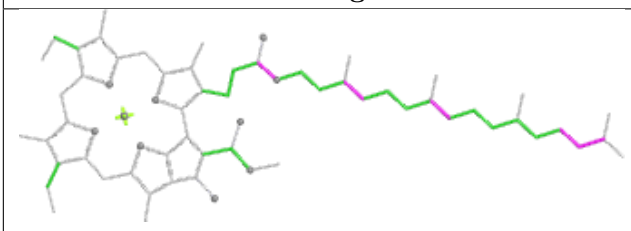
Ligand CLA a 407



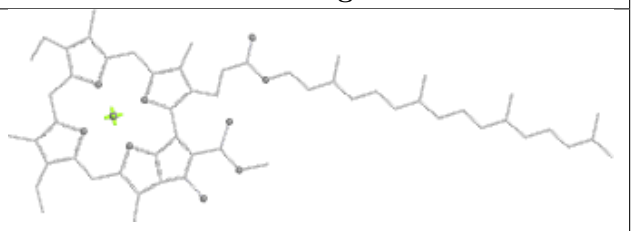
Bond lengths



Bond angles

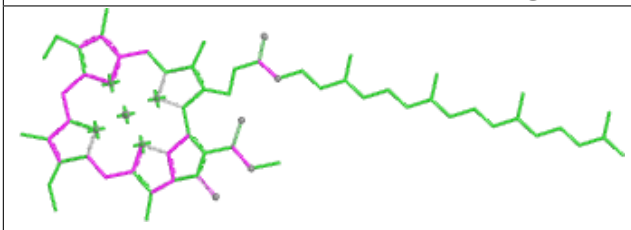


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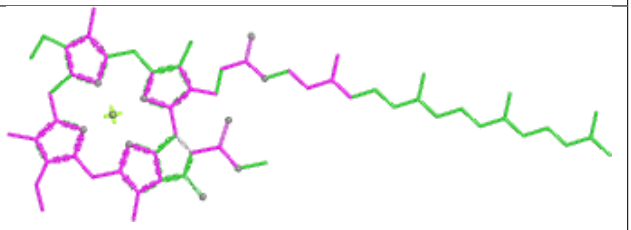


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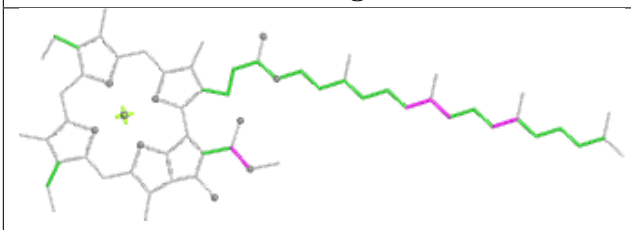
Ligand CLA C 514



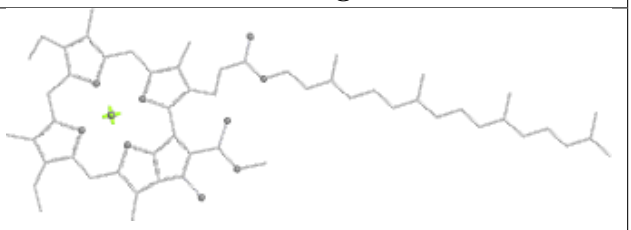
Bond lengths



Bond angles



Torsions

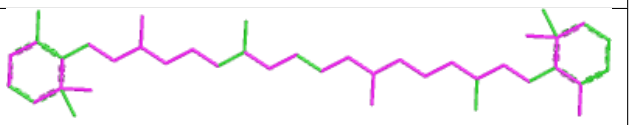


Rings

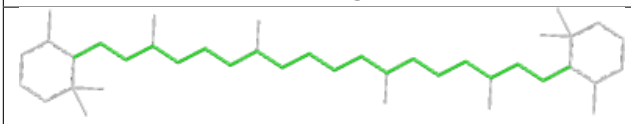
Ligand BCR k 101



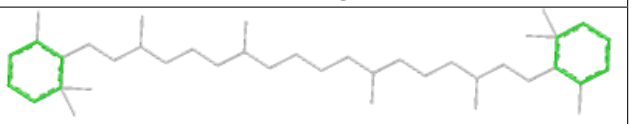
Bond lengths



Bond angles

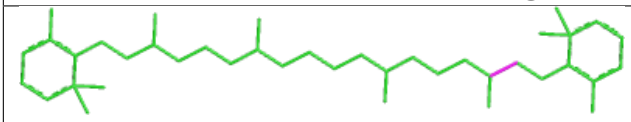


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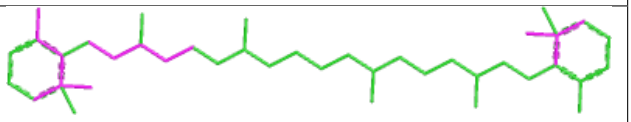


Rings

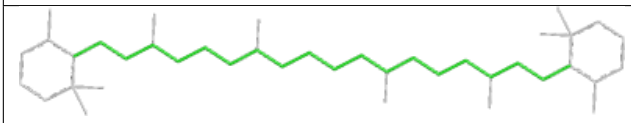
Ligand BCR C 516



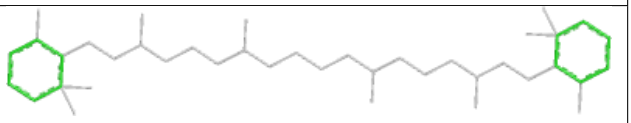
Bond lengths



Bond angles

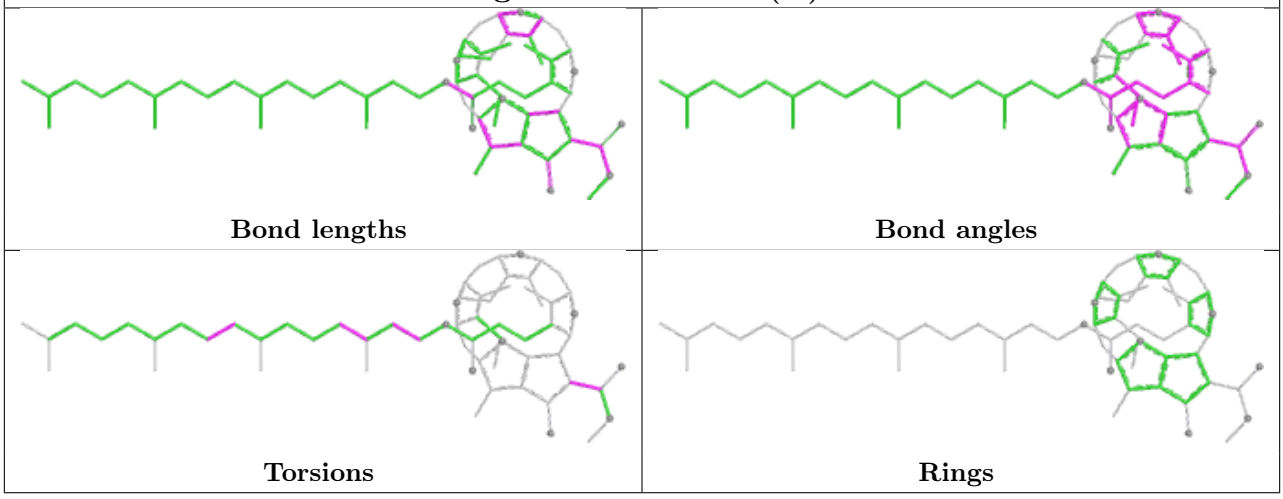


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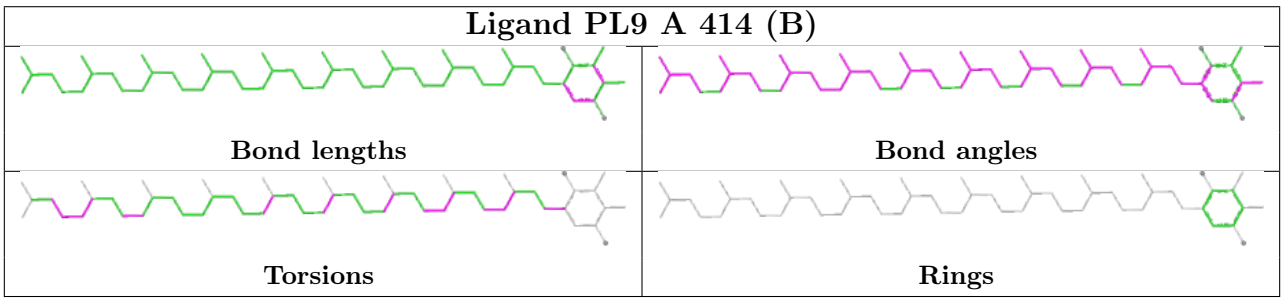


Rings

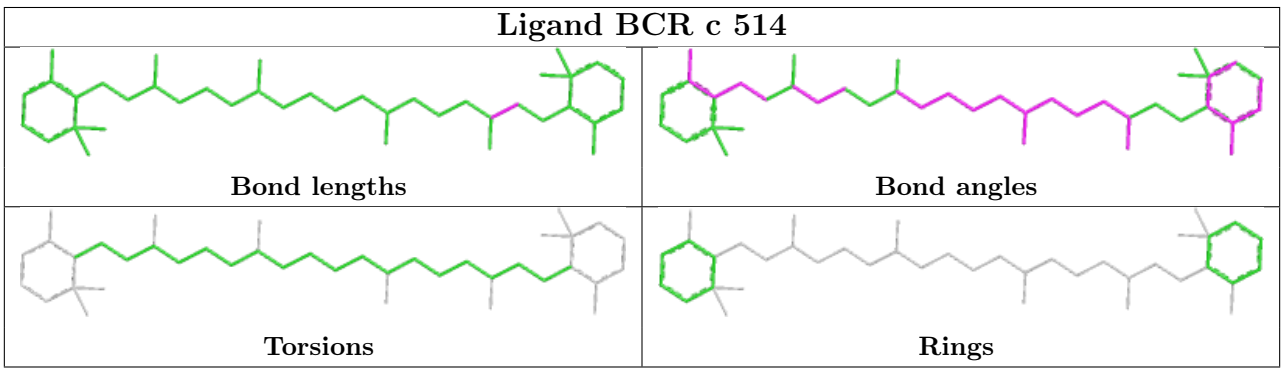
Ligand PHO a 406 (A)



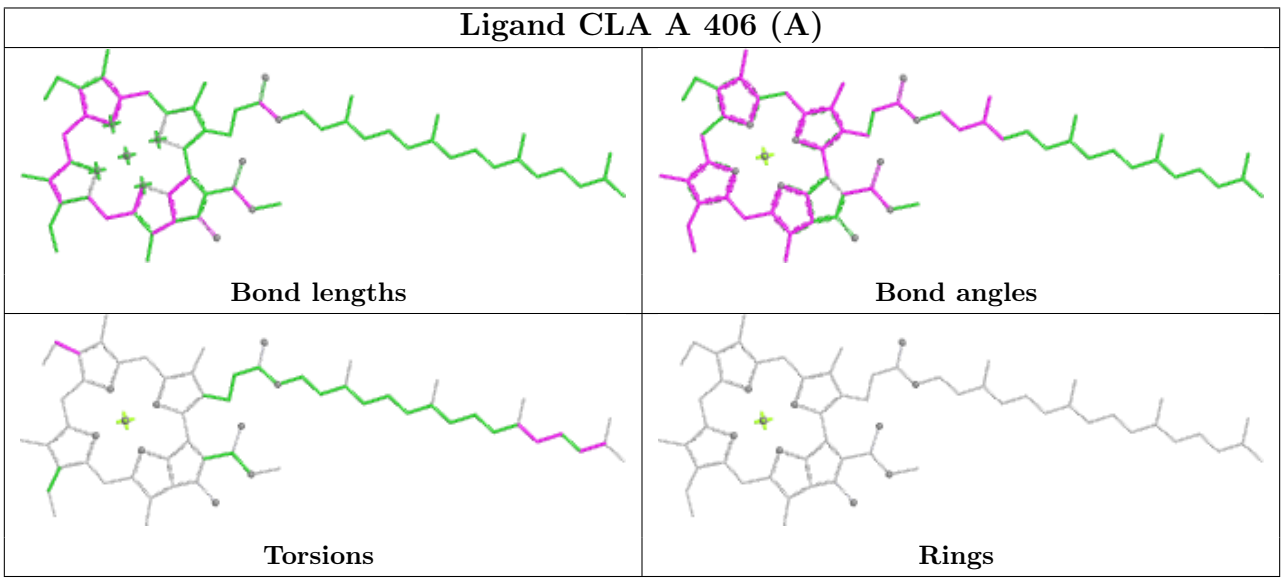
Ligand PL9 A 414 (B)



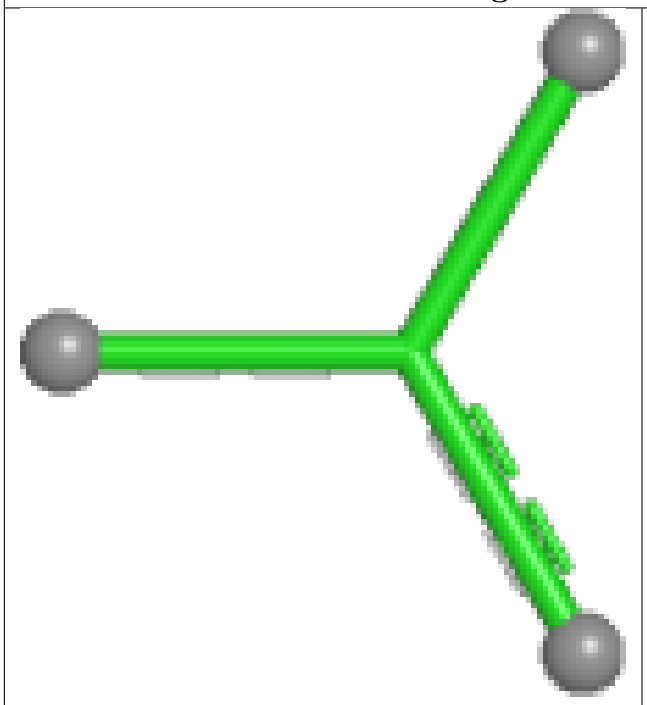
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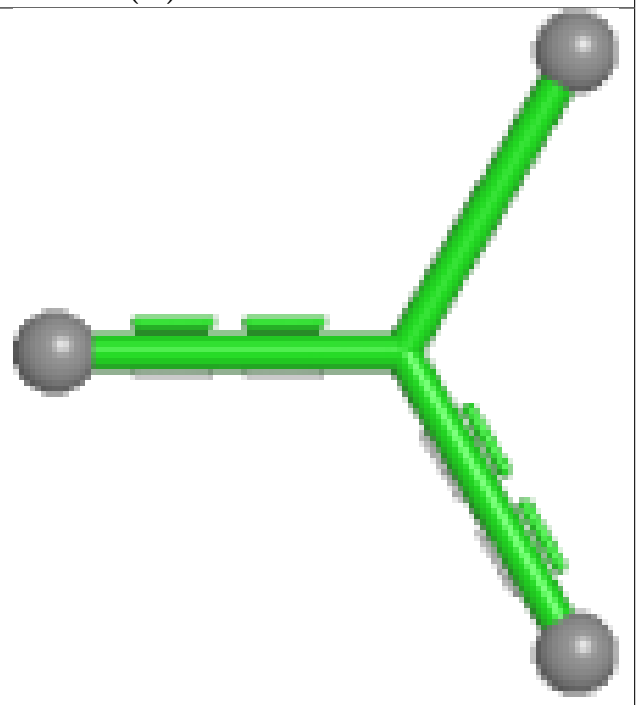
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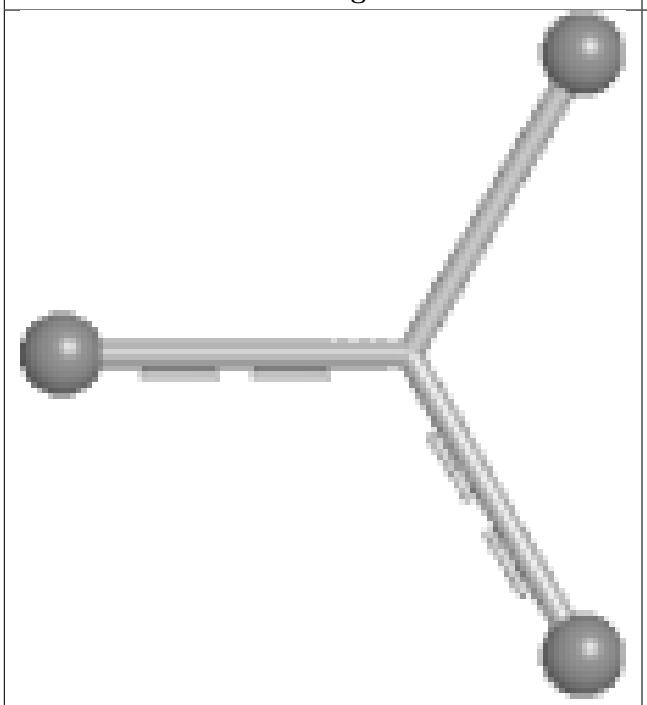
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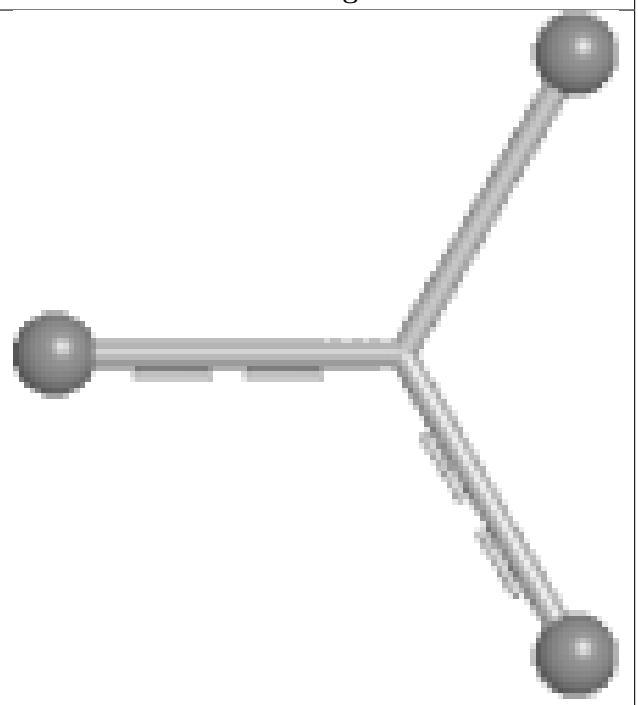
Bond lengths



Bond angles

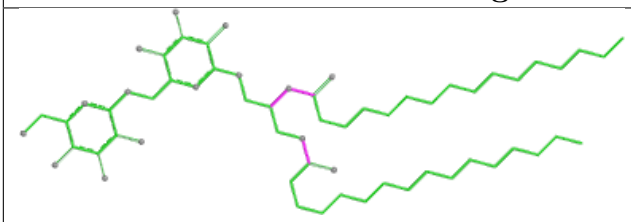


Torsions

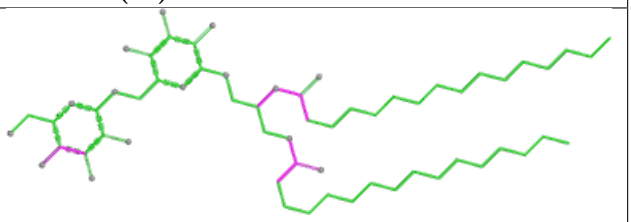


Rings

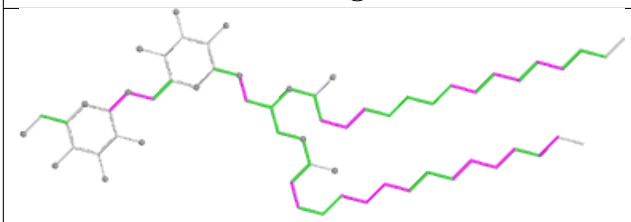
Ligand DGD c 517 (A)



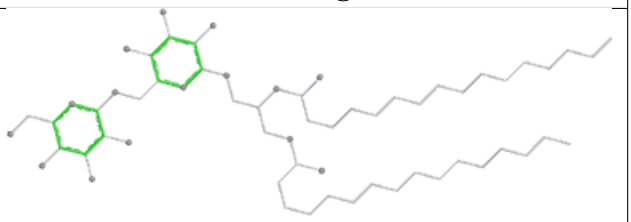
Bond lengths



Bond angles

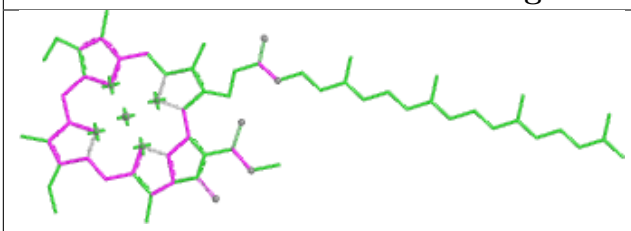


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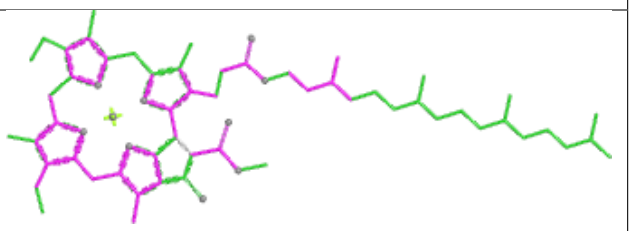


Rings

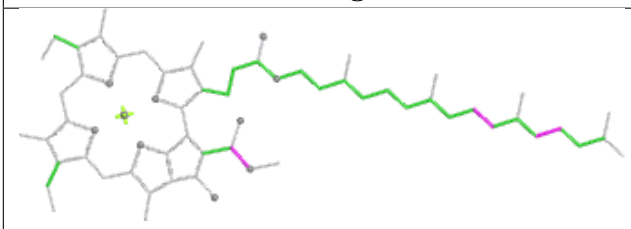
Ligand CLA C 509



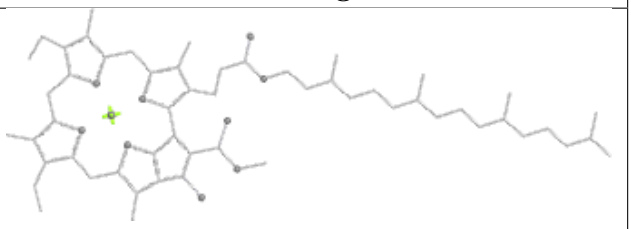
Bond lengths



Bond angles

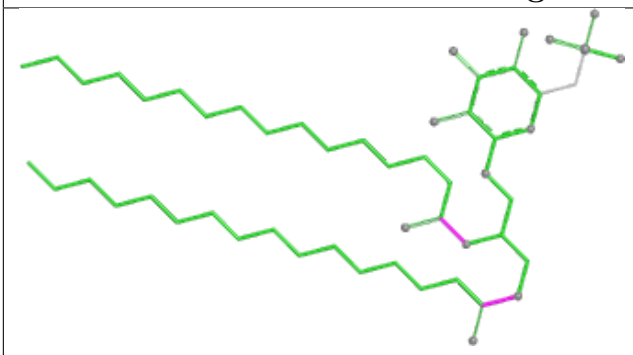


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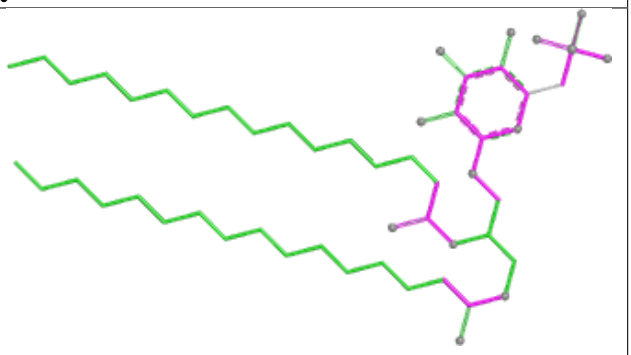


Rings

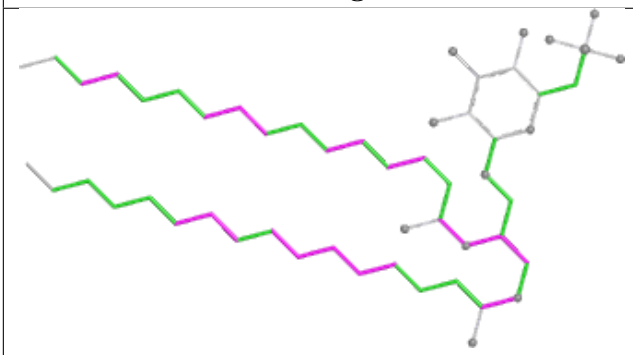
Ligand SQD b 620



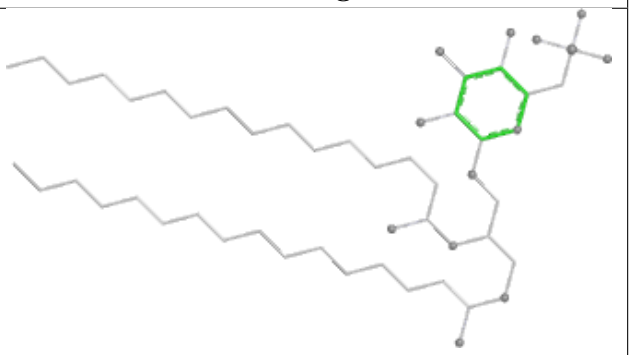
Bond lengths



Bond angles

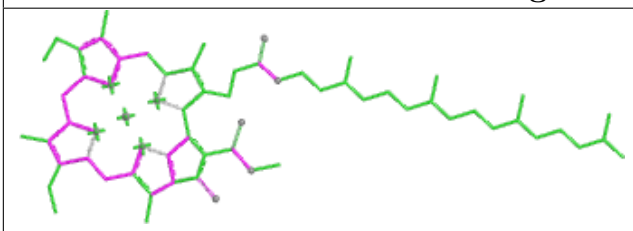


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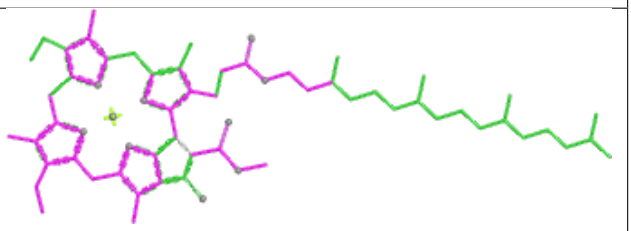


Rings

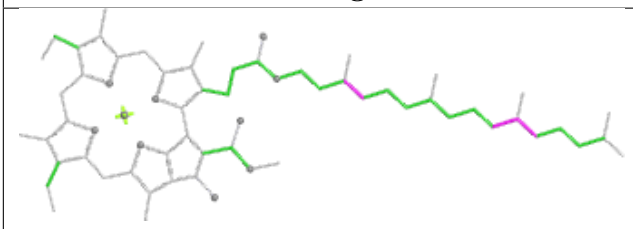
Ligand CLA c 504



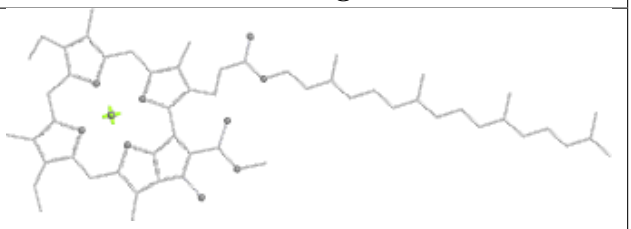
Bond lengths



Bond angles

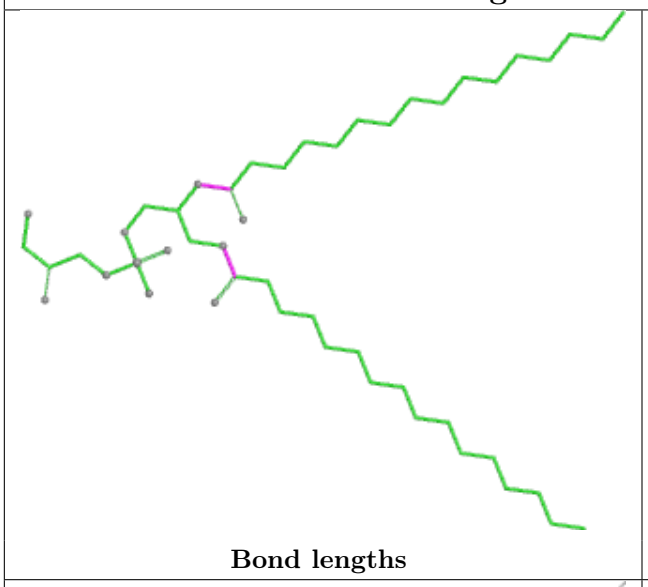


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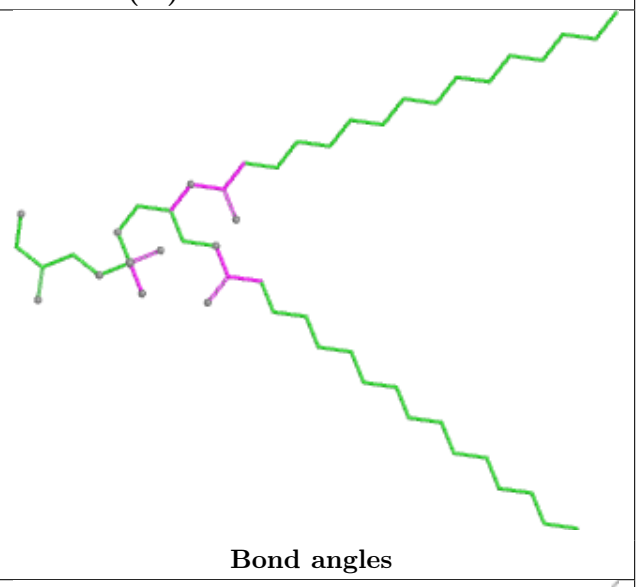


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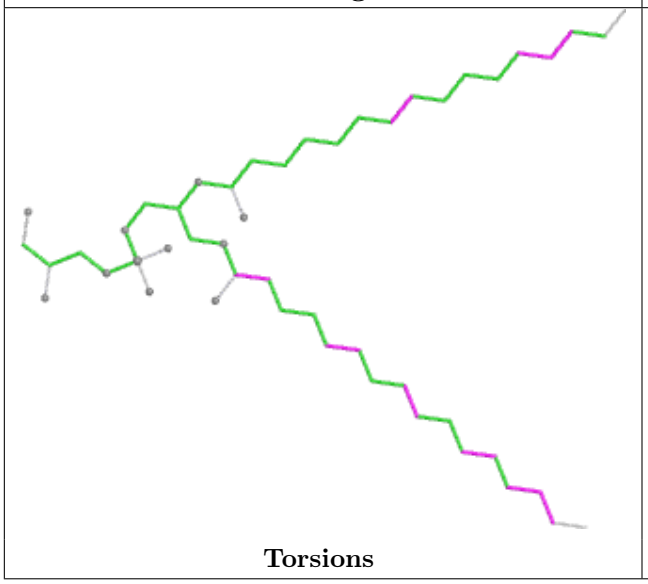
Ligand LHG A 419 (A)



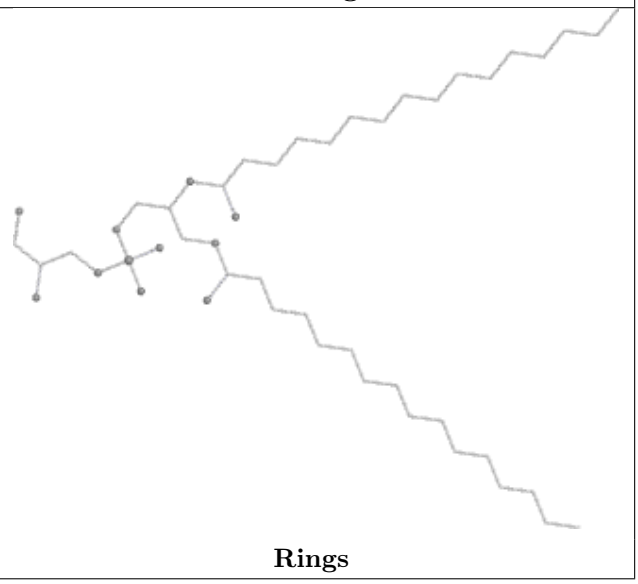
Bond lengths



Bond angles



Torsions

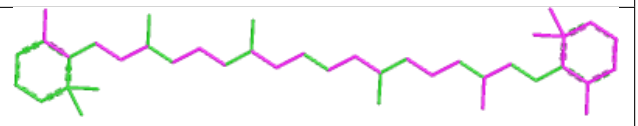


Rings

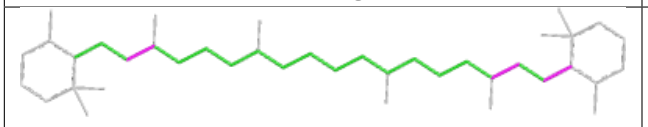
Ligand BCR d 406



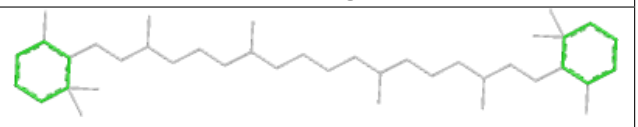
Bond lengths



Bond angles

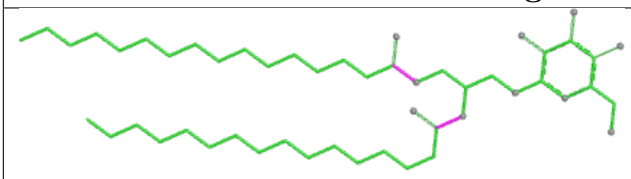


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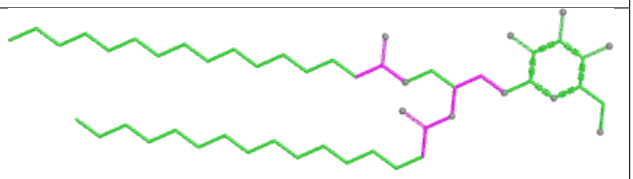


Rings

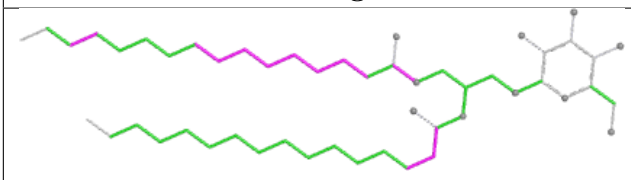
Ligand LMG c 519



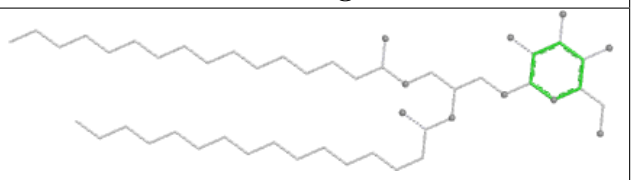
Bond lengths



Bond angles

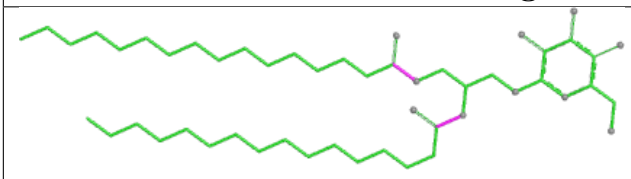


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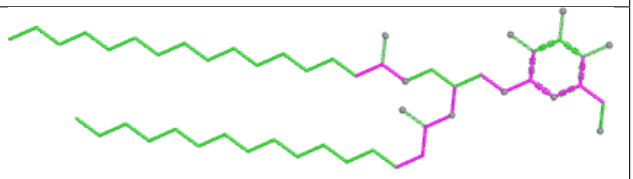


Rings

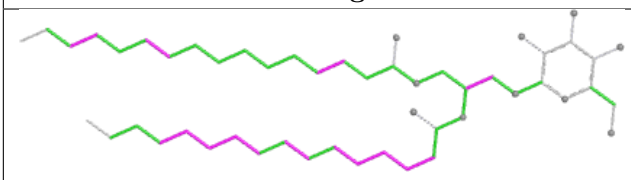
Ligand LMG C 501



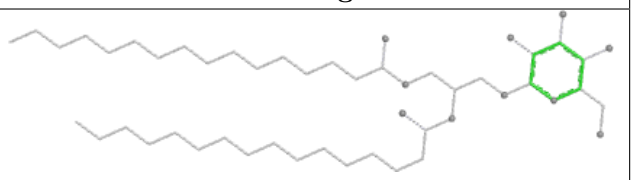
Bond lengths



Bond angles

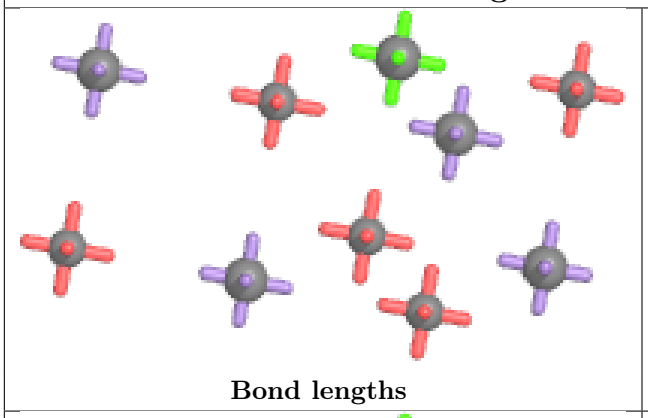


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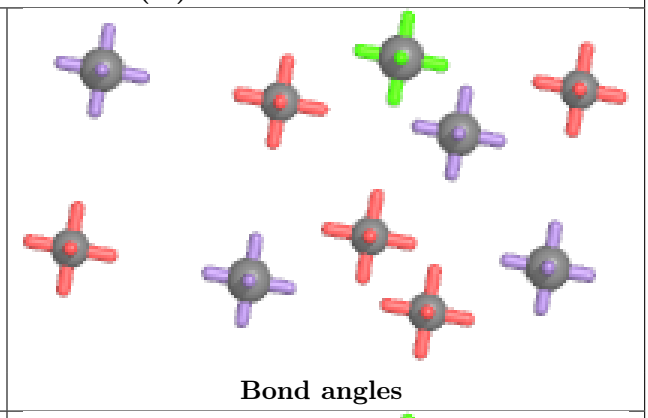


Rings

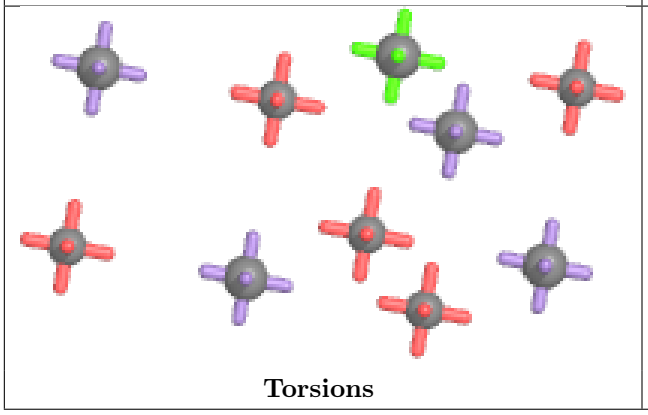
Ligand OEX A 413 (B)



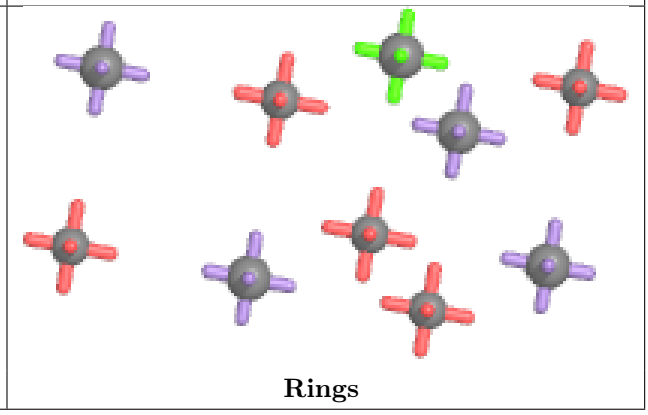
Bond lengths



Bond angles

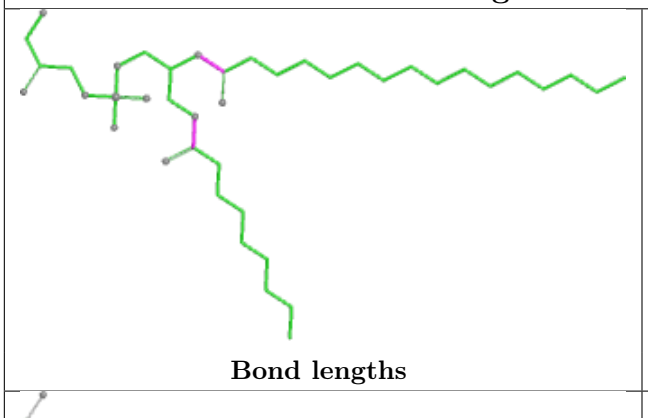


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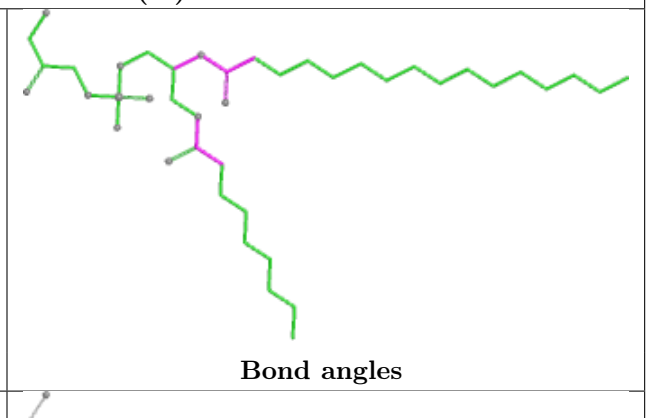


Rings

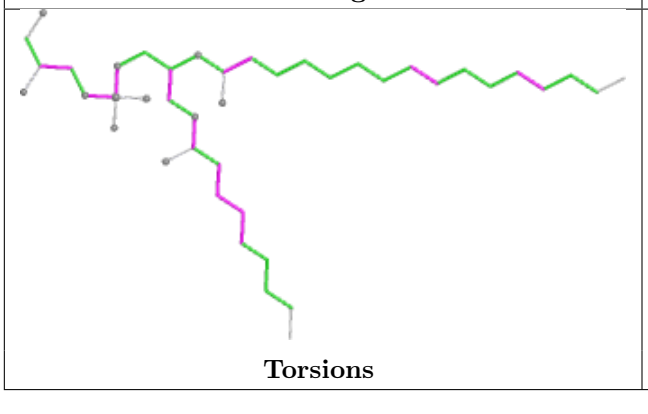
Ligand LHG E 101 (B)



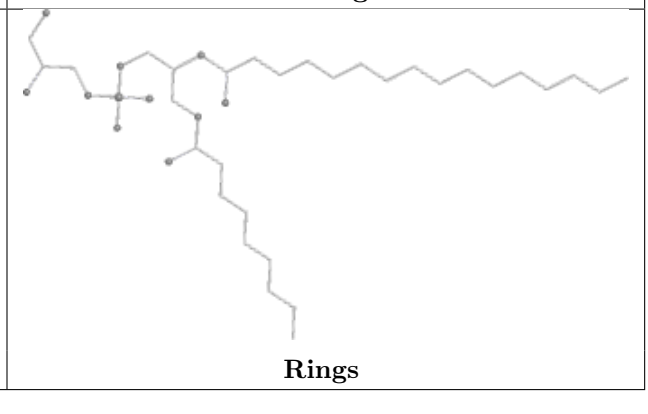
Bond lengths



Bond angles

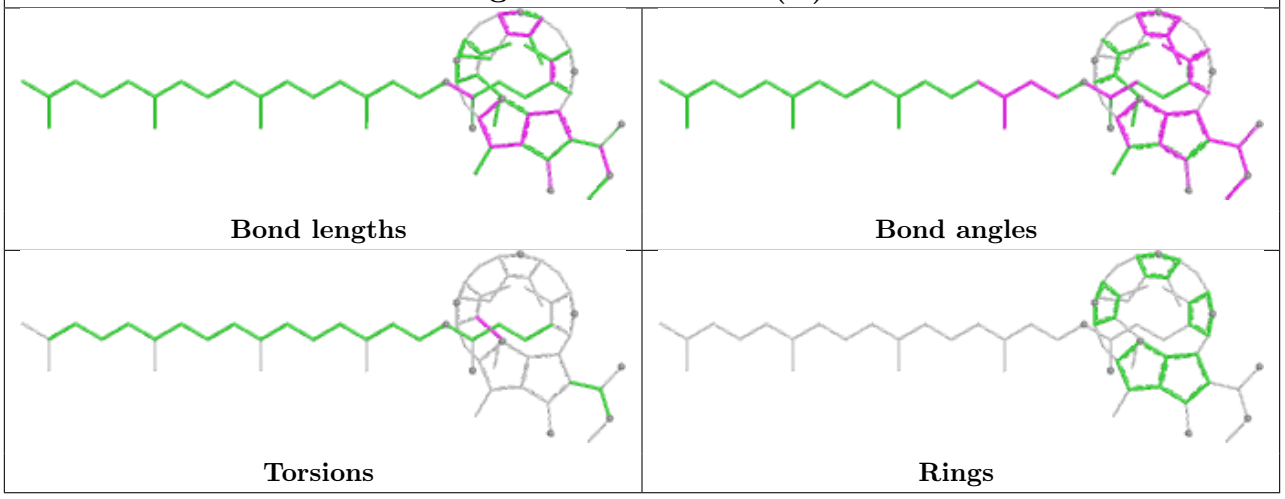


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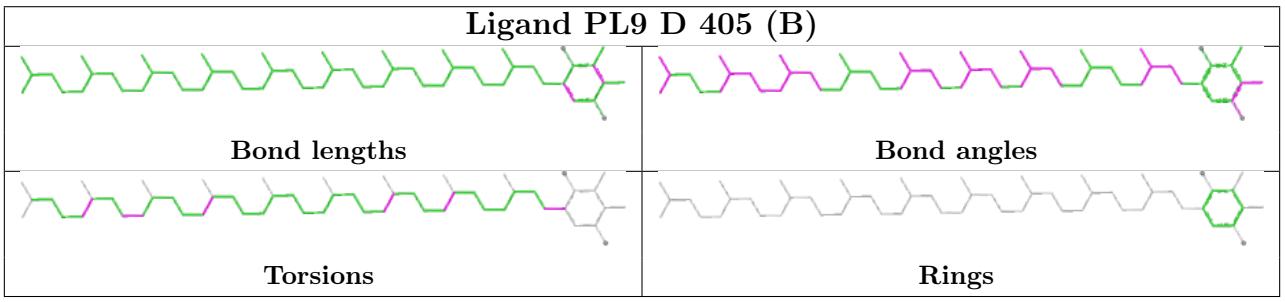


Rings

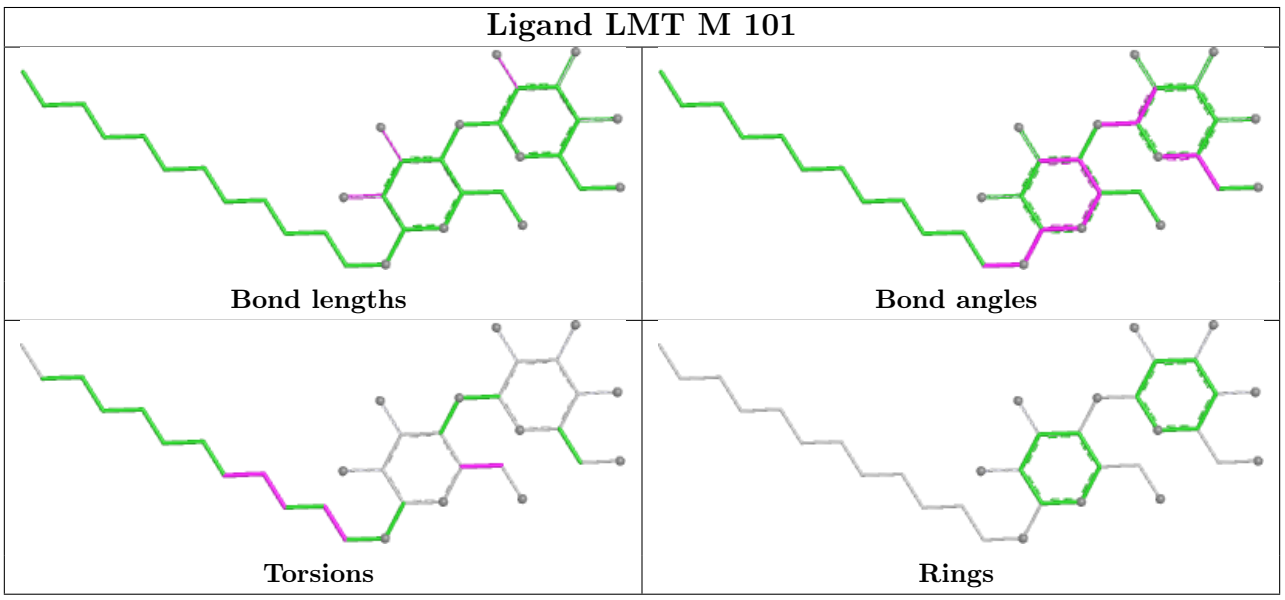
Ligand PHO A 416 (B)



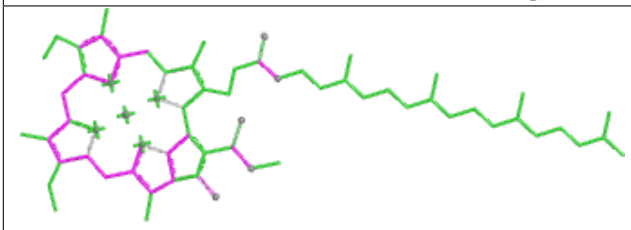
Ligand PL9 D 405 (B)



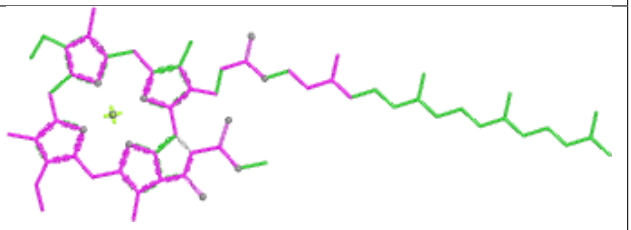
Ligand LMT M 101



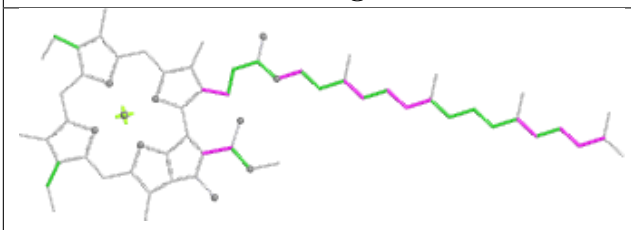
Ligand CLA C 507



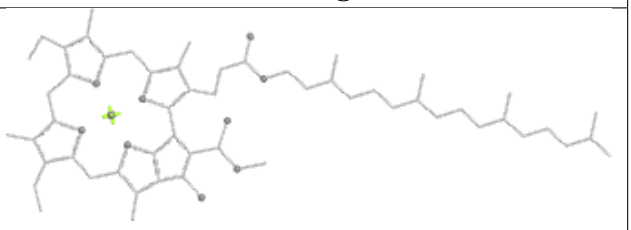
Bond lengths



Bond angles

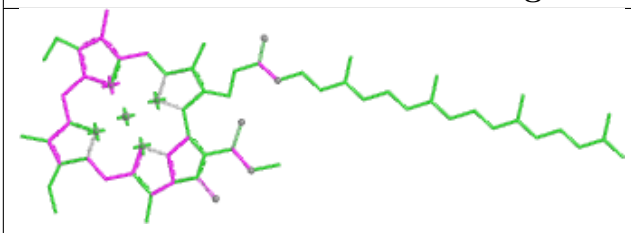


Torsions

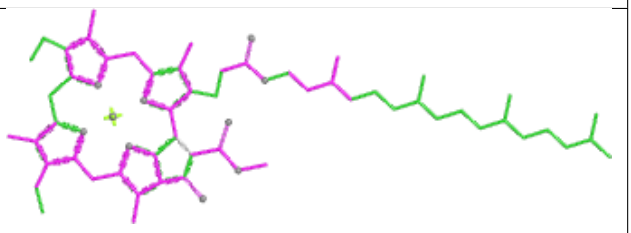


Rings

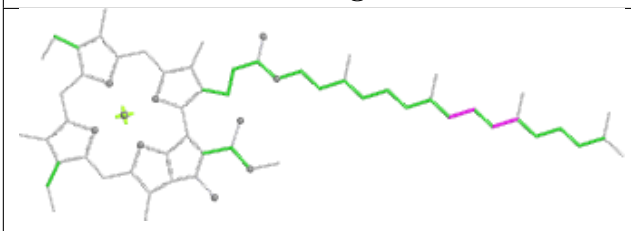
Ligand CLA B 611



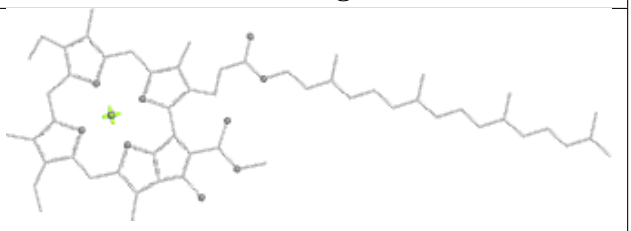
Bond lengths



Bond angles

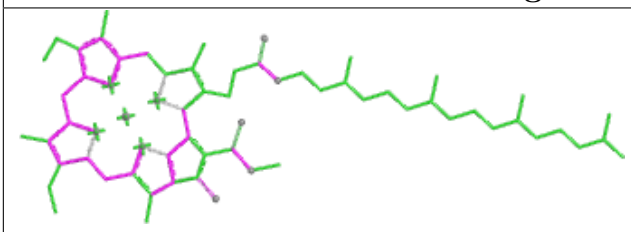


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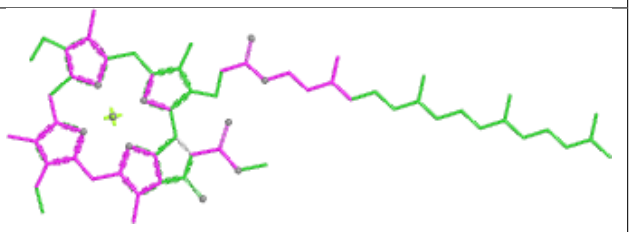


Rings

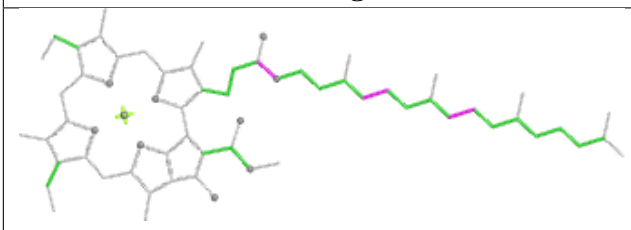
Ligand CLA C 512



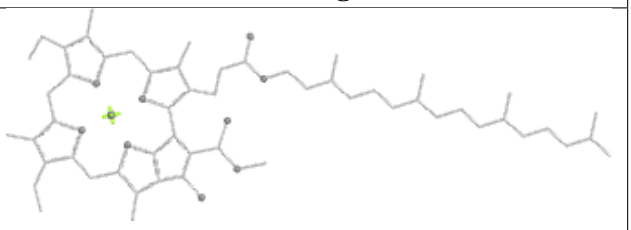
Bond lengths



Bond angles

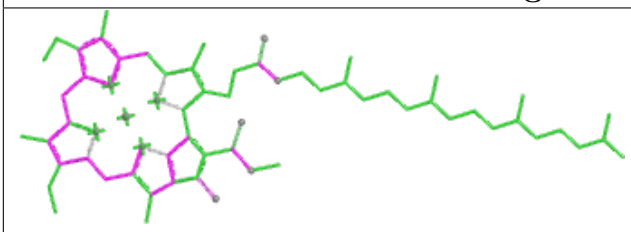


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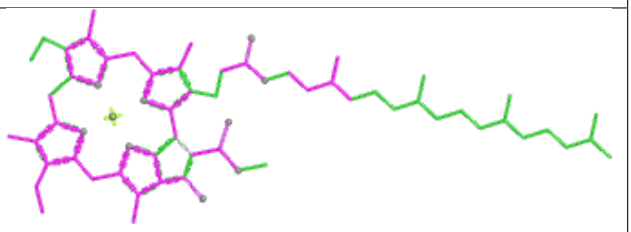


Rings

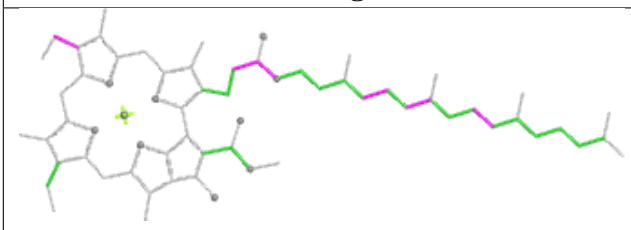
Ligand CLA C 513



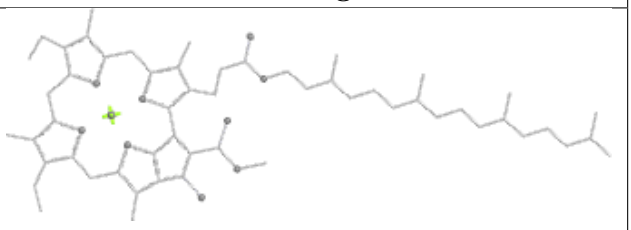
Bond lengths



Bond angles

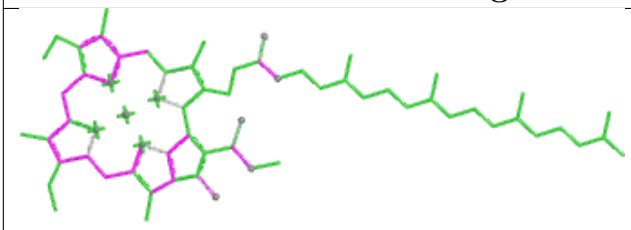


Torsions

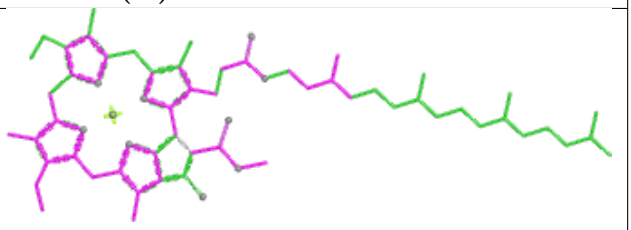


Rings

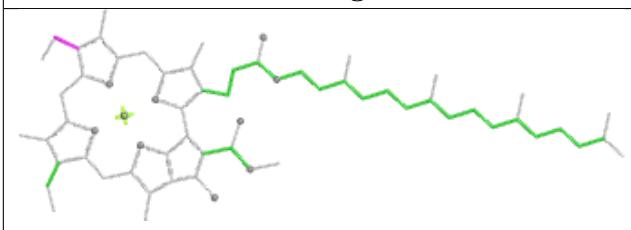
Ligand CLA D 402 (B)



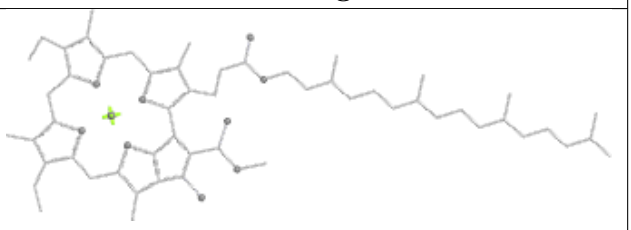
Bond lengths



Bond angles

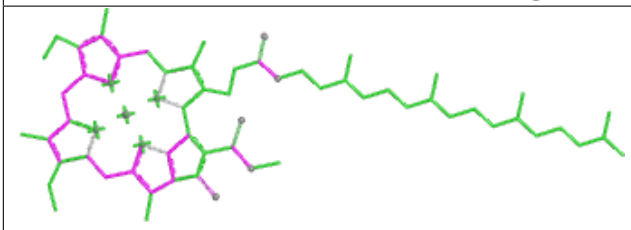


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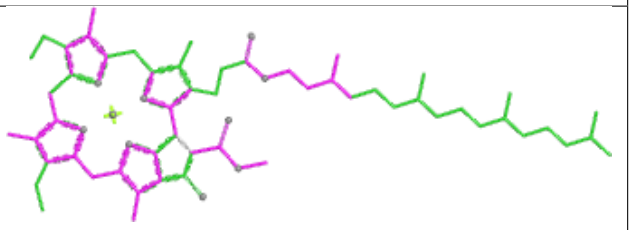


Rings

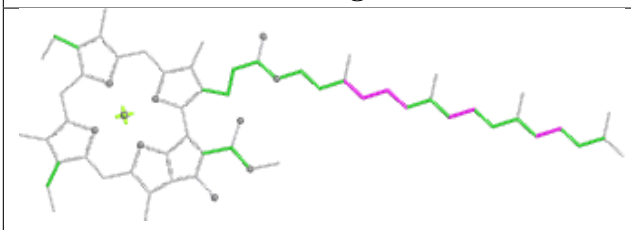
Ligand CLA b 605



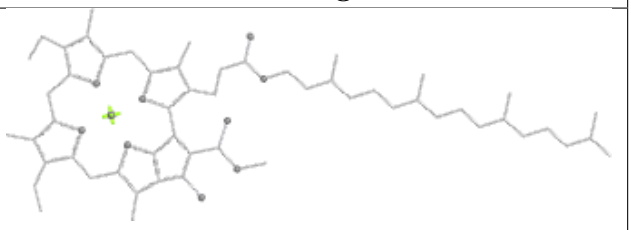
Bond lengths



Bond angles

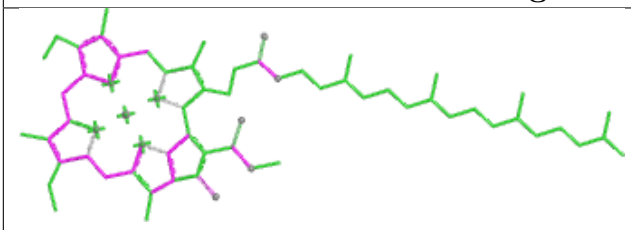


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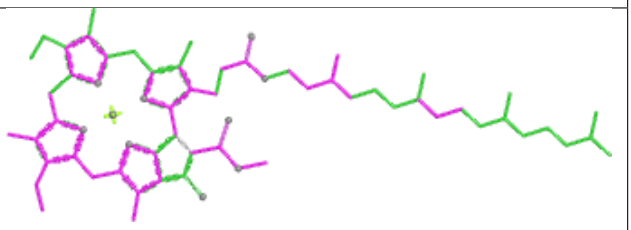


Rings

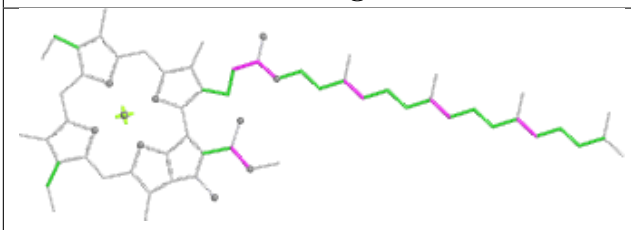
Ligand CLA c 510



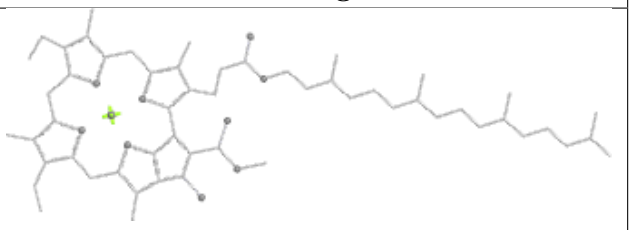
Bond lengths



Bond angles

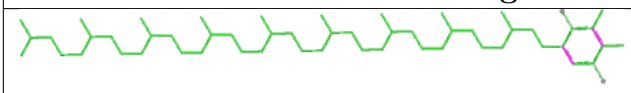


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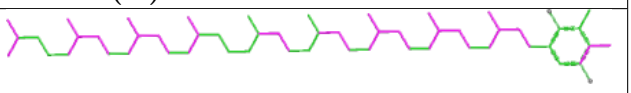


Rings

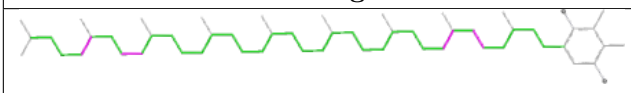
Ligand PL9 d 407 (B)



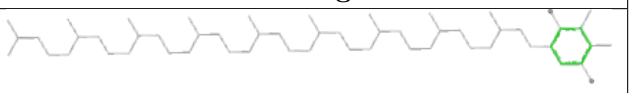
Bond lengths



Bond angles

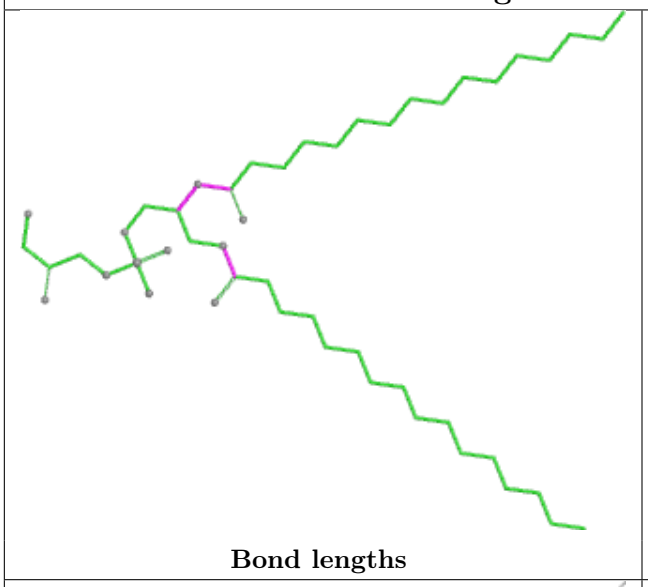


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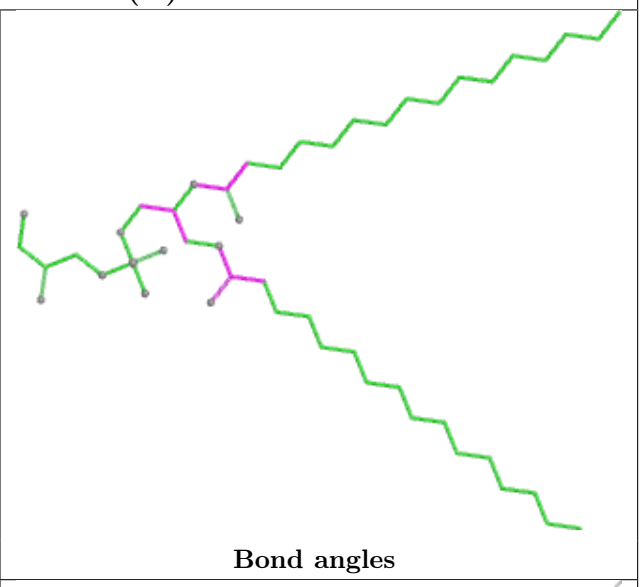


Rings

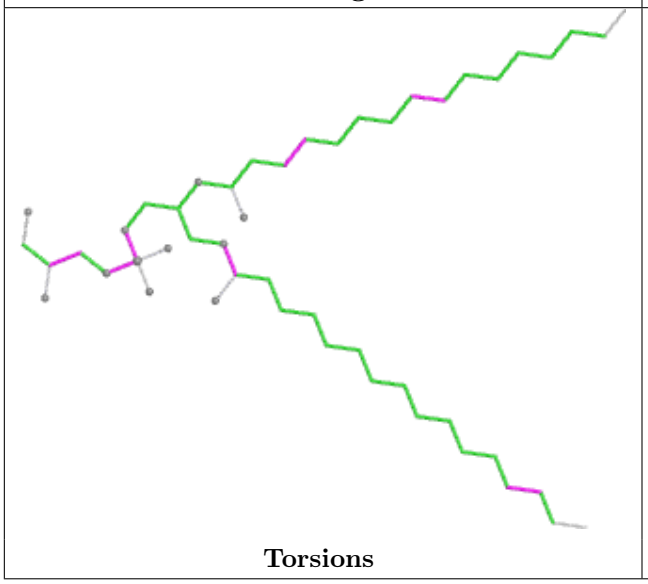
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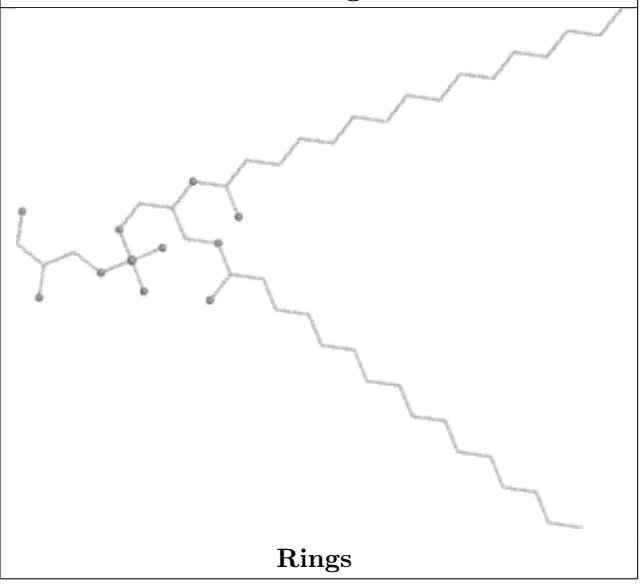
Bond lengths



Bond angles

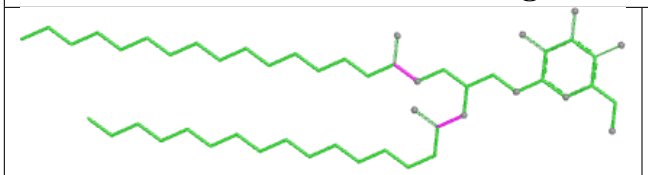


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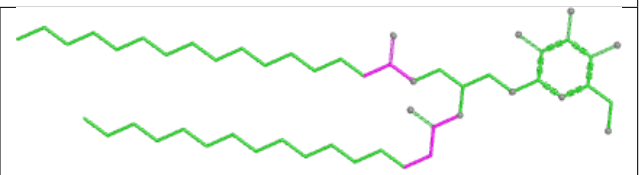


Rings

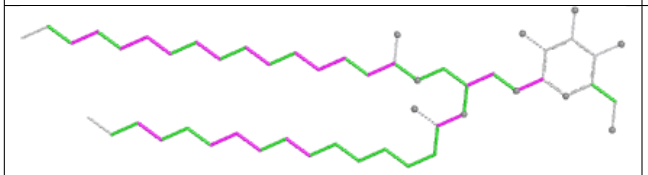
Ligand LMG B 620



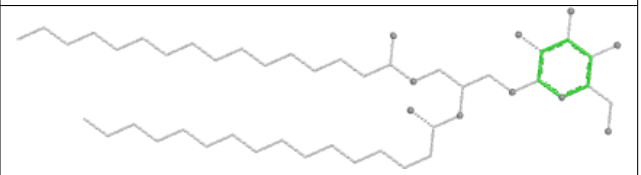
Bond lengths



Bond angles

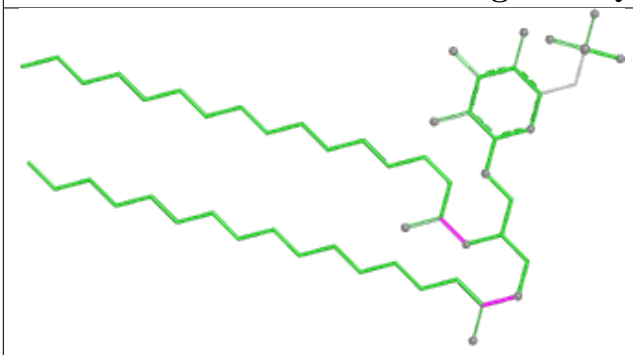


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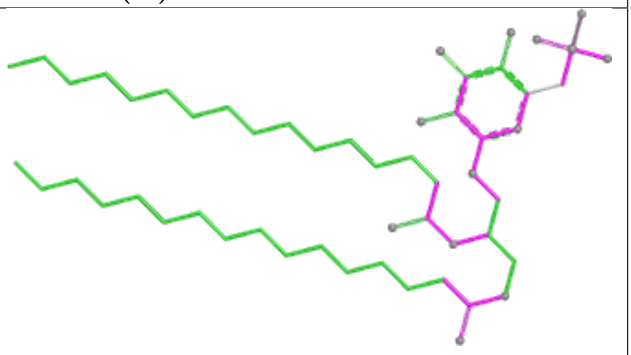


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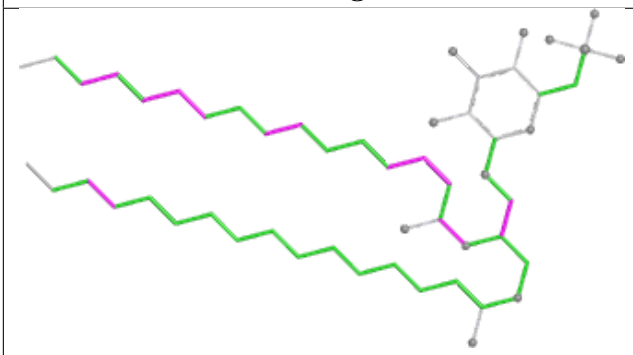
Ligand SQD A 410 (B)



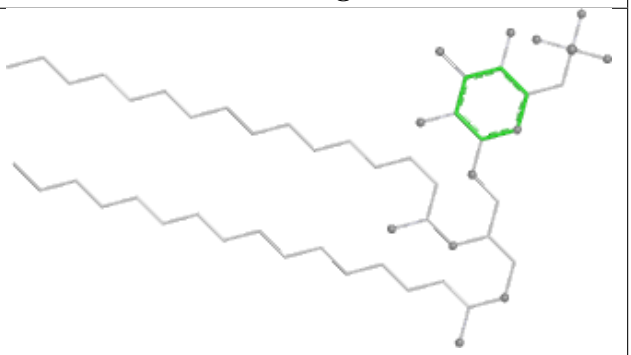
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Bond angles

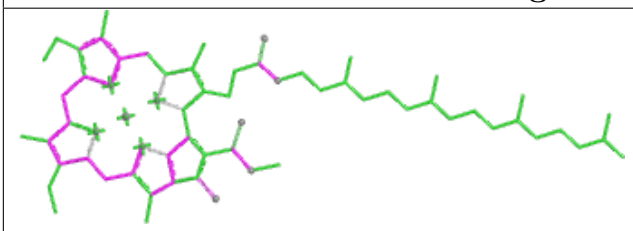


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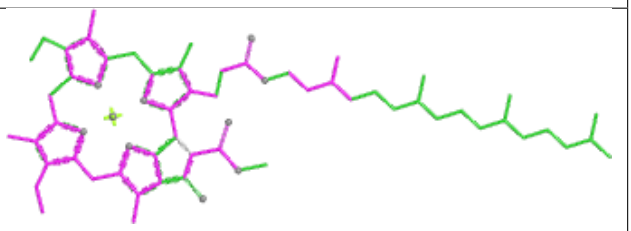


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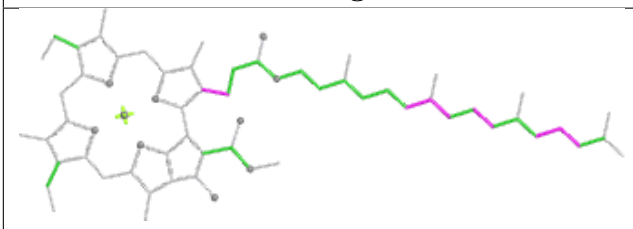
Ligand CLA c 506



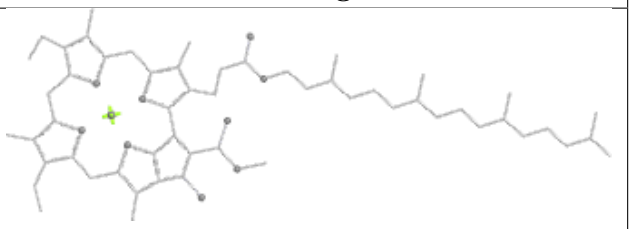
Bond lengths



Bond angles

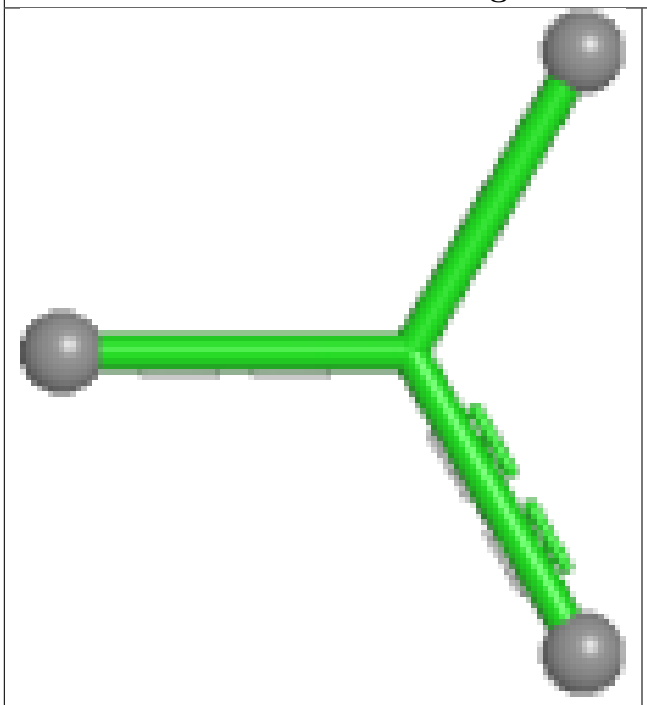


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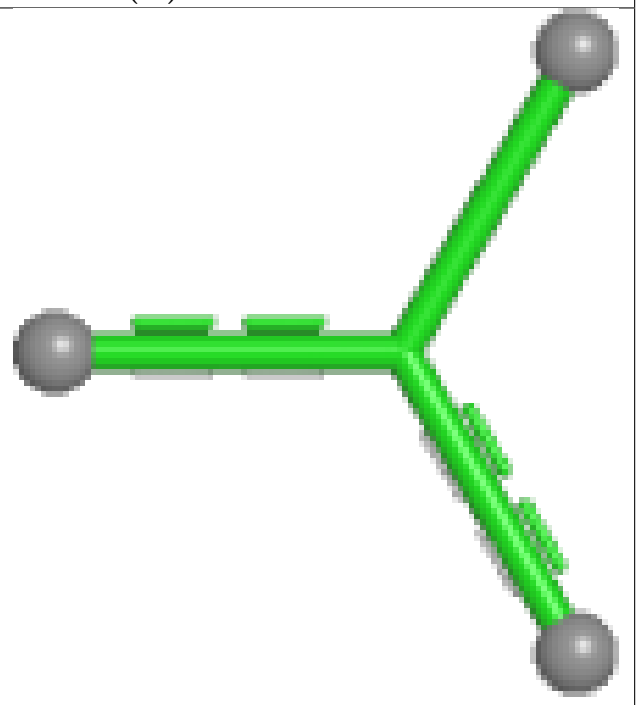


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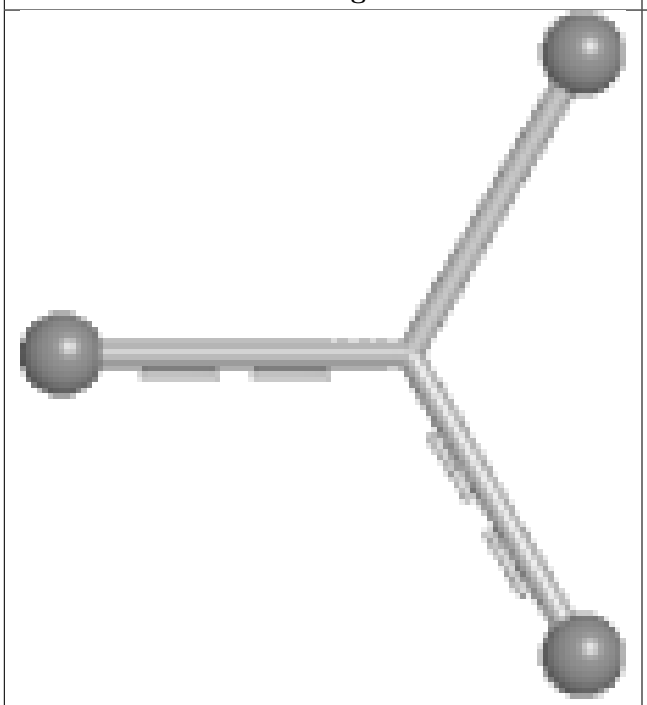
Ligand BCT D 401 (A)



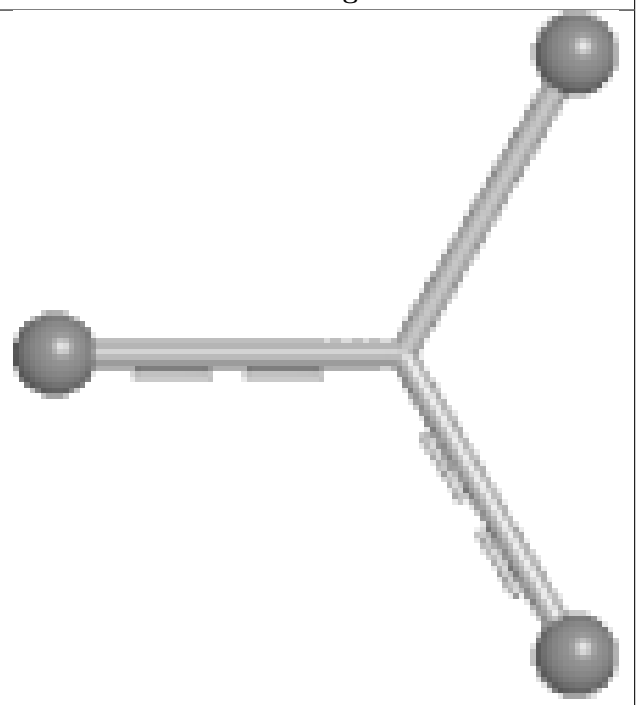
Bond lengths



Bond angles

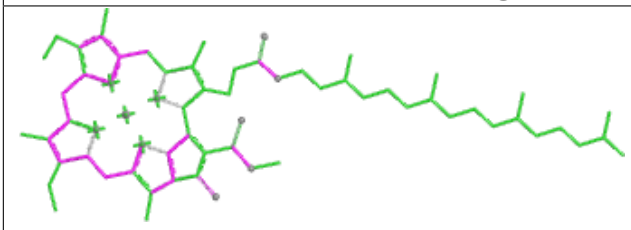


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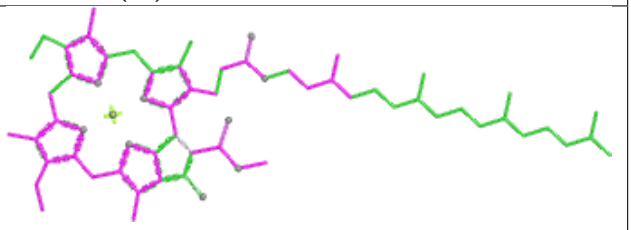


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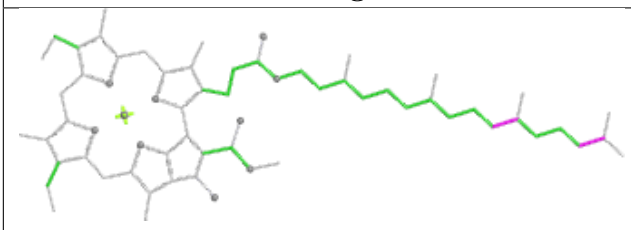
Ligand CLA d 404 (B)



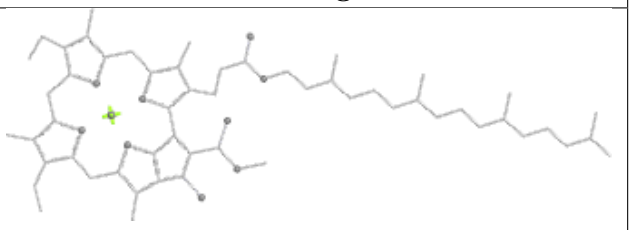
Bond lengths



Bond angles

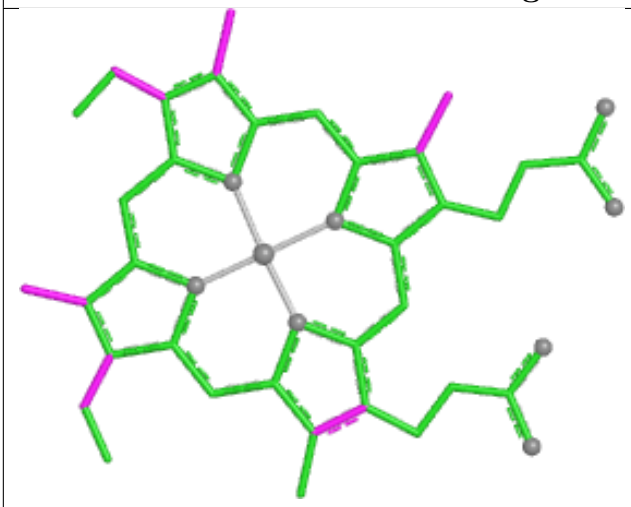


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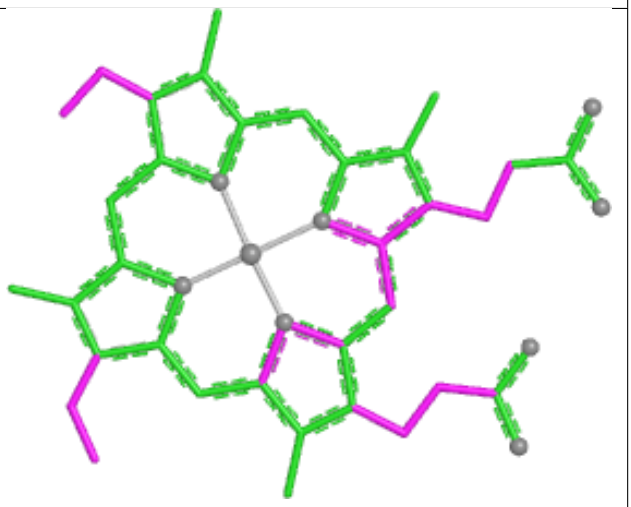


Rings

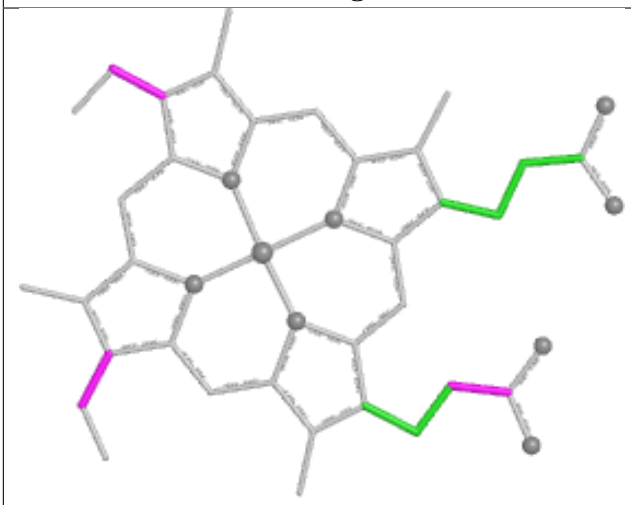
Ligand HEC V 201



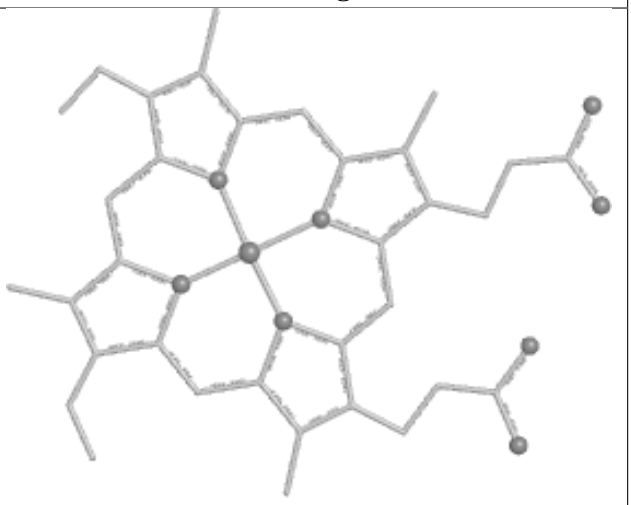
Bond lengths



Bond angles

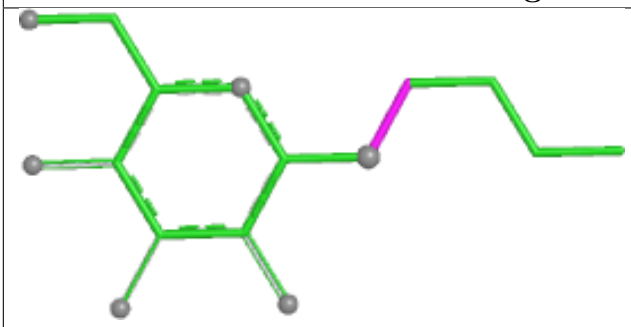


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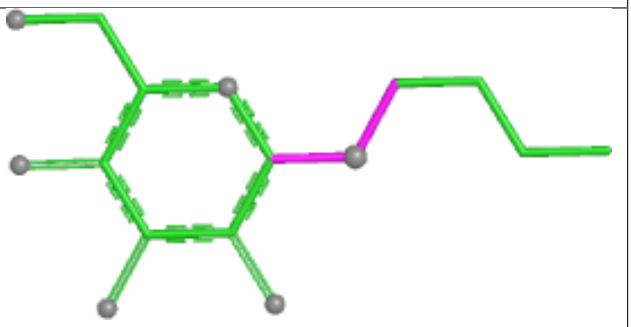


