Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 10:53 PM JST

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:

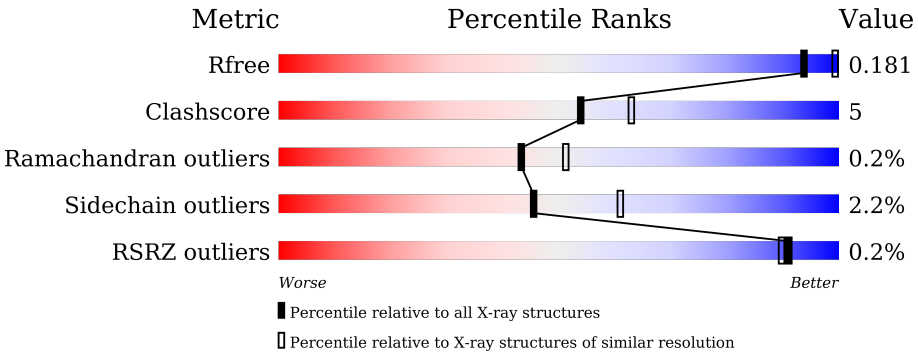
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 6% ·
1	a	344	89% 8% ·
2	B	505	93% 6%
2	b	505	91% 9%
3	C	455	91% 8% ·
3	c	455	90% 10%

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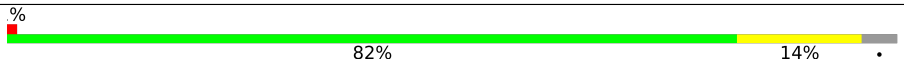
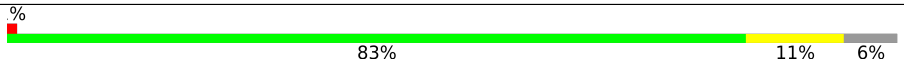
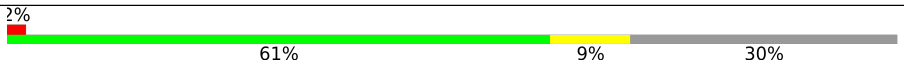
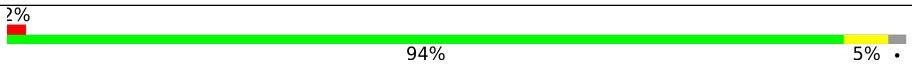
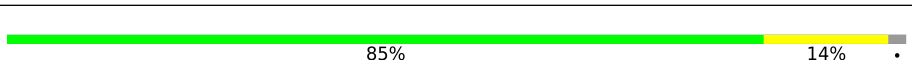
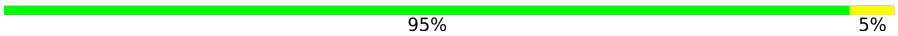
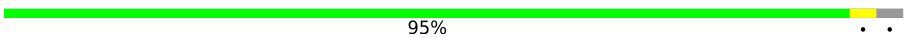
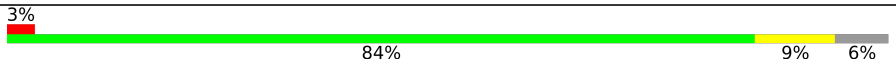
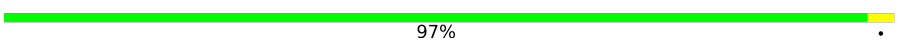
Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	91% 9%
17	X	40	90% 5% 5%
17	x	40	90% 5% 5%
18	Y	30	3% 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
27	GOL	A	418	-	-	X	-
27	GOL	a	418	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition (i)

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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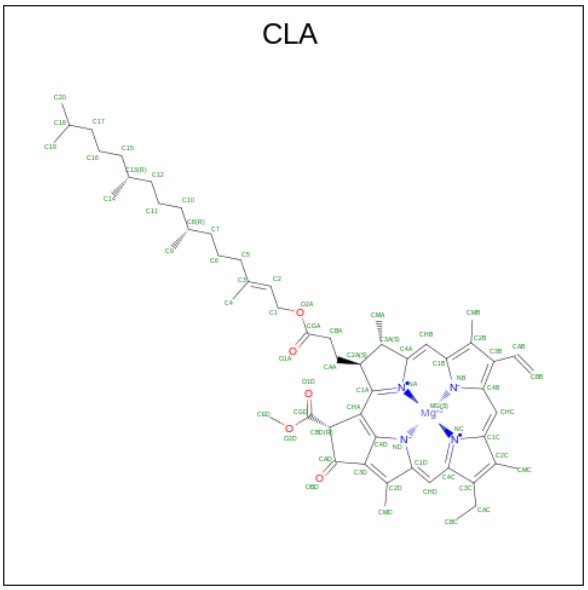
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2

- 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		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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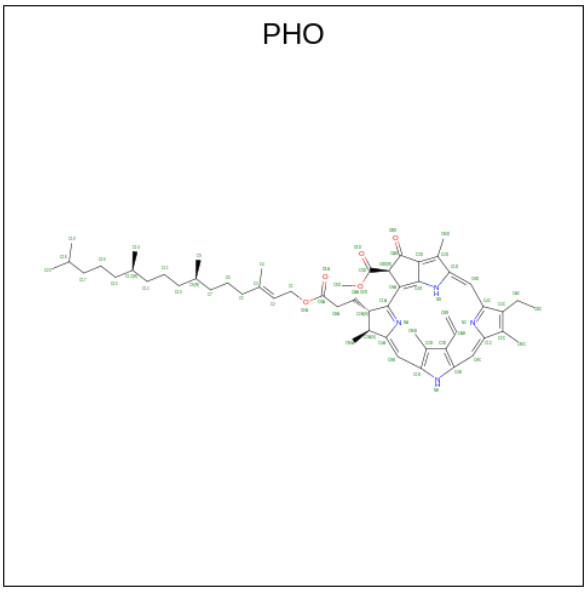
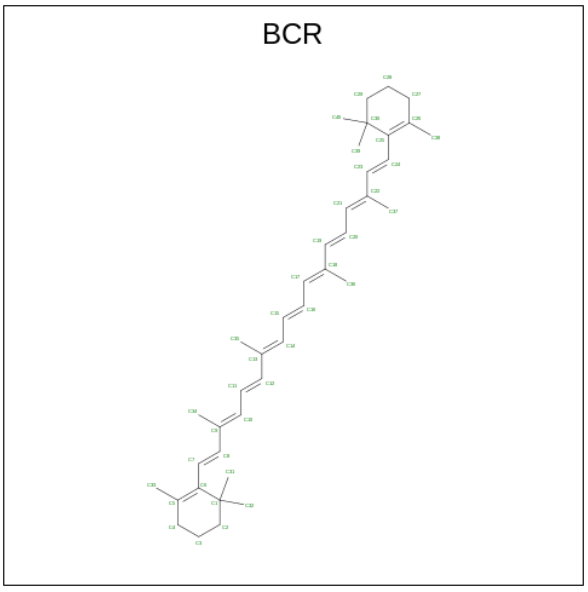
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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: $C_{55}H_{74}N_4O_5$).



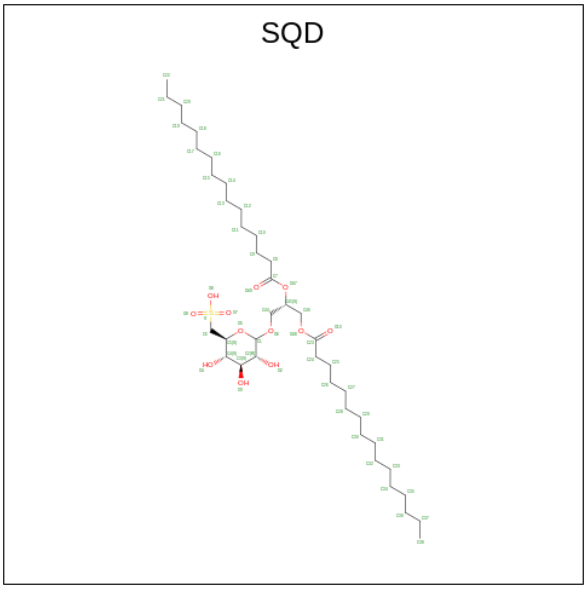
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	d	1	Total	C	N	O	0	1
			128	110	8	10		

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



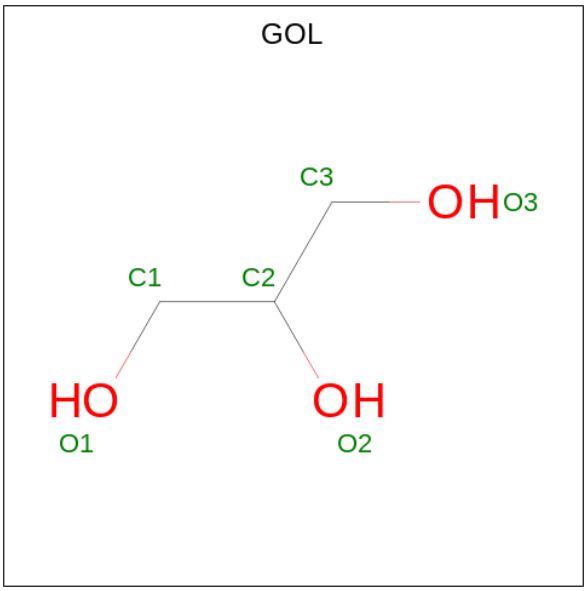
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total 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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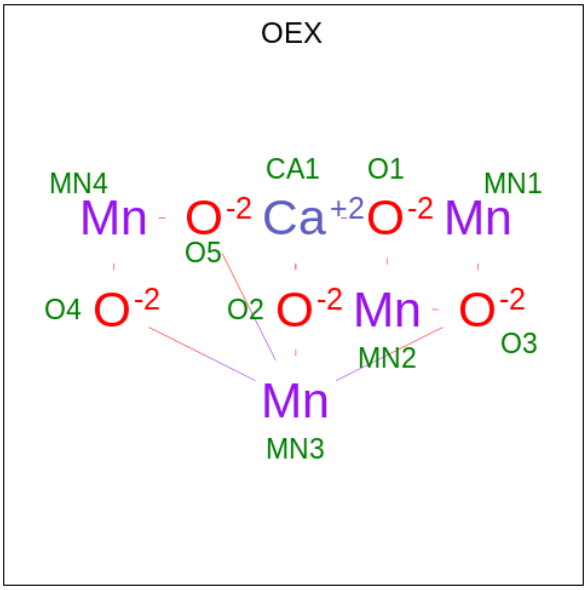
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 12 6 6	0	1
27	c	1	Total C O 6 3 3	0	0
27	d	1	Total C O 6 3 3	0	0
27	l	1	Total C O 12 6 6	0	1
27	o	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	v	1	Total C O 12 6 6	0	1

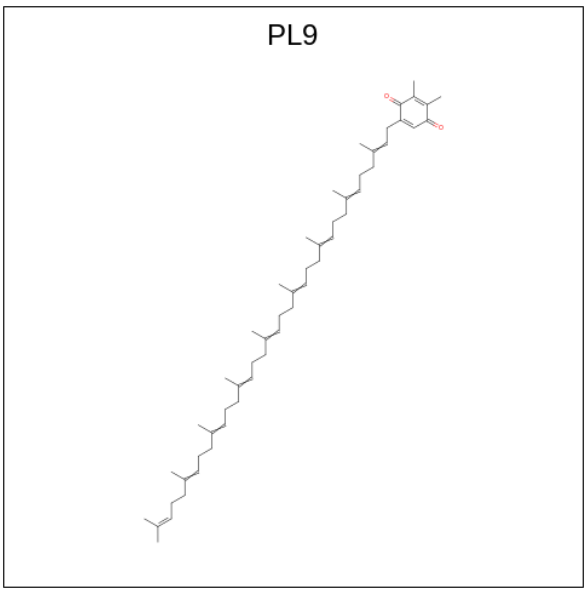
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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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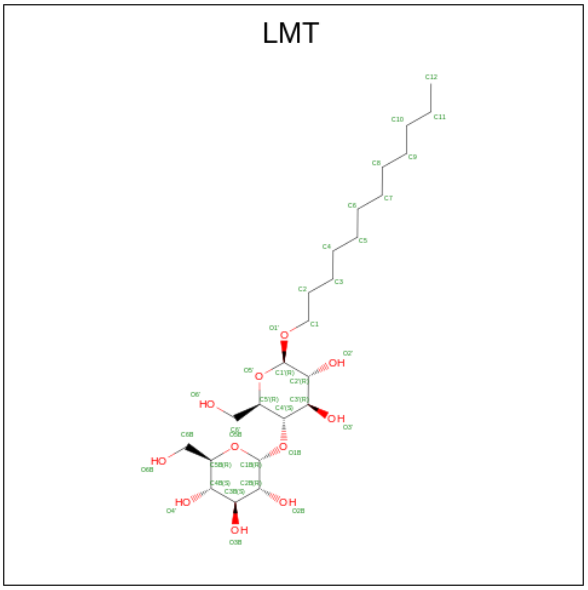
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 64 54 10	0	1
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- 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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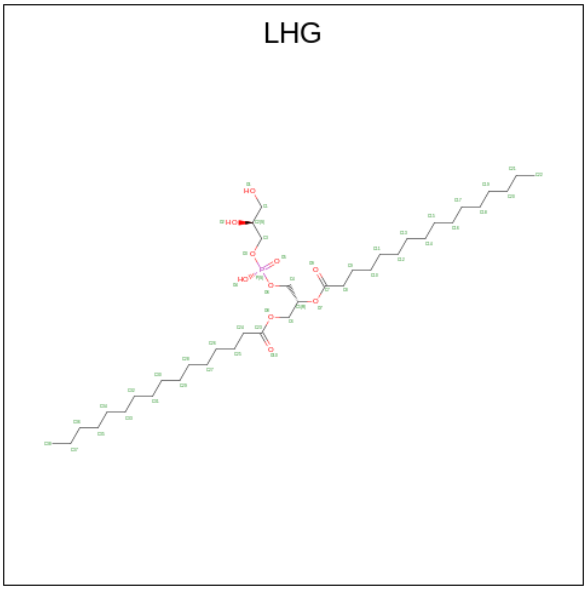
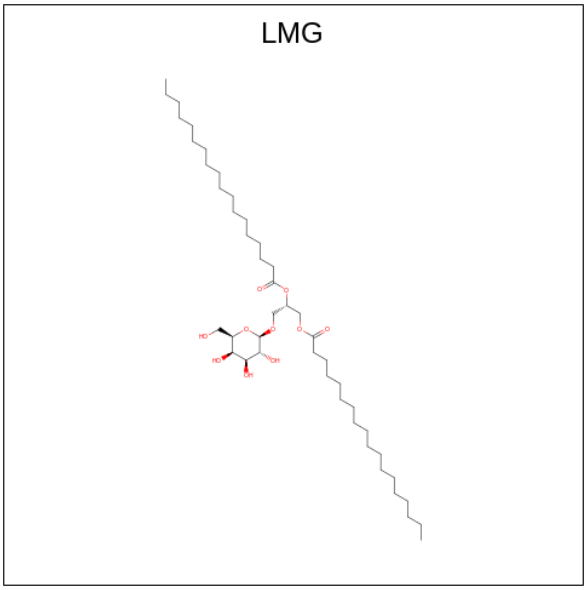
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 25 19 6	0	0
31	C	1	Total C O 35 24 11	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	T	1	Total C O 35 24 11	0	0
31	a	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 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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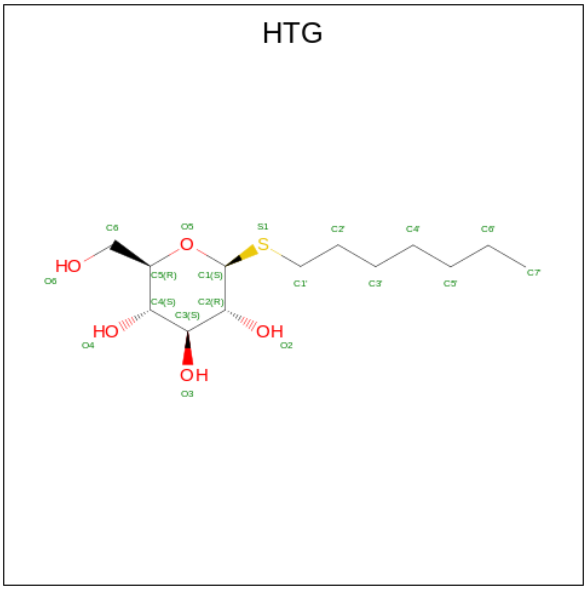
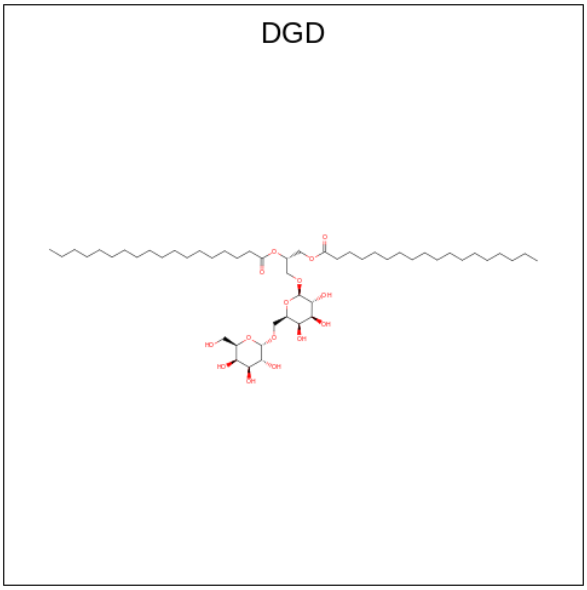
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	D	1	Total C O 51 41 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	m	1	Total C O 51 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: $C_{51}H_{96}O_{15}$).

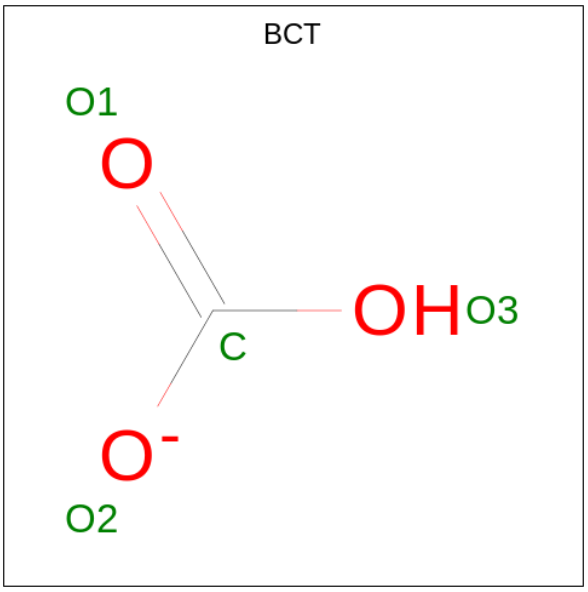


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

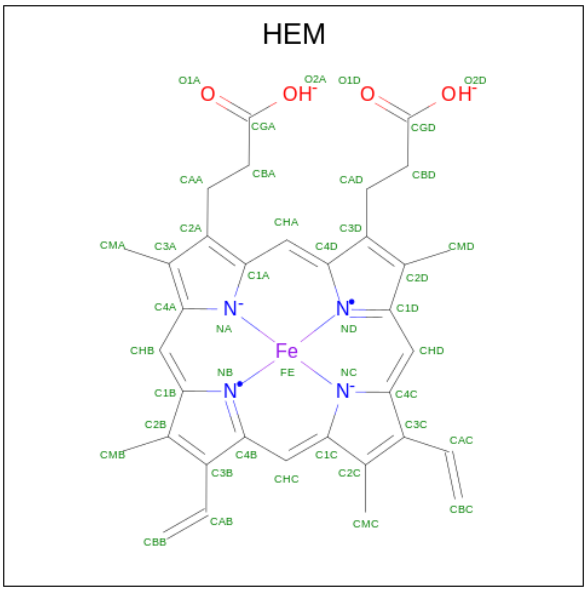
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

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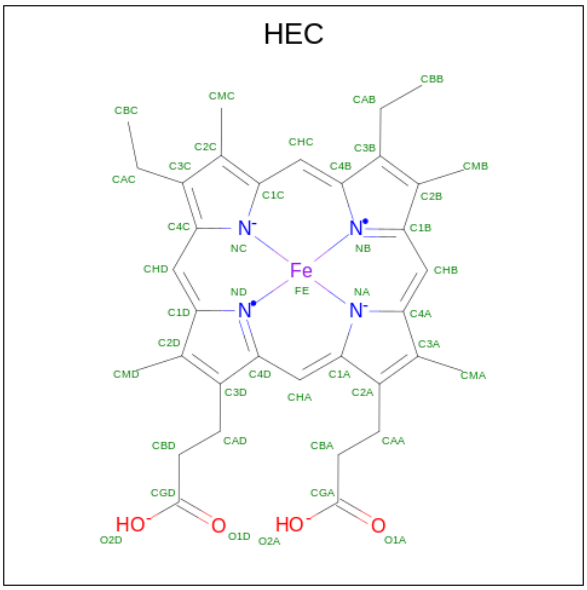
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 40 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 41 is water.

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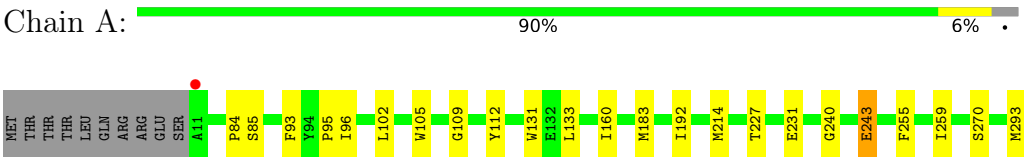
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	15	Total O 15 15	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	98	Total O 102 102	0	4
41	t	8	Total O 11 11	0	3
41	u	50	Total O 51 51	0	1
41	v	59	Total O 61 61	0	2
41	x	7	Total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

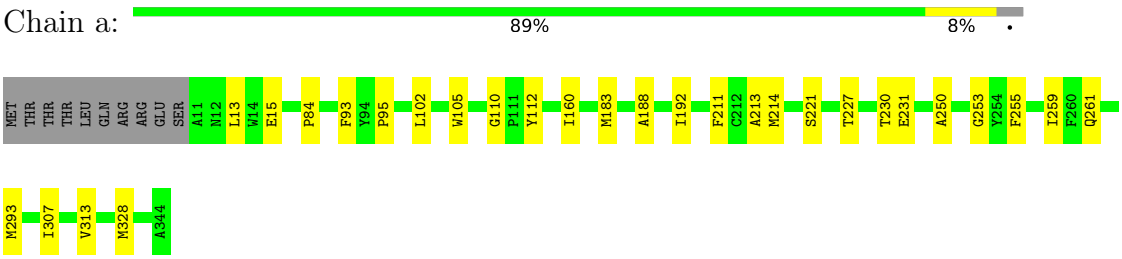
• Molecule 1: Photosystem II protein D1

Chain A:



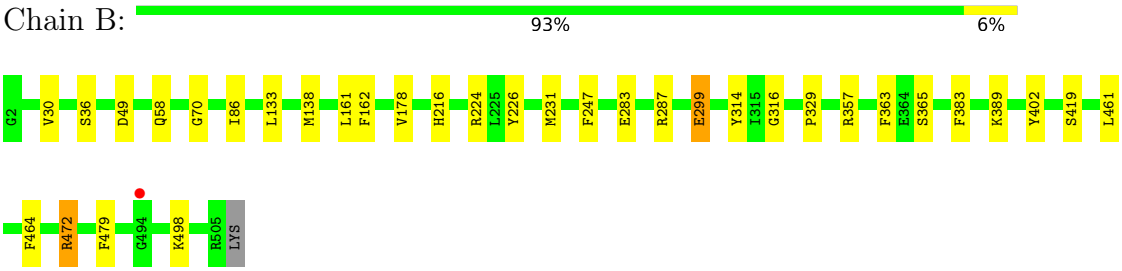
• Molecule 1: Photosystem II protein D1

Chain a:



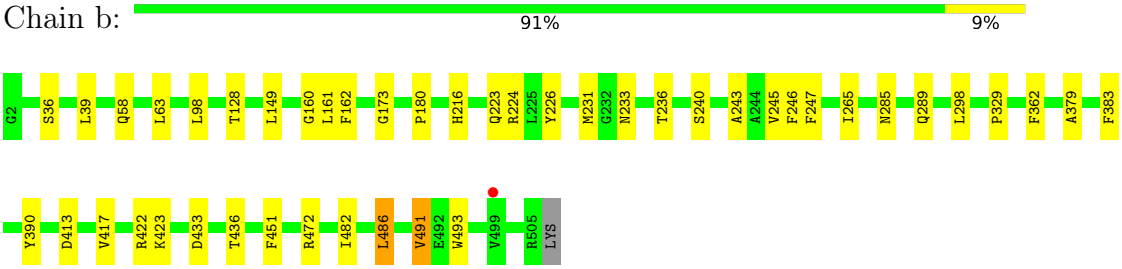
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



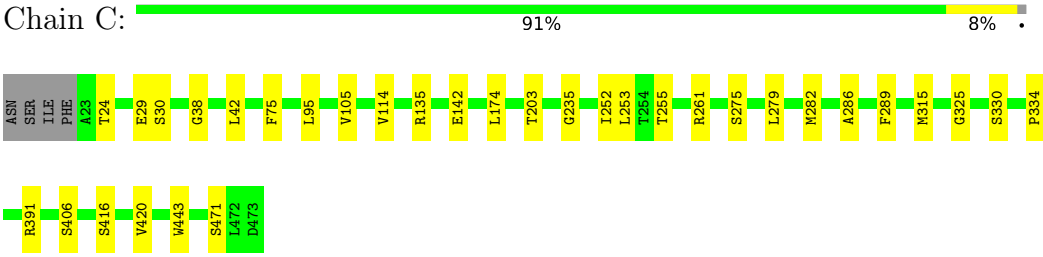
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



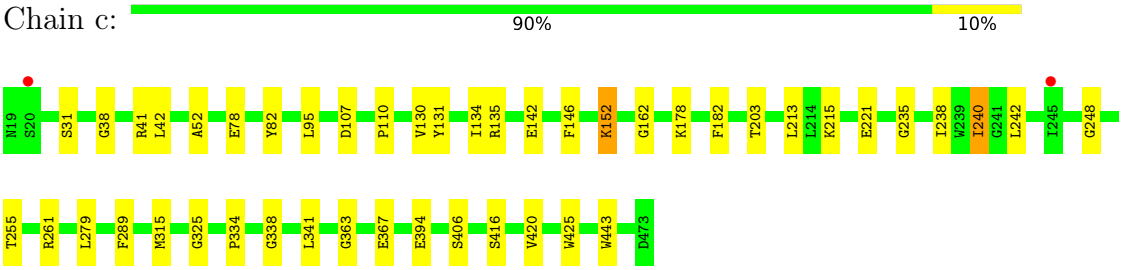
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



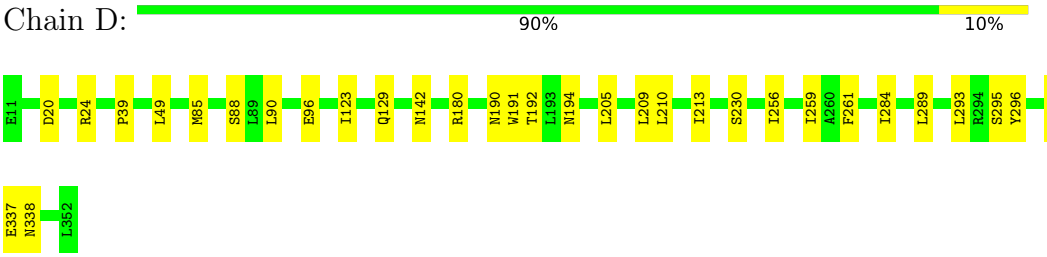
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



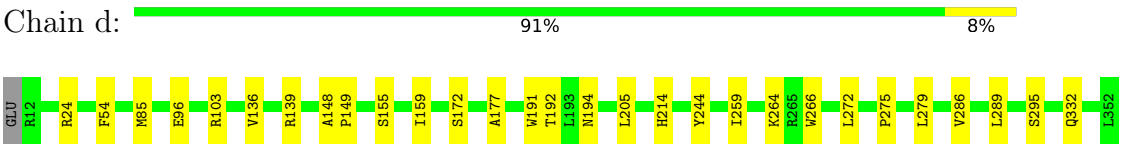
• Molecule 4: Photosystem II D2 protein

Chain D:



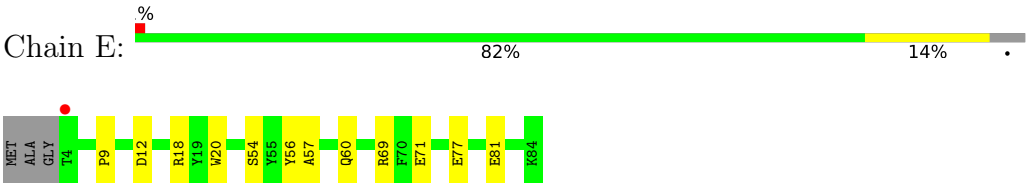
• Molecule 4: Photosystem II D2 protein

Chain d:



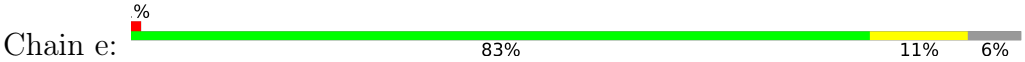
• Molecule 5: Cytochrome b559 subunit alpha

Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

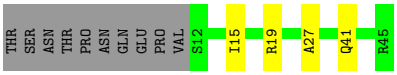




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

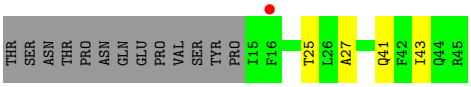




• Molecule 6: Cytochrome b559 subunit beta

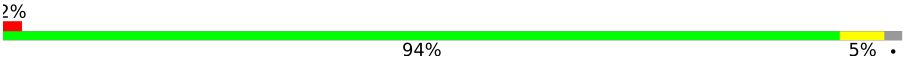
Chain f:

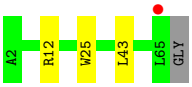




• Molecule 7: Photosystem II reaction center protein H

Chain H:

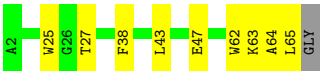




• Molecule 7: Photosystem II reaction center protein H

Chain h:

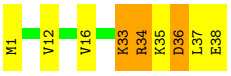




• Molecule 8: Photosystem II reaction center protein I

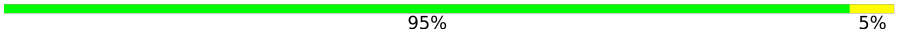
Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

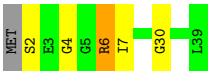




• Molecule 9: Photosystem II reaction center protein J

Chain J:

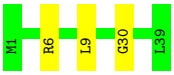




• Molecule 9: Photosystem II reaction center protein J

Chain j:

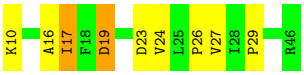




• Molecule 10: Photosystem II reaction center protein K

Chain K:

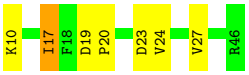




• Molecule 10: Photosystem II reaction center protein K

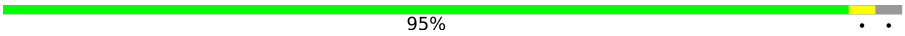
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

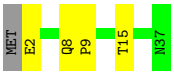




• Molecule 11: Photosystem II reaction center protein L

Chain l:





• Molecule 12: Photosystem II reaction center protein M

Chain M:

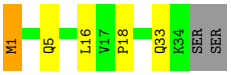




• Molecule 12: Photosystem II reaction center protein M

Chain m:

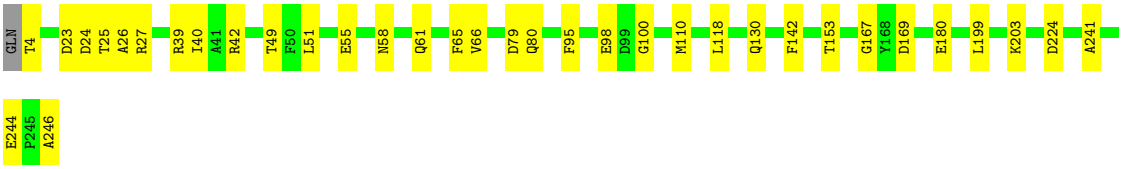




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

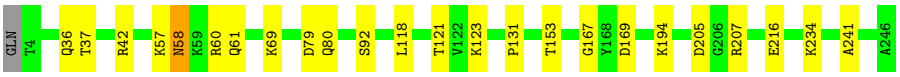




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

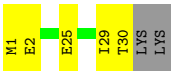




• Molecule 14: Photosystem II reaction center protein T

Chain T:

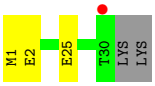




• Molecule 14: Photosystem II reaction center protein T

Chain t:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

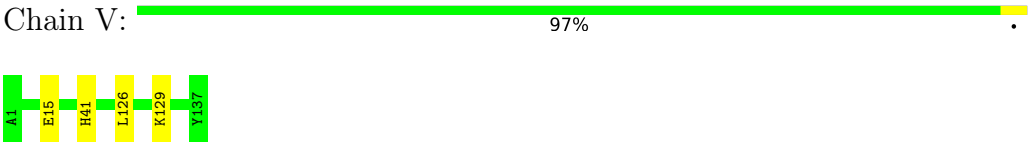
Chain u:





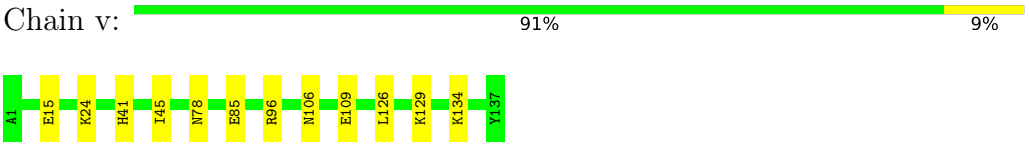
• Molecule 16: Cytochrome c-550

Chain V:



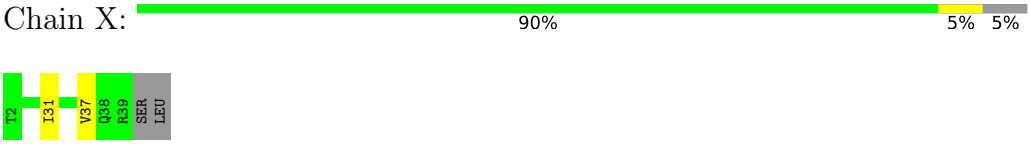
• Molecule 16: Cytochrome c-550

Chain v:



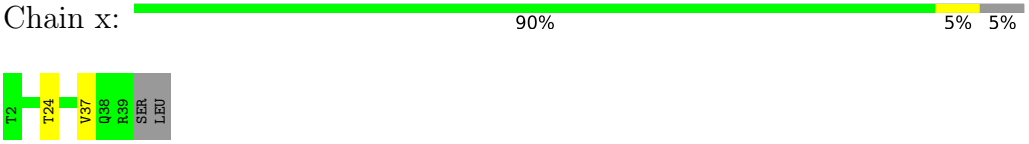
• Molecule 17: Photosystem II reaction center protein X

Chain X:



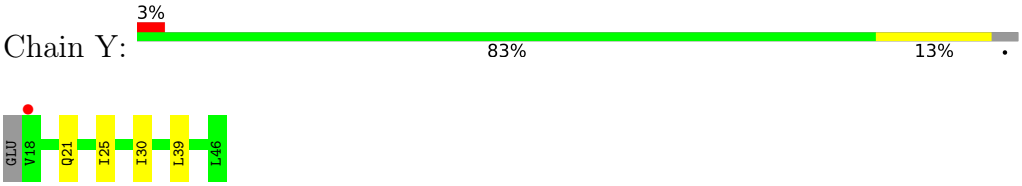
• Molecule 17: Photosystem II reaction center protein X

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



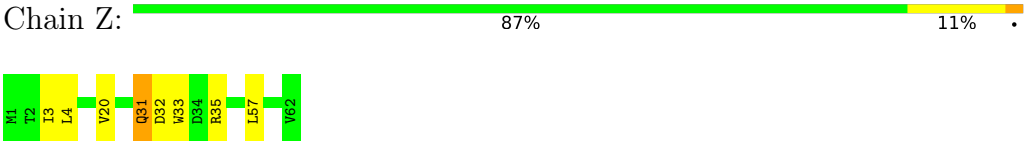
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



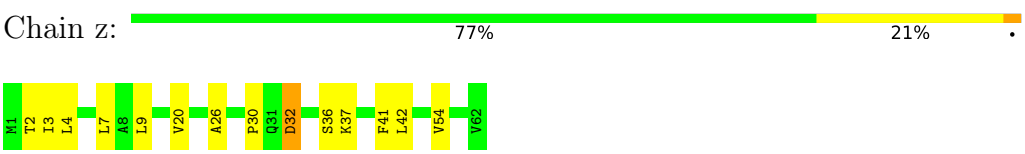
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



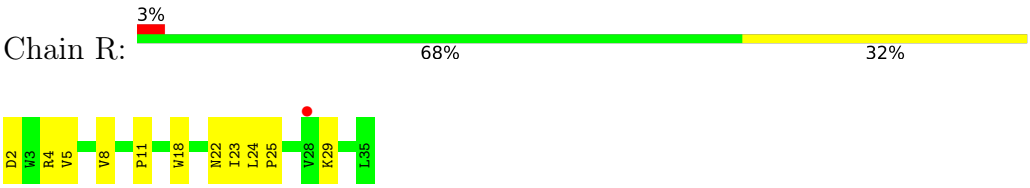
• Molecule 19: Photosystem II reaction center protein Z

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, HEM, PL9, LMT, OEX, FE2, PHO, FME, CLA, UNL, LMG, HEC, CA, SQD, BCR, MG, DGD, GOL, LHG, CL, HTG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	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

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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 (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.61	0	7,9,11	1.22	1 (14%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.21	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.14	0
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.40	2 (28%)
14	FME	t	1	14	8,9,10	0.72	0	7,9,11	1.72	2 (28%)

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	0.60	0	7,9,11	1.42	2 (28%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	CA-N-CN	-2.96	118.27	122.82
14	t	1	FME	O-C-CA	-2.50	118.23	124.78
14	T	1	FME	CG-CB-CA	2.28	119.29	112.95
12	m	1	FME	CA-N-CN	-2.27	119.34	122.82
14	T	1	FME	CA-N-CN	2.23	126.25	122.82
12	m	1	FME	O1-CN-N	-2.22	119.42	125.27
8	I	1	FME	O-C-CA	-2.19	119.03	124.78
12	M	1	FME	O-C-CA	-2.12	119.22	124.78

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	$\#\|Z\| > 2$
25	BCR	b	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.30	6 (10%)
23	CLA	C	514	3	69,73,73	2.03	19 (27%)	83,113,113	2.83	31 (37%)
23	CLA	c	503	3	69,73,73	2.07	19 (27%)	83,113,113	2.89	29 (34%)
23	CLA	c	509	3	69,73,73	2.03	19 (27%)	83,113,113	2.82	31 (37%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.40	10 (17%)
33	LMG	c	519	-	51,51,55	0.91	2 (3%)	59,59,63	1.12	5 (8%)
23	CLA	C	510	3	69,73,73	2.06	21 (30%)	83,113,113	2.84	31 (37%)
26	SQD	X	101	-	42,43,54	1.21	4 (9%)	51,54,65	2.16	13 (25%)
25	BCR	B	617	-	41,41,41	1.09	1 (2%)	56,56,56	1.31	8 (14%)
27	GOL	a	417	-	5,5,5	1.13	0	5,5,5	1.03	0
23	CLA	c	512	3	69,73,73	2.06	19 (27%)	83,113,113	2.85	30 (36%)
24	PHO	A	416[B]	-	58,69,69	2.75	14 (24%)	56,99,99	2.95	18 (32%)
23	CLA	B	605	2	69,73,73	2.00	18 (26%)	83,113,113	2.95	31 (37%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.57	15 (26%)
32	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	DGD	c	518	-	63,63,67	0.87	4 (6%)	77,77,81	1.04	5 (6%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.47	14 (25%)
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
32	LHG	D	406[B]	-	48,48,48	0.87	2 (4%)	51,54,54	0.97	3 (5%)
23	CLA	c	501	3	69,73,73	1.97	19 (27%)	83,113,113	2.92	30 (36%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.27	5 (8%)
38	HEM	E	102	6,5	50,50,50	1.53	7 (14%)	66,82,82	1.91	15 (22%)
23	CLA	b	608	2	69,73,73	2.01	20 (28%)	83,113,113	2.82	30 (36%)
28	OEX	a	412[A]	3,41,1	0,14,14	-	-	-		
32	LHG	b	629[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.05	3 (5%)
32	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.18	5 (9%)
27	GOL	b	624	-	5,5,5	1.11	1 (20%)	5,5,5	0.81	0
23	CLA	C	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.84	32 (38%)
31	LMT	F	101	-	36,36,36	1.06	1 (2%)	47,47,47	1.05	3 (6%)
26	SQD	a	411	-	53,54,54	1.06	3 (5%)	62,65,65	1.23	8 (12%)
31	LMT	b	627	-	25,25,36	0.90	1 (4%)	30,30,47	1.11	3 (10%)
23	CLA	C	513	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	34 (40%)
25	BCR	B	618	-	41,41,41	1.03	1 (2%)	56,56,56	1.38	8 (14%)
32	LHG	d	415[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
33	LMG	C	520	-	51,51,55	0.92	2 (3%)	59,59,63	1.14	7 (11%)
23	CLA	b	602	2	69,73,73	2.09	20 (28%)	83,113,113	2.91	35 (42%)
23	CLA	b	609	2	69,73,73	2.01	19 (27%)	83,113,113	2.79	31 (37%)
28	OEX	a	412[B]	3,41,1	0,14,14	-	-	-		
23	CLA	d	405	4	69,73,73	2.04	19 (27%)	83,113,113	2.82	30 (36%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
34	HTG	b	622	-	19,19,19	1.11	2 (10%)	23,24,24	1.94	8 (34%)
33	LMG	c	520	-	51,51,55	1.00	2 (3%)	59,59,63	1.35	8 (13%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.30	8 (14%)
23	CLA	B	603	2	69,73,73	1.99	20 (28%)	83,113,113	2.84	30 (36%)
28	OEX	A	413[A]	3,41,1	0,14,14	-	-	-		
24	PHO	a	406[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
29	PL9	a	413[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
27	GOL	C	523[B]	-	5,5,5	1.04	0	5,5,5	0.87	0
23	CLA	c	508	3	69,73,73	2.10	21 (30%)	83,113,113	2.77	27 (32%)
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.38	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	604	2	69,73,73	1.99	18 (26%)	83,113,113	2.83	27 (32%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
35	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.15	8 (10%)
23	CLA	b	610	41	69,73,73	2.02	20 (28%)	83,113,113	2.80	31 (37%)
24	PHO	a	406[B]	-	58,69,69	2.75	13 (22%)	56,99,99	2.72	17 (30%)
25	BCR	D	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.82	15 (26%)
29	PL9	a	413[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.96	22 (32%)
34	HTG	d	412	-	16,16,19	0.97	1 (6%)	20,21,24	1.52	1 (5%)
37	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	C	508	41	69,73,73	1.99	19 (27%)	83,113,113	2.79	29 (34%)
23	CLA	C	509	3	69,73,73	2.08	22 (31%)	83,113,113	2.75	27 (32%)
23	CLA	B	616	2	69,73,73	1.96	20 (28%)	83,113,113	2.89	30 (36%)
35	DGD	h	102	-	63,63,67	0.86	3 (4%)	77,77,81	1.08	4 (5%)
32	LHG	d	408[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.03	4 (7%)
23	CLA	a	405[B]	41	69,73,73	2.02	20 (28%)	83,113,113	2.86	30 (36%)
31	LMT	M	101	-	36,36,36	1.13	3 (8%)	47,47,47	1.18	4 (8%)
32	LHG	D	407[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.95	3 (5%)
23	CLA	C	504	3	69,73,73	2.01	20 (28%)	83,113,113	2.81	30 (36%)
24	PHO	A	416[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
32	LHG	d	409[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
31	LMT	e	101	-	36,36,36	1.02	4 (11%)	47,47,47	0.97	1 (2%)
37	BCT	d	401[B]	21	2,3,3	0.58	0	2,3,3	1.22	0
23	CLA	B	609	2	69,73,73	2.00	17 (24%)	83,113,113	2.84	29 (34%)
27	GOL	o	302	-	5,5,5	0.98	0	5,5,5	0.98	0
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	B	614	2	69,73,73	2.05	19 (27%)	83,113,113	2.96	30 (36%)
25	BCR	T	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.56	11 (19%)
23	CLA	b	613	2	69,73,73	1.91	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	b	611	2	69,73,73	1.96	19 (27%)	83,113,113	2.98	29 (34%)
26	SQD	l	101	-	53,54,54	1.06	4 (7%)	62,65,65	1.75	11 (17%)
23	CLA	d	402[B]	41	69,73,73	2.03	17 (24%)	83,113,113	2.84	33 (39%)
32	LHG	d	409[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.07	4 (7%)
27	GOL	b	628	-	5,5,5	0.41	0	5,5,5	1.41	1 (20%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.43	7 (12%)
25	BCR	b	619	-	41,41,41	1.11	1 (2%)	56,56,56	1.39	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
23	CLA	B	601	41	69,73,73	2.06	21 (30%)	83,113,113	2.87	29 (34%)
23	CLA	b	603	2	69,73,73	1.97	20 (28%)	83,113,113	2.86	33 (39%)
27	GOL	O	303	-	5,5,5	0.95	0	5,5,5	1.12	1 (20%)
25	BCR	t	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.60	13 (23%)
23	CLA	c	502	3	69,73,73	1.98	18 (26%)	83,113,113	2.70	26 (31%)
23	CLA	d	404[B]	4	69,73,73	1.97	20 (28%)	83,113,113	2.79	31 (37%)
25	BCR	B	619	-	41,41,41	1.08	1 (2%)	56,56,56	1.28	6 (10%)
31	LMT	A	417	-	36,36,36	0.94	2 (5%)	47,47,47	1.05	1 (2%)
25	BCR	K	102	-	41,41,41	1.07	1 (2%)	56,56,56	1.41	9 (16%)
34	HTG	C	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.39	2 (8%)
29	PL9	D	405[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.64	16 (23%)
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.48	9 (15%)
24	PHO	d	403[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
23	CLA	C	512	3	69,73,73	2.01	22 (31%)	83,113,113	2.75	28 (33%)
26	SQD	b	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.67	12 (19%)
33	LMG	B	620	-	51,51,55	0.92	2 (3%)	59,59,63	1.32	4 (6%)
34	HTG	b	625	-	19,19,19	1.07	2 (10%)	23,24,24	1.48	4 (17%)
23	CLA	C	506	3	69,73,73	2.00	19 (27%)	83,113,113	2.81	29 (34%)
27	GOL	a	410	-	5,5,5	0.96	0	5,5,5	0.98	0
24	PHO	d	403[B]	-	58,69,69	2.77	14 (24%)	56,99,99	2.93	16 (28%)
35	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	0.99	4 (5%)
23	CLA	B	610	41	69,73,73	2.05	19 (27%)	83,113,113	2.91	30 (36%)
27	GOL	a	418	-	5,5,5	1.41	1 (20%)	5,5,5	0.82	0
35	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.60	8 (14%)
23	CLA	c	510	3	69,73,73	2.02	20 (28%)	83,113,113	2.87	32 (38%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)
23	CLA	D	403	4	69,73,73	2.10	19 (27%)	83,113,113	2.80	34 (40%)
23	CLA	b	614	2	69,73,73	2.00	20 (28%)	83,113,113	2.99	32 (38%)
31	LMT	T	101	-	36,36,36	1.09	4 (11%)	47,47,47	1.08	2 (4%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.06	2 (4%)
34	HTG	D	410	-	16,16,19	1.05	2 (12%)	20,21,24	1.48	1 (5%)
31	LMT	B	627	-	36,36,36	1.18	4 (11%)	47,47,47	1.35	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	LMT	m	103	-	36,36,36	1.08	4 (11%)	47,47,47	1.08	3 (6%)
23	CLA	a	405[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
32	LHG	d	408[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
23	CLA	c	513	3	69,73,73	2.10	21 (30%)	83,113,113	2.85	31 (37%)
25	BCR	d	406	-	41,41,41	1.14	2 (4%)	56,56,56	1.87	15 (26%)
23	CLA	a	404[B]	1	69,73,73	1.99	20 (28%)	83,113,113	2.91	34 (40%)
27	GOL	v	202[B]	-	5,5,5	1.11	0	5,5,5	0.79	0
34	HTG	B	624	-	19,19,19	1.04	2 (10%)	23,24,24	1.24	3 (13%)
23	CLA	B	613	2	69,73,73	1.98	20 (28%)	83,113,113	2.75	30 (36%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
25	BCR	c	514	-	41,41,41	1.00	1 (2%)	56,56,56	1.70	14 (25%)
38	HEM	f	101	6,5	50,50,50	1.49	6 (12%)	66,82,82	1.77	11 (16%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
26	SQD	A	410[B]	-	53,54,54	0.92	3 (5%)	62,65,65	1.80	10 (16%)
27	GOL	B	626	-	5,5,5	1.07	0	5,5,5	0.93	0
40	HEC	v	201	16	50,50,50	1.79	8 (16%)	68,82,82	1.41	7 (10%)
23	CLA	d	402[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
27	GOL	A	411	-	5,5,5	1.20	0	5,5,5	0.67	0
27	GOL	d	414	-	5,5,5	1.06	0	5,5,5	0.91	0
23	CLA	A	405[B]	41	69,73,73	1.99	20 (28%)	83,113,113	2.81	35 (42%)
31	LMT	B	628	-	36,36,36	0.97	2 (5%)	47,47,47	1.17	5 (10%)
23	CLA	C	511	3	69,73,73	2.02	20 (28%)	83,113,113	2.89	33 (39%)
24	PHO	A	407[B]	-	58,69,69	2.72	11 (18%)	56,99,99	2.78	14 (25%)
25	BCR	a	408	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	9 (16%)
26	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.53	10 (19%)
33	LMG	d	413	39	51,51,55	0.88	2 (3%)	59,59,63	1.13	5 (8%)
35	DGD	c	516[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	5 (6%)
23	CLA	d	404[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
27	GOL	O	302	-	5,5,5	0.93	0	5,5,5	0.86	0
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.11	3 (6%)
40	HEC	V	201	16	50,50,50	1.81	8 (16%)	68,82,82	1.55	11 (16%)
27	GOL	D	412	-	5,5,5	1.44	1 (20%)	5,5,5	0.86	0
23	CLA	D	402[B]	4	69,73,73	2.02	20 (28%)	83,113,113	2.90	30 (36%)
25	BCR	C	515	-	41,41,41	1.06	1 (2%)	56,56,56	1.41	6 (10%)
27	GOL	c	525[A]	-	5,5,5	0.94	0	5,5,5	0.95	0

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	2.08	21 (30%)	83,113,113	2.84	33 (39%)
23	CLA	B	612	2	69,73,73	1.98	20 (28%)	83,113,113	2.85	29 (34%)
35	DGD	C	518[B]	-	63,63,67	0.88	2 (3%)	77,77,81	1.00	5 (6%)
23	CLA	C	503	3	69,73,73	2.03	20 (28%)	83,113,113	2.70	29 (34%)
27	GOL	c	525[B]	-	5,5,5	0.81	0	5,5,5	0.99	0
23	CLA	b	607	41	69,73,73	1.98	21 (30%)	83,113,113	2.70	28 (33%)
27	GOL	B	623	-	5,5,5	0.77	0	5,5,5	1.15	1 (20%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
31	LMT	b	621	-	25,25,36	0.96	2 (8%)	30,30,47	1.19	3 (10%)
32	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
23	CLA	c	505	3	69,73,73	2.04	19 (27%)	83,113,113	2.84	28 (33%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
27	GOL	V	203[B]	-	5,5,5	1.02	0	5,5,5	0.92	0
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
32	LHG	L	101[B]	-	48,48,48	0.92	3 (6%)	51,54,54	1.03	2 (3%)
23	CLA	c	506	3	69,73,73	2.00	20 (28%)	83,113,113	2.79	31 (37%)
23	CLA	c	511	3	69,73,73	2.07	20 (28%)	83,113,113	2.82	32 (38%)
23	CLA	A	404[B]	1	69,73,73	2.07	21 (30%)	83,113,113	2.85	30 (36%)
31	LMT	C	525	-	36,36,36	1.06	2 (5%)	47,47,47	1.16	4 (8%)
33	LMG	D	411	39	51,51,55	0.81	2 (3%)	59,59,63	1.07	4 (6%)
23	CLA	B	611	2	69,73,73	2.53	20 (28%)	83,113,113	4.03	33 (39%)
23	CLA	b	615	2	69,73,73	1.98	18 (26%)	83,113,113	2.85	30 (36%)
37	BCT	D	401[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	B	604	2	69,73,73	1.99	22 (31%)	83,113,113	2.70	30 (36%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	25 (36%)
23	CLA	b	605	2	69,73,73	1.95	20 (28%)	83,113,113	3.03	28 (33%)
27	GOL	o	303	-	5,5,5	1.02	1 (20%)	5,5,5	1.11	0
28	OEX	A	413[B]	3,41,1	0,14,14	-	-	-		
33	LMG	C	521	-	51,51,55	1.06	3 (5%)	59,59,63	1.35	7 (11%)
23	CLA	B	615	2	69,73,73	2.05	18 (26%)	83,113,113	2.86	30 (36%)
27	GOL	l	103[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
37	BCT	D	401[B]	21	2,3,3	0.61	0	2,3,3	1.25	0
29	PL9	d	407[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
23	CLA	B	606	2	69,73,73	1.96	18 (26%)	83,113,113	3.00	30 (36%)
35	DGD	c	516[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
34	HTG	B	622	-	19,19,19	0.77	1 (5%)	23,24,24	1.48	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	A	418	-	5,5,5	1.53	2 (40%)	5,5,5	1.10	1 (20%)
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
35	DGD	c	517[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
23	CLA	B	602	2	69,73,73	2.02	20 (28%)	83,113,113	2.87	31 (37%)
23	CLA	B	608	2	69,73,73	1.96	21 (30%)	83,113,113	2.82	34 (40%)
31	LMT	B	629	-	25,25,36	0.88	2 (8%)	30,30,47	1.19	3 (10%)
23	CLA	b	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.82	30 (36%)
27	GOL	l	103[B]	-	5,5,5	0.91	0	5,5,5	0.97	0
32	LHG	a	419[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
29	PL9	d	407[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.62	17 (25%)
23	CLA	D	402[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	a	407	1	69,73,73	1.99	19 (27%)	83,113,113	2.91	30 (36%)
23	CLA	b	606	2	69,73,73	1.98	19 (27%)	83,113,113	2.89	31 (37%)
31	LMT	a	416	-	36,36,36	1.01	2 (5%)	47,47,47	1.04	1 (2%)
25	BCR	Y	101	-	41,41,41	0.96	1 (2%)	56,56,56	1.78	14 (25%)
31	LMT	t	101	-	26,26,36	0.91	2 (7%)	31,31,47	1.26	1 (3%)
35	DGD	H	102	-	63,63,67	0.89	4 (6%)	77,77,81	1.05	5 (6%)
32	LHG	a	419[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.93	2 (4%)
35	DGD	c	517[B]	-	63,63,67	0.87	2 (3%)	77,77,81	0.92	4 (5%)
25	BCR	H	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.53	11 (19%)
23	CLA	B	607	41	69,73,73	1.93	19 (27%)	83,113,113	2.84	28 (33%)
23	CLA	c	507	41	69,73,73	2.03	19 (27%)	83,113,113	2.86	29 (34%)
35	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
32	LHG	d	415[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.08	5 (9%)
33	LMG	Z	101	-	37,37,55	1.00	2 (5%)	45,45,63	1.43	6 (13%)
27	GOL	c	526	-	5,5,5	1.10	0	5,5,5	0.99	0
23	CLA	b	601	41	69,73,73	2.10	20 (28%)	83,113,113	2.78	29 (34%)
26	SQD	A	412	-	53,54,54	1.03	3 (5%)	62,65,65	1.24	9 (14%)
23	CLA	C	505	41	69,73,73	1.98	20 (28%)	83,113,113	2.76	29 (34%)
33	LMG	a	415	-	51,51,55	0.92	2 (3%)	59,59,63	1.21	4 (6%)
34	HTG	V	202	-	11,11,19	0.31	0	15,15,24	1.07	1 (6%)
23	CLA	A	408	1	69,73,73	1.94	19 (27%)	83,113,113	2.94	35 (42%)
23	CLA	b	616	2	69,73,73	2.01	20 (28%)	83,113,113	3.00	32 (38%)
26	SQD	a	409[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
34	HTG	B	621	-	19,19,19	1.09	2 (10%)	23,24,24	1.63	4 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HTG	c	521	-	19,19,19	0.94	1 (5%)	23,24,24	1.54	2 (8%)
23	CLA	A	406[B]	41	69,73,73	2.05	18 (26%)	83,113,113	2.85	31 (37%)
34	HTG	b	623	-	19,19,19	1.05	1 (5%)	23,24,24	1.94	2 (8%)
23	CLA	C	507	3	69,73,73	2.04	21 (30%)	83,113,113	2.82	33 (39%)
26	SQD	a	409[B]	-	53,54,54	0.98	3 (5%)	62,65,65	1.63	12 (19%)

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
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	C	514	3	-	6/39/115/115	-
23	CLA	c	503	3	-	3/39/115/115	-
23	CLA	c	509	3	-	14/39/115/115	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
33	LMG	c	519	-	-	12/46/66/70	0/1/1/1
23	CLA	C	510	3	-	5/39/115/115	-
26	SQD	X	101	-	-	15/38/58/69	0/1/1/1
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	GOL	a	417	-	-	2/4/4/4	-
23	CLA	c	512	3	-	12/39/115/115	-
24	PHO	A	416[B]	-	-	1/37/103/103	0/5/6/6
23	CLA	B	605	2	-	8/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
32	LHG	b	629[A]	-	-	20/53/53/53	-
35	DGD	c	518	-	-	12/51/91/95	0/2/2/2
25	BCR	h	101	-	-	0/29/63/63	0/2/2/2
32	LHG	A	419[A]	-	-	10/53/53/53	-
32	LHG	D	406[B]	-	-	16/53/53/53	-
23	CLA	c	501	3	-	6/39/115/115	-
33	LMG	m	101	-	-	9/46/66/70	0/1/1/1
38	HEM	E	102	6,5	-	6/14/54/54	-
23	CLA	b	608	2	-	4/39/115/115	-
32	LHG	b	629[B]	-	-	18/53/53/53	-
32	LHG	A	419[B]	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	C	502	3	-	5/39/115/115	-
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
26	SQD	a	411	-	-	12/49/69/69	0/1/1/1
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
23	CLA	C	513	3	-	12/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
32	LHG	d	415[A]	-	-	13/53/53/53	-
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1
23	CLA	b	602	2	-	4/39/115/115	-
23	CLA	b	609	2	-	1/39/115/115	-
23	CLA	d	405	4	-	8/39/115/115	-
23	CLA	A	406[A]	41	-	7/39/115/115	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
33	LMG	c	520	-	-	8/46/66/70	0/1/1/1
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	B	603	2	-	7/39/115/115	-
29	PL9	a	413[A]	-	-	14/53/73/73	0/1/1/1
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
27	GOL	C	523[B]	-	-	0/4/4/4	-
23	CLA	c	508	3	-	4/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
23	CLA	b	604	2	-	10/39/115/115	-
32	LHG	D	407[A]	-	-	14/53/53/53	-
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	b	610	41	-	5/39/115/115	-
24	PHO	a	406[B]	-	-	5/37/103/103	0/5/6/6
25	BCR	D	404	-	-	4/29/63/63	0/2/2/2
29	PL9	a	413[B]	-	-	14/53/73/73	0/1/1/1
34	HTG	d	412	-	-	1/7/27/30	0/1/1/1
23	CLA	C	508	41	-	6/39/115/115	-
23	CLA	C	509	3	-	6/39/115/115	-
23	CLA	B	616	2	-	6/39/115/115	-
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	d	408[B]	-	-	13/53/53/53	-
23	CLA	a	405[B]	41	-	5/39/115/115	-
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
32	LHG	D	407[B]	-	-	12/53/53/53	-
23	CLA	C	504	3	-	2/39/115/115	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
32	LHG	d	409[A]	-	-	11/53/53/53	-
31	LMT	e	101	-	-	14/21/61/61	0/2/2/2
23	CLA	B	609	2	-	1/39/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-
32	LHG	D	406[A]	-	-	16/53/53/53	-
23	CLA	B	614	2	-	15/39/115/115	-
25	BCR	T	102	-	-	1/29/63/63	0/2/2/2
23	CLA	b	613	2	-	4/39/115/115	-
23	CLA	b	611	2	-	3/39/115/115	-
26	SQD	l	101	-	-	13/49/69/69	0/1/1/1
23	CLA	d	402[B]	41	-	4/39/115/115	-
32	LHG	d	409[B]	-	-	13/53/53/53	-
27	GOL	b	628	-	-	0/4/4/4	-
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
23	CLA	B	601	41	-	11/39/115/115	-
23	CLA	b	603	2	-	5/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
25	BCR	t	102	-	-	1/29/63/63	0/2/2/2
23	CLA	c	502	3	-	6/39/115/115	-
23	CLA	d	404[B]	4	-	4/39/115/115	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
31	LMT	A	417	-	-	8/21/61/61	0/2/2/2
25	BCR	K	102	-	-	3/29/63/63	0/2/2/2
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
33	LMG	C	501	-	-	14/46/66/70	0/1/1/1
24	PHO	d	403[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	C	512	3	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
33	LMG	B	620	-	-	17/46/66/70	0/1/1/1
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	C	506	3	-	4/39/115/115	-
27	GOL	a	410	-	-	4/4/4/4	-
24	PHO	d	403[B]	-	-	3/37/103/103	0/5/6/6
35	DGD	C	519	-	-	15/51/91/95	0/2/2/2
23	CLA	B	610	41	-	9/39/115/115	-
27	GOL	a	418	-	-	0/4/4/4	-
35	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	c	510	3	-	12/39/115/115	-
23	CLA	a	404[A]	1	-	3/39/115/115	-
23	CLA	D	403	4	-	15/39/115/115	-
23	CLA	b	614	2	-	14/39/115/115	-
31	LMT	T	101	-	-	9/21/61/61	0/2/2/2
27	GOL	v	202[A]	-	-	1/4/4/4	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
31	LMT	B	627	-	-	11/21/61/61	0/2/2/2
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2
23	CLA	a	405[A]	41	-	7/39/115/115	-
32	LHG	d	408[A]	-	-	13/53/53/53	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
23	CLA	c	513	3	-	7/39/115/115	-
25	BCR	d	406	-	-	5/29/63/63	0/2/2/2
23	CLA	a	404[B]	1	-	3/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
34	HTG	B	624	-	-	3/10/30/30	0/1/1/1
23	CLA	B	613	2	-	8/39/115/115	-
23	CLA	A	405[A]	41	-	4/39/115/115	-
25	BCR	c	514	-	-	1/29/63/63	0/2/2/2
38	HEM	f	101	6,5	-	8/14/54/54	-
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	B	626	-	-	3/4/4/4	-
40	HEC	v	201	16	1/1/3/7	5/14/54/54	-
23	CLA	d	402[A]	41	-	8/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
27	GOL	d	414	-	-	4/4/4/4	-
23	CLA	A	405[B]	41	-	5/39/115/115	-
31	LMT	B	628	-	-	11/21/61/61	0/2/2/2
23	CLA	C	511	3	-	13/39/115/115	-
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
33	LMG	d	413	39	-	9/46/66/70	0/1/1/1
35	DGD	c	516[B]	-	-	19/51/91/95	0/2/2/2
23	CLA	d	404[A]	4	-	2/39/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
32	LHG	E	101[B]	-	-	20/46/46/53	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
27	GOL	D	412	-	-	4/4/4/4	-
23	CLA	D	402[B]	4	-	2/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
27	GOL	c	525[A]	-	-	0/4/4/4	-
23	CLA	c	504	41	-	7/39/115/115	-
23	CLA	B	612	2	-	5/39/115/115	-
35	DGD	C	518[B]	-	-	16/51/91/95	0/2/2/2
23	CLA	C	503	3	-	9/39/115/115	-
27	GOL	c	525[B]	-	-	0/4/4/4	-
23	CLA	b	607	41	-	4/39/115/115	-
27	GOL	B	623	-	-	4/4/4/4	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
32	LHG	L	101[A]	-	-	19/53/53/53	-
23	CLA	c	505	3	-	7/39/115/115	-
23	CLA	A	404[A]	1	-	5/39/115/115	-
27	GOL	V	203[B]	-	-	2/4/4/4	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	L	101[B]	-	-	19/53/53/53	-
23	CLA	c	506	3	-	9/39/115/115	-
23	CLA	c	511	3	-	7/39/115/115	-
23	CLA	A	404[B]	1	-	2/39/115/115	-
31	LMT	C	525	-	-	15/21/61/61	0/2/2/2
33	LMG	D	411	39	-	10/46/66/70	0/1/1/1
23	CLA	B	611	2	-	2/39/115/115	-
23	CLA	b	615	2	-	8/39/115/115	-
23	CLA	B	604	2	-	2/39/115/115	-
29	PL9	A	414[B]	-	-	17/53/73/73	0/1/1/1
23	CLA	b	605	2	-	7/39/115/115	-
27	GOL	o	303	-	-	2/4/4/4	-
33	LMG	C	521	-	-	14/46/66/70	0/1/1/1
23	CLA	B	615	2	-	8/39/115/115	-
27	GOL	l	103[A]	-	-	2/4/4/4	-
29	PL9	d	407[A]	-	-	6/53/73/73	0/1/1/1
23	CLA	B	606	2	-	9/39/115/115	-
35	DGD	c	516[A]	-	-	20/51/91/95	0/2/2/2
34	HTG	B	622	-	-	2/10/30/30	0/1/1/1
27	GOL	A	418	-	-	2/4/4/4	-
32	LHG	E	101[A]	-	-	22/46/46/53	-
35	DGD	c	517[A]	-	-	17/51/91/95	0/2/2/2
23	CLA	B	602	2	-	11/39/115/115	-
23	CLA	B	608	2	-	3/39/115/115	-
31	LMT	B	629	-	-	11/17/37/61	0/1/1/2
23	CLA	b	612	2	-	4/39/115/115	-
27	GOL	l	103[B]	-	-	3/4/4/4	-
32	LHG	a	419[A]	-	-	16/46/46/53	-
29	PL9	d	407[B]	-	-	6/53/73/73	0/1/1/1
23	CLA	D	402[A]	4	-	0/39/115/115	-
23	CLA	a	407	1	-	9/39/115/115	-
23	CLA	b	606	2	-	13/39/115/115	-
31	LMT	a	416	-	-	11/21/61/61	0/2/2/2
25	BCR	Y	101	-	-	5/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
35	DGD	H	102	-	-	7/51/91/95	0/2/2/2
32	LHG	a	419[B]	-	-	16/46/46/53	-
35	DGD	c	517[B]	-	-	17/51/91/95	0/2/2/2
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
23	CLA	B	607	41	-	2/39/115/115	-
23	CLA	c	507	41	-	9/39/115/115	-
35	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
32	LHG	d	415[B]	-	-	11/53/53/53	-
33	LMG	Z	101	-	-	9/31/51/70	0/1/1/1
27	GOL	c	526	-	-	3/4/4/4	-
23	CLA	b	601	41	-	18/39/115/115	-
26	SQD	A	412	-	-	15/49/69/69	0/1/1/1
23	CLA	C	505	41	-	9/39/115/115	-
33	LMG	a	415	-	-	12/46/66/70	0/1/1/1
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
23	CLA	A	408	1	-	9/39/115/115	-
23	CLA	b	616	2	-	10/39/115/115	-
26	SQD	a	409[A]	-	-	10/49/69/69	0/1/1/1
34	HTG	B	621	-	-	3/10/30/30	0/1/1/1
34	HTG	c	521	-	-	2/10/30/30	0/1/1/1
23	CLA	A	406[B]	41	-	8/39/115/115	-
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
23	CLA	C	507	3	-	12/39/115/115	-
26	SQD	a	409[B]	-	-	11/49/69/69	0/1/1/1