Rings

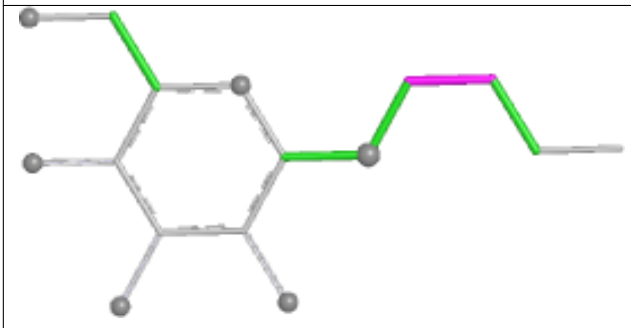
Ligand HTG d 412



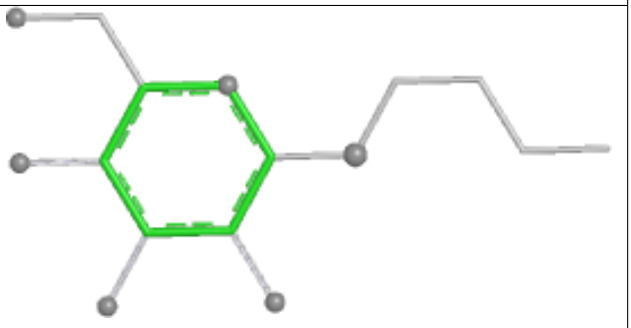
Bond lengths



Bond angles

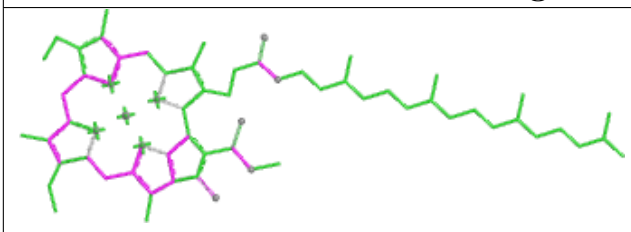


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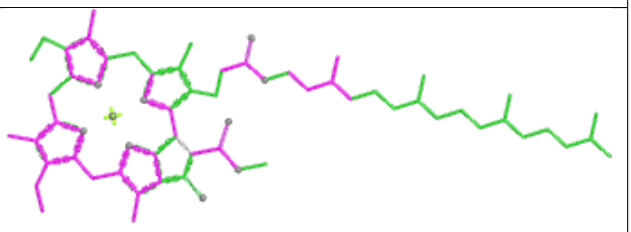


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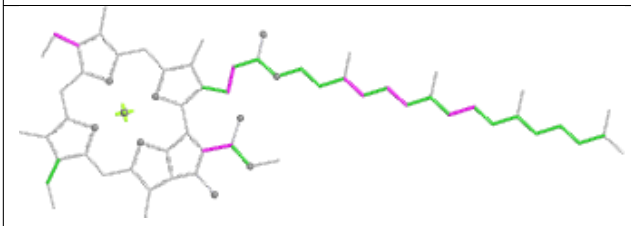
Ligand CLA c 507



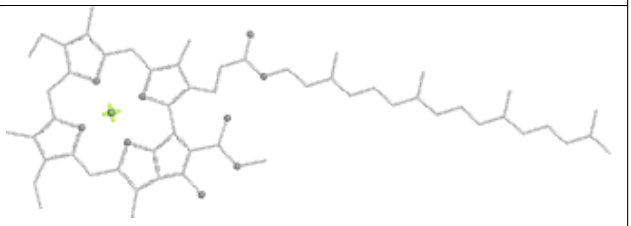
Bond lengths



Bond angles

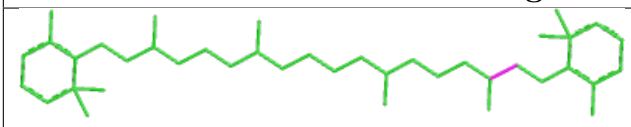


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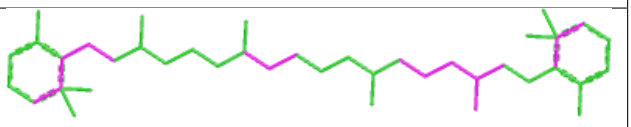


Rings

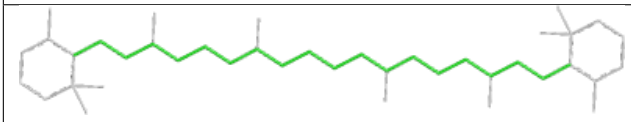
Ligand BCR b 618



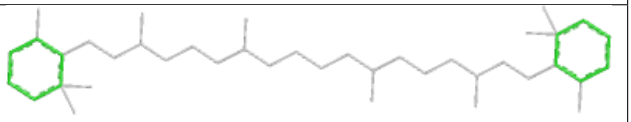
Bond lengths



Bond angles

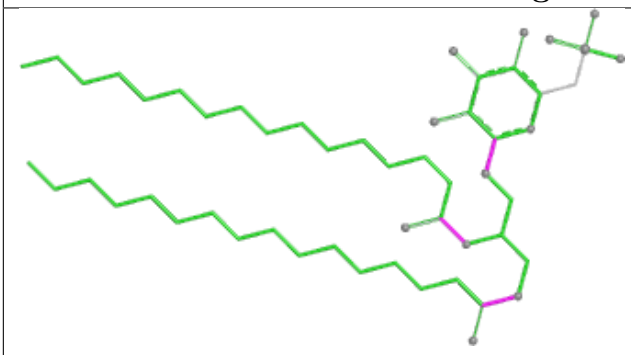


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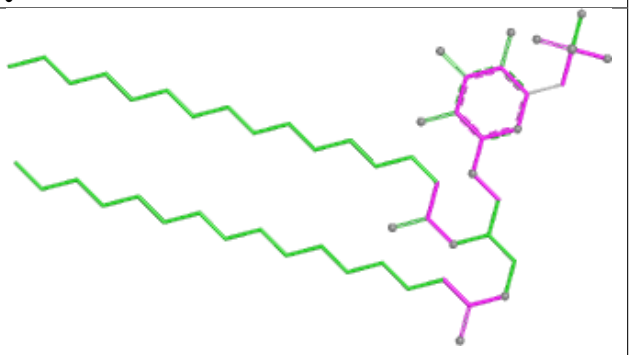


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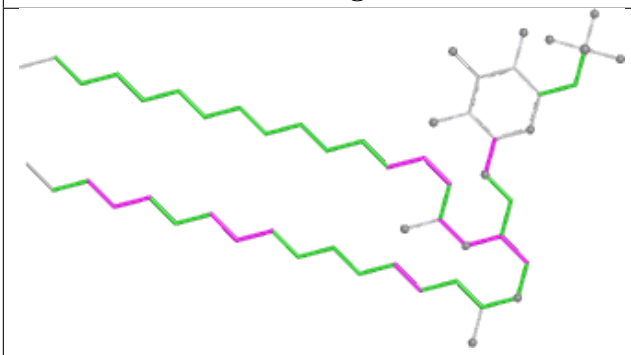
Ligand SQD l 101



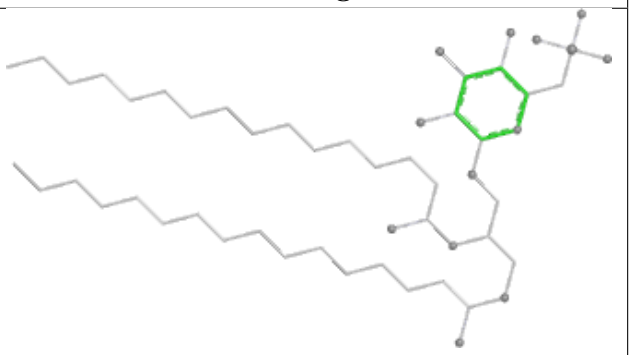
Bond lengths



Bond angles

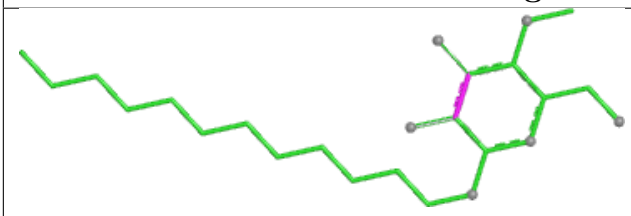


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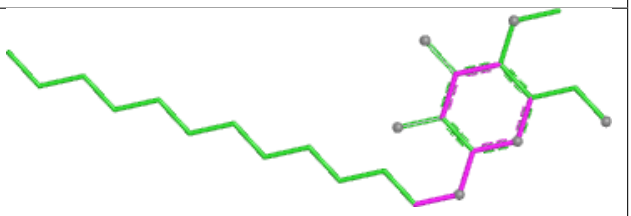


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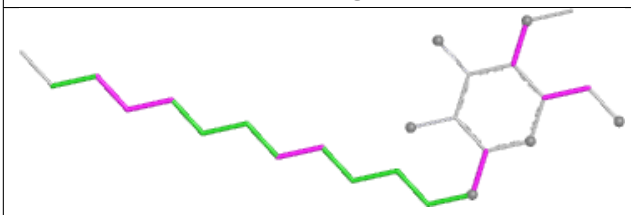
Ligand LMT b 621



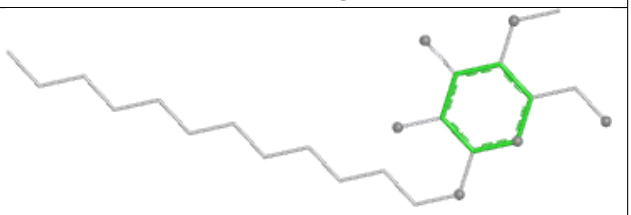
Bond lengths



Bond angles

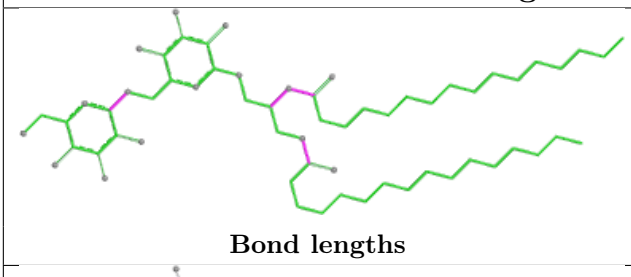


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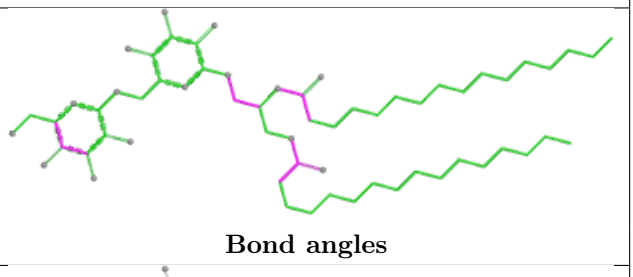


Rings

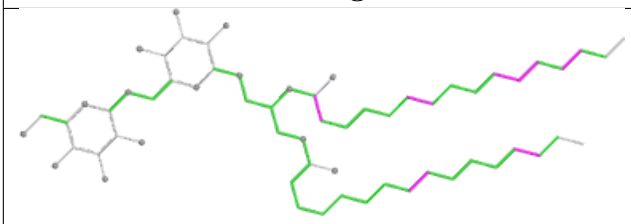
Ligand DGD H 102



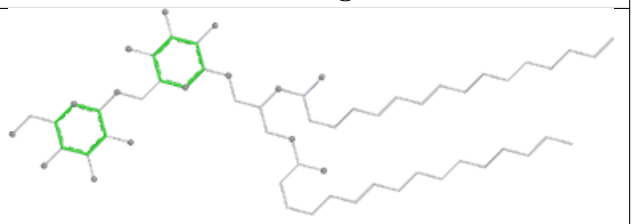
Bond lengths



Bond angles

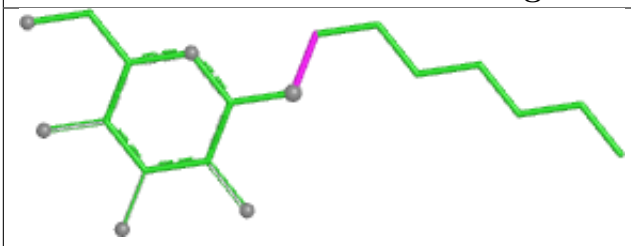


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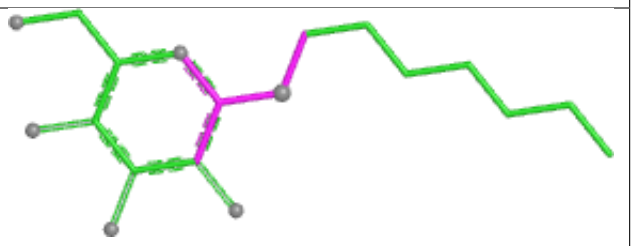


Rings

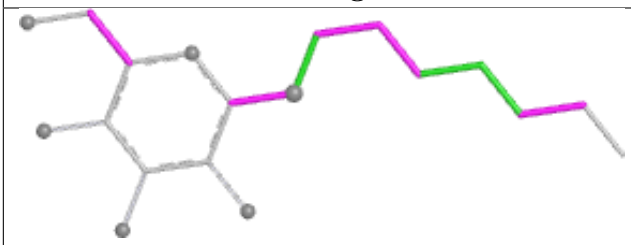
Ligand HTG b 623



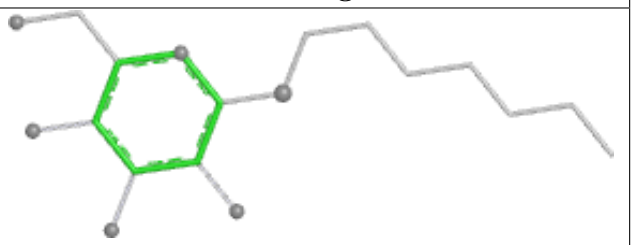
Bond lengths



Bond angles

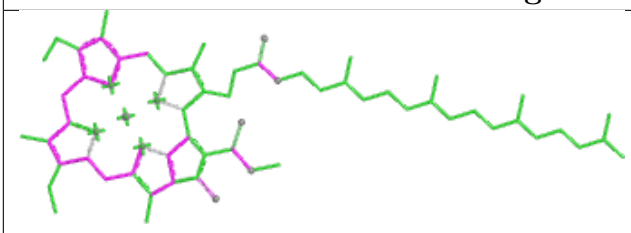


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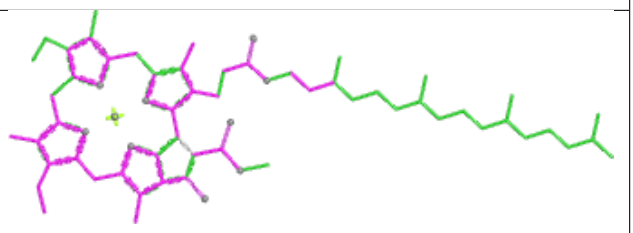


Rings

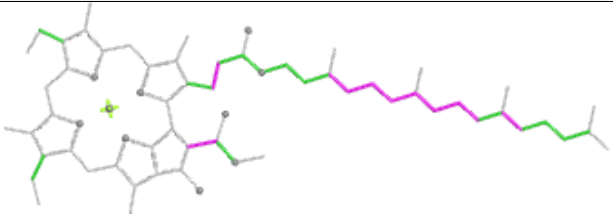
Ligand CLA B 614



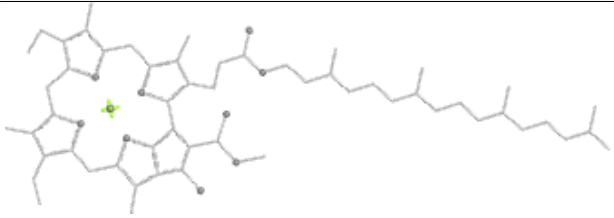
Bond lengths



Bond angles

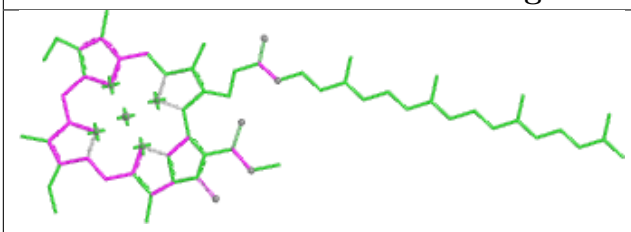


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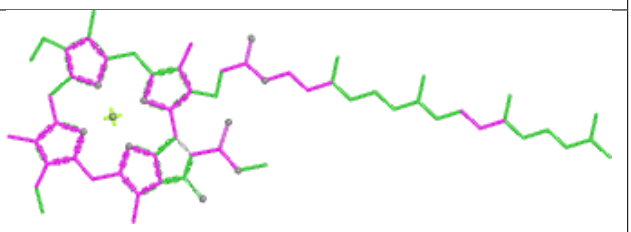


Rings

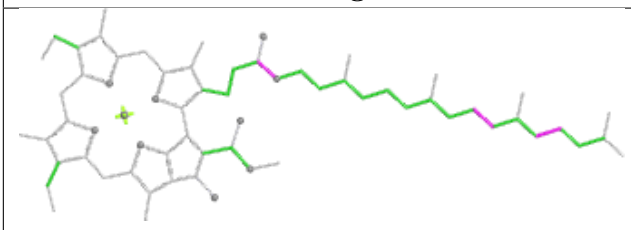
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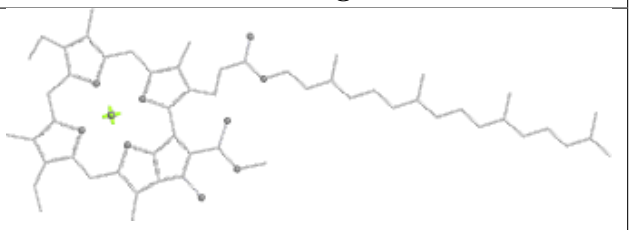
Bond lengths



Bond angles

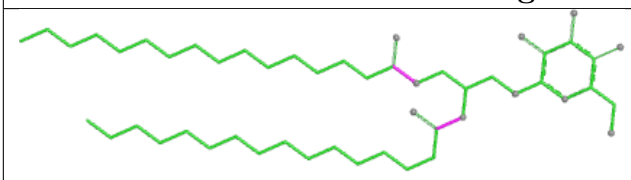


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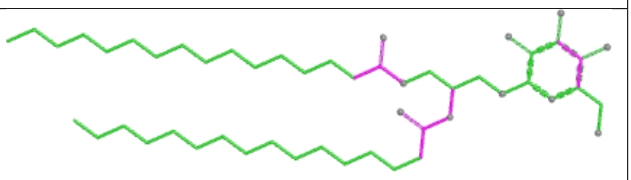


Rings

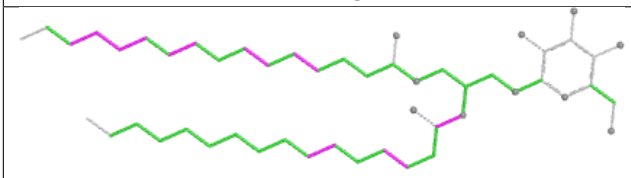
Ligand LMG m 101



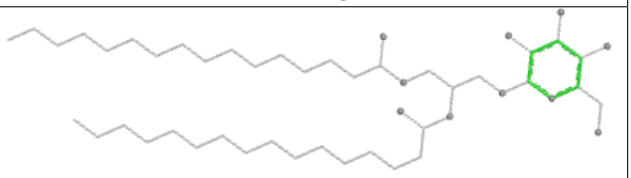
Bond lengths



Bond angles

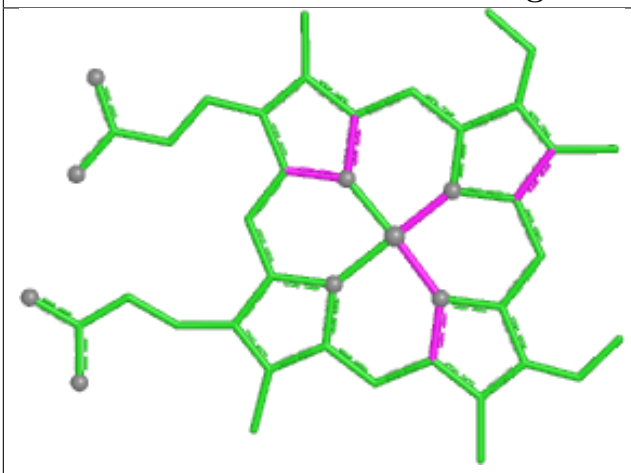


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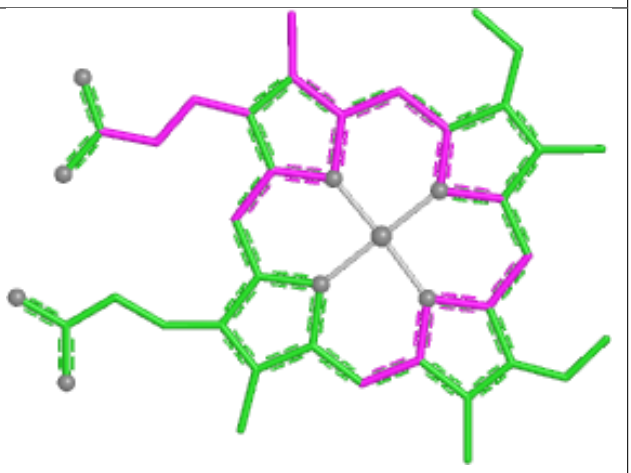


Rings

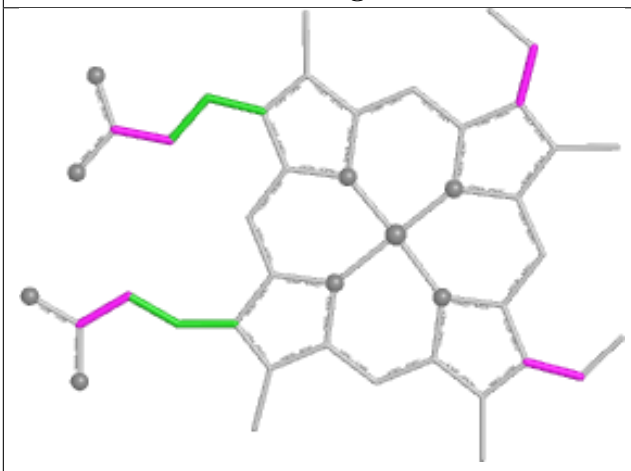
Ligand HEM f 101



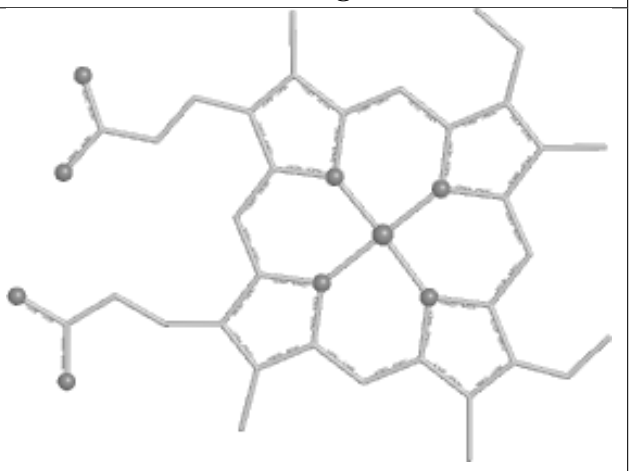
Bond lengths



Bond angles

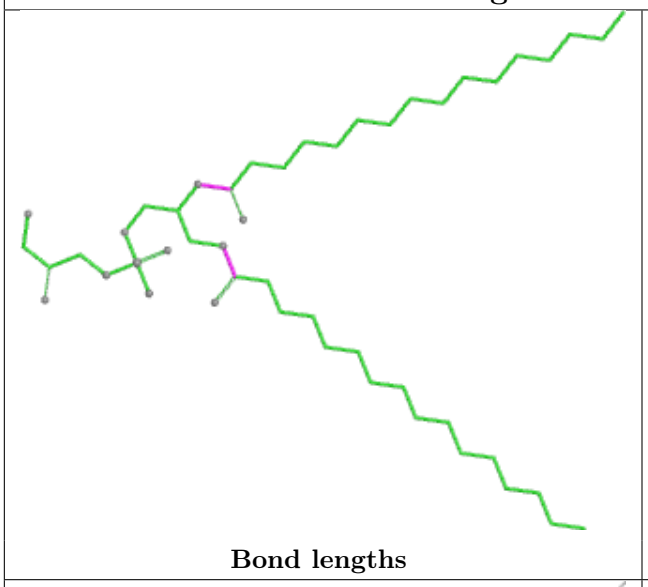


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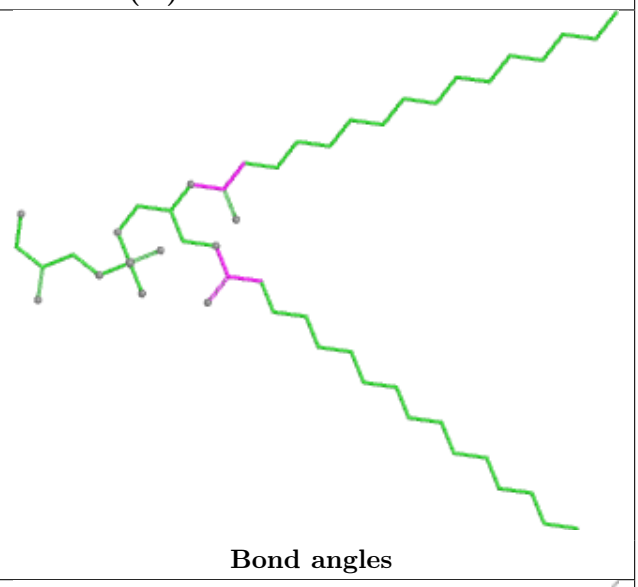


Rings

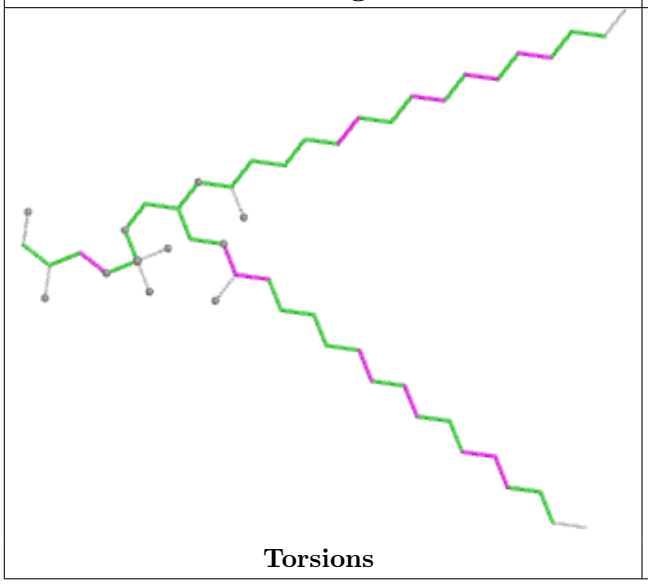
Ligand LHG D 407 (B)



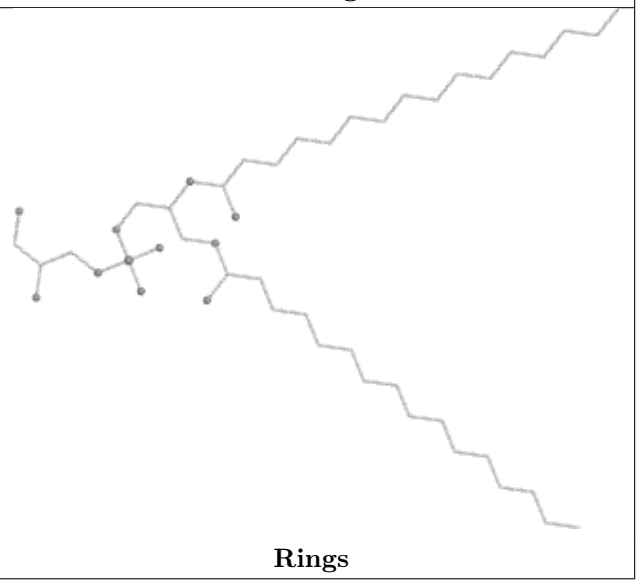
Bond lengths



Bond angles

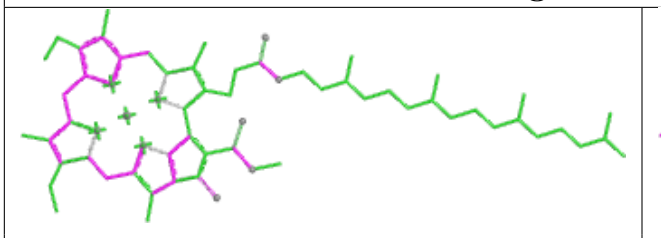


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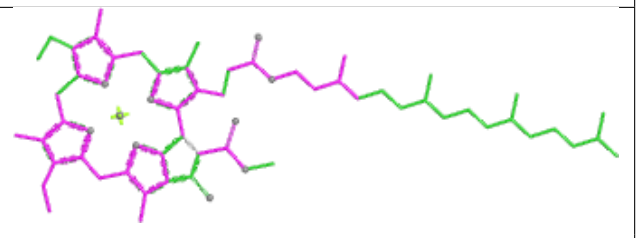


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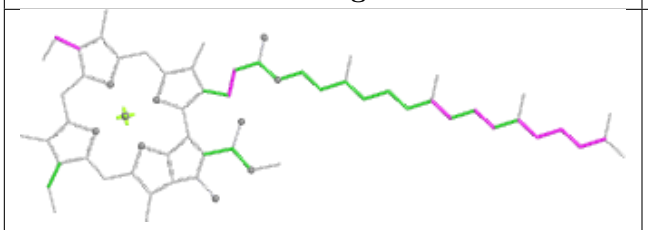
Ligand CLA b 606



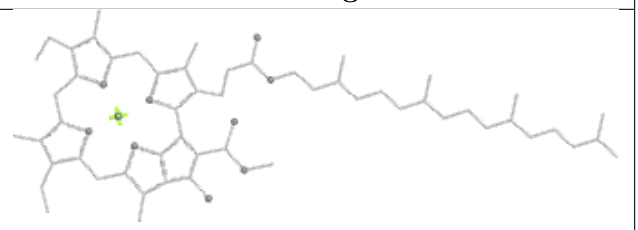
Bond lengths



Bond angles

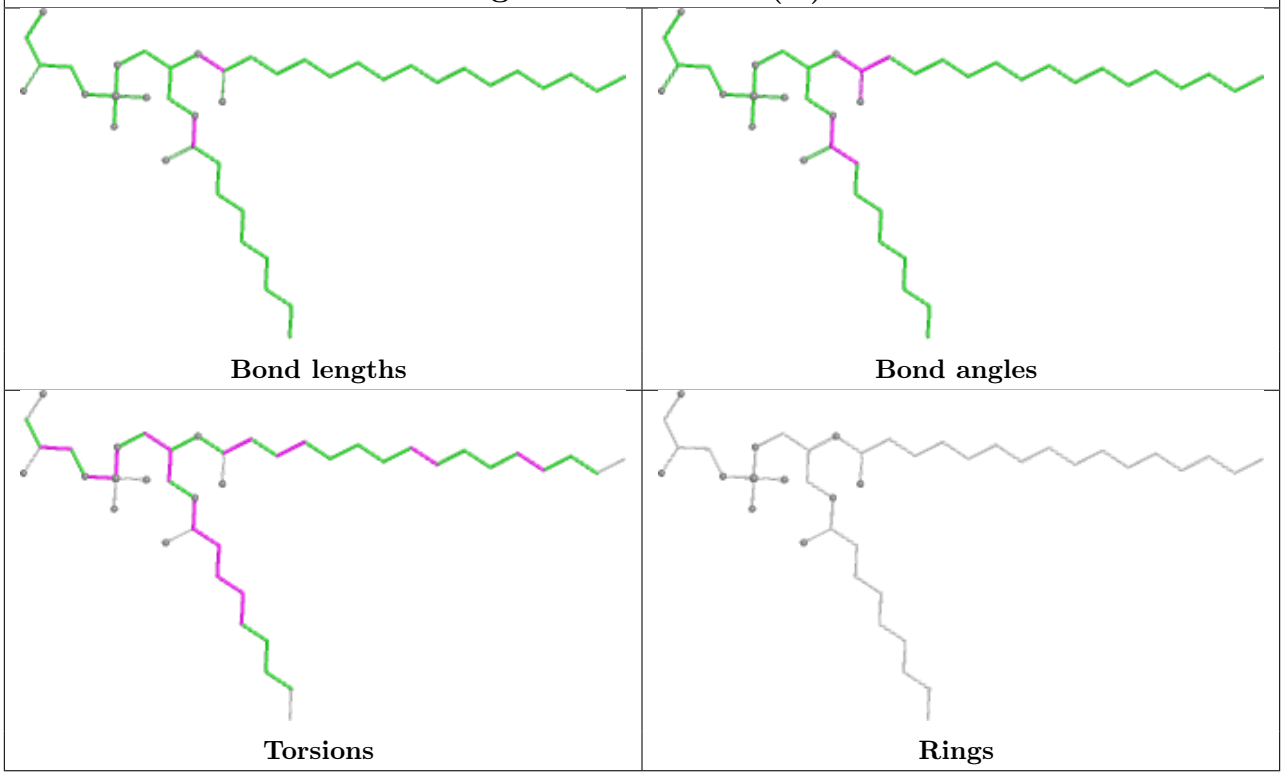


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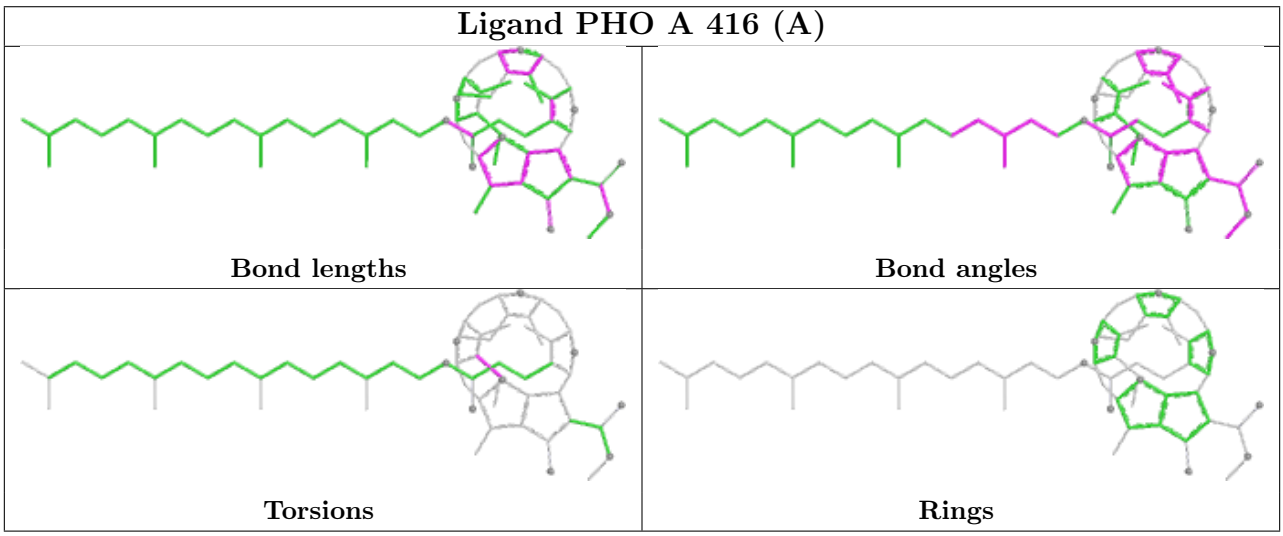


Rings

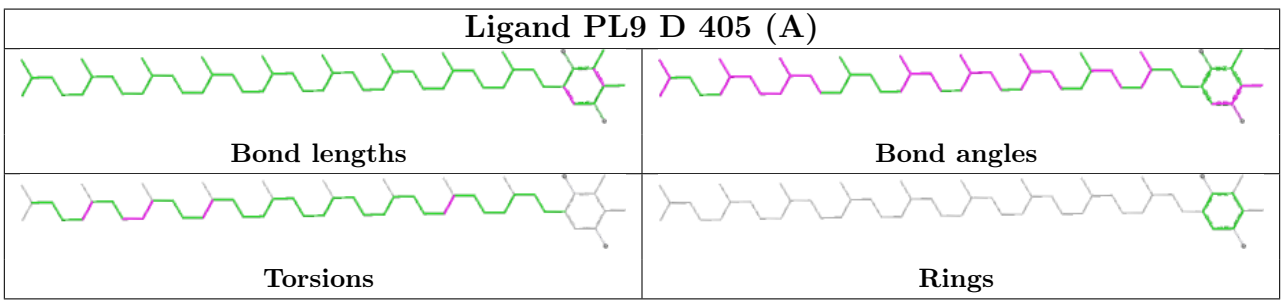
Ligand LHG E 101 (A)



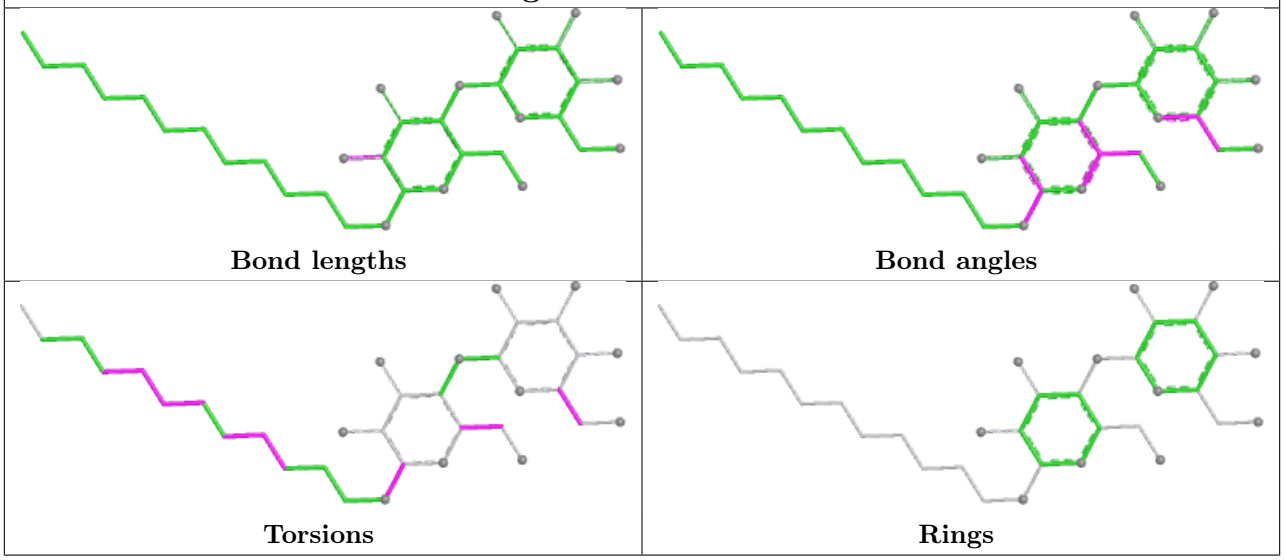
Ligand PHO A 416 (A)



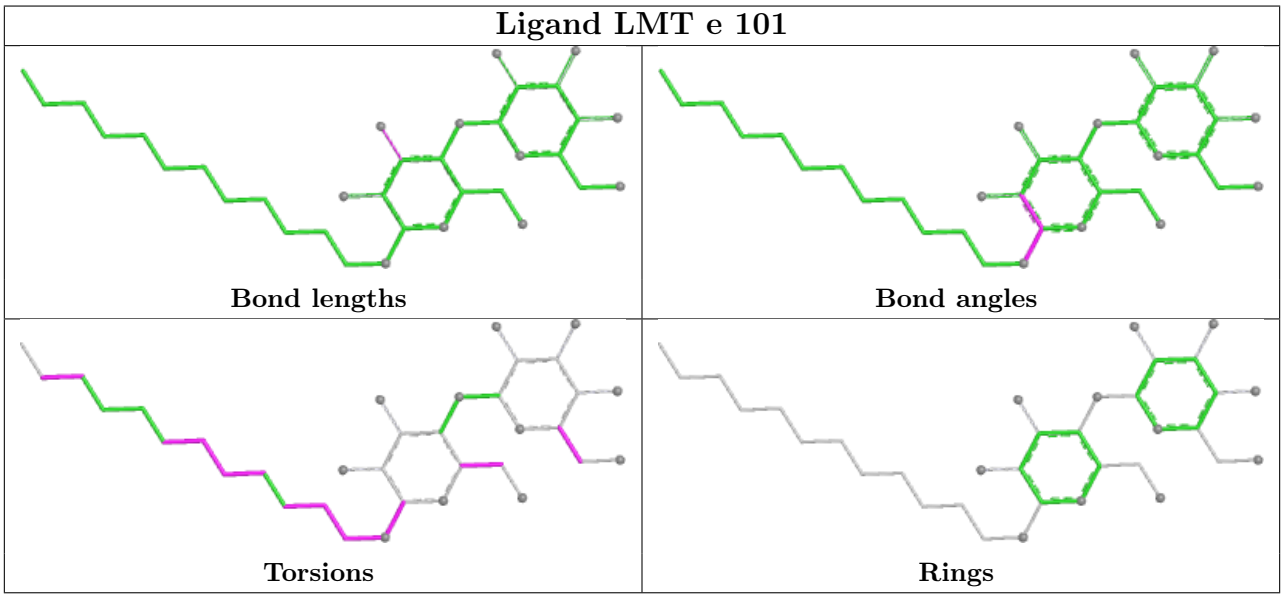
Ligand PL9 D 405 (A)



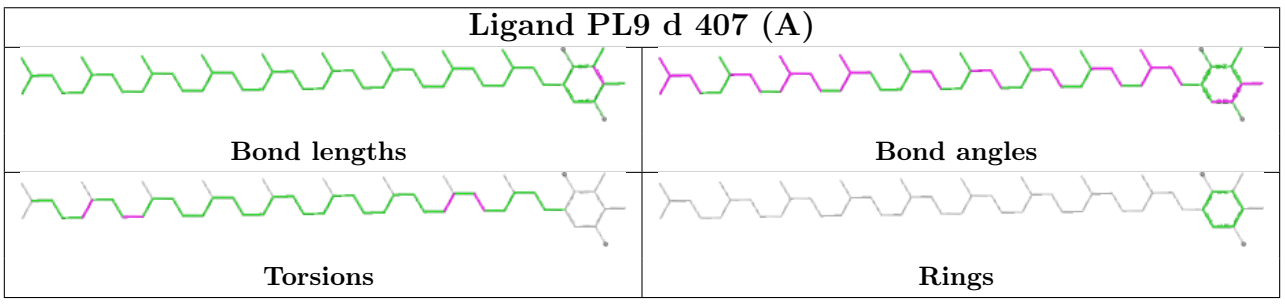
Ligand LMT B 628



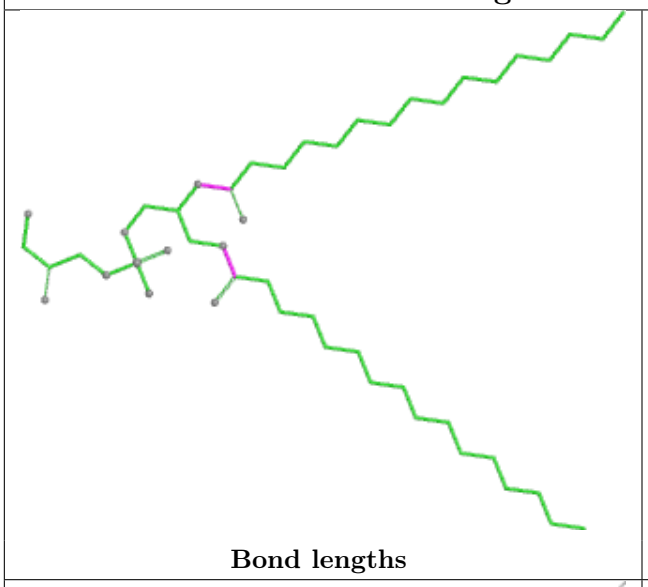
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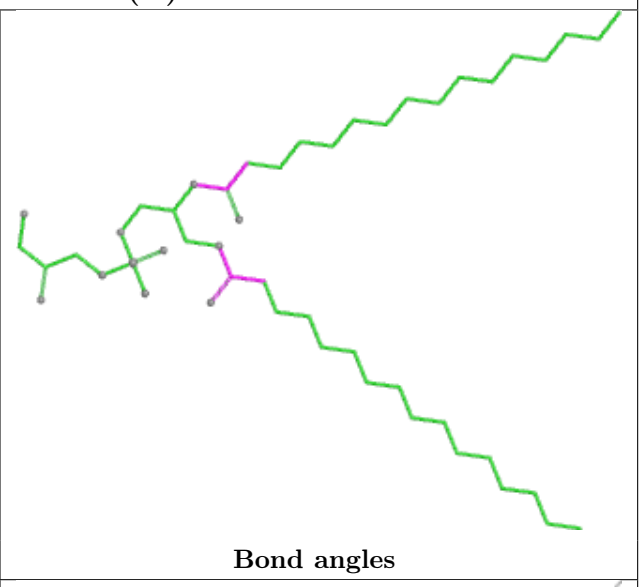
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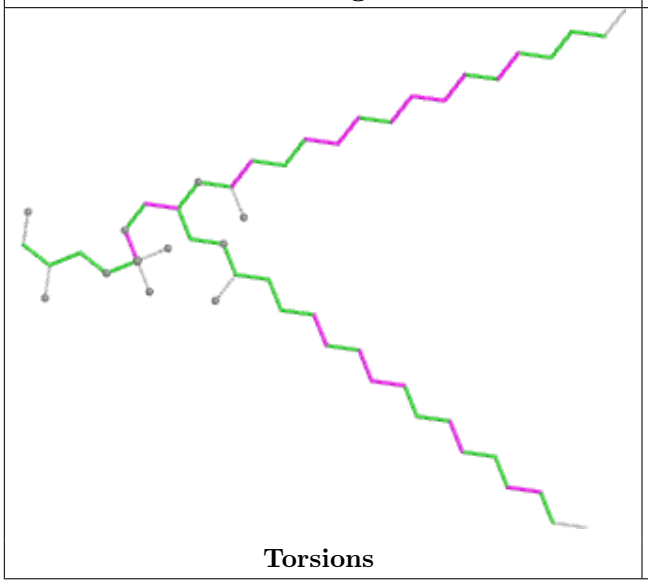
Ligand LHG b 629 (B)



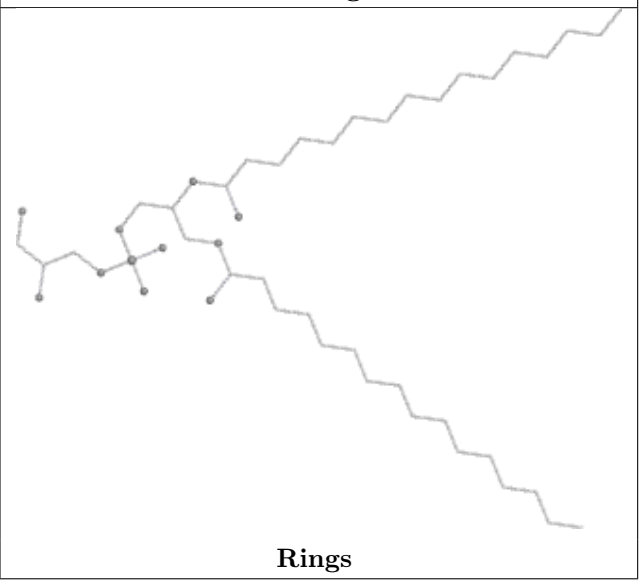
Bond lengths



Bond angles

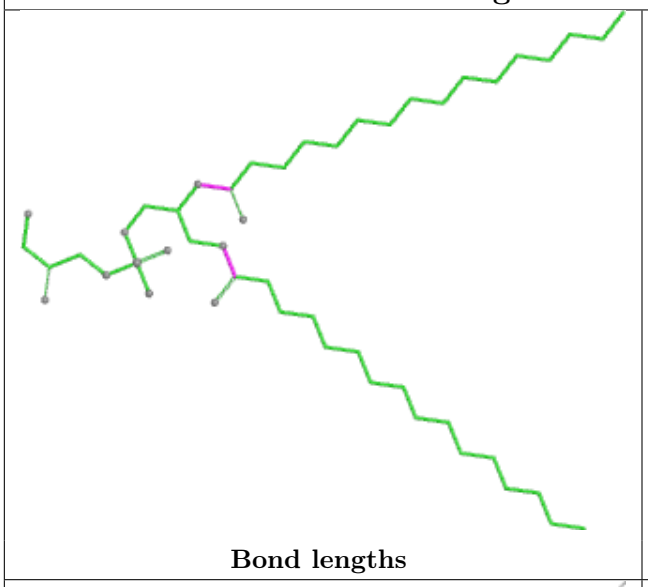


Torsions

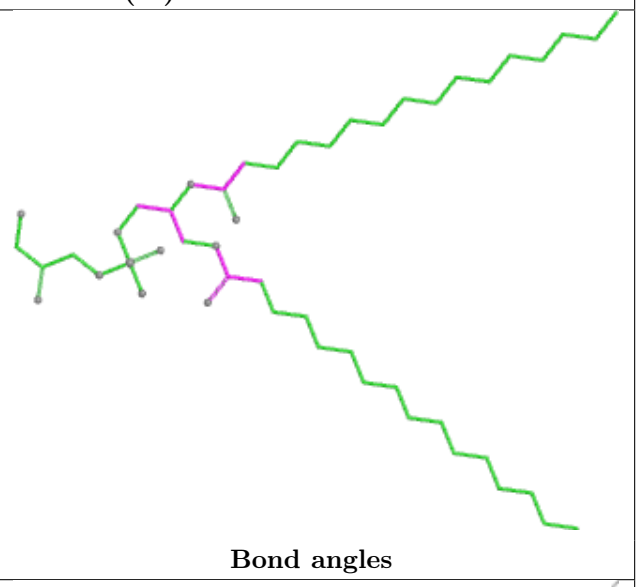


Rings

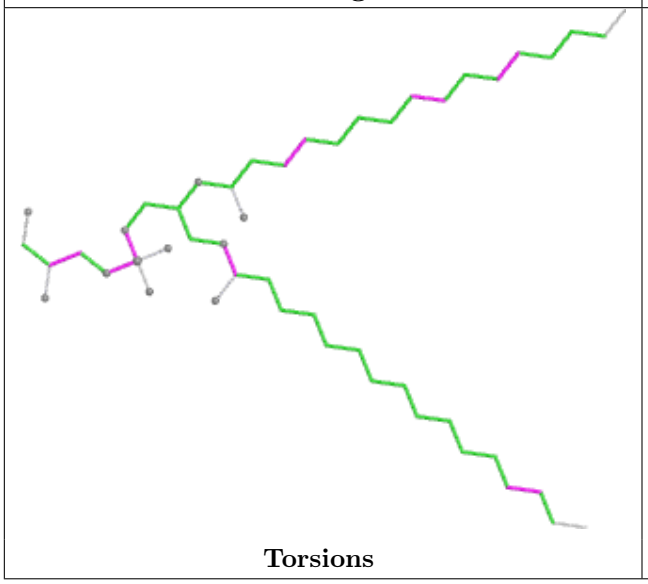
Ligand LHG d 408 (A)



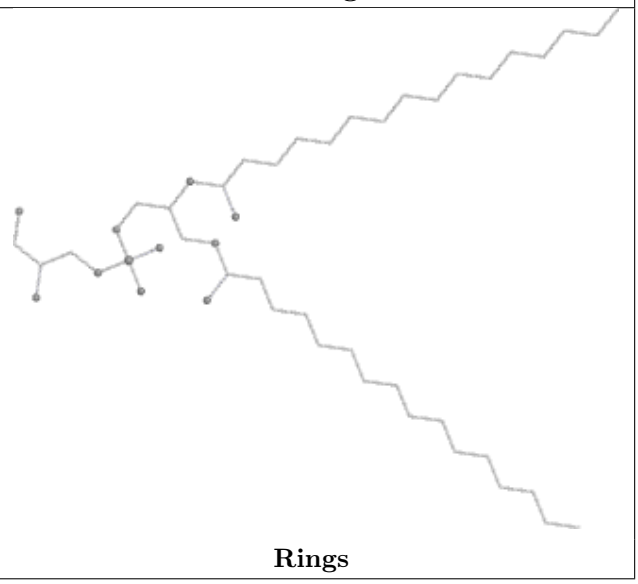
Bond lengths



Bond angles

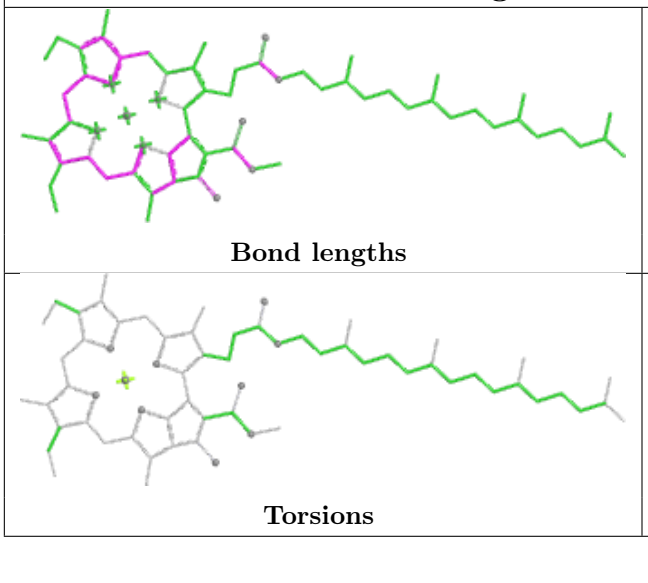


Torsions

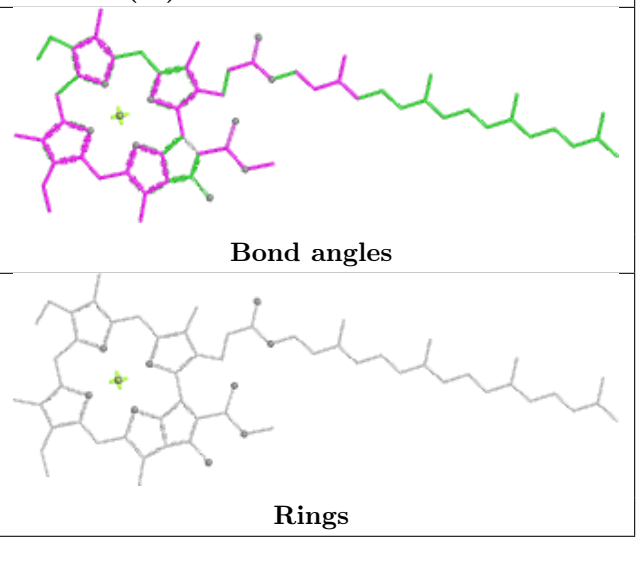


Rings

Ligand CLA D 402 (A)



Bond lengths

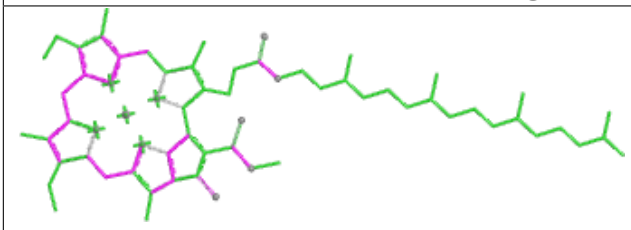


Bond angles

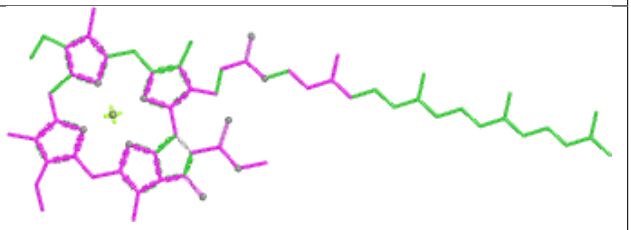
Torsions

Rings

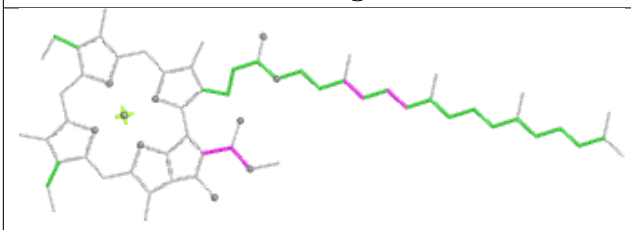
Ligand CLA B 605



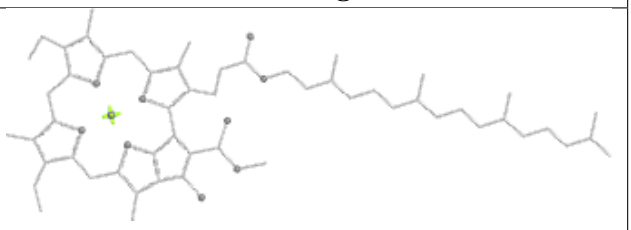
Bond lengths



Bond angles

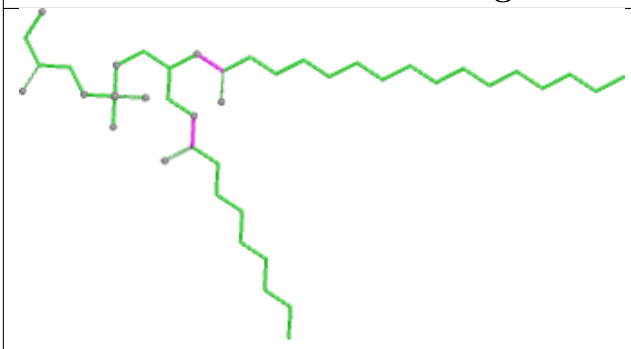


Torsions

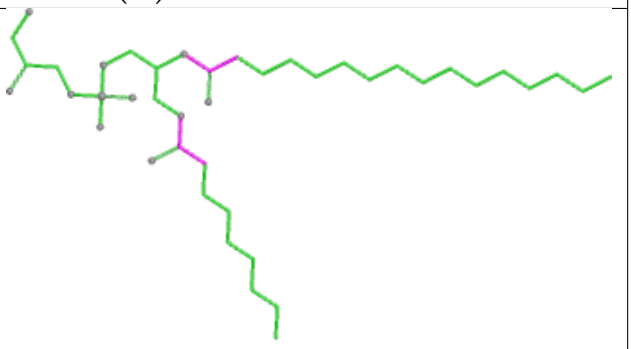


Rings

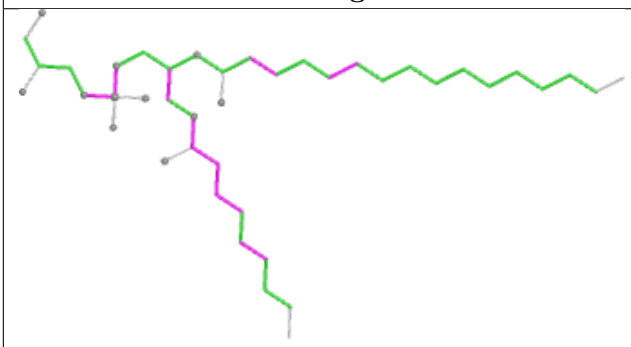
Ligand LHG a 419 (B)



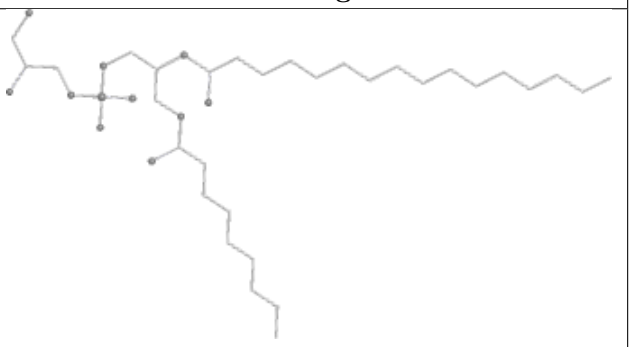
Bond lengths



Bond angles

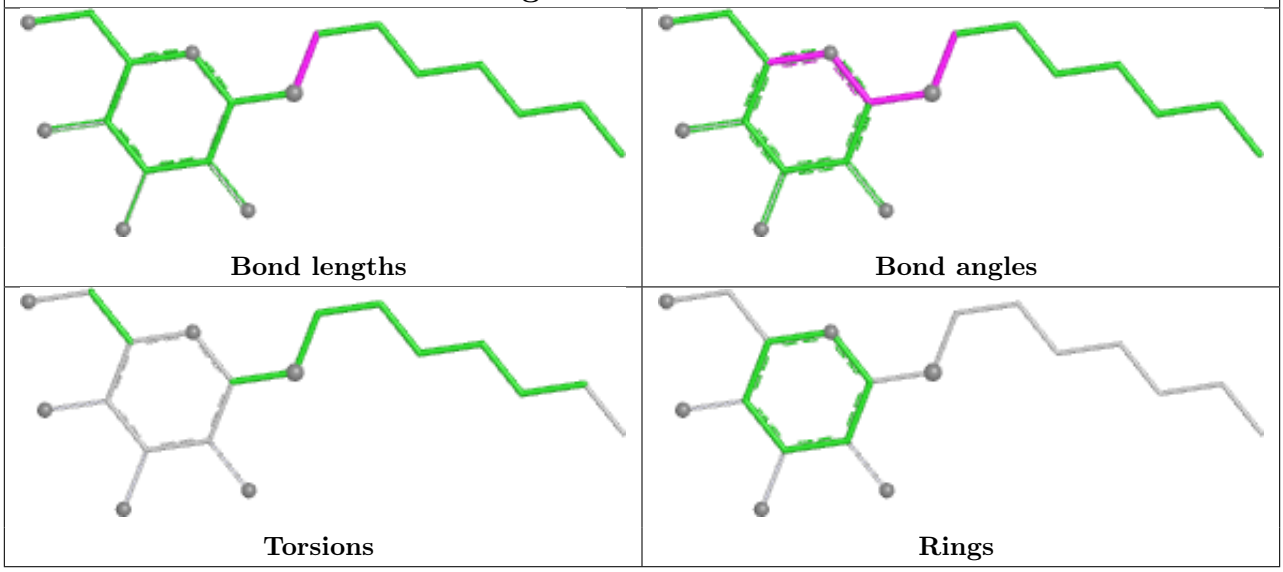


Torsions

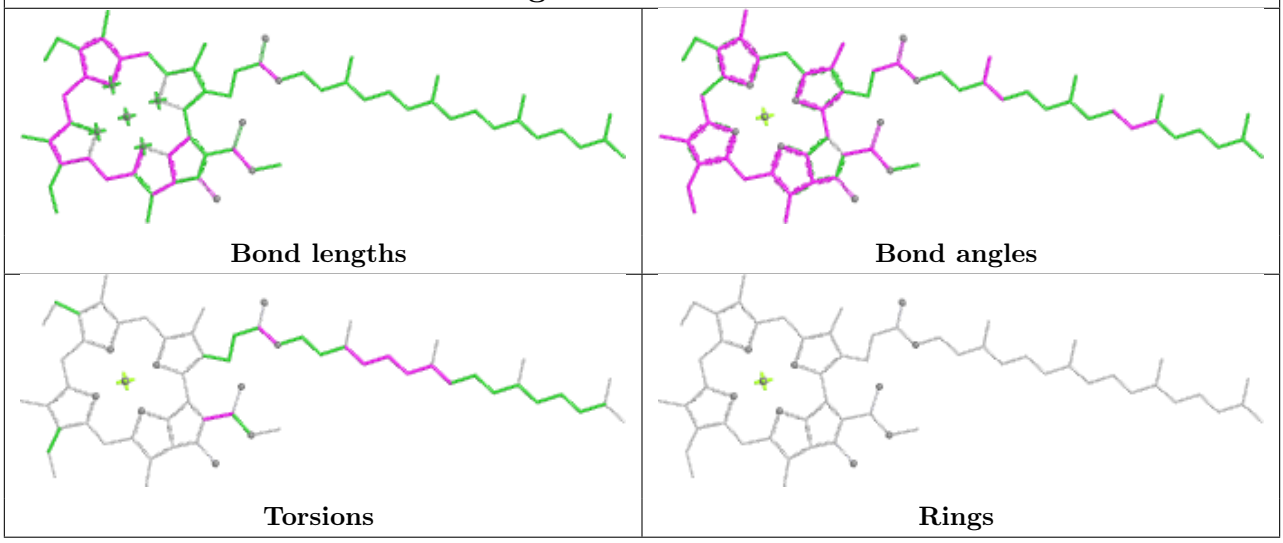


Rings

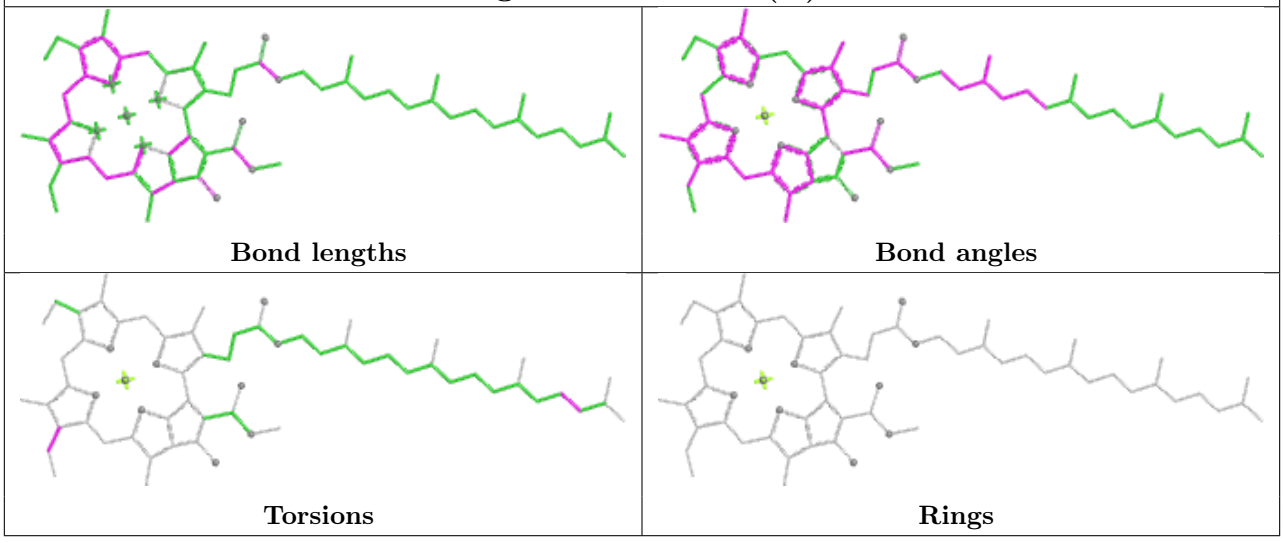
Ligand HTG C 522



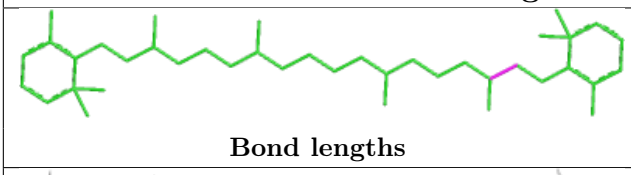
Ligand CLA b 616



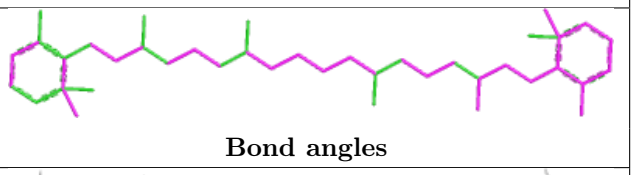
Ligand CLA a 404 (A)



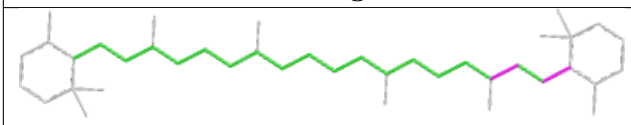
Ligand BCR D 404



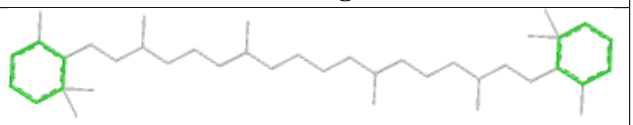
Bond lengths



Bond angles

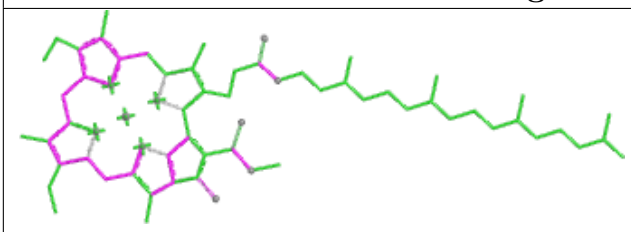


Torsions

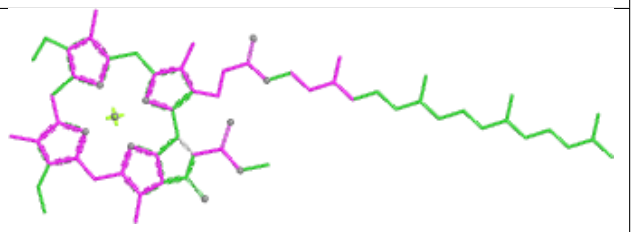


Rings

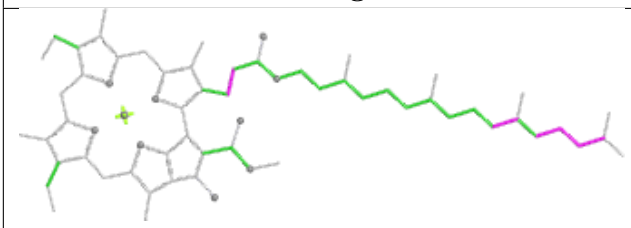
Ligand CLA b 610



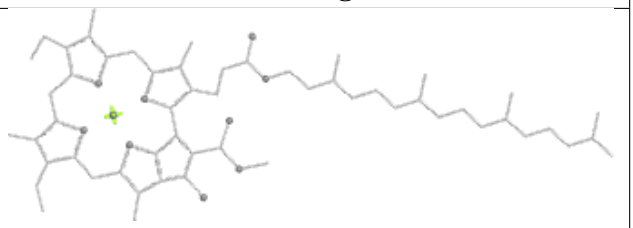
Bond lengths



Bond angles

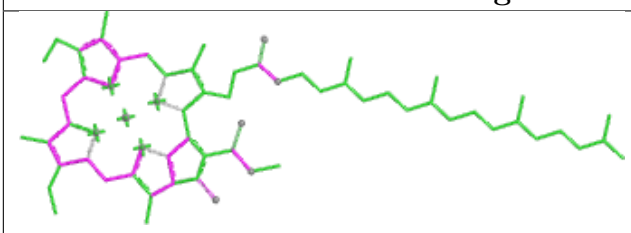


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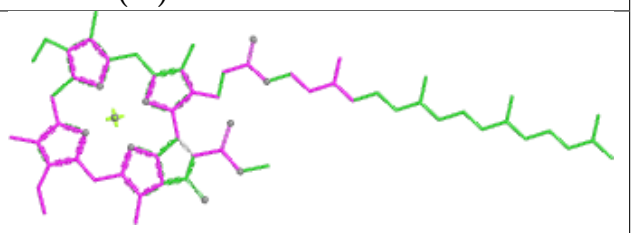


Rings

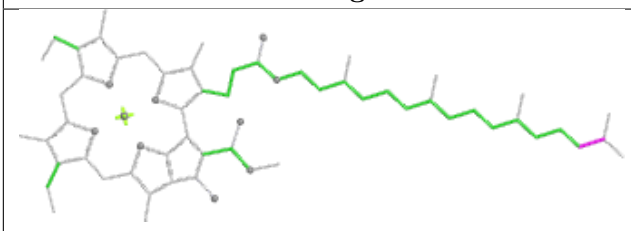
Ligand CLA d 404 (A)



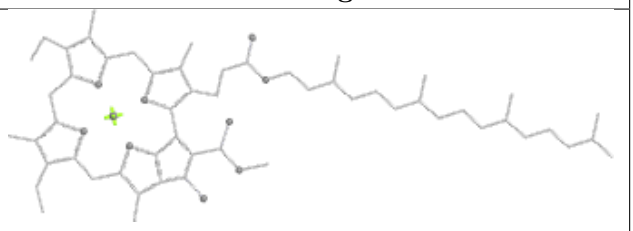
Bond lengths



Bond angles

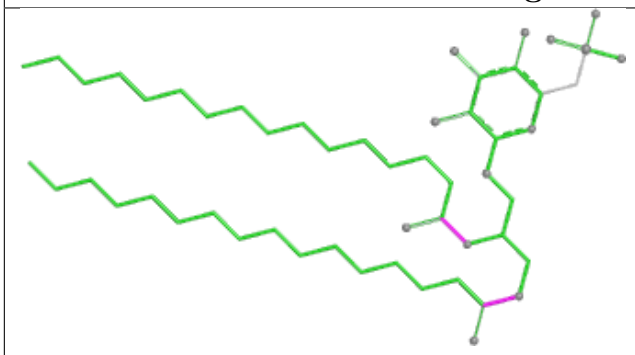


Torsions

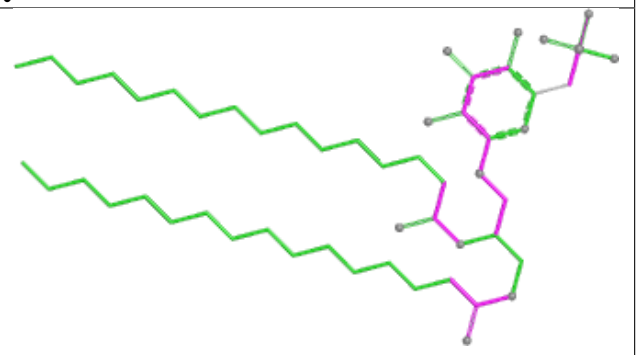


Rings

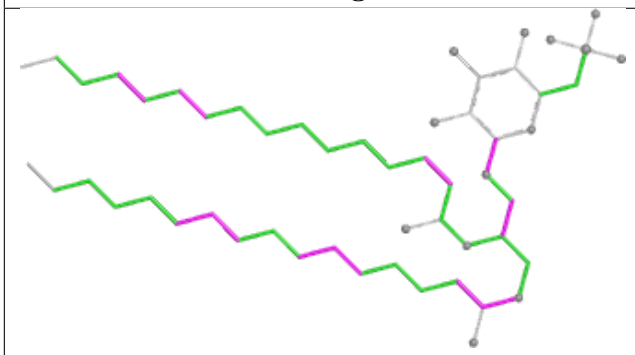
Ligand SQD A 412



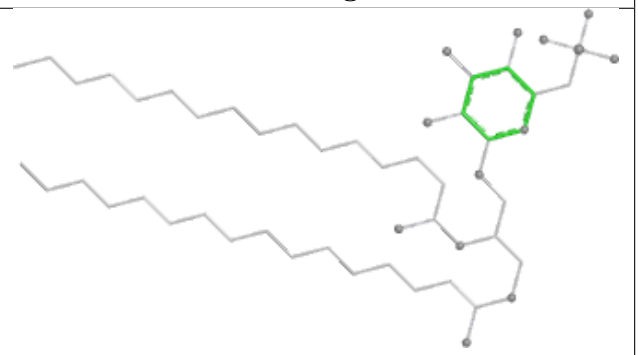
Bond lengths



Bond angles

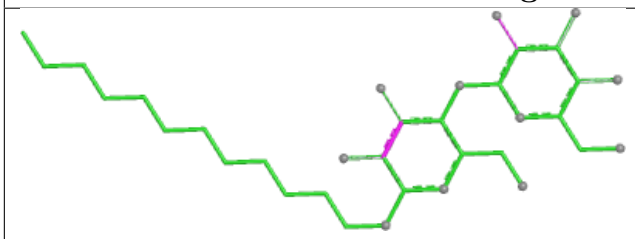


Torsions

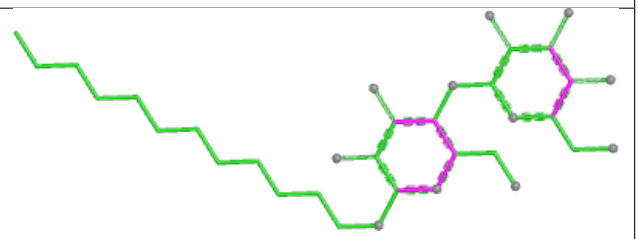


Rings

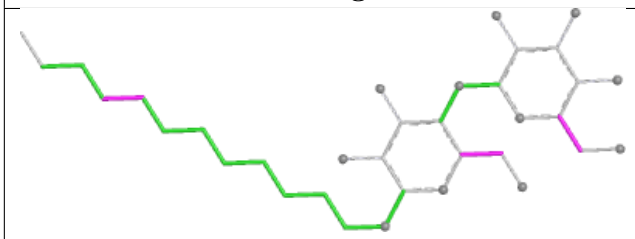
Ligand LMT m 103



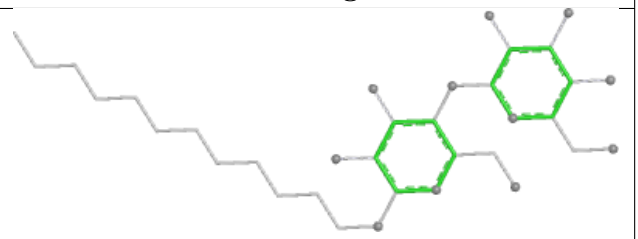
Bond lengths



Bond angles

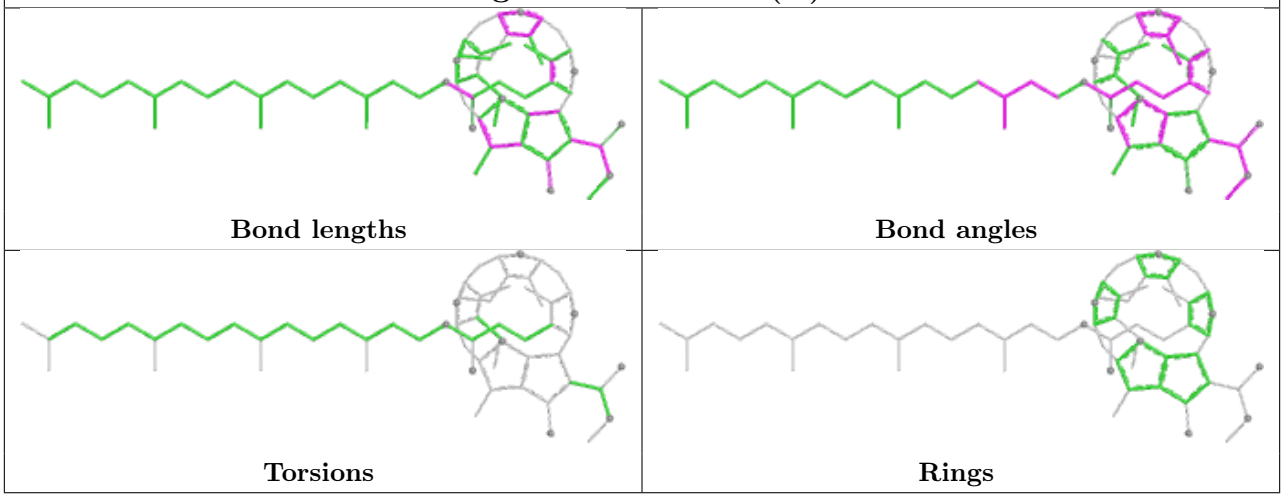


Torsions

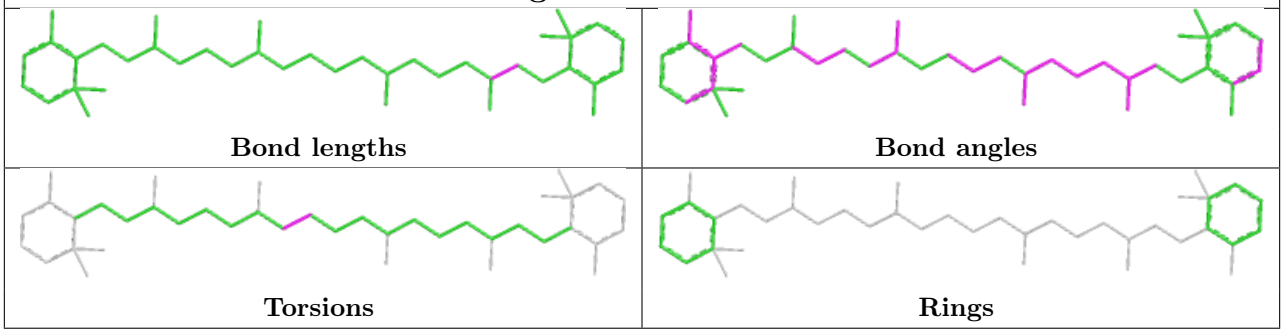


Rings

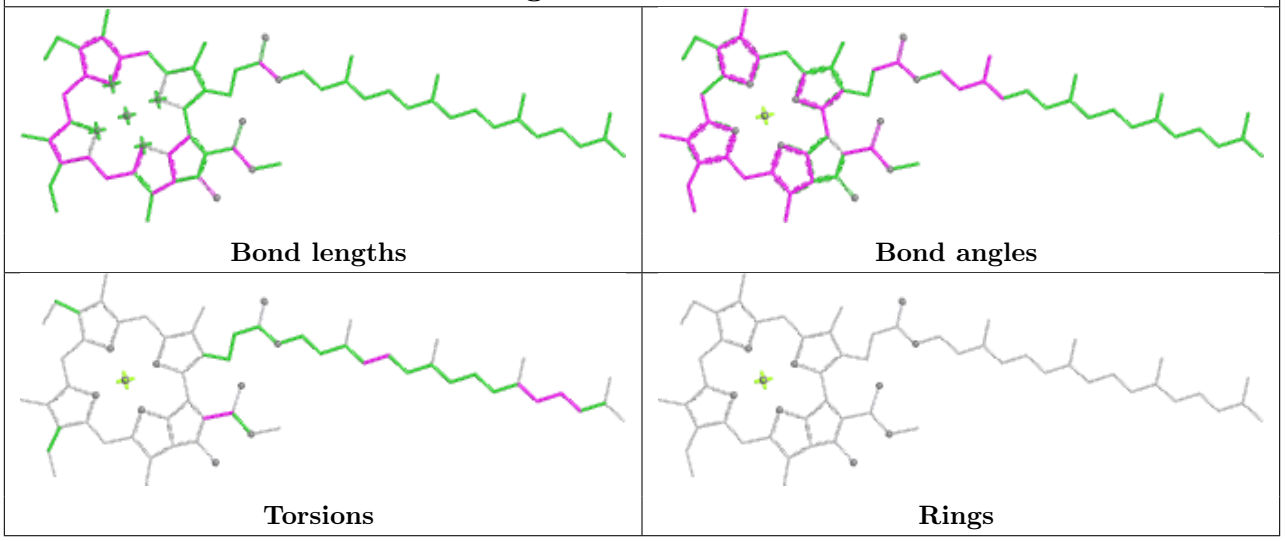
Ligand PHO d 403 (A)



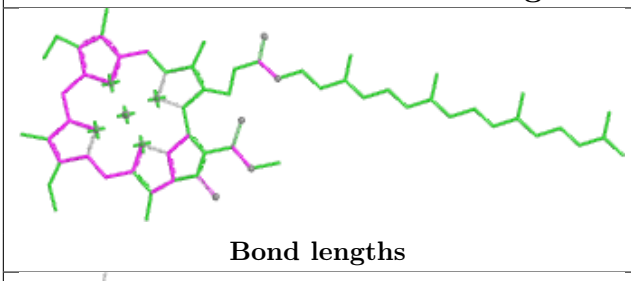
Ligand BCR t 102



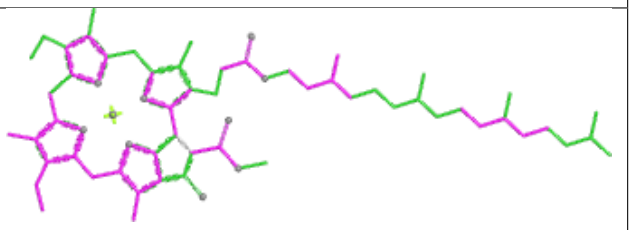
Ligand CLA C 503



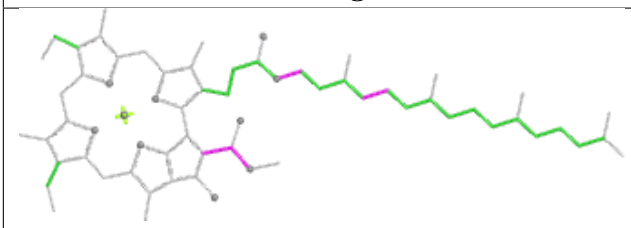
Ligand CLA C 510



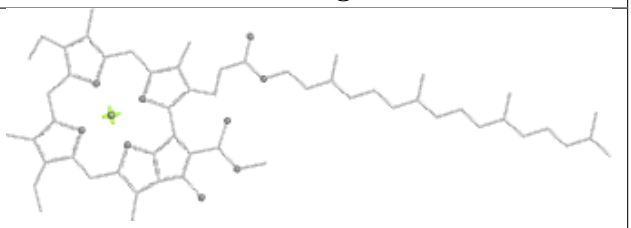
Bond lengths



Bond angles

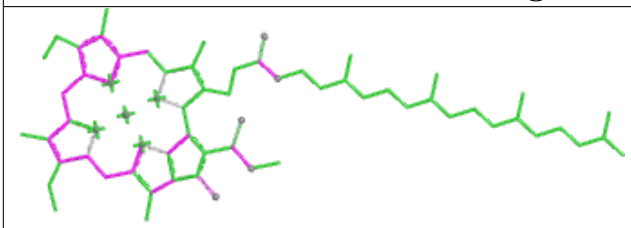


Torsions

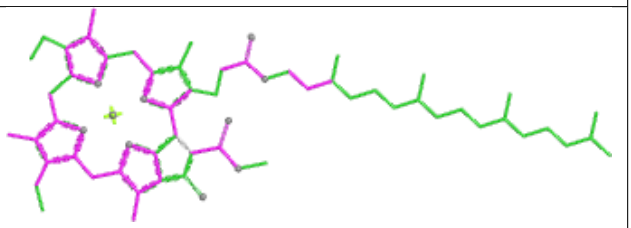


Rings

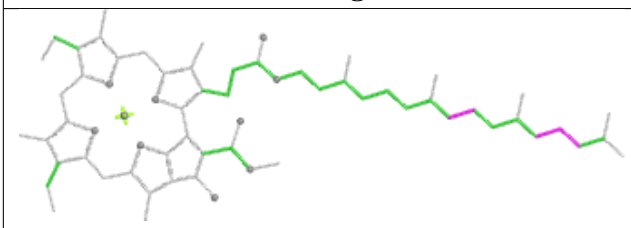
Ligand CLA b 611



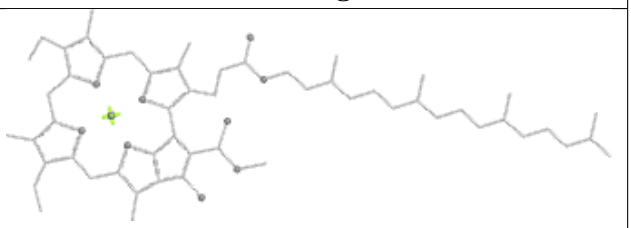
Bond lengths



Bond angles

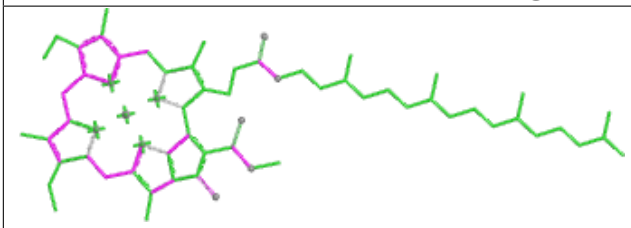


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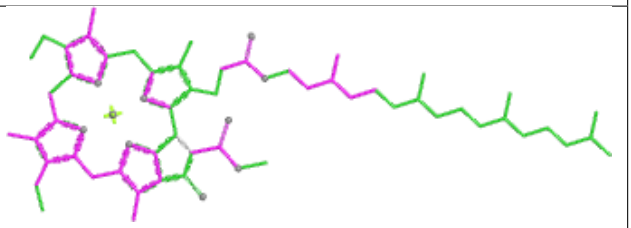


Rings

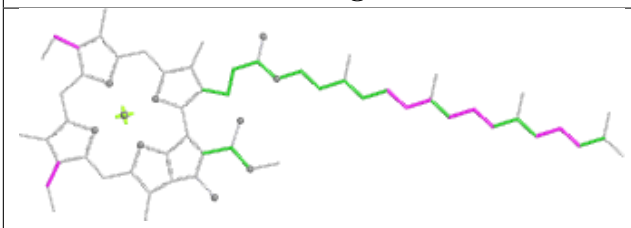
Ligand CLA b 604



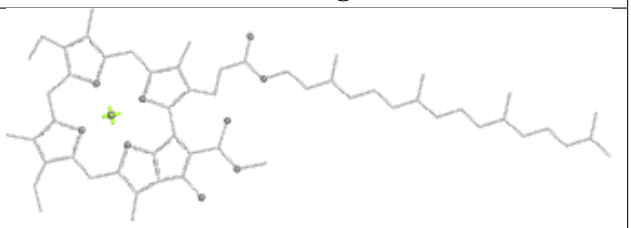
Bond lengths



Bond angles

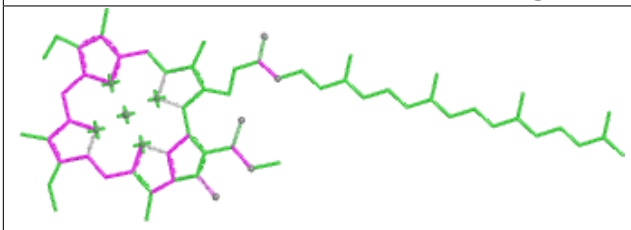


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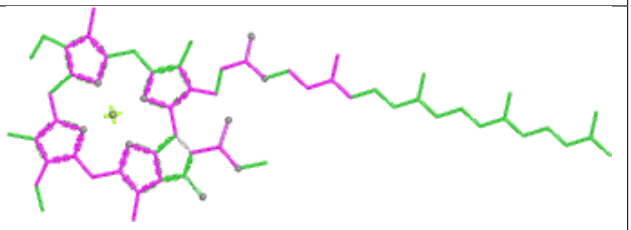


Rings

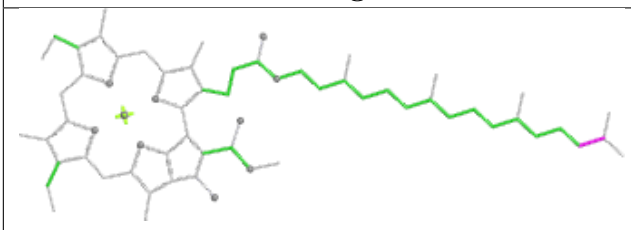
Ligand CLA c 508



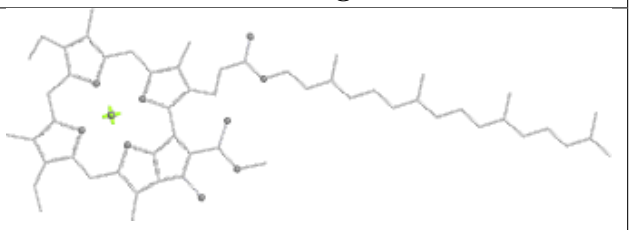
Bond lengths



Bond angles

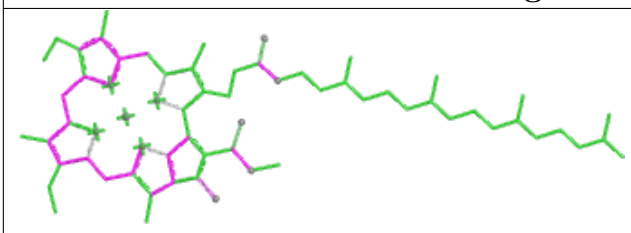


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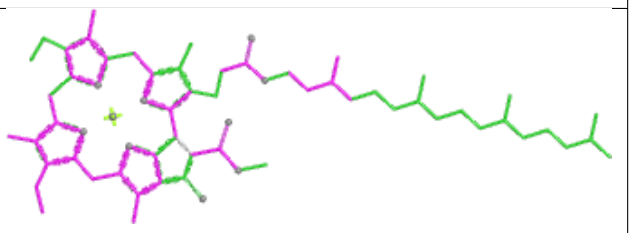