All (1885) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	406[B]	PHO	C1B-C2B	9.10	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	9.04	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	8.96	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	8.88	1.49	1.39
24	d	403[B]	PHO	C1D-C2D	8.80	1.49	1.39
24	d	403[A]	PHO	C1B-C2B	8.77	1.49	1.39
24	d	403[B]	PHO	C1B-C2B	8.71	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	416[A]	PHO	C1D-C2D	8.71	1.49	1.39
24	d	403[A]	PHO	C1D-C2D	8.58	1.49	1.39
24	A	416[B]	PHO	C1D-C2D	8.51	1.49	1.39
24	a	406[A]	PHO	C1D-C2D	8.45	1.48	1.39
24	a	406[B]	PHO	C1D-C2D	8.43	1.48	1.39
24	A	407[A]	PHO	C1B-C2B	8.30	1.48	1.39
24	A	416[A]	PHO	C1B-C2B	8.26	1.48	1.39
24	A	416[B]	PHO	C1B-C2B	8.12	1.48	1.39
40	v	201	HEC	C3D-C2D	8.03	1.53	1.36
40	V	201	HEC	C3D-C2D	7.27	1.52	1.36
24	d	403[A]	PHO	C3B-C4B	7.11	1.49	1.41
23	B	611	CLA	CMB-C2B	7.01	1.65	1.50
24	A	416[B]	PHO	C3B-C4B	6.88	1.49	1.41
24	d	403[B]	PHO	C3B-C4B	6.87	1.49	1.41
23	B	611	CLA	C1D-ND	6.87	1.46	1.37
24	A	416[A]	PHO	C3B-C4B	6.61	1.49	1.41
24	a	406[B]	PHO	C3B-C4B	6.60	1.49	1.41
23	B	611	CLA	C1B-C2B	6.58	1.58	1.43
24	a	406[A]	PHO	C3B-C4B	6.52	1.49	1.41
24	A	407[A]	PHO	C3B-C4B	6.43	1.48	1.41
24	A	416[B]	PHO	C4D-CHA	6.42	1.49	1.39
24	A	407[B]	PHO	C4D-CHA	6.39	1.49	1.39
24	a	406[B]	PHO	C4D-CHA	6.38	1.49	1.39
40	V	201	HEC	FE-ND	6.36	2.14	1.94
24	a	406[A]	PHO	C3B-C2B	6.36	1.49	1.40
24	A	416[A]	PHO	C4D-CHA	6.36	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.35	1.49	1.39
24	a	406[A]	PHO	C4D-CHA	6.34	1.49	1.39
24	d	403[B]	PHO	C3B-C2B	6.32	1.49	1.40
24	a	406[B]	PHO	C3B-C2B	6.25	1.49	1.40
24	A	416[B]	PHO	C3B-C2B	6.22	1.49	1.40
24	d	403[B]	PHO	C4D-CHA	6.21	1.49	1.39
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
24	A	407[B]	PHO	C3B-C2B	6.12	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	6.12	1.48	1.40
24	d	403[A]	PHO	C4D-CHA	6.09	1.49	1.39
24	A	416[A]	PHO	C3C-C2C	6.07	1.49	1.36
24	A	407[B]	PHO	C3C-C2C	6.04	1.49	1.36
24	A	407[B]	PHO	C3B-C4B	6.01	1.48	1.41
24	d	403[A]	PHO	C3C-C2C	5.98	1.49	1.36
24	d	403[A]	PHO	C3B-C2B	5.90	1.48	1.40
24	d	403[B]	PHO	C3C-C2C	5.83	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	416[B]	PHO	C3C-C2C	5.76	1.49	1.36
23	c	508	CLA	C3C-C2C	5.69	1.48	1.36
23	C	511	CLA	C1D-ND	5.69	1.44	1.37
24	a	406[B]	PHO	C3D-C2D	5.66	1.49	1.39
23	B	611	CLA	CHC-C1C	5.65	1.50	1.38
23	d	402[B]	CLA	C3C-C2C	5.64	1.48	1.36
23	C	504	CLA	C3C-C2C	5.60	1.48	1.36
24	a	406[B]	PHO	C3C-C2C	5.60	1.48	1.36
23	B	610	CLA	C3C-C2C	5.60	1.48	1.36
23	d	405	CLA	C3C-C2C	5.58	1.48	1.36
24	A	407[A]	PHO	C3C-C2C	5.58	1.48	1.36
23	A	404[B]	CLA	C1D-ND	5.57	1.44	1.37
23	c	505	CLA	C3C-C2C	5.55	1.48	1.36
23	c	511	CLA	C1D-ND	5.51	1.44	1.37
23	b	605	CLA	C3C-C2C	5.50	1.48	1.36
24	a	406[A]	PHO	C3C-C2C	5.49	1.48	1.36
23	b	601	CLA	C1D-ND	5.49	1.44	1.37
23	D	403	CLA	C3C-C2C	5.49	1.48	1.36
23	C	513	CLA	C3C-C2C	5.48	1.48	1.36
23	C	509	CLA	C3C-C2C	5.48	1.48	1.36
23	b	610	CLA	C3C-C2C	5.47	1.48	1.36
23	c	509	CLA	C3C-C2C	5.46	1.48	1.36
23	c	512	CLA	C3C-C2C	5.45	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
23	d	402[B]	CLA	C1D-ND	5.44	1.44	1.37
23	c	513	CLA	C1D-ND	5.44	1.44	1.37
24	a	406[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	c	503	CLA	C3C-C2C	5.39	1.48	1.36
23	b	612	CLA	C3C-C2C	5.39	1.48	1.36
23	C	509	CLA	C1D-ND	5.39	1.44	1.37
23	D	403	CLA	C1D-ND	5.38	1.44	1.37
23	B	605	CLA	C3C-C2C	5.37	1.48	1.36
23	c	504	CLA	C1D-ND	5.36	1.44	1.37
23	B	611	CLA	C3C-C2C	5.36	1.48	1.36
23	d	402[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	b	609	CLA	O2D-CGD	5.35	1.46	1.33
23	c	509	CLA	O2D-CGD	5.34	1.46	1.33
23	a	405[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	C	503	CLA	C1D-ND	5.33	1.44	1.37
23	C	514	CLA	C1D-ND	5.33	1.44	1.37
23	b	601	CLA	C3C-C2C	5.32	1.48	1.36
23	b	615	CLA	C3C-C2C	5.32	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.31	1.48	1.36
23	b	614	CLA	C3C-C2C	5.30	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.30	1.48	1.36
23	c	504	CLA	O2D-CGD	5.30	1.46	1.33
23	b	603	CLA	C3C-C2C	5.28	1.48	1.36
23	c	503	CLA	C1D-ND	5.28	1.44	1.37
24	d	403[A]	PHO	C3D-C2D	5.28	1.48	1.39
23	c	508	CLA	C1D-ND	5.27	1.44	1.37
23	A	408	CLA	C3C-C2C	5.26	1.47	1.36
23	a	405[B]	CLA	C3C-C2C	5.26	1.47	1.36
23	B	604	CLA	C3C-C2C	5.26	1.47	1.36
24	A	416[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	B	614	CLA	C1D-ND	5.24	1.44	1.37
23	C	505	CLA	C3C-C2C	5.24	1.47	1.36
23	B	608	CLA	C3C-C2C	5.23	1.47	1.36
23	B	603	CLA	C3C-C2C	5.23	1.47	1.36
23	d	404[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	D	402[B]	CLA	O2D-CGD	5.22	1.45	1.33
23	c	508	CLA	O2D-CGD	5.22	1.45	1.33
23	C	503	CLA	C3C-C2C	5.22	1.47	1.36
23	C	508	CLA	C3C-C2C	5.22	1.47	1.36
23	D	402[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	B	601	CLA	C3C-C2C	5.22	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	B	601	CLA	C1D-ND	5.21	1.44	1.37
23	b	602	CLA	C3C-C2C	5.20	1.47	1.36
23	B	606	CLA	C3C-C2C	5.20	1.47	1.36
23	B	616	CLA	C3C-C2C	5.19	1.47	1.36
23	d	404[B]	CLA	C3C-C2C	5.19	1.47	1.36
23	c	513	CLA	C3C-C2C	5.19	1.47	1.36
23	c	510	CLA	O2D-CGD	5.18	1.45	1.33
23	c	501	CLA	C1D-ND	5.18	1.44	1.37
23	d	402[B]	CLA	O2D-CGD	5.18	1.45	1.33
25	C	515	BCR	C23-C22	-5.18	1.34	1.45
23	C	510	CLA	C3C-C2C	5.17	1.47	1.36
23	C	511	CLA	C3C-C2C	5.17	1.47	1.36
23	D	402[B]	CLA	C3C-C2C	5.17	1.47	1.36
23	A	405[B]	CLA	C1D-ND	5.17	1.44	1.37
23	d	405	CLA	C1D-ND	5.16	1.44	1.37
23	d	402[A]	CLA	C1D-ND	5.16	1.44	1.37
23	C	509	CLA	O2D-CGD	5.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1D-ND	5.15	1.44	1.37
25	d	406	BCR	C23-C22	-5.15	1.34	1.45
23	c	507	CLA	C3C-C2C	5.15	1.47	1.36
24	A	416[B]	PHO	C3D-C2D	5.15	1.48	1.39
24	d	403[B]	PHO	C3D-C2D	5.15	1.48	1.39
23	b	616	CLA	C1D-ND	5.15	1.44	1.37
23	b	602	CLA	O2D-CGD	5.15	1.45	1.33
23	b	607	CLA	C3C-C2C	5.14	1.47	1.36
23	c	501	CLA	C3C-C2C	5.14	1.47	1.36
23	b	605	CLA	O2D-CGD	5.13	1.45	1.33
23	b	606	CLA	C3C-C2C	5.13	1.47	1.36
23	B	613	CLA	O2D-CGD	5.12	1.45	1.33
23	B	602	CLA	C3C-C2C	5.12	1.47	1.36
23	C	513	CLA	C1D-ND	5.12	1.44	1.37
23	B	614	CLA	C3C-C2C	5.11	1.47	1.36
23	C	512	CLA	O2D-CGD	5.11	1.45	1.33
24	d	403[B]	PHO	O2D-CGD	5.10	1.45	1.33
23	A	406[B]	CLA	C1D-ND	5.10	1.44	1.37
25	k	101	BCR	C23-C22	-5.10	1.35	1.45
23	B	601	CLA	O2A-CGA	5.10	1.48	1.33
23	c	510	CLA	C3C-C2C	5.10	1.47	1.36
23	c	506	CLA	C1D-ND	5.10	1.44	1.37
24	a	406[B]	PHO	O2D-CGD	5.09	1.45	1.33
23	B	615	CLA	C3C-C2C	5.09	1.47	1.36
23	C	510	CLA	C1D-ND	5.08	1.44	1.37
23	A	406[B]	CLA	O2D-CGD	5.08	1.45	1.33
23	C	507	CLA	O2D-CGD	5.08	1.45	1.33
23	c	511	CLA	C3C-C2C	5.07	1.47	1.36
24	A	416[B]	PHO	O2D-CGD	5.06	1.45	1.33
23	c	509	CLA	C1D-ND	5.06	1.44	1.37
23	c	502	CLA	C3C-C2C	5.06	1.47	1.36
23	B	601	CLA	O2D-CGD	5.06	1.45	1.33
23	B	609	CLA	C3C-C2C	5.06	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
23	b	603	CLA	O2D-CGD	5.05	1.45	1.33
23	B	605	CLA	C1D-ND	5.05	1.44	1.37
23	a	407	CLA	CHC-C1C	5.05	1.48	1.38
23	B	613	CLA	C1D-ND	5.04	1.44	1.37
23	B	615	CLA	C1D-ND	5.03	1.44	1.37
24	a	406[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	b	616	CLA	C3C-C2C	5.03	1.47	1.36
23	c	505	CLA	CHC-C1C	5.03	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHC-C1C	5.03	1.48	1.38
23	a	407	CLA	C3C-C2C	5.03	1.47	1.36
23	C	503	CLA	O2D-CGD	5.02	1.45	1.33
23	C	514	CLA	C3C-C2C	5.00	1.47	1.36
23	B	615	CLA	O2D-CGD	4.99	1.45	1.33
23	C	502	CLA	C3C-C2C	4.99	1.47	1.36
23	C	506	CLA	C3C-C2C	4.99	1.47	1.36
23	c	513	CLA	O2D-CGD	4.98	1.45	1.33
23	b	602	CLA	CHC-C1C	4.98	1.48	1.38
24	A	416[B]	PHO	OBD-CAD	4.98	1.29	1.22
23	d	402[A]	CLA	O2D-CGD	4.98	1.45	1.33
25	B	617	BCR	C23-C22	-4.97	1.35	1.45
23	b	602	CLA	C1D-ND	4.97	1.43	1.37
38	f	101	HEM	FE-NB	4.97	2.10	1.94
23	B	612	CLA	C3C-C2C	4.96	1.47	1.36
23	c	504	CLA	C3C-C2C	4.96	1.47	1.36
23	C	502	CLA	C1D-ND	4.96	1.43	1.37
23	b	604	CLA	C1D-ND	4.96	1.43	1.37
24	d	403[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	c	512	CLA	O2D-CGD	4.95	1.45	1.33
24	A	407[B]	PHO	C3D-C2D	4.95	1.48	1.39
23	c	512	CLA	C1D-ND	4.95	1.43	1.37
23	C	507	CLA	C3C-C2C	4.95	1.47	1.36
25	B	619	BCR	C23-C22	-4.94	1.35	1.45
23	C	502	CLA	CHC-C1C	4.94	1.48	1.38
23	A	405[B]	CLA	O2D-CGD	4.94	1.45	1.33
23	c	510	CLA	C1D-ND	4.94	1.43	1.37
23	c	506	CLA	O2D-CGD	4.93	1.45	1.33
23	a	405[B]	CLA	C1D-ND	4.93	1.43	1.37
23	b	613	CLA	CHC-C1C	4.93	1.48	1.38
23	c	506	CLA	C3C-C2C	4.93	1.47	1.36
23	B	609	CLA	O2D-CGD	4.93	1.45	1.33
24	A	416[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	b	611	CLA	C3C-C2C	4.90	1.47	1.36
23	C	506	CLA	CHC-C1C	4.90	1.48	1.38
24	A	407[A]	PHO	O2D-CGD	4.90	1.45	1.33
23	A	406[A]	CLA	O2D-CGD	4.90	1.45	1.33
23	B	607	CLA	C3C-C2C	4.90	1.47	1.36
23	B	616	CLA	CHC-C1C	4.90	1.48	1.38
23	b	610	CLA	CHC-C1C	4.89	1.48	1.38
23	C	510	CLA	O2D-CGD	4.89	1.45	1.33
23	c	502	CLA	C1D-ND	4.89	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	O2D-CGD	4.89	1.45	1.33
23	b	608	CLA	C3C-C2C	4.88	1.47	1.36
38	E	102	HEM	FE-NB	4.88	2.10	1.94
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
23	C	512	CLA	C3C-C2C	4.88	1.47	1.36
23	B	602	CLA	C1D-ND	4.88	1.43	1.37
23	c	511	CLA	O2D-CGD	4.88	1.45	1.33
25	K	102	BCR	C23-C22	-4.87	1.35	1.45
23	B	613	CLA	CHC-C1C	4.87	1.48	1.38
23	c	503	CLA	CHC-C1C	4.87	1.48	1.38
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	C	511	CLA	O2D-CGD	4.86	1.45	1.33
23	C	514	CLA	O2D-CGD	4.86	1.45	1.33
23	b	601	CLA	O2D-CGD	4.86	1.45	1.33
24	A	407[B]	PHO	O2D-CGD	4.85	1.45	1.33
23	C	504	CLA	CHC-C1C	4.85	1.48	1.38
26	X	101	SQD	O47-C7	4.85	1.48	1.34
23	C	504	CLA	C1D-ND	4.84	1.43	1.37
23	B	604	CLA	O2D-CGD	4.84	1.45	1.33
23	b	601	CLA	O2A-CGA	4.84	1.47	1.33
23	b	614	CLA	CHC-C1C	4.84	1.48	1.38
25	D	404	BCR	C23-C22	-4.84	1.35	1.45
24	d	403[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	b	605	CLA	C1D-ND	4.84	1.43	1.37
23	b	613	CLA	C3C-C2C	4.83	1.47	1.36
23	B	611	CLA	CHC-C4B	4.83	1.50	1.39
23	b	616	CLA	CHC-C1C	4.83	1.48	1.38
23	a	405[B]	CLA	O2D-CGD	4.83	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	4.83	1.45	1.33
23	A	405[B]	CLA	C3C-C2C	4.83	1.47	1.36
23	B	610	CLA	C1D-ND	4.83	1.43	1.37
23	C	508	CLA	CHC-C1C	4.82	1.48	1.38
23	c	507	CLA	O2D-CGD	4.82	1.45	1.33
25	T	102	BCR	C23-C22	-4.82	1.35	1.45
23	B	606	CLA	C1D-ND	4.80	1.43	1.37
23	D	402[A]	CLA	O2D-CGD	4.80	1.44	1.33
23	a	405[B]	CLA	CHC-C1C	4.80	1.48	1.38
23	c	512	CLA	CHC-C1C	4.79	1.48	1.38
23	b	604	CLA	C3C-C2C	4.79	1.46	1.36
24	d	403[B]	PHO	OBD-CAD	4.79	1.29	1.22
23	b	616	CLA	O2D-CGD	4.78	1.44	1.33
25	b	619	BCR	C23-C22	-4.78	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404[B]	CLA	O2D-CGD	4.77	1.44	1.33
25	c	514	BCR	C23-C22	-4.77	1.35	1.45
23	B	604	CLA	CHC-C1C	4.76	1.48	1.38
23	C	508	CLA	C1D-ND	4.76	1.43	1.37
23	b	609	CLA	CHC-C1C	4.76	1.48	1.38
23	b	615	CLA	O2D-CGD	4.76	1.44	1.33
23	B	602	CLA	CHC-C1C	4.76	1.48	1.38
23	b	614	CLA	O2D-CGD	4.75	1.44	1.33
23	C	506	CLA	C1D-ND	4.75	1.43	1.37
23	B	609	CLA	CHC-C1C	4.75	1.48	1.38
23	b	610	CLA	O2D-CGD	4.75	1.44	1.33
23	B	606	CLA	CHC-C1C	4.74	1.48	1.38
23	B	605	CLA	O2D-CGD	4.74	1.44	1.33
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	b	615	CLA	C1D-ND	4.72	1.43	1.37
23	c	502	CLA	O2D-CGD	4.72	1.44	1.33
25	b	617	BCR	C23-C22	-4.72	1.35	1.45
23	b	609	CLA	C3C-C2C	4.72	1.46	1.36
23	A	406[A]	CLA	CHC-C1C	4.72	1.48	1.38
23	b	606	CLA	C1D-ND	4.71	1.43	1.37
23	D	403	CLA	O2D-CGD	4.71	1.44	1.33
23	a	404[B]	CLA	C1D-ND	4.71	1.43	1.37
23	d	405	CLA	CHC-C1C	4.70	1.48	1.38
25	A	409	BCR	C23-C22	-4.70	1.35	1.45
23	D	403	CLA	CHD-C1D	4.70	1.47	1.38
23	b	611	CLA	O2D-CGD	4.69	1.44	1.33
33	c	520	LMG	O7-C10	4.69	1.47	1.34
23	b	606	CLA	CHC-C1C	4.69	1.48	1.38
23	b	609	CLA	C1D-ND	4.69	1.43	1.37
23	C	507	CLA	C1D-ND	4.69	1.43	1.37
25	C	516	BCR	C23-C22	-4.68	1.35	1.45
23	C	505	CLA	O2D-CGD	4.68	1.44	1.33
23	C	506	CLA	O2D-CGD	4.67	1.44	1.33
23	d	404[A]	CLA	O2D-CGD	4.66	1.44	1.33
23	C	513	CLA	O2D-CGD	4.66	1.44	1.33
23	B	602	CLA	O2D-CGD	4.66	1.44	1.33
23	D	403	CLA	CHC-C1C	4.66	1.48	1.38
23	b	611	CLA	C1D-ND	4.66	1.43	1.37
24	A	407[B]	PHO	OBD-CAD	4.65	1.28	1.22
23	B	615	CLA	CHC-C1C	4.65	1.48	1.38
23	c	505	CLA	O2D-CGD	4.65	1.44	1.33
23	A	406[B]	CLA	CHC-C1C	4.64	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C1D-ND	4.64	1.43	1.37
23	B	612	CLA	C1B-NB	-4.63	1.32	1.37
23	c	507	CLA	CHC-C1C	4.63	1.47	1.38
23	c	507	CLA	C1D-ND	4.63	1.43	1.37
23	b	606	CLA	O2D-CGD	4.63	1.44	1.33
25	t	102	BCR	C23-C22	-4.63	1.36	1.45
23	b	612	CLA	O2D-CGD	4.62	1.44	1.33
23	B	611	CLA	O2D-CGD	4.62	1.44	1.33
23	c	508	CLA	CHC-C1C	4.62	1.47	1.38
23	a	404[A]	CLA	C1D-ND	4.62	1.43	1.37
23	b	608	CLA	C1D-ND	4.61	1.43	1.37
23	B	601	CLA	CHC-C1C	4.61	1.47	1.38
23	b	604	CLA	CHC-C1C	4.61	1.47	1.38
23	b	613	CLA	O2D-CGD	4.60	1.44	1.33
23	b	608	CLA	O2D-CGD	4.59	1.44	1.33
25	c	515	BCR	C23-C22	-4.59	1.36	1.45
23	b	601	CLA	CHC-C1C	4.59	1.47	1.38
23	b	615	CLA	CHC-C1C	4.58	1.47	1.38
23	a	405[A]	CLA	CHC-C1C	4.58	1.47	1.38
23	A	408	CLA	O2D-CGD	4.58	1.44	1.33
23	c	511	CLA	CHC-C1C	4.57	1.47	1.38
33	C	521	LMG	O7-C10	4.57	1.47	1.34
25	y	101	BCR	C23-C22	-4.57	1.36	1.45
23	c	503	CLA	CHD-C1D	4.57	1.47	1.38
26	a	411	SQD	O48-C23	4.57	1.46	1.33
23	B	606	CLA	O2D-CGD	4.56	1.44	1.33
23	D	402[B]	CLA	CHC-C1C	4.56	1.47	1.38
23	b	607	CLA	O2D-CGD	4.55	1.44	1.33
23	d	405	CLA	O2D-CGD	4.55	1.44	1.33
23	A	405[A]	CLA	CHC-C1C	4.55	1.47	1.38
23	B	614	CLA	O2D-CGD	4.55	1.44	1.33
23	c	513	CLA	CHC-C1C	4.54	1.47	1.38
23	B	612	CLA	CHC-C1C	4.54	1.47	1.38
23	a	404[A]	CLA	O2D-CGD	4.54	1.44	1.33
33	C	521	LMG	O8-C28	4.54	1.46	1.33
23	B	605	CLA	CHC-C1C	4.54	1.47	1.38
25	h	101	BCR	C23-C22	-4.53	1.36	1.45
23	B	610	CLA	CHC-C1C	4.53	1.47	1.38
23	b	602	CLA	CHD-C1D	4.53	1.47	1.38
23	C	511	CLA	CHC-C1C	4.53	1.47	1.38
23	B	603	CLA	O2D-CGD	4.53	1.44	1.33
23	A	408	CLA	CHC-C1C	4.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	CHC-C1C	4.52	1.47	1.38
23	B	604	CLA	CHD-C1D	4.52	1.47	1.38
23	a	407	CLA	O2A-CGA	4.52	1.46	1.33
23	a	404[B]	CLA	O2D-CGD	4.52	1.44	1.33
23	b	612	CLA	CHC-C1C	4.52	1.47	1.38
23	c	513	CLA	CHD-C1D	4.52	1.47	1.38
23	B	613	CLA	C3C-C2C	4.52	1.46	1.36
23	B	614	CLA	CHC-C1C	4.52	1.47	1.38
23	c	504	CLA	CHC-C1C	4.51	1.47	1.38
23	d	405	CLA	CHD-C1D	4.51	1.47	1.38
23	B	608	CLA	O2D-CGD	4.51	1.44	1.33
23	B	616	CLA	O2D-CGD	4.51	1.44	1.33
26	l	101	SQD	O47-C7	4.51	1.47	1.34
23	c	501	CLA	CHC-C1C	4.50	1.47	1.38
23	c	512	CLA	O2A-CGA	4.50	1.46	1.33
23	D	402[B]	CLA	C1D-ND	4.50	1.43	1.37
23	b	601	CLA	CHD-C1D	4.50	1.47	1.38
23	a	405[A]	CLA	O2D-CGD	4.50	1.44	1.33
23	C	507	CLA	CHD-C1D	4.50	1.47	1.38
23	C	508	CLA	O2D-CGD	4.49	1.44	1.33
23	B	610	CLA	O2D-CGD	4.48	1.44	1.33
23	B	607	CLA	C1B-NB	-4.48	1.32	1.37
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
26	f	102	SQD	O47-C7	4.47	1.46	1.34
33	z	101	LMG	O8-C28	4.47	1.46	1.33
24	a	406[B]	PHO	OBD-CAD	4.46	1.28	1.22
23	A	404[B]	CLA	CHC-C1C	4.45	1.47	1.38
26	A	412	SQD	O48-C23	4.45	1.46	1.33
23	C	505	CLA	C1D-ND	4.45	1.43	1.37
23	C	514	CLA	CHC-C1C	4.45	1.47	1.38
23	b	611	CLA	CHC-C1C	4.44	1.47	1.38
23	c	505	CLA	C1D-ND	4.43	1.43	1.37
23	b	603	CLA	CHC-C1C	4.43	1.47	1.38
23	C	504	CLA	O2D-CGD	4.43	1.44	1.33
23	C	510	CLA	CHD-C1D	4.42	1.47	1.38
23	b	604	CLA	O2D-CGD	4.41	1.44	1.33
23	C	505	CLA	CHC-C1C	4.41	1.47	1.38
23	B	612	CLA	CHB-C1B	4.41	1.49	1.39
23	A	405[B]	CLA	CHC-C1C	4.40	1.47	1.38
23	d	402[A]	CLA	CHC-C1C	4.40	1.47	1.38
23	B	611	CLA	C4B-NB	-4.40	1.32	1.37
23	B	608	CLA	C1D-ND	4.40	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	CHD-C1D	4.40	1.46	1.38
32	E	101[B]	LHG	O8-C23	4.40	1.46	1.33
32	a	419[A]	LHG	O8-C23	4.39	1.46	1.33
23	A	408	CLA	O2A-CGA	4.39	1.46	1.33
23	b	607	CLA	CHD-C1D	4.39	1.46	1.38
23	d	402[A]	CLA	C3D-C2D	4.38	1.51	1.39
33	B	620	LMG	O8-C28	4.38	1.46	1.33
23	B	615	CLA	CHD-C1D	4.37	1.46	1.38
23	A	404[B]	CLA	CHD-C1D	4.37	1.46	1.38
25	a	408	BCR	C23-C22	-4.37	1.36	1.45
23	b	605	CLA	CHC-C1C	4.36	1.47	1.38
23	C	509	CLA	CHC-C1C	4.36	1.47	1.38
23	b	607	CLA	C1D-ND	4.36	1.43	1.37
23	c	513	CLA	O2A-CGA	4.36	1.46	1.33
23	B	616	CLA	C1D-ND	4.36	1.43	1.37
23	B	614	CLA	C4B-NB	-4.36	1.32	1.37
23	a	404[A]	CLA	CHC-C1C	4.36	1.47	1.38
24	a	406[A]	PHO	OBD-CAD	4.36	1.28	1.22
32	a	419[B]	LHG	O8-C23	4.35	1.46	1.33
25	H	101	BCR	C23-C22	-4.35	1.36	1.45
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33
26	b	620	SQD	O47-C7	4.34	1.46	1.34
23	B	607	CLA	CHC-C1C	4.34	1.47	1.38
23	d	404[B]	CLA	CHC-C1C	4.34	1.47	1.38
23	d	405	CLA	O2A-CGA	4.34	1.46	1.33
23	B	607	CLA	O2D-CGD	4.33	1.43	1.33
23	b	613	CLA	C1D-ND	4.33	1.43	1.37
25	Y	101	BCR	C23-C22	-4.32	1.36	1.45
23	c	510	CLA	CHC-C1C	4.32	1.47	1.38
23	c	502	CLA	O2A-CGA	4.32	1.46	1.33
24	A	416[A]	PHO	OBD-CAD	4.31	1.28	1.22
26	f	102	SQD	O48-C23	4.31	1.45	1.33
23	A	404[A]	CLA	CHC-C1C	4.31	1.47	1.38
32	d	409[A]	LHG	O8-C23	4.31	1.45	1.33
23	a	404[B]	CLA	CHC-C1C	4.31	1.47	1.38
23	c	511	CLA	CHD-C1D	4.31	1.46	1.38
23	c	510	CLA	CHB-C1B	4.30	1.49	1.39
23	A	406[B]	CLA	CHD-C1D	4.29	1.46	1.38
23	b	607	CLA	CHC-C1C	4.29	1.47	1.38
23	A	404[B]	CLA	CHD-C4C	4.29	1.49	1.39
23	B	615	CLA	O2A-CGA	4.29	1.45	1.33
23	b	611	CLA	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C1D-ND	4.28	1.43	1.37
23	C	503	CLA	CHD-C1D	4.27	1.46	1.38
23	c	507	CLA	CHD-C1D	4.27	1.46	1.38
23	d	402[B]	CLA	C3D-C2D	4.27	1.50	1.39
33	C	520	LMG	O8-C28	4.27	1.45	1.33
23	c	506	CLA	CHC-C1C	4.27	1.47	1.38
26	b	620	SQD	O48-C23	4.27	1.45	1.33
23	D	402[A]	CLA	C1D-ND	4.27	1.43	1.37
23	c	507	CLA	O2A-CGA	4.27	1.45	1.33
23	D	402[B]	CLA	O2A-CGA	4.26	1.45	1.33
23	C	514	CLA	CHD-C1D	4.26	1.46	1.38
23	C	514	CLA	O2A-CGA	4.25	1.45	1.33
23	C	509	CLA	C3D-C2D	4.25	1.50	1.39
23	D	402[A]	CLA	CHC-C1C	4.25	1.47	1.38
23	C	511	CLA	CHD-C4C	4.24	1.48	1.39
38	E	102	HEM	FE-NC	4.24	2.09	1.95
23	B	609	CLA	CHD-C1D	4.24	1.46	1.38
23	c	505	CLA	CHD-C1D	4.24	1.46	1.38
33	c	520	LMG	O8-C28	4.24	1.45	1.33
25	b	618	BCR	C23-C22	-4.24	1.36	1.45
23	A	408	CLA	C1D-ND	4.24	1.43	1.37
23	c	512	CLA	CHD-C1D	4.23	1.46	1.38
23	C	513	CLA	CHD-C1D	4.23	1.46	1.38
23	b	608	CLA	CHC-C1C	4.23	1.47	1.38
23	B	609	CLA	C1D-ND	4.23	1.43	1.37
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
32	d	409[B]	LHG	O8-C23	4.22	1.45	1.33
26	a	409[B]	SQD	O47-C7	4.22	1.46	1.34
23	D	402[A]	CLA	O2A-CGA	4.22	1.45	1.33
23	d	402[B]	CLA	CHC-C1C	4.22	1.47	1.38
23	C	506	CLA	CHD-C1D	4.22	1.46	1.38
23	c	505	CLA	CHC-C4B	4.22	1.48	1.39
23	B	610	CLA	OBD-CAD	4.22	1.29	1.22
23	b	610	CLA	CHD-C1D	4.21	1.46	1.38
33	m	101	LMG	O8-C28	4.21	1.45	1.33
23	B	614	CLA	CHD-C4C	4.21	1.48	1.39
23	B	610	CLA	C1B-NB	-4.21	1.32	1.37
23	d	402[B]	CLA	O2A-CGA	4.21	1.45	1.33
33	Z	101	LMG	O7-C10	4.20	1.46	1.34
23	A	405[B]	CLA	O2A-CGA	4.20	1.45	1.33
23	c	511	CLA	CHB-C1B	4.20	1.48	1.39
23	B	615	CLA	OBD-CAD	4.20	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	O2A-CGA	4.20	1.45	1.33
35	c	518	DGD	O1G-C1A	4.19	1.45	1.33
35	c	517[B]	DGD	O1G-C1A	4.19	1.45	1.33
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	c	503	CLA	O2A-CGA	4.18	1.45	1.33
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
23	b	604	CLA	CHD-C1D	4.18	1.46	1.38
23	c	511	CLA	O2A-CGA	4.18	1.45	1.33
23	C	512	CLA	CHD-C1D	4.18	1.46	1.38
23	B	609	CLA	O2A-CGA	4.18	1.45	1.33
23	c	502	CLA	CHC-C1C	4.17	1.47	1.38
23	b	602	CLA	CHD-C4C	4.17	1.48	1.39
23	c	506	CLA	O2A-CGA	4.17	1.45	1.33
23	b	610	CLA	C1D-ND	4.16	1.42	1.37
26	A	412	SQD	O47-C7	4.16	1.46	1.34
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	C	503	CLA	CHC-C1C	4.16	1.47	1.38
23	d	404[B]	CLA	O2A-CGA	4.16	1.45	1.33
23	b	602	CLA	CHC-C4B	4.15	1.48	1.39
23	a	405[A]	CLA	C1D-ND	4.15	1.42	1.37
23	C	506	CLA	CHB-C1B	4.15	1.48	1.39
26	l	101	SQD	O48-C23	4.15	1.45	1.33
23	c	503	CLA	CHD-C4C	4.15	1.48	1.39
23	c	508	CLA	CHD-C1D	4.15	1.46	1.38
32	a	419[B]	LHG	O7-C7	4.15	1.46	1.34
23	c	502	CLA	CHD-C1D	4.15	1.46	1.38
23	C	508	CLA	O2A-CGA	4.15	1.45	1.33
23	b	608	CLA	C3D-C2D	4.15	1.50	1.39
33	c	519	LMG	O7-C10	4.15	1.46	1.34
23	b	612	CLA	C1D-ND	4.14	1.42	1.37
24	A	407[A]	PHO	OBD-CAD	4.14	1.28	1.22
23	b	609	CLA	CHD-C1D	4.14	1.46	1.38
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
25	B	618	BCR	C23-C22	-4.13	1.37	1.45
23	B	605	CLA	CHC-C4B	4.13	1.48	1.39
23	b	612	CLA	CHB-C1B	4.13	1.48	1.39
32	a	419[A]	LHG	O7-C7	4.13	1.46	1.34
23	C	502	CLA	O2D-CGD	4.13	1.43	1.33
23	b	612	CLA	CHD-C1D	4.13	1.46	1.38
23	C	508	CLA	CHD-C1D	4.13	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404[A]	CLA	CHC-C1C	4.13	1.46	1.38
23	c	501	CLA	O2D-CGD	4.13	1.43	1.33
26	X	101	SQD	O48-C23	4.13	1.45	1.33
23	B	614	CLA	CHB-C1B	4.12	1.48	1.39
23	b	601	CLA	C3D-C2D	4.12	1.50	1.39
23	B	612	CLA	O2D-CGD	4.12	1.43	1.33
23	a	405[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	B	616	CLA	CHB-C1B	4.12	1.48	1.39
23	c	509	CLA	CHC-C1C	4.12	1.46	1.38
23	d	404[A]	CLA	CHB-C1B	4.11	1.48	1.39
38	f	101	HEM	FE-NC	4.11	2.09	1.95
23	B	615	CLA	C3D-C2D	4.11	1.50	1.39
23	b	611	CLA	CHB-C1B	4.11	1.48	1.39
23	b	616	CLA	O2A-CGA	4.11	1.45	1.33
23	B	611	CLA	C3B-C2B	4.11	1.55	1.41
32	L	101[B]	LHG	O8-C23	4.10	1.45	1.33
23	d	405	CLA	C3D-C2D	4.10	1.50	1.39
33	z	101	LMG	O7-C10	4.10	1.45	1.34
23	C	504	CLA	CHD-C1D	4.10	1.46	1.38
23	C	513	CLA	O2A-CGA	4.10	1.45	1.33
23	C	503	CLA	C3D-C2D	4.10	1.50	1.39
23	b	616	CLA	CHD-C1D	4.09	1.46	1.38
35	c	516[A]	DGD	O2G-C1B	4.09	1.45	1.34
33	C	501	LMG	O8-C28	4.09	1.45	1.33
23	B	603	CLA	CHC-C1C	4.09	1.46	1.38
23	d	402[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	D	403	CLA	C3D-C2D	4.08	1.50	1.39
23	b	601	CLA	CHD-C4C	4.08	1.48	1.39
23	C	510	CLA	O2A-CGA	4.08	1.45	1.33
23	C	509	CLA	OBD-CAD	4.08	1.29	1.22
23	B	602	CLA	CHD-C1D	4.08	1.46	1.38
23	c	501	CLA	CHD-C1D	4.07	1.46	1.38
23	b	608	CLA	O2A-CGA	4.07	1.45	1.33
33	a	415	LMG	O8-C28	4.07	1.45	1.33
23	B	611	CLA	CHD-C1D	4.07	1.46	1.38
26	a	409[A]	SQD	O47-C7	4.07	1.45	1.34
23	b	615	CLA	CHD-C1D	4.06	1.46	1.38
32	d	415[B]	LHG	O8-C23	4.06	1.45	1.33
23	B	614	CLA	O2A-CGA	4.06	1.45	1.33
23	c	506	CLA	CHD-C1D	4.06	1.46	1.38
23	c	503	CLA	O2D-CGD	4.06	1.43	1.33
35	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	CHD-C4C	4.06	1.48	1.39
23	D	402[A]	CLA	CHB-C1B	4.06	1.48	1.39
23	A	405[B]	CLA	C3D-C2D	4.06	1.50	1.39
23	C	505	CLA	CHD-C1D	4.06	1.46	1.38
35	C	518[B]	DGD	O1G-C1A	4.06	1.45	1.33
33	a	415	LMG	O7-C10	4.05	1.45	1.34
23	A	405[A]	CLA	C3D-C2D	4.05	1.50	1.39
23	d	404[A]	CLA	O2A-CGA	4.05	1.45	1.33
23	C	507	CLA	O2A-CGA	4.05	1.45	1.33
33	c	519	LMG	O8-C28	4.05	1.45	1.33
23	b	603	CLA	CHD-C1D	4.05	1.46	1.38
23	C	504	CLA	CHD-C4C	4.05	1.48	1.39
23	C	507	CLA	CHC-C1C	4.04	1.46	1.38
23	B	608	CLA	CHD-C1D	4.04	1.46	1.38
23	c	502	CLA	CHD-C4C	4.04	1.48	1.39
35	c	516[B]	DGD	O2G-C1B	4.04	1.45	1.34
23	d	404[B]	CLA	CHB-C1B	4.04	1.48	1.39
33	C	520	LMG	O7-C10	4.03	1.45	1.34
23	A	404[A]	CLA	CHD-C1D	4.03	1.46	1.38
23	C	512	CLA	O2A-CGA	4.03	1.45	1.33
23	b	607	CLA	C1B-NB	-4.03	1.32	1.37
23	b	604	CLA	CHC-C4B	4.03	1.48	1.39
32	D	407[B]	LHG	O7-C7	4.03	1.45	1.34
23	B	611	CLA	CHB-C1B	4.03	1.48	1.39
23	C	506	CLA	CHD-C4C	4.02	1.48	1.39
23	B	608	CLA	C3D-C2D	4.02	1.50	1.39
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
23	c	512	CLA	C3D-C2D	4.02	1.50	1.39
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	c	508	CLA	O2A-CGA	4.02	1.45	1.33
33	d	413	LMG	O8-C28	4.02	1.45	1.33
23	a	404[B]	CLA	CHD-C1D	4.02	1.46	1.38
23	d	404[B]	CLA	C1D-ND	4.02	1.42	1.37
23	B	603	CLA	CHB-C1B	4.02	1.48	1.39
33	C	501	LMG	O7-C10	4.01	1.45	1.34
23	a	405[B]	CLA	O2A-CGA	4.01	1.45	1.33
23	C	510	CLA	CHC-C1C	4.01	1.46	1.38
23	C	505	CLA	O2A-CGA	4.01	1.45	1.33
23	b	608	CLA	CHD-C1D	4.01	1.46	1.38
26	a	409[B]	SQD	O48-C23	4.01	1.45	1.33
23	C	502	CLA	O2A-CGA	4.00	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	502	CLA	C3D-C2D	4.00	1.50	1.39
23	c	504	CLA	C3D-C2D	4.00	1.50	1.39
23	D	403	CLA	CHC-C4B	4.00	1.48	1.39
26	a	411	SQD	O47-C7	4.00	1.45	1.34
23	c	509	CLA	O2A-CGA	3.99	1.45	1.33
23	a	404[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	c	503	CLA	CHC-C4B	3.99	1.48	1.39
23	a	407	CLA	C1D-ND	3.99	1.42	1.37
23	B	607	CLA	CHB-C1B	3.99	1.48	1.39
23	B	610	CLA	C3D-C2D	3.99	1.50	1.39
23	C	512	CLA	CHB-C1B	3.99	1.48	1.39
23	B	601	CLA	CHD-C1D	3.98	1.46	1.38
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
26	a	409[A]	SQD	O48-C23	3.98	1.45	1.33
23	c	501	CLA	CHD-C4C	3.98	1.48	1.39
23	c	507	CLA	CHD-C4C	3.97	1.48	1.39
23	b	616	CLA	CHC-C4B	3.96	1.48	1.39
35	h	102	DGD	O1G-C1A	3.96	1.44	1.33
23	c	509	CLA	CHD-C1D	3.96	1.46	1.38
23	A	406[B]	CLA	O2A-CGA	3.96	1.44	1.33
23	B	613	CLA	C3D-C2D	3.96	1.49	1.39
23	B	616	CLA	O2A-CGA	3.96	1.44	1.33
24	A	416[B]	PHO	O2A-CGA	3.96	1.44	1.33
23	c	505	CLA	CHD-C4C	3.96	1.48	1.39
23	a	404[A]	CLA	CHD-C4C	3.96	1.48	1.39
23	c	508	CLA	C3D-C2D	3.95	1.49	1.39
23	B	610	CLA	CHB-C1B	3.95	1.48	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	d	405	CLA	CHC-C4B	3.95	1.48	1.39
23	c	512	CLA	CHD-C4C	3.95	1.48	1.39
35	H	102	DGD	O1G-C1A	3.95	1.44	1.33
23	C	503	CLA	CHB-C1B	3.95	1.48	1.39
23	D	403	CLA	CHD-C4C	3.94	1.48	1.39
23	B	601	CLA	CHC-C4B	3.94	1.48	1.39
40	v	201	HEC	FE-ND	3.94	2.07	1.94
23	b	615	CLA	O2A-CGA	3.94	1.44	1.33
33	B	620	LMG	O7-C10	3.93	1.45	1.34
23	B	614	CLA	CHC-C4B	3.93	1.48	1.39
23	c	504	CLA	CHD-C1D	3.93	1.46	1.38
23	B	604	CLA	CHD-C4C	3.92	1.48	1.39
23	A	406[B]	CLA	OBD-CAD	3.92	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CHB-C1B	3.92	1.48	1.39
23	B	602	CLA	CHD-C4C	3.92	1.48	1.39
23	C	514	CLA	C3D-C2D	3.92	1.49	1.39
23	b	613	CLA	C3D-C2D	3.92	1.49	1.39
23	D	402[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	a	404[B]	CLA	CHD-C4C	3.92	1.48	1.39
23	C	514	CLA	CHD-C4C	3.92	1.48	1.39
23	b	614	CLA	C3D-C2D	3.92	1.49	1.39
23	b	606	CLA	CHD-C1D	3.91	1.46	1.38
23	B	613	CLA	CHB-C1B	3.91	1.48	1.39
23	C	511	CLA	O2A-CGA	3.91	1.44	1.33
23	c	502	CLA	CHB-C1B	3.91	1.48	1.39
23	B	609	CLA	C3D-C2D	3.91	1.49	1.39
23	C	507	CLA	CHD-C4C	3.91	1.48	1.39
32	D	407[A]	LHG	O8-C23	3.90	1.44	1.33
23	a	405[B]	CLA	CHD-C1D	3.90	1.46	1.38
23	B	615	CLA	CHB-C1B	3.90	1.48	1.39
23	D	402[B]	CLA	CHD-C1D	3.90	1.46	1.38
23	b	614	CLA	CHD-C4C	3.90	1.48	1.39
23	a	405[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	C	503	CLA	CHC-C4B	3.90	1.48	1.39
23	b	612	CLA	CHC-C4B	3.90	1.48	1.39
23	A	404[B]	CLA	C3D-C2D	3.90	1.49	1.39
23	D	402[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	B	616	CLA	C3D-C2D	3.89	1.49	1.39
23	D	403	CLA	CHB-C1B	3.89	1.48	1.39
35	C	519	DGD	O1G-C1A	3.89	1.44	1.33
23	B	602	CLA	C3D-C2D	3.89	1.49	1.39
32	L	101[B]	LHG	O7-C7	3.89	1.45	1.34
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
23	b	616	CLA	CHD-C4C	3.89	1.48	1.39
23	C	503	CLA	O2A-CGA	3.89	1.44	1.33
23	a	404[B]	CLA	O2A-CGA	3.88	1.44	1.33
23	C	505	CLA	CHB-C1B	3.88	1.48	1.39
23	B	604	CLA	OBD-CAD	3.88	1.29	1.22
23	c	505	CLA	CHB-C1B	3.88	1.48	1.39
23	C	508	CLA	CHC-C4B	3.88	1.48	1.39
26	A	410[B]	SQD	O48-C23	3.88	1.44	1.33
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
24	A	407[B]	PHO	O2A-CGA	3.88	1.44	1.33
23	c	508	CLA	OBD-CAD	3.87	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[B]	CLA	CHD-C1D	3.87	1.45	1.38
23	d	404[A]	CLA	C1B-NB	-3.87	1.33	1.37
23	D	402[B]	CLA	CHB-C1B	3.87	1.48	1.39
23	b	611	CLA	CHD-C4C	3.87	1.48	1.39
23	b	615	CLA	CHD-C4C	3.87	1.48	1.39
23	A	406[B]	CLA	C3D-C2D	3.87	1.49	1.39
23	b	605	CLA	CHD-C1D	3.87	1.45	1.38
23	C	509	CLA	CHD-C1D	3.87	1.45	1.38
32	b	629[B]	LHG	O7-C7	3.86	1.45	1.34
23	B	613	CLA	C1B-NB	-3.86	1.33	1.37
24	A	416[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	C	512	CLA	C1D-ND	3.86	1.42	1.37
23	b	613	CLA	O2A-CGA	3.86	1.44	1.33
23	B	611	CLA	O2A-CGA	3.85	1.44	1.33
32	D	406[B]	LHG	O7-C7	3.85	1.45	1.34
23	B	606	CLA	CHB-C1B	3.85	1.48	1.39
23	B	610	CLA	CHD-C1D	3.85	1.45	1.38
32	d	408[B]	LHG	O7-C7	3.85	1.45	1.34
23	B	606	CLA	O2A-CGA	3.85	1.44	1.33
23	a	405[B]	CLA	OBD-CAD	3.85	1.29	1.22
23	B	604	CLA	C1D-ND	3.85	1.42	1.37
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
23	B	613	CLA	CHD-C1D	3.85	1.45	1.38
23	C	509	CLA	CHB-C1B	3.85	1.48	1.39
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	c	506	CLA	C3D-C2D	3.84	1.49	1.39
23	c	513	CLA	C3D-C2D	3.84	1.49	1.39
23	D	402[B]	CLA	CHD-C4C	3.84	1.48	1.39
23	B	609	CLA	CHC-C4B	3.84	1.48	1.39
32	D	407[B]	LHG	O8-C23	3.84	1.44	1.33
32	L	101[A]	LHG	O8-C23	3.84	1.44	1.33
23	C	513	CLA	C3D-C2D	3.84	1.49	1.39
23	b	604	CLA	C3D-C2D	3.84	1.49	1.39
32	d	409[B]	LHG	O7-C7	3.84	1.45	1.34
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
23	C	510	CLA	CHD-C4C	3.84	1.48	1.39
35	C	518[B]	DGD	O2G-C1B	3.84	1.45	1.34
35	c	517[A]	DGD	O1G-C1A	3.83	1.44	1.33
23	c	509	CLA	CHB-C1B	3.83	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	C	510	CLA	OBD-CAD	3.83	1.29	1.22
23	A	408	CLA	CHD-C1D	3.83	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	CHB-C1B	3.83	1.48	1.39
23	c	508	CLA	CHB-C1B	3.83	1.48	1.39
23	b	604	CLA	CHD-C4C	3.83	1.48	1.39
23	B	605	CLA	C3D-C2D	3.83	1.49	1.39
24	d	403[A]	PHO	O2A-CGA	3.83	1.44	1.33
23	b	610	CLA	CHC-C4B	3.82	1.48	1.39
23	c	510	CLA	CHD-C4C	3.82	1.48	1.39
23	c	510	CLA	O2A-CGA	3.82	1.44	1.33
32	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
23	c	507	CLA	C3D-C2D	3.82	1.49	1.39
23	C	502	CLA	CHC-C4B	3.82	1.48	1.39
23	B	604	CLA	CHB-C1B	3.82	1.48	1.39
23	B	603	CLA	C3D-C2D	3.82	1.49	1.39
23	a	404[B]	CLA	C3D-C2D	3.81	1.49	1.39
23	c	506	CLA	CHB-C1B	3.81	1.48	1.39
40	v	201	HEC	FE-NB	3.81	2.06	1.94
23	B	603	CLA	O2A-CGA	3.81	1.44	1.33
23	B	608	CLA	CHC-C1C	3.81	1.46	1.38
23	b	602	CLA	C3D-C2D	3.81	1.49	1.39
23	C	510	CLA	C3D-C2D	3.81	1.49	1.39
23	c	506	CLA	CHD-C4C	3.81	1.47	1.39
23	a	407	CLA	CHC-C4B	3.81	1.48	1.39
23	A	406[B]	CLA	CHD-C4C	3.81	1.47	1.39
23	b	603	CLA	C3D-C2D	3.81	1.49	1.39
23	B	602	CLA	CHC-C4B	3.81	1.47	1.39
23	d	404[A]	CLA	CHD-C1D	3.81	1.45	1.38
35	c	516[B]	DGD	O1G-C1A	3.81	1.44	1.33
23	b	609	CLA	OBD-CAD	3.81	1.29	1.22
23	c	512	CLA	CHC-C4B	3.80	1.47	1.39
23	b	614	CLA	CHD-C1D	3.80	1.45	1.38
23	B	611	CLA	C1C-C2C	3.80	1.51	1.44
23	B	612	CLA	C4B-NB	-3.80	1.33	1.37
23	B	612	CLA	C1D-ND	3.80	1.42	1.37
23	a	405[B]	CLA	C3D-C2D	3.80	1.49	1.39
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
23	A	406[A]	CLA	CHC-C4B	3.80	1.47	1.39
23	d	402[A]	CLA	CHD-C1D	3.80	1.45	1.38
35	c	517[B]	DGD	O2G-C1B	3.79	1.45	1.34
23	b	612	CLA	C3D-C2D	3.79	1.49	1.39
23	A	408	CLA	CHD-C4C	3.79	1.47	1.39
23	b	609	CLA	C3D-C2D	3.79	1.49	1.39
23	C	513	CLA	CHD-C4C	3.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	CHC-C4B	3.79	1.47	1.39
23	C	512	CLA	CHD-C4C	3.79	1.47	1.39
23	B	603	CLA	CHD-C1D	3.78	1.45	1.38
23	B	605	CLA	CHD-C1D	3.78	1.45	1.38
23	A	405[A]	CLA	CHB-C1B	3.78	1.47	1.39
23	c	507	CLA	OBD-CAD	3.78	1.29	1.22
23	C	511	CLA	CHD-C1D	3.78	1.45	1.38
23	b	610	CLA	OBD-CAD	3.78	1.29	1.22
23	d	404[B]	CLA	CHD-C1D	3.78	1.45	1.38
35	C	517[B]	DGD	O1G-C1A	3.78	1.44	1.33
23	b	608	CLA	CHB-C1B	3.78	1.47	1.39
23	c	501	CLA	O2A-CGA	3.77	1.44	1.33
23	B	611	CLA	CHD-C4C	3.77	1.47	1.39
23	B	605	CLA	CHB-C1B	3.77	1.47	1.39
23	d	402[A]	CLA	OBD-CAD	3.77	1.29	1.22
23	b	615	CLA	C3D-C2D	3.77	1.49	1.39
23	b	611	CLA	CHD-C1D	3.77	1.45	1.38
23	c	513	CLA	CHB-C1B	3.77	1.47	1.39
23	b	610	CLA	CHD-C4C	3.76	1.47	1.39
23	B	606	CLA	CHC-C4B	3.76	1.47	1.39
23	c	501	CLA	C3D-C2D	3.76	1.49	1.39
23	c	504	CLA	O2A-CGA	3.76	1.44	1.33
23	C	505	CLA	C3D-C2D	3.76	1.49	1.39
23	B	611	CLA	OBD-CAD	3.76	1.29	1.22
23	a	405[B]	CLA	CHD-C4C	3.76	1.47	1.39
23	B	612	CLA	CHD-C1D	3.76	1.45	1.38
23	d	405	CLA	CHB-C1B	3.76	1.47	1.39
23	b	616	CLA	C3D-C2D	3.76	1.49	1.39
23	B	602	CLA	CHB-C1B	3.76	1.47	1.39
23	c	511	CLA	CHD-C4C	3.76	1.47	1.39
23	B	610	CLA	CHD-C4C	3.75	1.47	1.39
23	a	405[A]	CLA	CHB-C1B	3.75	1.47	1.39
23	D	402[B]	CLA	C3D-C2D	3.75	1.49	1.39
23	B	607	CLA	CHD-C1D	3.75	1.45	1.38
23	A	404[B]	CLA	C1B-NB	-3.75	1.33	1.37
35	h	102	DGD	O2G-C1B	3.75	1.44	1.34
23	b	603	CLA	CHD-C4C	3.75	1.47	1.39
32	d	415[A]	LHG	O8-C23	3.75	1.44	1.33
34	b	623	HTG	C1'-S1	-3.75	1.76	1.81
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
33	m	101	LMG	O7-C10	3.74	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	OBD-CAD	3.74	1.28	1.22
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	A	405[B]	CLA	CHB-C1B	3.74	1.47	1.39
23	B	611	CLA	C3B-C4B	3.73	1.51	1.42
23	C	507	CLA	C3D-C2D	3.73	1.49	1.39
32	A	419[B]	LHG	O8-C23	3.73	1.44	1.33
23	C	510	CLA	CHB-C1B	3.73	1.47	1.39
23	A	405[B]	CLA	CHD-C1D	3.73	1.45	1.38
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	c	508	CLA	CHD-C4C	3.73	1.47	1.39
23	b	606	CLA	O2A-CGA	3.73	1.44	1.33
23	B	609	CLA	CHD-C4C	3.73	1.47	1.39
33	d	413	LMG	O7-C10	3.73	1.44	1.34
23	D	402[A]	CLA	C1B-NB	-3.72	1.33	1.37
32	d	408[A]	LHG	O7-C7	3.72	1.44	1.34
23	C	512	CLA	C3D-C2D	3.72	1.49	1.39
23	A	405[A]	CLA	CHD-C1D	3.72	1.45	1.38
23	c	507	CLA	CHC-C4B	3.72	1.47	1.39
23	D	403	CLA	O2A-CGA	3.72	1.44	1.33
23	a	404[B]	CLA	CHB-C1B	3.72	1.47	1.39
23	B	601	CLA	C3D-C2D	3.72	1.49	1.39
23	C	507	CLA	C4B-NB	-3.71	1.33	1.37
35	C	518[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	C	512	CLA	C4B-NB	-3.71	1.33	1.37
23	d	404[B]	CLA	CHD-C4C	3.71	1.47	1.39
34	B	621	HTG	C1'-S1	-3.71	1.76	1.81
32	d	415[B]	LHG	O7-C7	3.71	1.44	1.34
23	c	509	CLA	C3D-C2D	3.71	1.49	1.39
23	C	511	CLA	CHB-C1B	3.71	1.47	1.39
23	b	602	CLA	O2A-CGA	3.71	1.44	1.33
23	B	605	CLA	O2A-CGA	3.70	1.44	1.33
23	B	606	CLA	CHD-C1D	3.70	1.45	1.38
23	d	402[B]	CLA	CHD-C4C	3.70	1.47	1.39
23	c	505	CLA	O2A-CGA	3.70	1.44	1.33
23	a	407	CLA	CHD-C1D	3.70	1.45	1.38
23	c	510	CLA	CHD-C1D	3.70	1.45	1.38
23	a	404[A]	CLA	CHB-C1B	3.69	1.47	1.39
23	C	503	CLA	CHD-C4C	3.69	1.47	1.39
23	C	508	CLA	C3D-C2D	3.69	1.49	1.39
23	c	504	CLA	CHD-C4C	3.69	1.47	1.39
23	b	608	CLA	C1B-NB	-3.69	1.33	1.37
23	C	504	CLA	CHB-C1B	3.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	a	405[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	b	606	CLA	CHB-C1B	3.68	1.47	1.39
23	A	404[A]	CLA	C4B-NB	-3.68	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	C	507	CLA	CHB-C1B	3.67	1.47	1.39
23	c	509	CLA	CHD-C4C	3.67	1.47	1.39
23	b	604	CLA	CHB-C1B	3.67	1.47	1.39
23	A	406[A]	CLA	C1B-NB	-3.67	1.33	1.37
23	c	501	CLA	CHC-C4B	3.67	1.47	1.39
23	a	404[B]	CLA	OBD-CAD	3.67	1.28	1.22
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	b	608	CLA	OBD-CAD	3.66	1.28	1.22
23	c	510	CLA	C3D-C2D	3.66	1.49	1.39
23	A	405[B]	CLA	C1B-NB	-3.66	1.33	1.37
23	a	404[A]	CLA	C3D-C2D	3.66	1.49	1.39
23	a	407	CLA	CHB-C1B	3.66	1.47	1.39
23	c	509	CLA	C4B-NB	-3.66	1.33	1.37
23	C	502	CLA	CHD-C4C	3.66	1.47	1.39
32	d	409[A]	LHG	O7-C7	3.66	1.44	1.34
23	b	605	CLA	CHD-C4C	3.66	1.47	1.39
23	A	405[A]	CLA	C1B-NB	-3.66	1.33	1.37
23	b	615	CLA	CHC-C4B	3.66	1.47	1.39
23	C	504	CLA	C3D-C2D	3.65	1.49	1.39
23	c	507	CLA	CHB-C1B	3.65	1.47	1.39
23	A	405[B]	CLA	CHD-C4C	3.65	1.47	1.39
23	B	607	CLA	CHD-C4C	3.65	1.47	1.39
23	b	614	CLA	CHC-C4B	3.65	1.47	1.39
23	C	506	CLA	O2A-CGA	3.64	1.44	1.33
23	b	609	CLA	O2A-CGA	3.64	1.44	1.33
23	D	402[B]	CLA	OBD-CAD	3.64	1.28	1.22
23	b	606	CLA	C3D-C2D	3.64	1.49	1.39
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
23	b	606	CLA	CHD-C4C	3.64	1.47	1.39
23	a	407	CLA	CHD-C4C	3.64	1.47	1.39
23	b	602	CLA	OBD-CAD	3.64	1.28	1.22
23	c	502	CLA	OBD-CAD	3.64	1.28	1.22
23	b	606	CLA	OBD-CAD	3.64	1.28	1.22
23	c	511	CLA	C3D-C2D	3.63	1.49	1.39
23	B	610	CLA	CHC-C4B	3.63	1.47	1.39
34	B	624	HTG	C1'-S1	-3.63	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	d	402[B]	CLA	C1B-NB	-3.63	1.33	1.37
23	d	405	CLA	CHD-C4C	3.63	1.47	1.39
23	B	609	CLA	CHB-C1B	3.63	1.47	1.39
23	b	610	CLA	C3D-C2D	3.63	1.49	1.39
23	b	614	CLA	CHB-C1B	3.63	1.47	1.39
23	B	615	CLA	CHD-C4C	3.63	1.47	1.39
23	b	601	CLA	OBD-CAD	3.63	1.28	1.22
23	C	505	CLA	CHD-C4C	3.62	1.47	1.39
23	B	601	CLA	CHD-C4C	3.62	1.47	1.39
23	b	603	CLA	CHC-C4B	3.62	1.47	1.39
35	c	516[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	C	510	CLA	C4B-NB	-3.62	1.33	1.37
23	d	402[A]	CLA	CHD-C4C	3.62	1.47	1.39
32	d	408[B]	LHG	O8-C23	3.62	1.43	1.33
32	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	B	604	CLA	CHC-C4B	3.62	1.47	1.39
23	B	608	CLA	CHD-C4C	3.61	1.47	1.39
23	a	404[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	606	CLA	CHC-C4B	3.61	1.47	1.39
23	B	607	CLA	CHC-C4B	3.61	1.47	1.39
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	613	CLA	CHD-C1D	3.61	1.45	1.38
34	b	622	HTG	C1'-S1	-3.60	1.76	1.81
32	b	629[B]	LHG	O8-C23	3.60	1.43	1.33
23	b	608	CLA	CHD-C4C	3.60	1.47	1.39
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	B	603	CLA	CHC-C4B	3.60	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
35	c	518	DGD	O2G-C1B	3.59	1.44	1.34
23	C	503	CLA	C4B-NB	-3.59	1.33	1.37
23	C	508	CLA	CHB-C1B	3.59	1.47	1.39
23	B	616	CLA	CHC-C4B	3.59	1.47	1.39
32	D	406[B]	LHG	O8-C23	3.59	1.43	1.33
23	b	611	CLA	C3D-C2D	3.59	1.48	1.39
23	c	505	CLA	C3D-C2D	3.59	1.48	1.39
23	C	507	CLA	OBD-CAD	3.59	1.28	1.22
23	b	605	CLA	CHC-C4B	3.59	1.47	1.39
23	B	608	CLA	O2A-CGA	3.58	1.43	1.33
26	A	410[B]	SQD	O47-C7	3.58	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	514	CLA	OBD-CAD	3.58	1.28	1.22
23	a	405[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	b	613	CLA	CHC-C4B	3.58	1.47	1.39
23	B	613	CLA	CHD-C4C	3.58	1.47	1.39
23	C	505	CLA	CHC-C4B	3.58	1.47	1.39
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	608	CLA	CHB-C1B	3.58	1.47	1.39
23	C	511	CLA	C3D-C2D	3.57	1.48	1.39
23	B	609	CLA	C3B-C4B	3.57	1.51	1.42
23	d	404[A]	CLA	CHD-C4C	3.57	1.47	1.39
32	A	419[B]	LHG	O7-C7	3.57	1.44	1.34
23	b	614	CLA	C1B-NB	-3.57	1.33	1.37
23	B	601	CLA	CHB-C1B	3.57	1.47	1.39
23	D	403	CLA	OBD-CAD	3.57	1.28	1.22
23	b	614	CLA	O2A-CGA	3.57	1.43	1.33
23	C	502	CLA	C3D-C2D	3.57	1.48	1.39
23	c	509	CLA	C1B-NB	-3.57	1.33	1.37
23	c	512	CLA	OBD-CAD	3.56	1.28	1.22
23	C	503	CLA	OBD-CAD	3.56	1.28	1.22
23	B	607	CLA	O2A-CGA	3.56	1.43	1.33
24	a	406[B]	PHO	O2A-CGA	3.56	1.43	1.33
23	C	502	CLA	C1B-NB	-3.56	1.33	1.37
23	A	405[A]	CLA	CHD-C4C	3.56	1.47	1.39
23	A	405[A]	CLA	CHC-C4B	3.56	1.47	1.39
23	A	404[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	C	502	CLA	CHB-C1B	3.55	1.47	1.39
23	C	506	CLA	CHC-C4B	3.55	1.47	1.39
35	C	517[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	d	404[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	605	CLA	CHD-C4C	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	B	603	CLA	CHD-C4C	3.55	1.47	1.39
23	b	607	CLA	C3D-C2D	3.54	1.48	1.39
23	c	511	CLA	OBD-CAD	3.54	1.28	1.22
23	a	405[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	C	507	CLA	C1B-NB	-3.54	1.33	1.37
35	c	517[A]	DGD	O2G-C1B	3.53	1.44	1.34
23	c	508	CLA	CHC-C4B	3.53	1.47	1.39
23	C	513	CLA	OBD-CAD	3.53	1.28	1.22
33	D	411	LMG	O8-C28	3.53	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C3D-C2D	3.53	1.48	1.39
23	C	511	CLA	C4B-NB	-3.53	1.33	1.37
32	d	408[A]	LHG	O8-C23	3.53	1.43	1.33
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	b	601	CLA	CHC-C4B	3.52	1.47	1.39
23	B	603	CLA	OBD-CAD	3.52	1.28	1.22
23	d	404[B]	CLA	C3D-C2D	3.52	1.48	1.39
40	v	201	HEC	FE-NC	3.52	2.07	1.95
23	b	615	CLA	C1B-NB	-3.52	1.33	1.37
23	c	506	CLA	OBD-CAD	3.52	1.28	1.22
23	B	607	CLA	C1D-ND	3.52	1.42	1.37
32	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
23	A	406[B]	CLA	CHB-C1B	3.52	1.47	1.39
23	b	603	CLA	O2A-CGA	3.52	1.43	1.33
23	B	614	CLA	CHD-C1D	3.51	1.45	1.38
23	b	601	CLA	CHB-C1B	3.51	1.47	1.39
23	b	602	CLA	C1B-NB	-3.51	1.33	1.37
23	B	612	CLA	CHC-C4B	3.51	1.47	1.39
23	b	615	CLA	OBD-CAD	3.51	1.28	1.22
23	A	406[B]	CLA	CHC-C4B	3.50	1.47	1.39
32	d	415[A]	LHG	O7-C7	3.50	1.44	1.34
23	c	504	CLA	C1B-NB	-3.50	1.33	1.37
23	b	607	CLA	CHC-C4B	3.50	1.47	1.39
23	B	612	CLA	O2A-CGA	3.50	1.43	1.33
23	C	511	CLA	C1B-NB	-3.50	1.33	1.37
23	a	407	CLA	C1B-NB	-3.50	1.33	1.37
23	C	508	CLA	CHD-C4C	3.50	1.47	1.39
23	c	503	CLA	C3D-C2D	3.50	1.48	1.39
32	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
32	b	629[A]	LHG	O8-C23	3.49	1.43	1.33
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	C	509	CLA	CHD-C4C	3.49	1.47	1.39
23	d	404[B]	CLA	CHC-C4B	3.49	1.47	1.39
23	b	608	CLA	C4B-NB	-3.48	1.33	1.37
23	c	513	CLA	C1B-NB	-3.48	1.33	1.37
23	c	504	CLA	CHB-C1B	3.48	1.47	1.39
23	d	402[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	c	513	CLA	OBD-CAD	3.48	1.28	1.22
23	c	504	CLA	OBD-CAD	3.47	1.28	1.22
23	b	609	CLA	CHD-C4C	3.47	1.47	1.39
23	b	603	CLA	OBD-CAD	3.47	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C3B-C4B	3.47	1.50	1.42
23	d	402[A]	CLA	CHC-C4B	3.47	1.47	1.39
23	b	604	CLA	OBD-CAD	3.47	1.28	1.22
23	B	616	CLA	CHD-C1D	3.47	1.45	1.38
23	B	606	CLA	C3D-C2D	3.46	1.48	1.39
35	C	519	DGD	O2G-C1B	3.46	1.44	1.34
23	B	601	CLA	OBD-CAD	3.46	1.28	1.22
23	A	405[B]	CLA	CHC-C4B	3.45	1.47	1.39
23	B	603	CLA	C1B-NB	-3.45	1.33	1.37
23	B	611	CLA	C3D-C2D	3.45	1.48	1.39
23	C	512	CLA	CHC-C4B	3.44	1.47	1.39
23	b	605	CLA	CHB-C1B	3.44	1.47	1.39
23	C	510	CLA	C1B-NB	-3.44	1.33	1.37
23	b	603	CLA	CHB-C1B	3.44	1.47	1.39
23	b	607	CLA	CHD-C4C	3.44	1.47	1.39
23	D	402[A]	CLA	C3D-C2D	3.43	1.48	1.39
23	a	407	CLA	C3D-C2D	3.43	1.48	1.39
23	A	406[A]	CLA	CHB-C1B	3.43	1.47	1.39
23	B	607	CLA	OBD-CAD	3.42	1.28	1.22
23	d	404[A]	CLA	CHC-C4B	3.42	1.47	1.39
23	b	604	CLA	O2A-CGA	3.42	1.43	1.33
23	B	613	CLA	OBD-CAD	3.42	1.28	1.22
23	d	402[B]	CLA	CHB-C1B	3.41	1.47	1.39
23	A	408	CLA	C3D-C2D	3.41	1.48	1.39
23	d	404[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	b	610	CLA	C1B-NB	-3.41	1.33	1.37
23	B	602	CLA	C1B-NB	-3.41	1.33	1.37
23	a	404[B]	CLA	C1B-NB	-3.41	1.33	1.37
23	c	513	CLA	CHC-C4B	3.40	1.47	1.39
23	B	612	CLA	C3D-C2D	3.40	1.48	1.39
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	616	CLA	OBD-CAD	3.40	1.28	1.22
23	b	613	CLA	CHB-C1B	3.40	1.47	1.39
38	E	102	HEM	C1B-NB	-3.40	1.34	1.40
23	c	511	CLA	CHC-C4B	3.40	1.47	1.39
23	B	606	CLA	C4B-NB	-3.39	1.33	1.37
23	c	507	CLA	C1B-NB	-3.39	1.33	1.37
24	a	406[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	c	509	CLA	OBD-CAD	3.38	1.28	1.22
23	D	403	CLA	C3B-C4B	3.38	1.50	1.42
23	c	503	CLA	C3B-C4B	3.38	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C4B-NB	-3.37	1.33	1.37
23	b	602	CLA	C3B-C4B	3.37	1.50	1.42
23	b	612	CLA	CHD-C4C	3.37	1.46	1.39
23	C	504	CLA	OBD-CAD	3.36	1.28	1.22
23	a	404[A]	CLA	CHC-C4B	3.36	1.46	1.39
23	d	402[A]	CLA	C1B-NB	-3.36	1.33	1.37
23	B	604	CLA	O2A-CGA	3.36	1.43	1.33
23	B	605	CLA	C4B-NB	-3.36	1.33	1.37
38	f	101	HEM	C4D-ND	-3.36	1.34	1.40
23	b	602	CLA	C1C-C2C	3.35	1.51	1.44
23	b	605	CLA	O2A-CGA	3.35	1.43	1.33
23	b	604	CLA	C1B-NB	-3.35	1.33	1.37
23	c	513	CLA	C4B-NB	-3.35	1.33	1.37
23	B	609	CLA	C1B-NB	-3.35	1.33	1.37
23	C	506	CLA	C3D-C2D	3.35	1.48	1.39
23	D	402[B]	CLA	C1B-NB	-3.34	1.33	1.37
23	A	408	CLA	CHC-C4B	3.34	1.46	1.39
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	C	514	CLA	C4B-NB	-3.34	1.33	1.37
23	D	402[A]	CLA	CHC-C4B	3.33	1.46	1.39
23	c	505	CLA	OBD-CAD	3.33	1.28	1.22
23	C	506	CLA	OBD-CAD	3.33	1.28	1.22
38	f	101	HEM	C1B-NB	-3.32	1.34	1.40
23	c	505	CLA	C1B-NB	-3.32	1.33	1.37
23	C	514	CLA	CHC-C4B	3.32	1.46	1.39
23	c	510	CLA	OBD-CAD	3.32	1.28	1.22
23	B	607	CLA	C3D-C2D	3.32	1.48	1.39
23	d	405	CLA	OBD-CAD	3.31	1.28	1.22
23	b	613	CLA	C1B-NB	-3.31	1.33	1.37
23	B	606	CLA	CHD-C4C	3.31	1.46	1.39
23	b	605	CLA	OBD-CAD	3.31	1.28	1.22
23	B	615	CLA	CHC-C4B	3.31	1.46	1.39
23	C	505	CLA	C1B-NB	-3.31	1.33	1.37
23	a	404[B]	CLA	C4B-NB	-3.30	1.33	1.37
23	C	509	CLA	CHC-C4B	3.30	1.46	1.39
23	a	404[A]	CLA	C1B-NB	-3.30	1.33	1.37
23	B	614	CLA	C3D-C2D	3.29	1.48	1.39
23	A	405[B]	CLA	OBD-CAD	3.29	1.28	1.22
23	c	511	CLA	C1B-C2B	3.29	1.51	1.43
23	C	510	CLA	CHC-C4B	3.29	1.46	1.39
23	c	506	CLA	C1B-NB	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404[B]	CLA	C4B-NB	-3.28	1.33	1.37
23	b	612	CLA	O2A-CGA	3.28	1.42	1.33
23	b	610	CLA	O2A-CGA	3.28	1.42	1.33
23	b	612	CLA	C4B-NB	-3.27	1.33	1.37
23	d	404[A]	CLA	C1D-ND	3.27	1.41	1.37
23	c	502	CLA	CHC-C4B	3.27	1.46	1.39
23	c	506	CLA	CHC-C4B	3.27	1.46	1.39
23	B	602	CLA	OBD-CAD	3.27	1.28	1.22
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	c	504	CLA	C4B-NB	-3.26	1.33	1.37
23	b	616	CLA	C3B-C4B	3.26	1.50	1.42
23	d	404[B]	CLA	C1B-NB	-3.25	1.33	1.37
33	D	411	LMG	O7-C10	3.25	1.43	1.34
23	A	408	CLA	OBD-CAD	3.24	1.28	1.22
23	C	513	CLA	CHB-C1B	3.24	1.46	1.39
23	a	405[A]	CLA	CHC-C4B	3.24	1.46	1.39
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	C	514	CLA	C1B-NB	-3.23	1.33	1.37
23	B	612	CLA	CHD-C4C	3.23	1.46	1.39
23	b	616	CLA	CHB-C1B	3.22	1.46	1.39
34	b	625	HTG	C1'-S1	-3.22	1.77	1.81
23	C	506	CLA	C1B-NB	-3.22	1.33	1.37
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	C	508	CLA	C4B-NB	-3.20	1.33	1.37
23	a	404[B]	CLA	CHC-C4B	3.20	1.46	1.39
34	D	410	HTG	C1'-S1	-3.20	1.77	1.81
23	B	616	CLA	CHD-C4C	3.20	1.46	1.39
23	A	405[A]	CLA	C3B-C4B	3.20	1.50	1.42
23	b	613	CLA	CHD-C4C	3.20	1.46	1.39
23	d	402[B]	CLA	CHC-C4B	3.19	1.46	1.39
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	c	510	CLA	C1C-C2C	3.18	1.50	1.44
23	C	506	CLA	C1B-C2B	3.17	1.50	1.43
23	B	608	CLA	C1B-NB	-3.17	1.33	1.37
23	D	402[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	b	606	CLA	C1B-NB	-3.17	1.33	1.37
23	c	510	CLA	C1B-NB	-3.17	1.33	1.37
23	B	604	CLA	C1B-NB	-3.17	1.33	1.37
23	a	404[A]	CLA	C4B-NB	-3.17	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	605	CLA	C3B-C4B	3.17	1.50	1.42
23	B	604	CLA	C3D-C2D	3.16	1.47	1.39
23	b	613	CLA	C4B-NB	-3.16	1.33	1.37
23	B	612	CLA	C1C-C2C	3.16	1.50	1.44
23	b	601	CLA	C1B-NB	-3.16	1.33	1.37
38	E	102	HEM	C4D-ND	-3.16	1.34	1.40
23	A	404[A]	CLA	CHC-C4B	3.15	1.46	1.39
23	A	406[B]	CLA	C4B-NB	-3.15	1.33	1.37
23	D	403	CLA	C1C-C2C	3.15	1.50	1.44
23	b	602	CLA	CHB-C1B	3.14	1.46	1.39
23	C	502	CLA	C3B-C4B	3.14	1.50	1.42
34	c	521	HTG	C1'-S1	-3.14	1.77	1.81
23	B	616	CLA	C1B-NB	-3.13	1.33	1.37
23	A	406[A]	CLA	C3B-C4B	3.13	1.50	1.42
23	A	404[B]	CLA	C4B-NB	-3.12	1.33	1.37
23	C	506	CLA	C3B-C4B	3.12	1.50	1.42
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
34	d	412	HTG	C1'-S1	-3.12	1.77	1.81
23	B	609	CLA	OBD-CAD	3.11	1.27	1.22
24	A	416[A]	PHO	CHA-CBD	-3.10	1.47	1.51
23	A	404[B]	CLA	CHC-C4B	3.10	1.46	1.39
23	A	404[A]	CLA	C1B-NB	-3.09	1.34	1.37
24	A	416[B]	PHO	CHA-CBD	-3.09	1.47	1.51
23	a	405[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	A	408	CLA	CHB-C1B	3.09	1.46	1.39
23	B	613	CLA	O2A-CGA	3.09	1.42	1.33
23	d	405	CLA	C3B-C4B	3.09	1.50	1.42
23	b	604	CLA	C1B-C2B	3.08	1.50	1.43
23	B	602	CLA	C1C-C2C	3.08	1.50	1.44
23	a	404[A]	CLA	O2A-CGA	3.07	1.42	1.33
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	505	CLA	OBD-CAD	3.07	1.27	1.22
23	A	406[B]	CLA	C3B-C4B	3.06	1.49	1.42
23	a	407	CLA	C3B-C4B	3.06	1.49	1.42
23	b	607	CLA	O2A-CGA	3.06	1.42	1.33
23	C	513	CLA	C3B-C4B	3.06	1.49	1.42
23	B	616	CLA	C4B-NB	-3.06	1.34	1.37
23	a	405[B]	CLA	C3B-C4B	3.05	1.49	1.42
23	c	511	CLA	C4B-NB	-3.05	1.34	1.37
34	C	522	HTG	C1'-S1	-3.05	1.77	1.81
23	a	407	CLA	C1C-C2C	3.05	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	b	625	HTG	C1-S1	-3.05	1.76	1.80
23	a	405[A]	CLA	C3B-C4B	3.05	1.49	1.42
23	B	610	CLA	C3B-C4B	3.04	1.49	1.42
23	b	605	CLA	C1B-NB	-3.04	1.34	1.37
23	c	507	CLA	C4B-NB	-3.04	1.34	1.37
23	C	507	CLA	CHC-C4B	3.03	1.46	1.39
23	c	508	CLA	C4B-NB	-3.03	1.34	1.37
23	B	601	CLA	C3B-C4B	3.03	1.49	1.42
23	b	601	CLA	C3B-C4B	3.03	1.49	1.42
23	c	504	CLA	C1B-C2B	3.02	1.50	1.43
23	c	502	CLA	C4B-NB	-3.02	1.34	1.37
23	A	406[B]	CLA	C1B-NB	-3.01	1.34	1.37
23	b	607	CLA	C1B-C2B	3.01	1.50	1.43
23	b	609	CLA	C1B-NB	-3.01	1.34	1.37
23	c	512	CLA	C3B-C4B	3.01	1.49	1.42
23	D	402[B]	CLA	C4B-NB	-3.01	1.34	1.37
23	C	508	CLA	C1B-NB	-3.00	1.34	1.37
23	c	509	CLA	CHC-C4B	3.00	1.46	1.39
23	c	512	CLA	C1B-NB	-3.00	1.34	1.37
23	b	606	CLA	C3B-C4B	3.00	1.49	1.42
23	B	605	CLA	C1B-NB	-2.99	1.34	1.37
23	b	612	CLA	C1C-C2C	2.99	1.50	1.44
23	b	603	CLA	C3B-C4B	2.99	1.49	1.42
23	d	404[A]	CLA	C4B-NB	-2.99	1.34	1.37
23	B	604	CLA	C1B-C2B	2.98	1.50	1.43
23	c	504	CLA	C1C-C2C	2.98	1.50	1.44
23	A	408	CLA	C1B-NB	-2.97	1.34	1.37
23	b	609	CLA	C3B-C4B	2.97	1.49	1.42
23	C	504	CLA	C3B-C4B	2.96	1.49	1.42
23	c	503	CLA	OBD-CAD	2.96	1.27	1.22
23	C	512	CLA	C4D-CHA	2.96	1.48	1.38
23	a	407	CLA	OBD-CAD	2.96	1.27	1.22
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	C	513	CLA	C1B-NB	-2.96	1.34	1.37
23	d	402[A]	CLA	C3B-C4B	2.96	1.49	1.42
23	C	511	CLA	CHC-C4B	2.95	1.46	1.39
23	b	611	CLA	C1B-C2B	2.95	1.50	1.43
23	D	403	CLA	C4C-C3C	2.95	1.50	1.45
23	b	606	CLA	C4B-NB	-2.95	1.34	1.37
23	C	507	CLA	C4C-C3C	2.95	1.50	1.45
23	c	506	CLA	C4B-NB	-2.95	1.34	1.37
23	b	611	CLA	OBD-CAD	2.95	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	C1B-C2B	2.94	1.50	1.43
23	B	606	CLA	OBD-CAD	2.94	1.27	1.22
23	c	503	CLA	C1B-NB	-2.94	1.34	1.37
23	B	603	CLA	C4B-NB	-2.94	1.34	1.37
23	b	611	CLA	C1B-NB	-2.93	1.34	1.37
23	c	506	CLA	C1B-C2B	2.93	1.50	1.43
23	B	614	CLA	OBD-CAD	2.93	1.27	1.22
23	b	612	CLA	C1B-C2B	2.93	1.50	1.43
23	B	614	CLA	C1B-NB	-2.93	1.34	1.37
23	c	503	CLA	C4B-NB	-2.92	1.34	1.37
23	B	615	CLA	C1B-C2B	2.92	1.50	1.43
23	B	616	CLA	OBD-CAD	2.91	1.27	1.22
23	A	404[B]	CLA	C4C-C3C	2.91	1.50	1.45
23	B	607	CLA	C4D-CHA	2.91	1.48	1.38
23	B	601	CLA	C1B-NB	-2.91	1.34	1.37
23	A	405[B]	CLA	C3B-C4B	2.91	1.49	1.42
23	B	608	CLA	OBD-CAD	2.90	1.27	1.22
23	D	403	CLA	C1B-NB	-2.90	1.34	1.37
23	B	605	CLA	OBD-CAD	2.90	1.27	1.22
23	B	611	CLA	MG-NB	2.89	2.11	2.05
23	C	505	CLA	C4D-CHA	2.89	1.48	1.38
23	c	509	CLA	C1B-C2B	2.89	1.50	1.43
23	C	505	CLA	C4B-NB	-2.89	1.34	1.37
23	B	610	CLA	C4D-CHA	2.89	1.48	1.38
23	B	615	CLA	C1C-C2C	2.89	1.50	1.44
23	a	405[B]	CLA	C4B-NB	-2.88	1.34	1.37
23	c	501	CLA	OBD-CAD	2.88	1.27	1.22
23	b	607	CLA	OBD-CAD	2.87	1.27	1.22
23	A	406[A]	CLA	C4B-NB	-2.87	1.34	1.37
23	b	614	CLA	C4B-NB	-2.87	1.34	1.37
23	b	604	CLA	C4D-CHA	2.86	1.48	1.38
23	B	615	CLA	C3B-C4B	2.86	1.49	1.42
23	b	611	CLA	C4B-NB	-2.85	1.34	1.37
23	c	510	CLA	C1B-C2B	2.84	1.50	1.43
23	c	508	CLA	C4C-C3C	2.84	1.49	1.45
23	b	603	CLA	C4B-NB	-2.84	1.34	1.37
23	c	513	CLA	C3B-C4B	2.84	1.49	1.42
23	B	606	CLA	C1C-C2C	2.84	1.50	1.44
23	c	502	CLA	C1B-NB	-2.84	1.34	1.37
23	c	511	CLA	C1B-NB	-2.83	1.34	1.37
23	C	513	CLA	C1C-C2C	2.83	1.50	1.44
26	a	409[B]	SQD	C6-S	-2.83	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402[A]	CLA	C1B-C2B	2.83	1.49	1.43
24	A	407[A]	PHO	CBD-CGD	-2.83	1.48	1.52
23	B	606	CLA	C3B-C4B	2.83	1.49	1.42
23	B	608	CLA	C4D-CHA	2.82	1.48	1.38
23	c	501	CLA	C3B-C4B	2.82	1.49	1.42
23	b	605	CLA	C3B-C4B	2.82	1.49	1.42
23	b	607	CLA	C4B-NB	-2.82	1.34	1.37
23	b	613	CLA	C1B-C2B	2.82	1.49	1.43
23	b	614	CLA	C3B-C4B	2.82	1.49	1.42
23	c	510	CLA	C3B-C4B	2.82	1.49	1.42
23	a	405[B]	CLA	C1B-NB	-2.82	1.34	1.37
23	c	503	CLA	C1C-C2C	2.82	1.50	1.44
23	B	601	CLA	C4B-NB	-2.82	1.34	1.37
23	C	504	CLA	C1B-NB	-2.81	1.34	1.37
23	b	613	CLA	C4D-CHA	2.81	1.48	1.38
23	C	505	CLA	C1B-C2B	2.80	1.49	1.43
35	H	102	DGD	O5D-C1E	2.80	1.45	1.40
23	C	509	CLA	C1B-NB	-2.80	1.34	1.37
23	C	510	CLA	C1B-C2B	2.80	1.49	1.43
23	B	606	CLA	C1B-NB	-2.80	1.34	1.37
23	b	603	CLA	C1B-C2B	2.80	1.49	1.43
24	d	403[B]	PHO	C3A-C2A	-2.79	1.52	1.54
23	B	616	CLA	C1B-C2B	2.79	1.49	1.43
23	c	502	CLA	C1B-C2B	2.79	1.49	1.43
23	D	403	CLA	C1B-C2B	2.79	1.49	1.43
23	d	402[B]	CLA	C3B-C4B	2.79	1.49	1.42
23	b	614	CLA	C1B-C2B	2.79	1.49	1.43
23	a	405[B]	CLA	C1C-C2C	2.78	1.49	1.44
23	a	405[B]	CLA	C1B-C2B	2.78	1.49	1.43
23	b	612	CLA	C1B-NB	-2.77	1.34	1.37
23	C	508	CLA	C4D-CHA	2.77	1.48	1.38
23	c	513	CLA	C1B-C2B	2.77	1.49	1.43
23	b	607	CLA	C1C-C2C	2.77	1.49	1.44
23	C	507	CLA	C1B-C2B	2.77	1.49	1.43
23	A	408	CLA	C1B-C2B	2.77	1.49	1.43
23	d	402[B]	CLA	C1B-C2B	2.77	1.49	1.43
29	A	414[A]	PL9	C6-C5	2.76	1.49	1.35
23	C	512	CLA	C3B-C4B	2.76	1.49	1.42
23	c	504	CLA	C1C-NC	-2.76	1.33	1.37
23	b	616	CLA	C1B-NB	-2.76	1.34	1.37
23	c	501	CLA	C4C-C3C	2.75	1.49	1.45
26	A	410[B]	SQD	C6-S	-2.75	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	413[A]	PL9	C6-C5	2.75	1.49	1.35
23	B	614	CLA	C4D-CHA	2.75	1.48	1.38
23	A	404[A]	CLA	C1B-C2B	2.75	1.49	1.43
23	b	616	CLA	C1C-C2C	2.75	1.49	1.44
23	b	610	CLA	C3B-C4B	2.75	1.49	1.42
23	B	612	CLA	C1B-C2B	2.74	1.49	1.43
23	b	601	CLA	C4B-NB	-2.74	1.34	1.37
23	B	615	CLA	C1B-NB	-2.74	1.34	1.37
29	A	414[B]	PL9	C6-C5	2.74	1.49	1.35
23	C	509	CLA	C1B-C2B	2.74	1.49	1.43
26	a	409[A]	SQD	C6-S	-2.73	1.67	1.77
23	b	607	CLA	C4C-C3C	2.73	1.49	1.45
23	A	405[A]	CLA	C4B-NB	-2.73	1.34	1.37
23	b	609	CLA	C4B-NB	-2.73	1.34	1.37
23	c	507	CLA	C1B-C2B	2.73	1.49	1.43
23	c	508	CLA	C1C-C2C	2.73	1.49	1.44
26	A	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	b	604	CLA	C3B-C4B	2.73	1.49	1.42
33	Z	101	LMG	O8-C28	2.73	1.46	1.33
23	C	511	CLA	C4C-C3C	2.72	1.49	1.45
23	A	406[A]	CLA	C4D-CHA	2.72	1.48	1.38
23	a	405[A]	CLA	C1C-C2C	2.72	1.49	1.44
23	B	612	CLA	C4D-CHA	2.72	1.48	1.38
23	d	402[A]	CLA	C1B-C2B	2.72	1.49	1.43
23	c	508	CLA	C3B-C4B	2.72	1.49	1.42
23	C	509	CLA	C4B-NB	-2.72	1.34	1.37
23	b	612	CLA	C3B-C4B	2.72	1.49	1.42
23	B	607	CLA	C1B-C2B	2.72	1.49	1.43
23	B	615	CLA	C4D-CHA	2.72	1.48	1.38
23	C	512	CLA	C1B-NB	-2.72	1.34	1.37
23	C	502	CLA	C4D-CHA	2.72	1.48	1.38
23	C	502	CLA	C1C-C2C	2.71	1.49	1.44
23	D	402[A]	CLA	C4D-CHA	2.71	1.48	1.38
29	a	413[B]	PL9	C6-C5	2.71	1.49	1.35
26	A	412	SQD	C6-S	-2.71	1.67	1.77
23	B	602	CLA	C1B-C2B	2.71	1.49	1.43
23	B	613	CLA	C4D-CHA	2.70	1.48	1.38
23	b	609	CLA	C4D-CHA	2.70	1.48	1.38
23	A	404[B]	CLA	C4D-CHA	2.70	1.48	1.38
23	A	408	CLA	C3B-C4B	2.70	1.49	1.42
23	C	512	CLA	C1C-C2C	2.70	1.49	1.44
23	C	510	CLA	C3B-C4B	2.69	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C4B-NB	-2.69	1.34	1.37
23	A	406[B]	CLA	C1B-C2B	2.69	1.49	1.43
23	C	514	CLA	C1B-C2B	2.69	1.49	1.43
23	c	501	CLA	C1B-C2B	2.69	1.49	1.43
23	B	610	CLA	C1B-C2B	2.69	1.49	1.43
23	A	408	CLA	C3D-C4D	-2.69	1.38	1.44
23	C	506	CLA	C4C-C3C	2.69	1.49	1.45
23	b	602	CLA	C4C-C3C	2.69	1.49	1.45
23	c	505	CLA	C1B-C2B	2.68	1.49	1.43
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
23	C	510	CLA	C1C-C2C	2.68	1.49	1.44
23	b	616	CLA	C1B-C2B	2.68	1.49	1.43
23	b	607	CLA	C4D-CHA	2.68	1.47	1.38
23	c	512	CLA	C4D-CHA	2.68	1.47	1.38
23	c	503	CLA	C1B-C2B	2.68	1.49	1.43
23	c	511	CLA	C4D-CHA	2.68	1.47	1.38
23	B	613	CLA	C1C-C2C	2.68	1.49	1.44
23	C	504	CLA	C4B-NB	-2.68	1.34	1.37
23	a	405[A]	CLA	C1B-C2B	2.68	1.49	1.43
23	A	404[B]	CLA	C1B-C2B	2.67	1.49	1.43
23	b	609	CLA	C1B-C2B	2.67	1.49	1.43
23	B	616	CLA	C4D-CHA	2.67	1.47	1.38
23	B	614	CLA	C3B-C4B	2.67	1.49	1.42
23	B	604	CLA	C3B-C4B	2.67	1.49	1.42
23	B	605	CLA	C1B-C2B	2.67	1.49	1.43
23	c	507	CLA	C4D-CHA	2.67	1.47	1.38
23	c	501	CLA	C4D-CHA	2.67	1.47	1.38
23	B	607	CLA	C1C-C2C	2.66	1.49	1.44
23	a	404[B]	CLA	C1B-C2B	2.66	1.49	1.43
23	b	610	CLA	C1C-C2C	2.66	1.49	1.44
23	A	408	CLA	C4B-NB	-2.66	1.34	1.37
23	a	404[A]	CLA	C1B-C2B	2.66	1.49	1.43
23	B	605	CLA	C4D-CHA	2.66	1.47	1.38
23	c	510	CLA	C4D-CHA	2.65	1.47	1.38
23	a	407	CLA	C4B-NB	-2.65	1.34	1.37
23	d	404[A]	CLA	C1B-C2B	2.65	1.49	1.43
23	C	508	CLA	C1C-C2C	2.65	1.49	1.44
23	B	602	CLA	C3B-C4B	2.65	1.49	1.42
23	c	513	CLA	C1C-C2C	2.64	1.49	1.44
23	C	513	CLA	C4D-CHA	2.64	1.47	1.38
23	B	604	CLA	C4D-CHA	2.64	1.47	1.38
23	b	611	CLA	C4C-C3C	2.64	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C1C-C2C	2.64	1.49	1.44
23	B	614	CLA	C3D-C4D	-2.64	1.38	1.44
23	C	505	CLA	C1C-C2C	2.64	1.49	1.44
26	f	102	SQD	C6-S	-2.64	1.67	1.77
23	B	604	CLA	C4B-NB	-2.64	1.34	1.37
23	A	405[B]	CLA	C1B-C2B	2.63	1.49	1.43
23	C	503	CLA	C3B-C4B	2.63	1.48	1.42
23	c	508	CLA	C1B-C2B	2.63	1.49	1.43
23	a	405[A]	CLA	C4B-NB	-2.63	1.34	1.37
40	V	201	HEC	CAC-C3C	2.62	1.57	1.51
23	b	608	CLA	C3B-C4B	2.62	1.48	1.42
23	b	610	CLA	C4D-CHA	2.62	1.47	1.38
23	B	614	CLA	C1B-C2B	2.62	1.49	1.43
23	a	405[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	c	511	CLA	C1C-C2C	2.62	1.49	1.44
23	C	513	CLA	C4B-NB	-2.62	1.34	1.37
23	B	607	CLA	C3D-C4D	-2.62	1.38	1.44
23	A	405[A]	CLA	C1B-C2B	2.62	1.49	1.43
23	C	503	CLA	C1B-C2B	2.62	1.49	1.43
23	c	508	CLA	C4D-CHA	2.62	1.47	1.38
40	V	201	HEC	FE-NC	2.62	2.04	1.95
23	c	505	CLA	C4C-C3C	2.61	1.49	1.45
23	B	616	CLA	C1C-C2C	2.61	1.49	1.44
23	A	408	CLA	C4D-CHA	2.60	1.47	1.38
27	a	418	GOL	C1-C2	2.60	1.62	1.51
23	D	402[B]	CLA	C1B-C2B	2.60	1.49	1.43
31	M	101	LMT	O2'-C2'	-2.60	1.36	1.43
23	C	507	CLA	C4D-CHA	2.60	1.47	1.38
23	B	610	CLA	C1C-C2C	2.60	1.49	1.44
23	B	602	CLA	C4B-NB	-2.60	1.34	1.37
23	b	611	CLA	C1C-C2C	2.60	1.49	1.44
23	B	603	CLA	C1B-C2B	2.60	1.49	1.43
23	d	405	CLA	C4B-NB	-2.60	1.34	1.37
23	C	511	CLA	C1B-C2B	2.59	1.49	1.43
23	c	507	CLA	C1C-C2C	2.59	1.49	1.44
23	B	613	CLA	C1B-C2B	2.59	1.49	1.43
38	E	102	HEM	C1C-C2C	-2.59	1.40	1.45
26	b	620	SQD	C6-S	-2.59	1.67	1.77
23	b	615	CLA	C4B-NB	-2.59	1.34	1.37
23	C	512	CLA	C1B-C2B	2.59	1.49	1.43
24	A	416[B]	PHO	C3A-C2A	-2.59	1.52	1.54
23	B	610	CLA	C4C-C3C	2.59	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	411	SQD	C6-S	-2.59	1.67	1.77
23	d	404[B]	CLA	C4D-CHA	2.59	1.47	1.38
23	C	509	CLA	C4C-C3C	2.58	1.49	1.45
23	d	405	CLA	C4D-CHA	2.58	1.47	1.38
31	t	101	LMT	O3'-C3'	-2.58	1.36	1.43
23	C	514	CLA	C4D-CHA	2.58	1.47	1.38
23	C	504	CLA	C1C-C2C	2.57	1.49	1.44
23	C	508	CLA	C1B-C2B	2.57	1.49	1.43
23	a	404[A]	CLA	C3B-C4B	2.57	1.48	1.42
23	C	502	CLA	OBD-CAD	2.57	1.26	1.22
31	C	525	LMT	O3'-C3'	-2.57	1.36	1.43
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	615	CLA	C4D-CHA	2.56	1.47	1.38
23	C	509	CLA	C4D-CHA	2.56	1.47	1.38
23	d	405	CLA	C1C-C2C	2.56	1.49	1.44
23	B	609	CLA	C1B-C2B	2.56	1.49	1.43
23	B	601	CLA	C1C-C2C	2.56	1.49	1.44
23	d	404[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	B	613	CLA	C4B-NB	-2.56	1.34	1.37
23	C	503	CLA	C1B-NB	-2.56	1.34	1.37
23	c	509	CLA	C4D-CHA	2.55	1.47	1.38
23	b	605	CLA	C4D-CHA	2.55	1.47	1.38
23	c	504	CLA	C4D-CHA	2.55	1.47	1.38
23	b	615	CLA	C1B-C2B	2.55	1.49	1.43
23	A	405[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	b	606	CLA	C4D-CHA	2.55	1.47	1.38
23	c	512	CLA	C1B-C2B	2.55	1.49	1.43
23	b	601	CLA	C4D-CHA	2.55	1.47	1.38
24	d	403[A]	PHO	C3A-C2A	-2.55	1.52	1.54
23	c	505	CLA	C1C-C2C	2.55	1.49	1.44
23	B	609	CLA	C4D-CHA	2.54	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.54	1.47	1.38
23	c	501	CLA	C4B-NB	-2.54	1.34	1.37
23	C	510	CLA	C4D-CHA	2.54	1.47	1.38
23	B	606	CLA	C4D-CHA	2.54	1.47	1.38
23	C	502	CLA	C1B-C2B	2.53	1.49	1.43
23	b	611	CLA	C3B-C4B	2.53	1.48	1.42
23	C	511	CLA	C4D-CHA	2.53	1.47	1.38
23	b	612	CLA	C4D-CHA	2.53	1.47	1.38
23	B	608	CLA	C1B-C2B	2.53	1.49	1.43
23	c	503	CLA	C3D-C4D	-2.53	1.38	1.44
23	B	616	CLA	C3B-C2B	2.53	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	C1C-C2C	2.53	1.49	1.44
40	v	201	HEC	CAC-C3C	2.53	1.57	1.51
23	c	508	CLA	C1B-NB	-2.52	1.34	1.37
23	b	612	CLA	C4C-C3C	2.52	1.49	1.45
23	C	507	CLA	C3D-C4D	-2.52	1.38	1.44
23	B	608	CLA	C3B-C4B	2.52	1.48	1.42
23	C	509	CLA	C3B-C2B	2.52	1.49	1.41
23	c	509	CLA	C4C-C3C	2.52	1.49	1.45
23	A	406[B]	CLA	C4D-CHA	2.52	1.47	1.38
23	d	404[B]	CLA	C1B-C2B	2.52	1.49	1.43
23	b	614	CLA	C3D-C4D	-2.51	1.38	1.44
23	c	503	CLA	C4D-CHA	2.51	1.47	1.38
26	l	101	SQD	C6-S	-2.51	1.68	1.77
23	b	610	CLA	C1B-C2B	2.51	1.49	1.43
31	M	101	LMT	O2B-C2B	-2.51	1.37	1.43
23	B	609	CLA	C1C-C2C	2.51	1.49	1.44
23	C	506	CLA	C4D-CHA	2.51	1.47	1.38
23	C	504	CLA	C4D-CHA	2.50	1.47	1.38
23	D	402[B]	CLA	C1C-C2C	2.50	1.49	1.44
23	d	402[B]	CLA	C4D-CHA	2.50	1.47	1.38
23	b	605	CLA	C1B-C2B	2.50	1.49	1.43
23	B	605	CLA	C1C-C2C	2.50	1.49	1.44
23	A	405[B]	CLA	C4B-NB	-2.49	1.34	1.37
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	a	404[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	c	506	CLA	C4D-CHA	2.49	1.47	1.38
23	B	602	CLA	C4D-CHA	2.49	1.47	1.38
23	c	510	CLA	C4B-NB	-2.49	1.34	1.37
23	c	505	CLA	C4D-CHA	2.49	1.47	1.38
31	B	627	LMT	O3'-C3'	-2.49	1.37	1.43
31	T	101	LMT	O3'-C3'	-2.49	1.37	1.43
34	B	624	HTG	C1-S1	-2.49	1.76	1.80
23	b	603	CLA	C4D-CHA	2.49	1.47	1.38
23	d	404[B]	CLA	C4C-C3C	2.48	1.49	1.45
23	b	608	CLA	C3D-C4D	-2.48	1.38	1.44
23	b	606	CLA	C3D-C4D	-2.48	1.38	1.44
23	a	404[B]	CLA	C4D-CHA	2.48	1.47	1.38
23	b	601	CLA	C1C-C2C	2.48	1.49	1.44
23	a	404[A]	CLA	C4D-CHA	2.48	1.47	1.38
31	m	103	LMT	O2B-C2B	-2.48	1.37	1.43
23	d	402[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	B	611	CLA	C4D-CHA	2.47	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C4C-C3C	2.47	1.49	1.45
23	b	609	CLA	C1C-C2C	2.47	1.49	1.44
31	B	627	LMT	C3'-C2'	2.47	1.58	1.52
29	D	405[B]	PL9	C6-C5	2.47	1.48	1.35
23	c	505	CLA	C4B-NB	-2.47	1.34	1.37
38	f	101	HEM	C1C-C2C	-2.47	1.40	1.45
23	c	502	CLA	C4D-CHA	2.47	1.47	1.38
23	B	606	CLA	C1B-C2B	2.47	1.49	1.43
23	c	502	CLA	C3B-C2B	2.47	1.49	1.41
23	B	614	CLA	C1C-C2C	2.47	1.49	1.44
23	b	606	CLA	C1B-C2B	2.46	1.49	1.43
23	B	603	CLA	C3B-C4B	2.46	1.48	1.42
23	b	616	CLA	C4B-NB	-2.46	1.34	1.37
31	B	629	LMT	O3'-C3'	-2.46	1.37	1.43
23	C	513	CLA	C3D-C4D	-2.46	1.38	1.44
23	c	513	CLA	C4D-CHA	2.46	1.47	1.38
26	X	101	SQD	C6-S	-2.46	1.68	1.77
23	b	608	CLA	C4D-CHA	2.46	1.47	1.38
23	C	512	CLA	C3B-C2B	2.45	1.49	1.41
23	C	506	CLA	C1C-C2C	2.45	1.49	1.44
23	b	606	CLA	C1C-C2C	2.45	1.49	1.44
23	B	601	CLA	C1B-C2B	2.45	1.49	1.43
23	C	509	CLA	C1C-C2C	2.45	1.49	1.44
23	D	402[B]	CLA	C4C-C3C	2.45	1.49	1.45
23	b	615	CLA	C3B-C4B	2.45	1.48	1.42
23	b	616	CLA	C4D-CHA	2.45	1.47	1.38
23	b	602	CLA	C4B-NB	-2.44	1.34	1.37
23	b	608	CLA	C1B-C2B	2.44	1.49	1.43
23	C	511	CLA	C1C-C2C	2.44	1.49	1.44
23	b	605	CLA	C4B-NB	-2.44	1.34	1.37
23	a	405[A]	CLA	C3D-C4D	-2.44	1.38	1.44
31	C	525	LMT	O2'-C2'	-2.44	1.37	1.43
23	b	614	CLA	C4D-CHA	2.44	1.47	1.38
23	A	406[A]	CLA	C1B-C2B	2.44	1.49	1.43
23	D	402[B]	CLA	C4D-CHA	2.44	1.47	1.38
23	a	404[B]	CLA	C4C-C3C	2.44	1.49	1.45
23	B	603	CLA	C4C-C3C	2.44	1.49	1.45
23	A	406[B]	CLA	C1C-C2C	2.43	1.49	1.44
23	A	404[B]	CLA	C3B-C4B	2.43	1.48	1.42
23	C	507	CLA	C3B-C4B	2.43	1.48	1.42
33	C	521	LMG	O1-C1	2.43	1.44	1.40
23	B	606	CLA	C3D-C4D	-2.43	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42
23	B	608	CLA	C3B-C2B	2.42	1.49	1.41
23	b	613	CLA	C3B-C4B	2.42	1.48	1.42
23	C	505	CLA	C4C-C3C	2.42	1.49	1.45
23	c	504	CLA	C4C-C3C	2.42	1.49	1.45
23	c	509	CLA	C3B-C4B	2.42	1.48	1.42
31	e	101	LMT	O3'-C3'	-2.42	1.37	1.43
23	C	512	CLA	C3D-C4D	-2.42	1.38	1.44
23	b	604	CLA	C4B-NB	-2.42	1.34	1.37
23	A	405[B]	CLA	C3D-C4D	-2.42	1.38	1.44
23	B	602	CLA	C3D-C4D	-2.41	1.38	1.44
23	c	504	CLA	C3B-C4B	2.41	1.48	1.42
23	B	601	CLA	C4D-CHA	2.41	1.47	1.38
23	A	405[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	A	406[A]	CLA	C1C-C2C	2.41	1.49	1.44
35	C	519	DGD	O2G-C2G	-2.41	1.40	1.46
29	d	407[B]	PL9	C6-C5	2.41	1.47	1.35
23	C	514	CLA	C3B-C4B	2.41	1.48	1.42
31	b	621	LMT	C3'-C2'	2.41	1.58	1.52
23	c	501	CLA	C1B-NB	-2.41	1.34	1.37
23	B	605	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	504	CLA	C3D-C4D	-2.40	1.38	1.44
23	b	602	CLA	C3D-C4D	-2.40	1.38	1.44
23	A	405[B]	CLA	C1C-C2C	2.40	1.49	1.44
23	c	508	CLA	C3B-C2B	2.40	1.49	1.41
23	C	514	CLA	C3B-C2B	2.40	1.49	1.41
23	b	610	CLA	C3D-C4D	-2.40	1.38	1.44
23	D	402[A]	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	610	CLA	C4C-C3C	2.39	1.49	1.45
23	b	608	CLA	C1C-C2C	2.39	1.49	1.44
23	d	402[B]	CLA	C4B-NB	-2.39	1.34	1.37
23	a	407	CLA	C4D-CHA	2.39	1.46	1.38
23	b	602	CLA	C4D-CHA	2.39	1.46	1.38
23	B	612	CLA	C3B-C2B	2.39	1.49	1.41
23	b	612	CLA	C3B-C2B	2.39	1.49	1.41
23	b	603	CLA	C1C-C2C	2.39	1.49	1.44
23	b	601	CLA	C3B-C2B	2.39	1.49	1.41
23	b	616	CLA	C3D-C4D	-2.39	1.38	1.44
23	D	403	CLA	C4D-CHA	2.39	1.46	1.38
23	C	514	CLA	C1C-C2C	2.39	1.49	1.44
23	c	511	CLA	C3B-C4B	2.38	1.48	1.42
23	C	505	CLA	C3B-C4B	2.38	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	CMC-C2C	2.38	1.55	1.50
23	C	511	CLA	C3D-C4D	-2.38	1.38	1.44
23	d	404[A]	CLA	C4D-CHA	2.38	1.46	1.38
27	A	418	GOL	C3-C2	2.38	1.61	1.51
23	b	615	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	615	CLA	C4C-C3C	2.37	1.49	1.45
23	a	405[B]	CLA	C3D-C4D	-2.37	1.38	1.44
23	C	510	CLA	C3B-C2B	2.37	1.49	1.41
23	a	404[B]	CLA	C1C-C2C	2.37	1.49	1.44
23	B	603	CLA	C3B-C2B	2.37	1.49	1.41
23	C	512	CLA	C4C-C3C	2.36	1.49	1.45
34	B	622	HTG	C1'-S1	-2.36	1.78	1.81
23	B	613	CLA	C3B-C2B	2.36	1.49	1.41
23	B	616	CLA	C3B-C4B	2.36	1.48	1.42
23	c	510	CLA	C4C-C3C	2.36	1.49	1.45
23	b	613	CLA	C3B-C2B	2.36	1.49	1.41
23	b	610	CLA	C4B-NB	-2.35	1.34	1.37
23	c	506	CLA	C3B-C4B	2.35	1.48	1.42
23	C	504	CLA	C1B-C2B	2.35	1.48	1.43
23	B	610	CLA	C3D-C4D	-2.35	1.38	1.44
29	d	407[A]	PL9	C6-C5	2.35	1.47	1.35
23	b	614	CLA	C1C-C2C	2.35	1.49	1.44
23	A	408	CLA	C3B-C2B	2.35	1.49	1.41
23	c	504	CLA	C3B-C2B	2.35	1.49	1.41
23	B	616	CLA	C3D-C4D	-2.35	1.38	1.44
23	c	506	CLA	C4C-C3C	2.35	1.49	1.45
27	A	418	GOL	O2-C2	-2.35	1.36	1.43
23	d	404[B]	CLA	C3D-C4D	-2.35	1.38	1.44
24	A	416[A]	PHO	C3D-C4D	-2.35	1.37	1.41
24	A	416[A]	PHO	C3A-C2A	-2.34	1.52	1.54
23	C	509	CLA	C3B-C4B	2.34	1.48	1.42
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
23	b	613	CLA	OBD-CAD	2.34	1.26	1.22
23	b	603	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	510	CLA	C4C-C3C	2.34	1.49	1.45
24	d	403[B]	PHO	C4B-NB	-2.34	1.34	1.38
23	b	608	CLA	C3B-C2B	2.34	1.49	1.41
29	D	405[A]	PL9	C6-C5	2.34	1.47	1.35
23	b	604	CLA	C1C-C2C	2.34	1.49	1.44
23	D	402[B]	CLA	C3D-C4D	-2.34	1.38	1.44
23	c	506	CLA	C3D-C4D	-2.34	1.38	1.44
23	C	513	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C4B-NB	-2.34	1.34	1.37
26	X	101	SQD	O6-C1	2.33	1.44	1.40
23	c	511	CLA	C3B-C2B	2.33	1.49	1.41
34	B	621	HTG	O5-C1	2.33	1.46	1.42
23	b	612	CLA	C3D-C4D	-2.33	1.38	1.44
23	a	404[B]	CLA	C3B-C2B	2.33	1.49	1.41
23	C	508	CLA	C4C-C3C	2.33	1.49	1.45
23	c	501	CLA	C3D-C4D	-2.33	1.38	1.44
24	a	406[A]	PHO	CBD-CGD	-2.33	1.49	1.52
23	b	603	CLA	C3B-C2B	2.33	1.49	1.41
23	c	510	CLA	C3B-C2B	2.33	1.49	1.41
23	a	404[A]	CLA	C3B-C2B	2.32	1.49	1.41
23	B	608	CLA	C1C-NC	-2.32	1.34	1.37
23	A	404[A]	CLA	C3B-C2B	2.32	1.49	1.41
31	a	416	LMT	O3'-C3'	-2.32	1.37	1.43
23	b	611	CLA	C4D-CHA	2.32	1.46	1.38
23	c	513	CLA	C3D-C4D	-2.32	1.38	1.44
23	b	614	CLA	C3B-C2B	2.32	1.49	1.41
40	V	201	HEC	CMC-C2C	2.32	1.55	1.50
23	c	501	CLA	C1C-C2C	2.32	1.49	1.44
31	M	101	LMT	O3'-C3'	-2.32	1.37	1.43
23	c	513	CLA	C4C-C3C	2.32	1.49	1.45
23	B	609	CLA	C3D-C4D	-2.32	1.38	1.44
34	b	622	HTG	O5-C1	2.32	1.46	1.42
23	C	511	CLA	C3B-C4B	2.32	1.48	1.42
23	b	609	CLA	C3D-C4D	-2.32	1.38	1.44
38	f	101	HEM	C1D-ND	-2.31	1.34	1.38
23	A	406[B]	CLA	C3D-C4D	-2.31	1.39	1.44
31	F	101	LMT	O3'-C3'	-2.31	1.37	1.43
23	d	405	CLA	C1B-C2B	2.31	1.48	1.43
23	d	404[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	d	404[A]	CLA	C3D-C4D	-2.30	1.39	1.44
23	D	403	CLA	C4B-NB	-2.30	1.35	1.37
23	B	603	CLA	C4D-CHA	2.30	1.46	1.38
23	B	613	CLA	C4C-C3C	2.30	1.49	1.45
35	h	102	DGD	O5D-C1E	2.30	1.44	1.40
23	d	405	CLA	C1B-NB	-2.29	1.35	1.37
23	b	611	CLA	C3B-C2B	2.29	1.48	1.41
23	A	404[B]	CLA	C3D-C4D	-2.28	1.39	1.44
23	C	503	CLA	C3B-C2B	2.28	1.48	1.41
23	C	505	CLA	C3B-C2B	2.28	1.48	1.41
24	A	416[B]	PHO	C4B-NB	-2.28	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	502	CLA	C3D-C4D	-2.28	1.39	1.44
23	c	503	CLA	C4C-C3C	2.28	1.49	1.45
23	d	404[B]	CLA	C3B-C4B	2.28	1.48	1.42
23	c	512	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	615	CLA	MG-NA	2.27	2.11	2.06
23	a	404[B]	CLA	C3B-C4B	2.27	1.48	1.42
23	B	602	CLA	C3B-C2B	2.27	1.48	1.41
23	C	506	CLA	C3D-C4D	-2.26	1.39	1.44
29	D	405[B]	PL9	C2-C3	2.26	1.40	1.34
23	b	613	CLA	C1C-C2C	2.26	1.48	1.44
24	A	416[A]	PHO	C4B-NB	-2.26	1.34	1.38
23	c	507	CLA	C3B-C4B	2.26	1.48	1.42
23	c	511	CLA	C4C-C3C	2.26	1.48	1.45
31	A	417	LMT	O2'-C2'	-2.25	1.37	1.43
23	C	505	CLA	C3D-C4D	-2.25	1.39	1.44
23	c	502	CLA	C3B-C4B	2.25	1.48	1.42
23	c	512	CLA	C1C-C2C	2.25	1.48	1.44
23	a	404[A]	CLA	C1C-C2C	2.25	1.48	1.44
24	a	406[B]	PHO	C4B-NB	-2.25	1.34	1.38
23	b	601	CLA	C4C-C3C	2.25	1.48	1.45
23	B	613	CLA	C3B-C4B	2.25	1.48	1.42
23	C	508	CLA	C3D-C4D	-2.25	1.39	1.44
23	d	405	CLA	C4C-C3C	2.25	1.48	1.45
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
31	B	628	LMT	O2'-C2'	-2.24	1.37	1.43
23	C	509	CLA	C1C-NC	-2.24	1.34	1.37
23	b	604	CLA	C3B-C2B	2.24	1.48	1.41
35	c	518	DGD	O2G-C2G	-2.24	1.41	1.46
23	d	404[A]	CLA	C3B-C4B	2.24	1.48	1.42
23	B	602	CLA	C4C-C3C	2.24	1.48	1.45
23	b	605	CLA	C1C-C2C	2.24	1.48	1.44
23	B	603	CLA	C1C-C2C	2.23	1.48	1.44
23	B	608	CLA	C1C-C2C	2.23	1.48	1.44
23	B	601	CLA	C3B-C2B	2.23	1.48	1.41
23	d	404[B]	CLA	C3B-C2B	2.23	1.48	1.41
23	C	514	CLA	C3D-C4D	-2.23	1.39	1.44
23	C	507	CLA	C1D-C2D	2.22	1.49	1.45
23	C	512	CLA	C1C-NC	-2.22	1.34	1.37
23	a	405[B]	CLA	C4C-C3C	2.22	1.48	1.45
23	B	601	CLA	C4C-C3C	2.21	1.48	1.45
23	C	513	CLA	C3B-C2B	2.21	1.48	1.41
23	b	607	CLA	C3D-C4D	-2.21	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	402[B]	CLA	C3B-C2B	2.21	1.48	1.41
35	C	518[A]	DGD	O5D-C1E	2.21	1.44	1.40
23	D	402[A]	CLA	C4C-C3C	2.21	1.48	1.45
23	c	508	CLA	C3D-C4D	-2.21	1.39	1.44
27	D	412	GOL	O2-C2	-2.21	1.36	1.43
40	V	201	HEC	FE-NB	2.21	2.01	1.94
23	c	506	CLA	C3B-C2B	2.21	1.48	1.41
31	m	103	LMT	C3'-C2'	2.20	1.57	1.52
23	d	402[A]	CLA	C4B-NB	-2.20	1.35	1.37
23	C	510	CLA	C3D-C4D	-2.20	1.39	1.44
23	B	601	CLA	C1C-NC	-2.20	1.34	1.37
23	B	604	CLA	C3D-C4D	-2.20	1.39	1.44
23	B	613	CLA	C3D-C4D	-2.20	1.39	1.44
24	A	416[A]	PHO	C1D-ND	-2.20	1.34	1.38
23	B	604	CLA	C1C-C2C	2.19	1.48	1.44
23	D	402[A]	CLA	C3B-C2B	2.19	1.48	1.41
23	B	610	CLA	C4B-NB	-2.19	1.35	1.37
23	C	503	CLA	C4D-CHA	2.19	1.46	1.38
23	D	402[B]	CLA	C3B-C4B	2.19	1.47	1.42
23	c	505	CLA	C3D-C4D	-2.19	1.39	1.44
29	a	413[A]	PL9	C2-C3	2.19	1.40	1.34
23	b	607	CLA	C3B-C4B	2.19	1.47	1.42
31	T	101	LMT	O2'-C2'	-2.19	1.37	1.43
23	c	509	CLA	C3B-C2B	2.19	1.48	1.41
24	A	407[B]	PHO	CBD-CGD	-2.19	1.49	1.52
31	T	101	LMT	O3B-C3B	-2.18	1.37	1.43
23	b	608	CLA	C4C-C3C	2.18	1.48	1.45
23	d	404[B]	CLA	C1C-C2C	2.18	1.48	1.44
24	a	406[B]	PHO	C1D-ND	-2.18	1.34	1.38
40	V	201	HEC	CMB-C2B	2.18	1.55	1.50
35	H	102	DGD	O2G-C2G	-2.18	1.41	1.46
23	c	507	CLA	C3D-C4D	-2.17	1.39	1.44
24	A	416[B]	PHO	C3D-C4D	-2.17	1.38	1.41
23	B	612	CLA	C1C-NC	-2.17	1.34	1.37
23	B	614	CLA	C4C-C3C	2.17	1.48	1.45
38	E	102	HEM	C3B-C4B	2.17	1.49	1.44
23	c	504	CLA	C3D-C4D	-2.17	1.39	1.44
23	b	610	CLA	C3B-C2B	2.16	1.48	1.41
23	B	608	CLA	C3D-C4D	-2.16	1.39	1.44
23	A	404[B]	CLA	C3B-C2B	2.16	1.48	1.41
23	B	616	CLA	C1C-NC	-2.16	1.34	1.37
23	D	402[A]	CLA	C3B-C4B	2.16	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	417	LMT	O3'-C3'	-2.16	1.37	1.43
25	d	406	BCR	C30-C25	-2.15	1.50	1.53
23	b	603	CLA	C1B-NB	-2.15	1.35	1.37
23	A	404[B]	CLA	C1C-C2C	2.15	1.48	1.44
23	A	408	CLA	C1C-NC	-2.15	1.34	1.37
29	a	413[B]	PL9	C2-C3	2.14	1.40	1.34
24	a	406[A]	PHO	C4B-NB	-2.14	1.34	1.38
23	b	614	CLA	C4C-C3C	2.14	1.48	1.45
23	B	601	CLA	C3D-C4D	-2.14	1.39	1.44
23	C	513	CLA	C4C-C3C	2.14	1.48	1.45
29	d	407[B]	PL9	C2-C3	2.14	1.40	1.34
23	b	606	CLA	C3B-C2B	2.14	1.48	1.41
23	c	513	CLA	C3B-C2B	2.14	1.48	1.41
23	c	502	CLA	C3D-C4D	-2.13	1.39	1.44
23	A	404[B]	CLA	C1D-C2D	2.13	1.49	1.45
24	d	403[A]	PHO	C4B-NB	-2.13	1.34	1.38
23	c	510	CLA	C3D-C4D	-2.13	1.39	1.44
23	b	601	CLA	C1B-C2B	2.13	1.48	1.43
24	A	407[A]	PHO	C4B-NB	-2.12	1.34	1.38
29	A	414[A]	PL9	C2-C1	-2.12	1.39	1.44
23	C	511	CLA	C3B-C2B	2.12	1.48	1.41
23	B	611	CLA	C3D-C4D	-2.12	1.39	1.44
31	a	416	LMT	O2'-C2'	-2.12	1.38	1.43
23	C	510	CLA	C1C-NC	-2.12	1.34	1.37
23	c	509	CLA	C3D-C4D	-2.12	1.39	1.44
31	b	627	LMT	O3'-C3'	-2.12	1.38	1.43
31	B	627	LMT	O5'-C5'	-2.12	1.39	1.44
23	d	402[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	B	604	CLA	C1A-CHA	2.12	1.51	1.43
23	c	512	CLA	C4C-C3C	2.12	1.48	1.45
23	B	604	CLA	MG-NA	2.11	2.11	2.06
34	D	410	HTG	C1-S1	-2.11	1.77	1.80
23	B	612	CLA	C3B-C4B	2.11	1.47	1.42
23	b	613	CLA	C3D-C4D	-2.11	1.39	1.44
23	C	502	CLA	C4C-C3C	2.11	1.48	1.45
40	V	201	HEC	CMA-C3A	2.11	1.55	1.50
23	C	503	CLA	C4C-C3C	2.11	1.48	1.45
23	c	507	CLA	C1D-C2D	2.11	1.49	1.45
35	c	518	DGD	O5D-C1E	2.10	1.43	1.40
23	b	605	CLA	C3D-C4D	-2.10	1.39	1.44
23	C	504	CLA	C4C-C3C	2.10	1.48	1.45
23	C	509	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	627	LMT	O4'-C4B	-2.10	1.38	1.43
26	l	101	SQD	O6-C1	2.10	1.43	1.40
24	A	407[A]	PHO	C1B-NB	-2.09	1.34	1.38
23	C	504	CLA	C3B-C2B	2.09	1.48	1.41
23	A	405[B]	CLA	C3B-C2B	2.09	1.48	1.41
31	e	101	LMT	O2B-C2B	-2.09	1.38	1.43
23	c	506	CLA	C1C-C2C	2.09	1.48	1.44
23	B	603	CLA	C3D-C4D	-2.09	1.39	1.44
23	b	613	CLA	C4C-C3C	2.09	1.48	1.45
23	C	506	CLA	C4B-NB	-2.09	1.35	1.37
23	a	405[A]	CLA	C4C-C3C	2.08	1.48	1.45
40	v	201	HEC	CAB-C3B	2.08	1.56	1.51
23	A	405[B]	CLA	C4C-C3C	2.08	1.48	1.45
23	C	502	CLA	C3B-C2B	2.08	1.48	1.41
24	d	403[B]	PHO	C1B-NB	-2.08	1.34	1.38
23	B	604	CLA	C4C-C3C	2.08	1.48	1.45
23	B	607	CLA	C4C-C3C	2.08	1.48	1.45
23	d	404[A]	CLA	C3B-C2B	2.07	1.48	1.41
23	b	605	CLA	C1D-C2D	2.07	1.49	1.45
23	B	604	CLA	C3B-C2B	2.07	1.48	1.41
23	b	607	CLA	C3B-C2B	2.07	1.48	1.41
38	E	102	HEM	C1D-ND	-2.07	1.34	1.38
31	T	101	LMT	O1'-C1'	-2.07	1.36	1.40
23	b	609	CLA	C1C-NC	-2.07	1.34	1.37
23	b	605	CLA	C3B-C2B	2.07	1.48	1.41
24	a	406[B]	PHO	C3A-C2A	-2.07	1.52	1.54
23	B	615	CLA	C4B-NB	-2.07	1.35	1.37
24	A	407[A]	PHO	C1D-ND	-2.07	1.34	1.38
31	B	628	LMT	O3'-C3'	-2.06	1.38	1.43
23	C	507	CLA	C3B-C2B	2.06	1.48	1.41
23	a	404[B]	CLA	C3D-C4D	-2.06	1.39	1.44
40	v	201	HEC	CMD-C2D	2.06	1.55	1.50
23	c	513	CLA	C1D-C2D	2.06	1.49	1.45
31	e	101	LMT	O3B-C3B	-2.06	1.38	1.43
23	B	612	CLA	C4C-C3C	2.06	1.48	1.45
23	b	616	CLA	C3B-C2B	2.06	1.48	1.41
23	c	508	CLA	C1C-NC	-2.06	1.34	1.37
31	b	621	LMT	O3'-C3'	-2.06	1.38	1.43
23	a	407	CLA	C3B-C2B	2.05	1.48	1.41
23	d	405	CLA	C3D-C4D	-2.05	1.39	1.44
23	b	607	CLA	C1A-CHA	2.05	1.51	1.43
23	a	407	CLA	C4C-C3C	2.05	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1C-NC	-2.05	1.34	1.37
29	D	405[A]	PL9	C2-C3	2.04	1.40	1.34
23	C	508	CLA	C3B-C4B	2.04	1.47	1.42
27	o	303	GOL	C1-C2	2.04	1.60	1.51
24	d	403[A]	PHO	C1B-NB	-2.03	1.34	1.38
23	D	403	CLA	C3D-C4D	-2.03	1.39	1.44
31	e	101	LMT	O2'-C2'	-2.03	1.38	1.43
23	C	503	CLA	C3D-C4D	-2.03	1.39	1.44
23	C	512	CLA	C1A-CHA	2.03	1.51	1.43
23	b	616	CLA	C4C-C3C	2.03	1.48	1.45
32	L	101[B]	LHG	O7-C5	-2.02	1.41	1.46
32	b	629[A]	LHG	O7-C5	-2.02	1.41	1.46
23	B	607	CLA	C3B-C2B	2.02	1.48	1.41
23	C	509	CLA	C1A-CHA	2.02	1.51	1.43
31	B	629	LMT	O2'-C2'	-2.02	1.38	1.43
23	b	602	CLA	CHB-C4A	-2.02	1.32	1.37
23	d	402[B]	CLA	C1C-C2C	2.02	1.48	1.44
23	b	603	CLA	C4C-C3C	2.02	1.48	1.45
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
23	b	602	CLA	C1B-C2B	2.02	1.48	1.43
27	b	624	GOL	C3-C2	2.02	1.60	1.51
31	m	103	LMT	O3B-C3B	-2.02	1.38	1.43
31	m	103	LMT	O3'-C3'	-2.01	1.38	1.43
29	A	414[B]	PL9	C2-C1	-2.01	1.39	1.44
31	t	101	LMT	O2'-C2'	-2.01	1.38	1.43
24	d	403[B]	PHO	C1D-ND	-2.01	1.34	1.38
23	b	601	CLA	C3D-C4D	-2.00	1.39	1.44
23	a	405[B]	CLA	C3B-C2B	2.00	1.48	1.41
24	d	403[A]	PHO	CBD-CGD	-2.00	1.49	1.52

All (3324) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	17.33	121.85	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.61	90.73	107.16
24	d	403[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	d	403[B]	PHO	C2D-C1D-ND	11.76	117.64	109.53
24	A	416[B]	PHO	C2D-C1D-ND	11.64	117.56	109.53
24	A	407[B]	PHO	C2D-C1D-ND	11.45	117.43	109.53
24	A	407[A]	PHO	C2D-C1D-ND	11.43	117.42	109.53
23	B	611	CLA	C1D-ND-C4D	-11.26	98.34	106.33
24	a	406[A]	PHO	C2D-C1D-ND	11.21	117.26	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406[B]	PHO	C2D-C1D-ND	10.98	117.11	109.53
23	B	612	CLA	C1D-ND-C4D	-10.94	98.56	106.33
24	A	416[A]	PHO	C2D-C1D-ND	10.73	116.93	109.53
23	B	611	CLA	CHB-C1B-NB	-10.49	113.15	124.26
23	b	605	CLA	C1D-ND-C4D	-10.47	98.90	106.33
23	a	407	CLA	C1D-ND-C4D	-10.35	98.99	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-10.11	99.15	106.33
23	b	611	CLA	C1D-ND-C4D	-9.98	99.25	106.33
23	B	614	CLA	C1D-ND-C4D	-9.87	99.33	106.33
23	B	601	CLA	C1D-ND-C4D	-9.78	99.39	106.33
23	B	611	CLA	C2D-C1D-ND	9.77	117.31	110.10
23	a	405[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	B	612	CLA	C2D-C1D-ND	9.67	117.23	110.10
23	c	503	CLA	C1D-ND-C4D	-9.66	99.47	106.33
23	c	511	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	a	407	CLA	C2D-C1D-ND	9.62	117.19	110.10
23	B	606	CLA	C1D-ND-C4D	-9.60	99.51	106.33
23	c	501	CLA	C1D-ND-C4D	-9.60	99.52	106.33
23	B	615	CLA	C1D-ND-C4D	-9.59	99.52	106.33
23	A	408	CLA	C1D-ND-C4D	-9.55	99.55	106.33
23	c	505	CLA	C1D-ND-C4D	-9.50	99.59	106.33
23	B	602	CLA	C1D-ND-C4D	-9.47	99.60	106.33
23	b	605	CLA	C2D-C1D-ND	9.46	117.08	110.10
23	B	606	CLA	C2D-C1D-ND	9.44	117.06	110.10
23	C	502	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	B	607	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	C	504	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	C	506	CLA	C1D-ND-C4D	-9.34	99.70	106.33
23	b	611	CLA	C2D-C1D-ND	9.33	116.98	110.10
23	b	616	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	B	605	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	c	506	CLA	C1D-ND-C4D	-9.26	99.75	106.33
23	C	514	CLA	C1D-ND-C4D	-9.25	99.76	106.33
23	b	615	CLA	C1D-ND-C4D	-9.25	99.77	106.33
23	d	405	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	B	609	CLA	C1D-ND-C4D	-9.19	99.81	106.33
23	b	614	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	c	513	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	D	402[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	606	CLA	C1D-ND-C4D	-9.14	99.84	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	C1D-ND-C4D	-9.12	99.85	106.33
23	b	610	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	A	405[A]	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	C	511	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	a	404[B]	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	b	612	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	d	404[B]	CLA	C1D-ND-C4D	-9.07	99.89	106.33
23	A	405[A]	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	d	404[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	B	616	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	b	603	CLA	C1D-ND-C4D	-8.98	99.95	106.33
23	a	404[A]	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	613	CLA	C2D-C1D-ND	8.94	116.69	110.10
23	b	601	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	D	402[B]	CLA	C1D-ND-C4D	-8.92	99.99	106.33
23	B	607	CLA	C2D-C1D-ND	8.92	116.68	110.10
23	d	402[B]	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	b	614	CLA	C2D-C1D-ND	8.89	116.65	110.10
23	B	610	CLA	C2D-C1D-ND	8.87	116.64	110.10
23	c	504	CLA	C1D-ND-C4D	-8.85	100.05	106.33
23	C	510	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	B	615	CLA	C2D-C1D-ND	8.83	116.61	110.10
23	B	616	CLA	C2D-C1D-ND	8.83	116.61	110.10
23	c	510	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	C	505	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	c	509	CLA	C1D-ND-C4D	-8.82	100.07	106.33
23	a	405[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	B	610	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	a	405[B]	CLA	C2D-C1D-ND	8.80	116.59	110.10
23	b	602	CLA	C1D-ND-C4D	-8.79	100.09	106.33
23	c	501	CLA	C2D-C1D-ND	8.75	116.55	110.10
23	B	605	CLA	C2D-C1D-ND	8.75	116.55	110.10
23	C	512	CLA	C1D-ND-C4D	-8.70	100.15	106.33
23	b	607	CLA	C1D-ND-C4D	-8.68	100.17	106.33
23	B	614	CLA	C2D-C1D-ND	8.67	116.49	110.10
23	d	402[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	C	508	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	C	509	CLA	C1D-ND-C4D	-8.65	100.19	106.33
23	B	613	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	A	406[A]	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	B	603	CLA	C1D-ND-C4D	-8.60	100.23	106.33
23	C	503	CLA	C1D-ND-C4D	-8.60	100.23	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	C2D-C1D-ND	8.59	116.43	110.10
23	A	405[B]	CLA	C1D-ND-C4D	-8.58	100.24	106.33
23	c	502	CLA	C1D-ND-C4D	-8.55	100.26	106.33
23	c	512	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	C	505	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	d	402[A]	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	B	608	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	A	408	CLA	C2D-C1D-ND	8.52	116.38	110.10
23	b	608	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	D	403	CLA	C1D-ND-C4D	-8.52	100.29	106.33
23	b	616	CLA	C2D-C1D-ND	8.48	116.36	110.10
23	D	402[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	C	507	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	c	512	CLA	C2B-C1B-NB	8.46	115.90	110.23
23	B	601	CLA	C2D-C1D-ND	8.45	116.33	110.10
23	c	511	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	B	602	CLA	C2D-C1D-ND	8.40	116.29	110.10
23	c	507	CLA	C1D-ND-C4D	-8.38	100.38	106.33
23	d	402[B]	CLA	C2D-C1D-ND	8.36	116.26	110.10
23	b	602	CLA	C2B-C1B-NB	8.32	115.81	110.23
23	c	508	CLA	C2D-C1D-ND	8.31	116.23	110.10
23	b	615	CLA	C2D-C1D-ND	8.31	116.23	110.10
23	d	405	CLA	C2D-C1D-ND	8.30	116.22	110.10
23	A	404[B]	CLA	C1D-ND-C4D	-8.29	100.45	106.33
23	b	613	CLA	C1D-ND-C4D	-8.27	100.46	106.33
23	c	508	CLA	C1D-ND-C4D	-8.26	100.47	106.33
23	b	604	CLA	C1D-ND-C4D	-8.25	100.47	106.33
23	B	609	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	C	502	CLA	C2D-C1D-ND	8.23	116.17	110.10
23	C	513	CLA	C2B-C1B-NB	8.20	115.73	110.23
23	C	512	CLA	C2D-C1D-ND	8.18	116.13	110.10
23	A	405[B]	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	C	513	CLA	C1D-ND-C4D	-8.16	100.54	106.33
23	C	514	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	b	607	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	B	604	CLA	C1D-ND-C4D	-8.14	100.55	106.33
23	c	510	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	A	406[B]	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	c	503	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	c	506	CLA	C2D-C1D-ND	8.10	116.07	110.10
23	b	609	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	502	CLA	C2D-C1D-ND	8.08	116.06	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	C2D-C1D-ND	8.06	116.05	110.10
23	A	408	CLA	C2B-C1B-NB	8.05	115.63	110.23
23	b	614	CLA	C2B-C1B-NB	8.04	115.62	110.23
23	B	603	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	a	404[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	C	508	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	C	509	CLA	C2D-C1D-ND	7.93	115.94	110.10
23	d	404[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	b	604	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	C	510	CLA	C2D-C1D-ND	7.91	115.93	110.10
23	c	504	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	c	509	CLA	C2D-C1D-ND	7.87	115.90	110.10
23	a	404[B]	CLA	C2D-C1D-ND	7.86	115.90	110.10
23	b	610	CLA	C2D-C1D-ND	7.86	115.90	110.10
23	c	505	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	B	608	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	d	405	CLA	C2B-C1B-NB	7.85	115.49	110.23
23	D	402[B]	CLA	C2D-C1D-ND	7.83	115.87	110.10
23	b	606	CLA	C2D-C1D-ND	7.81	115.86	110.10
23	c	512	CLA	C2D-C1D-ND	7.76	115.82	110.10
23	b	601	CLA	C2D-C1D-ND	7.74	115.81	110.10
23	A	404[B]	CLA	C2B-C1B-NB	7.73	115.42	110.23
23	B	601	CLA	C2B-C1B-NB	7.70	115.39	110.23
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	b	612	CLA	C2D-C1D-ND	7.69	115.77	110.10
23	b	606	CLA	C2B-C1B-NB	7.69	115.39	110.23
23	C	503	CLA	C2D-C1D-ND	7.68	115.76	110.10
23	b	603	CLA	C2D-C1D-ND	7.63	115.73	110.10
23	d	404[B]	CLA	C2D-C1D-ND	7.63	115.73	110.10
23	b	608	CLA	C2D-C1D-ND	7.63	115.73	110.10
34	b	623	HTG	C1'-S1-C1	7.62	114.34	100.09
23	c	507	CLA	C2D-C1D-ND	7.61	115.71	110.10
23	c	513	CLA	C2D-C1D-ND	7.60	115.70	110.10
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	D	403	CLA	C2B-C1B-NB	7.53	115.28	110.23
23	c	513	CLA	C2B-C1B-NB	7.51	115.27	110.23
23	B	608	CLA	C2B-C1B-NB	7.50	115.26	110.23
23	b	616	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	b	603	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	C	514	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	b	601	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	c	503	CLA	C2B-C1B-NB	7.48	115.25	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[B]	CLA	C2B-C1B-NB	7.47	115.24	110.23
23	B	611	CLA	CMB-C2B-C1B	7.47	136.75	125.37
23	c	501	CLA	CHD-C1D-ND	-7.47	117.59	124.45
23	C	506	CLA	C2D-C1D-ND	7.46	115.61	110.10
23	D	403	CLA	C2D-C1D-ND	7.45	115.60	110.10
24	A	407[B]	PHO	O2D-CGD-CBD	7.45	120.44	111.00
23	C	511	CLA	C2D-C1D-ND	7.44	115.58	110.10
23	B	606	CLA	CMD-C2D-C1D	7.43	137.80	124.71
23	a	404[B]	CLA	C2B-C1B-NB	7.42	115.20	110.23
23	c	503	CLA	C4A-NA-C1A	-7.39	103.38	106.71
23	b	602	CLA	C4A-NA-C1A	-7.39	103.39	106.71
24	A	416[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	B	611	CLA	CHD-C4C-C3C	-7.35	114.03	124.84
23	c	501	CLA	CMD-C2D-C1D	7.35	137.67	124.71
23	D	402[B]	CLA	C4A-NA-C1A	-7.32	103.41	106.71
24	A	416[B]	PHO	O2D-CGD-CBD	7.32	120.27	111.00
23	c	505	CLA	C2B-C1B-NB	7.32	115.14	110.23
23	C	511	CLA	CMD-C2D-C1D	7.31	137.59	124.71
23	B	610	CLA	O2D-CGD-CBD	7.26	124.17	111.27
23	B	616	CLA	CHD-C4C-C3C	-7.24	114.19	124.84
23	C	511	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	d	403[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
23	b	616	CLA	C4A-NA-C1A	-7.20	103.47	106.71
24	A	416[B]	PHO	C4D-ND-C1D	-7.20	101.50	108.83
23	A	404[A]	CLA	C2B-C1B-NB	7.20	115.06	110.23
23	B	616	CLA	O2D-CGD-CBD	7.19	124.04	111.27
23	C	513	CLA	C4A-NA-C1A	-7.18	103.48	106.71
24	a	406[B]	PHO	O2D-CGD-CBD	7.18	120.10	111.00
24	a	406[A]	PHO	O2D-CGD-CBD	7.16	120.07	111.00
23	b	608	CLA	C2B-C1B-NB	7.16	115.03	110.23
26	X	101	SQD	O6-C1-C2	7.16	119.48	108.30
23	C	504	CLA	C4A-NA-C1A	-7.15	103.49	106.71
24	a	406[A]	PHO	C1C-C2C-C3C	-7.15	102.67	108.61
23	B	605	CLA	CHD-C4C-C3C	-7.14	114.34	124.84
24	d	403[B]	PHO	O2D-CGD-CBD	7.14	120.04	111.00
23	c	504	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	C	513	CLA	C2D-C1D-ND	7.14	115.36	110.10
23	C	507	CLA	C2D-C1D-ND	7.13	115.36	110.10
23	c	507	CLA	O2D-CGD-CBD	7.13	123.93	111.27
24	A	416[A]	PHO	C2B-C1B-NB	7.12	114.44	109.53
23	C	512	CLA	C2B-C1B-NB	7.12	115.00	110.23
24	d	403[A]	PHO	C2B-C1B-NB	7.11	114.44	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	A	406[A]	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	C	510	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	d	402[B]	CLA	C2B-C1B-NB	7.10	114.99	110.23
23	C	504	CLA	C2B-C1B-NB	7.09	114.99	110.23
24	A	416[B]	PHO	C2B-C1B-NB	7.09	114.42	109.53
23	b	605	CLA	CHD-C4C-C3C	-7.08	114.43	124.84
24	d	403[A]	PHO	C4D-ND-C1D	-7.08	101.62	108.83
23	b	611	CLA	C2B-C1B-NB	7.05	114.96	110.23
23	B	614	CLA	C2B-C1B-NB	7.02	114.94	110.23
23	b	602	CLA	C2D-C1D-ND	7.00	115.26	110.10
23	a	404[A]	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	C	503	CLA	C2B-C1B-NB	6.97	114.90	110.23
23	B	611	CLA	CMD-C2D-C1D	6.96	136.98	124.71
24	d	403[B]	PHO	C4D-ND-C1D	-6.96	101.75	108.83
24	A	407[B]	PHO	C4D-ND-C1D	-6.95	101.76	108.83
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	B	614	CLA	CMD-C2D-C1D	6.91	136.89	124.71
23	a	407	CLA	C2B-C1B-NB	6.91	114.86	110.23
24	d	403[A]	PHO	C1C-C2C-C3C	-6.90	102.87	108.61
23	C	507	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	b	615	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	b	616	CLA	O2D-CGD-CBD	6.86	123.46	111.27
40	V	201	HEC	C1D-ND-C4D	6.86	112.16	105.07
23	B	609	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	a	405[A]	CLA	C2B-C1B-NB	6.86	114.83	110.23
24	d	403[B]	PHO	C2B-C1B-NB	6.86	114.26	109.53
24	A	407[A]	PHO	C4D-ND-C1D	-6.85	101.86	108.83
23	D	402[B]	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	B	604	CLA	C2D-C1D-ND	6.83	115.14	110.10
23	b	616	CLA	CHD-C4C-C3C	-6.83	114.80	124.84
23	A	404[B]	CLA	CMD-C2D-C1D	6.83	136.75	124.71
23	b	605	CLA	C2B-C1B-NB	6.82	114.81	110.23
23	c	510	CLA	C2B-C1B-NB	6.82	114.80	110.23
23	B	615	CLA	C4A-NA-C1A	-6.82	103.64	106.71
23	B	606	CLA	CHD-C1D-ND	-6.79	118.22	124.45
23	C	507	CLA	CMD-C2D-C1D	6.78	136.66	124.71
23	B	610	CLA	C2B-C1B-NB	6.78	114.77	110.23
23	a	407	CLA	CHD-C4C-C3C	-6.75	114.92	124.84
23	c	508	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	c	503	CLA	CMD-C2D-C1D	6.74	136.59	124.71
23	a	405[B]	CLA	C2B-C1B-NB	6.74	114.75	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	C4A-NA-C1A	-6.74	103.68	106.71
23	B	612	CLA	CHD-C4C-C3C	-6.74	114.94	124.84
23	b	615	CLA	C4A-NA-C1A	-6.73	103.68	106.71
23	C	508	CLA	CMD-C2D-C1D	6.72	136.56	124.71
23	b	611	CLA	CMD-C2D-C1D	6.71	136.54	124.71
23	b	613	CLA	C2B-C1B-NB	6.71	114.73	110.23
23	c	502	CLA	C2C-C1C-NC	6.70	116.25	109.97
23	A	405[A]	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	c	513	CLA	CMD-C2D-C1D	6.69	136.50	124.71
23	C	506	CLA	CMD-C2D-C1D	6.68	136.49	124.71
23	B	603	CLA	O2D-CGD-CBD	6.68	123.14	111.27
23	d	402[A]	CLA	C2B-C1B-NB	6.67	114.71	110.23
23	C	507	CLA	C2C-C1C-NC	6.66	116.21	109.97
23	b	605	CLA	CHD-C1D-ND	-6.66	118.33	124.45
23	C	509	CLA	C2C-C1C-NC	6.65	116.21	109.97
23	c	507	CLA	CHD-C1D-ND	-6.65	118.34	124.45
23	C	502	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	B	606	CLA	C4A-NA-C1A	-6.64	103.72	106.71
23	B	609	CLA	C4A-NA-C1A	-6.64	103.72	106.71
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	605	CLA	CMD-C2D-C1D	6.61	136.35	124.71
24	a	406[B]	PHO	C1C-C2C-C3C	-6.60	103.13	108.61
23	c	507	CLA	CMD-C2D-C1D	6.59	136.33	124.71
24	A	407[B]	PHO	C1C-C2C-C3C	-6.59	103.13	108.61
23	C	505	CLA	C2C-C1C-NC	6.59	116.14	109.97
23	C	504	CLA	CMD-C2D-C1D	6.58	136.31	124.71
24	A	416[A]	PHO	C1C-C2C-C3C	-6.58	103.14	108.61
23	c	501	CLA	C2B-C1B-NB	6.56	114.63	110.23
23	A	408	CLA	CHD-C1D-ND	-6.53	118.45	124.45
23	D	402[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	b	609	CLA	CHD-C4C-C3C	-6.52	115.26	124.84
23	d	404[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	A	404[B]	CLA	CHD-C1D-ND	-6.51	118.47	124.45
23	B	613	CLA	C2B-C1B-NB	6.51	114.59	110.23
23	A	404[B]	CLA	C2D-C1D-ND	6.50	114.90	110.10
23	b	606	CLA	CHD-C4C-C3C	-6.50	115.29	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
23	B	615	CLA	CHD-C4C-C3C	-6.48	115.32	124.84
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
26	X	101	SQD	O47-C7-C8	6.45	125.41	111.50
23	c	509	CLA	C2B-C1B-NB	6.45	114.56	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403[B]	PHO	C1C-C2C-C3C	-6.45	103.25	108.61
23	A	408	CLA	CMD-C2D-C1D	6.44	136.07	124.71
23	b	614	CLA	O2D-CGD-CBD	6.44	122.72	111.27
23	B	605	CLA	C2B-C1B-NB	6.44	114.55	110.23
23	C	506	CLA	C2B-C1B-NB	6.43	114.54	110.23
23	b	613	CLA	CHD-C4C-C3C	-6.43	115.39	124.84
23	b	606	CLA	CMD-C2D-C1D	6.42	136.04	124.71
23	B	609	CLA	CMD-C2D-C1D	6.42	136.03	124.71
24	a	406[B]	PHO	C2B-C1B-NB	6.42	113.96	109.53
24	A	416[A]	PHO	C4D-ND-C1D	-6.42	102.30	108.83
24	a	406[A]	PHO	C2B-C1B-NB	6.41	113.95	109.53
23	B	604	CLA	C2C-C1C-NC	6.41	115.98	109.97
23	a	404[B]	CLA	C2C-C1C-NC	6.40	115.97	109.97
23	B	605	CLA	CMD-C2D-C1D	6.40	135.98	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-6.38	103.84	106.71
23	b	604	CLA	C2B-C1B-NB	6.38	114.51	110.23
23	d	404[B]	CLA	C2C-C1C-NC	6.37	115.94	109.97
23	B	602	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
23	b	601	CLA	O2D-CGD-CBD	6.37	122.59	111.27
23	b	607	CLA	C2C-C1C-NC	6.36	115.93	109.97
23	b	615	CLA	CMD-C2D-C1D	6.36	135.92	124.71
23	C	508	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
23	B	616	CLA	C2B-C1B-NB	6.35	114.49	110.23
23	C	513	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
24	a	406[A]	PHO	C4D-ND-C1D	-6.34	102.38	108.83
23	C	509	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	a	405[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	b	610	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
23	D	402[B]	CLA	CMD-C2D-C1D	6.31	135.84	124.71
23	c	502	CLA	C2B-C1B-NB	6.31	114.46	110.23
23	a	405[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	a	405[B]	CLA	CHD-C1D-ND	-6.30	118.67	124.45
23	b	604	CLA	C2C-C1C-NC	6.29	115.87	109.97
23	A	405[B]	CLA	C2B-C1B-NB	6.29	114.45	110.23
23	b	611	CLA	CHD-C4C-C3C	-6.29	115.60	124.84
23	C	512	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	D	402[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	a	404[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	c	510	CLA	CHD-C4C-C3C	-6.26	115.64	124.84
23	c	504	CLA	CHD-C1D-ND	-6.25	118.71	124.45
24	A	407[A]	PHO	C2B-C1B-NB	6.25	113.84	109.53
23	c	513	CLA	CHD-C1D-ND	-6.24	118.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	O2D-CGD-CBD	6.24	122.36	111.27
23	d	405	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	b	612	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	B	615	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	c	503	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
23	B	601	CLA	CHD-C4C-C3C	-6.23	115.68	124.84
23	C	504	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
23	B	601	CLA	CMD-C2D-C1D	6.22	135.68	124.71
23	d	402[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	b	614	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	c	505	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	c	505	CLA	O2D-CGD-CBD	6.21	122.30	111.27
23	b	606	CLA	C4A-NA-C1A	-6.21	103.92	106.71
23	B	615	CLA	C2B-C1B-NB	6.20	114.39	110.23
23	c	508	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	a	404[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	d	404[B]	CLA	CMD-C2D-C1D	6.19	135.62	124.71
23	C	510	CLA	CMD-C2D-C1D	6.19	135.62	124.71
23	c	505	CLA	C4A-NA-C1A	-6.18	103.93	106.71
23	c	504	CLA	CMD-C2D-C1D	6.17	135.59	124.71
40	v	201	HEC	C1D-ND-C4D	6.17	111.44	105.07
23	c	506	CLA	CMD-C2D-C1D	6.17	135.58	124.71
23	b	603	CLA	C4A-NA-C1A	-6.16	103.94	106.71
23	D	402[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	B	609	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	b	601	CLA	C4A-NA-C1A	-6.16	103.94	106.71
23	c	510	CLA	CMD-C2D-C1D	6.16	135.57	124.71
23	c	503	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	B	609	CLA	CHD-C4C-C3C	-6.15	115.79	124.84
24	A	407[A]	PHO	C1C-C2C-C3C	-6.15	103.49	108.61
23	c	512	CLA	C4A-NA-C1A	-6.15	103.94	106.71
23	b	606	CLA	CHD-C1D-ND	-6.15	118.80	124.45
23	c	511	CLA	C2B-C1B-NB	6.14	114.35	110.23
23	A	405[B]	CLA	CMD-C2D-C1D	6.14	135.53	124.71
23	b	601	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	b	616	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	b	611	CLA	CHD-C1D-ND	-6.12	118.83	124.45
23	A	404[B]	CLA	C2C-C1C-NC	6.12	115.70	109.97
23	B	601	CLA	O2D-CGD-CBD	6.11	122.13	111.27
23	d	402[B]	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	d	404[B]	CLA	C2B-C1B-NB	6.11	114.33	110.23
34	D	410	HTG	C1'-S1-C1	6.11	111.51	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	B	607	CLA	CHD-C4C-C3C	-6.10	115.87	124.84
23	d	405	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	b	607	CLA	CMD-C2D-C1D	6.10	135.46	124.71
23	a	405[B]	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
34	c	521	HTG	C1'-S1-C1	6.08	111.47	100.09
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	C	511	CLA	O2D-CGD-CBD	6.07	122.06	111.27
23	c	509	CLA	CMD-C2D-C1D	6.06	135.39	124.71
23	C	507	CLA	CHD-C1D-ND	-6.05	118.89	124.45
23	c	507	CLA	C2B-C1B-NB	6.05	114.29	110.23
23	c	507	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
23	C	511	CLA	CHD-C1D-ND	-6.03	118.91	124.45
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	A	406[B]	CLA	CHD-C1D-ND	-6.03	118.91	124.45
23	d	404[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
24	a	406[B]	PHO	C4D-ND-C1D	-6.03	102.70	108.83
23	b	609	CLA	C2B-C1B-NB	6.02	114.27	110.23
23	D	402[B]	CLA	CHD-C1D-ND	-6.02	118.92	124.45
23	c	504	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	B	610	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	C	514	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	b	610	CLA	C2B-C1B-NB	6.01	114.26	110.23
23	C	502	CLA	CMD-C2D-C1D	6.00	135.29	124.71
23	C	502	CLA	CHD-C4C-C3C	-6.00	116.03	124.84
23	b	608	CLA	C4A-NA-C1A	-5.99	104.01	106.71
23	D	402[B]	CLA	C2C-C1C-NC	5.99	115.58	109.97
23	C	513	CLA	CMD-C2D-C1D	5.99	135.27	124.71
23	b	613	CLA	C2C-C1C-NC	5.99	115.58	109.97
25	Y	101	BCR	C33-C5-C6	-5.99	117.81	124.53
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	a	405[B]	CLA	CMD-C2D-C1D	5.98	135.25	124.71
24	A	416[B]	PHO	C1C-C2C-C3C	-5.97	103.64	108.61
23	c	502	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	c	505	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
23	c	511	CLA	CMD-C2D-C1D	5.96	135.21	124.71
23	a	404[B]	CLA	C4A-NA-C1A	-5.96	104.03	106.71
23	b	605	CLA	O2D-CGD-CBD	5.95	121.84	111.27
23	A	405[B]	CLA	C2C-C1C-NC	5.95	115.55	109.97
23	A	406[B]	CLA	CMD-C2D-C1D	5.95	135.19	124.71
23	c	506	CLA	C2C-C1C-NC	5.94	115.54	109.97
23	c	509	CLA	C2C-C1C-NC	5.94	115.54	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	CMD-C2D-C1D	5.94	135.18	124.71
23	B	606	CLA	C2B-C1B-NB	5.94	114.21	110.23
23	b	612	CLA	C2B-C1B-NB	5.92	114.20	110.23
23	B	615	CLA	CMD-C2D-C1D	5.91	135.13	124.71
23	B	612	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	B	604	CLA	C2B-C1B-NB	5.91	114.19	110.23
23	C	505	CLA	C2B-C1B-NB	5.91	114.19	110.23
23	B	605	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	C	511	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	b	608	CLA	CHD-C4C-C3C	-5.90	116.16	124.84
23	b	612	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	b	610	CLA	CMD-C2D-C1D	5.90	135.11	124.71
23	C	509	CLA	C2B-C1B-NB	5.90	114.19	110.23
23	A	405[B]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414[A]	PL9	C7-C8-C9	-5.89	116.99	126.79
23	A	404[A]	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	A	406[A]	CLA	CHD-C1D-ND	-5.88	119.05	124.45
23	b	602	CLA	O2D-CGD-CBD	5.88	121.71	111.27
23	B	611	CLA	C3D-C2D-C1D	-5.87	97.82	105.83
23	b	615	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
26	A	410[B]	SQD	O6-C1-C2	5.87	117.46	108.30
23	D	402[A]	CLA	C2B-C1B-NB	5.87	114.17	110.23
23	C	508	CLA	O2D-CGD-CBD	5.86	121.67	111.27
23	B	603	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	a	404[B]	CLA	CHD-C1D-ND	-5.84	119.08	124.45
23	a	404[B]	CLA	CMD-C2D-C1D	5.84	135.01	124.71
23	B	603	CLA	C2C-C1C-NC	5.84	115.44	109.97
23	b	604	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
23	B	613	CLA	CHD-C4C-C3C	-5.82	116.28	124.84
23	C	502	CLA	O2D-CGD-CBD	5.82	121.61	111.27
23	A	406[B]	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
23	A	404[A]	CLA	CHD-C1D-ND	-5.81	119.11	124.45
26	l	101	SQD	O6-C1-C2	5.81	117.38	108.30
23	d	402[B]	CLA	C2C-C1C-NC	5.81	115.42	109.97
23	d	402[B]	CLA	CHD-C1D-ND	-5.81	119.12	124.45
23	C	510	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	b	601	CLA	CHD-C1D-ND	-5.80	119.12	124.45
23	c	506	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	b	602	CLA	CMD-C2D-C1D	5.80	134.93	124.71
23	b	601	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
23	C	504	CLA	CHD-C1D-ND	-5.79	119.13	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMD-C2D-C1D	5.79	134.92	124.71
23	c	506	CLA	CHD-C1D-ND	-5.79	119.13	124.45
23	b	602	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	b	611	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	B	616	CLA	C3C-C4C-NC	5.78	117.05	110.57
23	b	614	CLA	CMD-C2D-C1D	5.78	134.89	124.71
23	C	503	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	B	605	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	C	508	CLA	C2B-C1B-NB	5.77	114.10	110.23
23	c	508	CLA	CMD-C2D-C1D	5.76	134.87	124.71
23	A	405[B]	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	d	405	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	a	404[A]	CLA	CMD-C2D-C1D	5.75	134.84	124.71
23	d	402[A]	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	B	608	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	c	506	CLA	C2B-C1B-NB	5.74	114.08	110.23
23	c	512	CLA	CHD-C4C-C3C	-5.74	116.40	124.84
23	B	606	CLA	C3D-C2D-C1D	-5.74	98.00	105.83
23	b	603	CLA	CHD-C4C-C3C	-5.73	116.41	124.84
23	b	615	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	B	607	CLA	C2C-C1C-NC	5.72	115.33	109.97
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	B	601	CLA	CHD-C1D-ND	-5.71	119.20	124.45
23	c	509	CLA	C1-C2-C3	-5.70	116.18	126.04
34	d	412	HTG	C1'-S1-C1	5.70	110.76	100.09
23	c	507	CLA	C4A-NA-C1A	-5.70	104.14	106.71
23	c	508	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	D	403	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
23	C	506	CLA	CHD-C1D-ND	-5.69	119.23	124.45
23	B	614	CLA	O2D-CGD-CBD	5.69	121.37	111.27
34	B	622	HTG	C1'-S1-C1	5.69	110.72	100.09
23	D	402[B]	CLA	CHD-C4C-C3C	-5.68	116.49	124.84
23	C	514	CLA	CHD-C1D-ND	-5.68	119.23	124.45
23	C	514	CLA	CMD-C2D-C1D	5.68	134.72	124.71
23	d	402[B]	CLA	CMD-C2D-C1D	5.68	134.72	124.71
23	b	611	CLA	O2D-CGD-CBD	5.68	121.35	111.27
23	B	614	CLA	CHD-C1D-ND	-5.67	119.24	124.45
23	B	606	CLA	O2D-CGD-CBD	5.67	121.35	111.27
23	b	602	CLA	CHD-C1D-ND	-5.67	119.24	124.45
23	d	404[A]	CLA	C2B-C1B-NB	5.67	114.03	110.23
23	c	505	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	B	608	CLA	C2C-C1C-NC	5.66	115.28	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	C4A-NA-C1A	-5.65	104.16	106.71
23	A	408	CLA	CHD-C4C-C3C	-5.65	116.53	124.84
23	d	404[B]	CLA	CHD-C1D-ND	-5.65	119.26	124.45
23	c	513	CLA	C4A-NA-C1A	-5.65	104.17	106.71
23	c	512	CLA	O2D-CGD-CBD	5.64	121.30	111.27
23	b	609	CLA	CMD-C2D-C1D	5.64	134.66	124.71
23	d	404[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	b	608	CLA	C2C-C1C-NC	5.64	115.25	109.97
23	B	604	CLA	CMD-C2D-C1D	5.63	134.63	124.71
23	c	509	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	C	506	CLA	CHD-C4C-C3C	-5.62	116.58	124.84
23	B	604	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
23	d	402[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	B	613	CLA	CMD-C2D-C1D	5.60	134.58	124.71
24	A	407[B]	PHO	C2B-C1B-NB	5.60	113.39	109.53
23	C	502	CLA	CHD-C1D-ND	-5.60	119.31	124.45
23	D	403	CLA	CMD-C2D-C1D	5.59	134.57	124.71
23	C	505	CLA	CMD-C2D-C1D	5.59	134.57	124.71
23	C	506	CLA	C2C-C1C-NC	5.59	115.20	109.97
23	C	505	CLA	CHD-C1D-ND	-5.58	119.33	124.45
26	a	409[A]	SQD	O6-C1-C2	5.58	117.02	108.30
23	A	405[A]	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	d	404[B]	CLA	C4A-NA-C1A	-5.57	104.20	106.71
23	B	603	CLA	C2B-C1B-NB	5.56	113.96	110.23
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	C	510	CLA	CHD-C1D-ND	-5.56	119.34	124.45
23	a	404[B]	CLA	CHD-C4C-C3C	-5.56	116.66	124.84
23	b	610	CLA	O2D-CGD-CBD	5.56	121.15	111.27
23	d	404[A]	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	a	405[A]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	b	607	CLA	CHD-C4C-C3C	-5.55	116.68	124.84
23	C	503	CLA	C2C-C1C-NC	5.55	115.17	109.97
23	d	404[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	b	605	CLA	C3D-C2D-C1D	-5.54	98.26	105.83
23	C	506	CLA	C4A-NA-C1A	-5.54	104.22	106.71
25	t	102	BCR	C33-C5-C6	-5.54	118.31	124.53
23	c	513	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	c	507	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	b	612	CLA	C4A-NA-C1A	-5.53	104.22	106.71
23	B	603	CLA	CMD-C2D-C1D	5.52	134.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	C	514	CLA	C2C-C1C-NC	5.51	115.13	109.97
23	C	510	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	c	501	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	B	602	CLA	O2D-CGD-CBD	5.49	121.02	111.27
23	c	511	CLA	CHD-C1D-ND	-5.48	119.42	124.45
23	c	513	CLA	C2C-C1C-NC	5.47	115.10	109.97
23	B	608	CLA	O2D-CGD-CBD	5.47	120.99	111.27
38	E	102	HEM	CAD-CBD-CGD	5.47	125.37	113.60
23	c	512	CLA	CMD-C2D-C1D	5.45	134.32	124.71
23	C	508	CLA	C2C-C1C-NC	5.45	115.08	109.97
23	a	405[B]	CLA	C4A-NA-C1A	-5.45	104.26	106.71
23	b	608	CLA	O2D-CGD-CBD	5.45	120.95	111.27
23	C	505	CLA	CHD-C4C-C3C	-5.45	116.83	124.84
23	b	613	CLA	C3C-C4C-NC	5.44	116.68	110.57
23	d	402[A]	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	c	504	CLA	O2D-CGD-CBD	5.44	120.93	111.27
23	C	508	CLA	CHD-C1D-ND	-5.43	119.46	124.45
23	A	408	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	a	407	CLA	CHD-C1D-ND	-5.42	119.48	124.45
23	C	511	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	d	404[B]	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	B	607	CLA	CHD-C1D-ND	-5.41	119.49	124.45
23	B	602	CLA	C4A-NA-C1A	-5.41	104.28	106.71
23	C	503	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	b	604	CLA	C4A-NA-C1A	-5.40	104.28	106.71
25	b	617	BCR	C7-C8-C9	-5.39	118.09	126.23
26	b	620	SQD	O6-C1-C2	5.39	116.72	108.30
23	d	405	CLA	O2D-CGD-CBD	5.39	120.84	111.27
23	a	404[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	c	510	CLA	C2C-C1C-NC	5.38	115.02	109.97
23	b	615	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	B	613	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	B	607	CLA	C2B-C1B-NB	5.37	113.83	110.23
23	B	604	CLA	O2D-CGD-CBD	5.37	120.81	111.27
23	C	512	CLA	C2C-C1C-NC	5.37	115.00	109.97
24	d	403[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	B	612	CLA	C3C-C4C-NC	5.36	116.59	110.57
23	A	406[B]	CLA	C2C-C1C-NC	5.36	115.00	109.97
25	D	404	BCR	C7-C8-C9	-5.36	118.14	126.23
23	D	403	CLA	CHD-C1D-ND	-5.36	119.53	124.45
23	b	603	CLA	CHD-C1D-ND	-5.36	119.53	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	CHD-C1D-ND	-5.35	119.53	124.45
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
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	608	CLA	C4A-NA-C1A	-5.35	104.30	106.71
23	B	614	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
23	B	611	CLA	CHD-C1D-ND	-5.34	119.54	124.45
23	C	513	CLA	O2D-CGD-CBD	5.34	120.76	111.27
23	a	405[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	b	603	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	A	406[A]	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	C	507	CLA	CHD-C4C-C3C	-5.32	117.02	124.84
23	B	614	CLA	C2C-C1C-NC	5.32	114.96	109.97
23	B	605	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
23	b	603	CLA	CMD-C2D-C1D	5.32	134.08	124.71
23	C	506	CLA	O2D-CGD-CBD	5.32	120.72	111.27
23	c	512	CLA	CHD-C1D-ND	-5.32	119.57	124.45
23	b	611	CLA	C3D-C2D-C1D	-5.32	98.58	105.83
23	c	508	CLA	C4A-NA-C1A	-5.32	104.32	106.71
23	b	609	CLA	CHD-C1D-ND	-5.31	119.57	124.45
23	B	616	CLA	C4A-NA-C1A	-5.31	104.32	106.71
23	a	404[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	B	602	CLA	CMD-C2D-C1D	5.29	134.03	124.71
23	D	403	CLA	C4A-NA-C1A	-5.29	104.33	106.71
23	C	509	CLA	C3C-C4C-NC	5.29	116.50	110.57
23	B	605	CLA	C2C-C1C-NC	5.28	114.92	109.97
23	D	403	CLA	O2D-CGD-CBD	5.28	120.65	111.27
23	B	614	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	B	611	CLA	CMC-C2C-C1C	5.27	133.07	125.04
23	c	501	CLA	C3D-C2D-C1D	-5.27	98.63	105.83
26	X	101	SQD	C1-O5-C5	-5.27	103.35	113.69
23	b	613	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	b	612	CLA	C3C-C4C-NC	5.26	116.47	110.57
23	b	608	CLA	CHD-C1D-ND	-5.25	119.63	124.45
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	b	607	CLA	C2B-C1B-NB	5.25	113.75	110.23
23	B	602	CLA	C2C-C1C-NC	5.25	114.89	109.97
23	B	610	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
23	B	607	CLA	O2D-CGD-CBD	5.24	120.58	111.27
23	A	408	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	b	604	CLA	CMD-C2D-C1D	5.23	133.92	124.71
23	c	512	CLA	C3B-C2B-C1B	-5.22	100.86	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	409[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	C	509	CLA	CMD-C2D-C1D	5.21	133.89	124.71
24	A	416[B]	PHO	C3D-C4D-ND	5.20	114.81	107.72
23	b	608	CLA	CMD-C2D-C1D	5.20	133.88	124.71
29	A	414[B]	PL9	C7-C8-C9	-5.20	118.14	126.79
26	l	101	SQD	O47-C7-C8	5.20	122.70	111.50
23	C	512	CLA	CHD-C1D-ND	-5.19	119.68	124.45
23	B	610	CLA	CHD-C1D-ND	-5.19	119.69	124.45
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	d	402[A]	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	B	606	CLA	C2C-C1C-NC	5.18	114.82	109.97
24	A	407[A]	PHO	C3D-C4D-ND	5.17	114.77	107.72
23	B	607	CLA	C4A-NA-C1A	-5.17	104.38	106.71
23	b	614	CLA	C2C-C1C-NC	5.17	114.81	109.97
23	B	603	CLA	CHD-C1D-ND	-5.16	119.71	124.45
34	C	522	HTG	C1'-S1-C1	5.16	109.75	100.09
23	A	408	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
23	C	509	CLA	O2D-CGD-CBD	5.16	120.43	111.27
23	b	605	CLA	C2C-C1C-NC	5.16	114.80	109.97
23	B	603	CLA	C4A-NA-C1A	-5.15	104.39	106.71
23	c	501	CLA	CHD-C4C-C3C	-5.15	117.28	124.84
23	C	513	CLA	C3B-C2B-C1B	-5.13	100.97	107.16
23	b	605	CLA	C4A-NA-C1A	-5.12	104.40	106.71
23	c	511	CLA	C2C-C1C-NC	5.12	114.77	109.97
24	A	407[B]	PHO	C3D-C4D-ND	5.12	114.70	107.72
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.71
26	a	409[B]	SQD	O6-C1-C2	5.12	116.30	108.30
23	B	609	CLA	C2C-C1C-NC	5.11	114.76	109.97
26	A	410[B]	SQD	C1-O5-C5	-5.11	103.66	113.69
23	A	405[B]	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
23	b	614	CLA	CHD-C1D-ND	-5.11	119.76	124.45
23	C	514	CLA	C3B-C2B-C1B	-5.10	101.00	107.16
23	B	607	CLA	CMD-C2D-C1D	5.10	133.71	124.71
23	B	612	CLA	CMD-C2D-C1D	5.10	133.71	124.71
23	c	504	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	c	502	CLA	C1C-C2C-C3C	-5.10	101.60	106.96
23	C	510	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	b	609	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	d	403[A]	PHO	C3D-C4D-ND	5.09	114.66	107.72
23	b	604	CLA	CHD-C1D-ND	-5.08	119.79	124.45
23	b	616	CLA	C3D-C2D-C1D	-5.08	98.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	509	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	B	611	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	b	612	CLA	O2D-CGD-CBD	5.07	120.27	111.27
23	B	616	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
23	B	608	CLA	CHD-C1D-ND	-5.07	119.80	124.45
23	c	504	CLA	C2C-C1C-NC	5.07	114.72	109.97
23	B	610	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	C	505	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	c	502	CLA	O2D-CGD-CBD	5.05	120.25	111.27
23	b	607	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	B	607	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	C	503	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
23	b	603	CLA	O2D-CGD-CBD	5.04	120.22	111.27
33	B	620	LMG	O7-C10-C11	5.03	122.34	111.50
23	B	614	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
24	d	403[B]	PHO	C1-C2-C3	-5.02	117.35	126.04
23	b	604	CLA	C1-C2-C3	-5.02	117.36	126.04
23	b	614	CLA	C3B-C2B-C1B	-5.02	101.10	107.16
23	c	504	CLA	C3B-C2B-C1B	-5.02	101.11	107.16
23	B	604	CLA	C3C-C4C-NC	5.01	116.19	110.57
23	b	607	CLA	CHD-C1D-ND	-5.01	119.85	124.45
26	a	409[B]	SQD	O47-C7-C8	5.01	122.30	111.50
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
24	d	403[B]	PHO	C3D-C4D-ND	5.01	114.55	107.72
23	b	606	CLA	O2D-CGD-CBD	5.00	120.16	111.27
23	A	408	CLA	C3B-C2B-C1B	-5.00	101.13	107.16
23	A	404[B]	CLA	CHD-C4C-C3C	-4.98	117.51	124.84
23	B	602	CLA	CHD-C1D-ND	-4.98	119.88	124.45
23	A	406[B]	CLA	C4A-NA-C1A	-4.98	104.47	106.71
23	b	607	CLA	C3C-C4C-NC	4.97	116.15	110.57
23	B	604	CLA	C4A-NA-C1A	-4.96	104.48	106.71
23	C	508	CLA	C3B-C2B-C1B	-4.96	101.18	107.16
23	b	610	CLA	C2C-C1C-NC	4.96	114.61	109.97
23	C	512	CLA	C3B-C2B-C1B	-4.95	101.18	107.16
23	a	407	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	a	407	CLA	O2D-CGD-CBD	4.95	120.07	111.27
23	b	610	CLA	C4A-NA-C1A	-4.95	104.48	106.71
23	b	613	CLA	CMD-C2D-C1D	4.95	133.44	124.71
38	f	101	HEM	CHC-C4B-NB	4.95	129.79	124.42
23	c	503	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	a	407	CLA	CMD-C2D-C1D	4.95	133.43	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	C3C-C4C-NC	4.94	116.11	110.57
23	a	405[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	B	601	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	B	608	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
23	D	403	CLA	C2C-C1C-NC	4.93	114.59	109.97
23	a	405[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
24	A	416[A]	PHO	C3D-C4D-ND	4.91	114.42	107.72
23	C	513	CLA	CHD-C1D-ND	-4.91	119.94	124.45
23	c	505	CLA	C2C-C1C-NC	4.91	114.57	109.97
26	b	620	SQD	O47-C7-C8	4.91	122.08	111.50
23	C	512	CLA	O2D-CGD-CBD	4.90	119.97	111.27
23	d	402[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	A	404[A]	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
23	B	616	CLA	C2C-C1C-NC	4.88	114.55	109.97
38	E	102	HEM	CHC-C4B-NB	4.88	129.72	124.42
23	a	405[B]	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
23	C	514	CLA	O2D-CGD-CBD	4.88	119.93	111.27
23	b	606	CLA	C2C-C1C-NC	4.88	114.54	109.97
23	c	511	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	b	610	CLA	CHD-C1D-ND	-4.87	119.98	124.45
23	B	605	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	C	510	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	a	405[B]	CLA	O2D-CGD-CBD	4.87	119.91	111.27
23	C	508	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	C	505	CLA	O2D-CGD-CBD	4.86	119.90	111.27
23	C	503	CLA	CMD-C2D-C1D	4.86	133.28	124.71
23	C	510	CLA	C3B-C2B-C1B	-4.86	101.30	107.16
23	c	505	CLA	C3C-C4C-NC	4.85	116.01	110.57
23	B	608	CLA	CMD-C2D-C1D	4.85	133.26	124.71
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	a	404[B]	CLA	C3B-C2B-C1B	-4.84	101.31	107.16
23	c	501	CLA	O2D-CGD-CBD	4.84	119.87	111.27
23	A	405[B]	CLA	C1C-C2C-C3C	-4.84	101.86	106.96
23	d	402[B]	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
34	b	622	HTG	C1-O5-C5	4.84	121.50	112.58
23	B	612	CLA	C2C-C1C-NC	4.84	114.50	109.97
23	c	506	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
23	c	503	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	B	601	CLA	C3B-C2B-C1B	-4.83	101.34	107.16
23	b	612	CLA	C1-C2-C3	-4.83	117.70	126.04
23	c	504	CLA	C3D-C2D-C1D	-4.82	99.25	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CMD-C2D-C1D	4.82	133.21	124.71
23	B	612	CLA	CHD-C1D-ND	-4.82	120.03	124.45
23	b	609	CLA	C4A-NA-C1A	-4.81	104.54	106.71
23	B	615	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	c	506	CLA	C4A-NA-C1A	-4.81	104.55	106.71
23	d	405	CLA	C3B-C2B-C1B	-4.80	101.37	107.16
23	b	609	CLA	C1-C2-C3	-4.80	117.75	126.04
23	b	615	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
24	a	406[B]	PHO	C3D-C4D-ND	4.79	114.25	107.72
23	C	508	CLA	C3C-C4C-NC	4.79	115.94	110.57
25	y	101	BCR	C33-C5-C6	-4.79	119.15	124.53
23	b	604	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	A	406[B]	CLA	O2D-CGD-CBD	4.78	119.77	111.27
23	b	603	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
23	b	609	CLA	C3C-C4C-NC	4.78	115.93	110.57
23	B	603	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	B	616	CLA	O2D-CGD-O1D	-4.77	114.52	123.84
23	C	502	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	A	406[B]	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	b	610	CLA	C1-C2-C3	-4.75	117.83	126.04
23	C	504	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	D	402[B]	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	c	513	CLA	C3B-C2B-C1B	-4.74	101.43	107.16
23	b	602	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
25	d	406	BCR	C7-C8-C9	-4.74	119.07	126.23
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	C	505	CLA	C3C-C4C-NC	4.74	115.89	110.57
23	b	611	CLA	C3C-C4C-NC	4.74	115.89	110.57
23	b	605	CLA	C3D-C4D-ND	4.74	117.90	110.24
23	A	404[B]	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
23	C	511	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
23	d	404[B]	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	b	613	CLA	C3B-C2B-C1B	-4.72	101.47	107.16
23	B	615	CLA	C2C-C1C-NC	4.71	114.39	109.97
23	B	603	CLA	C3C-C4C-NC	4.71	115.86	110.57
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	405[A]	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
23	d	405	CLA	C2C-C1C-NC	4.71	114.39	109.97
23	c	507	CLA	C3B-C2B-C1B	-4.71	101.48	107.16
23	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	C	507	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
23	b	606	CLA	C3B-C2B-C1B	-4.70	101.48	107.16
23	a	407	CLA	C3C-C4C-NC	4.70	115.84	110.57
24	A	416[B]	PHO	C1-C2-C3	-4.70	117.92	126.04
26	f	102	SQD	O47-C7-C8	4.70	121.62	111.50
23	b	601	CLA	C2C-C1C-NC	4.69	114.37	109.97
23	B	612	CLA	C3D-C4D-ND	4.69	117.83	110.24
23	B	601	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	B	606	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	C	502	CLA	C2C-C1C-NC	4.69	114.36	109.97
23	B	602	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	d	402[B]	CLA	C4A-NA-C1A	-4.68	104.60	106.71
26	X	101	SQD	O8-S-C6	4.68	113.20	105.74
23	a	405[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	b	605	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
23	B	613	CLA	O2D-CGD-CBD	4.68	119.59	111.27
33	C	501	LMG	O1-C1-C2	4.68	115.61	108.30
29	a	413[B]	PL9	C7-C3-C4	4.68	120.68	116.88
23	C	504	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
23	b	611	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
24	a	406[A]	PHO	C3D-C4D-ND	4.67	114.08	107.72
23	b	612	CLA	CMD-C2D-C1D	4.67	132.94	124.71
23	d	404[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	b	610	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	b	609	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
33	d	413	LMG	O7-C10-C11	4.66	121.54	111.50
23	c	512	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	B	616	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
23	C	511	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
26	A	410[B]	SQD	C1-C2-C3	-4.65	100.31	110.00
23	A	405[B]	CLA	C4A-NA-C1A	-4.65	104.61	106.71
23	B	602	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
23	D	403	CLA	CMB-C2B-C1B	4.64	132.44	125.37
23	C	507	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	D	402[B]	CLA	C1-C2-C3	-4.63	118.03	126.04
23	c	507	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	D	402[B]	CLA	C3C-C4C-NC	4.63	115.77	110.57
25	c	514	BCR	C11-C10-C9	-4.63	120.70	127.31
23	c	509	CLA	CHD-C1D-ND	-4.63	120.20	124.45
25	H	101	BCR	C38-C26-C25	-4.63	119.33	124.53
23	b	614	CLA	O2D-CGD-O1D	-4.63	114.79	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	c	511	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
23	a	405[B]	CLA	C3D-C4D-ND	4.63	117.72	110.24
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	502	CLA	CMD-C2D-C1D	4.62	132.86	124.71
23	c	510	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	c	502	CLA	C3B-C2B-C1B	-4.61	101.59	107.16
23	B	608	CLA	C3C-C4C-NC	4.61	115.75	110.57
23	C	512	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	C	505	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
29	a	413[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	B	611	CLA	C4A-NA-C1A	-4.60	104.64	106.71
26	b	620	SQD	C1-O5-C5	-4.60	104.66	113.69
23	C	506	CLA	C3C-C4C-NC	4.60	115.73	110.57
23	B	610	CLA	C4A-NA-C1A	-4.59	104.64	106.71
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	A	406[B]	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	c	502	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	a	405[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	B	609	CLA	C3C-C4C-NC	4.58	115.70	110.57
23	c	508	CLA	CHD-C1D-ND	-4.57	120.25	124.45
23	c	509	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	c	509	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
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	d	402[B]	CLA	O2D-CGD-CBD	4.57	119.39	111.27
23	b	608	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
23	C	503	CLA	O2D-CGD-CBD	4.57	119.38	111.27
23	B	603	CLA	O2D-CGD-O1D	-4.56	114.92	123.84
23	b	606	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
33	C	501	LMG	C7-O1-C1	-4.56	104.83	113.74
23	D	402[A]	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	A	406[A]	CLA	C3D-C4D-ND	4.55	117.61	110.24
23	c	508	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
23	c	512	CLA	C2C-C1C-NC	4.55	114.23	109.97
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	b	605	CLA	C3C-C4C-NC	4.54	115.67	110.57
23	c	508	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	c	510	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	b	601	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
23	d	402[B]	CLA	C1C-C2C-C3C	-4.54	102.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C1C-C2C-C3C	-4.53	102.19	106.96
23	c	510	CLA	O2D-CGD-CBD	4.53	119.32	111.27
23	C	512	CLA	C3C-C4C-NC	4.53	115.65	110.57
23	c	508	CLA	O2D-CGD-CBD	4.53	119.32	111.27
26	f	102	SQD	C1-O5-C5	4.53	122.58	113.69
23	b	611	CLA	C4A-NA-C1A	-4.53	104.67	106.71
29	A	414[B]	PL9	C32-C33-C34	-4.53	116.75	127.66
23	c	501	CLA	C4A-NA-C1A	-4.53	104.67	106.71
24	A	416[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
23	C	509	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	b	613	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	c	501	CLA	CMB-C2B-C1B	4.51	132.25	125.37
23	c	505	CLA	C3D-C4D-ND	4.51	117.54	110.24
23	c	508	CLA	C1-C2-C3	-4.51	118.24	126.04
23	a	405[B]	CLA	C2C-C1C-NC	4.51	114.20	109.97
23	C	507	CLA	C4A-NA-C1A	-4.51	104.68	106.71
23	b	602	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	D	402[B]	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	d	402[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	c	502	CLA	CHD-C1D-ND	-4.48	120.33	124.45
23	a	404[A]	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	C	513	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	C	509	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	b	602	CLA	C3D-C4D-ND	4.48	117.48	110.24
23	C	507	CLA	O2D-CGD-CBD	4.47	119.22	111.27
23	C	507	CLA	C1C-C2C-C3C	-4.47	102.25	106.96
23	B	613	CLA	CHD-C1D-ND	-4.47	120.35	124.45
23	a	407	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	c	503	CLA	O2D-CGD-CBD	4.46	119.19	111.27
23	a	405[B]	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
23	C	513	CLA	C2C-C1C-NC	4.46	114.15	109.97
23	A	406[B]	CLA	C3D-C4D-ND	4.46	117.45	110.24
23	B	605	CLA	C3C-C4C-NC	4.46	115.57	110.57
23	c	501	CLA	O2D-CGD-O1D	-4.46	115.13	123.84
23	C	503	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	B	609	CLA	C3D-C4D-ND	4.46	117.44	110.24
23	B	607	CLA	C1C-C2C-C3C	-4.45	102.27	106.96
23	B	602	CLA	C3D-C4D-ND	4.45	117.44	110.24
23	b	601	CLA	C3B-C2B-C1B	-4.45	101.78	107.16
23	C	504	CLA	O2D-CGD-CBD	4.45	119.18	111.27
23	D	403	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	b	603	CLA	C3D-C4D-ND	4.45	117.44	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	C2C-C1C-NC	4.45	114.14	109.97
23	a	407	CLA	C3D-C4D-ND	4.45	117.43	110.24
23	b	604	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	d	404[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	B	612	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	B	605	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	B	611	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	a	407	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	c	510	CLA	C1-C2-C3	-4.44	118.37	126.04
23	d	404[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	B	602	CLA	C3C-C4C-NC	4.44	115.55	110.57
23	b	612	CLA	CHD-C1D-ND	-4.44	120.38	124.45
23	C	513	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	B	611	CLA	C1D-CHD-C4C	-4.43	116.50	126.06
23	B	607	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	c	503	CLA	C3B-C2B-C1B	-4.42	101.82	107.16
23	C	506	CLA	CMB-C2B-C1B	4.42	132.10	125.37
23	b	616	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
23	c	505	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
23	b	611	CLA	C3D-C4D-ND	4.41	117.38	110.24
23	c	506	CLA	C3D-C4D-ND	4.41	117.38	110.24
23	d	404[B]	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	c	507	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
23	B	613	CLA	C1-C2-C3	-4.41	118.42	126.04
23	c	503	CLA	C1D-CHD-C4C	-4.40	116.58	126.06
23	b	616	CLA	C1D-CHD-C4C	-4.39	116.58	126.06
23	D	402[A]	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
33	c	520	LMG	O6-C5-C4	4.39	117.67	109.69
23	d	402[A]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	b	612	CLA	C3B-C2B-C1B	-4.39	101.87	107.16
23	C	506	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	d	404[B]	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
23	b	602	CLA	C3C-C4C-NC	4.38	115.48	110.57
29	a	413[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	B	611	CLA	C3D-C4D-ND	4.38	117.32	110.24
23	b	613	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	B	604	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
23	b	615	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
23	d	405	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	B	601	CLA	C3C-C4C-NC	4.37	115.47	110.57
23	b	612	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	C	508	CLA	C4A-NA-C1A	-4.37	104.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	C1-C2-C3	-4.37	118.49	126.04
23	d	404[B]	CLA	C1C-C2C-C3C	-4.36	102.37	106.96
23	b	603	CLA	C1D-CHD-C4C	-4.36	116.65	126.06
23	b	601	CLA	C3D-C4D-ND	4.36	117.29	110.24
23	c	510	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
23	B	615	CLA	C3D-C4D-ND	4.36	117.29	110.24
23	B	601	CLA	C3D-C4D-ND	4.36	117.29	110.24
23	C	511	CLA	C1-C2-C3	-4.36	118.51	126.04
23	b	608	CLA	CMC-C2C-C1C	4.34	131.65	125.04
23	B	615	CLA	C3C-C4C-NC	4.34	115.44	110.57
33	a	415	LMG	O7-C10-C11	4.34	120.85	111.50
23	c	513	CLA	C3D-C4D-ND	4.34	117.25	110.24
23	b	610	CLA	C3D-C2D-C1D	-4.33	99.92	105.83
25	H	101	BCR	C16-C17-C18	-4.33	121.13	127.31
23	a	404[B]	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	A	404[B]	CLA	C1C-C2C-C3C	-4.33	102.41	106.96
23	C	503	CLA	C3D-C2D-C1D	-4.33	99.93	105.83
23	B	613	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
23	C	509	CLA	C1-C2-C3	-4.32	118.56	126.04
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	D	403	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
23	B	612	CLA	O2D-CGD-O1D	-4.32	115.39	123.84
23	a	404[B]	CLA	C1C-C2C-C3C	-4.32	102.42	106.96
23	B	601	CLA	C4A-NA-C1A	-4.32	104.76	106.71
38	E	102	HEM	C4C-NC-C1C	4.32	109.58	105.35
23	B	615	CLA	CMB-C2B-C1B	4.32	131.94	125.37
23	A	408	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.52	110.52
23	D	402[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	a	404[B]	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	b	603	CLA	C3C-C4C-NC	4.30	115.40	110.57
23	b	604	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
23	A	404[B]	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	C	504	CLA	C3D-C4D-ND	4.30	117.19	110.24
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
32	E	101[B]	LHG	O7-C7-C8	4.29	120.76	111.50
23	b	610	CLA	C3D-C4D-ND	4.29	117.19	110.24
23	c	503	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	A	404[B]	CLA	C3B-C4B-NB	4.29	114.49	110.52
23	C	504	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	c	513	CLA	O2D-CGD-CBD	4.29	118.89	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CHD-C1D-ND	-4.29	120.51	124.45
23	a	404[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	b	616	CLA	C3C-C4C-NC	4.28	115.38	110.57
23	B	606	CLA	C3B-C2B-C1B	-4.28	101.99	107.16
23	b	615	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	B	610	CLA	O2A-CGA-CBA	4.28	125.34	111.91
23	B	604	CLA	C1-C2-C3	-4.28	118.64	126.04
23	B	610	CLA	C3C-C4C-NC	4.28	115.37	110.57
38	E	102	HEM	C1B-NB-C4B	4.27	109.48	105.07
23	C	511	CLA	C1C-C2C-C3C	-4.27	102.47	106.96
23	c	513	CLA	C1D-CHD-C4C	-4.27	116.85	126.06
25	Y	101	BCR	C16-C17-C18	-4.27	121.22	127.31
23	a	404[B]	CLA	C3B-C4B-NB	4.27	114.47	110.52
23	a	405[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	A	404[B]	CLA	C3D-C2D-C1D	-4.25	100.03	105.83
23	C	511	CLA	C4A-NA-C1A	-4.25	104.80	106.71
23	c	509	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
23	c	501	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
23	d	405	CLA	C4A-NA-C1A	-4.24	104.80	106.71
23	D	402[B]	CLA	O2D-CGD-CBD	4.24	118.80	111.27
23	C	511	CLA	C3D-C4D-ND	4.24	117.10	110.24
23	c	504	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	C	503	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	C	502	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	a	404[B]	CLA	C3C-C4C-NC	4.23	115.32	110.57
23	D	402[B]	CLA	C3D-C4D-ND	4.23	117.09	110.24
23	C	514	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	C	503	CLA	C3C-C4C-NC	4.23	115.31	110.57
23	C	507	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	C	505	CLA	C4A-NA-C1A	-4.23	104.81	106.71
23	c	507	CLA	C3C-C4C-NC	4.22	115.31	110.57
23	c	511	CLA	C3C-C4C-NC	4.22	115.31	110.57
23	d	402[B]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	404[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	b	607	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
26	A	410[B]	SQD	O9-S-C6	4.22	111.95	106.94
23	a	405[A]	CLA	C3B-C2B-C1B	-4.21	102.07	107.16
23	b	606	CLA	C3C-C4C-NC	4.21	115.30	110.57
23	b	609	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	C	506	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
23	c	511	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	B	609	CLA	O2D-CGD-CBD	4.21	118.75	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C3D-C4D-ND	4.21	117.04	110.24
23	c	511	CLA	C3B-C4B-NB	4.21	114.42	110.52
23	a	404[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	D	403	CLA	C3D-C4D-ND	4.21	117.04	110.24
33	C	521	LMG	O6-C5-C4	4.20	117.31	109.69
23	d	404[B]	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	B	605	CLA	C1D-CHD-C4C	-4.19	117.01	126.06
23	c	501	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	c	505	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
23	A	406[B]	CLA	C1C-C2C-C3C	-4.19	102.55	106.96
33	C	501	LMG	O7-C10-C11	4.19	120.53	111.50
23	b	615	CLA	C1D-CHD-C4C	-4.19	117.02	126.06
26	a	409[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	b	606	CLA	C3D-C4D-ND	4.19	117.01	110.24
23	A	405[B]	CLA	O2D-CGD-CBD	4.19	118.70	111.27
23	C	506	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
23	C	509	CLA	C3B-C4B-NB	4.18	114.39	110.52
31	t	101	LMT	C3'-C4'-C5'	-4.18	101.35	110.93
23	c	505	CLA	O2D-CGD-O1D	-4.18	115.67	123.84
23	a	404[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	B	608	CLA	C3D-C4D-ND	4.17	116.99	110.24
23	C	513	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
23	b	615	CLA	C3D-C4D-ND	4.17	116.98	110.24
29	a	413[B]	PL9	C7-C8-C9	-4.17	119.86	126.79
23	d	402[B]	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
23	D	403	CLA	C3B-C2B-C1B	-4.16	102.14	107.16
23	C	502	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	B	607	CLA	C3D-C4D-ND	4.16	116.96	110.24
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	C	504	CLA	C1D-CHD-C4C	-4.16	117.09	126.06
23	C	508	CLA	CMB-C2B-C1B	4.15	131.70	125.37
33	Z	101	LMG	O7-C10-C11	4.15	120.45	111.50
23	B	604	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	b	614	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
23	C	514	CLA	C3C-C4C-NC	4.15	115.23	110.57
23	B	612	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	d	404[B]	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	b	610	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
23	b	603	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	b	604	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
23	B	608	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
23	a	404[B]	CLA	CAA-C2A-C3A	-4.15	101.43	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	101	HEM	C4C-NC-C1C	4.14	109.41	105.35
23	C	505	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
23	D	402[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	c	501	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
23	c	511	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	B	604	CLA	CHD-C1D-ND	-4.13	120.66	124.45
23	C	512	CLA	C4A-NA-C1A	-4.13	104.85	106.71
23	a	404[B]	CLA	C1D-CHD-C4C	-4.13	117.14	126.06
23	C	514	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
23	B	603	CLA	C1D-CHD-C4C	-4.13	117.15	126.06
23	c	508	CLA	C1C-C2C-C3C	-4.13	102.62	106.96
23	c	513	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	b	607	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	c	503	CLA	C3C-C4C-NC	4.12	115.20	110.57
23	b	614	CLA	C4A-NA-C1A	-4.12	104.85	106.71
23	B	605	CLA	C4-C3-C5	4.12	122.21	115.27
23	B	605	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	b	614	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	A	404[B]	CLA	O2D-CGD-CBD	4.12	118.59	111.27
23	c	504	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	d	402[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
29	A	414[A]	PL9	C7-C3-C2	-4.12	117.89	123.30
23	d	404[A]	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	d	404[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
23	b	605	CLA	O2D-CGD-O1D	-4.11	115.80	123.84
23	c	502	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
23	B	614	CLA	C1-C2-C3	-4.10	118.95	126.04
23	b	616	CLA	C2C-C1C-NC	4.10	113.81	109.97
23	b	616	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	B	614	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	c	506	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
23	C	511	CLA	C3B-C4B-NB	4.10	114.31	110.52
23	b	606	CLA	C4-C3-C5	4.09	122.16	115.27
23	a	404[A]	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	b	614	CLA	C3C-C4C-NC	4.09	115.16	110.57
23	b	602	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
31	B	627	LMT	C1'-O5'-C5'	-4.09	105.67	113.69
23	B	616	CLA	C3D-C4D-ND	4.08	116.84	110.24
25	d	406	BCR	C15-C14-C13	-4.08	121.49	127.31
23	A	404[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
23	D	403	CLA	C3C-C4C-NC	4.08	115.14	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
35	C	517[A]	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	B	615	CLA	C3B-C2B-C1B	-4.08	102.24	107.16
23	A	404[B]	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
26	a	409[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
26	A	410[B]	SQD	C44-O6-C1	-4.07	105.78	113.74
23	c	509	CLA	C3B-C4B-NB	4.07	114.29	110.52
23	b	602	CLA	O2D-CGD-O1D	-4.07	115.88	123.84
23	b	611	CLA	C3B-C4B-NB	4.07	114.29	110.52
23	D	402[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	C	509	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
23	B	613	CLA	CAC-C3C-C4C	4.07	130.09	124.81
23	c	506	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	b	606	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
23	C	509	CLA	C3D-C4D-ND	4.06	116.81	110.24
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
23	C	512	CLA	C3D-C4D-ND	4.06	116.80	110.24
23	d	402[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
38	E	102	HEM	CHD-C4C-NC	4.06	128.83	124.44
23	c	506	CLA	C3B-C4B-NB	4.06	114.28	110.52
23	c	512	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	B	603	CLA	CAC-C3C-C4C	4.05	130.07	124.81
33	m	101	LMG	O7-C10-C11	4.05	120.23	111.50
23	C	503	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	c	502	CLA	C3D-C4D-ND	4.04	116.77	110.24
23	d	402[B]	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
23	B	602	CLA	C1D-CHD-C4C	-4.04	117.35	126.06
33	c	520	LMG	O7-C10-C11	4.04	120.20	111.50
23	a	405[B]	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	A	404[B]	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
33	C	520	LMG	O7-C10-C11	4.03	120.19	111.50
26	l	101	SQD	C3-C4-C5	4.03	117.43	110.24
23	b	603	CLA	CAA-C2A-C3A	-4.02	101.78	112.78
23	b	609	CLA	O2D-CGD-CBD	4.02	118.41	111.27
23	d	402[B]	CLA	CAA-C2A-C3A	-4.02	101.78	112.78
23	b	603	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
23	b	616	CLA	CMB-C2B-C1B	4.02	131.49	125.37
23	B	610	CLA	CAA-C2A-C3A	-4.01	101.79	112.78
23	c	510	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	D	403	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	d	402[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	B	612	CLA	C2B-C1B-NB	4.01	112.92	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	601	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
23	B	614	CLA	C3D-C4D-ND	4.01	116.72	110.24
34	B	621	HTG	O5-C1-C2	4.00	115.35	110.31
23	C	505	CLA	C3D-C4D-ND	4.00	116.71	110.24
33	C	521	LMG	O7-C10-C11	4.00	120.11	111.50
23	d	404[A]	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
23	b	616	CLA	O2D-CGD-O1D	-4.00	116.03	123.84
23	c	506	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	B	606	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	d	402[A]	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
23	C	508	CLA	C1D-CHD-C4C	-3.99	117.46	126.06
23	B	601	CLA	C1D-CHD-C4C	-3.98	117.46	126.06
23	B	610	CLA	C3D-C4D-ND	3.98	116.68	110.24
23	C	510	CLA	C3C-C4C-NC	3.98	115.04	110.57
23	c	509	CLA	C3D-C4D-ND	3.98	116.67	110.24
29	a	413[B]	PL9	C32-C33-C34	-3.97	118.09	127.66
23	C	510	CLA	C3D-C4D-ND	3.97	116.67	110.24
23	D	402[B]	CLA	C1C-C2C-C3C	-3.97	102.78	106.96
29	a	413[B]	PL9	C7-C3-C2	-3.96	118.09	123.30
23	B	603	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
23	B	612	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	C	507	CLA	C3B-C4B-NB	3.95	114.18	110.52
23	b	604	CLA	C3B-C4B-NB	3.95	114.18	110.52
23	a	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	606	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
26	X	101	SQD	C44-O6-C1	-3.95	106.02	113.74
23	c	511	CLA	C4A-NA-C1A	-3.95	104.93	106.71
23	C	511	CLA	C1D-CHD-C4C	-3.95	117.54	126.06
23	A	406[A]	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
23	A	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	B	604	CLA	C1D-CHD-C4C	-3.95	117.55	126.06
32	d	409[B]	LHG	O7-C7-C8	3.94	120.00	111.50
23	b	607	CLA	O2D-CGD-CBD	3.94	118.27	111.27
23	B	611	CLA	CHD-C4C-NC	3.94	130.41	124.20
29	d	407[A]	PL9	C42-C43-C44	-3.93	118.19	127.66
23	b	607	CLA	C3B-C2B-C1B	-3.93	102.41	107.16
23	C	512	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
23	B	616	CLA	C4C-C3C-C2C	-3.93	101.17	106.90
23	b	612	CLA	C3D-C2D-C1D	-3.93	100.47	105.83
23	D	402[A]	CLA	C1-C2-C3	-3.93	119.25	126.04
23	a	405[A]	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	b	606	CLA	O2D-CGD-O1D	-3.93	116.16	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	612	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	B	605	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
23	A	405[B]	CLA	C3B-C2B-C1B	-3.92	102.43	107.16
23	c	509	CLA	C3C-C4C-NC	3.92	114.97	110.57
23	c	512	CLA	C1D-CHD-C4C	-3.92	117.61	126.06
23	c	504	CLA	C3B-C4B-NB	3.92	114.15	110.52
26	a	409[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
33	c	519	LMG	O7-C10-C11	3.91	119.93	111.50
23	A	405[A]	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
29	A	414[A]	PL9	C7-C3-C4	3.91	120.05	116.88
23	A	405[B]	CLA	C3D-C4D-ND	3.91	116.56	110.24
23	C	502	CLA	C3C-C4C-NC	3.90	114.95	110.57
23	b	604	CLA	CMC-C2C-C1C	3.90	130.98	125.04
23	C	508	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	B	610	CLA	CMB-C2B-C1B	3.90	131.31	125.37
23	B	610	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
23	c	502	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	B	603	CLA	C3D-C4D-ND	3.90	116.54	110.24
23	b	607	CLA	C3B-C4B-NB	3.90	114.13	110.52
29	a	413[A]	PL9	C32-C33-C34	-3.89	118.28	127.66
23	b	613	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
23	C	513	CLA	C3D-C4D-ND	3.89	116.53	110.24
23	c	510	CLA	CMC-C2C-C1C	3.89	130.96	125.04
23	d	402[B]	CLA	C3C-C4C-NC	3.89	114.93	110.57
23	b	615	CLA	O2D-CGD-CBD	3.88	118.17	111.27
23	C	505	CLA	C3B-C4B-NB	3.88	114.12	110.52
32	A	419[A]	LHG	O8-C23-O10	-3.88	113.79	123.59
35	c	516[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	A	405[A]	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	d	405	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	B	602	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	c	507	CLA	C3D-C4D-ND	3.88	116.52	110.24
23	B	607	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
23	b	610	CLA	C1D-CHD-C4C	-3.88	117.69	126.06
23	C	514	CLA	C4A-NA-C1A	-3.88	104.96	106.71
23	c	510	CLA	C3D-C4D-ND	3.88	116.51	110.24
23	C	513	CLA	C1-C2-C3	-3.87	119.34	126.04
25	T	102	BCR	C15-C16-C17	-3.87	115.55	123.47
29	A	414[B]	PL9	C7-C3-C4	3.87	120.02	116.88
23	d	402[A]	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
23	C	507	CLA	C3C-C4C-NC	3.87	114.91	110.57
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
23	A	406[B]	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	B	615	CLA	C1C-C2C-C3C	-3.86	102.89	106.96
23	b	609	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
23	B	616	CLA	C1D-CHD-C4C	-3.86	117.73	126.06
23	b	616	CLA	O2A-CGA-CBA	3.86	124.02	111.91
23	c	507	CLA	CMB-C2B-C1B	3.86	131.25	125.37
23	A	405[B]	CLA	CAA-C2A-C3A	-3.86	102.22	112.78
35	C	518[B]	DGD	O2G-C1B-C2B	3.86	119.81	111.50
23	c	502	CLA	O2D-CGD-O1D	-3.85	116.30	123.84
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	B	604	CLA	C3D-C4D-ND	3.85	116.47	110.24
26	A	412	SQD	O47-C7-C8	3.85	119.80	111.50
25	b	617	BCR	C33-C5-C6	-3.85	120.21	124.53
34	b	622	HTG	C1'-S1-C1	3.84	107.28	100.09
23	C	509	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
24	A	407[B]	PHO	C1A-C2A-C3A	-3.84	99.18	102.84
23	b	608	CLA	C1D-CHD-C4C	-3.84	117.78	126.06
23	C	510	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
29	a	413[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
23	B	606	CLA	C3D-C4D-ND	3.83	116.44	110.24
23	C	514	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	C	502	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
23	b	610	CLA	O2A-CGA-CBA	3.83	123.92	111.91
33	c	520	LMG	C3-C4-C5	3.83	117.06	110.24
23	A	408	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	c	506	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	a	404[B]	CLA	O2D-CGD-CBD	3.82	118.06	111.27
23	b	611	CLA	C1-C2-C3	-3.81	119.44	126.04
23	C	506	CLA	CAC-C3C-C4C	3.81	129.76	124.81
23	c	507	CLA	CMC-C2C-C1C	3.81	130.84	125.04
23	c	508	CLA	C3D-C4D-ND	3.81	116.40	110.24
29	A	414[B]	PL9	C7-C3-C2	-3.81	118.29	123.30
25	C	515	BCR	C7-C8-C9	-3.80	120.49	126.23
23	B	614	CLA	C3C-C4C-NC	3.80	114.84	110.57
23	d	402[A]	CLA	CMB-C2B-C1B	3.80	131.16	125.37
25	d	406	BCR	C40-C30-C25	-3.80	104.14	110.30
32	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	416[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
25	B	618	BCR	C29-C30-C25	3.80	116.33	110.48
23	C	513	CLA	C4-C3-C5	3.80	121.66	115.27
23	c	506	CLA	C1-C2-C3	-3.79	119.48	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	407	CLA	C1D-CHD-C4C	-3.79	117.88	126.06
23	b	614	CLA	C1-C2-C3	-3.79	119.49	126.04
23	B	605	CLA	CMB-C2B-C1B	3.79	131.14	125.37
23	B	610	CLA	C3B-C2B-C1B	-3.79	102.59	107.16
23	c	502	CLA	C3B-C4B-NB	3.79	114.03	110.52
33	Z	101	LMG	C1-C2-C3	3.78	117.88	110.00
23	b	609	CLA	C3B-C2B-C1B	-3.78	102.59	107.16
23	C	510	CLA	C1D-CHD-C4C	-3.78	117.90	126.06
23	c	512	CLA	C1-C2-C3	-3.78	119.50	126.04
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74
23	b	604	CLA	C3D-C4D-ND	3.78	116.35	110.24
23	A	408	CLA	C3B-C4B-NB	3.78	114.02	110.52
23	C	502	CLA	C3B-C2B-C1B	-3.77	102.61	107.16
23	b	601	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	c	501	CLA	C1-C2-C3	-3.77	119.52	126.04
23	B	615	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
23	A	405[B]	CLA	C1D-CHD-C4C	-3.76	117.94	126.06
26	a	411	SQD	O47-C7-C8	3.76	119.61	111.50
23	A	406[B]	CLA	CMB-C2B-C1B	3.76	131.09	125.37
24	d	403[A]	PHO	C4-C3-C5	3.76	121.59	115.27
23	B	610	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	d	405	CLA	CMB-C2B-C1B	3.75	131.09	125.37
23	c	505	CLA	C4C-C3C-C2C	-3.75	101.43	106.90
23	A	408	CLA	C3C-C4C-NC	3.75	114.78	110.57
23	b	613	CLA	C1-C2-C3	-3.75	119.56	126.04
23	c	512	CLA	C3C-C4C-NC	3.75	114.77	110.57
23	A	408	CLA	O2D-CGD-CBD	3.74	117.92	111.27
23	c	510	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
23	b	609	CLA	CAC-C3C-C4C	3.74	129.66	124.81
29	a	413[A]	PL9	C15-C14-C16	3.74	121.56	115.27
23	B	605	CLA	CHD-C4C-NC	3.74	130.09	124.20
23	a	407	CLA	CMC-C2C-C1C	3.73	130.73	125.04
23	A	408	CLA	C1-C2-C3	-3.73	119.58	126.04
25	d	406	BCR	C29-C30-C25	3.73	116.23	110.48
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	B	602	CLA	C1C-C2C-C3C	-3.73	103.04	106.96
23	d	402[B]	CLA	C3B-C4B-NB	3.73	113.97	110.52
23	b	612	CLA	CAC-C3C-C4C	3.72	129.64	124.81
23	c	511	CLA	O2D-CGD-O1D	-3.72	116.56	123.84
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	101	BCR	C29-C30-C25	3.72	116.20	110.48
23	c	513	CLA	C1C-C2C-C3C	-3.71	103.05	106.96
23	c	513	CLA	C3B-C4B-NB	3.71	113.96	110.52
23	B	614	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
25	K	102	BCR	C7-C8-C9	-3.71	120.63	126.23
23	c	509	CLA	C4A-NA-C1A	-3.71	105.04	106.71
23	A	406[B]	CLA	C1D-CHD-C4C	-3.71	118.06	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	c	509	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	a	407	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	C	509	CLA	C4C-C3C-C2C	-3.70	101.51	106.90
23	B	613	CLA	C4A-NA-C1A	-3.70	105.04	106.71
23	c	502	CLA	C4A-NA-C1A	-3.69	105.05	106.71
35	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
25	k	101	BCR	C7-C8-C9	-3.69	120.65	126.23
23	C	510	CLA	C3B-C4B-NB	3.69	113.94	110.52
23	c	506	CLA	C1D-CHD-C4C	-3.69	118.10	126.06
23	B	604	CLA	C3D-C2D-C1D	-3.69	100.80	105.83
23	b	612	CLA	C1D-CHD-C4C	-3.69	118.11	126.06
34	b	625	HTG	C1-O5-C5	3.69	119.38	112.58
26	a	409[B]	SQD	C1-C2-C3	-3.68	102.33	110.00
23	b	602	CLA	C1D-CHD-C4C	-3.68	118.11	126.06
23	b	613	CLA	C3B-C4B-NB	3.68	113.93	110.52
32	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.50
29	D	405[B]	PL9	C42-C43-C44	-3.68	118.80	127.66
23	b	603	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
23	A	406[A]	CLA	CMB-C2B-C1B	3.68	130.97	125.37
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
23	b	608	CLA	C3B-C4B-NB	3.67	113.92	110.52
23	B	607	CLA	CMC-C2C-C1C	3.67	130.62	125.04
23	a	404[A]	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	B	608	CLA	C3B-C4B-NB	3.66	113.92	110.52
23	b	611	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	C	509	CLA	C1D-CHD-C4C	-3.66	118.16	126.06
23	B	612	CLA	C4C-C3C-C2C	-3.66	101.56	106.90
40	V	201	HEC	CBD-CAD-C3D	-3.66	102.47	112.63
23	C	509	CLA	C4A-NA-C1A	-3.65	105.06	106.71
32	b	629[B]	LHG	O7-C7-C8	3.65	119.38	111.50
23	b	612	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
23	c	505	CLA	CMB-C2B-C1B	3.65	130.93	125.37
23	A	405[B]	CLA	C3C-C4C-NC	3.65	114.66	110.57
23	C	514	CLA	C3B-C4B-NB	3.65	113.90	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	C3D-C4D-ND	3.64	116.13	110.24
38	f	101	HEM	C1B-NB-C4B	3.64	108.83	105.07
23	c	504	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
23	d	405	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
23	D	402[A]	CLA	C3B-C4B-NB	3.64	113.89	110.52
25	T	102	BCR	C16-C17-C18	-3.64	122.12	127.31
23	C	507	CLA	C1-C2-C3	-3.64	119.75	126.04
23	a	405[B]	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	b	612	CLA	C4-C3-C5	3.63	121.38	115.27
23	B	609	CLA	C3B-C2B-C1B	-3.63	102.78	107.16
23	c	501	CLA	C3C-C4C-NC	3.63	114.64	110.57
26	a	409[A]	SQD	O9-S-C6	3.63	111.25	106.94
23	b	603	CLA	C3B-C4B-NB	3.62	113.87	110.52
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	b	612	CLA	CMC-C2C-C1C	3.62	130.55	125.04
23	b	605	CLA	CHD-C4C-NC	3.62	129.90	124.20
38	f	101	HEM	CAD-CBD-CGD	3.62	121.39	113.60
32	A	419[B]	LHG	O7-C7-C8	3.62	119.29	111.50
23	c	507	CLA	O2D-CGD-O1D	-3.61	116.77	123.84
23	b	606	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
25	D	404	BCR	C38-C26-C25	-3.61	120.47	124.53
25	C	515	BCR	C33-C5-C6	-3.61	120.48	124.53
32	d	415[B]	LHG	O7-C7-C8	3.60	119.26	111.50
23	C	507	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
34	B	624	HTG	C1'-S1-C1	3.60	106.82	100.09
24	A	416[A]	PHO	C4D-CHA-CBD	3.59	110.14	108.52
23	B	613	CLA	C3B-C4B-NB	3.59	113.85	110.52
25	C	516	BCR	C7-C8-C9	-3.59	120.81	126.23
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
29	A	414[B]	PL9	C37-C38-C39	-3.58	119.03	127.66
23	d	404[A]	CLA	C3B-C4B-NB	3.58	113.84	110.52
25	B	617	BCR	C33-C5-C6	-3.58	120.51	124.53
23	B	612	CLA	CAC-C3C-C4C	3.58	129.46	124.81
23	c	508	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	b	604	CLA	O2D-CGD-O1D	-3.58	116.84	123.84
23	b	602	CLA	CAA-C2A-C3A	-3.58	102.98	112.78
35	c	516[B]	DGD	O2G-C1B-C2B	3.58	119.21	111.50
29	a	413[B]	PL9	C15-C14-C16	3.58	121.29	115.27
23	B	608	CLA	C4C-C3C-C2C	-3.58	101.69	106.90
23	C	506	CLA	C1D-CHD-C4C	-3.57	118.35	126.06
23	B	603	CLA	C1C-C2C-C3C	-3.57	103.20	106.96
23	C	510	CLA	CMC-C2C-C1C	3.57	130.48	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C1-C2-C3	-3.57	119.87	126.04
23	b	616	CLA	CHD-C4C-NC	3.56	129.82	124.20
38	f	101	HEM	CHA-C4D-ND	3.56	128.77	124.37
23	D	403	CLA	C1C-C2C-C3C	-3.56	103.21	106.96
23	B	610	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
23	b	613	CLA	C3D-C4D-ND	3.56	116.00	110.24
25	y	101	BCR	C15-C14-C13	-3.56	122.23	127.31
24	d	403[B]	PHO	C4-C3-C5	3.56	121.26	115.27
23	d	404[A]	CLA	C1-C2-C3	-3.56	119.89	126.04
23	b	615	CLA	CMB-C2B-C1B	3.56	130.79	125.37
23	B	616	CLA	C3B-C4B-NB	3.56	113.81	110.52
23	B	615	CLA	CED-O2D-CGD	3.55	123.98	115.94
23	B	615	CLA	CMC-C2C-C1C	3.55	130.45	125.04
23	b	605	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	c	504	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	B	608	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
23	C	512	CLA	O2D-CGD-O1D	-3.55	116.90	123.84
23	b	612	CLA	C3B-C4B-NB	3.55	113.81	110.52
23	c	510	CLA	C3B-C4B-NB	3.55	113.81	110.52
29	d	407[A]	PL9	C40-C39-C41	3.55	121.23	115.27
29	a	413[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
23	B	609	CLA	CMB-C2B-C1B	3.54	130.76	125.37
23	B	611	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
23	B	609	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
25	K	102	BCR	C38-C26-C25	-3.53	120.56	124.53
25	b	619	BCR	C24-C23-C22	-3.53	120.90	126.23
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	b	610	CLA	C4C-C3C-C2C	-3.53	101.76	106.90
23	b	614	CLA	C3B-C4B-NB	3.52	113.78	110.52
33	a	415	LMG	C7-O1-C1	-3.52	106.85	113.74
23	c	506	CLA	CAC-C3C-C4C	3.52	129.38	124.81
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66
23	b	615	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
23	A	408	CLA	CAA-C2A-C3A	-3.51	103.16	112.78
23	A	405[B]	CLA	CBC-CAC-C3C	-3.51	102.75	112.43
35	c	517[B]	DGD	O2G-C1B-C2B	3.51	119.07	111.50
29	A	414[A]	PL9	C15-C14-C16	3.51	121.18	115.27
23	A	404[A]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	c	503	CLA	CMB-C2B-C1B	3.51	130.71	125.37
23	b	604	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
26	a	409[B]	SQD	C44-O6-C1	-3.50	106.90	113.74
29	D	405[A]	PL9	C53-C6-C1	3.50	122.15	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	CMB-C2B-C1B	3.50	130.70	125.37
23	B	613	CLA	O2A-CGA-O1A	-3.50	114.77	123.59
23	c	504	CLA	C1-O2A-CGA	3.49	125.61	116.44
23	a	405[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	b	613	CLA	C1D-CHD-C4C	-3.48	118.54	126.06
29	D	405[B]	PL9	C10-C9-C11	3.48	121.13	115.27
23	B	606	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
23	B	607	CLA	C3B-C4B-NB	3.48	113.75	110.52
29	a	413[A]	PL9	C30-C29-C31	3.48	121.13	115.27
23	A	404[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
29	a	413[B]	PL9	C27-C28-C29	-3.48	119.28	127.66
23	B	603	CLA	CAA-C2A-C3A	-3.48	103.25	112.78
23	A	405[B]	CLA	CMC-C2C-C1C	3.48	130.33	125.04
31	A	417	LMT	O5B-C5B-C4B	3.48	116.01	109.69
23	b	608	CLA	C3C-C4C-NC	3.48	114.47	110.57
29	D	405[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
23	B	607	CLA	C1D-CHD-C4C	-3.47	118.57	126.06
23	C	502	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	613	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	a	404[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	d	404[B]	CLA	C1D-CHD-C4C	-3.47	118.58	126.06
23	c	508	CLA	C3B-C4B-NB	3.46	113.73	110.52
23	B	603	CLA	C3B-C4B-NB	3.46	113.73	110.52
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	d	404[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	b	604	CLA	CAC-C3C-C4C	3.46	129.30	124.81
23	B	614	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	b	612	CLA	C4C-C3C-C2C	-3.46	101.86	106.90
23	B	602	CLA	O2D-CGD-O1D	-3.46	117.08	123.84
23	D	402[B]	CLA	C3B-C4B-NB	3.46	113.72	110.52
29	D	405[B]	PL9	C25-C24-C26	3.46	121.08	115.27
25	d	406	BCR	C38-C26-C25	-3.45	120.65	124.53
23	d	404[B]	CLA	O2A-CGA-CBA	3.45	122.74	111.91
23	a	405[B]	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
29	A	414[B]	PL9	C22-C23-C24	-3.45	119.36	127.66
23	b	602	CLA	CMC-C2C-C1C	3.44	130.28	125.04
34	V	202	HTG	C1-O5-C5	3.44	116.86	112.19
23	B	602	CLA	CAA-C2A-C3A	-3.44	103.36	112.78
23	A	406[B]	CLA	C3B-C4B-NB	3.44	113.71	110.52
23	d	404[B]	CLA	C3B-C4B-NB	3.44	113.70	110.52
26	l	101	SQD	O7-S-C6	3.43	111.02	106.94
23	b	607	CLA	C1D-CHD-C4C	-3.43	118.65	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[B]	CLA	CMB-C2B-C1B	3.43	130.60	125.37
23	C	503	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
33	Z	101	LMG	O6-C1-C2	3.43	117.61	110.35
32	L	101[B]	LHG	O7-C7-C8	3.43	118.89	111.50
23	B	614	CLA	CMC-C2C-C1C	3.43	130.26	125.04
25	a	408	BCR	C38-C26-C25	-3.43	120.68	124.53
25	C	515	BCR	C15-C14-C13	-3.42	122.42	127.31
23	a	404[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
29	a	413[A]	PL9	C35-C34-C36	3.41	121.01	115.27
25	D	404	BCR	C10-C11-C12	-3.41	112.58	123.22
23	C	507	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
23	C	508	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	B	613	CLA	C1D-CHD-C4C	-3.41	118.71	126.06
23	C	512	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
33	C	521	LMG	C3-C4-C5	3.41	116.32	110.24
29	d	407[B]	PL9	C40-C39-C41	3.40	120.99	115.27
23	C	509	CLA	O2D-CGD-O1D	-3.40	117.19	123.84
23	B	606	CLA	O2A-CGA-O1A	-3.40	115.02	123.59
23	C	508	CLA	O2D-CGD-O1D	-3.40	117.20	123.84
25	A	409	BCR	C24-C23-C22	-3.40	121.10	126.23
23	c	512	CLA	C4-C3-C5	3.40	120.98	115.27
26	l	101	SQD	C1-O5-C5	-3.39	107.03	113.69
23	B	612	CLA	CMC-C2C-C1C	3.39	130.21	125.04
23	c	503	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	b	613	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
29	D	405[A]	PL9	C25-C24-C26	3.39	120.97	115.27
23	C	508	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
32	A	419[B]	LHG	C5-O7-C7	-3.38	109.46	117.79
23	b	610	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
23	b	611	CLA	C1D-CHD-C4C	-3.38	118.77	126.06
23	C	506	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
23	A	404[B]	CLA	C3C-C4C-NC	3.38	114.36	110.57
33	B	620	LMG	O8-C28-C29	3.38	122.50	111.91
23	C	510	CLA	CAC-C3C-C4C	3.37	129.19	124.81
23	B	601	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
23	B	605	CLA	O2A-CGA-O1A	-3.37	115.08	123.59
25	b	619	BCR	C11-C10-C9	-3.37	122.50	127.31
35	c	517[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	d	405	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
23	c	507	CLA	C4-C3-C5	3.37	120.94	115.27
23	B	604	CLA	C3B-C4B-NB	3.37	113.64	110.52
33	z	101	LMG	O7-C10-C11	3.37	118.76	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	O2A-CGA-O1A	-3.37	115.10	123.59
25	b	618	BCR	C37-C22-C21	-3.36	118.22	122.92
23	B	609	CLA	CMC-C2C-C1C	3.36	130.15	125.04
23	b	612	CLA	C2A-C1A-CHA	-3.35	118.00	123.86
23	B	608	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
23	b	616	CLA	C4C-C3C-C2C	-3.34	102.02	106.90
35	C	517[B]	DGD	O2G-C1B-C2B	3.34	118.70	111.50
29	A	414[B]	PL9	C15-C14-C16	3.34	120.89	115.27
26	a	411	SQD	O7-S-C6	3.34	110.91	106.94
23	c	511	CLA	C4-C3-C5	3.34	120.89	115.27
23	B	614	CLA	C3B-C4B-NB	3.34	113.61	110.52
23	C	511	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	d	405	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	b	609	CLA	CMC-C2C-C1C	3.33	130.12	125.04
23	b	609	CLA	C3B-C4B-NB	3.33	113.61	110.52
23	B	607	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
25	B	618	BCR	C15-C14-C13	-3.33	122.56	127.31
38	f	101	HEM	CHD-C4C-NC	3.33	128.04	124.44
23	d	404[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	b	602	CLA	CAC-C3C-C4C	3.33	129.13	124.81
23	B	609	CLA	C1D-CHD-C4C	-3.33	118.88	126.06
23	C	511	CLA	C3C-C4C-NC	3.33	114.30	110.57
23	B	613	CLA	C4-C3-C5	3.32	120.86	115.27
23	b	608	CLA	C1-C2-C3	-3.32	120.30	126.04
23	C	512	CLA	C3B-C4B-NB	3.32	113.59	110.52
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	A	406[A]	CLA	C3B-C4B-NB	3.32	113.59	110.52
25	c	514	BCR	C15-C14-C13	-3.31	122.58	127.31
23	c	509	CLA	CHC-C1C-C2C	-3.31	117.53	126.73
23	c	502	CLA	CHC-C1C-C2C	-3.31	117.53	126.73
23	a	404[B]	CLA	C4-C3-C5	3.31	120.84	115.27
23	B	603	CLA	CMC-C2C-C1C	3.31	130.08	125.04
23	B	607	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
23	c	507	CLA	C1D-CHD-C4C	-3.31	118.92	126.06
23	b	601	CLA	O2D-CGD-O1D	-3.31	117.38	123.84
34	B	621	HTG	C1'-S1-C1	3.30	106.27	100.09
23	b	606	CLA	CHD-C4C-NC	3.30	129.41	124.20
29	a	413[B]	PL9	C30-C29-C31	3.30	120.83	115.27
26	a	411	SQD	O48-C23-C24	3.30	122.27	111.91
25	h	101	BCR	C38-C26-C25	-3.30	120.82	124.53
23	B	603	CLA	C4C-C3C-C2C	-3.30	102.08	106.90
23	C	505	CLA	O2D-CGD-O1D	-3.30	117.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	415[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
24	A	416[B]	PHO	C1A-C2A-C3A	-3.30	99.70	102.84
23	C	504	CLA	C4C-C3C-C2C	-3.30	102.09	106.90
38	E	102	HEM	CHB-C1B-NB	3.29	128.44	124.37
25	T	102	BCR	C11-C10-C9	-3.29	122.61	127.31
23	b	607	CLA	C4A-NA-C1A	-3.29	105.23	106.71
32	d	409[A]	LHG	O7-C7-C8	3.29	118.59	111.50
23	C	507	CLA	CAC-C3C-C4C	3.29	129.08	124.81
23	c	510	CLA	C4-C3-C5	3.29	120.81	115.27
23	B	611	CLA	CHB-C4A-NA	3.29	129.06	124.51
26	a	409[B]	SQD	C1-O5-C5	-3.29	107.23	113.69
23	B	601	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	c	511	CLA	CHD-C4C-NC	3.28	129.38	124.20
23	c	503	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	c	508	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
26	l	101	SQD	O9-S-C6	3.28	110.84	106.94
25	Y	101	BCR	C15-C14-C13	-3.28	122.63	127.31
23	C	512	CLA	C4C-C3C-C2C	-3.28	102.11	106.90
23	d	404[B]	CLA	C1-C2-C3	-3.28	120.37	126.04
23	b	608	CLA	CHD-C4C-NC	3.28	129.37	124.20
23	b	609	CLA	CBC-CAC-C3C	-3.28	103.39	112.43
23	C	507	CLA	CHC-C1C-C2C	-3.27	117.64	126.73
23	b	608	CLA	CBC-CAC-C3C	-3.27	103.41	112.43
23	B	608	CLA	CAC-C3C-C4C	3.27	129.05	124.81
23	B	604	CLA	CMB-C2B-C1B	3.26	130.34	125.37
38	E	102	HEM	CBD-CAD-C3D	-3.26	103.56	112.63
23	C	511	CLA	C4-C3-C5	3.26	120.76	115.27
23	b	608	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	c	505	CLA	CAC-C3C-C4C	3.26	129.04	124.81
23	B	606	CLA	CMC-C2C-C1C	3.26	130.00	125.04
23	B	611	CLA	CAC-C3C-C4C	3.26	129.04	124.81
23	B	614	CLA	O2A-CGA-CBA	3.26	122.12	111.91
23	C	504	CLA	O2A-CGA-O1A	-3.26	115.38	123.59
23	B	609	CLA	CBC-CAC-C3C	-3.25	103.47	112.43
32	d	415[A]	LHG	O7-C7-C8	3.25	118.50	111.50
25	d	406	BCR	C16-C17-C18	-3.25	122.68	127.31
23	b	609	CLA	CMB-C2B-C1B	3.24	130.31	125.37
23	b	603	CLA	C4-C3-C5	3.24	120.73	115.27
23	c	512	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	b	602	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
23	A	404[B]	CLA	CHC-C1C-C2C	-3.24	117.72	126.73
26	A	410[B]	SQD	O47-C7-C8	3.24	118.48	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	C1-C2-C3	-3.24	120.44	126.04
25	D	404	BCR	C28-C27-C26	-3.24	108.30	114.08
23	b	615	CLA	C3B-C4B-NB	3.24	113.52	110.52
33	c	520	LMG	C9-C8-C7	-3.24	104.13	111.79
23	b	613	CLA	O2D-CGD-CBD	3.24	117.02	111.27
38	f	101	HEM	CHD-C1D-ND	3.24	127.93	124.42
32	d	415[B]	LHG	O8-C23-C24	3.23	122.05	111.91
23	b	604	CLA	CMB-C2B-C1B	3.23	130.29	125.37
32	A	419[B]	LHG	O8-C23-O10	-3.23	115.44	123.59
23	c	505	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
23	c	509	CLA	CAC-C3C-C4C	3.23	129.00	124.81
23	B	607	CLA	CBC-CAC-C3C	-3.23	103.53	112.43
23	A	405[A]	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	D	403	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	A	408	CLA	C1D-CHD-C4C	-3.22	119.10	126.06
23	a	404[B]	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
25	c	514	BCR	C16-C17-C18	-3.22	122.71	127.31
24	d	403[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	b	611	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
23	b	614	CLA	CMB-C2B-C1B	3.22	130.27	125.37
23	C	506	CLA	C4C-C3C-C2C	-3.22	102.21	106.90
32	d	415[A]	LHG	O8-C23-C24	3.22	122.00	111.91
23	b	609	CLA	C4C-C3C-C2C	-3.21	102.21	106.90
23	a	407	CLA	CAA-C2A-C3A	-3.21	103.98	112.78
23	B	614	CLA	CHD-C4C-NC	3.21	129.26	124.20
40	V	201	HEC	CAD-CBD-CGD	-3.21	106.69	113.60
23	B	603	CLA	C4-C3-C5	3.21	120.67	115.27
23	C	505	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
23	B	614	CLA	O2A-CGA-O1A	-3.20	115.50	123.59
25	D	404	BCR	C16-C17-C18	-3.20	122.74	127.31
23	b	609	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
23	c	511	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
34	b	625	HTG	O5-C5-C4	3.20	115.51	109.69
23	b	608	CLA	CAC-C3C-C4C	3.20	128.96	124.81
23	b	603	CLA	C2A-C1A-CHA	-3.19	118.27	123.86
23	B	615	CLA	CHD-C4C-NC	3.19	129.24	124.20
23	D	402[B]	CLA	C1D-CHD-C4C	-3.19	119.17	126.06
23	B	605	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
23	a	404[A]	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
23	B	601	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
23	C	511	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
23	c	511	CLA	C4C-C3C-C2C	-3.19	102.25	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	a	407	CLA	CHD-C4C-NC	3.19	129.23	124.20
25	D	404	BCR	C29-C30-C25	3.19	115.39	110.48
23	b	614	CLA	O2A-CGA-O1A	-3.19	115.55	123.59
23	C	509	CLA	CHC-C1C-C2C	-3.19	117.88	126.73
23	C	513	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
29	A	414[B]	PL9	C27-C28-C29	-3.19	119.99	127.66
29	a	413[A]	PL9	C17-C18-C19	-3.19	119.99	127.66
23	C	502	CLA	CBC-CAC-C3C	-3.18	103.65	112.43
23	B	613	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
25	B	619	BCR	C24-C23-C22	-3.18	121.43	126.23
23	c	504	CLA	C4C-C3C-C2C	-3.18	102.26	106.90
26	l	101	SQD	O48-C23-C24	3.18	121.88	111.91
23	A	405[B]	CLA	C3B-C4B-NB	3.18	113.46	110.52
23	A	406[A]	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
29	A	414[A]	PL9	C27-C28-C29	-3.18	120.01	127.66
23	D	402[B]	CLA	CAC-C3C-C4C	3.18	128.93	124.81
23	d	402[B]	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	B	610	CLA	CAA-CBA-CGA	-3.18	103.97	113.25
23	B	611	CLA	C2A-C1A-CHA	-3.18	118.31	123.86
25	d	406	BCR	C10-C11-C12	-3.17	113.31	123.22
23	B	611	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
29	a	413[B]	PL9	C37-C38-C39	-3.17	120.02	127.66
23	B	602	CLA	C3B-C4B-NB	3.17	113.46	110.52
29	a	413[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	b	605	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
26	b	620	SQD	O7-S-C6	3.17	110.70	106.94
23	D	402[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	c	512	CLA	O2A-CGA-CBA	3.17	121.85	111.91
26	X	101	SQD	C1-C2-C3	-3.17	103.40	110.00
23	b	615	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	B	615	CLA	O2D-CGD-CBD	3.16	116.89	111.27
23	d	402[B]	CLA	CMB-C2B-C1B	3.16	130.19	125.37
38	f	101	HEM	C4D-ND-C1D	3.16	108.34	105.07
23	B	610	CLA	O2A-CGA-O1A	-3.16	115.61	123.59
23	b	610	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
23	a	404[B]	CLA	CAA-C2A-C1A	-3.16	101.62	111.97
23	B	607	CLA	C4-C3-C5	3.16	120.58	115.27
23	B	610	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
23	C	514	CLA	CBC-CAC-C3C	-3.16	103.73	112.43
34	b	622	HTG	O2-C2-C1	3.16	116.07	110.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	525	LMT	O5B-C5B-C4B	3.16	115.43	109.69
29	d	407[B]	PL9	C7-C8-C9	-3.16	121.54	126.79
24	A	416[A]	PHO	C4-C3-C5	3.15	120.58	115.27
23	b	611	CLA	C4C-C3C-C2C	-3.15	102.30	106.90
23	b	615	CLA	C4-C3-C5	3.15	120.58	115.27
23	d	402[A]	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	A	405[A]	CLA	CMB-C2B-C1B	3.15	130.17	125.37
32	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79
23	D	403	CLA	CAC-C3C-C4C	3.15	128.90	124.81
32	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
23	a	407	CLA	C4-C3-C5	3.15	120.56	115.27
23	d	404[B]	CLA	C4-C3-C5	3.15	120.56	115.27
23	A	405[B]	CLA	CHD-C4C-NC	3.15	129.16	124.20
23	B	610	CLA	C3B-C4B-NB	3.14	113.43	110.52
23	B	616	CLA	CAC-C3C-C4C	3.14	128.89	124.81
31	B	627	LMT	O1'-C1'-C2'	3.14	113.21	108.30
23	B	608	CLA	CMA-C3A-C4A	-3.14	103.34	111.77
23	B	604	CLA	O2A-CGA-O1A	-3.14	115.68	123.59
23	c	509	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
23	b	601	CLA	C1C-C2C-C3C	-3.14	103.66	106.96
23	b	612	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
23	d	402[A]	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	a	405[A]	CLA	CHD-C4C-NC	3.13	129.13	124.20
29	a	413[B]	PL9	C25-C24-C26	3.13	120.53	115.27
29	d	407[B]	PL9	C42-C43-C44	-3.13	120.13	127.66
23	a	405[A]	CLA	C1-C2-C3	-3.13	120.64	126.04
23	d	404[A]	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
23	b	614	CLA	CHD-C4C-NC	3.12	129.13	124.20
23	C	513	CLA	C1C-C2C-C3C	-3.12	103.67	106.96
23	b	611	CLA	CHC-C1C-C2C	-3.12	118.06	126.73
23	c	501	CLA	C3B-C4B-NB	3.12	113.41	110.52
23	b	616	CLA	CBC-CAC-C3C	-3.12	103.83	112.43
25	b	618	BCR	C29-C30-C25	3.12	115.28	110.48
29	D	405[A]	PL9	C51-C49-C50	3.12	121.49	114.60
24	A	416[B]	PHO	C4-C3-C5	3.12	120.51	115.27
23	c	506	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
23	c	503	CLA	CHD-C4C-NC	3.11	129.11	124.20
23	b	613	CLA	CHC-C1C-C2C	-3.11	118.09	126.73
23	b	610	CLA	O2A-CGA-O1A	-3.11	115.74	123.59
23	B	612	CLA	C1C-C2C-C3C	-3.11	103.69	106.96
23	b	607	CLA	CAC-C3C-C4C	3.11	128.84	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414[B]	PL9	C20-C19-C21	3.11	120.50	115.27
29	D	405[A]	PL9	C10-C9-C11	3.11	120.50	115.27
23	A	408	CLA	CBC-CAC-C3C	-3.10	103.87	112.43
23	c	501	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
33	C	521	LMG	O8-C28-C29	3.10	121.63	111.91
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
23	b	616	CLA	C3B-C4B-NB	3.10	113.39	110.52
24	d	403[B]	PHO	CMB-C2B-C3B	3.09	130.47	124.68
23	B	614	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	b	614	CLA	CHC-C1C-C2C	-3.09	118.14	126.73
32	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	b	615	CLA	CHC-C1C-C2C	-3.09	118.15	126.73
23	b	610	CLA	CMB-C2B-C1B	3.09	130.07	125.37
23	D	402[B]	CLA	CMC-C2C-C1C	3.09	129.74	125.04
24	d	403[A]	PHO	CMB-C2B-C3B	3.08	130.44	124.68
29	a	413[A]	PL9	C10-C9-C11	3.08	120.45	115.27
23	B	613	CLA	CMC-C2C-C1C	3.08	129.73	125.04
23	C	503	CLA	CMB-C2B-C1B	3.08	130.06	125.37
23	A	406[B]	CLA	O2A-CGA-O1A	-3.08	115.82	123.59
26	b	620	SQD	O8-S-C6	3.08	110.65	105.74
24	a	406[B]	PHO	O2A-CGA-CBA	3.08	121.57	111.91
23	B	601	CLA	CAC-C3C-C4C	3.08	128.80	124.81
31	b	627	LMT	C3'-C4'-C5'	-3.07	103.88	110.93
29	A	414[B]	PL9	C17-C18-C19	-3.07	120.26	127.66
23	d	402[B]	CLA	CHC-C1C-C2C	-3.07	118.19	126.73
23	a	405[B]	CLA	CMC-C2C-C1C	3.07	129.72	125.04
23	a	404[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
23	a	407	CLA	C3B-C4B-NB	3.07	113.36	110.52
32	a	419[B]	LHG	O7-C7-C8	3.07	118.11	111.50
33	c	519	LMG	O1-C7-C8	-3.07	103.50	110.90
23	b	607	CLA	CBC-CAC-C3C	-3.07	103.98	112.43
29	A	414[B]	PL9	C10-C9-C11	3.06	120.43	115.27
23	B	606	CLA	O2A-CGA-CBA	3.06	121.52	111.91
23	c	501	CLA	CAC-C3C-C4C	3.06	128.78	124.81
25	h	101	BCR	C7-C8-C9	-3.06	121.61	126.23
23	b	601	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
29	d	407[B]	PL9	C10-C9-C11	3.06	120.41	115.27
23	a	405[B]	CLA	CHD-C4C-NC	3.06	129.02	124.20
23	b	613	CLA	O2A-CGA-O1A	-3.06	115.88	123.59
23	C	502	CLA	CHD-C4C-NC	3.06	129.02	124.20
32	d	408[B]	LHG	O7-C7-C8	3.05	118.08	111.50
29	d	407[A]	PL9	C10-C9-C11	3.05	120.41	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	b	619	BCR	C38-C26-C25	-3.05	121.10	124.53
23	B	603	CLA	CHC-C1C-C2C	-3.05	118.25	126.73
23	a	404[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	B	613	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	D	402[A]	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	405[A]	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	a	405[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	c	510	CLA	CAC-C3C-C4C	3.05	128.77	124.81
23	b	605	CLA	CMB-C2B-C1B	3.05	130.01	125.37
26	b	620	SQD	C3-C4-C5	3.05	115.68	110.24
23	d	404[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
23	A	405[B]	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
25	D	404	BCR	C37-C22-C23	3.04	122.87	118.08
23	d	404[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	B	605	CLA	CMC-C2C-C1C	3.04	129.67	125.04
23	c	509	CLA	C1-O2A-CGA	3.04	124.42	116.44
29	a	413[B]	PL9	C35-C34-C36	3.04	120.38	115.27
23	c	502	CLA	CHD-C4C-NC	3.04	128.99	124.20
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	C	503	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
23	B	602	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	d	404[A]	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	A	406[A]	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	B	612	CLA	C11-C12-C13	-3.03	106.13	115.92
23	D	402[B]	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
26	f	102	SQD	O5-C1-C2	3.03	116.76	110.35
23	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
26	A	412	SQD	O48-C23-C24	3.03	121.41	111.91
23	c	503	CLA	C1-C2-C3	-3.03	120.81	126.04
23	B	615	CLA	C3B-C4B-NB	3.02	113.32	110.52
23	d	404[A]	CLA	C4-C3-C5	3.02	120.36	115.27
29	a	413[B]	PL9	C22-C23-C24	-3.02	120.38	127.66
35	c	518	DGD	O2G-C1B-C2B	3.02	118.01	111.50
29	d	407[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
23	C	505	CLA	C1-O2A-CGA	3.02	124.36	116.44
23	D	402[B]	CLA	O2A-CGA-CBA	3.02	121.38	111.91
23	b	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	C	504	CLA	C4-C3-C5	3.02	120.34	115.27
23	C	503	CLA	C3B-C4B-NB	3.01	113.31	110.52
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
29	a	413[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
25	T	102	BCR	C2-C1-C6	3.01	115.12	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	CMC-C2C-C1C	3.01	129.62	125.04
23	a	404[B]	CLA	C1-C2-C3	-3.01	120.84	126.04
32	d	408[A]	LHG	O7-C7-C8	3.01	117.99	111.50
23	D	402[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	b	607	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
29	a	413[B]	PL9	C17-C18-C19	-3.01	120.42	127.66
23	B	609	CLA	C4C-C3C-C2C	-3.00	102.52	106.90
23	d	404[B]	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	C	504	CLA	CHD-C4C-NC	3.00	128.93	124.20
29	d	407[B]	PL9	C37-C38-C39	-3.00	120.44	127.66
26	a	409[B]	SQD	C45-O47-C7	-3.00	110.41	117.79
33	C	520	LMG	O8-C28-C29	3.00	121.31	111.91
38	f	101	HEM	CHB-C1B-NB	3.00	128.07	124.37
23	A	405[A]	CLA	CHD-C4C-NC	3.00	128.93	124.20
26	a	409[A]	SQD	C45-O47-C7	-3.00	110.42	117.79
25	H	101	BCR	C37-C22-C21	-3.00	118.73	122.92
23	c	513	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	b	606	CLA	C3B-C4B-NB	2.99	113.29	110.52
23	C	506	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
23	d	402[B]	CLA	CBC-CAC-C3C	-2.99	104.19	112.43
23	A	404[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	C	514	CLA	C1-C2-C3	-2.99	120.87	126.04
23	C	512	CLA	C4-C3-C5	2.99	120.30	115.27
23	B	604	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	c	508	CLA	CMB-C2B-C1B	2.99	129.92	125.37
32	D	407[A]	LHG	O8-C23-C24	2.98	121.27	111.91
23	B	607	CLA	CMB-C2B-C1B	2.98	129.91	125.37
23	b	614	CLA	CHB-C1B-NB	-2.98	121.10	124.26
29	D	405[B]	PL9	C17-C18-C19	-2.98	120.49	127.66
23	b	607	CLA	C4C-C3C-C2C	-2.98	102.56	106.90
23	A	408	CLA	O2A-CGA-CBA	2.97	121.24	111.91
23	C	513	CLA	CHD-C4C-NC	2.97	128.89	124.20
23	c	509	CLA	O2A-CGA-CBA	2.97	121.23	111.91
34	b	622	HTG	O5-C5-C4	2.97	115.09	109.69
32	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	a	405[B]	CLA	CMB-C2B-C1B	2.97	129.89	125.37
23	b	601	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	a	407	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
25	C	516	BCR	C11-C10-C9	-2.97	123.07	127.31
23	b	615	CLA	C11-C10-C8	-2.97	106.32	115.92
23	c	503	CLA	CMC-C2C-C1C	2.97	129.56	125.04
23	A	404[B]	CLA	O2A-CGA-CBA	2.97	121.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
33	m	101	LMG	O8-C28-C29	2.97	121.21	111.91
23	c	503	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	A	405[B]	CLA	C4-C3-C5	2.96	120.26	115.27
24	A	416[B]	PHO	C4D-CHA-CBD	2.96	109.86	108.52
23	b	602	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
25	b	619	BCR	C39-C30-C25	-2.96	105.49	110.30
23	C	511	CLA	O2A-CGA-CBA	2.96	121.20	111.91
23	a	407	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	c	503	CLA	C3B-C4B-NB	2.96	113.26	110.52
23	B	606	CLA	CHD-C4C-NC	2.96	128.87	124.20
25	B	619	BCR	C38-C26-C25	-2.96	121.20	124.53
23	B	615	CLA	C4-C3-C5	2.96	120.25	115.27
23	c	513	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	a	405[B]	CLA	C1-C2-C3	-2.96	120.93	126.04
23	b	614	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	b	601	CLA	C1-O2A-CGA	2.95	124.19	116.44
23	D	403	CLA	C4-C3-C5	2.95	120.24	115.27
23	b	601	CLA	C4-C3-C5	2.95	120.24	115.27
35	h	102	DGD	O1G-C1A-C2A	2.95	121.17	111.91
32	D	406[B]	LHG	O7-C7-C8	2.95	117.86	111.50
23	c	502	CLA	CMB-C2B-C1B	2.95	129.87	125.37
23	d	402[A]	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
23	A	408	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
23	b	610	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	D	403	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
25	B	618	BCR	C37-C22-C21	-2.95	118.79	122.92
25	k	101	BCR	C24-C23-C22	-2.95	121.78	126.23
33	z	101	LMG	O8-C28-C29	2.95	121.16	111.91
25	Y	101	BCR	C38-C26-C25	-2.95	121.22	124.53
25	C	516	BCR	C33-C5-C6	-2.95	121.22	124.53
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
23	B	601	CLA	CHD-C4C-NC	2.95	128.84	124.20
23	C	502	CLA	CAC-C3C-C4C	2.94	128.63	124.81
23	A	406[B]	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
23	d	404[B]	CLA	O2A-CGA-O1A	-2.94	116.17	123.59
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
23	C	505	CLA	CHC-C1C-C2C	-2.94	118.56	126.73
23	a	405[B]	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
23	b	613	CLA	O2A-CGA-CBA	2.94	121.13	111.91
32	D	407[B]	LHG	O7-C7-C8	2.94	117.83	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C3B-C4B-NB	2.94	113.24	110.52
23	C	513	CLA	O2A-CGA-CBA	2.94	121.12	111.91
35	C	519	DGD	O1G-C1A-C2A	2.94	121.12	111.91
32	a	419[A]	LHG	O7-C7-C8	2.94	117.83	111.50
25	y	101	BCR	C38-C26-C25	-2.94	121.23	124.53
23	A	406[A]	CLA	CHD-C4C-NC	2.93	128.83	124.20
29	A	414[A]	PL9	C17-C18-C19	-2.93	120.59	127.66
23	B	604	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
32	D	406[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
23	D	403	CLA	CHC-C1C-C2C	-2.93	118.58	126.73
23	c	512	CLA	CHD-C4C-NC	2.93	128.82	124.20
29	d	407[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
32	d	415[B]	LHG	O8-C23-O10	-2.93	116.19	123.59
23	A	406[B]	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	C	503	CLA	C2A-C1A-CHA	-2.93	118.74	123.86
35	h	102	DGD	O2G-C1B-C2B	2.93	117.81	111.50
23	C	511	CLA	CHD-C4C-NC	2.93	128.81	124.20
29	d	407[A]	PL9	C27-C28-C29	-2.93	120.61	127.66
23	B	606	CLA	CMB-C2B-C1B	2.93	129.82	125.37
23	A	404[A]	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	C	506	CLA	CMC-C2C-C1C	2.92	129.49	125.04
23	D	402[B]	CLA	C4-C3-C5	2.92	120.19	115.27
23	b	609	CLA	CHD-C4C-NC	2.92	128.81	124.20
23	C	514	CLA	CMC-C2C-C1C	2.92	129.49	125.04
33	a	415	LMG	C8-O7-C10	-2.92	110.59	117.79
23	d	405	CLA	C4-C3-C5	2.92	120.19	115.27
33	D	411	LMG	O7-C10-C11	2.92	117.80	111.50
23	d	402[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	b	602	CLA	C11-C12-C13	-2.92	106.48	115.92
23	c	512	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	A	406[A]	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	A	406[B]	CLA	CHD-C4C-NC	2.92	128.80	124.20
29	A	414[B]	PL9	C30-C29-C31	2.92	120.18	115.27
26	f	102	SQD	C4-C3-C2	-2.92	105.73	110.82
29	d	407[A]	PL9	C53-C6-C1	2.92	120.95	114.99
26	A	412	SQD	O8-S-C6	2.92	110.39	105.74
23	c	504	CLA	CHD-C4C-NC	2.92	128.80	124.20
29	a	413[A]	PL9	C22-C23-C24	-2.92	120.64	127.66
23	B	605	CLA	CBC-CAC-C3C	-2.91	104.39	112.43
23	C	511	CLA	O2A-CGA-O1A	-2.91	116.24	123.59
23	b	610	CLA	C4-C3-C5	2.91	120.17	115.27
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	616	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
32	D	407[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
23	c	512	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	A	406[B]	CLA	CAA-C2A-C3A	-2.91	104.82	112.78
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
23	b	604	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
23	a	404[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	a	413[B]	PL9	C10-C9-C11	2.90	120.15	115.27
29	A	414[B]	PL9	C40-C39-C41	2.90	120.15	115.27
23	a	405[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
31	B	628	LMT	O1'-C1'-C2'	2.90	112.83	108.30
34	b	623	HTG	O5-C1-C2	2.90	113.96	110.31
23	c	506	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
26	A	410[B]	SQD	O48-C23-C24	2.90	121.01	111.91
23	d	402[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
23	a	405[A]	CLA	CMB-C2B-C1B	2.89	129.78	125.37
33	c	519	LMG	O8-C28-C29	2.89	120.99	111.91
23	C	514	CLA	CHD-C4C-NC	2.89	128.76	124.20
23	A	408	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
23	c	508	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
23	b	606	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
23	d	405	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	C	510	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	a	405[B]	CLA	C3B-C4B-NB	2.89	113.20	110.52
23	c	504	CLA	CBC-CAC-C3C	-2.89	104.47	112.43
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
25	k	101	BCR	C39-C30-C25	-2.89	105.62	110.30
23	c	513	CLA	CAA-C2A-C3A	-2.89	104.88	112.78
23	C	505	CLA	CBC-CAC-C3C	-2.89	104.48	112.43
40	V	201	HEC	C4B-NB-C1B	2.88	108.05	105.07
23	c	510	CLA	O2A-CGA-CBA	2.88	120.96	111.91
23	c	508	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	A	405[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	D	402[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	C	503	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
23	c	505	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
23	B	616	CLA	CHD-C4C-NC	2.88	128.74	124.20
29	D	405[B]	PL9	C40-C39-C41	2.88	120.11	115.27
23	C	512	CLA	CHD-C4C-NC	2.88	128.74	124.20
23	a	407	CLA	O2A-CGA-CBA	2.88	120.94	111.91
23	c	506	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
23	C	502	CLA	CMC-C2C-C1C	2.87	129.42	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	CHD-C4C-NC	2.87	128.73	124.20
24	a	406[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	D	402[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
25	t	102	BCR	C15-C16-C17	-2.87	117.60	123.47
29	D	405[B]	PL9	C51-C49-C50	2.87	120.94	114.60
23	A	404[B]	CLA	C2A-C1A-CHA	-2.87	118.84	123.86
23	c	513	CLA	O2A-CGA-CBA	2.87	120.91	111.91
23	B	606	CLA	CBC-CAC-C3C	-2.87	104.53	112.43
23	d	404[B]	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
23	B	616	CLA	C1-O2A-CGA	2.86	123.96	116.44
29	a	413[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
23	B	608	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
23	b	607	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	b	614	CLA	CAC-C3C-C4C	2.86	128.52	124.81
23	B	609	CLA	C3B-C4B-NB	2.86	113.17	110.52
23	C	505	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	b	614	CLA	CMC-C2C-C1C	2.86	129.39	125.04
23	C	513	CLA	CMA-C3A-C4A	-2.86	104.09	111.77
26	a	409[B]	SQD	O8-S-C6	2.85	110.28	105.74
23	d	404[B]	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
24	a	406[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	c	510	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	c	509	CLA	O2A-C1-C2	2.85	116.12	108.64
23	A	408	CLA	CHD-C4C-NC	2.85	128.69	124.20
32	b	629[A]	LHG	O8-C23-C24	2.85	120.84	111.91
32	E	101[B]	LHG	O8-C23-C24	2.85	120.84	111.91
23	c	502	CLA	CBC-CAC-C3C	-2.85	104.59	112.43
29	a	413[B]	PL9	C42-C43-C44	-2.84	120.81	127.66
23	b	614	CLA	CBC-CAC-C3C	-2.84	104.59	112.43
23	A	408	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
23	d	405	CLA	CHD-C4C-NC	2.84	128.68	124.20
24	a	406[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
23	C	511	CLA	CAC-C3C-C4C	2.84	128.49	124.81
23	C	510	CLA	O2A-CGA-CBA	2.84	120.82	111.91
23	B	605	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	c	511	CLA	CMB-C2B-C1B	2.84	129.69	125.37
23	B	608	CLA	CHB-C4A-NA	2.83	128.43	124.51
23	b	607	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
23	a	404[B]	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	b	606	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
23	C	505	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
23	B	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
23	C	507	CLA	O2A-CGA-CBA	2.83	120.78	111.91
23	C	510	CLA	CHD-C4C-NC	2.83	128.66	124.20
23	B	604	CLA	C6-C7-C8	-2.82	106.79	115.92
40	v	201	HEC	CHA-C4D-ND	2.82	127.48	124.42
23	b	602	CLA	C1-C2-C3	-2.82	121.17	126.04
35	c	516[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	c	506	CLA	CMC-C2C-C1C	2.82	129.33	125.04
23	b	610	CLA	CHD-C4C-NC	2.81	128.64	124.20
26	l	101	SQD	O48-C23-O10	-2.81	116.49	123.59
23	c	508	CLA	CAA-C2A-C3A	-2.81	105.07	112.78
25	D	404	BCR	C3-C4-C5	-2.81	109.06	114.08
25	y	101	BCR	C10-C11-C12	-2.81	114.45	123.22
23	c	506	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	C	514	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
23	B	606	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
23	B	610	CLA	CHD-C4C-NC	2.81	128.62	124.20
23	B	612	CLA	O2A-CGA-CBA	2.80	120.71	111.91
23	b	608	CLA	CHC-C1C-C2C	-2.80	118.95	126.73
23	C	507	CLA	C4-C3-C5	2.80	119.98	115.27
34	B	621	HTG	C1-O5-C5	2.80	117.74	112.58
23	B	606	CLA	C4-C3-C5	2.80	119.98	115.27
23	c	509	CLA	C4-C3-C5	2.80	119.98	115.27
23	B	609	CLA	C1-C2-C3	-2.80	121.21	126.04
23	B	602	CLA	C4C-C3C-C2C	-2.80	102.82	106.90
23	B	607	CLA	O2A-CGA-O1A	-2.80	116.53	123.59
23	d	404[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.73
23	C	505	CLA	CAC-C3C-C4C	2.79	128.44	124.81
35	C	517[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
38	E	102	HEM	CHD-C1D-ND	2.79	127.45	124.42
23	C	503	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
29	D	405[B]	PL9	C53-C6-C1	2.79	120.70	114.99
23	a	405[B]	CLA	C4-C3-C5	2.79	119.97	115.27
23	c	510	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
32	b	629[B]	LHG	O8-C23-C24	2.79	120.67	111.91
35	c	516[B]	DGD	C3G-C2G-C1G	-2.79	105.19	111.79
38	E	102	HEM	CHA-C4D-ND	2.79	127.81	124.37
23	B	615	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	D	404	BCR	C40-C30-C25	-2.79	105.78	110.30
23	A	406[A]	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
23	b	603	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
23	a	404[B]	CLA	C4C-C3C-C2C	-2.79	102.84	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	617	BCR	C11-C10-C9	-2.79	123.33	127.31
32	D	407[A]	LHG	O7-C7-C8	2.79	117.50	111.50
23	B	607	CLA	CHD-C4C-NC	2.79	128.59	124.20
26	l	101	SQD	C4-C3-C2	2.79	115.69	110.82
23	c	509	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
23	B	615	CLA	C11-C10-C8	-2.78	106.92	115.92
26	a	409[A]	SQD	O47-C7-O49	-2.78	116.98	123.70
23	d	405	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
23	B	611	CLA	C1-C2-C3	-2.78	121.23	126.04
23	C	504	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
23	B	614	CLA	CHC-C1C-C2C	-2.78	119.02	126.73
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
23	C	502	CLA	C3B-C4B-NB	2.78	113.09	110.52
31	B	627	LMT	C2'-C3'-C4'	2.78	116.02	109.68
29	d	407[B]	PL9	C53-C6-C1	2.78	120.67	114.99
23	D	402[B]	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
23	b	602	CLA	CMB-C2B-C1B	2.77	129.59	125.37
23	A	408	CLA	CMB-C2B-C1B	2.77	129.59	125.37
40	V	201	HEC	CBC-CAC-C3C	2.77	120.07	112.43
23	C	507	CLA	CMC-C2C-C1C	2.77	129.26	125.04
40	v	201	HEC	CBD-CAD-C3D	-2.77	104.93	112.63
25	h	101	BCR	C24-C23-C22	-2.77	122.05	126.23
23	c	501	CLA	C4-C3-C5	2.77	119.93	115.27
32	D	406[B]	LHG	O8-C23-O10	-2.77	116.60	123.59
33	D	411	LMG	O8-C28-O10	-2.77	116.60	123.59
23	A	404[B]	CLA	CAA-C2A-C1A	-2.77	102.90	111.97
23	b	605	CLA	CHC-C1C-C2C	-2.77	119.04	126.73
23	b	605	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
23	c	507	CLA	O2A-CGA-CBA	2.77	120.59	111.91
26	A	412	SQD	C4-C3-C2	-2.77	106.00	110.82
23	b	603	CLA	CMB-C2B-C1B	2.76	129.58	125.37
23	b	601	CLA	CHC-C1C-C2C	-2.76	119.05	126.73
23	C	508	CLA	C4-C3-C5	2.76	119.92	115.27
24	A	416[B]	PHO	O2D-CGD-O1D	-2.76	118.44	123.84
23	a	404[B]	CLA	O2A-CGA-CBA	2.76	120.57	111.91
35	H	102	DGD	O1G-C1A-C2A	2.76	120.57	111.91
29	a	413[A]	PL9	C53-C6-C1	2.76	120.64	114.99
23	C	503	CLA	CAC-C3C-C4C	2.76	128.39	124.81
23	c	512	CLA	CAC-C3C-C4C	2.76	128.39	124.81
31	M	101	LMT	C1'-O5'-C5'	-2.76	108.27	113.69
23	C	502	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
23	C	510	CLA	C16-C15-C13	-2.76	107.00	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	CMC-C2C-C1C	2.76	129.24	125.04
25	c	515	BCR	C11-C10-C9	-2.75	123.38	127.31
23	b	615	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
33	C	501	LMG	C6-C5-C4	2.75	119.45	113.00
23	b	605	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	C	508	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	b	615	CLA	O2A-CGA-O1A	-2.75	116.65	123.59
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
23	C	504	CLA	CMB-C2B-C1B	2.75	129.56	125.37
23	B	613	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
38	f	101	HEM	CBD-CAD-C3D	-2.75	104.99	112.63
23	c	501	CLA	C1D-CHD-C4C	-2.75	120.13	126.06
23	B	610	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
23	C	514	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
23	C	507	CLA	CBC-CAC-C3C	-2.75	104.86	112.43
23	C	510	CLA	O2A-CGA-O1A	-2.75	116.66	123.59
23	d	404[B]	CLA	C2A-C1A-CHA	-2.75	119.06	123.86
23	B	604	CLA	CMC-C2C-C1C	2.74	129.22	125.04
23	C	507	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
23	b	606	CLA	O2A-CGA-O1A	-2.74	116.67	123.59
26	X	101	SQD	O5-C1-O6	2.74	116.47	109.97
31	b	621	LMT	C1'-O5'-C5'	-2.74	108.31	113.69
23	b	611	CLA	C2A-C1A-CHA	-2.74	119.06	123.86
23	C	507	CLA	O2A-CGA-O1A	-2.74	116.68	123.59
23	B	615	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	c	501	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
35	H	102	DGD	O1G-C1A-O1A	-2.74	116.68	123.59
32	A	419[B]	LHG	O8-C23-C24	2.74	120.50	111.91
29	d	407[B]	PL9	C27-C28-C29	-2.74	121.07	127.66
23	b	611	CLA	CHD-C4C-NC	2.74	128.51	124.20
29	A	414[A]	PL9	C10-C9-C8	-2.74	116.66	123.68
23	A	404[A]	CLA	CAC-C3C-C4C	2.73	128.36	124.81
23	B	614	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
35	C	517[B]	DGD	O3G-C3G-C2G	-2.73	104.30	110.90
23	B	601	CLA	CMB-C2B-C1B	2.73	129.53	125.37
23	b	614	CLA	O2A-CGA-CBA	2.73	120.48	111.91
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	b	609	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
35	C	517[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
23	B	609	CLA	CHD-C4C-NC	2.73	128.50	124.20
26	A	410[B]	SQD	O8-S-C6	2.73	110.09	105.74
23	C	508	CLA	CHC-C1C-C2C	-2.73	119.15	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	402[B]	CLA	O2A-CGA-O1A	-2.73	116.71	123.59
32	d	409[A]	LHG	O8-C23-C24	2.73	120.46	111.91
23	C	503	CLA	C4C-C3C-C2C	-2.73	102.92	106.90
23	C	514	CLA	O2A-CGA-CBA	2.72	120.46	111.91
23	d	402[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	b	607	CLA	CMC-C2C-C1C	2.72	129.18	125.04
29	D	405[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	402[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	B	603	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
23	B	605	CLA	C1-C2-C3	-2.72	121.34	126.04
23	b	616	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	B	629	LMT	O1'-C1'-C2'	2.72	112.55	108.30
23	C	510	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
32	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
23	b	603	CLA	O2A-CGA-CBA	2.72	120.43	111.91
24	A	407[B]	PHO	O1D-CGD-CBD	-2.72	120.22	124.74
25	b	618	BCR	C37-C22-C23	2.72	122.36	118.08
25	c	514	BCR	C20-C21-C22	-2.72	123.44	127.31
23	a	407	CLA	CBC-CAC-C3C	-2.71	104.95	112.43
23	d	405	CLA	CHC-C1C-C2C	-2.71	119.19	126.73
23	b	605	CLA	CMC-C2C-C1C	2.71	129.17	125.04
23	C	503	CLA	O2A-CGA-CBA	2.71	120.42	111.91
29	d	407[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
32	D	407[B]	LHG	O8-C23-C24	2.71	120.42	111.91
23	B	604	CLA	O2A-CGA-CBA	2.71	120.41	111.91
23	a	405[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	c	515	BCR	C37-C22-C21	-2.71	119.13	122.92
23	B	612	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	c	505	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
24	a	406[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
29	a	413[B]	PL9	C53-C6-C1	2.71	120.52	114.99
23	A	406[A]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	b	601	CLA	C3B-C4B-NB	2.70	113.02	110.52
23	c	506	CLA	CMB-C2B-C1B	2.70	129.49	125.37
23	A	404[A]	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
25	d	406	BCR	C21-C20-C19	-2.70	114.78	123.22
23	C	510	CLA	CHB-C1B-NB	-2.70	121.39	124.26
26	a	411	SQD	C3-C4-C5	2.70	115.06	110.24
23	B	609	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	b	611	CLA	O2A-CGA-O1A	-2.70	116.78	123.59
31	a	416	LMT	C3'-C4'-C5'	-2.70	104.73	110.93
23	B	615	CLA	C6-C7-C8	-2.70	107.19	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	E	102	HEM	CBA-CAA-C2A	-2.70	105.13	112.63
23	c	513	CLA	C1-C2-C3	-2.70	121.38	126.04
23	c	513	CLA	CHC-C1C-C2C	-2.70	119.23	126.73
23	c	509	CLA	CHD-C4C-NC	2.70	128.46	124.20
35	C	518[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	D	402[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	b	606	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	C	502	CLA	C1-O2A-CGA	2.69	123.51	116.44
23	b	606	CLA	CBC-CAC-C3C	-2.69	105.01	112.43
33	Z	101	LMG	C4-C3-C2	2.69	115.52	110.82
23	B	616	CLA	O2A-CGA-CBA	2.69	120.35	111.91
26	f	102	SQD	O5-C5-C4	2.69	114.58	109.69
23	b	604	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	B	603	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
31	T	101	LMT	C1'-O5'-C5'	-2.69	108.41	113.69
23	A	406[B]	CLA	O2A-CGA-CBA	2.69	120.34	111.91
23	b	612	CLA	CHC-C1C-C2C	-2.68	119.28	126.73
24	a	406[B]	PHO	O2A-CGA-O1A	-2.68	116.82	123.59
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	B	601	CLA	C3B-C4B-NB	2.68	113.00	110.52
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
25	y	101	BCR	C24-C23-C22	-2.68	122.19	126.23
23	B	607	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
23	B	612	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
23	d	402[B]	CLA	O2A-CGA-CBA	2.68	120.31	111.91
23	a	405[A]	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
25	k	101	BCR	C15-C14-C13	-2.68	123.49	127.31
23	A	404[B]	CLA	C1-C2-C3	-2.68	121.41	126.04
32	d	409[B]	LHG	O8-C23-C24	2.68	120.31	111.91
32	a	419[A]	LHG	O8-C23-C24	2.68	120.30	111.91
24	d	403[A]	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
23	d	405	CLA	C2A-C1A-CHA	-2.68	119.18	123.86
25	t	102	BCR	C11-C10-C9	-2.68	123.49	127.31
35	c	516[A]	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	405[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
23	b	615	CLA	CHD-C4C-NC	2.67	128.42	124.20
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
23	b	615	CLA	CAC-C3C-C4C	2.67	128.28	124.81
23	b	616	CLA	CMC-C2C-C1C	2.67	129.11	125.04
23	b	603	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
23	B	614	CLA	CBC-CAC-C3C	-2.67	105.07	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	CHC-C1C-C2C	-2.67	119.31	126.73
23	B	601	CLA	CHC-C1C-C2C	-2.67	119.32	126.73
23	c	504	CLA	CMB-C2B-C1B	2.67	129.43	125.37
23	c	510	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
23	A	406[B]	CLA	C4-C3-C5	2.67	119.76	115.27
23	a	405[B]	CLA	CAA-C2A-C3A	-2.66	105.48	112.78
23	D	402[B]	CLA	C2A-C1A-CHA	-2.66	119.20	123.86
23	A	405[B]	CLA	CMA-C3A-C2A	-2.66	103.08	113.83
23	C	502	CLA	C4C-C3C-C2C	-2.66	103.02	106.90
25	t	102	BCR	C21-C20-C19	-2.66	114.91	123.22
23	c	504	CLA	O2A-CGA-O1A	-2.66	116.87	123.59
25	t	102	BCR	C1-C6-C7	2.66	123.31	115.78
25	B	617	BCR	C15-C14-C13	-2.66	123.51	127.31
23	b	601	CLA	CAC-C3C-C4C	2.66	128.26	124.81
26	f	102	SQD	O8-S-C6	2.66	109.98	105.74
23	D	403	CLA	CHD-C4C-NC	2.66	128.39	124.20
25	c	514	BCR	C36-C18-C17	-2.66	119.20	122.92
23	a	405[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	c	503	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
31	B	627	LMT	C4B-C3B-C2B	2.66	115.46	110.82
25	b	617	BCR	C24-C23-C22	-2.65	122.22	126.23
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59
23	A	406[B]	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	C	512	CLA	CMC-C2C-C1C	2.65	129.08	125.04
29	D	405[B]	PL9	C20-C19-C21	2.65	119.73	115.27
23	a	404[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
23	b	602	CLA	CMA-C3A-C4A	-2.65	104.64	111.77
23	c	510	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
33	C	501	LMG	C1-O6-C5	-2.65	108.48	113.69
23	d	405	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
29	D	405[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	b	604	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
23	a	405[B]	CLA	CAC-C3C-C4C	2.65	128.24	124.81
33	m	101	LMG	C8-O7-C10	-2.65	111.28	117.79
25	k	101	BCR	C38-C26-C25	-2.65	121.56	124.53
23	D	403	CLA	CMC-C2C-C1C	2.65	129.07	125.04
26	X	101	SQD	O47-C7-O49	-2.64	117.31	123.70
29	A	414[B]	PL9	C35-C34-C36	2.64	119.72	115.27
29	D	405[B]	PL9	C37-C38-C39	-2.64	121.30	127.66
23	A	408	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	B	605	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
25	H	101	BCR	C7-C8-C9	-2.64	122.24	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	CAC-C3C-C4C	2.64	128.24	124.81
23	B	613	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
26	f	102	SQD	O48-C23-C24	2.64	120.19	111.91
23	b	604	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	b	606	CLA	CAA-C2A-C3A	-2.64	105.55	112.78
23	B	602	CLA	CMA-C3A-C4A	-2.64	104.68	111.77
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	B	602	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
25	B	618	BCR	C37-C22-C23	2.64	122.23	118.08
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
23	c	511	CLA	CMC-C2C-C1C	2.63	129.05	125.04
31	C	525	LMT	O5'-C5'-C6'	2.63	112.98	106.44
23	c	504	CLA	CMC-C2C-C1C	2.63	129.05	125.04
24	A	416[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
25	b	618	BCR	C15-C14-C13	-2.63	123.55	127.31
25	k	101	BCR	C2-C1-C6	2.63	114.53	110.48
23	C	513	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
23	c	511	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	C	514	CLA	C4C-C3C-C2C	-2.63	103.06	106.90
23	C	513	CLA	CMC-C2C-C1C	2.63	129.04	125.04
23	c	504	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
24	A	407[B]	PHO	CMA-C3A-C4A	-2.63	108.62	114.38
23	A	406[B]	CLA	CBC-CAC-C3C	-2.63	105.19	112.43
25	d	406	BCR	C28-C27-C26	-2.63	109.39	114.08
23	B	614	CLA	C4C-C3C-C2C	-2.62	103.07	106.90
23	c	509	CLA	CHB-C1B-NB	-2.62	121.48	124.26
23	B	602	CLA	CAC-C3C-C4C	2.62	128.21	124.81
29	A	414[B]	PL9	C12-C13-C14	-2.62	121.34	127.66
33	c	520	LMG	O8-C28-C29	2.62	120.14	111.91
26	X	101	SQD	O48-C23-C24	2.62	120.14	111.91
23	b	603	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
23	d	404[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
27	b	628	GOL	C3-C2-C1	-2.62	101.52	111.70
23	C	514	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	C	503	CLA	CHD-C4C-NC	2.62	128.33	124.20
32	a	419[B]	LHG	O8-C23-C24	2.62	120.12	111.91
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
25	Y	101	BCR	C36-C18-C17	-2.61	119.26	122.92
23	C	506	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
23	b	616	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
23	C	512	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
23	B	601	CLA	C1-O2A-CGA	2.61	123.29	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
23	C	508	CLA	C1-C2-C3	-2.61	121.53	126.04
32	D	406[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	C	514	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
23	C	504	CLA	CHC-C1C-C2C	-2.61	119.49	126.73
23	a	404[B]	CLA	CMA-C3A-C4A	-2.61	104.77	111.77
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.50
23	b	616	CLA	CAC-C3C-C4C	2.61	128.19	124.81
23	a	404[B]	CLA	C2A-C1A-CHA	-2.60	119.30	123.86
32	d	408[B]	LHG	O8-C23-O10	-2.60	117.02	123.59
23	A	408	CLA	CHB-C4A-NA	2.60	128.11	124.51
32	L	101[A]	LHG	O8-C23-C24	2.60	120.06	111.91
23	b	612	CLA	O2A-CGA-CBA	2.60	120.06	111.91
35	c	516[B]	DGD	O3G-C3G-C2G	-2.60	104.63	110.90
29	a	413[B]	PL9	C40-C39-C41	2.60	119.64	115.27
23	C	513	CLA	O2A-CGA-O1A	-2.59	117.04	123.59
23	b	605	CLA	C1-O2A-CGA	2.59	123.25	116.44
23	B	601	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	d	402[A]	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	A	405[A]	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	C	514	CLA	C4-C3-C5	2.59	119.63	115.27
35	c	518	DGD	O1G-C1A-C2A	2.59	120.04	111.91
23	B	616	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
25	h	101	BCR	C37-C22-C21	-2.59	119.30	122.92
23	C	513	CLA	CMB-C2B-C1B	2.59	129.31	125.37
23	b	607	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
23	A	404[B]	CLA	CAC-C3C-C4C	2.59	128.17	124.81
23	C	503	CLA	C4-C3-C5	2.59	119.62	115.27
23	a	404[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
25	c	514	BCR	C33-C5-C6	-2.59	121.62	124.53
35	C	517[B]	DGD	O5D-C6D-C5D	-2.58	104.27	109.05
23	a	405[B]	CLA	CHC-C1C-C2C	-2.58	119.55	126.73
23	c	506	CLA	O2A-CGA-O1A	-2.58	117.07	123.59
23	B	605	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
23	c	507	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
29	d	407[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
33	D	411	LMG	O8-C28-C29	2.58	120.00	111.91
25	c	515	BCR	C37-C22-C23	2.58	122.14	118.08
25	T	102	BCR	C12-C13-C14	-2.58	114.99	118.94
29	a	413[B]	PL9	C20-C19-C21	2.58	119.60	115.27
23	b	605	CLA	C1-C2-C3	-2.57	121.59	126.04
23	d	405	CLA	CAC-C3C-C4C	2.57	128.15	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	A	406[B]	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
23	c	513	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
24	a	406[B]	PHO	O2D-CGD-O1D	-2.57	118.81	123.84
23	d	402[B]	CLA	C4C-C3C-C2C	-2.57	103.15	106.90
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	D	402[B]	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
25	c	514	BCR	C37-C22-C21	-2.57	119.33	122.92
25	Y	101	BCR	C10-C11-C12	-2.57	115.20	123.22
23	b	602	CLA	C2A-C1A-CHA	-2.57	119.37	123.86
23	c	504	CLA	CAC-C3C-C4C	2.57	128.14	124.81
31	T	101	LMT	C3'-C4'-C5'	-2.57	105.04	110.93
23	D	403	CLA	O2A-CGA-CBA	2.57	119.96	111.91
23	A	408	CLA	C4-C3-C5	2.57	119.59	115.27
23	C	504	CLA	CAC-C3C-C4C	2.56	128.13	124.81
23	D	402[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
31	M	101	LMT	C3'-C4'-C5'	-2.56	105.05	110.93
23	D	402[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
35	c	516[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
23	D	403	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
23	b	608	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	c	508	CLA	C4-C3-C5	2.56	119.58	115.27
23	C	513	CLA	CAC-C3C-C4C	2.56	128.13	124.81
23	c	507	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
23	B	608	CLA	C11-C12-C13	-2.56	107.65	115.92
23	c	502	CLA	CMC-C2C-C1C	2.56	128.94	125.04
23	C	504	CLA	O2A-CGA-CBA	2.56	119.93	111.91
23	C	503	CLA	CMC-C2C-C1C	2.56	128.93	125.04
23	a	405[B]	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
23	B	609	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	b	611	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	c	511	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	c	507	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
23	B	611	CLA	O2A-CGA-O1A	-2.55	117.15	123.59
23	c	503	CLA	C4-C3-C5	2.55	119.57	115.27
31	F	101	LMT	C1'-O5'-C5'	-2.55	108.69	113.69
23	B	606	CLA	C3B-C4B-NB	2.55	112.88	110.52
31	B	629	LMT	C3'-C4'-C5'	-2.55	105.09	110.93
24	a	406[B]	PHO	C1A-C2A-C3A	-2.55	100.42	102.84
25	t	102	BCR	C37-C22-C23	2.55	122.09	118.08
26	a	411	SQD	C1-O5-C5	2.55	118.69	113.69
25	A	409	BCR	C40-C30-C25	-2.55	106.17	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C4-C3-C5	2.55	119.55	115.27
26	a	409[B]	SQD	O9-S-C6	2.55	109.96	106.94
35	C	518[B]	DGD	C2G-O2G-C1B	-2.54	111.53	117.79
23	c	510	CLA	C11-C10-C8	-2.54	107.70	115.92
23	C	509	CLA	O2A-CGA-CBA	2.54	119.89	111.91
23	b	603	CLA	CBC-CAC-C3C	-2.54	105.42	112.43
23	d	405	CLA	CBC-CAC-C3C	-2.54	105.42	112.43
23	A	405[B]	CLA	CAC-C3C-C4C	2.54	128.11	124.81
34	b	622	HTG	O5-C1-C2	2.54	113.51	110.31
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
24	a	406[B]	PHO	CMB-C2B-C3B	2.54	129.43	124.68
23	c	511	CLA	C1-C2-C3	-2.54	121.65	126.04
24	d	403[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	b	613	CLA	C4-C3-C5	2.54	119.54	115.27
23	b	611	CLA	CAC-C3C-C4C	2.54	128.10	124.81
25	a	408	BCR	C37-C22-C21	-2.54	119.37	122.92
29	D	405[B]	PL9	C45-C44-C46	2.53	119.53	115.27
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
23	c	507	CLA	C3B-C4B-NB	2.53	112.86	110.52
23	C	504	CLA	C1-C2-C3	-2.53	121.67	126.04
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	603	CLA	CHD-C4C-NC	2.53	128.19	124.20
23	c	506	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	b	602	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	a	407	CLA	CMA-C3A-C2A	-2.52	103.64	113.83
23	a	405[A]	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	C	513	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	A	406[A]	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
26	A	412	SQD	C1-C2-C3	-2.52	104.75	110.00
23	B	613	CLA	CBC-CAC-C3C	-2.52	105.48	112.43
31	B	628	LMT	O5'-C5'-C4'	2.52	115.07	109.75
23	C	512	CLA	CAC-C3C-C4C	2.52	128.08	124.81
33	d	413	LMG	C7-O1-C1	-2.52	108.82	113.74
23	b	604	CLA	C4-C3-C5	2.52	119.51	115.27
23	A	404[B]	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
35	h	102	DGD	O1G-C1A-O1A	-2.52	117.24	123.59
23	c	505	CLA	O2A-CGA-CBA	2.52	119.80	111.91
24	A	416[B]	PHO	CMB-C2B-C3B	2.52	129.38	124.68
23	c	506	CLA	C4-C3-C5	2.52	119.50	115.27
24	d	403[B]	PHO	O2D-CGD-O1D	-2.51	118.92	123.84
40	v	201	HEC	C4B-NB-C1B	2.51	107.67	105.07
23	c	504	CLA	O2D-CGD-O1D	-2.51	118.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	413[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	d	402[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	b	611	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	B	615	CLA	C1-O2A-CGA	2.51	123.03	116.44
38	E	102	HEM	O2A-CGA-CBA	2.51	122.10	114.03
25	C	516	BCR	C32-C1-C6	-2.51	106.23	110.30
24	A	407[A]	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407[A]	PHO	CMB-C2B-C3B	2.51	129.37	124.68
23	C	507	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	a	405[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
25	t	102	BCR	C20-C21-C22	-2.51	123.73	127.31
29	d	407[B]	PL9	C36-C37-C38	-2.51	103.64	111.88
23	d	402[B]	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
23	B	603	CLA	O2A-CGA-CBA	2.51	119.77	111.91
23	C	502	CLA	C4-C3-C5	2.51	119.48	115.27
29	d	407[B]	PL9	C17-C18-C19	-2.50	121.63	127.66
33	C	501	LMG	C8-O7-C10	-2.50	111.62	117.79
29	a	413[B]	PL9	C47-C48-C49	-2.50	119.19	127.75
25	B	617	BCR	C7-C8-C9	-2.50	122.45	126.23
25	d	406	BCR	C33-C5-C6	-2.50	121.72	124.53
23	b	607	CLA	C4-C3-C5	2.50	119.48	115.27
25	T	102	BCR	C33-C5-C6	-2.50	121.72	124.53
25	a	408	BCR	C29-C30-C25	2.50	114.33	110.48
23	A	404[B]	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
23	a	404[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
29	D	405[B]	PL9	C27-C28-C29	-2.50	121.65	127.66
23	d	405	CLA	O2A-CGA-CBA	2.49	119.74	111.91
23	C	510	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
29	d	407[B]	PL9	C20-C19-C21	2.49	119.47	115.27
23	C	510	CLA	C11-C12-C13	-2.49	107.86	115.92
23	C	511	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
35	h	102	DGD	O4D-C4D-C3D	-2.49	104.59	110.35
25	a	408	BCR	C7-C8-C9	-2.49	122.47	126.23
23	a	405[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	b	610	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
23	a	405[B]	CLA	O2A-CGA-O1A	-2.49	117.31	123.59
23	C	513	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	d	407[B]	PL9	C22-C23-C24	-2.49	121.67	127.66
23	A	404[B]	CLA	CHD-C4C-NC	2.49	128.12	124.20
23	b	614	CLA	C4-C3-C5	2.49	119.45	115.27
24	a	406[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
38	f	101	HEM	CMD-C2D-C1D	2.48	128.82	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403[B]	PHO	C4A-C3A-C2A	-2.48	100.48	102.84
23	B	615	CLA	CHC-C1C-C2C	-2.48	119.83	126.73
23	b	614	CLA	CMA-C3A-C4A	-2.48	105.10	111.77
26	b	620	SQD	O9-S-C6	2.48	109.89	106.94
23	c	502	CLA	O2A-CGA-CBA	2.48	119.70	111.91
23	A	405[B]	CLA	OBD-CAD-C3D	-2.48	122.55	128.52
25	H	101	BCR	C10-C11-C12	-2.48	115.48	123.22
23	B	604	CLA	CAC-C3C-C4C	2.48	128.03	124.81
35	C	517[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	407[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
25	D	404	BCR	C15-C14-C13	-2.48	123.77	127.31
23	C	512	CLA	C1-O2A-CGA	2.48	122.95	116.44
23	A	405[B]	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
23	b	610	CLA	CAA-CBA-CGA	-2.48	106.02	113.25
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
25	Y	101	BCR	C15-C16-C17	-2.47	118.41	123.47
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
32	D	407[B]	LHG	O8-C23-O10	-2.47	117.35	123.59
29	A	414[B]	PL9	C42-C43-C44	-2.47	121.70	127.66
23	A	404[B]	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
23	B	607	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
23	a	407	CLA	CMB-C2B-C1B	2.47	129.13	125.37
23	b	609	CLA	C16-C15-C13	-2.47	107.93	115.92
23	B	601	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	504	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	513	CLA	CHD-C4C-NC	2.47	128.10	124.20
23	c	503	CLA	CAC-C3C-C4C	2.47	128.01	124.81
23	c	512	CLA	CMC-C2C-C1C	2.47	128.80	125.04
23	b	613	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
40	V	201	HEC	C3D-C4D-ND	-2.47	107.97	110.36
23	b	602	CLA	CHB-C1B-C2B	-2.46	120.28	127.24
23	c	512	CLA	C3B-C4B-NB	2.46	112.80	110.52
23	C	503	CLA	CBC-CAC-C3C	-2.46	105.64	112.43
32	d	408[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
23	c	501	CLA	CHD-C4C-NC	2.46	128.08	124.20
35	C	517[B]	DGD	C2G-O2G-C1B	-2.46	111.73	117.79
23	C	506	CLA	CHB-C1B-NB	-2.46	121.65	124.26
26	a	409[A]	SQD	O7-S-C6	2.46	109.86	106.94
24	A	416[B]	PHO	CED-O2D-CGD	2.46	121.50	115.94
23	d	402[B]	CLA	C1-C2-C3	-2.46	121.79	126.04
38	E	102	HEM	O2D-CGD-CBD	2.46	121.92	114.03
29	A	414[B]	PL9	C53-C6-C1	2.46	120.01	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CHD-C4C-NC	2.45	128.07	124.20
23	d	402[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	C	506	CLA	O2A-CGA-CBA	2.45	119.59	111.91
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
25	h	101	BCR	C36-C18-C17	-2.45	119.49	122.92
26	f	102	SQD	O47-C7-O49	-2.45	117.79	123.70
29	a	413[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	B	602	CLA	CHC-C1C-C2C	-2.45	119.93	126.73
25	a	408	BCR	C20-C21-C22	-2.45	123.82	127.31
23	a	405[B]	CLA	O2A-CGA-CBA	2.45	119.58	111.91
23	c	501	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
23	c	503	CLA	CHC-C1C-C2C	-2.45	119.94	126.73
23	B	611	CLA	CMB-C2B-C3B	2.45	132.51	126.59
29	D	405[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
29	a	413[A]	PL9	C20-C19-C21	2.44	119.38	115.27
25	K	102	BCR	C24-C23-C22	-2.44	122.54	126.23
23	B	606	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
23	D	403	CLA	CMA-C3A-C4A	-2.44	105.21	111.77
23	c	501	CLA	CBC-CAC-C3C	-2.44	105.71	112.43
23	B	603	CLA	CMA-C3A-C2A	-2.44	103.99	113.83
23	A	405[A]	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
23	a	404[A]	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	K	102	BCR	C36-C18-C19	2.43	121.91	118.08
35	c	517[B]	DGD	O1G-C1A-C2A	2.43	119.54	111.91
24	a	406[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
25	c	515	BCR	C2-C1-C6	2.43	114.22	110.48
23	C	514	CLA	CMB-C2B-C1B	2.43	129.07	125.37
23	c	501	CLA	CMC-C2C-C1C	2.43	128.74	125.04
25	Y	101	BCR	C36-C18-C19	2.43	121.90	118.08
23	b	611	CLA	CMB-C2B-C1B	2.43	129.06	125.37
23	C	508	CLA	O2A-CGA-CBA	2.43	119.52	111.91
23	A	405[B]	CLA	CHB-C1B-NB	-2.43	121.69	124.26
23	C	502	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
29	d	407[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
24	A	407[B]	PHO	O2A-CGA-CBA	2.42	119.51	111.91
25	H	101	BCR	C33-C5-C6	-2.42	121.81	124.53
25	A	409	BCR	C8-C7-C6	-2.42	120.40	127.20
25	T	102	BCR	C35-C13-C12	2.42	121.89	118.08
31	m	103	LMT	C3'-C4'-C5'	-2.42	105.38	110.93
23	C	514	CLA	CHB-C1B-NB	-2.42	121.70	124.26
26	a	409[B]	SQD	O47-C7-O49	-2.42	117.86	123.70
23	C	506	CLA	C4-C3-C5	2.42	119.34	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	H	102	DGD	O2G-C1B-C2B	2.42	116.71	111.50
26	a	409[A]	SQD	O8-S-C6	2.41	109.59	105.74
31	C	525	LMT	O1'-C1'-C2'	2.41	112.07	108.30
23	B	608	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
23	b	614	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68
23	B	611	CLA	C3B-C4B-NB	2.41	112.75	110.52
29	A	414[B]	PL9	C45-C44-C46	2.41	119.33	115.27
23	b	612	CLA	CHB-C1B-NB	-2.41	121.70	124.26
23	B	615	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
23	C	504	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
23	d	405	CLA	C3B-C4B-NB	2.41	112.75	110.52
23	a	405[B]	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
26	b	620	SQD	C1-C2-C3	-2.41	104.98	110.00
23	B	606	CLA	C7-C6-C5	-2.41	106.82	113.36
23	D	402[B]	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
23	a	404[B]	CLA	CHD-C4C-NC	2.41	128.00	124.20
23	c	506	CLA	O2A-CGA-CBA	2.41	119.46	111.91
23	B	616	CLA	CHC-C1C-C2C	-2.41	120.05	126.73
23	c	507	CLA	CBC-CAC-C3C	-2.41	105.80	112.43
23	b	605	CLA	C4-C3-C5	2.41	119.32	115.27
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
35	C	517[B]	DGD	C3G-C2G-C1G	-2.40	106.10	111.79
33	C	520	LMG	O8-C28-O10	-2.40	117.52	123.59
23	B	611	CLA	OBD-CAD-C3D	-2.40	122.73	128.52
23	A	408	CLA	CMA-C3A-C2A	-2.40	104.13	113.83
31	B	629	LMT	O5'-C5'-C4'	2.40	114.82	109.75
26	a	411	SQD	O48-C23-O10	-2.40	117.54	123.59
23	C	509	CLA	CHD-C4C-NC	2.40	127.98	124.20
25	B	617	BCR	C29-C30-C25	2.40	114.17	110.48
23	b	607	CLA	C1-O2A-CGA	2.40	122.73	116.44
25	k	101	BCR	C11-C10-C9	-2.39	123.89	127.31
23	b	603	CLA	C7-C6-C5	-2.39	106.86	113.36
23	D	403	CLA	C2A-C1A-CHA	-2.39	119.67	123.86
23	b	609	CLA	C7-C6-C5	-2.39	106.86	113.36
23	B	608	CLA	CAA-C2A-C3A	-2.39	106.22	112.78
32	D	406[B]	LHG	O8-C23-C24	2.39	119.41	111.91
25	b	618	BCR	C2-C1-C6	2.39	114.16	110.48
25	H	101	BCR	C36-C18-C17	-2.39	119.58	122.92
23	B	604	CLA	C11-C12-C13	-2.39	108.20	115.92
23	A	408	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
23	d	402[B]	CLA	C2A-C1A-CHA	-2.38	119.69	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	CHB-C4A-NA	2.38	127.81	124.51
33	c	519	LMG	C8-O7-C10	-2.38	111.93	117.79
23	B	612	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
32	L	101[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
23	b	607	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	c	510	CLA	C4-C3-C2	-2.38	117.58	123.68
23	b	616	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	B	608	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
23	B	610	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
29	a	413[A]	PL9	C10-C9-C8	-2.38	117.58	123.68
23	B	604	CLA	O1D-CGD-CBD	-2.38	119.62	124.48
25	d	406	BCR	C39-C30-C25	-2.38	106.44	110.30
26	A	410[B]	SQD	O48-C23-O10	-2.38	117.60	123.59
29	d	407[A]	PL9	C7-C8-C9	-2.38	122.84	126.79
23	B	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	C	516	BCR	C29-C30-C25	2.38	114.14	110.48
29	D	405[A]	PL9	C45-C44-C46	2.38	119.27	115.27
23	B	608	CLA	CMC-C2C-C1C	2.37	128.66	125.04
25	c	514	BCR	C28-C27-C26	-2.37	109.84	114.08
23	B	608	CLA	C11-C10-C8	-2.37	108.25	115.92
23	d	402[B]	CLA	CHB-C1B-NB	-2.37	121.75	124.26
23	C	507	CLA	CMB-C2B-C1B	2.37	128.98	125.37
26	X	101	SQD	C46-C45-C44	-2.37	106.18	111.79
23	D	403	CLA	CHB-C1B-NB	-2.37	121.75	124.26
23	a	404[B]	CLA	C7-C6-C5	-2.37	106.93	113.36
23	b	616	CLA	C4-C3-C5	2.37	119.25	115.27
23	C	512	CLA	CMB-C2B-C1B	2.37	128.97	125.37
25	h	101	BCR	C16-C15-C14	-2.37	118.63	123.47
40	V	201	HEC	CHA-C1A-NA	2.37	127.00	124.44
35	c	516[B]	DGD	O6D-C1D-O3G	-2.37	104.37	109.97
23	b	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
32	A	419[B]	LHG	O7-C7-O9	-2.37	117.98	123.70
23	b	613	CLA	CHD-C4C-NC	2.36	127.93	124.20
23	d	402[B]	CLA	CHB-C4A-NA	2.36	127.78	124.51
31	B	628	LMT	O5'-C5'-C6'	2.36	112.31	106.44
32	d	415[B]	LHG	C5-O7-C7	-2.36	111.97	117.79
25	c	515	BCR	C21-C20-C19	-2.36	115.84	123.22
23	C	513	CLA	C2A-C1A-CHA	-2.36	119.73	123.86
23	B	601	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	c	513	CLA	CBC-CAC-C3C	-2.36	105.92	112.43
25	C	515	BCR	C16-C17-C18	-2.36	123.94	127.31
29	A	414[B]	PL9	C10-C9-C8	-2.36	117.63	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	405[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
23	c	505	CLA	CHD-C4C-NC	2.36	127.92	124.20
23	B	609	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
23	A	408	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	c	509	CLA	CMB-C2B-C1B	2.36	128.96	125.37
23	c	507	CLA	C1-C2-C3	-2.36	121.97	126.04
34	B	624	HTG	C3-C4-C5	2.36	114.44	110.24
33	C	520	LMG	C8-O7-C10	-2.36	111.99	117.79
23	b	615	CLA	O2A-CGA-CBA	2.36	119.30	111.91
25	h	101	BCR	C16-C17-C18	-2.35	123.95	127.31
23	d	404[B]	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	D	405[B]	PL9	C30-C29-C31	2.35	119.23	115.27
24	A	416[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
29	a	413[B]	PL9	C45-C44-C46	2.35	119.23	115.27
23	b	603	CLA	CMC-C2C-C1C	2.35	128.62	125.04
24	a	406[B]	PHO	CBA-CAA-C2A	-2.35	106.94	113.81
25	B	619	BCR	C29-C30-C25	2.35	114.10	110.48
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	c	504	CLA	CED-O2D-CGD	2.35	121.25	115.94
35	C	518[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44
29	a	413[A]	PL9	C45-C44-C46	2.35	119.22	115.27
25	t	102	BCR	C7-C6-C5	-2.35	115.78	121.46
23	d	402[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	C	504	CLA	CBC-CAC-C3C	-2.35	105.96	112.43
25	a	408	BCR	C15-C16-C17	-2.35	118.67	123.47
25	c	515	BCR	C7-C8-C9	-2.35	122.69	126.23
23	b	606	CLA	CMB-C2B-C1B	2.34	128.94	125.37
25	Y	101	BCR	C34-C9-C8	2.34	121.77	118.08
23	d	404[B]	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
32	d	408[B]	LHG	O8-C23-C24	2.34	119.26	111.91
23	B	616	CLA	CBC-CAC-C3C	-2.34	105.97	112.43
26	a	409[B]	SQD	O48-C23-C24	2.34	119.26	111.91
23	B	612	CLA	CHC-C1C-C2C	-2.34	120.22	126.73
23	c	511	CLA	CMA-C3A-C4A	2.34	118.07	111.77
23	c	503	CLA	O2A-CGA-CBA	2.34	119.25	111.91
24	A	416[B]	PHO	O2A-CGA-CBA	2.34	119.25	111.91
25	Y	101	BCR	C1-C6-C7	2.34	122.40	115.78
35	C	518[B]	DGD	O1G-C1A-C2A	2.34	119.25	111.91
23	B	605	CLA	CED-O2D-CGD	2.34	121.23	115.94
23	B	601	CLA	CMC-C2C-C1C	2.34	128.60	125.04
38	E	102	HEM	C4D-ND-C1D	2.34	107.49	105.07
23	c	510	CLA	CBC-CAC-C3C	-2.34	105.99	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	102	BCR	C21-C20-C19	-2.34	115.93	123.22
35	C	517[B]	DGD	O1G-C1A-O1A	-2.34	117.70	123.59
23	b	606	CLA	C1-O2A-CGA	2.33	122.57	116.44
23	b	606	CLA	O2A-CGA-CBA	2.33	119.23	111.91
23	B	603	CLA	CHD-C4C-NC	2.33	127.88	124.20
34	c	521	HTG	O5-C1-C2	2.33	113.25	110.31
23	d	402[B]	CLA	CMA-C3A-C2A	-2.33	104.42	113.83
24	A	407[B]	PHO	C1-C2-C3	-2.33	122.01	126.04
23	c	508	CLA	O2A-CGA-CBA	2.33	119.22	111.91
23	c	513	CLA	CMB-C2B-C1B	2.33	128.92	125.37
23	D	402[A]	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	c	508	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	c	506	CLA	CAA-C2A-C3A	-2.33	106.40	112.78
23	C	509	CLA	C4-C3-C5	2.33	119.19	115.27
23	d	402[A]	CLA	C1-O2A-CGA	2.33	122.56	116.44
25	c	515	BCR	C32-C1-C6	-2.33	106.52	110.30
23	C	511	CLA	CMB-C2B-C1B	2.33	128.92	125.37
25	b	617	BCR	C29-C30-C25	2.33	114.07	110.48
23	B	612	CLA	C3B-C4B-NB	2.33	112.68	110.52
24	A	416[B]	PHO	CMA-C3A-C4A	-2.33	109.28	114.38
25	c	514	BCR	C38-C26-C25	-2.33	121.91	124.53
29	a	413[A]	PL9	C35-C34-C33	-2.33	117.70	123.68
35	C	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
35	c	517[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
23	B	602	CLA	CMB-C2B-C1B	2.33	128.91	125.37
23	C	506	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
23	c	510	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
32	d	408[A]	LHG	O8-C23-C24	2.33	119.21	111.91
23	C	509	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
35	c	516[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
24	d	403[B]	PHO	C1A-C2A-C3A	-2.32	100.63	102.84
40	v	201	HEC	C4A-NA-C1A	2.32	107.62	105.35
23	b	612	CLA	CHD-C4C-NC	2.32	127.86	124.20
25	Y	101	BCR	C37-C22-C23	2.32	121.73	118.08
23	B	608	CLA	CHD-C4C-NC	2.32	127.86	124.20
23	a	405[A]	CLA	C4-C3-C5	2.32	119.17	115.27
23	c	503	CLA	CBC-CAC-C3C	-2.32	106.04	112.43
23	d	405	CLA	CHB-C4A-NA	2.32	127.72	124.51
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
26	a	411	SQD	O5-C5-C4	2.32	113.90	109.69
25	y	101	BCR	C16-C17-C18	-2.32	124.00	127.31
26	a	409[A]	SQD	O48-C23-C24	2.32	119.17	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	403	CLA	C1-C2-C3	-2.31	122.04	126.04
23	b	602	CLA	O2A-CGA-CBA	2.31	119.17	111.91
25	B	618	BCR	C38-C26-C25	-2.31	121.93	124.53
24	d	403[B]	PHO	CBA-CAA-C2A	-2.31	107.05	113.81
25	K	102	BCR	C20-C21-C22	-2.31	124.01	127.31
23	b	602	CLA	CHC-C1C-C2C	-2.31	120.31	126.73
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
25	h	101	BCR	C20-C21-C22	-2.31	124.01	127.31
34	b	625	HTG	C1'-S1-C1	2.31	104.41	100.09
23	c	507	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
23	b	602	CLA	C11-C10-C8	-2.31	108.46	115.92
24	A	407[B]	PHO	O2D-CGD-O1D	-2.31	119.33	123.84
23	A	404[B]	CLA	CMC-C2C-C1C	2.31	128.55	125.04
25	h	101	BCR	C34-C9-C8	2.31	121.71	118.08
25	k	101	BCR	C3-C4-C5	-2.31	109.96	114.08
33	B	620	LMG	C12-C11-C10	-2.31	105.24	113.62
23	D	403	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
29	d	407[B]	PL9	C45-C44-C46	2.30	119.15	115.27
25	c	514	BCR	C36-C18-C19	2.30	121.71	118.08
23	d	404[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
24	a	406[B]	PHO	CMC-C2C-C1C	2.30	129.08	124.73
29	D	405[B]	PL9	C7-C8-C9	-2.30	122.96	126.79
23	A	406[B]	CLA	C1-C2-C3	-2.30	122.06	126.04
23	A	405[B]	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
23	d	404[B]	CLA	CBC-CAC-C3C	-2.30	106.08	112.43
23	B	612	CLA	C1-C2-C3	-2.30	122.06	126.04
25	y	101	BCR	C21-C20-C19	-2.30	116.03	123.22
23	d	404[B]	CLA	CHD-C4C-NC	2.30	127.83	124.20
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
33	d	413	LMG	O7-C10-O9	-2.30	118.14	123.70
23	B	614	CLA	OBD-CAD-C3D	-2.30	122.98	128.52
23	A	405[B]	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
23	c	505	CLA	C4-C3-C5	2.30	119.14	115.27
23	b	603	CLA	C5-C3-C2	-2.30	116.46	121.12
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	B	605	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
23	c	513	CLA	CHB-C1B-NB	-2.30	121.83	124.26
23	B	610	CLA	CMC-C2C-C1C	2.30	128.53	125.04
23	C	505	CLA	CHB-C1B-NB	-2.30	121.83	124.26
23	B	602	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	c	515	BCR	C20-C21-C22	-2.29	124.03	127.31
34	B	621	HTG	O2-C2-C3	-2.29	105.04	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	620	SQD	O48-C23-C24	2.29	119.11	111.91
23	c	504	CLA	O2A-CGA-CBA	2.29	119.11	111.91
23	c	504	CLA	CHB-C1B-NB	-2.29	121.83	124.26
23	c	513	CLA	C4-C3-C5	2.29	119.13	115.27
23	A	406[B]	CLA	CMA-C3A-C2A	-2.29	104.58	113.83
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
24	d	403[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
35	C	517[B]	DGD	O6D-C1D-O3G	-2.29	104.55	109.97
31	B	628	LMT	O5B-C5B-C6B	2.29	112.13	106.44
23	C	514	CLA	CAC-C3C-C4C	2.29	127.78	124.81
32	d	409[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
23	a	405[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	B	602	CLA	C11-C12-C13	-2.28	108.53	115.92
23	b	606	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
35	H	102	DGD	O3G-C3G-C2G	-2.28	105.39	110.90
23	C	512	CLA	C1-C2-C3	-2.28	122.10	126.04
26	A	412	SQD	O48-C23-O10	-2.28	117.83	123.59
23	C	505	CLA	C4-C3-C5	2.28	119.11	115.27
26	a	411	SQD	O8-S-C6	2.28	109.37	105.74
23	C	511	CLA	C2A-C1A-CHA	-2.28	119.88	123.86
23	B	608	CLA	C1-C2-C3	-2.28	122.10	126.04
24	a	406[B]	PHO	CMA-C3A-C4A	-2.28	109.39	114.38
23	d	402[B]	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
25	h	101	BCR	C10-C11-C12	-2.28	116.11	123.22
35	c	516[B]	DGD	C2G-O2G-C1B	-2.27	112.19	117.79
23	C	511	CLA	CMC-C2C-C1C	2.27	128.50	125.04
35	C	519	DGD	O2G-C1B-C2B	2.27	116.40	111.50
23	b	604	CLA	CHD-C4C-NC	2.27	127.78	124.20
23	a	404[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	d	402[B]	CLA	C1-O2A-CGA	2.27	122.40	116.44
23	A	405[B]	CLA	C1-C2-C3	-2.27	122.11	126.04
29	d	407[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
32	b	629[B]	LHG	O8-C23-O10	-2.27	117.86	123.59
23	c	513	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
26	l	101	SQD	C44-O6-C1	-2.27	109.31	113.74
29	A	414[B]	PL9	C47-C48-C49	-2.27	120.00	127.75
25	k	101	BCR	C32-C1-C6	-2.27	106.62	110.30
40	V	201	HEC	CBA-CAA-C2A	-2.27	106.33	112.63
23	A	406[B]	CLA	CMA-C3A-C4A	-2.27	105.68	111.77
24	A	416[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
23	c	512	CLA	CBA-CAA-C2A	-2.27	107.17	113.86
23	c	502	CLA	C1-O2A-CGA	2.27	122.39	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C3B-C4B-NB	2.27	112.62	110.52
25	c	514	BCR	C8-C7-C6	-2.27	120.84	127.20
23	b	610	CLA	C3B-C4B-NB	2.27	112.62	110.52
32	d	408[B]	LHG	C6-C5-C4	-2.26	106.44	111.79
23	B	610	CLA	CHB-C4A-NA	2.26	127.64	124.51
35	c	518	DGD	O3G-C3G-C2G	-2.26	105.44	110.90
32	d	415[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
23	c	513	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
23	D	402[A]	CLA	C4-C3-C5	2.26	119.07	115.27
34	B	624	HTG	O5-C5-C4	2.26	113.80	109.69
32	d	408[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
25	A	409	BCR	C16-C17-C18	-2.26	124.09	127.31
31	m	103	LMT	C3B-C4B-C5B	-2.26	106.21	110.24
25	c	515	BCR	C33-C5-C6	-2.26	121.99	124.53
23	a	404[B]	CLA	CAC-C3C-C4C	2.26	127.74	124.81
23	a	405[B]	CLA	CBC-CAC-C3C	-2.26	106.21	112.43
33	C	521	LMG	C9-C8-C7	-2.26	106.45	111.79
25	B	618	BCR	C2-C1-C6	2.26	113.95	110.48
25	B	619	BCR	C21-C20-C19	-2.26	116.17	123.22
32	b	629[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
27	A	418	GOL	C3-C2-C1	-2.26	102.93	111.70
24	d	403[A]	PHO	C4-C3-C2	-2.26	117.89	123.68
23	B	604	CLA	C6-C5-C3	-2.25	107.55	113.45
23	B	612	CLA	C4A-NA-C1A	-2.25	105.69	106.71
23	c	510	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
23	b	602	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
29	D	405[A]	PL9	C20-C19-C21	2.25	119.05	115.27
25	a	408	BCR	C3-C4-C5	-2.25	110.06	114.08
25	k	101	BCR	C10-C11-C12	-2.25	116.20	123.22
24	A	416[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68
23	b	603	CLA	CAC-C3C-C4C	2.25	127.72	124.81
25	k	101	BCR	C16-C17-C18	-2.25	124.11	127.31
32	L	101[B]	LHG	O8-C23-C24	2.25	118.95	111.91
25	k	101	BCR	C34-C9-C8	2.24	121.61	118.08
23	C	512	CLA	O2A-CGA-CBA	2.24	118.95	111.91
23	b	601	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
25	d	406	BCR	C40-C30-C39	2.24	115.42	108.53
23	D	402[B]	CLA	CHD-C4C-NC	2.24	127.74	124.20
29	d	407[B]	PL9	C51-C49-C50	2.24	119.56	114.60
29	A	414[B]	PL9	C25-C24-C26	2.24	119.04	115.27
23	b	610	CLA	CMA-C3A-C4A	-2.24	105.75	111.77
40	V	201	HEC	CHA-C4D-ND	2.24	126.85	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
23	c	505	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
32	E	101[B]	LHG	O7-C7-O9	-2.24	118.29	123.70
23	b	608	CLA	C11-C12-C13	-2.24	108.69	115.92
33	C	521	LMG	O1-C1-C2	2.24	111.80	108.30
23	C	514	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
24	A	407[B]	PHO	O2A-CGA-O1A	-2.24	117.95	123.59
33	c	520	LMG	O8-C28-O10	-2.23	117.95	123.59
29	D	405[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
40	v	201	HEC	CAD-CBD-CGD	-2.23	108.80	113.60
29	A	414[B]	PL9	C35-C34-C33	-2.23	117.95	123.68
29	A	414[B]	PL9	C51-C49-C50	2.23	119.53	114.60
23	B	603	CLA	C7-C6-C5	-2.23	107.30	113.36
23	c	504	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
29	D	405[B]	PL9	C22-C23-C24	-2.23	122.29	127.66
23	a	404[B]	CLA	O2A-CGA-O1A	-2.23	117.97	123.59
25	a	408	BCR	C11-C10-C9	-2.23	124.13	127.31
26	A	410[B]	SQD	O9-S-O7	-2.23	106.24	113.95
40	V	201	HEC	C2A-C1A-NA	-2.23	108.16	110.32
23	b	602	CLA	CAA-CBA-CGA	-2.23	106.74	113.25
23	b	615	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
23	b	613	CLA	CHB-C4A-NA	2.23	127.59	124.51
25	K	102	BCR	C35-C13-C14	-2.23	119.80	122.92
34	b	625	HTG	C1-C2-C3	-2.23	106.19	110.59
29	d	407[B]	PL9	C35-C34-C36	2.23	119.02	115.27
23	C	506	CLA	CHA-C1A-NA	-2.23	121.30	126.40
25	c	514	BCR	C29-C30-C25	2.22	113.91	110.48
23	a	404[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
24	d	403[B]	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
23	b	606	CLA	C1-C2-C3	-2.22	122.20	126.04
26	A	410[A]	SQD	O8-S-C6	2.22	109.28	105.74
23	C	505	CLA	CMB-C2B-C1B	2.22	128.75	125.37
23	B	602	CLA	CMA-C3A-C2A	-2.22	104.86	113.83
23	c	511	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
29	d	407[B]	PL9	C15-C14-C16	2.22	119.01	115.27
23	B	608	CLA	CMB-C2B-C1B	2.22	128.75	125.37
23	B	611	CLA	C4-C3-C5	2.22	119.00	115.27
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	h	101	BCR	C11-C10-C9	-2.22	124.14	127.31
23	b	609	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
25	b	617	BCR	C20-C21-C22	-2.22	124.15	127.31
33	d	413	LMG	O8-C28-C29	2.22	118.86	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
35	C	517[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
23	b	601	CLA	O2A-CGA-CBA	2.22	118.86	111.91
35	c	517[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
23	B	612	CLA	C1-O2A-CGA	2.21	122.25	116.44
23	A	406[B]	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	D	404	BCR	C21-C20-C19	-2.21	116.31	123.22
23	C	506	CLA	CHD-C4C-NC	2.21	127.69	124.20
25	C	516	BCR	C39-C30-C25	-2.21	106.71	110.30
23	B	608	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	b	613	CLA	CMB-C2B-C1B	2.21	128.74	125.37
23	c	505	CLA	CMC-C2C-C1C	2.21	128.41	125.04
25	b	619	BCR	C34-C9-C10	-2.21	119.83	122.92
24	a	406[B]	PHO	O1D-CGD-CBD	-2.21	121.06	124.74
23	C	508	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
23	D	403	CLA	CHB-C4A-NA	2.21	127.57	124.51
23	A	408	CLA	CMA-C3A-C4A	-2.21	105.83	111.77
23	C	507	CLA	CGD-CBD-CAD	-2.21	103.58	110.73
25	T	102	BCR	C3-C4-C5	-2.21	110.13	114.08
23	B	609	CLA	C16-C15-C13	-2.21	108.78	115.92
25	C	515	BCR	C24-C23-C22	-2.21	122.90	126.23
23	b	609	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	A	407[A]	PHO	C1-C2-C3	-2.20	122.24	126.04
23	a	405[A]	CLA	CAC-C3C-C4C	2.20	127.67	124.81
26	b	620	SQD	C44-O6-C1	-2.20	109.44	113.74
34	C	522	HTG	C1-O5-C5	2.20	116.64	112.58
23	b	608	CLA	O2A-CGA-CBA	2.20	118.81	111.91
23	b	607	CLA	CMB-C2B-C1B	2.20	128.72	125.37
23	c	505	CLA	C3B-C4B-NB	2.20	112.55	110.52
23	D	402[B]	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
23	D	403	CLA	CBC-CAC-C3C	-2.20	106.38	112.43
23	B	606	CLA	OBD-CAD-C3D	-2.20	123.24	128.52
24	A	416[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
23	a	407	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
23	B	611	CLA	C1C-C2C-C3C	-2.19	104.65	106.96
23	c	511	CLA	C1-O2A-CGA	2.19	122.20	116.44
23	d	404[B]	CLA	CMC-C2C-C1C	2.19	128.38	125.04
23	C	504	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
23	c	501	CLA	O2A-CGA-CBA	2.19	118.79	111.91
23	c	509	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
23	C	505	CLA	C2A-C1A-CHA	-2.19	120.03	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	521	LMG	C1-C2-C3	-2.19	105.43	110.00
26	X	101	SQD	O48-C23-O10	-2.19	118.07	123.59
24	a	406[B]	PHO	OBD-CAD-C3D	-2.19	124.35	127.98
29	D	405[B]	PL9	C36-C37-C38	-2.19	104.69	111.88
23	B	604	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
23	b	608	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
23	B	605	CLA	O2A-CGA-CBA	2.19	118.77	111.91
23	C	509	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
25	Y	101	BCR	C7-C6-C5	-2.19	116.17	121.46
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
35	C	518[B]	DGD	O1G-C1A-O1A	-2.18	118.08	123.59
26	a	409[A]	SQD	O9-S-O7	-2.18	106.39	113.95
23	C	509	CLA	CAC-C3C-C4C	2.18	127.64	124.81
26	b	620	SQD	O47-C7-O49	-2.18	118.43	123.70
23	b	608	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	c	502	CLA	C4C-C3C-C2C	-2.18	103.72	106.90
29	a	413[B]	PL9	C35-C34-C33	-2.18	118.08	123.68
23	c	510	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
23	b	601	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
34	b	622	HTG	O2-C2-C3	-2.18	105.31	110.35
29	d	407[A]	PL9	C51-C49-C50	2.18	119.42	114.60
23	b	601	CLA	CHB-C1B-C2B	-2.18	121.08	127.24
23	d	404[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	B	608	CLA	CMA-C3A-C2A	-2.18	105.04	113.83
23	c	511	CLA	CHB-C1B-NB	-2.18	121.95	124.26
33	B	620	LMG	O8-C28-O10	-2.18	118.10	123.59
35	c	517[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
25	c	514	BCR	C34-C9-C10	-2.17	119.88	122.92
24	d	403[B]	PHO	CED-O2D-CGD	2.17	120.85	115.94
26	f	102	SQD	O7-S-C6	2.17	109.52	106.94
26	b	620	SQD	O5-C1-C2	-2.17	105.76	110.35
31	m	103	LMT	C1'-O5'-C5'	-2.17	109.43	113.69
23	C	511	CLA	CHB-C4A-NA	2.17	127.51	124.51
24	a	406[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
26	X	101	SQD	O8-S-O7	-2.17	105.98	111.27
32	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24
23	B	616	CLA	C4-C3-C2	-2.17	118.12	123.68
27	O	303	GOL	C3-C2-C1	-2.17	103.28	111.70
23	c	509	CLA	C4-C3-C2	-2.17	118.12	123.68
23	b	608	CLA	C4C-C3C-C2C	-2.16	103.74	106.90
33	c	519	LMG	O8-C28-O10	-2.16	118.13	123.59
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	525	LMT	O5'-C5'-C4'	2.16	114.31	109.75
35	C	519	DGD	O3G-C3G-C2G	-2.16	105.68	110.90
25	t	102	BCR	C35-C13-C12	2.16	121.48	118.08
25	k	101	BCR	C36-C18-C19	2.16	121.48	118.08
23	c	506	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
25	y	101	BCR	C40-C30-C25	-2.16	106.80	110.30
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	d	405	CLA	C1-O2A-CGA	2.16	122.10	116.44
33	C	501	LMG	C12-C11-C10	-2.16	105.78	113.62
23	d	402[B]	CLA	C4-C3-C5	2.16	118.90	115.27
23	B	613	CLA	CHD-C4C-NC	2.16	127.60	124.20
23	b	610	CLA	CMC-C2C-C1C	2.15	128.32	125.04
25	B	619	BCR	C10-C11-C12	-2.15	116.50	123.22
31	M	101	LMT	O5B-C5B-C6B	2.15	111.79	106.44
23	d	402[B]	CLA	CAC-C3C-C2C	2.15	131.21	127.53
27	B	623	GOL	C3-C2-C1	-2.15	103.34	111.70
35	c	518	DGD	O2G-C1B-O1B	-2.15	118.50	123.70
40	v	201	HEC	CMD-C2D-C1D	2.15	128.31	125.04
35	C	518[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	c	502	CLA	C1-C2-C3	-2.15	122.33	126.04
31	B	627	LMT	C1B-C2B-C3B	2.15	114.47	110.00
33	a	415	LMG	O8-C28-C29	2.15	118.65	111.91
35	c	516[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
31	e	101	LMT	O1'-C1'-C2'	2.15	111.66	108.30
25	B	617	BCR	C21-C20-C19	-2.15	116.52	123.22
23	C	508	CLA	CAC-C3C-C4C	2.15	127.60	124.81
23	C	513	CLA	C4-C3-C2	-2.15	118.17	123.68
25	T	102	BCR	C1-C6-C7	2.15	121.85	115.78
29	d	407[A]	PL9	C35-C34-C36	2.15	118.88	115.27
38	E	102	HEM	C4A-NA-C1A	2.15	107.45	105.35
25	D	404	BCR	C15-C16-C17	-2.14	119.08	123.47
25	C	515	BCR	C38-C26-C25	-2.14	122.12	124.53
23	c	501	CLA	C2A-C1A-CHA	-2.14	120.11	123.86
25	D	404	BCR	C24-C23-C22	-2.14	123.00	126.23
23	A	404[B]	CLA	CMA-C3A-C2A	-2.14	105.19	113.83
25	B	619	BCR	C34-C9-C8	2.14	121.45	118.08
23	B	607	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
26	X	101	SQD	O7-S-C6	2.14	109.48	106.94
23	b	606	CLA	CHB-C1B-C2B	-2.14	121.19	127.24
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27
25	K	102	BCR	C15-C14-C13	-2.14	124.26	127.31
31	b	621	LMT	C1-O1'-C1'	2.14	117.39	113.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	C6-C7-C8	-2.14	109.00	115.92
25	B	617	BCR	C16-C17-C18	-2.14	124.26	127.31
23	B	610	CLA	CHB-C1B-NB	-2.14	121.99	124.26
40	V	201	HEC	C4A-NA-C1A	2.14	107.44	105.35
23	a	407	CLA	CHC-C1C-C2C	-2.14	120.79	126.73
23	C	511	CLA	CHB-C1B-NB	-2.14	122.00	124.26
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
23	a	404[B]	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	B	606	CLA	C2A-C1A-CHA	-2.13	120.13	123.86
25	Y	101	BCR	C28-C27-C26	-2.13	110.27	114.08
25	B	618	BCR	C10-C11-C12	-2.13	116.56	123.22
25	b	618	BCR	C8-C7-C6	-2.13	121.22	127.20
25	h	101	BCR	C36-C18-C19	2.13	121.43	118.08
29	a	413[B]	PL9	C51-C49-C50	2.13	119.31	114.60
23	c	504	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
24	A	407[B]	PHO	C4-C3-C5	2.13	118.85	115.27
23	b	616	CLA	CHC-C4B-NB	-2.13	122.00	124.26
23	B	611	CLA	C2C-C1C-NC	2.13	111.97	109.97
35	C	517[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
35	c	517[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
25	d	406	BCR	C29-C28-C27	-2.13	106.63	111.38
23	b	601	CLA	CAA-C2A-C3A	-2.13	106.96	112.78
23	B	608	CLA	O2A-CGA-CBA	2.13	118.58	111.91
23	C	511	CLA	CBC-CAC-C3C	-2.13	106.57	112.43
29	D	405[B]	PL9	C42-C41-C39	-2.13	105.98	112.98
23	C	513	CLA	OBD-CAD-C3D	-2.12	123.41	128.52
23	C	513	CLA	C3B-C4B-NB	2.12	112.49	110.52
25	a	408	BCR	C24-C23-C22	-2.12	123.03	126.23
23	d	404[B]	CLA	CMB-C2B-C1B	2.12	128.60	125.37
23	B	606	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
24	d	403[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
23	c	503	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
35	C	517[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
23	b	605	CLA	CED-O2D-CGD	2.12	120.73	115.94
23	C	504	CLA	CHB-C1B-C2B	-2.12	121.25	127.24
23	C	508	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
23	c	509	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
33	m	101	LMG	O8-C28-O10	-2.12	118.24	123.59
23	B	609	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
23	B	616	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
23	C	502	CLA	C11-C12-C13	-2.12	109.07	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C4-C3-C2	-2.12	118.24	123.68
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
23	C	502	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
23	c	505	CLA	CHB-C1B-NB	-2.11	122.02	124.26
31	M	101	LMT	C1-O1'-C1'	2.11	117.35	113.84
26	A	412	SQD	O6-C44-C45	-2.11	105.80	110.90
26	l	101	SQD	O5-C1-C2	-2.11	105.88	110.35
23	A	408	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
26	A	412	SQD	O6-C1-C2	2.11	111.60	108.30
23	C	504	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	a	407	CLA	C2A-C1A-CHA	-2.11	120.17	123.86
23	B	615	CLA	CHA-C1A-NA	-2.11	121.57	126.40
25	H	101	BCR	C37-C22-C23	2.11	121.39	118.08
24	A	416[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
25	D	404	BCR	C30-C25-C24	2.10	121.73	115.78
25	b	619	BCR	C16-C15-C14	-2.10	119.17	123.47
33	m	101	LMG	C3-C4-C5	2.10	113.99	110.24
23	c	512	CLA	CHA-C1A-NA	-2.10	121.58	126.40
23	b	615	CLA	C6-C7-C8	-2.10	109.12	115.92
29	a	413[B]	PL9	C10-C9-C8	-2.10	118.29	123.68
29	d	407[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
23	C	513	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
23	C	502	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
32	b	629[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
23	b	613	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
23	a	404[B]	CLA	CMC-C2C-C1C	2.10	128.24	125.04
35	H	102	DGD	C3E-C4E-C5E	-2.10	106.50	110.24
31	F	101	LMT	C3B-C4B-C5B	-2.10	106.50	110.24
25	b	619	BCR	C21-C20-C19	-2.10	116.67	123.22
23	A	405[B]	CLA	O2A-CGA-CBA	2.10	118.48	111.91
23	c	512	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
38	E	102	HEM	CHA-C1A-NA	2.09	127.70	123.85
32	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
26	A	412	SQD	O7-S-C6	2.09	109.43	106.94
23	D	402[A]	CLA	CMB-C2B-C1B	2.09	128.56	125.37
29	A	414[B]	PL9	C2-C3-C4	2.09	121.68	118.80
25	Y	101	BCR	C3-C4-C5	-2.09	110.34	114.08
31	b	627	LMT	O1'-C1'-C2'	2.09	111.57	108.30
23	C	510	CLA	C4-C3-C5	2.09	118.79	115.27
35	C	517[B]	DGD	O1G-C1A-C2A	2.09	118.47	111.91
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36
25	d	406	BCR	C37-C22-C23	2.09	121.37	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	Z	101	LMG	C9-C8-C7	-2.09	106.85	111.79
23	B	613	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	c	505	CLA	C2A-C1A-CHA	-2.09	120.21	123.86
23	A	405[B]	CLA	C4C-C3C-C2C	-2.09	103.86	106.90
23	b	601	CLA	CMC-C2C-C1C	2.08	128.21	125.04
23	b	616	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
23	d	404[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
23	c	510	CLA	CED-O2D-CGD	2.08	120.65	115.94
23	a	404[B]	CLA	CMA-C3A-C2A	-2.08	105.42	113.83
23	c	504	CLA	C1-C2-C3	-2.08	122.44	126.04
26	a	409[B]	SQD	C3-C4-C5	2.08	113.95	110.24
23	A	405[B]	CLA	CAA-CBA-CGA	2.08	119.33	113.25
23	B	611	CLA	CMA-C3A-C2A	-2.08	105.44	113.83
33	C	520	LMG	O1-C7-C8	-2.08	105.89	110.90
25	b	617	BCR	C21-C20-C19	-2.08	116.74	123.22
31	b	627	LMT	C1'-O5'-C5'	-2.08	109.61	113.69
23	b	610	CLA	CAC-C3C-C2C	2.07	131.08	127.53
23	C	502	CLA	O2A-CGA-CBA	2.07	118.42	111.91
23	c	508	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
23	b	616	CLA	C11-C12-C13	-2.07	109.22	115.92
23	B	616	CLA	CMB-C2B-C3B	2.07	131.61	126.59
23	B	614	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
23	b	615	CLA	CHA-C1A-NA	-2.07	121.65	126.40
25	K	102	BCR	C39-C30-C25	-2.07	106.94	110.30
25	D	404	BCR	C29-C28-C27	-2.07	106.75	111.38
23	c	511	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
23	C	513	CLA	CBC-CAC-C3C	-2.07	106.72	112.43
25	K	102	BCR	C29-C30-C25	2.07	113.67	110.48
35	C	518[B]	DGD	O2G-C1B-O1B	-2.07	118.70	123.70
24	A	416[B]	PHO	OBD-CAD-C3D	-2.07	124.54	127.98
23	A	408	CLA	C11-C12-C13	-2.07	109.23	115.92
26	f	102	SQD	O48-C23-O10	-2.07	118.37	123.59
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405[A]	PL9	C12-C13-C14	-2.07	122.68	127.66
25	A	409	BCR	C11-C10-C9	-2.07	124.36	127.31
24	A	416[B]	PHO	O1D-CGD-CBD	-2.07	121.30	124.74
23	b	609	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
29	d	407[B]	PL9	C36-C34-C33	-2.07	116.93	121.12
25	c	515	BCR	C15-C16-C17	-2.07	119.24	123.47
29	D	405[A]	PL9	C30-C29-C31	2.07	118.75	115.27
23	b	612	CLA	CMB-C2B-C1B	2.07	128.52	125.37
29	a	413[A]	PL9	C51-C49-C50	2.07	119.17	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	OBD-CAD-C3D	-2.07	123.55	128.52
25	A	409	BCR	C33-C5-C6	-2.07	122.21	124.53
23	B	604	CLA	CED-O2D-CGD	2.07	120.61	115.94
29	A	414[B]	PL9	C37-C36-C34	-2.07	106.18	112.98
29	D	405[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
33	c	520	LMG	C1-O6-C5	2.06	117.74	113.69
25	t	102	BCR	C28-C27-C26	-2.06	110.39	114.08
23	D	402[B]	CLA	CED-O2D-CGD	2.06	120.60	115.94
23	c	511	CLA	C11-C10-C8	-2.06	109.25	115.92
25	T	102	BCR	C15-C14-C13	2.06	130.25	127.31
23	B	612	CLA	CMA-C3A-C2A	-2.06	105.51	113.83
32	d	409[B]	LHG	O8-C23-O10	-2.06	118.39	123.59
24	d	403[B]	PHO	C4-C3-C2	-2.06	118.39	123.68
25	B	617	BCR	C37-C22-C23	2.06	121.32	118.08
25	c	514	BCR	C15-C16-C17	-2.06	119.25	123.47
23	b	609	CLA	CHA-C1A-NA	-2.06	121.68	126.40
23	B	611	CLA	CED-O2D-CGD	2.06	120.59	115.94
23	A	404[B]	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
23	b	609	CLA	O2A-CGA-CBA	2.06	118.36	111.91
23	C	508	CLA	CBB-CAB-C3B	-2.06	117.39	127.62
25	B	618	BCR	C28-C27-C26	-2.05	110.41	114.08
23	C	504	CLA	C3B-C4B-NB	2.05	112.42	110.52
29	d	407[B]	PL9	C12-C13-C14	-2.05	122.71	127.66
25	t	102	BCR	C33-C5-C4	2.05	117.56	113.62
35	C	517[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	C	505	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
34	b	622	HTG	C6-C5-C4	-2.05	108.20	113.00
23	b	611	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
25	H	101	BCR	C31-C1-C6	-2.05	106.97	110.30
23	A	404[A]	CLA	CHB-C4A-NA	2.05	127.34	124.51
33	C	520	LMG	O7-C10-O9	-2.05	118.75	123.70
23	b	610	CLA	C4-C3-C2	-2.05	118.42	123.68
23	B	613	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
23	C	505	CLA	C1-C2-C3	-2.05	122.50	126.04
23	D	403	CLA	CMA-C3A-C2A	-2.04	105.58	113.83
33	C	501	LMG	O8-C28-C29	2.04	118.32	111.91
32	D	407[A]	LHG	O4-P-O5	2.04	122.34	112.24
23	C	508	CLA	C3B-C4B-NB	2.04	112.41	110.52
33	d	413	LMG	C8-O7-C10	-2.04	112.76	117.79
23	B	616	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	409	BCR	C15-C14-C13	-2.04	124.40	127.31
23	c	507	CLA	CAC-C3C-C4C	2.04	127.46	124.81
25	h	101	BCR	C29-C30-C25	2.04	113.62	110.48
23	C	511	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
25	H	101	BCR	C16-C15-C14	-2.04	119.30	123.47
23	C	507	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	C	509	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
23	B	602	CLA	C1-O2A-CGA	2.04	121.79	116.44
23	c	506	CLA	CGD-CBD-CAD	-2.04	104.14	110.73
23	b	612	CLA	OBD-CAD-C3D	-2.04	123.62	128.52
34	B	622	HTG	C1-C2-C3	2.04	114.61	110.59
23	C	502	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
31	b	621	LMT	C2'-C3'-C4'	2.03	114.33	109.68
23	b	611	CLA	CHB-C1B-NB	-2.03	122.10	124.26
35	c	517[B]	DGD	C2G-O2G-C1B	-2.03	112.78	117.79
23	b	605	CLA	CAC-C3C-C2C	2.03	131.01	127.53
23	d	404[B]	CLA	CED-O2D-CGD	2.03	120.53	115.94
25	d	406	BCR	C38-C26-C27	2.03	117.52	113.62
26	a	409[B]	SQD	O48-C23-O10	-2.03	118.46	123.59
23	a	404[A]	CLA	CMB-C2B-C3B	2.03	131.51	126.59
23	B	602	CLA	C1-C2-C3	-2.03	122.53	126.04
23	B	611	CLA	O2A-CGA-CBA	2.03	118.28	111.91
23	a	407	CLA	CAC-C3C-C4C	2.03	127.44	124.81
23	d	402[A]	CLA	CAC-C3C-C2C	2.03	131.00	127.53
26	a	409[A]	SQD	O48-C23-O10	-2.03	118.47	123.59
23	B	601	CLA	CHB-C1B-NB	-2.03	122.11	124.26
25	C	516	BCR	C2-C1-C6	2.03	113.60	110.48
23	C	507	CLA	OBD-CAD-C3D	-2.03	123.64	128.52
24	a	406[A]	PHO	CBC-CAC-C3C	-2.03	109.91	112.88
23	B	603	CLA	C2A-C3A-C4A	-2.03	98.59	101.87
25	t	102	BCR	C2-C1-C6	2.03	113.60	110.48
29	d	407[A]	PL9	C45-C44-C46	2.03	118.68	115.27
23	B	610	CLA	CAC-C3C-C4C	2.03	127.44	124.81
32	d	409[B]	LHG	C5-O7-C7	-2.03	112.81	117.79
23	b	614	CLA	CED-O2D-CGD	2.02	120.52	115.94
23	B	607	CLA	CAC-C3C-C4C	2.02	127.44	124.81
23	B	615	CLA	CAC-C3C-C4C	2.02	127.44	124.81
33	Z	101	LMG	C1-O6-C5	2.02	117.66	113.69
23	C	502	CLA	C1-C2-C3	-2.02	122.54	126.04
32	d	415[B]	LHG	O7-C7-O9	-2.02	118.81	123.70
25	h	101	BCR	C33-C5-C6	-2.02	122.25	124.53
24	A	416[B]	PHO	C4A-C3A-C2A	-2.02	100.91	102.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[B]	CLA	CED-O2D-CGD	2.02	120.52	115.94
33	c	520	LMG	C1-C2-C3	-2.02	105.78	110.00
23	B	614	CLA	CHB-C1B-C2B	-2.02	121.52	127.24
23	b	608	CLA	C4-C3-C5	2.02	118.67	115.27
33	D	411	LMG	C9-C8-C7	-2.02	107.00	111.79
33	C	520	LMG	O1-C1-C2	-2.02	105.15	108.30
23	c	508	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
34	b	622	HTG	C3-C4-C5	2.02	113.84	110.24
24	d	403[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91
25	k	101	BCR	C20-C21-C22	-2.02	124.43	127.31
23	b	602	CLA	C1-O2A-CGA	2.02	121.74	116.44
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
33	C	501	LMG	O6-C1-O1	-2.02	105.19	109.97
23	b	603	CLA	CHB-C4A-NA	2.02	127.30	124.51
24	A	416[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
31	B	628	LMT	C3B-C4B-C5B	-2.01	106.65	110.24
23	d	404[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
24	a	406[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
25	H	101	BCR	C20-C21-C22	-2.01	124.44	127.31
37	D	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
23	a	404[B]	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
23	D	402[A]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
37	d	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
23	b	602	CLA	CHB-C4A-NA	2.01	127.29	124.51
25	t	102	BCR	C37-C22-C21	-2.01	120.11	122.92
24	a	406[B]	PHO	CAC-C3C-C4C	2.01	129.36	124.27
29	D	405[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
23	c	501	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
25	b	617	BCR	C15-C16-C17	-2.01	119.36	123.47
35	C	519	DGD	O1G-C1A-O1A	-2.01	118.53	123.59
23	b	616	CLA	OBD-CAD-C3D	-2.01	123.69	128.52
23	b	615	CLA	C1-C2-C3	-2.01	122.57	126.04
25	A	409	BCR	C37-C22-C21	-2.01	120.11	122.92
35	c	517[B]	DGD	O6E-C1E-O5D	-2.00	105.23	109.97
23	C	510	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
23	B	601	CLA	CBC-CAC-C3C	-2.00	106.91	112.43
35	c	518	DGD	O3G-C1D-C2D	-2.00	105.18	108.30
31	F	101	LMT	C2'-C3'-C4'	2.00	114.25	109.68
23	B	605	CLA	CAA-C2A-C3A	-2.00	107.30	112.78