Rings

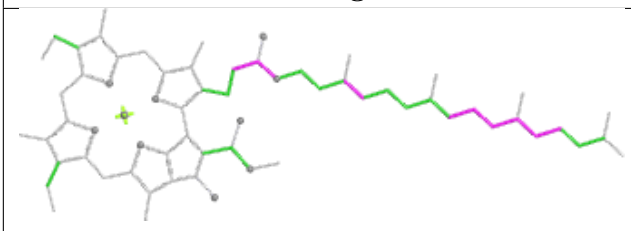
Ligand CLA C 511



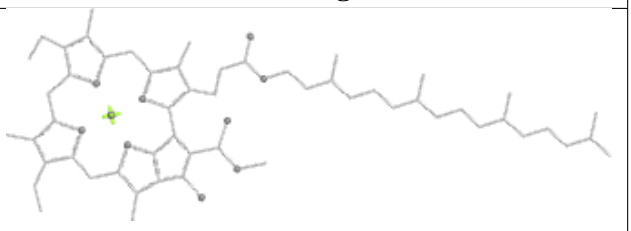
Bond lengths



Bond angles

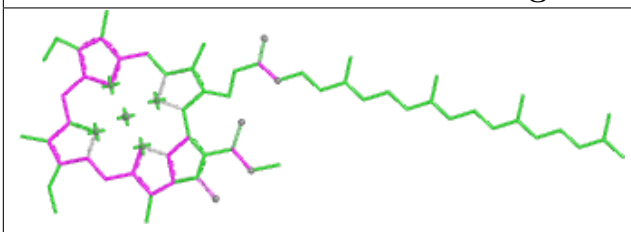


Torsions

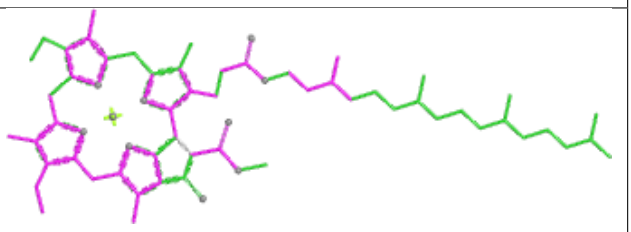


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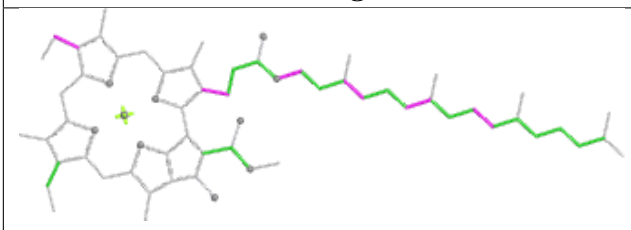
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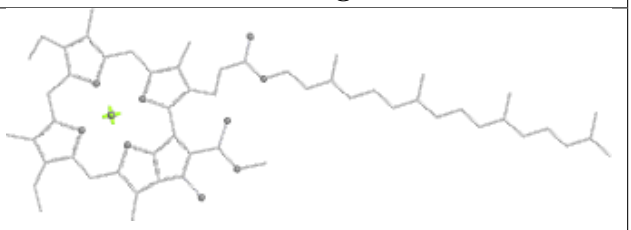
Bond lengths



Bond angles

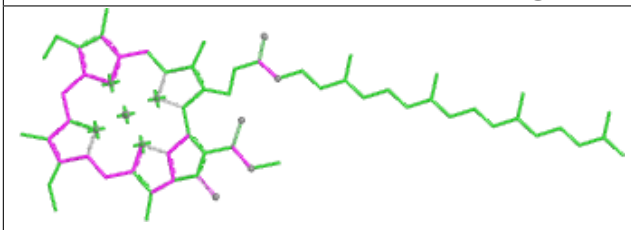


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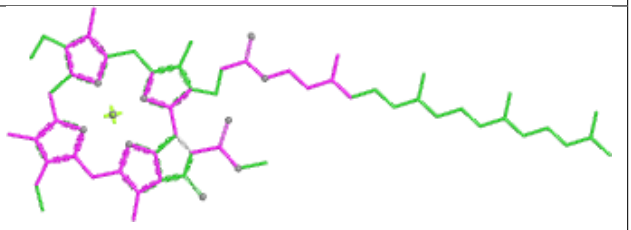


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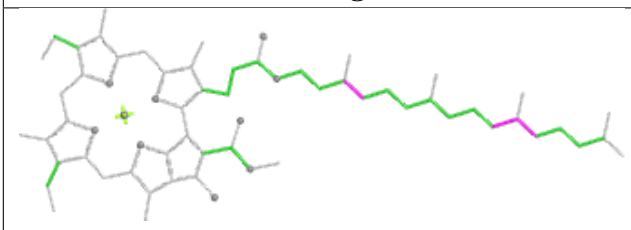
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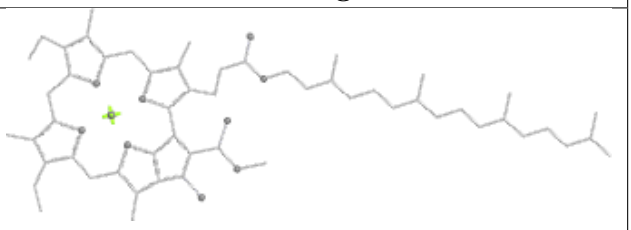
Bond lengths



Bond angles



Torsions

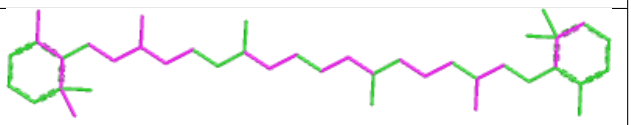


Rings

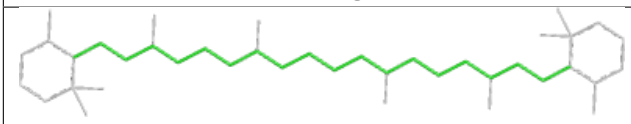
Ligand BCR B 617



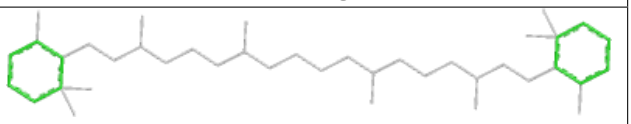
Bond lengths



Bond angles

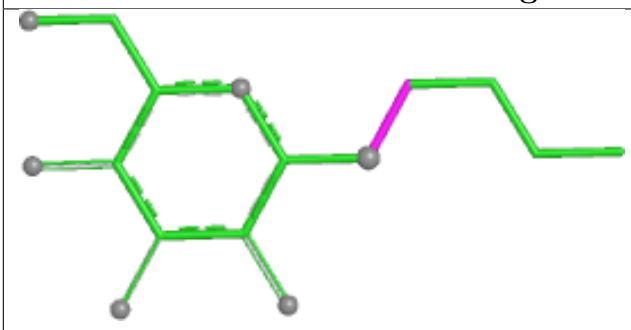


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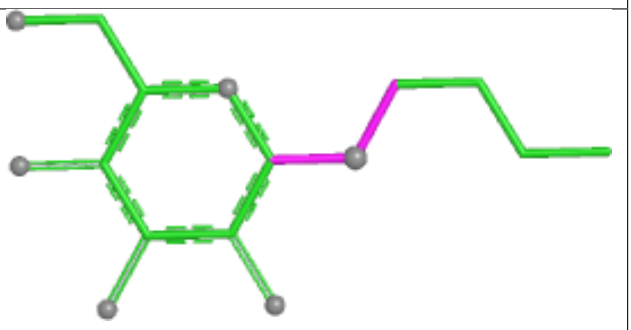


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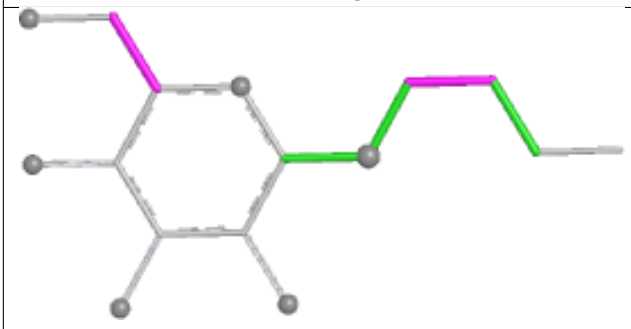
Ligand HTG D 410



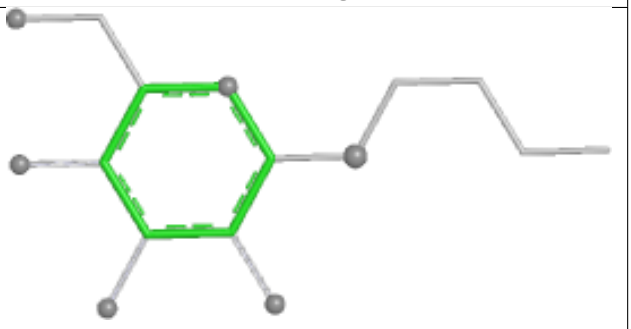
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Bond angles

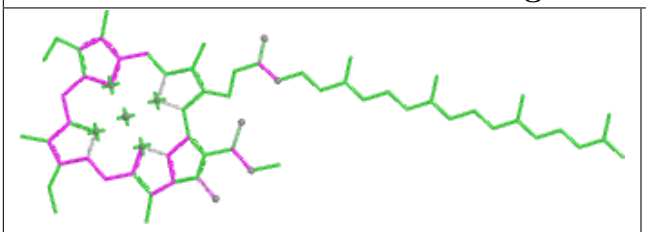


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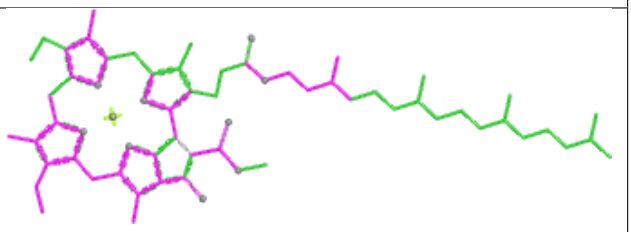


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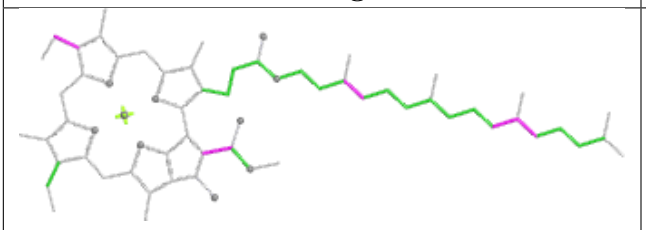
Ligand CLA C 505



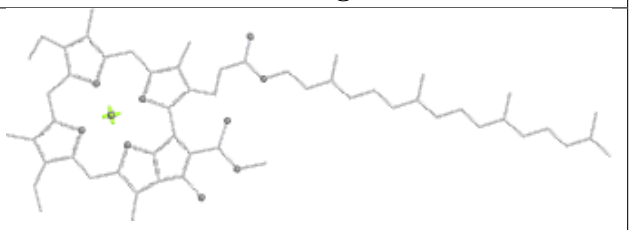
Bond lengths



Bond angles

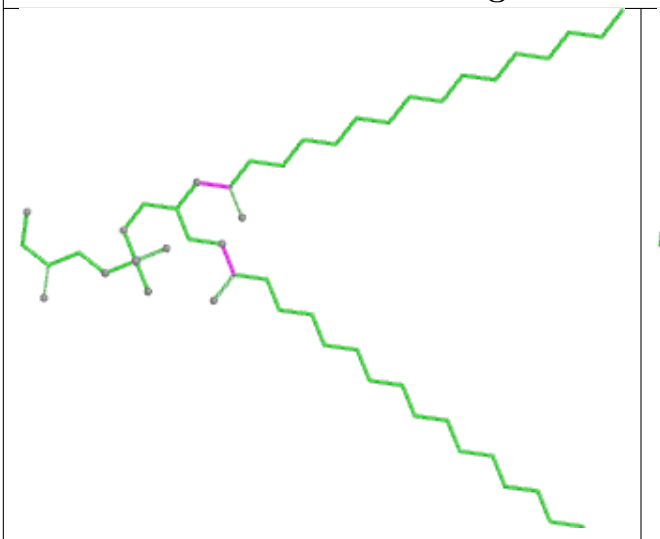


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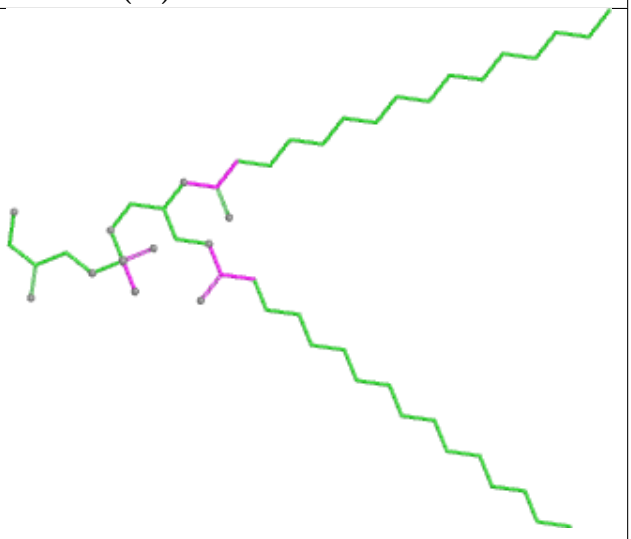


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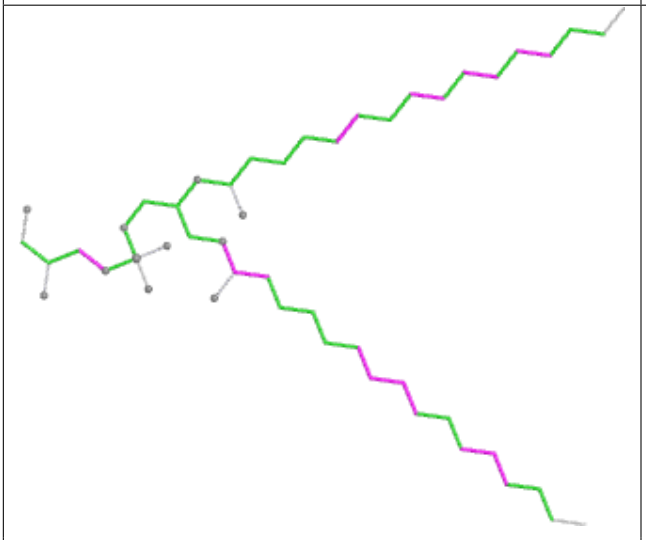
Ligand LHG D 407 (A)



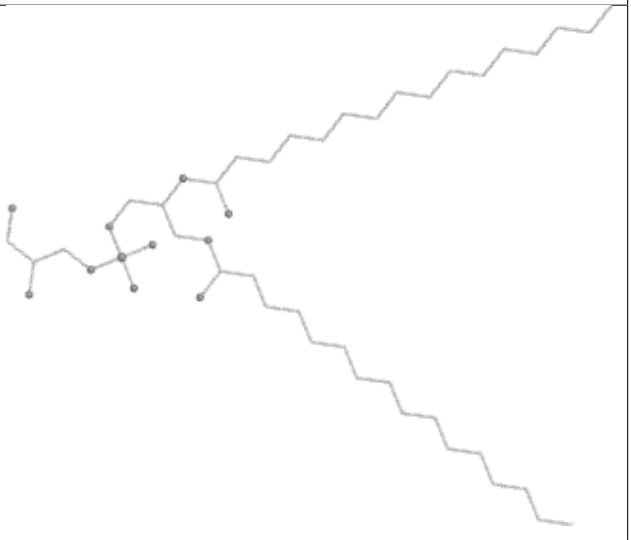
Bond lengths



Bond angles

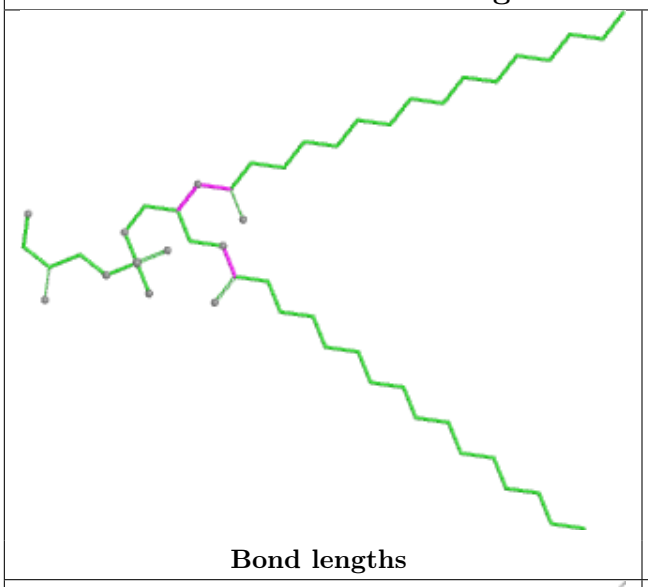


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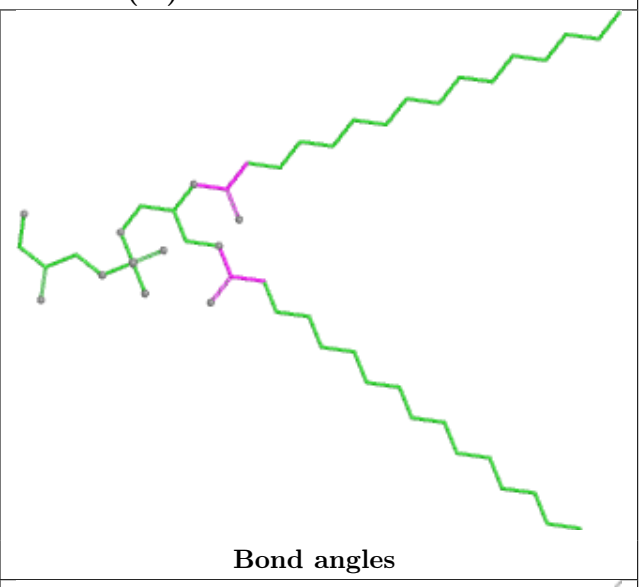


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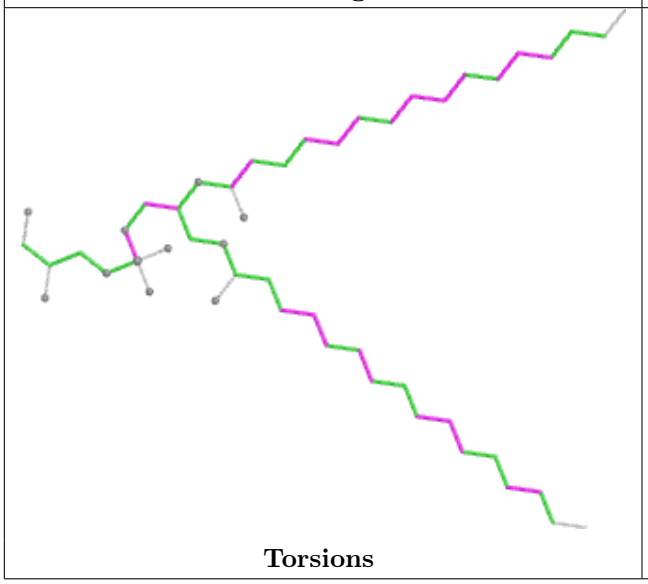
Ligand LHG b 629 (A)



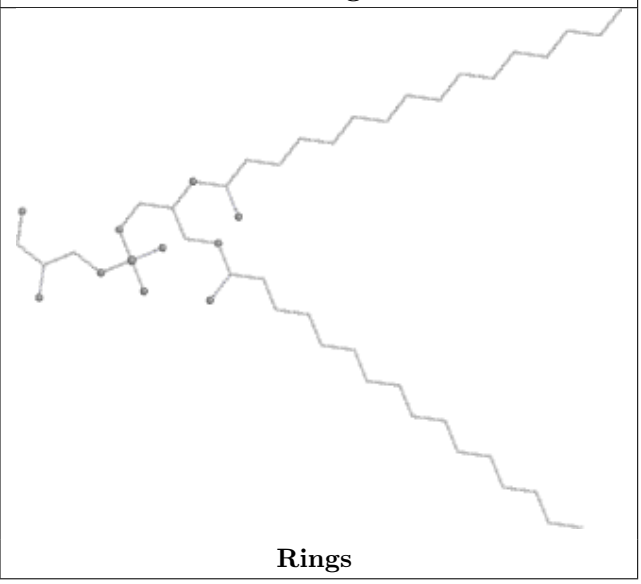
Bond lengths



Bond angles

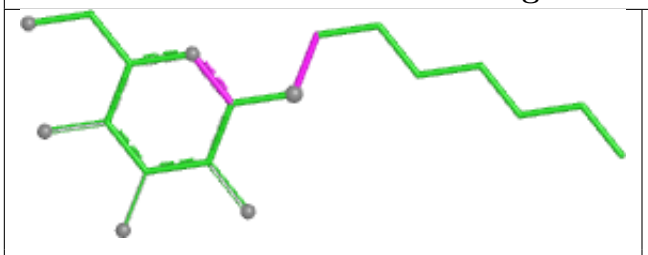


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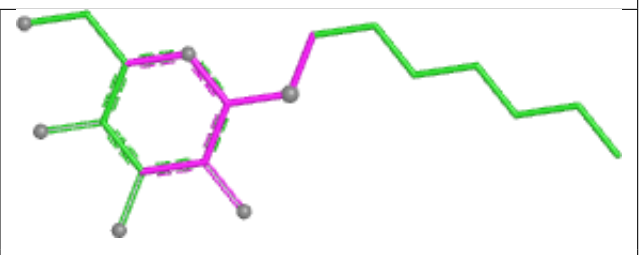


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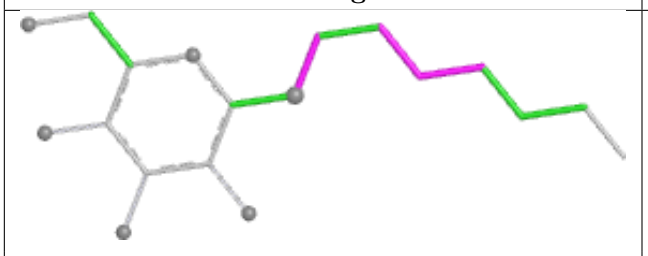
Ligand HTG B 621



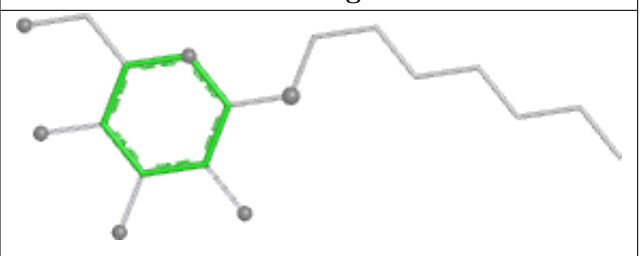
Bond lengths



Bond angles

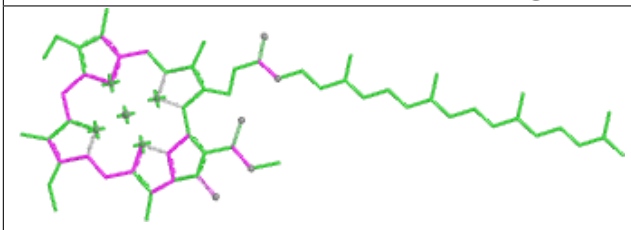


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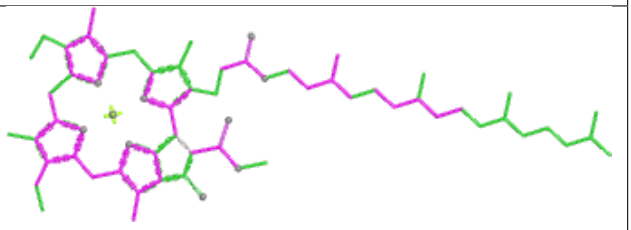


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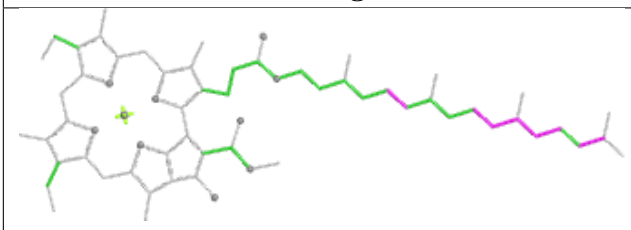
Ligand CLA b 615



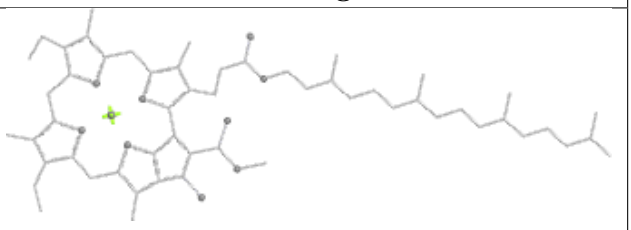
Bond lengths



Bond angles

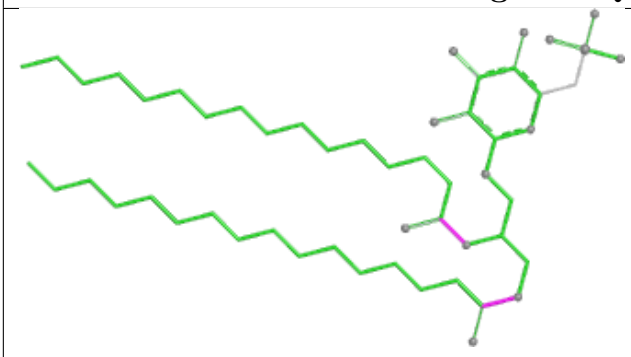


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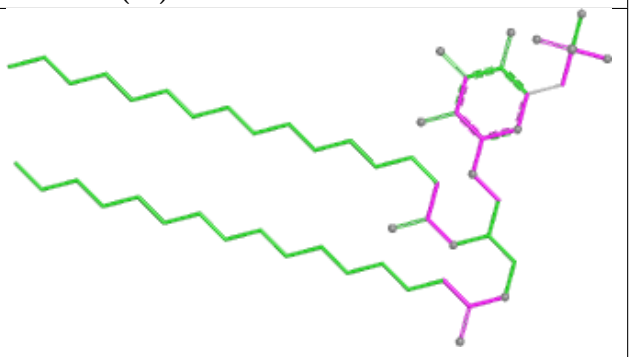


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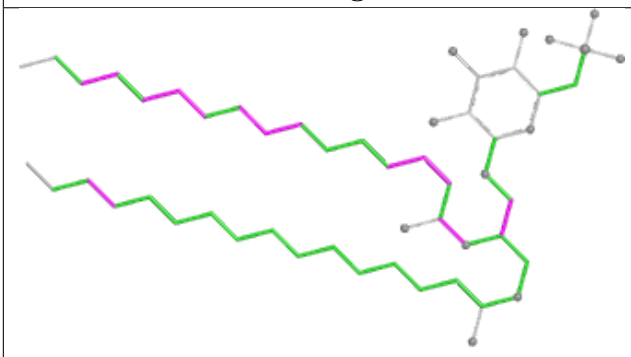
Ligand SQD A 410 (A)



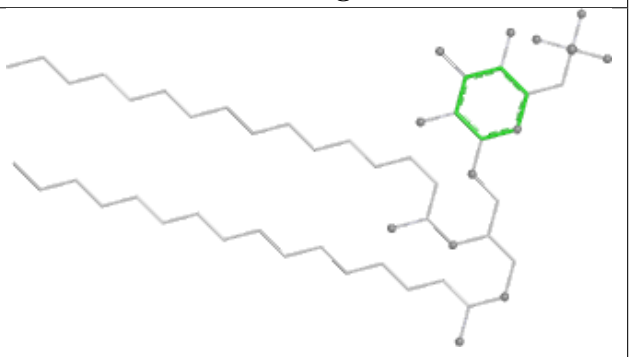
Bond lengths



Bond angles

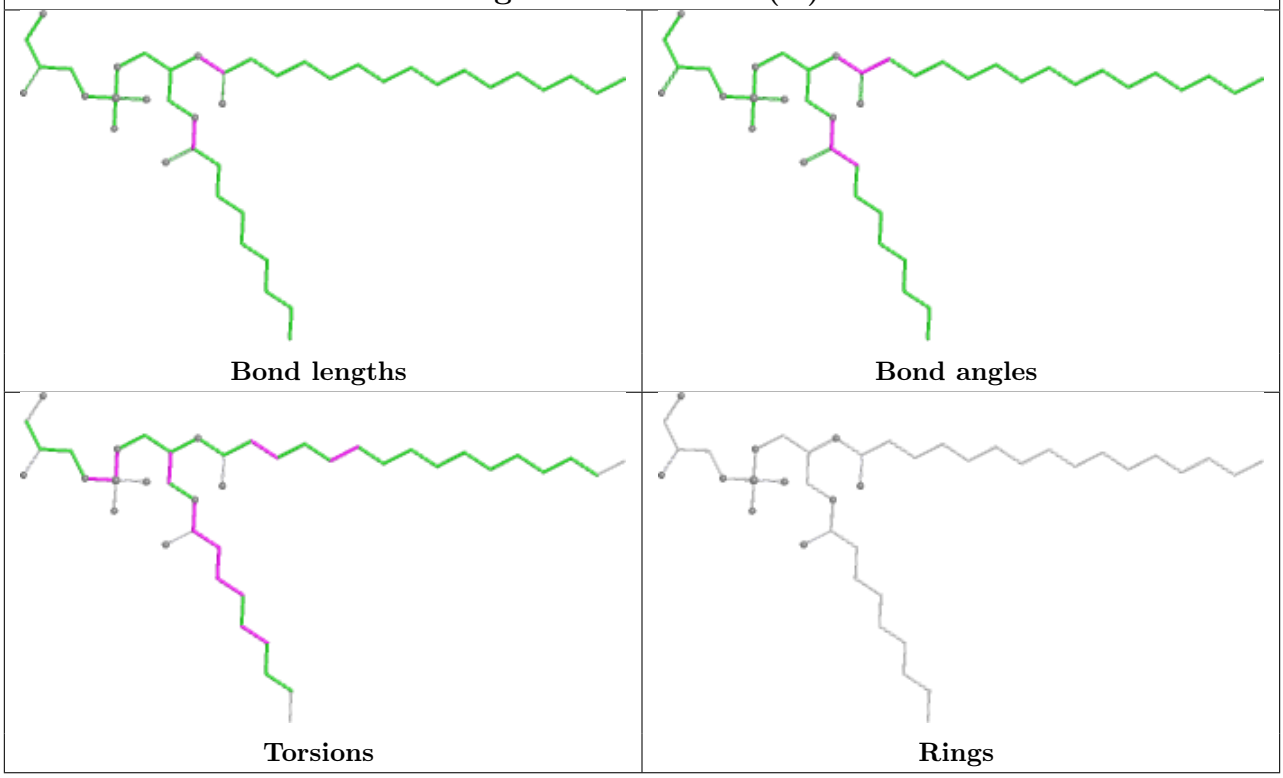


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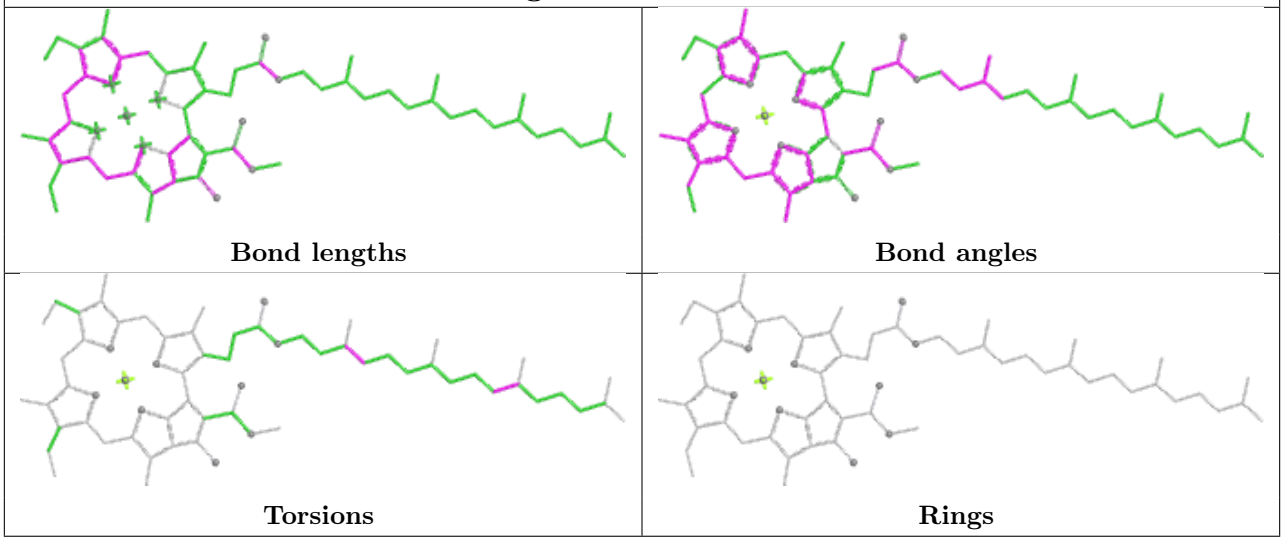


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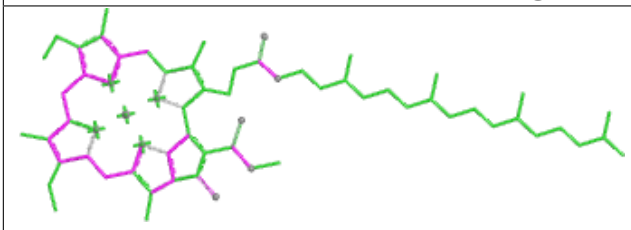
Ligand LHG a 419 (A)



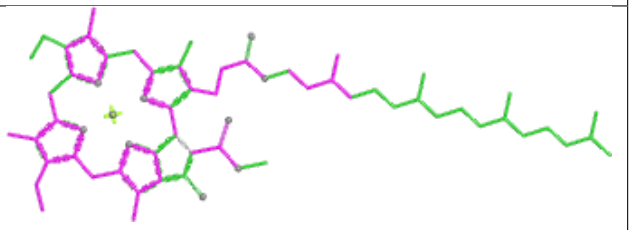
Ligand CLA C 506



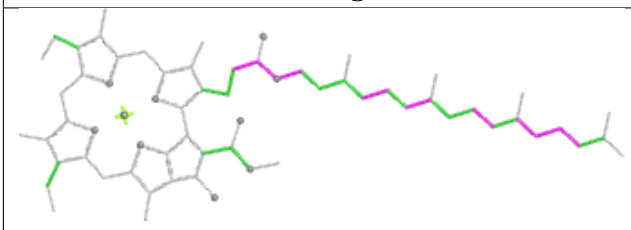
Ligand CLA c 512



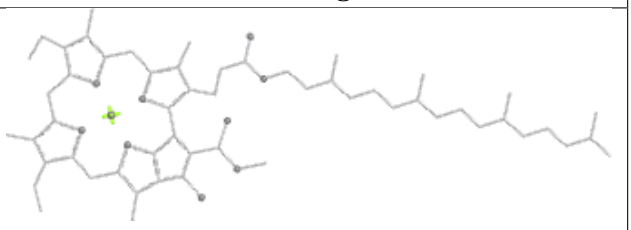
Bond lengths



Bond angles

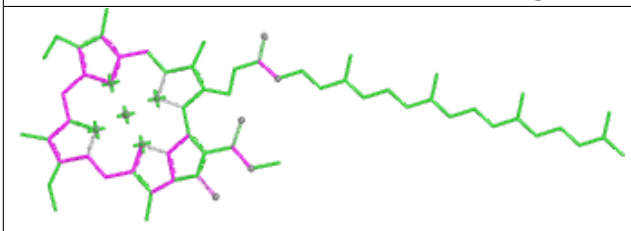


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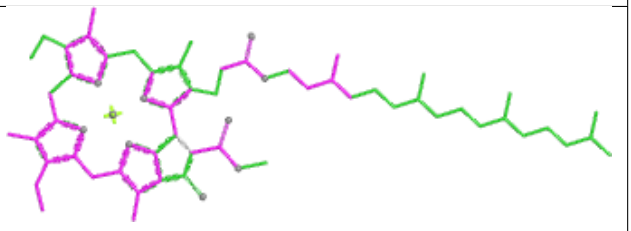


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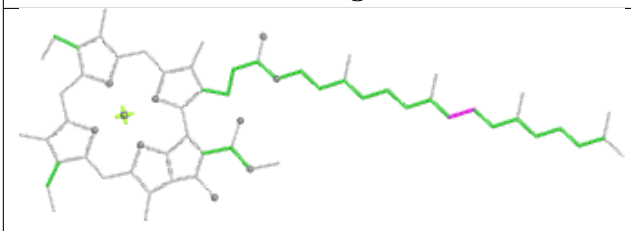
Ligand CLA c 503



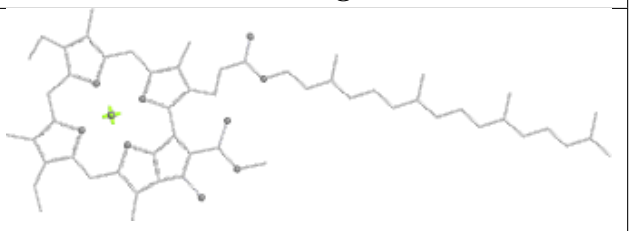
Bond lengths



Bond angles

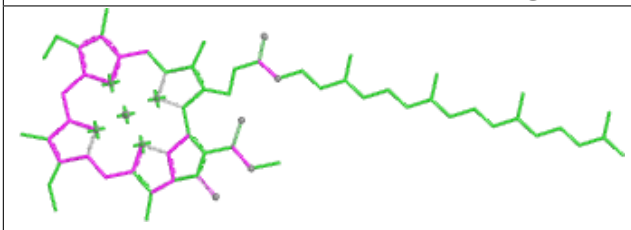


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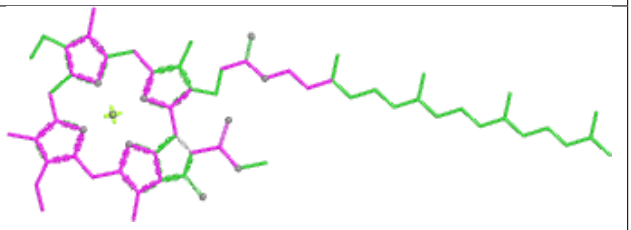


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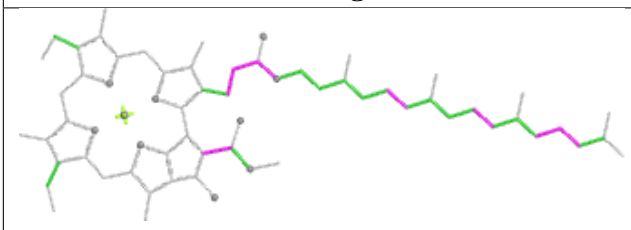
Ligand CLA B 601



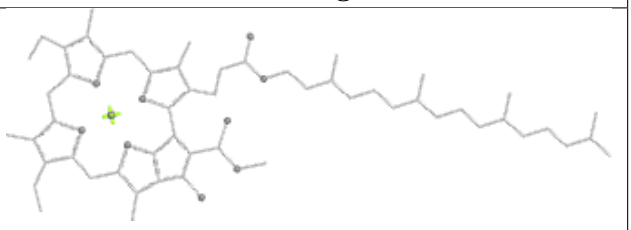
Bond lengths



Bond angles

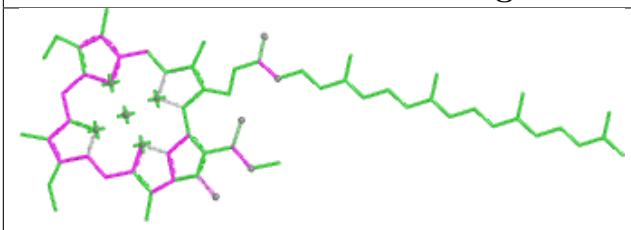


Torsions

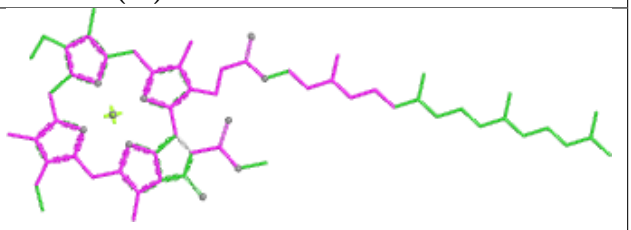


Rings

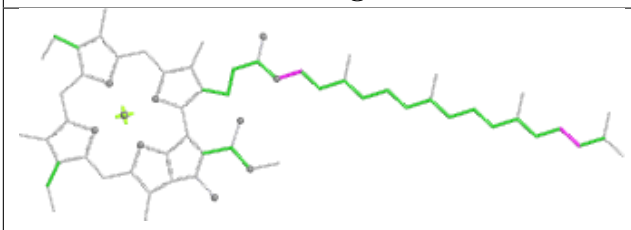
Ligand CLA a 404 (B)



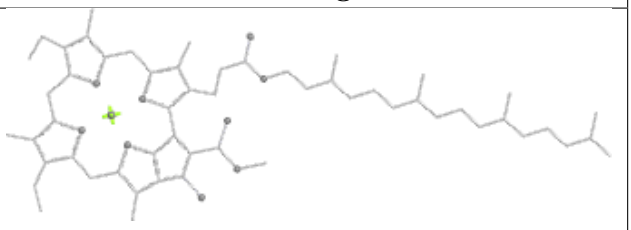
Bond lengths



Bond angles

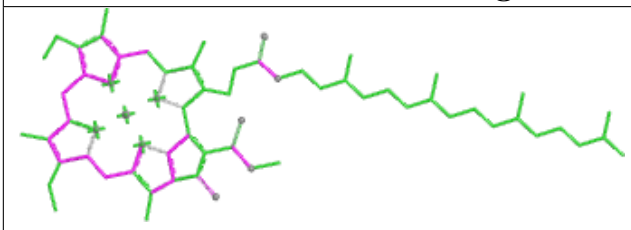


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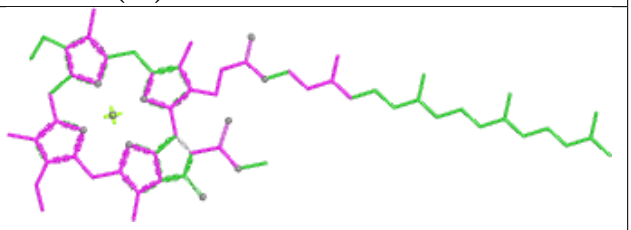


Rings

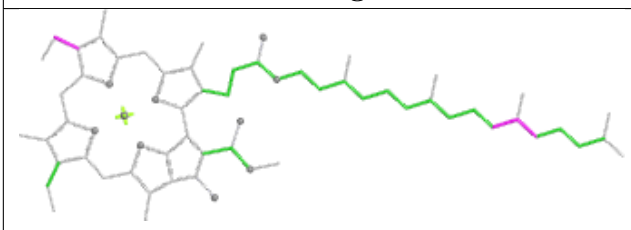
Ligand CLA a 405 (A)



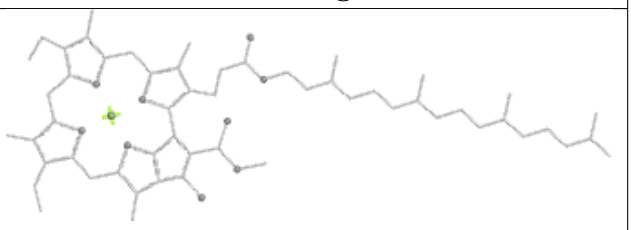
Bond lengths



Bond angles

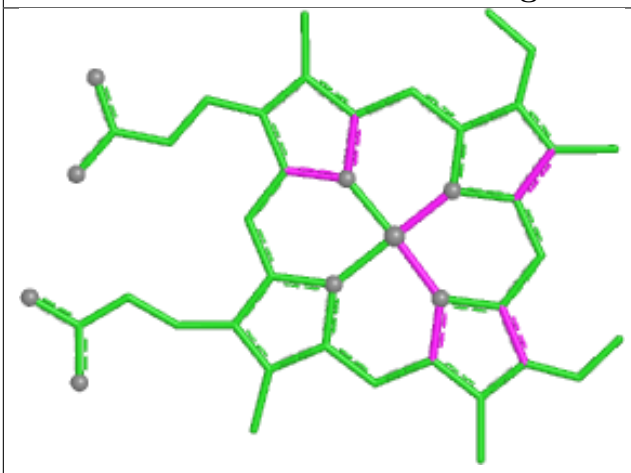


Torsions

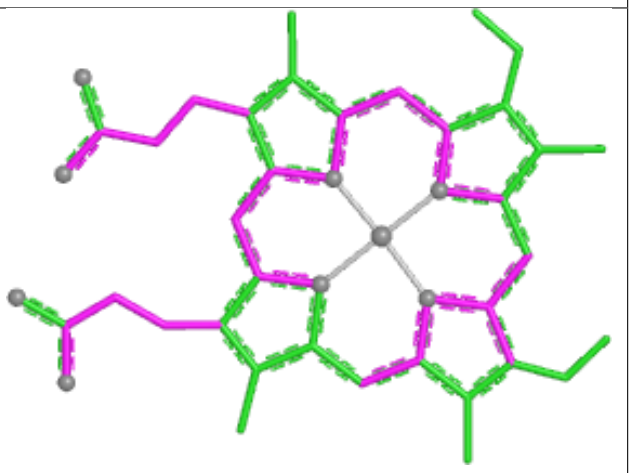


Rings

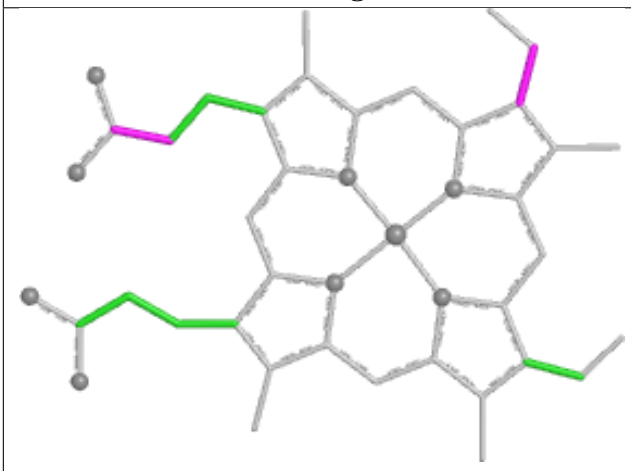
Ligand HEM E 102



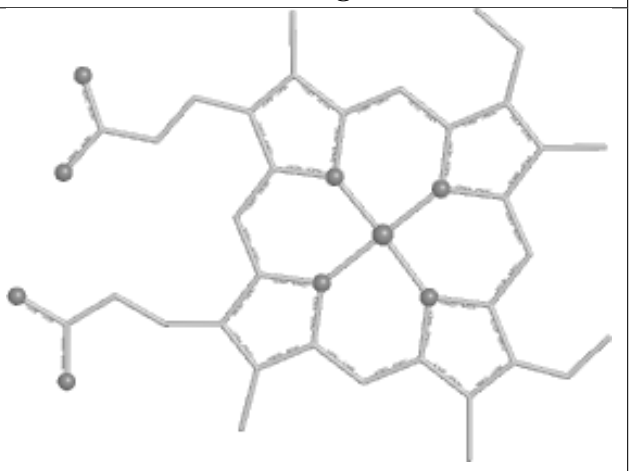
Bond lengths



Bond angles

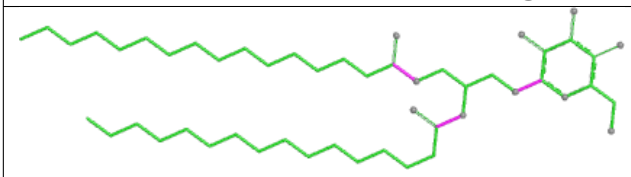


Torsions

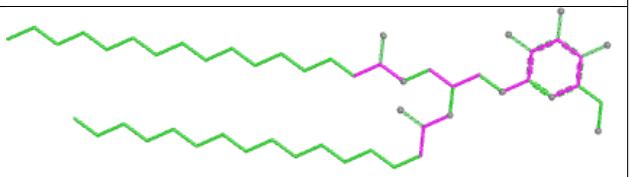


Rings

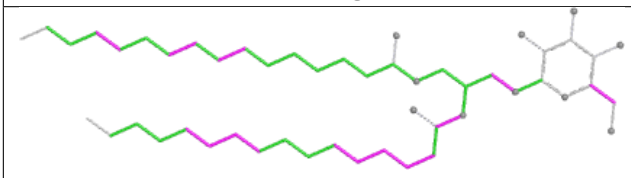
Ligand LMG C 521



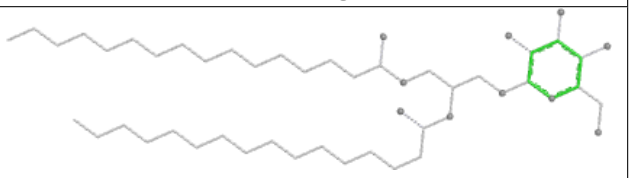
Bond lengths



Bond angles



Torsions

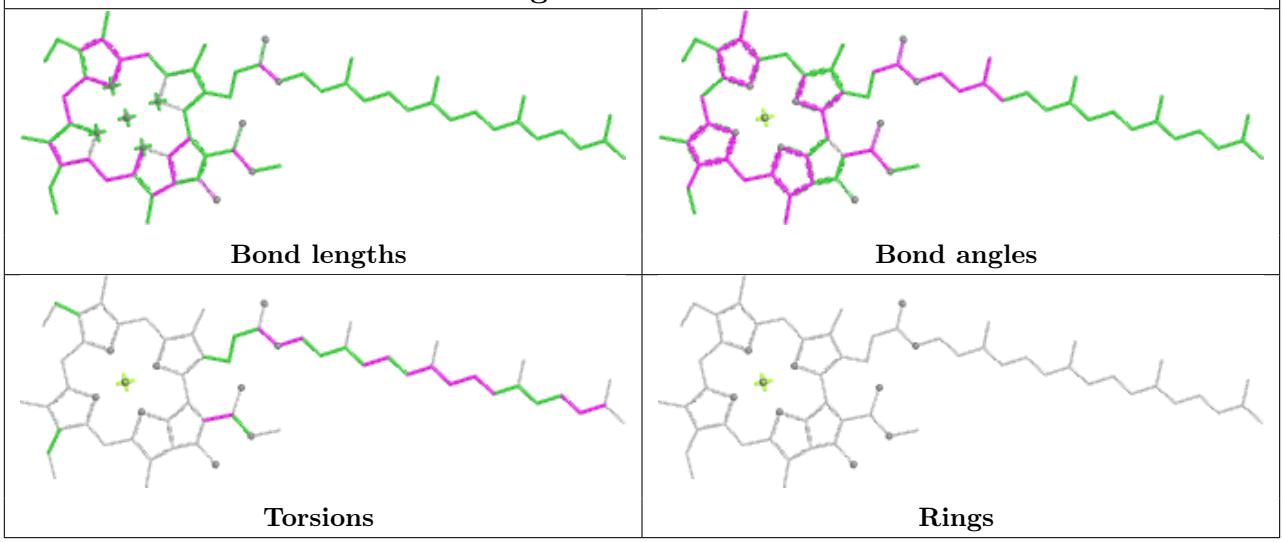


Rings

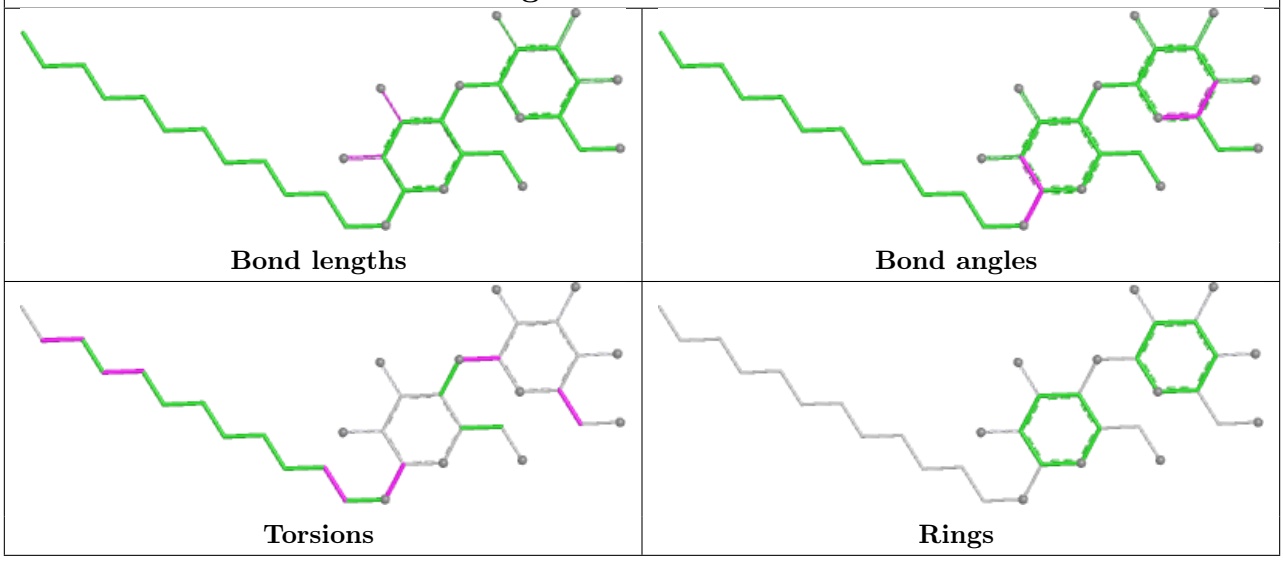
Ligand PL9 a 413 (B)



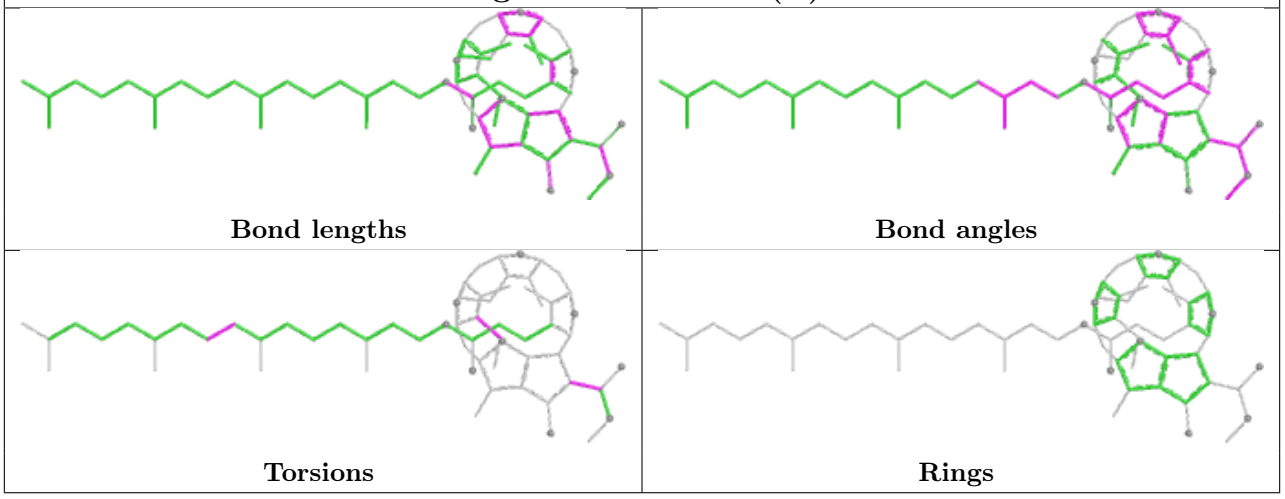
Ligand CLA c 509



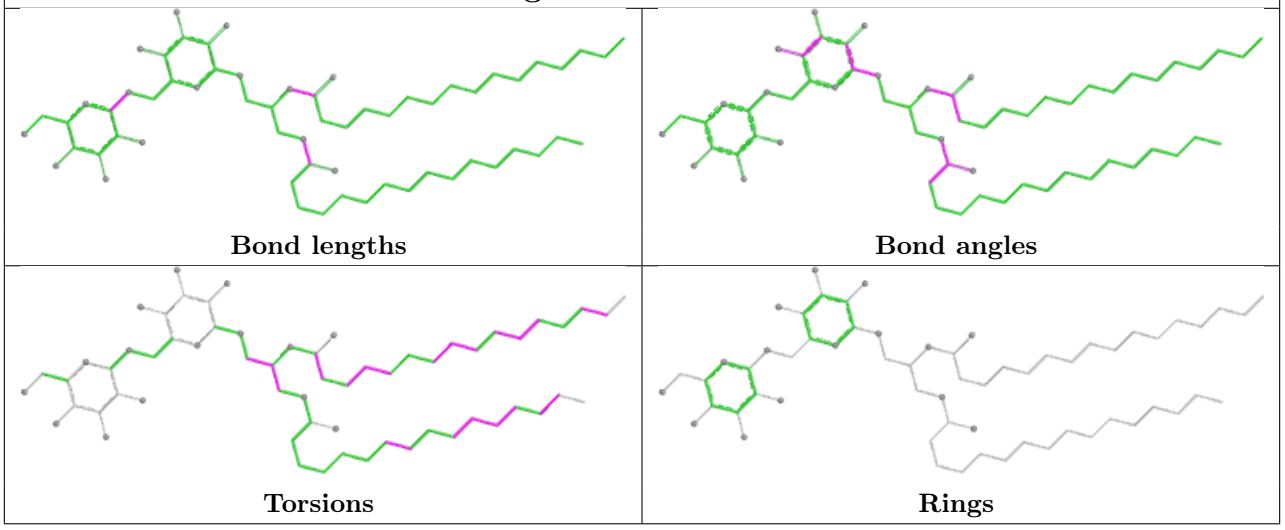
Ligand LMT A 417



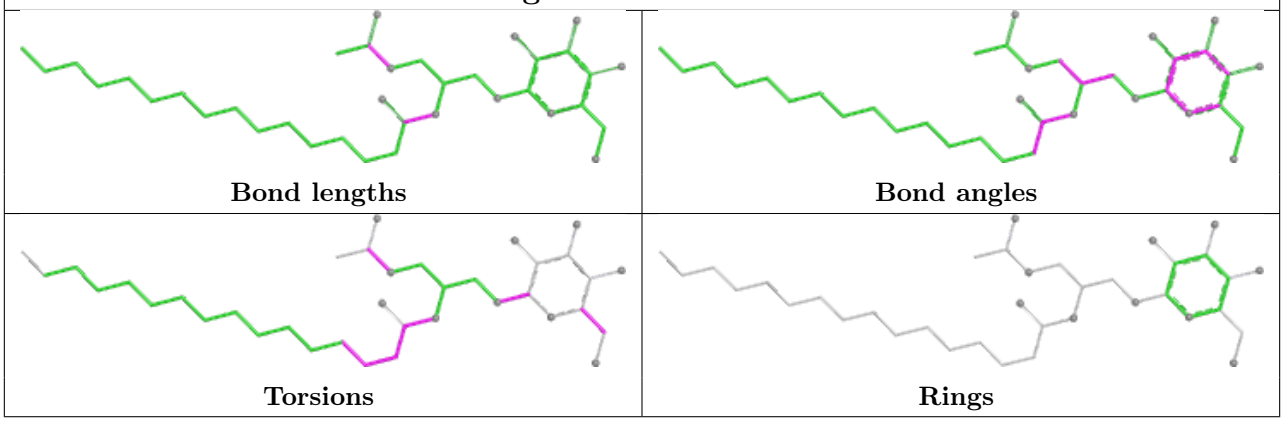
Ligand PHO d 403 (B)



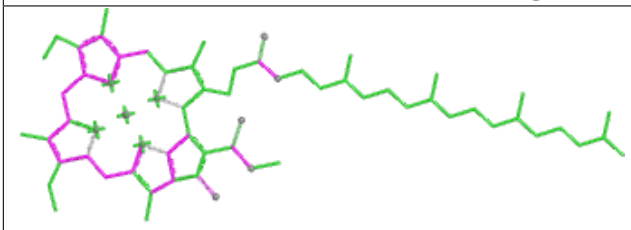
Ligand DGD h 102



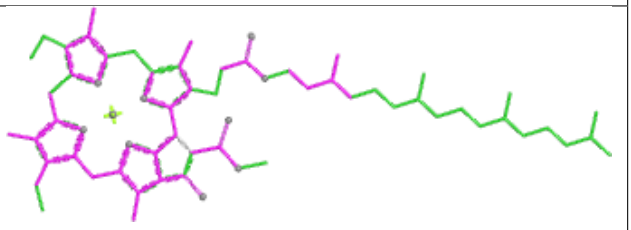
Ligand LMG Z 101



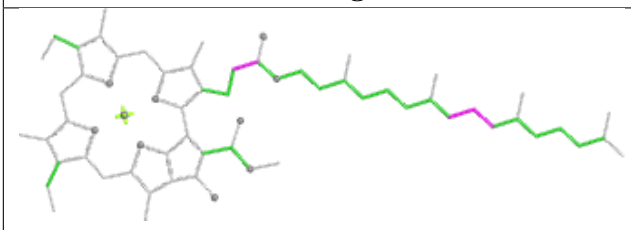
Ligand CLA b 612



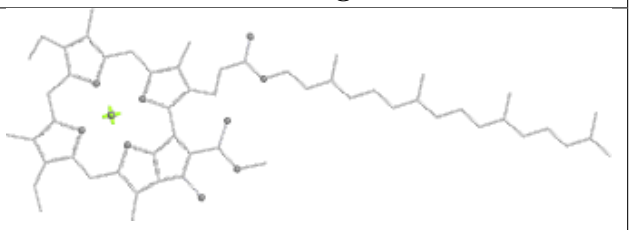
Bond lengths



Bond angles

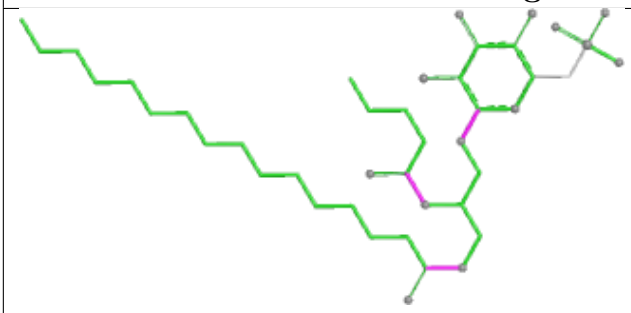


Torsions

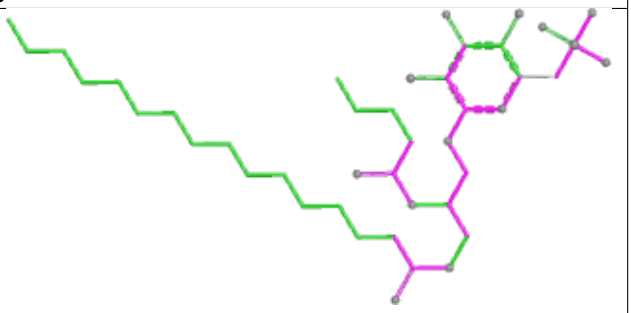


Rings

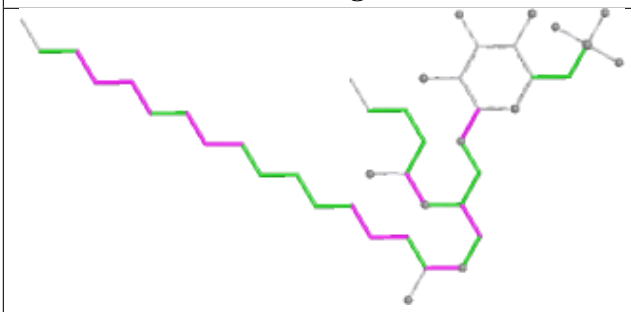
Ligand SQD X 101



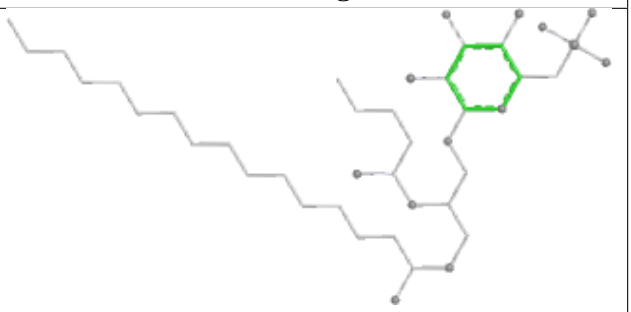
Bond lengths



Bond angles

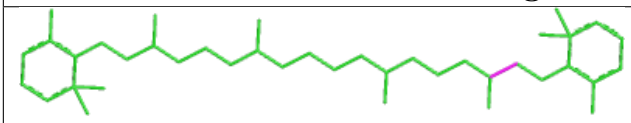


Torsions

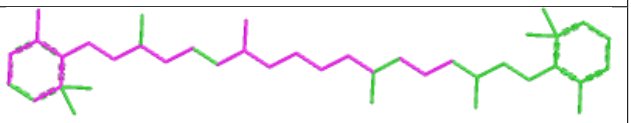


Rings

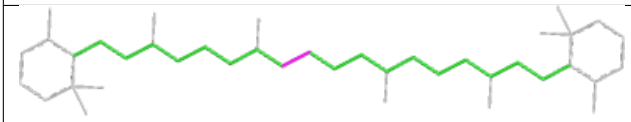
Ligand BCR T 102



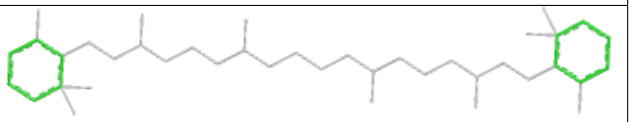
Bond lengths



Bond angles

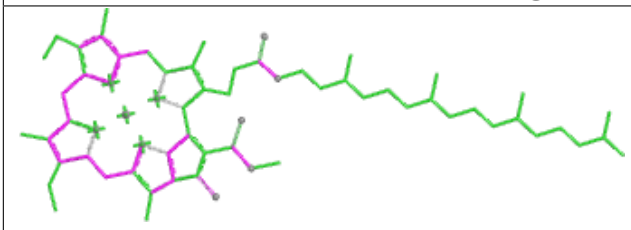


Torsions

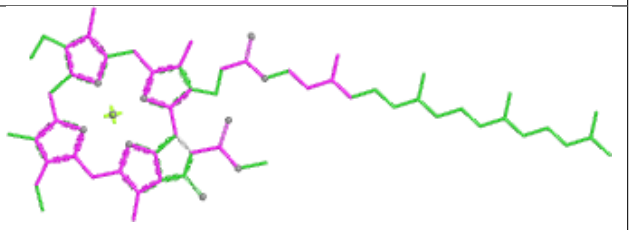


Rings

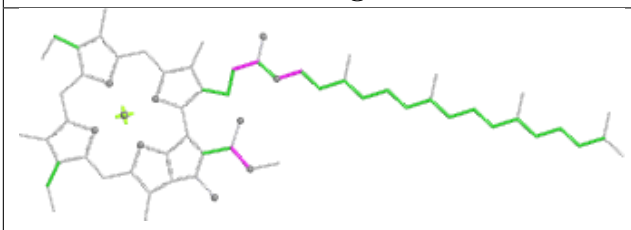
Ligand CLA b 613



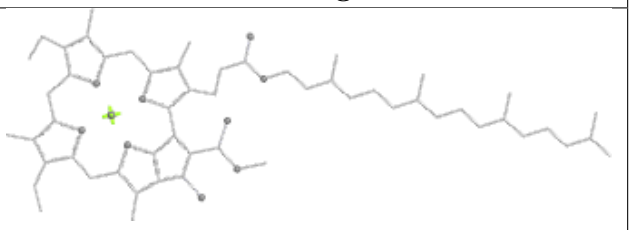
Bond lengths



Bond angles

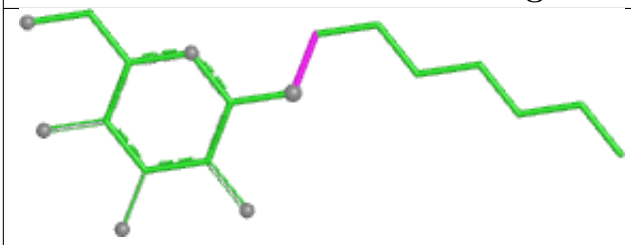


Torsions

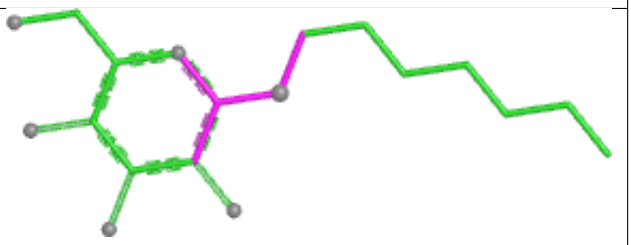


Rings

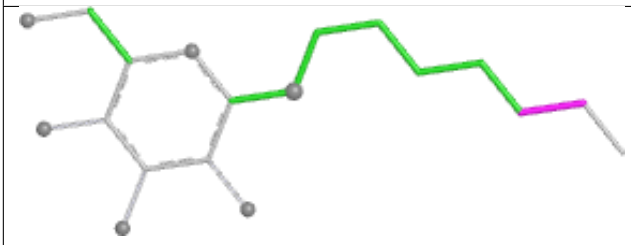
Ligand HTG c 521



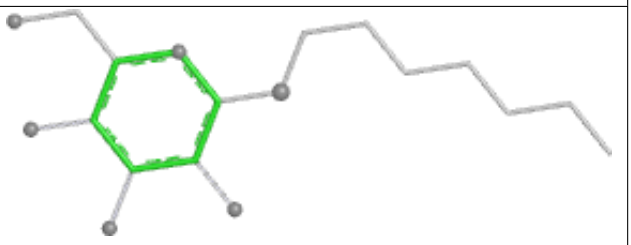
Bond lengths



Bond angles

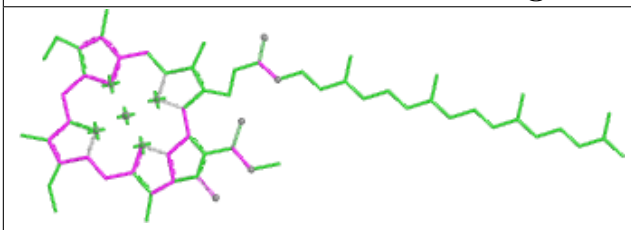


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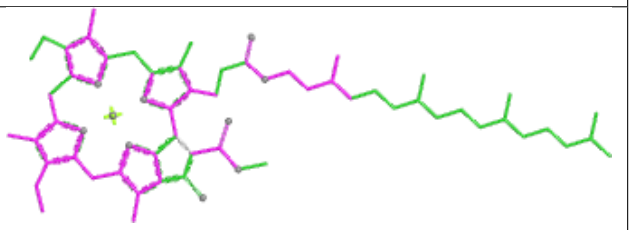


Rings

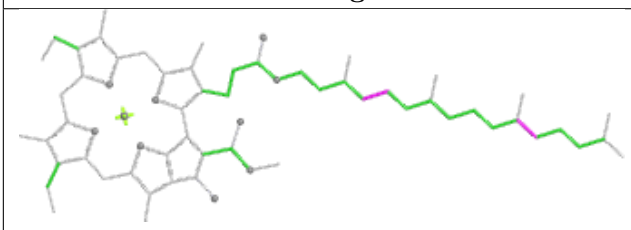
Ligand CLA b 607



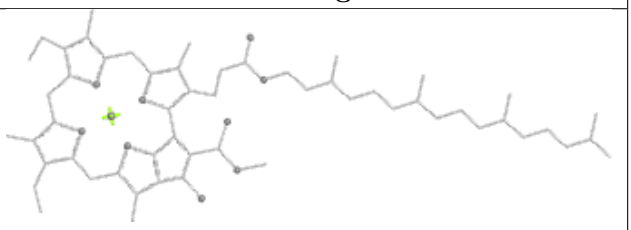
Bond lengths



Bond angles

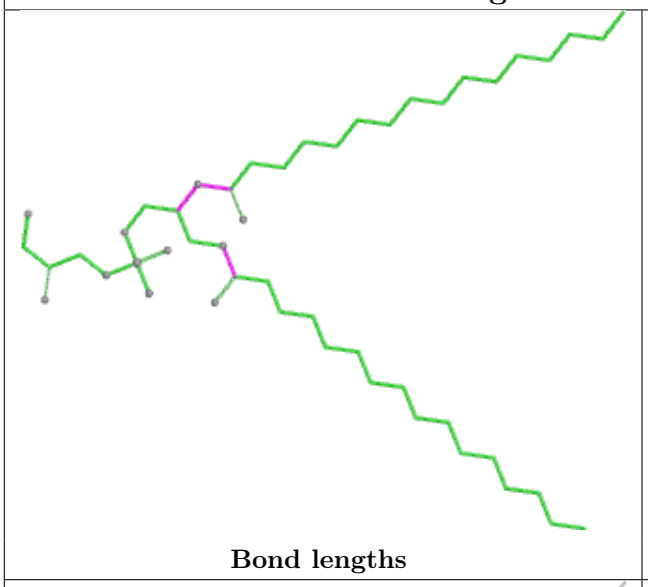


Torsions

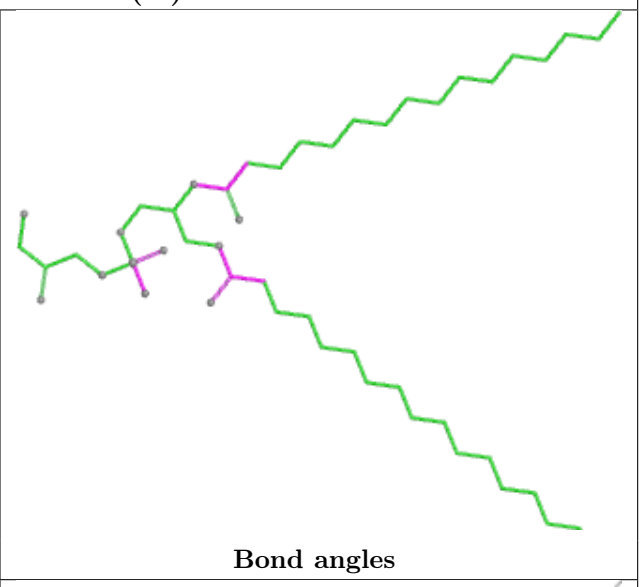


Rings

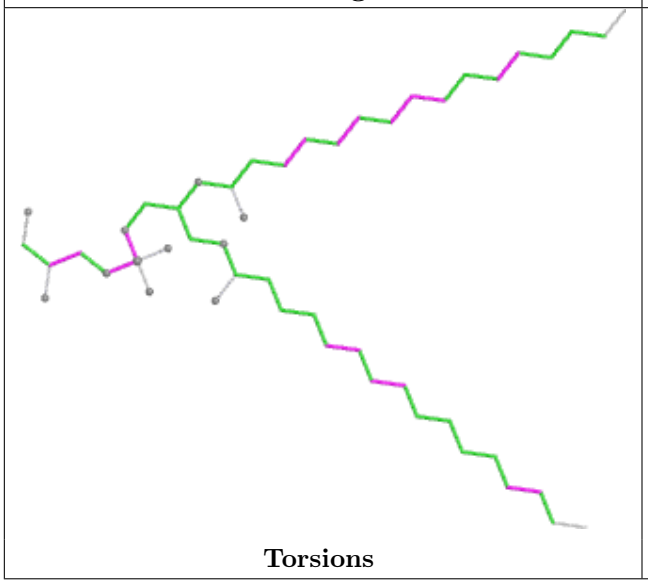
Ligand LHG D 406 (A)



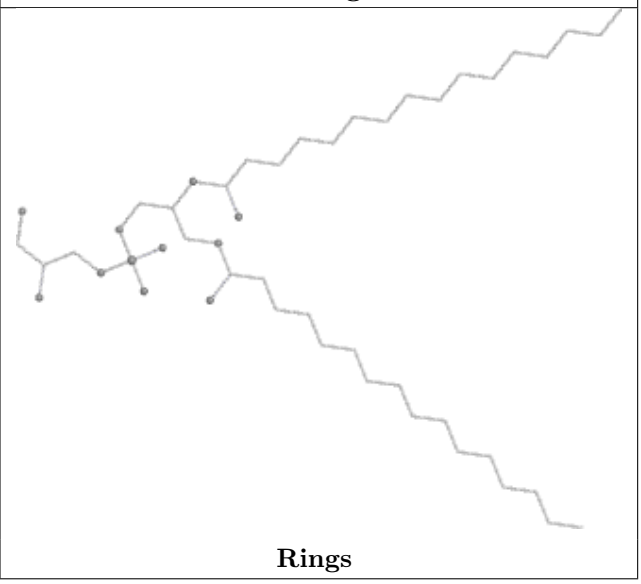
Bond lengths



Bond angles



Torsions

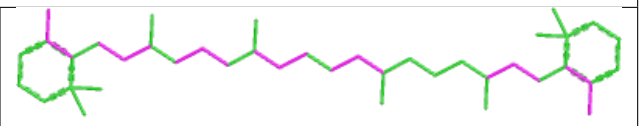


Rings

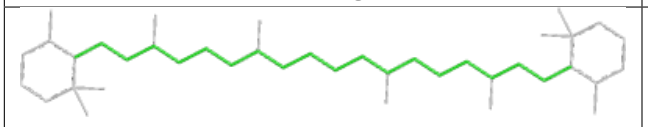
Ligand BCR C 515



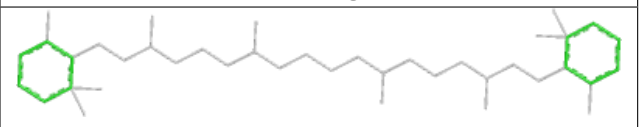
Bond lengths



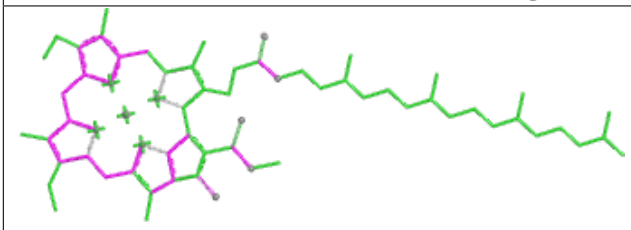
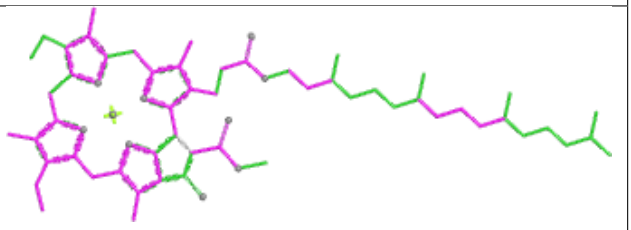
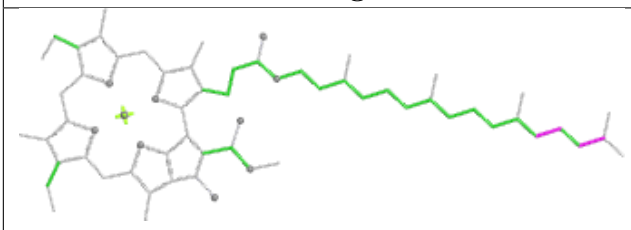
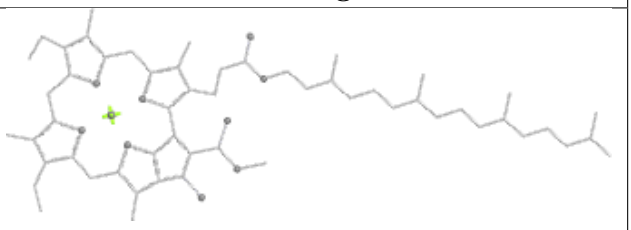
Bond angles

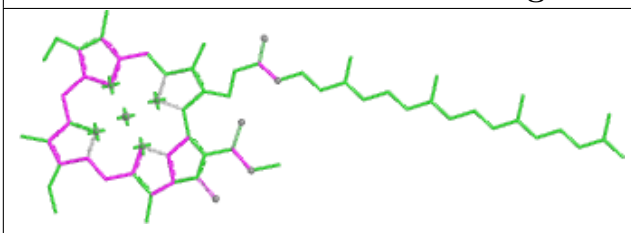
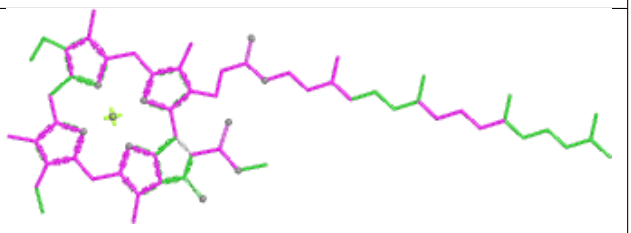
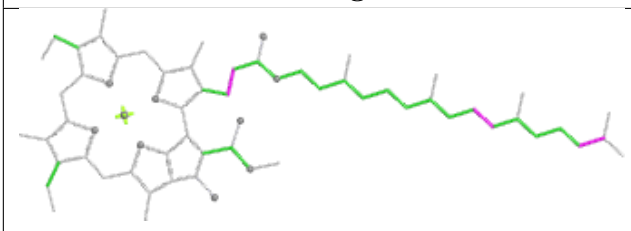
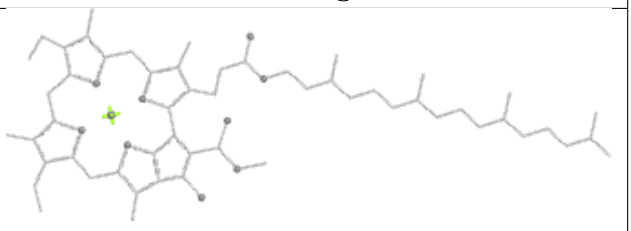


Torsions

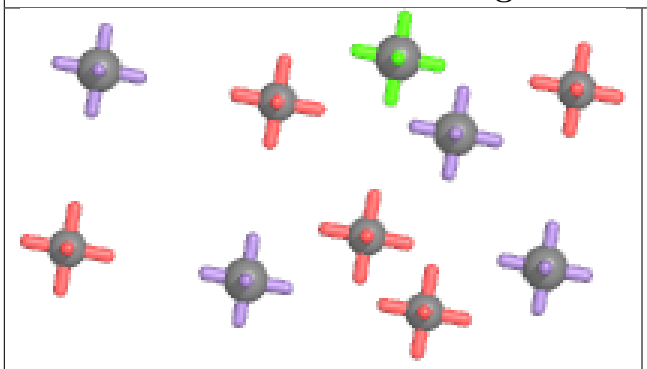


Rings

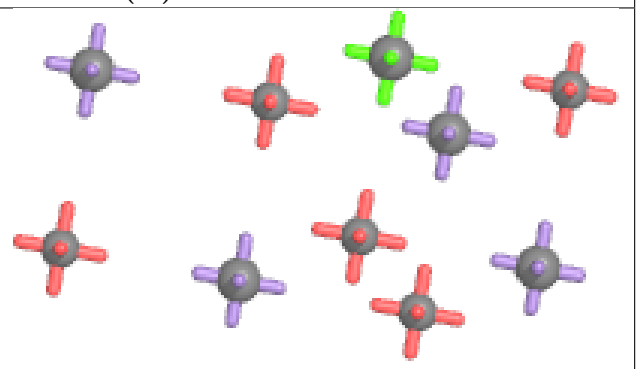
Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

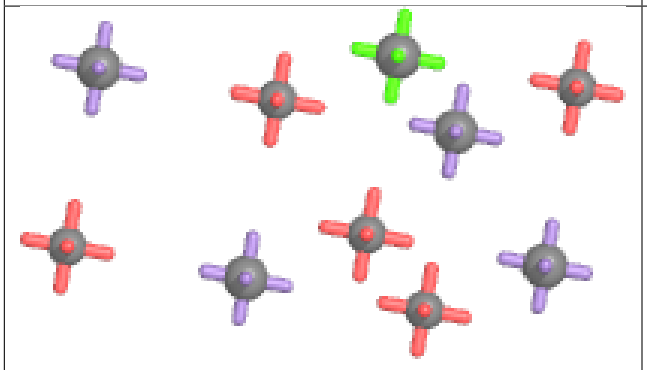
Ligand OEX a 412 (B)



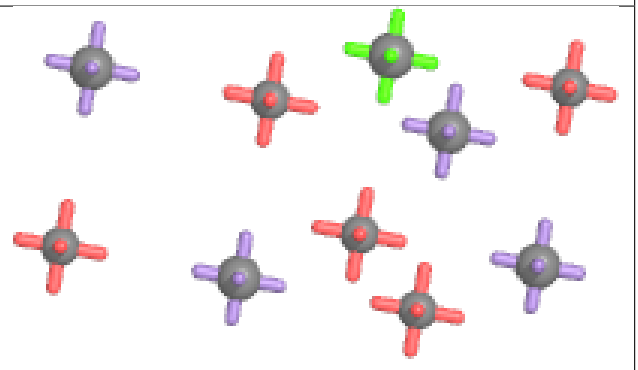
Bond lengths



Bond angles

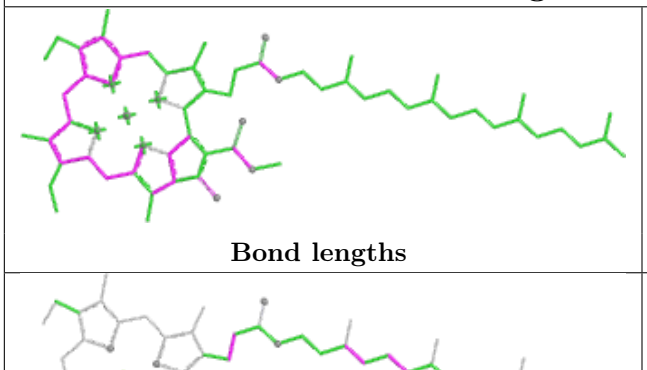


Torsions

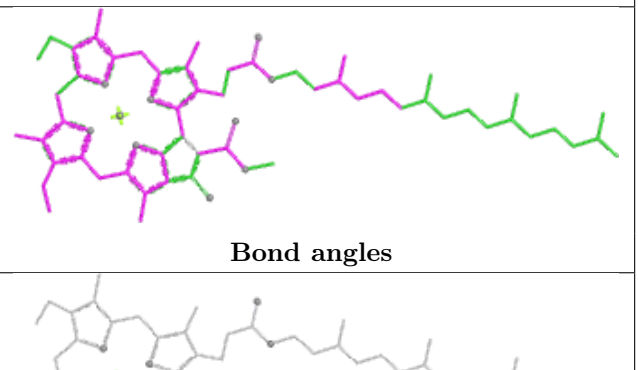


Rings

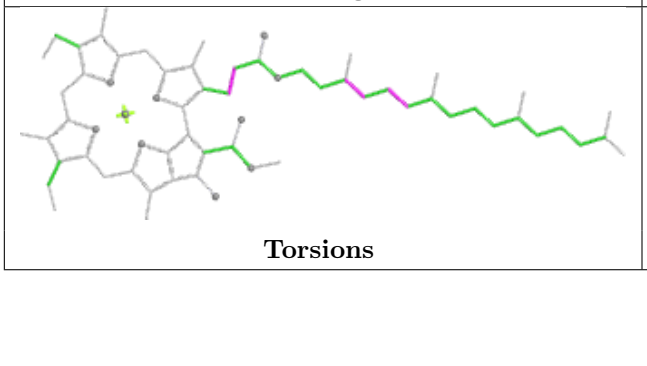
Ligand CLA b 603



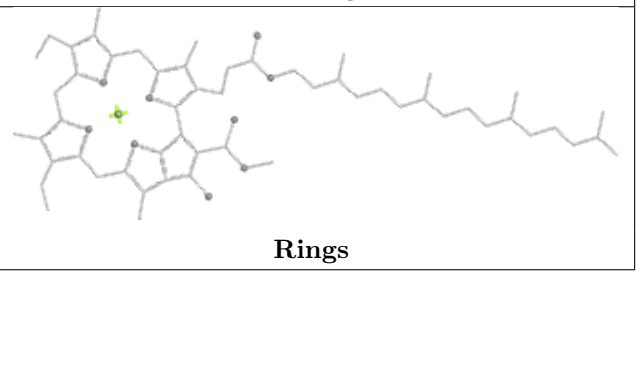
Bond lengths



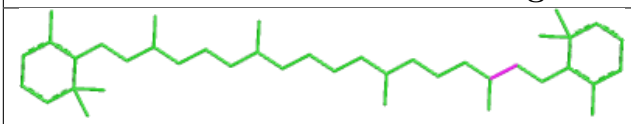
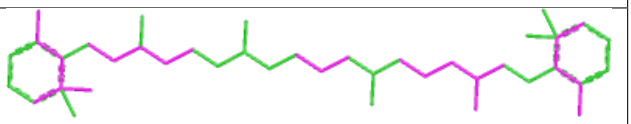
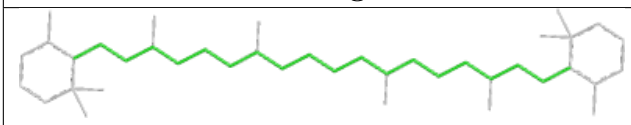
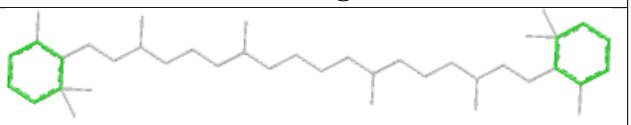
Bond angles