All (2) chirality outliers are listed below:

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

All (1647) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C14-C13-C15-C16
23	C	508	CLA	C2B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	b	605	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	C2B-C3B-CAB-CBB
23	c	507	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2B-C3B-CAB-CBB
23	c	513	CLA	C4B-C3B-CAB-CBB
23	d	405	CLA	C2-C3-C5-C6
23	d	405	CLA	C4-C3-C5-C6
25	b	617	BCR	C1-C6-C7-C8
25	y	101	BCR	C1-C6-C7-C8
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	X	101	SQD	C2-C1-O6-C44
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

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Mol	Chain	Res	Type	Atoms
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
27	o	303	GOL	C1-C2-C3-O3
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	413[A]	PL9	C9-C11-C12-C13
29	a	413[A]	PL9	C14-C16-C17-C18
29	a	413[A]	PL9	C25-C24-C26-C27
29	a	413[B]	PL9	C9-C11-C12-C13
29	a	413[B]	PL9	C14-C16-C17-C18
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	B	628	LMT	C2'-C1'-O1'-C1
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
31	t	101	LMT	C2-C1-O1'-C1'
32	D	406[A]	LHG	O2-C2-C3-O3
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5

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

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Mol	Chain	Res	Type	Atoms
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
34	B	621	HTG	C2'-C1'-S1-C1
38	E	102	HEM	C2C-C3C-CAC-CBC
38	E	102	HEM	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
31	T	101	LMT	O5'-C5'-C6'-O6'
31	a	416	LMT	O5B-C5B-C6B-O6B
23	C	505	CLA	C4-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
29	a	413[B]	PL9	C25-C24-C26-C27
31	T	101	LMT	C4B-C5B-C6B-O6B
23	a	407	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C18-C19-C21-C22
23	b	616	CLA	C3-C5-C6-C7
23	c	512	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	O5-C5-C6-O6
34	b	625	HTG	S1-C1'-C2'-C3'
33	C	521	LMG	O9-C10-O7-C8
31	B	627	LMT	C4'-C5'-C6'-O6'
31	m	103	LMT	C4B-C5B-C6B-O6B
31	b	621	LMT	O5'-C5'-C6'-O6'
23	C	504	CLA	CBD-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
32	d	408[B]	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
33	C	521	LMG	O6-C5-C6-O5
26	A	410[B]	SQD	C8-C7-O47-C45
23	C	514	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CBD-CGD-O2D-CED
23	c	511	CLA	CBD-CGD-O2D-CED
33	c	520	LMG	C4-C5-C6-O5
31	B	628	LMT	C4B-C5B-C6B-O6B
34	D	410	HTG	C4-C5-C6-O6
31	B	627	LMT	C6-C7-C8-C9
34	D	410	HTG	S1-C1'-C2'-C3'
31	C	525	LMT	O5B-C5B-C6B-O6B
31	C	525	LMT	O5'-C5'-C6'-O6'
31	b	627	LMT	O5'-C5'-C6'-O6'
34	b	625	HTG	O5-C5-C6-O6
31	T	101	LMT	C4'-C5'-C6'-O6'
31	a	416	LMT	C4B-C5B-C6B-O6B
33	c	520	LMG	O6-C5-C6-O5
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
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[A]	PL9	C30-C29-C31-C32
29	a	413[B]	PL9	C15-C14-C16-C17
29	a	413[B]	PL9	C30-C29-C31-C32
31	F	101	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	507	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C13-C14-C16-C17
29	a	413[A]	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
29	a	413[B]	PL9	C13-C14-C16-C17
29	a	413[B]	PL9	C28-C29-C31-C32
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
40	v	201	HEC	C2C-C3C-CAC-CBC
31	B	627	LMT	O5B-C5B-C6B-O6B
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'
26	l	101	SQD	O5-C1-O6-C44
29	D	405[A]	PL9	C39-C41-C42-C43
23	a	407	CLA	CBA-CGA-O2A-C1
31	B	627	LMT	O5'-C5'-C6'-O6'
31	t	101	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	C4'-C5'-C6'-O6'
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	408[A]	LHG	C1-C2-C3-O3
23	C	502	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
33	B	620	LMG	C39-C40-C41-C42
35	c	517[B]	DGD	C1B-C2B-C3B-C4B
32	D	407[A]	LHG	C33-C34-C35-C36
31	C	525	LMT	C4B-C5B-C6B-O6B
26	X	101	SQD	C23-C24-C25-C26
31	B	629	LMT	C2'-C1'-O1'-C1
31	C	525	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
31	m	103	LMT	O5B-C5B-C6B-O6B
31	B	627	LMT	C4B-C5B-C6B-O6B
31	b	627	LMT	C4'-C5'-C6'-O6'
23	C	505	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	B	613	CLA	C11-C12-C13-C14
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

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Mol	Chain	Res	Type	Atoms
23	c	504	CLA	C11-C12-C13-C14
23	c	509	CLA	C11-C10-C8-C9
33	B	620	LMG	C15-C16-C17-C18
23	B	601	CLA	C10-C11-C12-C13
25	D	404	BCR	C37-C22-C23-C24
25	K	102	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C34
34	d	412	HTG	S1-C1'-C2'-C3'
25	b	619	BCR	C7-C8-C9-C10
26	l	101	SQD	C7-C8-C9-C10
23	b	611	CLA	C15-C16-C17-C18
23	c	512	CLA	C15-C16-C17-C18
23	A	408	CLA	C5-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
33	d	413	LMG	C10-C11-C12-C13
34	b	623	HTG	C1'-C2'-C3'-C4'
23	B	601	CLA	C5-C6-C7-C8
23	B	606	CLA	C10-C11-C12-C13
23	B	614	CLA	C8-C10-C11-C12
23	C	508	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
27	O	303	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
31	a	416	LMT	O1'-C1-C2-C3
35	C	519	DGD	C6B-C7B-C8B-C9B
34	B	624	HTG	O5-C5-C6-O6
32	E	101[A]	LHG	C23-C24-C25-C26
33	Z	101	LMG	C10-C11-C12-C13
35	c	517[A]	DGD	C1B-C2B-C3B-C4B
31	C	525	LMT	O1'-C1-C2-C3
32	D	407[B]	LHG	C33-C34-C35-C36
23	A	408	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C7
25	T	102	BCR	C13-C14-C15-C16
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	b	605	CLA	C8-C10-C11-C12
23	c	513	CLA	C10-C11-C12-C13
40	V	201	HEC	C2C-C3C-CAC-CBC
23	a	407	CLA	O1A-CGA-O2A-C1
31	C	525	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
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	C	503	CLA	C13-C15-C16-C17
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
26	l	101	SQD	C30-C31-C32-C33
31	e	101	LMT	O5B-C5B-C6B-O6B
31	e	101	LMT	O5'-C5'-C6'-O6'
23	D	403	CLA	C10-C11-C12-C13
40	v	201	HEC	C4C-C3C-CAC-CBC
23	B	614	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
31	C	525	LMT	C5'-C4'-O1B-C1B
35	C	519	DGD	CAB-CBB-CCB-CDB
23	B	602	CLA	C13-C15-C16-C17
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
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O3
32	a	419[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C4-O6-P-O3
32	a	419[B]	LHG	C3-O3-P-O6
32	a	419[B]	LHG	C4-O6-P-O3
32	d	408[A]	LHG	C3-O3-P-O6
32	d	408[B]	LHG	C4-O6-P-O3
31	M	101	LMT	O5'-C5'-C6'-O6'
31	m	103	LMT	O5'-C5'-C6'-O6'
23	c	509	CLA	O1A-CGA-O2A-C1
40	V	201	HEC	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
34	b	622	HTG	S1-C1'-C2'-C3'
26	A	410[A]	SQD	C7-C8-C9-C10
32	D	406[A]	LHG	C1-C2-C3-O3
32	d	408[B]	LHG	C1-C2-C3-O3
33	B	620	LMG	O9-C10-O7-C8
23	D	403	CLA	C4-C3-C5-C6
23	c	504	CLA	C4-C3-C5-C6
23	B	603	CLA	C13-C15-C16-C17
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
23	c	509	CLA	CBA-CGA-O2A-C1
31	B	627	LMT	C5'-C4'-O1B-C1B
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
35	h	102	DGD	C6B-C7B-C8B-C9B
31	B	629	LMT	C4'-C5'-C6'-O6'
26	A	410[A]	SQD	C15-C16-C17-C18
26	X	101	SQD	C30-C31-C32-C33
32	L	101[A]	LHG	C12-C13-C14-C15
33	C	521	LMG	C18-C19-C20-C21
34	B	622	HTG	C3'-C4'-C5'-C6'
35	c	516[B]	DGD	C2B-C3B-C4B-C5B
33	B	620	LMG	C11-C10-O7-C8
23	b	606	CLA	C15-C16-C17-C18
23	c	506	CLA	C15-C16-C17-C18
34	B	621	HTG	C1'-C2'-C3'-C4'
26	A	410[B]	SQD	C15-C16-C17-C18
31	e	101	LMT	C4-C5-C6-C7
31	t	101	LMT	C4-C5-C6-C7
32	L	101[A]	LHG	C17-C18-C19-C20
32	d	415[A]	LHG	C16-C17-C18-C19
33	a	415	LMG	C30-C31-C32-C33
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
23	B	603	CLA	C16-C17-C18-C20
23	a	407	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
34	B	624	HTG	S1-C1'-C2'-C3'
32	D	406[B]	LHG	C16-C17-C18-C19
33	B	620	LMG	C17-C18-C19-C20
34	b	622	HTG	C3'-C4'-C5'-C6'

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Mol	Chain	Res	Type	Atoms
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	516[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
26	f	102	SQD	C32-C33-C34-C35
31	C	525	LMT	C3-C4-C5-C6
32	D	407[B]	LHG	C32-C33-C34-C35
33	B	620	LMG	C34-C35-C36-C37
33	m	101	LMG	C35-C36-C37-C38
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
31	B	629	LMT	C3-C4-C5-C6
33	C	521	LMG	C17-C18-C19-C20
35	c	516[A]	DGD	C2B-C3B-C4B-C5B
31	A	417	LMT	O1'-C1-C2-C3
32	L	101[B]	LHG	C12-C13-C14-C15
33	D	411	LMG	C35-C36-C37-C38
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
26	A	412	SQD	C2-C1-O6-C44
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	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
26	X	101	SQD	C24-C25-C26-C27
33	D	411	LMG	C19-C20-C21-C22
33	a	415	LMG	C34-C35-C36-C37
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	H	102	DGD	C5B-C6B-C7B-C8B
35	c	516[A]	DGD	C9A-CAA-CBA-CCA
23	B	615	CLA	C16-C17-C18-C19
23	c	508	CLA	C16-C17-C18-C19
23	d	405	CLA	C16-C17-C18-C20
29	A	414[A]	PL9	C45-C44-C46-C47
29	D	405[B]	PL9	C15-C14-C16-C17
32	D	406[A]	LHG	C16-C17-C18-C19
32	a	419[A]	LHG	C26-C27-C28-C29
32	b	629[A]	LHG	C14-C15-C16-C17
32	b	629[B]	LHG	C14-C15-C16-C17
34	b	622	HTG	C2'-C3'-C4'-C5'
29	d	407[A]	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
23	a	405[A]	CLA	C11-C12-C13-C14
23	a	405[B]	CLA	C11-C12-C13-C14
23	c	504	CLA	C14-C13-C15-C16
40	V	201	HEC	C4C-C3C-CAC-CBC
26	A	410[B]	SQD	C7-C8-C9-C10
31	b	627	LMT	C7-C8-C9-C10
31	e	101	LMT	C5-C6-C7-C8
32	D	407[A]	LHG	C32-C33-C34-C35
32	L	101[A]	LHG	C15-C16-C17-C18
32	a	419[B]	LHG	C26-C27-C28-C29
32	d	408[B]	LHG	C34-C35-C36-C37
32	d	415[B]	LHG	C16-C17-C18-C19
33	D	411	LMG	C30-C31-C32-C33
23	A	406[B]	CLA	C13-C15-C16-C17
31	B	629	LMT	C11-C10-C9-C8
32	d	415[A]	LHG	C32-C33-C34-C35
33	C	501	LMG	C17-C18-C19-C20
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
35	c	518	DGD	CBB-CCB-CDB-CEB
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	v	202[B]	GOL	O1-C1-C2-C3
32	A	419[B]	LHG	O1-C1-C2-C3
25	D	404	BCR	C21-C22-C23-C24
23	B	602	CLA	C15-C16-C17-C18
32	L	101[A]	LHG	C25-C26-C27-C28
33	C	520	LMG	C16-C17-C18-C19
32	E	101[B]	LHG	C23-C24-C25-C26
33	C	501	LMG	C10-C11-C12-C13
33	a	415	LMG	C10-C11-C12-C13
26	A	412	SQD	C17-C18-C19-C20
31	B	627	LMT	C5-C6-C7-C8
31	B	628	LMT	C2-C3-C4-C5
31	B	629	LMT	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	A	419[A]	LHG	C34-C35-C36-C37
32	A	419[B]	LHG	C34-C35-C36-C37
32	L	101[B]	LHG	C25-C26-C27-C28
32	d	408[A]	LHG	C11-C10-C9-C8
33	C	501	LMG	C12-C13-C14-C15
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
33	Z	101	LMG	O6-C5-C6-O5
23	B	602	CLA	C4B-C3B-CAB-CBB
23	B	610	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	509	CLA	C16-C17-C18-C20
31	t	101	LMT	C4'-C5'-C6'-O6'
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
26	A	410[A]	SQD	C12-C13-C14-C15
26	a	411	SQD	C25-C26-C27-C28
33	C	501	LMG	C36-C37-C38-C39
33	a	415	LMG	C21-C22-C23-C24
31	b	627	LMT	C5-C6-C7-C8
32	L	101[A]	LHG	C13-C14-C15-C16
32	L	101[B]	LHG	C17-C18-C19-C20
32	d	408[A]	LHG	C34-C35-C36-C37
33	c	519	LMG	C34-C35-C36-C37
33	d	413	LMG	C29-C30-C31-C32
33	m	101	LMG	C39-C40-C41-C42
26	X	101	SQD	C29-C30-C31-C32
32	d	409[A]	LHG	C27-C28-C29-C30
35	c	516[B]	DGD	C2A-C1A-O1G-C1G
35	c	516[B]	DGD	O6D-C5D-C6D-O5D
33	c	519	LMG	C31-C32-C33-C34
23	B	608	CLA	C13-C15-C16-C17
23	C	513	CLA	C10-C11-C12-C13
31	C	525	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
35	h	102	DGD	C2B-C3B-C4B-C5B
35	h	102	DGD	C3B-C4B-C5B-C6B
35	h	102	DGD	CAB-CBB-CCB-CDB
23	B	603	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	b	615	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
31	B	628	LMT	C5-C6-C7-C8
32	A	419[A]	LHG	C12-C13-C14-C15
32	b	629[A]	LHG	C16-C17-C18-C19
32	b	629[B]	LHG	C16-C17-C18-C19
31	C	525	LMT	C1-C2-C3-C4
23	C	509	CLA	CBD-CGD-O2D-CED
31	m	103	LMT	C7-C8-C9-C10
32	E	101[A]	LHG	C24-C25-C26-C27
32	E	101[B]	LHG	C24-C25-C26-C27
33	m	101	LMG	C38-C39-C40-C41
35	c	516[A]	DGD	O6D-C5D-C6D-O5D
26	b	620	SQD	C31-C32-C33-C34
23	c	505	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C45-C44-C46-C47
29	d	407[A]	PL9	C15-C14-C16-C17
35	c	516[A]	DGD	C2A-C1A-O1G-C1G
23	c	505	CLA	C2-C3-C5-C6
24	a	406[B]	PHO	C2-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[A]	PL9	C43-C44-C46-C47
29	A	414[B]	PL9	C12-C11-C9-C8
29	D	405[A]	PL9	C13-C14-C16-C17
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
23	C	504	CLA	O1D-CGD-O2D-CED
31	b	621	LMT	C3'-C4'-O1B-C1B
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
32	A	419[B]	LHG	C12-C13-C14-C15
32	D	407[B]	LHG	C15-C16-C17-C18
32	d	409[B]	LHG	C27-C28-C29-C30
35	c	517[A]	DGD	CBB-CCB-CDB-CEB
35	h	102	DGD	C7B-C8B-C9B-CAB
31	a	416	LMT	C1-C2-C3-C4
23	B	602	CLA	C2B-C3B-CAB-CBB
23	a	405[A]	CLA	C2B-C3B-CAB-CBB
32	D	407[A]	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
35	c	516[A]	DGD	C5A-C6A-C7A-C8A
31	e	101	LMT	C1-C2-C3-C4
26	l	101	SQD	C11-C10-C9-C8
31	T	101	LMT	C7-C8-C9-C10
33	C	501	LMG	C19-C20-C21-C22
33	c	519	LMG	C33-C34-C35-C36
35	c	516[A]	DGD	CAA-CBA-CCA-CDA
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
31	b	627	LMT	C3-C4-C5-C6
32	d	415[A]	LHG	C29-C30-C31-C32
34	B	621	HTG	C2'-C3'-C4'-C5'
35	h	102	DGD	C9A-CAA-CBA-CCA
23	C	507	CLA	C5-C6-C7-C8
35	c	516[A]	DGD	C7A-C8A-C9A-CAA
23	d	405	CLA	C16-C17-C18-C19
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
33	C	520	LMG	C17-C18-C19-C20
33	D	411	LMG	C12-C13-C14-C15
35	h	102	DGD	CAA-CBA-CCA-CDA
23	C	503	CLA	C15-C16-C17-C18
31	B	628	LMT	C6-C7-C8-C9
35	c	516[B]	DGD	C5A-C6A-C7A-C8A
35	c	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
24	a	406[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C15-C14-C16-C17
29	d	407[B]	PL9	C15-C14-C16-C17
23	C	505	CLA	C12-C13-C15-C16
23	C	511	CLA	C11-C12-C13-C15
23	a	405[A]	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	606	CLA	C12-C13-C15-C16
23	c	504	CLA	C12-C13-C15-C16
23	C	512	CLA	C3-C5-C6-C7
35	c	516[B]	DGD	O1A-C1A-O1G-C1G
26	b	620	SQD	C14-C15-C16-C17
23	B	605	CLA	C5-C6-C7-C8
33	m	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
23	c	512	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
32	D	407[A]	LHG	C29-C30-C31-C32
35	H	102	DGD	C7A-C8A-C9A-CAA
23	b	614	CLA	C10-C11-C12-C13
23	c	507	CLA	C5-C6-C7-C8
32	D	406[A]	LHG	C13-C14-C15-C16
32	d	415[B]	LHG	C32-C33-C34-C35
35	c	516[B]	DGD	C7A-C8A-C9A-CAA
26	a	411	SQD	C31-C32-C33-C34
26	f	102	SQD	C25-C26-C27-C28
32	d	415[B]	LHG	C29-C30-C31-C32
33	c	519	LMG	C28-C29-C30-C31
23	c	511	CLA	O1D-CGD-O2D-CED
23	b	604	CLA	C15-C16-C17-C18
23	c	511	CLA	C8-C10-C11-C12
38	f	101	HEM	C2C-C3C-CAC-CBC
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	c	516[A]	DGD	O1A-C1A-O1G-C1G
23	c	501	CLA	CBD-CGD-O2D-CED
35	c	516[B]	DGD	C4D-C5D-C6D-O5D
26	A	412	SQD	O5-C1-O6-C44
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
26	a	409[A]	SQD	C9-C10-C11-C12
35	c	516[B]	DGD	CAA-CBA-CCA-CDA
33	m	101	LMG	C11-C10-O7-C8
26	b	620	SQD	C13-C14-C15-C16
33	D	411	LMG	C36-C37-C38-C39
38	f	101	HEM	C4C-C3C-CAC-CBC
23	B	615	CLA	C5-C6-C7-C8
23	c	510	CLA	CBD-CGD-O2D-CED
26	a	409[B]	SQD	C9-C10-C11-C12
33	C	521	LMG	C19-C20-C21-C22
35	c	517[B]	DGD	C4A-C5A-C6A-C7A
23	c	509	CLA	C3-C5-C6-C7
31	M	101	LMT	C3-C4-C5-C6
33	C	521	LMG	C13-C14-C15-C16
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
26	l	101	SQD	C34-C35-C36-C37
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
23	c	508	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
32	D	406[B]	LHG	C12-C13-C14-C15
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
23	D	403	CLA	C2-C3-C5-C6
29	D	405[B]	PL9	C13-C14-C16-C17
29	d	407[B]	PL9	C13-C14-C16-C17
29	D	405[B]	PL9	C4-C3-C7-C8
23	B	606	CLA	C11-C10-C8-C9
23	C	505	CLA	C14-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
26	b	620	SQD	C28-C29-C30-C31
32	b	629[A]	LHG	C13-C14-C15-C16
33	C	501	LMG	C11-C12-C13-C14
34	b	623	HTG	O5-C5-C6-O6
25	d	406	BCR	C7-C8-C9-C34
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	B	610	CLA	C16-C17-C18-C20
32	D	407[A]	LHG	C17-C18-C19-C20
23	A	406[A]	CLA	C13-C15-C16-C17
35	c	517[B]	DGD	C6A-C7A-C8A-C9A
26	A	410[B]	SQD	C11-C10-C9-C8
26	A	412	SQD	C26-C27-C28-C29
26	a	411	SQD	C16-C17-C18-C19
31	C	525	LMT	C4-C5-C6-C7
31	a	416	LMT	C2-C3-C4-C5
32	L	101[B]	LHG	C13-C14-C15-C16
32	b	629[B]	LHG	C27-C28-C29-C30
33	m	101	LMG	C14-C15-C16-C17
35	c	518	DGD	CBA-CCA-CDA-CEA
23	A	404[A]	CLA	C13-C15-C16-C17
23	d	404[A]	CLA	C16-C17-C18-C20
32	d	409[A]	LHG	C25-C26-C27-C28
32	d	409[B]	LHG	C28-C29-C30-C31
35	H	102	DGD	CCB-CDB-CEB-CFB
35	c	516[B]	DGD	O6E-C5E-C6E-O5E
31	C	525	LMT	C3'-C4'-O1B-C1B
23	b	601	CLA	C8-C10-C11-C12
23	C	511	CLA	C4-C3-C5-C6
23	c	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	C27-C28-C29-C30
26	b	620	SQD	C26-C27-C28-C29
31	t	101	LMT	O1'-C1-C2-C3
32	d	409[B]	LHG	C25-C26-C27-C28
31	b	621	LMT	C11-C10-C9-C8
31	t	101	LMT	C7-C8-C9-C10
35	c	517[A]	DGD	C4A-C5A-C6A-C7A
23	B	614	CLA	C5-C6-C7-C8
33	d	413	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
26	A	410[A]	SQD	O6-C44-C45-C46
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
31	a	416	LMT	C3-C4-C5-C6
32	E	101[B]	LHG	C4-C5-C6-O8
32	d	409[B]	LHG	C34-C35-C36-C37
23	B	615	CLA	C10-C11-C12-C13
31	F	101	LMT	C4-C5-C6-C7
32	E	101[A]	LHG	C25-C26-C27-C28
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
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
26	b	620	SQD	C11-C10-C9-C8
33	a	415	LMG	C35-C36-C37-C38
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
23	A	404[B]	CLA	C13-C15-C16-C17
23	C	511	CLA	C10-C11-C12-C13
32	D	407[B]	LHG	C29-C30-C31-C32
32	d	415[B]	LHG	C24-C25-C26-C27
33	C	520	LMG	C36-C37-C38-C39
35	c	516[A]	DGD	C4D-C5D-C6D-O5D
33	C	520	LMG	C34-C35-C36-C37
33	m	101	LMG	C37-C38-C39-C40
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
35	C	518[B]	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C16-C17-C18-C20
23	C	514	CLA	O1D-CGD-O2D-CED
33	C	501	LMG	C13-C14-C15-C16
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
31	B	627	LMT	C3'-C4'-O1B-C1B
23	C	507	CLA	C15-C16-C17-C18
33	C	501	LMG	C20-C21-C22-C23
34	b	625	HTG	C4-C5-C6-O6
23	A	405[A]	CLA	C15-C16-C17-C18
23	b	610	CLA	C15-C16-C17-C18
33	D	411	LMG	O6-C5-C6-O5
35	c	516[A]	DGD	O6E-C5E-C6E-O5E
29	A	414[B]	PL9	C12-C11-C9-C10
29	a	413[A]	PL9	C12-C11-C9-C10
31	a	416	LMT	C9-C10-C11-C12
35	h	102	DGD	CDB-CEB-CFB-CGB
23	C	511	CLA	C2-C3-C5-C6
23	C	513	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	C10-C11-C12-C13
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
32	d	409[B]	LHG	C29-C30-C31-C32
32	d	415[A]	LHG	C33-C34-C35-C36
26	b	620	SQD	C46-C45-O47-C7
26	l	101	SQD	C46-C45-O47-C7
23	C	510	CLA	C2-C1-O2A-CGA
32	d	409[A]	LHG	C34-C35-C36-C37
23	D	403	CLA	O1D-CGD-O2D-CED
26	a	409[A]	SQD	C12-C13-C14-C15
32	D	406[A]	LHG	C12-C13-C14-C15
32	b	629[B]	LHG	C13-C14-C15-C16
23	B	601	CLA	C13-C15-C16-C17
31	e	101	LMT	C3-C4-C5-C6
32	D	407[B]	LHG	C17-C18-C19-C20
23	c	512	CLA	O1A-CGA-O2A-C1
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
23	B	613	CLA	C13-C15-C16-C17
26	b	620	SQD	C18-C19-C20-C21
26	b	620	SQD	O10-C23-O48-C46
26	b	620	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
23	b	605	CLA	C5-C6-C7-C8
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
33	d	413	LMG	C11-C12-C13-C14
34	c	521	HTG	C4'-C5'-C6'-C7'
23	C	502	CLA	O1D-CGD-O2D-CED
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
23	d	404[A]	CLA	C16-C17-C18-C19
32	d	409[A]	LHG	C29-C30-C31-C32
29	a	413[B]	PL9	C12-C11-C9-C10
33	C	521	LMG	C35-C36-C37-C38
23	A	406[A]	CLA	C12-C13-C15-C16
23	B	602	CLA	C6-C7-C8-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C10-C8-C7
23	B	614	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	511	CLA	C12-C13-C15-C16
23	D	403	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	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	B	602	CLA	C11-C12-C13-C14
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	D	403	CLA	C14-C13-C15-C16
23	b	601	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	512	CLA	C6-C7-C8-C9
23	B	605	CLA	CBD-CGD-O2D-CED
32	d	409[A]	LHG	C28-C29-C30-C31
32	D	407[B]	LHG	C24-C23-O8-C6
26	a	409[B]	SQD	C12-C13-C14-C15
32	b	629[A]	LHG	C27-C28-C29-C30
33	a	415	LMG	C29-C30-C31-C32
23	c	512	CLA	C10-C11-C12-C13
32	d	415[B]	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
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
32	E	101[A]	LHG	O6-C4-C5-C6
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
32	D	406[A]	LHG	C10-C11-C12-C13
32	D	407[A]	LHG	C13-C14-C15-C16
32	d	409[A]	LHG	C9-C10-C11-C12
31	B	629	LMT	O1'-C1-C2-C3
29	d	407[A]	PL9	C45-C44-C46-C47
23	B	610	CLA	C13-C15-C16-C17
31	b	621	LMT	C3-C4-C5-C6
32	A	419[A]	LHG	C26-C27-C28-C29
32	d	408[A]	LHG	C13-C14-C15-C16
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
34	B	624	HTG	C4'-C5'-C6'-C7'
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
23	c	506	CLA	C3A-C2A-CAA-CBA
31	C	525	LMT	C5-C6-C7-C8
32	A	419[B]	LHG	C26-C27-C28-C29
23	C	510	CLA	O1D-CGD-O2D-CED
31	b	627	LMT	C2-C1-O1'-C1'
31	e	101	LMT	C2-C1-O1'-C1'
31	M	101	LMT	O1'-C1-C2-C3
32	E	101[B]	LHG	C25-C26-C27-C28
32	D	406[B]	LHG	C11-C10-C9-C8
33	c	520	LMG	C29-C28-O8-C9
35	c	517[A]	DGD	CDA-CEA-CFA-CGA
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
32	D	407[B]	LHG	C13-C14-C15-C16
32	L	101[A]	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
32	a	419[A]	LHG	C10-C11-C12-C13
32	b	629[A]	LHG	C12-C13-C14-C15
24	a	406[A]	PHO	O2A-C1-C2-C3
32	d	408[B]	LHG	C11-C10-C9-C8
33	C	520	LMG	C31-C32-C33-C34
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
23	C	513	CLA	O1A-CGA-O2A-C1
24	a	406[A]	PHO	C4-C3-C5-C6
23	d	404[B]	CLA	C16-C17-C18-C20
29	A	414[B]	PL9	C43-C44-C46-C47
29	D	405[A]	PL9	C43-C44-C46-C47
31	e	101	LMT	C9-C10-C11-C12
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
32	D	406[B]	LHG	C26-C27-C28-C29
35	c	517[B]	DGD	C9B-CAB-CBB-CCB
32	a	419[A]	LHG	C7-C8-C9-C10
23	B	602	CLA	C3-C5-C6-C7
23	B	601	CLA	C2A-CAA-CBA-CGA
27	B	626	GOL	O1-C1-C2-O2
27	o	302	GOL	O2-C2-C3-O3
32	A	419[B]	LHG	O1-C1-C2-O2
26	A	410[B]	SQD	C12-C13-C14-C15
32	E	101[A]	LHG	O6-C4-C5-O7
26	X	101	SQD	C24-C23-O48-C46
32	D	407[B]	LHG	O10-C23-O8-C6
33	z	101	LMG	C10-C11-C12-C13
23	A	406[A]	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C19
32	b	629[A]	LHG	C31-C32-C33-C34
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
23	A	406[B]	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
33	C	520	LMG	C37-C38-C39-C40
33	Z	101	LMG	C11-C12-C13-C14
26	X	101	SQD	C32-C33-C34-C35
23	B	607	CLA	C3-C5-C6-C7
23	C	509	CLA	O1D-CGD-O2D-CED
26	a	409[A]	SQD	C34-C35-C36-C37
33	z	101	LMG	C14-C15-C16-C17
26	a	409[A]	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	O47-C45-C46-O48
23	d	405	CLA	CBA-CGA-O2A-C1
23	c	509	CLA	C15-C16-C17-C18
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
32	E	101[A]	LHG	C17-C18-C19-C20
29	a	413[A]	PL9	C24-C26-C27-C28
32	D	407[A]	LHG	C10-C11-C12-C13
35	C	519	DGD	CDB-CEB-CFB-CGB
23	a	404[B]	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
26	l	101	SQD	C24-C25-C26-C27
32	L	101[B]	LHG	C15-C16-C17-C18
23	c	512	CLA	C13-C15-C16-C17
23	B	614	CLA	C14-C13-C15-C16
23	a	405[B]	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
31	M	101	LMT	C2-C3-C4-C5
32	b	629[B]	LHG	C12-C13-C14-C15
31	A	417	LMT	C7-C8-C9-C10
32	D	406[B]	LHG	C10-C11-C12-C13
32	a	419[B]	LHG	C10-C11-C12-C13
23	A	405[B]	CLA	C15-C16-C17-C18
23	c	509	CLA	C10-C11-C12-C13
33	z	101	LMG	C20-C21-C22-C23
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
25	D	404	BCR	C23-C24-C25-C26
25	D	404	BCR	C23-C24-C25-C30
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
23	b	601	CLA	CAA-CBA-CGA-O2A
32	d	415[A]	LHG	C25-C26-C27-C28
34	b	623	HTG	S1-C1'-C2'-C3'
25	K	102	BCR	C7-C8-C9-C10
25	d	406	BCR	C7-C8-C9-C10
23	b	601	CLA	C13-C15-C16-C17
32	d	415[B]	LHG	C25-C26-C27-C28
23	A	406[B]	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	514	CLA	C11-C10-C8-C7
23	b	604	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
23	c	506	CLA	C11-C10-C8-C7
23	c	510	CLA	C11-C10-C8-C7
24	a	406[A]	PHO	C2-C3-C5-C6
32	L	101[A]	LHG	C11-C10-C9-C8
32	d	415[A]	LHG	C24-C25-C26-C27
33	c	519	LMG	C10-C11-C12-C13
32	b	629[A]	LHG	C34-C35-C36-C37
23	C	511	CLA	O1A-CGA-O2A-C1
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
34	b	623	HTG	O5-C1-S1-C1'
34	c	521	HTG	C2'-C1'-S1-C1
32	d	409[B]	LHG	C9-C10-C11-C12
35	h	102	DGD	CDA-CEA-CFA-CGA
23	d	404[B]	CLA	C16-C17-C18-C19
23	C	512	CLA	C8-C10-C11-C12
35	c	518	DGD	C2A-C1A-O1G-C1G
33	B	620	LMG	C36-C37-C38-C39
35	C	519	DGD	C7B-C8B-C9B-CAB
23	b	604	CLA	C10-C11-C12-C13
26	a	409[B]	SQD	C27-C28-C29-C30
23	A	404[B]	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	501	CLA	CAD-CBD-CGD-O2D
23	c	503	CLA	CAD-CBD-CGD-O2D
23	c	510	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
38	f	101	HEM	C2B-C3B-CAB-CBB
23	b	607	CLA	C3-C5-C6-C7
31	B	628	LMT	C3-C4-C5-C6
32	E	101[A]	LHG	C13-C14-C15-C16
33	c	519	LMG	C29-C30-C31-C32
33	a	415	LMG	O8-C28-C29-C30
26	a	409[A]	SQD	C27-C28-C29-C30
32	d	415[B]	LHG	C27-C28-C29-C30
33	d	413	LMG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
23	c	511	CLA	O1A-CGA-O2A-C1
26	A	412	SQD	C24-C23-O48-C46
32	D	406[A]	LHG	C34-C35-C36-C37
35	c	516[B]	DGD	O6E-C1E-O5D-C6D
26	a	409[B]	SQD	O6-C44-C45-C46
32	D	407[B]	LHG	C2-C3-O3-P
32	E	101[A]	LHG	C4-C5-C6-O8
32	d	409[B]	LHG	C2-C3-O3-P
23	B	601	CLA	O1A-CGA-O2A-C1
32	L	101[B]	LHG	O6-C4-C5-O7
32	b	629[A]	LHG	O6-C4-C5-O7
23	C	510	CLA	C3-C5-C6-C7
31	T	101	LMT	C1-C2-C3-C4
23	B	606	CLA	C8-C10-C11-C12
32	E	101[B]	LHG	C17-C18-C19-C20
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	C9B-CAB-CBB-CCB
23	C	507	CLA	C16-C17-C18-C20
35	c	518	DGD	C2B-C3B-C4B-C5B
32	E	101[B]	LHG	C1-C2-C3-O3
31	b	627	LMT	C1-C2-C3-C4
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O1D
32	E	101[B]	LHG	C13-C14-C15-C16
35	C	519	DGD	CBA-CCA-CDA-CEA
23	c	511	CLA	C3-C5-C6-C7
23	d	405	CLA	O1A-CGA-O2A-C1
33	c	520	LMG	O10-C28-O8-C9
33	C	521	LMG	C4-C5-C6-O5
31	b	627	LMT	C6-C7-C8-C9
40	V	201	HEC	C4B-C3B-CAB-CBB
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
33	C	501	LMG	C39-C40-C41-C42
23	b	602	CLA	C10-C11-C12-C13
32	d	408[B]	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
27	c	526	GOL	O1-C1-C2-O2
31	F	101	LMT	C6-C7-C8-C9
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
23	c	510	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C45-C44-C46-C47
32	D	407[B]	LHG	C27-C28-C29-C30
33	C	501	LMG	C18-C19-C20-C21
35	c	517[A]	DGD	C1A-C2A-C3A-C4A
40	v	201	HEC	C2B-C3B-CAB-CBB
23	B	605	CLA	C11-C12-C13-C14
23	B	610	CLA	C14-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C9
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
35	H	102	DGD	CCA-CDA-CEA-CFA
35	c	518	DGD	O1A-C1A-O1G-C1G
23	c	507	CLA	C2A-CAA-CBA-CGA
32	L	101[B]	LHG	C24-C25-C26-C27
32	L	101[B]	LHG	C27-C28-C29-C30
26	X	101	SQD	O10-C23-O48-C46
26	A	412	SQD	C7-C8-C9-C10
27	o	302	GOL	C1-C2-C3-O3
23	b	612	CLA	C8-C10-C11-C12
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
23	B	605	CLA	O1D-CGD-O2D-CED
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
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
23	A	406[B]	CLA	C16-C17-C18-C20
23	b	608	CLA	C2-C1-O2A-CGA
23	b	601	CLA	CBA-CGA-O2A-C1
32	d	409[A]	LHG	C24-C23-O8-C6
32	A	419[A]	LHG	C32-C33-C34-C35
32	D	406[A]	LHG	C4-O6-P-O3
32	d	415[A]	LHG	C3-O3-P-O6
32	a	419[A]	LHG	C23-C24-C25-C26
26	a	409[A]	SQD	C35-C36-C37-C38
23	B	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C3-C5-C6-C7
32	D	407[A]	LHG	C2-C3-O3-P
32	d	409[A]	LHG	C2-C3-O3-P
32	b	629[B]	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
32	D	406[A]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	419[A]	LHG	C4-O6-P-O4
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
26	f	102	SQD	C23-C24-C25-C26
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
31	b	627	LMT	O1'-C1-C2-C3
35	c	516[A]	DGD	O6E-C1E-O5D-C6D
32	L	101[A]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
26	X	101	SQD	C34-C35-C36-C37
31	B	627	LMT	C9-C10-C11-C12
32	A	419[B]	LHG	C18-C19-C20-C21
32	d	415[A]	LHG	C27-C28-C29-C30
32	d	415[B]	LHG	C13-C14-C15-C16
33	D	411	LMG	C18-C19-C20-C21
35	c	516[A]	DGD	CCB-CDB-CEB-CFB
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	502	CLA	CAD-CBD-CGD-O1D
26	A	412	SQD	O10-C23-O48-C46
23	C	513	CLA	C3-C5-C6-C7
33	C	520	LMG	C29-C30-C31-C32
32	D	407[A]	LHG	C24-C23-O8-C6
23	c	501	CLA	O1D-CGD-O2D-CED
32	E	101[A]	LHG	C1-C2-C3-O3
23	b	616	CLA	C5-C6-C7-C8
26	a	409[B]	SQD	C34-C35-C36-C37
23	B	610	CLA	C12-C13-C15-C16
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C2-C3-C5-C6
23	C	507	CLA	C3A-C2A-CAA-CBA
23	b	615	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	509	CLA	C6-C7-C8-C10
23	c	509	CLA	C11-C10-C8-C7
23	d	404[B]	CLA	C11-C12-C13-C15
32	a	419[B]	LHG	C23-C24-C25-C26
32	b	629[B]	LHG	O6-C4-C5-O7
23	b	605	CLA	C13-C15-C16-C17
32	d	409[A]	LHG	O10-C23-O8-C6
26	a	409[B]	SQD	C35-C36-C37-C38
23	B	601	CLA	CAA-CBA-CGA-O2A
35	C	518[A]	DGD	C1A-C2A-C3A-C4A
31	B	629	LMT	C6-C7-C8-C9
32	D	407[A]	LHG	O10-C23-O8-C6
35	c	516[A]	DGD	C8B-C9B-CAB-CBB
23	c	507	CLA	C8-C10-C11-C12
26	A	410[A]	SQD	C34-C35-C36-C37
23	b	601	CLA	O1A-CGA-O2A-C1
26	l	101	SQD	O47-C45-C46-O48
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
26	a	409[A]	SQD	C11-C12-C13-C14
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
23	B	601	CLA	C15-C16-C17-C18
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
24	a	406[B]	PHO	C8-C10-C11-C12
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
35	C	518[B]	DGD	C3B-C4B-C5B-C6B
35	H	102	DGD	O2G-C1B-C2B-C3B
32	L	101[B]	LHG	C11-C12-C13-C14
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	b	615	CLA	C14-C13-C15-C16
31	B	629	LMT	C2-C3-C4-C5
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
31	A	417	LMT	O5B-C5B-C6B-O6B
27	v	202[B]	GOL	O1-C1-C2-O2
24	a	406[A]	PHO	C8-C10-C11-C12
23	B	611	CLA	C8-C10-C11-C12
32	b	629[B]	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C30-C31-C32-C33
23	A	406[A]	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	D	402[B]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
32	d	409[B]	LHG	O10-C23-O8-C6
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
23	D	403	CLA	C8-C10-C11-C12
23	d	402[B]	CLA	C15-C16-C17-C18
32	d	415[A]	LHG	C34-C35-C36-C37
31	a	416	LMT	O5'-C5'-C6'-O6'
31	A	417	LMT	C9-C10-C11-C12
32	d	408[B]	LHG	C13-C14-C15-C16
32	d	409[A]	LHG	C32-C33-C34-C35
35	c	516[B]	DGD	C1A-C2A-C3A-C4A
23	C	502	CLA	C2A-CAA-CBA-CGA
26	A	412	SQD	C15-C16-C17-C18
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
26	A	410[A]	SQD	C16-C17-C18-C19
35	c	517[B]	DGD	C1A-C2A-C3A-C4A
32	d	408[A]	LHG	O10-C23-O8-C6
32	L	101[A]	LHG	O6-C4-C5-O7
23	C	506	CLA	C4-C3-C5-C6
25	d	406	BCR	C23-C24-C25-C26
25	d	406	BCR	C23-C24-C25-C30
29	A	414[A]	PL9	C28-C29-C31-C32
35	h	102	DGD	CBA-CCA-CDA-CEA
32	d	408[A]	LHG	C24-C23-O8-C6
23	d	402[A]	CLA	C4C-C3C-CAC-CBC
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
33	B	620	LMG	C37-C38-C39-C40
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	518	DGD	CDA-CEA-CFA-CGA
33	Z	101	LMG	C2-C1-O1-C7
35	c	516[A]	DGD	C2E-C1E-O5D-C6D
35	c	516[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
32	L	101[A]	LHG	C26-C27-C28-C29
35	C	519	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
26	a	409[B]	SQD	C11-C12-C13-C14
33	B	620	LMG	C29-C30-C31-C32
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
35	h	102	DGD	C6A-C7A-C8A-C9A
32	d	415[B]	LHG	C3-O3-P-O6
32	L	101[B]	LHG	C23-C24-C25-C26
32	L	101[A]	LHG	C27-C28-C29-C30
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
32	d	409[B]	LHG	C32-C33-C34-C35
34	b	622	HTG	C1'-C2'-C3'-C4'
23	B	605	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C12-C13-C15
23	C	514	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C6-C7-C8-C10
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	502	CLA	C11-C12-C13-C15
35	c	516[B]	DGD	C4B-C5B-C6B-C7B
35	C	518[B]	DGD	C4E-C5E-C6E-O5E
23	a	407	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C10-C8-C9
23	c	509	CLA	C6-C7-C8-C9
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	b	629[B]	LHG	C31-C32-C33-C34
26	a	409[B]	SQD	C7-C8-C9-C10
35	c	516[A]	DGD	C4B-C5B-C6B-C7B
32	d	415[A]	LHG	C1-C2-C3-O3
23	C	511	CLA	C13-C15-C16-C17
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
23	B	603	CLA	C2-C3-C5-C6
29	a	413[B]	PL9	C43-C44-C46-C47
23	B	608	CLA	C16-C17-C18-C20
32	d	409[B]	LHG	C24-C23-O8-C6
23	b	614	CLA	CBD-CGD-O2D-CED
31	T	101	LMT	O1'-C1-C2-C3
32	d	409[A]	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
23	c	506	CLA	C13-C15-C16-C17
33	B	620	LMG	C32-C33-C34-C35
23	C	505	CLA	C4B-C3B-CAB-CBB
23	D	402[B]	CLA	C4B-C3B-CAB-CBB
31	a	416	LMT	O5'-C1'-O1'-C1
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
25	t	102	BCR	C13-C14-C15-C16
29	a	413[B]	PL9	C24-C26-C27-C28
32	a	419[B]	LHG	C7-C8-C9-C10
24	d	403[B]	PHO	C2C-C3C-CAC-CBC
38	f	101	HEM	C4B-C3B-CAB-CBB
26	A	410[A]	SQD	C11-C10-C9-C8
23	b	612	CLA	C10-C11-C12-C13
32	b	629[A]	LHG	C25-C26-C27-C28
23	b	613	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C8-C10-C11-C12
32	D	406[A]	LHG	C11-C10-C9-C8
34	b	623	HTG	C4'-C5'-C6'-C7'
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
26	X	101	SQD	O47-C45-C46-O48
32	a	419[A]	LHG	C24-C25-C26-C27
26	A	410[B]	SQD	C16-C17-C18-C19
38	E	102	HEM	CAD-CBD-CGD-O1D
23	C	502	CLA	C16-C17-C18-C20
23	d	402[B]	CLA	C4C-C3C-CAC-CBC
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
35	C	519	DGD	C8A-C9A-CAA-CBA
34	b	622	HTG	O5-C5-C6-O6
23	b	616	CLA	CBA-CGA-O2A-C1
31	b	621	LMT	C7-C8-C9-C10
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
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	a	405[A]	CLA	C6-C7-C8-C9
23	c	506	CLA	C6-C7-C8-C9
23	C	507	CLA	C16-C17-C18-C19
35	c	518	DGD	C6B-C7B-C8B-C9B

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Mol	Chain	Res	Type	Atoms
33	m	101	LMG	C32-C33-C34-C35
35	c	517[A]	DGD	C7B-C8B-C9B-CAB
32	L	101[A]	LHG	C23-C24-C25-C26
23	D	403	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
32	L	101[B]	LHG	C11-C10-C9-C8
24	a	406[B]	PHO	O2A-C1-C2-C3
33	B	620	LMG	O6-C1-O1-C7
33	a	415	LMG	C13-C14-C15-C16
25	Y	101	BCR	C37-C22-C23-C24
32	a	419[B]	LHG	C24-C25-C26-C27
23	d	402[A]	CLA	C15-C16-C17-C18
26	A	412	SQD	C30-C31-C32-C33
26	A	410[A]	SQD	C13-C14-C15-C16
29	a	413[B]	PL9	C45-C44-C46-C47
23	C	502	CLA	C1A-C2A-CAA-CBA
35	C	519	DGD	C4A-C5A-C6A-C7A
23	b	615	CLA	C11-C12-C13-C15
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
31	B	627	LMT	C1-C2-C3-C4
32	A	419[A]	LHG	C18-C19-C20-C21
32	b	629[A]	LHG	C17-C18-C19-C20
33	B	620	LMG	C18-C19-C20-C21
23	b	610	CLA	C13-C15-C16-C17
23	B	606	CLA	C16-C17-C18-C19
33	z	101	LMG	C13-C14-C15-C16
35	c	518	DGD	O6D-C5D-C6D-O5D
23	c	503	CLA	C8-C10-C11-C12
35	C	519	DGD	C6A-C7A-C8A-C9A
33	B	620	LMG	O8-C28-C29-C30
32	D	406[A]	LHG	C26-C27-C28-C29
35	C	519	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	CAA-CBA-CCA-CDA
35	c	516[B]	DGD	CBA-CCA-CDA-CEA
40	V	201	HEC	CAD-CBD-CGD-O1D
32	A	419[B]	LHG	C32-C33-C34-C35
32	d	408[A]	LHG	C16-C17-C18-C19
33	C	501	LMG	C29-C30-C31-C32
23	c	513	CLA	C4-C3-C5-C6
23	c	509	CLA	C8-C10-C11-C12
29	d	407[A]	PL9	C43-C44-C46-C47
23	c	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
23	c	501	CLA	C2B-C3B-CAB-CBB
38	E	102	HEM	CAD-CBD-CGD-O2D
23	b	615	CLA	C5-C6-C7-C8
23	c	506	CLA	C10-C11-C12-C13
23	C	503	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
31	a	416	LMT	C2'-C1'-O1'-C1
40	V	201	HEC	CAD-CBD-CGD-O2D
35	h	102	DGD	O1G-C1G-C2G-O2G
25	K	102	BCR	C19-C20-C21-C22
23	A	406[A]	CLA	C16-C17-C18-C19
35	C	519	DGD	C9A-CAA-CBA-CCA
31	e	101	LMT	O1'-C1-C2-C3
29	A	414[A]	PL9	C39-C41-C42-C43
29	A	414[B]	PL9	C39-C41-C42-C43
32	A	419[B]	LHG	C1-C2-C3-O3
29	a	413[A]	PL9	C45-C44-C46-C47
32	D	406[B]	LHG	C28-C29-C30-C31
23	c	512	CLA	C2-C1-O2A-CGA
23	b	615	CLA	C13-C15-C16-C17
23	A	408	CLA	C11-C12-C13-C14
23	C	505	CLA	C11-C12-C13-C14
23	c	502	CLA	C11-C12-C13-C14
23	d	405	CLA	C11-C12-C13-C14
32	b	629[B]	LHG	C9-C10-C11-C12
23	c	510	CLA	O1A-CGA-O2A-C1
32	A	419[A]	LHG	C29-C30-C31-C32
32	L	101[B]	LHG	C26-C27-C28-C29
33	C	521	LMG	C12-C13-C14-C15
35	c	516[A]	DGD	CAB-CBB-CCB-CDB
23	B	614	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	Y	101	BCR	C23-C24-C25-C30
25	c	514	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
33	z	101	LMG	O7-C10-C11-C12
35	H	102	DGD	CAB-CBB-CCB-CDB
23	b	615	CLA	C10-C11-C12-C13
27	d	414	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	l	103[A]	GOL	O1-C1-C2-C3
27	l	103[B]	GOL	C1-C2-C3-O3
27	v	202[A]	GOL	O1-C1-C2-C3
23	C	512	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	C4-C3-C5-C6
29	D	405[A]	PL9	C35-C34-C36-C37
29	D	405[B]	PL9	C35-C34-C36-C37
25	Y	101	BCR	C21-C22-C23-C24
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
31	A	417	LMT	C2B-C1B-O1B-C4'
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	c	516[B]	DGD	C5D-C6D-O5D-C1E
26	b	620	SQD	C10-C11-C12-C13
31	F	101	LMT	C2-C3-C4-C5
32	d	415[B]	LHG	C18-C19-C20-C21
35	c	518	DGD	CDB-CEB-CFB-CGB
23	A	404[A]	CLA	C16-C17-C18-C19
31	B	627	LMT	C7-C8-C9-C10
32	A	419[A]	LHG	C35-C36-C37-C38
38	f	101	HEM	CAA-CBA-CGA-O2A
31	e	101	LMT	C4B-C5B-C6B-O6B
38	f	101	HEM	CAD-CBD-CGD-O1D
23	b	604	CLA	C4B-C3B-CAB-CBB
32	b	629[A]	LHG	C10-C11-C12-C13
32	d	409[B]	LHG	C10-C11-C12-C13
29	A	414[B]	PL9	C25-C24-C26-C27
35	c	518	DGD	CAA-CBA-CCA-CDA
23	B	613	CLA	C11-C10-C8-C7
23	a	405[A]	CLA	C6-C7-C8-C10
23	c	510	CLA	C12-C13-C15-C16
23	B	613	CLA	C15-C16-C17-C18
32	L	101[A]	LHG	C16-C17-C18-C19
27	A	418	GOL	O1-C1-C2-O2
32	b	629[B]	LHG	C10-C11-C12-C13
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
23	C	508	CLA	C13-C15-C16-C17
33	C	521	LMG	C11-C12-C13-C14
23	a	407	CLA	C15-C16-C17-C18
35	c	517[B]	DGD	C5B-C6B-C7B-C8B
23	C	511	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	A	419[A]	LHG	O8-C23-C24-C25
32	b	629[B]	LHG	O7-C7-C8-C9
29	D	405[B]	PL9	C18-C19-C21-C22
35	c	517[A]	DGD	C9B-CAB-CBB-CCB
23	B	608	CLA	C16-C17-C18-C19
26	A	410[B]	SQD	C18-C19-C20-C21
34	B	622	HTG	C4'-C5'-C6'-C7'
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	a	405[B]	CLA	C14-C13-C15-C16
23	b	607	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
23	d	404[B]	CLA	C11-C12-C13-C14
32	A	419[B]	LHG	C30-C31-C32-C33
40	v	201	HEC	CAD-CBD-CGD-O2D
35	C	519	DGD	O1A-C1A-O1G-C1G
32	A	419[B]	LHG	O8-C23-C24-C25
32	L	101[B]	LHG	O7-C7-C8-C9
33	Z	101	LMG	O7-C10-C11-C12
35	h	102	DGD	O2G-C1B-C2B-C3B
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	a	404[B]	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	607	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	505	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	406[B]	PHO	CAD-CBD-CGD-O2D
24	d	403[A]	PHO	CAD-CBD-CGD-O2D
32	D	407[A]	LHG	C28-C29-C30-C31
32	b	629[A]	LHG	C30-C31-C32-C33
32	b	629[B]	LHG	C28-C29-C30-C31
32	L	101[A]	LHG	O7-C7-C8-C9
32	a	419[A]	LHG	O8-C23-C24-C25
26	l	101	SQD	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
29	A	414[A]	PL9	C25-C24-C26-C27
23	b	616	CLA	C2-C3-C5-C6
29	d	407[B]	PL9	C43-C44-C46-C47
25	d	406	BCR	C21-C22-C23-C24
33	C	520	LMG	C11-C12-C13-C14
40	v	201	HEC	CAD-CBD-CGD-O1D
23	B	612	CLA	O1A-CGA-O2A-C1
32	b	629[A]	LHG	O7-C7-C8-C9
33	c	519	LMG	C32-C33-C34-C35
35	C	519	DGD	CDA-CEA-CFA-CGA
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	602	CLA	O2A-C1-C2-C3
24	A	407[A]	PHO	O2A-C1-C2-C3
24	A	407[B]	PHO	O2A-C1-C2-C3
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
23	B	612	CLA	CBA-CGA-O2A-C1
23	D	403	CLA	CBA-CGA-O2A-C1
31	T	101	LMT	C4-C5-C6-C7
33	d	413	LMG	C16-C17-C18-C19
33	C	501	LMG	C15-C16-C17-C18
23	A	405[A]	CLA	CHA-CBD-CGD-O1D
23	A	405[A]	CLA	CHA-CBD-CGD-O2D
23	A	405[B]	CLA	CHA-CBD-CGD-O1D
23	A	405[B]	CLA	CHA-CBD-CGD-O2D
23	A	406[B]	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	502	CLA	CHA-CBD-CGD-O2D
23	c	507	CLA	CHA-CBD-CGD-O1D
23	c	507	CLA	CHA-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	d	402[A]	CLA	CHA-CBD-CGD-O1D
23	d	402[A]	CLA	CHA-CBD-CGD-O2D
26	A	410[B]	SQD	C34-C35-C36-C37
33	m	101	LMG	C11-C12-C13-C14
32	E	101[B]	LHG	O7-C7-C8-C9
33	c	519	LMG	O7-C10-C11-C12
32	A	419[A]	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
32	d	415[A]	LHG	C13-C14-C15-C16
33	c	519	LMG	C30-C31-C32-C33
33	c	520	LMG	O1-C7-C8-O7
35	C	518[A]	DGD	CAB-CBB-CCB-CDB
38	f	101	HEM	CAA-CBA-CGA-O1A
35	c	518	DGD	O6E-C5E-C6E-O5E
26	a	411	SQD	C26-C27-C28-C29
35	c	518	DGD	C9B-CAB-CBB-CCB
23	B	613	CLA	CAA-CBA-CGA-O2A
23	c	510	CLA	CAA-CBA-CGA-O2A
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
27	d	414	GOL	O2-C2-C3-O3
23	b	613	CLA	O1D-CGD-O2D-CED
26	a	411	SQD	O48-C23-C24-C25
23	b	604	CLA	C13-C15-C16-C17
23	C	507	CLA	C12-C13-C15-C16
23	b	607	CLA	C12-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C15
23	B	606	CLA	C16-C17-C18-C20
29	A	414[A]	PL9	C4-C3-C7-C8
23	C	513	CLA	CAA-CBA-CGA-O2A
23	A	408	CLA	C14-C13-C15-C16
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
32	A	419[B]	LHG	O10-C23-C24-C25
26	b	620	SQD	C30-C31-C32-C33
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
23	c	510	CLA	CBA-CGA-O2A-C1
32	a	419[B]	LHG	O8-C23-C24-C25
32	d	415[A]	LHG	C18-C19-C20-C21
33	Z	101	LMG	C29-C28-O8-C9
23	B	603	CLA	C2A-CAA-CBA-CGA
23	b	602	CLA	C2A-CAA-CBA-CGA
32	b	629[A]	LHG	C24-C25-C26-C27
35	c	517[B]	DGD	CBB-CCB-CDB-CEB
35	c	516[B]	DGD	C8B-C9B-CAB-CBB
26	f	102	SQD	C34-C35-C36-C37
32	A	419[B]	LHG	C17-C18-C19-C20
32	d	409[B]	LHG	C33-C34-C35-C36
35	C	518[B]	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
38	f	101	HEM	CAD-CBD-CGD-O2D
32	L	101[B]	LHG	O9-C7-C8-C9
26	b	620	SQD	C25-C26-C27-C28
33	B	620	LMG	C21-C22-C23-C24
27	A	418	GOL	O1-C1-C2-C3
27	B	626	GOL	O1-C1-C2-C3
27	l	103[A]	GOL	C1-C2-C3-O3
29	D	405[A]	PL9	C28-C29-C31-C32
26	a	411	SQD	C15-C16-C17-C18
35	C	519	DGD	C2A-C1A-O1G-C1G
32	D	406[B]	LHG	C32-C33-C34-C35
23	c	506	CLA	C1A-C2A-CAA-CBA
23	c	511	CLA	C1A-C2A-CAA-CBA
26	A	412	SQD	C31-C32-C33-C34
32	A	419[A]	LHG	O10-C23-C24-C25
32	b	629[B]	LHG	O9-C7-C8-C9
33	Z	101	LMG	O9-C10-C11-C12
29	A	414[B]	PL9	C46-C47-C48-C49
26	X	101	SQD	C33-C34-C35-C36
23	b	608	CLA	C13-C15-C16-C17
32	a	419[A]	LHG	O10-C23-C24-C25
32	a	419[B]	LHG	O10-C23-C24-C25
32	b	629[A]	LHG	O9-C7-C8-C9
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
33	D	411	LMG	O7-C10-C11-C12
35	c	516[A]	DGD	O2G-C1B-C2B-C3B
26	a	409[B]	SQD	C18-C19-C20-C21
33	d	413	LMG	C19-C20-C21-C22
23	B	602	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	c	503	CLA	C2A-CAA-CBA-CGA
26	f	102	SQD	C28-C29-C30-C31
33	C	521	LMG	C38-C39-C40-C41
23	c	510	CLA	CAA-CBA-CGA-O1A
33	c	519	LMG	C39-C40-C41-C42
23	b	613	CLA	CAA-CBA-CGA-O2A
32	E	101[A]	LHG	O7-C7-C8-C9
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
23	C	509	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C13-C15-C16-C17
32	L	101[B]	LHG	O9-C7-O7-C5
31	A	417	LMT	O5B-C1B-O1B-C4'
23	C	511	CLA	CAA-CBA-CGA-O1A
32	E	101[B]	LHG	O9-C7-C8-C9
32	D	406[B]	LHG	C34-C35-C36-C37
23	B	615	CLA	C8-C10-C11-C12
23	B	610	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C4B-C3B-CAB-CBB
23	c	501	CLA	C4B-C3B-CAB-CBB
23	c	502	CLA	C4B-C3B-CAB-CBB
32	d	408[A]	LHG	C4-O6-P-O5
32	d	415[B]	LHG	C3-O3-P-O5
23	A	408	CLA	C16-C17-C18-C19
23	B	616	CLA	C16-C17-C18-C20
33	B	620	LMG	C30-C31-C32-C33
23	B	613	CLA	CAA-CBA-CGA-O1A
23	C	513	CLA	CAA-CBA-CGA-O1A
23	b	601	CLA	CAA-CBA-CGA-O1A
31	e	101	LMT	C2B-C1B-O1B-C4'
32	L	101[A]	LHG	O9-C7-C8-C9
33	c	519	LMG	O10-C28-O8-C9
33	a	415	LMG	C14-C15-C16-C17
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
35	c	516[A]	DGD	C1A-C2A-C3A-C4A
23	b	603	CLA	C5-C6-C7-C8
32	D	407[B]	LHG	O8-C23-C24-C25
33	a	415	LMG	O10-C28-C29-C30
29	d	407[A]	PL9	C11-C12-C13-C14
33	d	413	LMG	C38-C39-C40-C41
23	A	406[B]	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
33	C	521	LMG	C10-C11-C12-C13
26	a	411	SQD	O10-C23-C24-C25
33	c	519	LMG	O9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	a	409[A]	SQD	C10-C11-C12-C13
23	b	612	CLA	CAA-CBA-CGA-O2A
23	A	405[B]	CLA	C13-C15-C16-C17
23	C	513	CLA	C11-C10-C8-C9
23	b	601	CLA	C11-C12-C13-C14
23	d	402[A]	CLA	C11-C12-C13-C14
31	a	416	LMT	C4'-C5'-C6'-O6'
23	c	512	CLA	CAA-CBA-CGA-O2A
26	A	412	SQD	O48-C23-C24-C25
32	D	407[A]	LHG	O8-C23-C24-C25
35	c	516[B]	DGD	O2G-C1B-C2B-C3B
32	d	409[B]	LHG	O8-C23-C24-C25
29	d	407[B]	PL9	C11-C12-C13-C14
23	B	612	CLA	C13-C15-C16-C17
23	B	615	CLA	C13-C15-C16-C17
26	a	409[A]	SQD	C19-C20-C21-C22
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	D	411	LMG	C34-C35-C36-C37
35	c	516[A]	DGD	CBA-CCA-CDA-CEA
23	B	615	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C7
23	b	608	CLA	C12-C13-C15-C16
23	b	614	CLA	C11-C10-C8-C7
38	E	102	HEM	CAA-CBA-CGA-O2A
32	E	101[A]	LHG	O8-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
33	B	620	LMG	O7-C10-C11-C12
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
32	D	406[A]	LHG	C28-C29-C30-C31
33	d	413	LMG	C28-C29-C30-C31
25	y	101	BCR	C21-C22-C23-C24
32	D	407[A]	LHG	O10-C23-C24-C25
32	E	101[B]	LHG	O10-C23-C24-C25
35	c	516[A]	DGD	O1B-C1B-C2B-C3B
31	B	628	LMT	C7-C8-C9-C10
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
31	m	103	LMT	C2-C1-O1'-C1'
23	c	512	CLA	CAA-CBA-CGA-O1A
33	D	411	LMG	O9-C10-C11-C12
23	C	512	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C29-C28-O8-C9
33	C	521	LMG	C33-C34-C35-C36
23	c	501	CLA	CAA-CBA-CGA-O2A
26	a	409[B]	SQD	O47-C7-C8-C9
35	c	517[B]	DGD	CDA-CEA-CFA-CGA
26	A	412	SQD	O10-C23-C24-C25
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[A]	LHG	O10-C23-C24-C25
24	d	403[B]	PHO	C8-C10-C11-C12
35	C	518[A]	DGD	O1B-C1B-C2B-C3B
35	C	518[B]	DGD	O1B-C1B-C2B-C3B
35	c	516[B]	DGD	O1B-C1B-C2B-C3B
33	c	520	LMG	O7-C10-C11-C12
38	E	102	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

171 monomers are involved in 360 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	618	BCR	4	0
23	C	514	CLA	1	0
23	c	503	CLA	3	0
23	c	509	CLA	3	0
33	c	519	LMG	1	0
23	C	510	CLA	2	0
26	X	101	SQD	2	0
25	B	617	BCR	1	0
27	a	417	GOL	1	0
23	c	512	CLA	7	0
24	A	416[B]	PHO	1	0
23	B	605	CLA	4	0
25	k	101	BCR	2	0
35	c	518	DGD	3	0
25	h	101	BCR	4	0
32	A	419[A]	LHG	2	0
32	D	406[B]	LHG	1	0
23	c	501	CLA	4	0
38	E	102	HEM	1	0
32	A	419[B]	LHG	1	0
23	C	502	CLA	6	0
26	a	411	SQD	2	0
23	C	513	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	618	BCR	4	0
23	b	602	CLA	2	0
23	b	609	CLA	4	0
23	d	405	CLA	2	0
23	A	406[A]	CLA	1	0
34	b	622	HTG	1	0
33	c	520	LMG	1	0
25	A	409	BCR	1	0
29	a	413[A]	PL9	5	0
23	c	508	CLA	8	0
25	C	516	BCR	1	0
23	b	604	CLA	2	0
32	D	407[A]	LHG	5	0
35	C	517[B]	DGD	3	0
24	a	406[B]	PHO	1	0
25	D	404	BCR	2	0
29	a	413[B]	PL9	6	0
23	C	508	CLA	2	0
23	C	509	CLA	3	0
23	B	616	CLA	4	0
35	h	102	DGD	2	0
32	d	408[B]	LHG	2	0
23	a	405[B]	CLA	2	0
31	M	101	LMT	1	0
32	D	407[B]	LHG	2	0
23	C	504	CLA	3	0
24	A	416[A]	PHO	1	0
32	d	409[A]	LHG	10	0
31	e	101	LMT	1	0
23	B	609	CLA	3	0
32	D	406[A]	LHG	2	0
23	B	614	CLA	3	0
25	T	102	BCR	7	0
23	b	613	CLA	2	0
26	l	101	SQD	1	0
23	d	402[B]	CLA	3	0
32	d	409[B]	LHG	10	0
27	b	628	GOL	1	0
25	b	617	BCR	1	0
25	b	619	BCR	5	0
23	B	601	CLA	4	0
27	O	303	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	t	102	BCR	4	0
23	c	502	CLA	2	0
23	d	404[B]	CLA	3	0
25	B	619	BCR	1	0
31	A	417	LMT	1	0
25	K	102	BCR	2	0
24	d	403[A]	PHO	2	0
23	C	512	CLA	2	0
26	b	620	SQD	3	0
33	B	620	LMG	1	0
34	b	625	HTG	1	0
23	C	506	CLA	4	0
24	d	403[B]	PHO	2	0
35	C	519	DGD	3	0
23	B	610	CLA	1	0
27	a	418	GOL	4	0
35	C	517[A]	DGD	2	0
25	y	101	BCR	2	0
23	a	404[A]	CLA	3	0
23	b	614	CLA	1	0
27	v	202[A]	GOL	1	0
33	z	101	LMG	2	0
23	a	405[A]	CLA	2	0
32	d	408[A]	LHG	3	0
26	A	410[A]	SQD	1	0
23	c	513	CLA	2	0
25	d	406	BCR	1	0
23	a	404[B]	CLA	3	0
27	v	202[B]	GOL	1	0
34	B	624	HTG	1	0
23	B	613	CLA	5	0
23	A	405[A]	CLA	4	0
25	c	514	BCR	3	0
38	f	101	HEM	2	0
24	A	407[A]	PHO	2	0
26	A	410[B]	SQD	2	0
27	B	626	GOL	1	0
23	d	402[A]	CLA	2	0
23	A	405[B]	CLA	3	0
31	B	628	LMT	1	0
23	C	511	CLA	3	0
24	A	407[B]	PHO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	a	408	BCR	1	0
33	d	413	LMG	4	0
35	c	516[B]	DGD	2	0
23	d	404[A]	CLA	2	0
27	O	302	GOL	1	0
32	E	101[B]	LHG	2	0
40	V	201	HEC	1	0
27	D	412	GOL	2	0
23	D	402[B]	CLA	3	0
25	C	515	BCR	2	0
23	c	504	CLA	2	0
23	B	612	CLA	1	0
35	C	518[B]	DGD	3	0
23	C	503	CLA	5	0
23	b	607	CLA	1	0
27	B	623	GOL	2	0
31	b	621	LMT	2	0
23	c	505	CLA	6	0
23	A	404[A]	CLA	5	0
29	A	414[A]	PL9	9	0
23	c	506	CLA	4	0
23	c	511	CLA	6	0
23	A	404[B]	CLA	2	0
31	C	525	LMT	1	0
23	b	615	CLA	1	0
23	B	604	CLA	1	0
29	A	414[B]	PL9	9	0
23	b	605	CLA	3	0
33	C	521	LMG	3	0
23	B	615	CLA	7	0
27	l	103[A]	GOL	1	0
23	B	606	CLA	2	0
35	c	516[A]	DGD	2	0
27	A	418	GOL	4	0
32	E	101[A]	LHG	5	0
35	c	517[A]	DGD	1	0
23	B	602	CLA	2	0
23	b	612	CLA	1	0
32	a	419[A]	LHG	4	0
29	d	407[B]	PL9	1	0
23	D	402[A]	CLA	3	0
23	a	407	CLA	5	0

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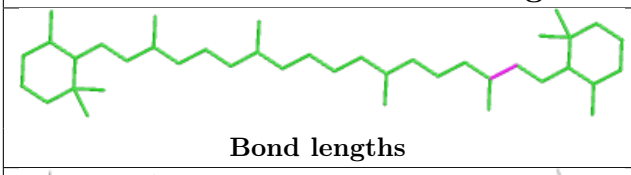
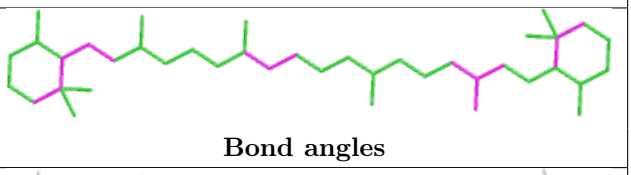
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	606	CLA	2	0
31	a	416	LMT	1	0
25	Y	101	BCR	2	0
31	t	101	LMT	1	0
35	H	102	DGD	1	0
32	a	419[B]	LHG	4	0
35	c	517[B]	DGD	1	0
25	H	101	BCR	1	0
23	c	507	CLA	3	0
35	C	518[A]	DGD	2	0
32	d	415[B]	LHG	1	0
33	Z	101	LMG	1	0
23	b	601	CLA	3	0
23	C	505	CLA	1	0
23	A	408	CLA	4	0
23	b	616	CLA	1	0
26	a	409[A]	SQD	5	0
34	B	621	HTG	1	0
34	c	521	HTG	1	0
23	A	406[B]	CLA	1	0
23	C	507	CLA	5	0
26	a	409[B]	SQD	5	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.

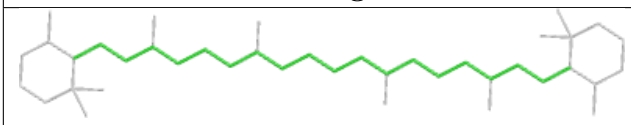
Ligand BCR b 618



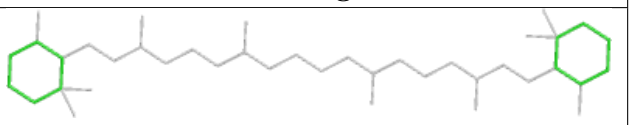
Bond lengths



Bond angles

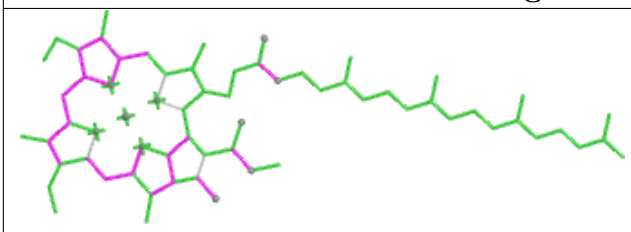


Torsions

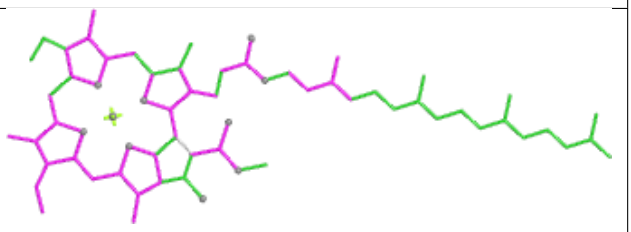


Rings

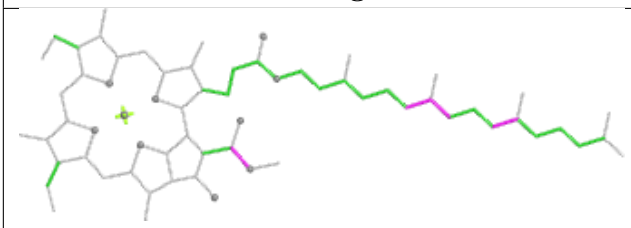
Ligand CLA C 514



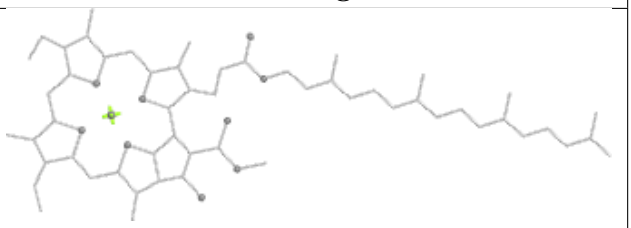
Bond lengths



Bond angles

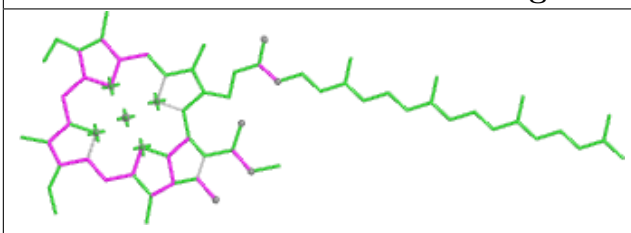


Torsions

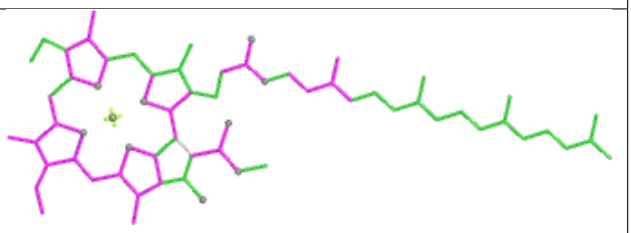


Rings

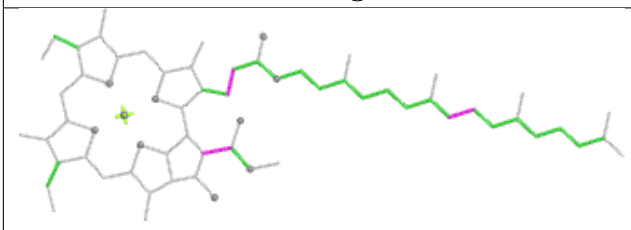
Ligand CLA c 503



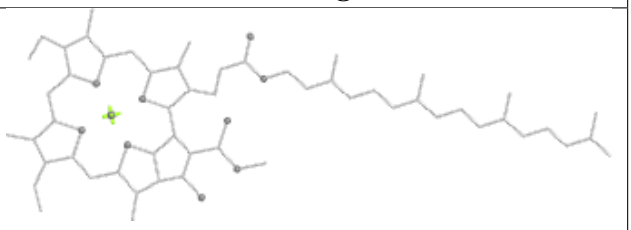
Bond lengths



Bond angles

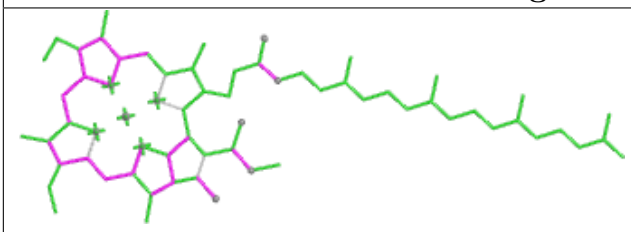


Torsions

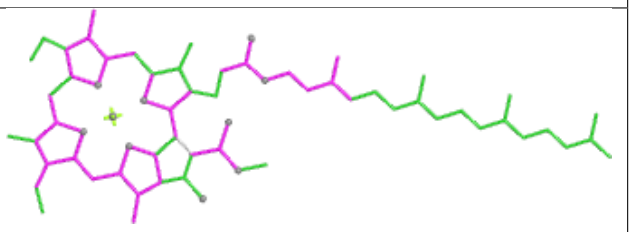


Rings

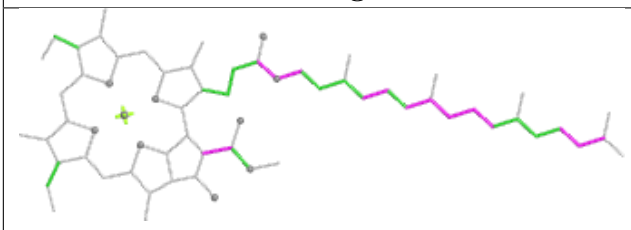
Ligand CLA c 509



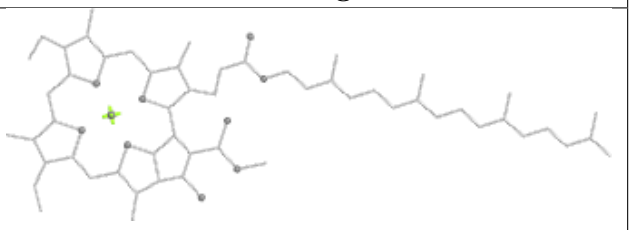
Bond lengths



Bond angles



Torsions

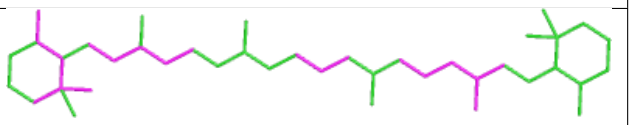


Rings

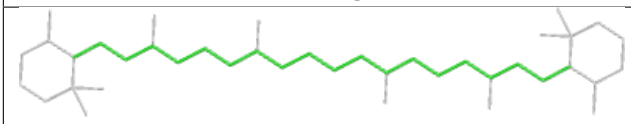
Ligand BCR c 515



Bond lengths



Bond angles



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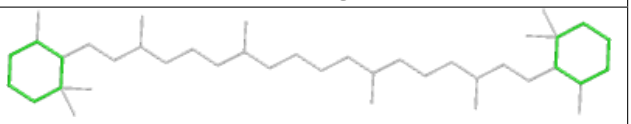
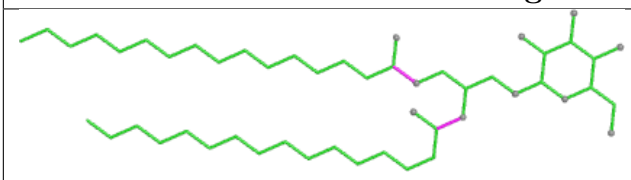
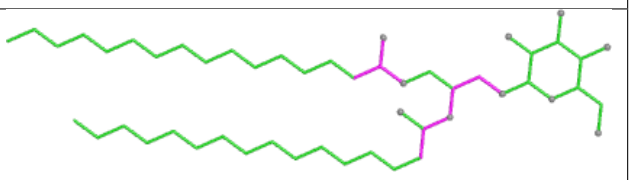


Rings

Ligand LMG c 519



Bond lengths



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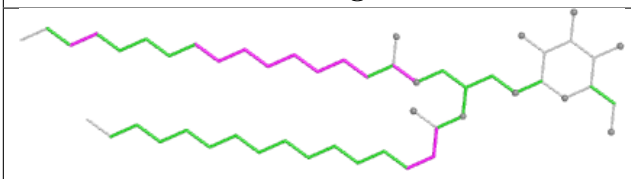

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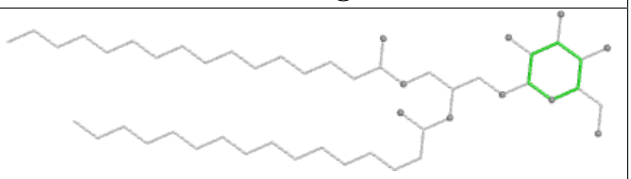
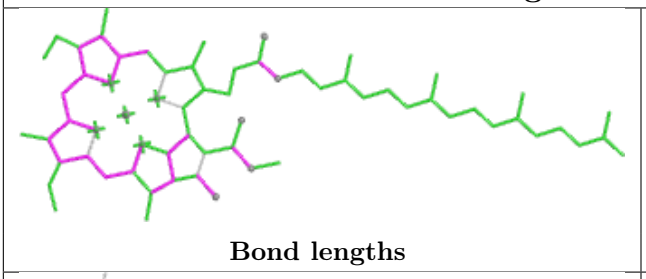
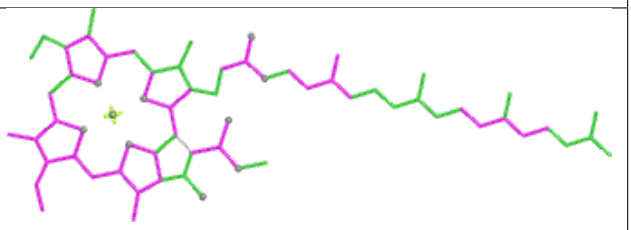


Rings

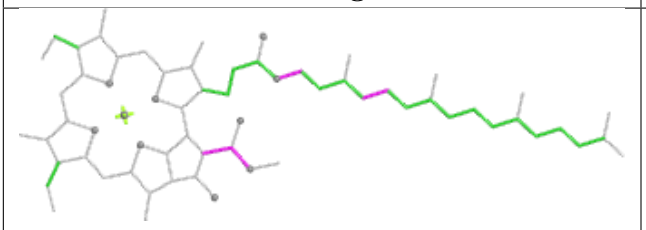
Ligand CLA C 510



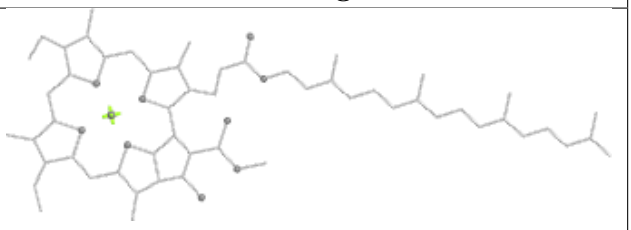
Bond lengths



Bond angles

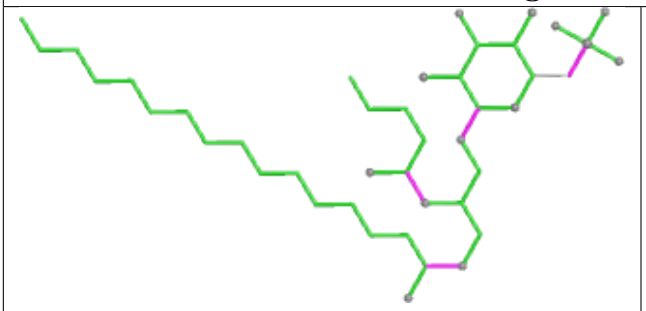


Torsions



Rings

Ligand SQD X 101



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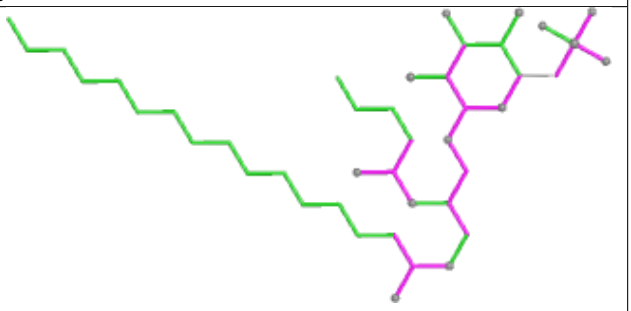
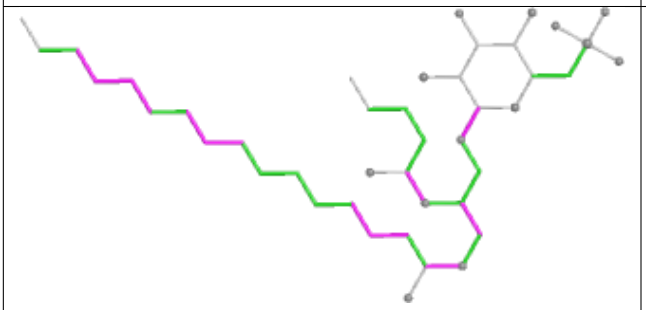
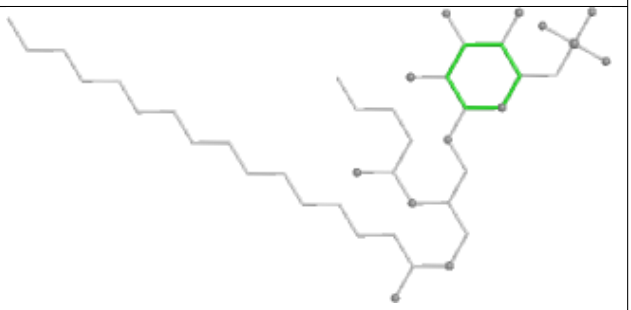


Bond angles

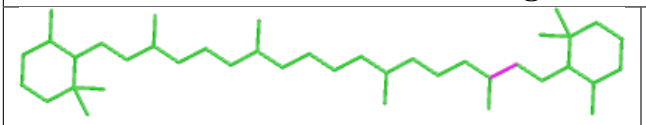


Torsions



Rings

Ligand BCR B 617



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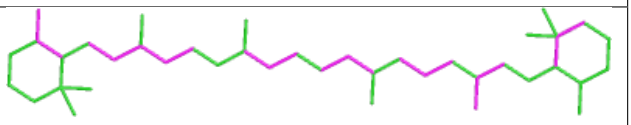
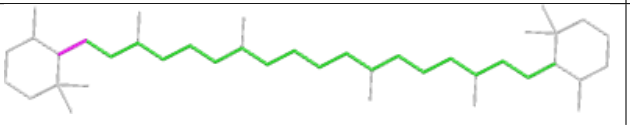


Bond angles



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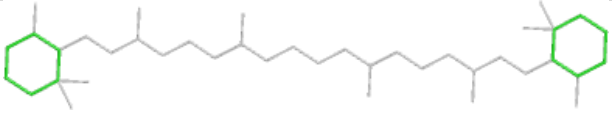
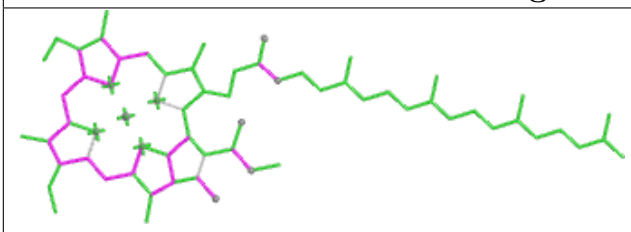


Rings

Ligand CLA c 512



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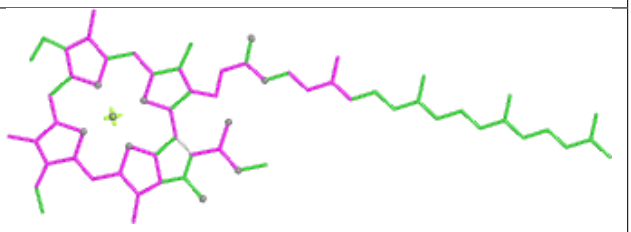

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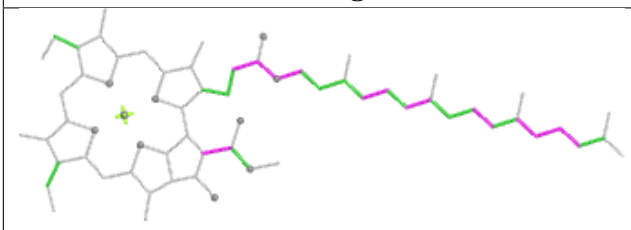

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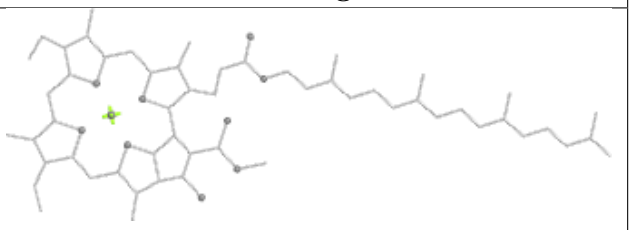
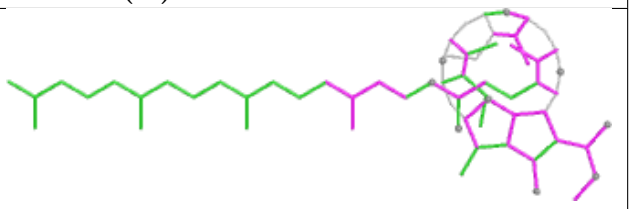


Rings

Ligand PHO A 416 (B)



Bond lengths



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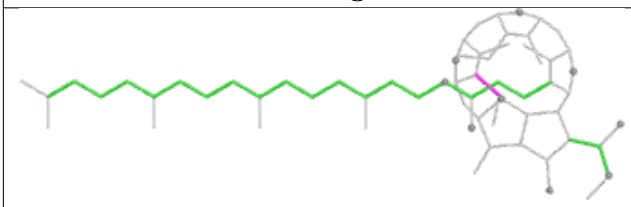

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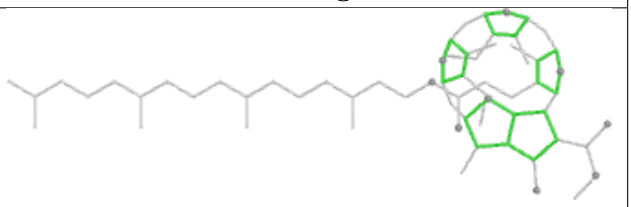
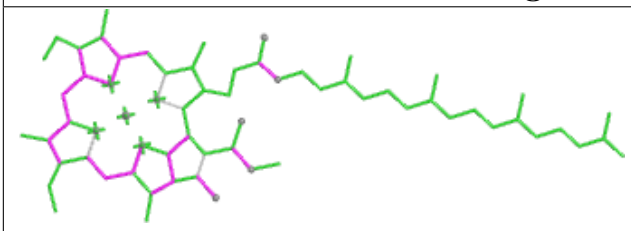


Rings

Ligand CLA B 605



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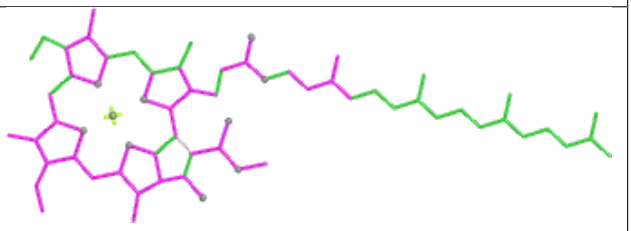
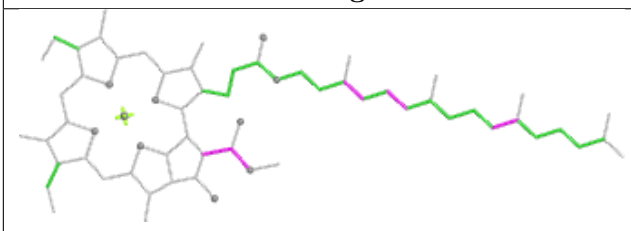


Bond angles



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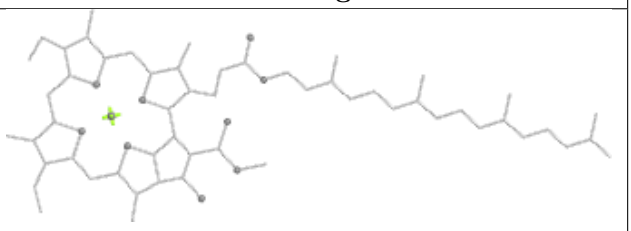
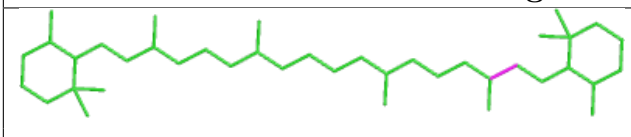


Rings

Ligand BCR k 101



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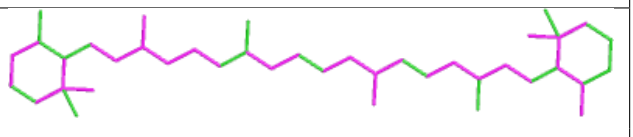
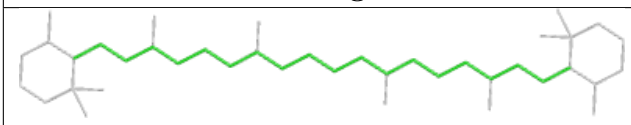


Bond angles



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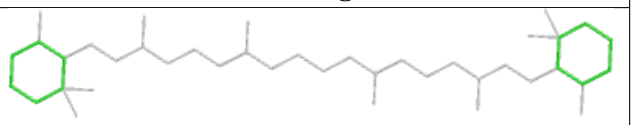
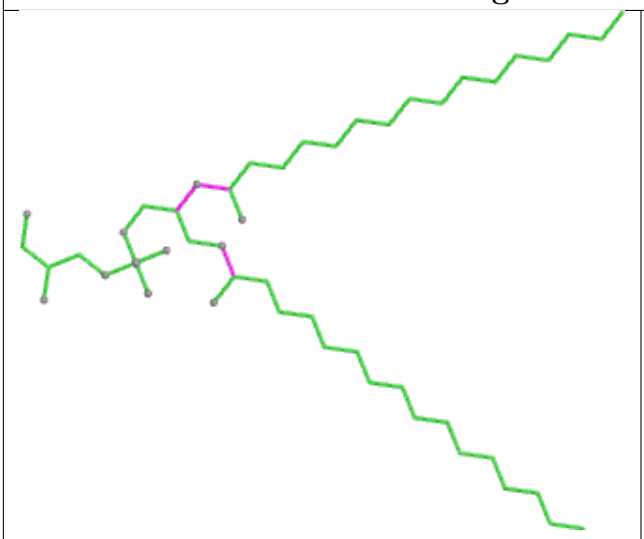


Rings

Ligand LHG b 629 (A)



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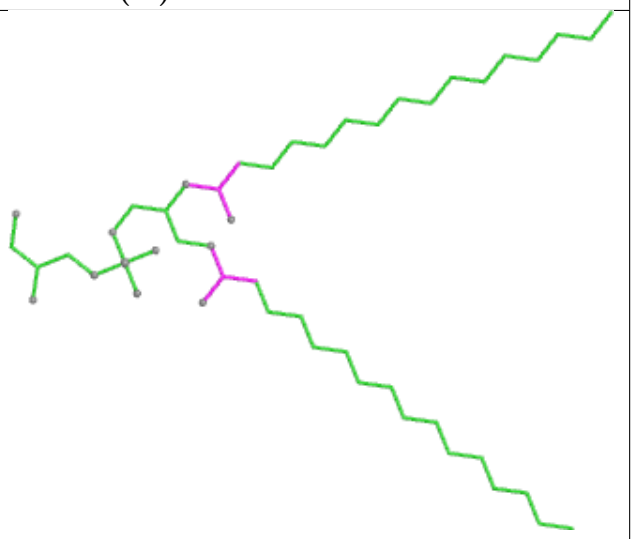
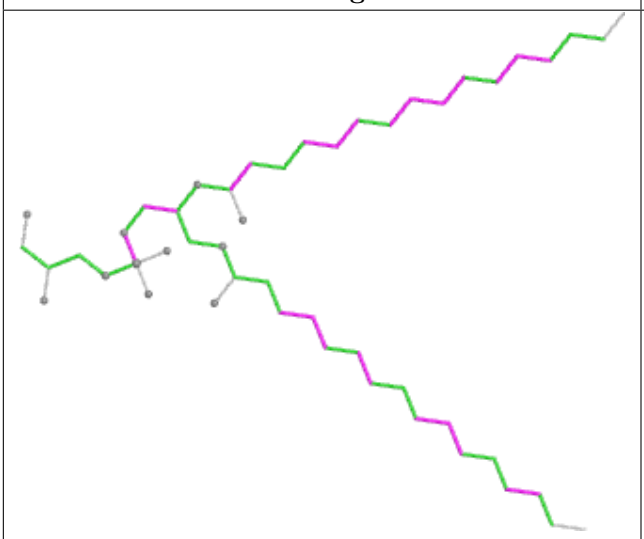


Bond angles



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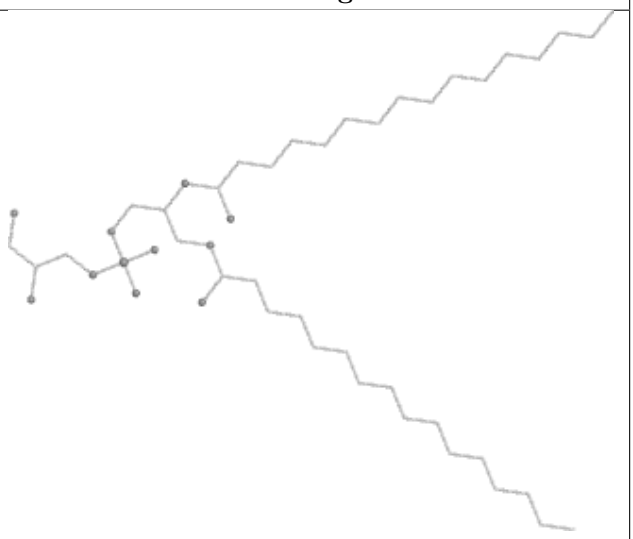
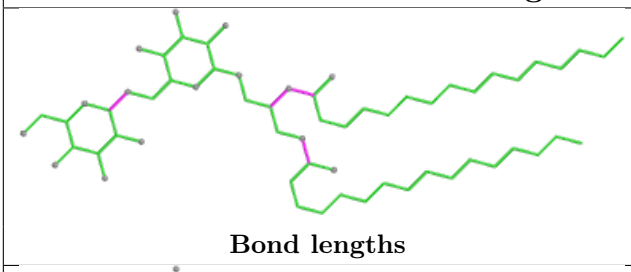


Rings

Ligand DGD c 518



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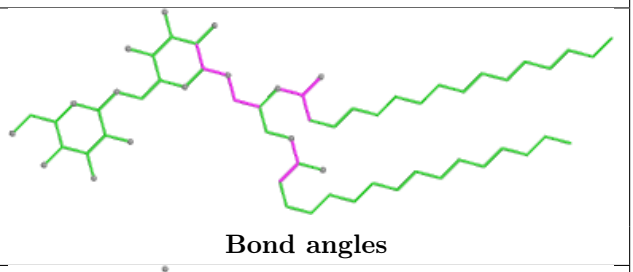
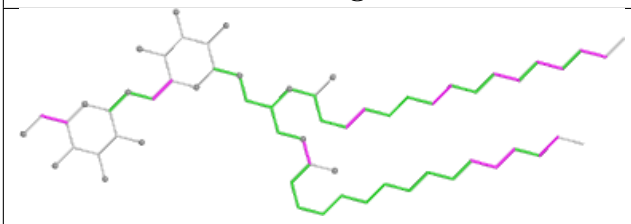


Bond angles



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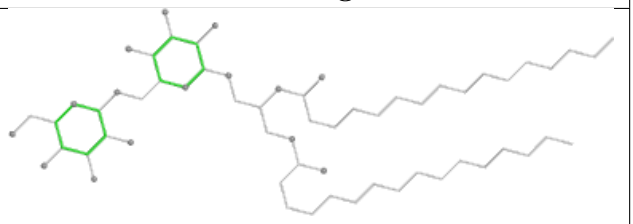
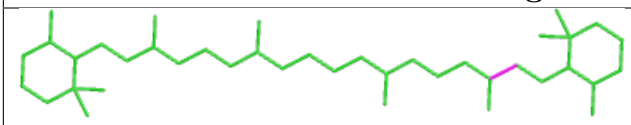


Rings

Ligand BCR h 101



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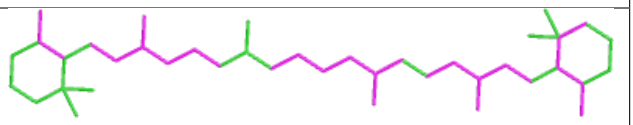
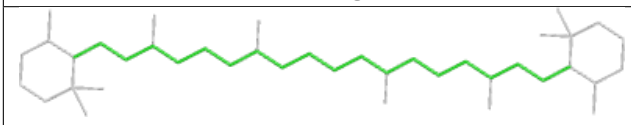


Bond angles



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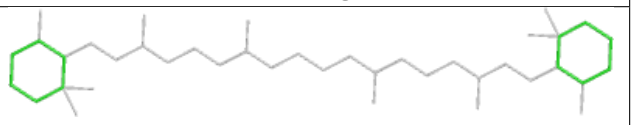
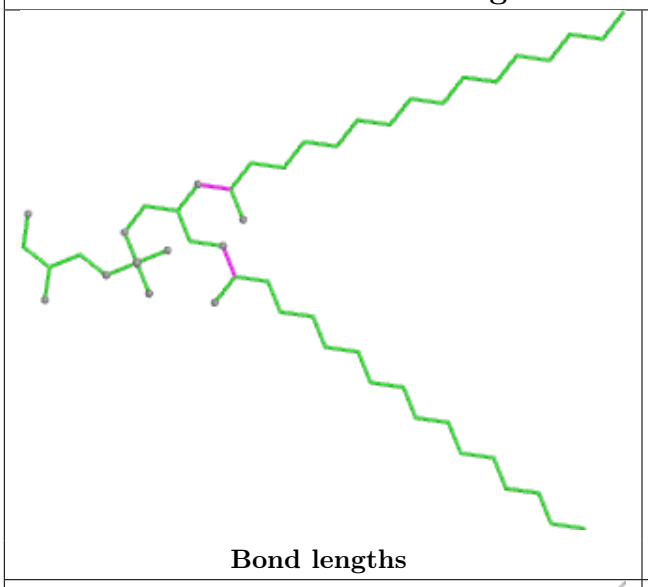


Rings

Ligand LHG A 419 (A)



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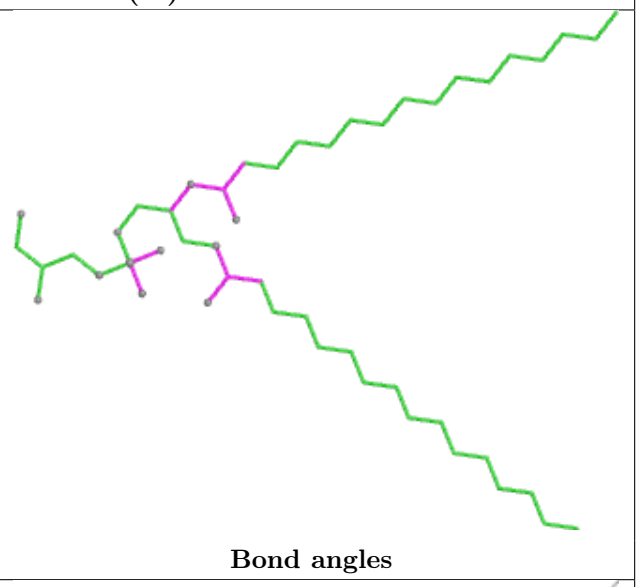
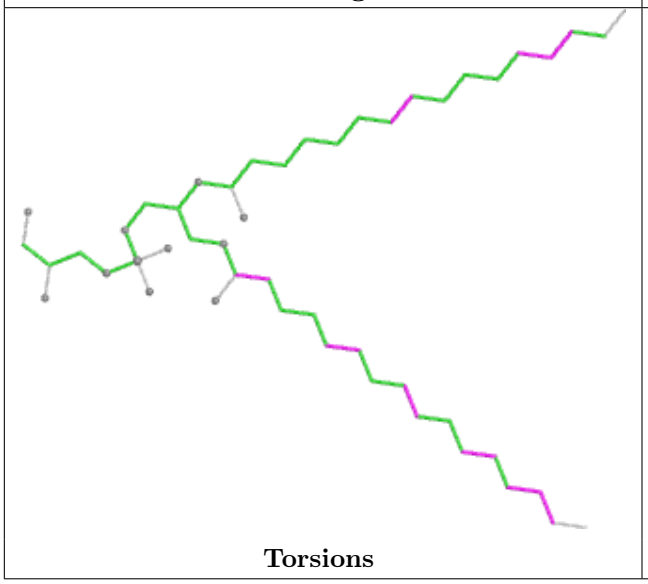


Bond angles



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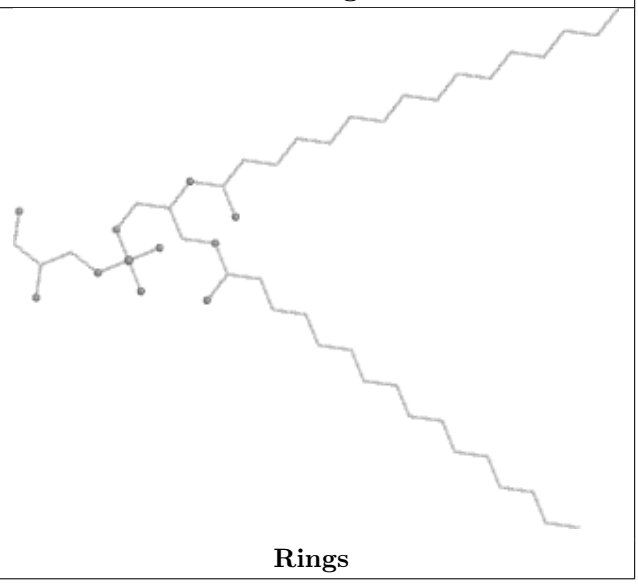
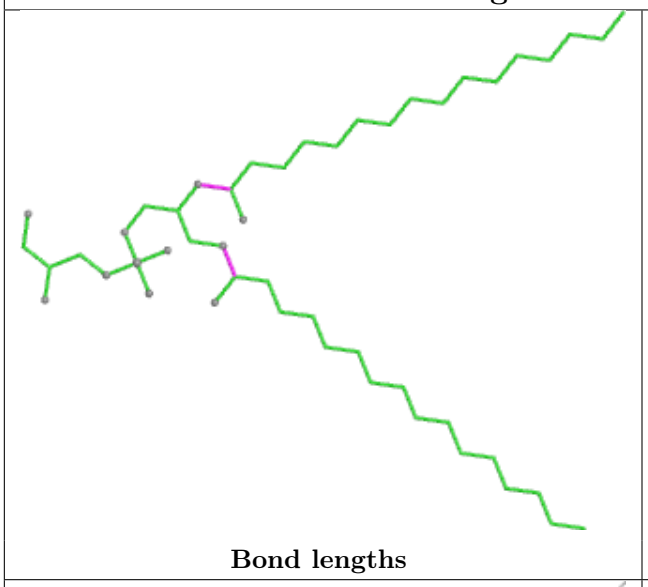


Rings

Ligand LHG D 406 (B)



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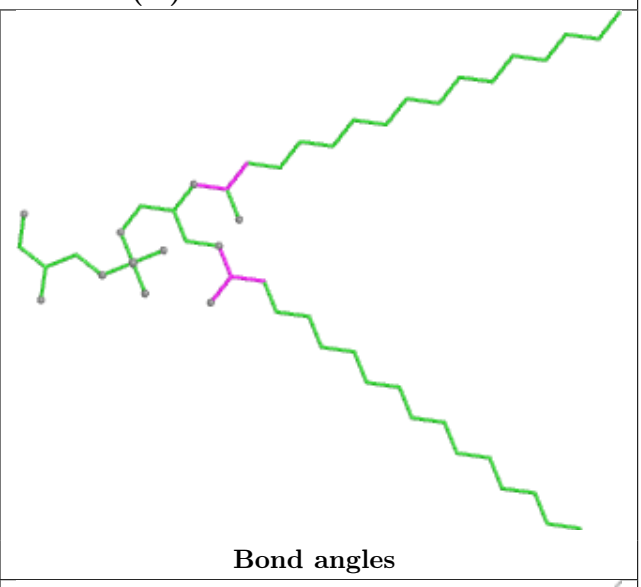
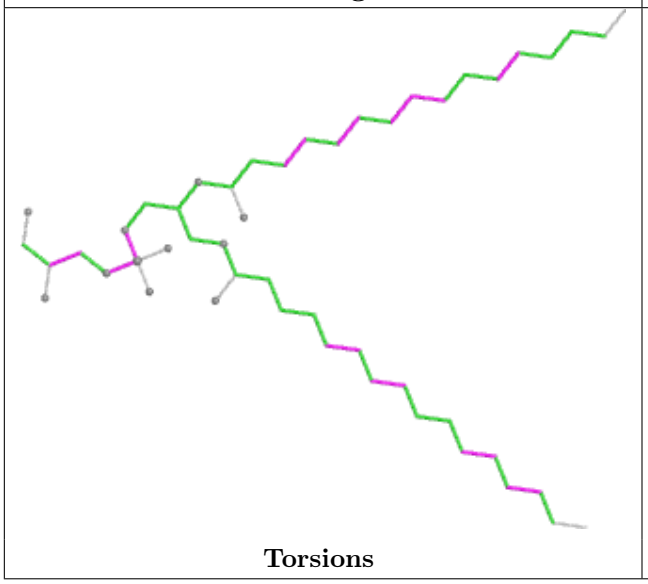


Bond angles



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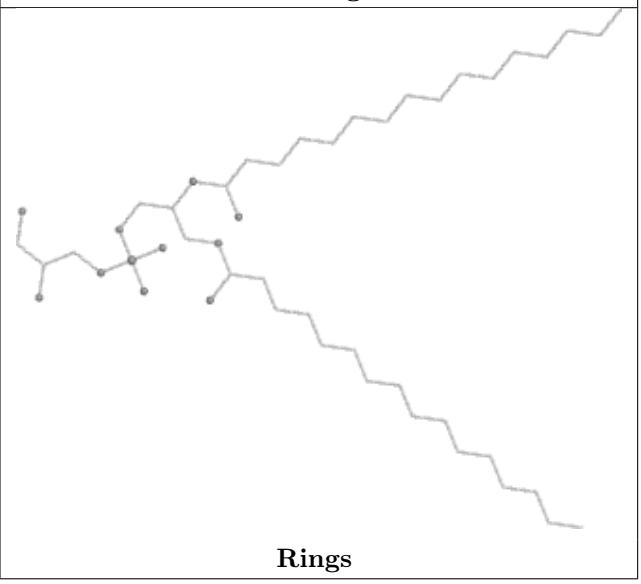
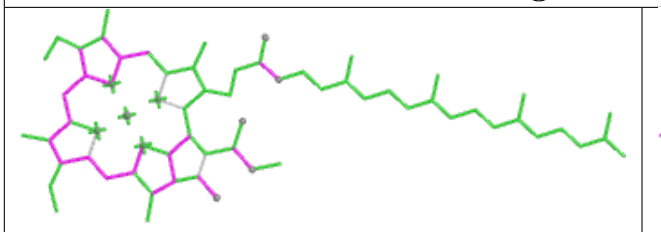


Rings

Ligand CLA c 501



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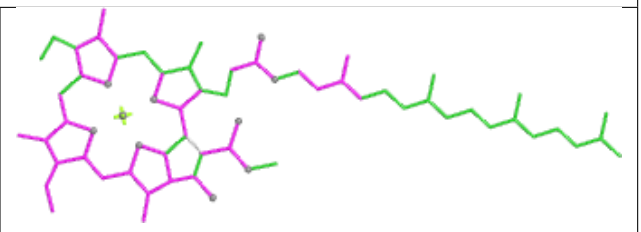
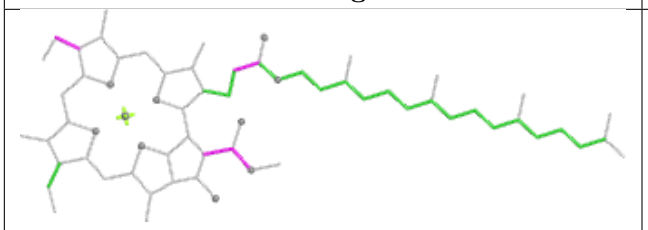


Bond angles



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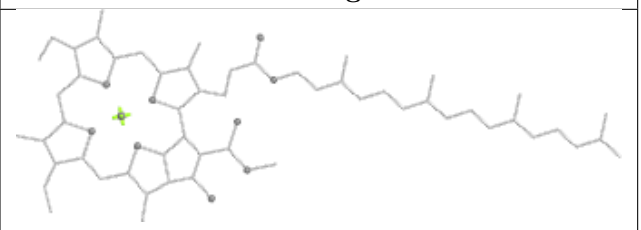
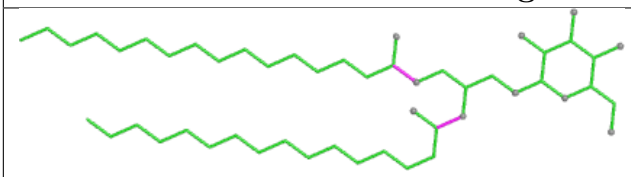


Rings

Ligand LMG m 101



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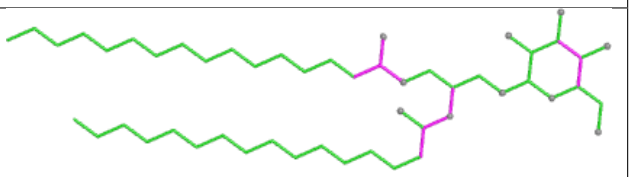
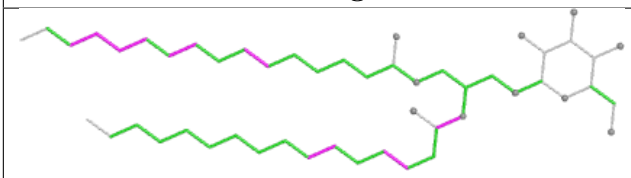


Bond angles



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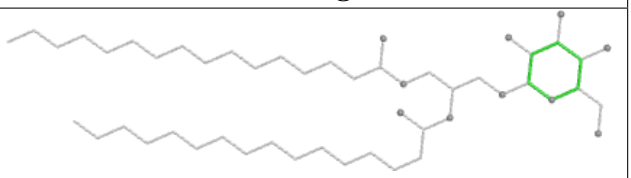
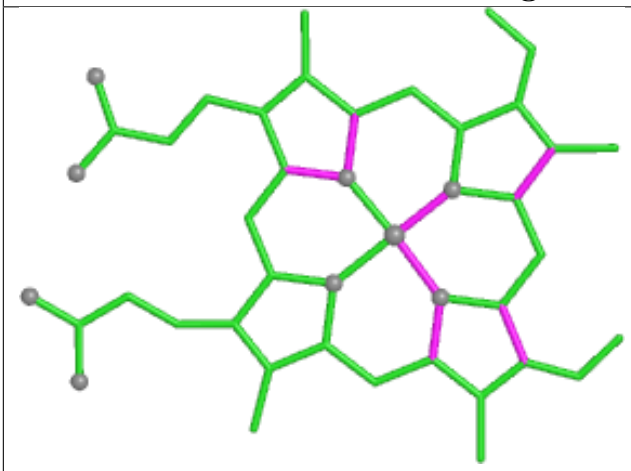


Rings

Ligand HEM E 102



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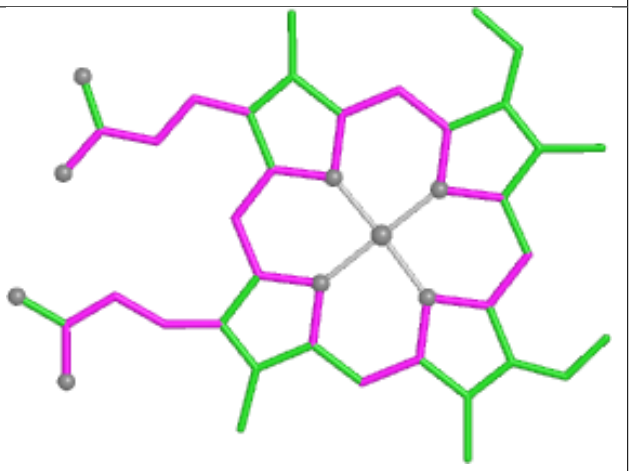
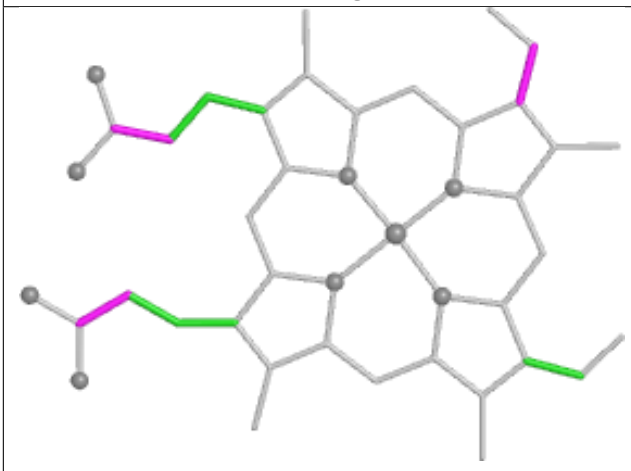


Bond angles



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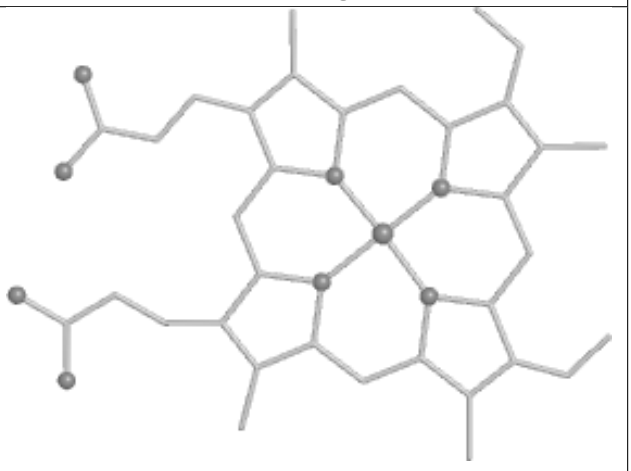
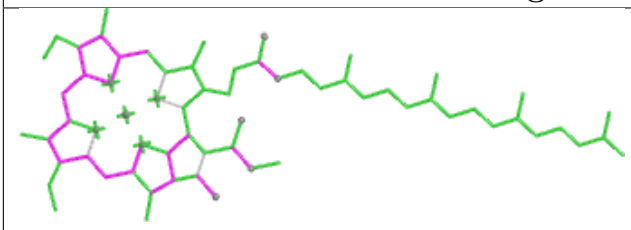
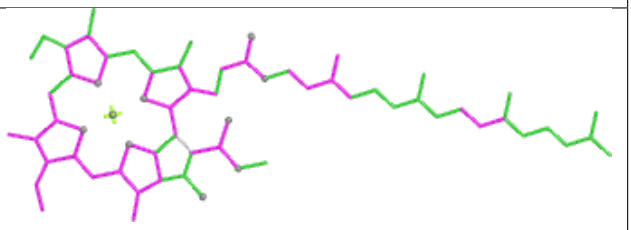


Rings

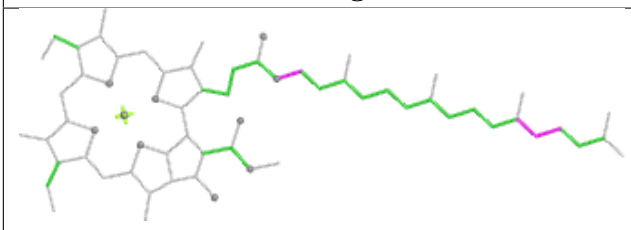
Ligand CLA b 608



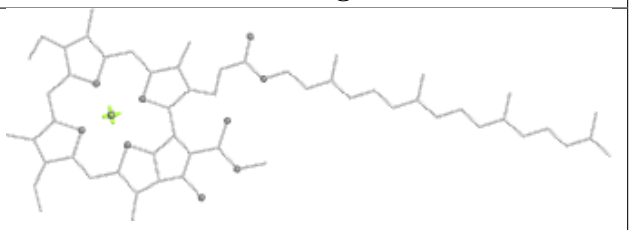
Bond lengths



Bond angles

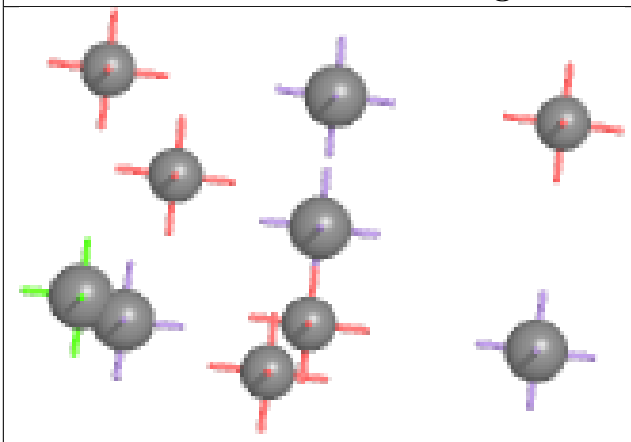


Torsions

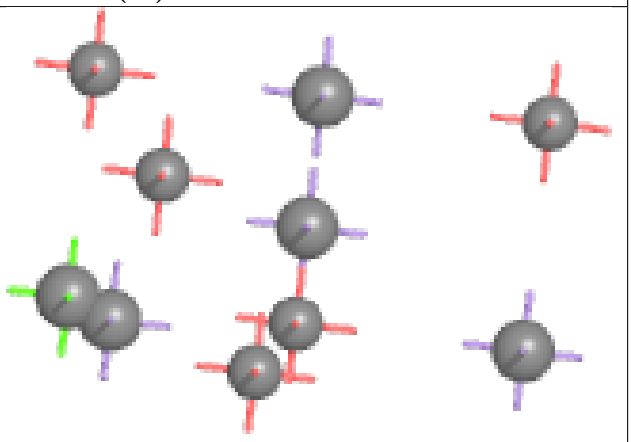


Rings

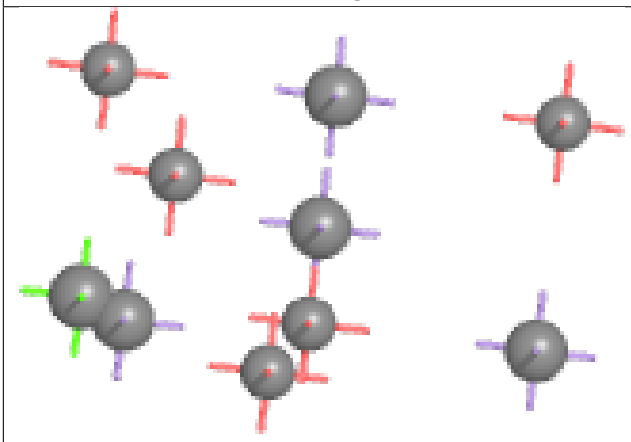
Ligand OEX a 412 (A)



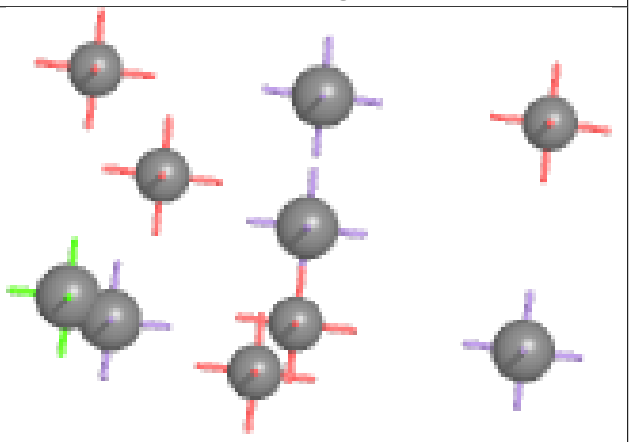
Bond lengths



Bond angles

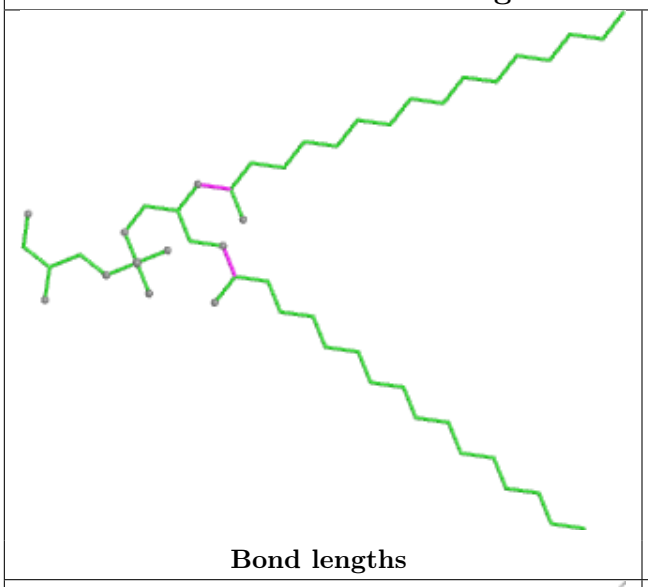


Torsions



Rings

Ligand LHG b 629 (B)



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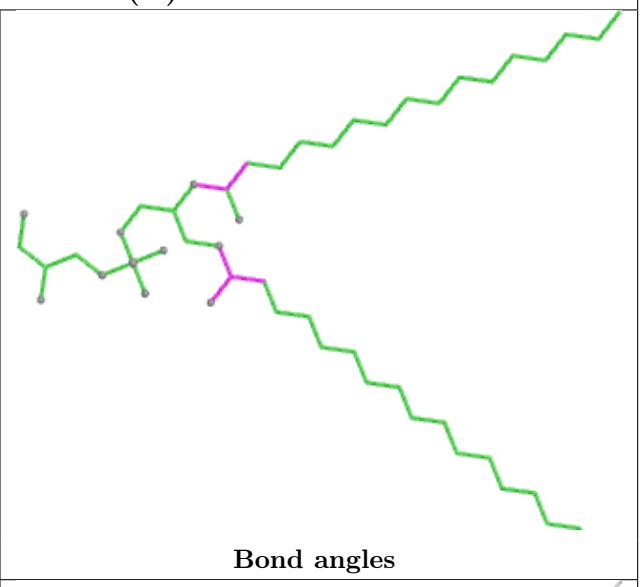
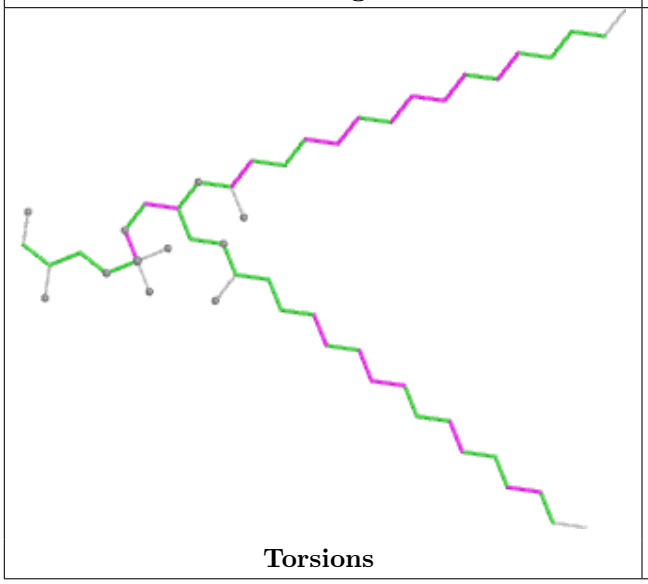


Bond angles



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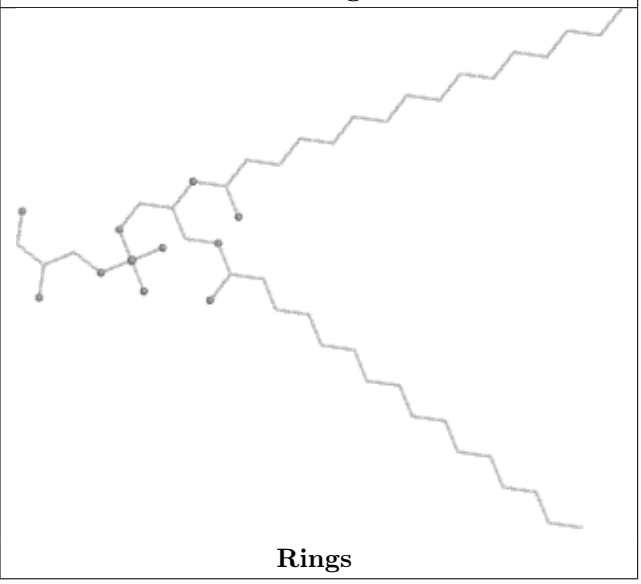
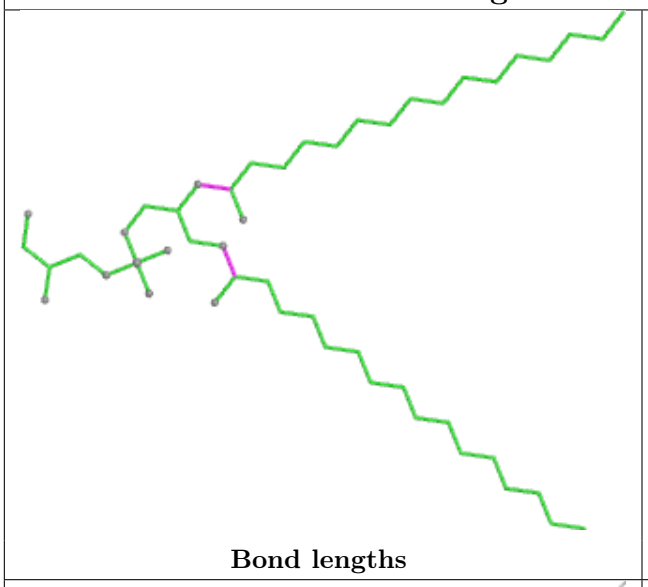


Rings

Ligand LHG A 419 (B)



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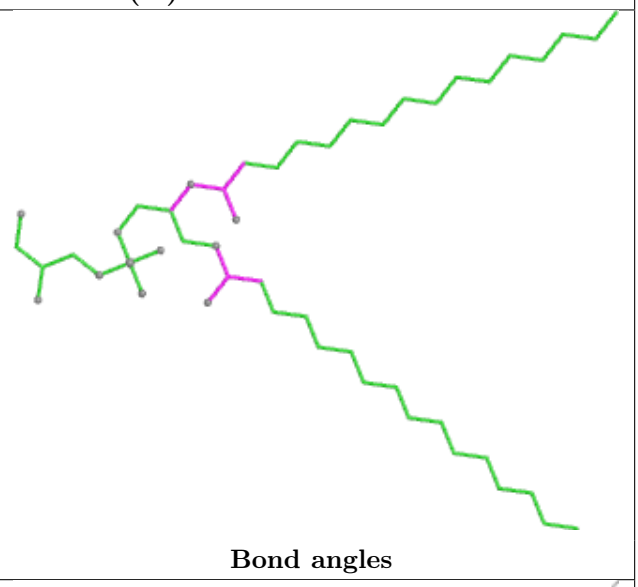
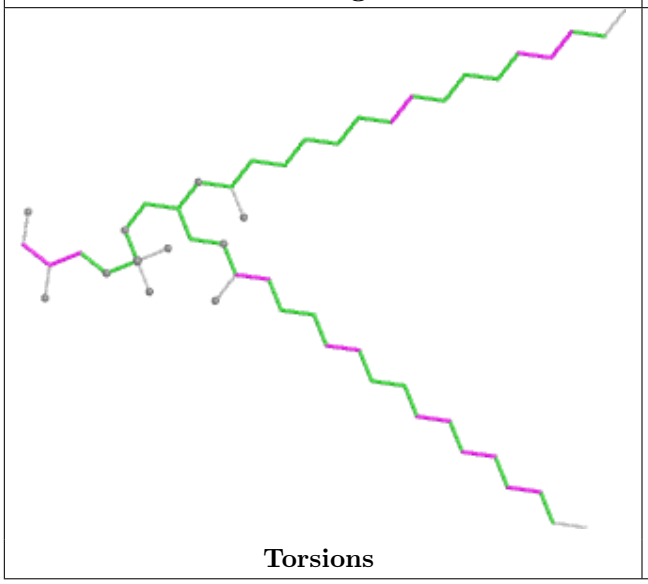
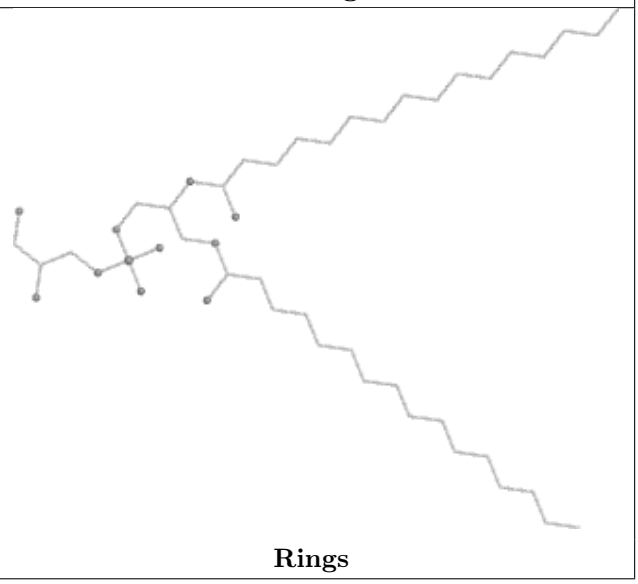


Bond angles

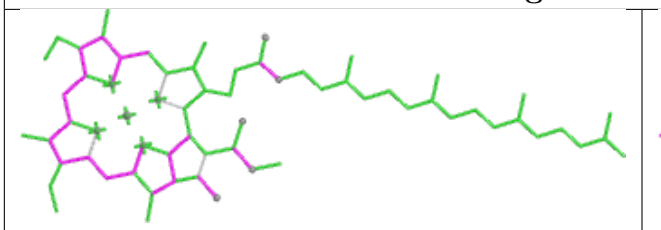


Torsions



Rings

Ligand CLA C 502



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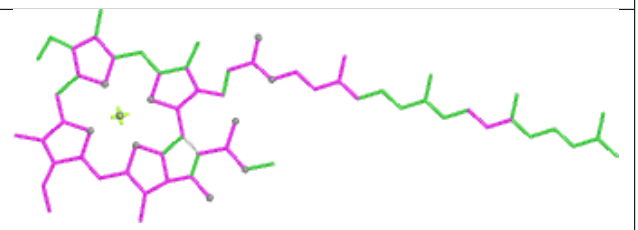
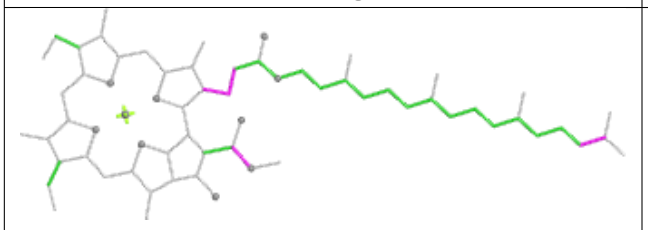


Bond angles



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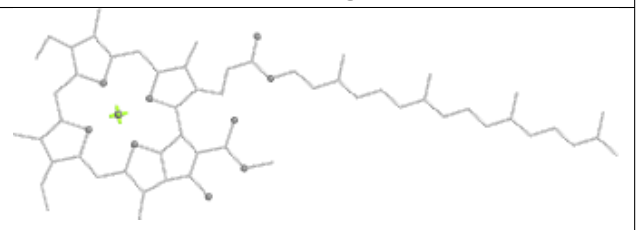
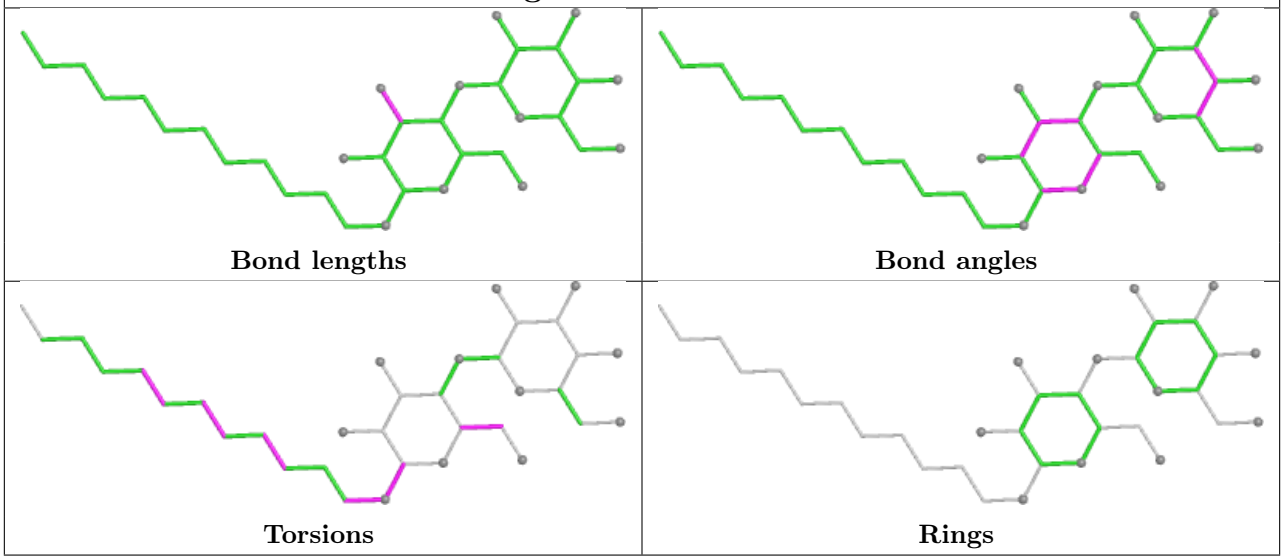
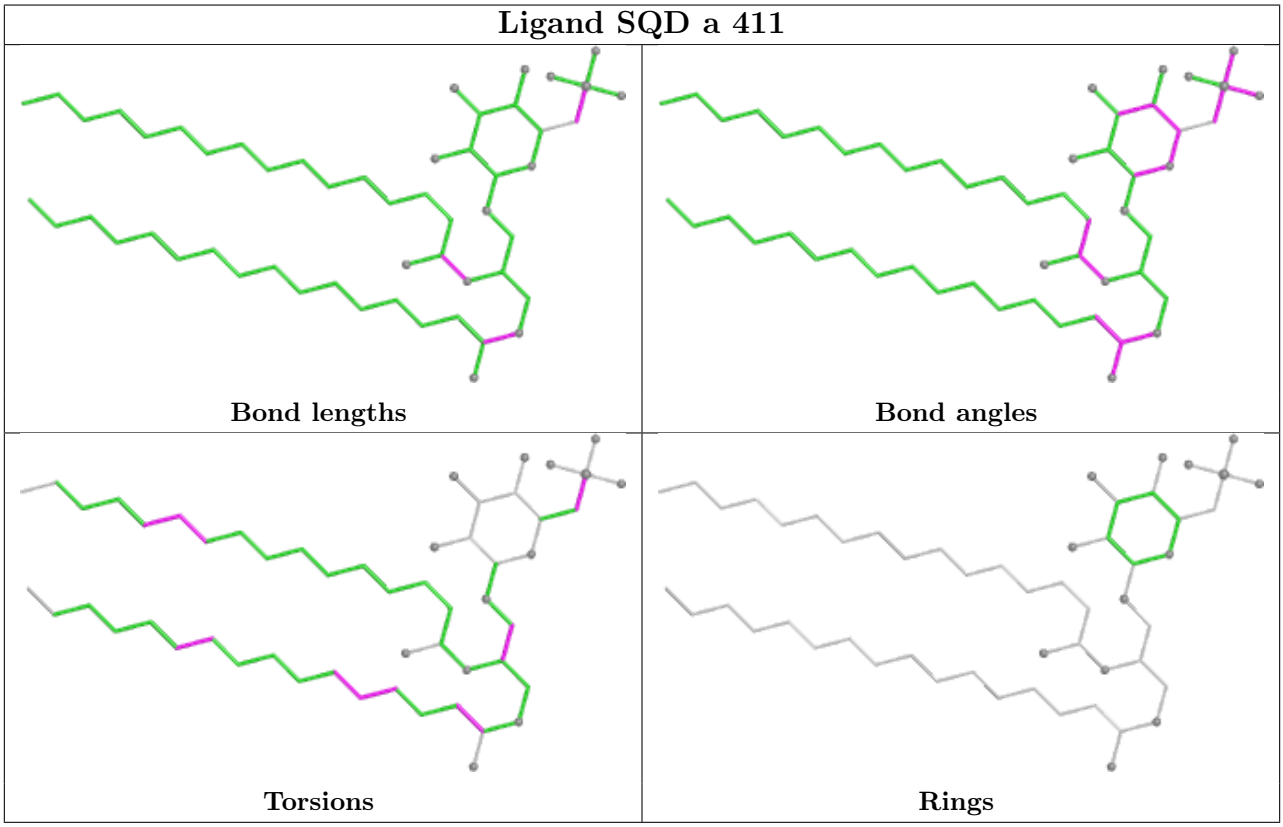


Rings

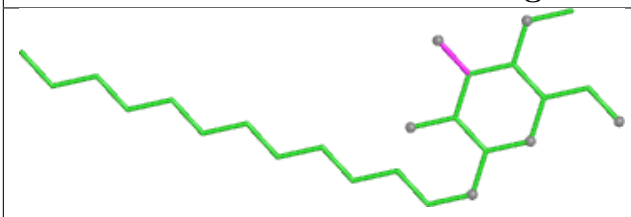
Ligand LMT F 101



Ligand SQD a 411



Ligand LMT b 627



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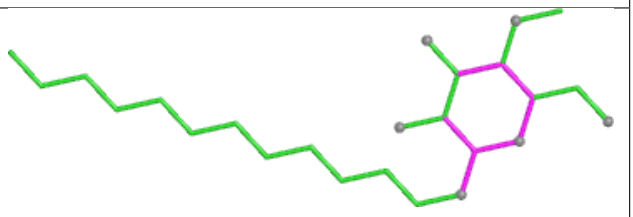
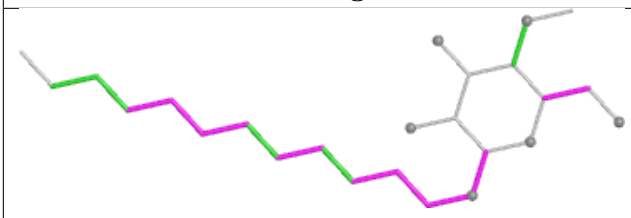


Bond angles



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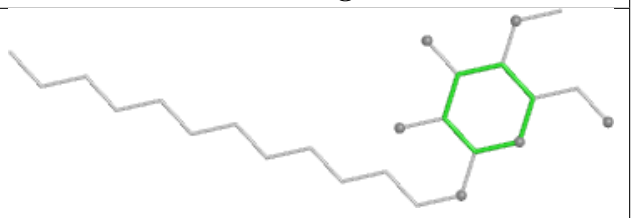
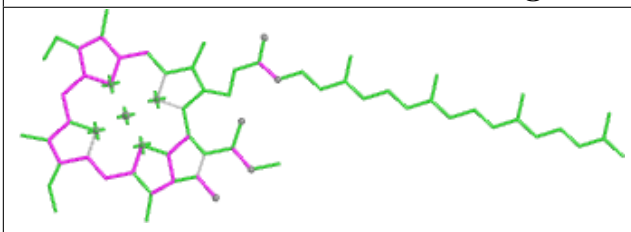


Rings

Ligand CLA C 513



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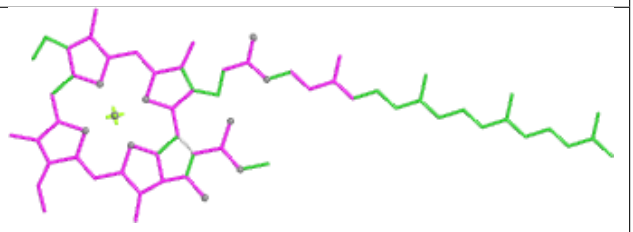
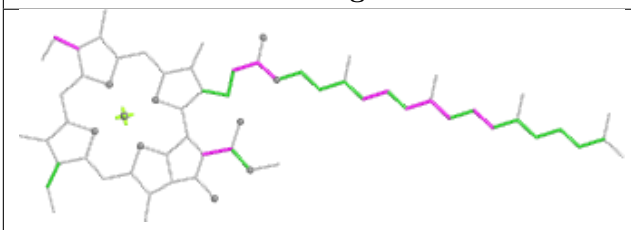


Bond angles



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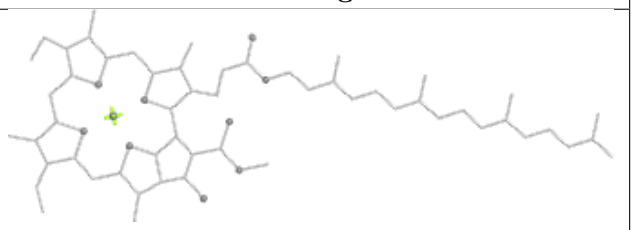
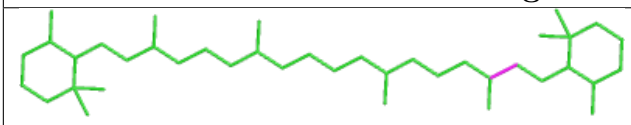


Rings

Ligand BCR B 618



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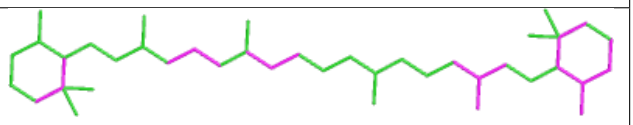
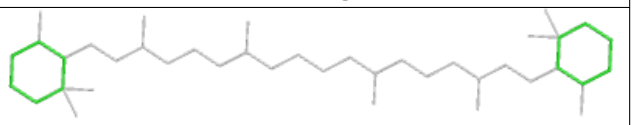


Bond angles

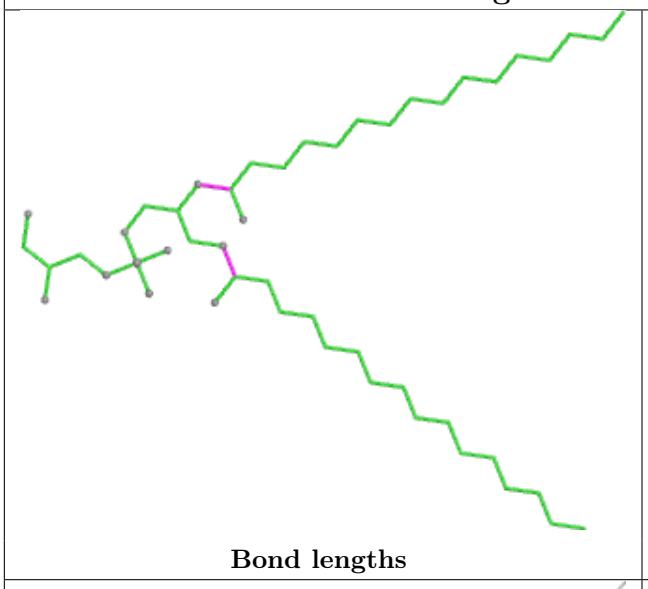


Torsions



Rings

Ligand LHG d 415 (A)



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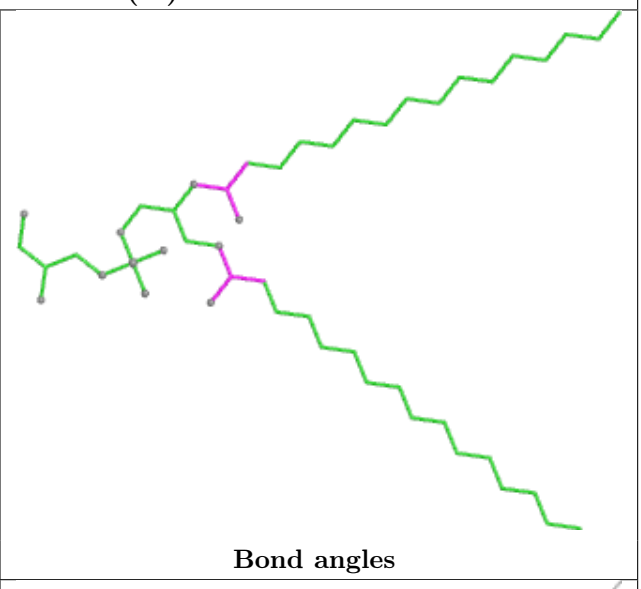
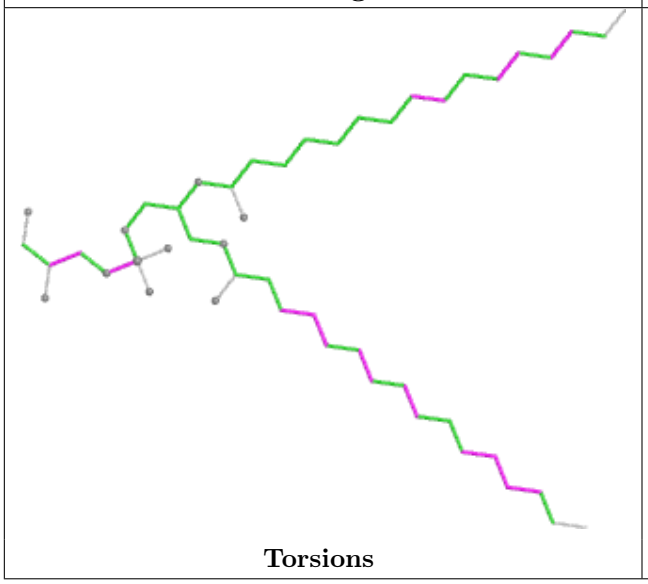


Bond angles



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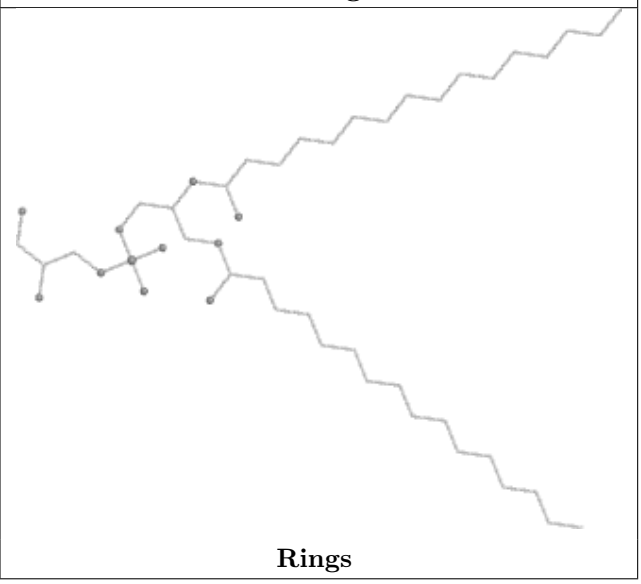
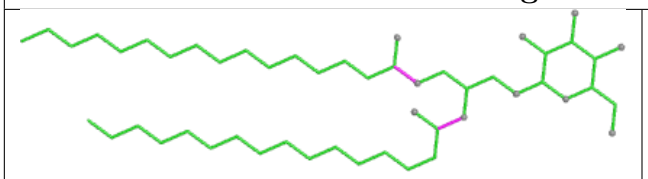


Rings

Ligand LMG C 520



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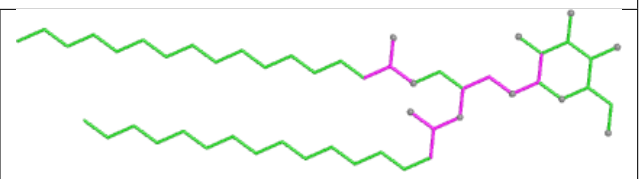
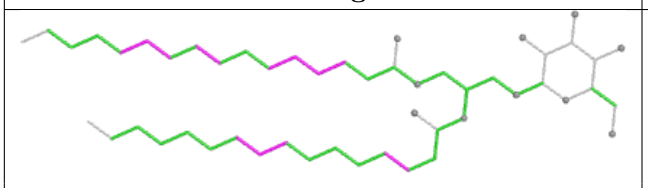


Bond angles



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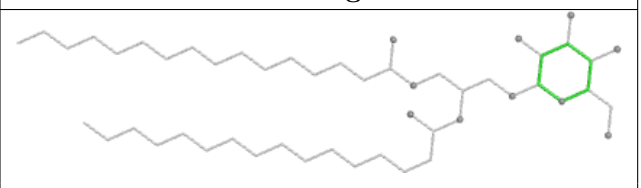
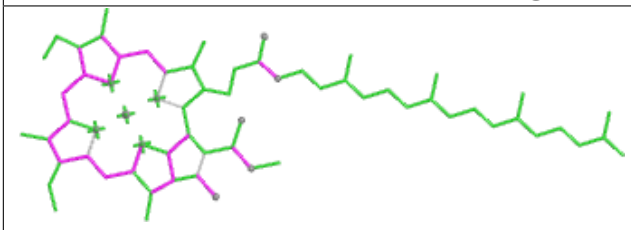


Rings

Ligand CLA b 602



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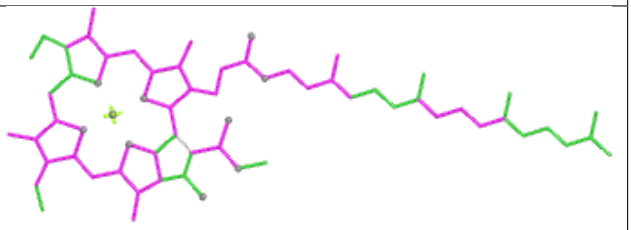
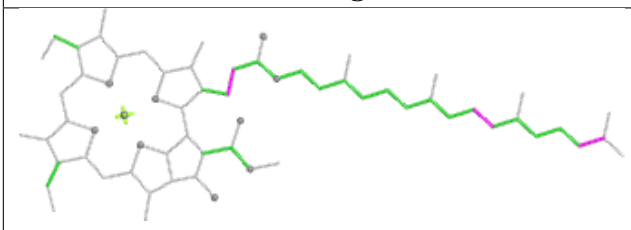


Bond angles



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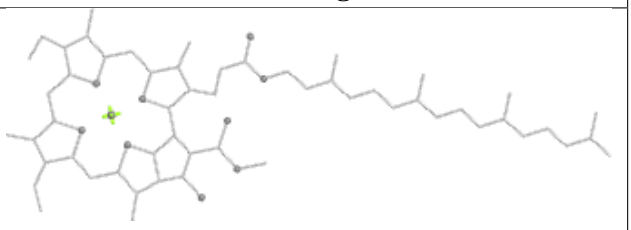
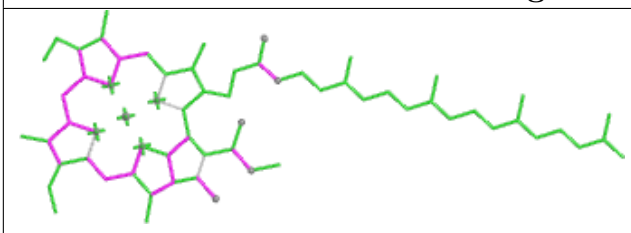


Rings

Ligand CLA b 609



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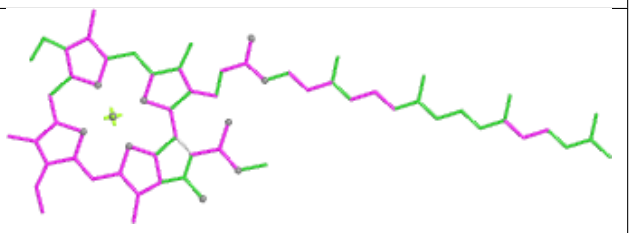
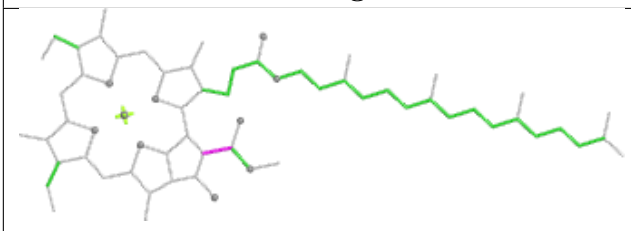


Bond angles



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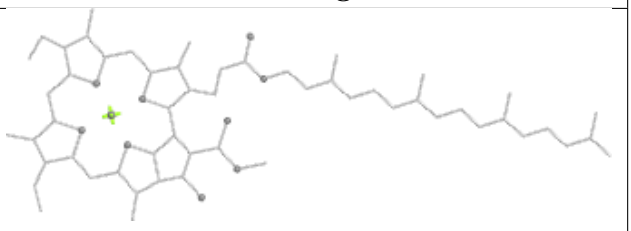
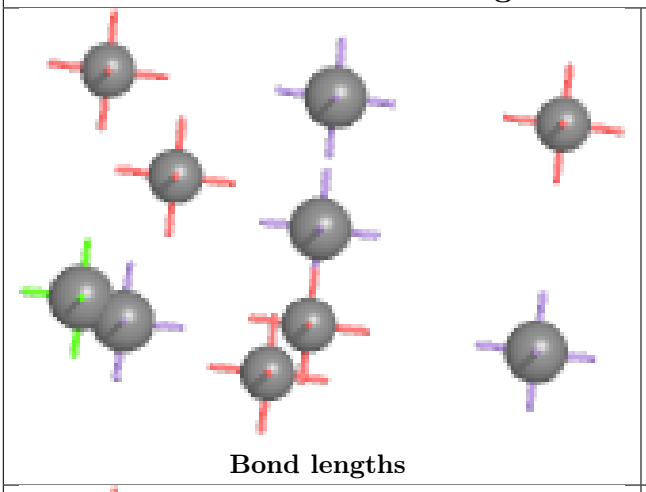


Rings

Ligand OEX a 412 (B)



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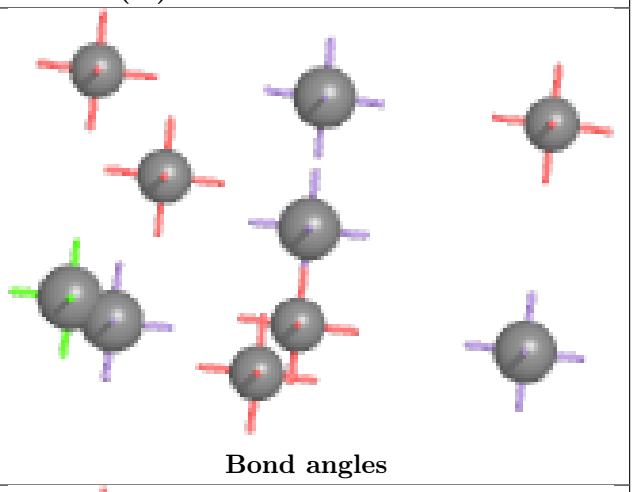
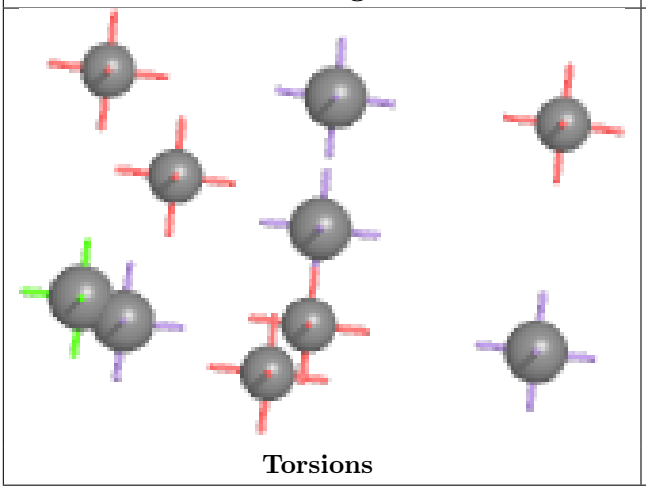
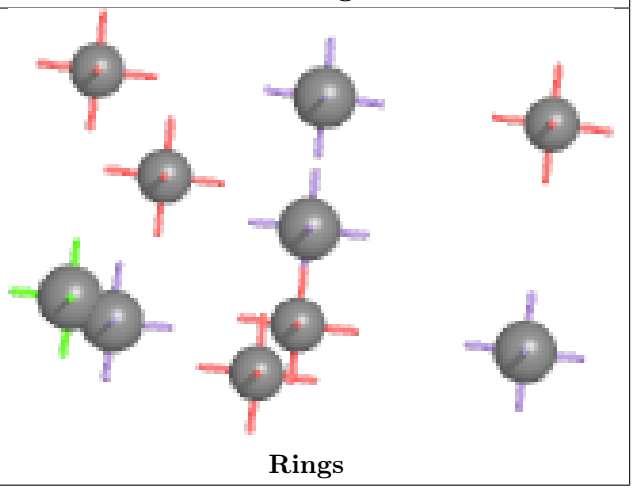


Bond angles

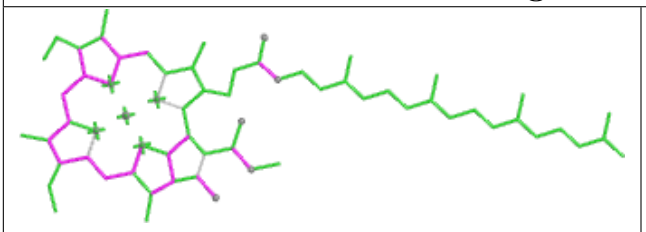


Torsions



Rings

Ligand CLA d 405



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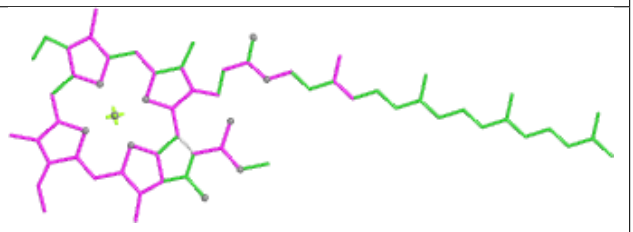
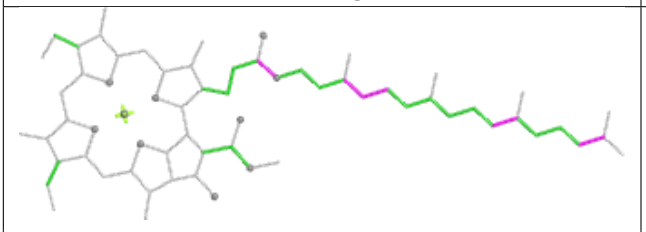


Bond angles



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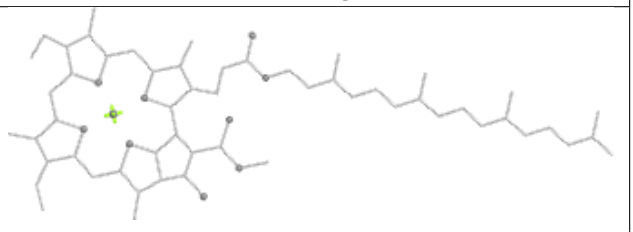
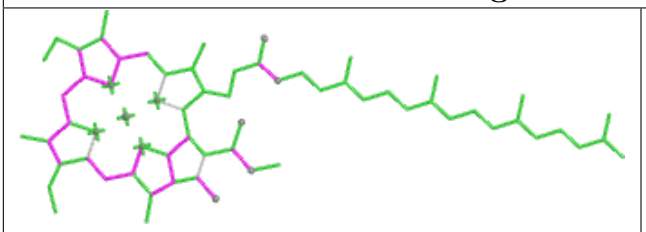
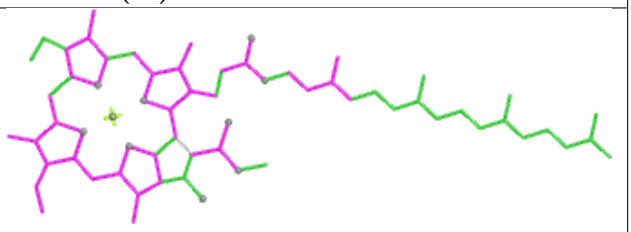


Rings

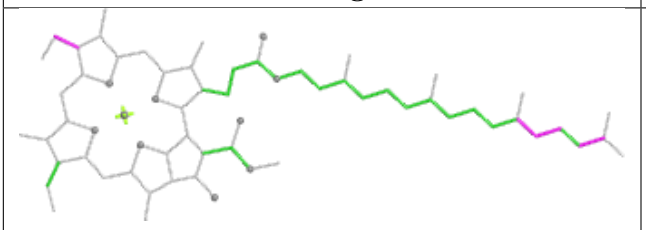
Ligand CLA A 406 (A)



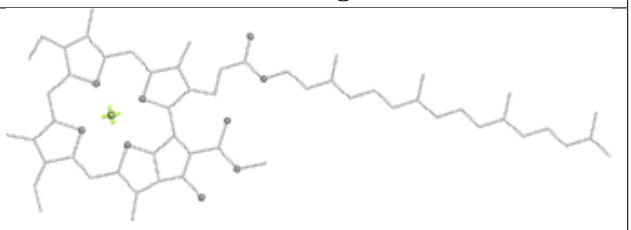
Bond lengths



Bond angles

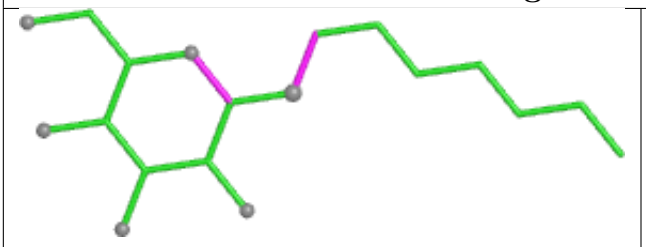


Torsions

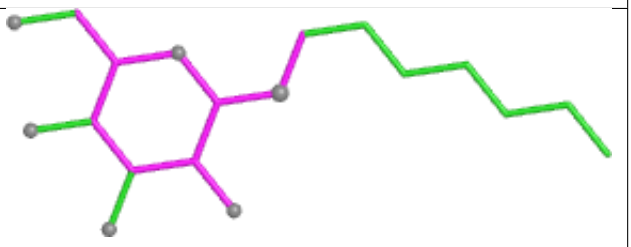


Rings

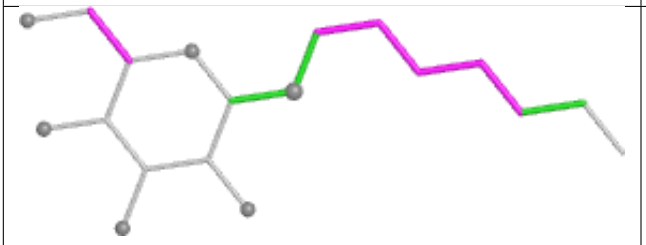
Ligand HTG b 622



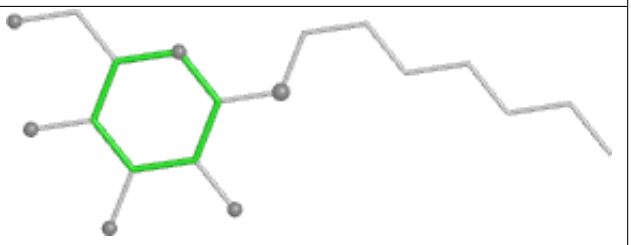
Bond lengths



Bond angles

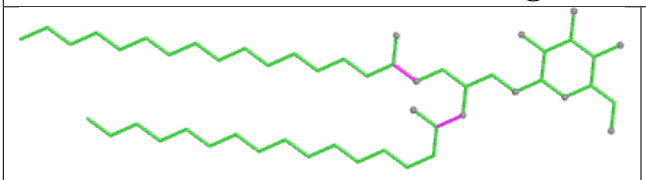


Torsions



Rings

Ligand LMG c 520



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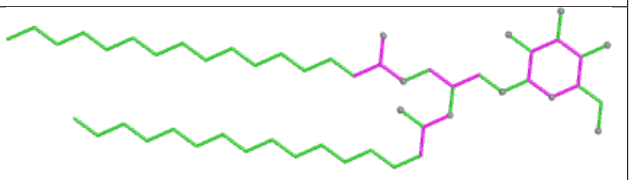
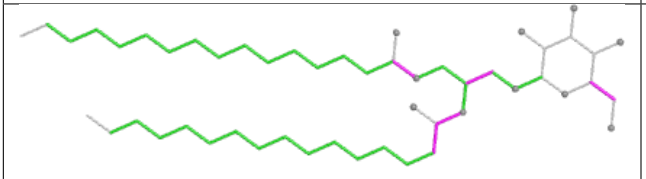


Bond angles



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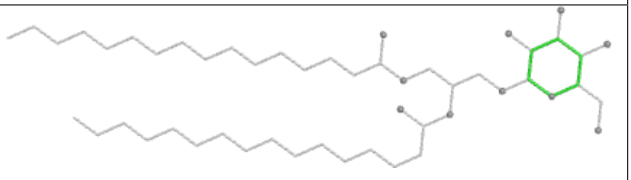
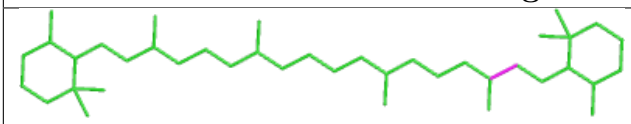


Rings

Ligand BCR A 409



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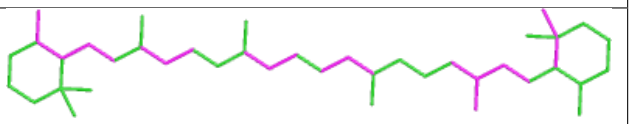
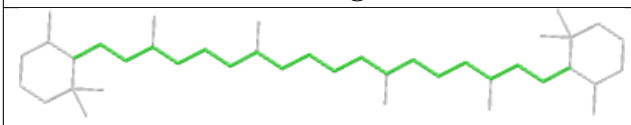


Bond angles



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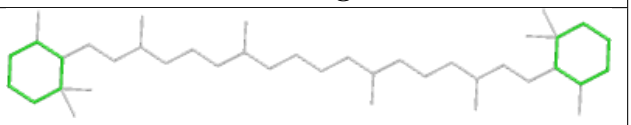
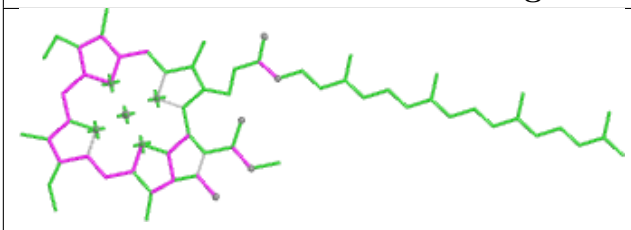


Rings

Ligand CLA B 603



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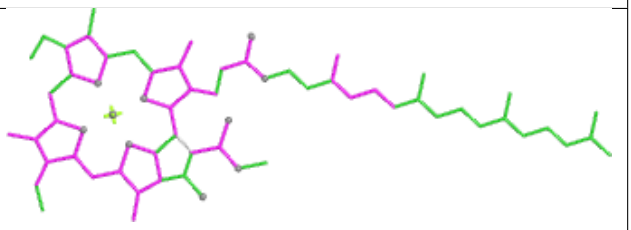
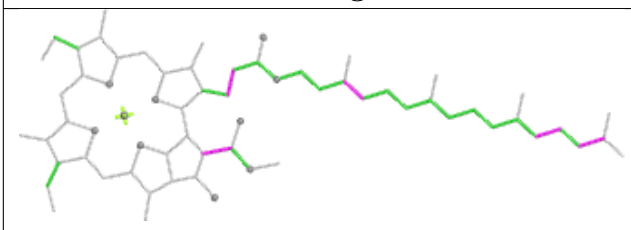


Bond angles



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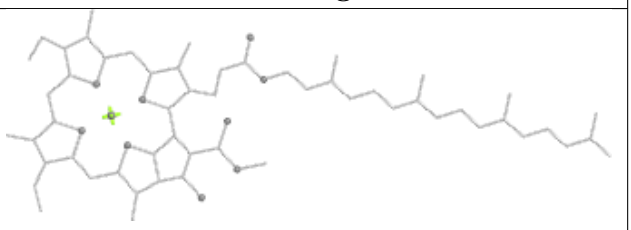
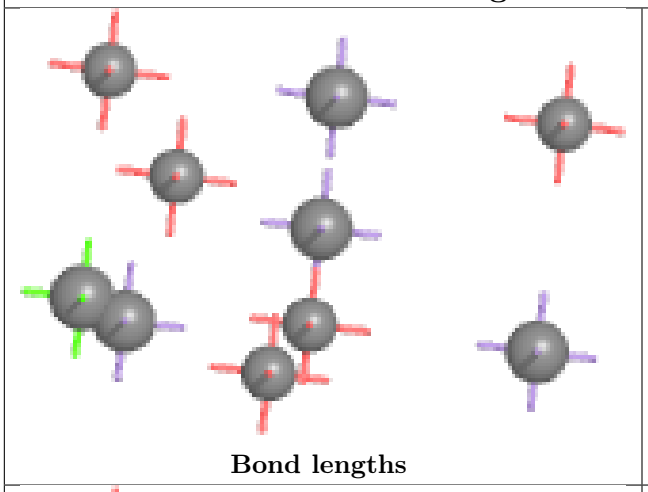


Rings

Ligand OEX A 413 (A)



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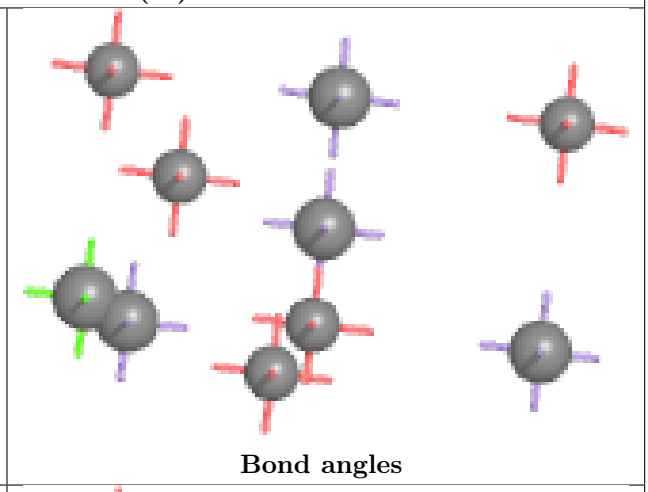

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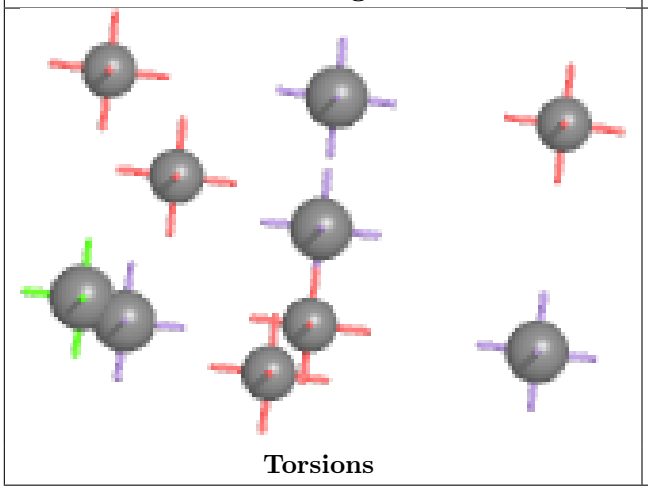

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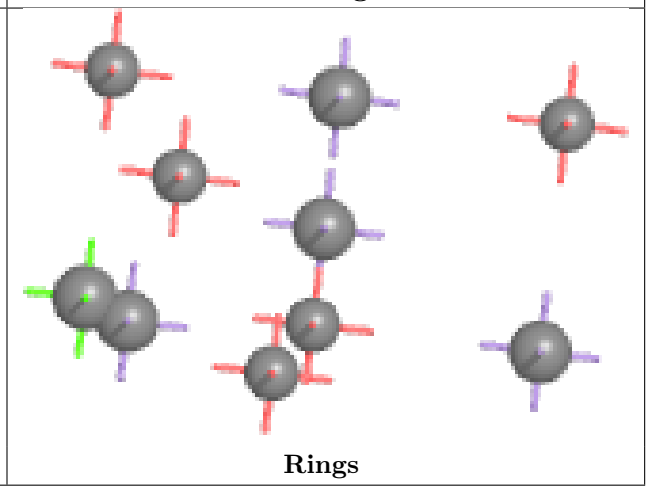
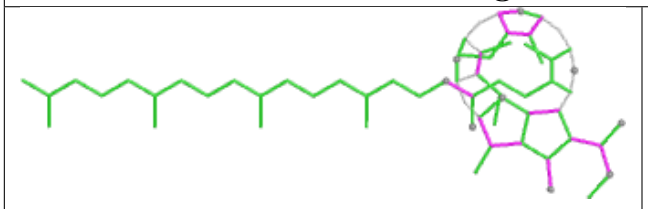


Rings

Ligand PHO a 406 (A)



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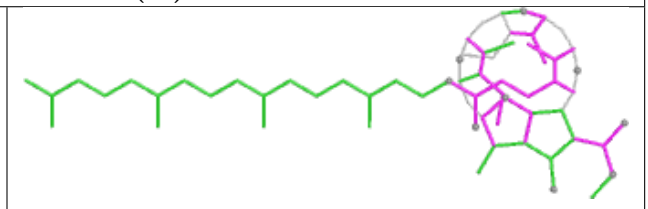
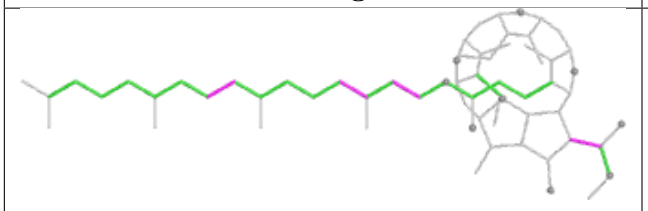


Bond angles



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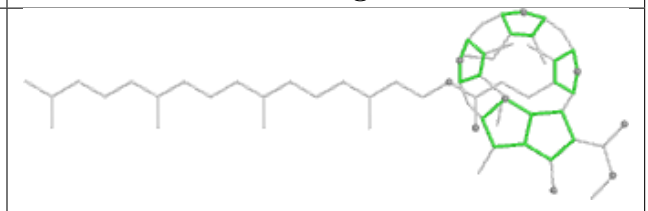
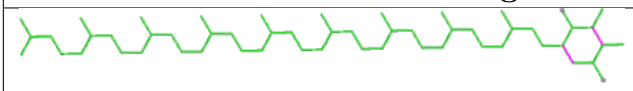


Rings

Ligand PL9 a 413 (A)



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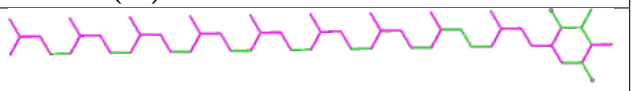
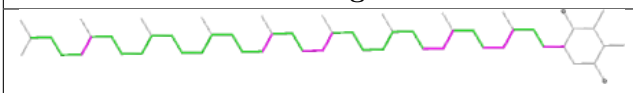


Bond angles



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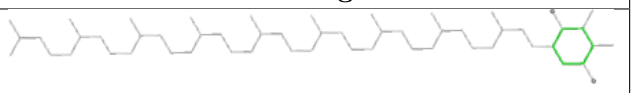
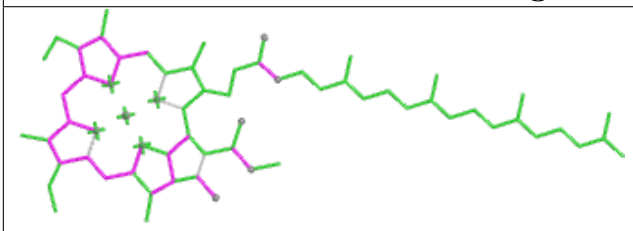


Rings

Ligand CLA c 508



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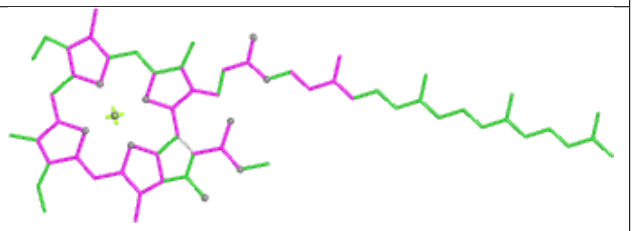
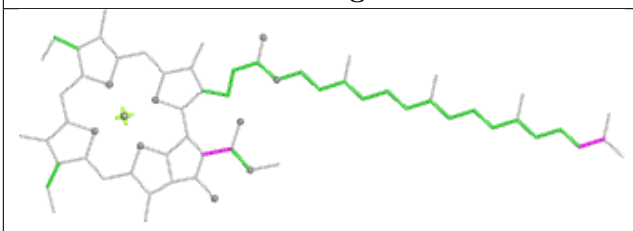


Bond angles



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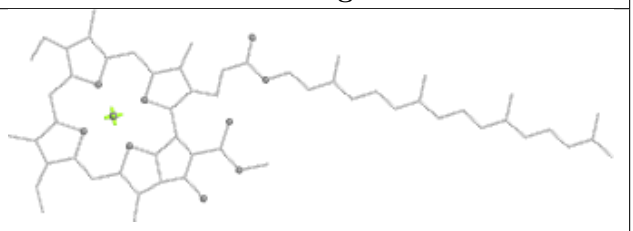
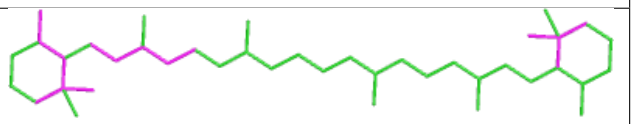


Rings

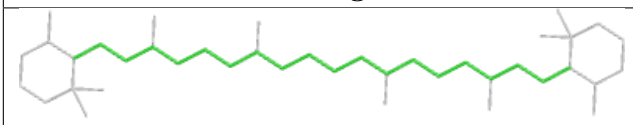
Ligand BCR C 516



Bond lengths



Bond angles



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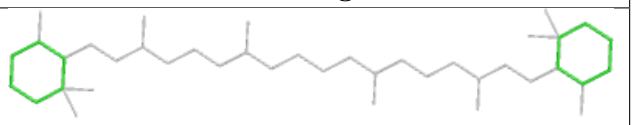
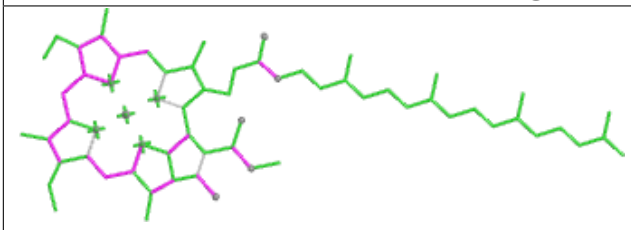


Rings

Ligand CLA b 604



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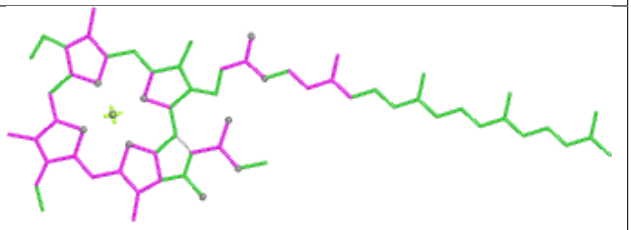
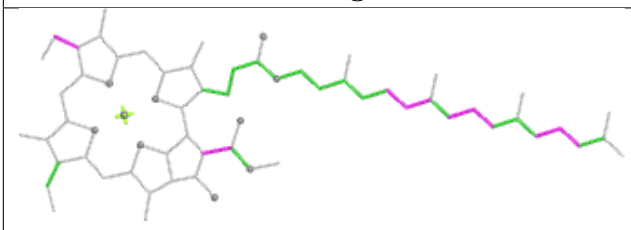


Bond angles



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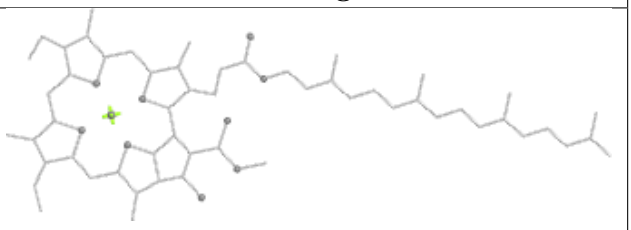
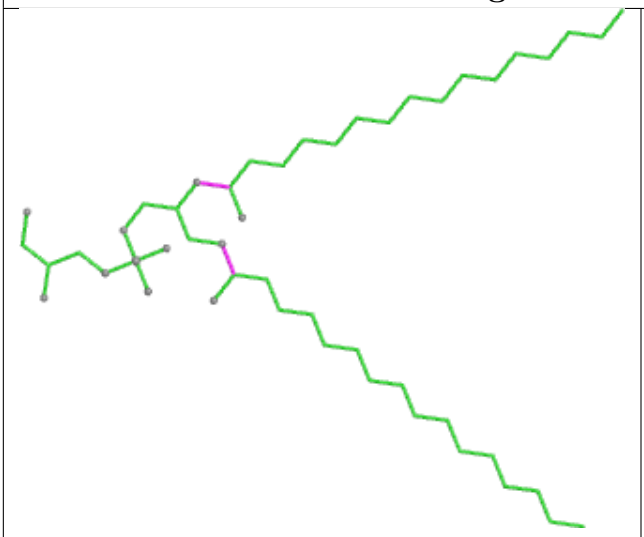


Rings

Ligand LHG D 407 (A)



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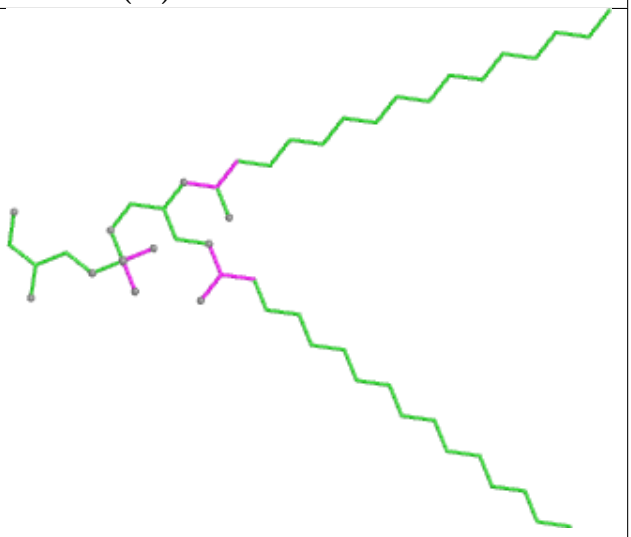
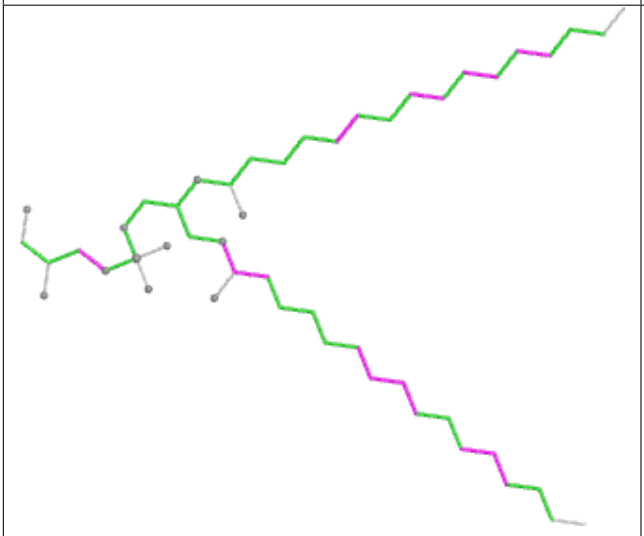


Bond angles



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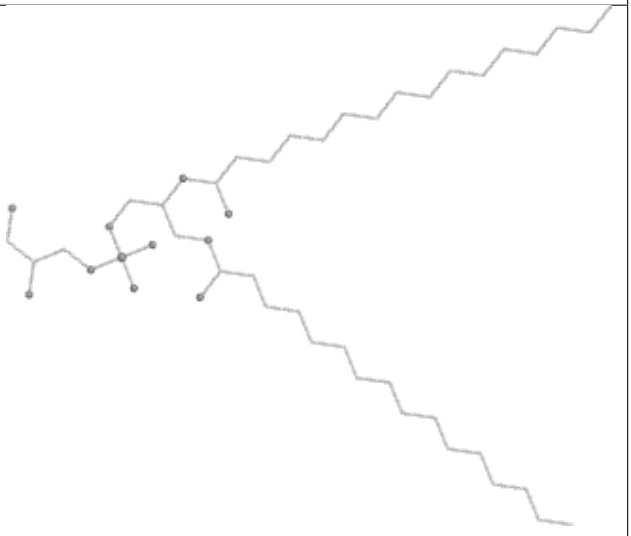
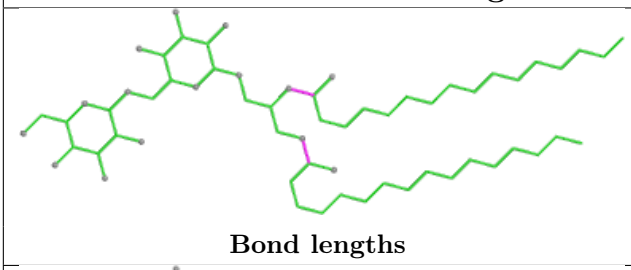


Rings

Ligand DGD C 517 (B)



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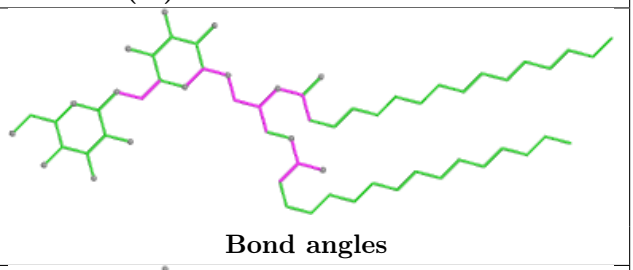
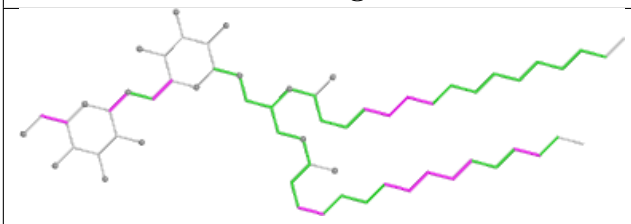


Bond angles



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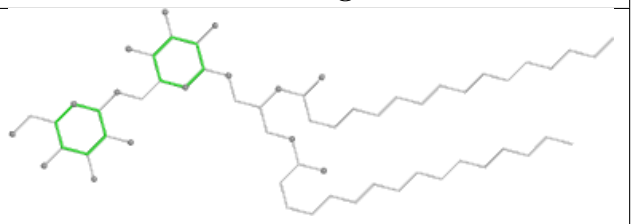
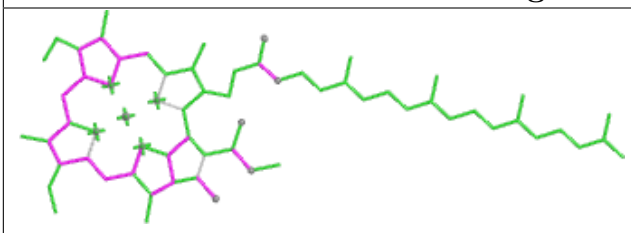


Rings

Ligand CLA b 610



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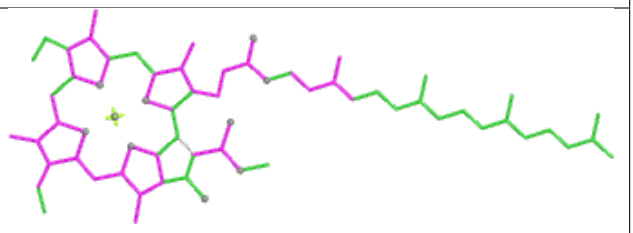
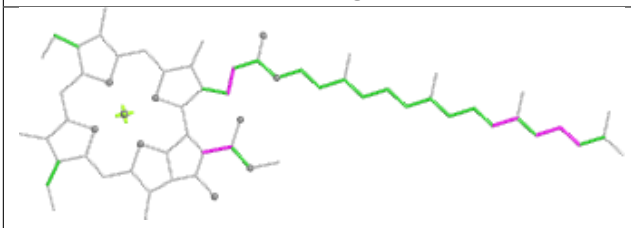


Bond angles



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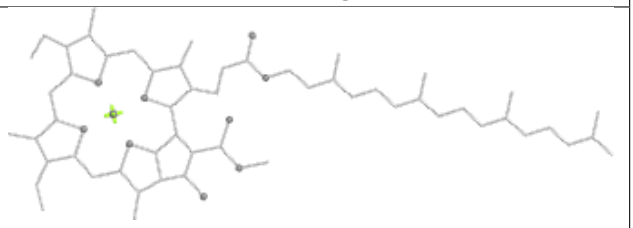
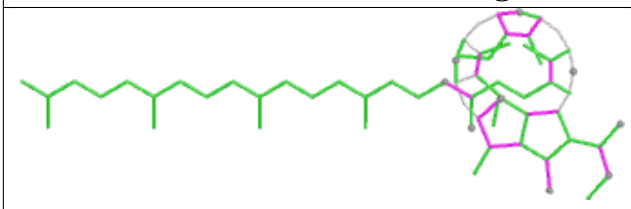
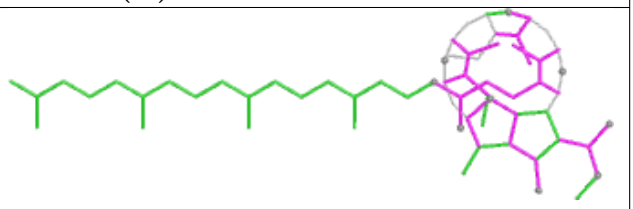


Rings

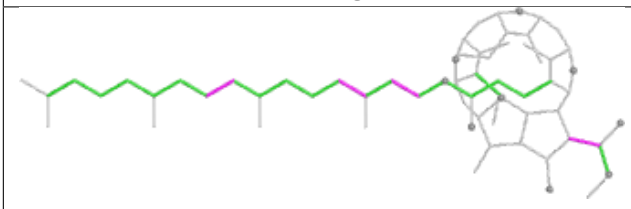
Ligand PHO a 406 (B)



Bond lengths



Bond angles



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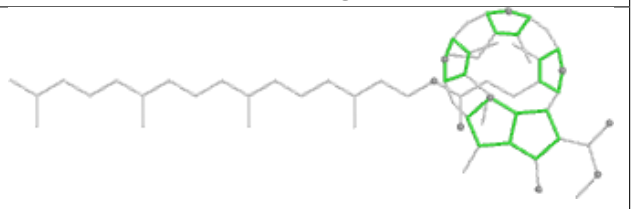
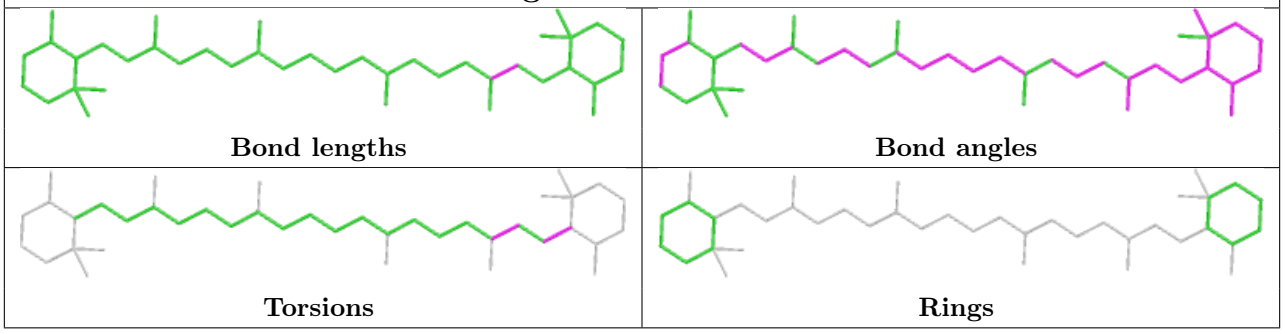
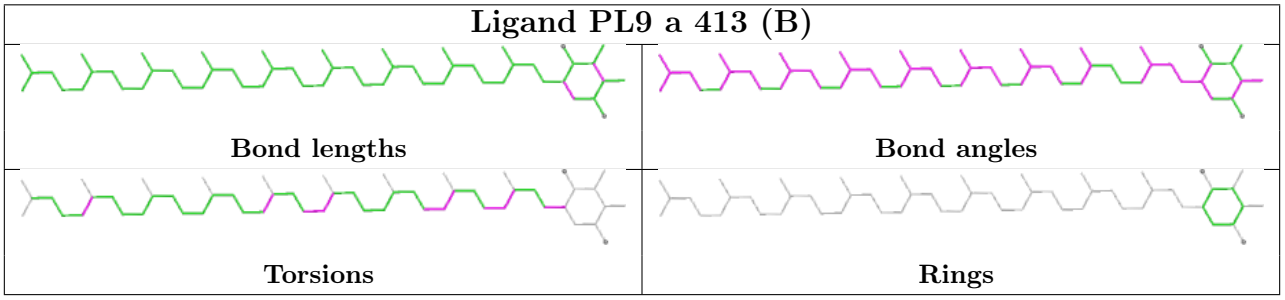