Torsions



Rings

Ligand BCR c 515	
 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.66	1 (0%) 90 88	21, 26, 59, 123	222 (66%)
1	a	334/344 (97%)	-0.63	0 100 100	22, 28, 65, 126	220 (65%)
2	B	504/505 (99%)	-0.59	1 (0%) 91 90	23, 54, 81, 117	22 (4%)
2	b	504/505 (99%)	-0.51	1 (0%) 91 90	24, 57, 92, 152	19 (3%)
3	C	451/455 (99%)	-0.61	0 100 100	23, 59, 79, 156	99 (21%)
3	c	455/455 (100%)	-0.53	2 (0%) 88 87	24, 66, 86, 130	101 (22%)
4	D	342/342 (100%)	-0.67	0 100 100	21, 47, 65, 139	115 (33%)
4	d	341/342 (99%)	-0.67	0 100 100	22, 51, 72, 137	119 (34%)
5	E	81/84 (96%)	-0.44	1 (1%) 76 74	54, 69, 99, 163	0
5	e	79/84 (94%)	-0.38	1 (1%) 75 73	32, 75, 114, 149	2 (2%)
6	F	34/44 (77%)	-0.59	0 100 100	54, 62, 88, 114	0
6	f	31/44 (70%)	-0.44	1 (3%) 50 47	55, 67, 95, 150	1 (3%)
7	H	64/65 (98%)	-0.35	1 (1%) 70 67	50, 62, 83, 108	0
7	h	64/65 (98%)	-0.47	0 100 100	40, 68, 92, 108	1 (1%)
8	I	37/38 (97%)	-0.32	0 100 100	55, 63, 124, 163	0
8	i	37/38 (97%)	-0.36	0 100 100	56, 65, 120, 147	0
9	J	38/39 (97%)	-0.34	0 100 100	52, 69, 123, 179	0
9	j	39/39 (100%)	-0.32	0 100 100	60, 75, 124, 168	0
10	K	37/37 (100%)	-0.66	0 100 100	60, 69, 88, 109	0
10	k	37/37 (100%)	-0.57	0 100 100	67, 74, 96, 112	0
11	L	36/37 (97%)	-0.63	0 100 100	24, 47, 100, 147	2 (5%)
11	l	36/37 (97%)	-0.61	0 100 100	25, 48, 100, 118	2 (5%)
12	M	32/36 (88%)	-0.63	0 100 100	28, 50, 74, 138	1 (3%)
12	m	33/36 (91%)	-0.54	0 100 100	24, 50, 70, 149	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.56	0 100 100	22, 64, 116, 182	10 (4%)
13	o	243/244 (99%)	-0.53	0 100 100	22, 66, 124, 170	8 (3%)
14	T	29/32 (90%)	-0.68	0 100 100	26, 48, 58, 66	6 (20%)
14	t	29/32 (90%)	-0.64	1 (3%) 48 45	28, 49, 64, 76	5 (17%)
15	U	96/104 (92%)	-0.64	0 100 100	26, 59, 90, 99	4 (4%)
15	u	97/104 (93%)	-0.65	0 100 100	28, 63, 83, 134	5 (5%)
16	V	137/137 (100%)	-0.72	0 100 100	23, 58, 83, 109	6 (4%)
16	v	137/137 (100%)	-0.62	0 100 100	27, 72, 102, 132	6 (4%)
17	X	38/40 (95%)	-0.31	0 100 100	35, 71, 91, 112	1 (2%)
17	x	38/40 (95%)	-0.11	0 100 100	63, 77, 123, 163	0
18	Y	29/30 (96%)	0.01	1 (3%) 48 45	67, 85, 126, 135	0
18	y	29/30 (96%)	-0.30	0 100 100	74, 91, 110, 120	0
19	Z	62/62 (100%)	-0.37	0 100 100	66, 80, 135, 166	0
19	z	62/62 (100%)	0.04	0 100 100	80, 94, 145, 194	0
20	R	34/34 (100%)	0.38	1 (2%) 53 50	81, 102, 132, 136	0
All	All	5283/5384 (98%)	-0.55	12 (0%) 91 90	21, 58, 99, 194	979 (18%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	3.8
5	e	79[A]	PHE	3.5
6	f	16[A]	PHE	3.0
14	t	30[A]	THR	2.6
2	B	494	GLY	2.5
2	b	499	VAL	2.5
18	Y	18	VAL	2.3
5	E	4	THR	2.3
20	R	28	VAL	2.3
3	c	20	SER	2.3
1	A	11	ALA	2.2
3	c	245[A]	ILE	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	48,58,67,71	0
8	FME	I	1	10/11	0.95	0.07	61,66,80,83	0
8	FME	i	1	10/11	0.97	0.07	54,69,78,87	0
12	FME	m	1	10/11	0.97	0.07	50,63,89,112	0
14	FME	t	1	10/11	0.97	0.07	44,50,62,79	0
12	FME	M	1	10/11	0.98	0.05	51,61,93,108	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	a	417	6/6	0.62	0.15	76,100,104,106	0
31	LMT	B	628	35/35	0.67	0.15	65,113,141,150	0
31	LMT	A	417	35/35	0.68	0.14	71,114,140,143	0
30	UNL	J	101	10/-	0.69	0.26	70,81,90,98	0
30	UNL	A	415	28/-	0.70	0.15	85,115,140,150	0
30	UNL	a	414	30/-	0.71	0.13	86,116,145,155	0
30	UNL	m	102	10/-	0.71	0.21	72,77,98,101	0
31	LMT	F	101	35/35	0.71	0.15	103,138,178,184	0
31	LMT	C	525	35/35	0.72	0.13	104,136,153,169	0
30	UNL	j	101	10/-	0.73	0.18	77,94,106,107	0
30	UNL	I	101	40/-	0.73	0.15	74,107,162,165	0
34	HTG	B	622	19/19	0.73	0.16	67,96,114,122	0
31	LMT	e	101	35/35	0.75	0.14	115,148,191,192	0
30	UNL	l	102	10/-	0.75	0.16	67,78,90,91	0
27	GOL	d	414	6/6	0.76	0.15	57,70,79,96	0
27	GOL	B	626	6/6	0.76	0.15	71,84,95,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	K	101[A]	34/-	0.77	0.14	90,112,124,131	34
31	LMT	a	416	35/35	0.77	0.12	109,138,151,159	0
30	UNL	K	101[B]	34/-	0.77	0.14	90,112,125,131	34
26	SQD	f	102	43/54	0.77	0.12	91,127,172,181	0
34	HTG	C	522	19/19	0.78	0.12	96,129,147,149	0
36	CA	F	102	1/1	0.78	0.23	127,127,127,127	0
31	LMT	b	621	25/35	0.79	0.12	76,107,158,168	0
30	UNL	i	101	40/-	0.79	0.13	77,110,160,169	0
33	LMG	C	521	51/55	0.79	0.11	62,121,157,168	0
30	UNL	b	626	33/-	0.80	0.12	66,95,158,169	0
30	UNL	D	409	40/-	0.80	0.13	66,88,144,152	0
27	GOL	l	103[B]	6/6	0.80	0.19	68,101,107,109	6
27	GOL	l	103[A]	6/6	0.80	0.19	68,100,106,109	6
30	UNL	d	411	36/-	0.81	0.11	68,96,141,147	0
27	GOL	o	302	6/6	0.81	0.17	84,107,119,119	0
30	UNL	c	524[A]	32/-	0.81	0.15	99,117,127,138	32
34	HTG	D	410	16/19	0.81	0.12	87,105,132,152	0
30	UNL	c	524[B]	32/-	0.81	0.15	99,117,127,138	32
27	GOL	O	303	6/6	0.82	0.14	84,100,106,113	0
27	GOL	b	624	6/6	0.82	0.16	94,98,109,114	0
34	HTG	V	202	11/19	0.82	0.09	80,105,120,125	0
27	GOL	o	303	6/6	0.82	0.15	86,92,104,113	0
32	LHG	a	419[A]	42/49	0.83	0.10	98,142,156,164	42
32	LHG	a	419[B]	42/49	0.83	0.10	98,142,157,164	42
30	UNL	B	625	33/-	0.83	0.14	56,114,143,148	0
34	HTG	c	521	19/19	0.83	0.09	115,128,145,146	0
34	HTG	d	412	16/19	0.83	0.11	89,122,141,160	0
31	LMT	B	627	35/35	0.83	0.12	65,99,135,143	0
34	HTG	b	623	19/19	0.84	0.11	90,135,161,168	0
26	SQD	a	411	54/54	0.84	0.10	67,96,137,148	0
31	LMT	T	101	35/35	0.84	0.11	73,125,172,177	0
27	GOL	O	302	6/6	0.84	0.09	78,90,102,112	0
29	PL9	A	414[B]	55/55	0.85	0.15	69,98,111,118	55
33	LMG	Z	101	37/55	0.85	0.14	72,120,148,167	0
26	SQD	A	412	54/54	0.85	0.10	62,92,128,150	0
27	GOL	a	418	6/6	0.85	0.14	57,81,81,85	0
29	PL9	A	414[A]	55/55	0.85	0.15	69,98,111,118	55
27	GOL	A	411	6/6	0.86	0.13	66,81,84,89	0
31	LMT	t	101	26/35	0.86	0.12	80,104,149,158	0
31	LMT	M	101	35/35	0.86	0.10	59,91,109,114	0
27	GOL	A	418	6/6	0.86	0.15	54,77,81,90	0
34	HTG	b	622	19/19	0.86	0.12	56,81,114,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LMT	B	629	25/35	0.86	0.12	59,92,142,167	0
33	LMG	c	520	51/55	0.86	0.10	74,137,172,177	0
27	GOL	c	526	6/6	0.86	0.17	99,110,125,131	0
33	LMG	z	101	39/55	0.86	0.13	76,130,154,170	0
36	CA	f	103	1/1	0.86	0.11	121,121,121,121	0
31	LMT	b	627	25/35	0.87	0.12	58,97,145,159	0
29	PL9	a	413[A]	55/55	0.87	0.15	90,111,123,128	55
31	LMT	m	103	35/35	0.87	0.10	66,90,104,112	0
29	PL9	a	413[B]	55/55	0.87	0.15	91,111,123,128	55
26	SQD	l	101	54/54	0.88	0.10	66,95,131,148	0
34	HTG	B	621	19/19	0.88	0.12	61,89,119,125	0
26	SQD	b	620	54/54	0.88	0.10	63,95,115,125	0
27	GOL	D	412	6/6	0.88	0.12	51,66,78,97	0
32	LHG	E	101[A]	42/49	0.88	0.12	76,105,120,125	42
32	LHG	E	101[B]	42/49	0.88	0.12	76,105,120,125	42
27	GOL	V	203[B]	6/6	0.89	0.13	57,68,74,76	6
27	GOL	a	410	6/6	0.89	0.12	71,81,93,94	0
26	SQD	X	101	43/54	0.89	0.11	66,107,130,146	0
27	GOL	V	203[A]	6/6	0.89	0.13	57,68,74,75	6
34	HTG	B	624	19/19	0.90	0.08	65,80,100,104	0
23	CLA	b	601	65/65	0.90	0.09	59,85,126,159	0
36	CA	o	301	1/1	0.90	0.07	112,112,112,112	0
33	LMG	C	501	51/55	0.91	0.09	69,90,112,127	0
23	CLA	B	601	65/65	0.91	0.09	56,77,115,157	0
30	UNL	D	408	17/-	0.91	0.10	60,73,105,123	0
23	CLA	c	513	65/65	0.92	0.09	63,93,130,151	0
33	LMG	a	415	51/55	0.92	0.08	68,94,111,120	0
33	LMG	c	519	51/55	0.92	0.09	63,94,131,156	0
27	GOL	C	523[A]	6/6	0.92	0.10	59,61,65,68	6
33	LMG	m	101	51/55	0.92	0.09	59,74,98,111	0
27	GOL	C	523[B]	6/6	0.92	0.10	59,62,66,68	6
27	GOL	v	202[A]	6/6	0.92	0.11	68,77,83,86	6
33	LMG	B	620	51/55	0.92	0.08	53,73,94,117	0
27	GOL	v	202[B]	6/6	0.92	0.11	68,78,83,86	6
33	LMG	C	520	51/55	0.92	0.09	58,84,122,126	0
26	SQD	A	410[B]	54/54	0.93	0.09	58,80,115,120	54
32	LHG	A	419[A]	49/49	0.93	0.10	52,66,87,92	49
32	LHG	A	419[B]	49/49	0.93	0.10	51,66,87,92	49
27	GOL	B	623	6/6	0.93	0.07	70,75,88,90	0
23	CLA	b	616	65/65	0.93	0.08	48,63,130,144	0
23	CLA	C	514	65/65	0.93	0.08	58,85,116,125	0
26	SQD	a	409[A]	54/54	0.93	0.09	62,83,118,123	54

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	d	410	17/-	0.93	0.09	71,85,109,115	0
26	SQD	a	409[B]	54/54	0.93	0.09	62,82,119,124	54
25	BCR	D	404	40/40	0.93	0.09	49,60,106,108	0
25	BCR	T	102	40/40	0.93	0.07	45,58,70,71	0
34	HTG	b	625	19/19	0.93	0.07	62,81,103,109	0
33	LMG	D	411	51/55	0.93	0.09	51,66,131,140	0
25	BCR	d	406	40/40	0.93	0.08	52,69,108,110	0
25	BCR	t	102	40/40	0.93	0.07	43,59,78,81	0
26	SQD	A	410[A]	54/54	0.93	0.09	58,80,115,119	54
33	LMG	d	413	51/55	0.93	0.08	56,71,116,148	0
25	BCR	K	102	40/40	0.94	0.09	56,65,77,79	0
23	CLA	c	504	65/65	0.94	0.07	52,65,111,135	0
32	LHG	d	415[A]	49/49	0.94	0.09	53,69,82,88	49
32	LHG	d	415[B]	49/49	0.94	0.09	53,70,82,88	49
23	CLA	c	512	65/65	0.94	0.09	61,81,131,143	0
23	CLA	C	507	65/65	0.94	0.08	55,69,122,147	0
29	PL9	D	405[A]	55/55	0.94	0.07	37,51,59,69	55
29	PL9	D	405[B]	55/55	0.94	0.07	37,50,59,70	55
25	BCR	y	101	40/40	0.94	0.07	56,71,81,98	0
23	CLA	d	405	65/65	0.94	0.09	50,65,130,150	0
25	BCR	C	515	40/40	0.94	0.07	56,74,89,91	0
32	LHG	D	407[A]	49/49	0.94	0.09	50,62,109,116	49
35	DGD	C	518[A]	62/66	0.94	0.08	51,64,117,124	62
35	DGD	C	518[B]	62/66	0.94	0.08	51,65,117,124	62
35	DGD	c	517[A]	62/66	0.94	0.08	57,68,122,137	62
35	DGD	c	517[B]	62/66	0.94	0.08	56,68,122,138	62
35	DGD	c	518	62/66	0.94	0.07	49,67,105,134	0
32	LHG	D	407[B]	49/49	0.94	0.09	50,61,109,116	49
23	CLA	C	505	65/65	0.94	0.08	42,57,101,129	0
25	BCR	H	101	40/40	0.94	0.08	51,65,84,90	0
23	CLA	B	616	65/65	0.95	0.09	47,61,132,140	0
23	CLA	c	506	65/65	0.95	0.08	51,69,125,143	0
23	CLA	c	507	65/65	0.95	0.08	52,69,87,93	0
23	CLA	A	408	65/65	0.95	0.08	43,52,131,147	0
23	CLA	B	603	65/65	0.95	0.07	42,54,72,82	0
23	CLA	C	509	65/65	0.95	0.07	47,56,129,144	0
25	BCR	A	409	40/40	0.95	0.07	38,52,66,70	0
25	BCR	B	618	40/40	0.95	0.06	41,56,71,86	0
25	BCR	B	619	40/40	0.95	0.07	47,59,93,95	0
23	CLA	C	513	65/65	0.95	0.08	55,72,115,136	0
23	CLA	B	606	65/65	0.95	0.08	44,58,119,129	0
23	CLA	D	403	65/65	0.95	0.08	46,59,127,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	a	405[A]	65/65	0.95	0.07	43,54,125,137	65
23	CLA	a	405[B]	65/65	0.95	0.07	43,54,125,137	65
25	BCR	Y	101	40/40	0.95	0.07	53,66,85,87	0
25	BCR	a	408	40/40	0.95	0.07	45,55,66,71	0
25	BCR	b	619	40/40	0.95	0.07	49,60,88,90	0
25	BCR	c	514	40/40	0.95	0.07	67,80,95,101	0
23	CLA	a	407	65/65	0.95	0.09	41,58,142,155	0
25	BCR	h	101	40/40	0.95	0.08	55,69,93,95	0
23	CLA	B	611	65/65	0.95	0.07	38,47,67,77	0
30	UNL	X	102	18/-	0.95	0.10	61,75,108,109	0
23	CLA	b	606	65/65	0.95	0.07	44,59,118,129	0
23	CLA	b	614	65/65	0.95	0.07	42,52,98,114	0
27	GOL	c	525[A]	6/6	0.95	0.07	64,69,73,75	6
27	GOL	c	525[B]	6/6	0.95	0.07	64,69,73,75	6
23	CLA	B	614	65/65	0.95	0.07	38,52,106,125	0
35	DGD	C	519	62/66	0.95	0.07	46,60,102,124	0
35	DGD	H	102	62/66	0.95	0.08	47,63,75,87	0
35	DGD	c	516[A]	62/66	0.95	0.07	48,64,102,111	62
35	DGD	c	516[B]	62/66	0.95	0.07	47,64,102,111	62
32	LHG	b	629[A]	49/49	0.95	0.08	52,60,69,95	49
32	LHG	b	629[B]	49/49	0.95	0.08	52,60,69,96	49
32	LHG	d	408[A]	49/49	0.95	0.08	51,59,73,79	49
35	DGD	h	102	62/66	0.95	0.08	53,67,78,85	0
32	LHG	d	408[B]	49/49	0.95	0.08	50,59,74,79	49
36	CA	O	301	1/1	0.95	0.04	105,105,105,105	0
32	LHG	d	409[A]	49/49	0.95	0.09	54,65,114,131	49
32	LHG	d	409[B]	49/49	0.95	0.09	54,65,114,132	49
25	BCR	k	101	40/40	0.96	0.08	58,74,86,88	0
23	CLA	A	404[A]	65/65	0.96	0.06	36,44,61,71	65
30	UNL	x	101	18/-	0.96	0.10	70,83,127,136	0
23	CLA	A	404[B]	65/65	0.96	0.06	36,44,63,72	65
23	CLA	c	508	65/65	0.96	0.07	45,64,124,146	0
23	CLA	B	602	65/65	0.96	0.06	48,56,73,86	0
23	CLA	C	502	65/65	0.96	0.06	50,61,73,77	0
23	CLA	C	504	65/65	0.96	0.06	46,61,73,80	0
24	PHO	A	416[A]	64/64	0.96	0.06	38,51,57,65	64
24	PHO	A	416[B]	64/64	0.96	0.06	38,51,57,65	64
24	PHO	d	403[A]	64/64	0.96	0.06	45,55,63,68	64
24	PHO	d	403[B]	64/64	0.96	0.06	44,55,62,68	64
23	CLA	A	406[A]	65/65	0.96	0.06	42,49,115,125	65
25	BCR	B	617	40/40	0.96	0.05	43,53,67,68	0
23	CLA	b	602	65/65	0.96	0.07	49,61,81,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
29	PL9	d	407[A]	55/55	0.96	0.07	40,52,62,70	55
29	PL9	d	407[B]	55/55	0.96	0.07	40,52,62,70	55
23	CLA	b	603	65/65	0.96	0.06	43,58,82,90	0
23	CLA	A	406[B]	65/65	0.96	0.06	42,49,116,126	65
32	LHG	D	406[A]	49/49	0.96	0.07	47,56,68,78	49
32	LHG	D	406[B]	49/49	0.96	0.07	47,56,68,79	49
25	BCR	C	516	40/40	0.96	0.06	50,64,75,84	0
35	DGD	C	517[A]	62/66	0.96	0.07	47,58,102,106	62
35	DGD	C	517[B]	62/66	0.96	0.07	46,58,102,106	62
23	CLA	b	607	65/65	0.96	0.06	39,48,78,90	0
23	CLA	b	609	65/65	0.96	0.07	47,65,79,92	0
23	CLA	b	611	65/65	0.96	0.06	39,52,72,76	0
23	CLA	b	612	65/65	0.96	0.07	39,54,66,74	0
23	CLA	C	508	65/65	0.96	0.07	49,63,85,98	0
23	CLA	B	607	65/65	0.96	0.06	35,49,78,84	0
25	BCR	b	617	40/40	0.96	0.06	46,56,63,70	0
25	BCR	b	618	40/40	0.96	0.06	47,57,76,86	0
23	CLA	c	501	65/65	0.96	0.07	54,66,79,93	0
23	CLA	c	503	65/65	0.96	0.06	47,71,83,94	0
25	BCR	c	515	40/40	0.96	0.06	57,65,78,79	0
27	GOL	b	628	6/6	0.96	0.07	84,88,96,97	0
36	CA	c	522	1/1	0.96	0.08	76,76,76,76	0
23	CLA	B	610	65/65	0.96	0.08	39,55,65,86	0
23	CLA	c	505	65/65	0.96	0.07	49,65,93,105	0
37	BCT	D	401[A]	4/4	0.96	0.07	56,59,60,66	4
37	BCT	D	401[B]	4/4	0.96	0.07	56,58,61,67	4
37	BCT	d	401[A]	4/4	0.96	0.07	59,61,71,78	4
37	BCT	d	401[B]	4/4	0.96	0.07	59,62,72,79	4
23	CLA	d	402[B]	65/65	0.97	0.05	41,46,61,71	65
23	CLA	d	404[A]	65/65	0.97	0.06	40,47,77,96	65
23	CLA	d	404[B]	65/65	0.97	0.06	40,47,77,96	65
23	CLA	C	506	65/65	0.97	0.06	43,63,91,104	0
23	CLA	B	605	65/65	0.97	0.06	39,49,67,84	0
23	CLA	b	604	65/65	0.97	0.07	40,52,99,123	0
24	PHO	a	406[A]	64/64	0.97	0.05	44,49,56,59	64
24	PHO	a	406[B]	64/64	0.97	0.05	44,49,56,59	64
23	CLA	b	605	65/65	0.97	0.07	39,51,76,85	0
23	CLA	B	612	65/65	0.97	0.06	37,51,61,75	0
23	CLA	B	613	65/65	0.97	0.06	41,48,97,114	0
23	CLA	b	608	65/65	0.97	0.05	43,56,79,92	0
23	CLA	C	510	65/65	0.97	0.07	47,59,83,91	0
23	CLA	b	610	65/65	0.97	0.06	48,57,68,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	511	65/65	0.97	0.06	49,58,80,87	0
23	CLA	C	512	65/65	0.97	0.07	51,64,81,84	0
32	LHG	L	101[A]	49/49	0.97	0.07	52,59,70,91	49
32	LHG	L	101[B]	49/49	0.97	0.07	52,59,70,91	49
23	CLA	b	613	65/65	0.97	0.05	41,50,84,100	0
23	CLA	A	405[A]	65/65	0.97	0.05	36,44,57,70	65
23	CLA	b	615	65/65	0.97	0.06	48,61,82,91	0
23	CLA	B	615	65/65	0.97	0.06	43,54,80,91	0
23	CLA	D	402[A]	65/65	0.97	0.07	37,44,68,81	65
23	CLA	c	502	65/65	0.97	0.06	46,61,94,106	0
23	CLA	D	402[B]	65/65	0.97	0.07	36,44,69,82	65
23	CLA	A	405[B]	65/65	0.97	0.05	36,44,57,70	65
23	CLA	a	404[A]	65/65	0.97	0.06	39,47,61,78	65
36	CA	C	524	1/1	0.97	0.05	72,72,72,72	0
23	CLA	a	404[B]	65/65	0.97	0.06	38,47,62,78	65
23	CLA	B	608	65/65	0.97	0.05	39,50,71,83	0
23	CLA	C	503	65/65	0.97	0.06	44,55,82,93	0
23	CLA	c	509	65/65	0.97	0.07	49,63,90,101	0
23	CLA	c	510	65/65	0.97	0.06	51,64,81,89	0
23	CLA	c	511	65/65	0.97	0.07	57,68,91,106	0
23	CLA	B	609	65/65	0.97	0.06	46,59,72,76	0
23	CLA	B	604	65/65	0.97	0.06	37,48,115,128	0
23	CLA	d	402[A]	65/65	0.97	0.05	42,47,61,71	65
22	CL	A	402[B]	1/1	0.98	0.06	43,43,43,43	1
24	PHO	A	407[A]	64/64	0.98	0.05	38,46,55,58	64
24	PHO	A	407[B]	64/64	0.98	0.05	38,46,55,58	64
22	CL	a	403[A]	1/1	0.98	0.08	52,52,52,52	1
22	CL	a	403[B]	1/1	0.98	0.08	52,52,52,52	1
22	CL	A	402[A]	1/1	0.98	0.06	43,43,43,43	1
38	HEM	f	101	43/43	0.98	0.08	60,79,110,137	0
40	HEC	V	201	43/43	0.98	0.06	41,51,57,61	0
40	HEC	v	201	43/43	0.98	0.07	53,62,69,75	0
28	OEX	A	413[A]	10/10	0.99	0.03	41,45,48,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	41,44,48,50	10
22	CL	A	403[A]	1/1	0.99	0.03	47,47,47,47	1
22	CL	A	403[B]	1/1	0.99	0.03	47,47,47,47	1
22	CL	a	402[A]	1/1	0.99	0.05	50,50,50,50	1
38	HEM	E	102	43/43	0.99	0.06	53,69,80,89	0
22	CL	a	402[B]	1/1	0.99	0.05	50,50,50,50	1
39	MG	J	102	1/1	0.99	0.03	60,60,60,60	0
39	MG	j	102	1/1	0.99	0.05	64,64,64,64	0
21	FE2	a	401[A]	1/1	0.99	0.02	55,55,55,55	1

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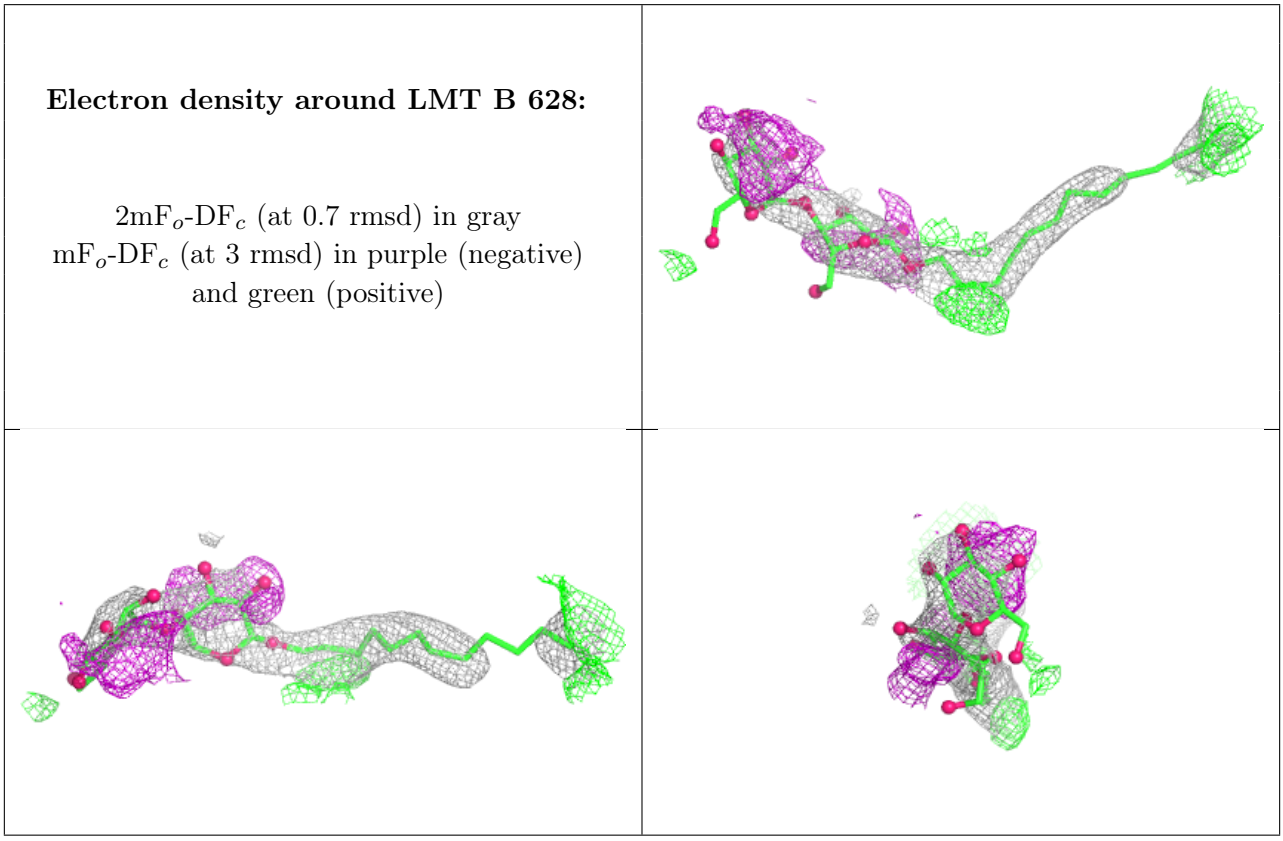
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	a	401[B]	1/1	0.99	0.02	54,54,54,54	1
28	OEX	a	412[B]	10/10	1.00	0.02	47,49,51,55	10
21	FE2	A	401[A]	1/1	1.00	0.01	51,51,51,51	1
36	CA	c	523	1/1	1.00	0.03	78,78,78,78	0
21	FE2	A	401[B]	1/1	1.00	0.01	52,52,52,52	1
28	OEX	a	412[A]	10/10	1.00	0.02	47,49,51,55	10

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

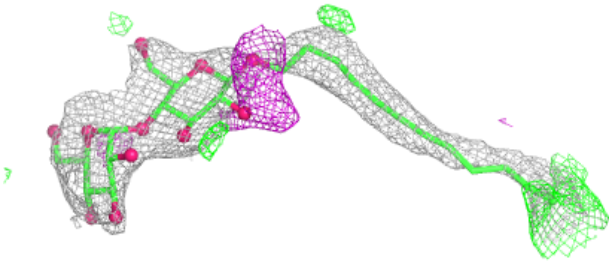
Electron density around LMT B 628:

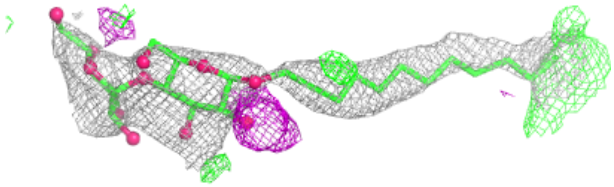
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

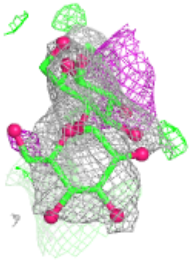


Electron density around LMT A 417:

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

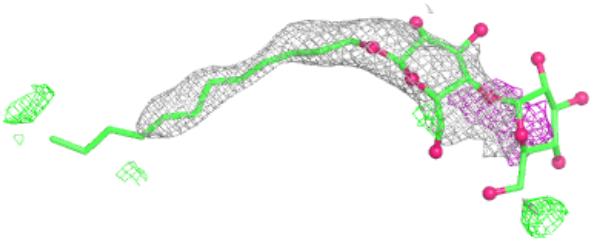


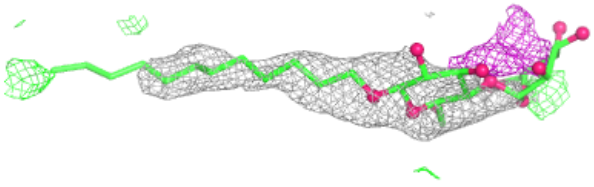


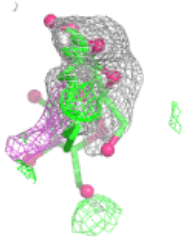


Electron density around LMT F 101:

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

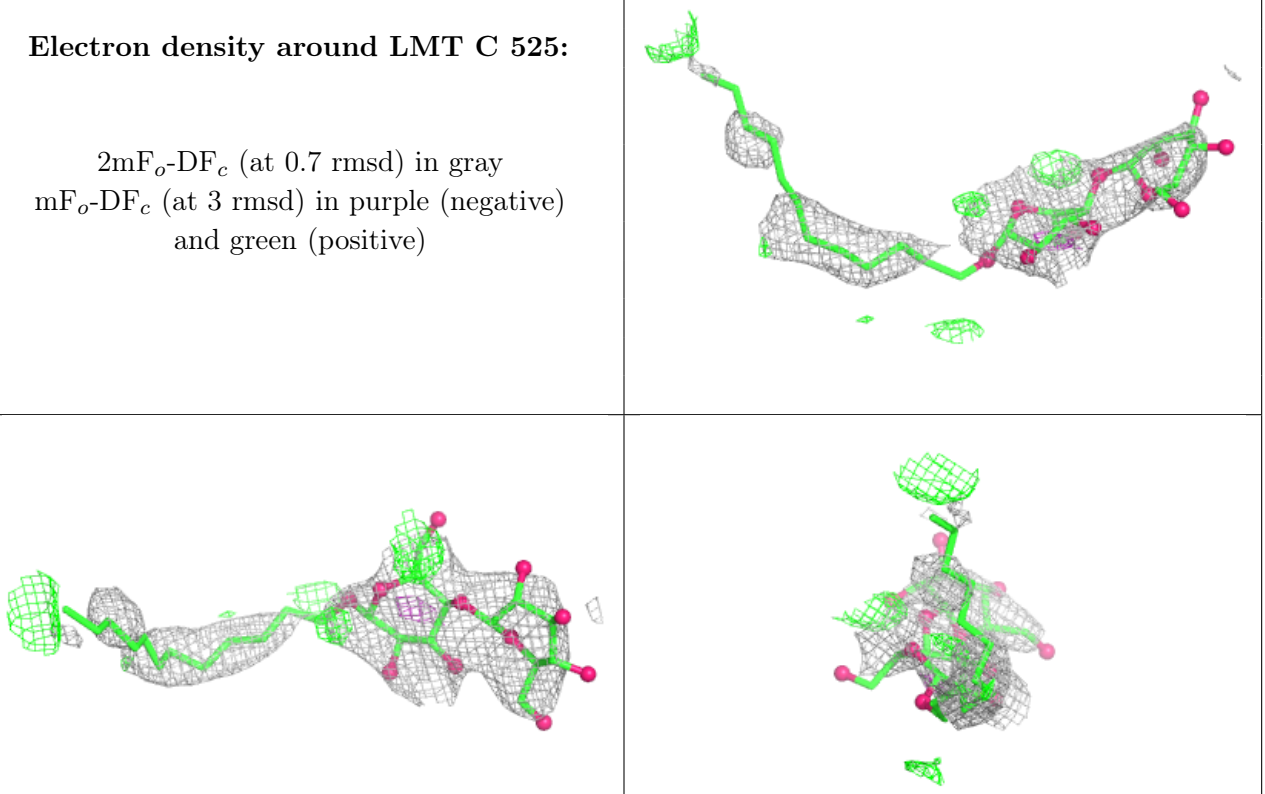






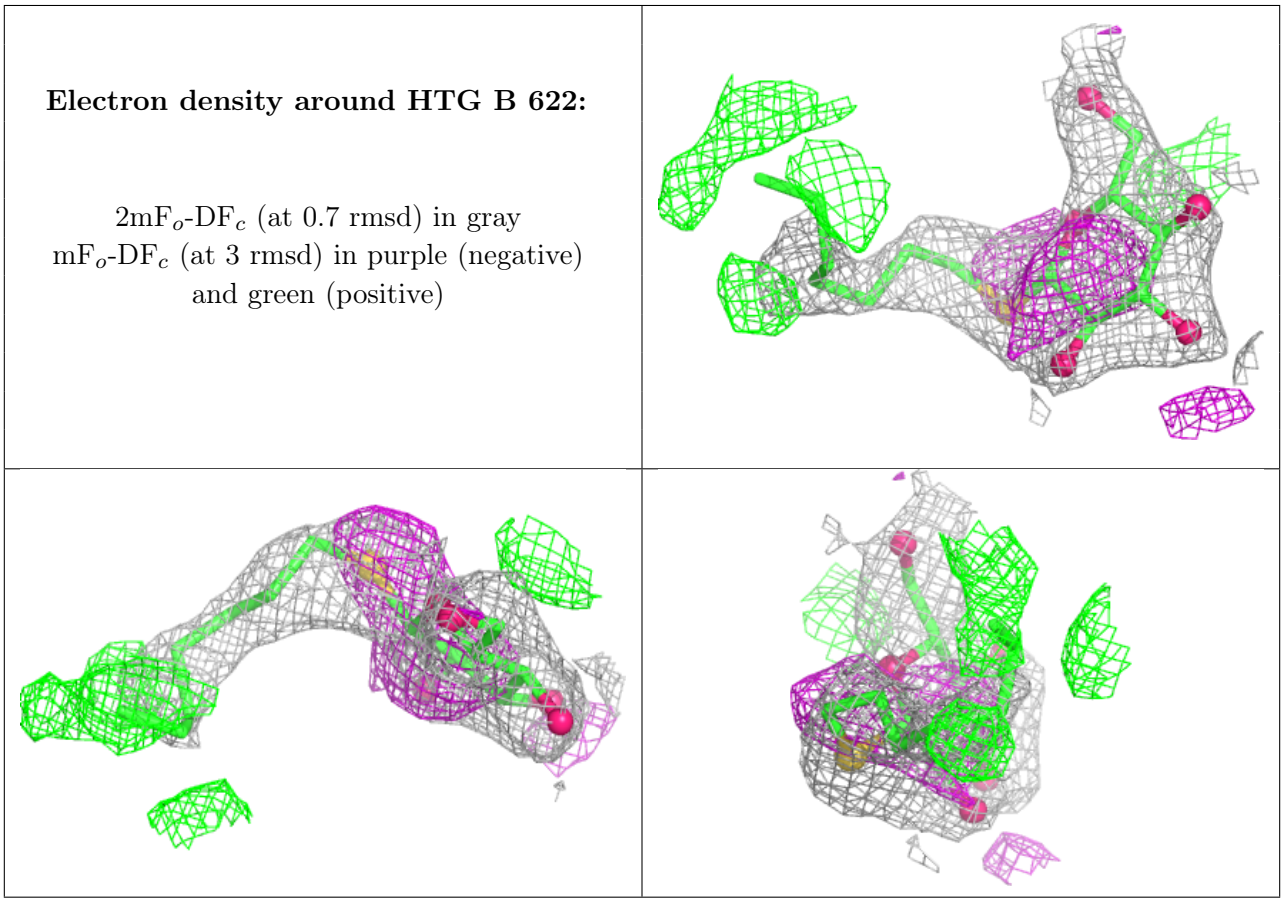
Electron density around LMT C 525:

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



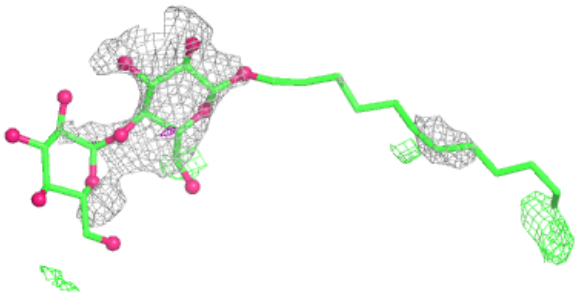
Electron density around HTG B 622:

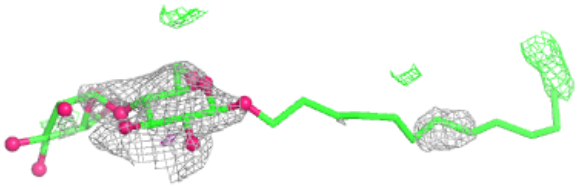
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

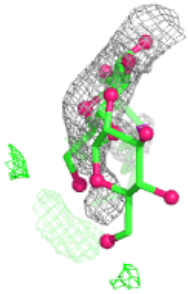


Electron density around LMT e 101:

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

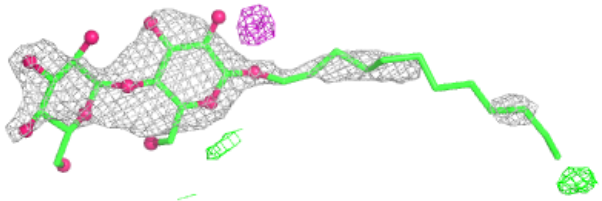


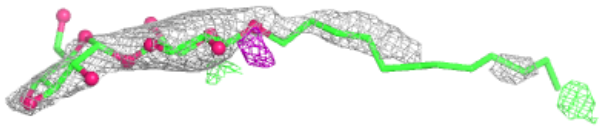




Electron density around LMT a 416:

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

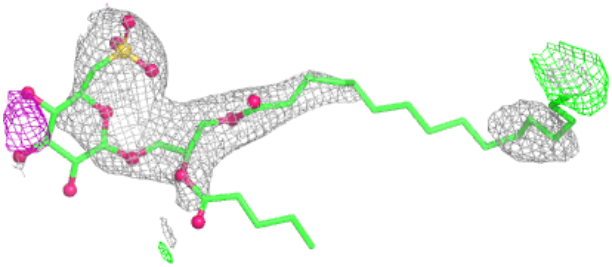


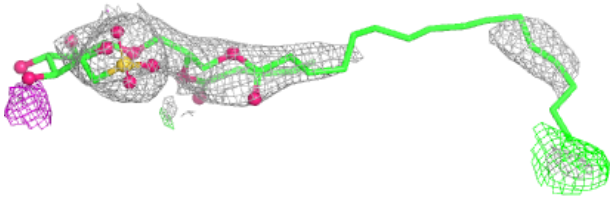


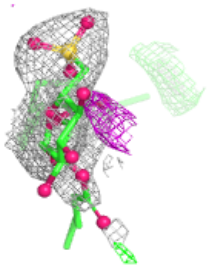


Electron density around SQD f 102:

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

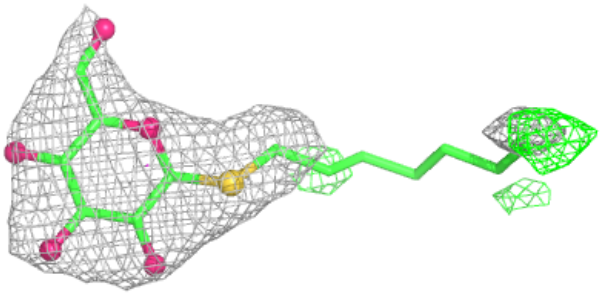


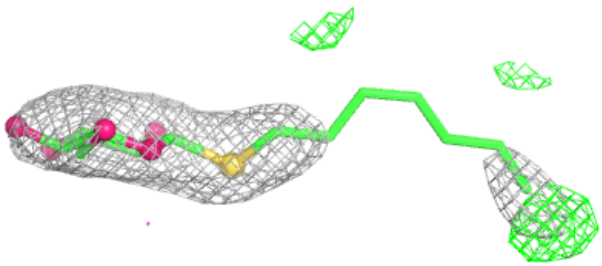


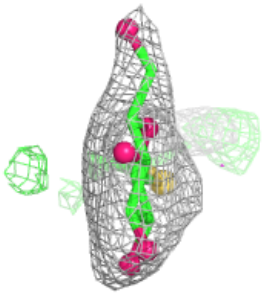


Electron density around HTG C 522:

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

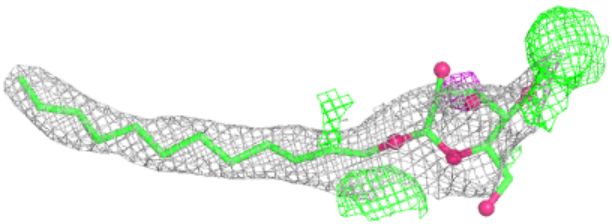


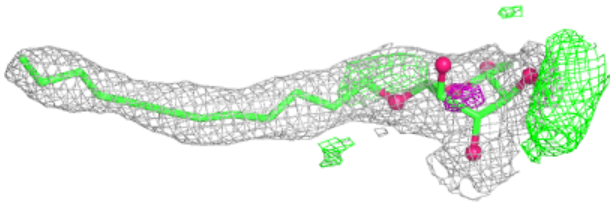


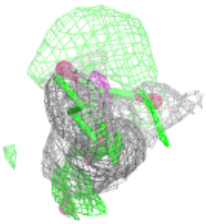


Electron density around LMT b 621:

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

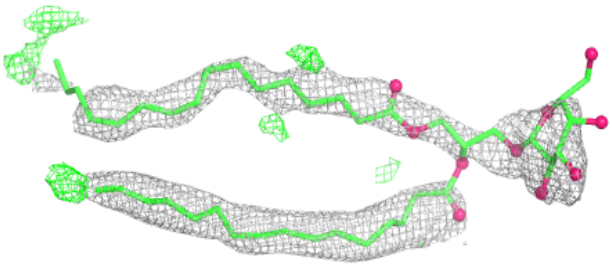


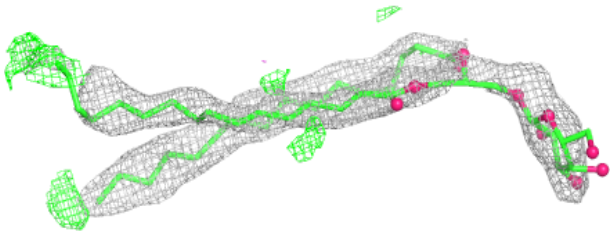


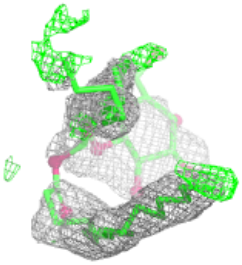


Electron density around LMG C 521:

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

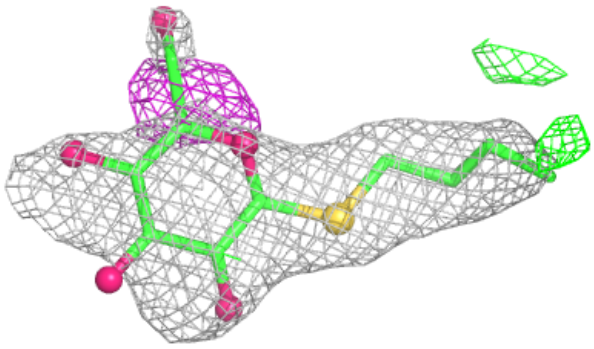


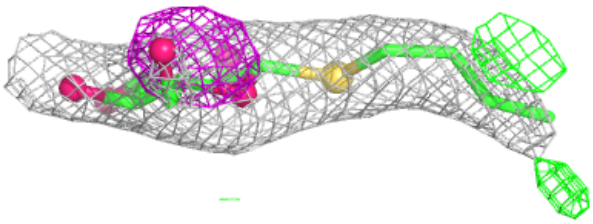


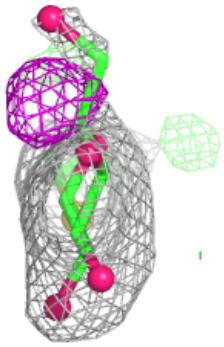


Electron density around HTG D 410:

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

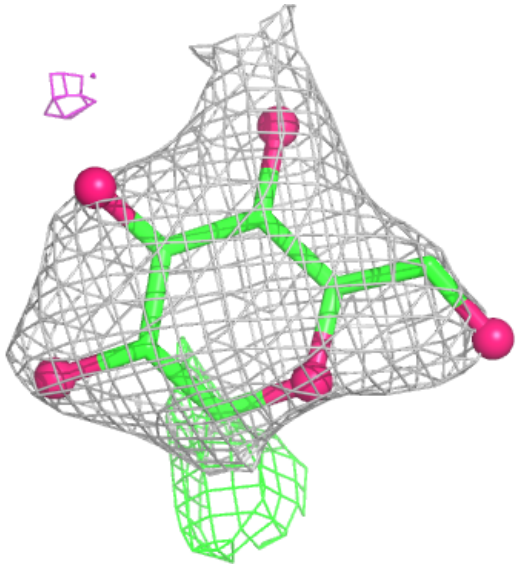


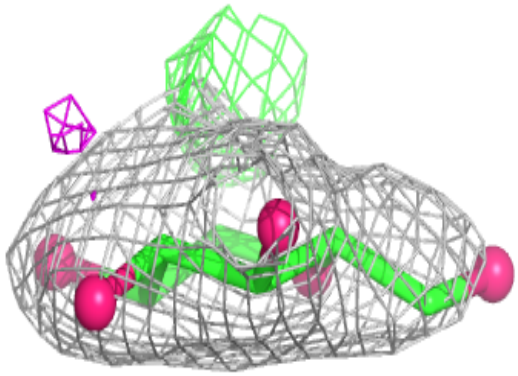


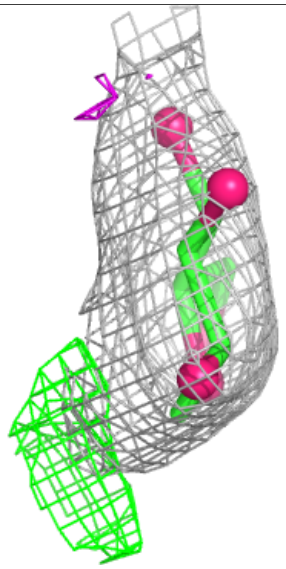


Electron density around HTG V 202:

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

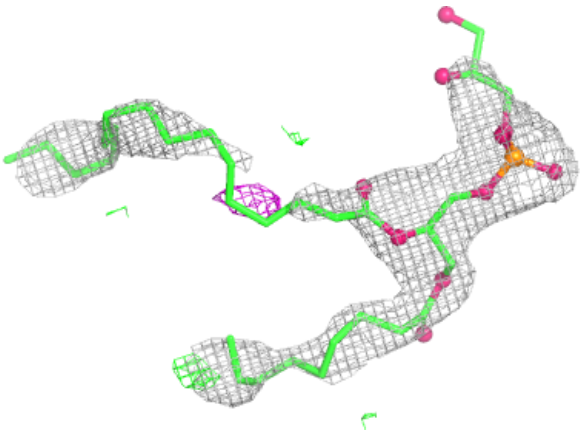


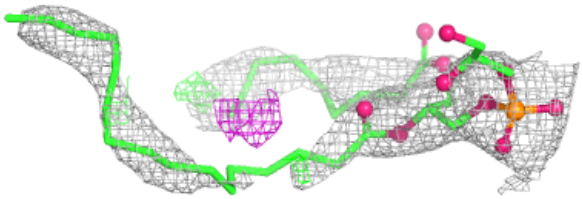


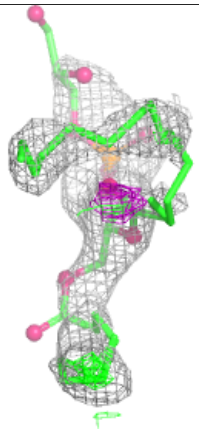


Electron density around LHG a 419 (A):

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

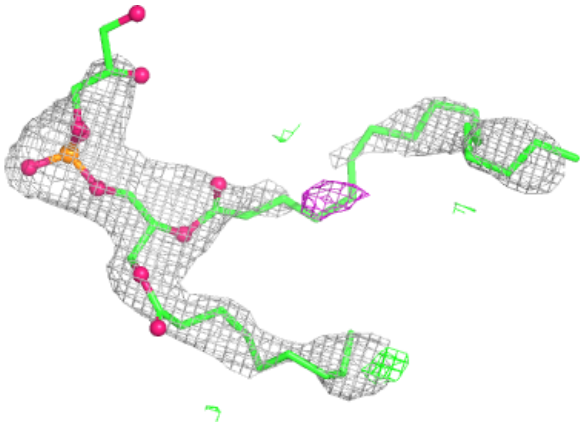


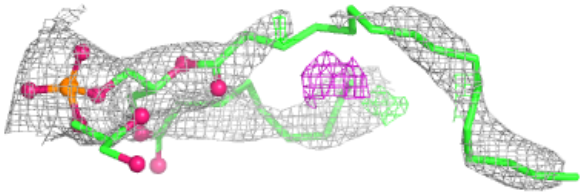


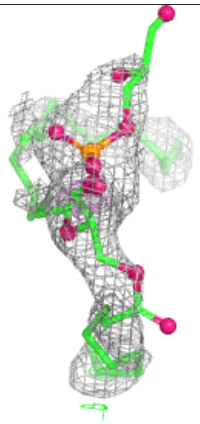


Electron density around LHG a 419 (B):

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

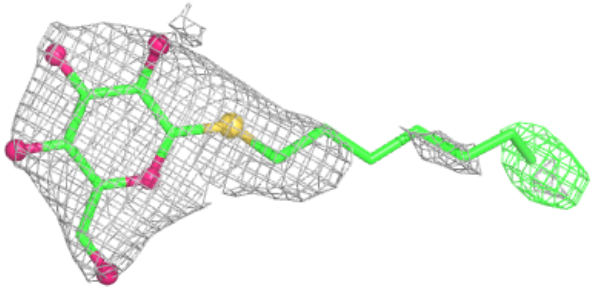


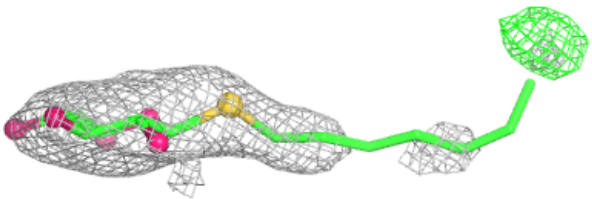


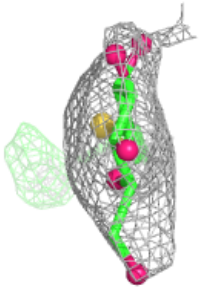


Electron density around HTG c 521:

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

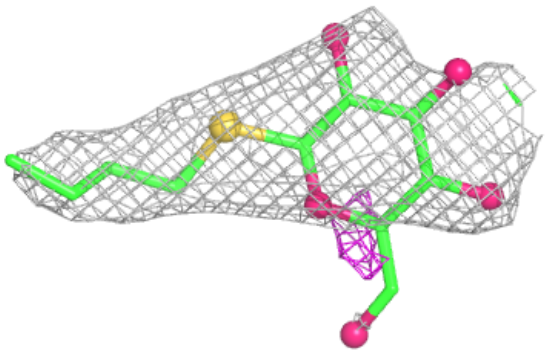


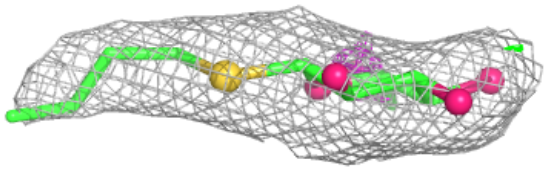


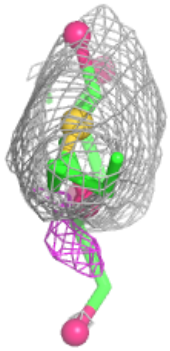


Electron density around HTG d 412:

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

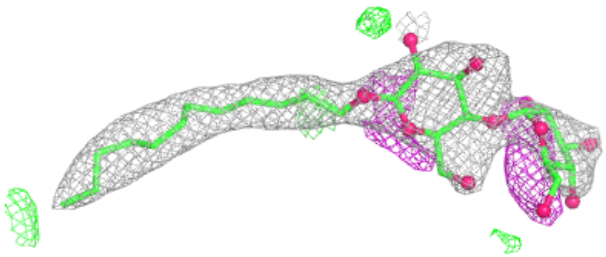


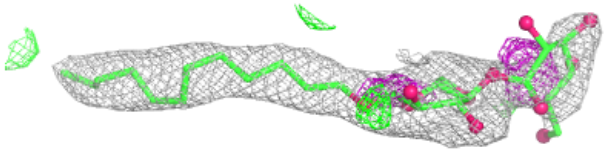


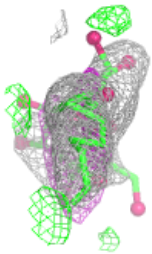


Electron density around LMT B 627:

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

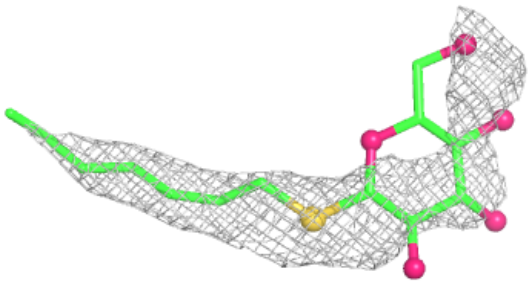


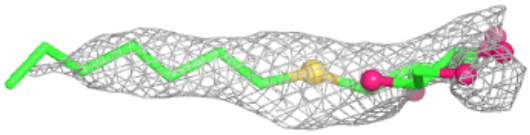


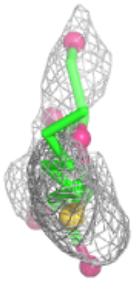


Electron density around HTG b 623:

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

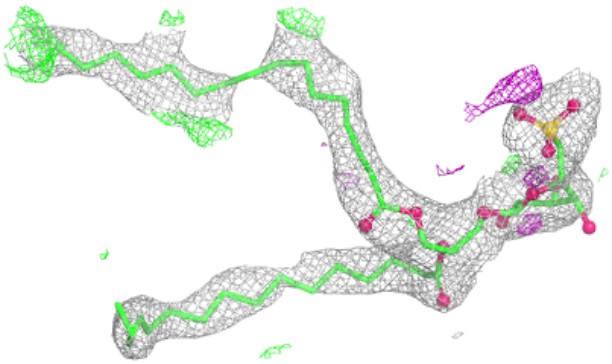


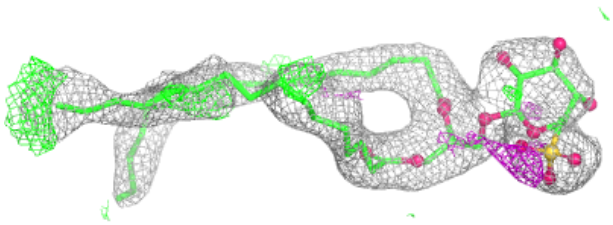


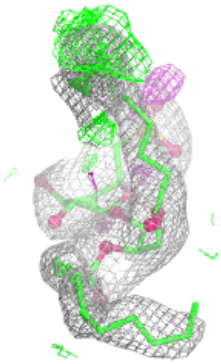


Electron density around SQD a 411:

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

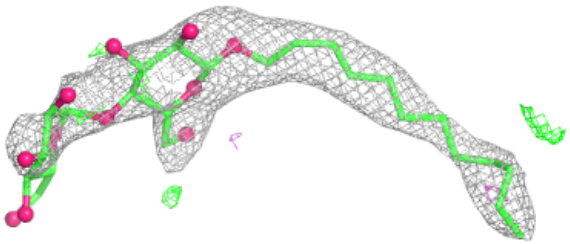


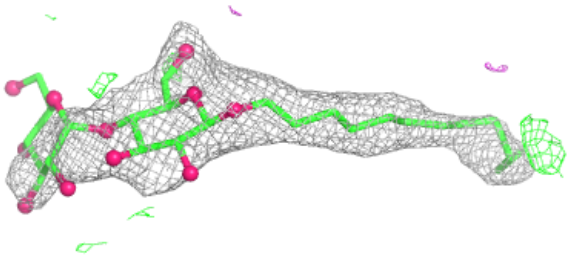


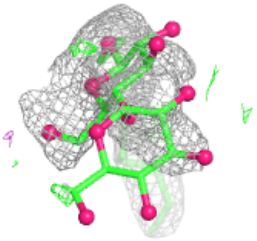


Electron density around LMT T 101:

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

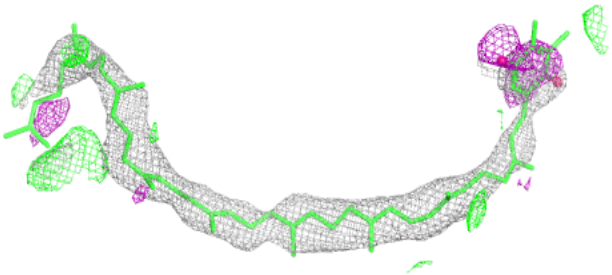


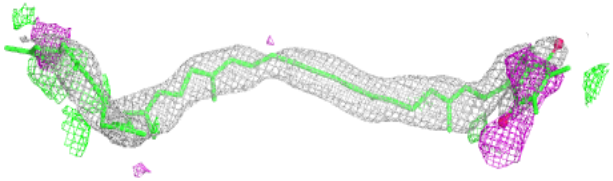


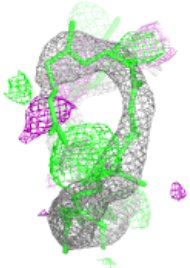


Electron density around PL9 A 414 (B):

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

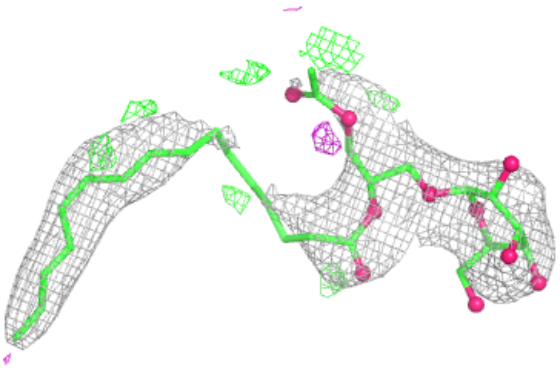


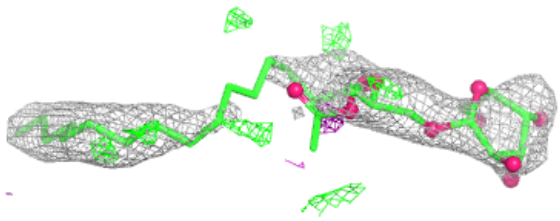


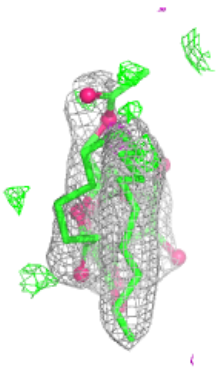


Electron density around LMG Z 101:

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

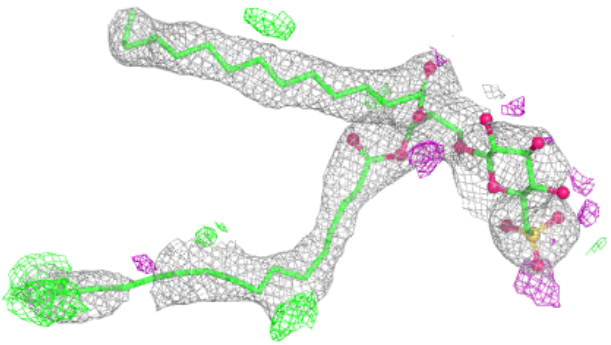


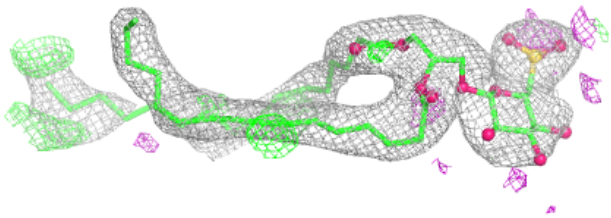


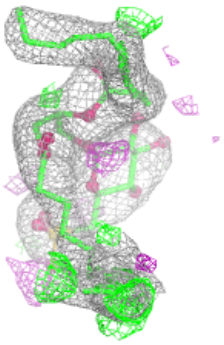


Electron density around SQD A 412:

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

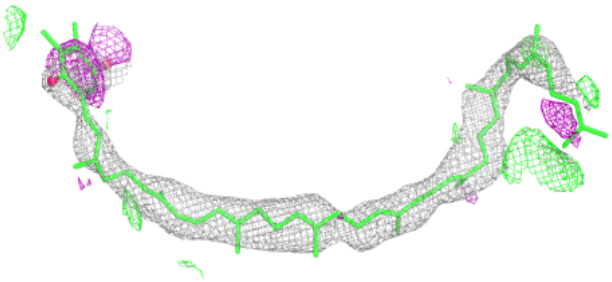


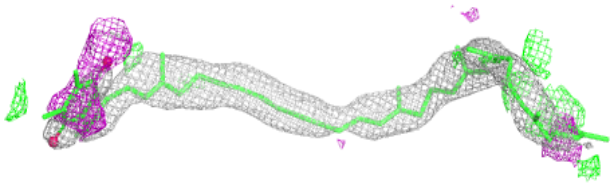


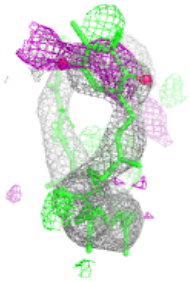


Electron density around PL9 A 414 (A):

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

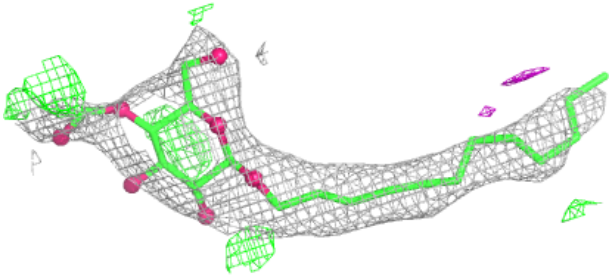


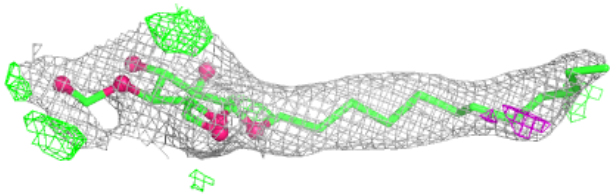


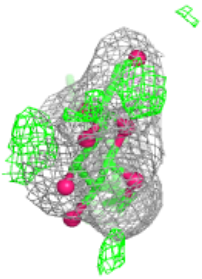


Electron density around LMT t 101:

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

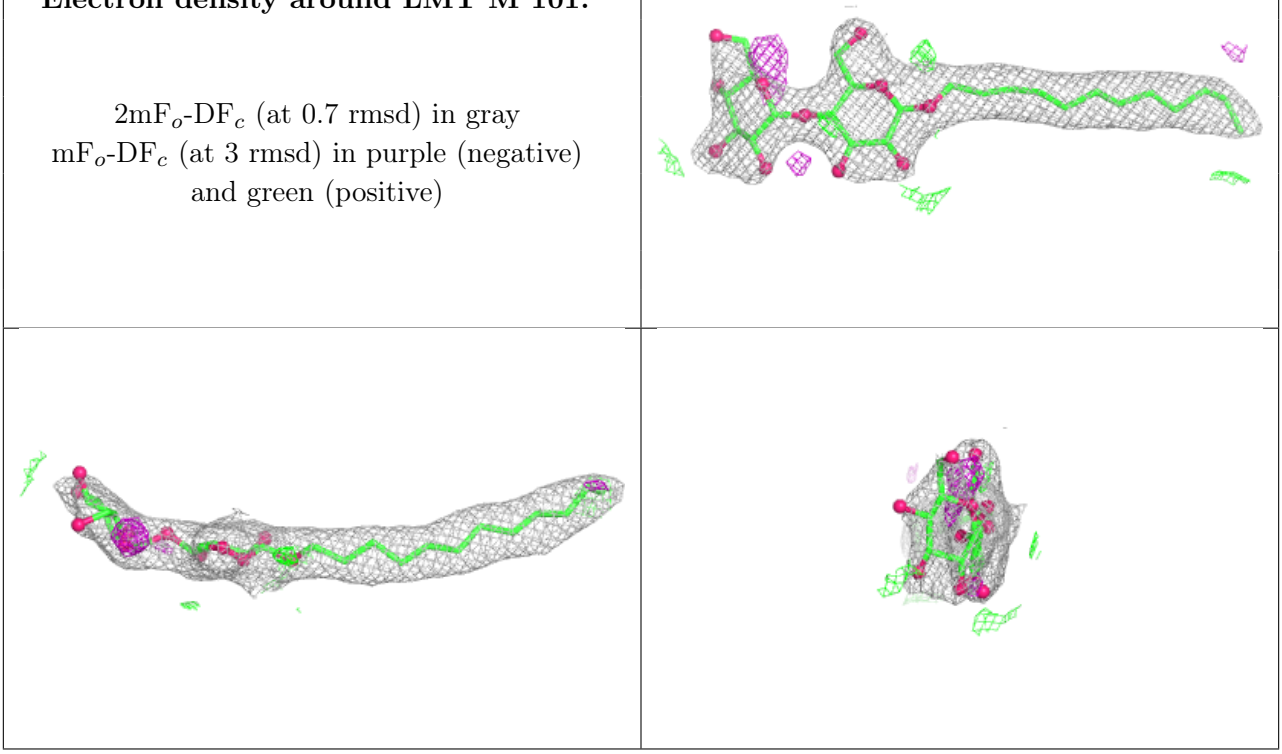






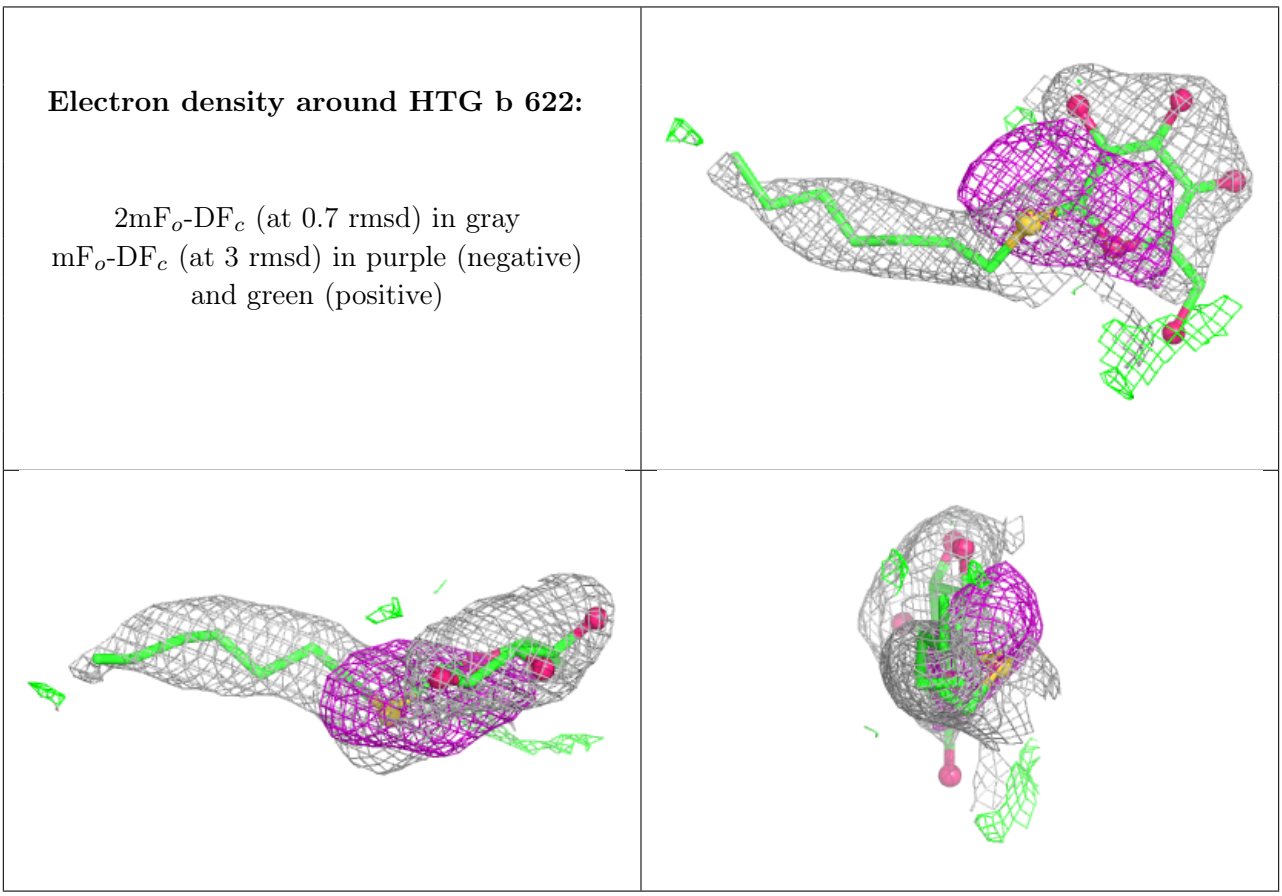
Electron density around LMT M 101:

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



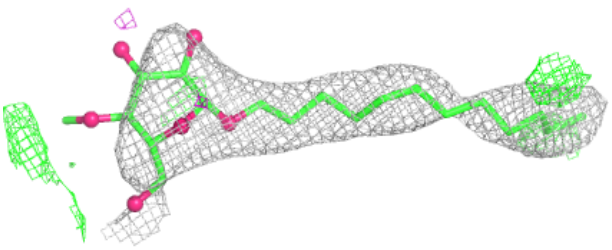
Electron density around HTG b 622:

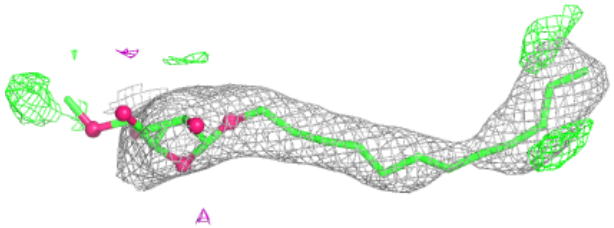
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

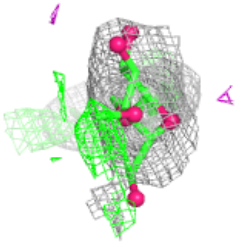


Electron density around LMT B 629:

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

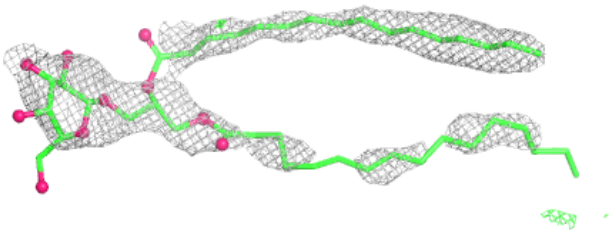


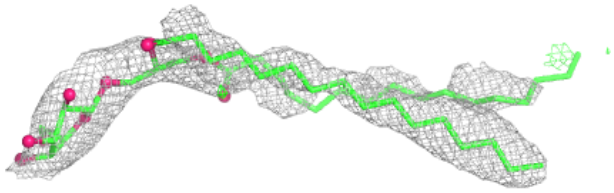


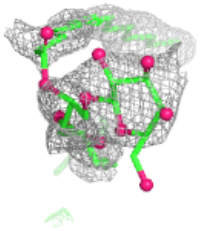


Electron density around LMG c 520:

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

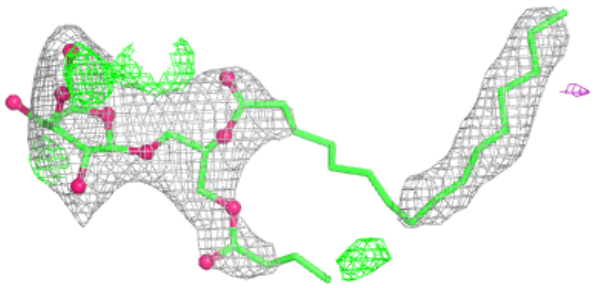


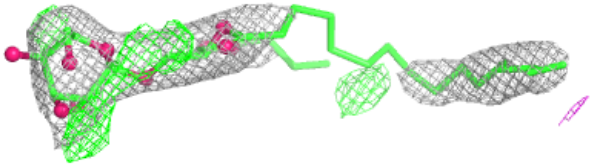


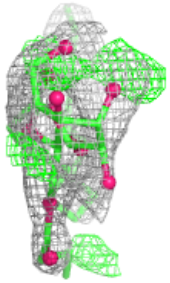


Electron density around LMG z 101:

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

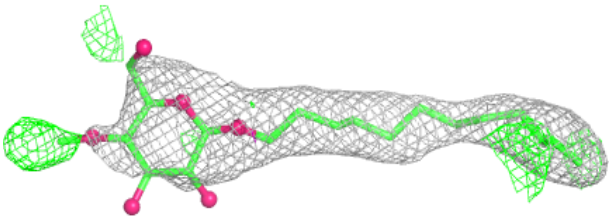


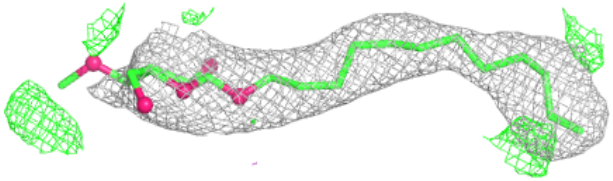


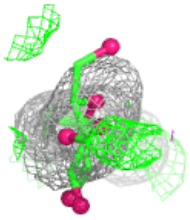


Electron density around LMT b 627:

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

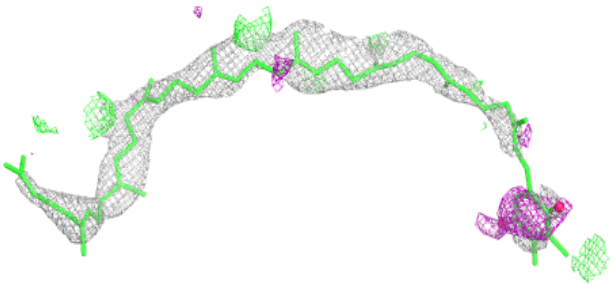


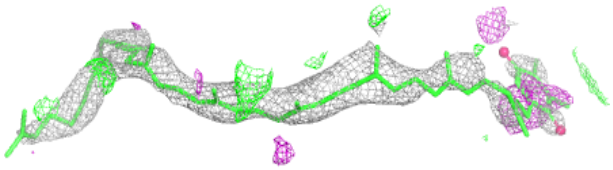


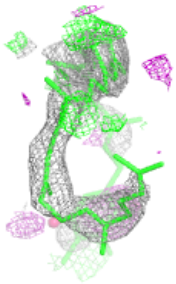


Electron density around PL9 a 413 (A):

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

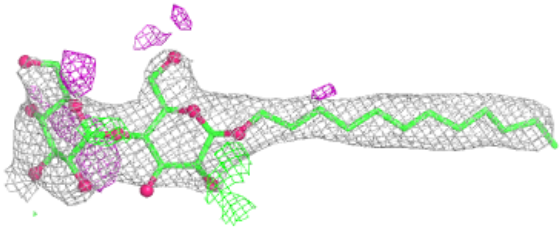


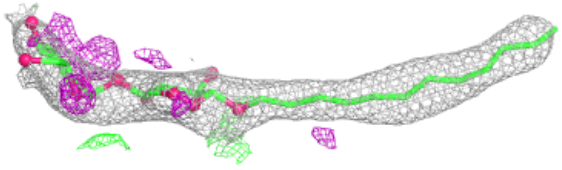


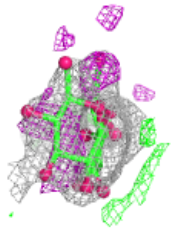


Electron density around LMT m 103:

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

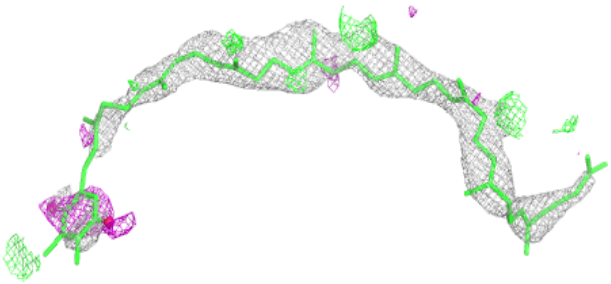


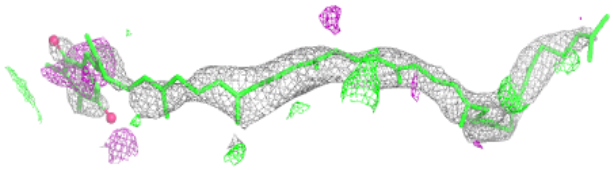


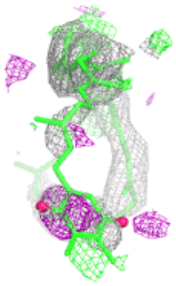


Electron density around PL9 a 413 (B):

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

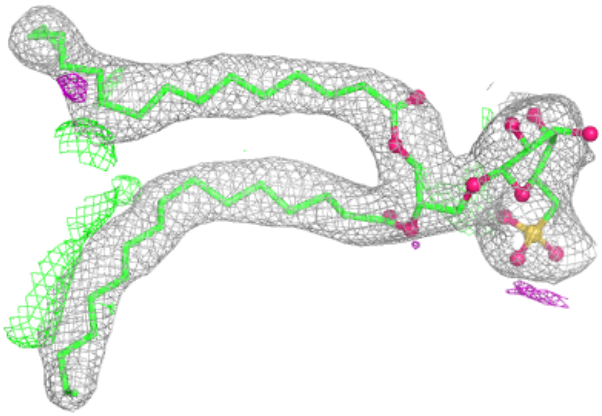


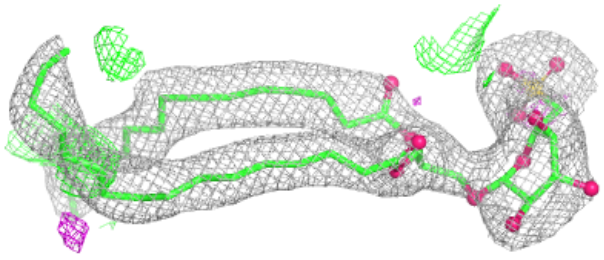


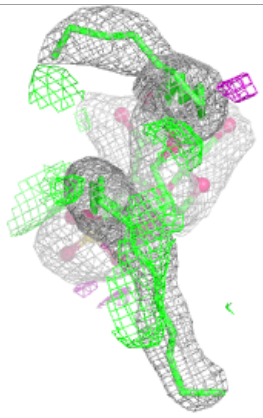


Electron density around SQD l 101:

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

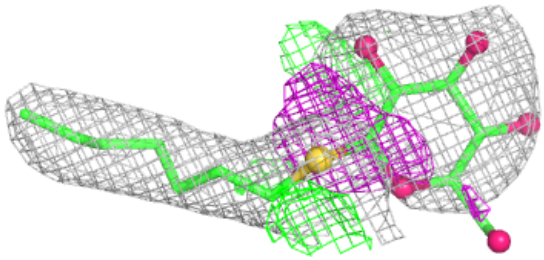


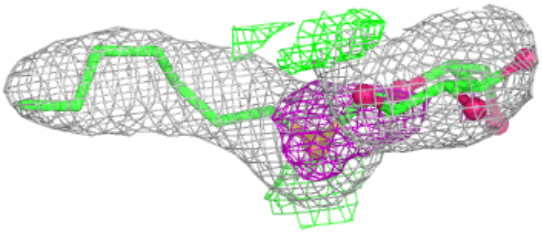


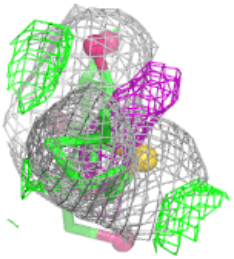


Electron density around HTG B 621:

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

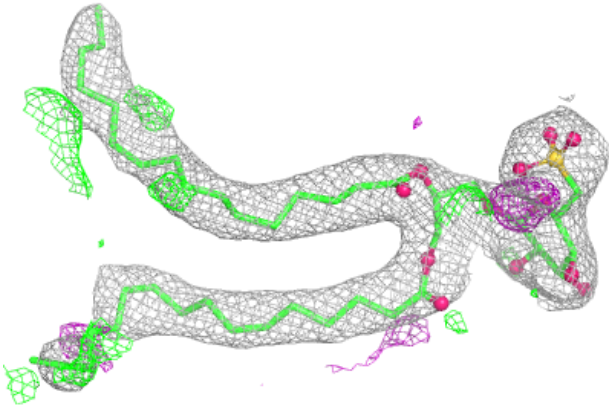


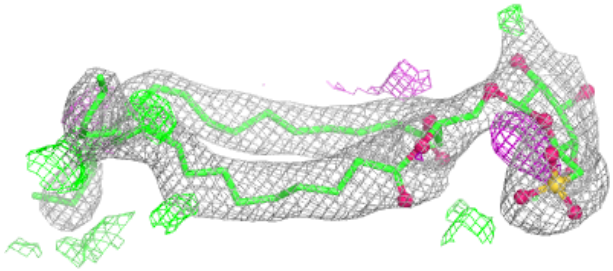


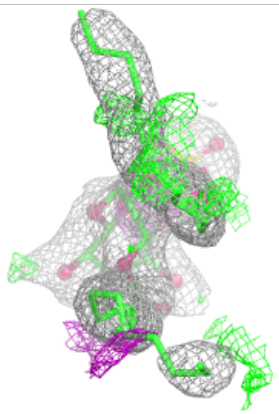


Electron density around SQD b 620:

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

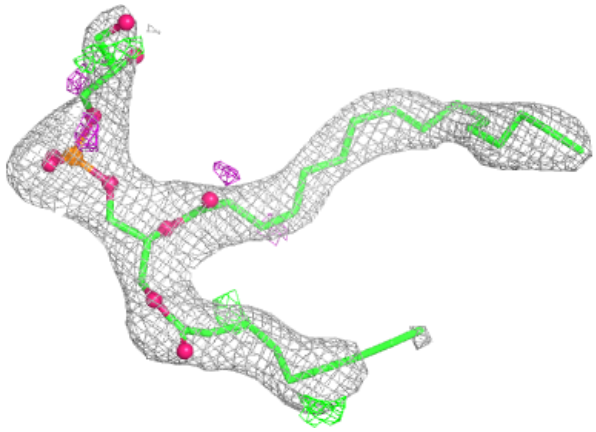


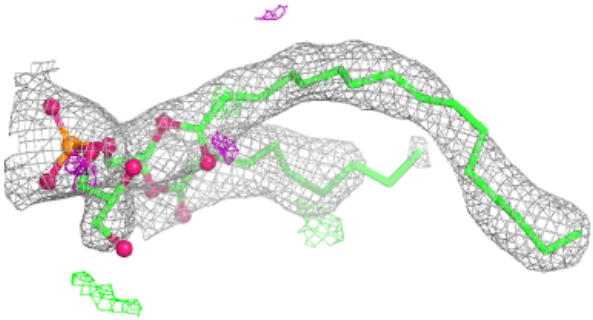




Electron density around LHG E 101 (A):

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

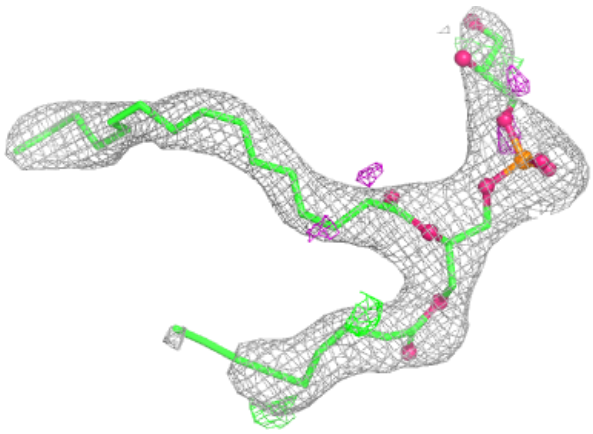


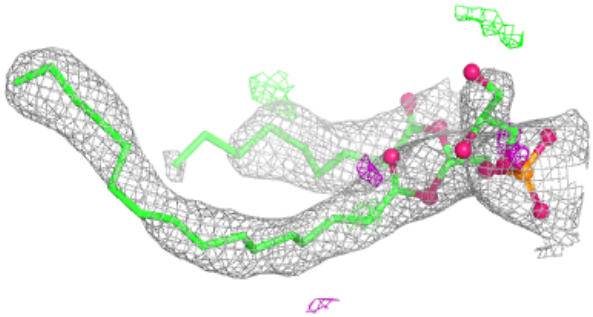




Electron density around LHG E 101 (B):

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

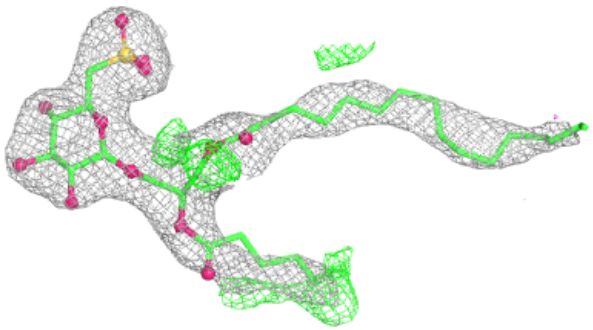


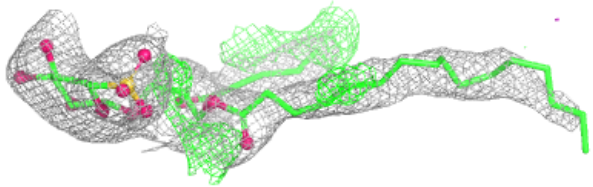


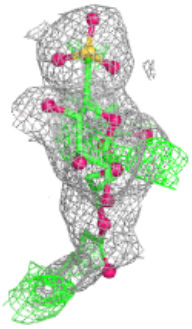


Electron density around SQD X 101:

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

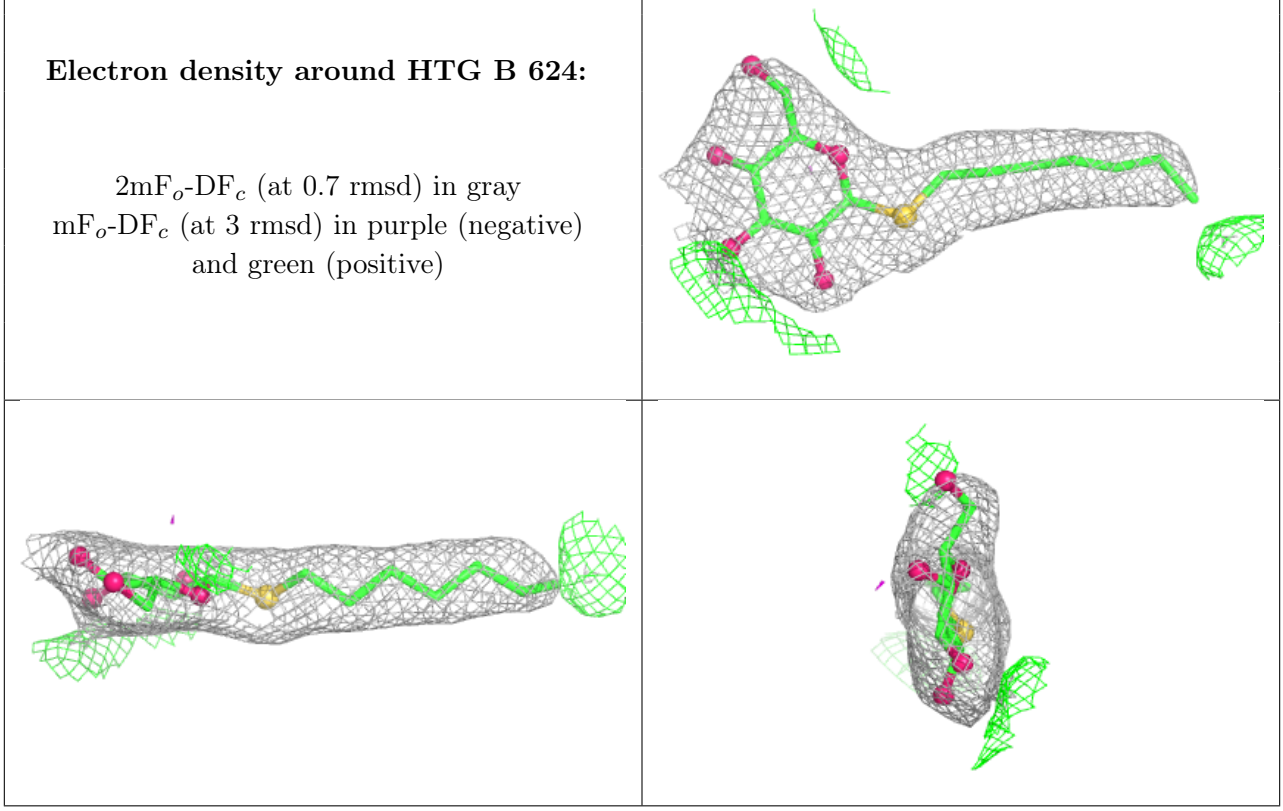






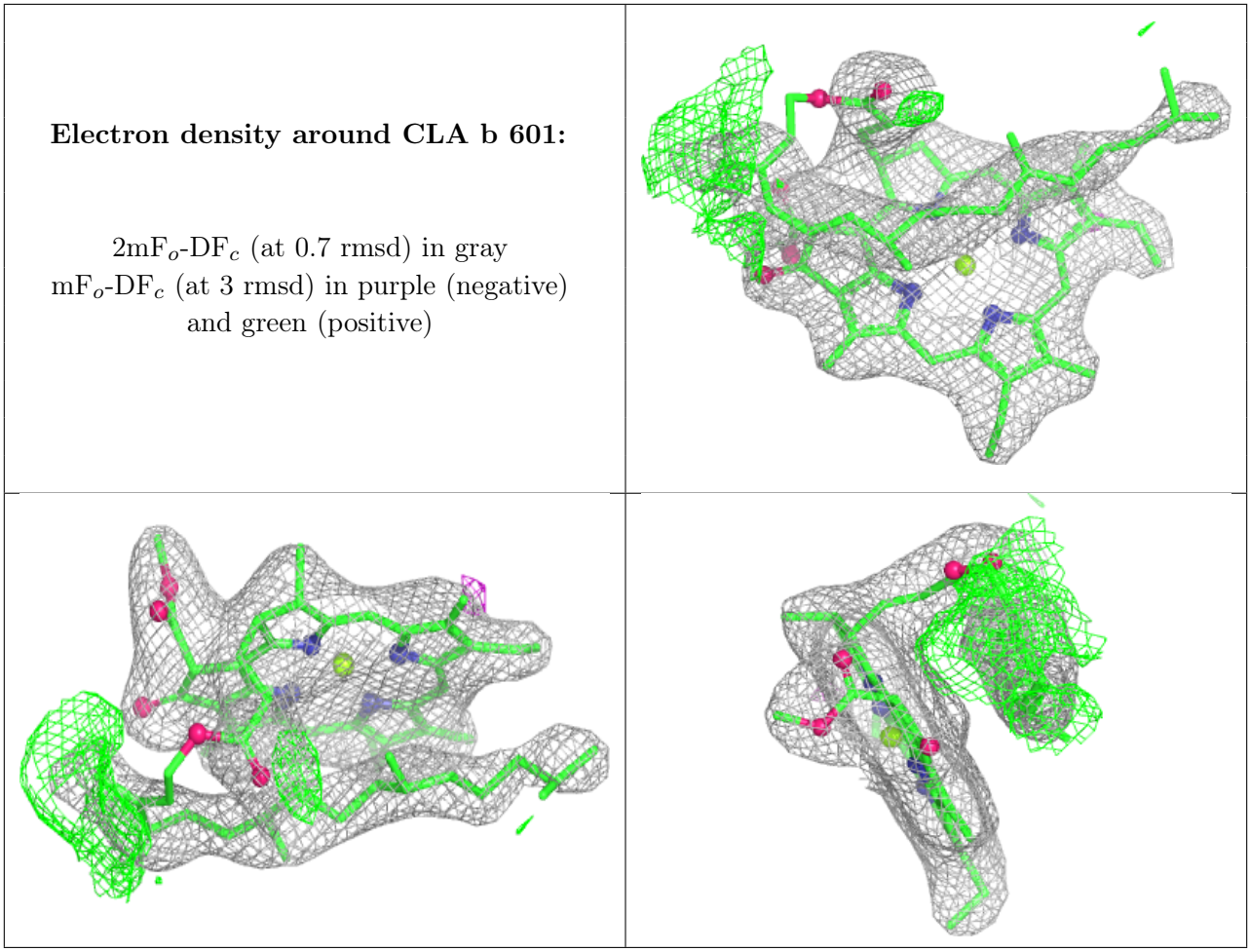
Electron density around HTG B 624:

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



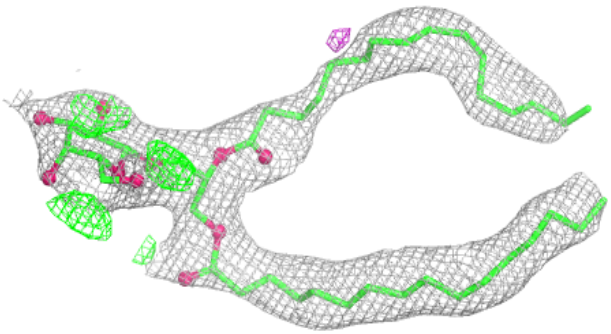
Electron density around CLA b 601:

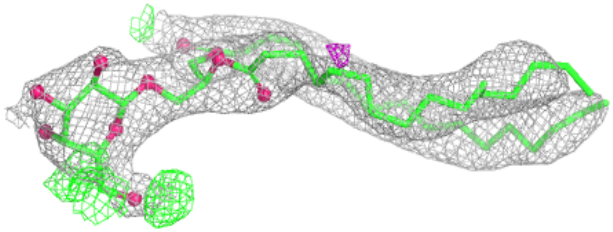
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

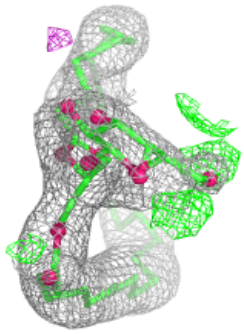


Electron density around LMG C 501:

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

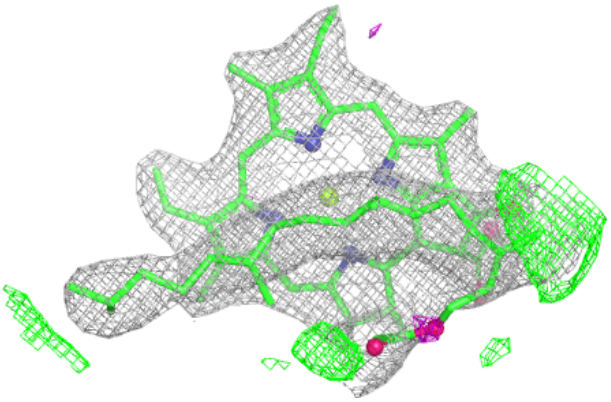


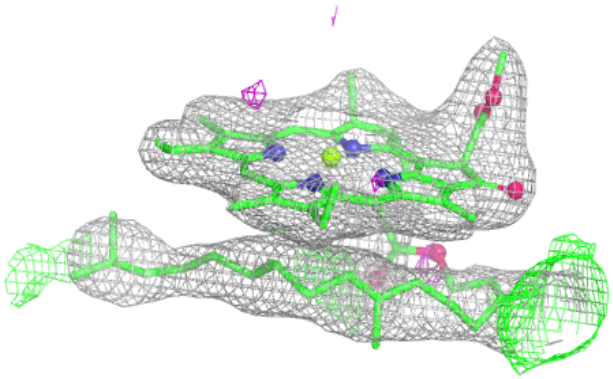


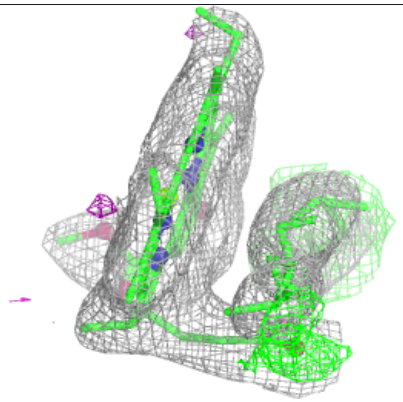


Electron density around CLA B 601:

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

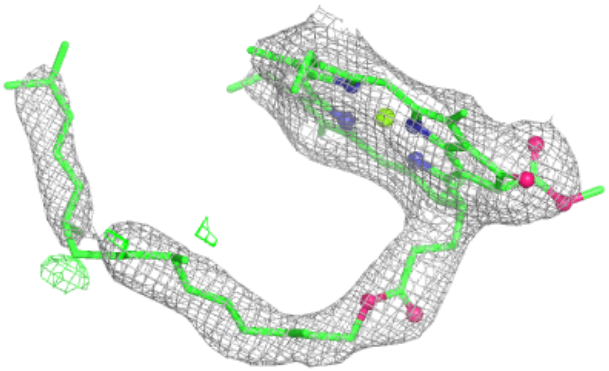


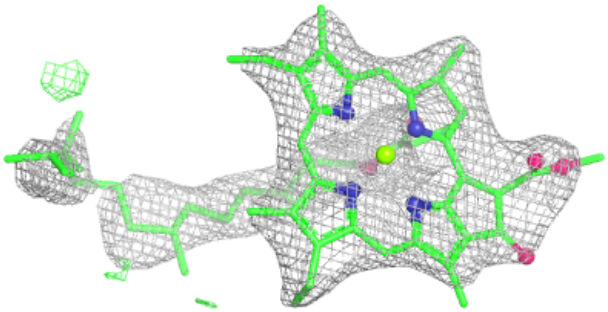


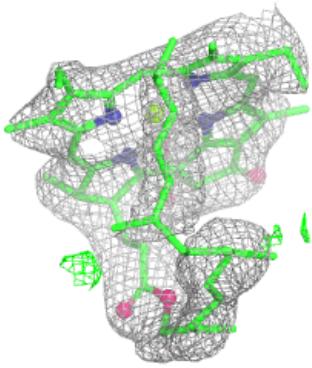


Electron density around CLA c 513:

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

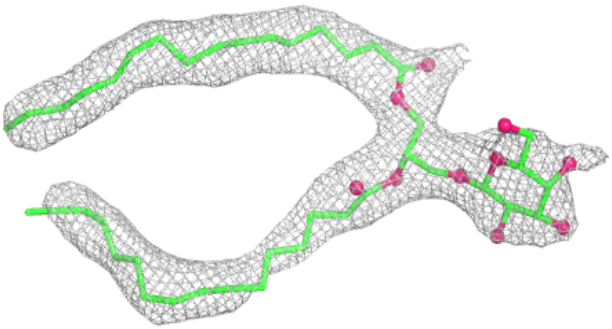


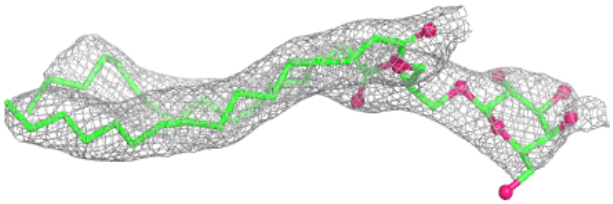


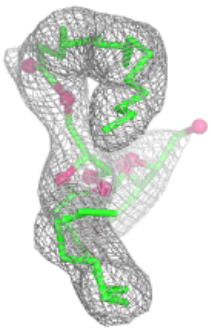


Electron density around LMG a 415:

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

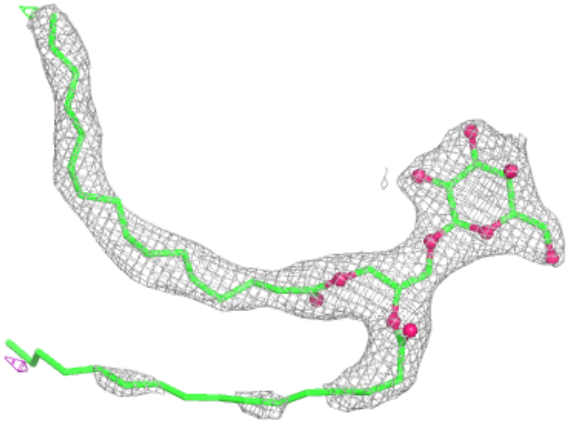


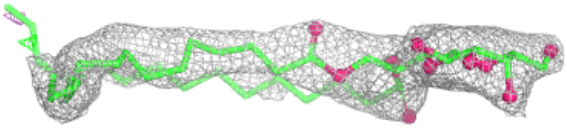


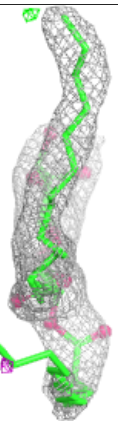


Electron density around LMG c 519:

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

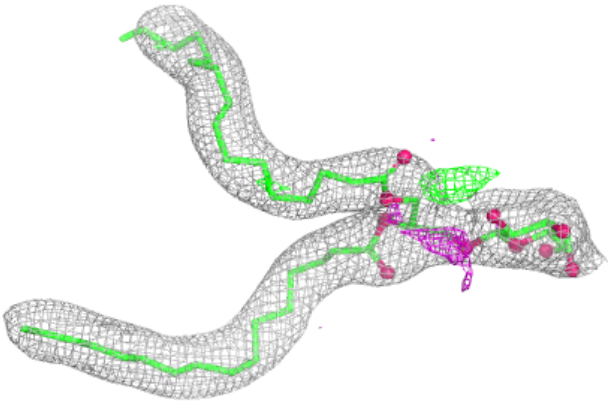


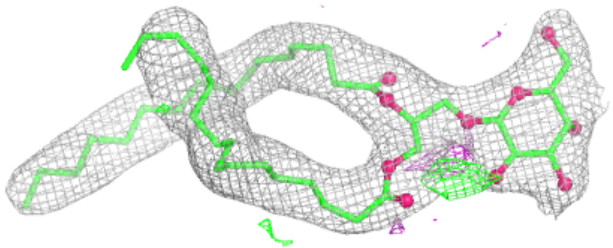


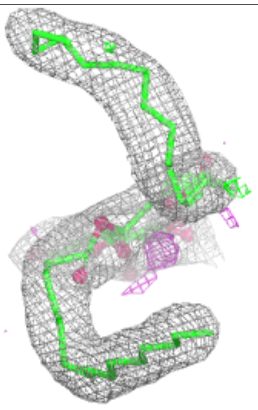


Electron density around LMG m 101:

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

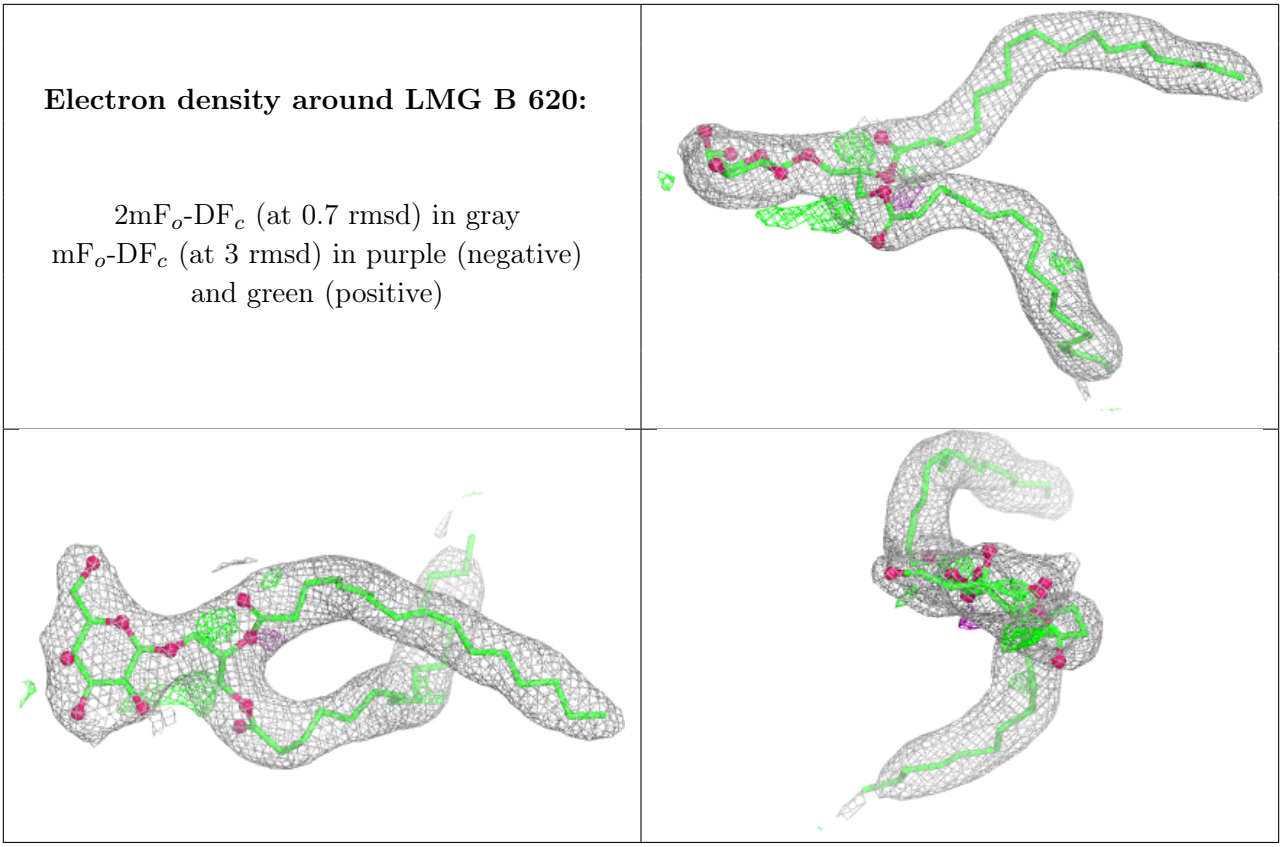






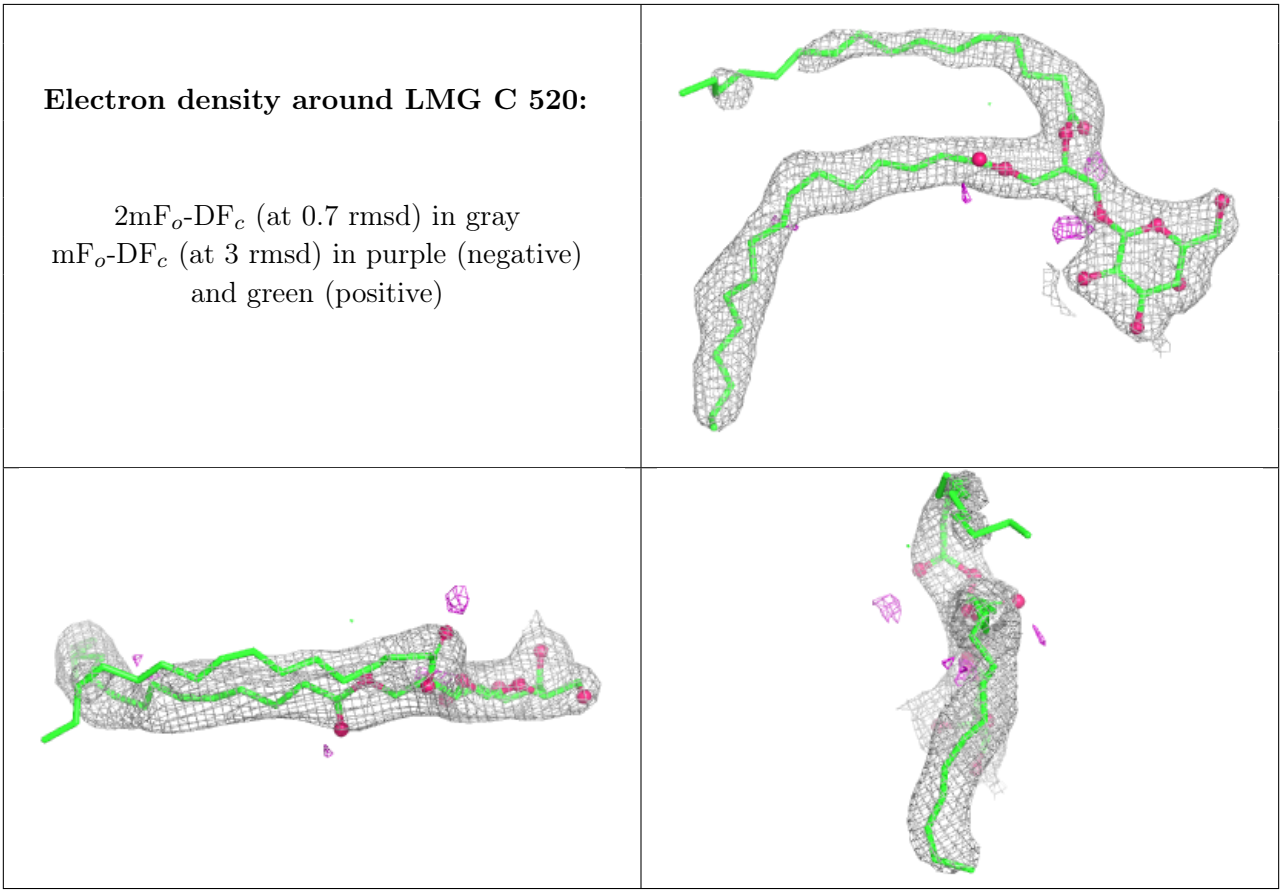
Electron density around LMG B 620:

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



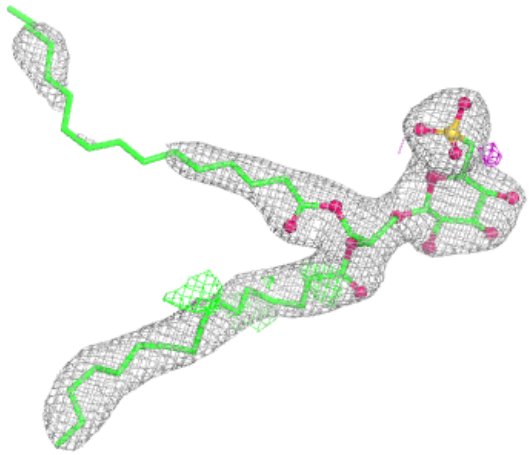
Electron density around LMG C 520:

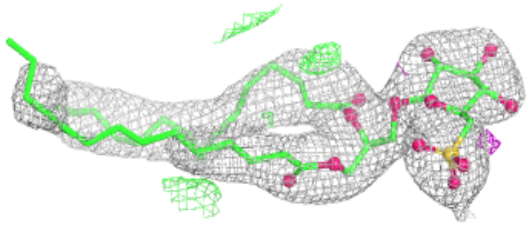
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

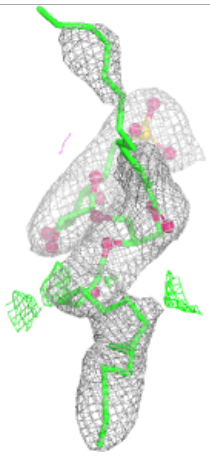


Electron density around SQD A 410 (B):

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

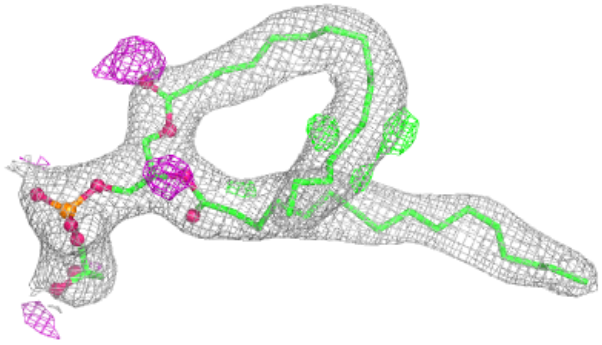


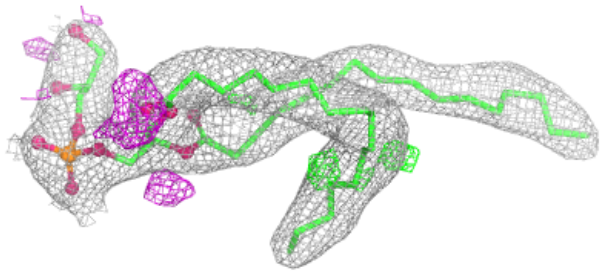


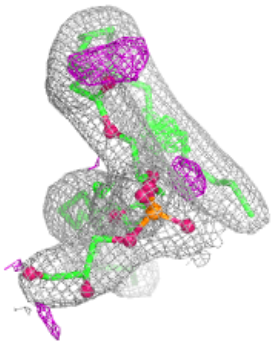


Electron density around LHG A 419 (A):

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

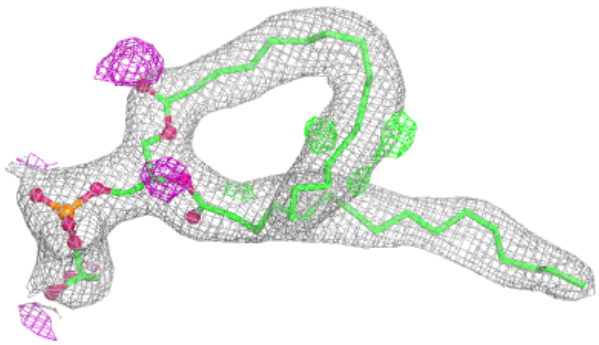


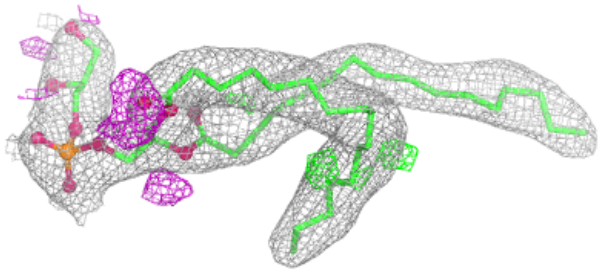




Electron density around LHG A 419 (B):

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

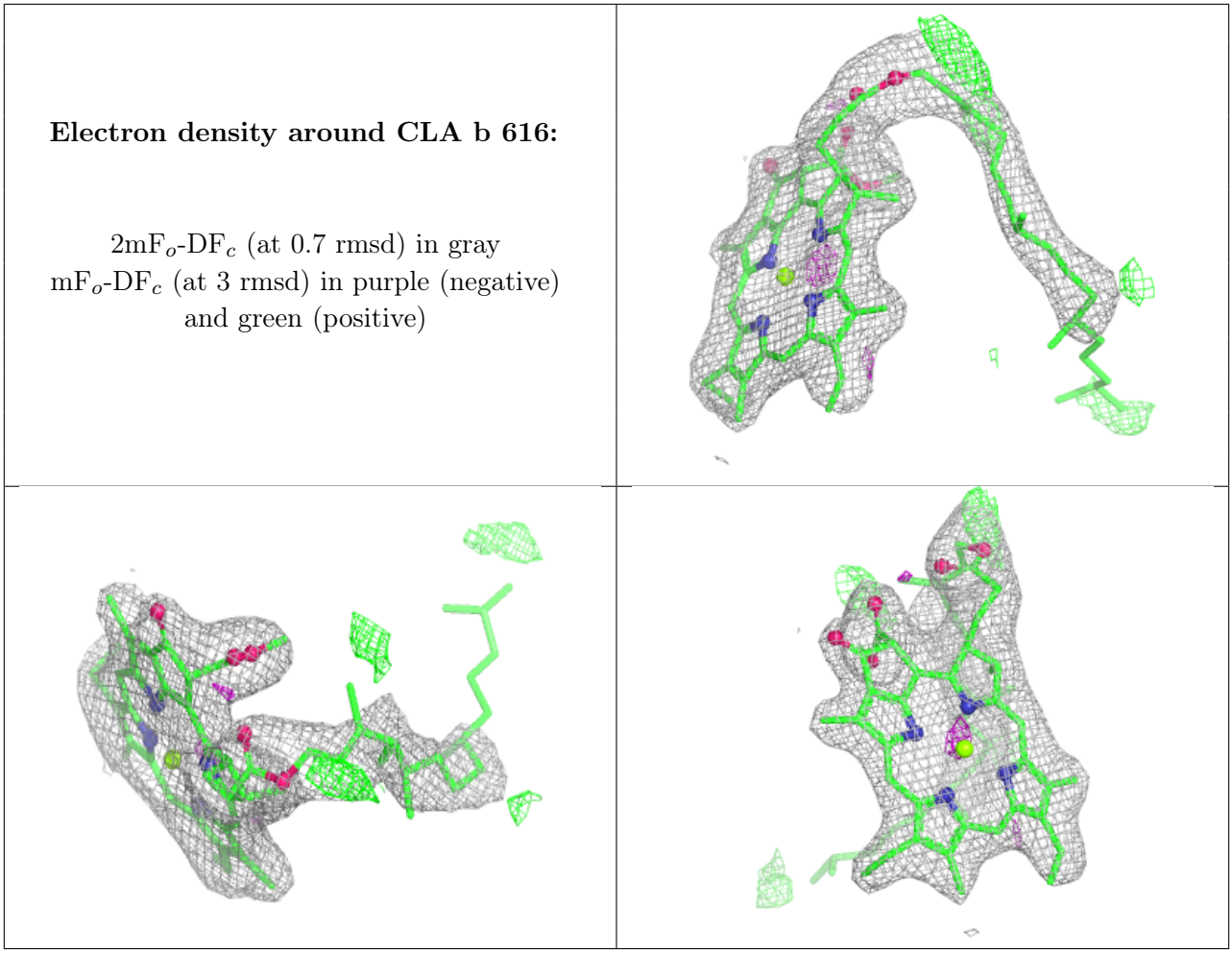






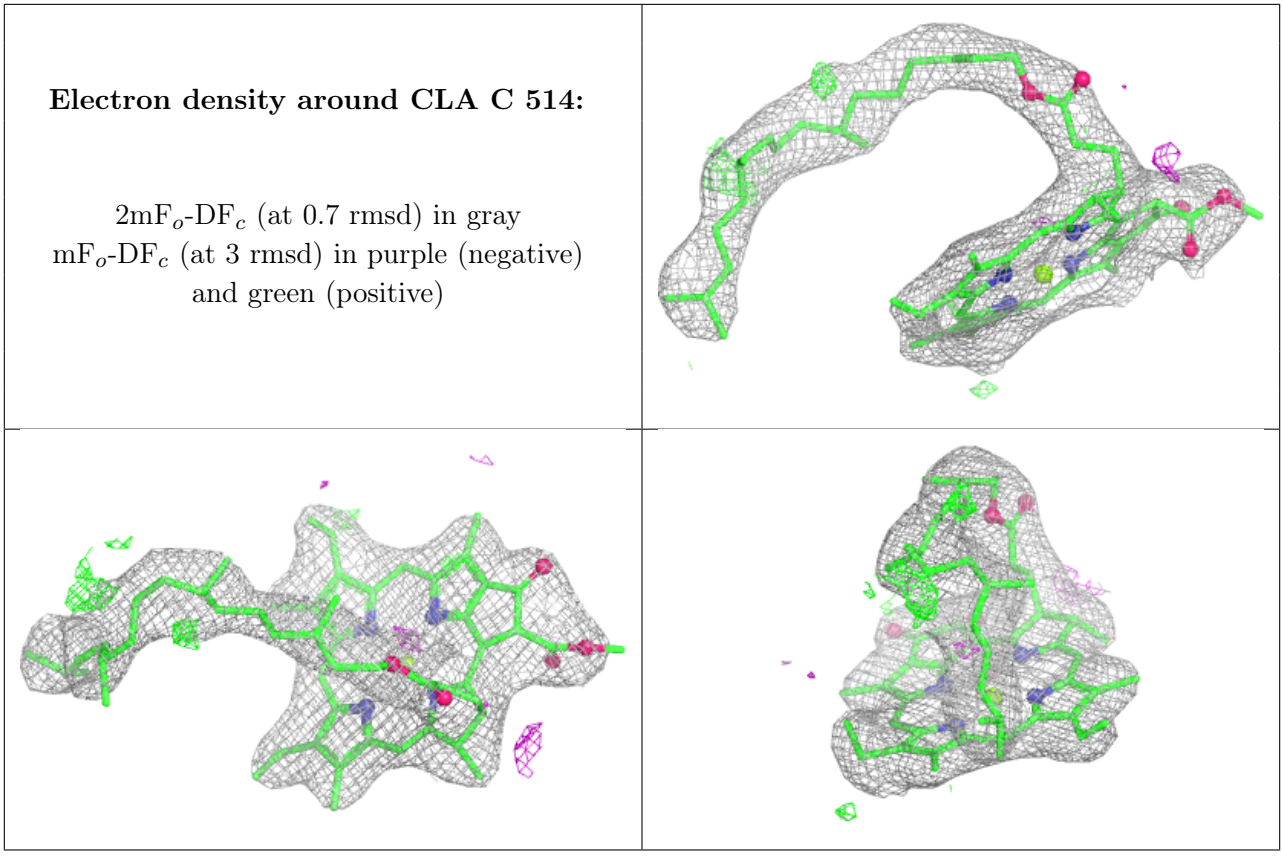
Electron density around CLA b 616:

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



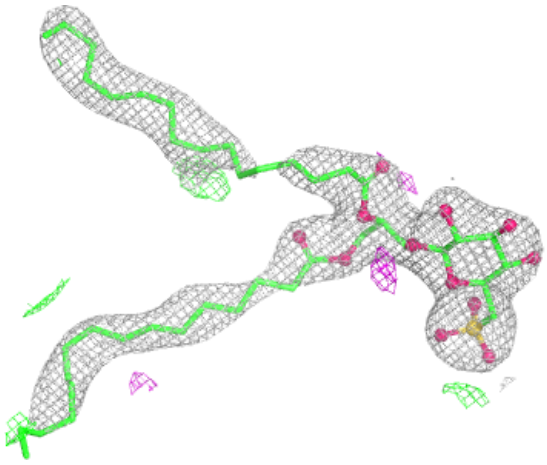
Electron density around CLA C 514:

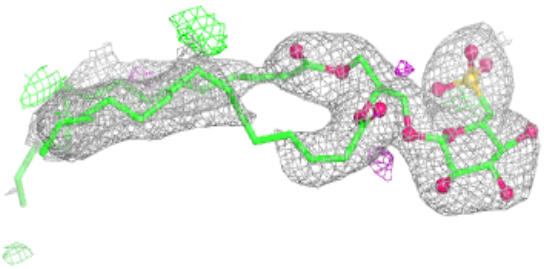
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

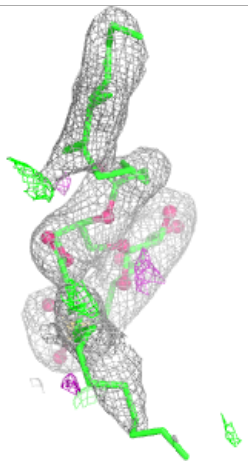


Electron density around SQD a 409 (A):

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

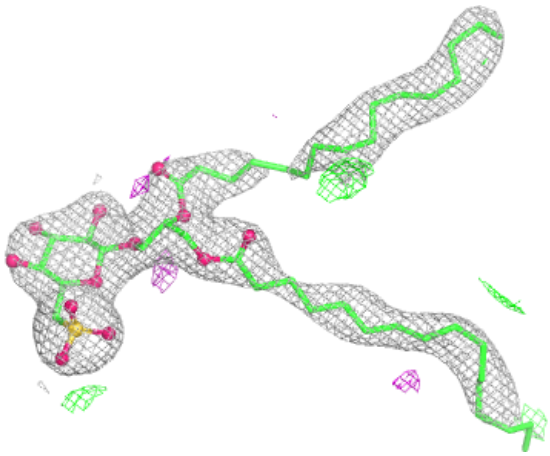


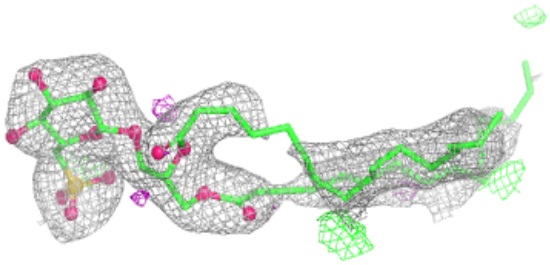


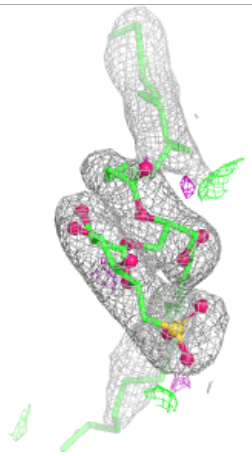


Electron density around SQD a 409 (B):

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

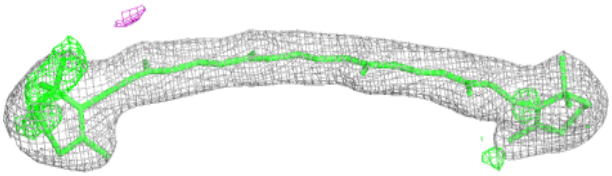


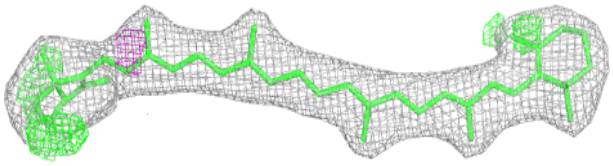


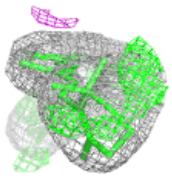


Electron density around BCR D 404:

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

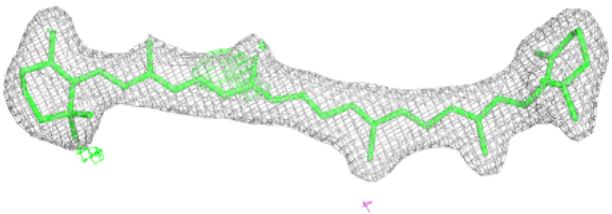


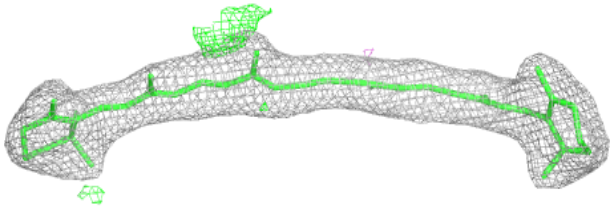


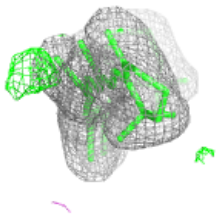


Electron density around BCR T 102:

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

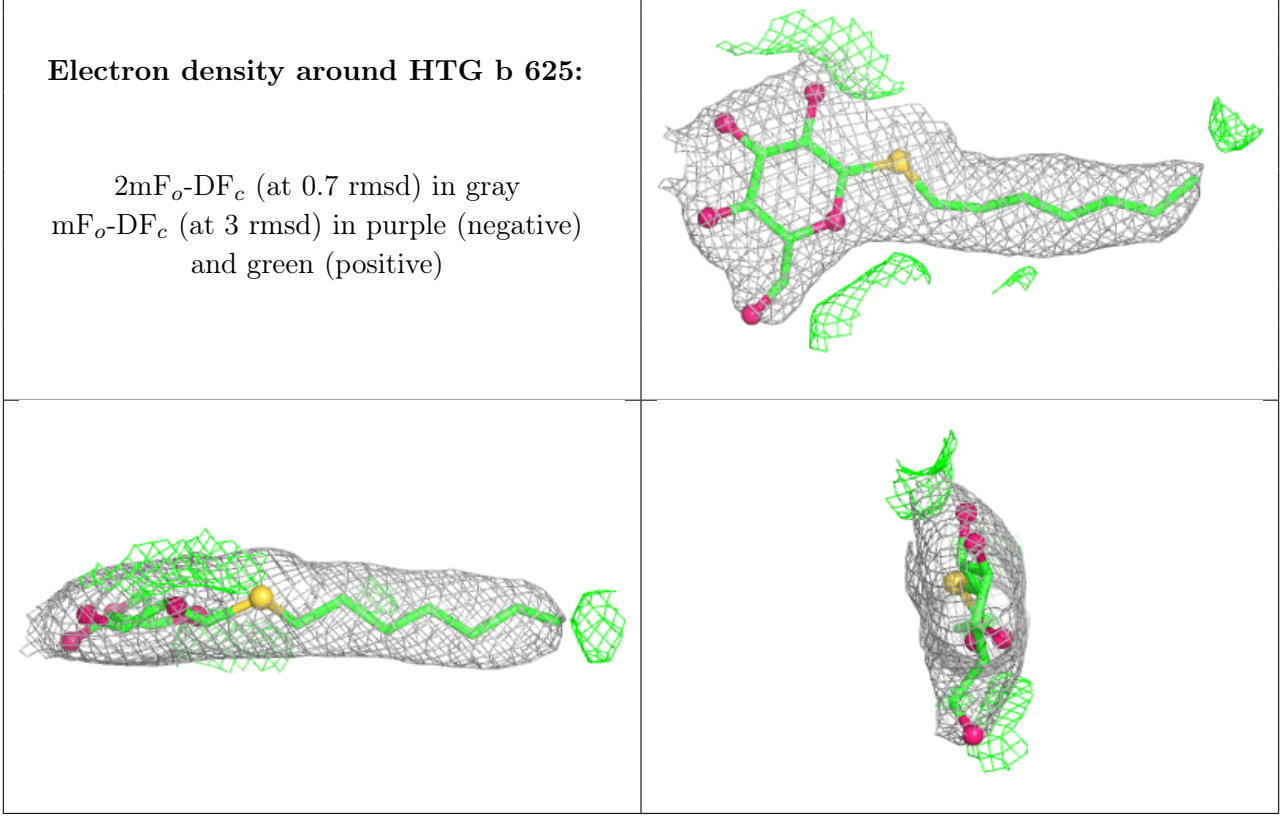






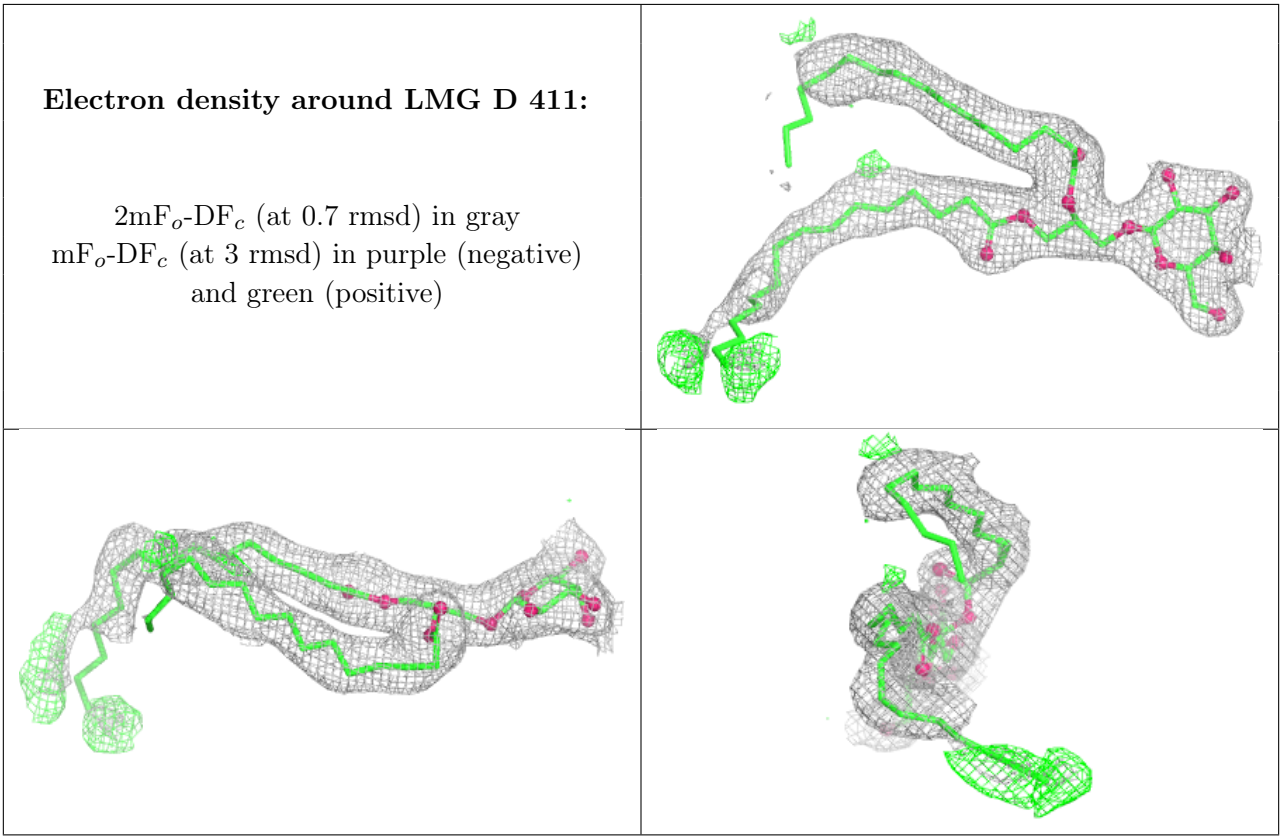
Electron density around HTG b 625:

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



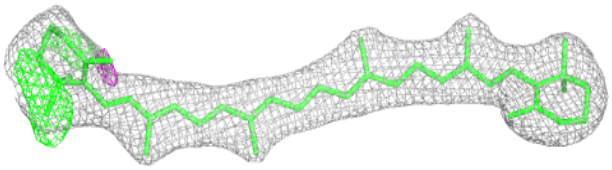
Electron density around LMG D 411:

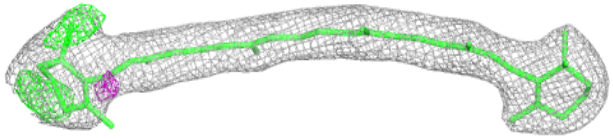
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

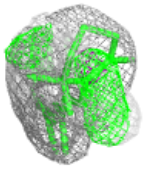


Electron density around BCR d 406:

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

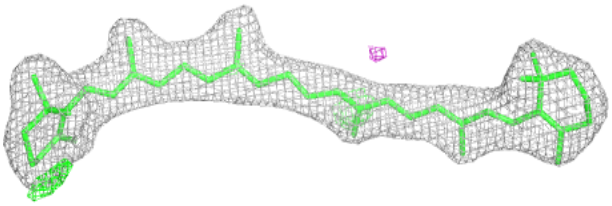


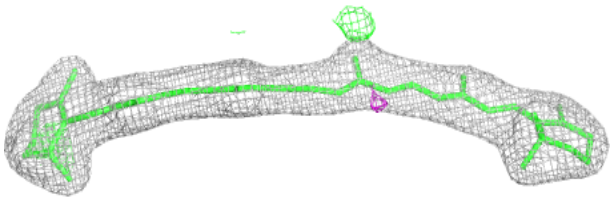


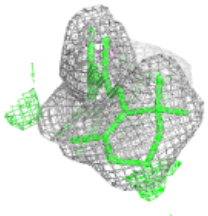


Electron density around BCR t 102:

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

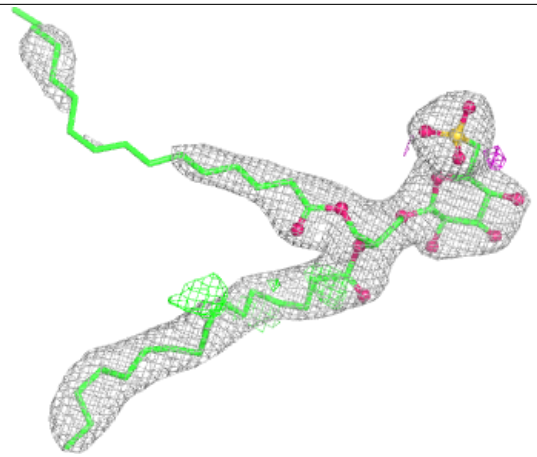


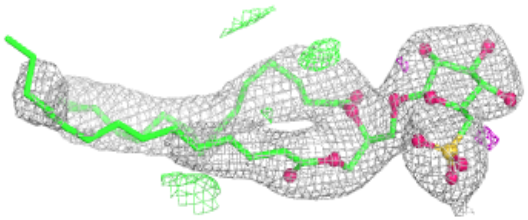


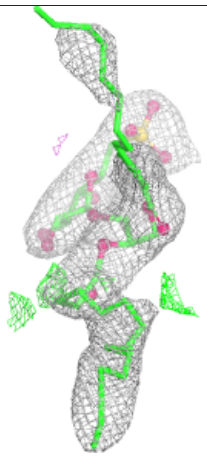


Electron density around SQD A 410 (A):

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

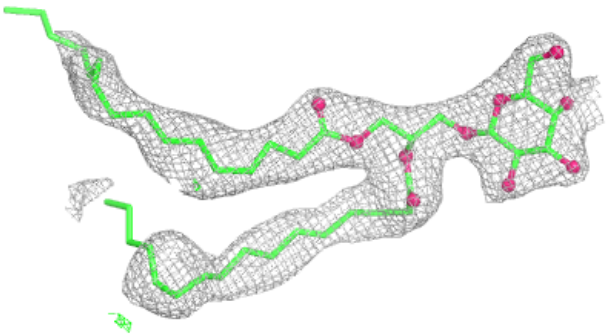


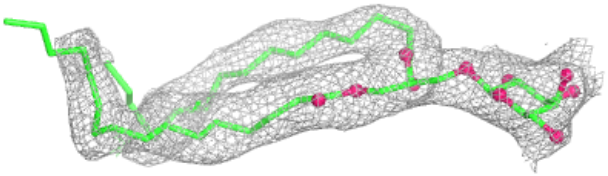


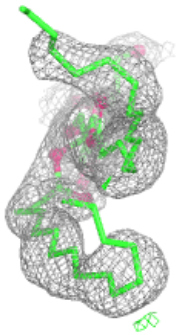


Electron density around LMG d 413:

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

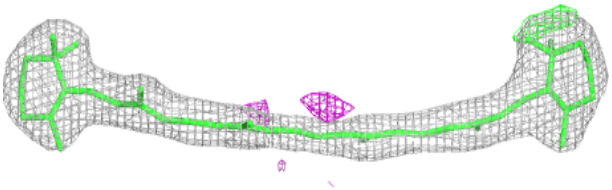


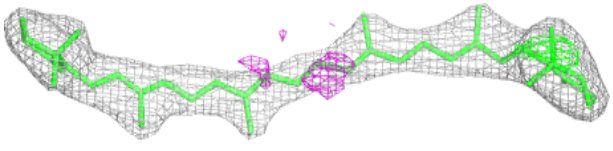


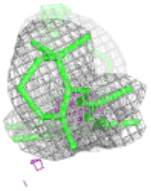


Electron density around BCR K 102:

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

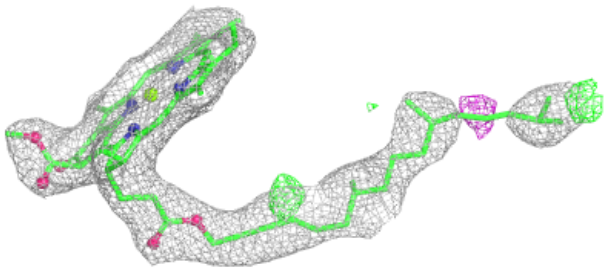


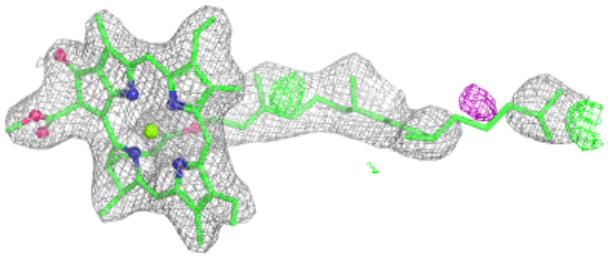


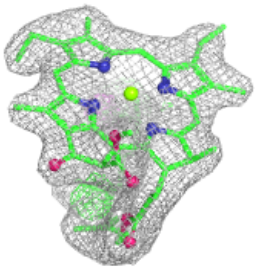


Electron density around CLA c 504:

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

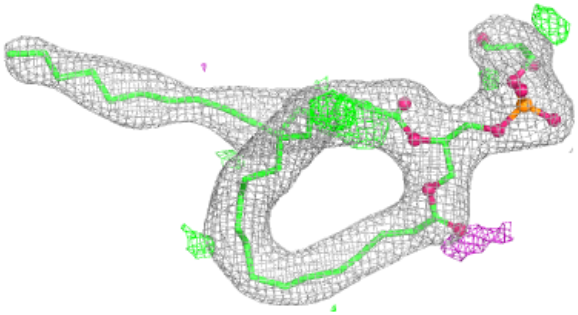


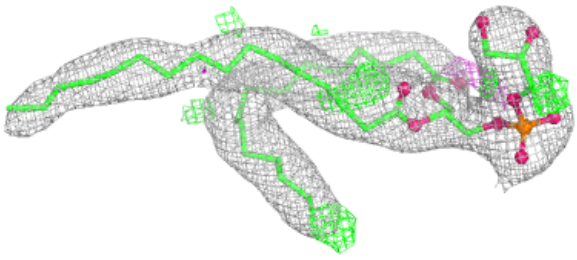


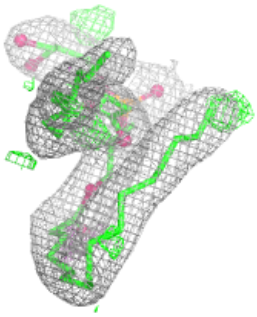


Electron density around LHG d 415 (A):

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

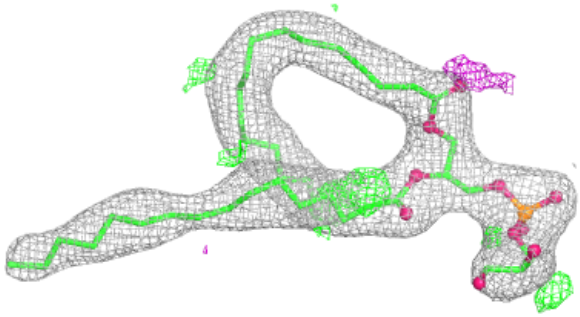


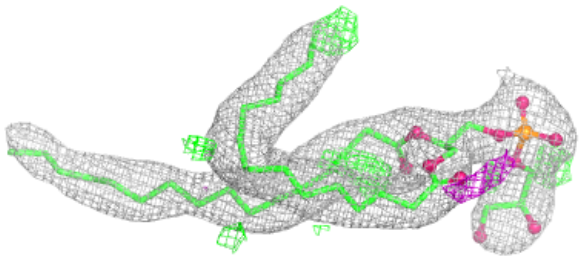


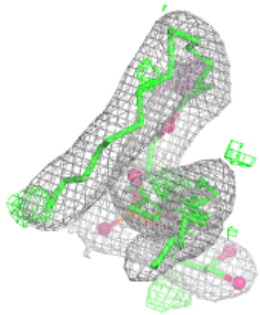


Electron density around LHG d 415 (B):

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

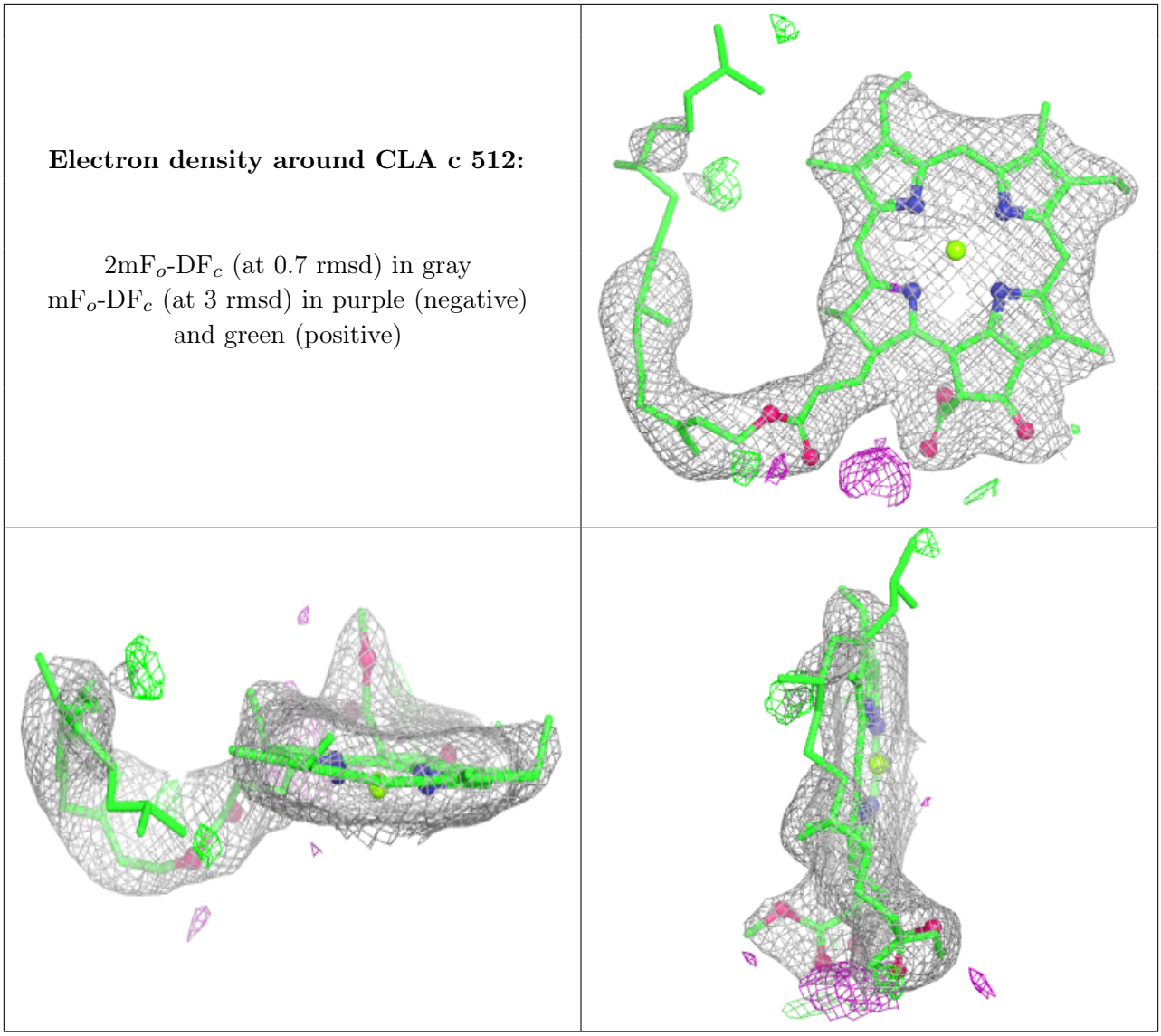






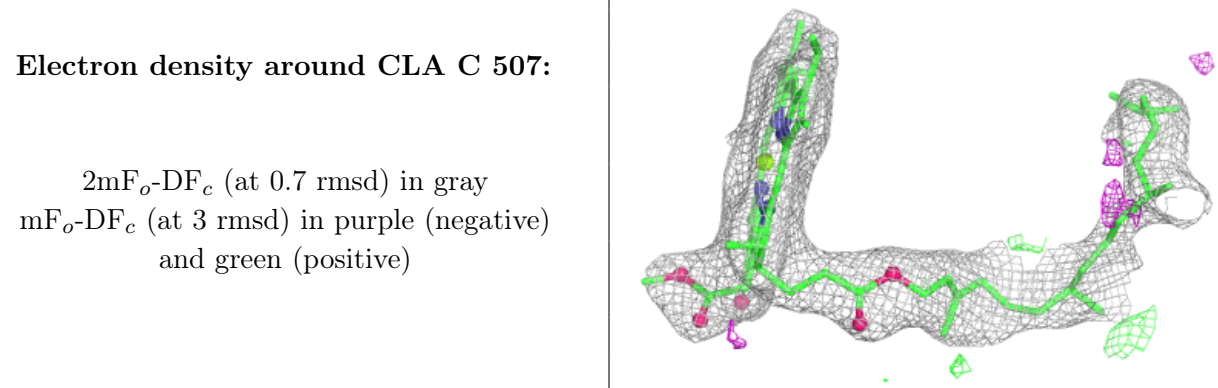
Electron density around CLA c 512:

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



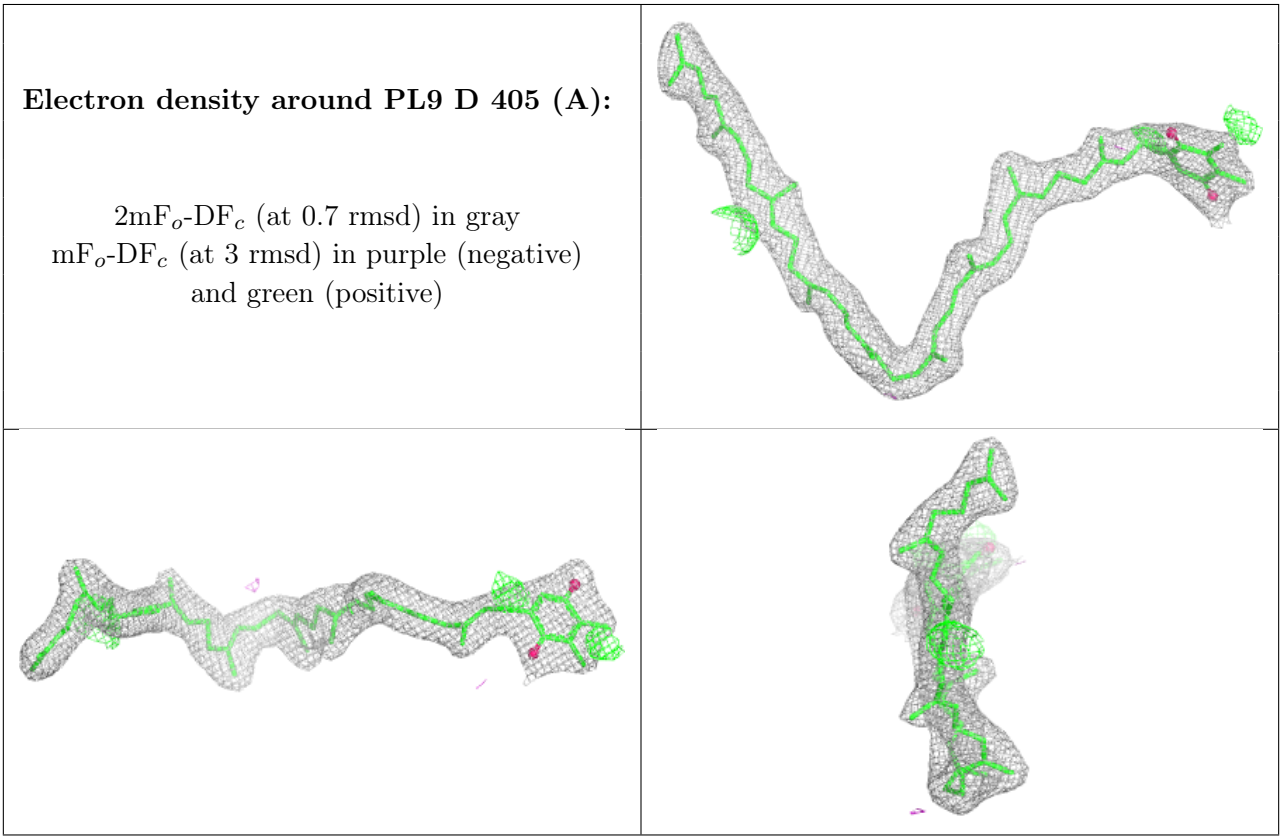
Electron density around CLA C 507:

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



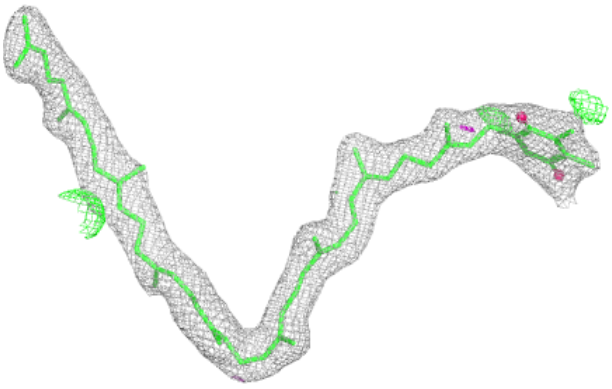
Electron density around PL9 D 405 (A):

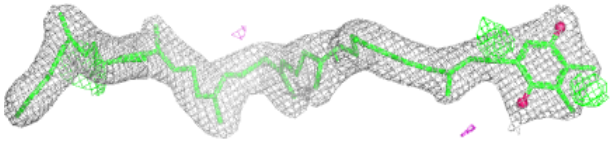
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

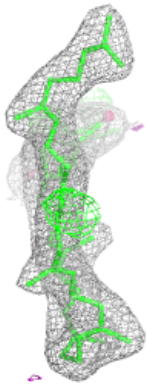


Electron density around PL9 D 405 (B):

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

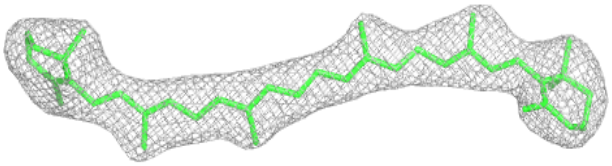


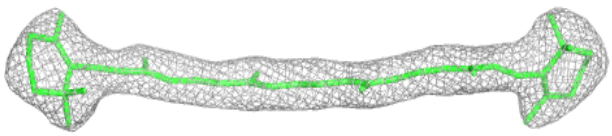


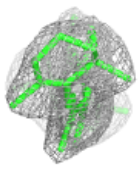


Electron density around BCR y 101:

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

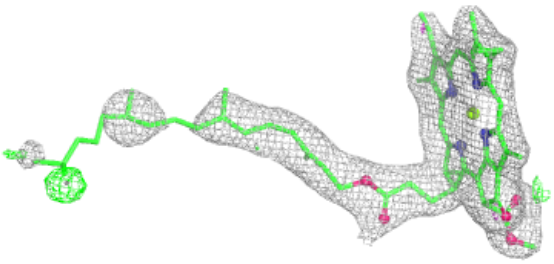


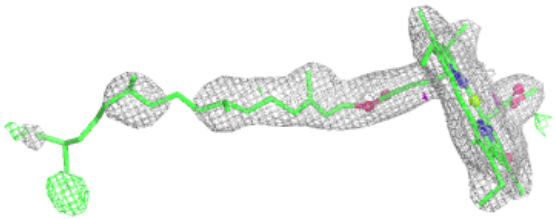


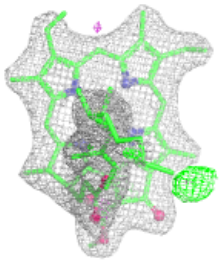


Electron density around CLA d 405:

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

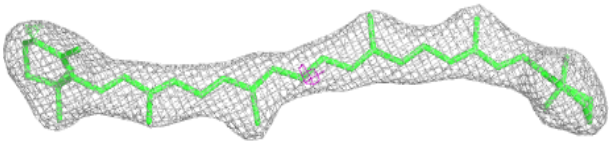


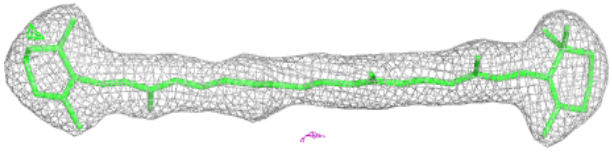


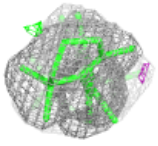


Electron density around BCR C 515:

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

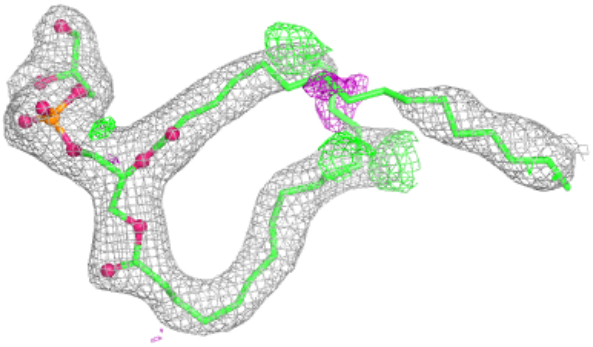


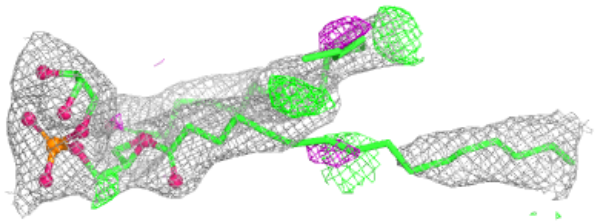


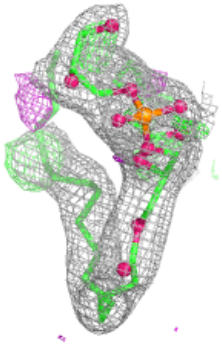


Electron density around LHG D 407 (A):

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

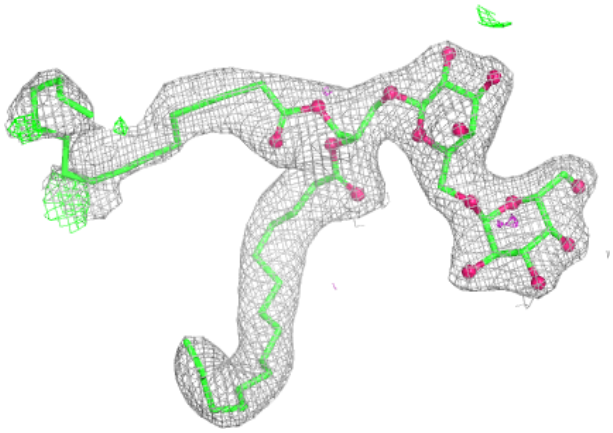


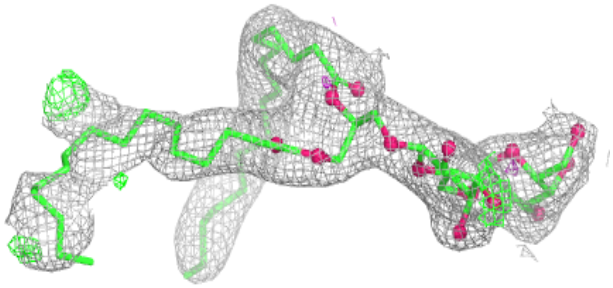


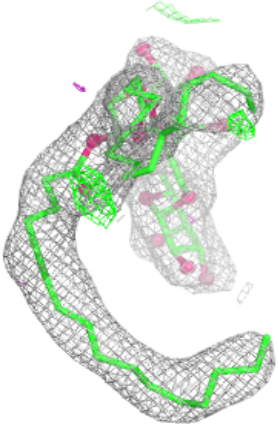


Electron density around DGD C 518 (A):

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

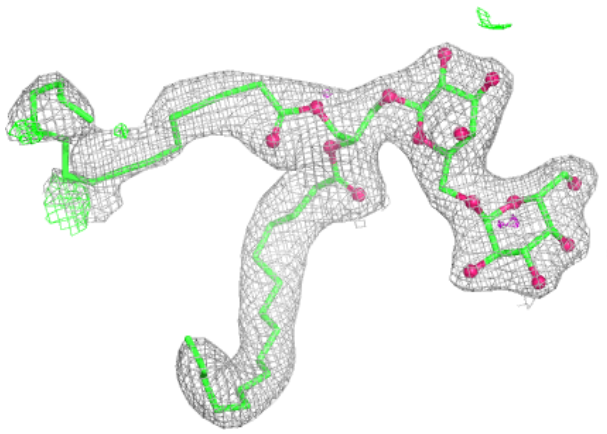


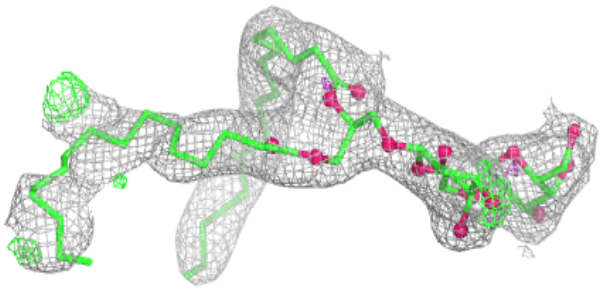


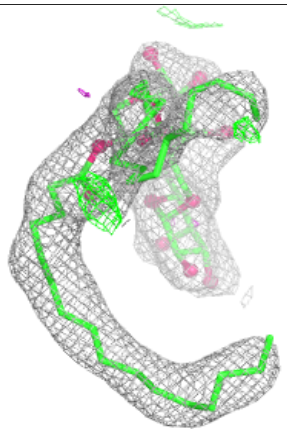


Electron density around DGD C 518 (B):

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

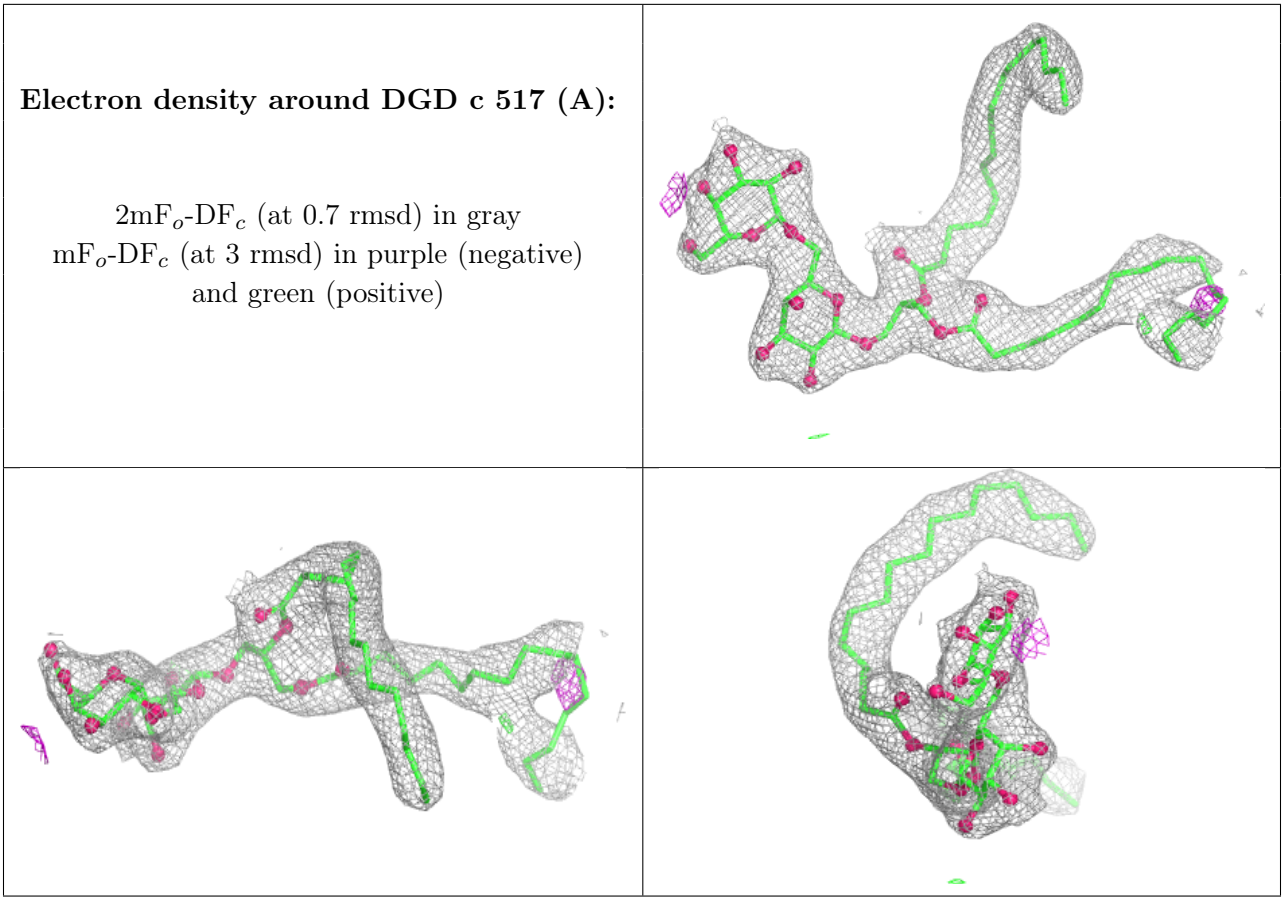






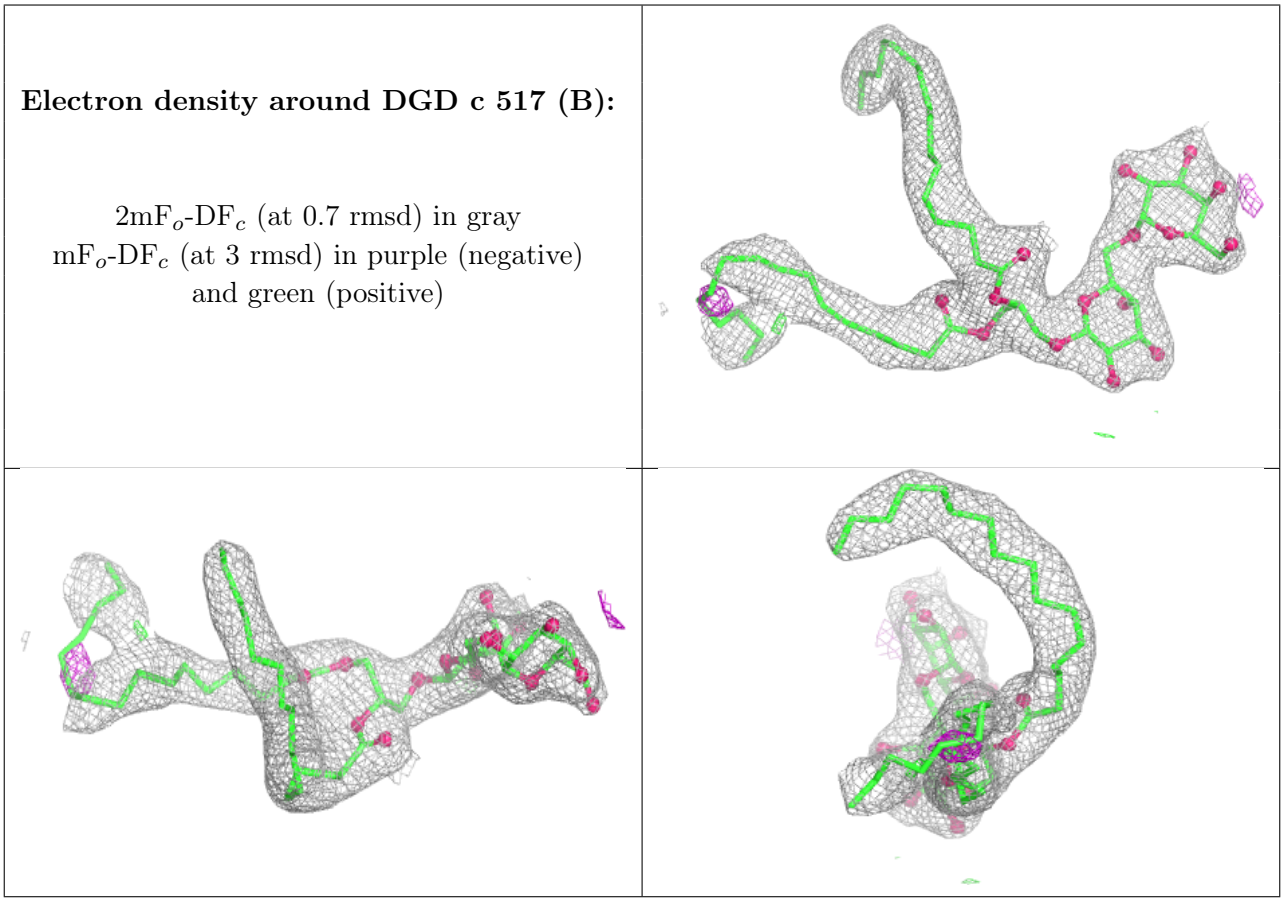
Electron density around DGD c 517 (A):

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



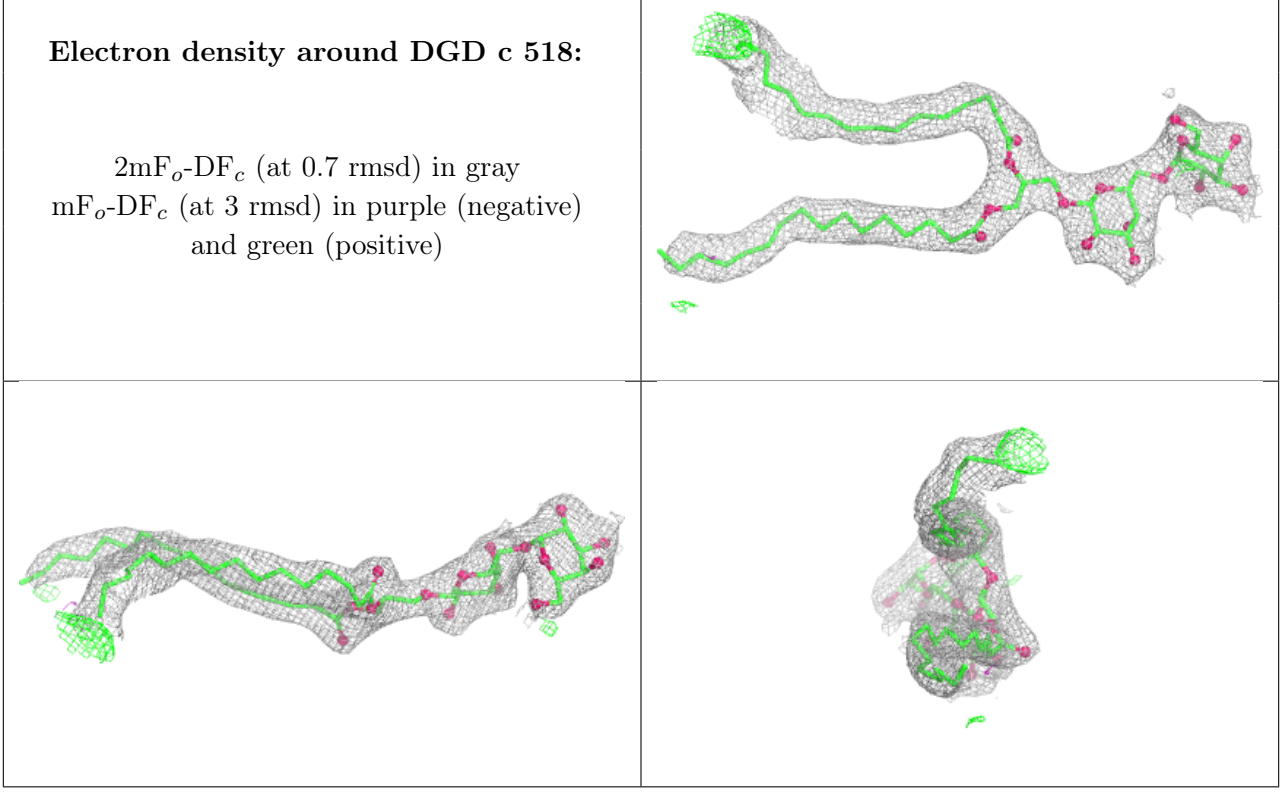
Electron density around DGD c 517 (B):

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



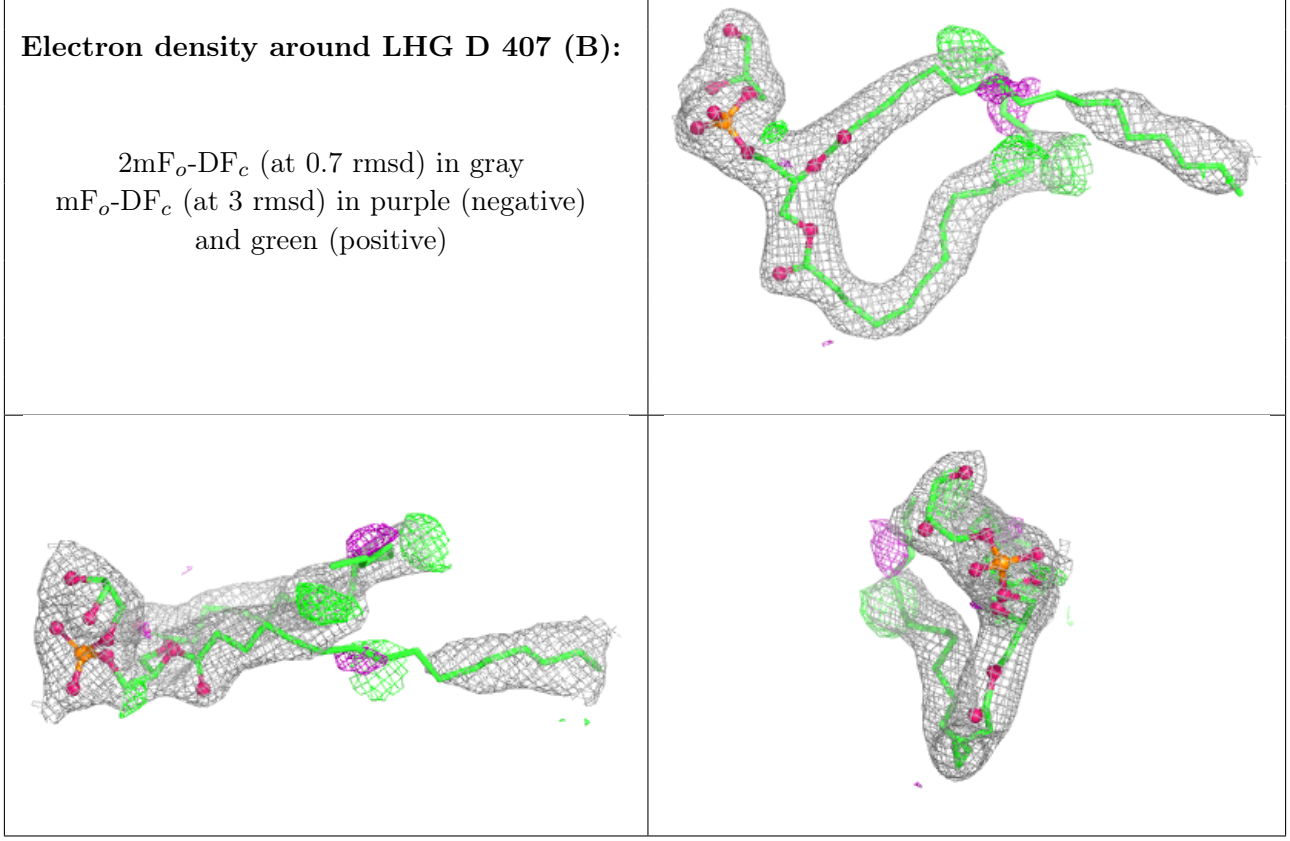
Electron density around DGD c 518:

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



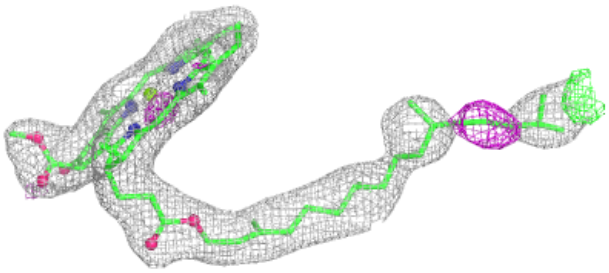
Electron density around LHG D 407 (B):

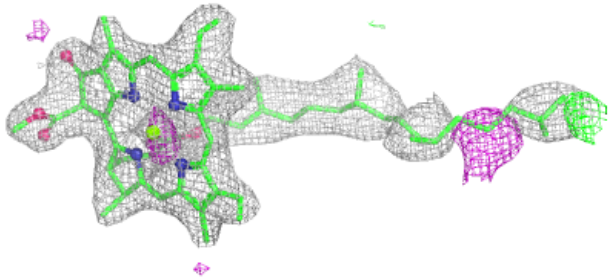
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

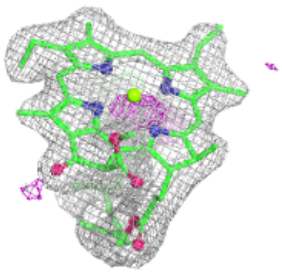


Electron density around CLA C 505:

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

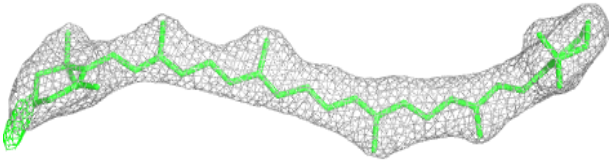


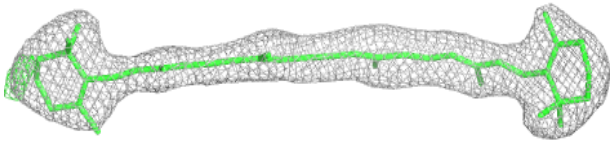


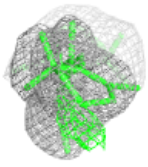


Electron density around BCR H 101:

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

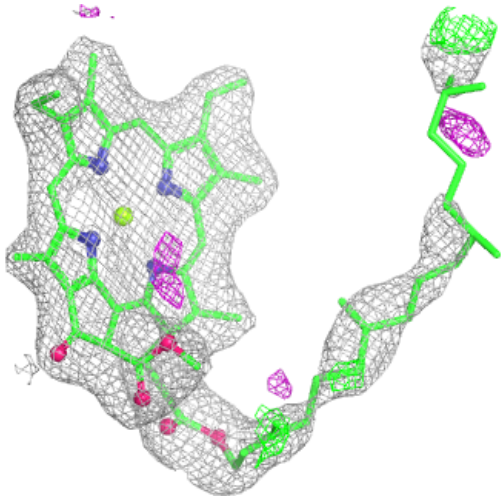


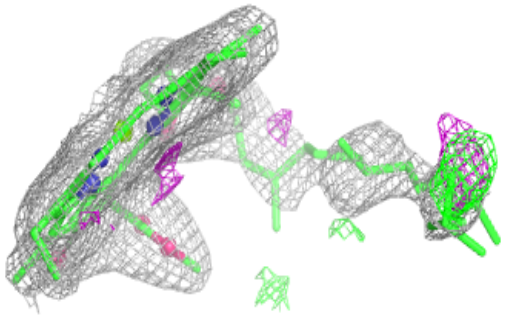


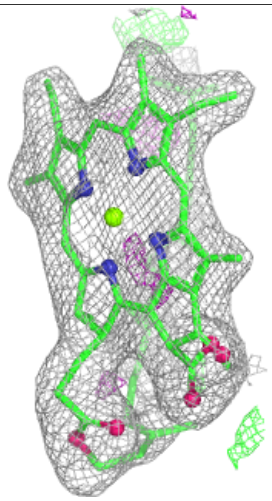


Electron density around CLA B 616:

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

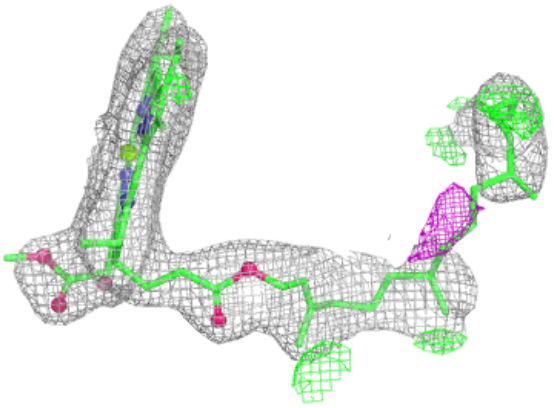


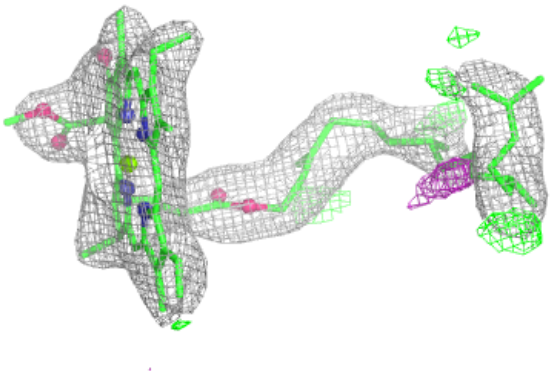


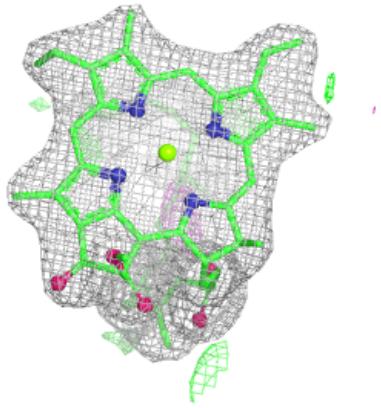


Electron density around CLA c 506:

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

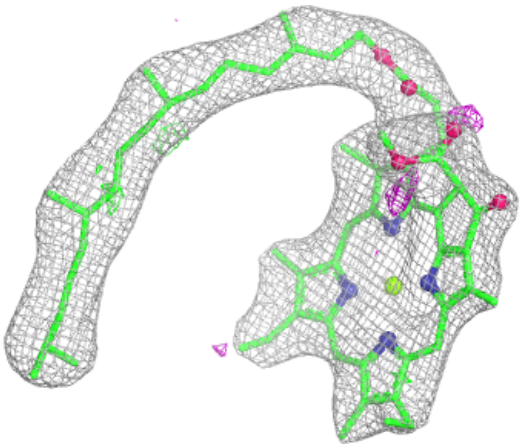


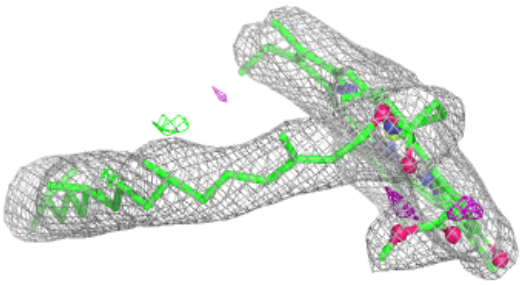


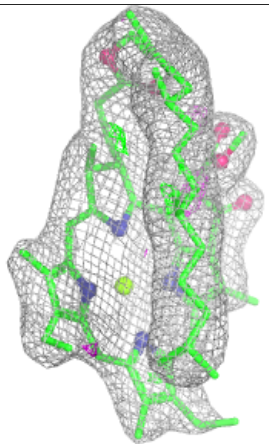


Electron density around CLA c 507:

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

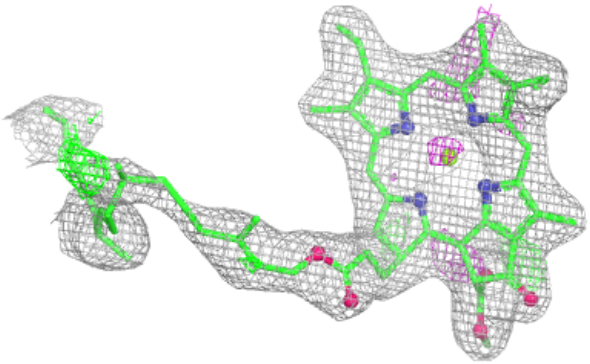


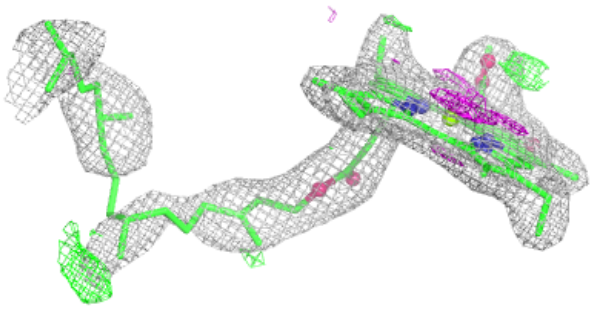




Electron density around CLA A 408:

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

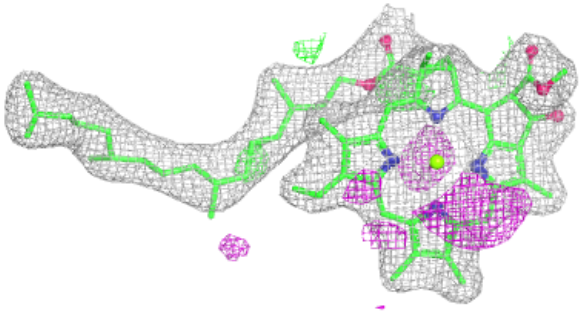


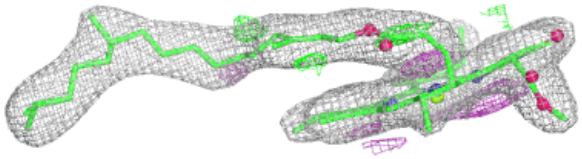


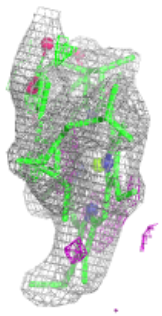


Electron density around CLA B 603:

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

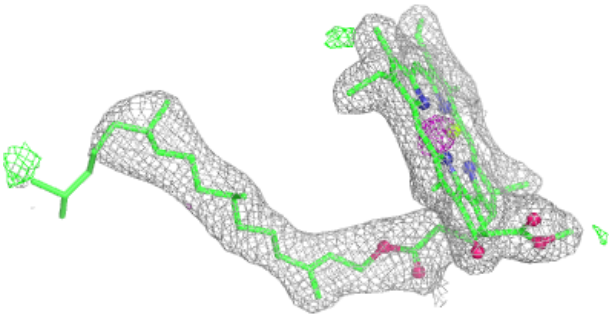


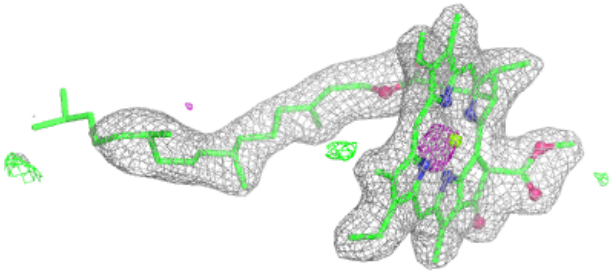


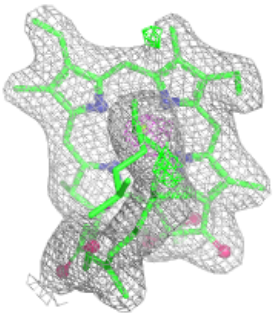


Electron density around CLA C 509:

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

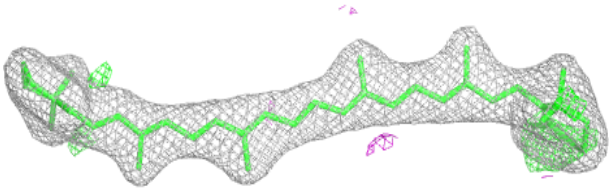


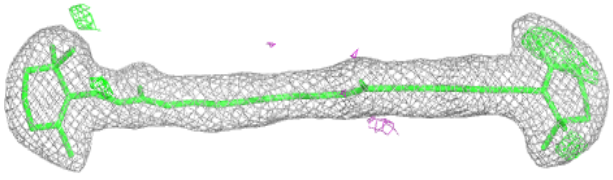


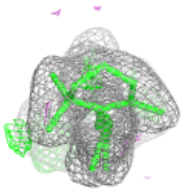


Electron density around BCR A 409:

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

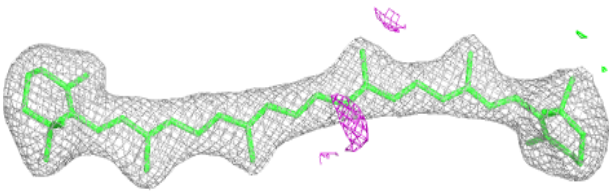


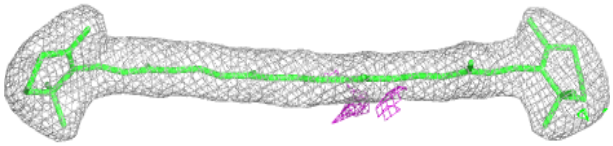


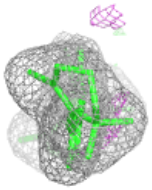


Electron density around BCR B 618:

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

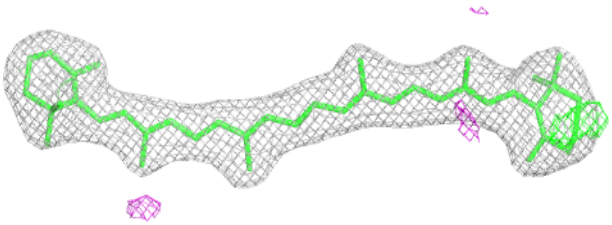


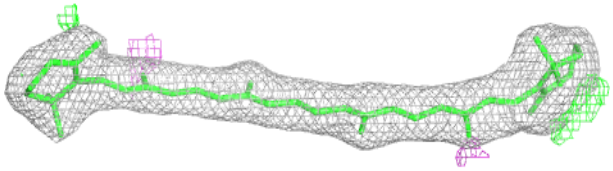


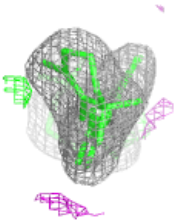


Electron density around BCR B 619:

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

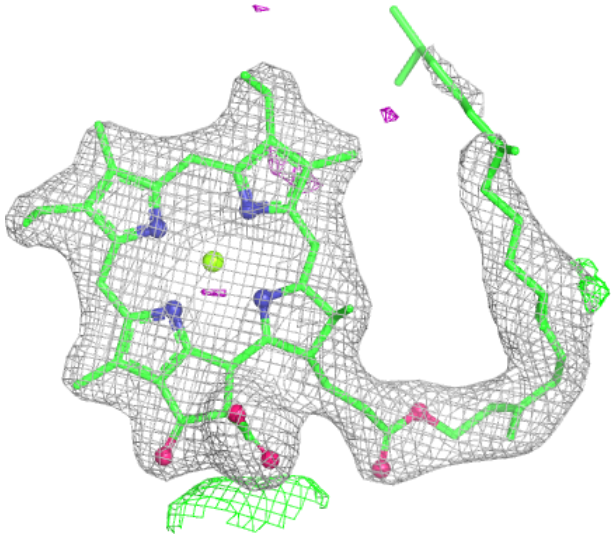


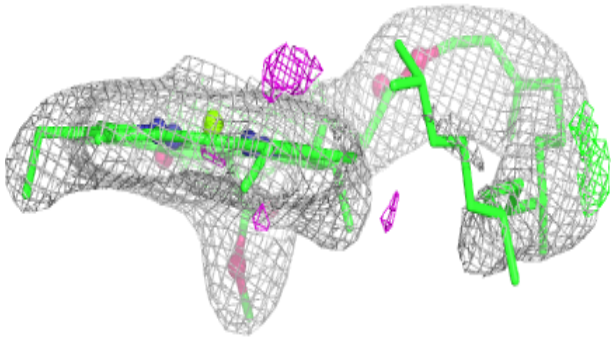


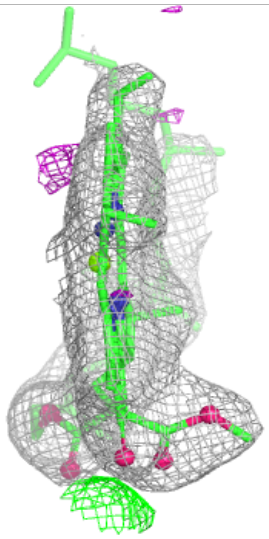


Electron density around CLA C 513:

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

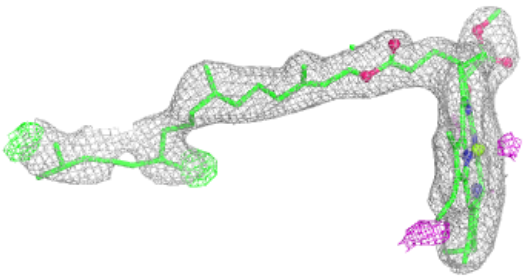


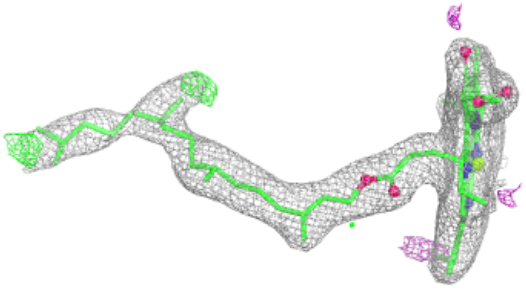


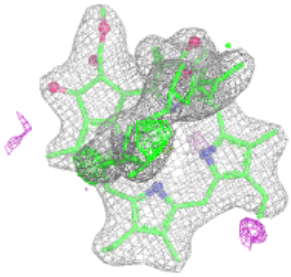


Electron density around CLA B 606:

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

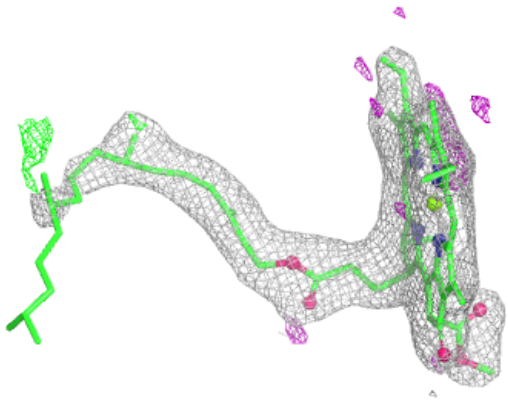


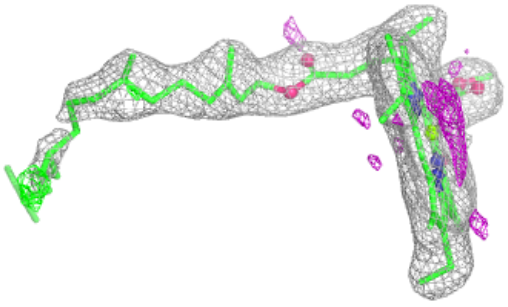


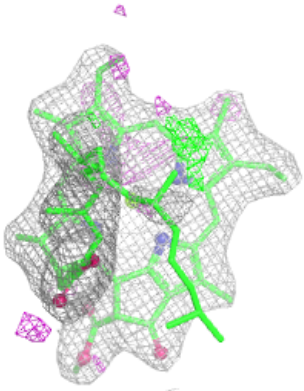


Electron density around CLA D 403:

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

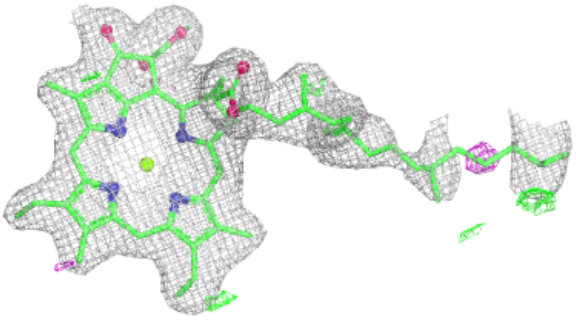


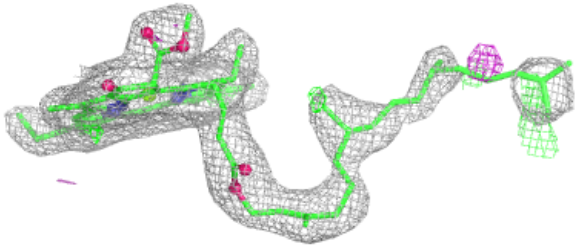


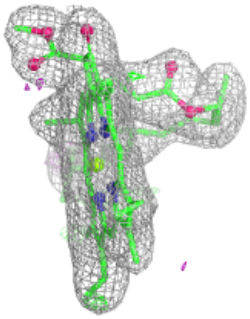


Electron density around CLA a 405 (A):

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

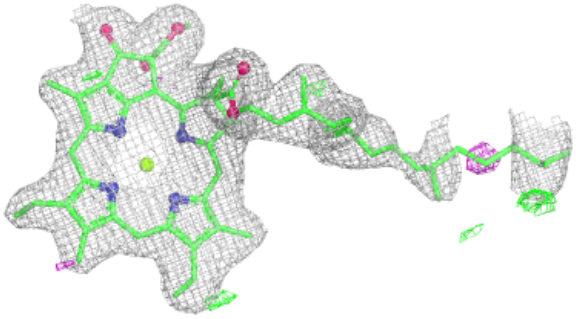


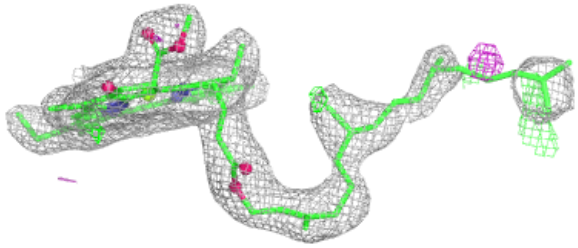


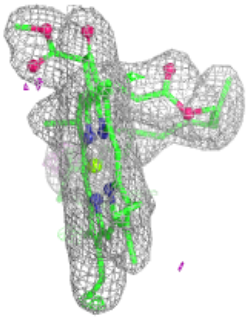


Electron density around CLA a 405 (B):

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

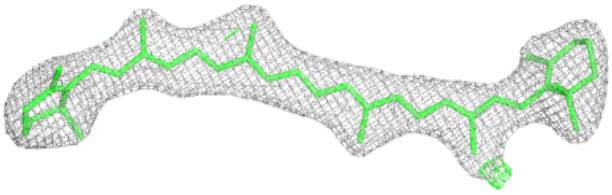


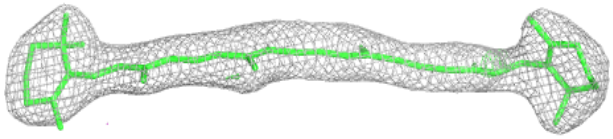


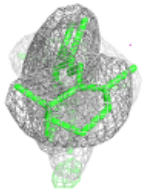


Electron density around BCR Y 101:

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

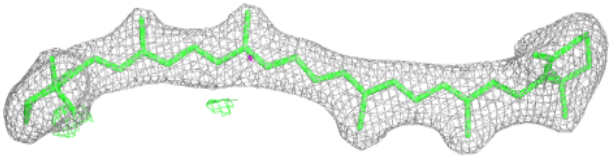


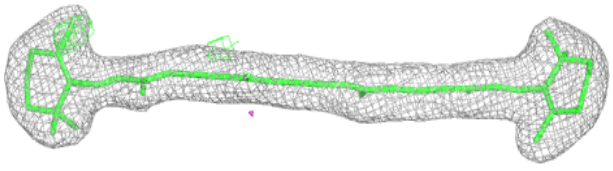


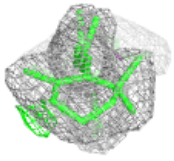


Electron density around BCR a 408:

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

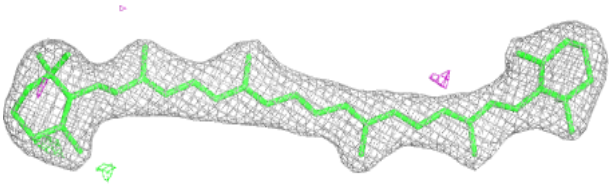


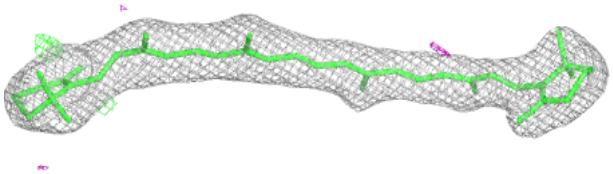


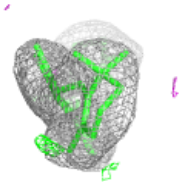


Electron density around BCR b 619:

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

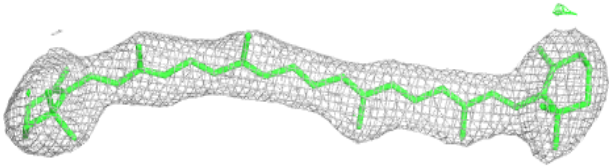


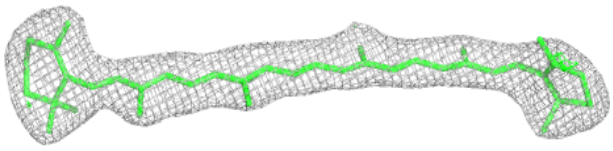


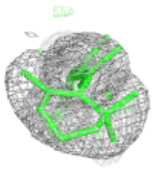


Electron density around BCR c 514:

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

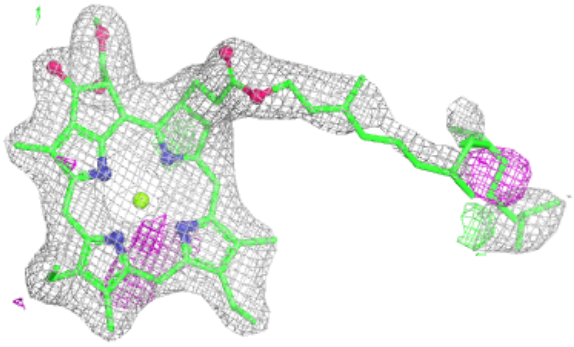


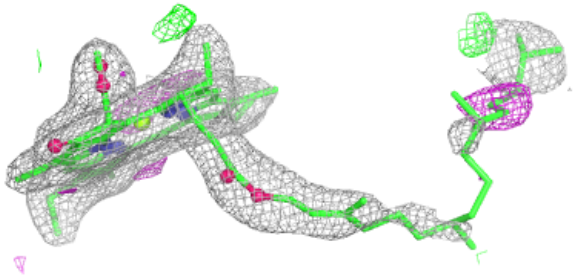


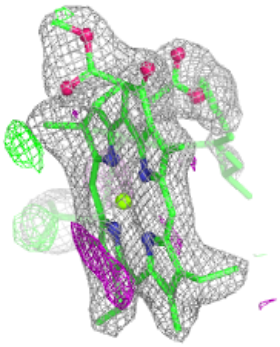


Electron density around CLA a 407:

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

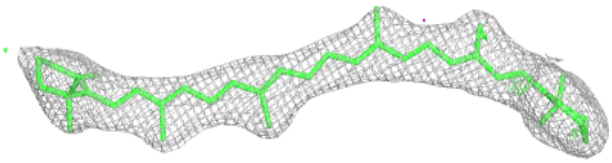


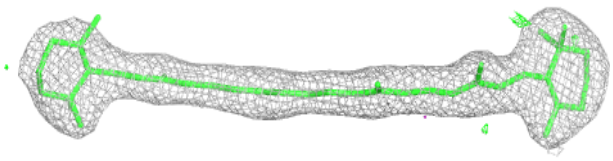


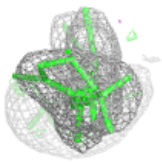


Electron density around BCR h 101:

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

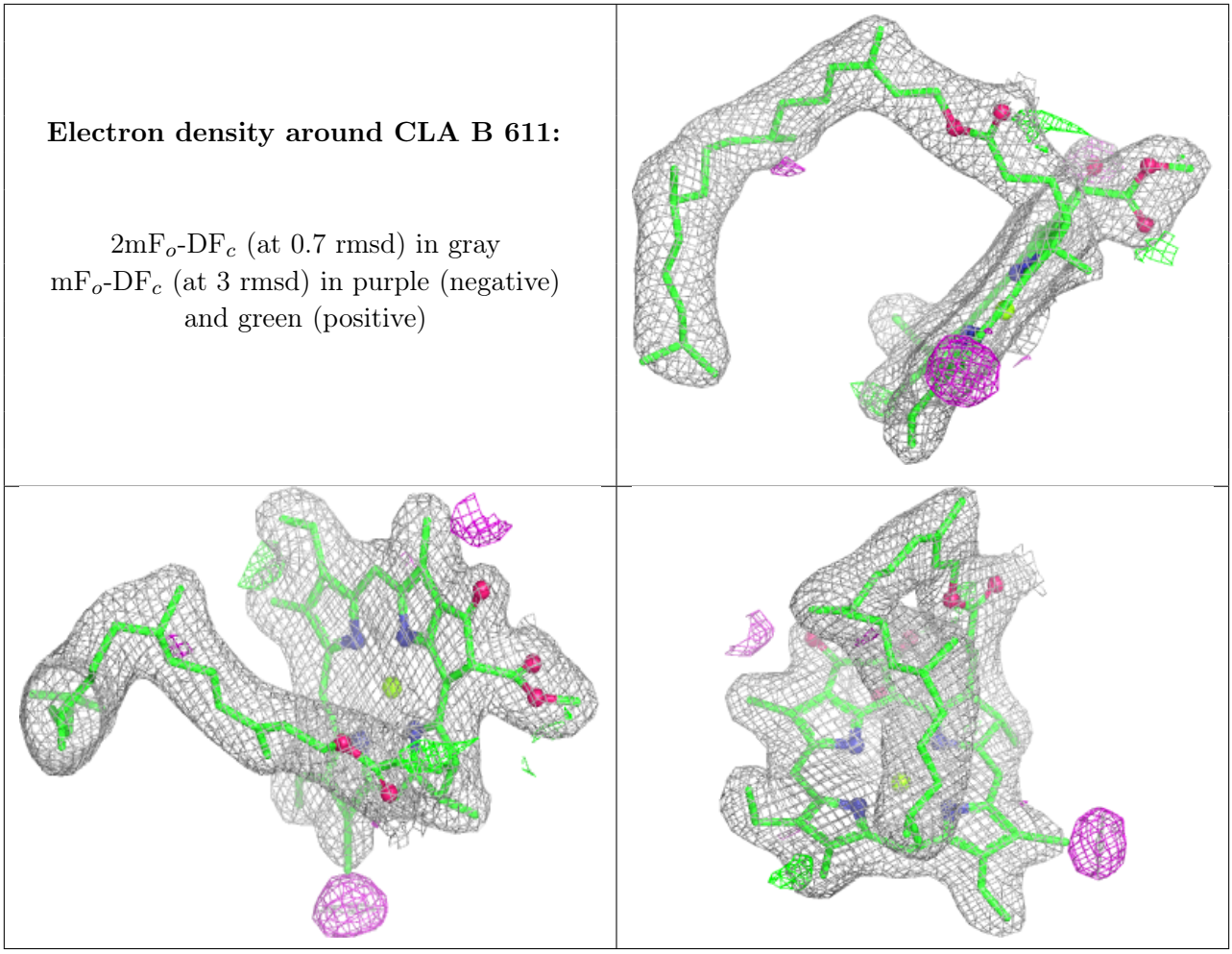






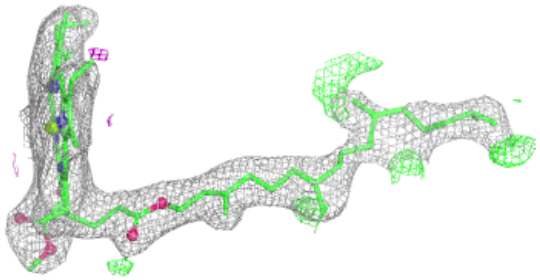
Electron density around CLA B 611:

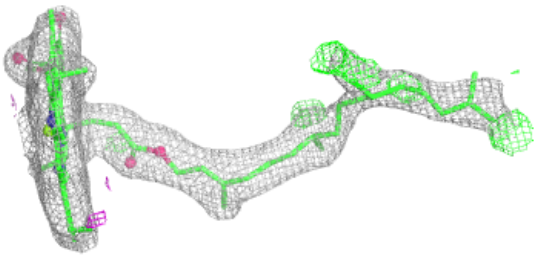
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

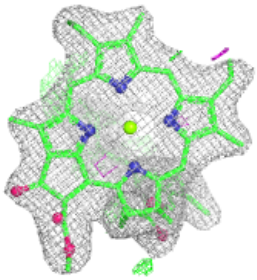


Electron density around CLA b 606:

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

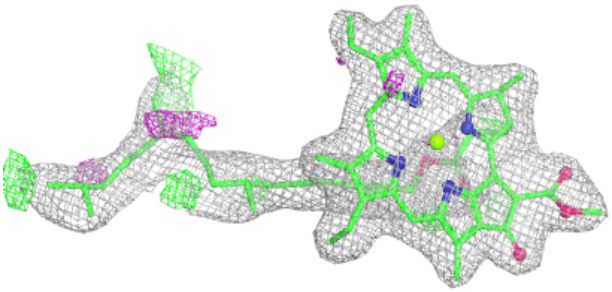


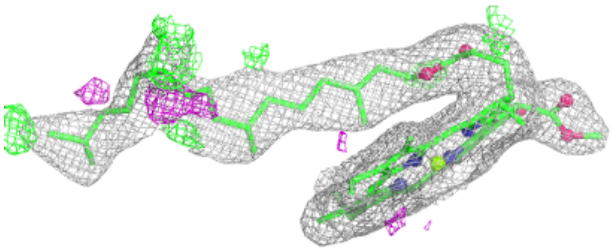




Electron density around CLA b 614:

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

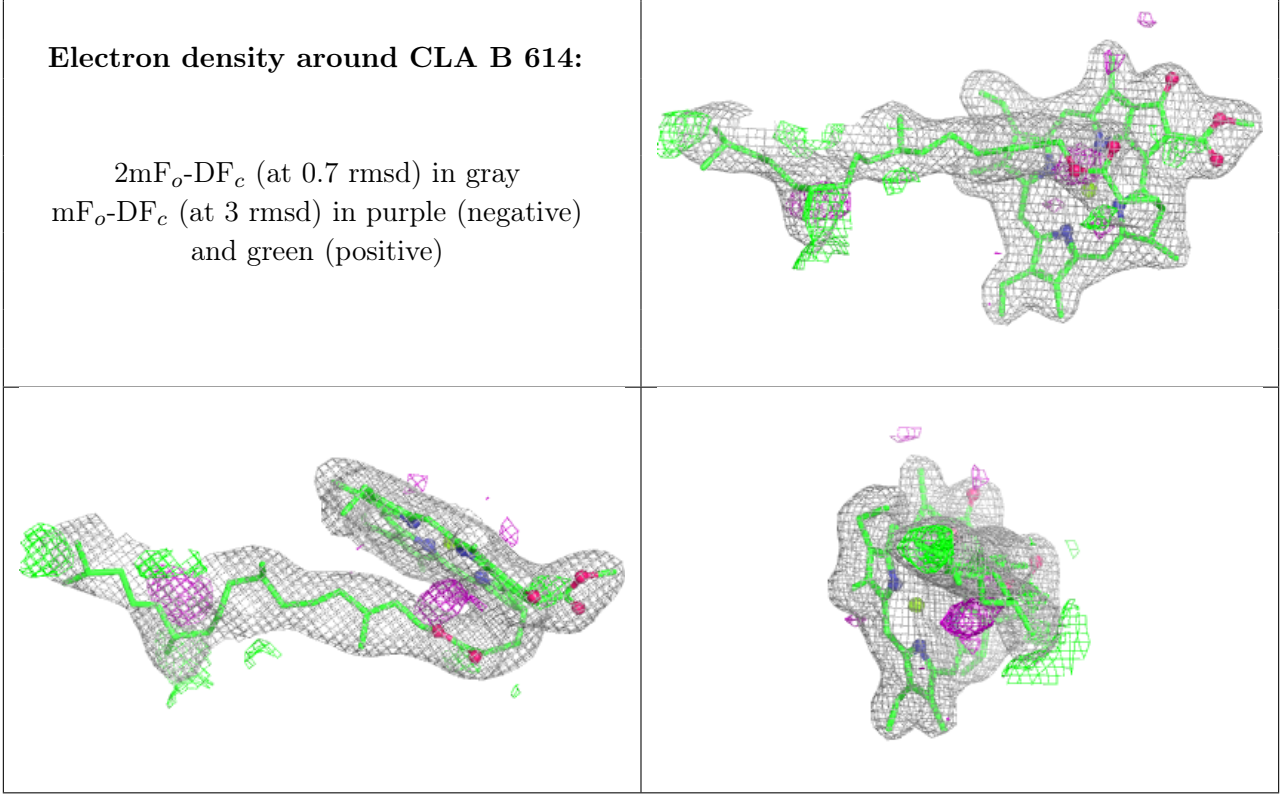






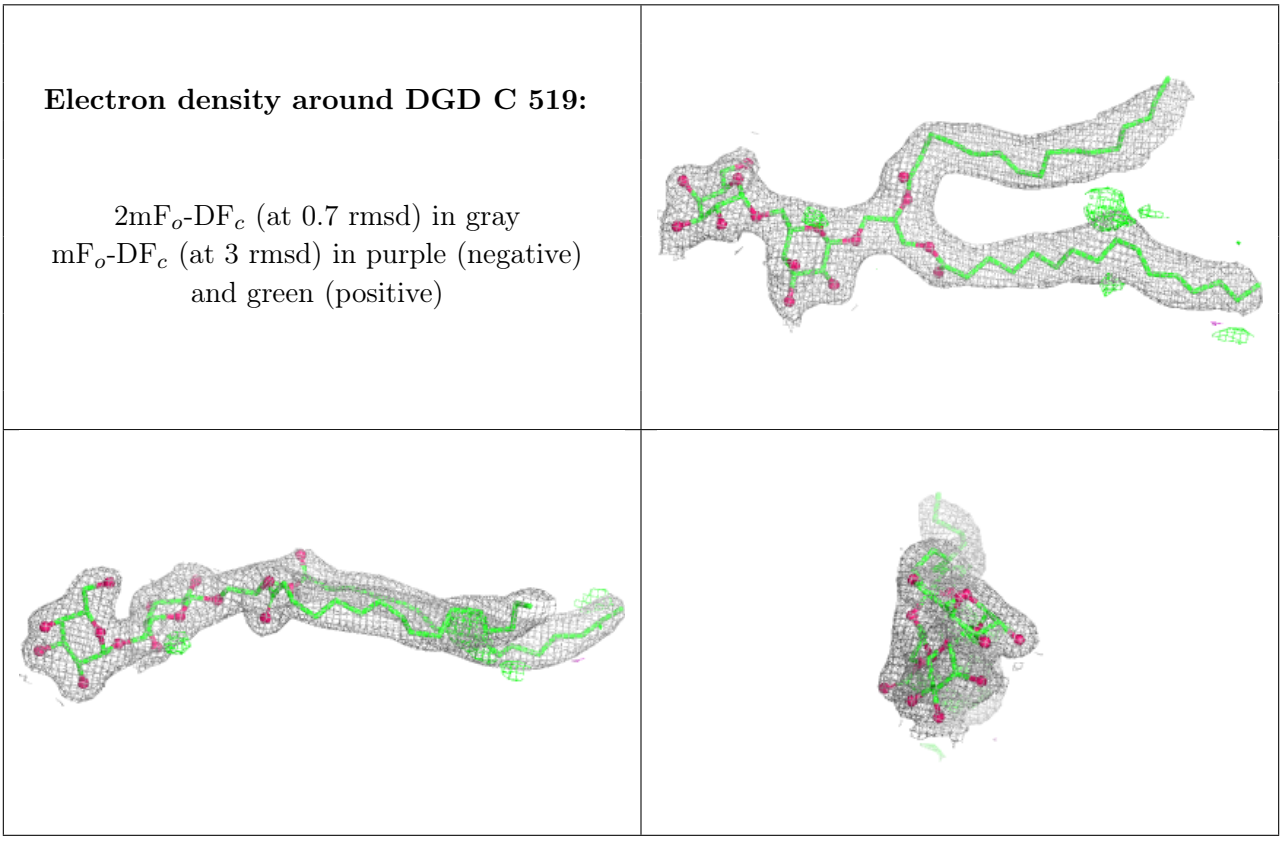
Electron density around CLA B 614:

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



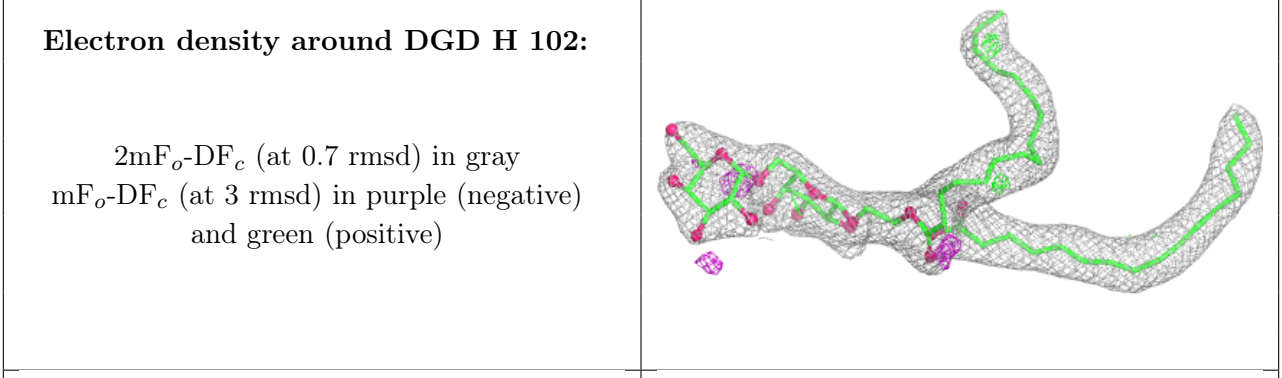
Electron density around DGD C 519:

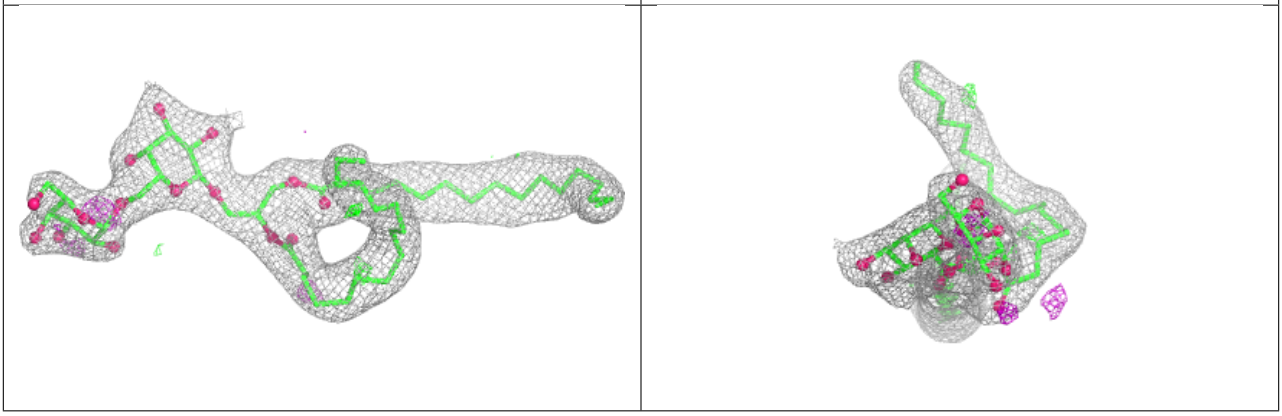
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD H 102:

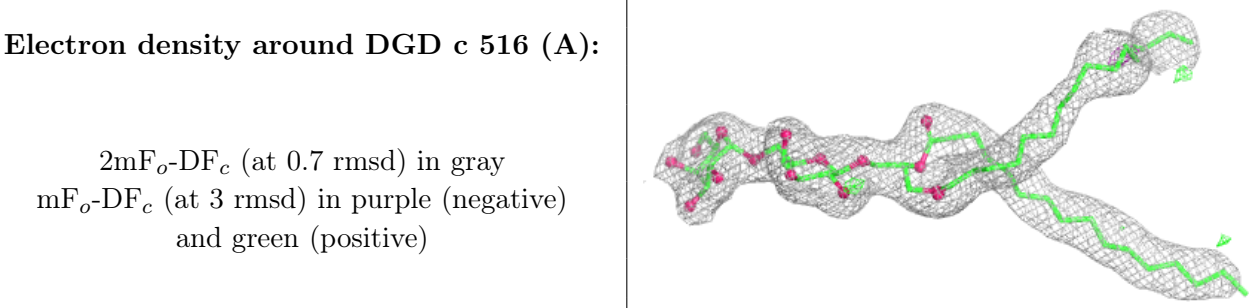
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

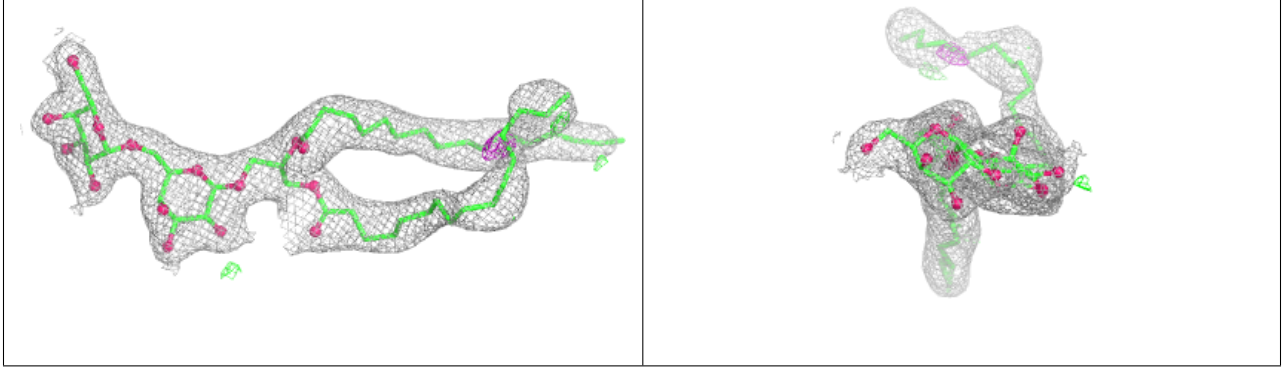




Electron density around DGD c 516 (A):

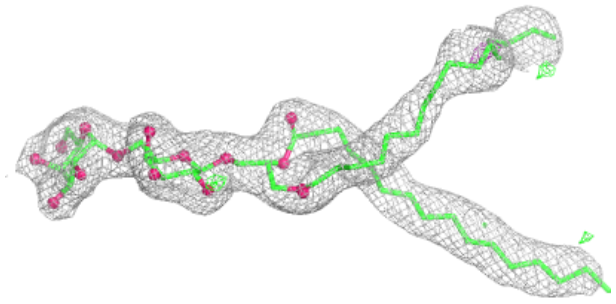
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

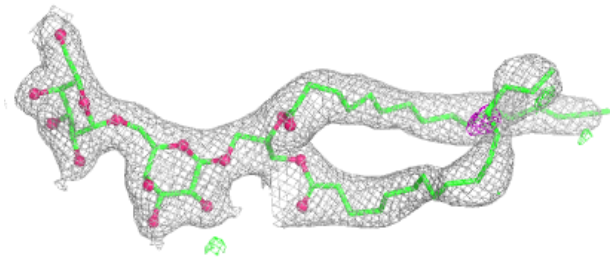


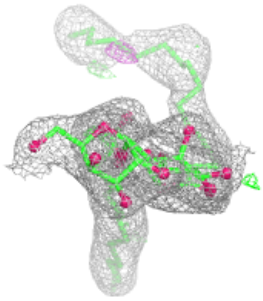


Electron density around DGD c 516 (B):

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

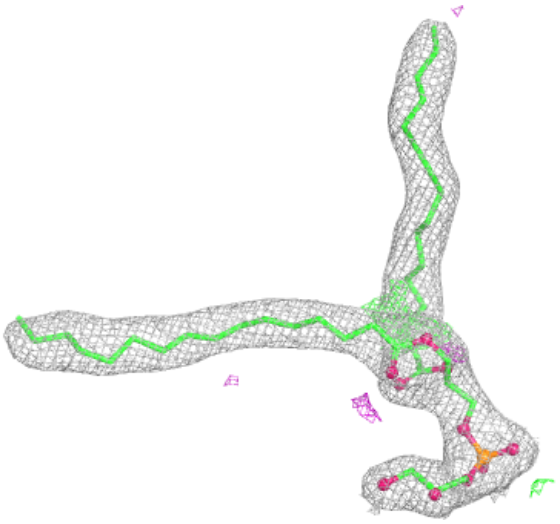


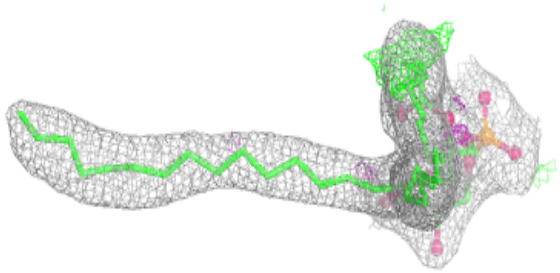


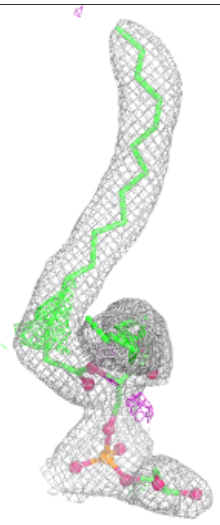


Electron density around LHG b 629 (A):

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

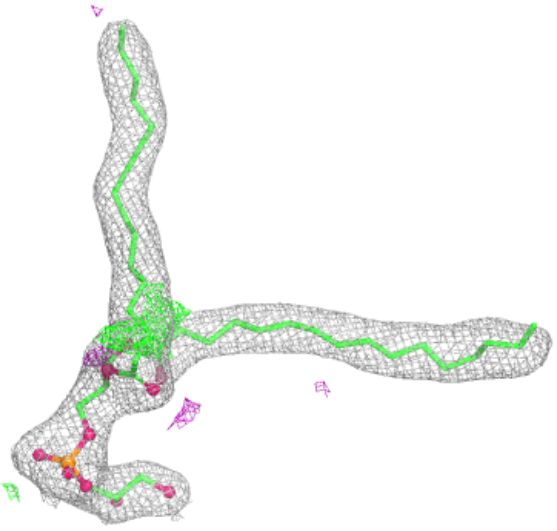


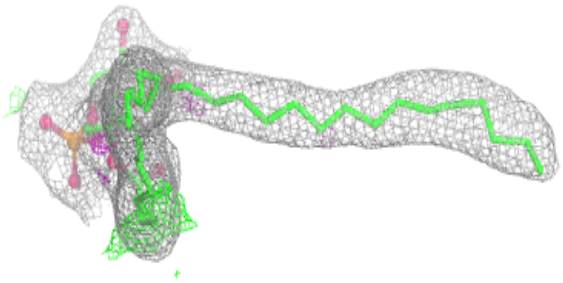


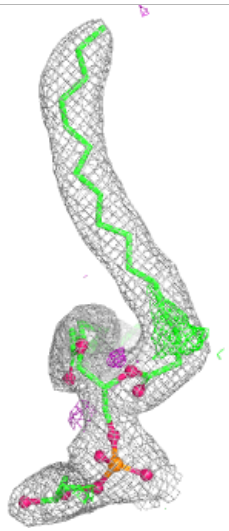


Electron density around LHG b 629 (B):

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

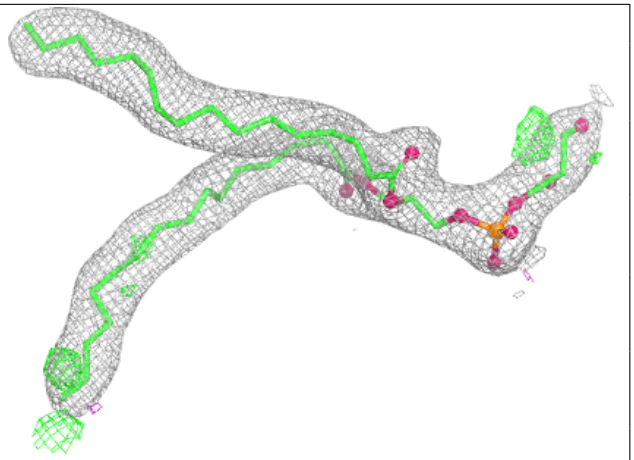


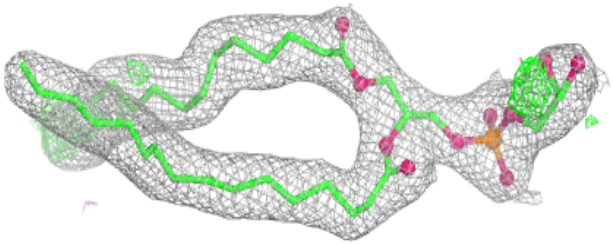


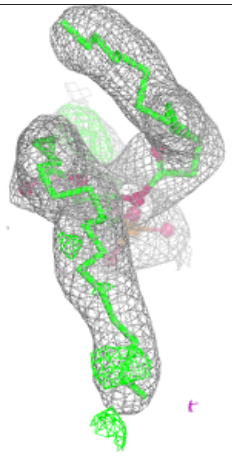


Electron density around LHG d 408 (A):

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

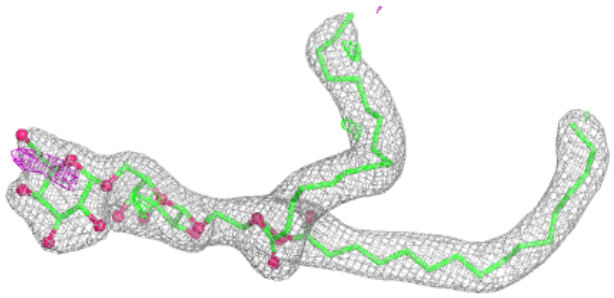


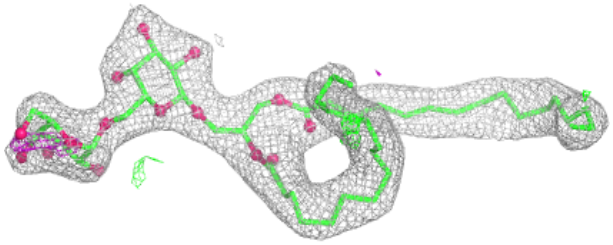




Electron density around DGD h 102:

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

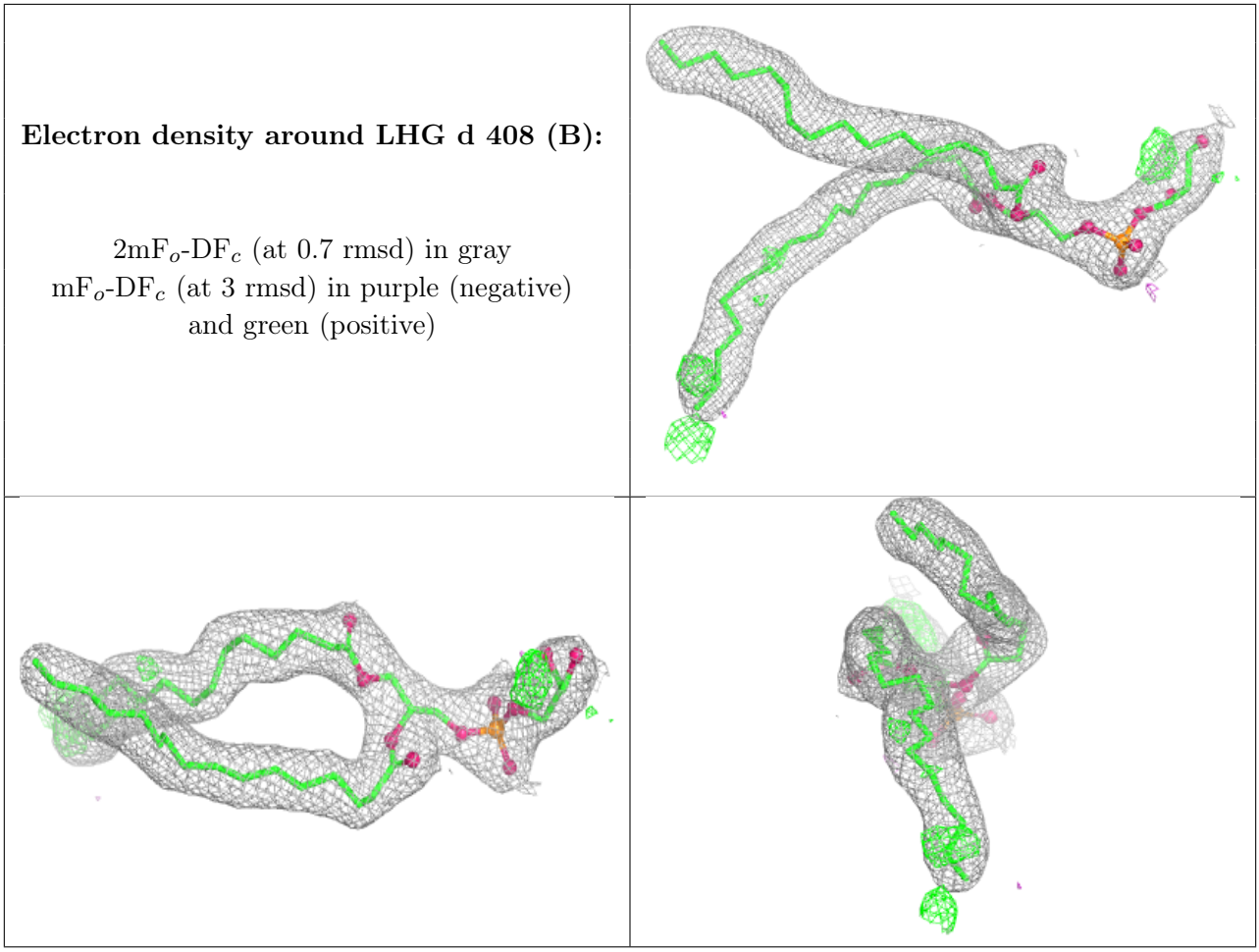






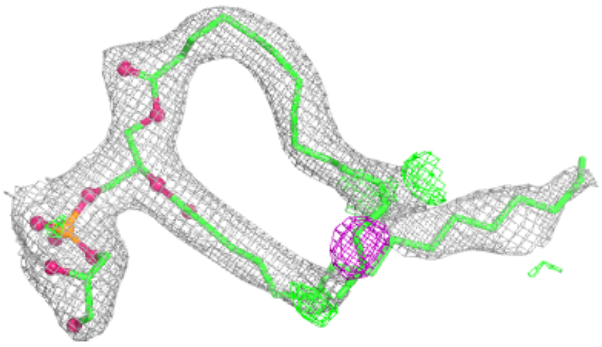
Electron density around LHG d 408 (B):

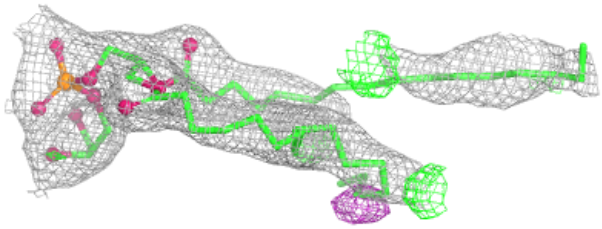
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

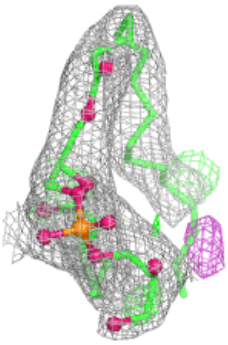


Electron density around LHG d 409 (A):

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

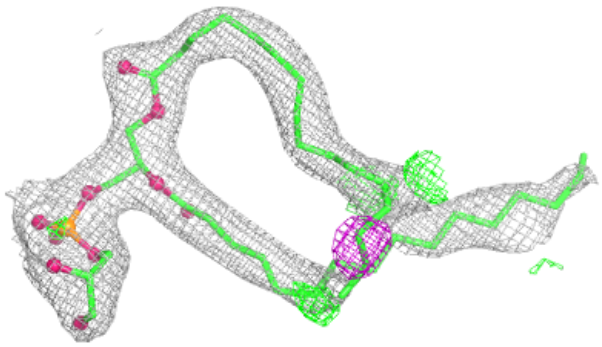


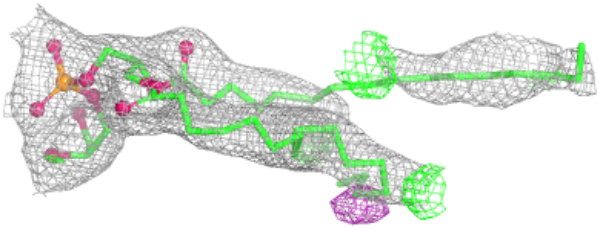


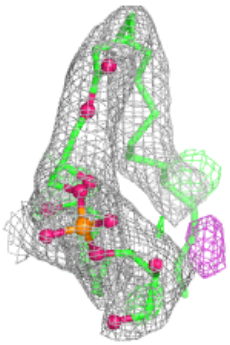


Electron density around LHG d 409 (B):

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

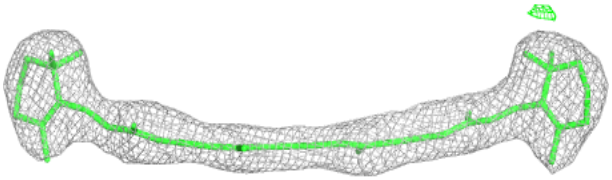


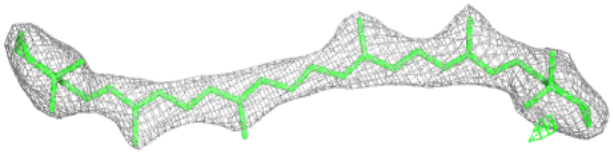


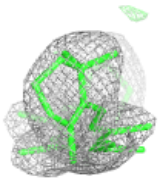


Electron density around BCR k 101:

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

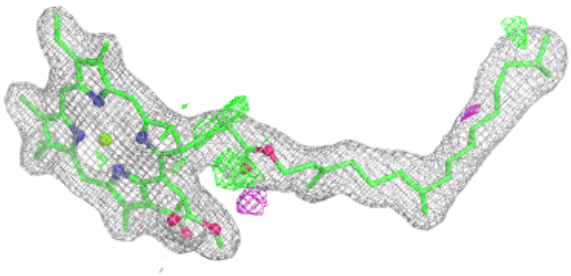


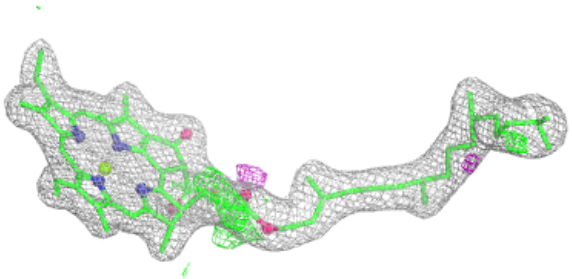




Electron density around CLA A 404 (A):

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

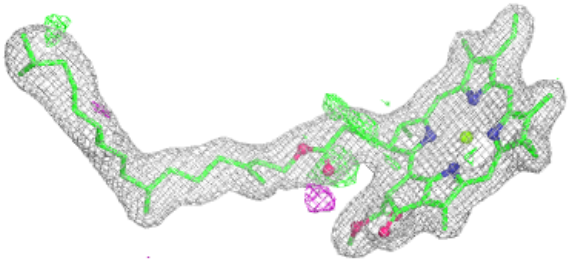


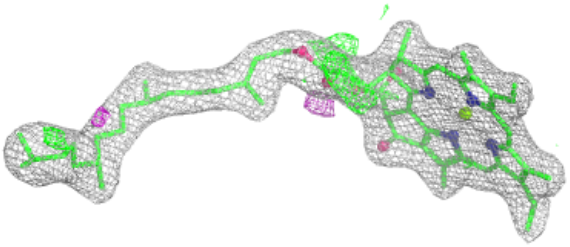


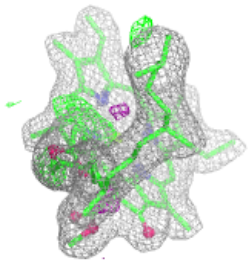


Electron density around CLA A 404 (B):

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

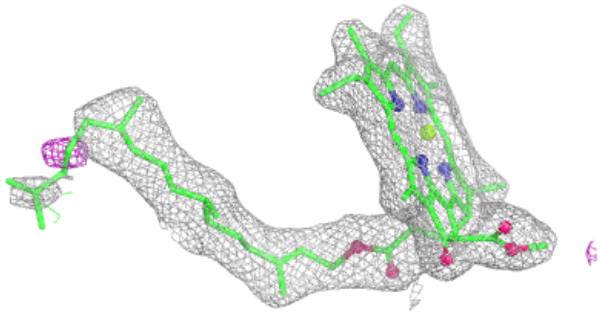


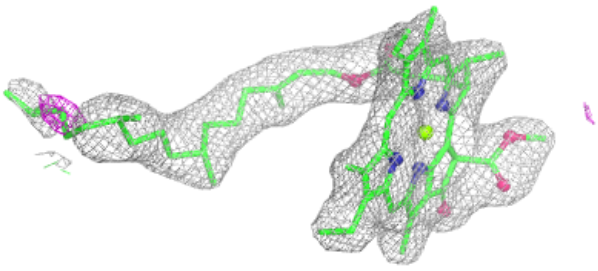


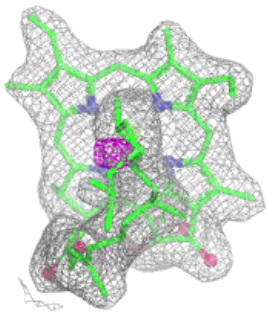


Electron density around CLA c 508:

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

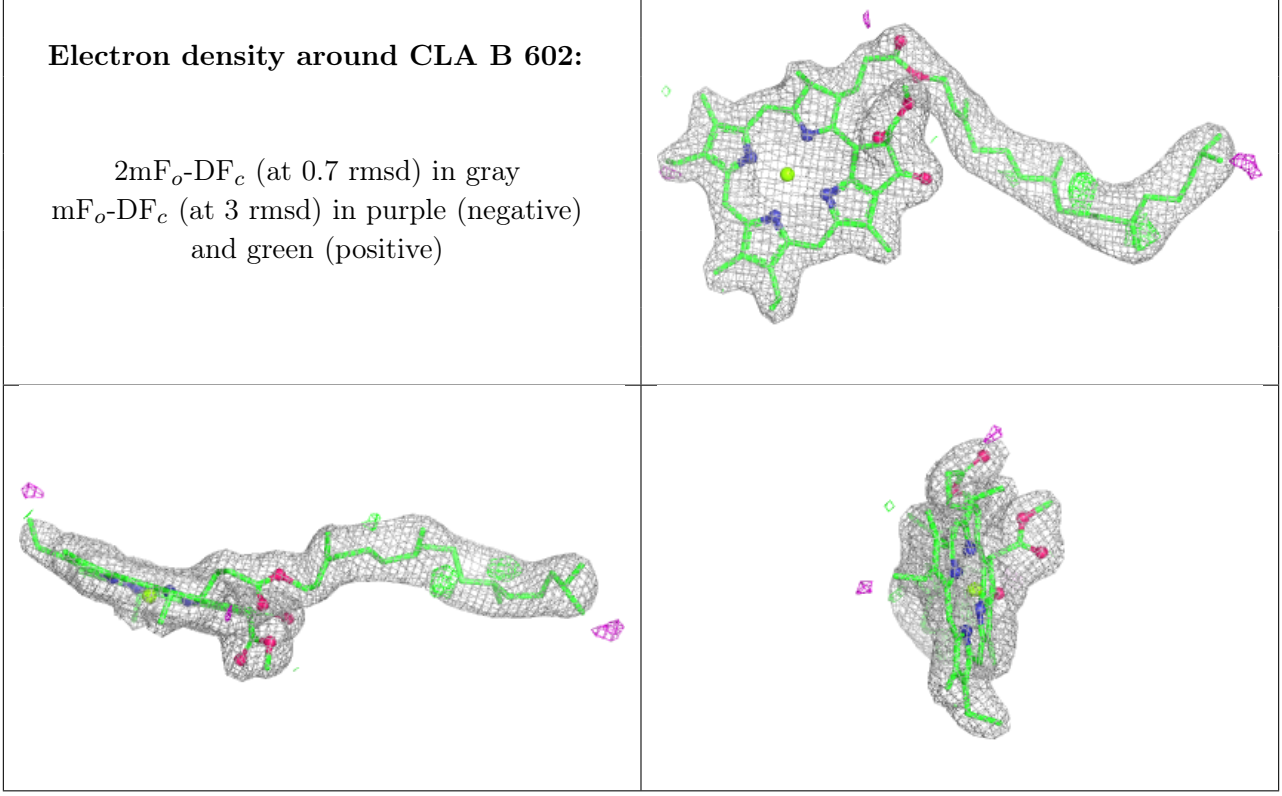






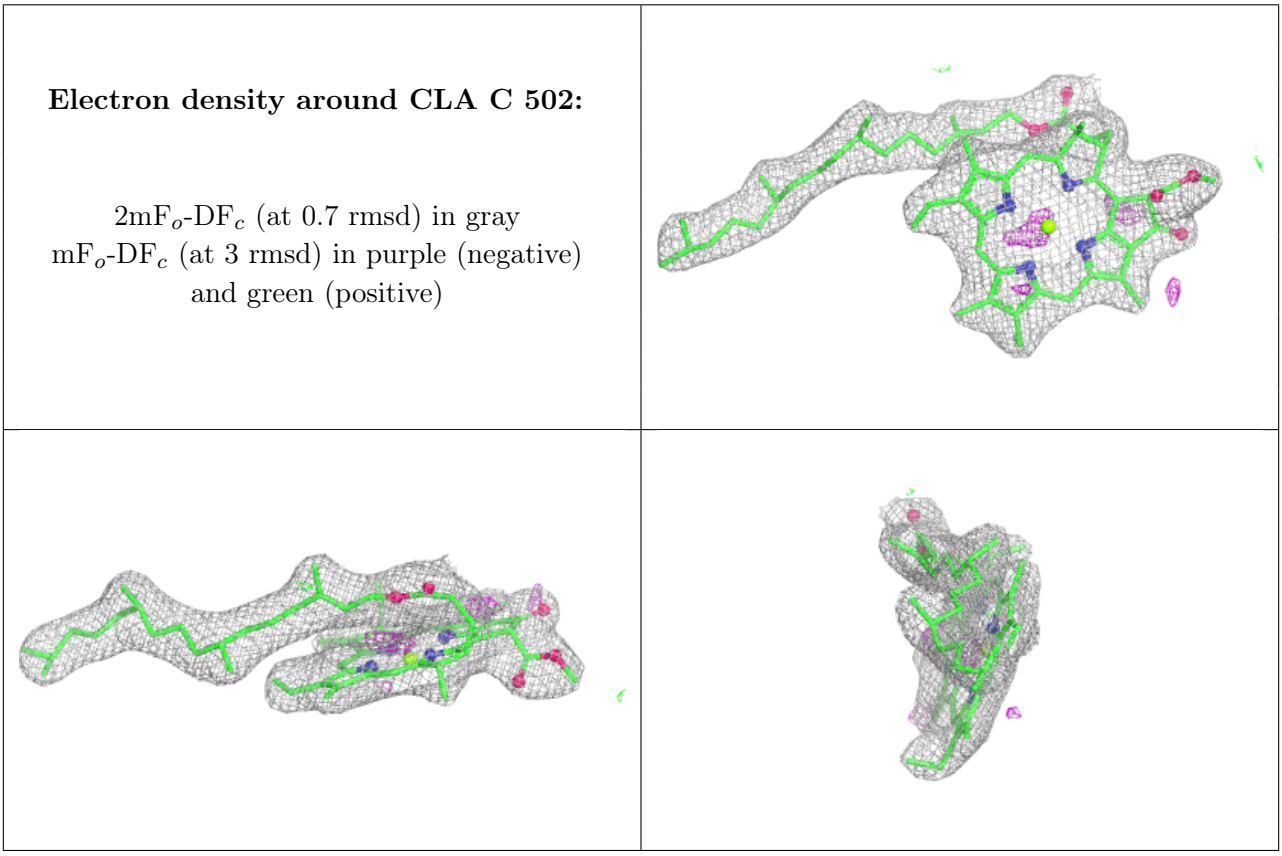
Electron density around CLA B 602:

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



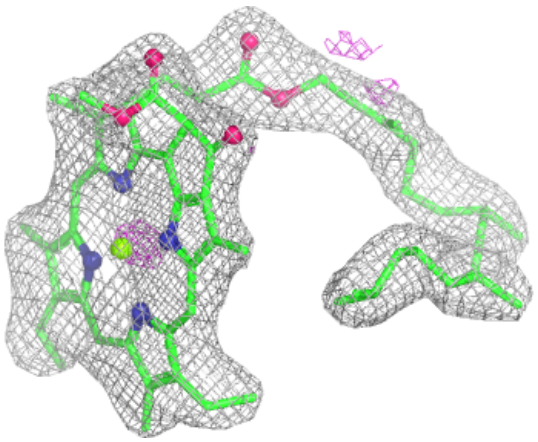
Electron density around CLA C 502:

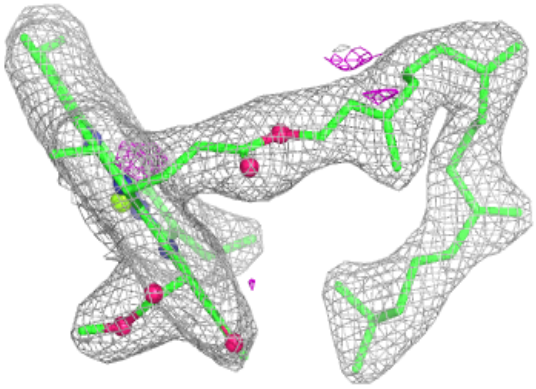
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

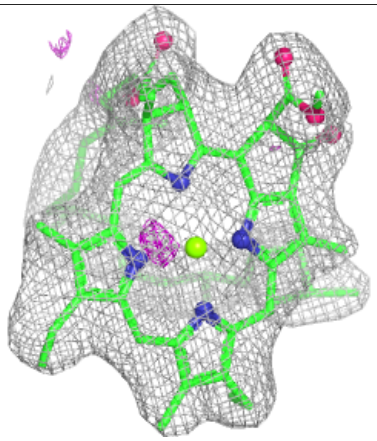


Electron density around CLA C 504:

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

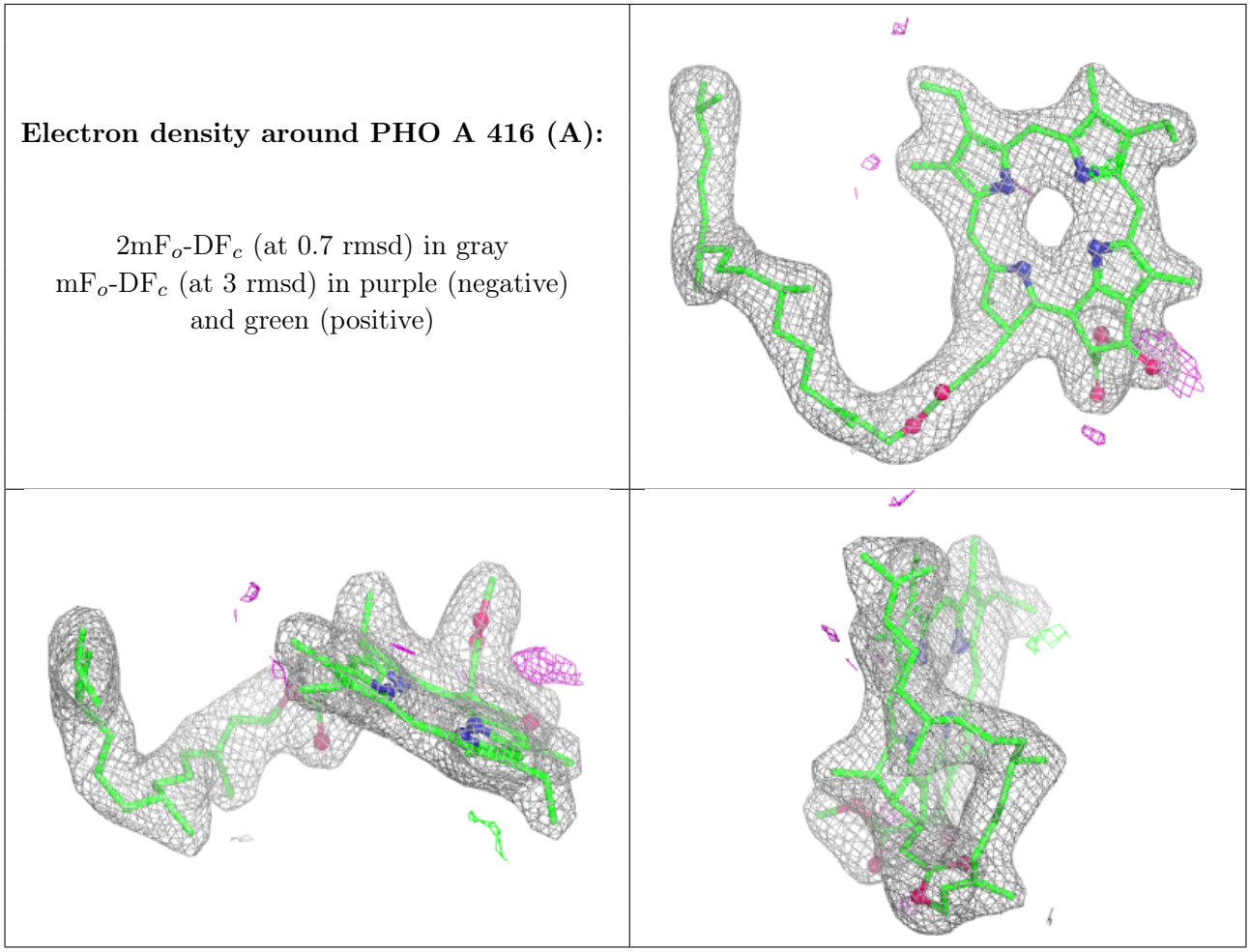






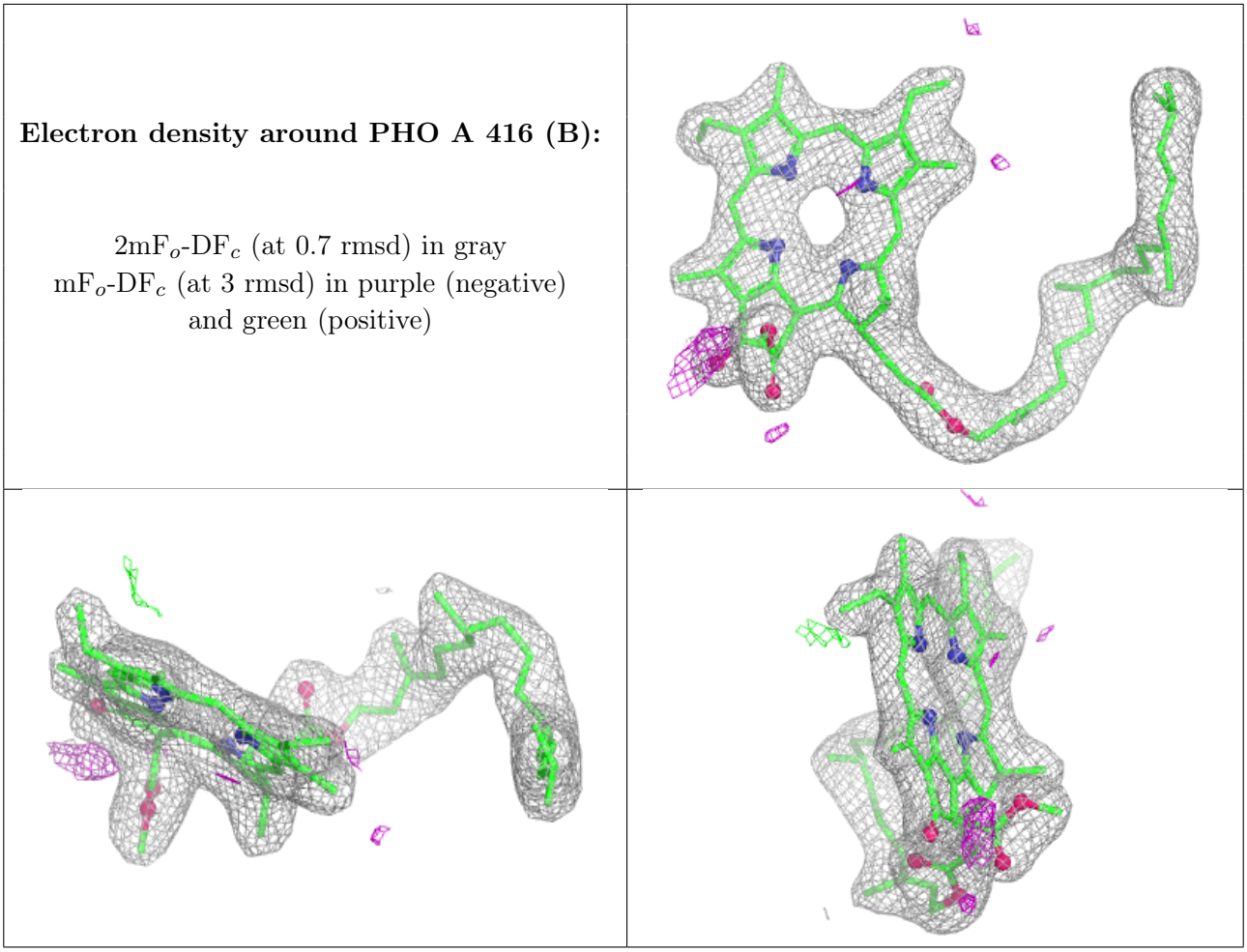
Electron density around PHO A 416 (A):

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



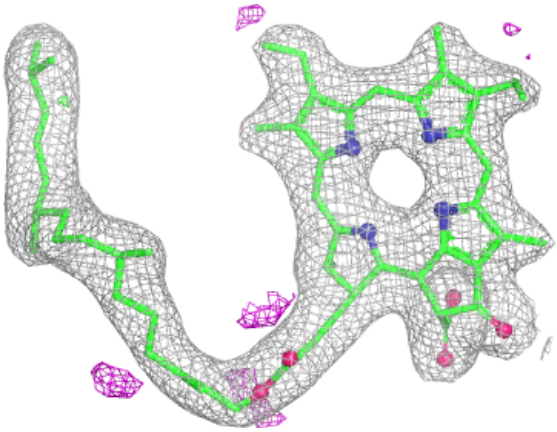
Electron density around PHO A 416 (B):

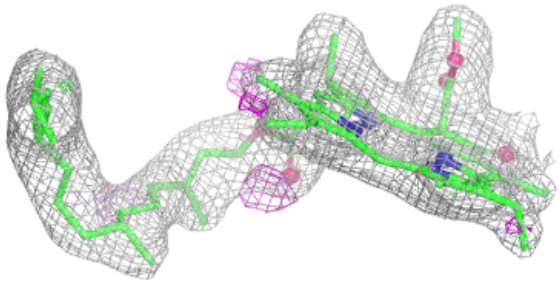
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

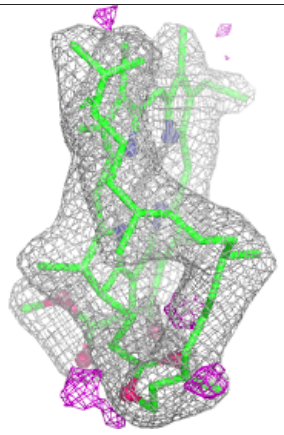


Electron density around PHO d 403 (A):

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

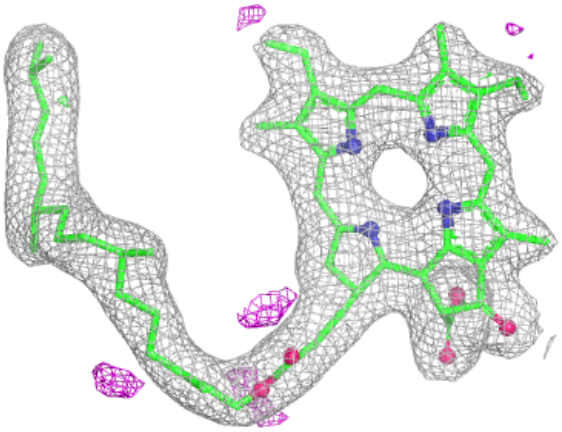


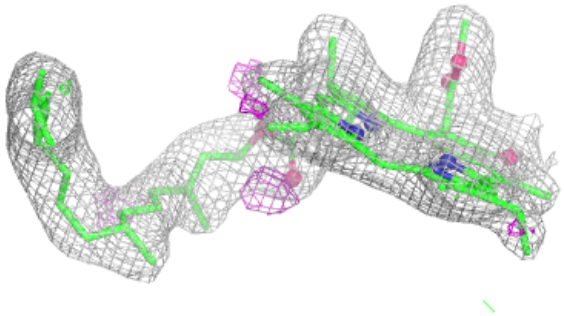


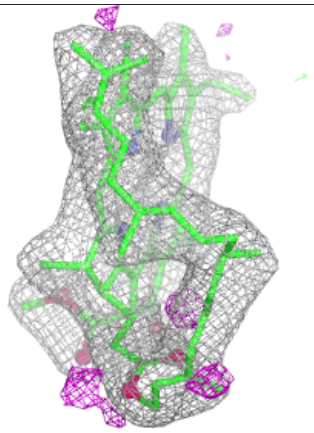


Electron density around PHO d 403 (B):

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

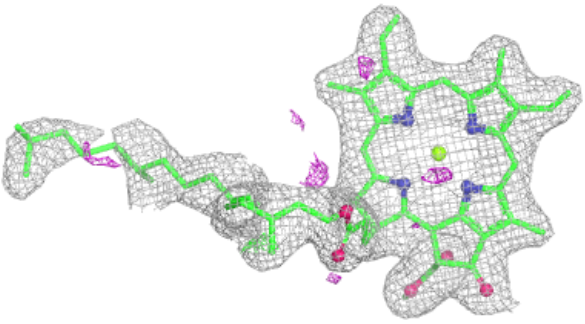


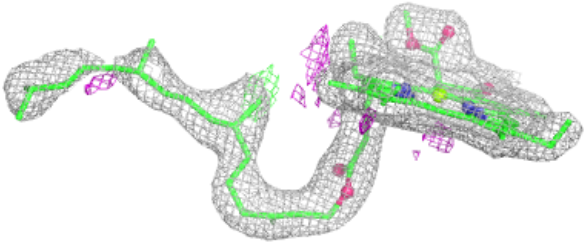


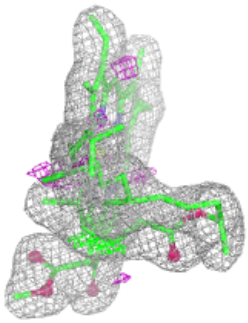


Electron density around CLA A 406 (A):

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

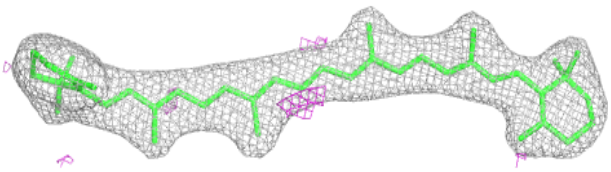


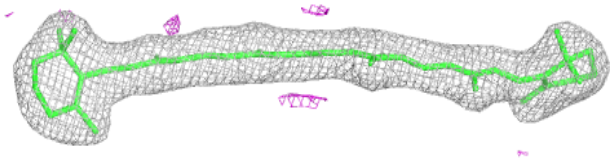


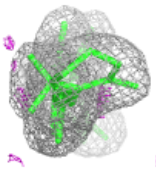


Electron density around BCR B 617:

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

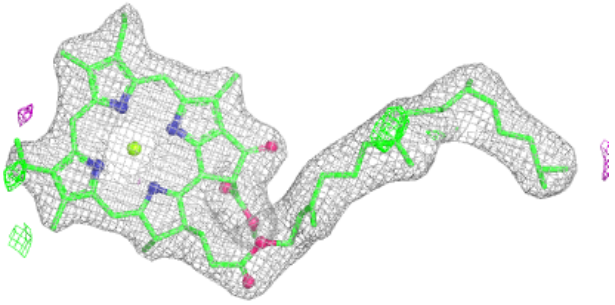


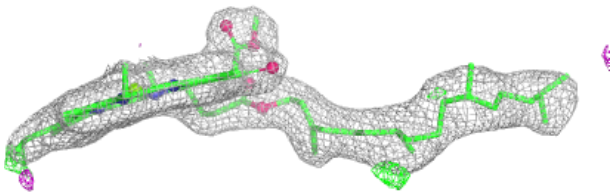


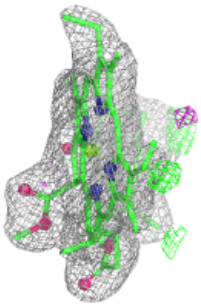


Electron density around CLA b 602:

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

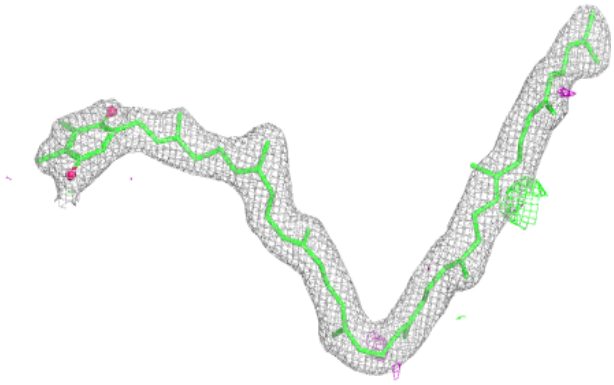


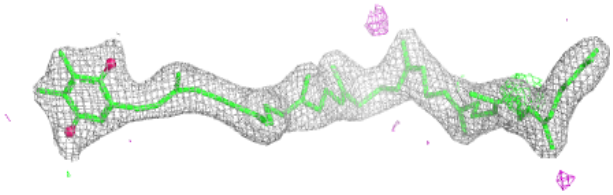




Electron density around PL9 d 407 (A):

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

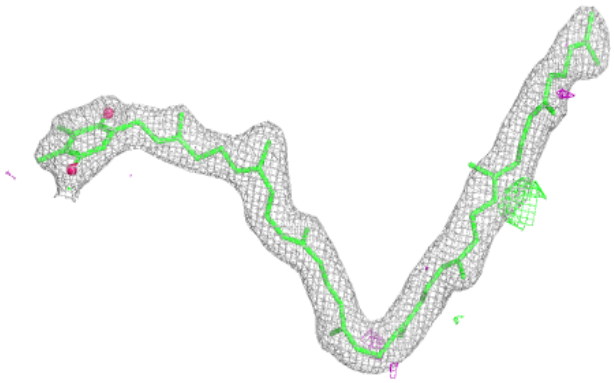


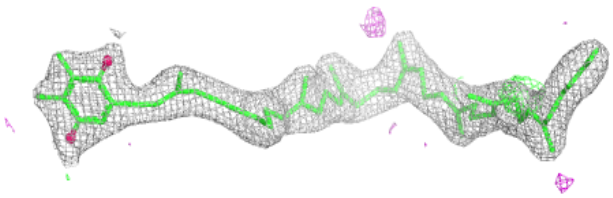




Electron density around PL9 d 407 (B):

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

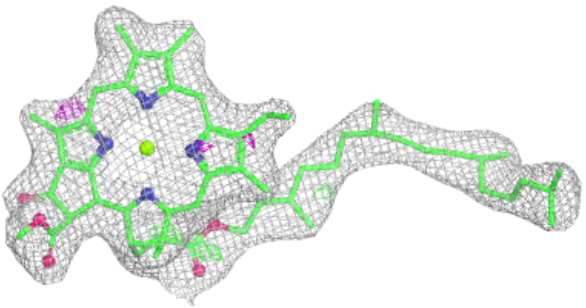


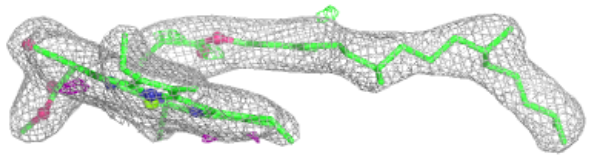


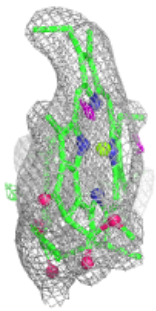


Electron density around CLA b 603:

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

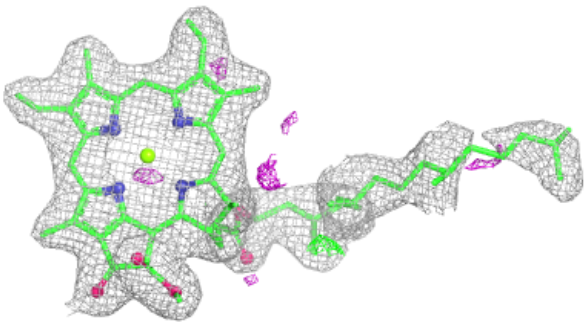


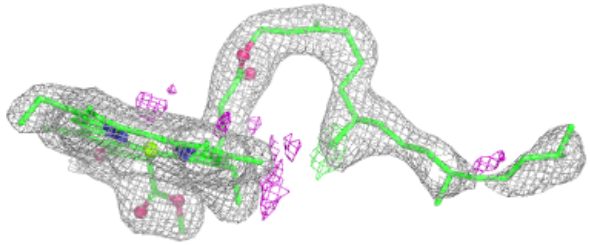




Electron density around CLA A 406 (B):