Rings

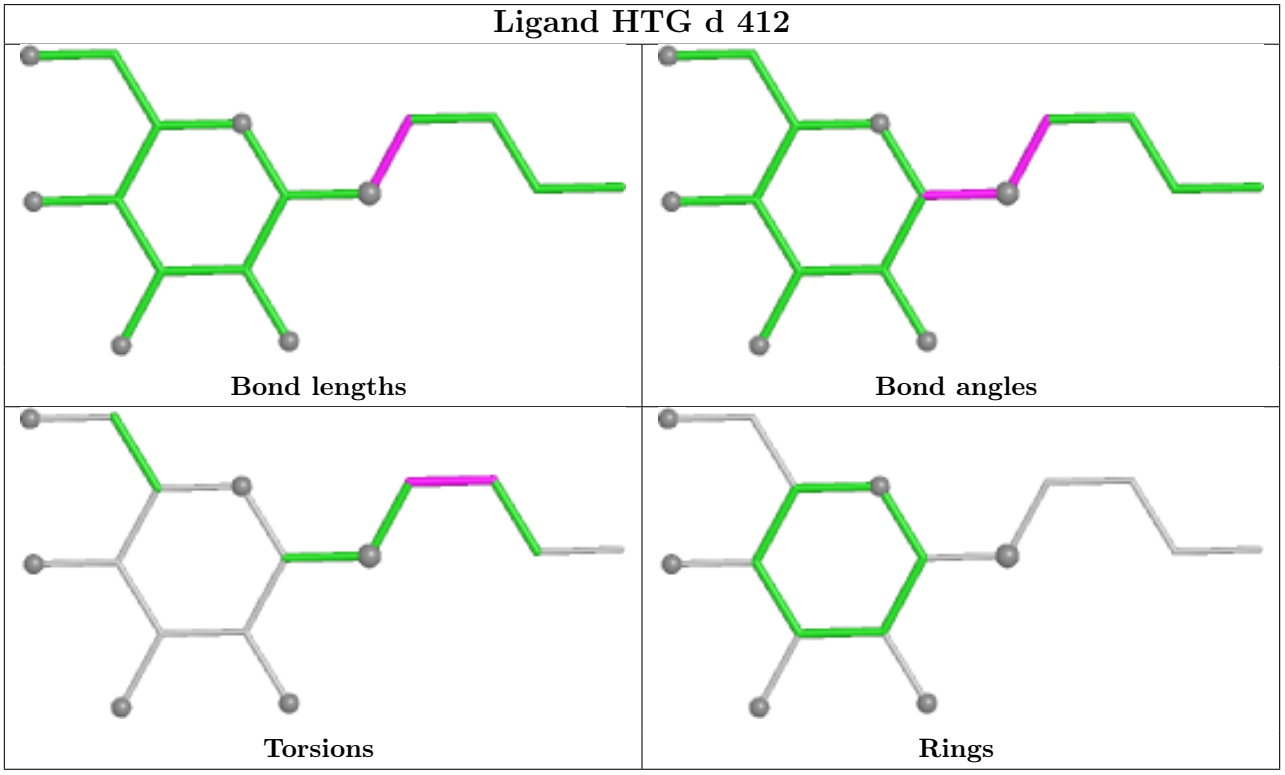
Ligand BCR D 404



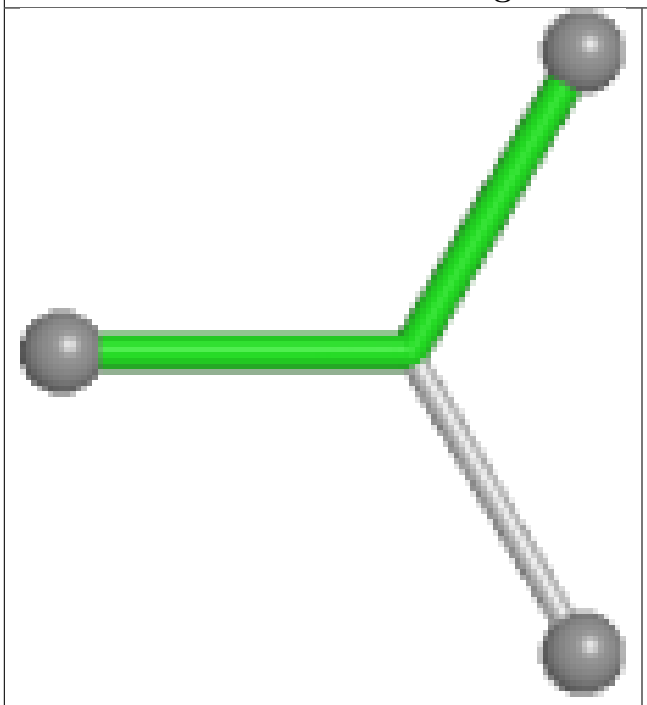
Ligand PL9 a 413 (B)



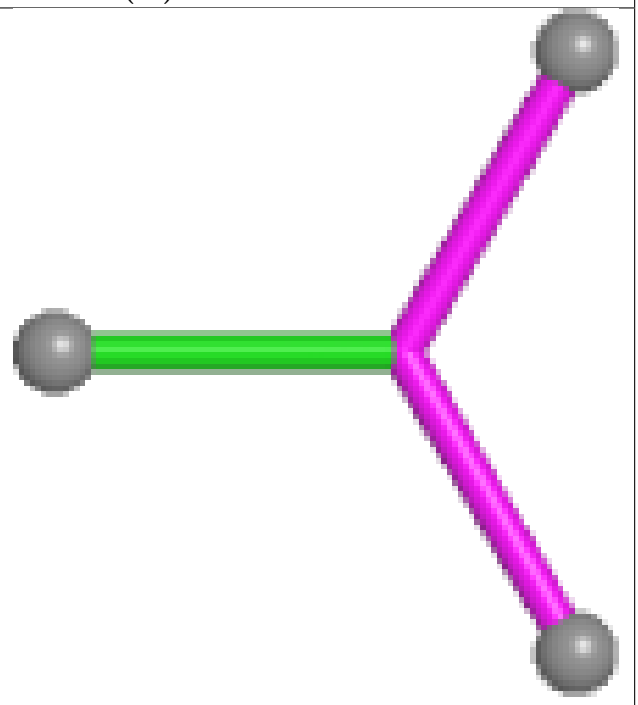
Ligand HTG d 412



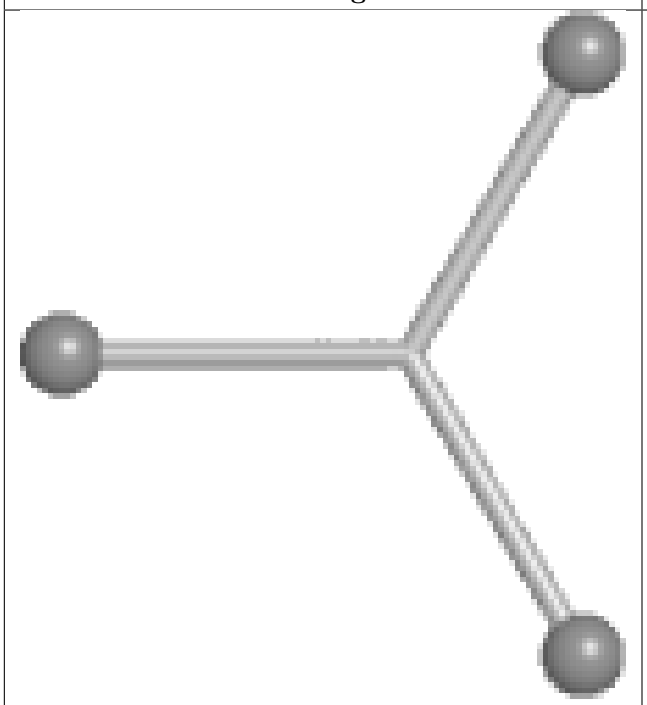
Ligand BCT d 401 (A)



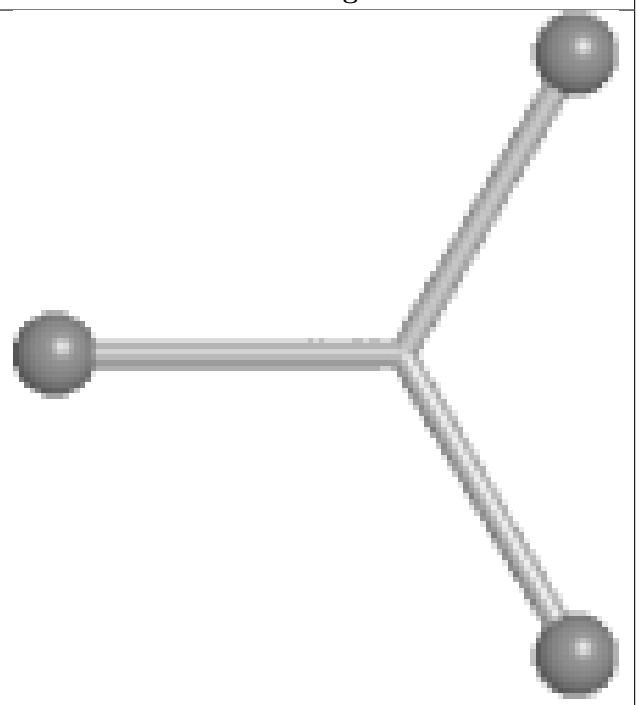
Bond lengths



Bond angles

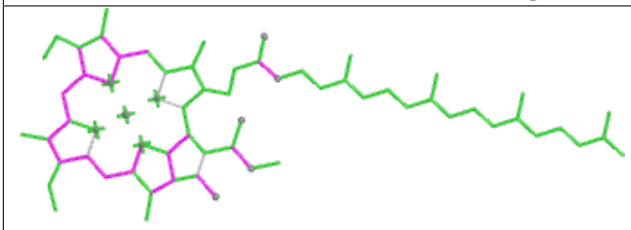


Torsions



Rings

Ligand CLA C 508



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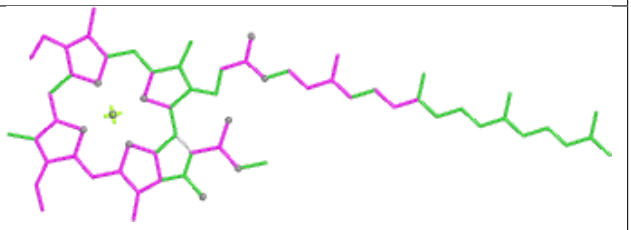
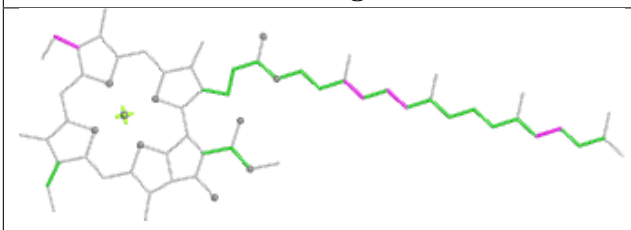


Bond angles



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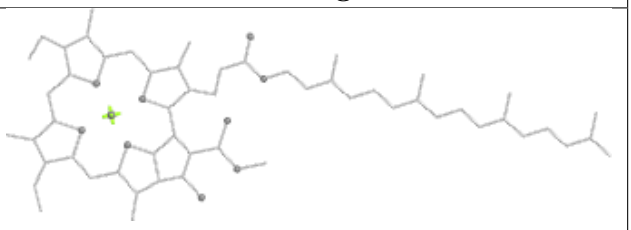
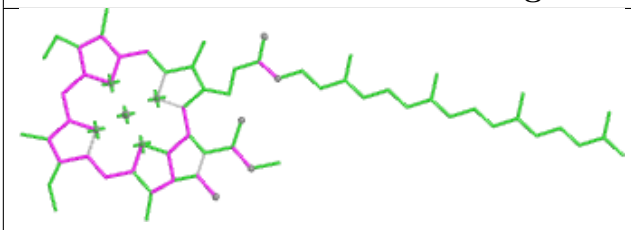
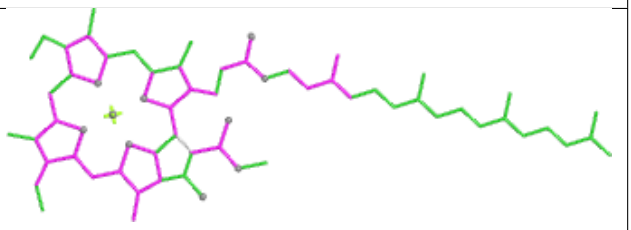


Rings

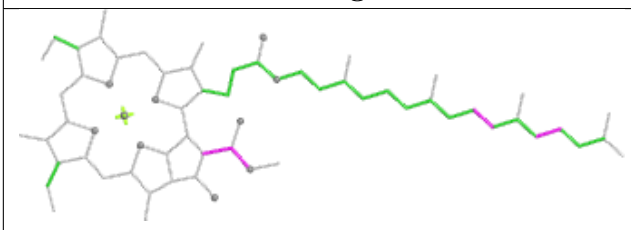
Ligand CLA C 509



Bond lengths



Bond angles



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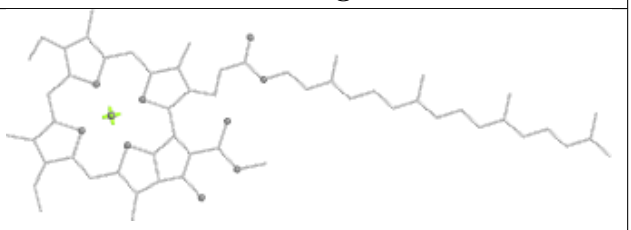
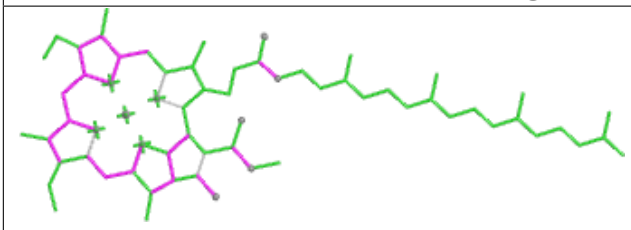


Rings

Ligand CLA B 616



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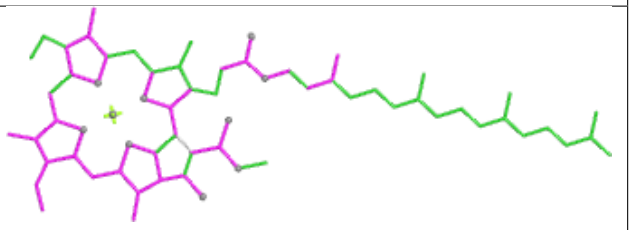
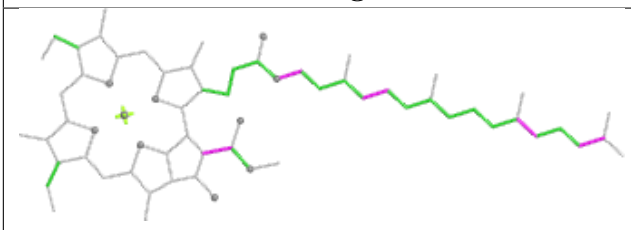
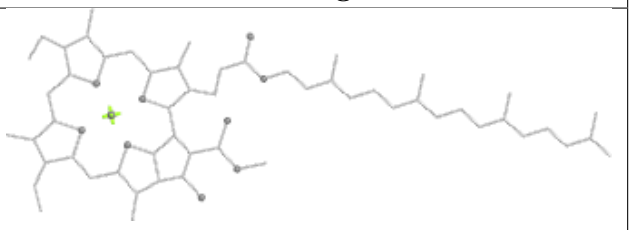


Bond angles

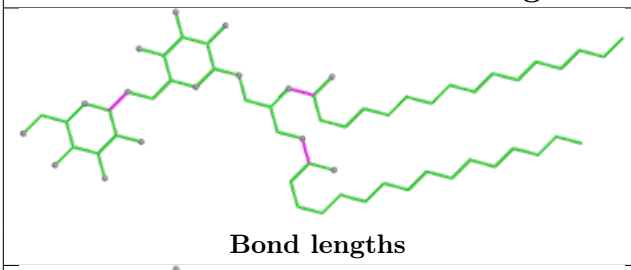


Torsions



Rings

Ligand DGD h 102



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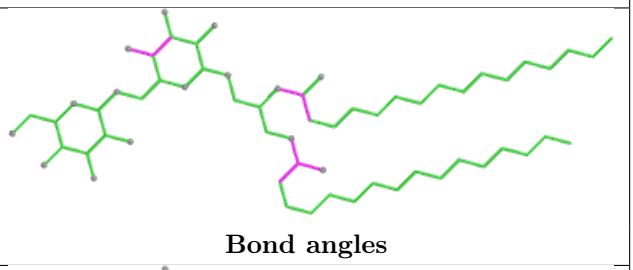
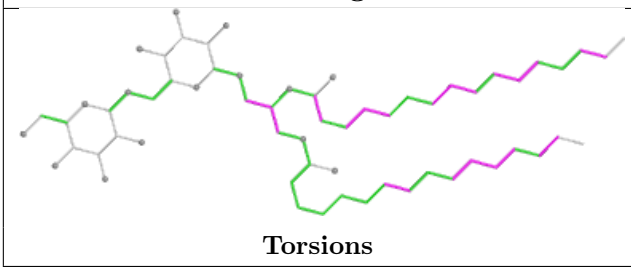


Bond angles



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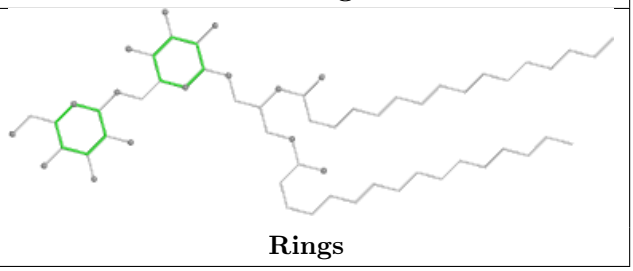
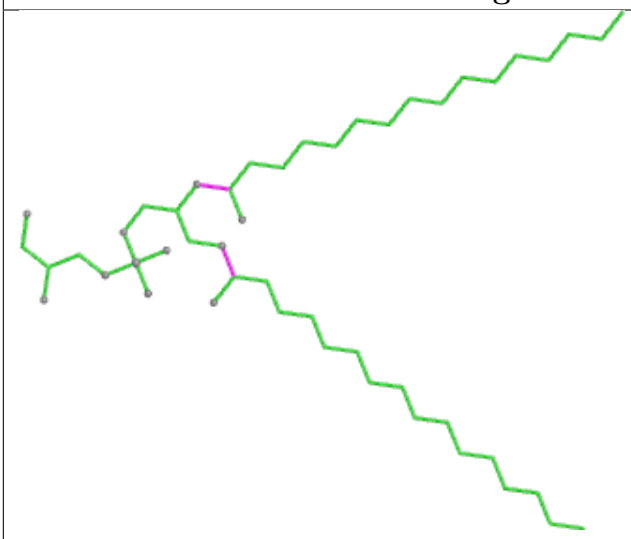


Rings

Ligand LHG d 408 (B)



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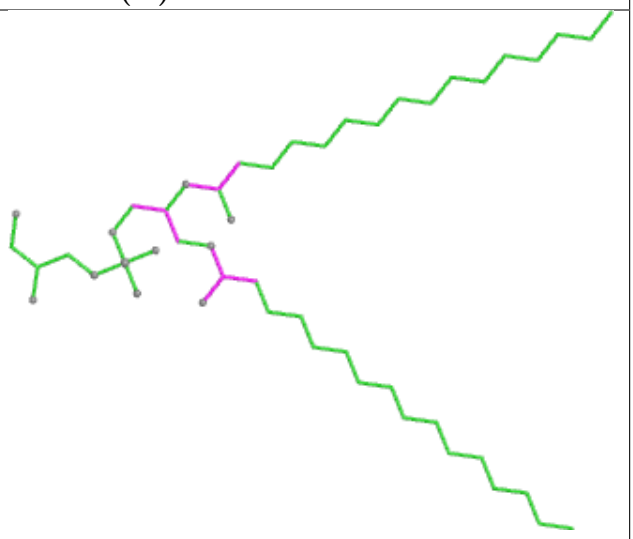
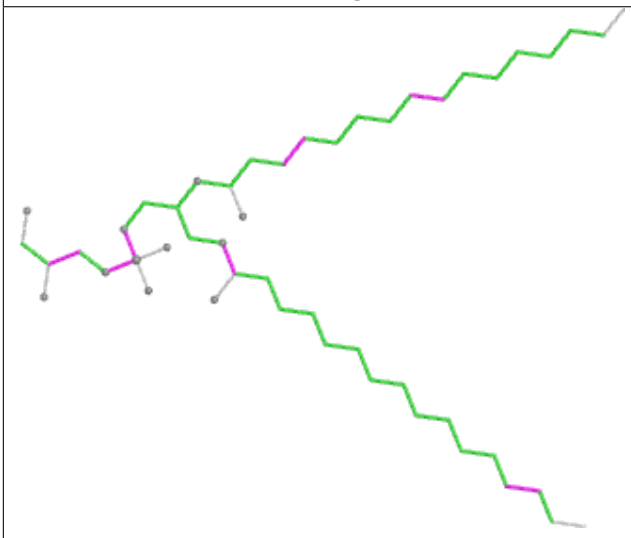


Bond angles



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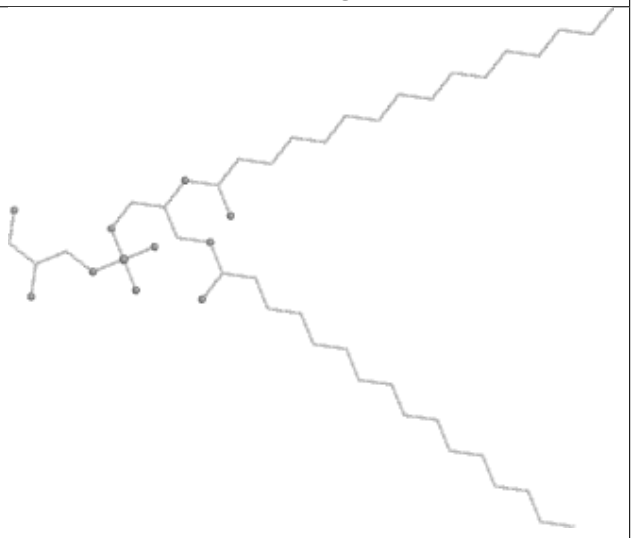
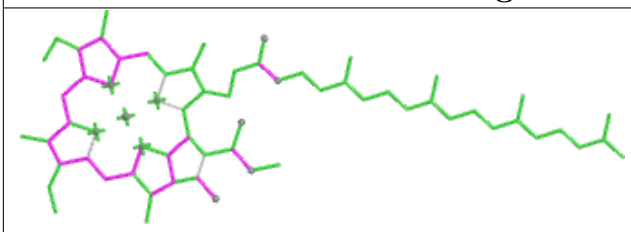


Rings

Ligand CLA a 405 (B)



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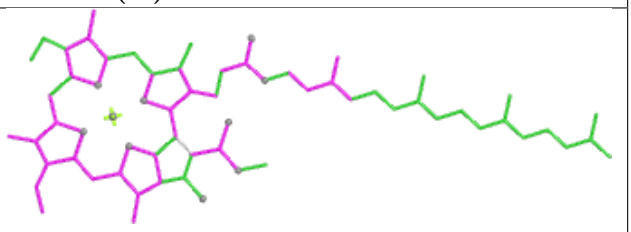
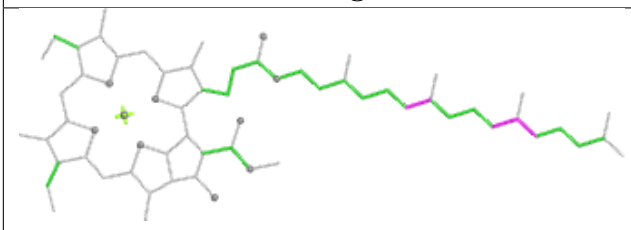
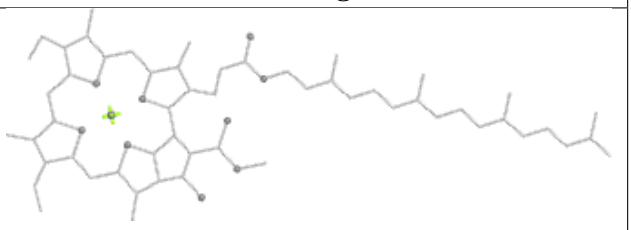


Bond angles

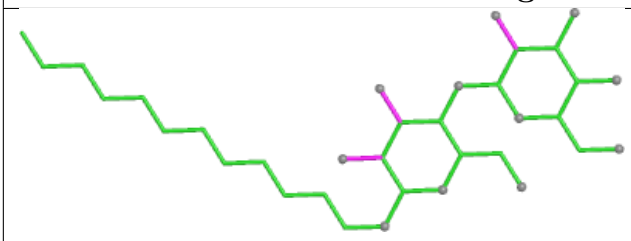


Torsions



Rings

Ligand LMT M 101



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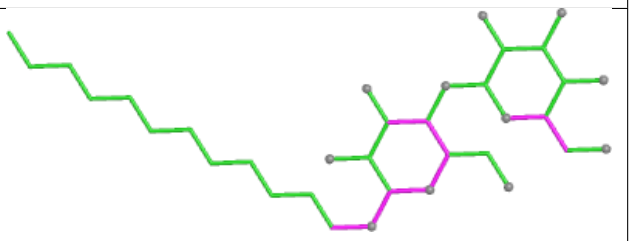
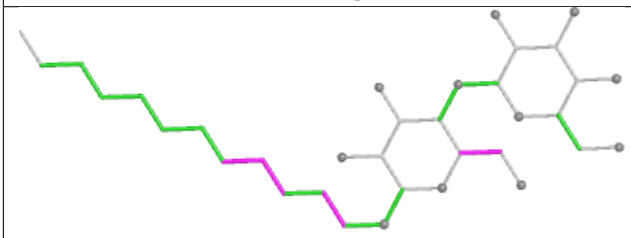


Bond angles



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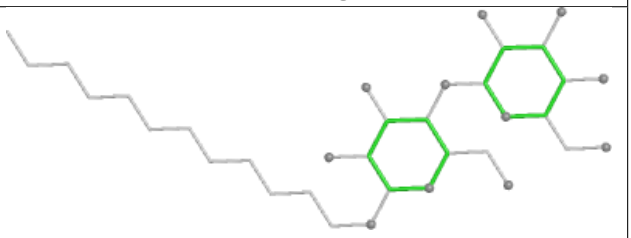
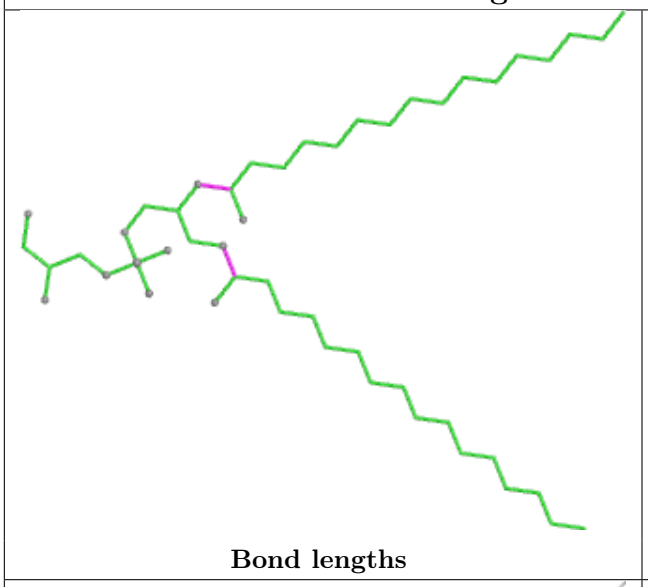


Rings

Ligand LHG D 407 (B)



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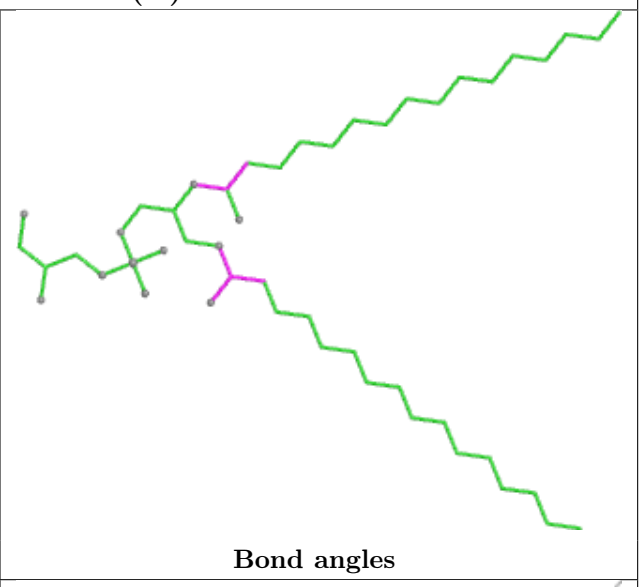
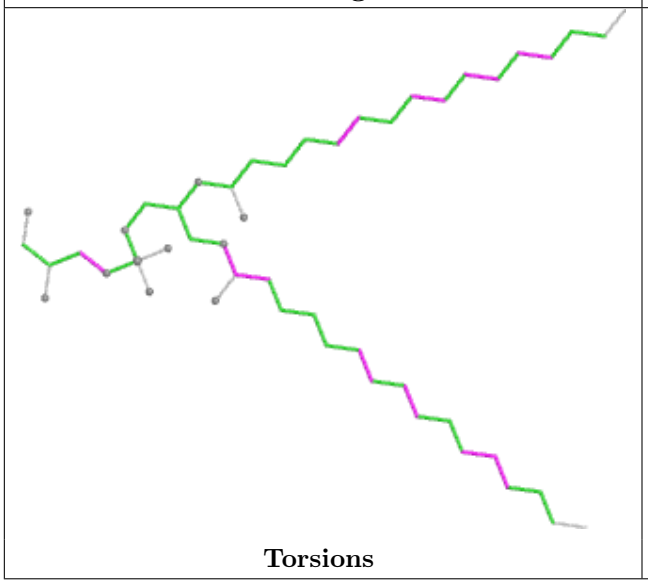
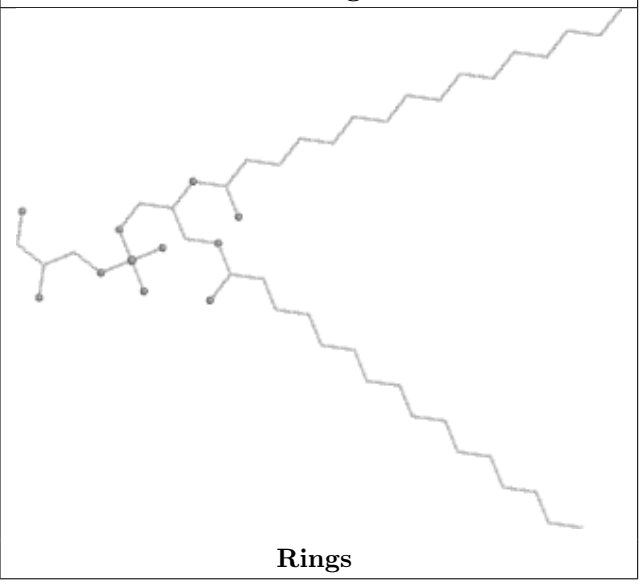


Bond angles

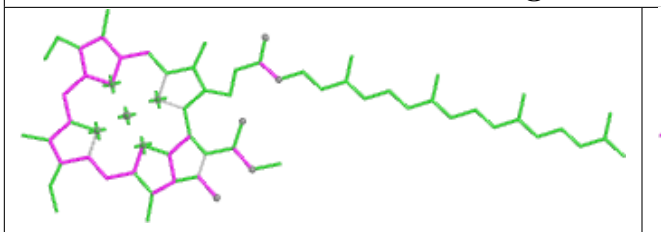


Torsions

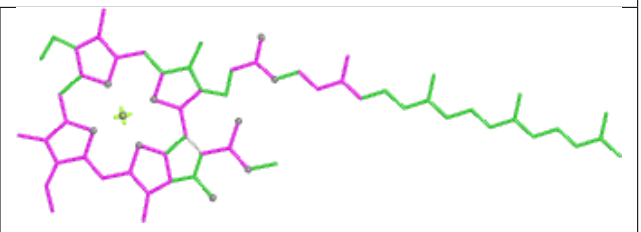


Rings

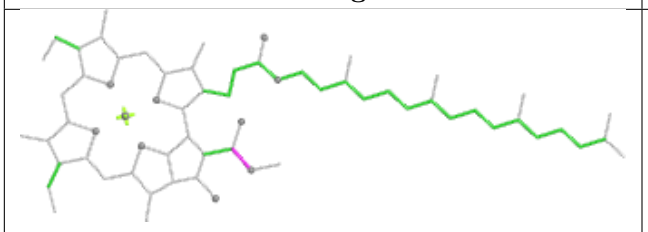
Ligand CLA C 504



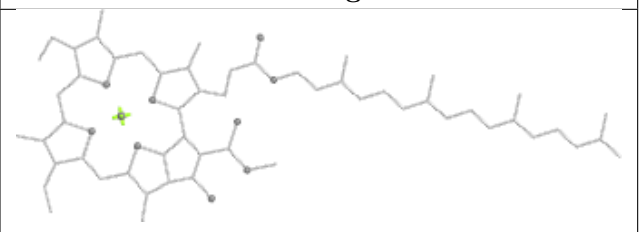
Bond lengths



Bond angles

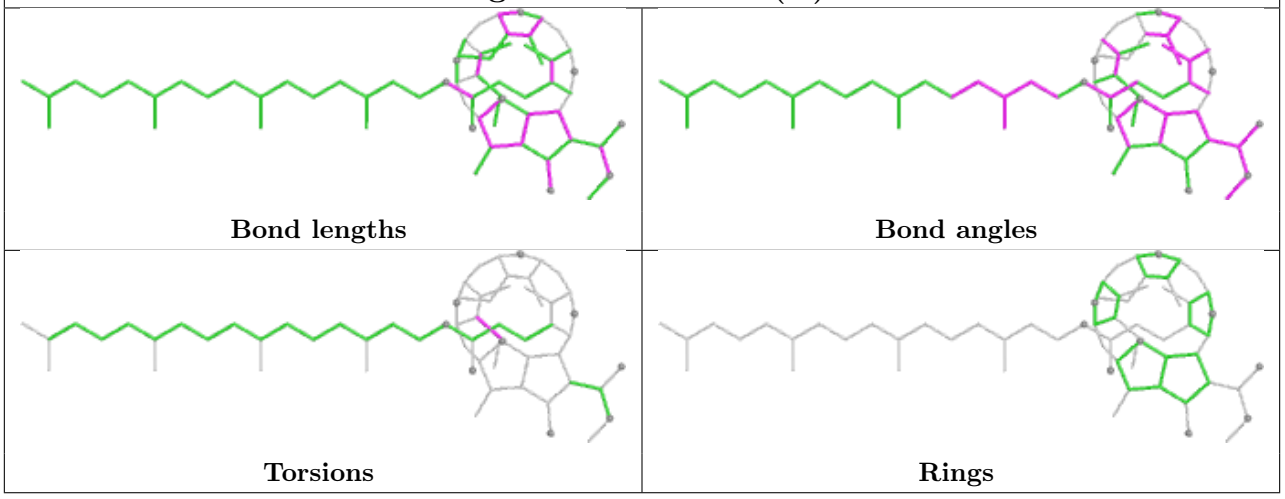


Torsions

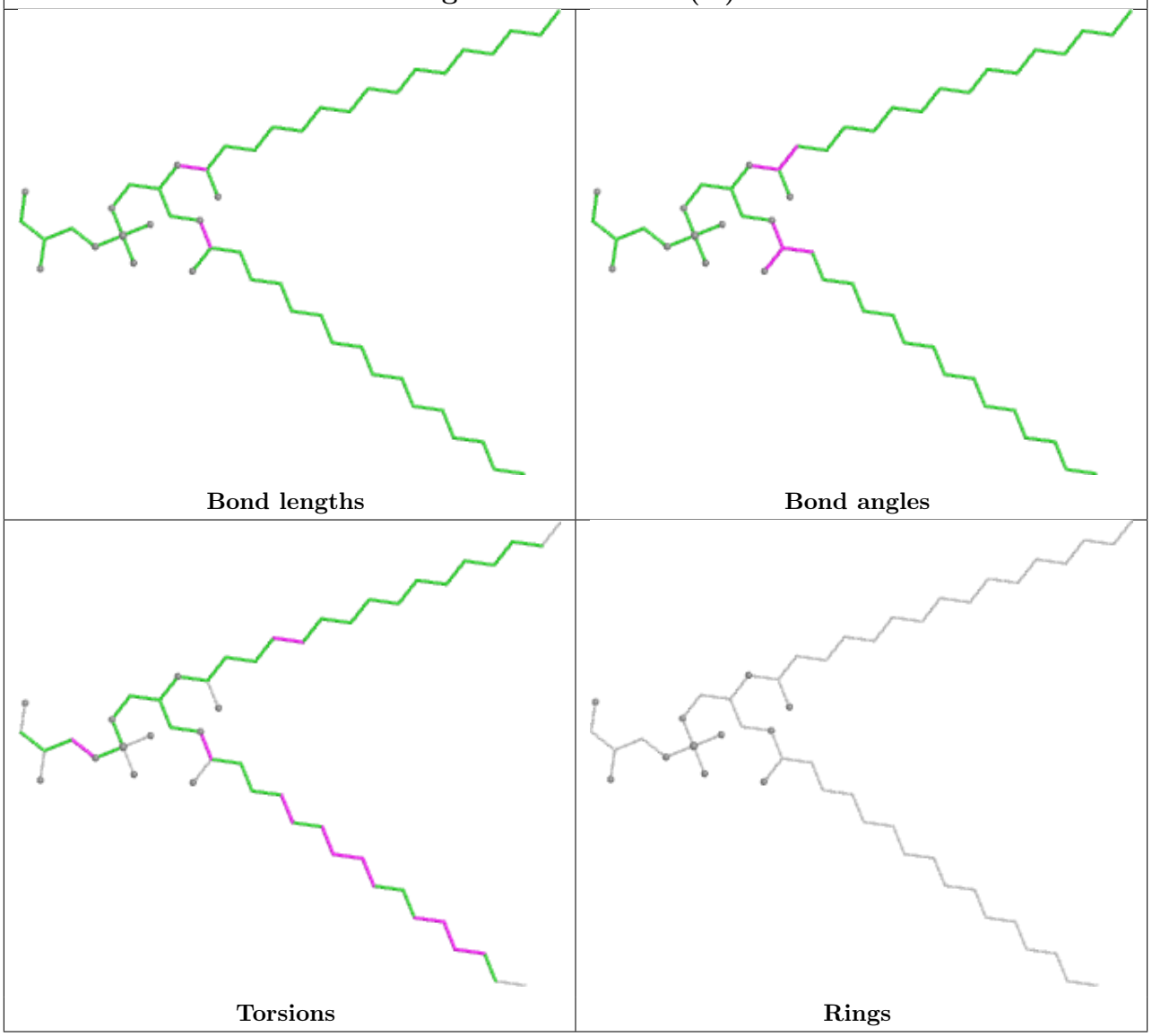


Rings

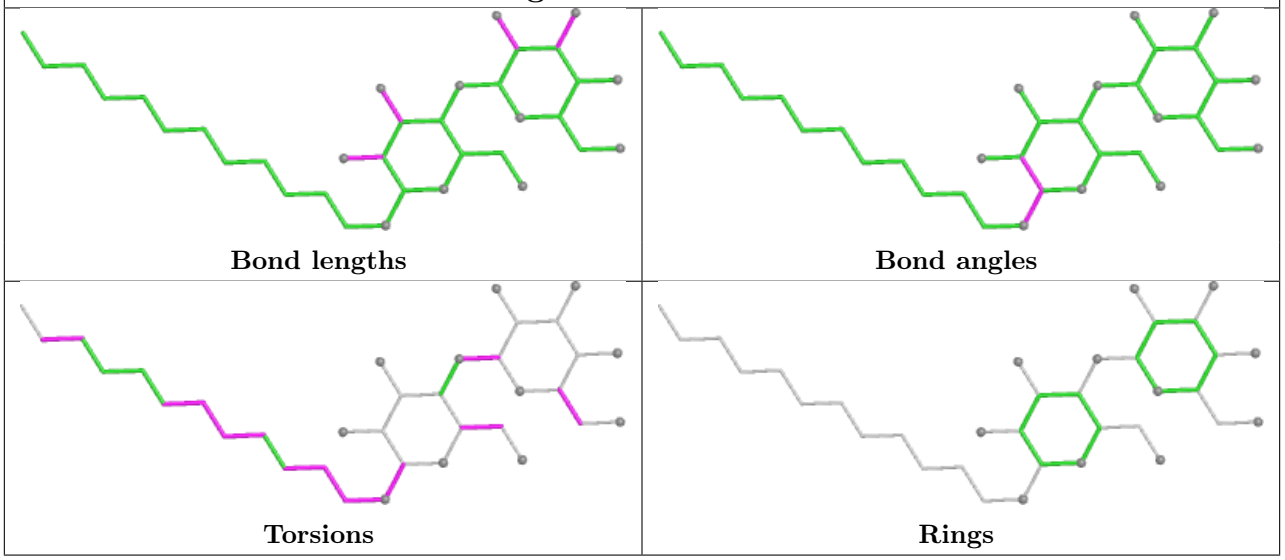
Ligand PHO A 416 (A)



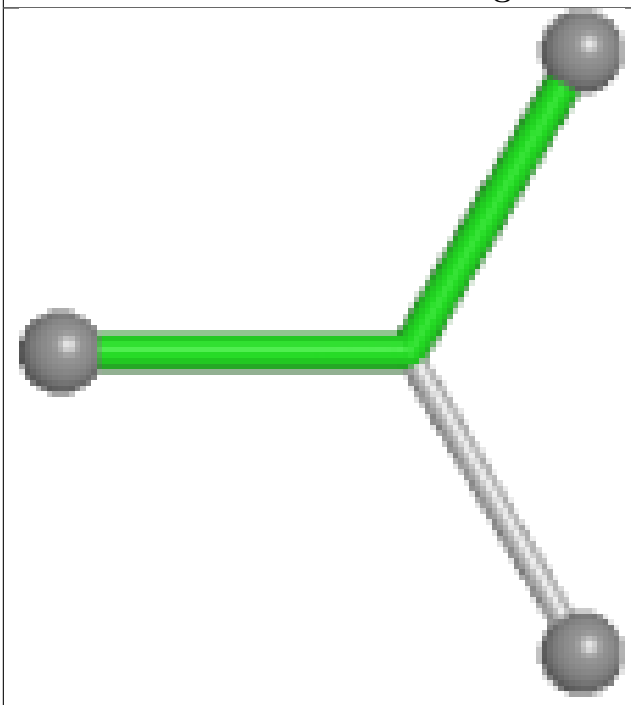
Ligand LHG d 409 (A)



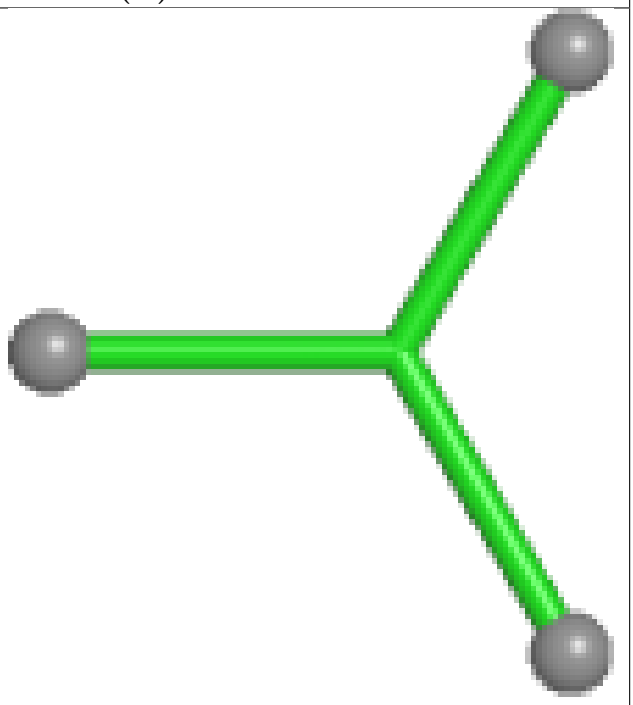
Ligand LMT e 101



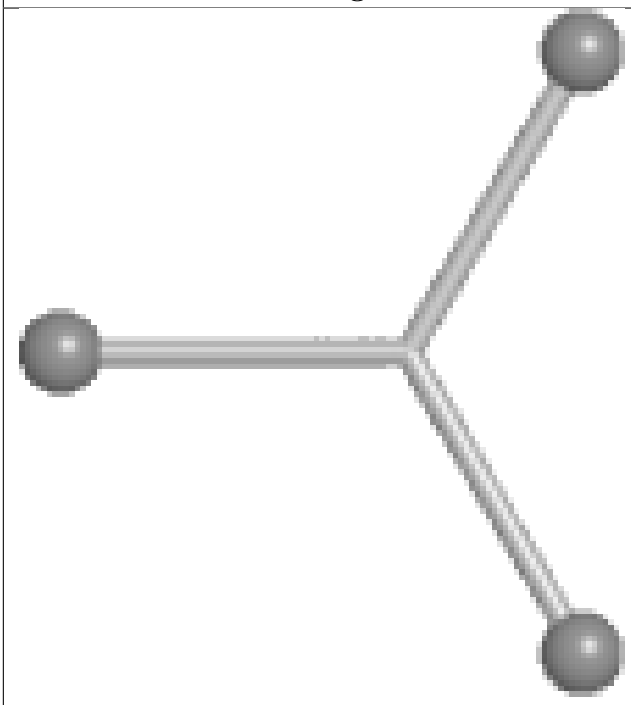
Ligand BCT d 401 (B)



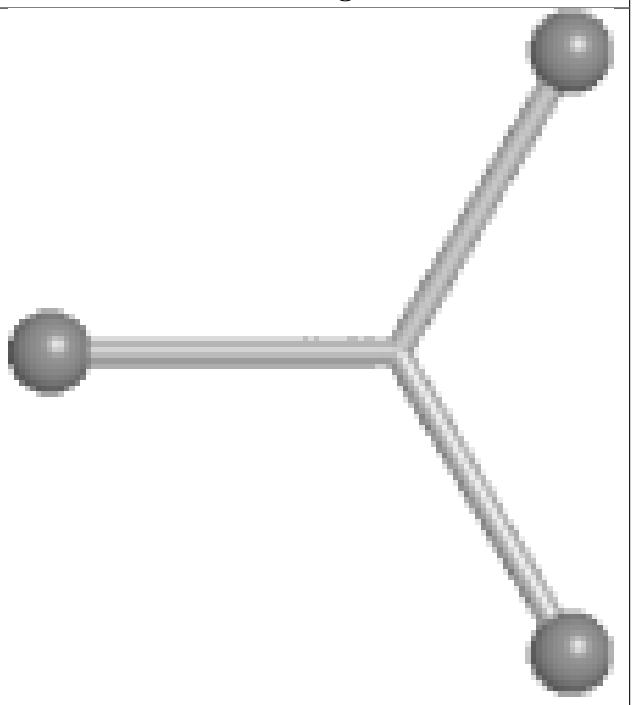
Bond lengths



Bond angles

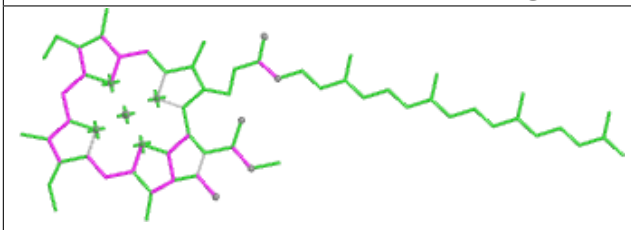


Torsions

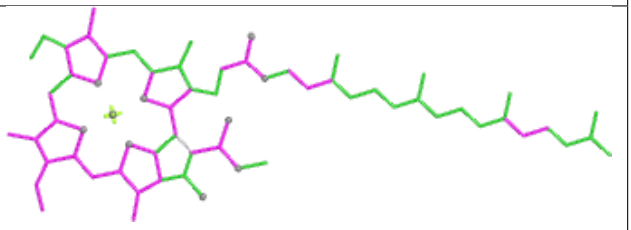


Rings

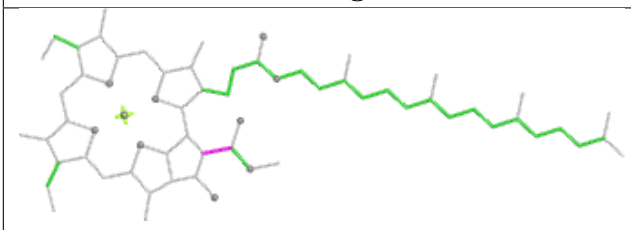
Ligand CLA B 609



Bond lengths



Bond angles



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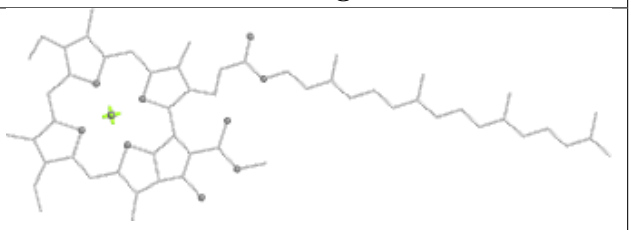
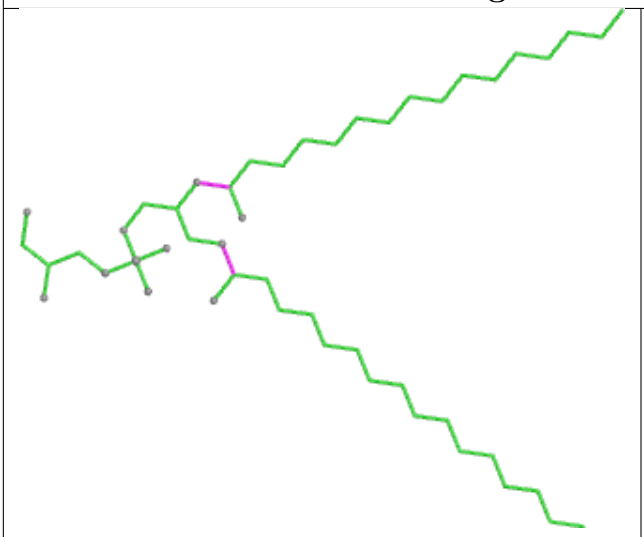
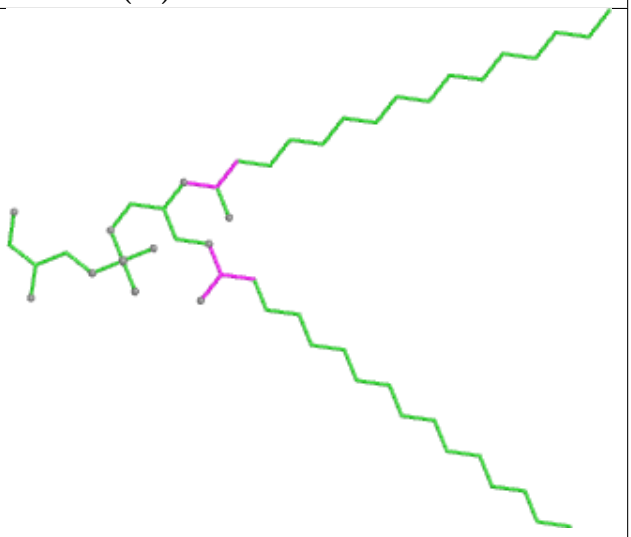


Rings

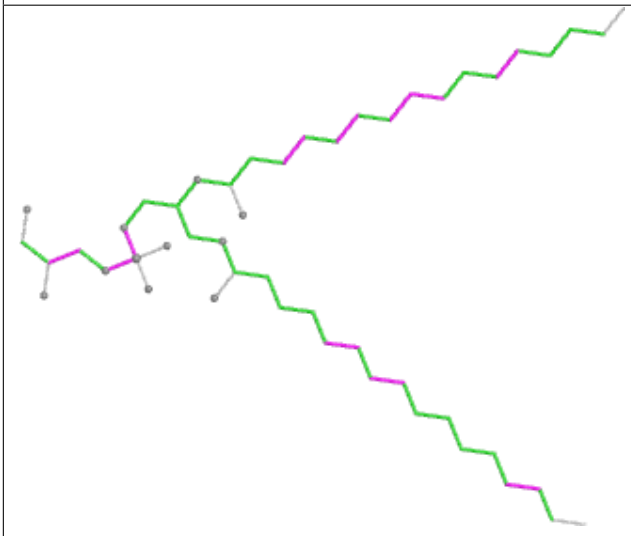
Ligand LHG D 406 (A)



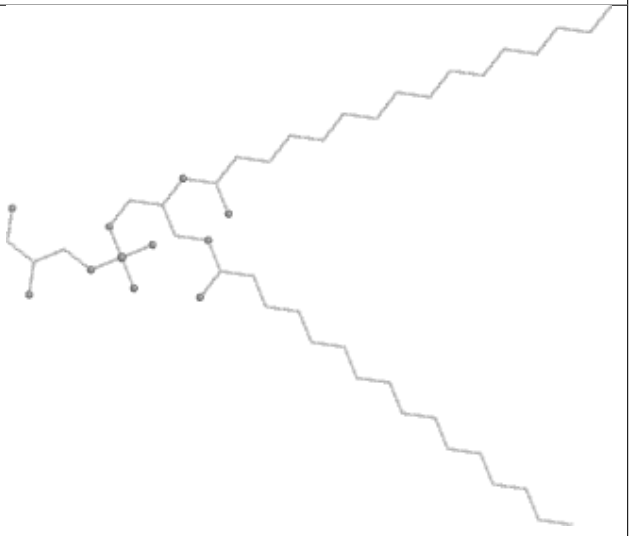
Bond lengths



Bond angles

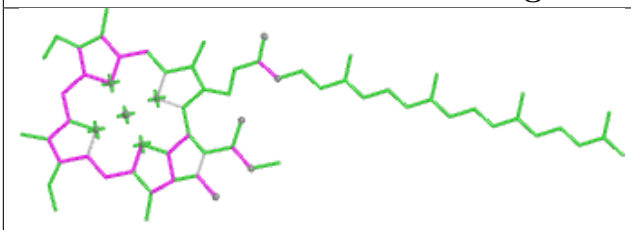


Torsions

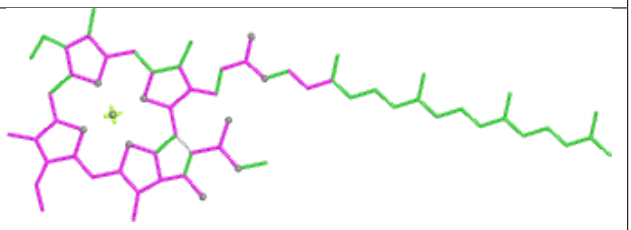


Rings

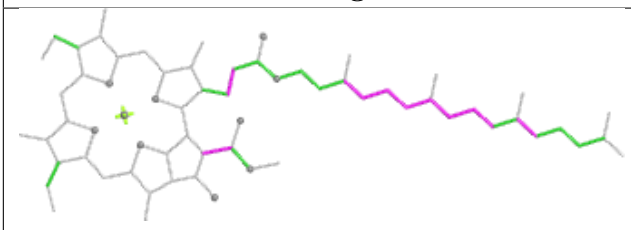
Ligand CLA B 614



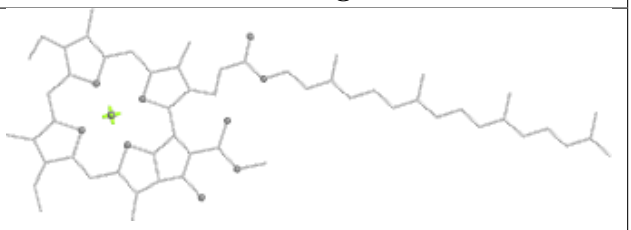
Bond lengths



Bond angles

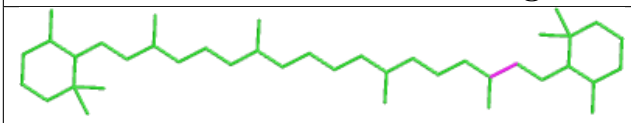


Torsions

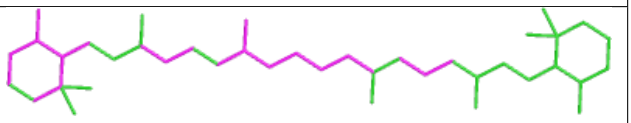


Rings

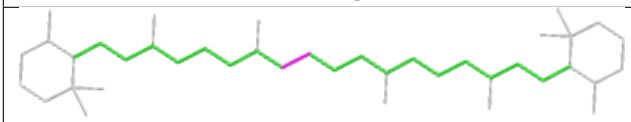
Ligand BCR T 102



Bond lengths



Bond angles



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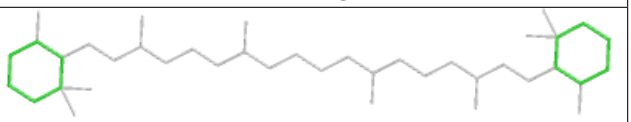
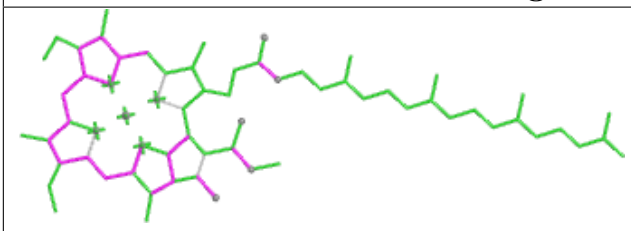


Rings

Ligand CLA b 613



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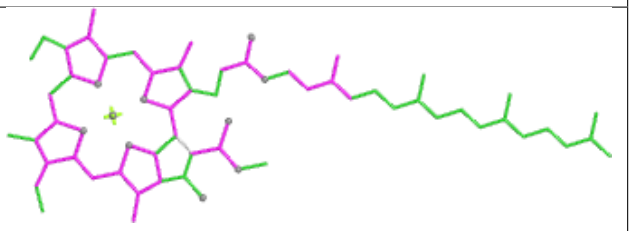
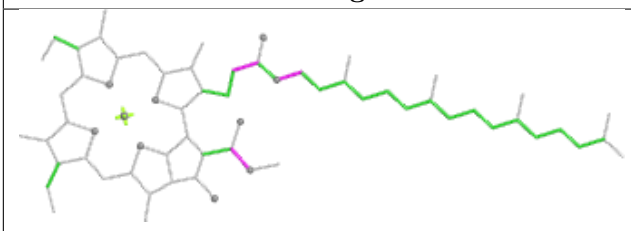


Bond angles



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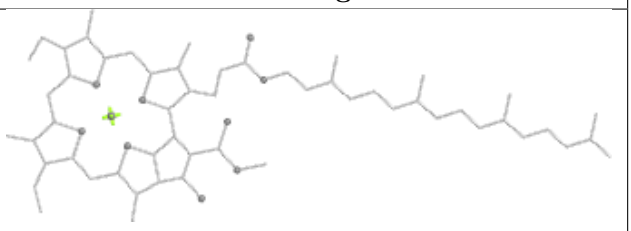
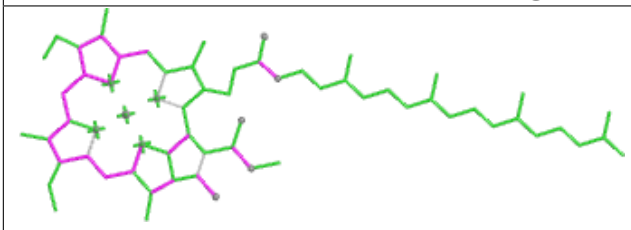


Rings

Ligand CLA b 611



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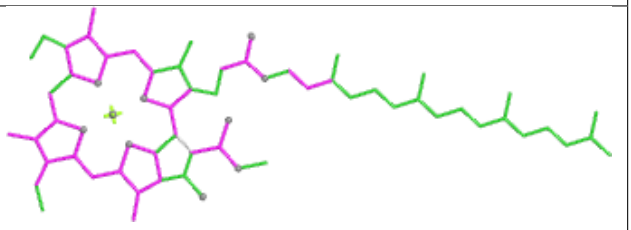
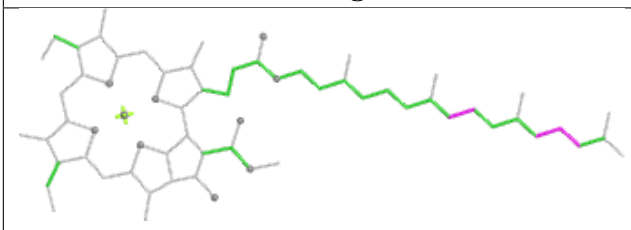


Bond angles



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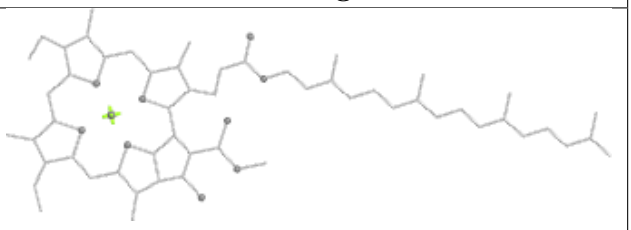
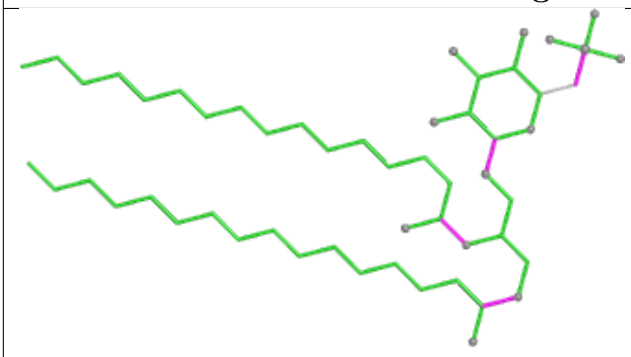


Rings

Ligand SQD l 101



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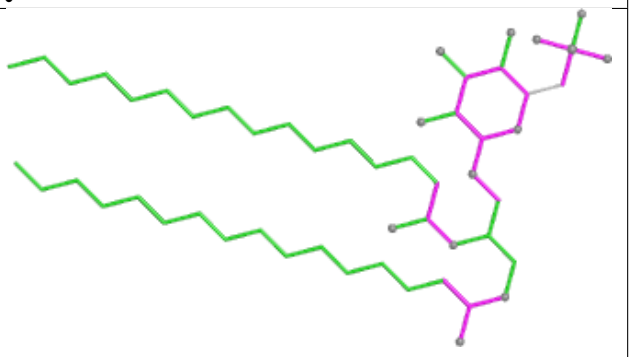
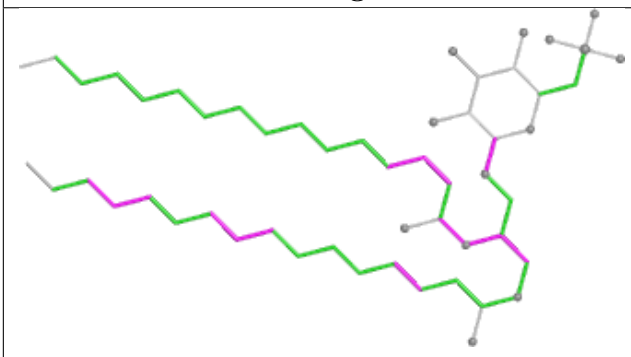


Bond angles



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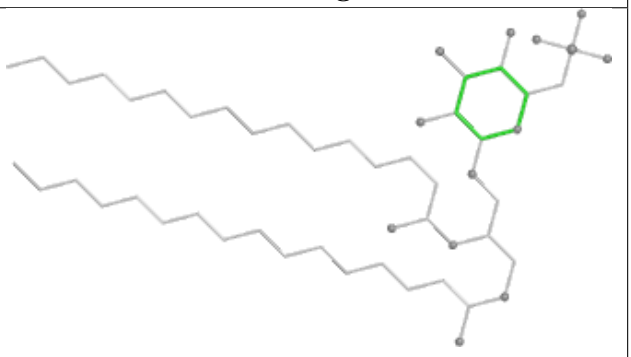
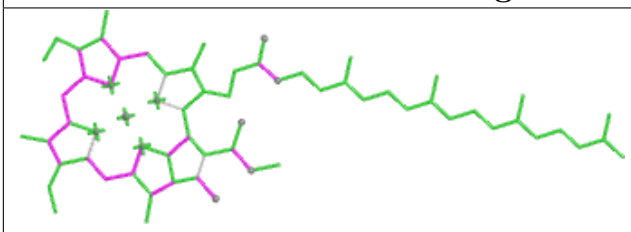


Rings

Ligand CLA d 402 (B)



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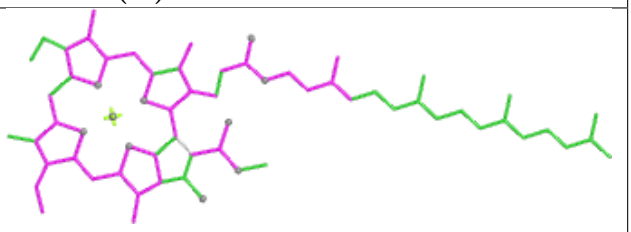
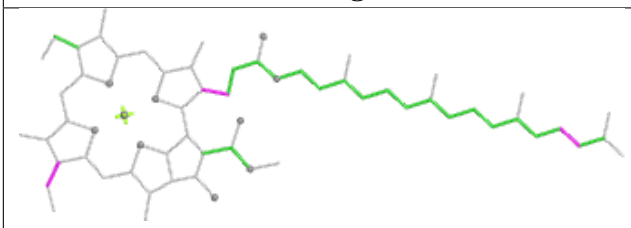


Bond angles



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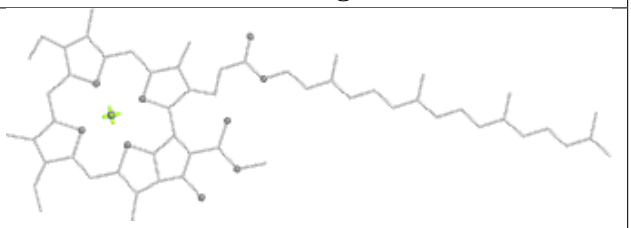
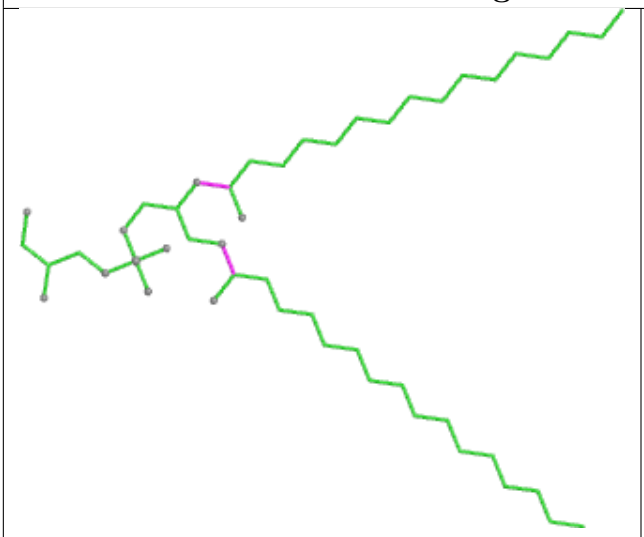


Rings

Ligand LHG d 409 (B)



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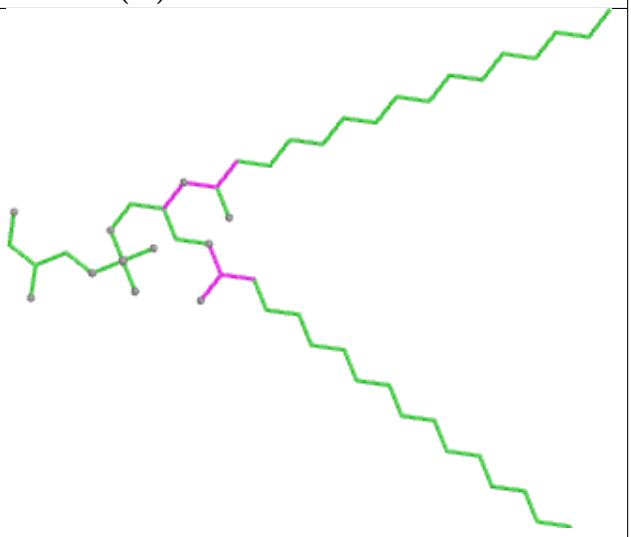
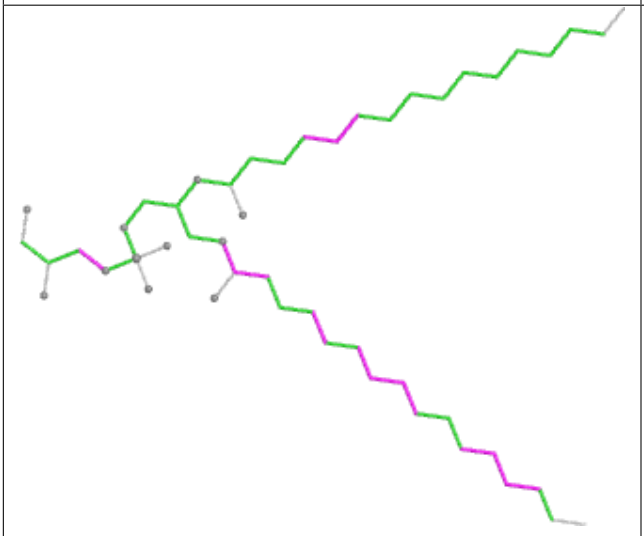


Bond angles



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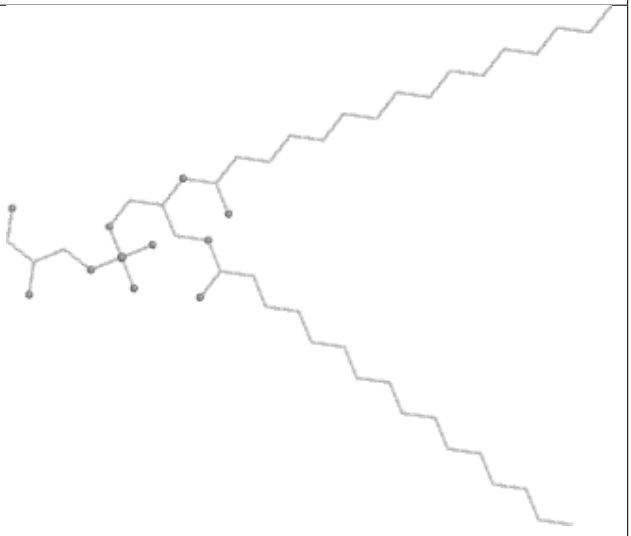
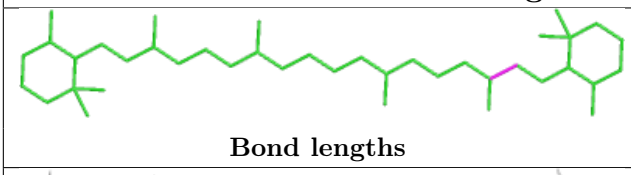


Rings

Ligand BCR b 617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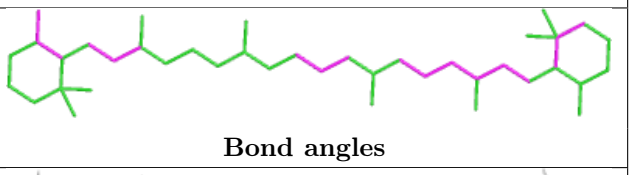
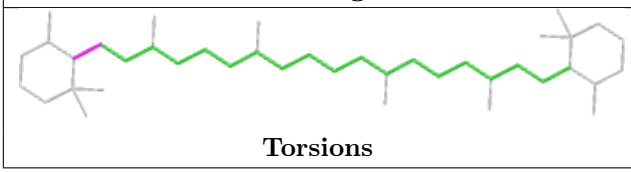

Bond angles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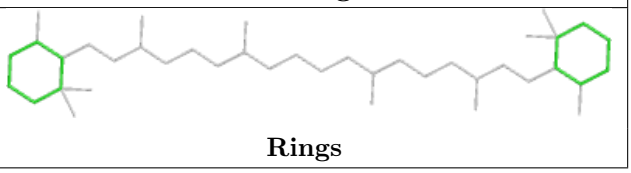
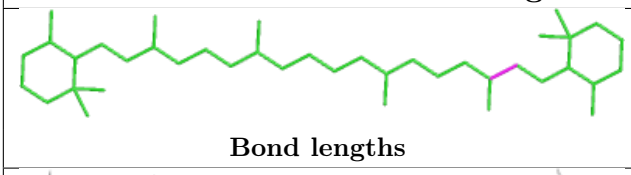

Rings

Ligand BCR b 619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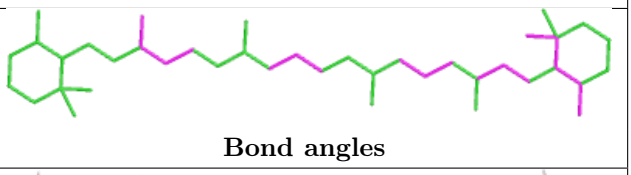
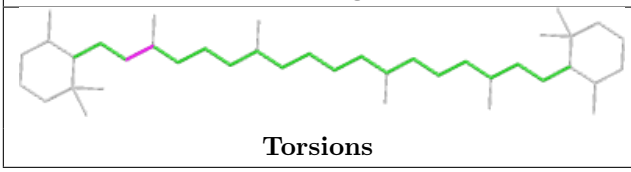

Bond angles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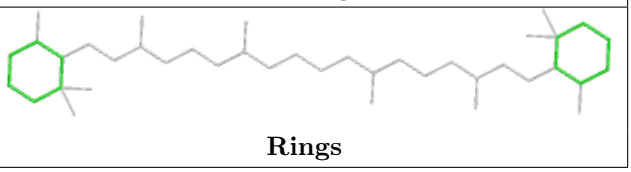
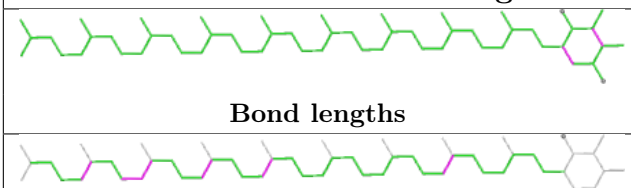

Rings

Ligand PL9 D 405 (A)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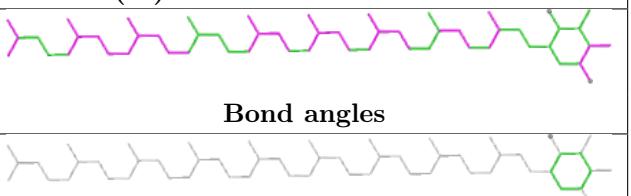
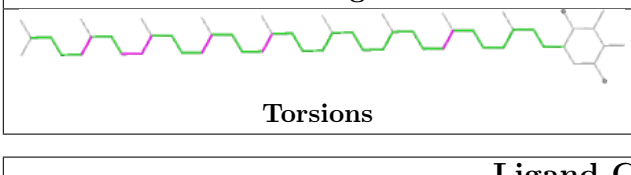

Bond angles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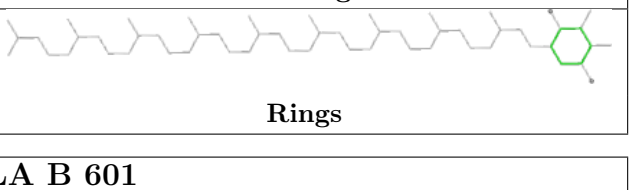
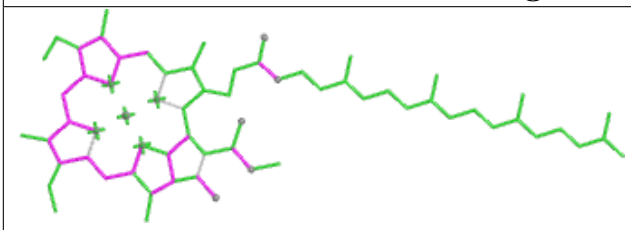

Rings

Ligand CLA B 601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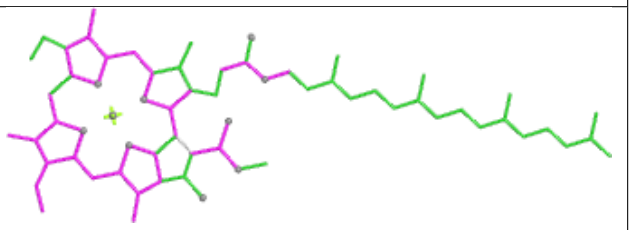
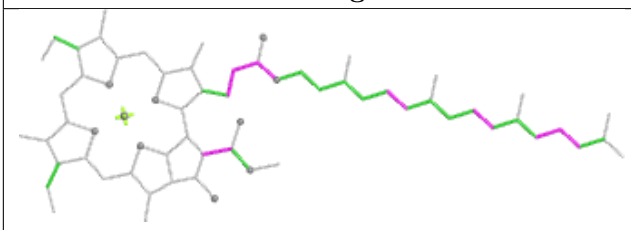

Bond angles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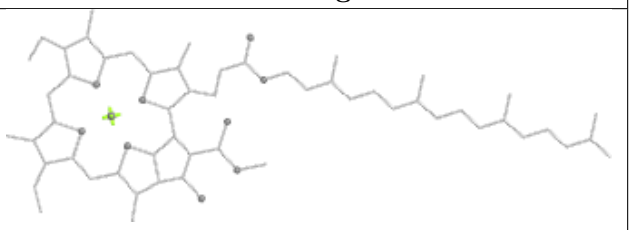
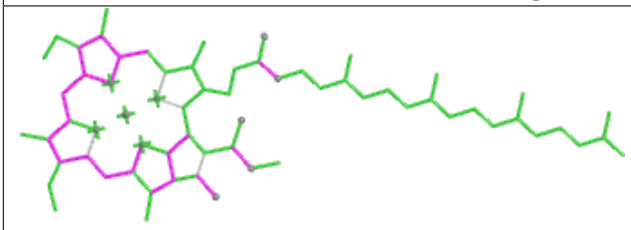

Rings

Ligand CLA b 603



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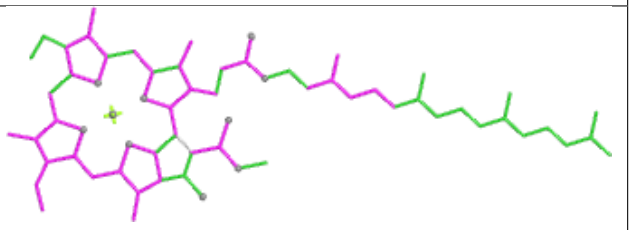
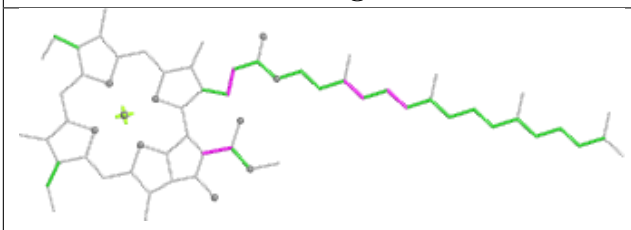


Bond angles



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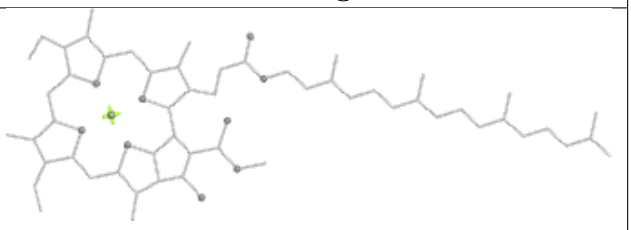
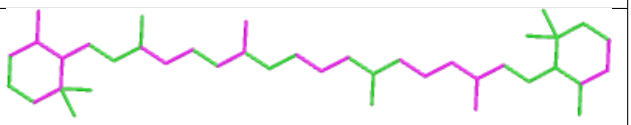


Rings

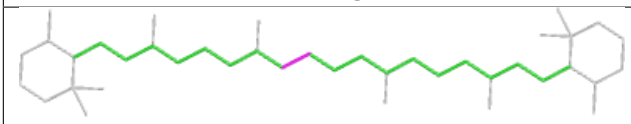
Ligand BCR t 102



Bond lengths



Bond angles



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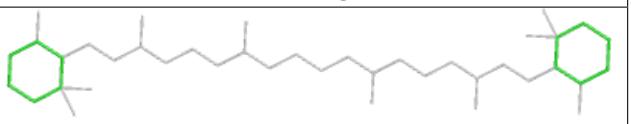
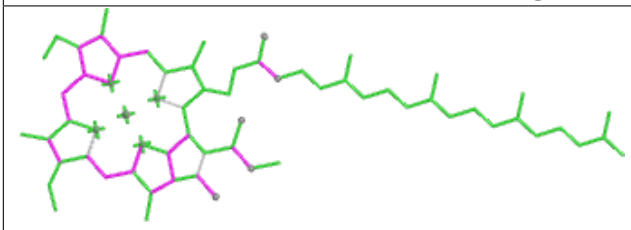


Rings

Ligand CLA c 502



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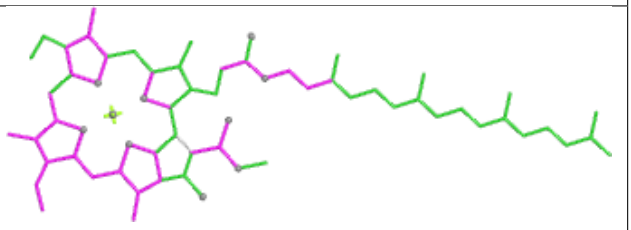
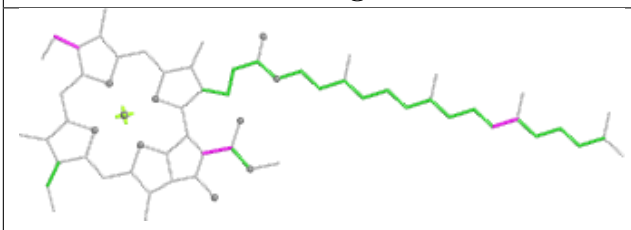


Bond angles



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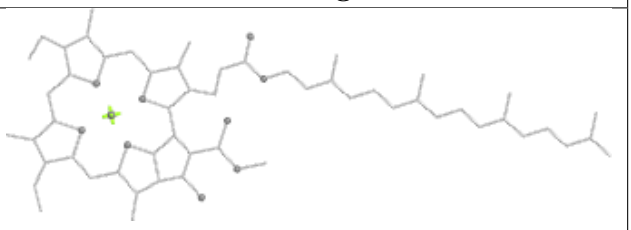
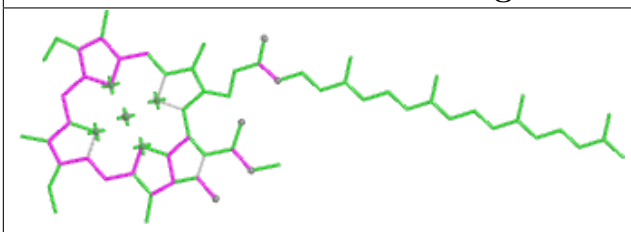


Rings

Ligand CLA d 404 (B)



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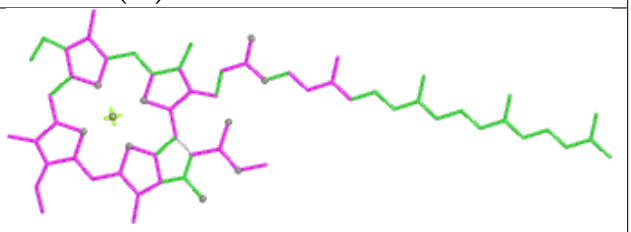
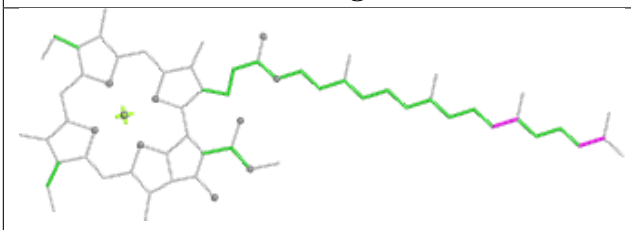


Bond angles



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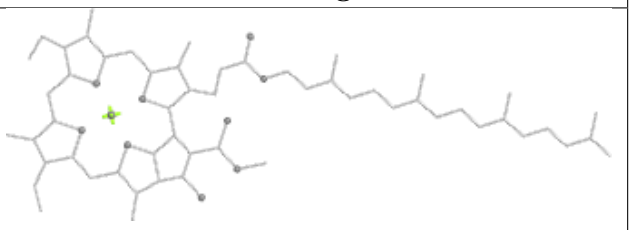
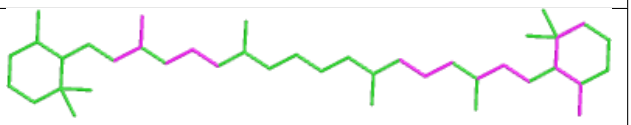


Rings

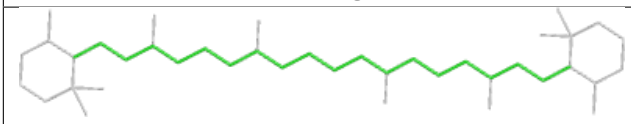
Ligand BCR B 619



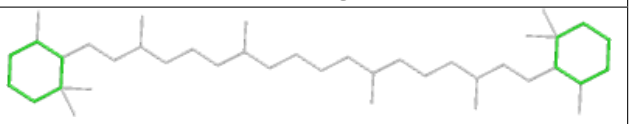
Bond lengths



Bond angles

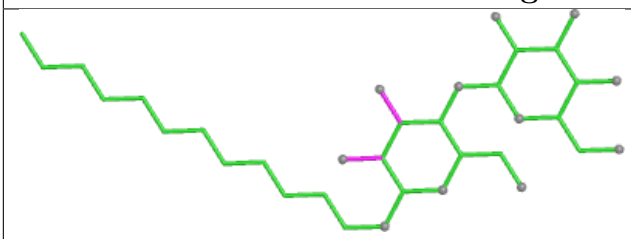


Torsions

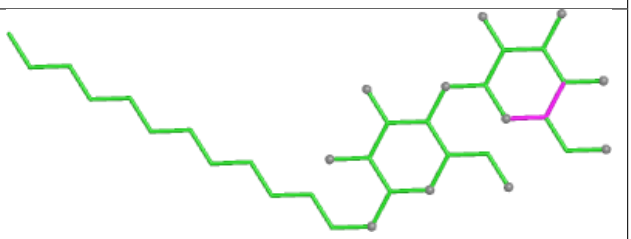


Rings

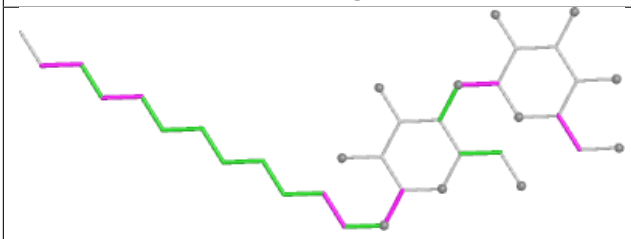
Ligand LMT A 417



Bond lengths



Bond angles



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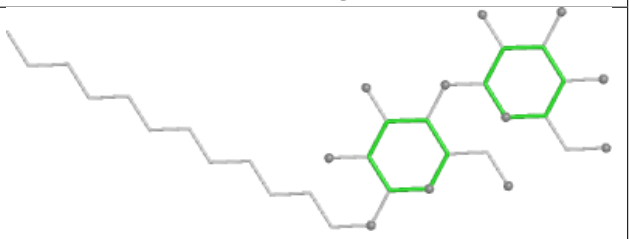
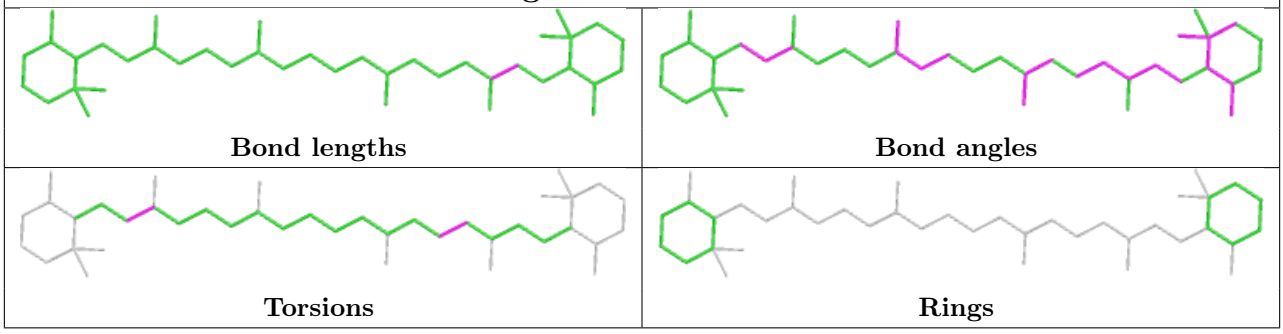
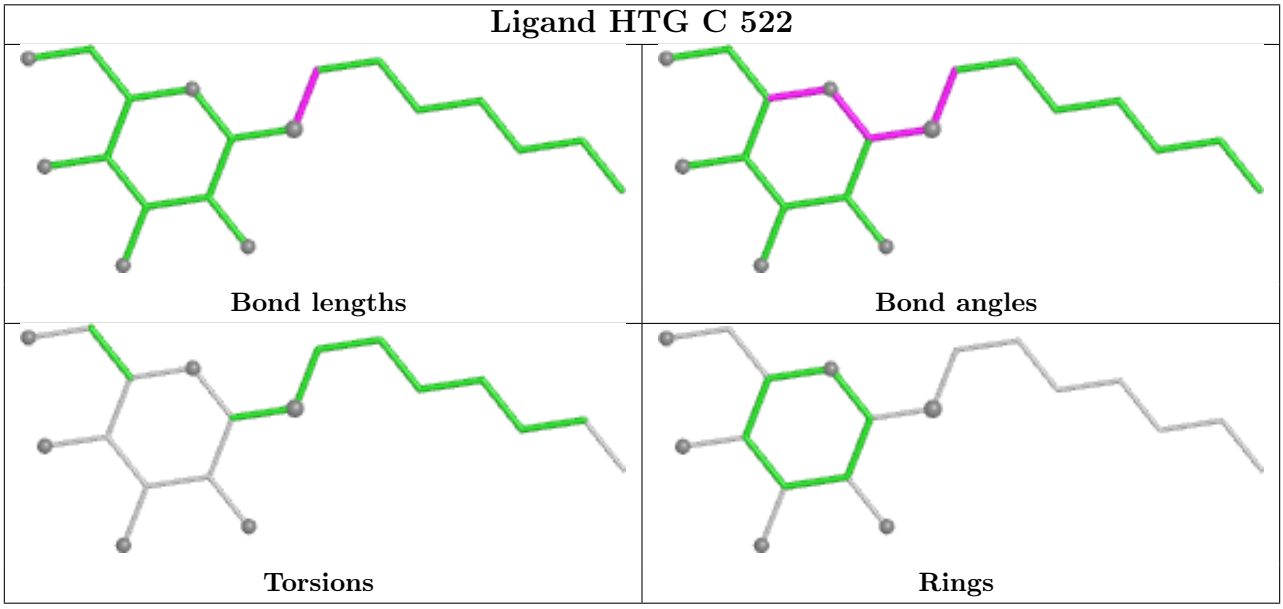


Rings

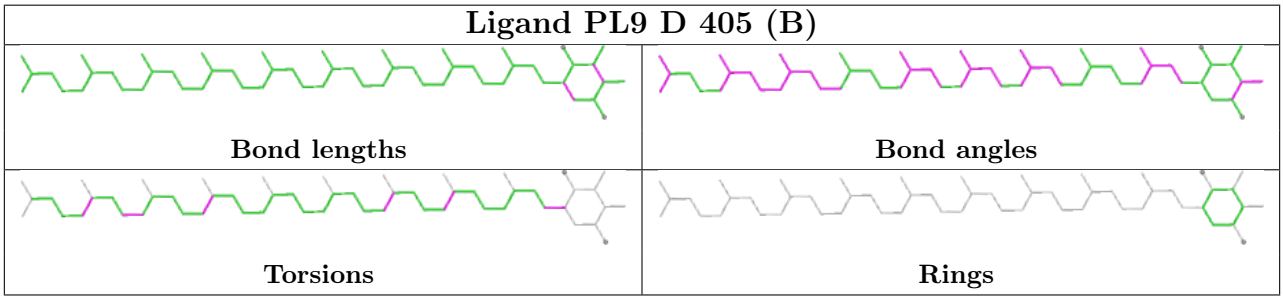
Ligand BCR K 102



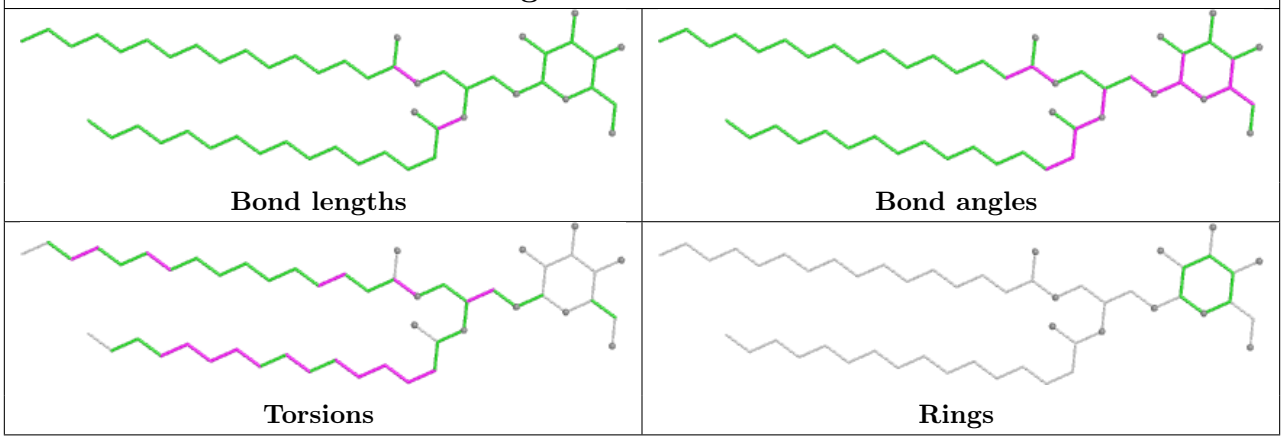
Ligand HTG C 522



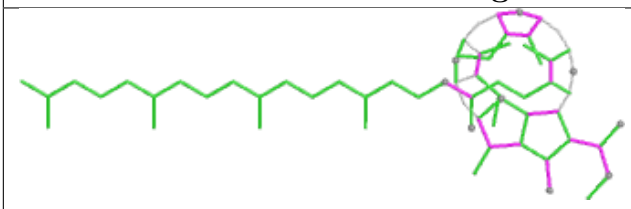
Ligand PL9 D 405 (B)



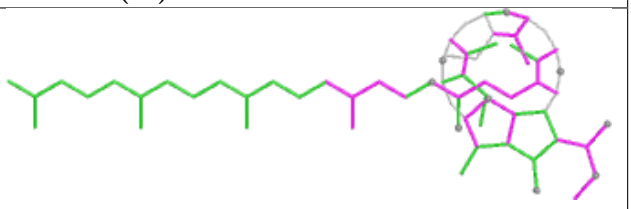
Ligand LMG C 501



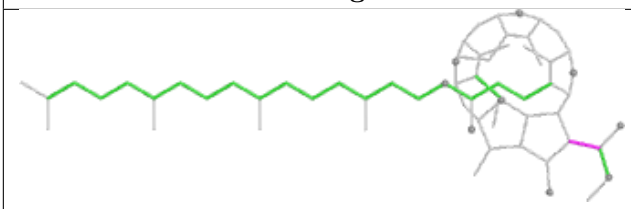
Ligand PHO d 403 (A)



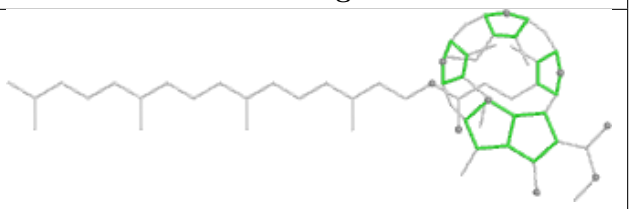
Bond lengths



Bond angles

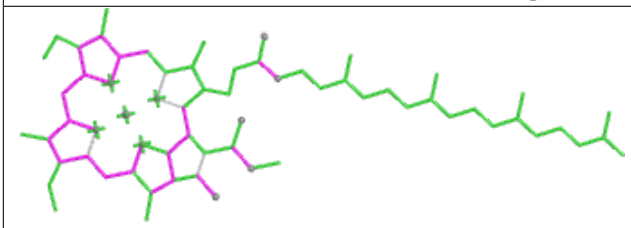


Torsions

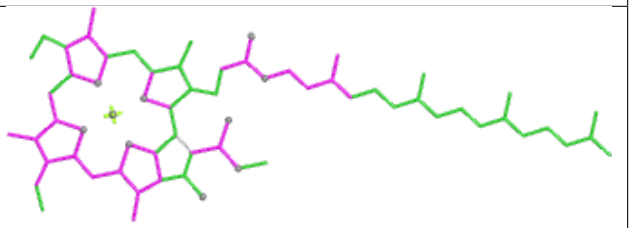


Rings

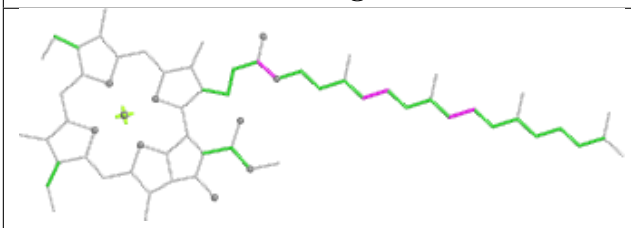
Ligand CLA C 512



Bond lengths



Bond angles



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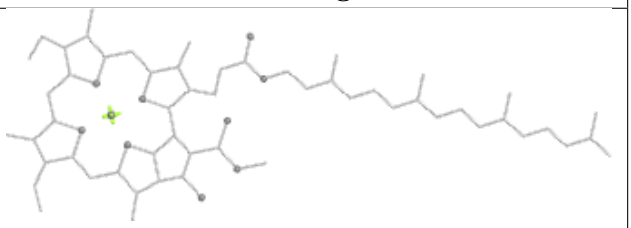
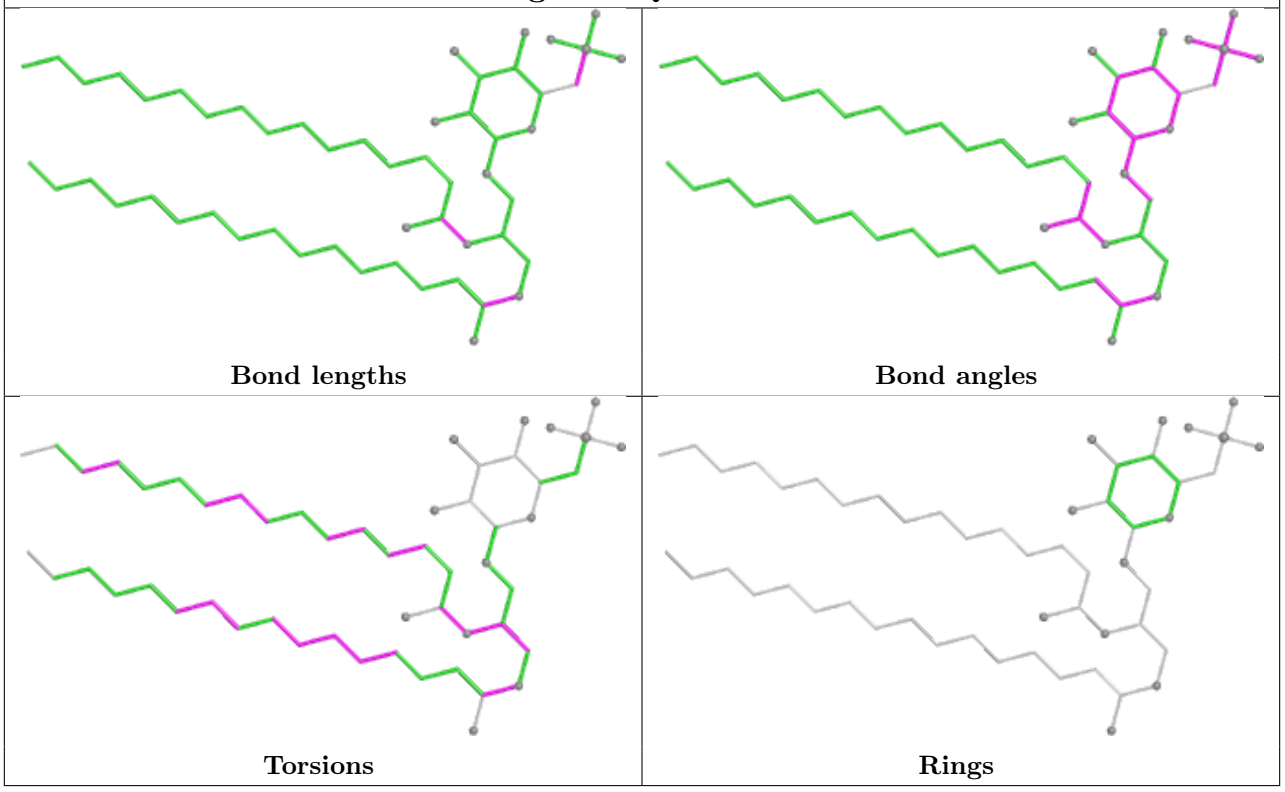
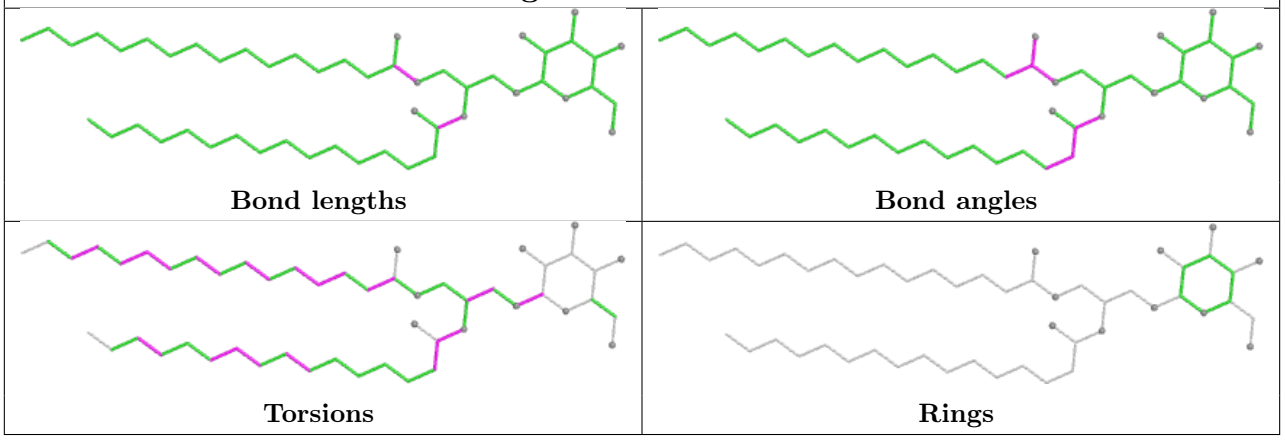


Rings

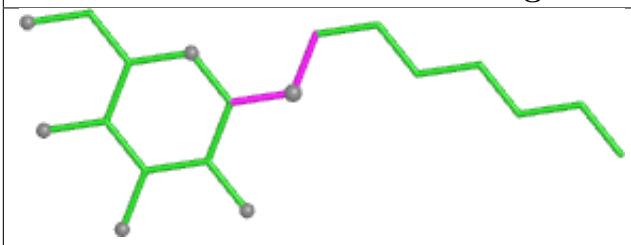
Ligand SQD b 620



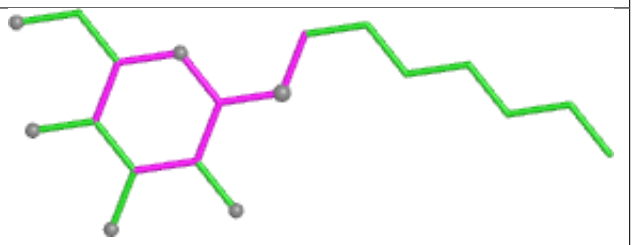
Ligand LMG B 620



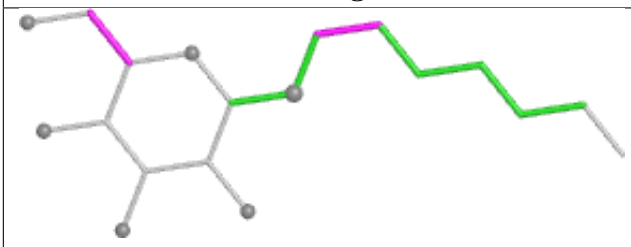
Ligand HTG b 625



Bond lengths



Bond angles



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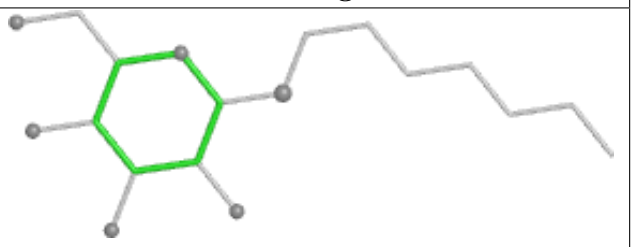
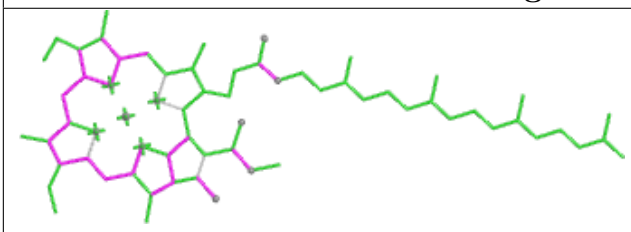


Rings

Ligand CLA C 506



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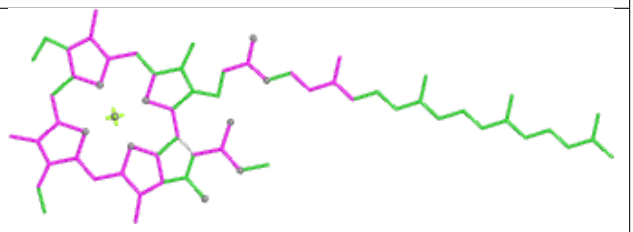
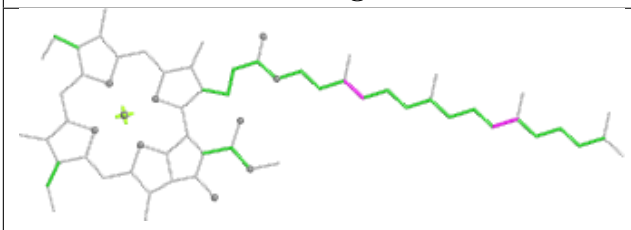


Bond angles



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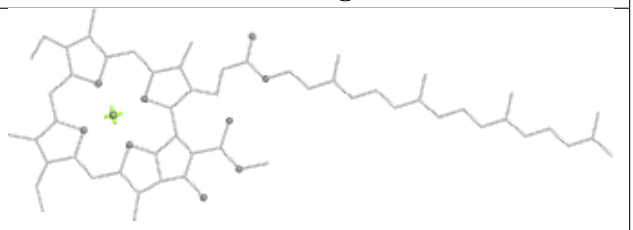
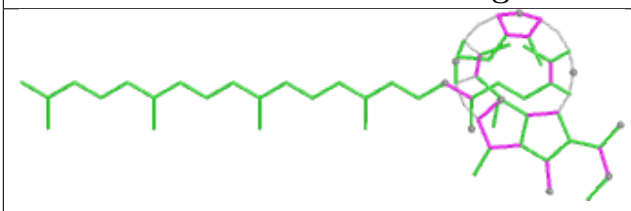


Rings

Ligand PHO d 403 (B)



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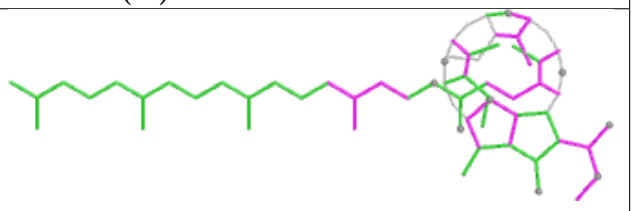
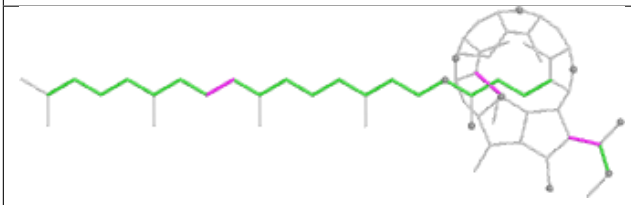


Bond angles



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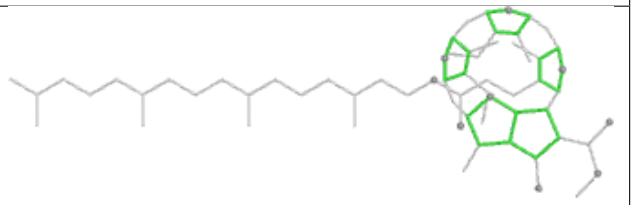
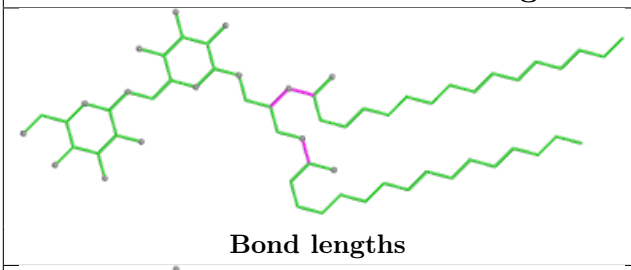


Rings

Ligand DGD C 519



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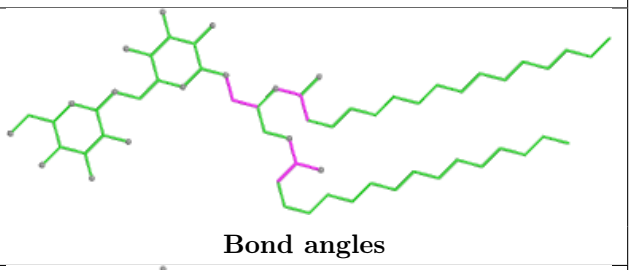
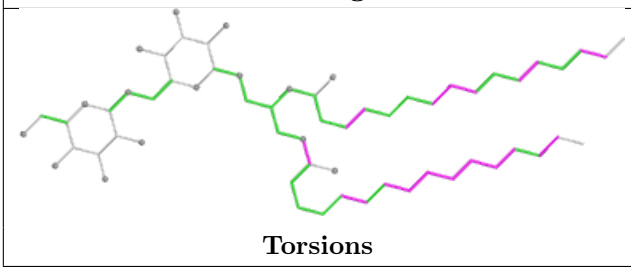


Bond angles



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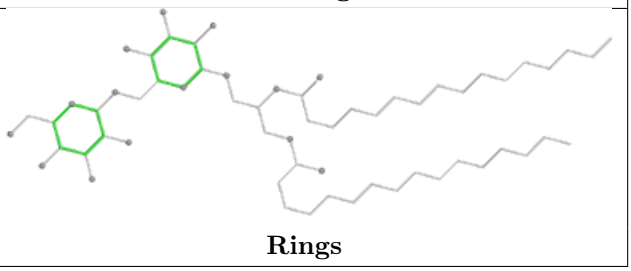
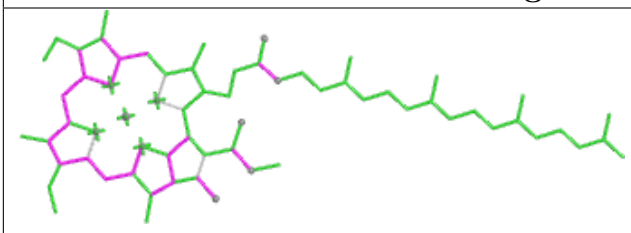


Rings

Ligand CLA B 610



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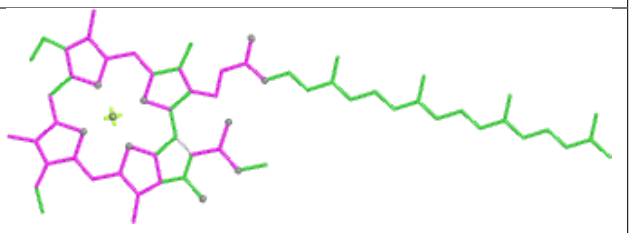
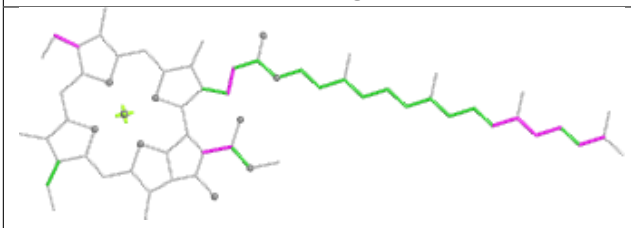


Bond angles



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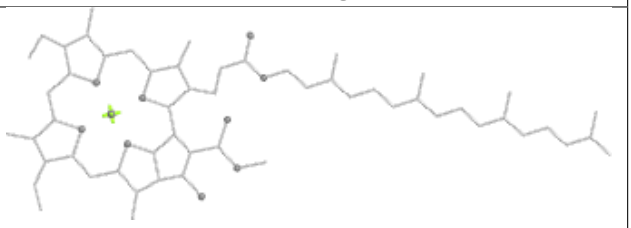
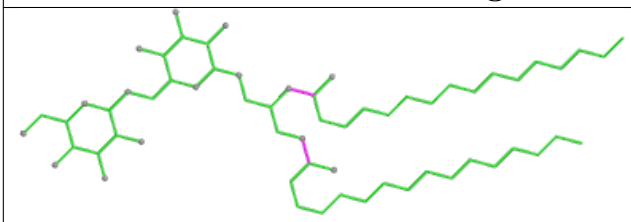


Rings

Ligand DGD C 517 (A)



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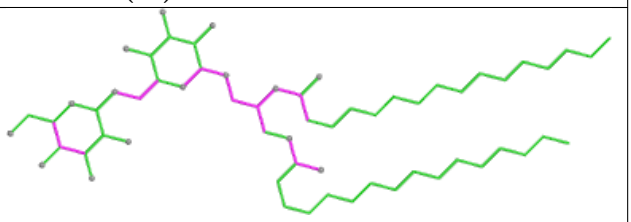
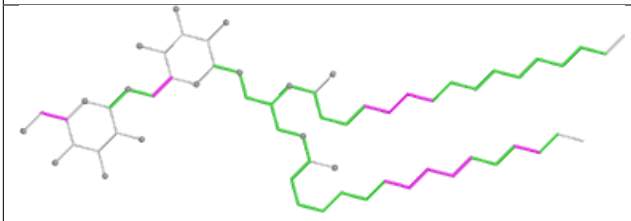


Bond angles



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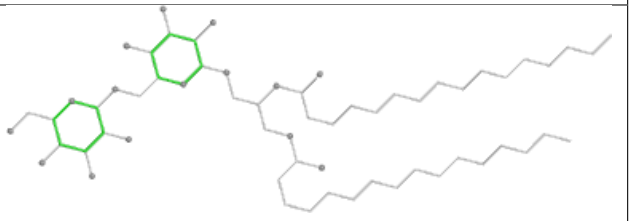
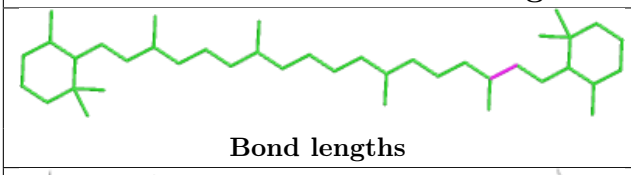


Rings

Ligand BCR y 101



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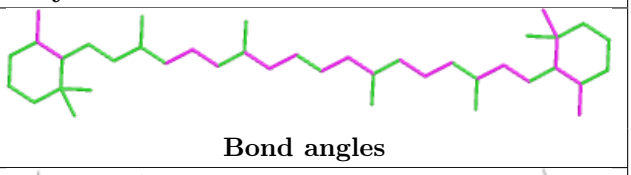
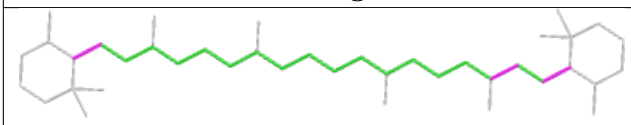


Bond angles



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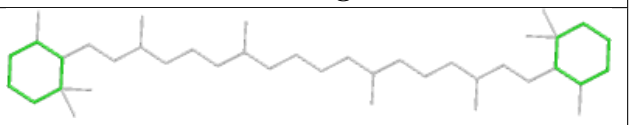
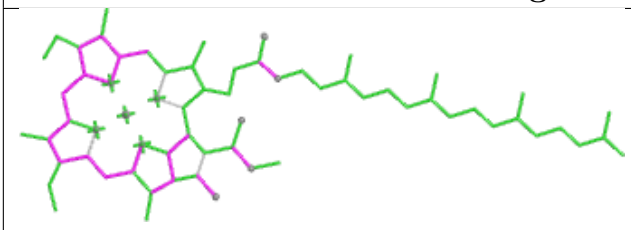
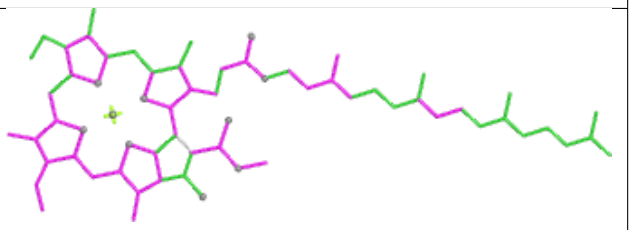


Rings

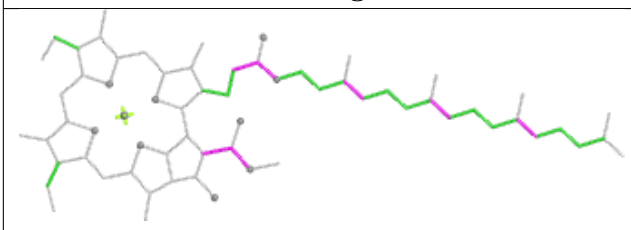
Ligand CLA c 510



Bond lengths



Bond angles



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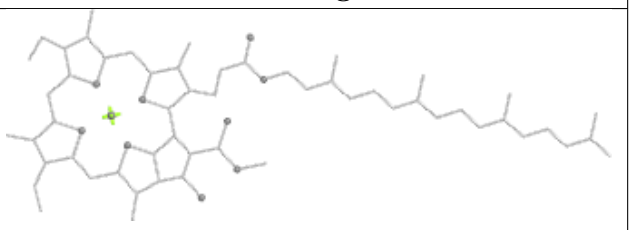
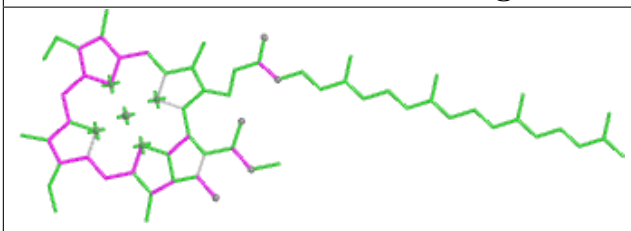


Rings

Ligand CLA a 404 (A)



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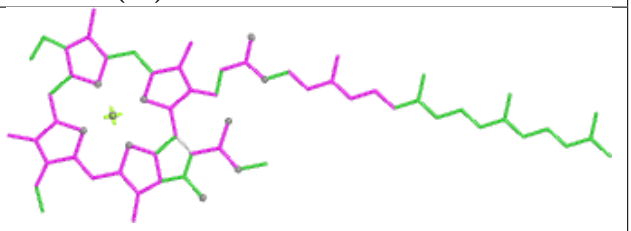
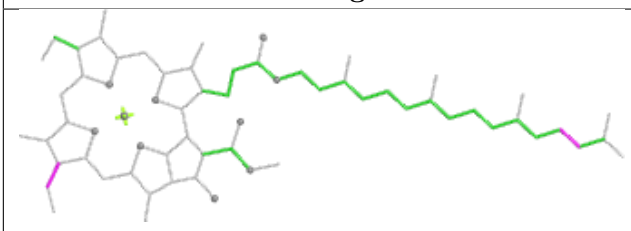


Bond angles



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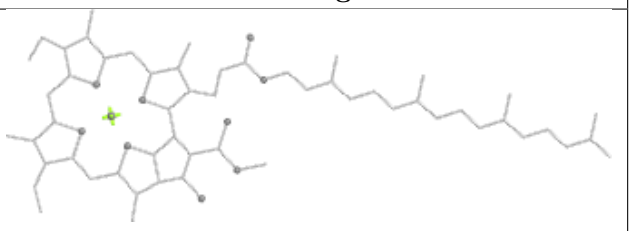
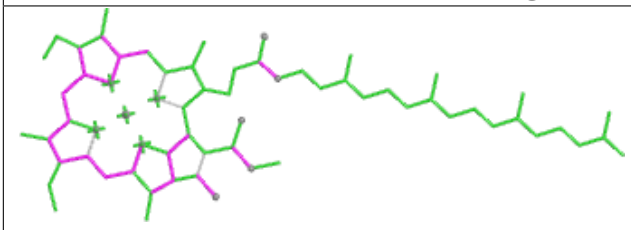


Rings

Ligand CLA D 403



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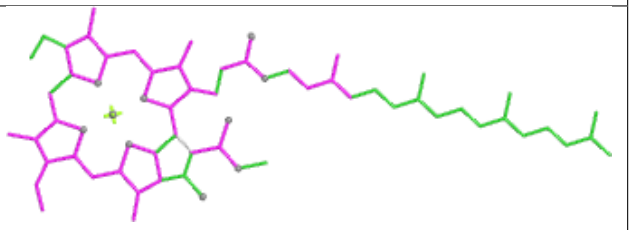
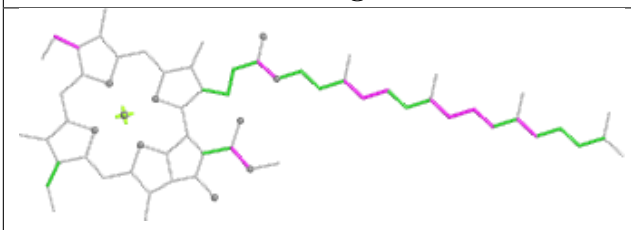
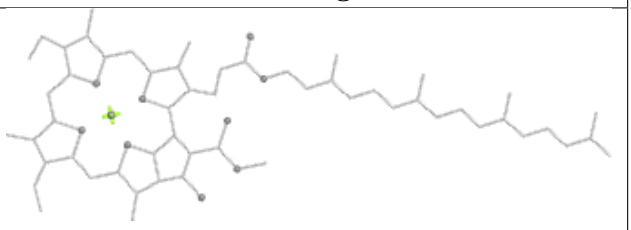


Bond angles

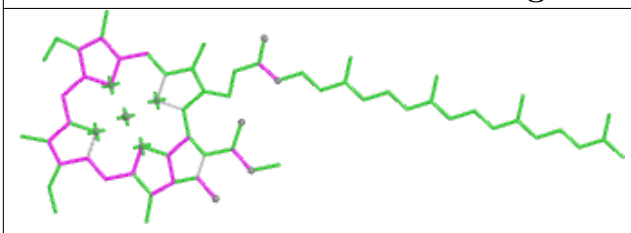


Torsions

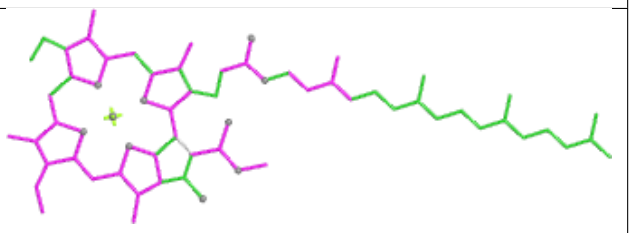


Rings

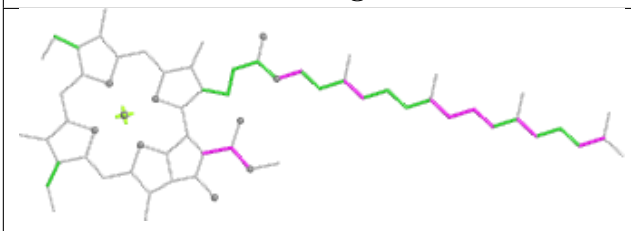
Ligand CLA b 614



Bond lengths



Bond angles



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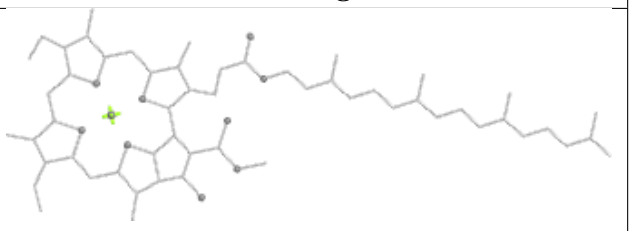
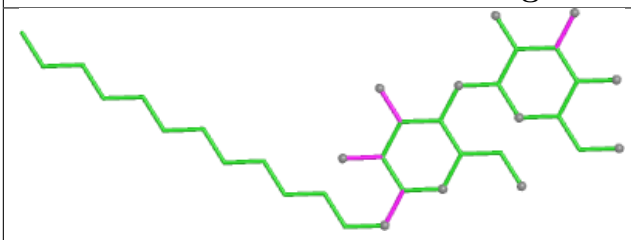


Rings

Ligand LMT T 101



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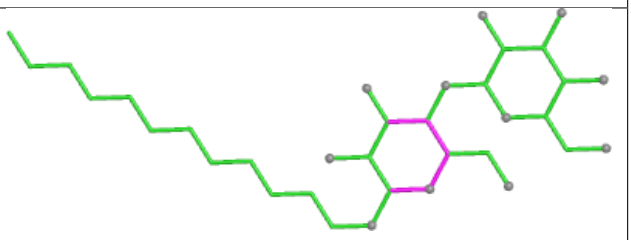
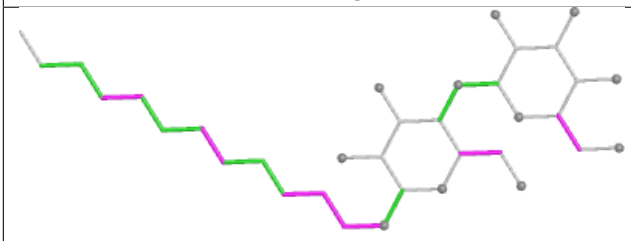


Bond angles



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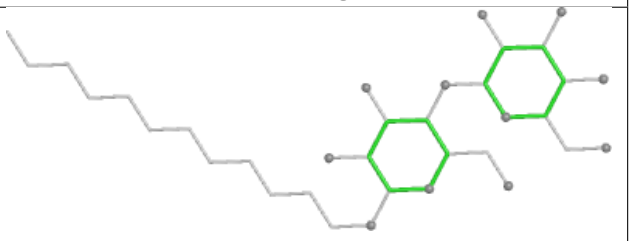
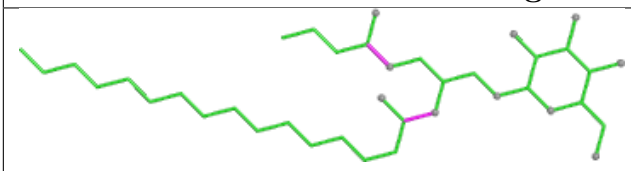


Rings

Ligand LMG z 101



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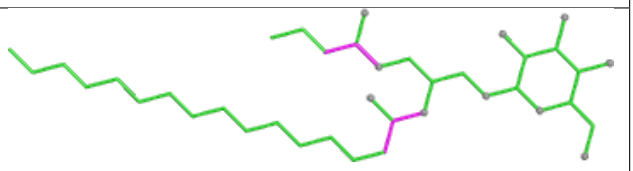
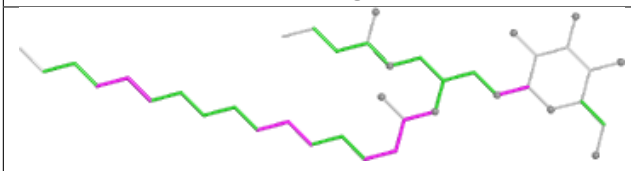


Bond angles



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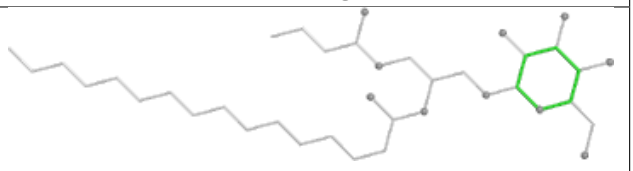
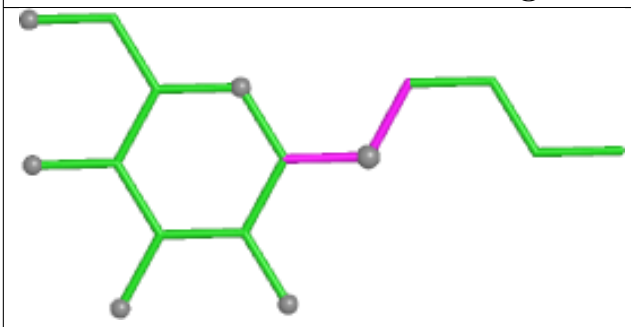


Rings

Ligand HTG D 410



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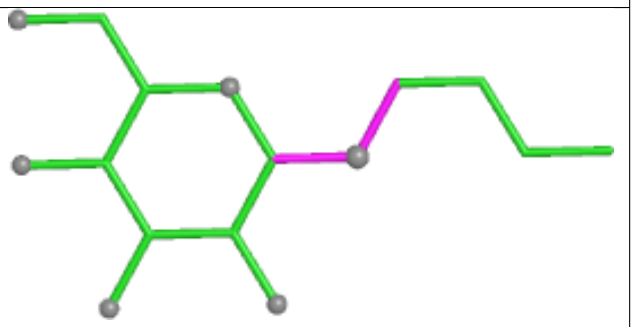
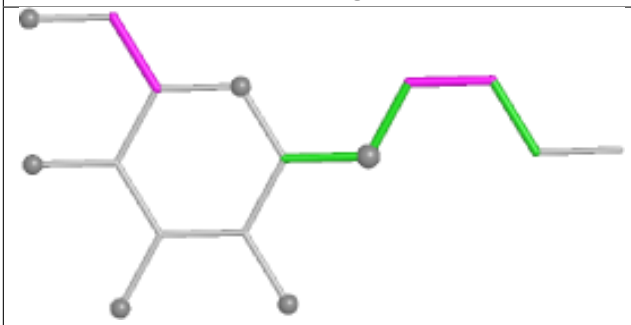


Bond angles



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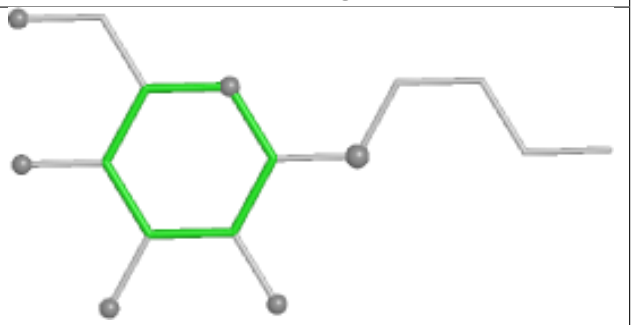
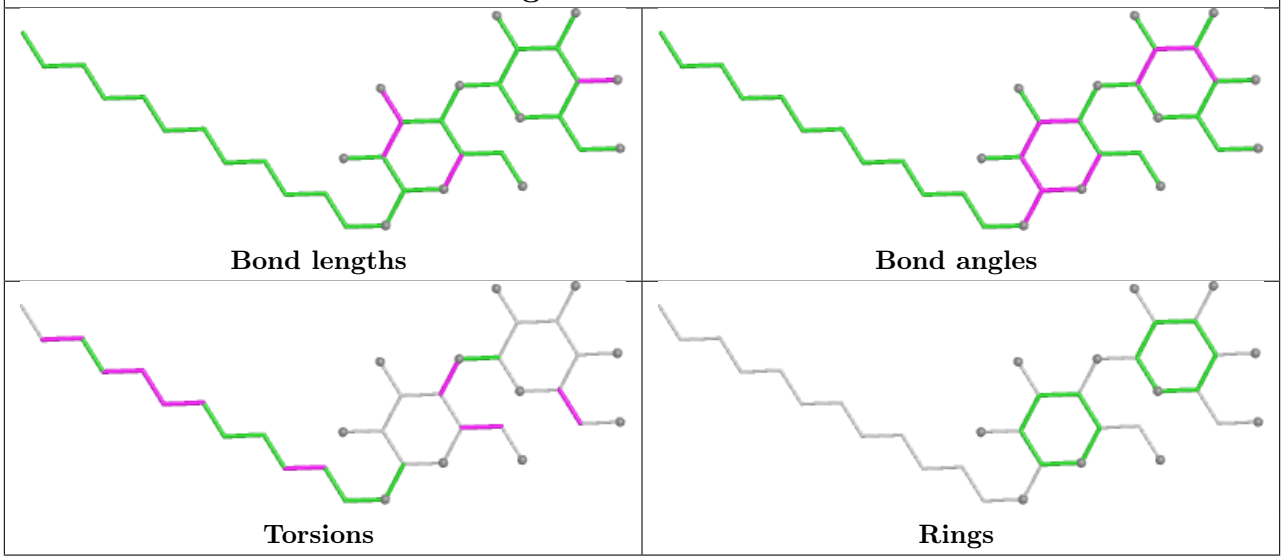
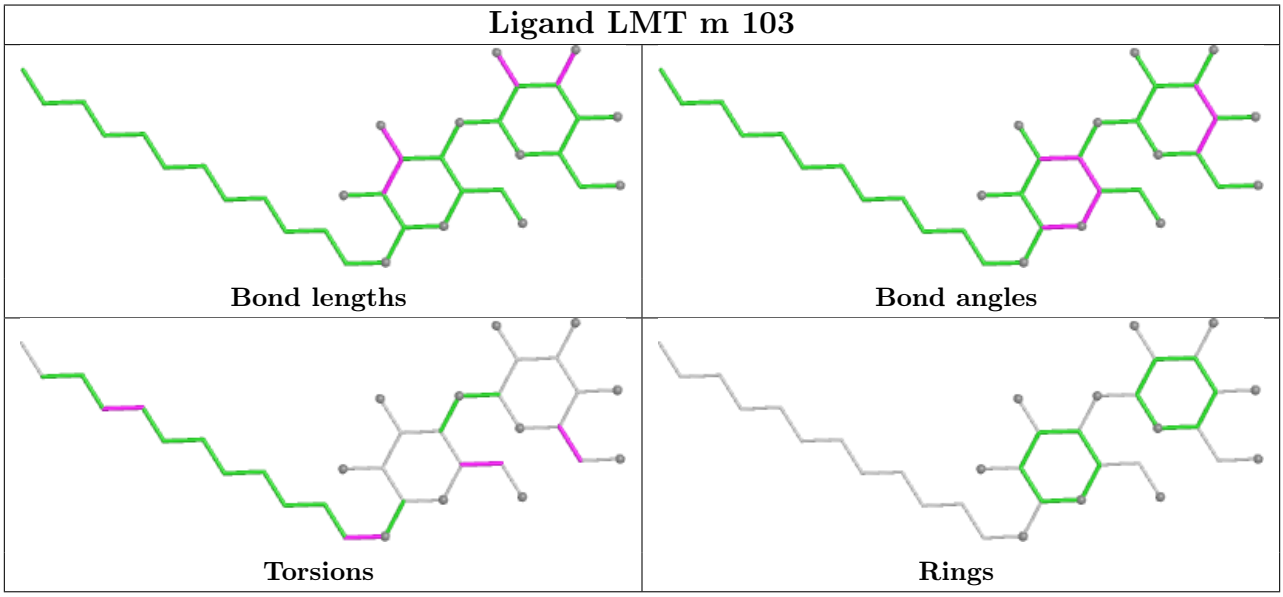


Rings

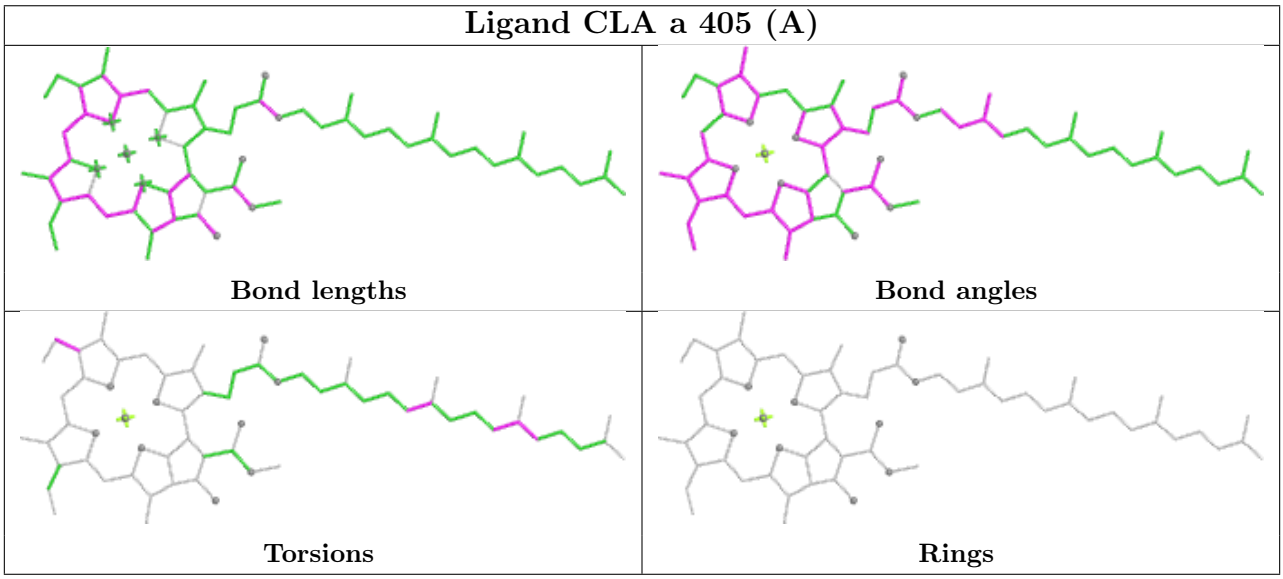
Ligand LMT B 627



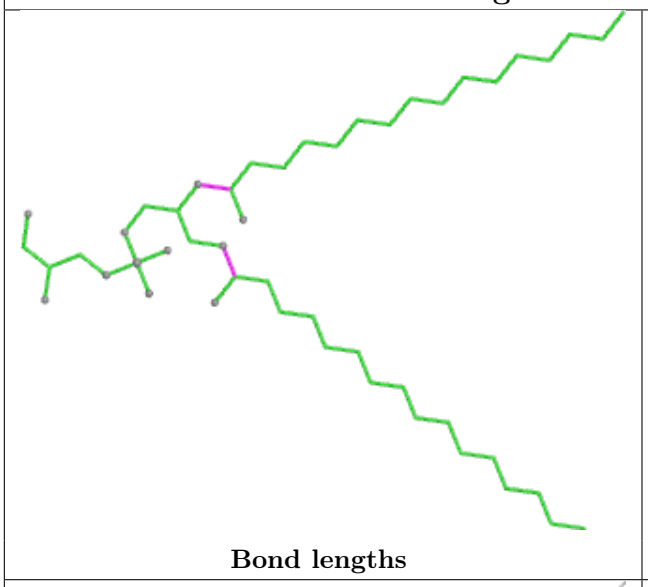
Ligand LMT m 103



Ligand CLA a 405 (A)



Ligand LHG d 408 (A)



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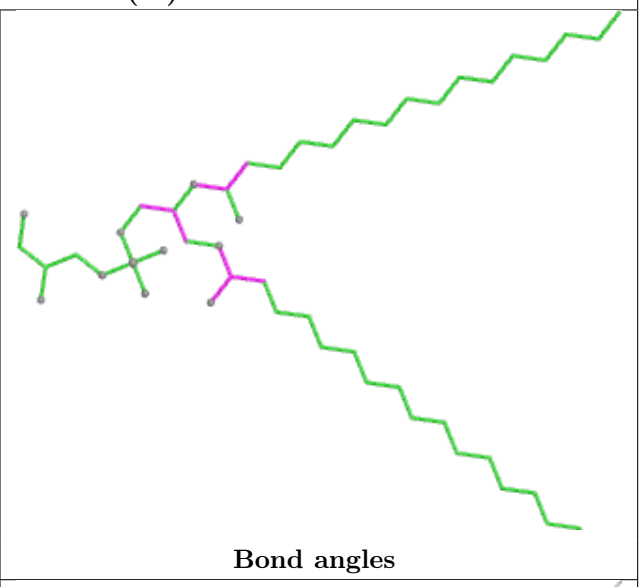
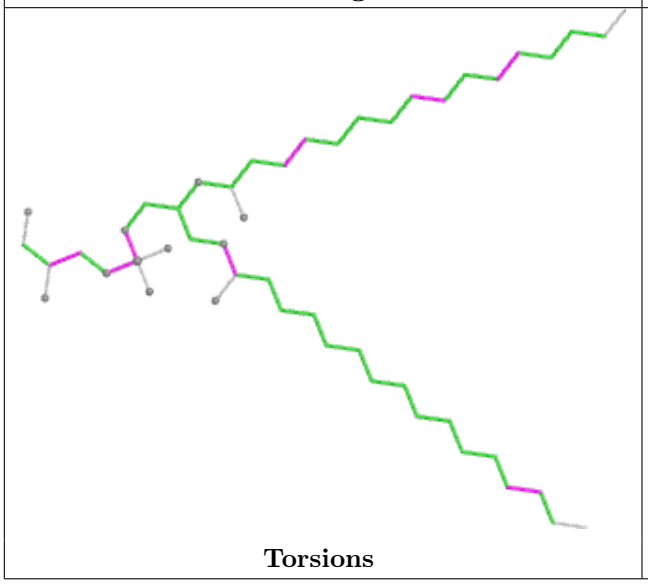
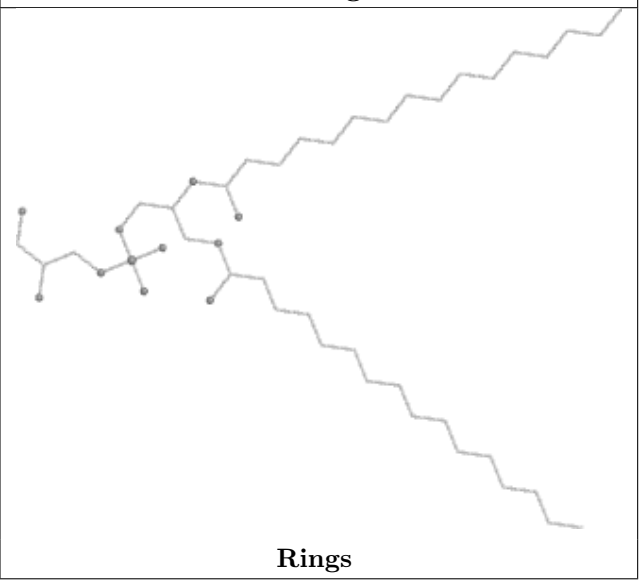


Bond angles

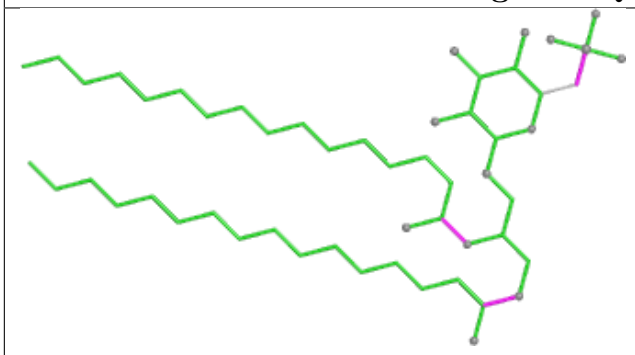


Torsions



Rings

Ligand SQD A 410 (A)



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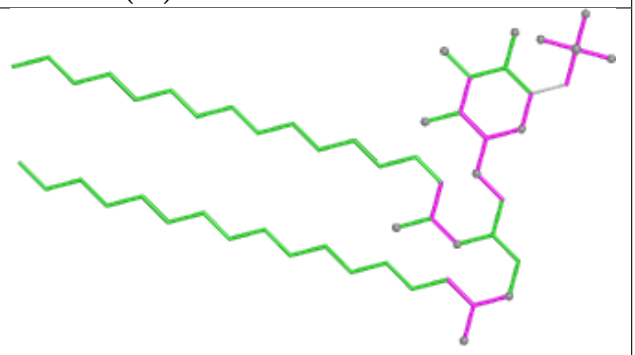
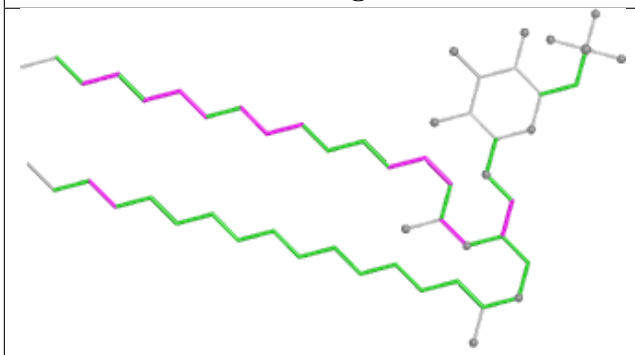


Bond angles



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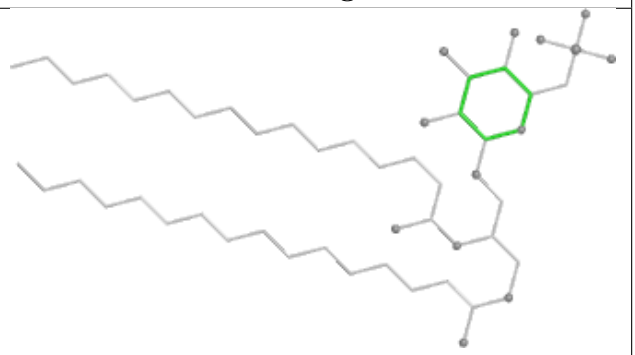
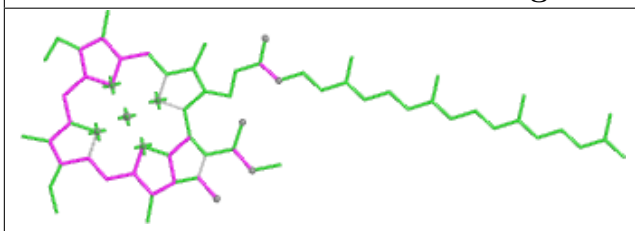


Rings

Ligand CLA c 513



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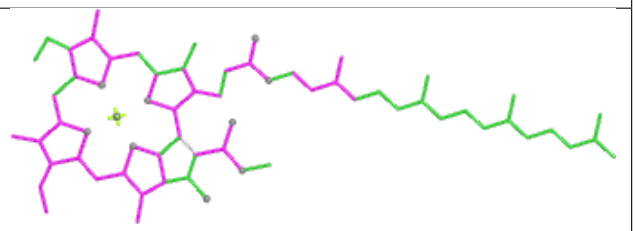
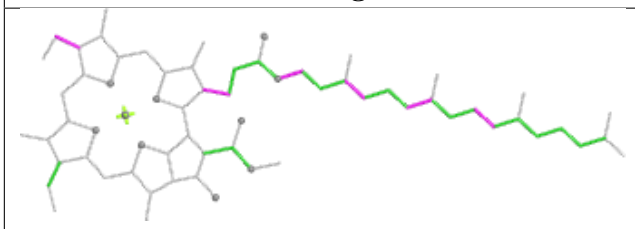


Bond angles



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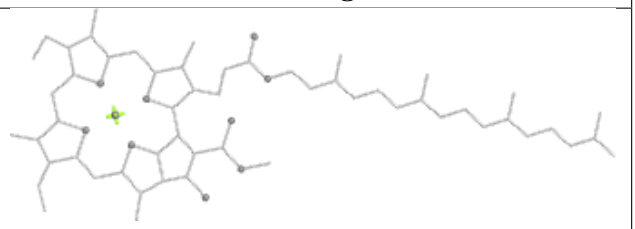
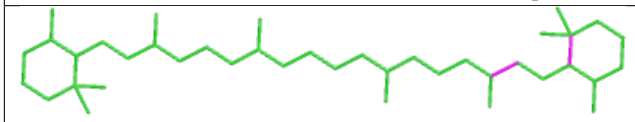


Rings

Ligand BCR d 406



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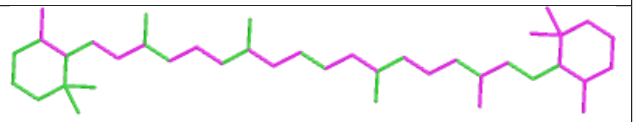
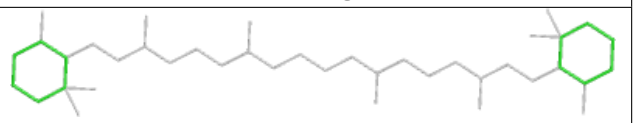


Bond angles

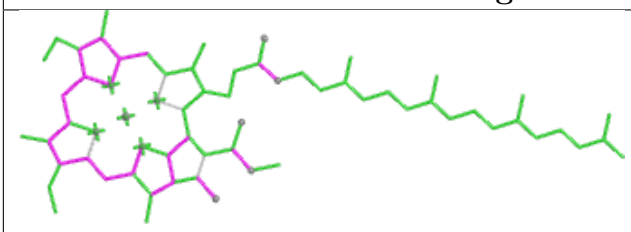


Torsions



Rings

Ligand CLA a 404 (B)



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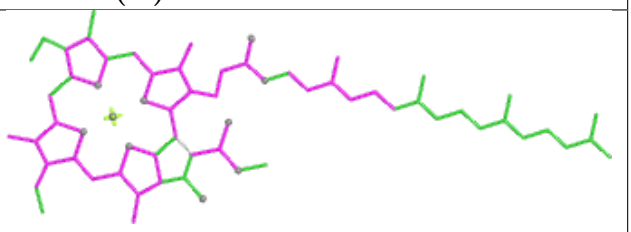
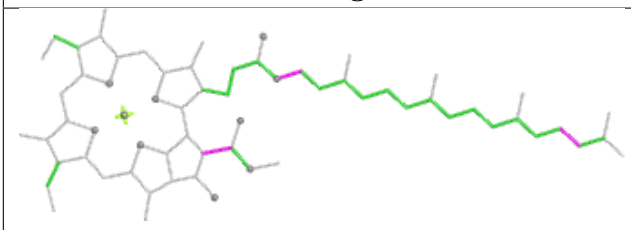


Bond angles



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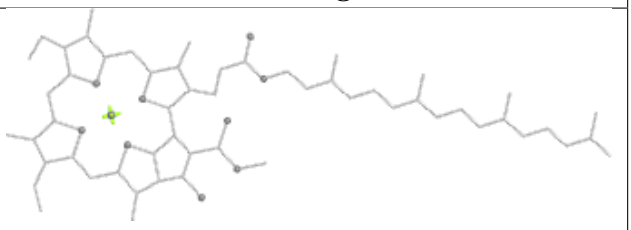
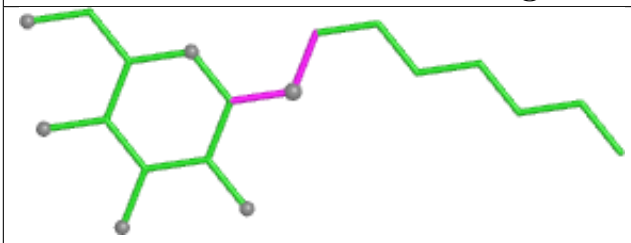


Rings

Ligand HTG B 624



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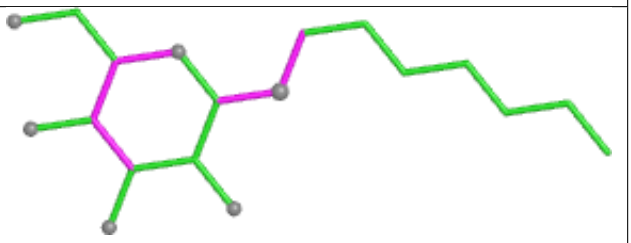
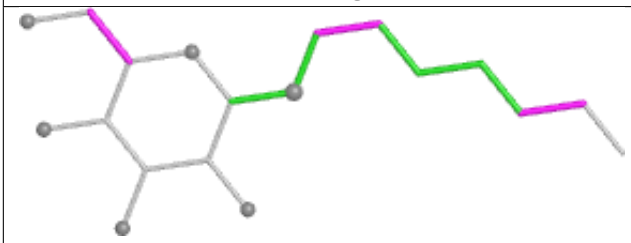


Bond angles



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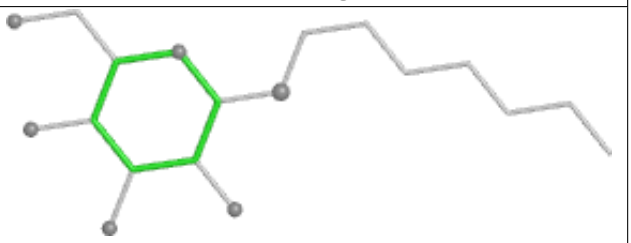
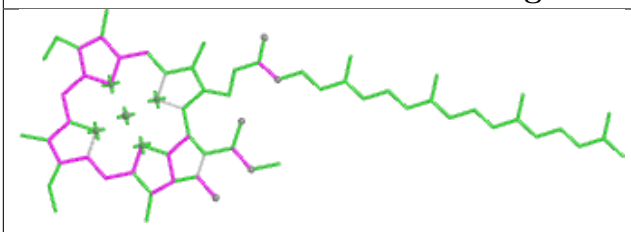


Rings

Ligand CLA B 613



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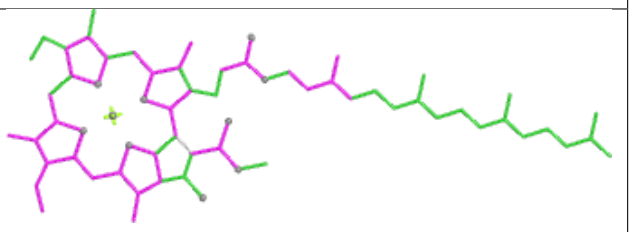
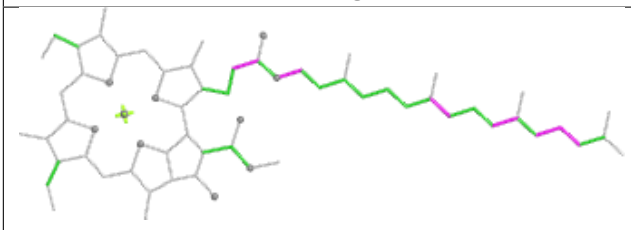


Bond angles



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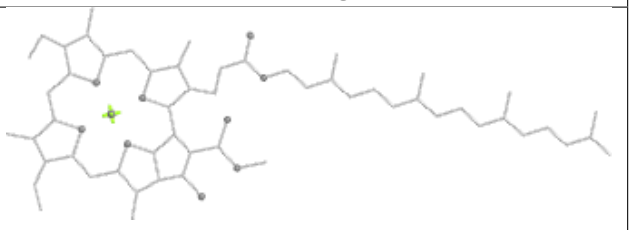
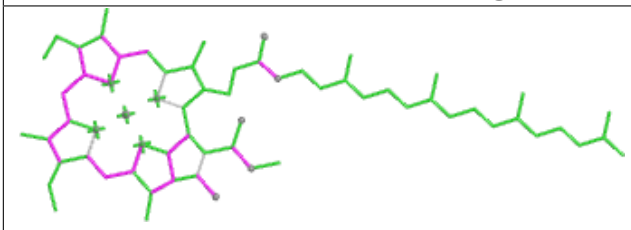


Rings

Ligand CLA A 405 (A)



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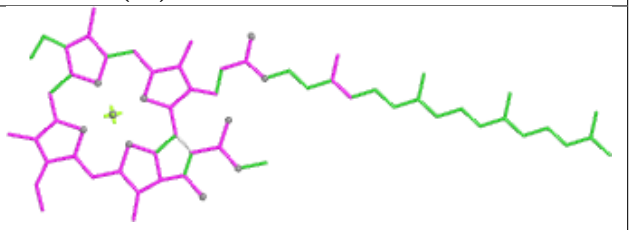
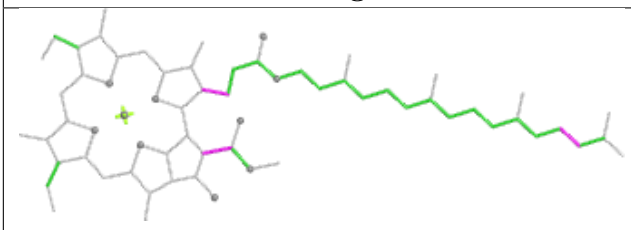


Bond angles



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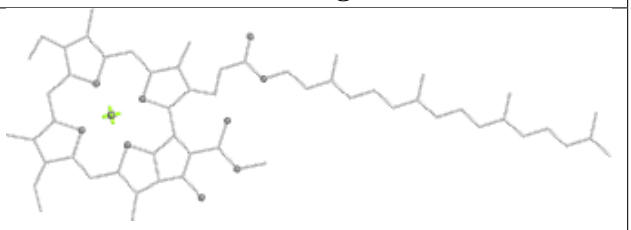


Rings

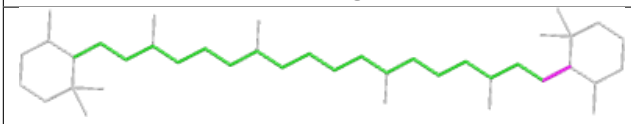
Ligand BCR c 514



Bond lengths



Bond angles



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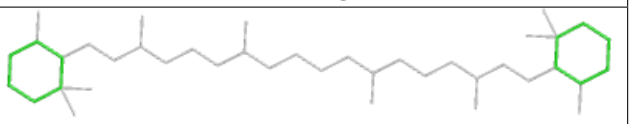
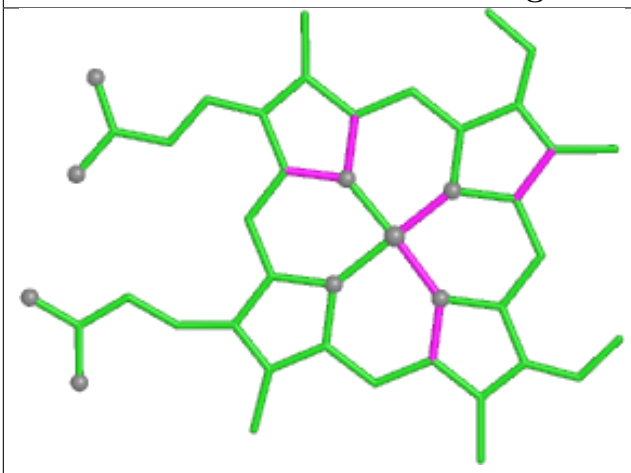
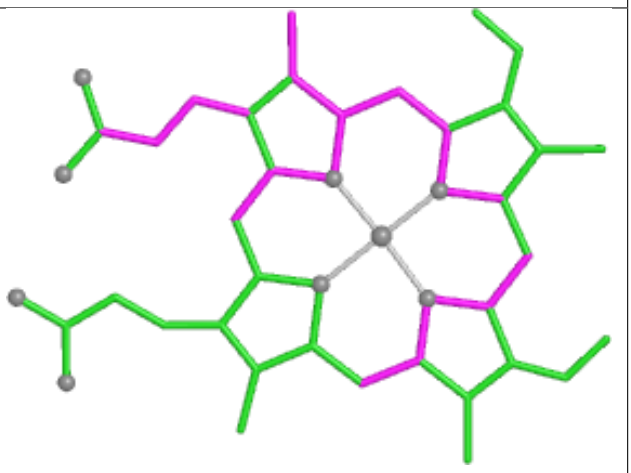


Rings

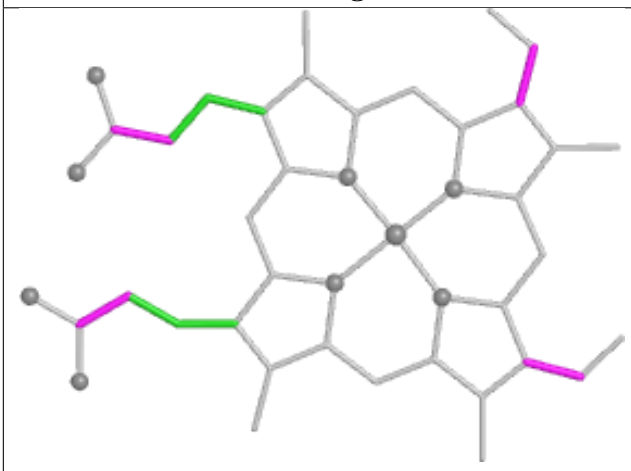
Ligand HEM f 101



Bond lengths



Bond angles



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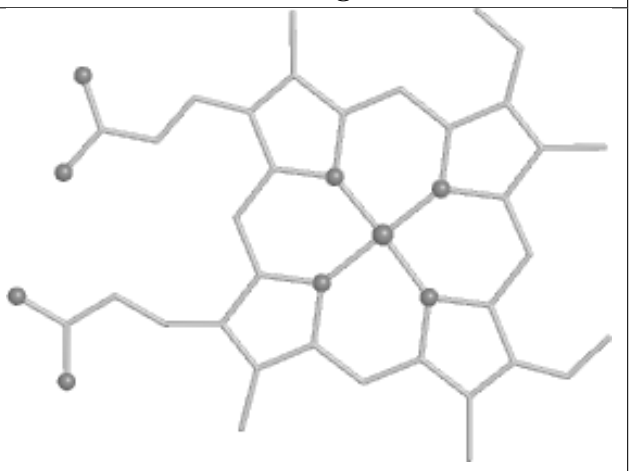
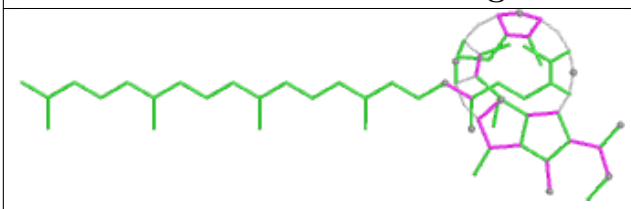
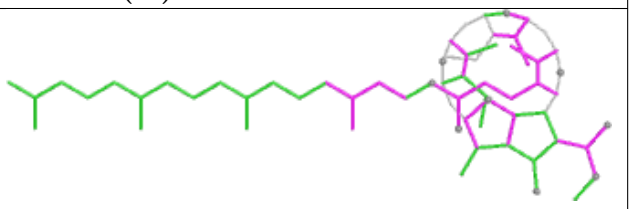


Rings

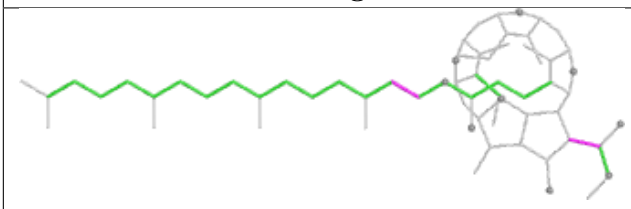
Ligand PHO A 407 (A)



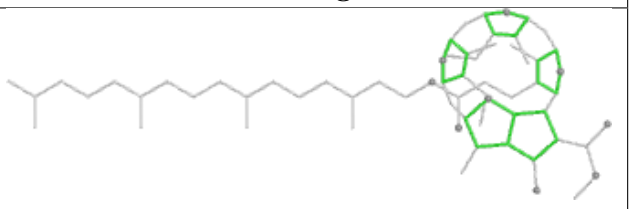
Bond lengths



Bond angles

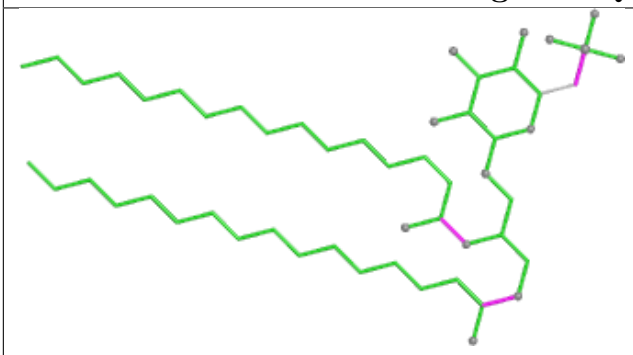


Torsions



Rings

Ligand SQD A 410 (B)



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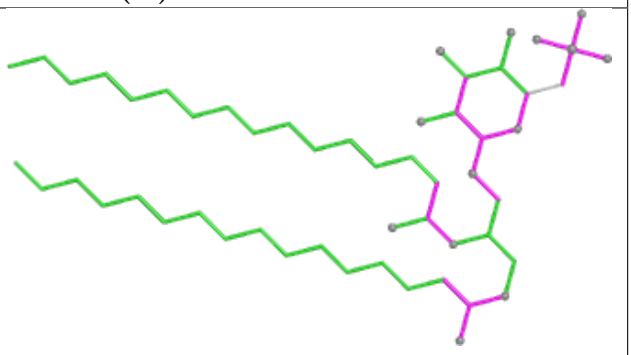
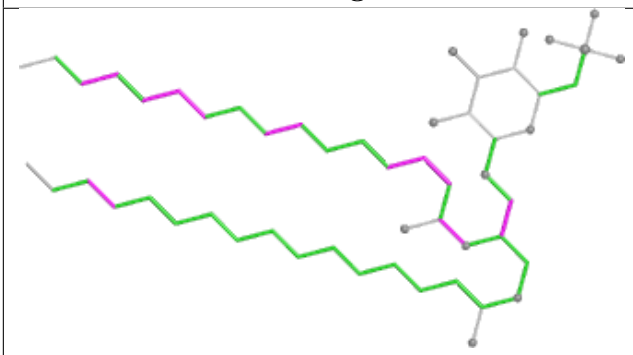


Bond angles



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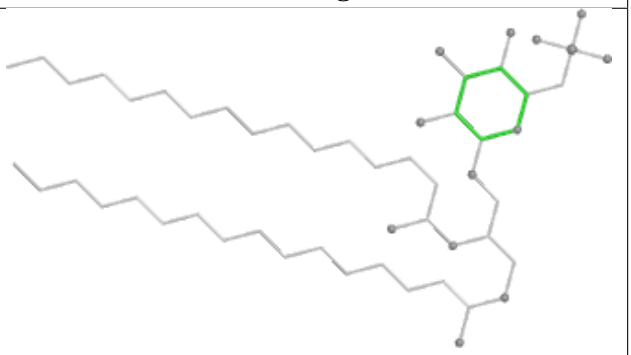
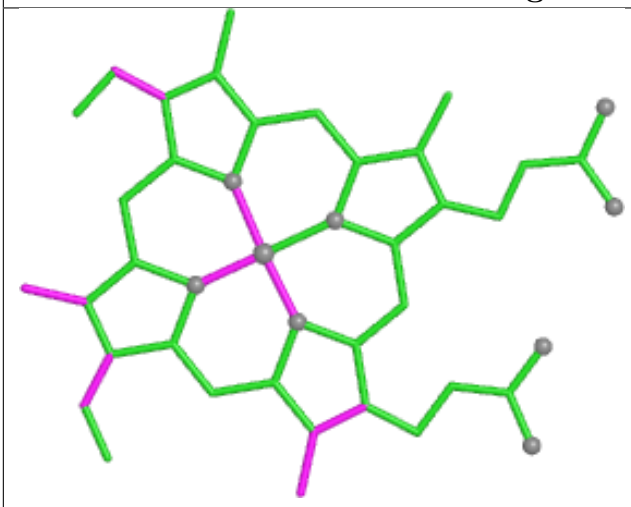


Rings

Ligand HEC v 201



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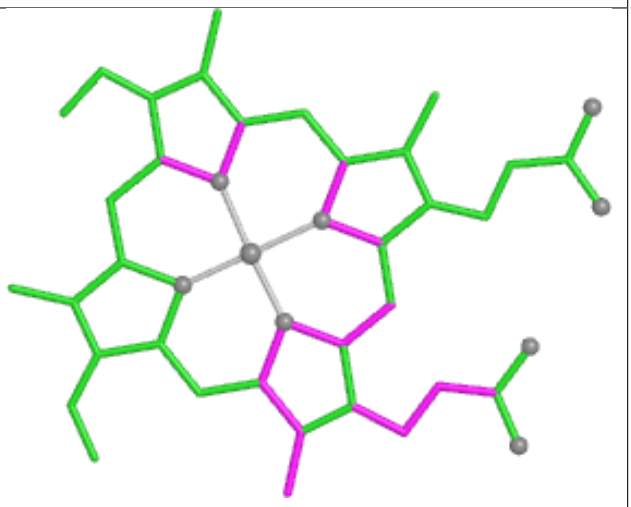
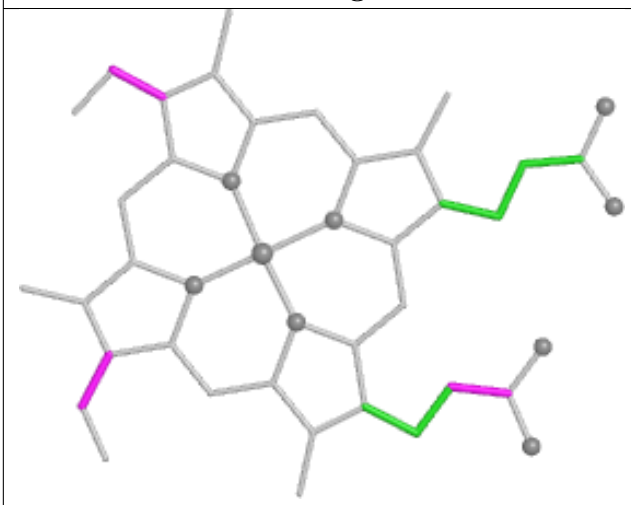


Bond angles



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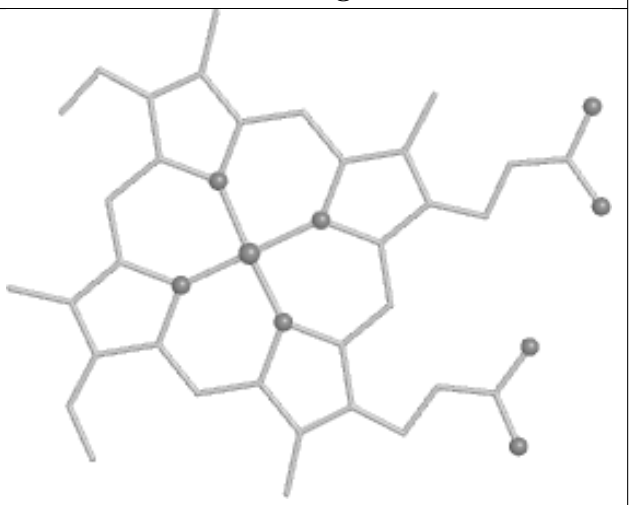
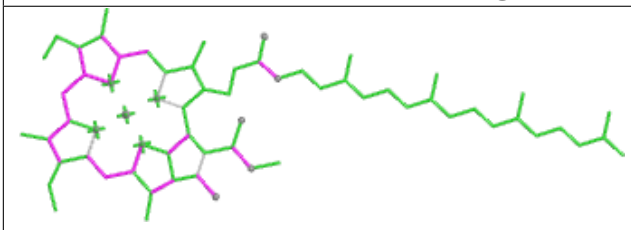


Rings

Ligand CLA d 402 (A)



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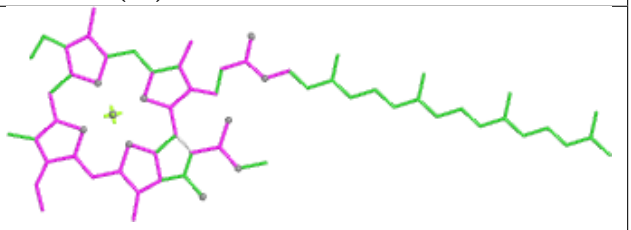
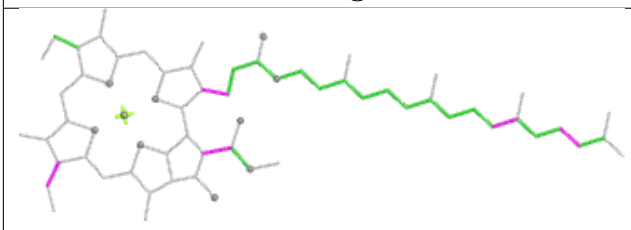


Bond angles



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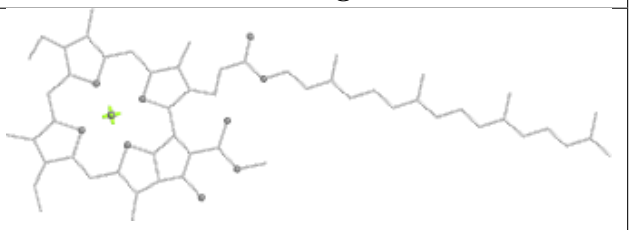
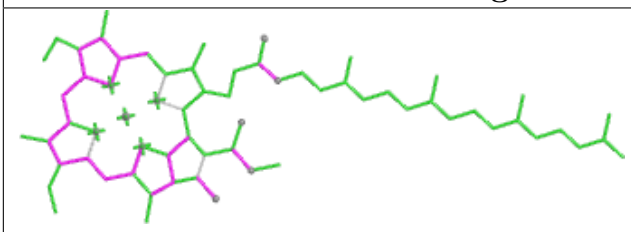


Rings

Ligand CLA A 405 (B)



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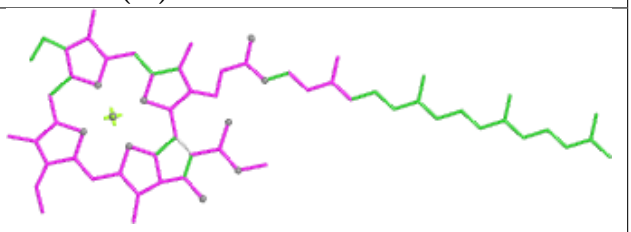
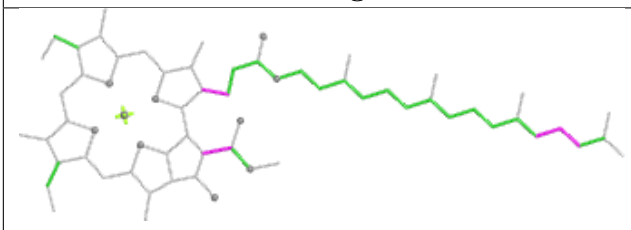


Bond angles



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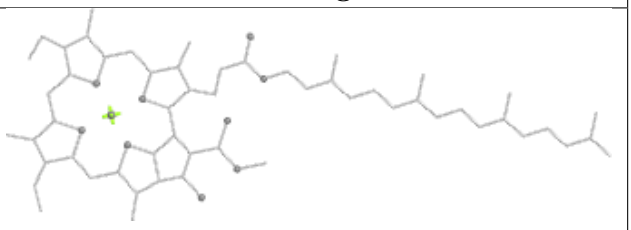
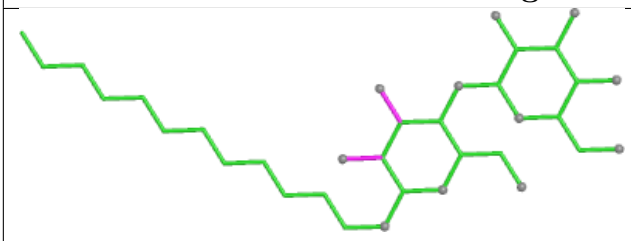


Rings

Ligand LMT B 628



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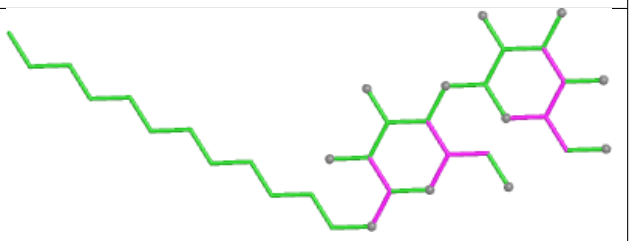
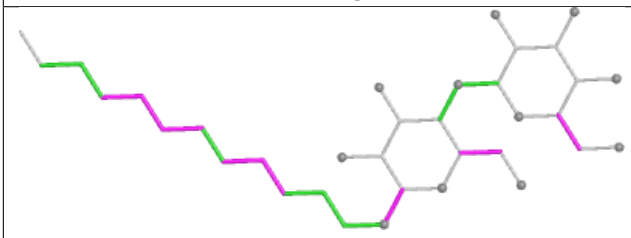


Bond angles



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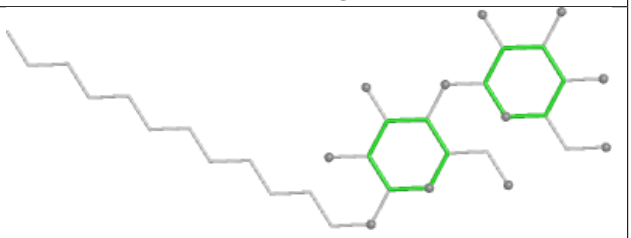
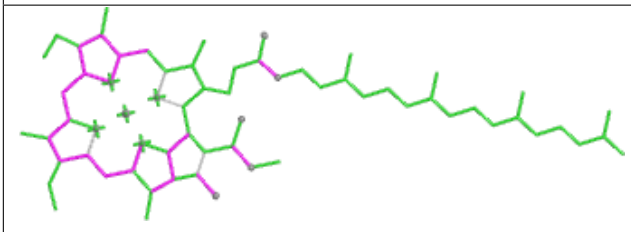


Rings

Ligand CLA C 511



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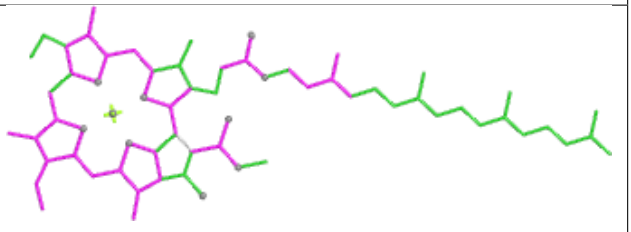
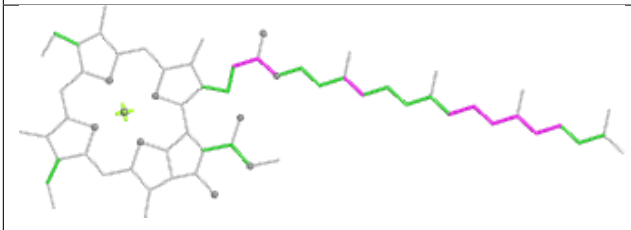


Bond angles



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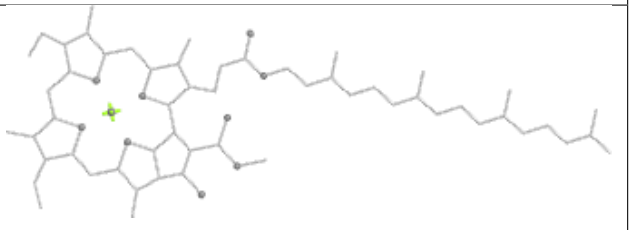
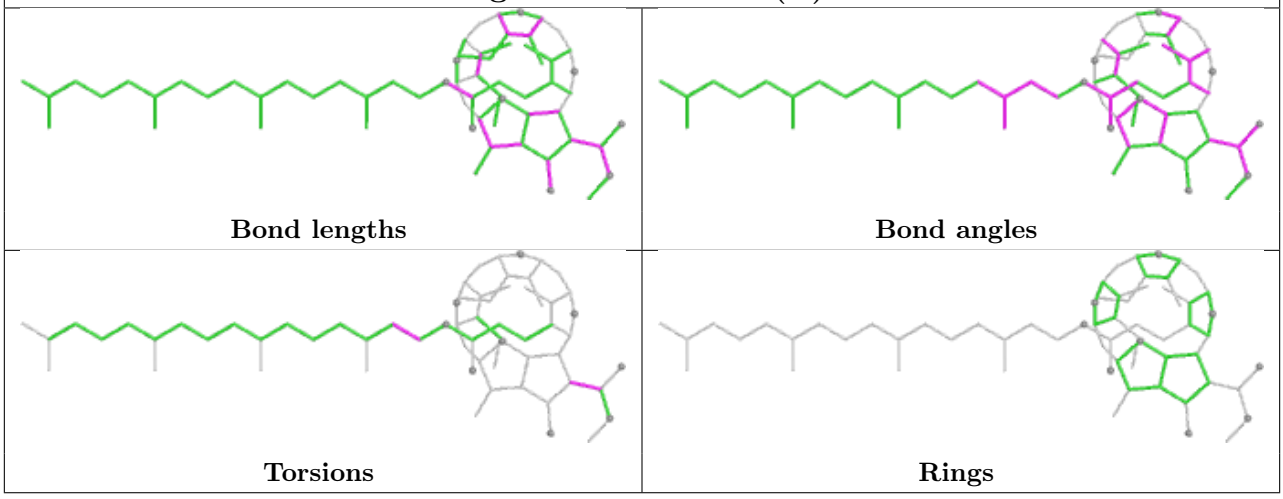
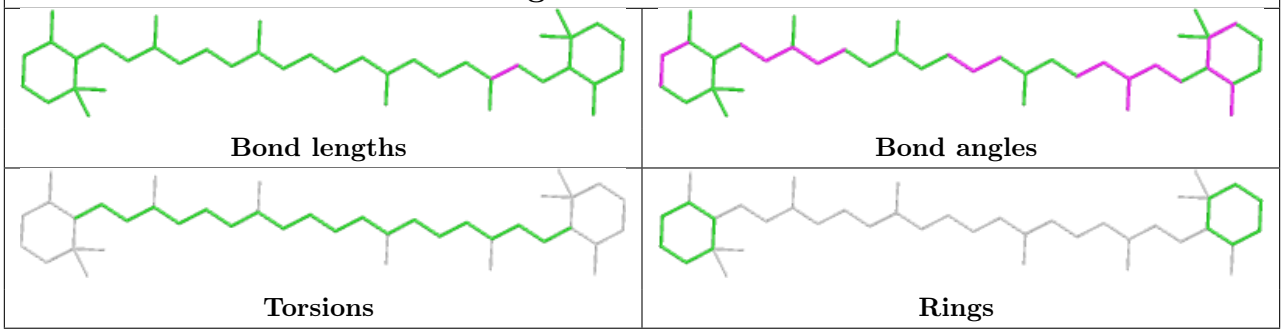


Rings

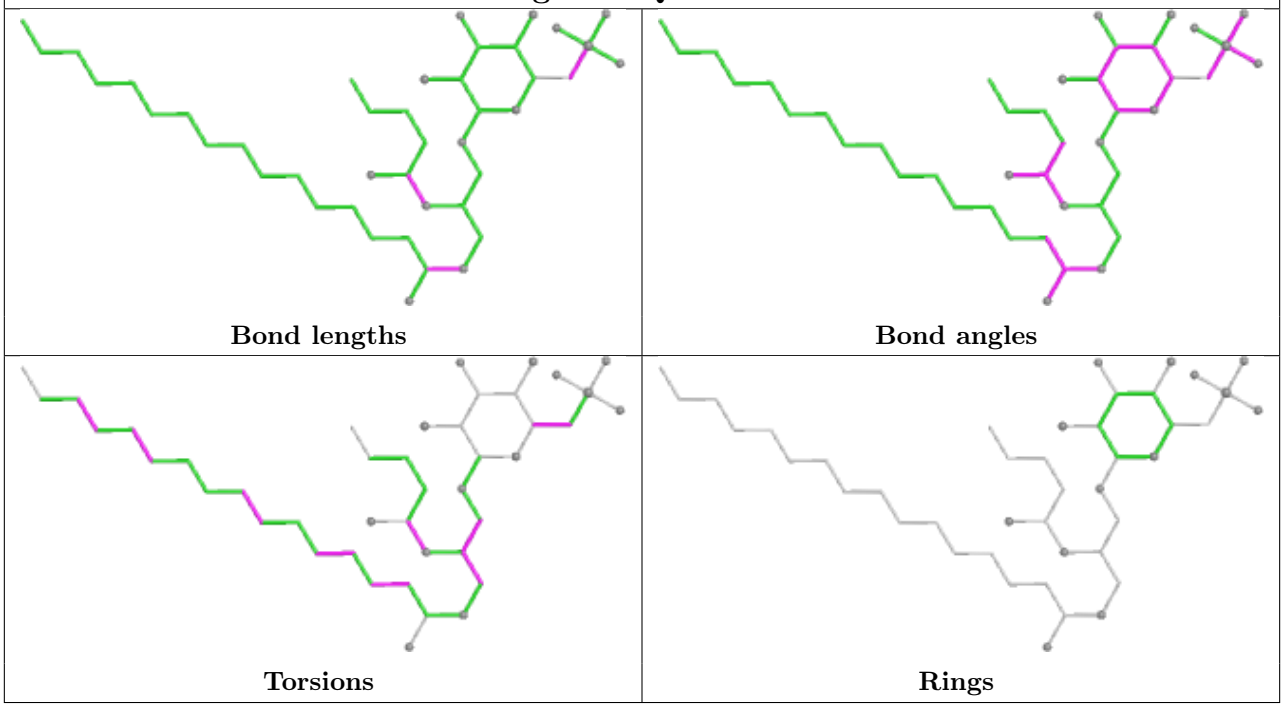
Ligand PHO A 407 (B)



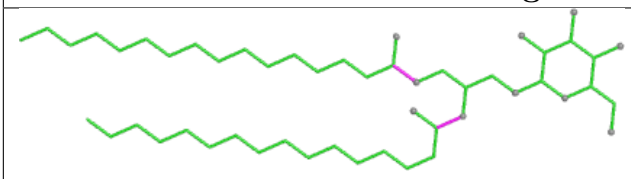
Ligand BCR a 408



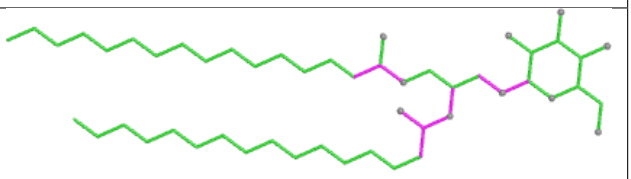
Ligand SQD f 102



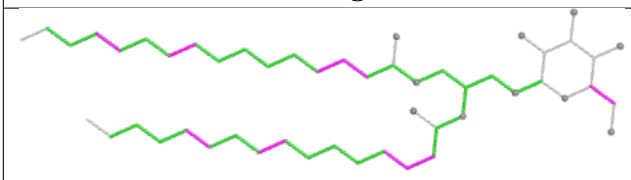
Ligand LMG d 413



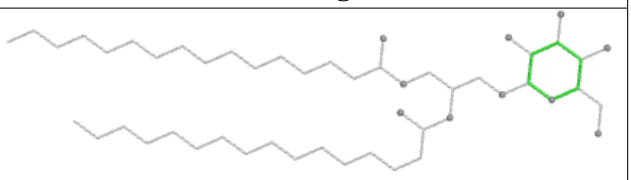
Bond lengths



Bond angles

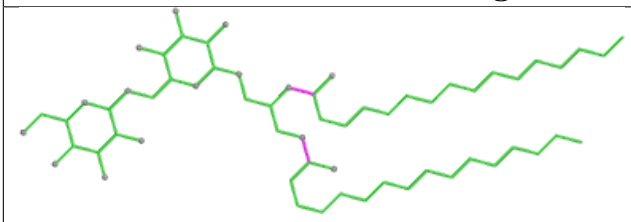


Torsions



Rings

Ligand DGD c 516 (B)



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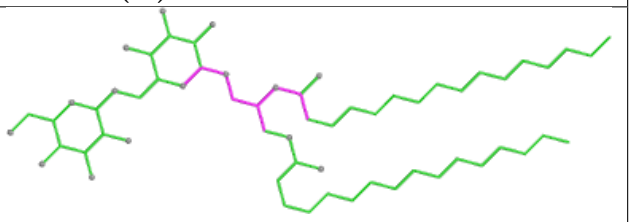
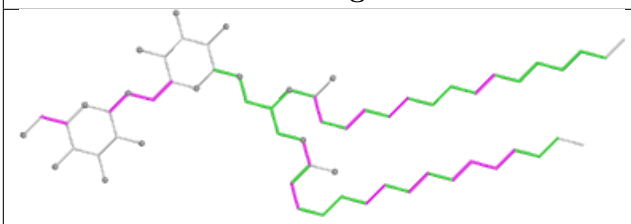


Bond angles



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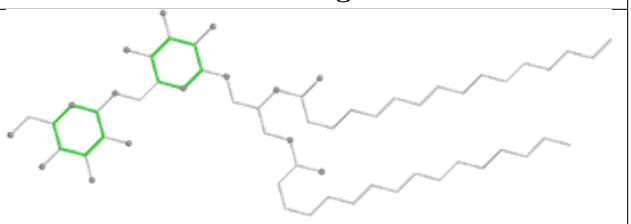
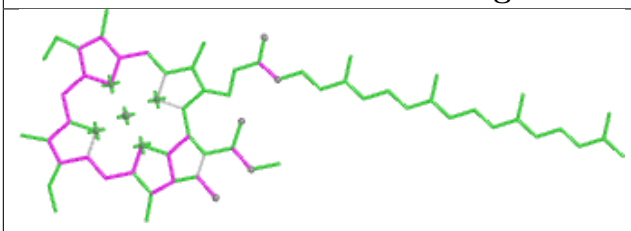


Rings

Ligand CLA d 404 (A)



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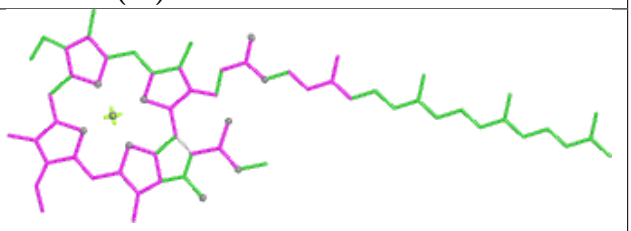
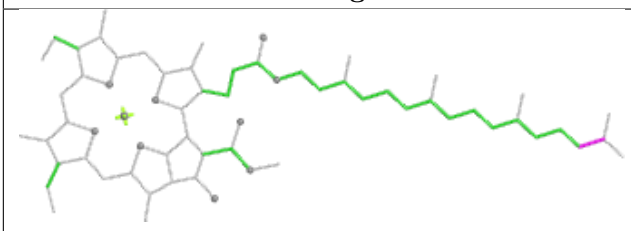


Bond angles



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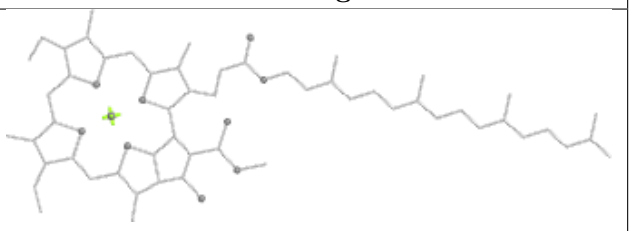
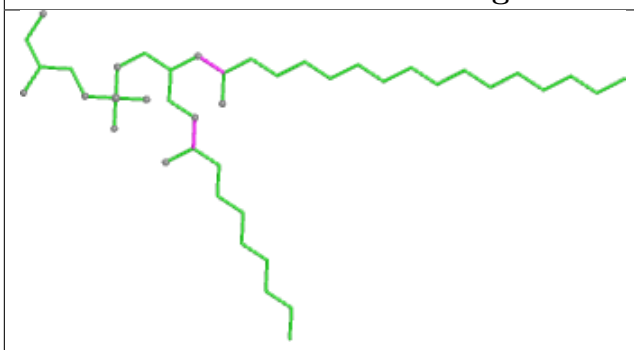


Rings

Ligand LHG E 101 (B)



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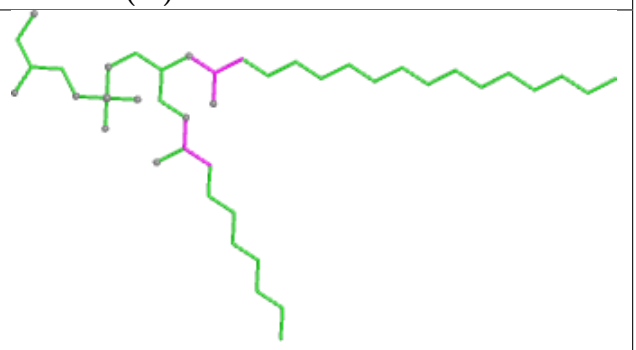
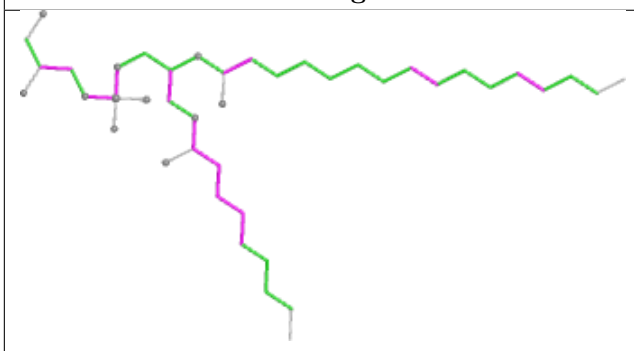


Bond angles



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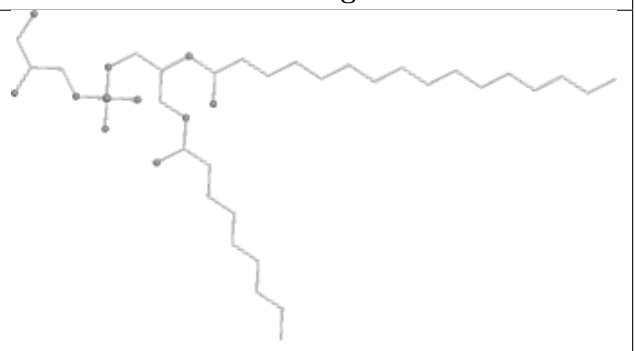
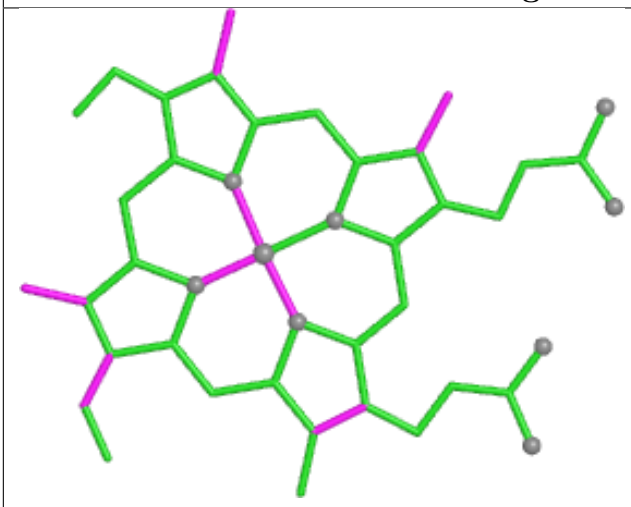


Rings

Ligand HEC V 201



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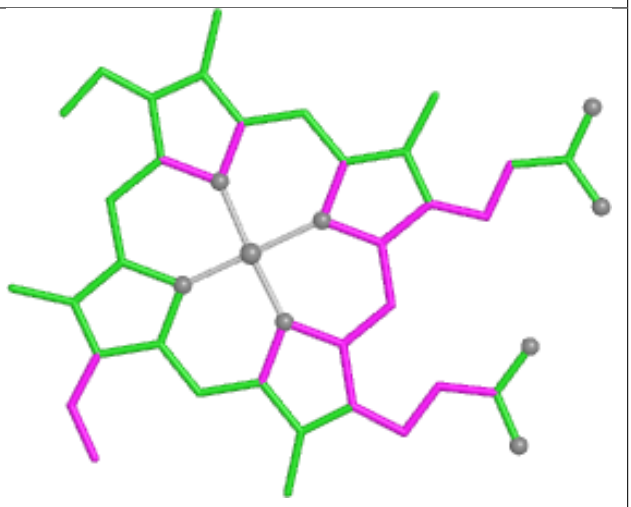
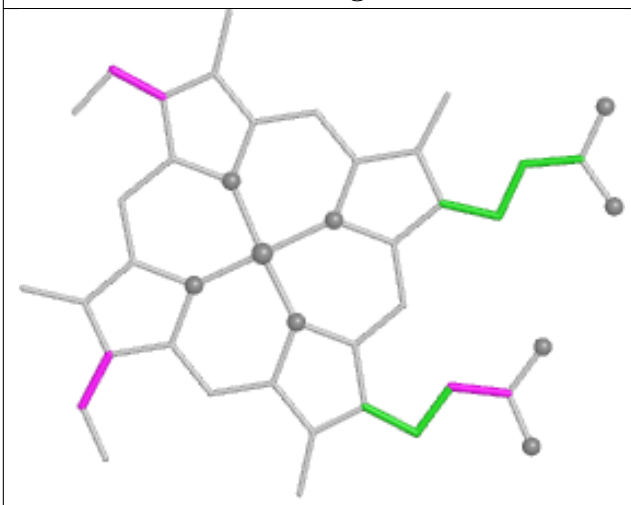


Bond angles



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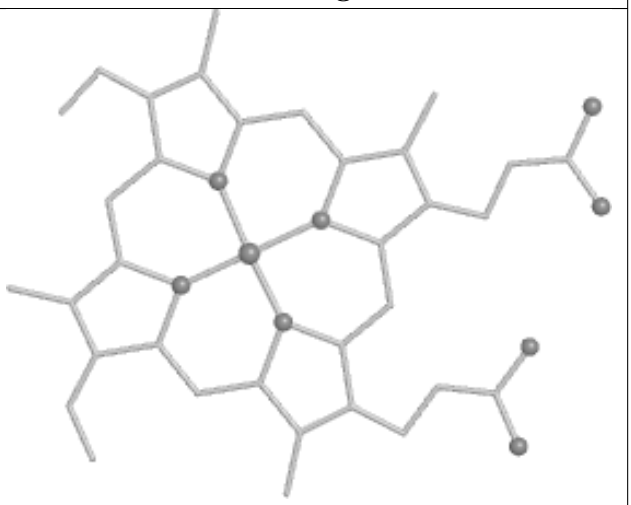
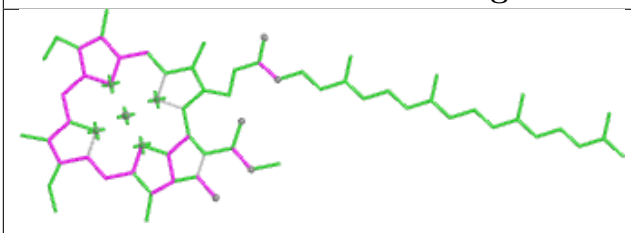


Rings

Ligand CLA D 402 (B)



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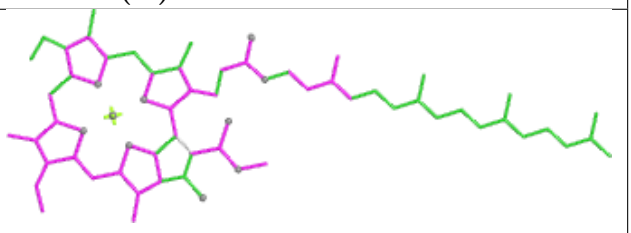
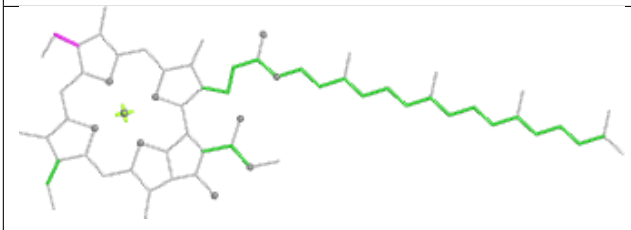


Bond angles



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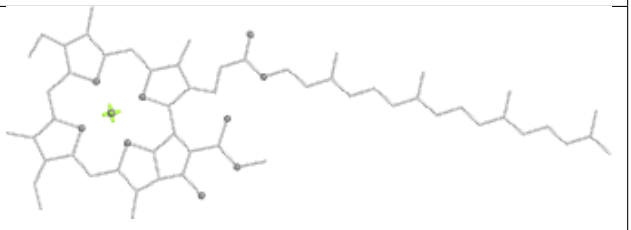
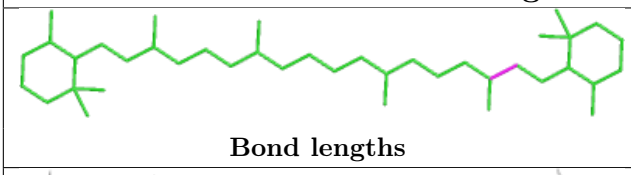
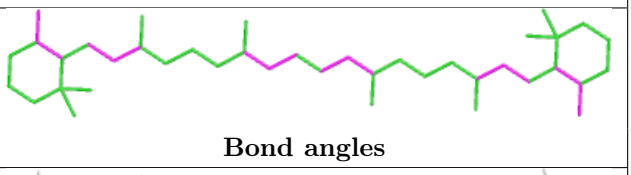


Rings

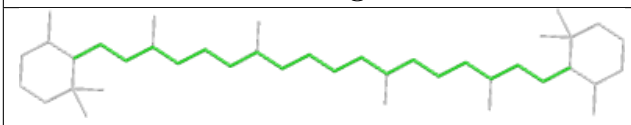
Ligand BCR C 515



Bond lengths



Bond angles



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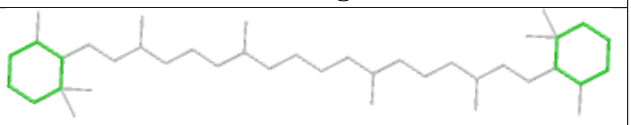
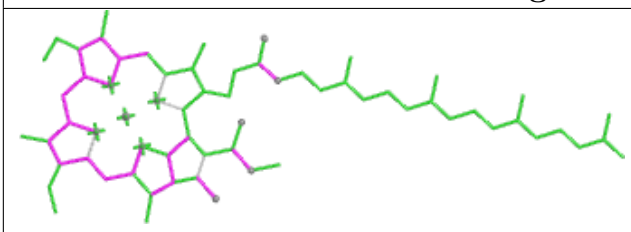
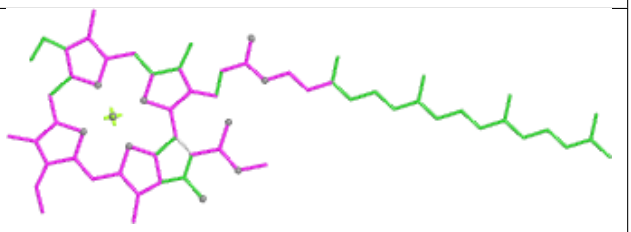


Rings

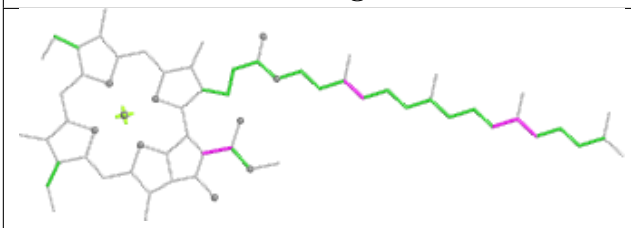
Ligand CLA c 504



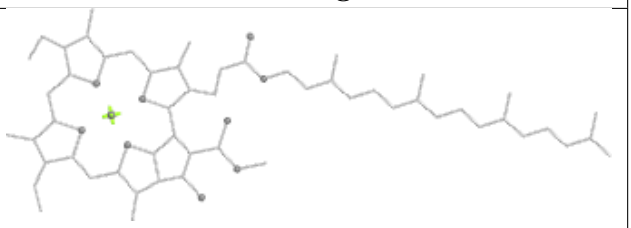
Bond lengths



Bond angles

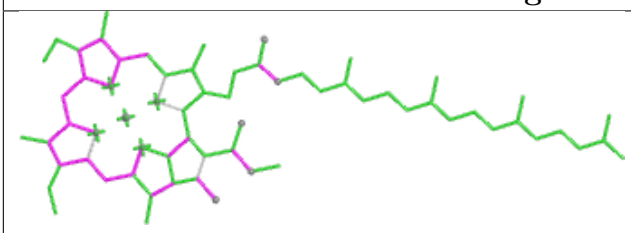


Torsions



Rings

Ligand CLA B 612



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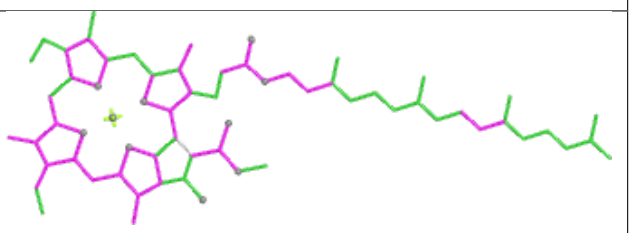
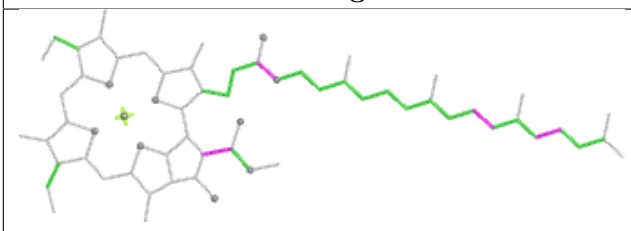


Bond angles



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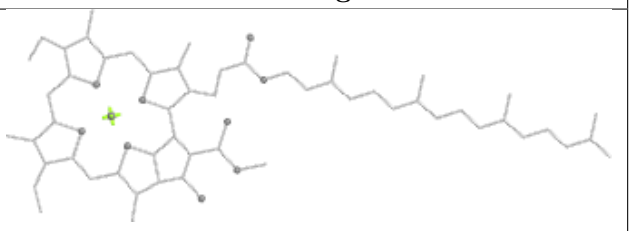
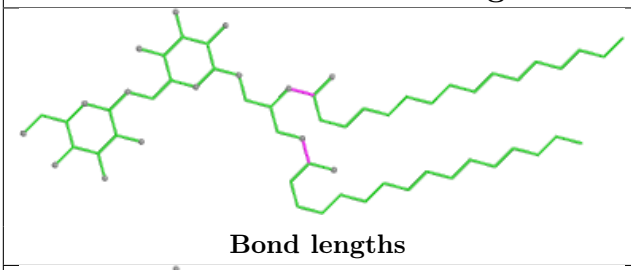


Rings

Ligand DGD C 518 (B)



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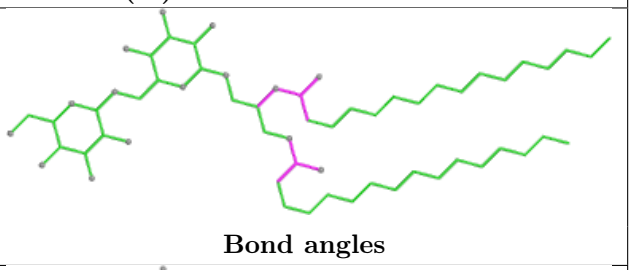
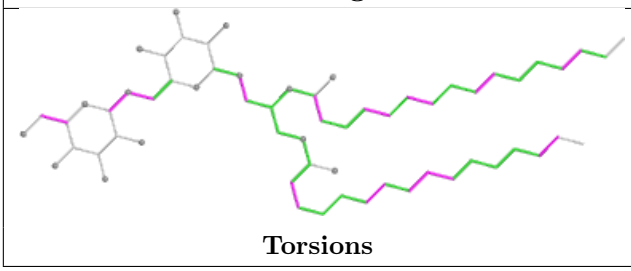


Bond angles



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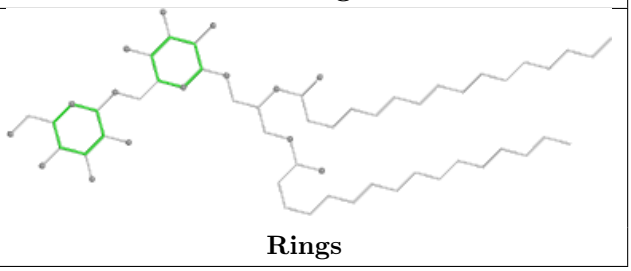
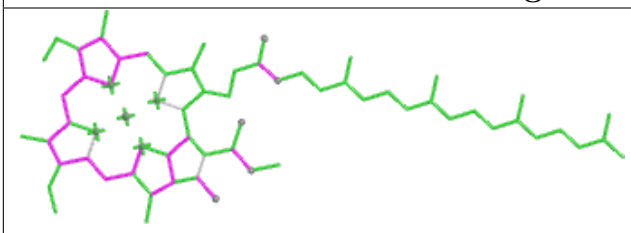


Rings

Ligand CLA C 503



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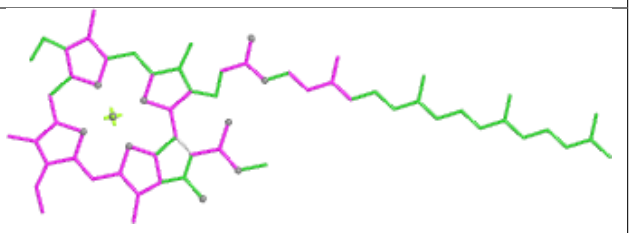
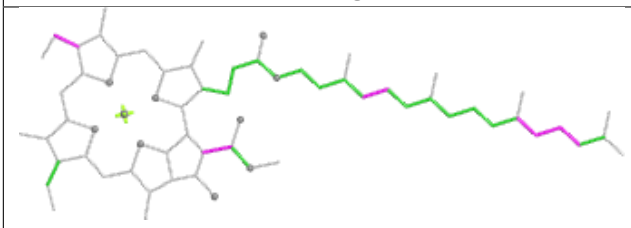


Bond angles



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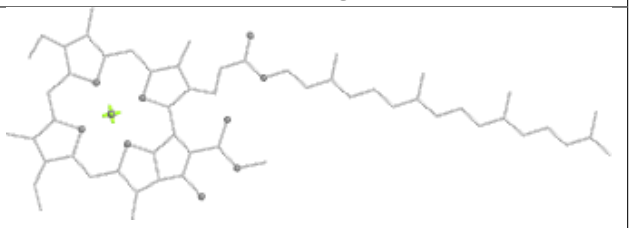
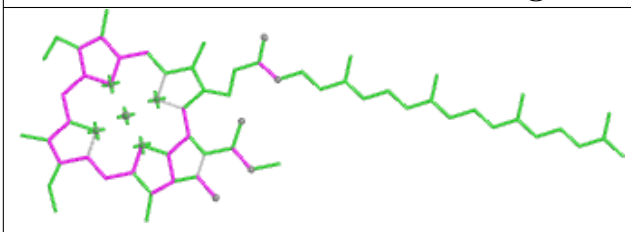


Rings

Ligand CLA b 607



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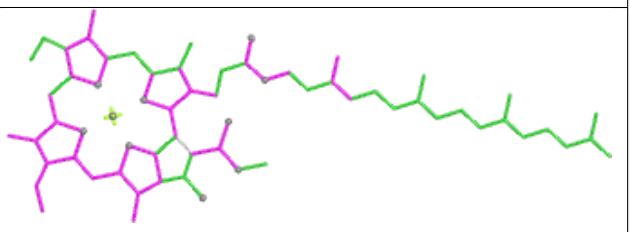
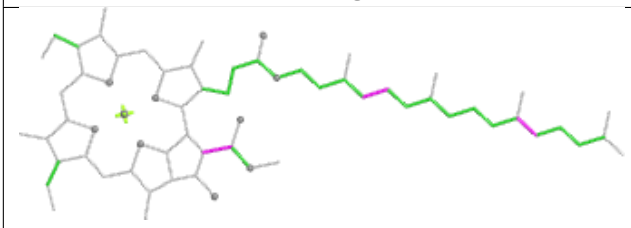


Bond angles



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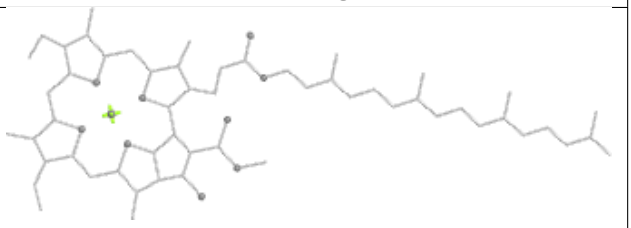
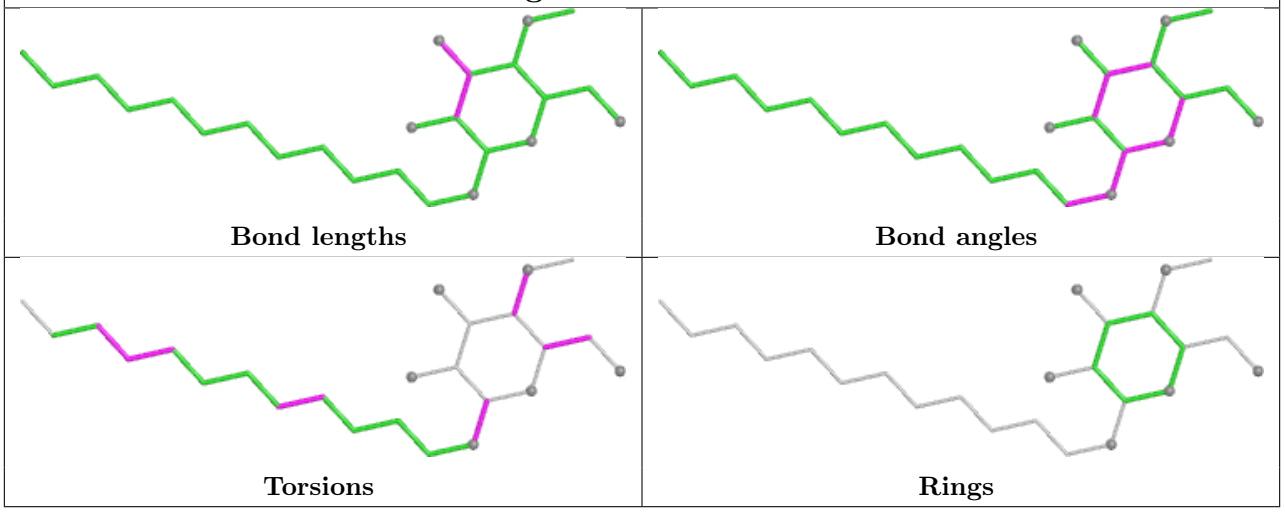
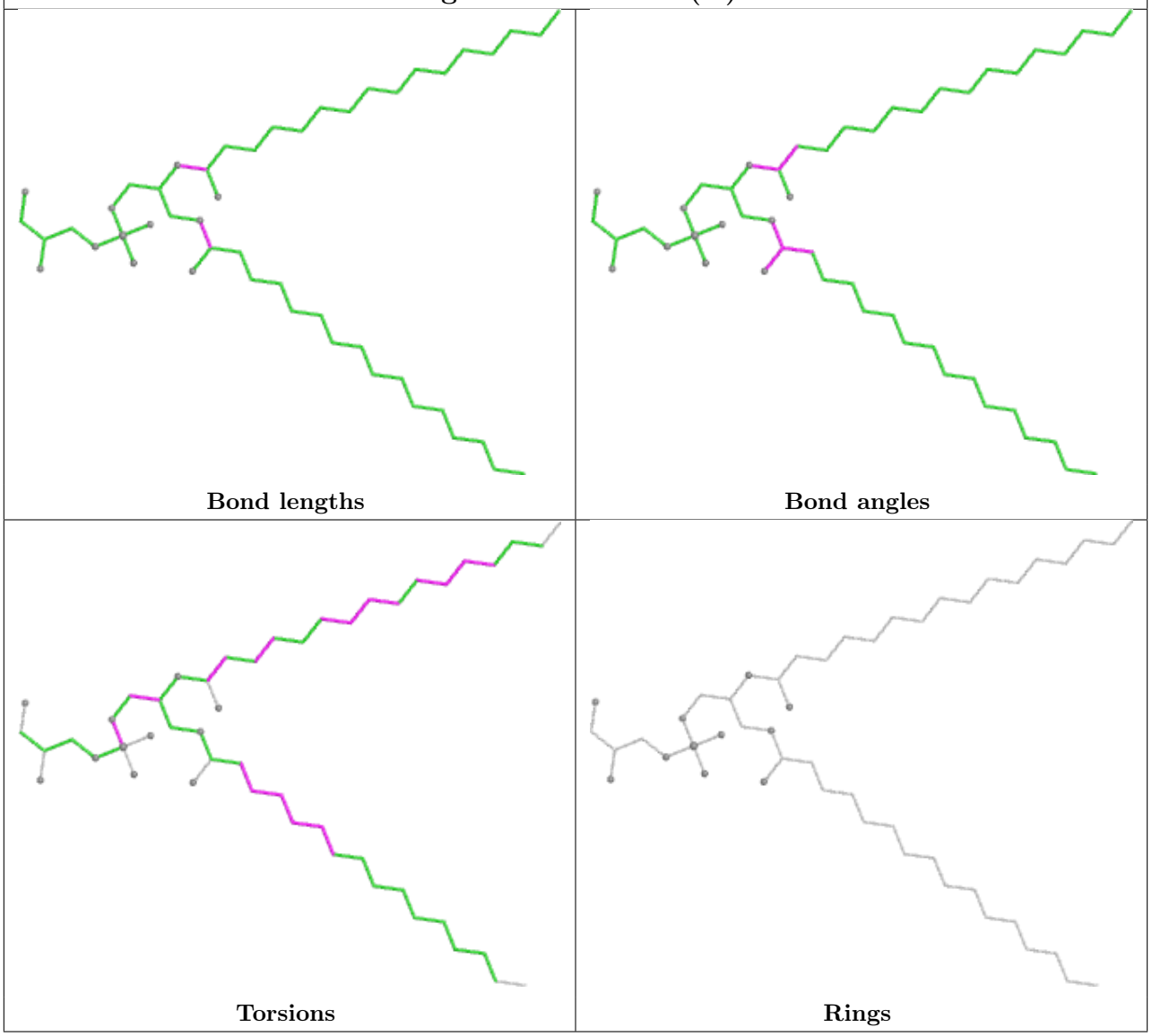


Rings

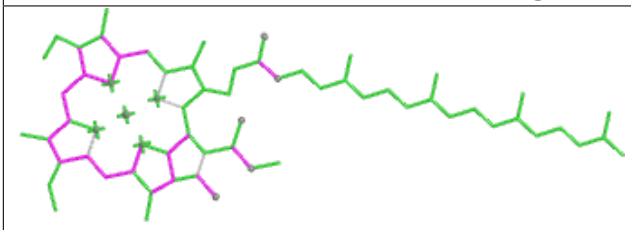
Ligand LMT b 621



Ligand LHG L 101 (A)



Ligand CLA c 505



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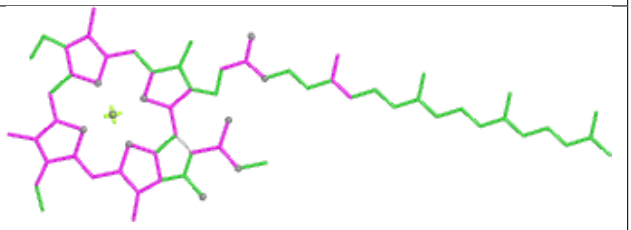
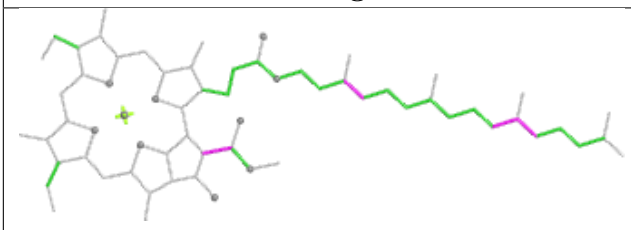


Bond angles



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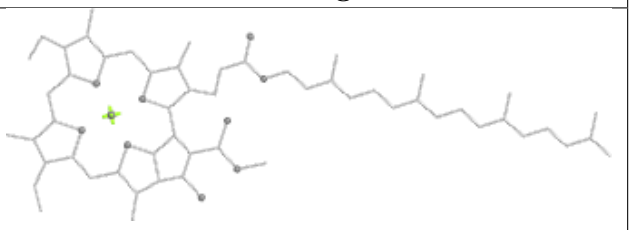
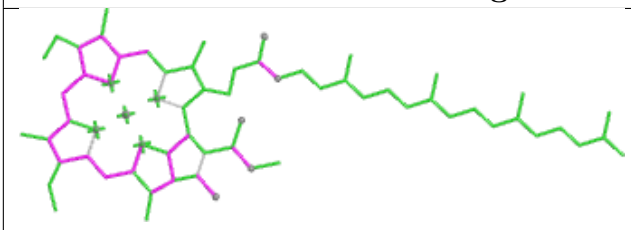


Rings

Ligand CLA A 404 (A)



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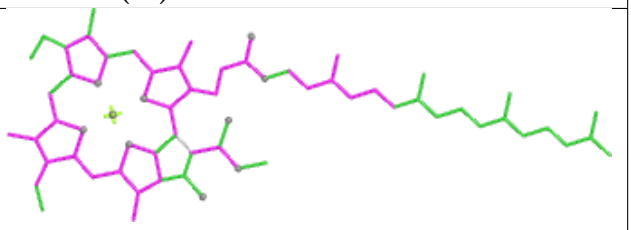
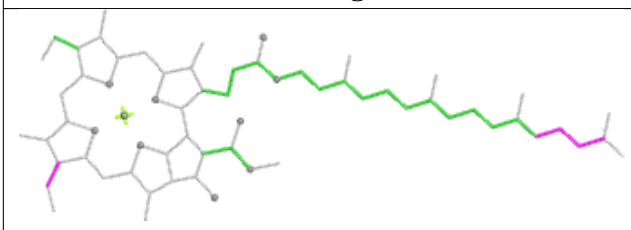


Bond angles



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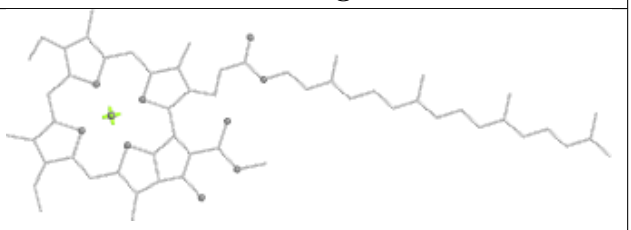
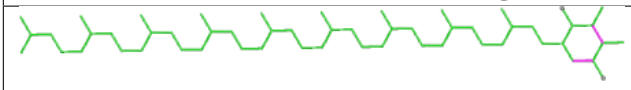


Rings

Ligand PL9 A 414 (A)



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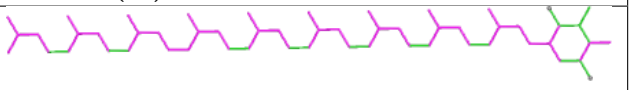
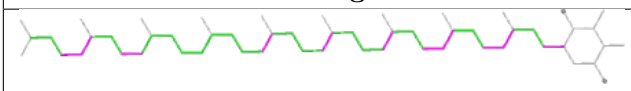
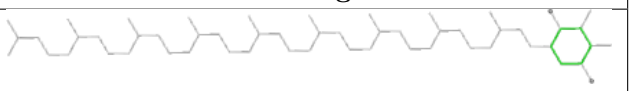


Bond angles

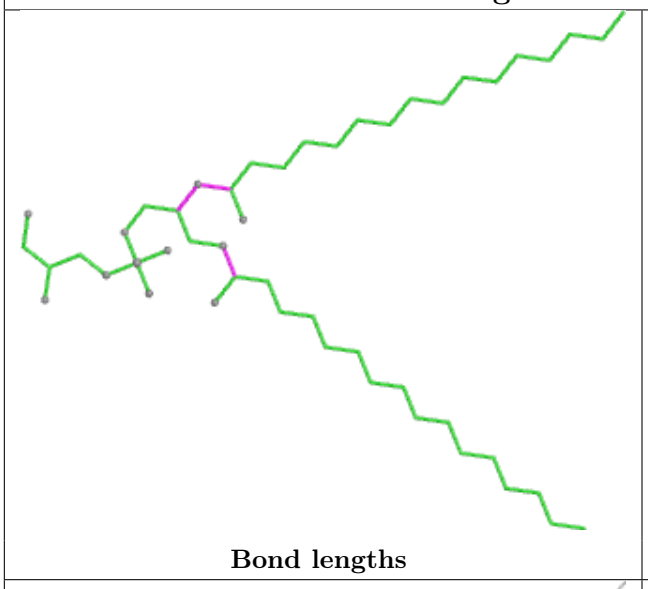


Torsions



Rings

Ligand LHG L 101 (B)



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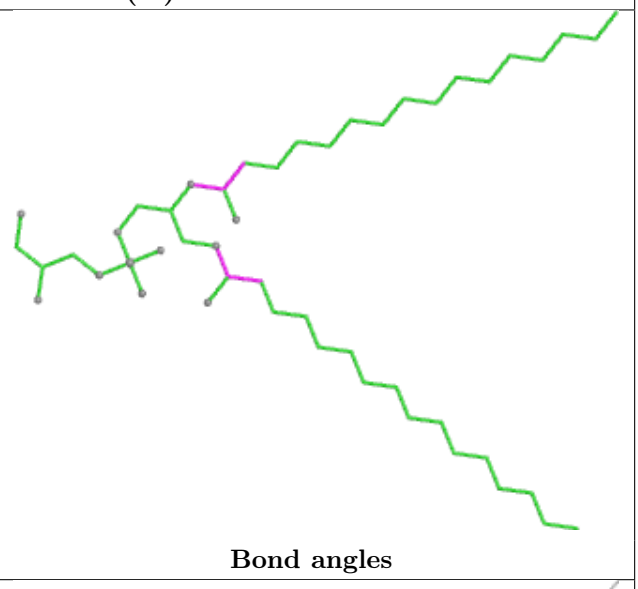
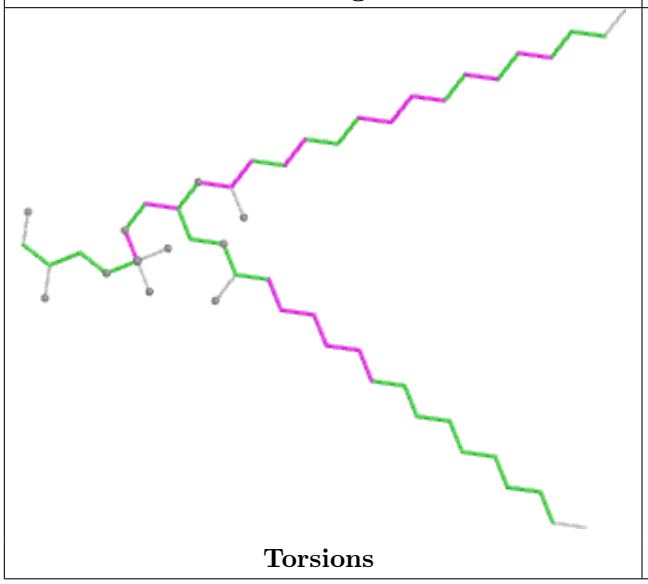


Bond angles



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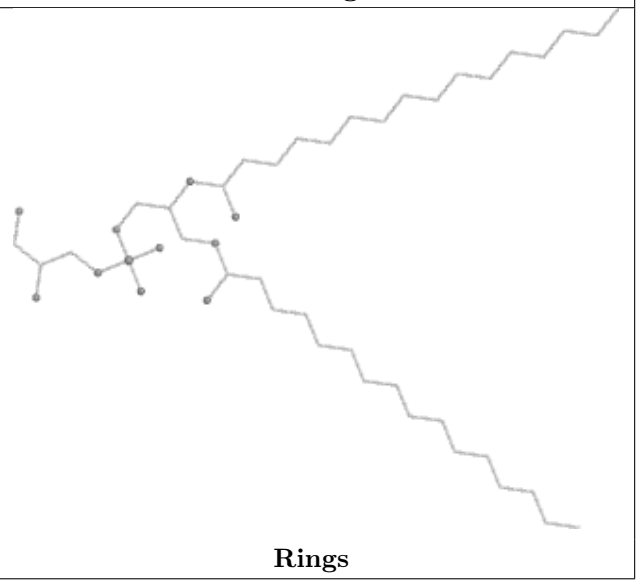
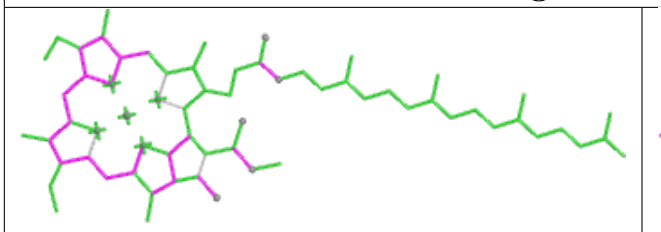


Rings

Ligand CLA c 506



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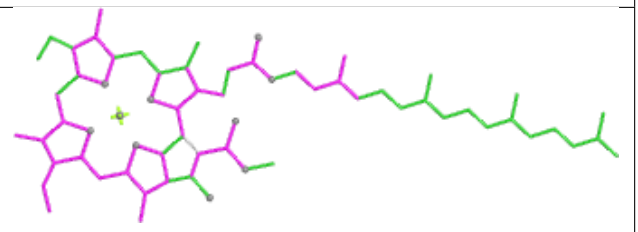
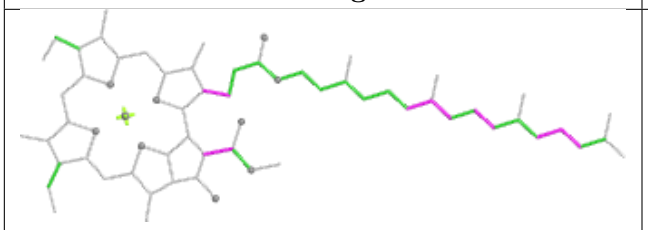


Bond angles



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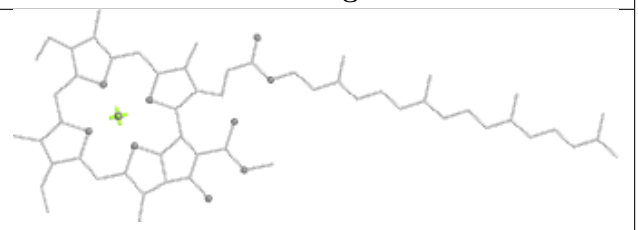
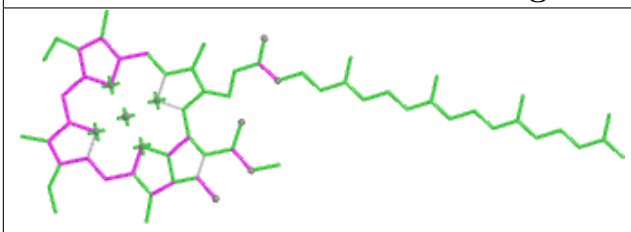


Rings

Ligand CLA c 511



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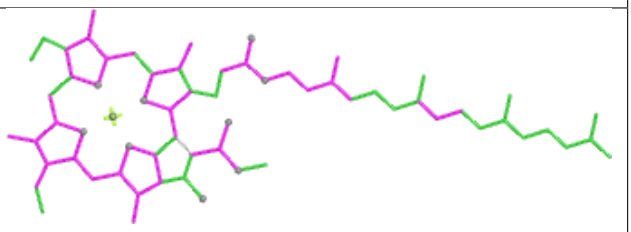
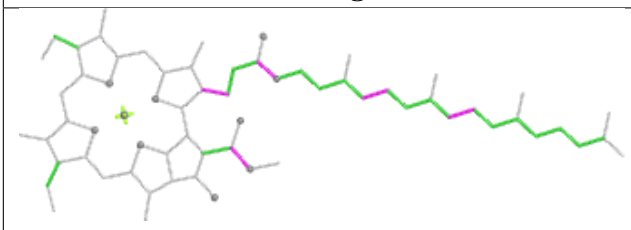


Bond angles



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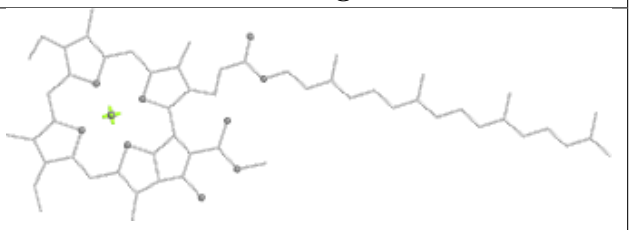
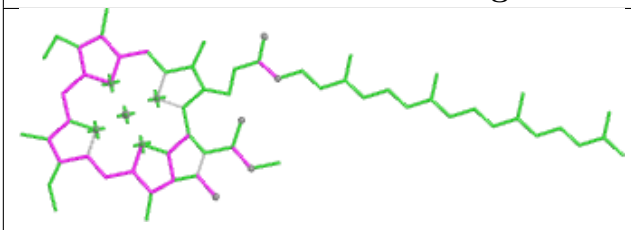


Rings

Ligand CLA A 404 (B)



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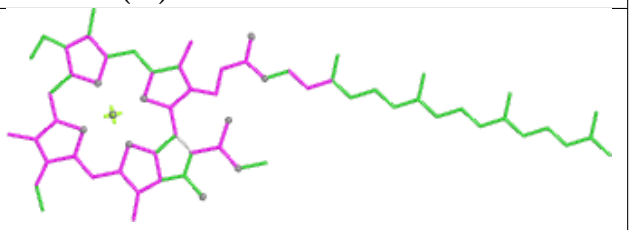
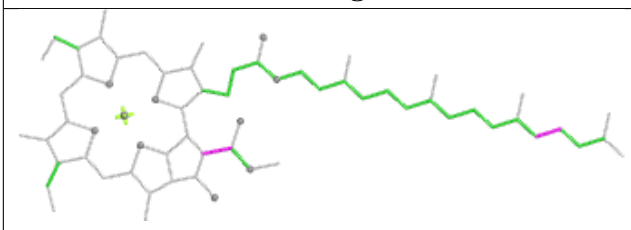


Bond angles



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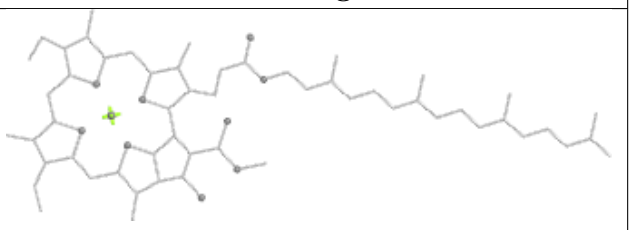
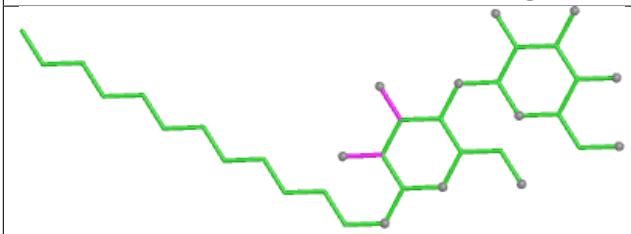
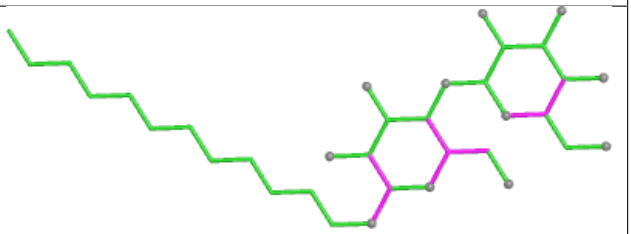


Rings

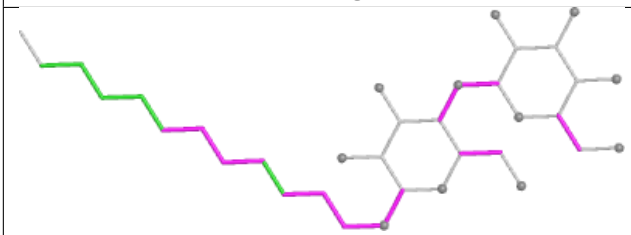
Ligand LMT C 525



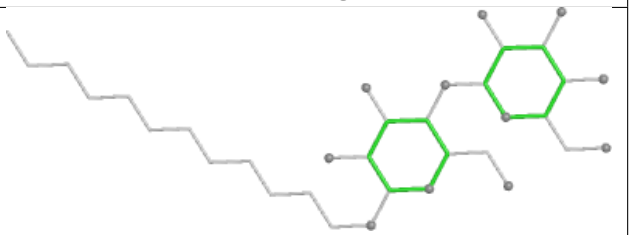
Bond lengths



Bond angles

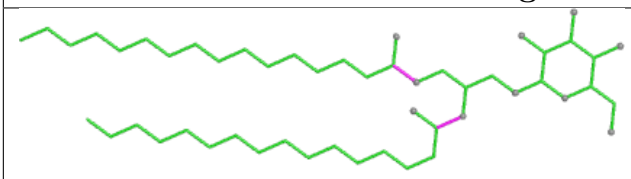


Torsions

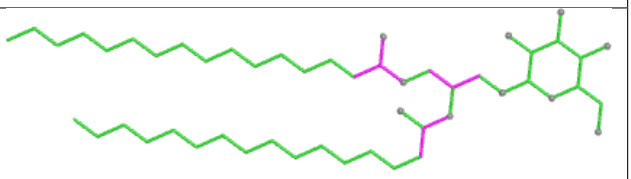


Rings

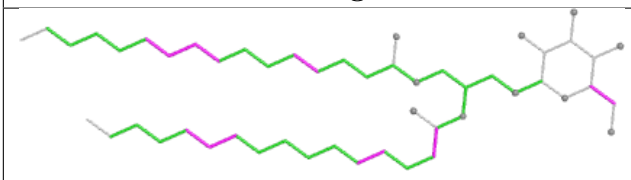
Ligand LMG D 411



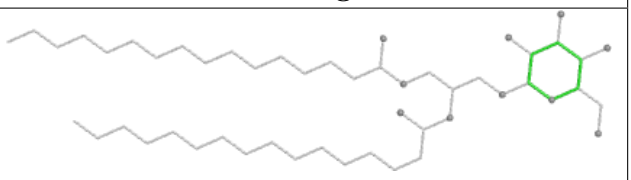
Bond lengths



Bond angles

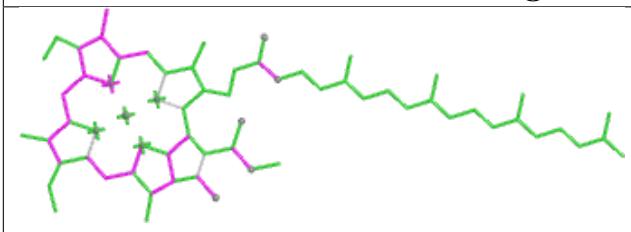


Torsions

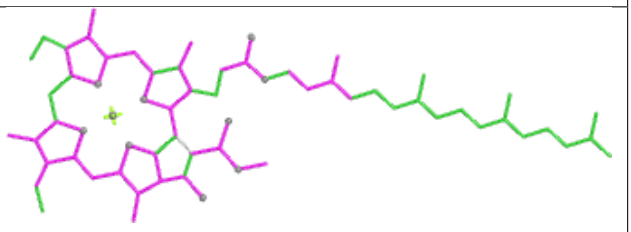


Rings

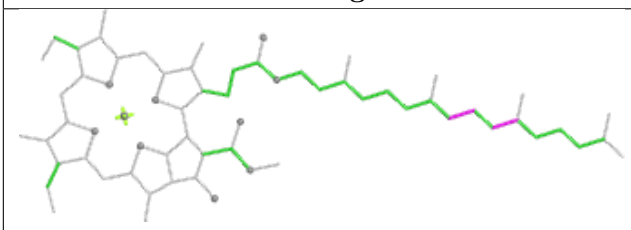
Ligand CLA B 611



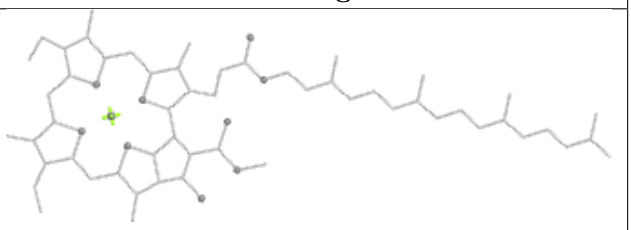
Bond lengths



Bond angles

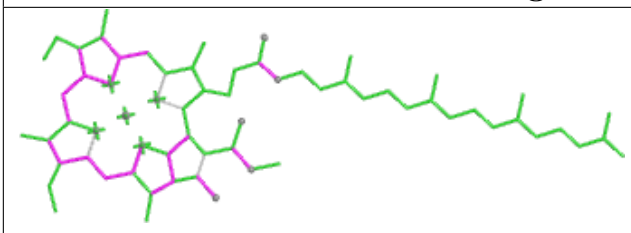


Torsions



Rings

Ligand CLA b 615



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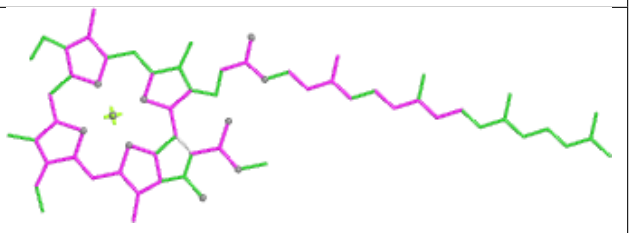
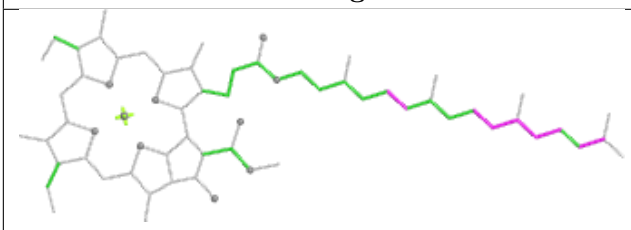