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

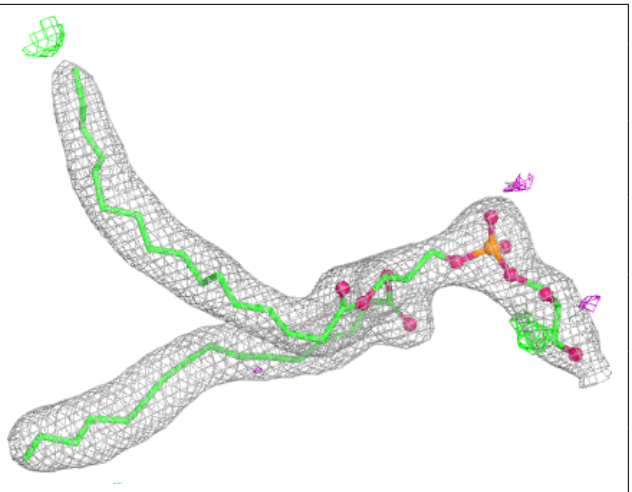


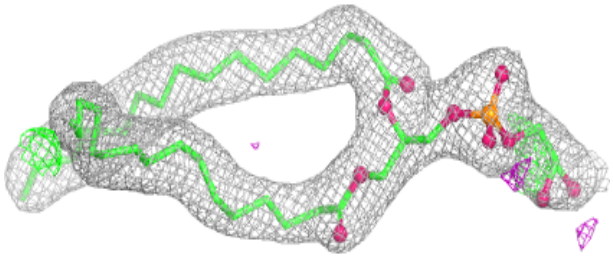


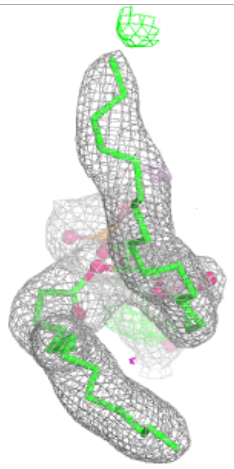


Electron density around LHG D 406 (A):

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

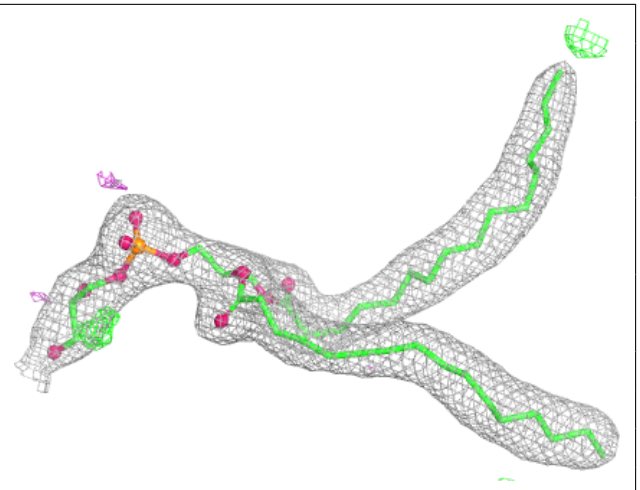


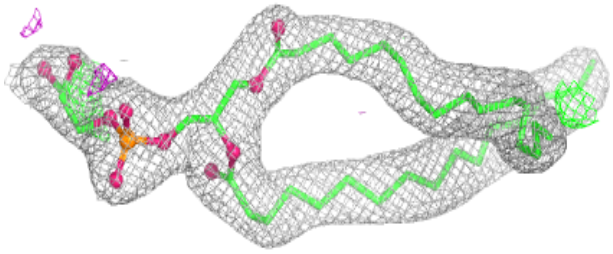


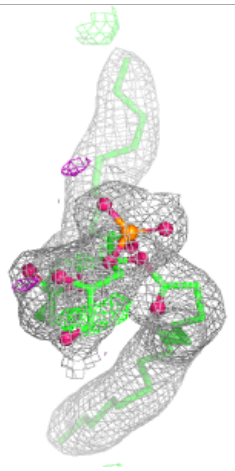


Electron density around LHG D 406 (B):

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

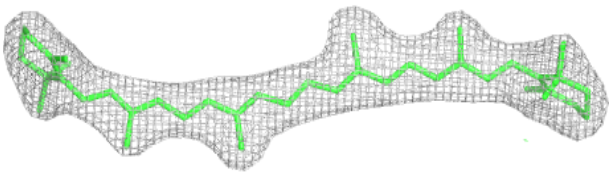


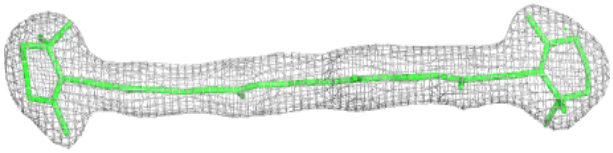


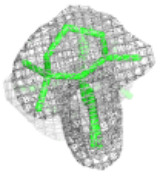


Electron density around BCR C 516:

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

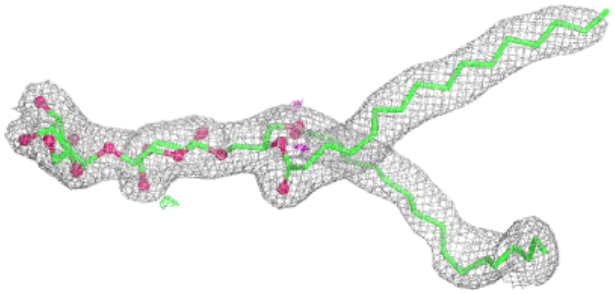


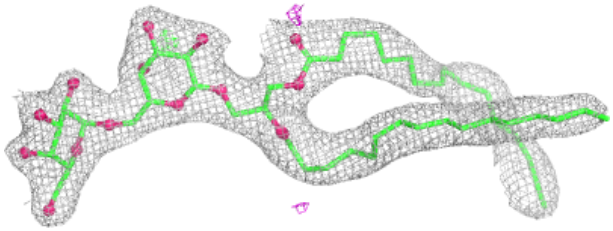


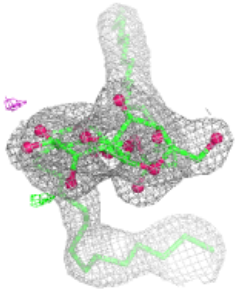


Electron density around DGD C 517 (A):

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

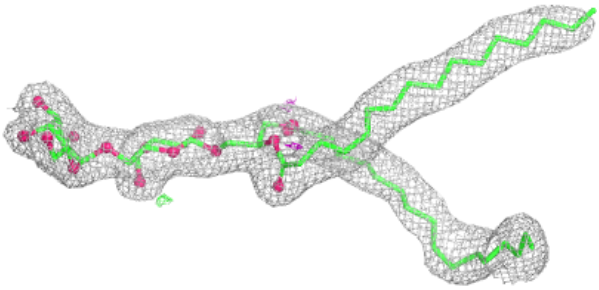


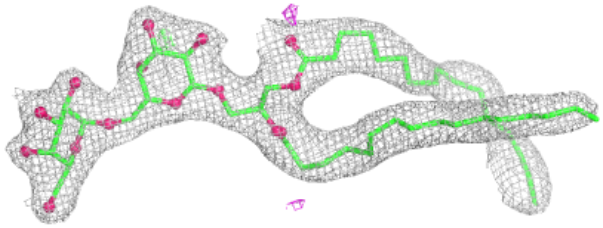


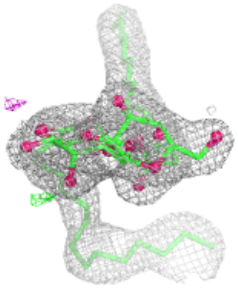


Electron density around DGD C 517 (B):

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

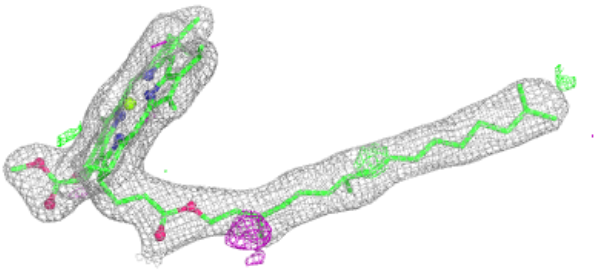


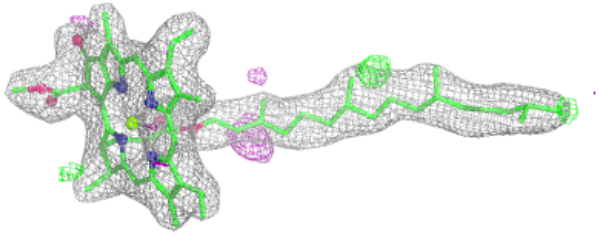


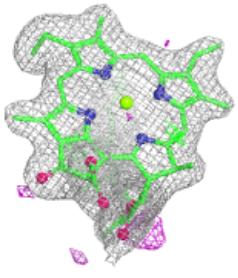


Electron density around CLA b 607:

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

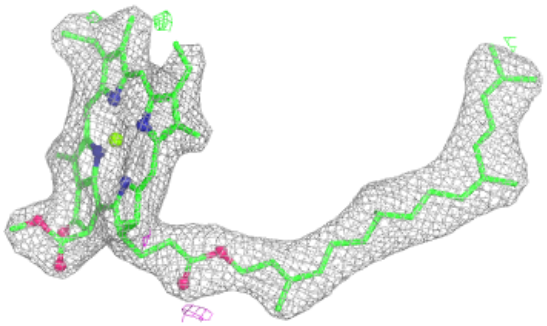


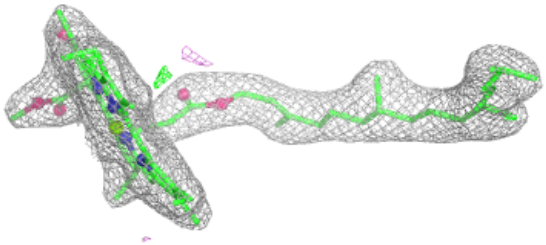


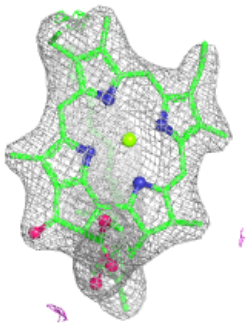


Electron density around CLA b 609:

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

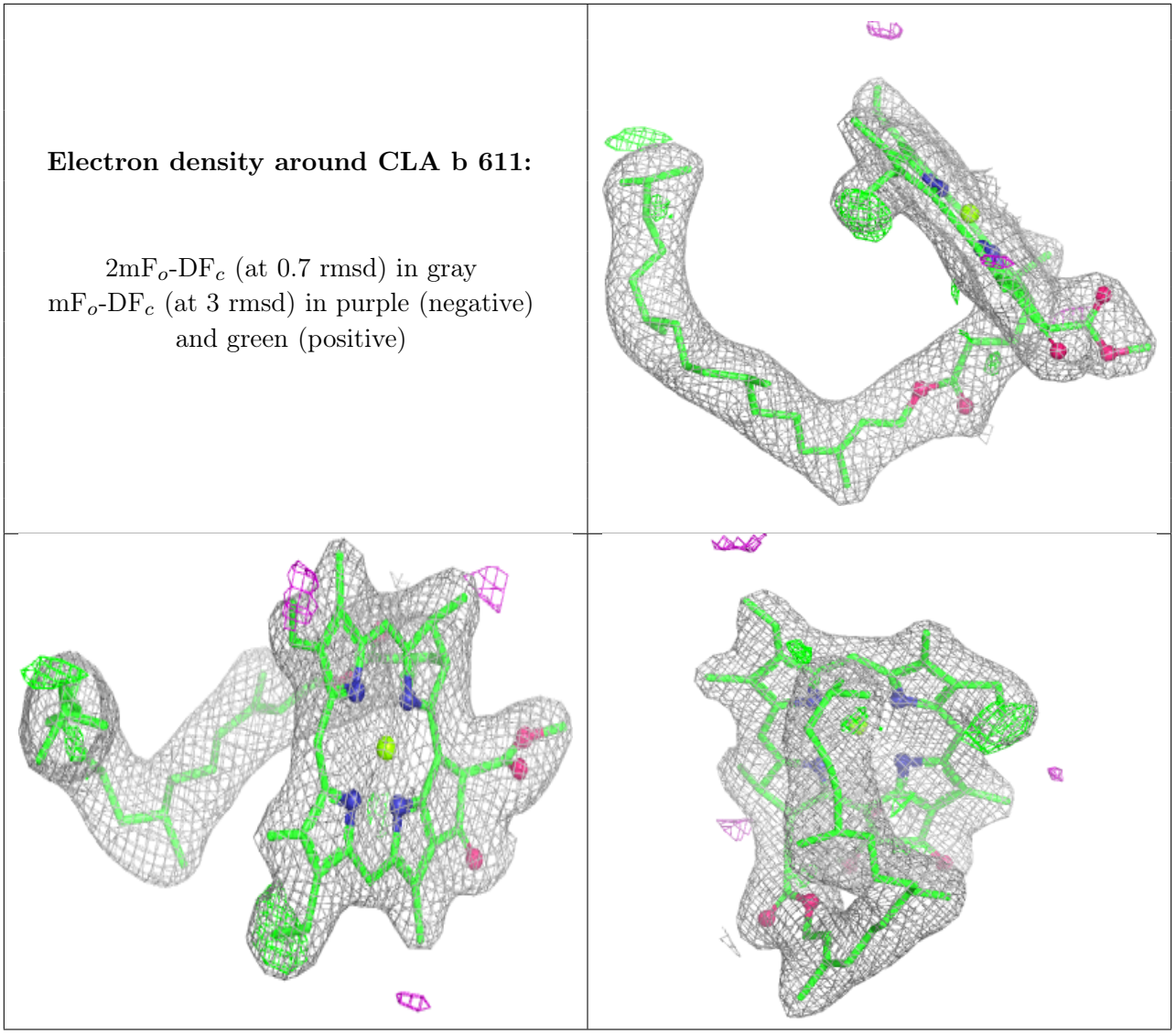






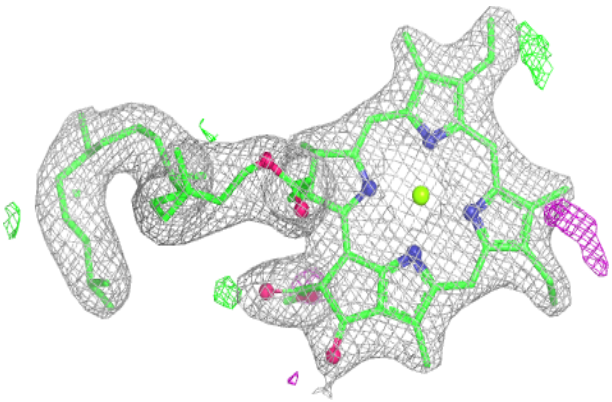
Electron density around CLA b 611:

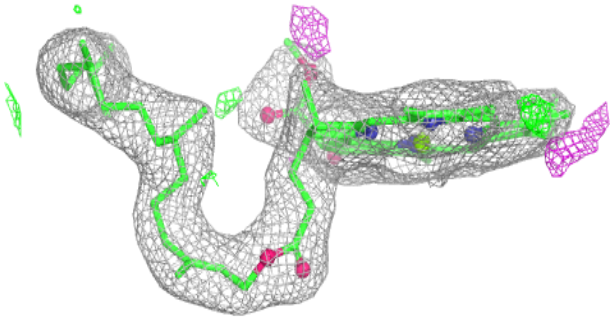
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

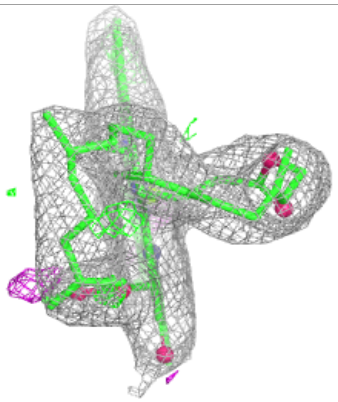


Electron density around CLA b 612:

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

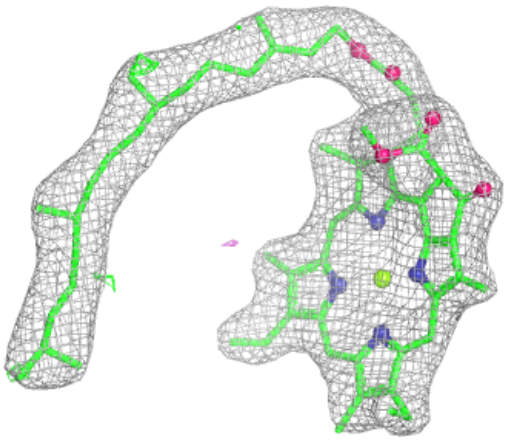


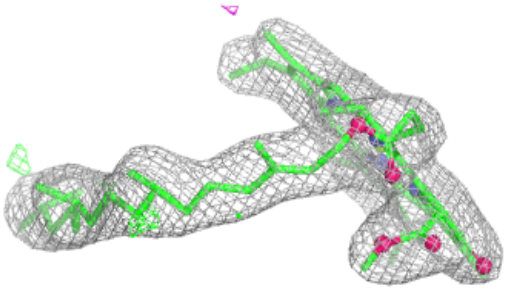


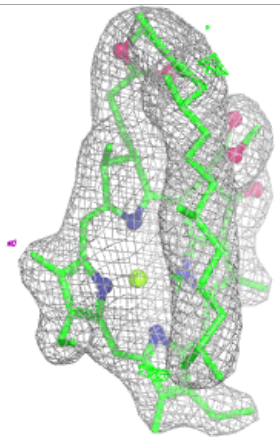


Electron density around CLA C 508:

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

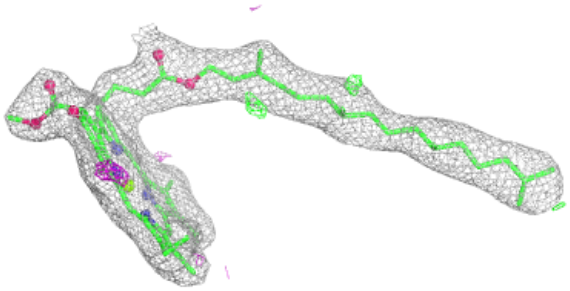


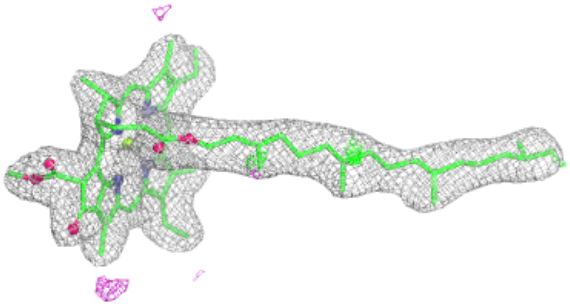


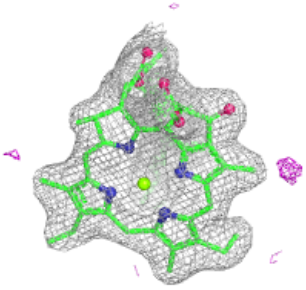


Electron density around CLA B 607:

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

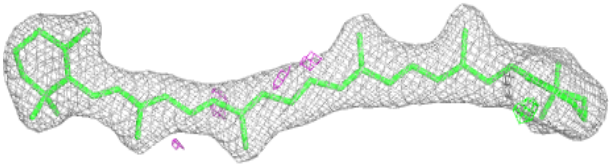


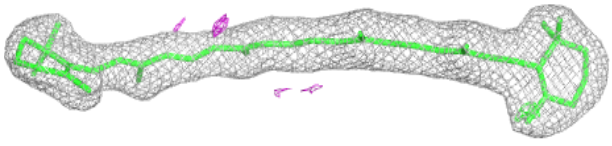


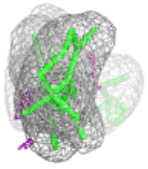


Electron density around BCR b 617:

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

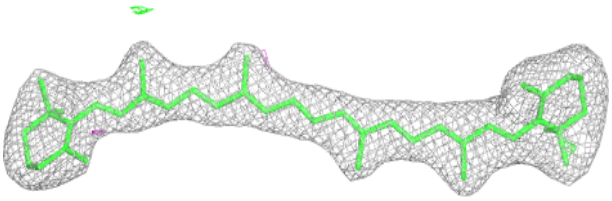


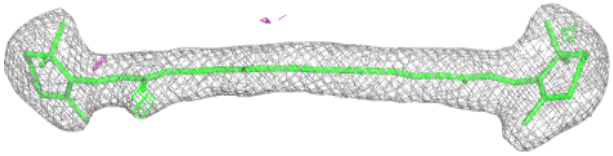


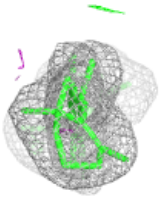


Electron density around BCR b 618:

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

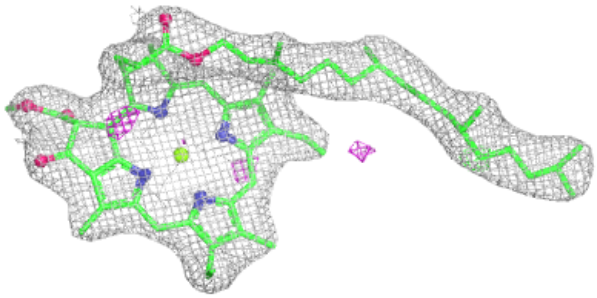


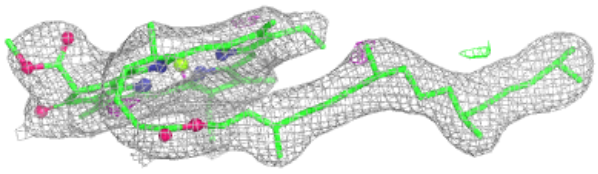


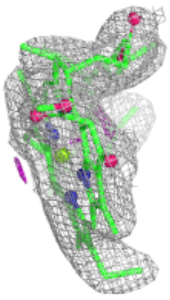


Electron density around CLA c 501:

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

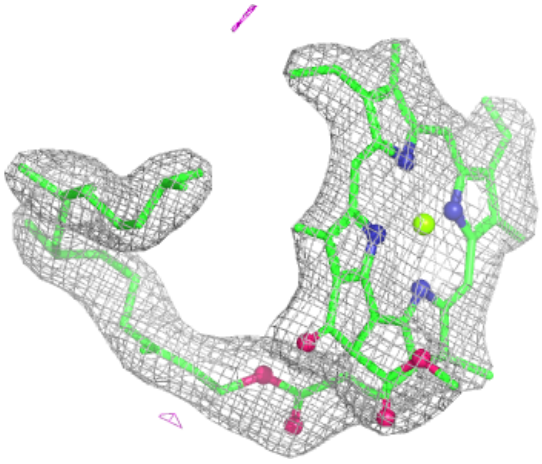


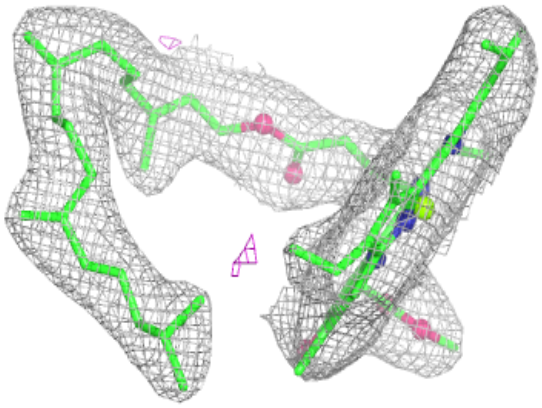


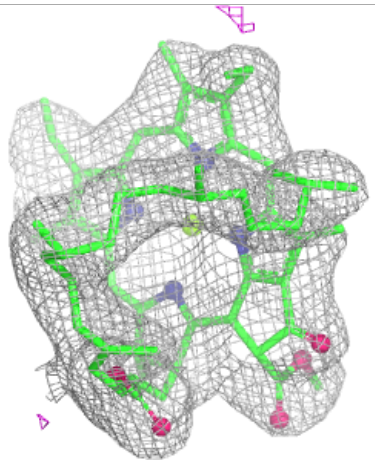


Electron density around CLA c 503:

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

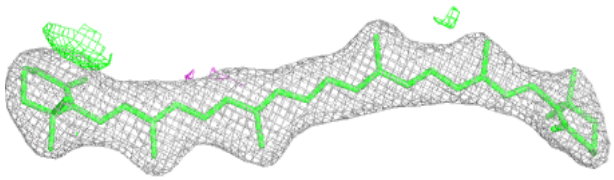


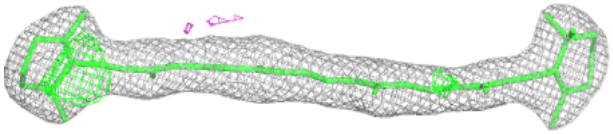


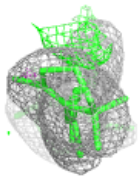


Electron density around BCR c 515:

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

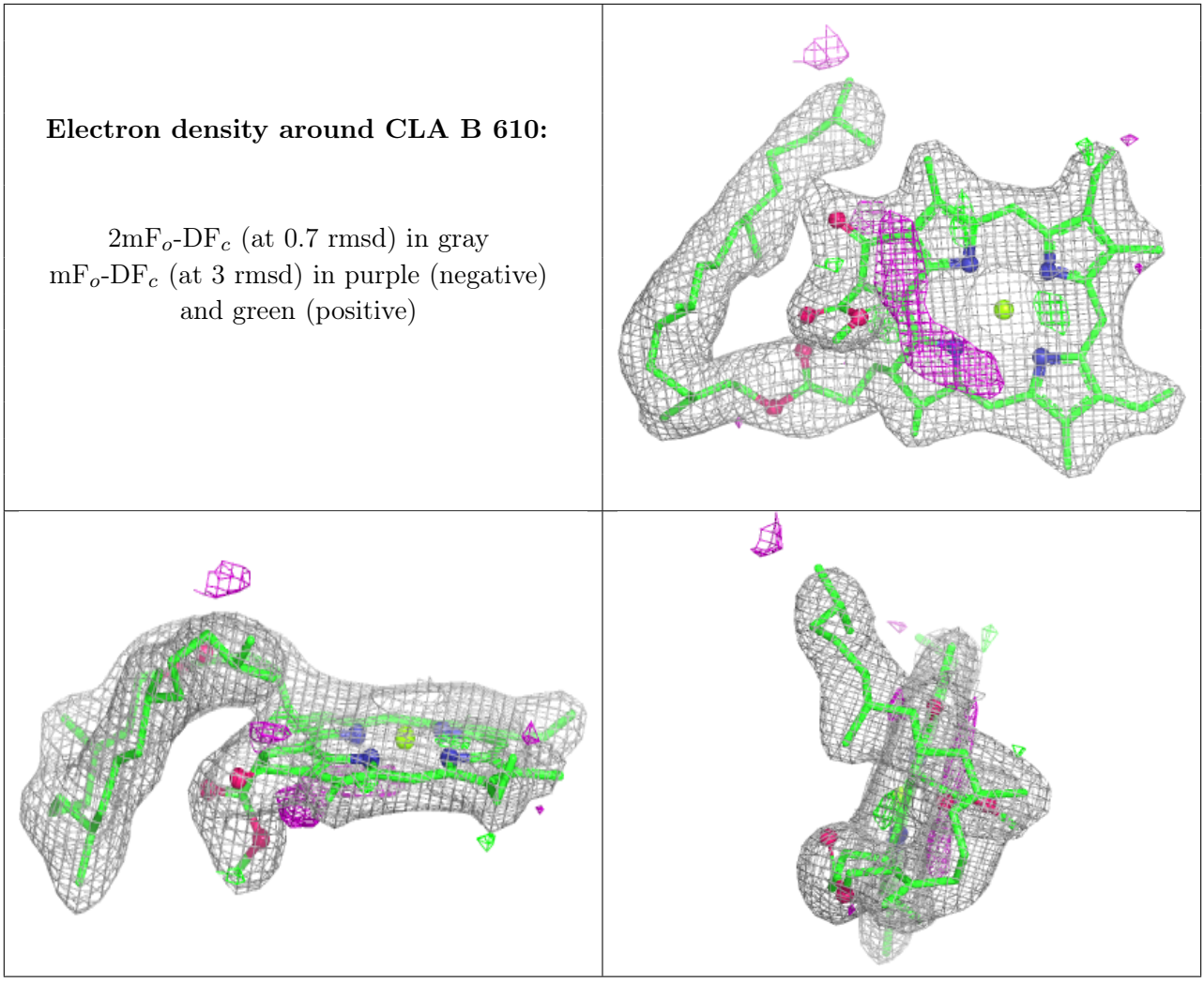






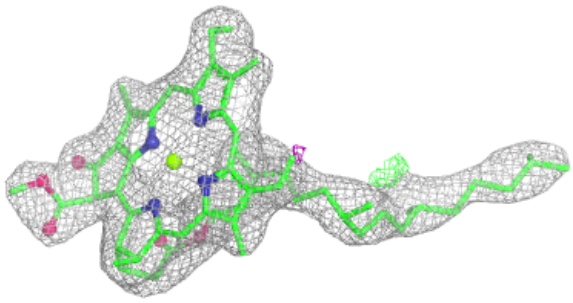
Electron density around CLA B 610:

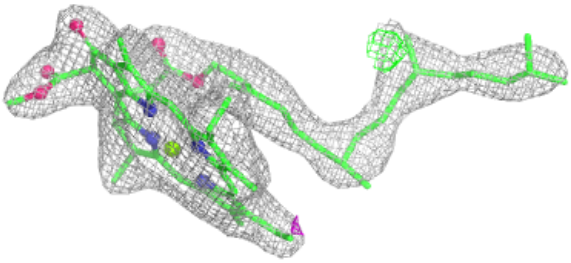
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

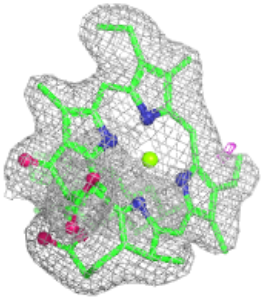


Electron density around CLA c 505:

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

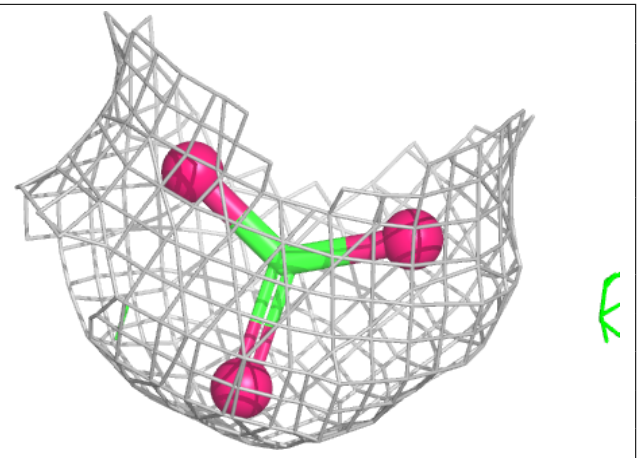


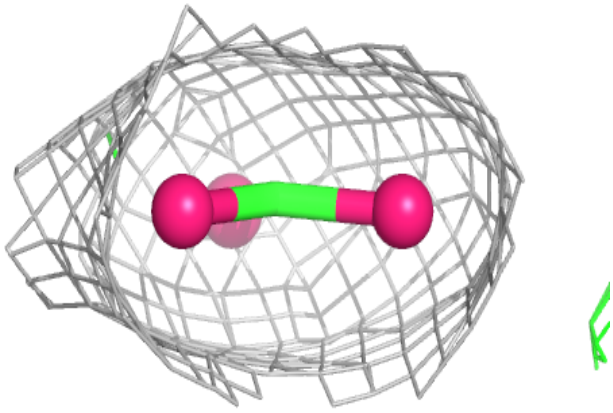


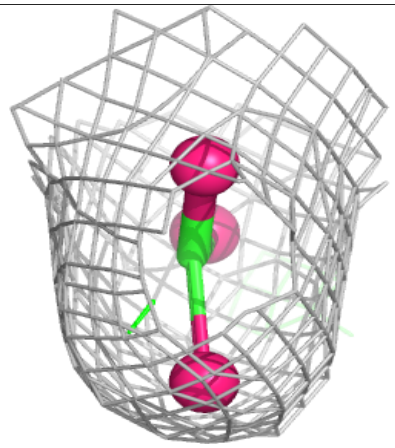


Electron density around BCT D 401 (A):

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

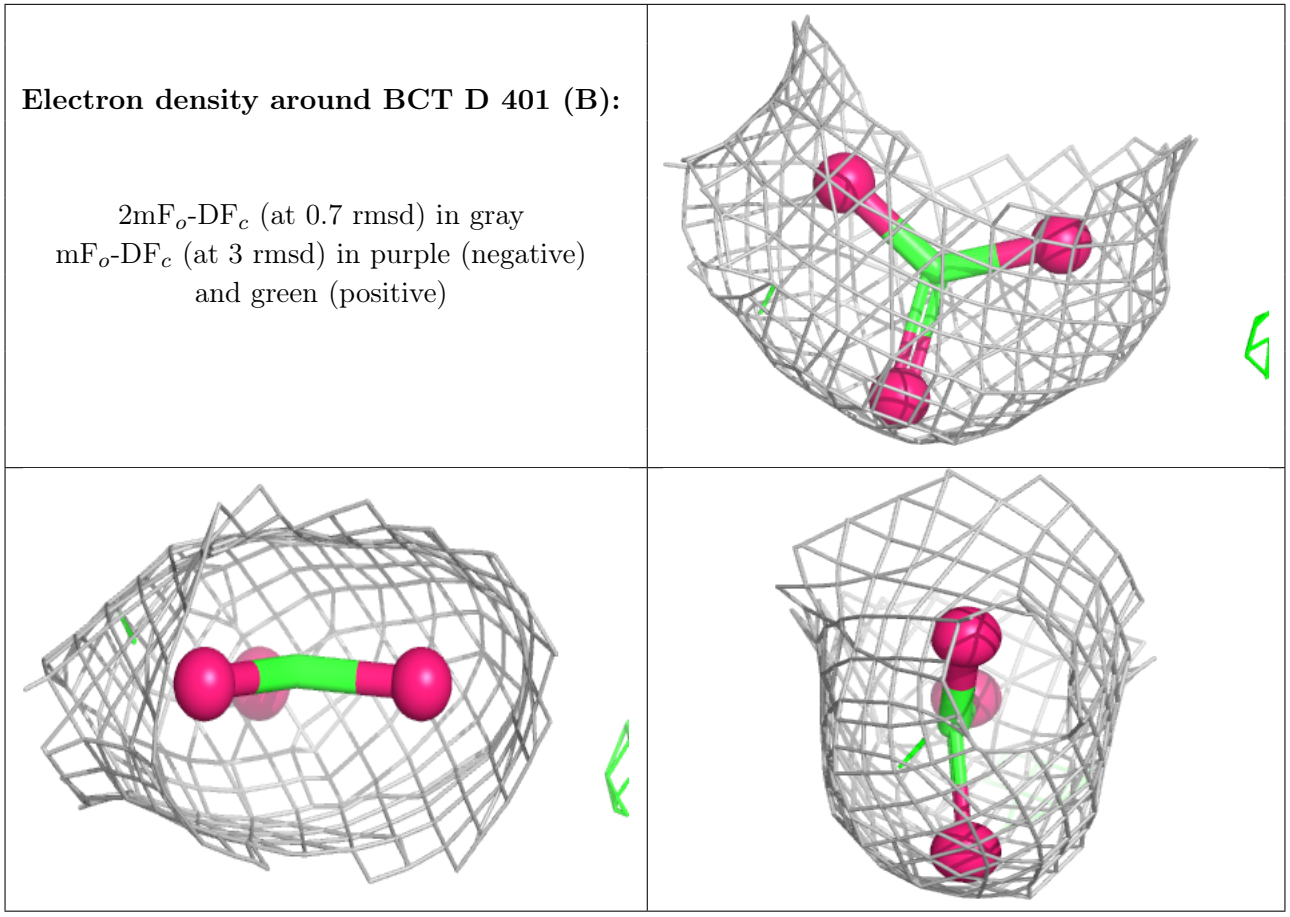






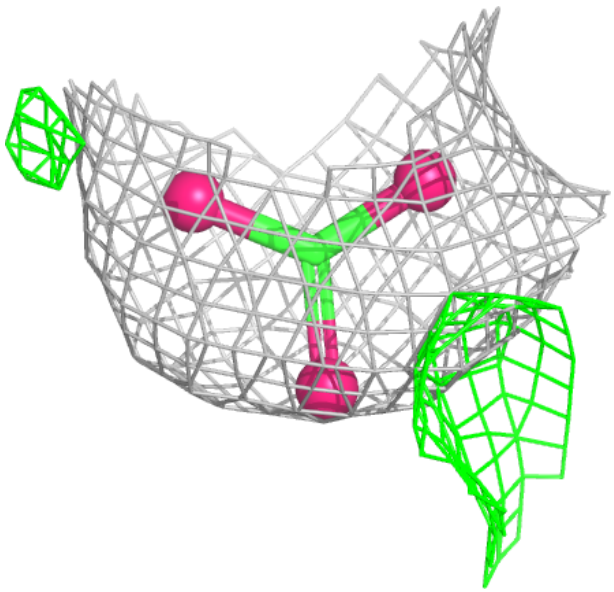
Electron density around BCT D 401 (B):

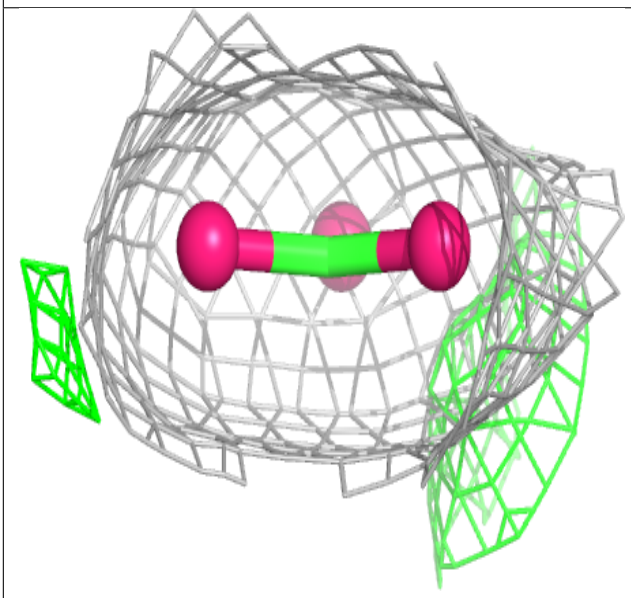
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

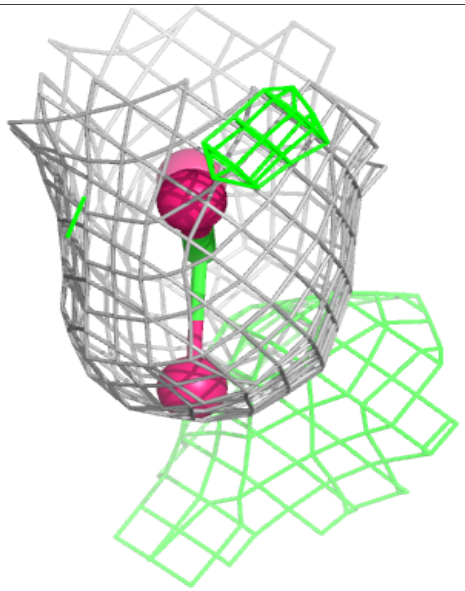


Electron density around BCT d 401 (A):

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

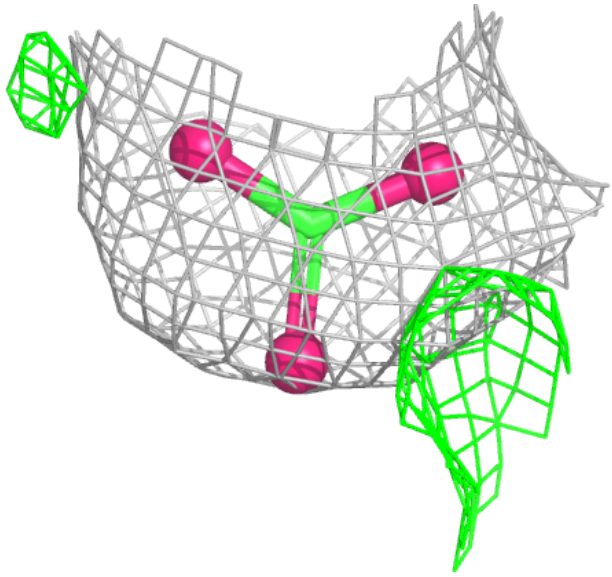


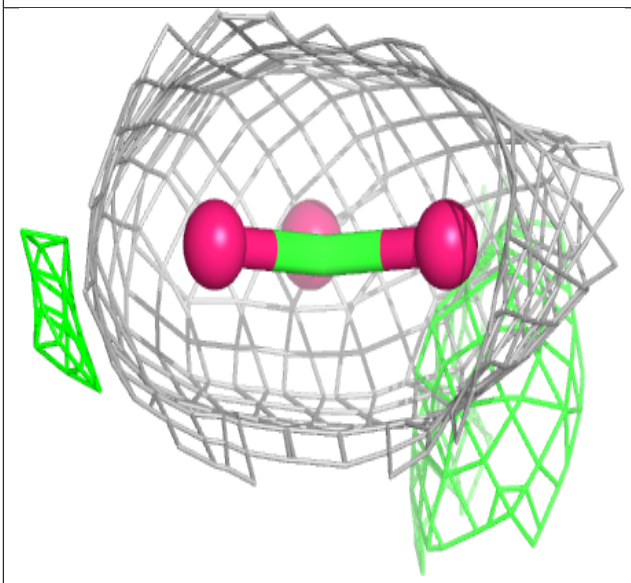


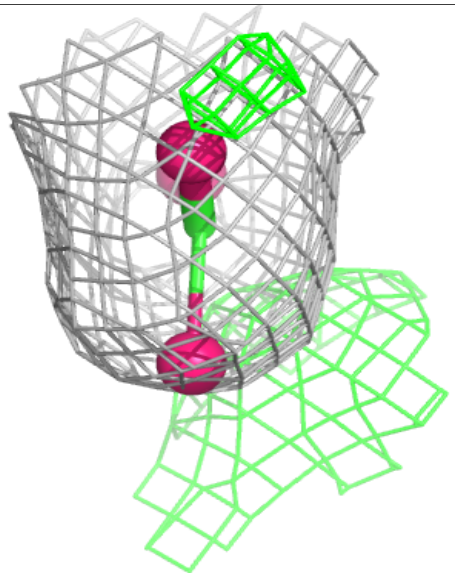


Electron density around BCT d 401 (B):

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

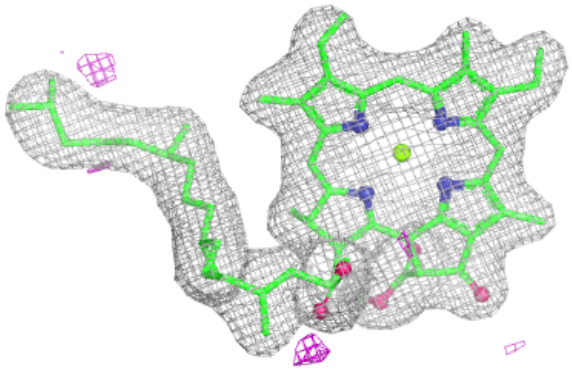


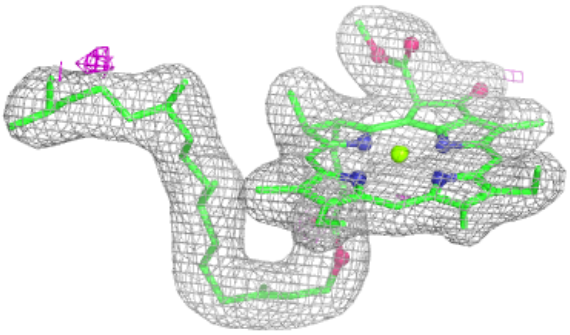


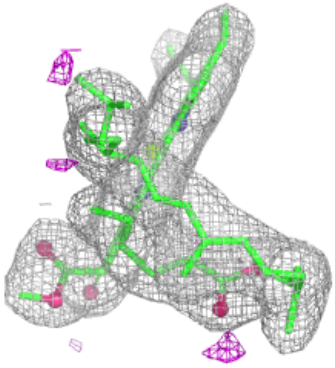


Electron density around CLA d 402 (B):

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

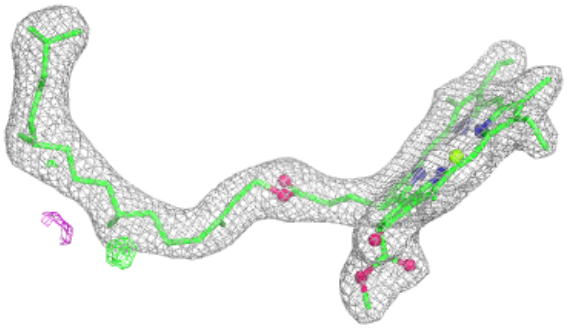


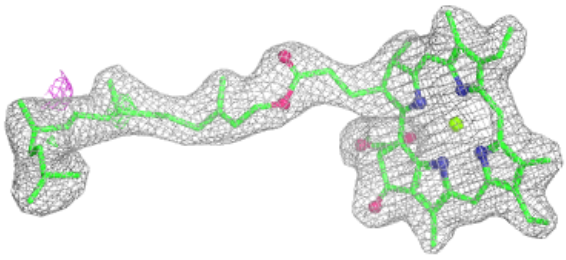


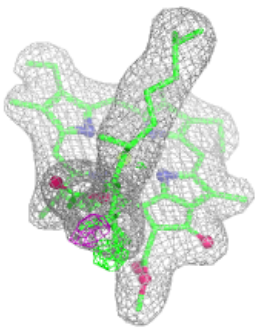


Electron density around CLA d 404 (A):

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

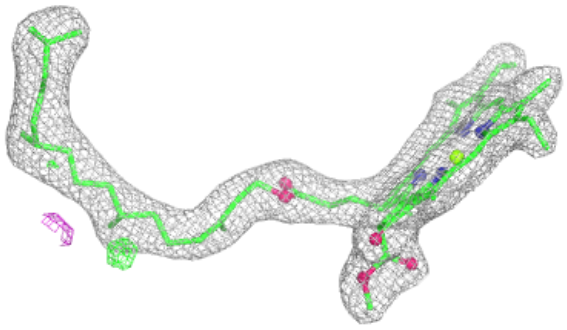


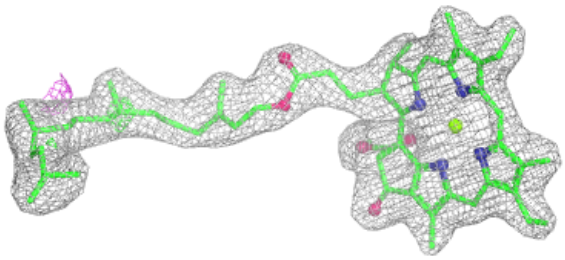


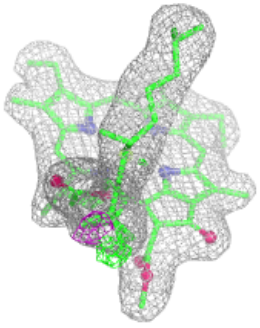


Electron density around CLA d 404 (B):

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

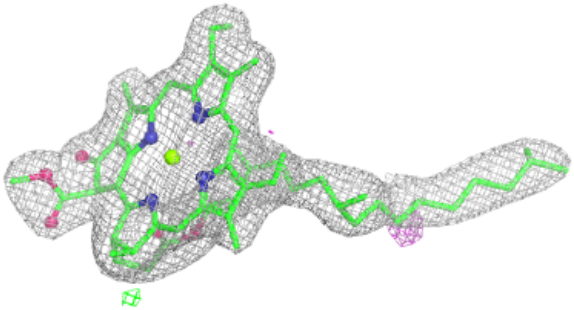


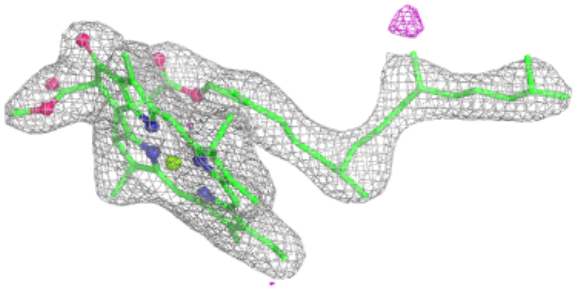


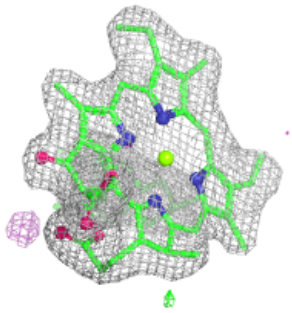


Electron density around CLA C 506:

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

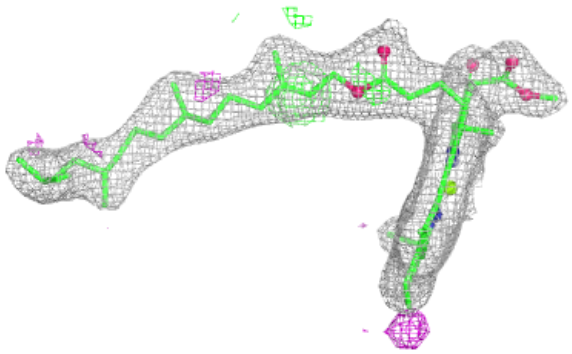


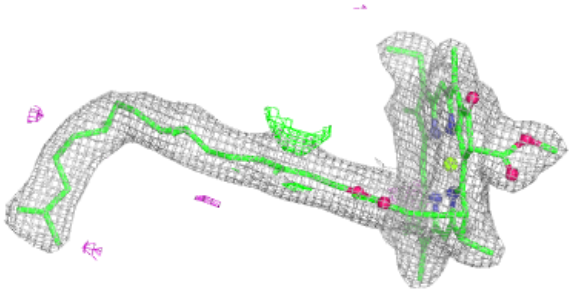


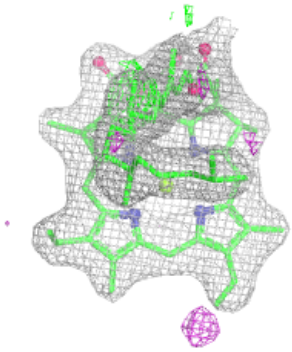


Electron density around CLA B 605:

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

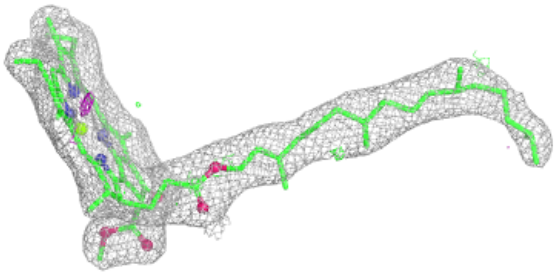


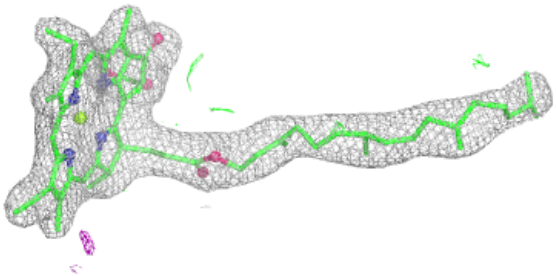


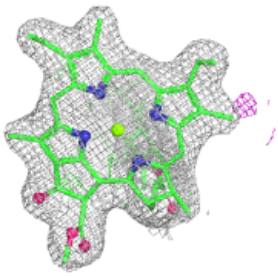


Electron density around CLA b 604:

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

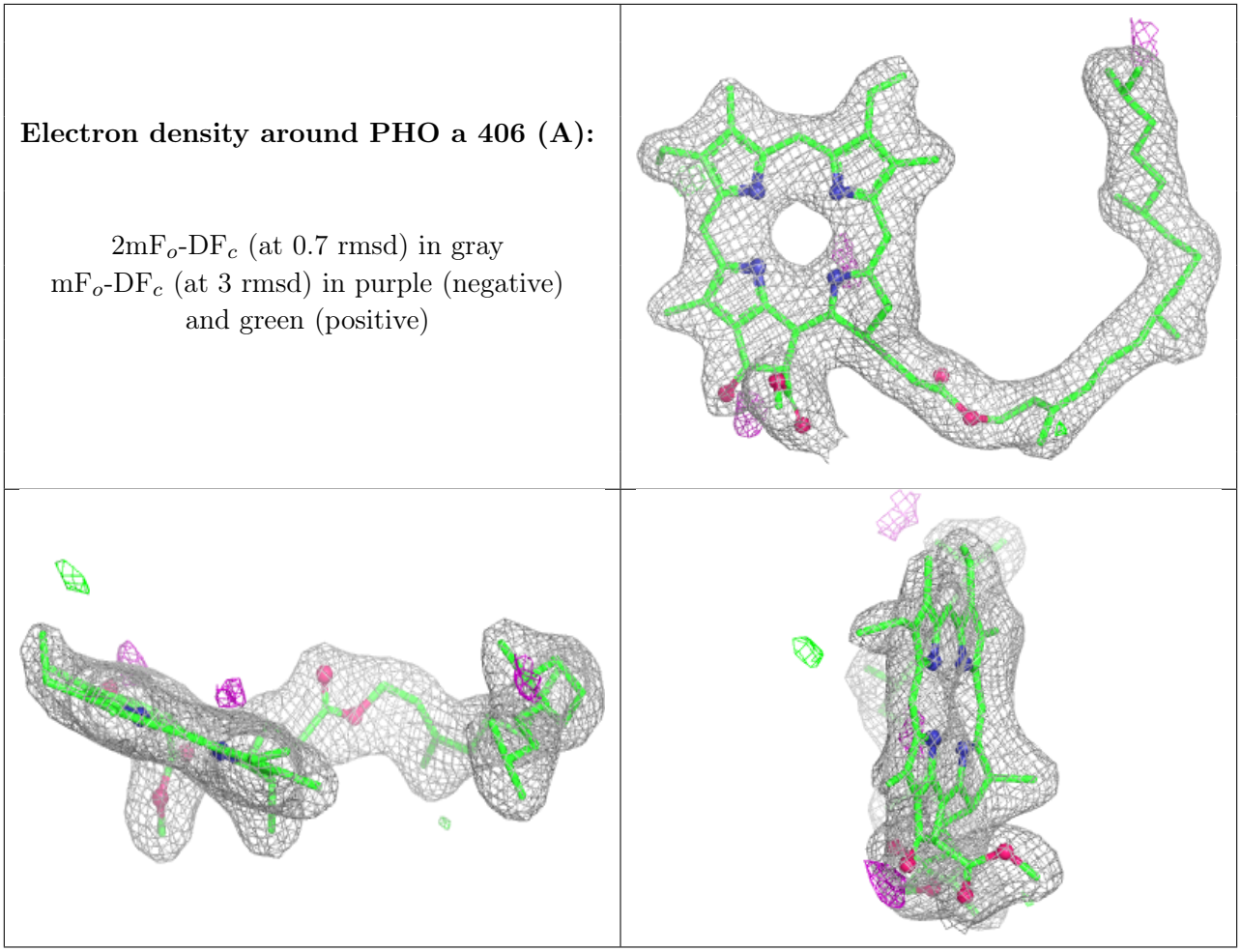






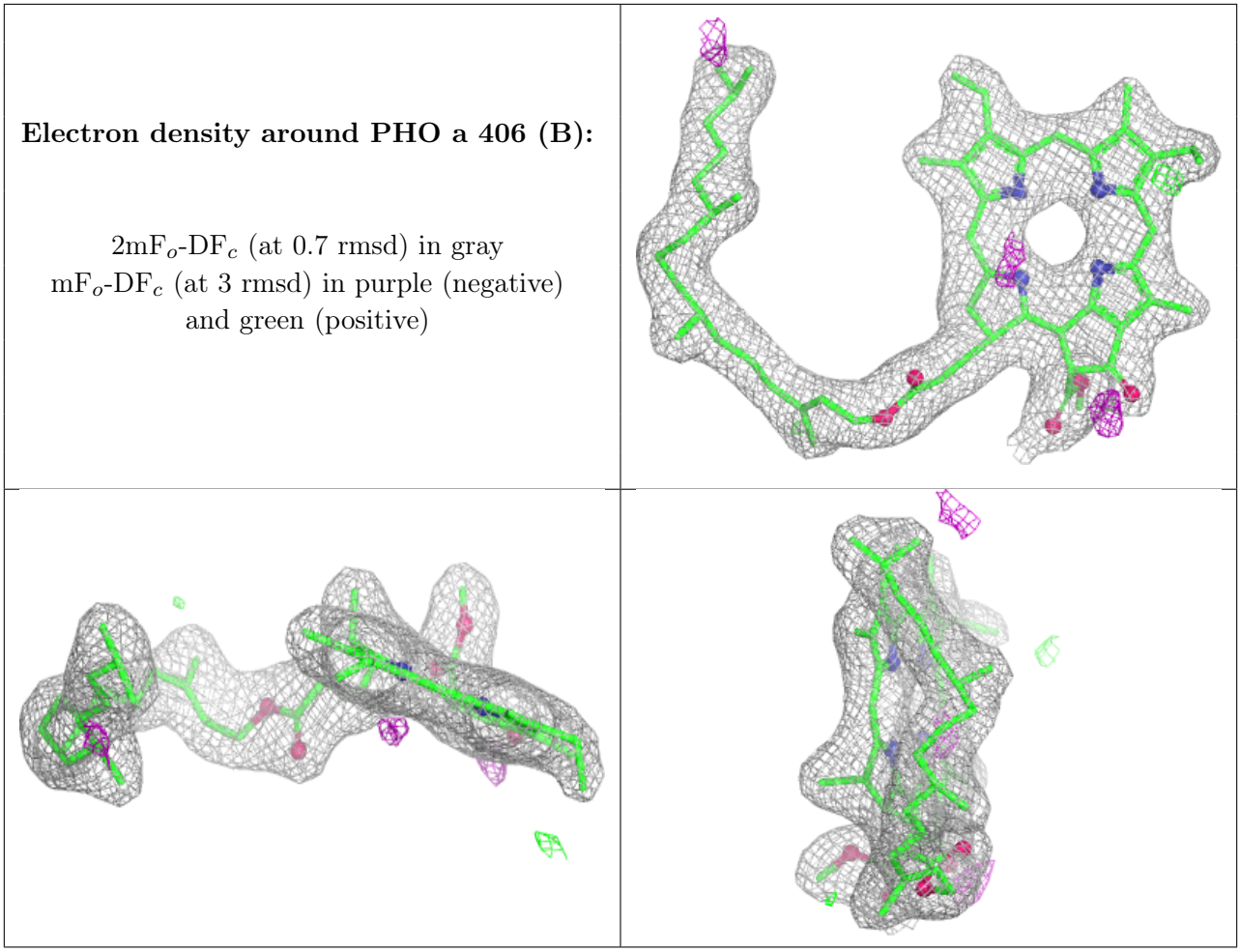
Electron density around PHO a 406 (A):

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



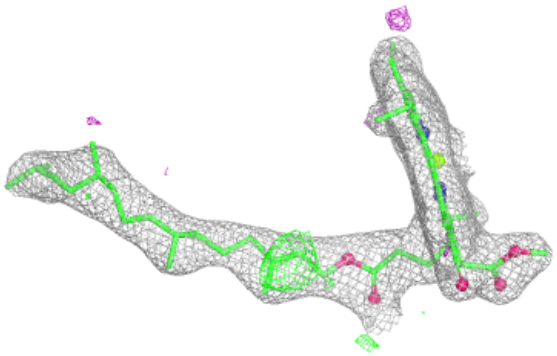
Electron density around PHO a 406 (B):

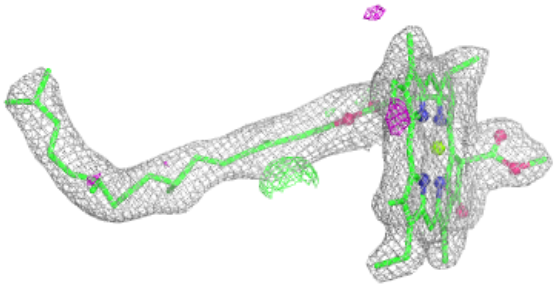
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

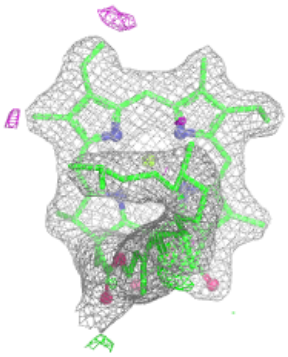


Electron density around CLA b 605:

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

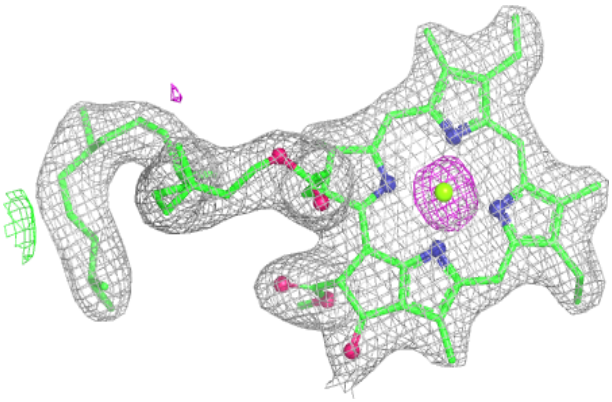


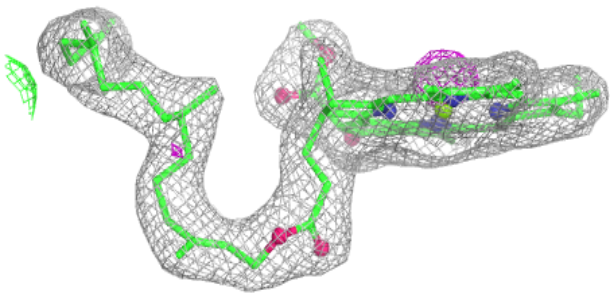


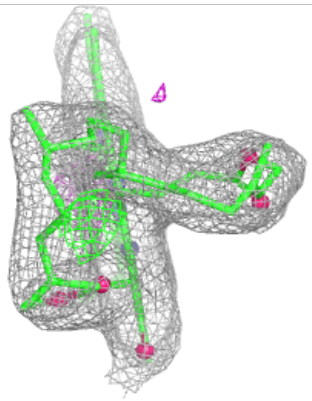


Electron density around CLA B 612:

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

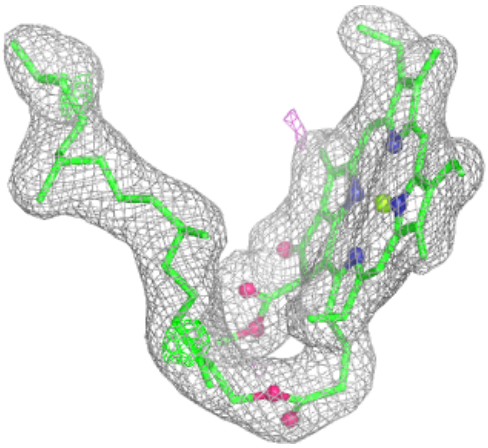


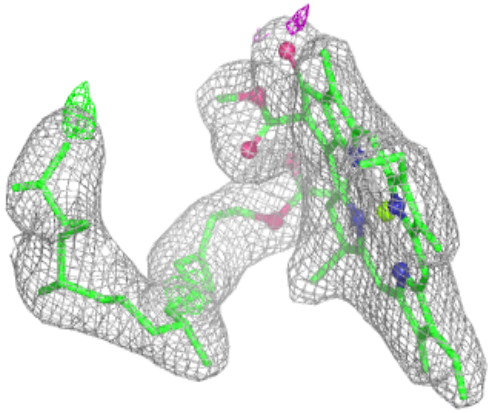




Electron density around CLA B 613:

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

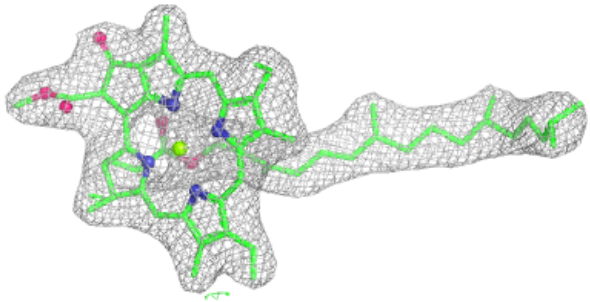


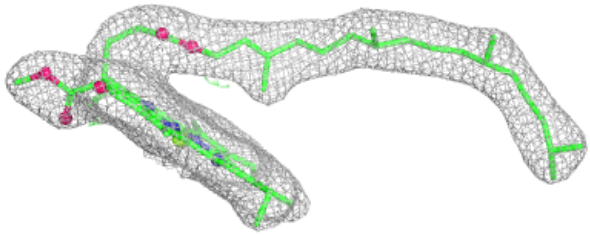


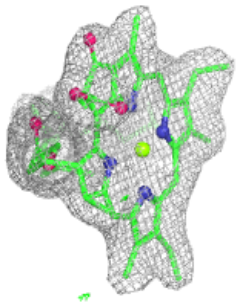


Electron density around CLA b 608:

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

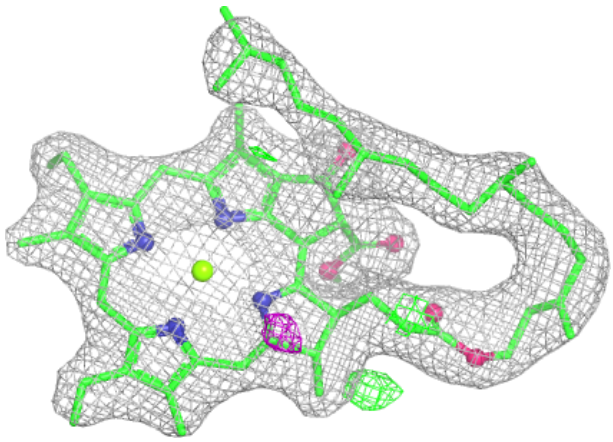


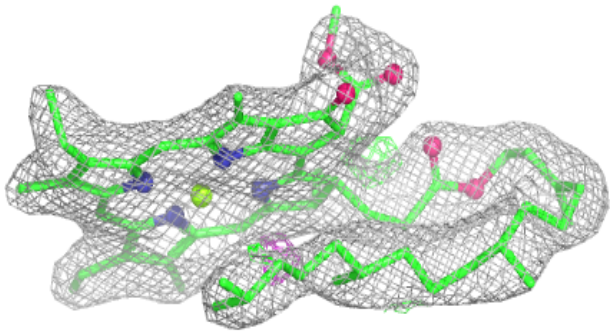


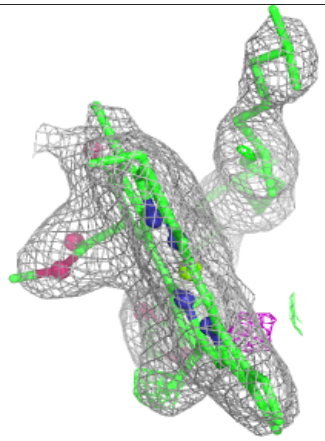


Electron density around CLA C 510:

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

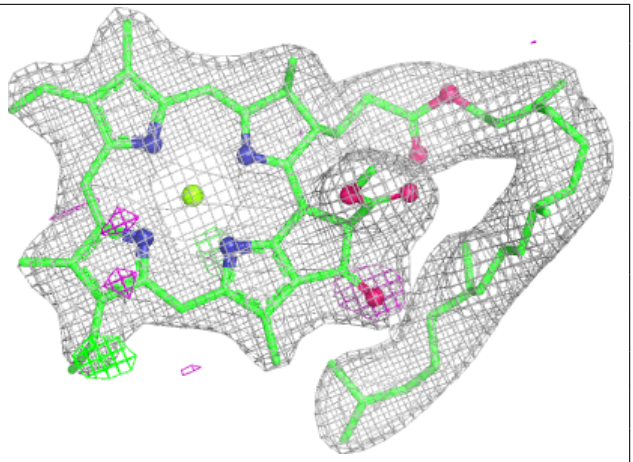


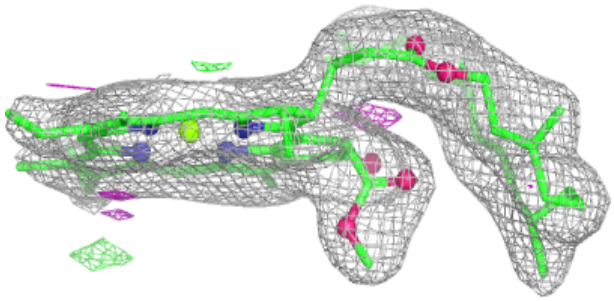


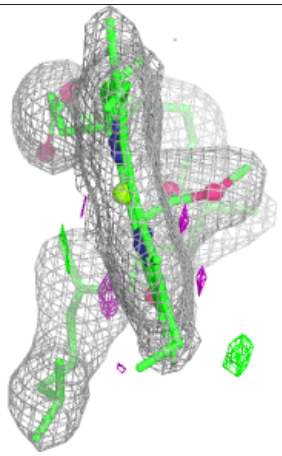


Electron density around CLA b 610:

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

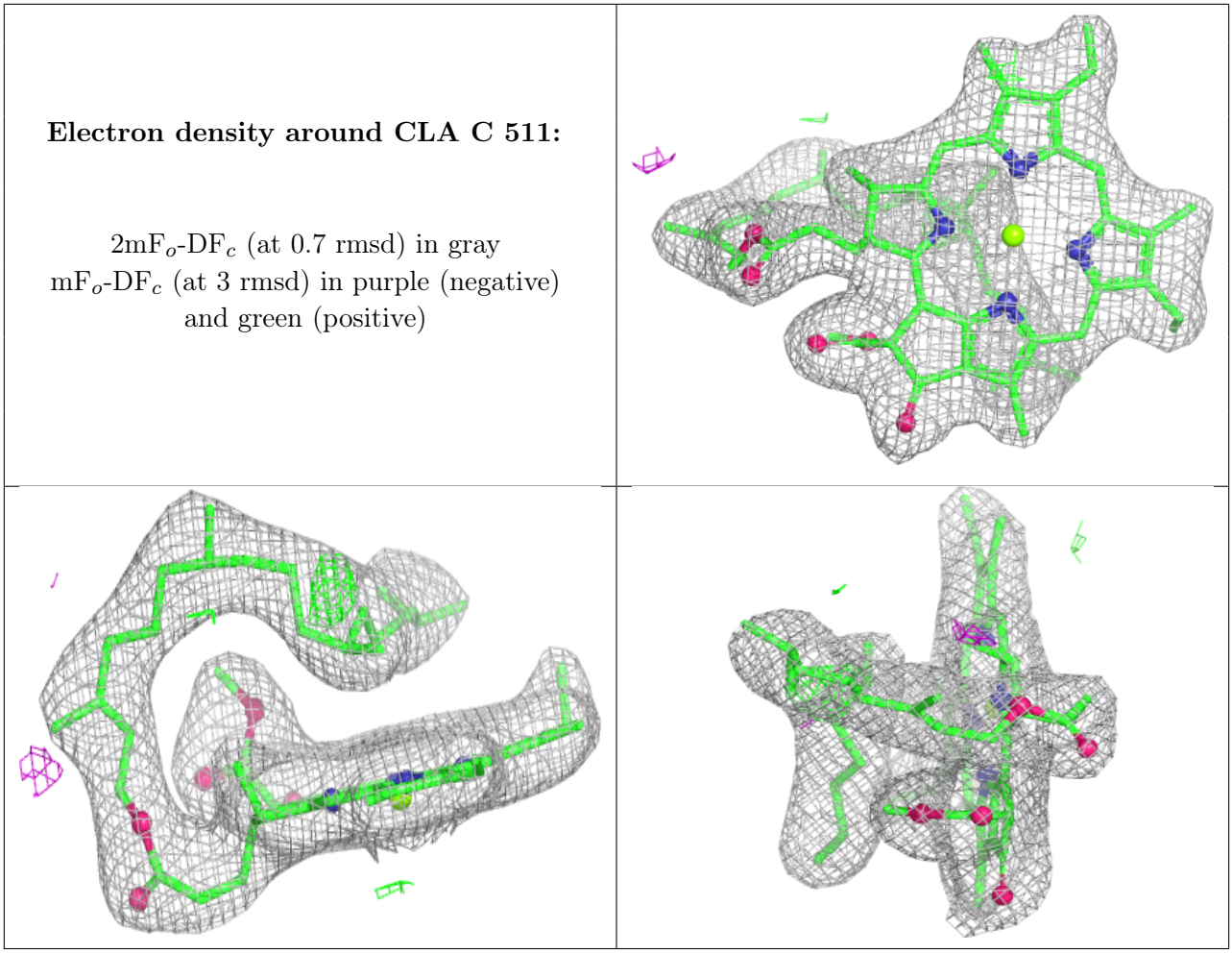






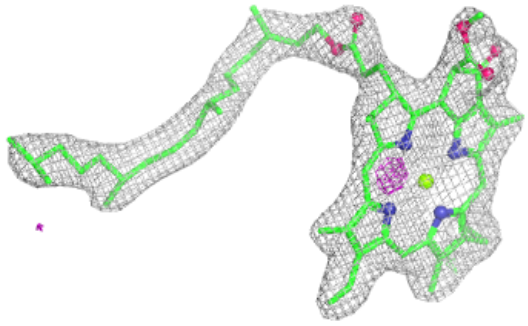
Electron density around CLA C 511:

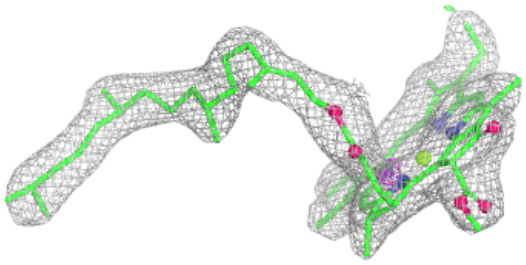
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

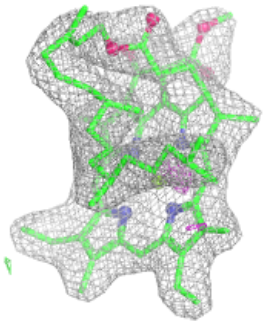


Electron density around CLA C 512:

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

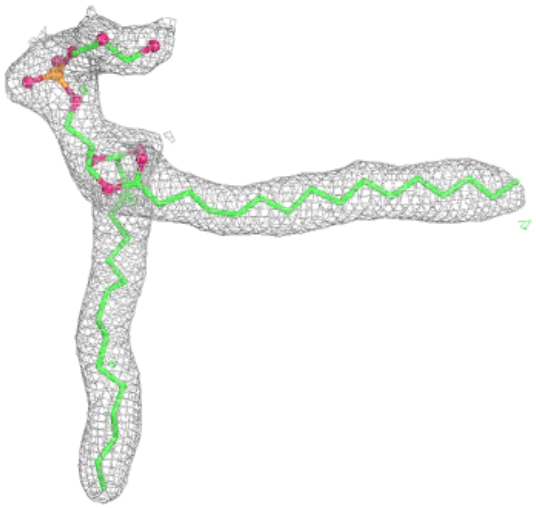


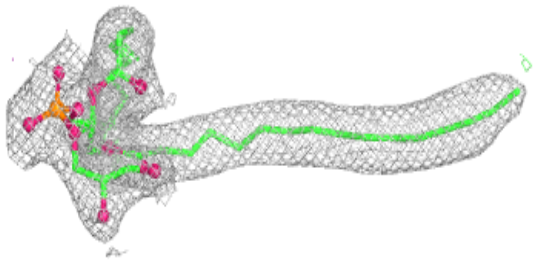


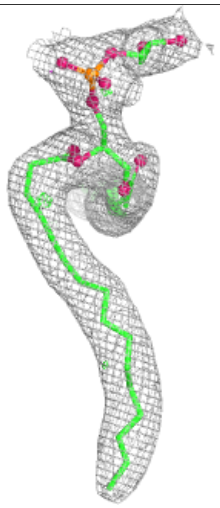


Electron density around LHG L 101 (A):

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

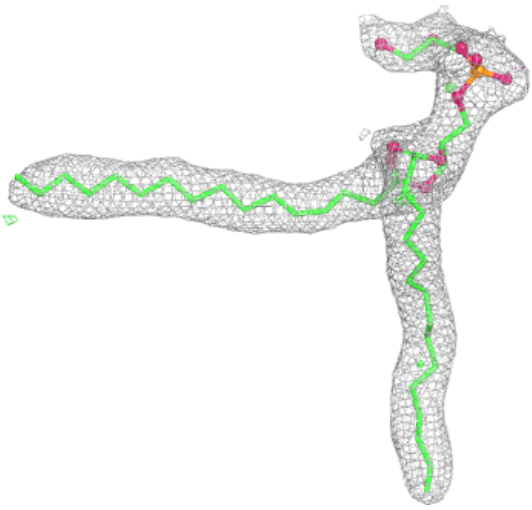


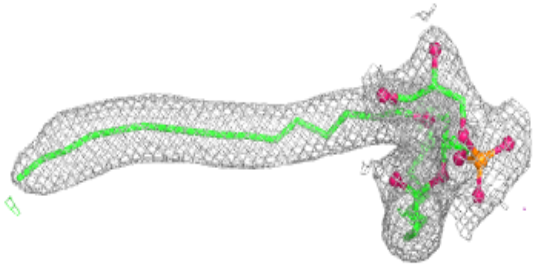


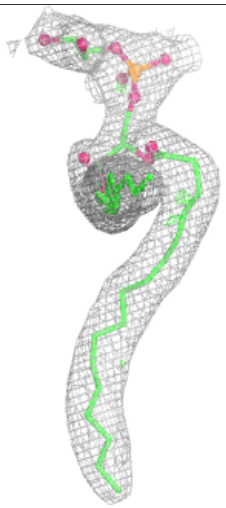


Electron density around LHG L 101 (B):

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

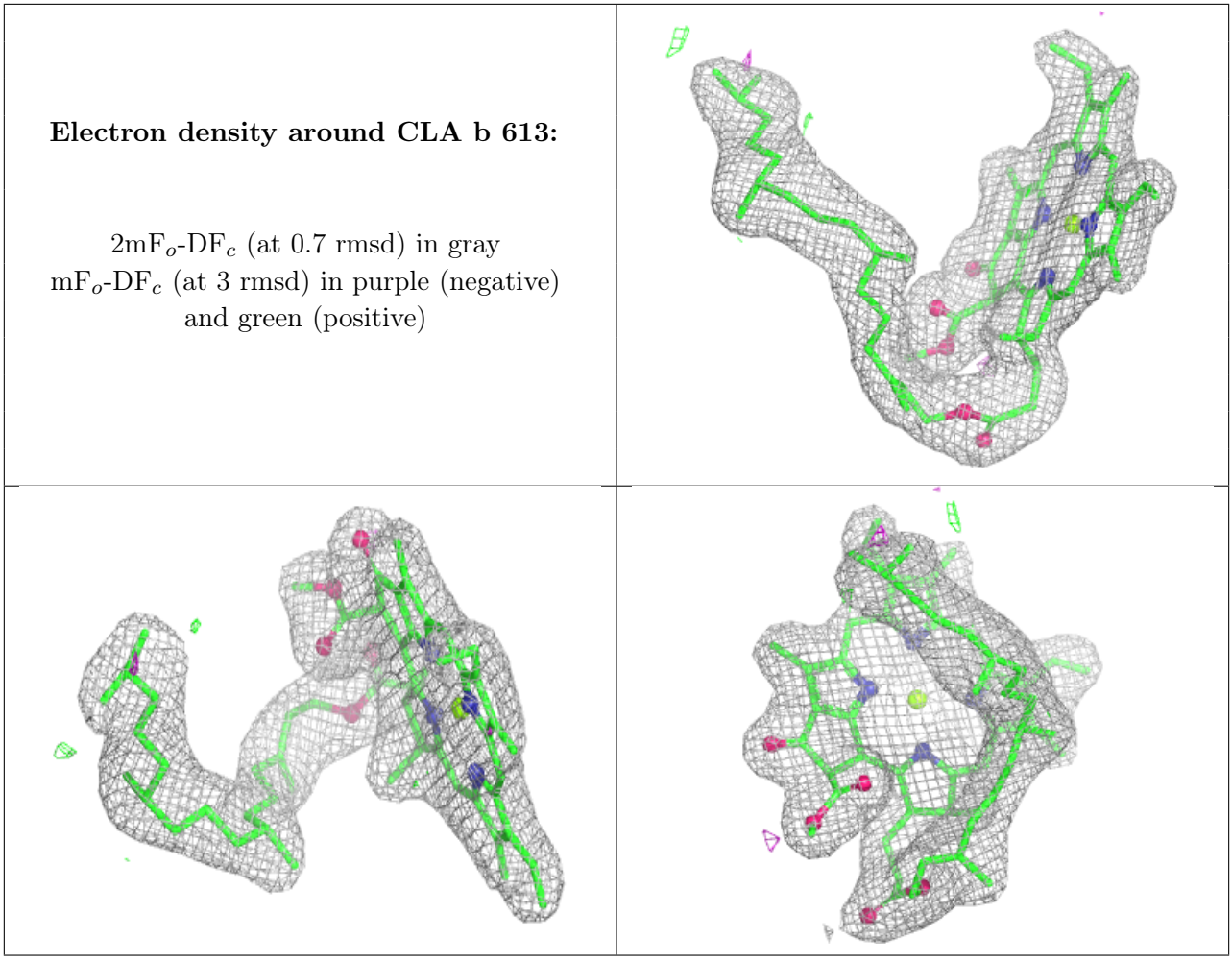






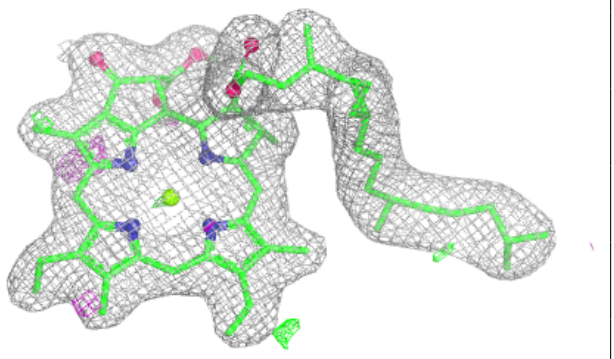
Electron density around CLA b 613:

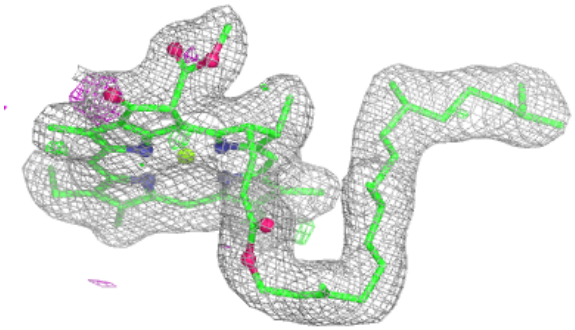
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

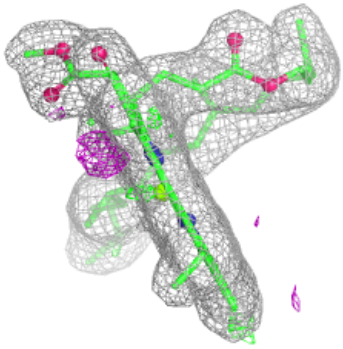


Electron density around CLA A 405 (A):

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

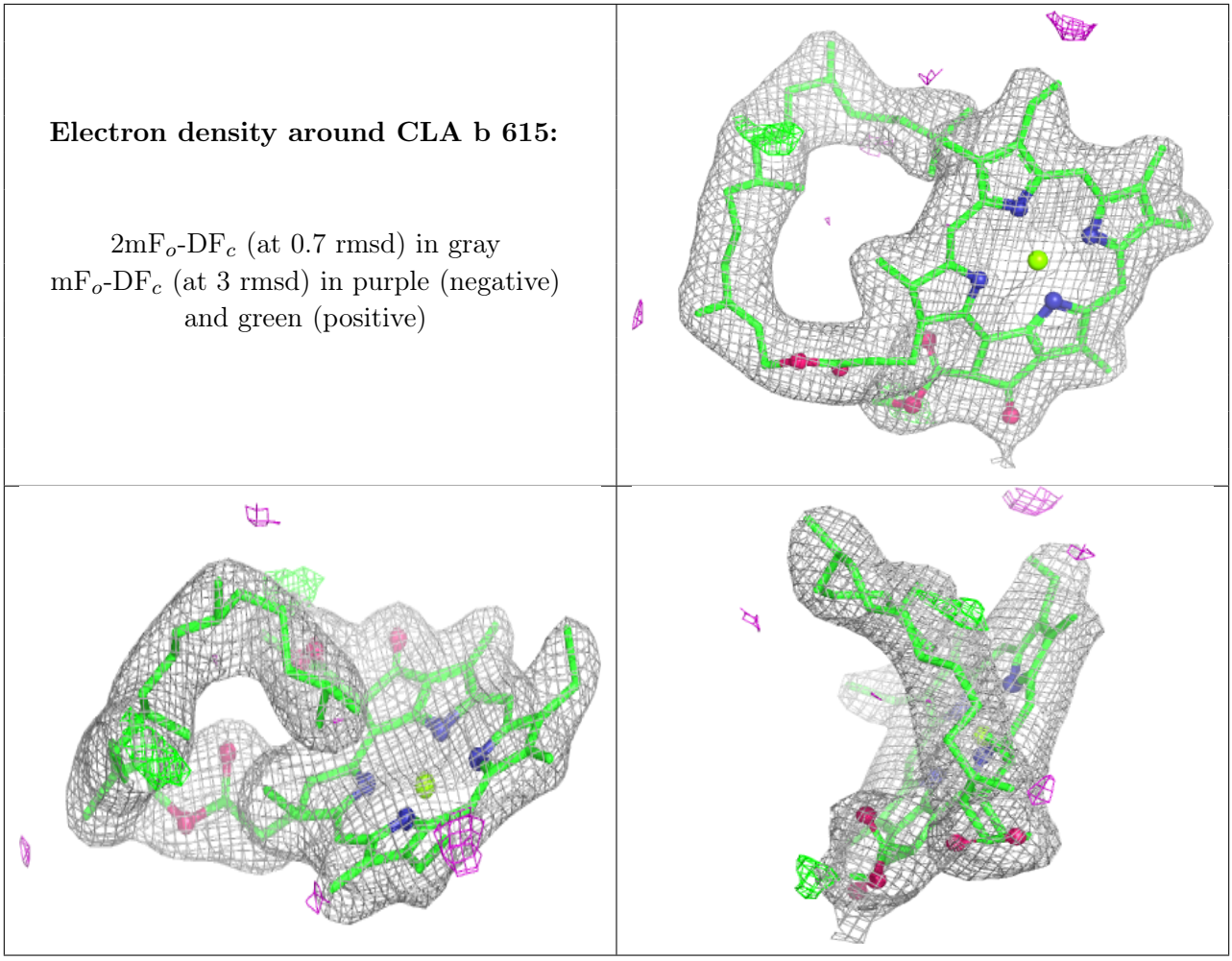






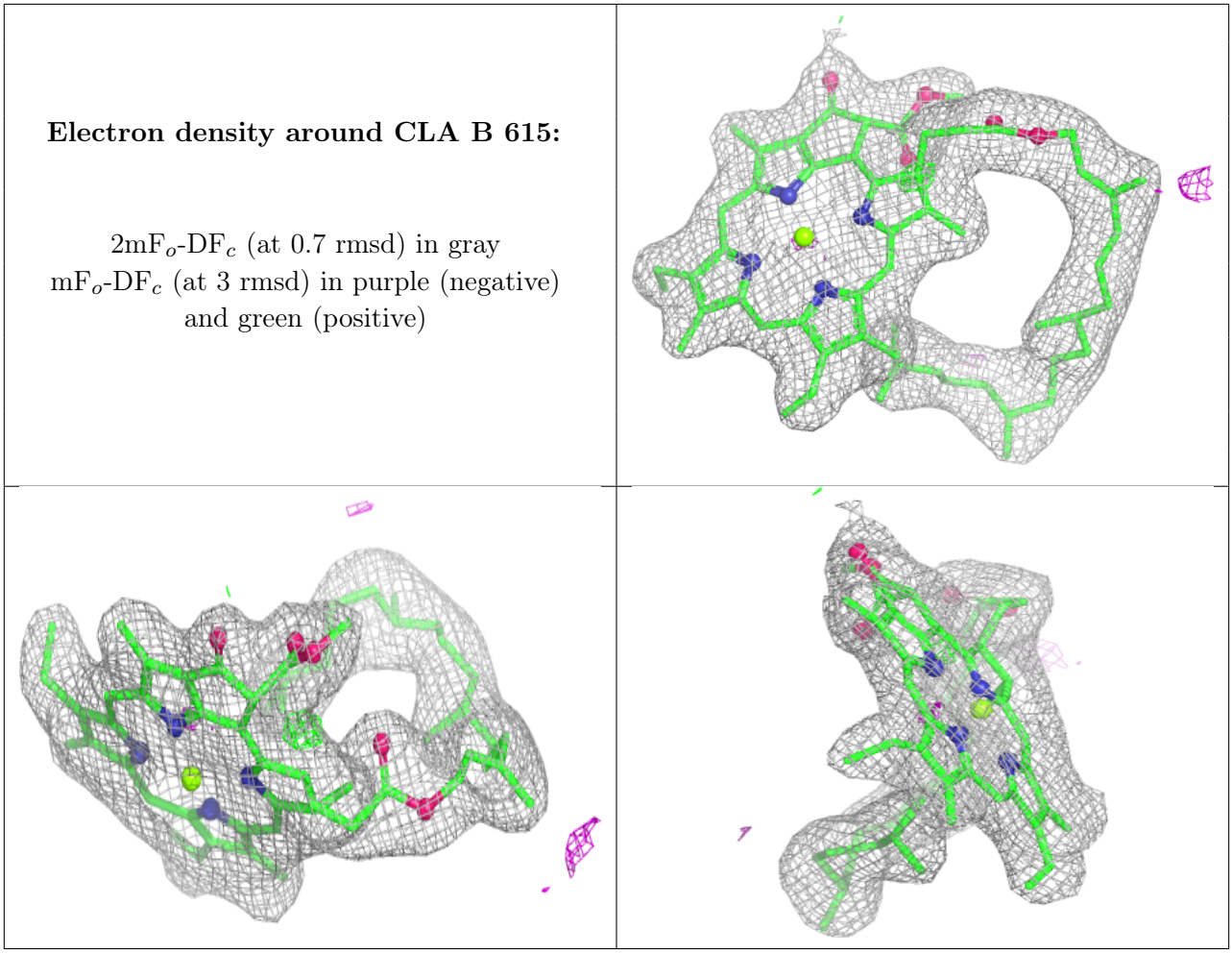
Electron density around CLA b 615:

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



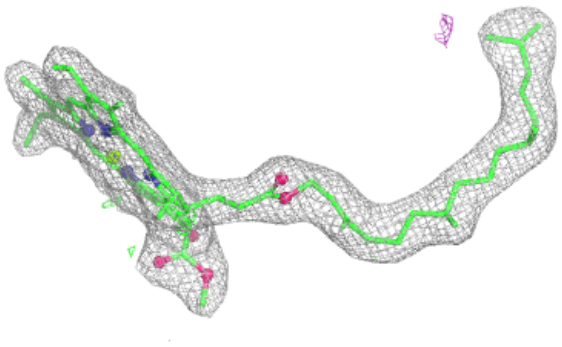
Electron density around CLA B 615:

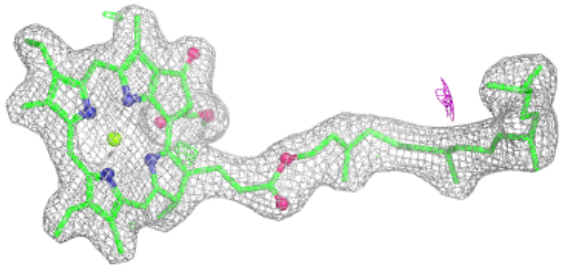
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

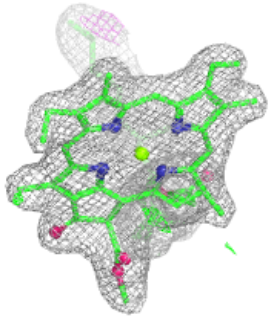


Electron density around CLA D 402 (A):

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

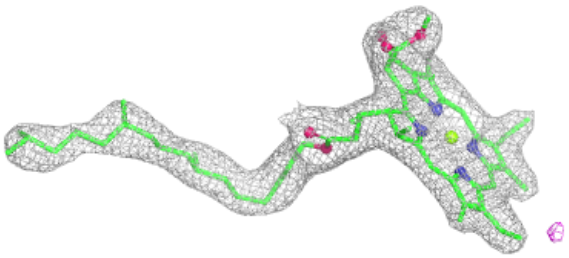


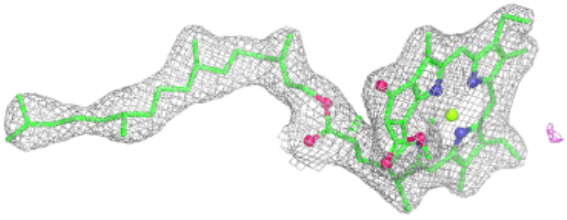


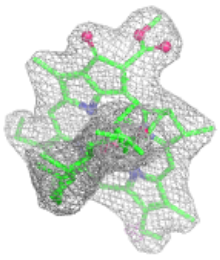


Electron density around CLA c 502:

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

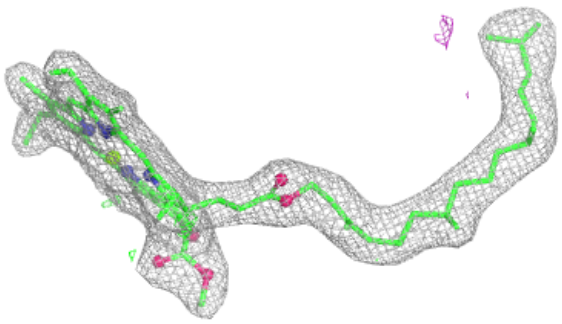


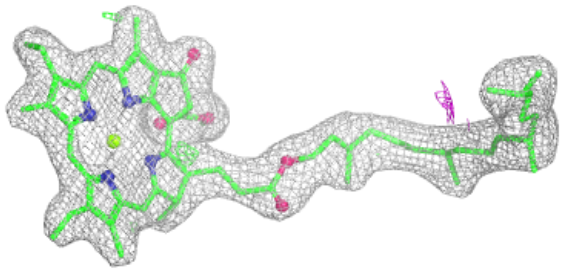


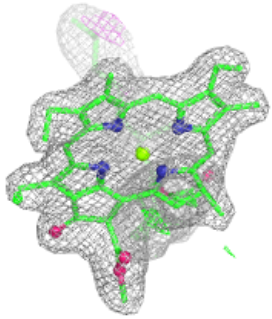


Electron density around CLA D 402 (B):

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

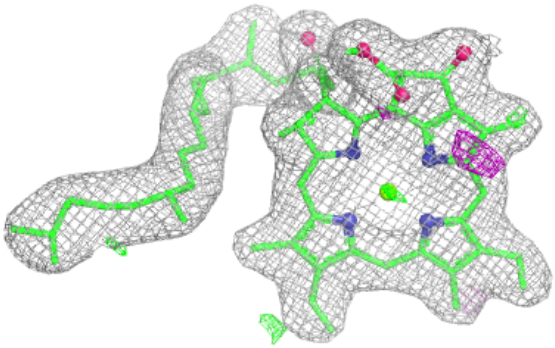


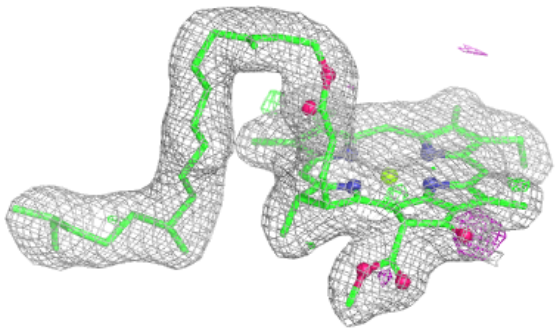


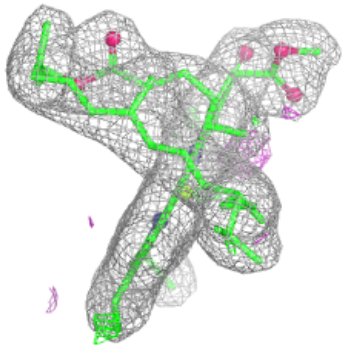


Electron density around CLA A 405 (B):

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

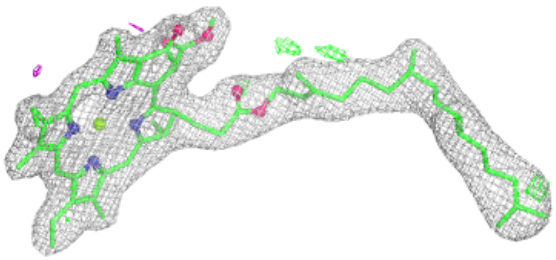


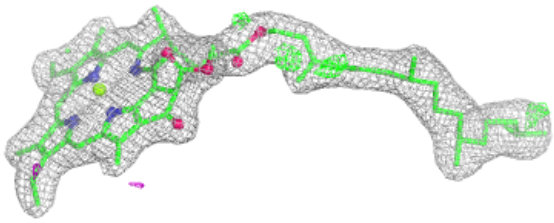


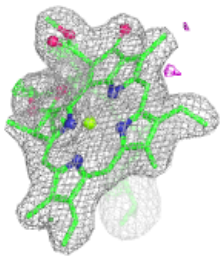


Electron density around CLA a 404 (A):

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

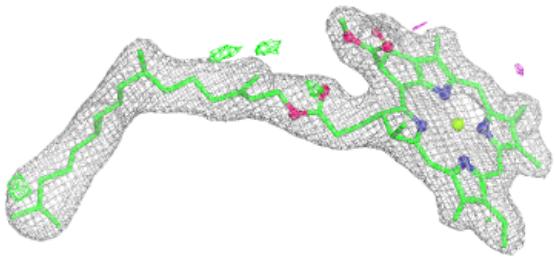


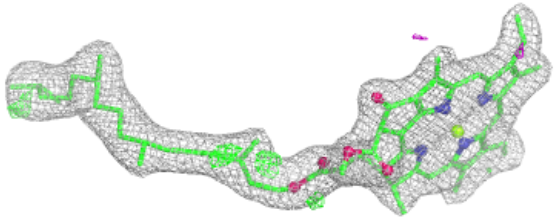


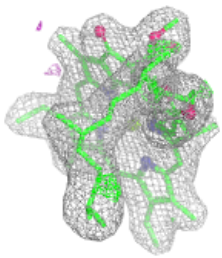


Electron density around CLA a 404 (B):

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

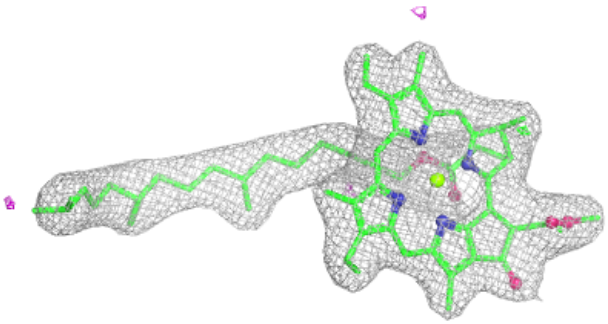


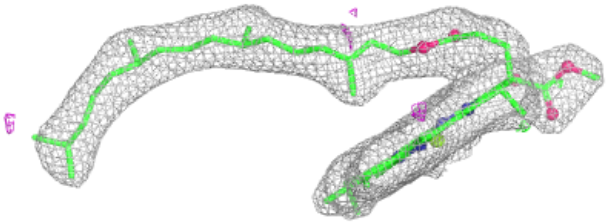




Electron density around CLA B 608:

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

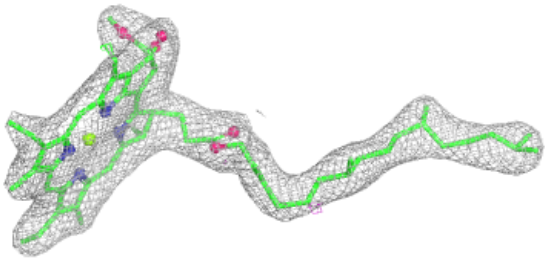


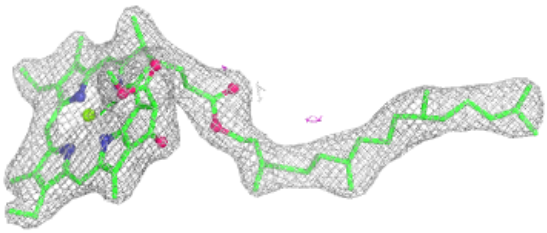


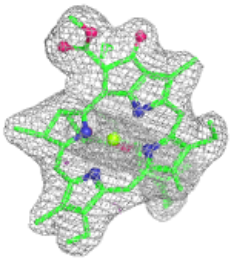


Electron density around CLA C 503:

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

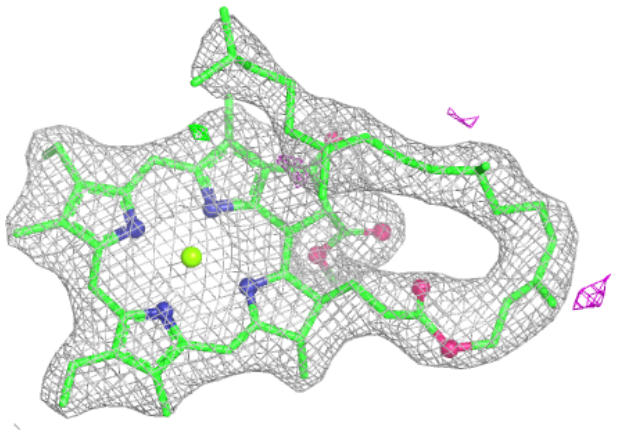


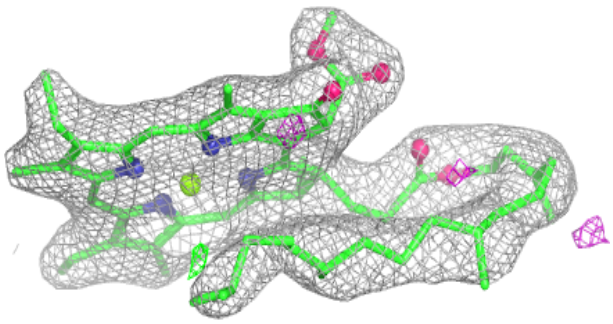


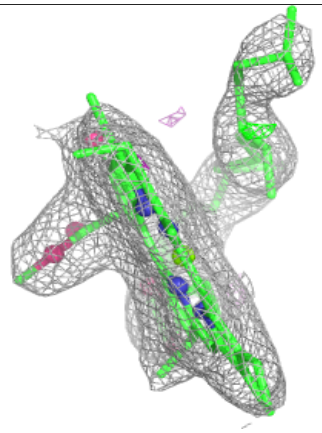


Electron density around CLA c 509:

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

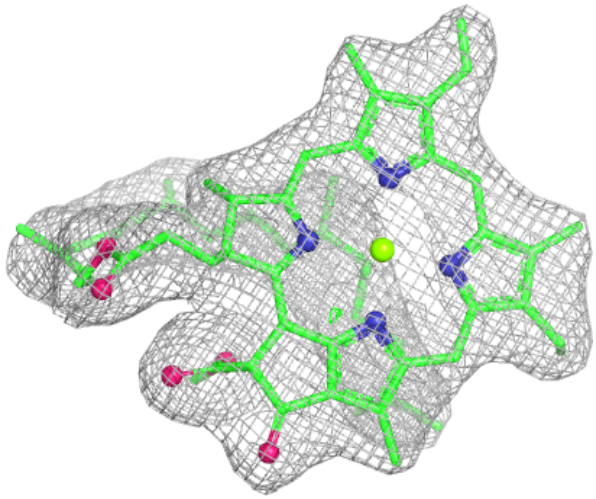


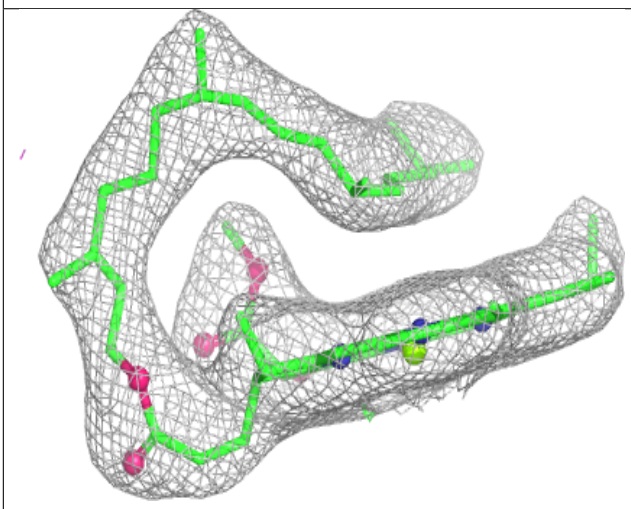


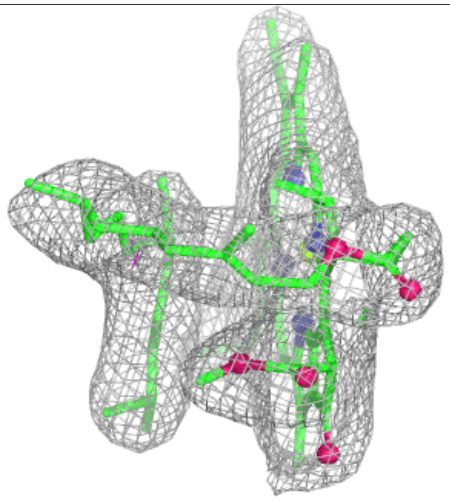


Electron density around CLA c 510:

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

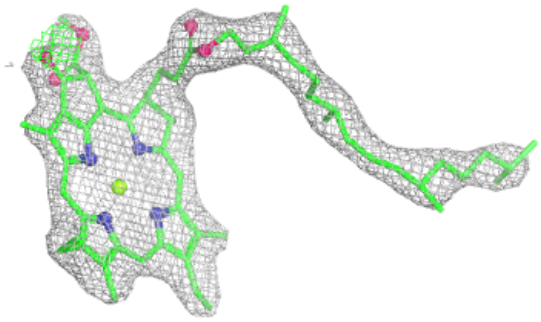


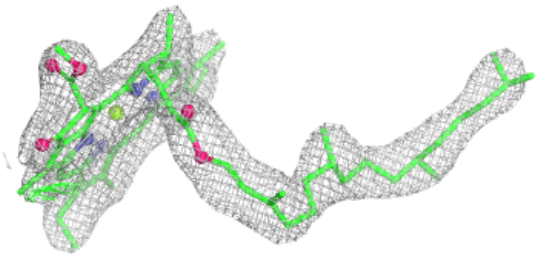


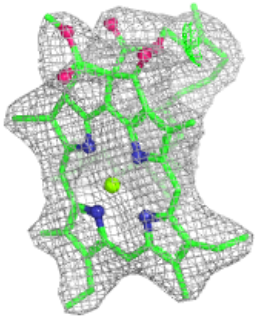


Electron density around CLA c 511:

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

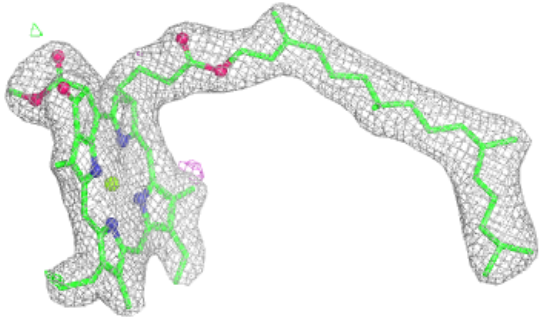


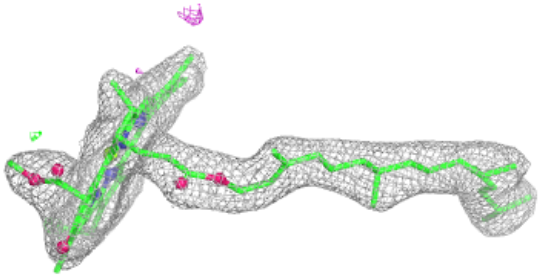


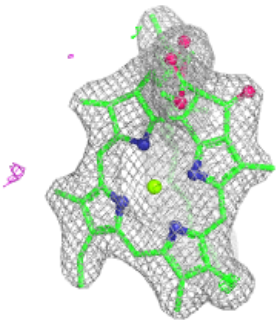


Electron density around CLA B 609:

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

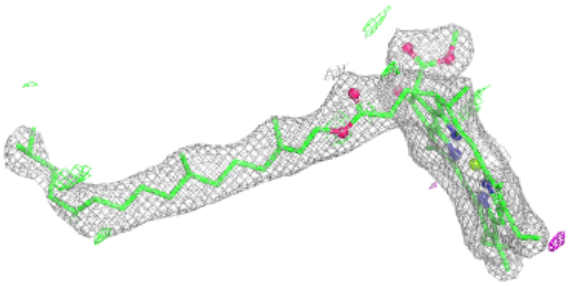


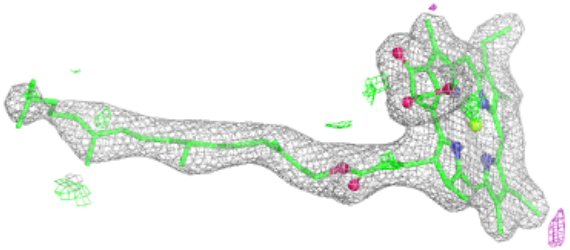


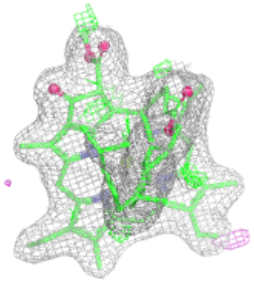


Electron density around CLA B 604:

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

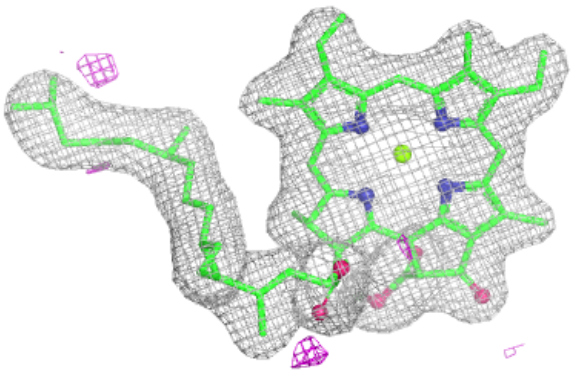


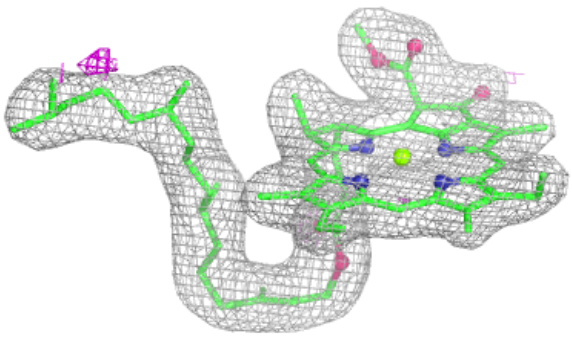


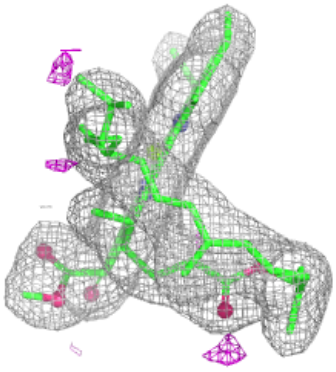


Electron density around CLA d 402 (A):

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

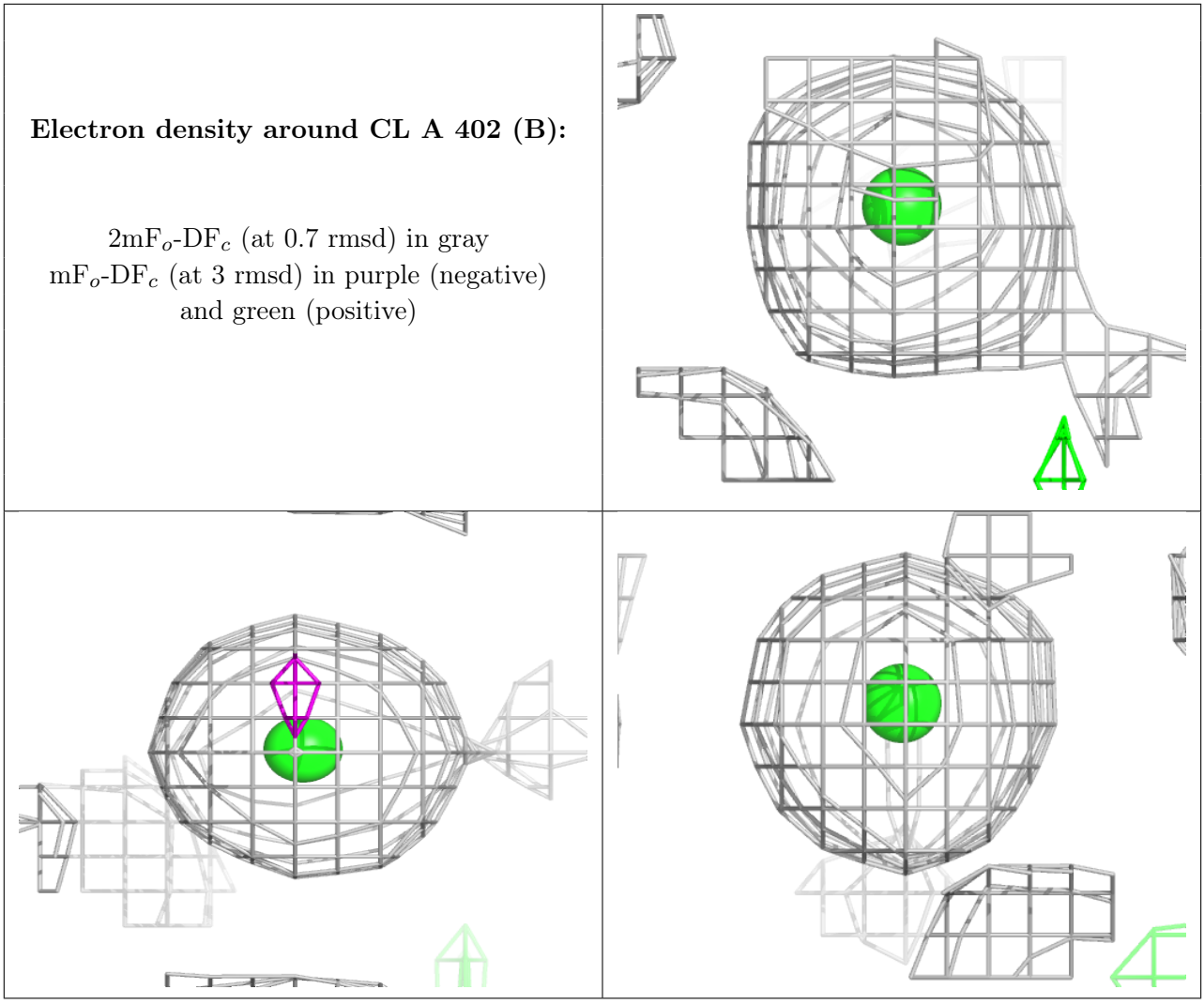






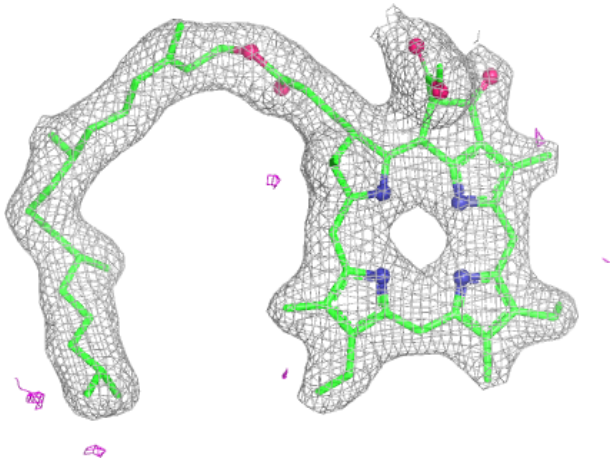
Electron density around CL A 402 (B):

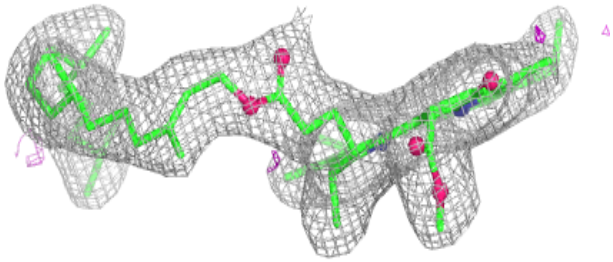
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

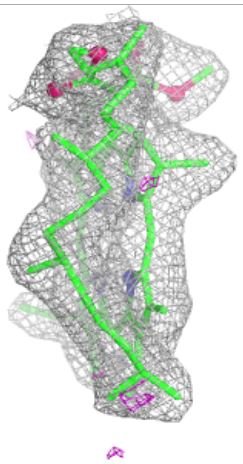


Electron density around PHO A 407 (A):

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

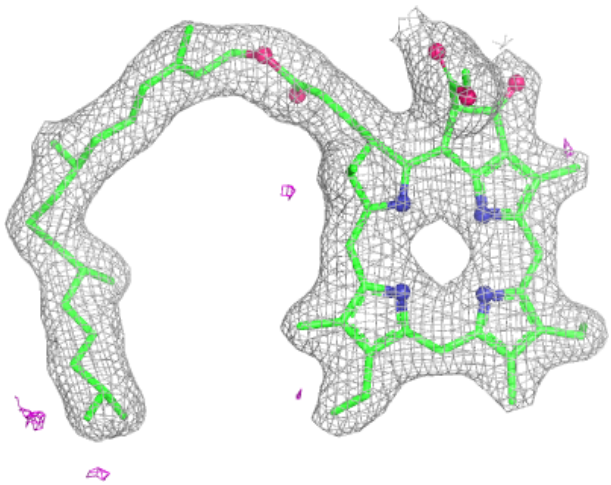


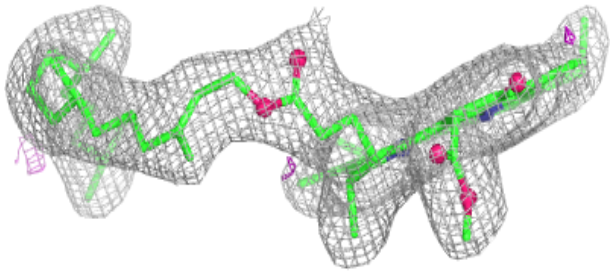


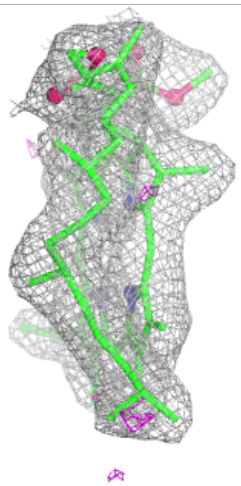


Electron density around PHO A 407 (B):

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

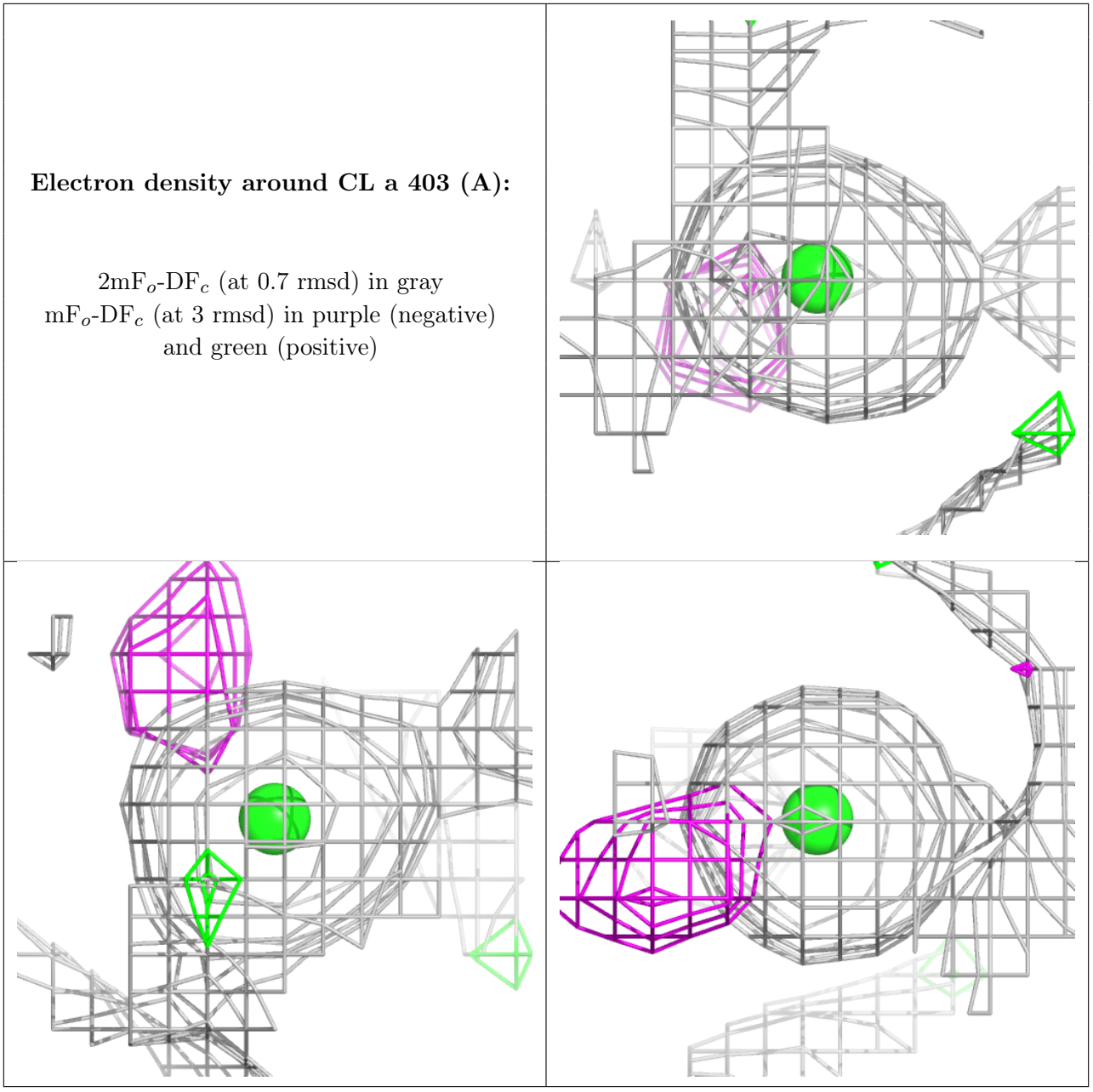






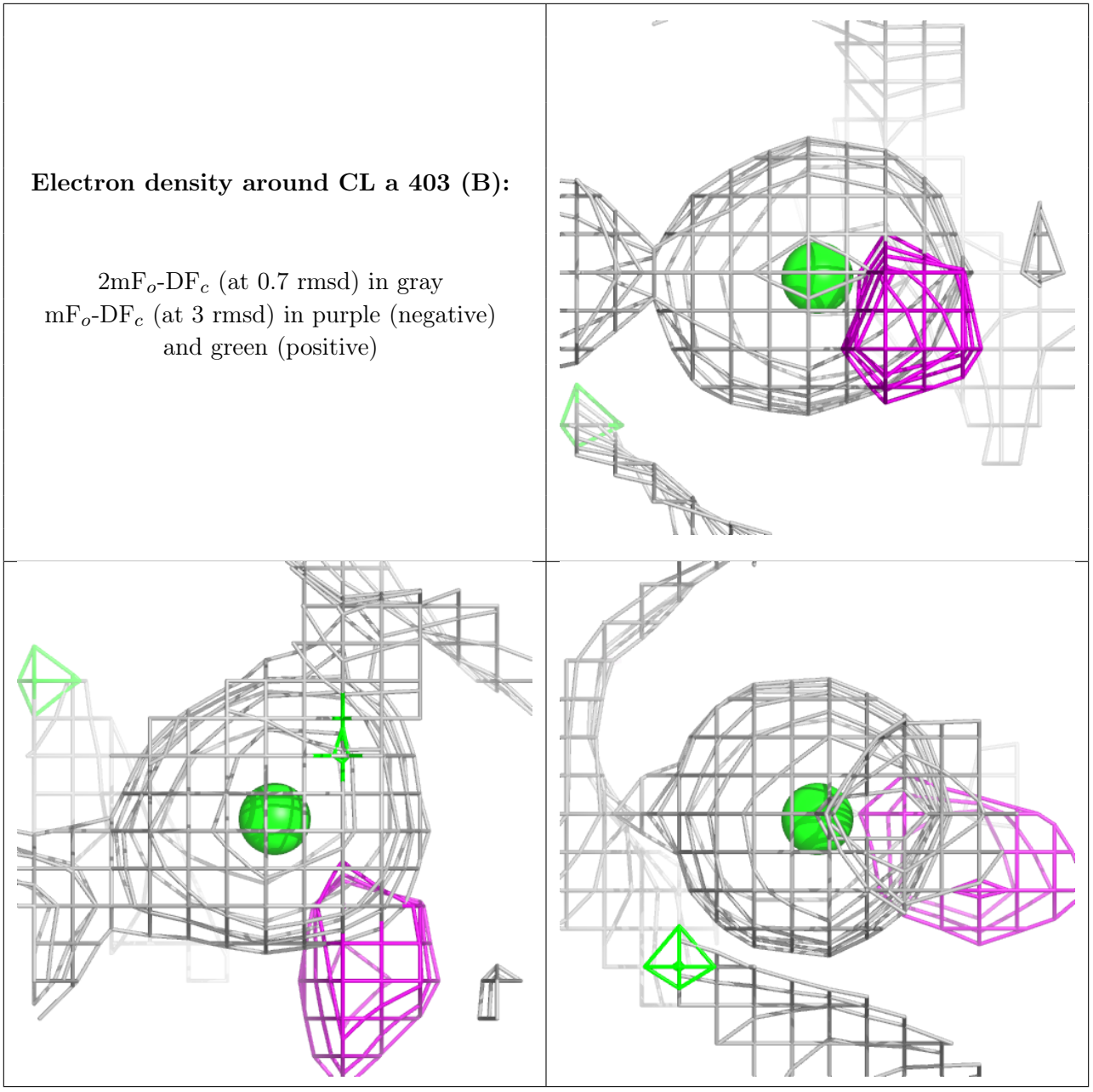
Electron density around CL a 403 (A):

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



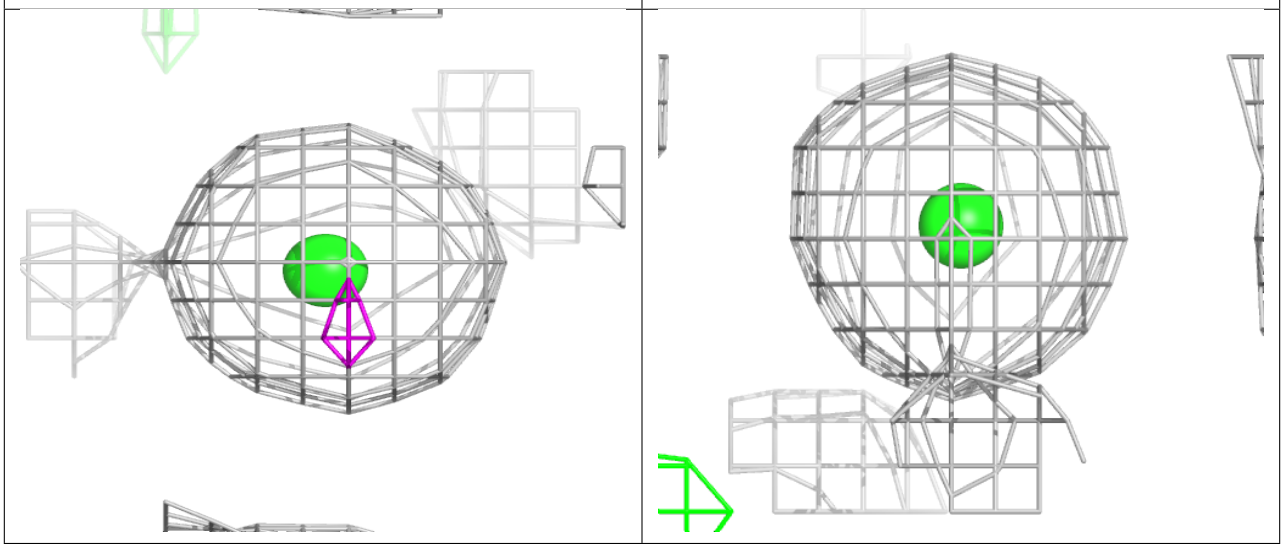
Electron density around CL a 403 (B):

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



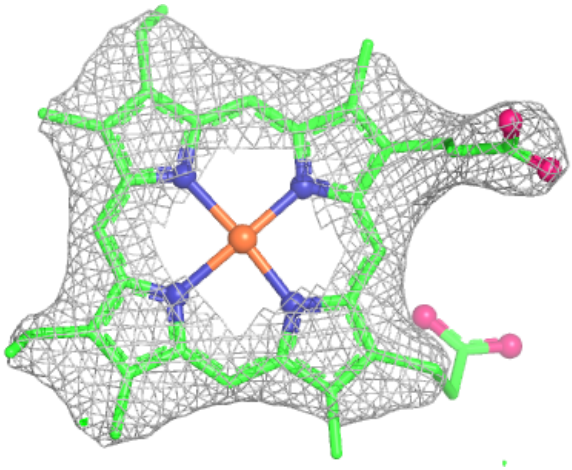
Electron density around CL A 402 (A):

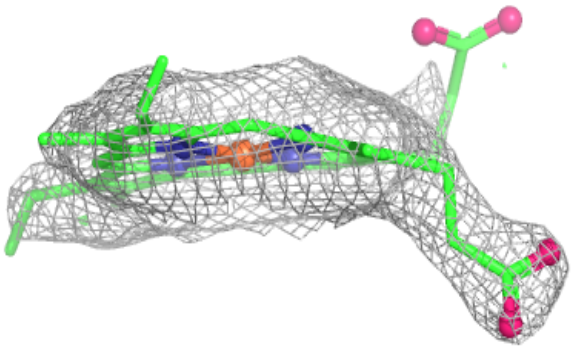
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

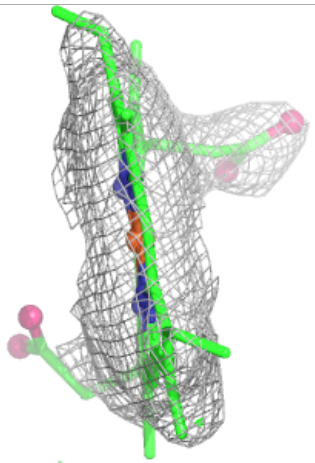


Electron density around HEM f 101:

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

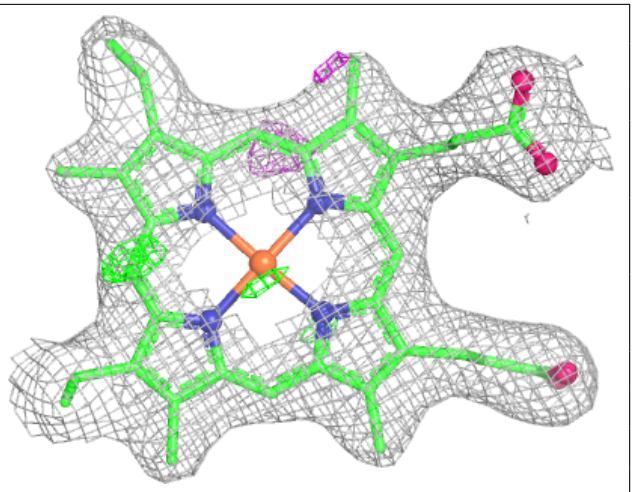


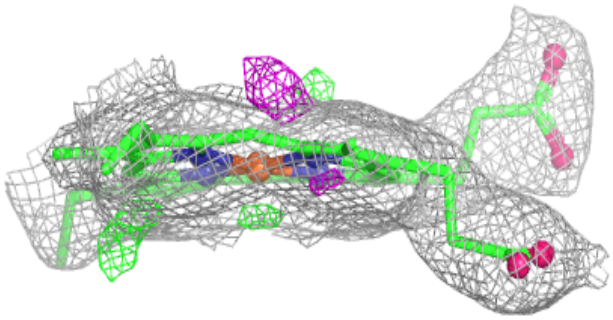


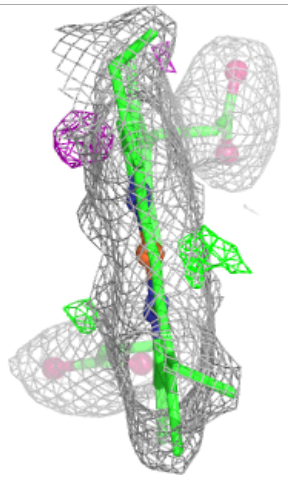


Electron density around HEC V 201:

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

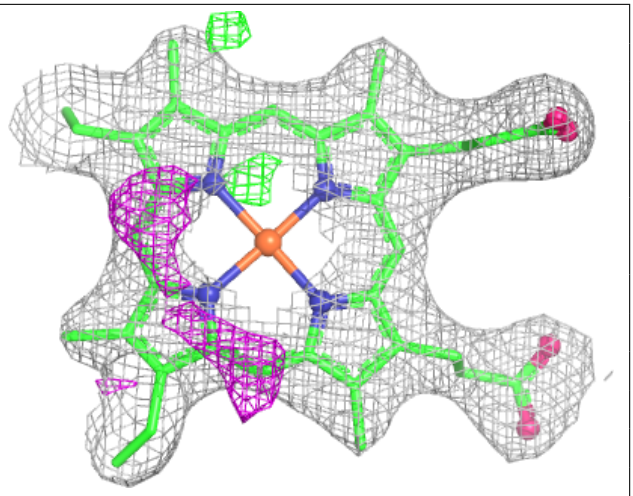


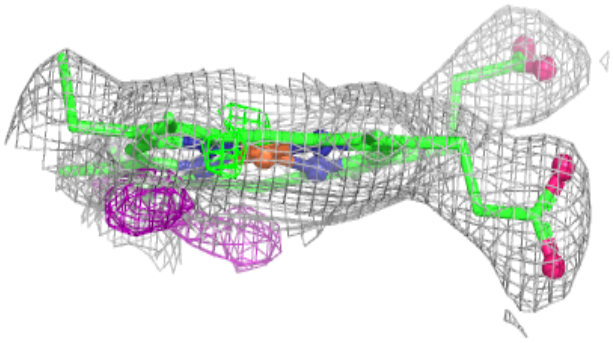


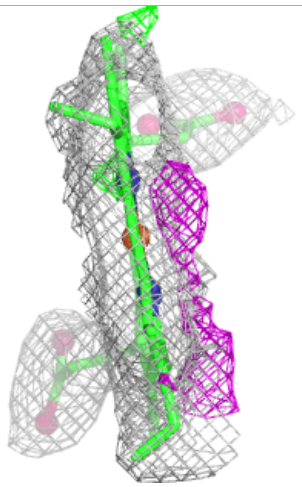


Electron density around HEC v 201:

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

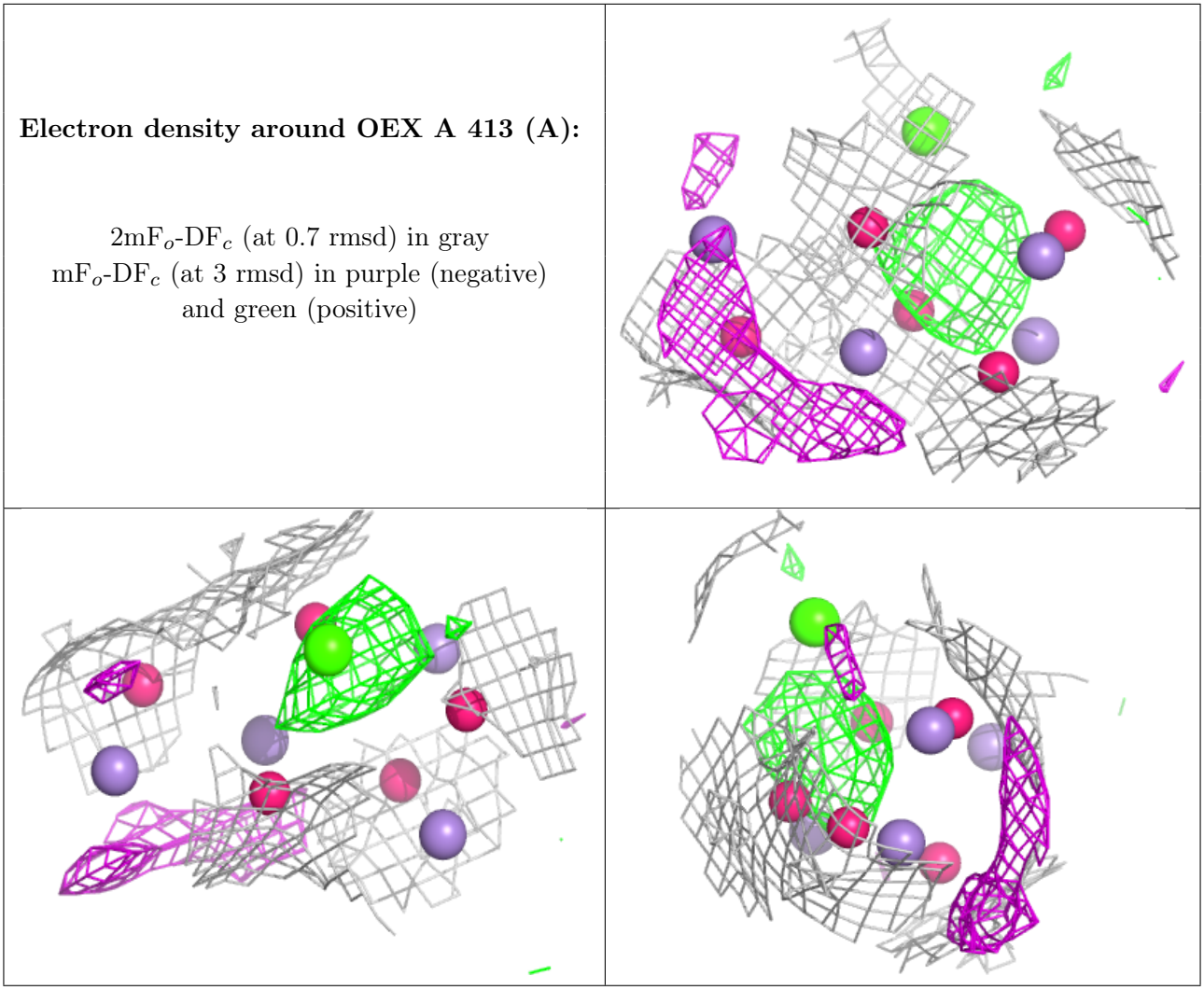






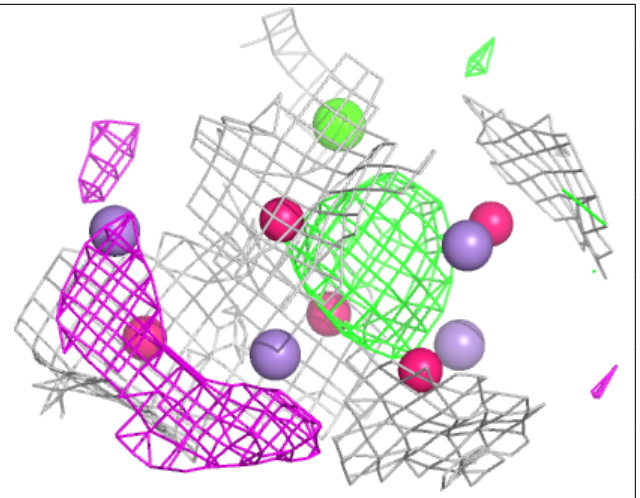
Electron density around OEX A 413 (A):

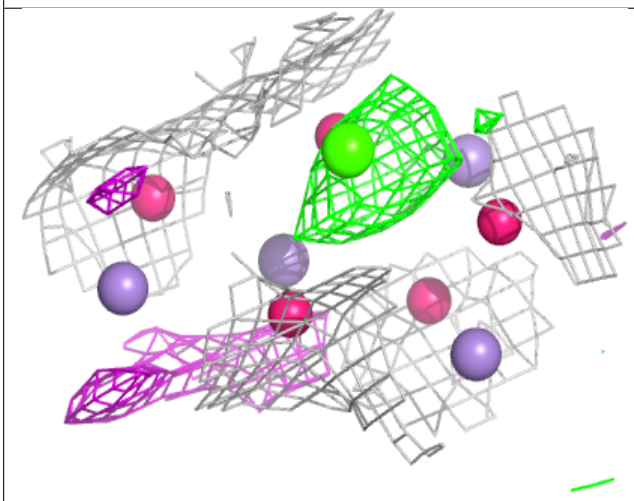
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

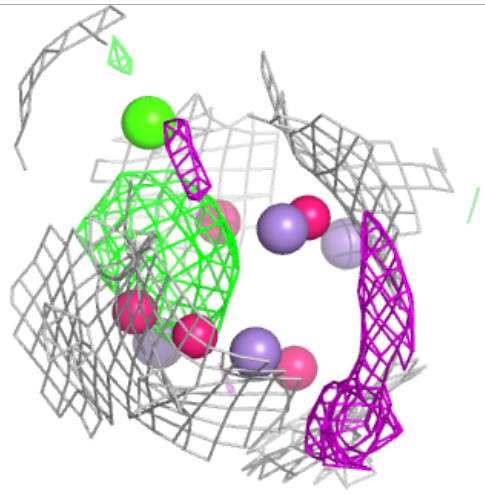


Electron density around OEX A 413 (B):

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

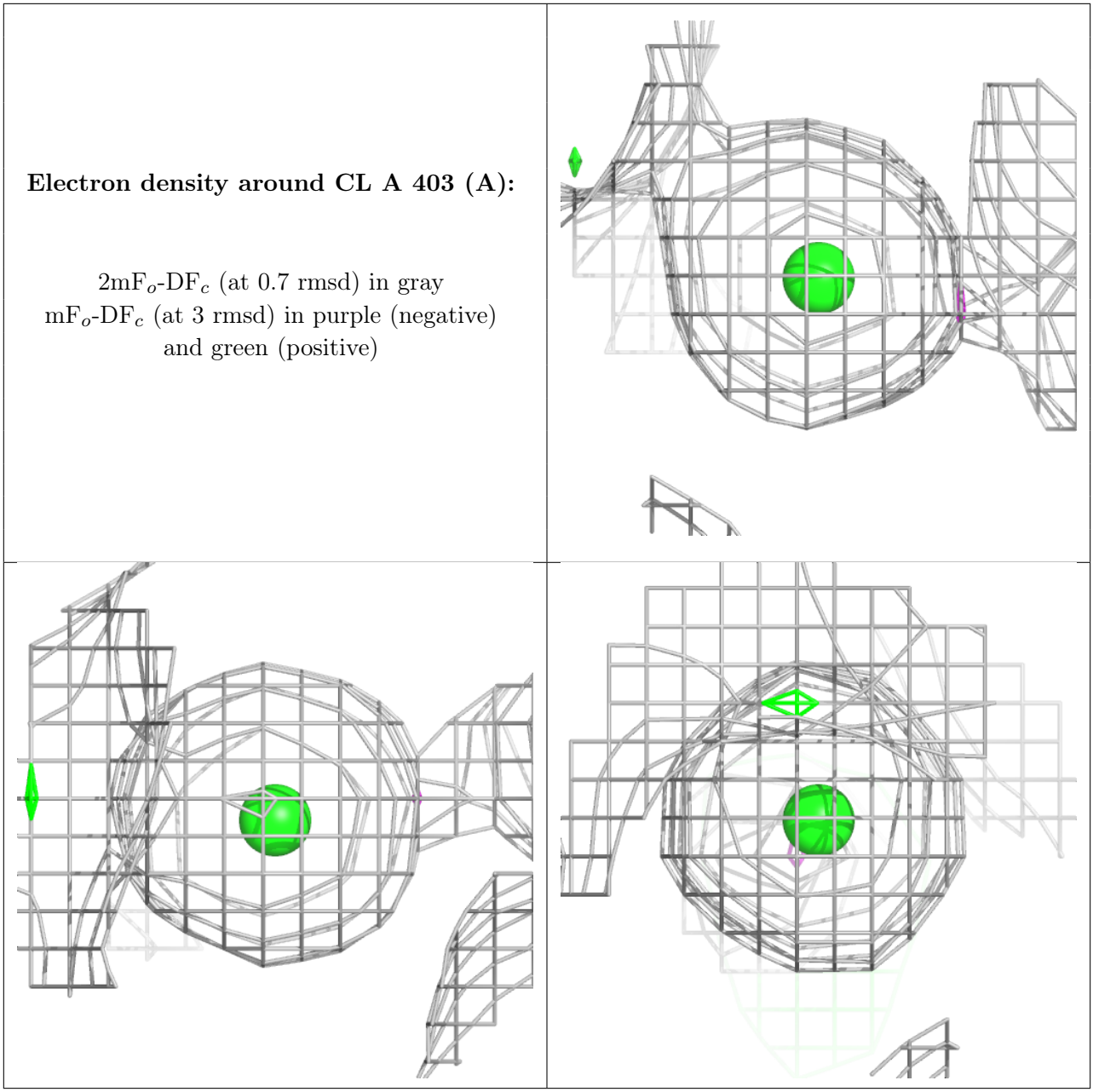






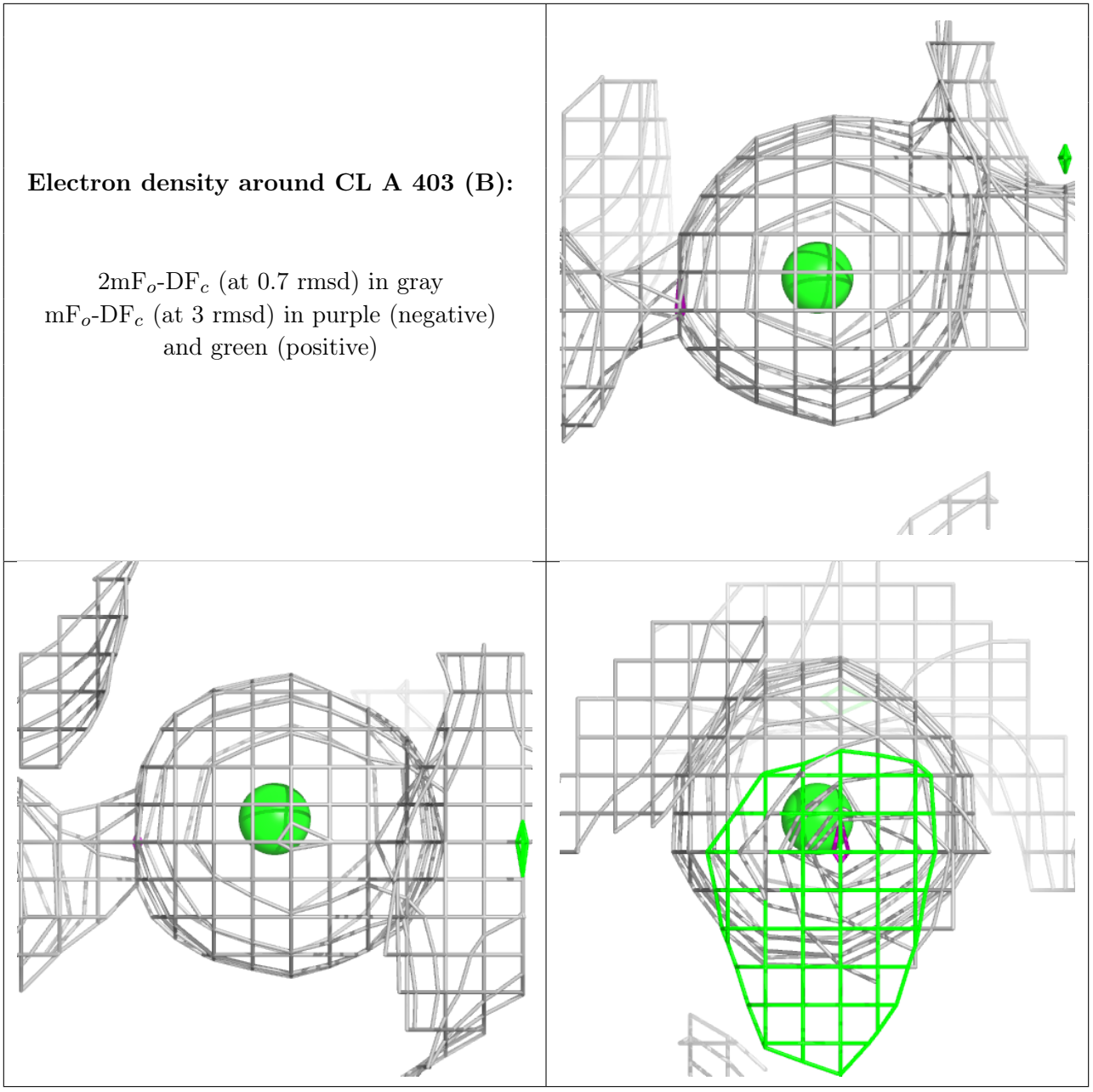
Electron density around CL A 403 (A):

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



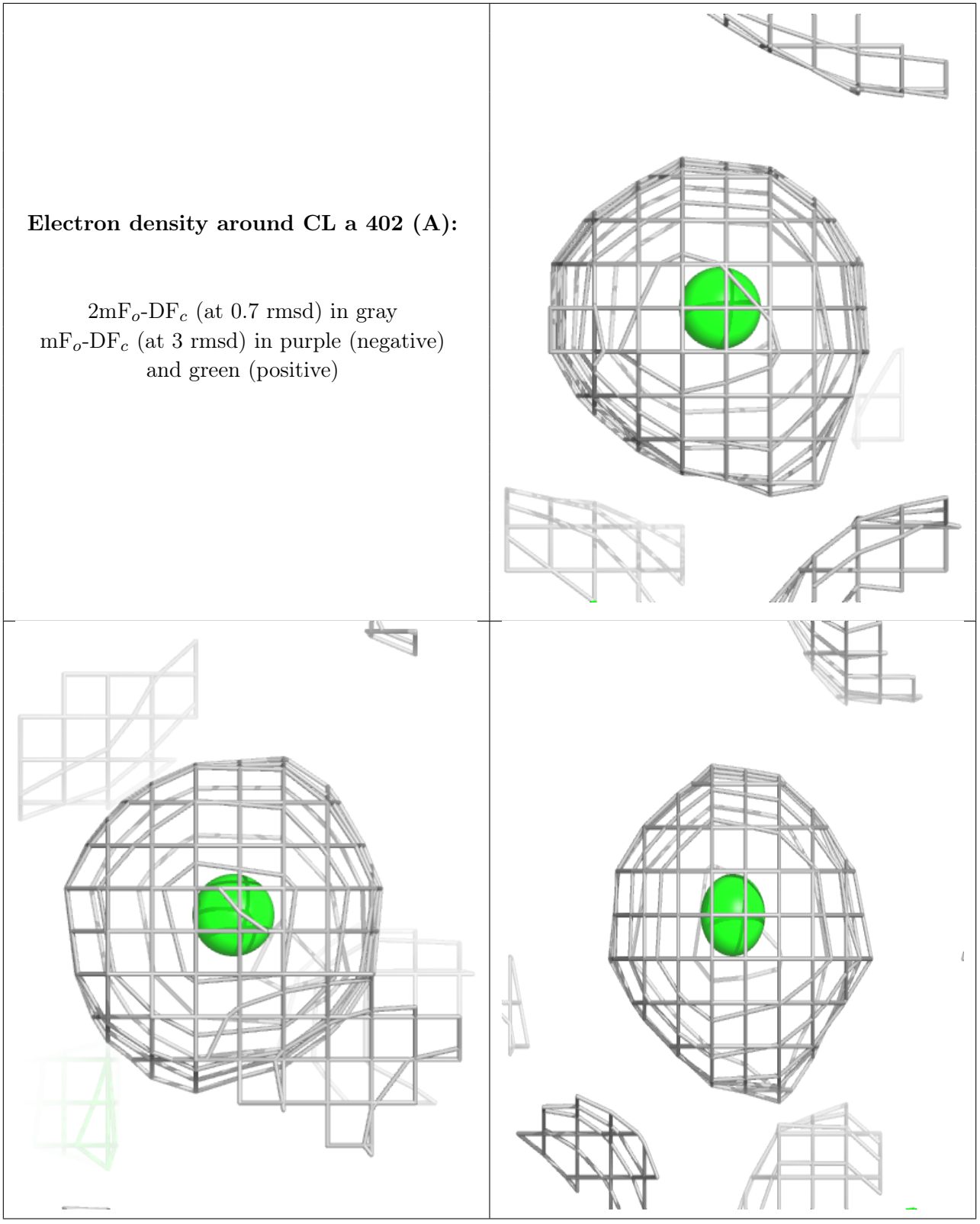
Electron density around CL A 403 (B):

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



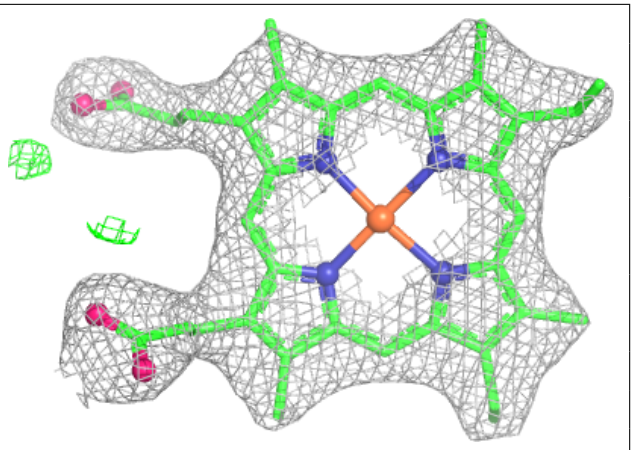
Electron density around CL a 402 (A):

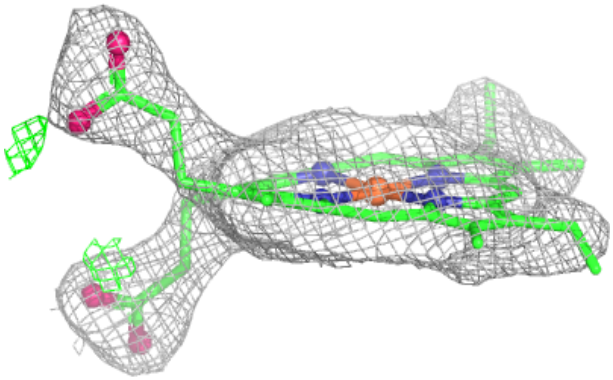
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

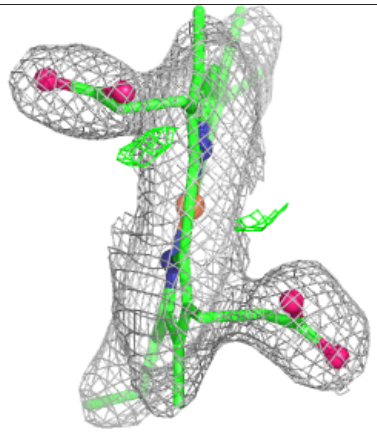


Electron density around HEM E 102:

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

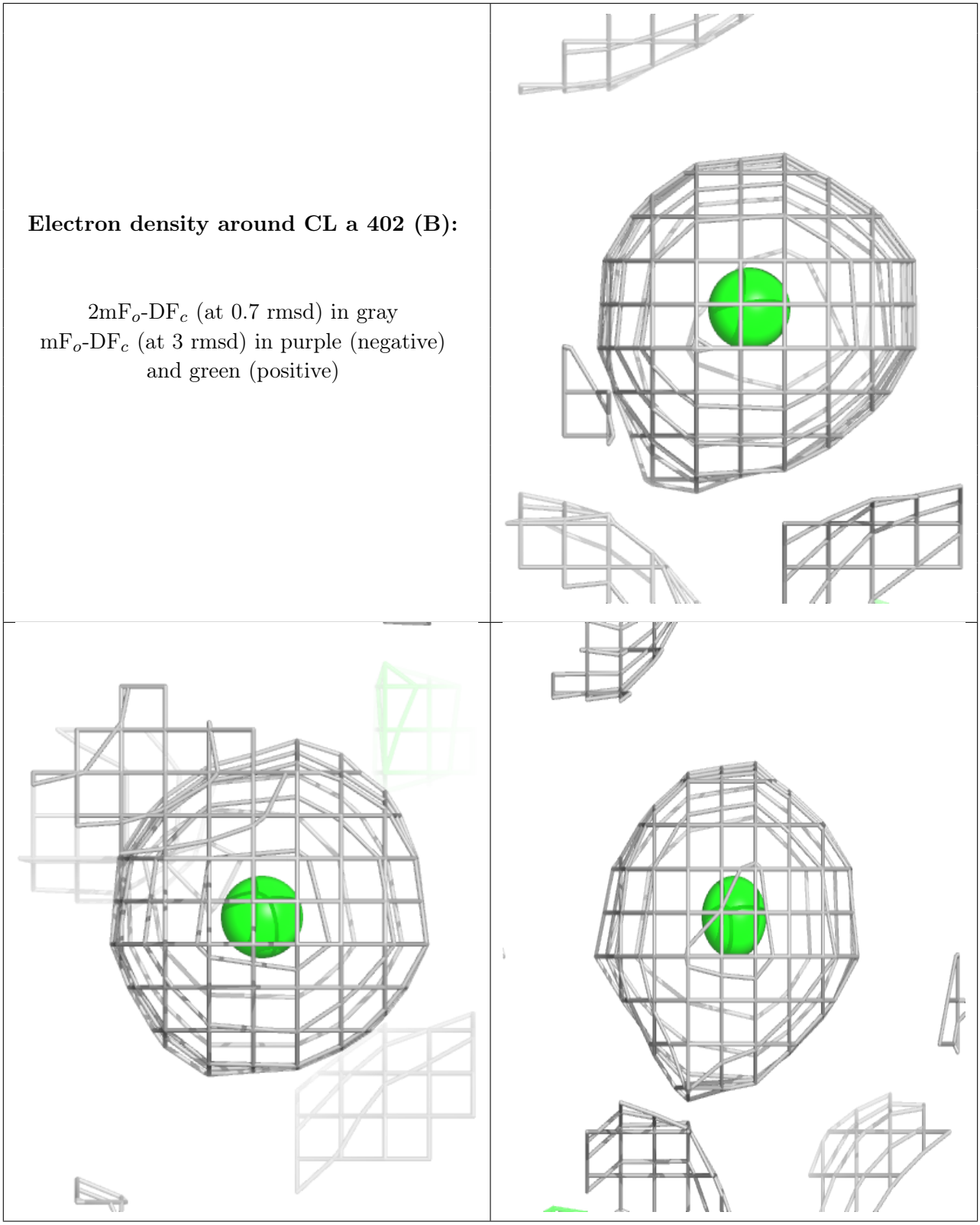






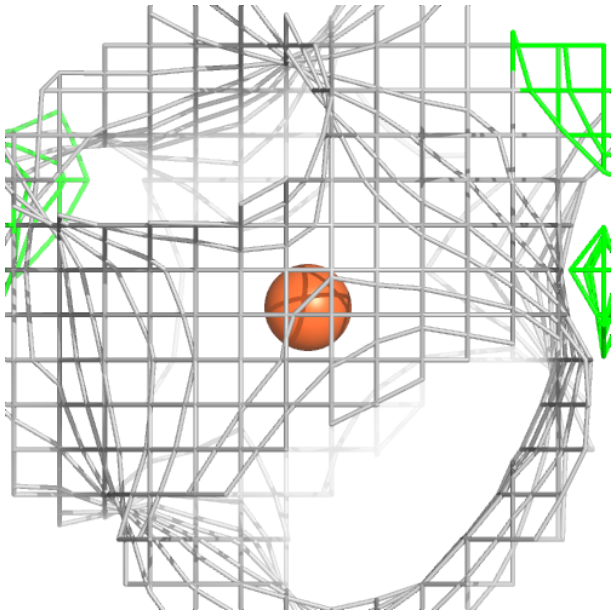
Electron density around CL a 402 (B):

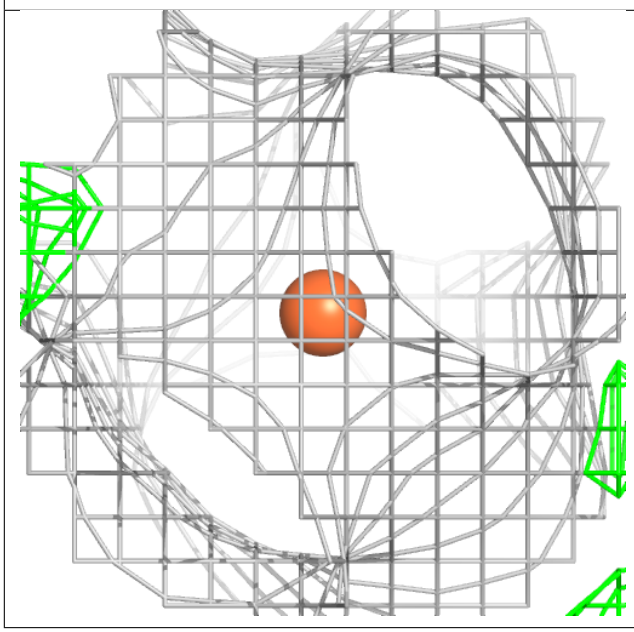
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

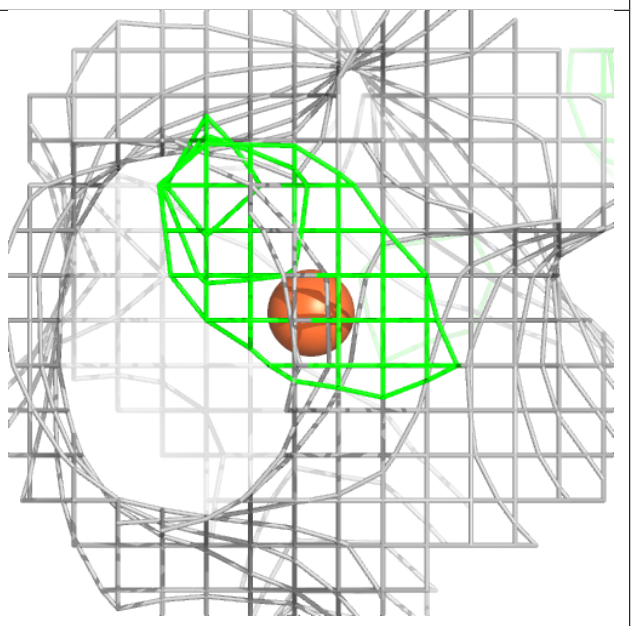


Electron density around FE2 a 401 (A):

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

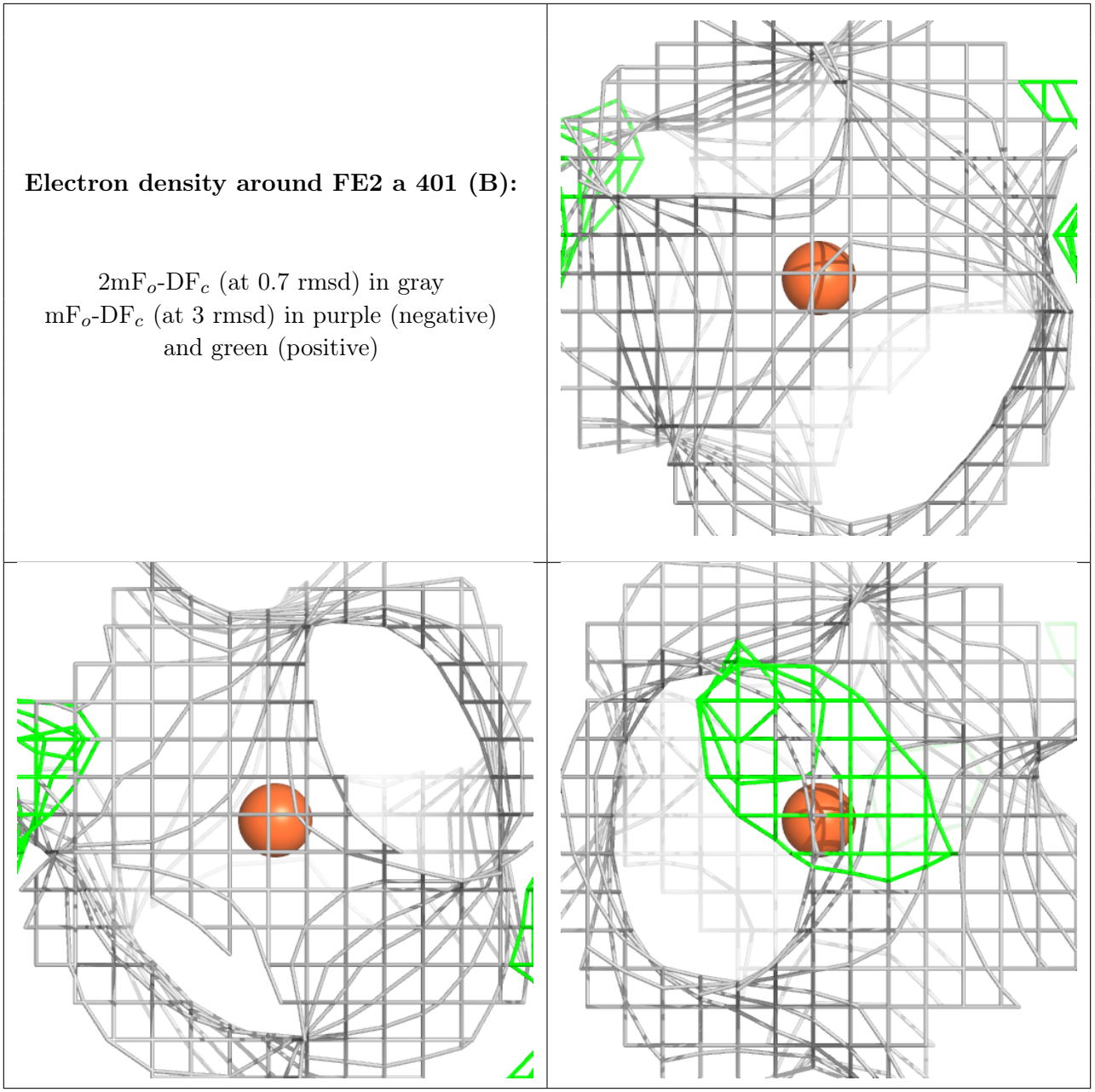






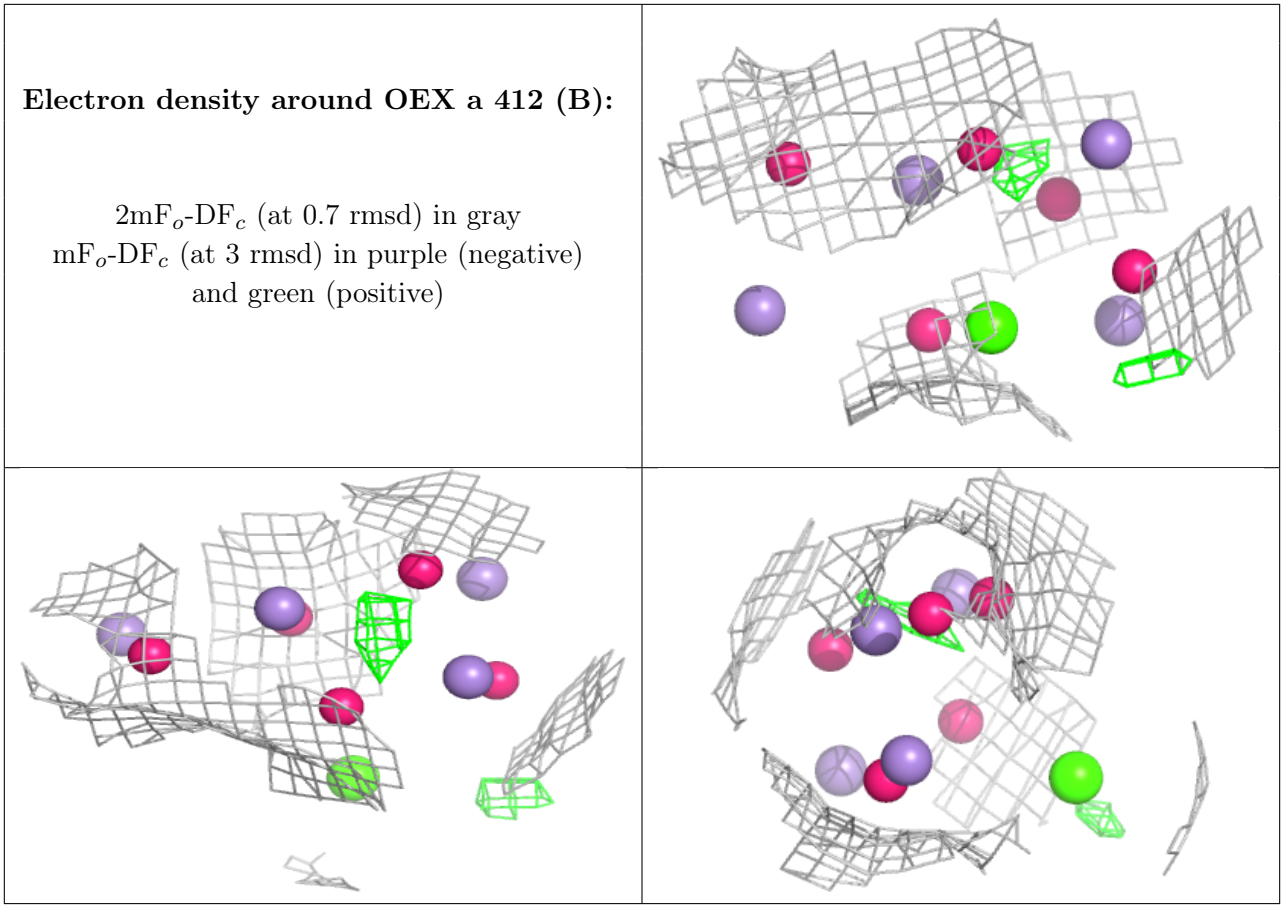
Electron density around FE2 a 401 (B):

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



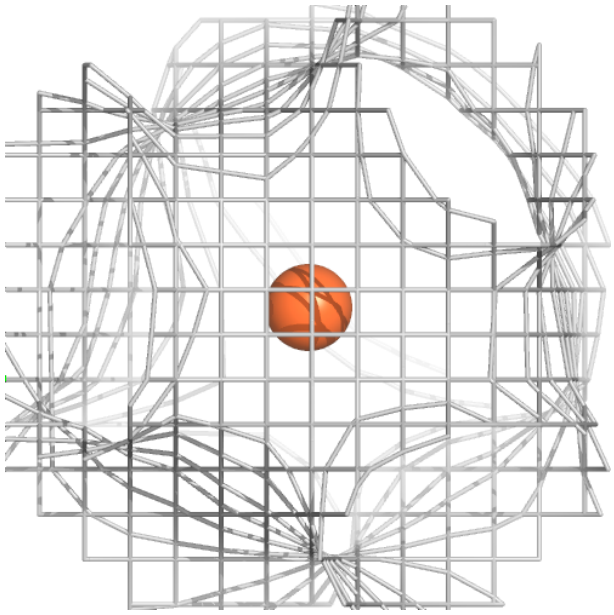
Electron density around OEX a 412 (B):

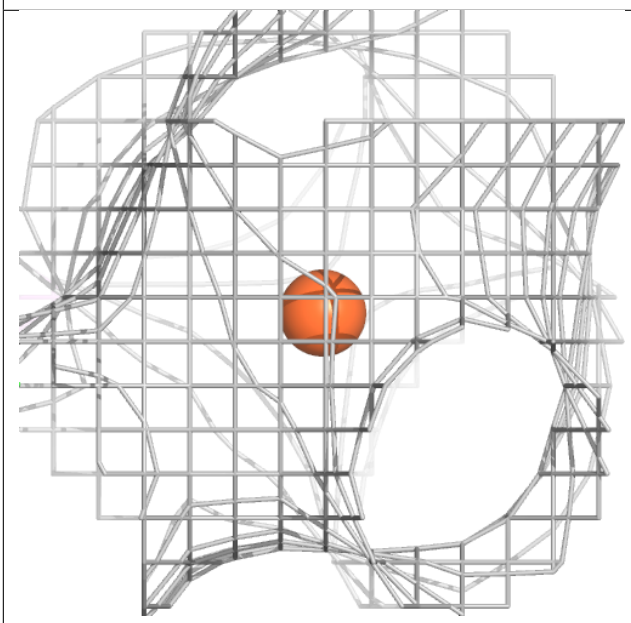
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

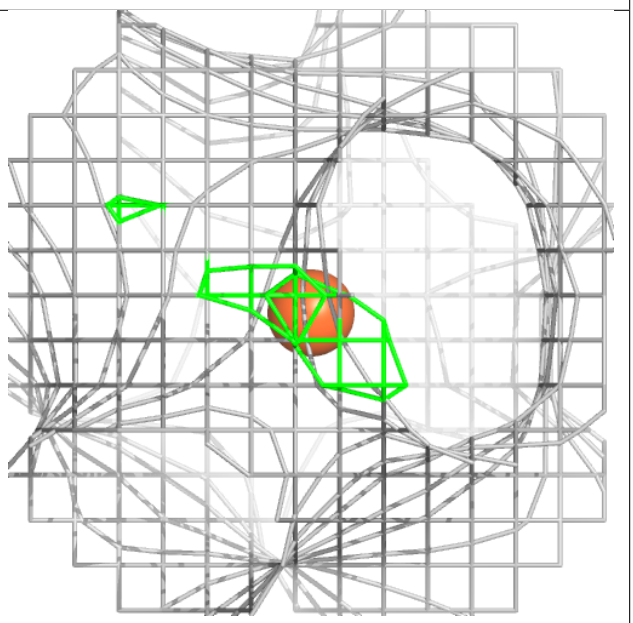


Electron density around FE2 A 401 (A):

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

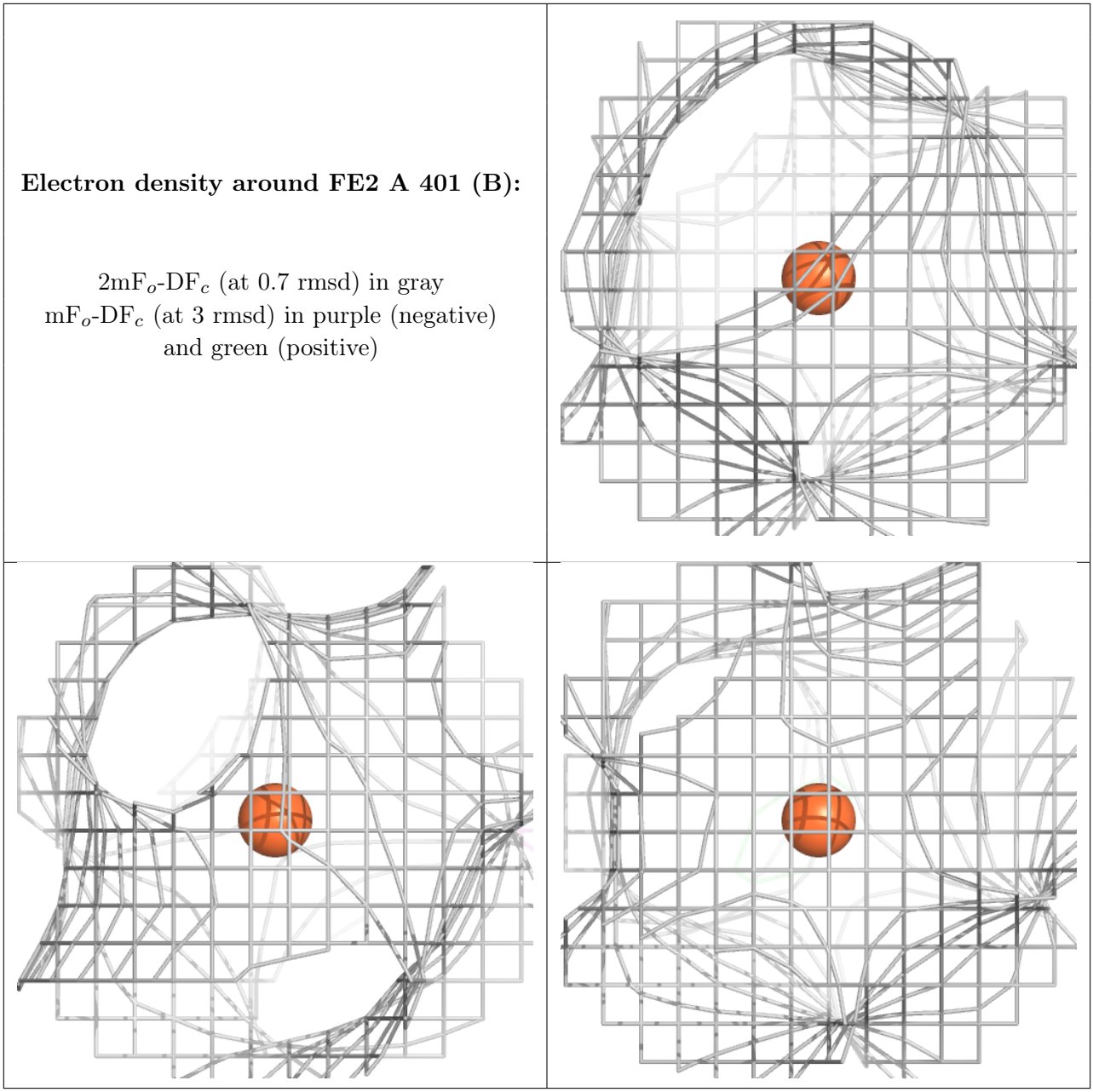






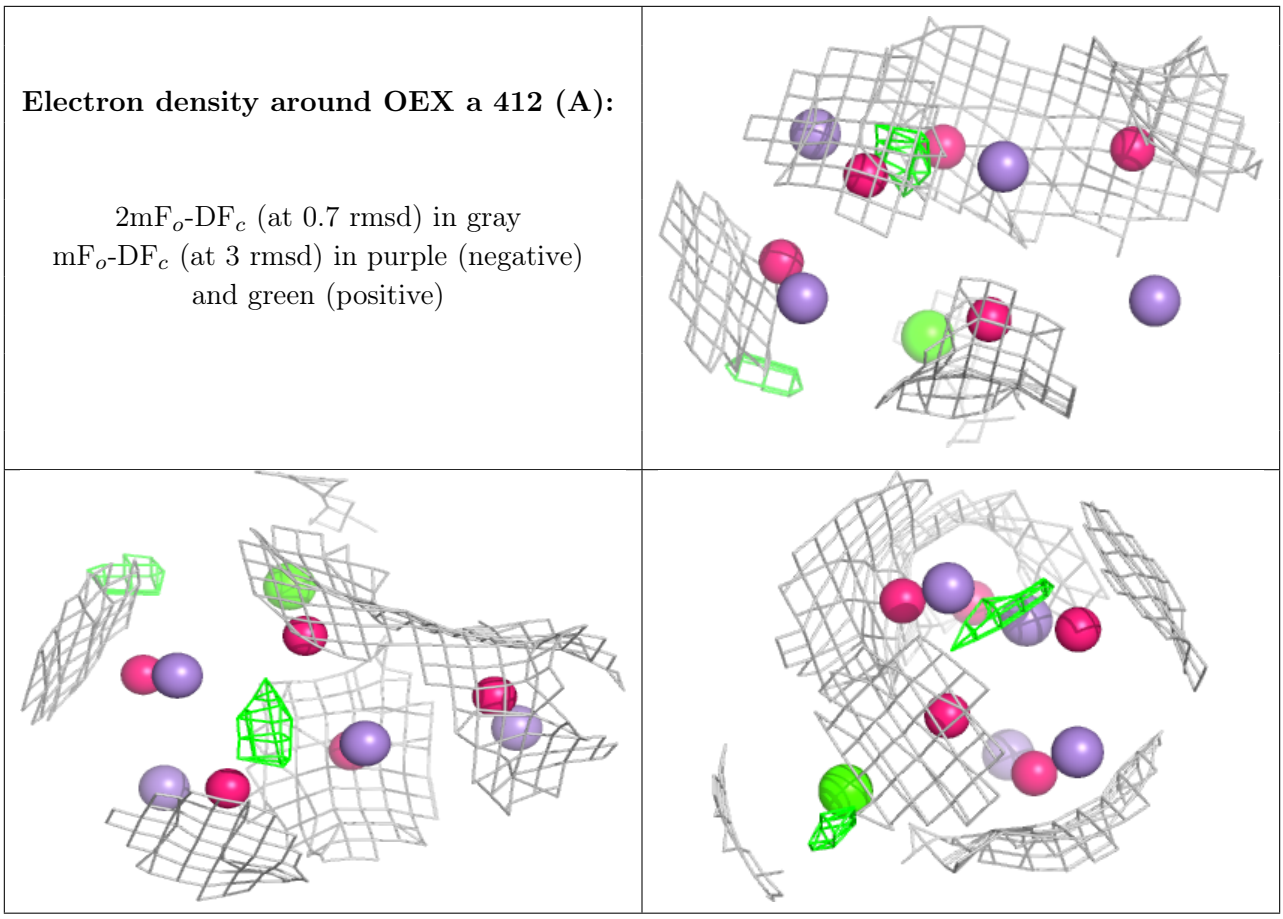
Electron density around FE2 A 401 (B):

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



Electron density around OEX a 412 (A):

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



6.5 Other polymers

There are no such residues in this entry.