Bond angles



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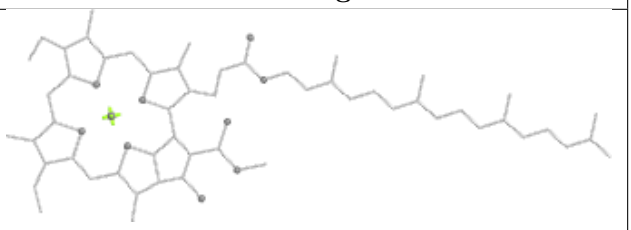
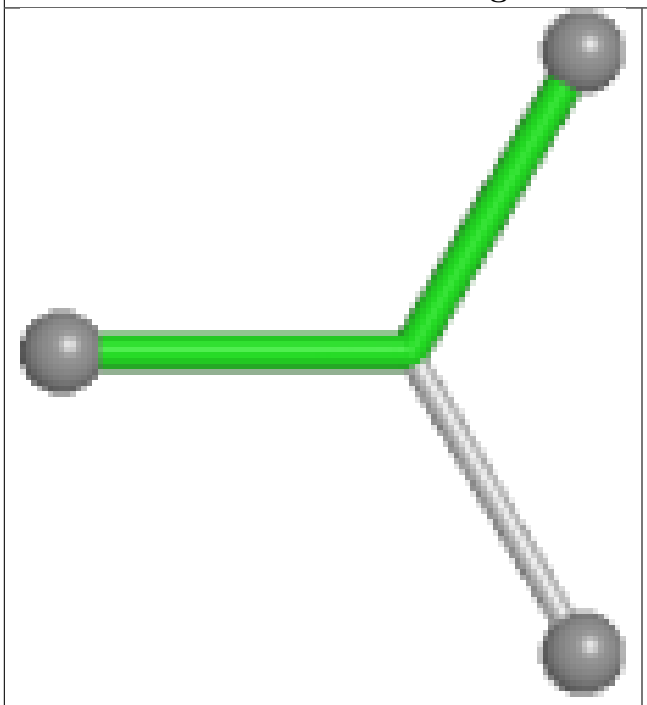


Rings

Ligand BCT D 401 (A)



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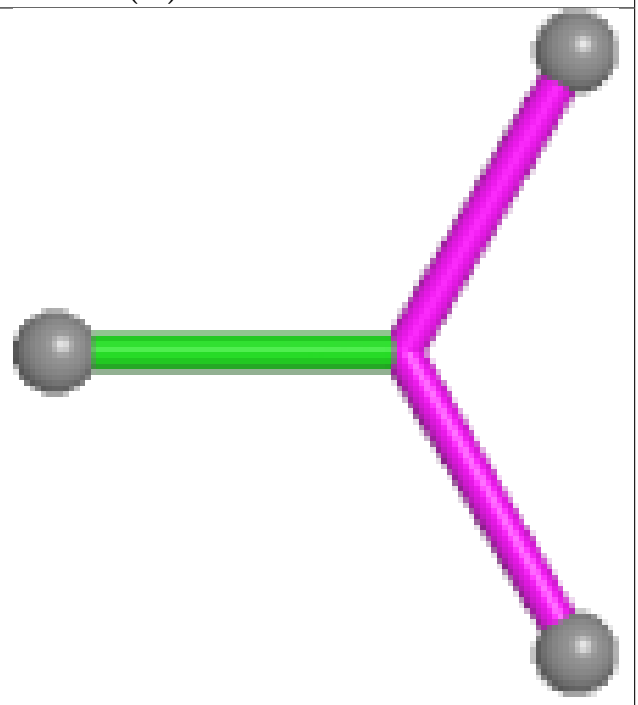
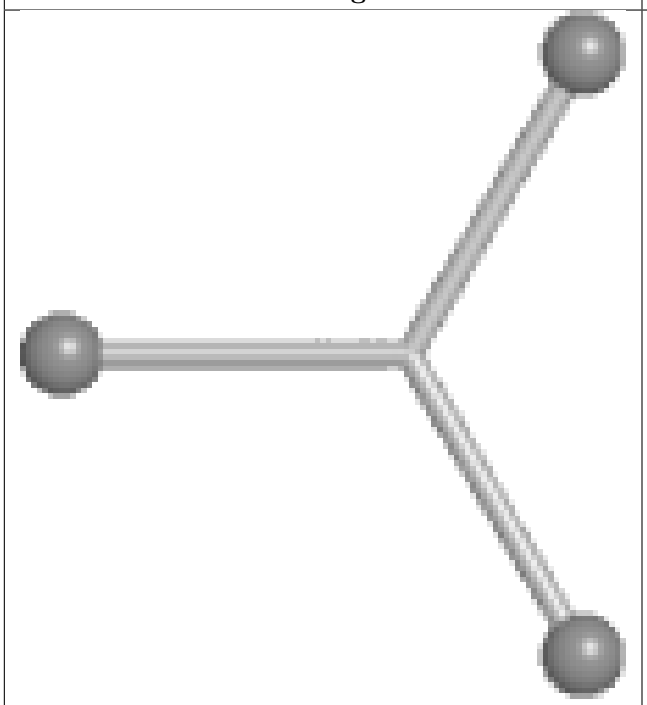


Bond angles



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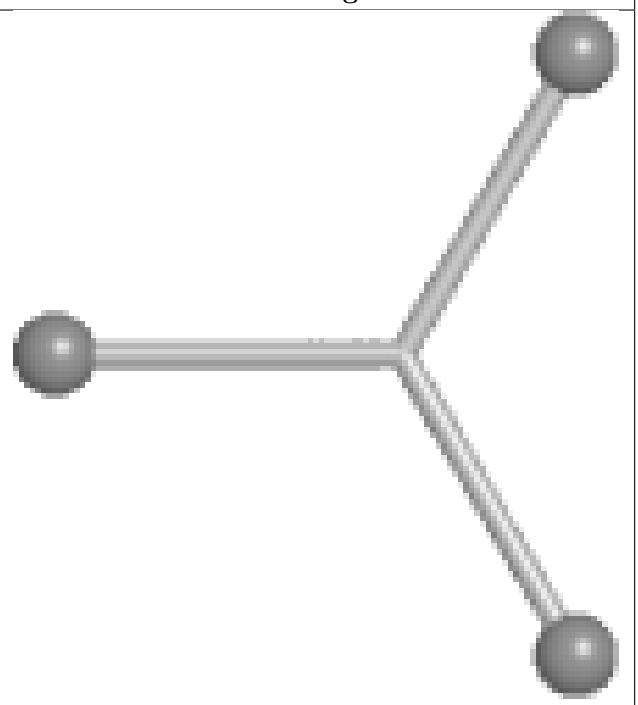
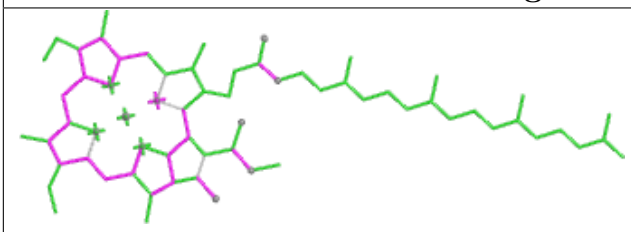
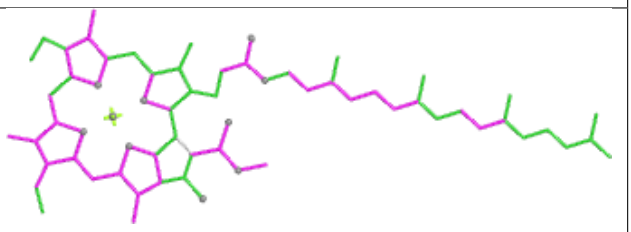


Rings

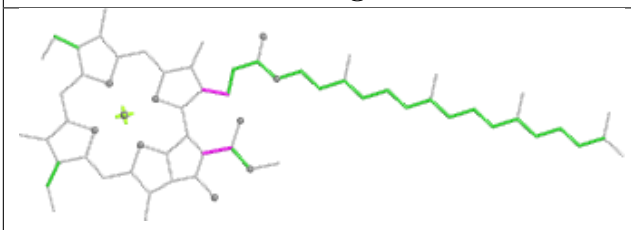
Ligand CLA B 604



Bond lengths



Bond angles



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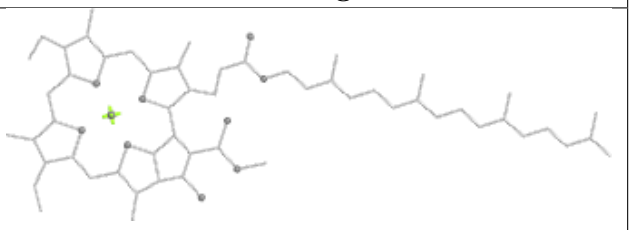
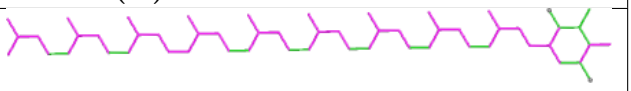


Rings

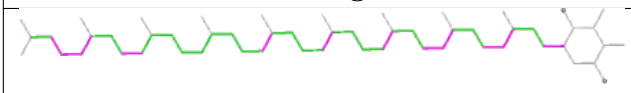
Ligand PL9 A 414 (B)



Bond lengths



Bond angles



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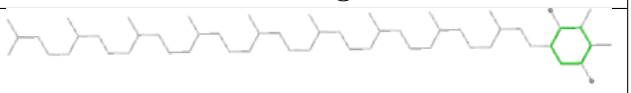
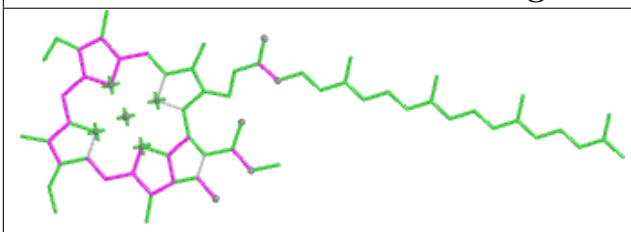
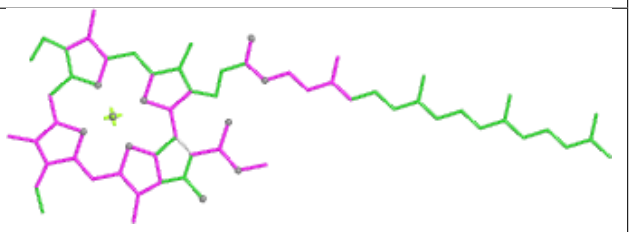


Rings

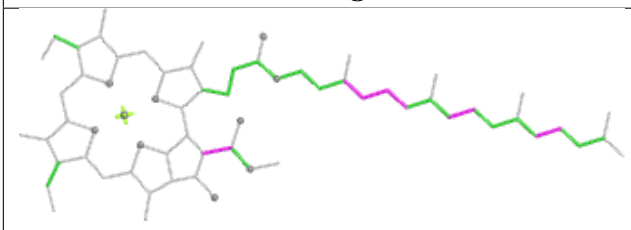
Ligand CLA b 605



Bond lengths



Bond angles



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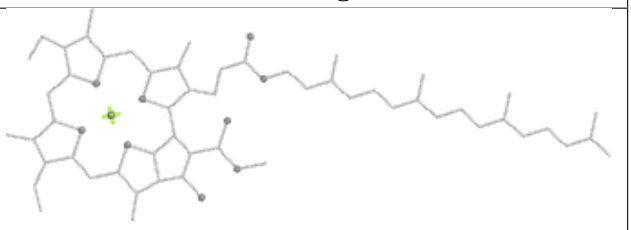
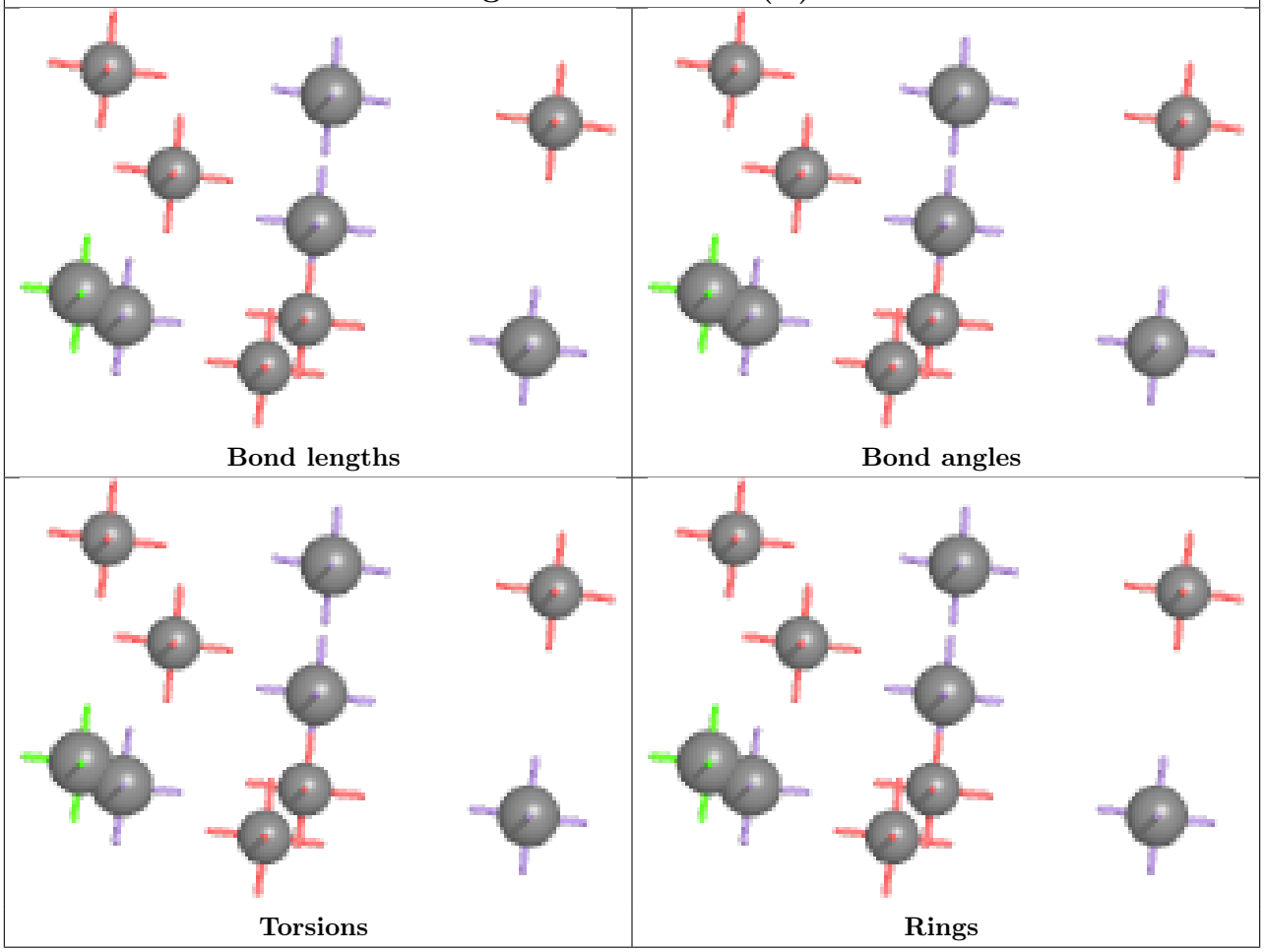
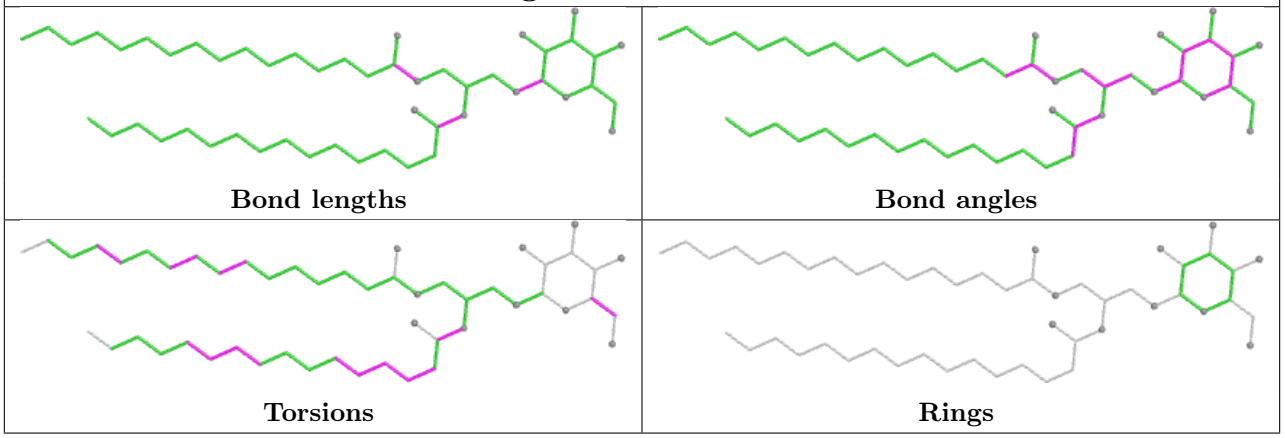


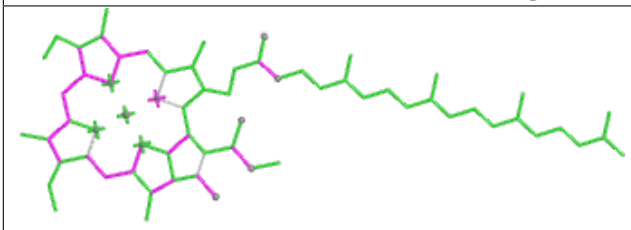
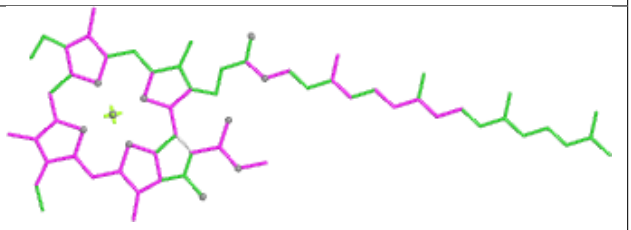
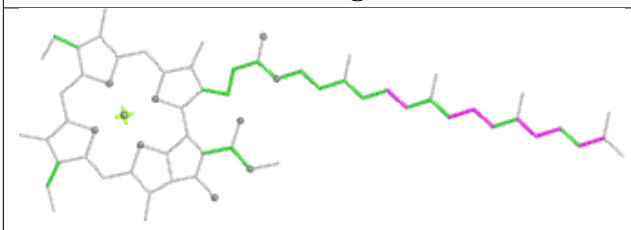
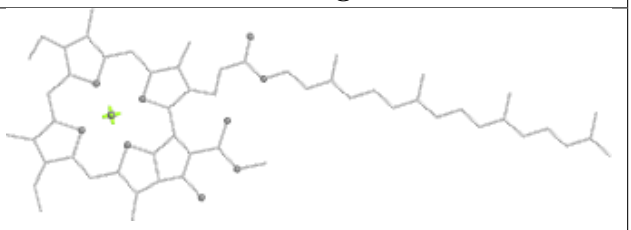
Rings

Ligand OEX A 413 (B)

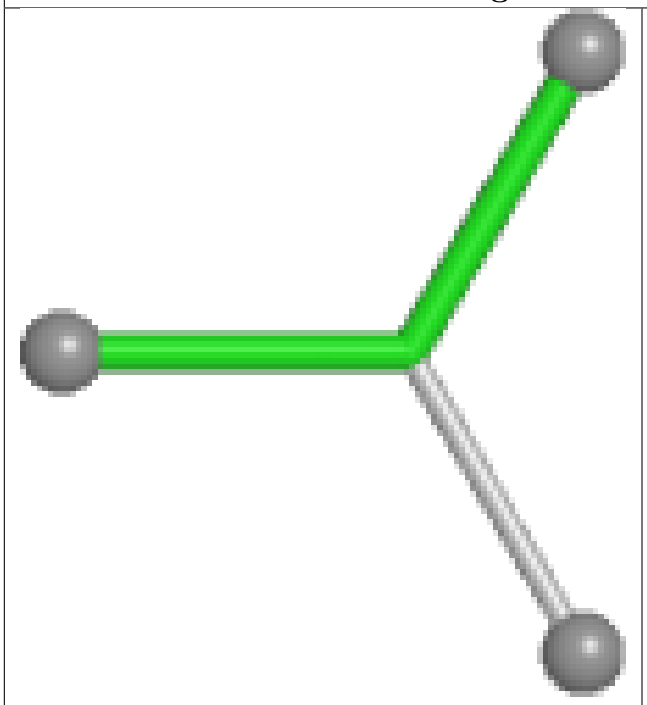


Ligand LMG C 521



Ligand CLA B 615	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand BCT D 401 (B)



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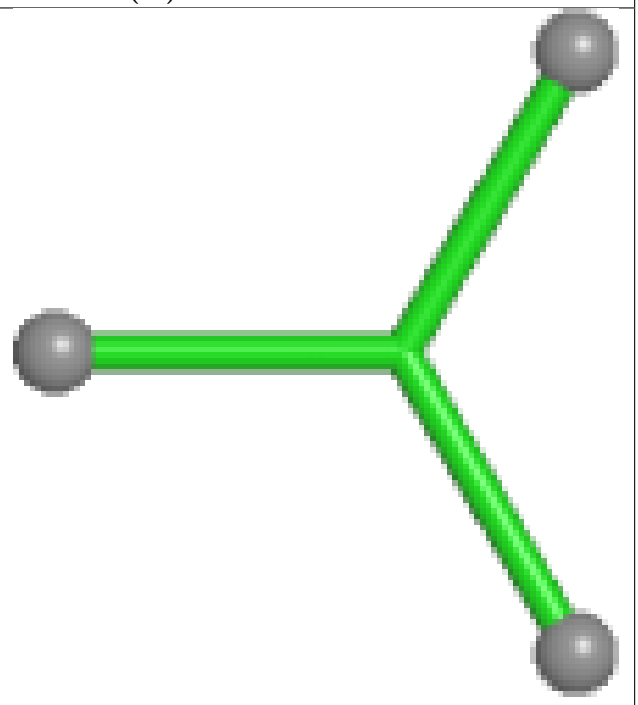
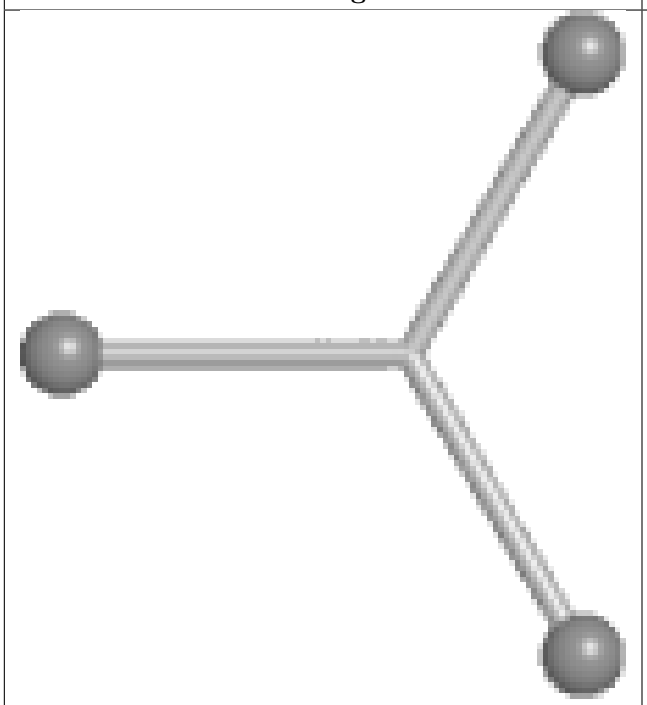
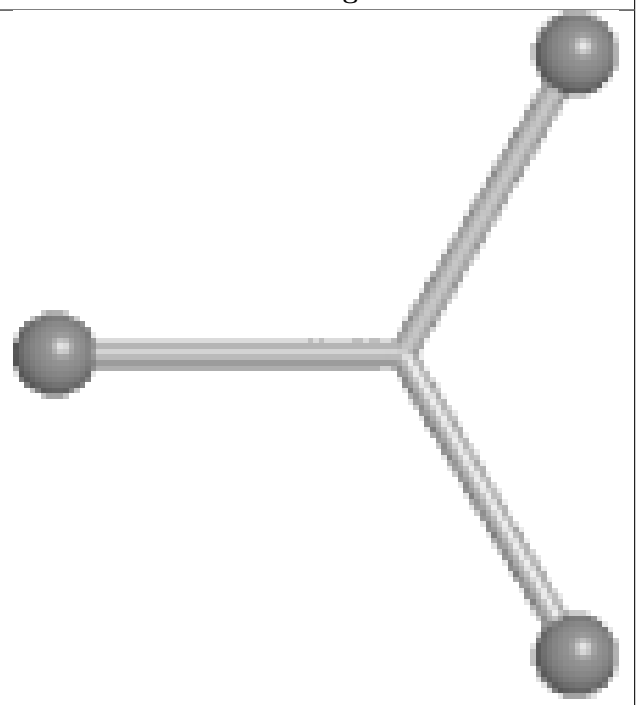


Bond angles

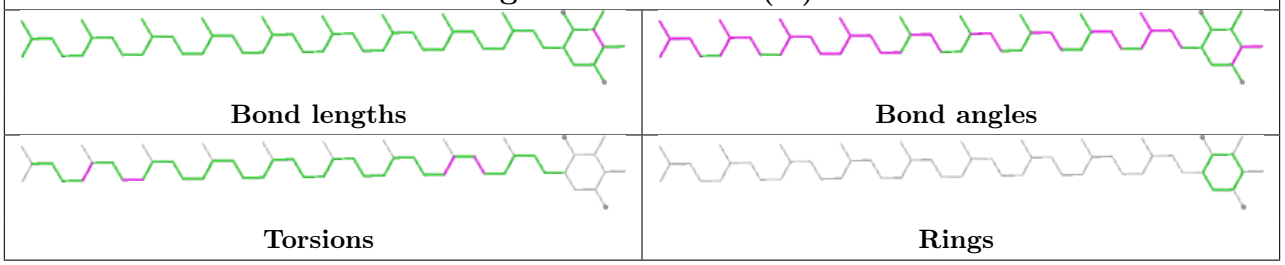


Torsions

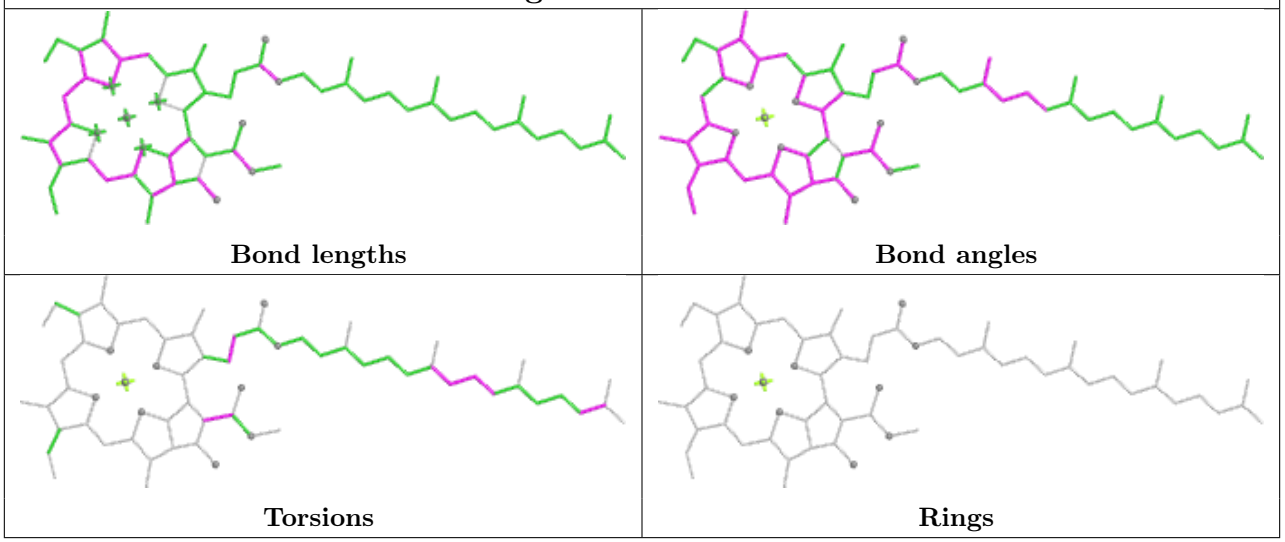


Rings

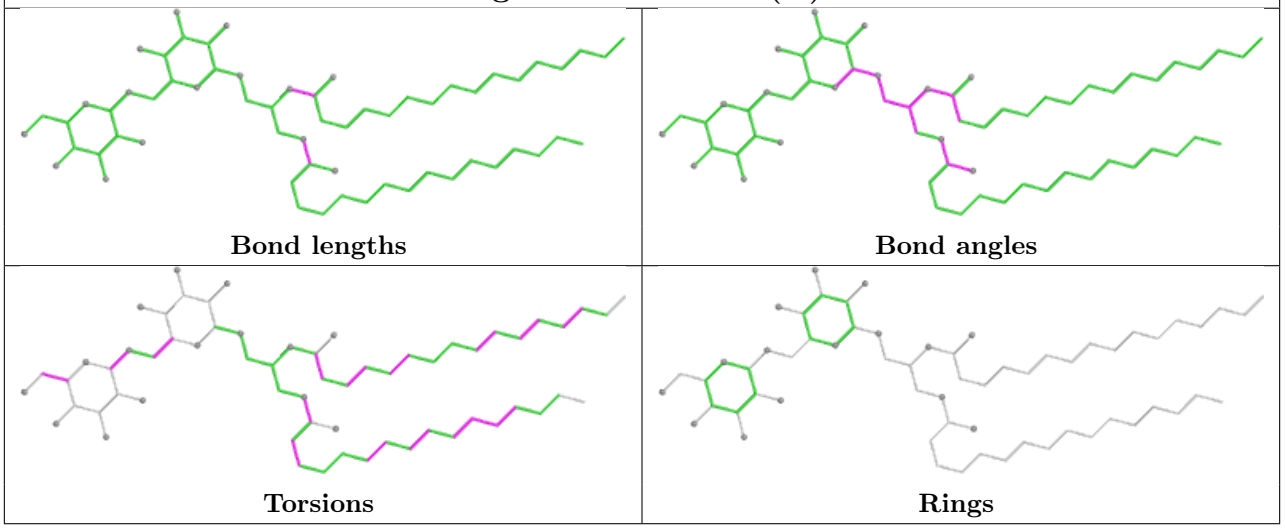
Ligand PL9 d 407 (A)



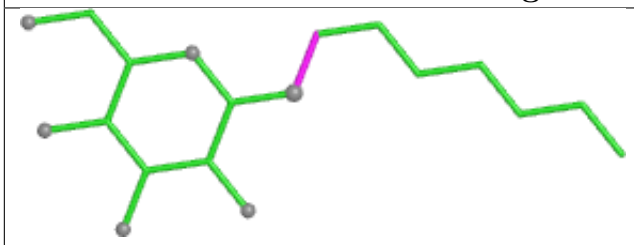
Ligand CLA B 606



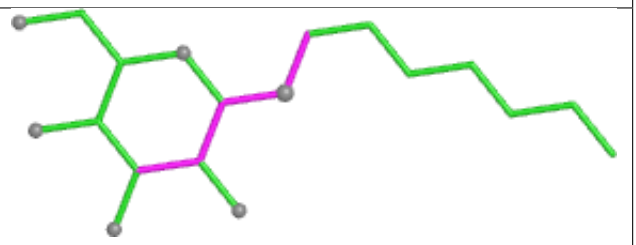
Ligand DGD c 516 (A)



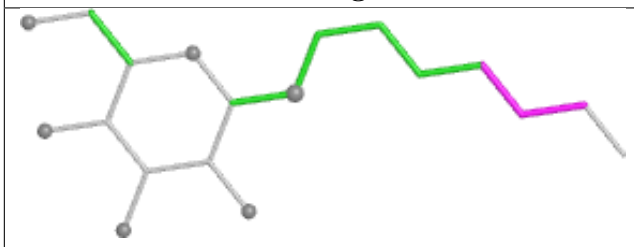
Ligand HTG B 622



Bond lengths



Bond angles



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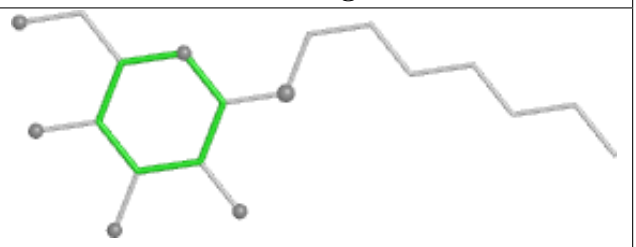
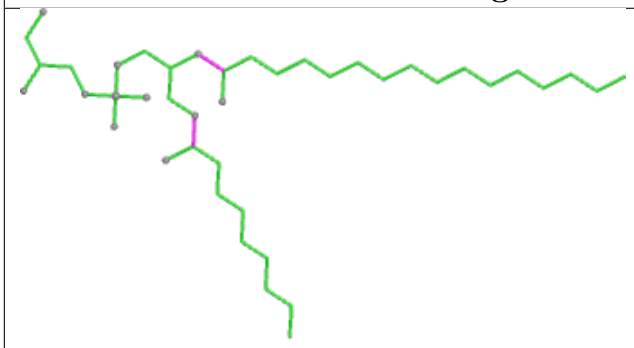


Rings

Ligand LHG E 101 (A)



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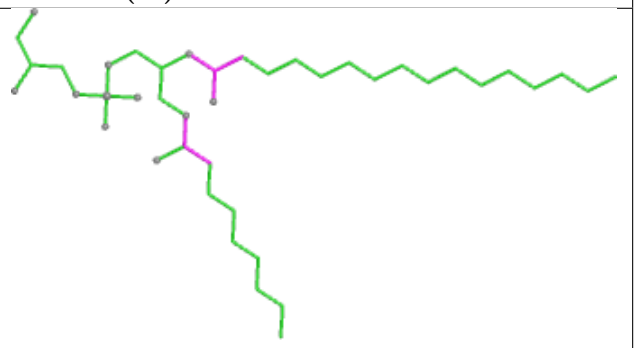
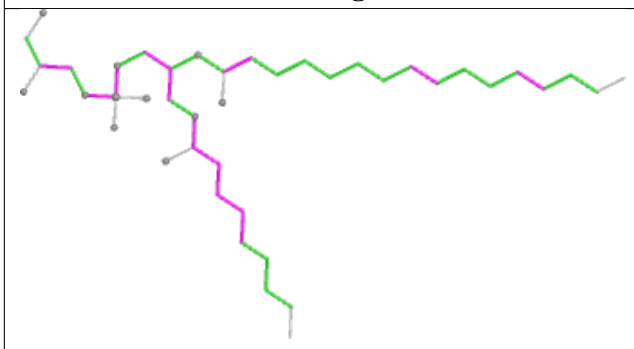


Bond angles



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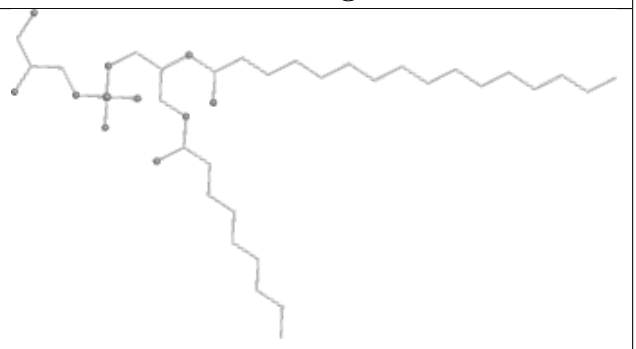
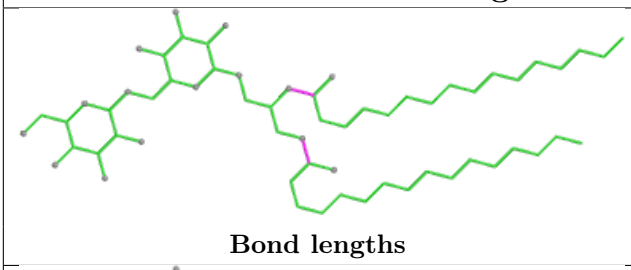
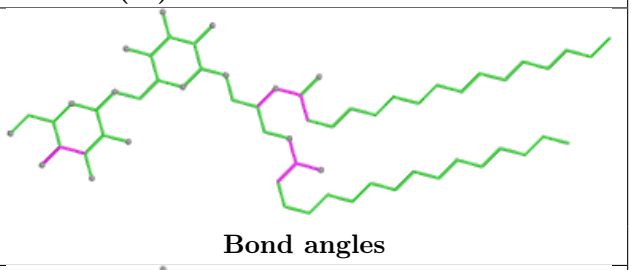


Rings

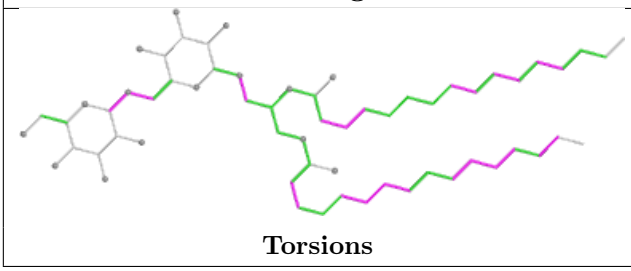
Ligand DGD c 517 (A)



Bond lengths



Bond angles



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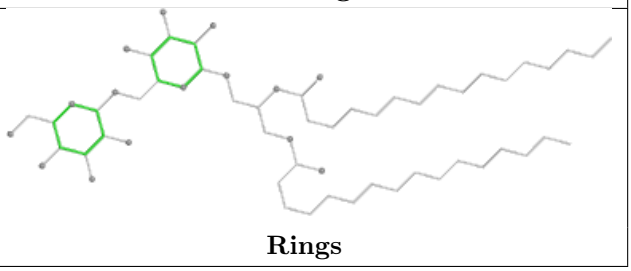
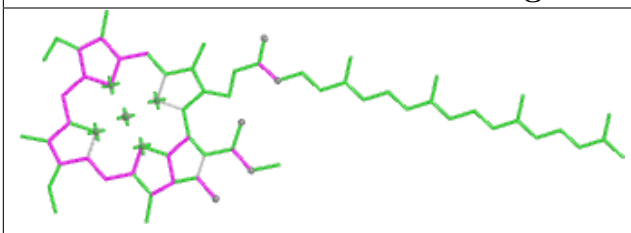
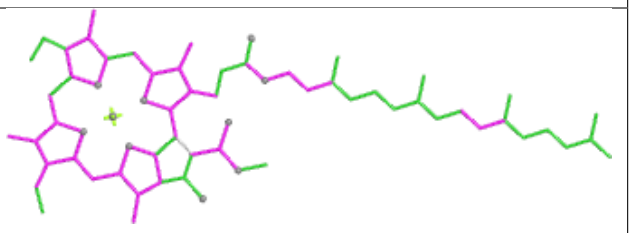


Rings

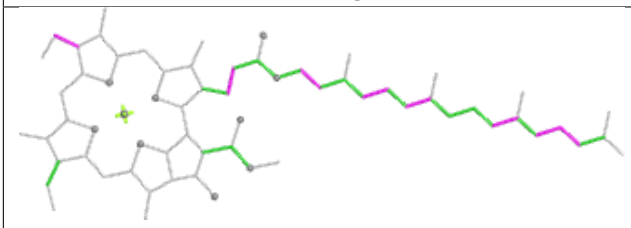
Ligand CLA B 602



Bond lengths



Bond angles



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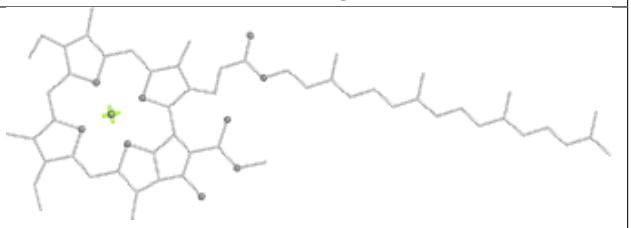
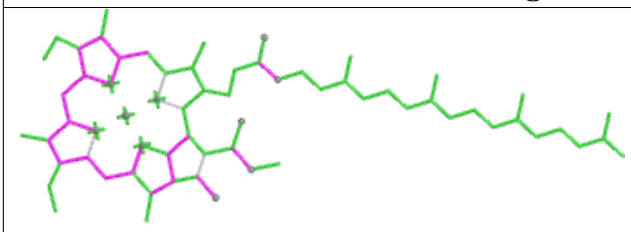


Rings

Ligand CLA B 608



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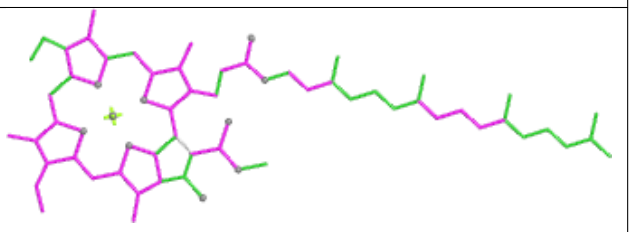
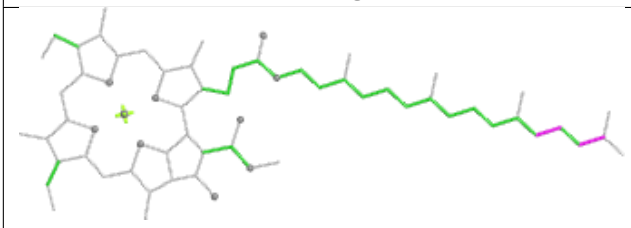
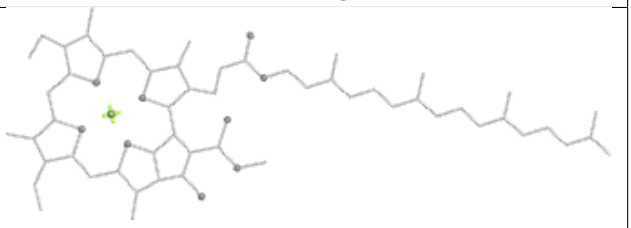


Bond angles

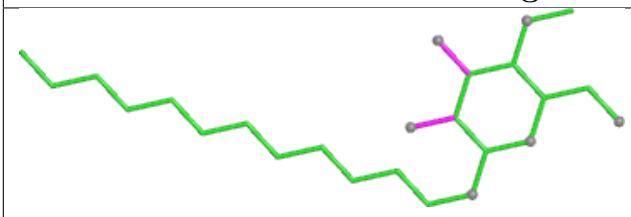


Torsions

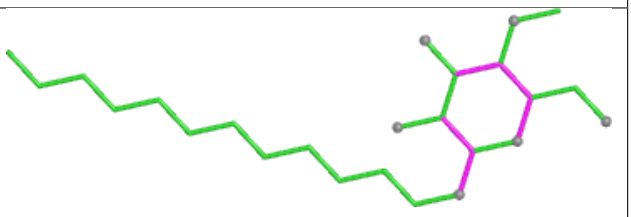


Rings

Ligand LMT B 629



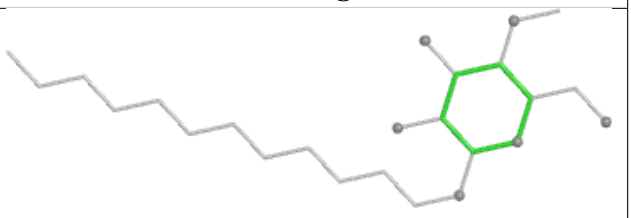
Bond lengths



Bond angles

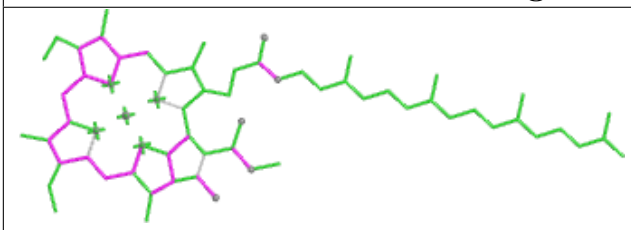


Torsions

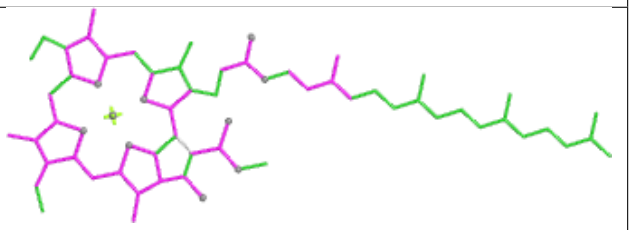


Rings

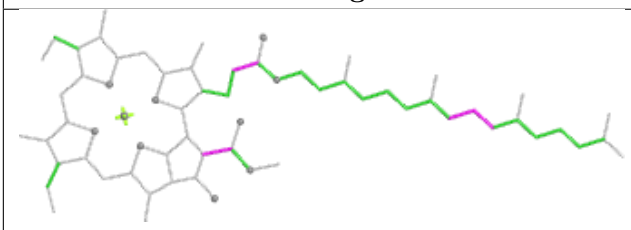
Ligand CLA b 612



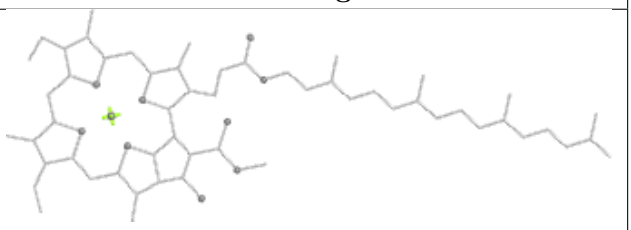
Bond lengths



Bond angles

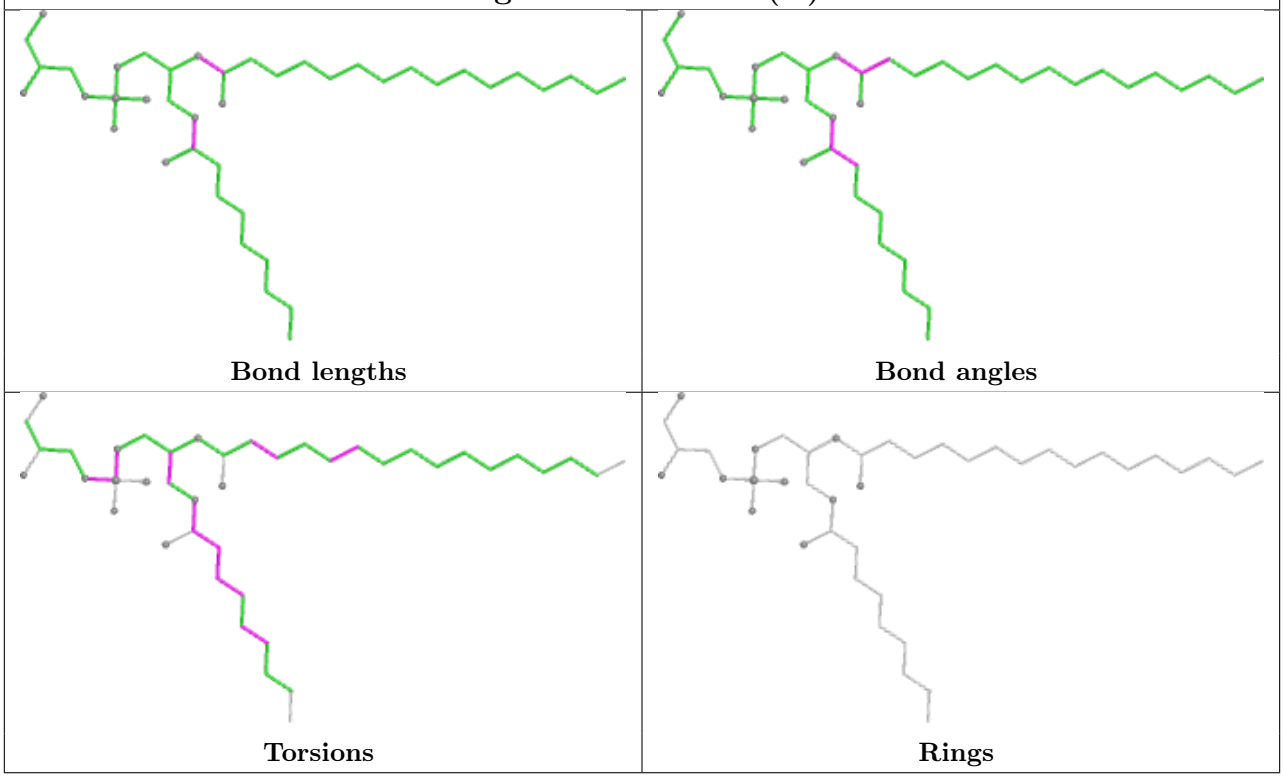


Torsions

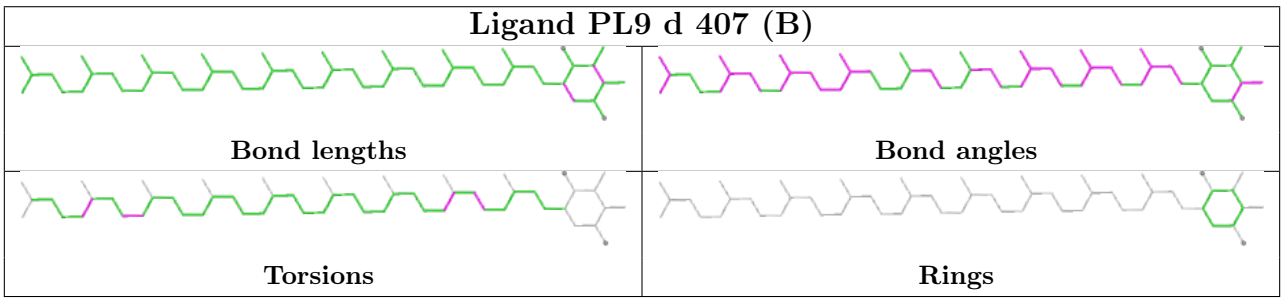


Rings

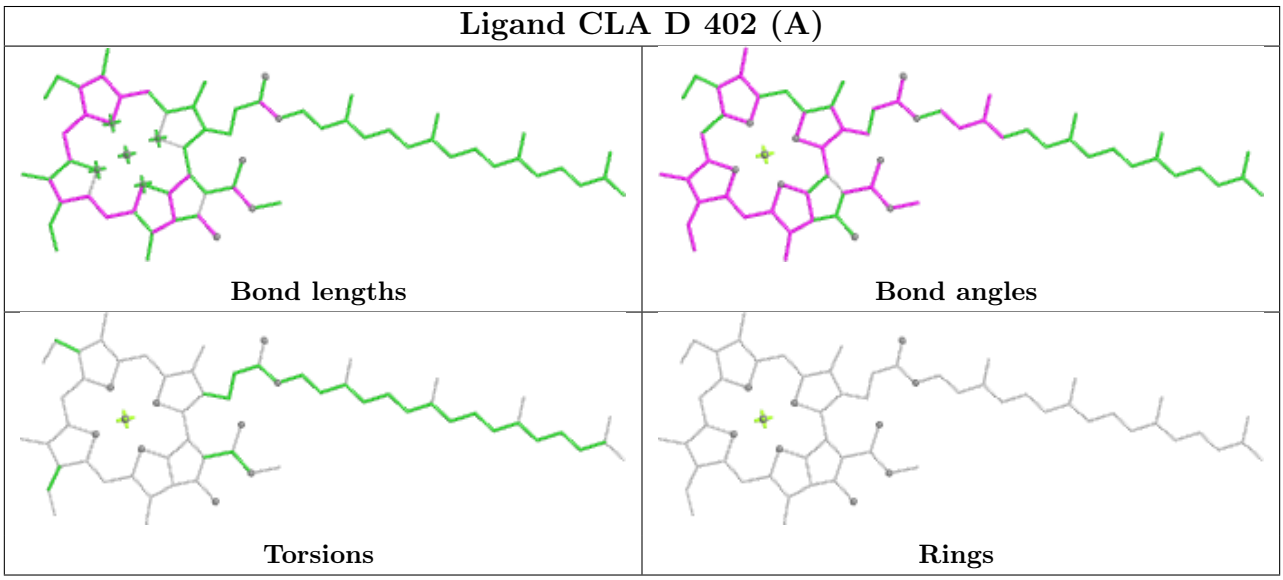
Ligand LHG a 419 (A)



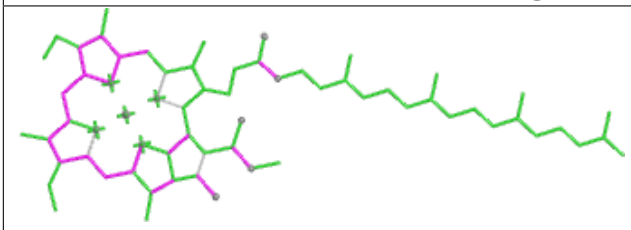
Ligand PL9 d 407 (B)



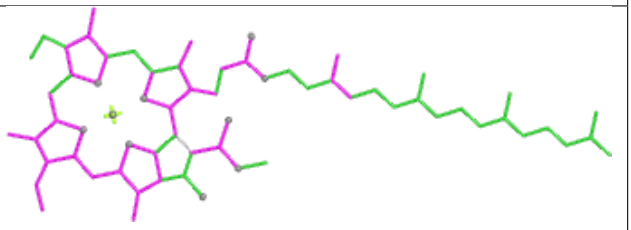
Ligand CLA D 402 (A)



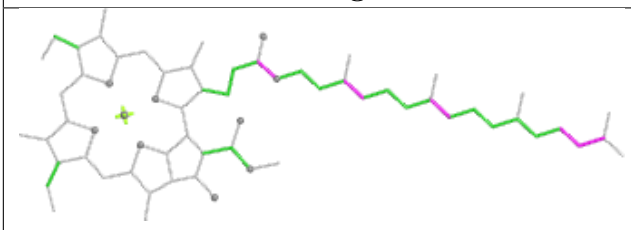
Ligand CLA a 407



Bond lengths



Bond angles



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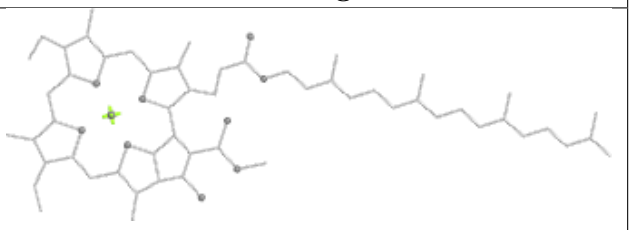
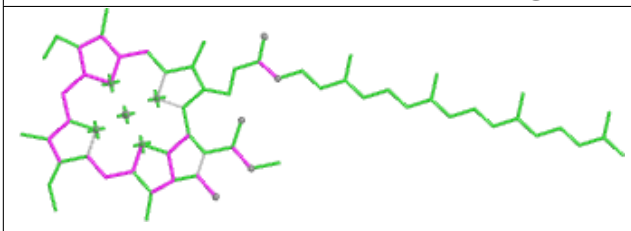
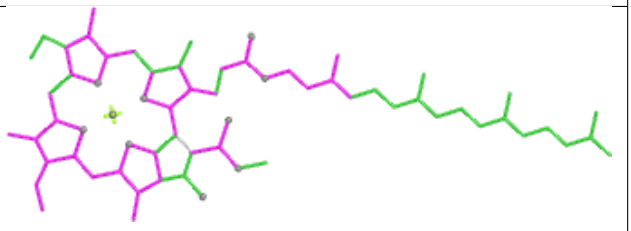


Rings

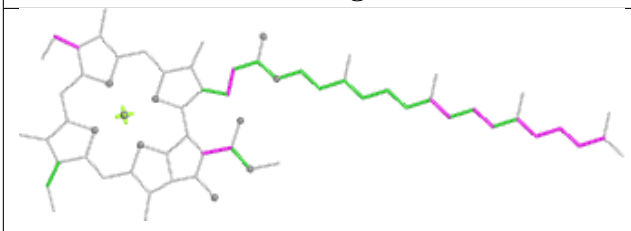
Ligand CLA b 606



Bond lengths



Bond angles



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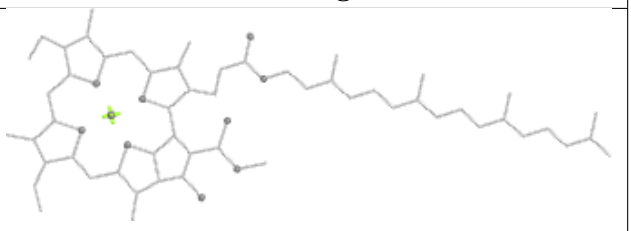
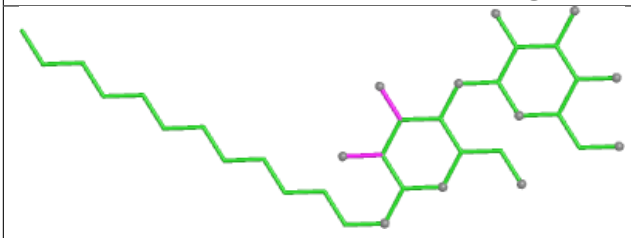


Rings

Ligand LMT a 416



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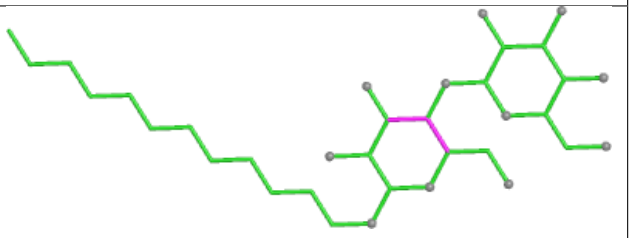
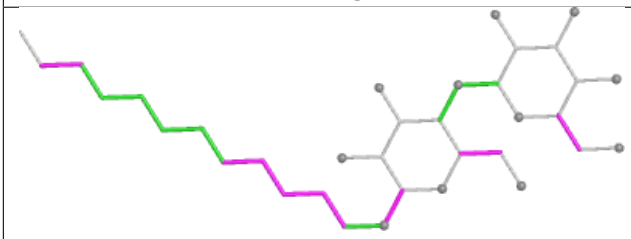


Bond angles



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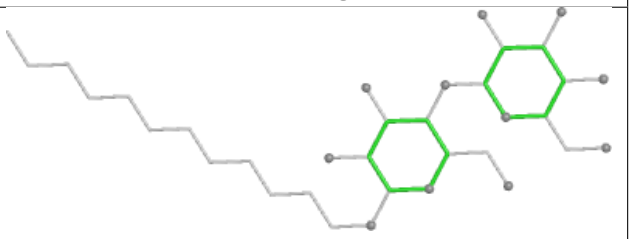
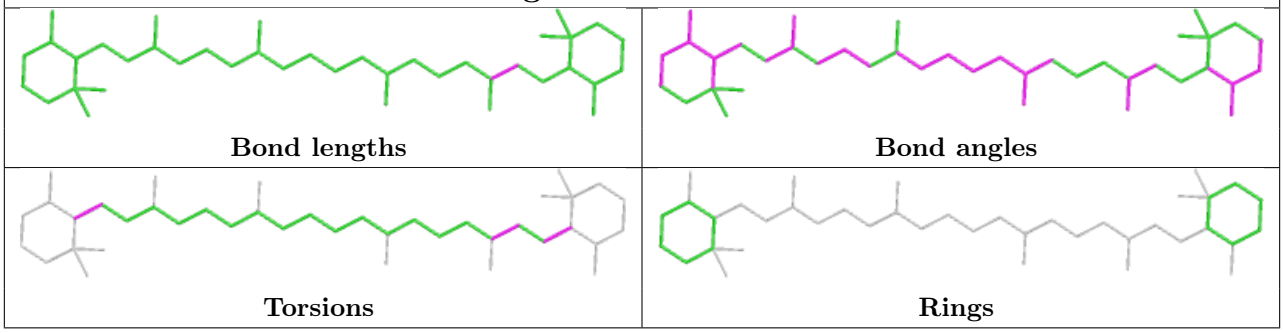
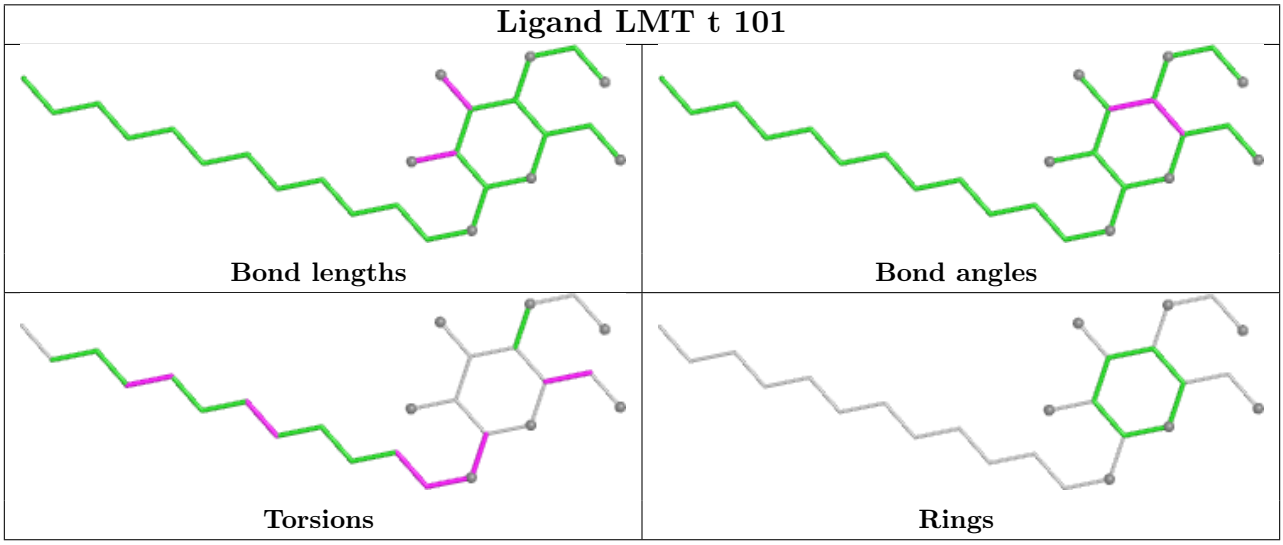


Rings

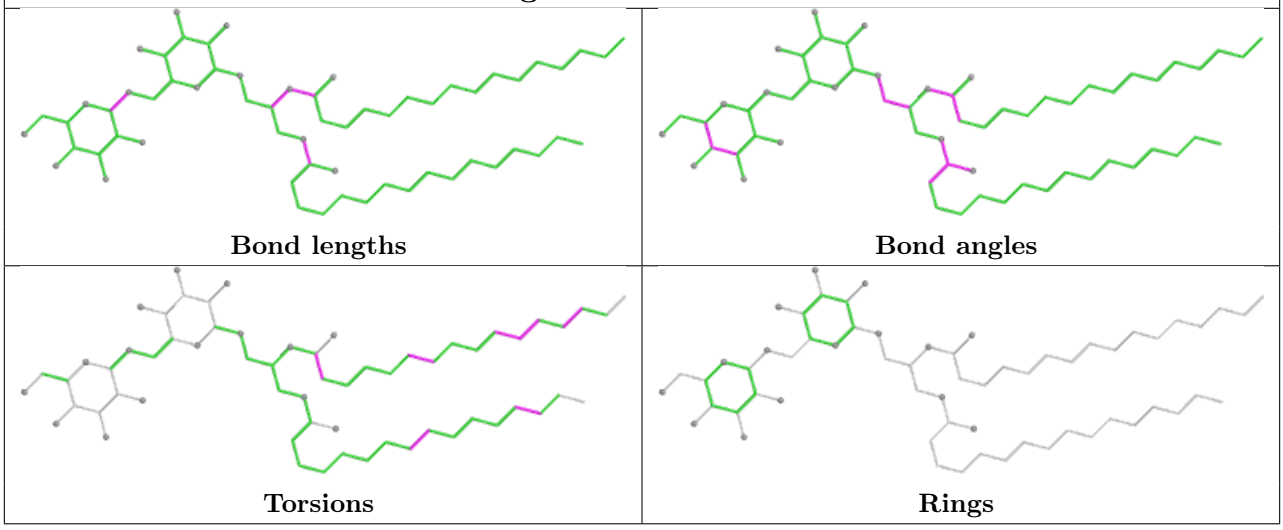
Ligand BCR Y 101



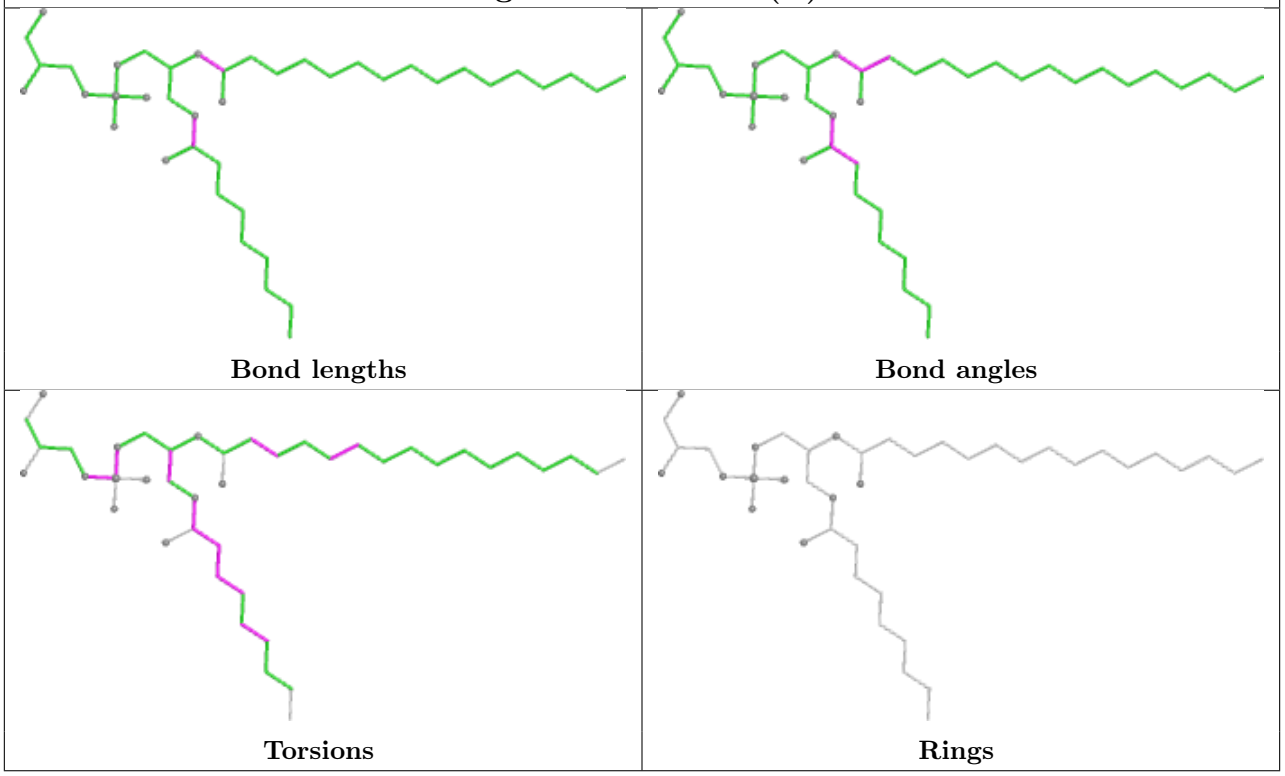
Ligand LMT t 101



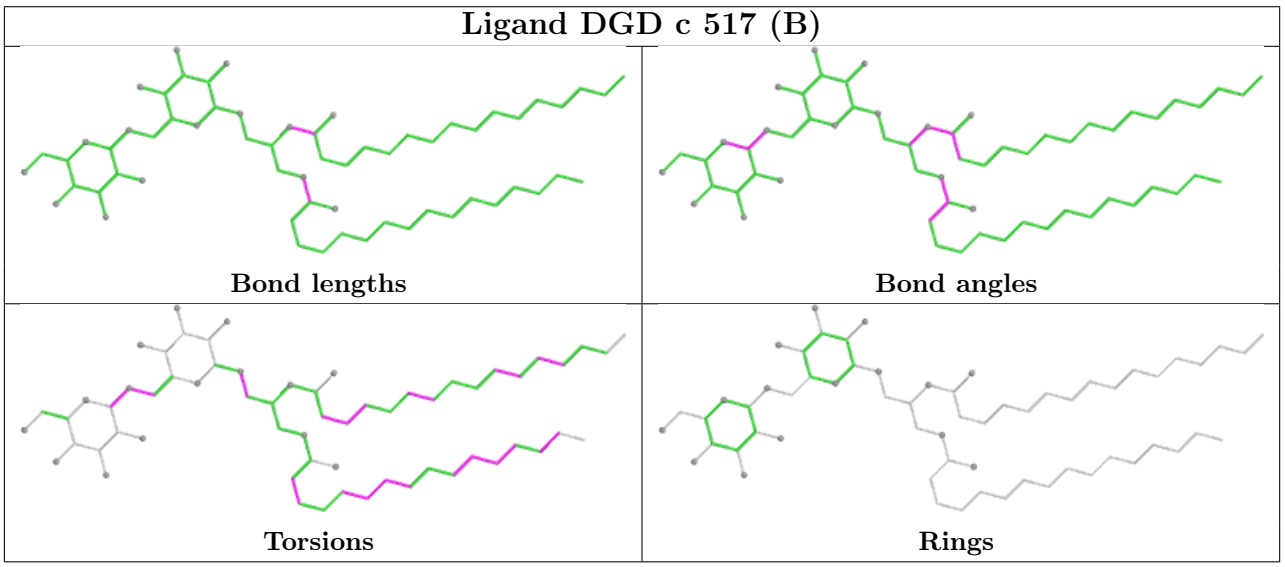
Ligand DGD H 102



Ligand LHG a 419 (B)



Ligand DGD c 517 (B)



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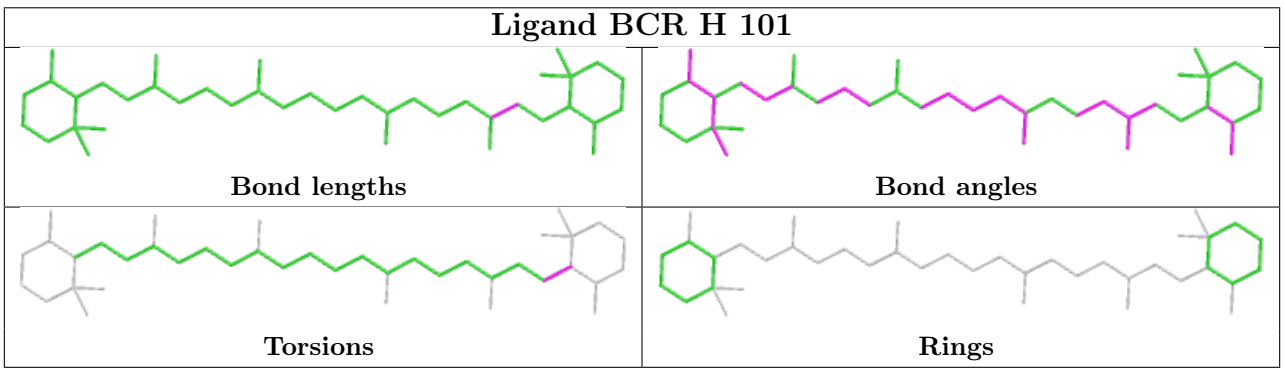
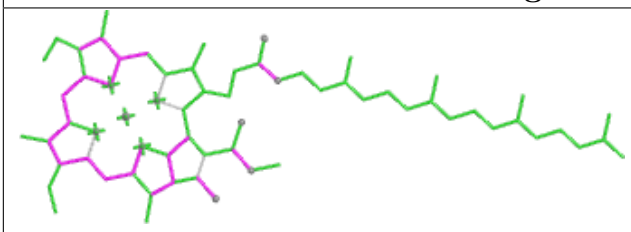
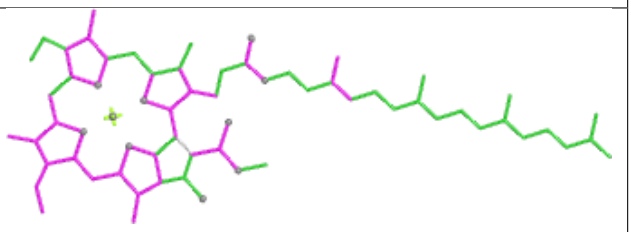


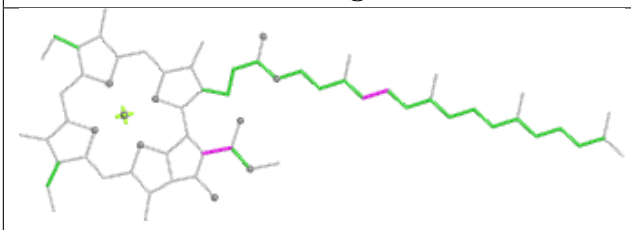
Ligand CLA B 607



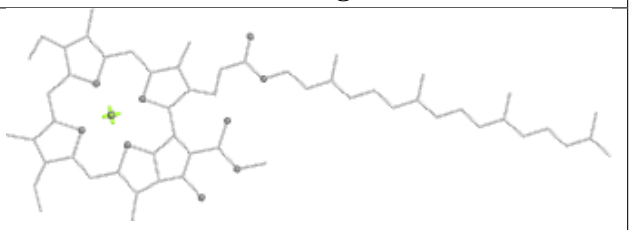
Bond lengths



Bond angles

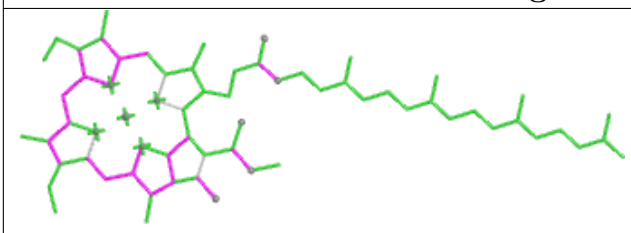


Torsions



Rings

Ligand CLA c 507



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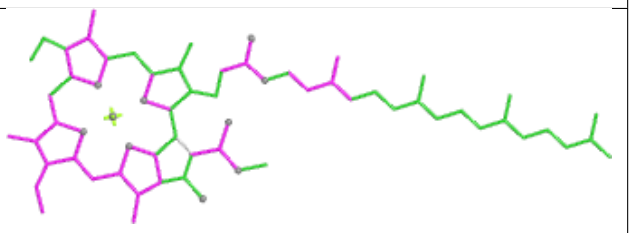
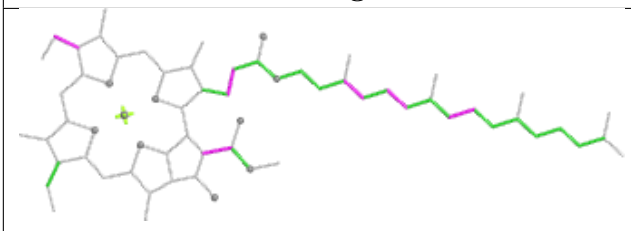


Bond angles



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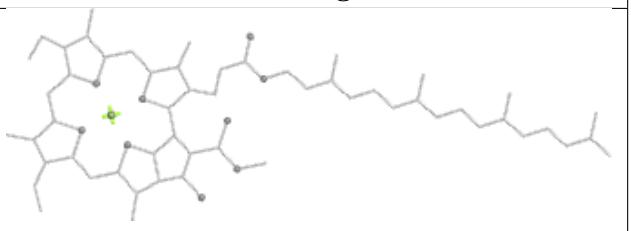
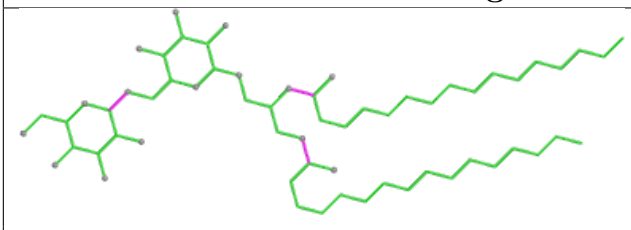


Rings

Ligand DGD C 518 (A)



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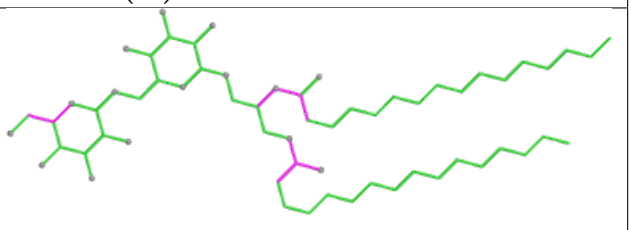
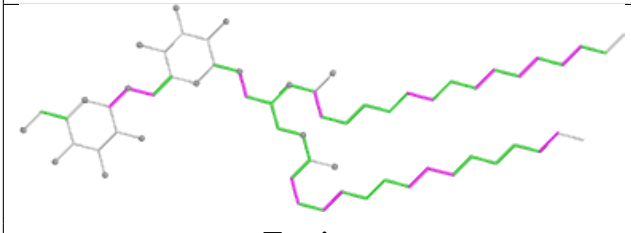
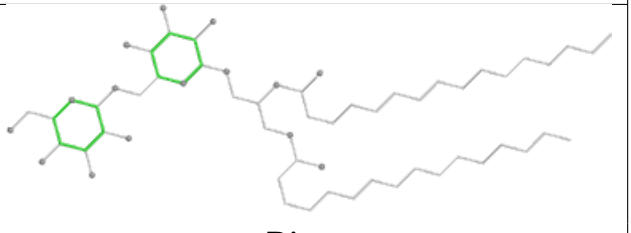


Bond angles

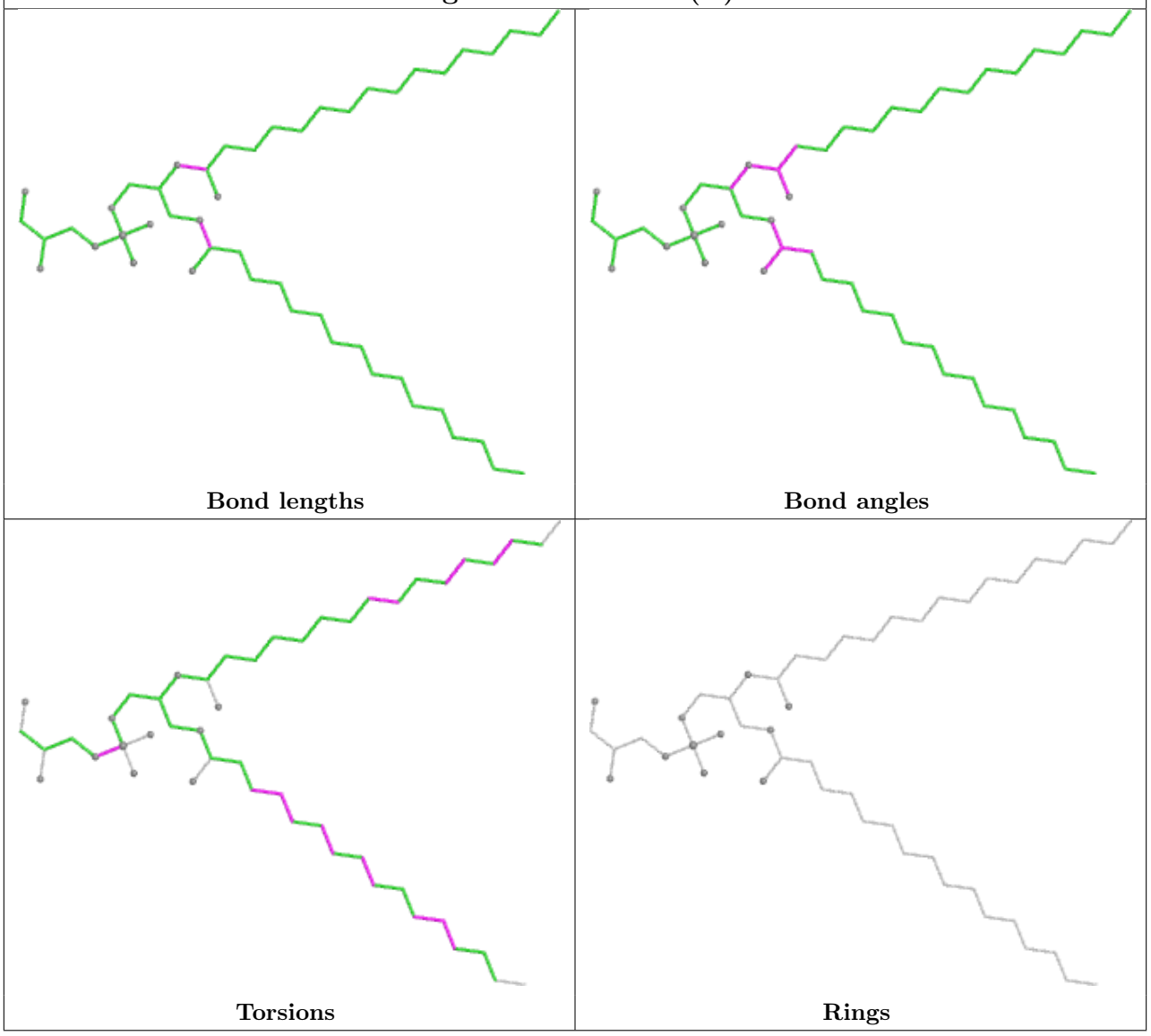


Torsions

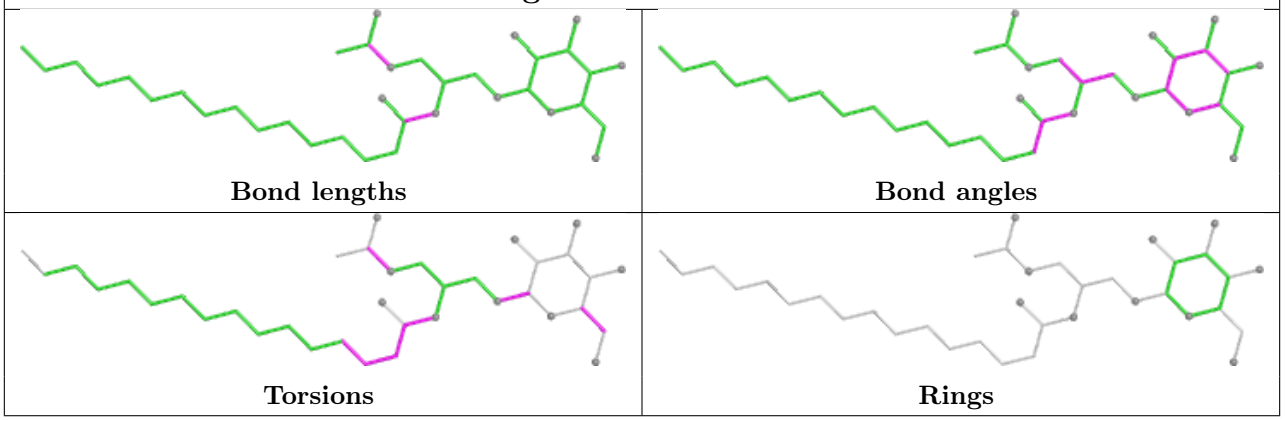


Rings

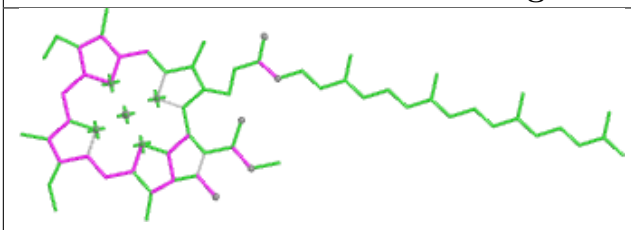
Ligand LHG d 415 (B)



Ligand LMG Z 101



Ligand CLA b 601



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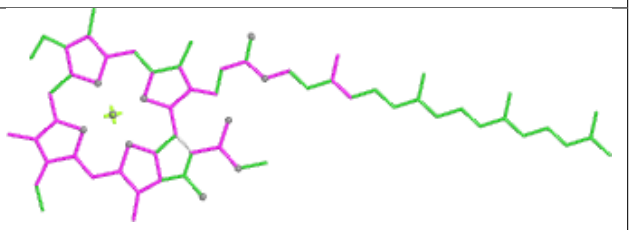
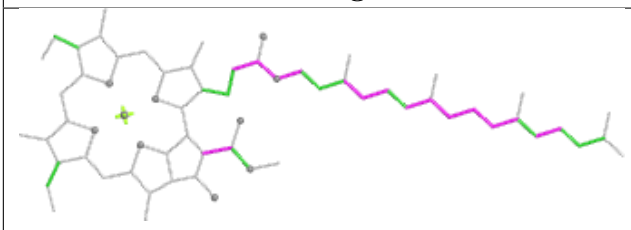


Bond angles



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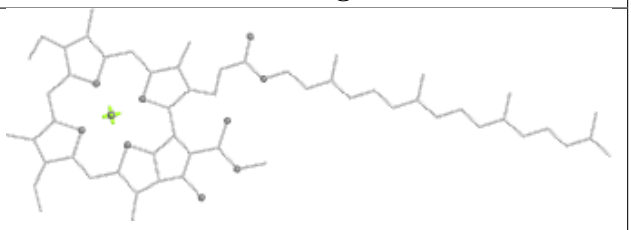
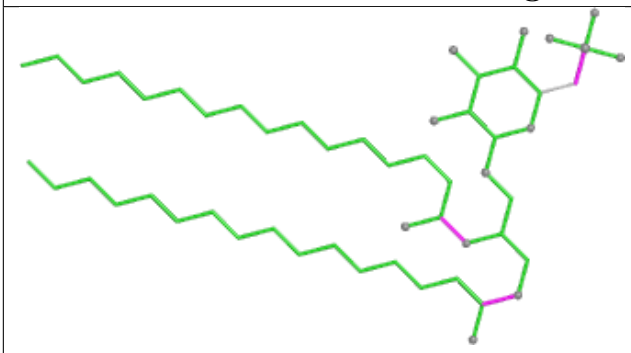


Rings

Ligand SQD A 412



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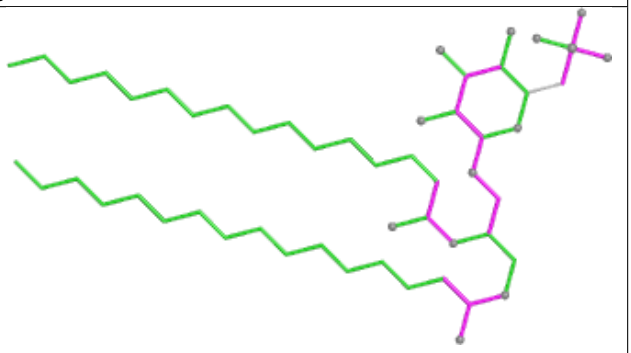
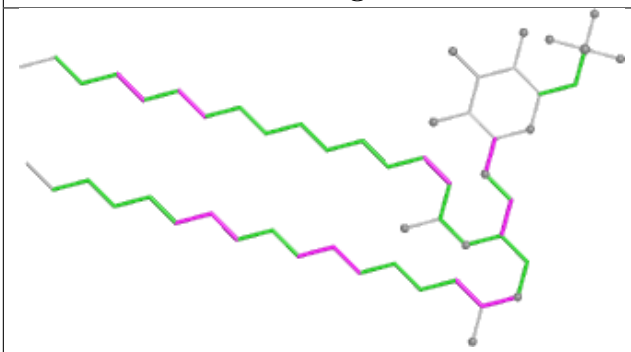


Bond angles



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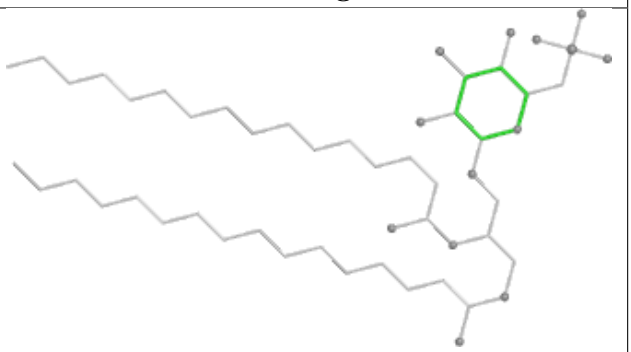
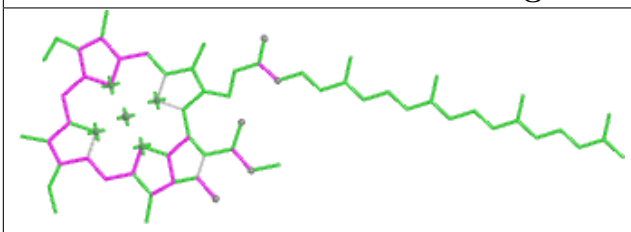
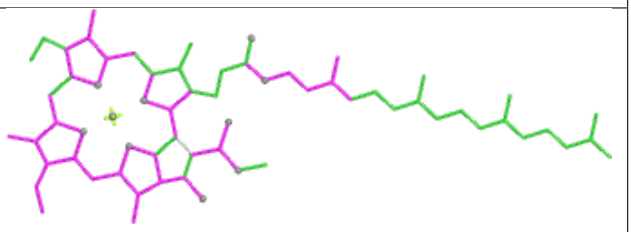


Rings

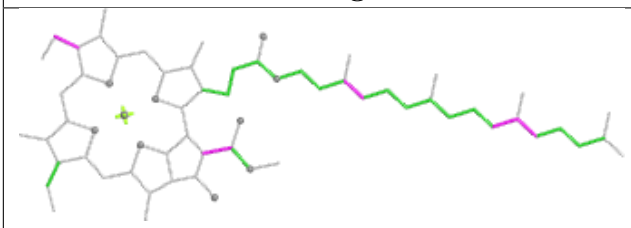
Ligand CLA C 505



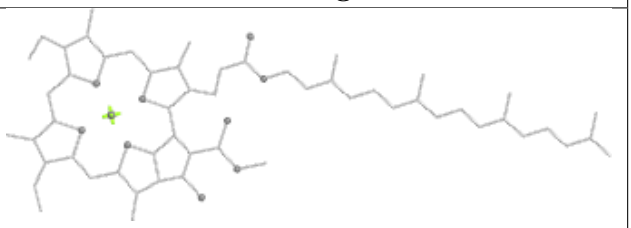
Bond lengths



Bond angles

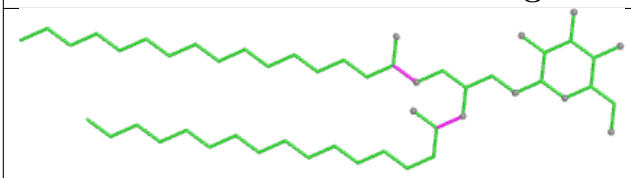


Torsions

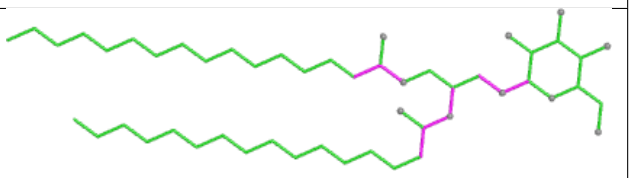


Rings

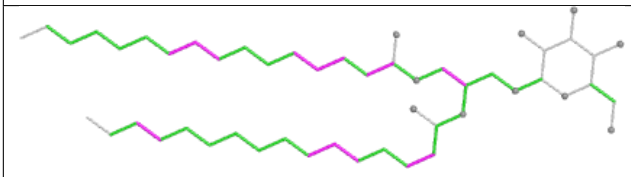
Ligand LMG a 415



Bond lengths



Bond angles



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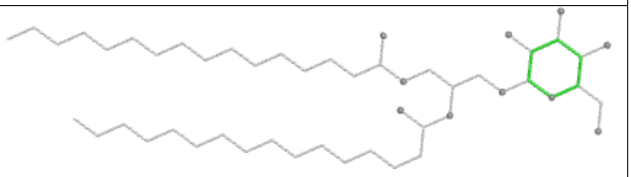
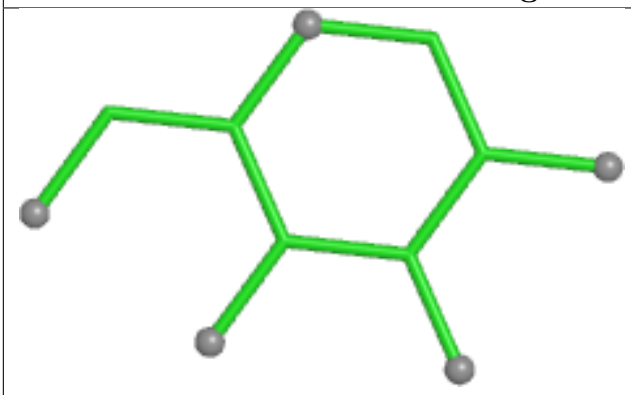
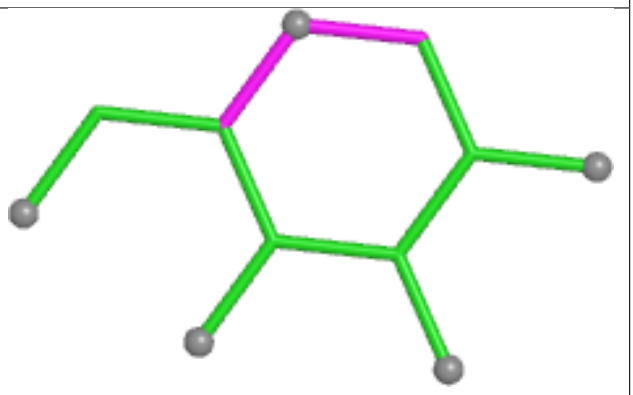


Rings

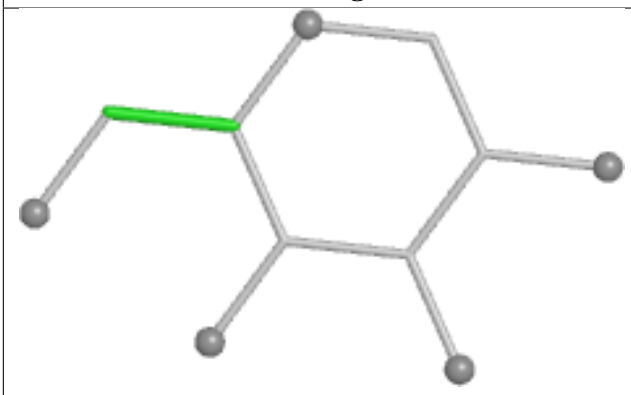
Ligand HTG V 202



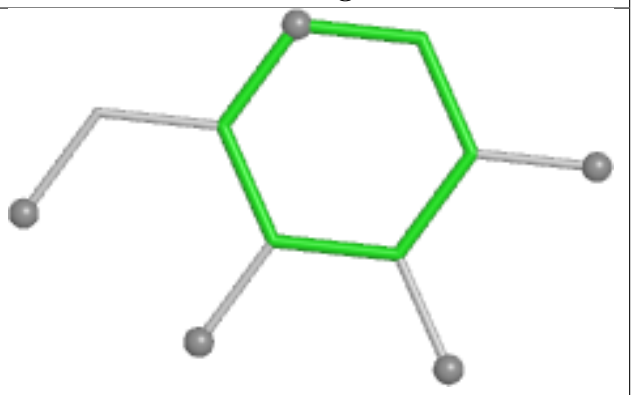
Bond lengths



Bond angles

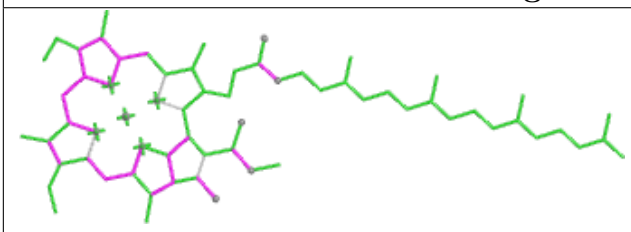


Torsions

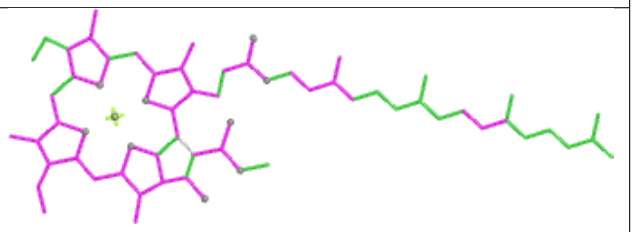


Rings

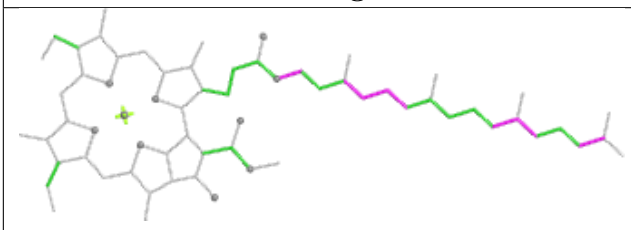
Ligand CLA A 408



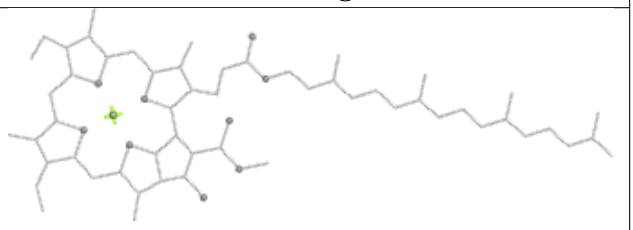
Bond lengths



Bond angles

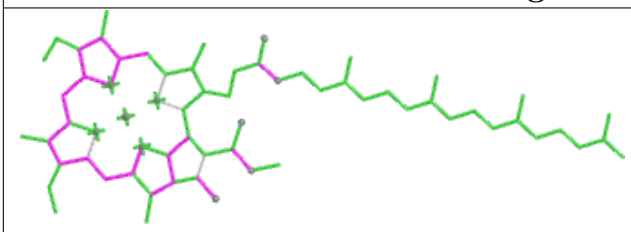


Torsions

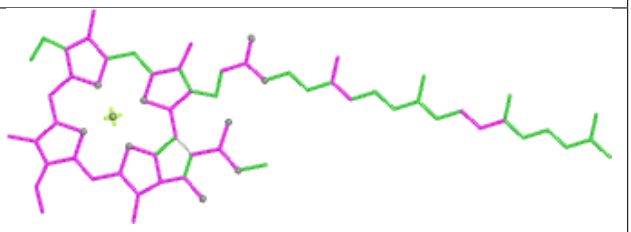


Rings

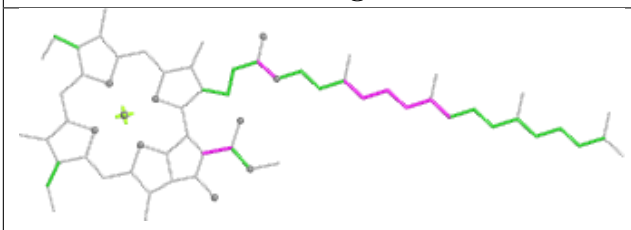
Ligand CLA b 616



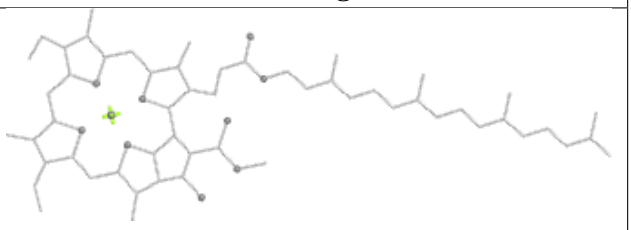
Bond lengths



Bond angles

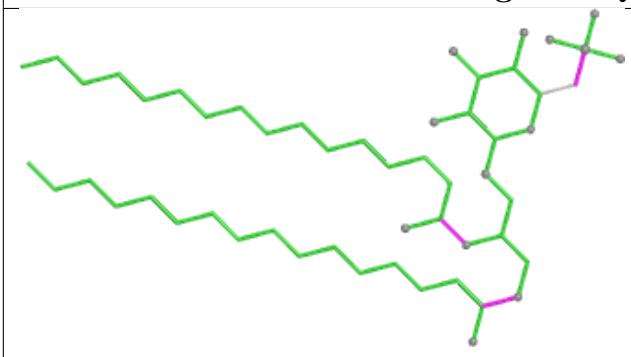


Torsions

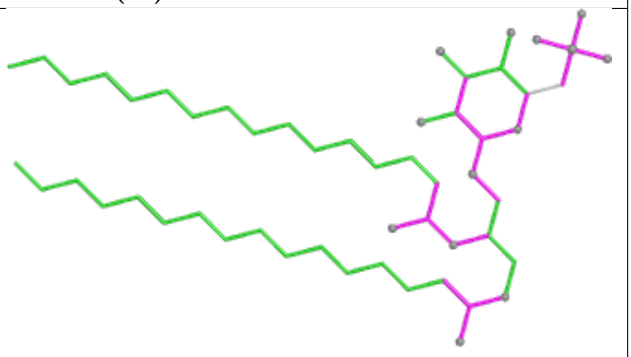


Rings

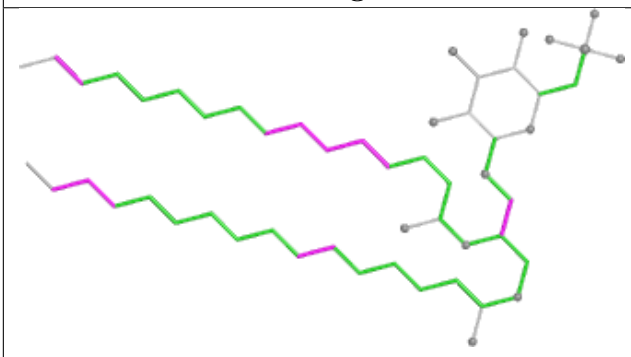
Ligand SQD a 409 (A)



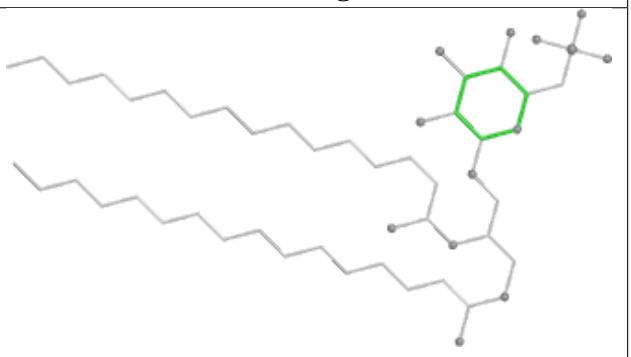
Bond lengths



Bond angles

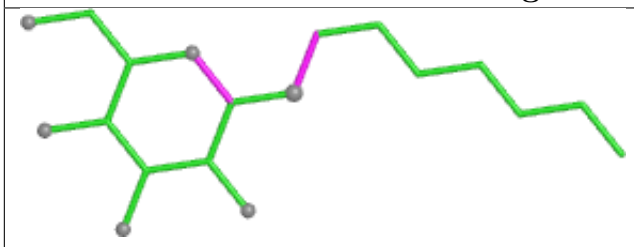


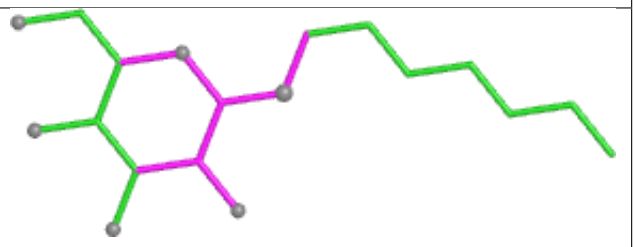
Torsions

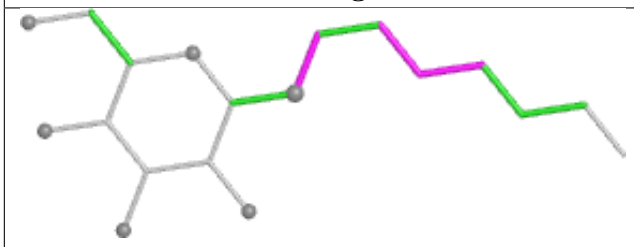


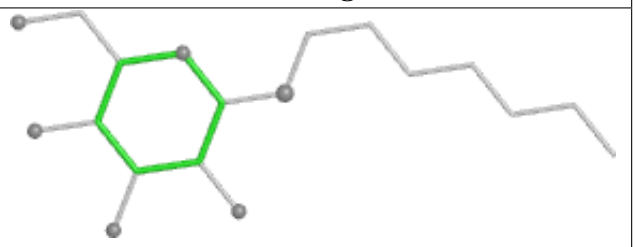
Rings

Ligand HTG B 621

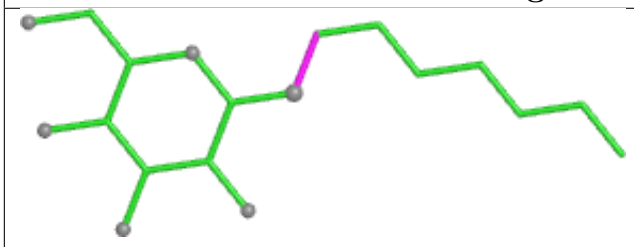

Bond lengths

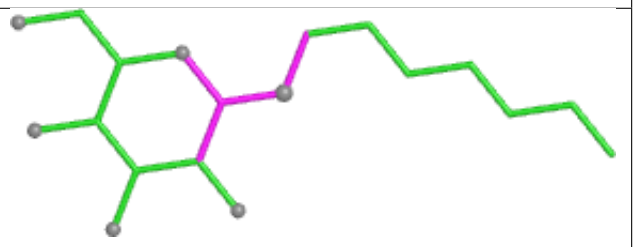

Bond angles

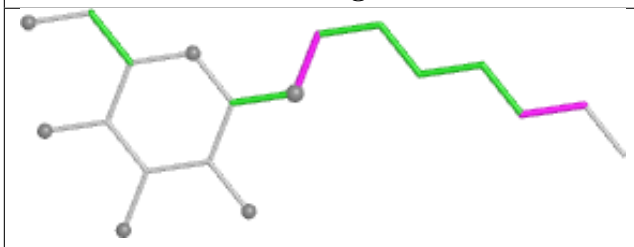

Torsions

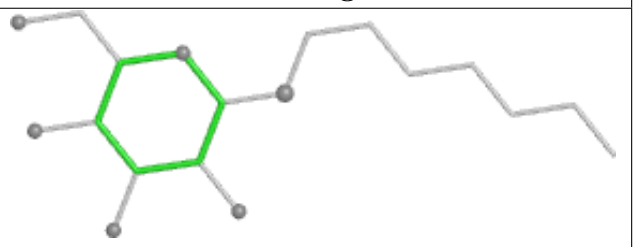

Rings

Ligand HTG c 521

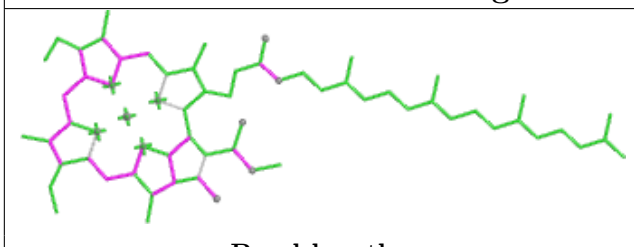

Bond lengths

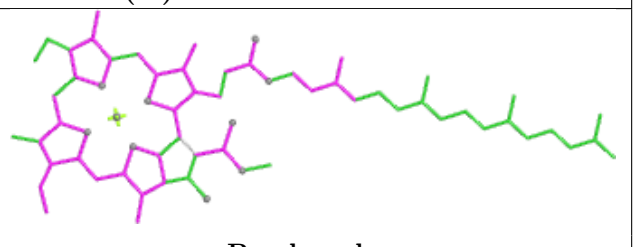

Bond angles

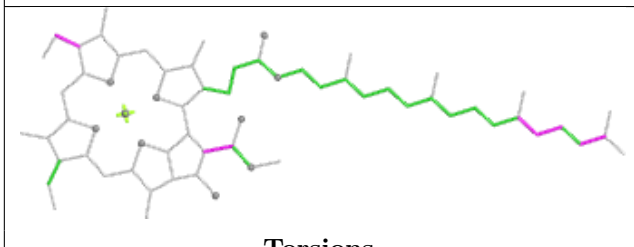

Torsions

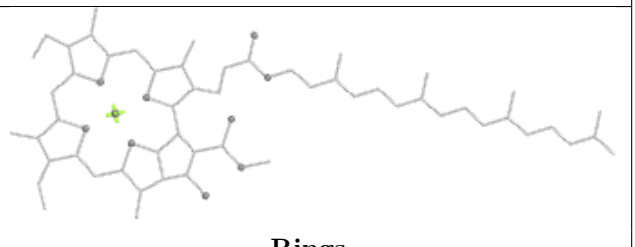

Rings

Ligand CLA A 406 (B)

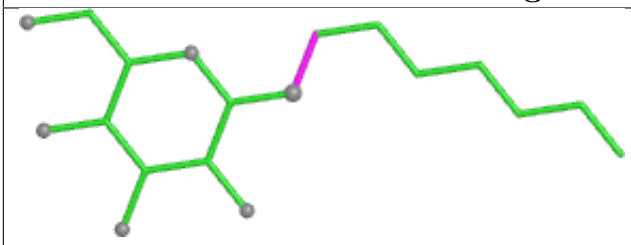

Bond lengths


Bond angles

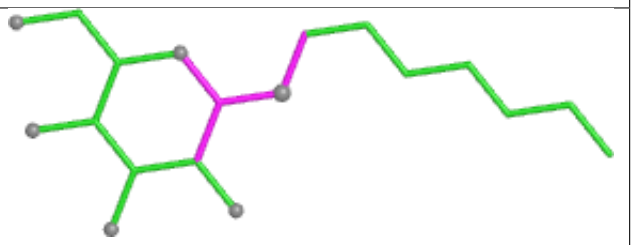

Torsions


Rings

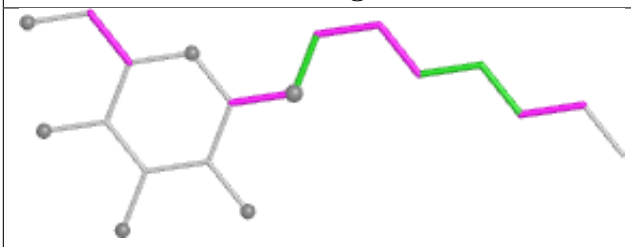
Ligand HTG b 623



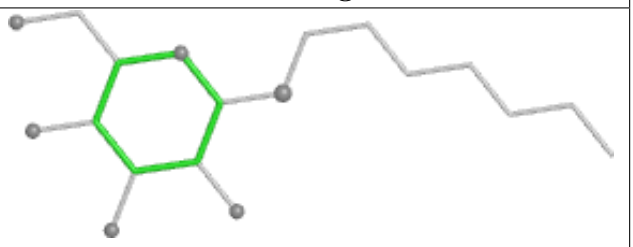
Bond lengths



Bond angles

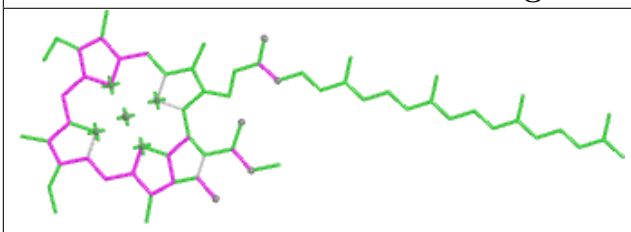


Torsions

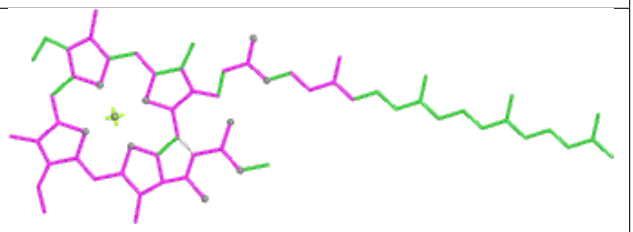


Rings

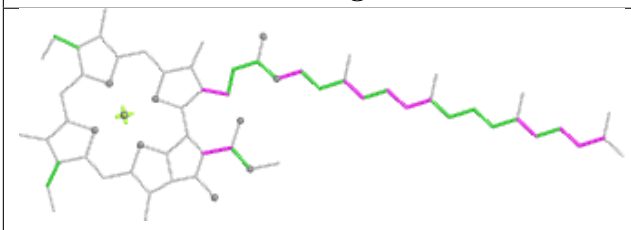
Ligand CLA C 507



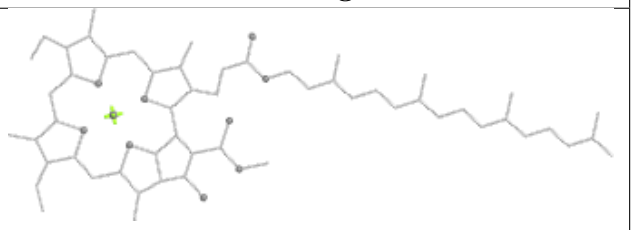
Bond lengths



Bond angles

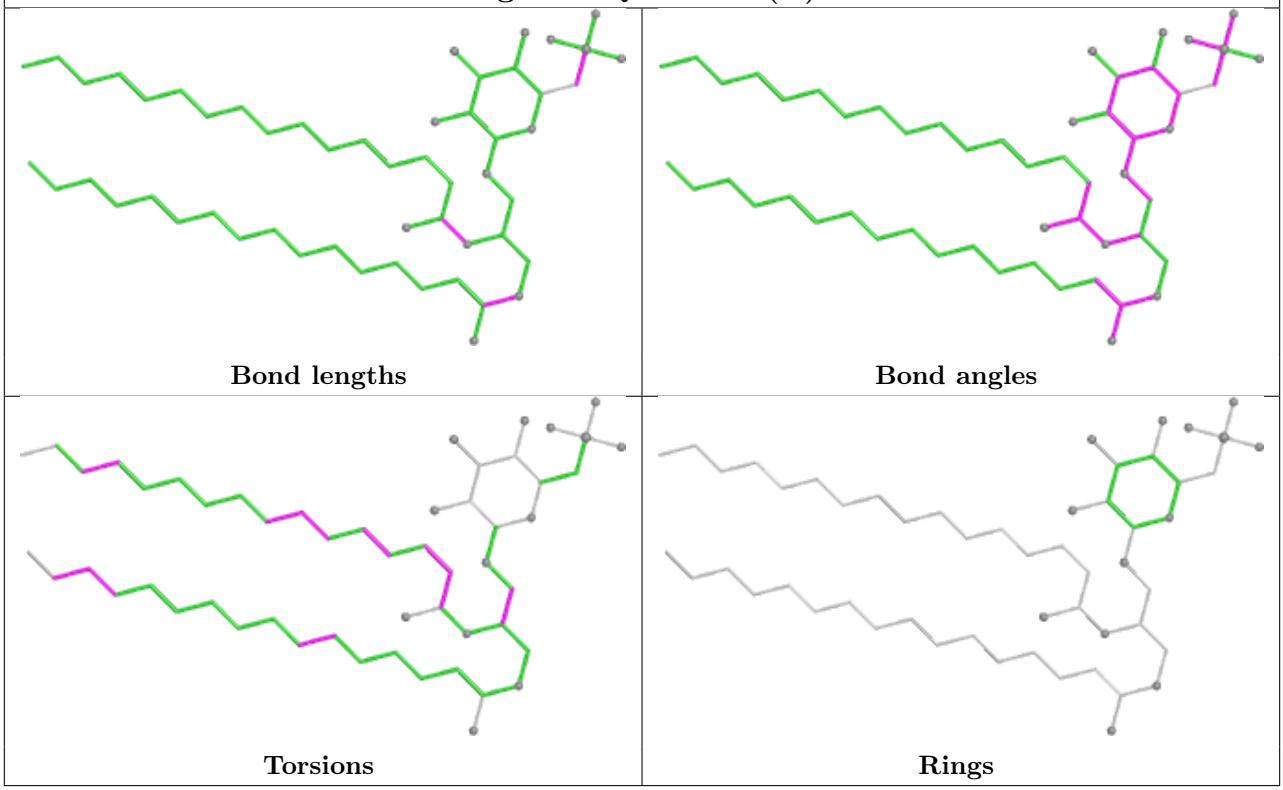


Torsions



Rings

Ligand SQD a 409 (B)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.66	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	a	417	6/6	0.62	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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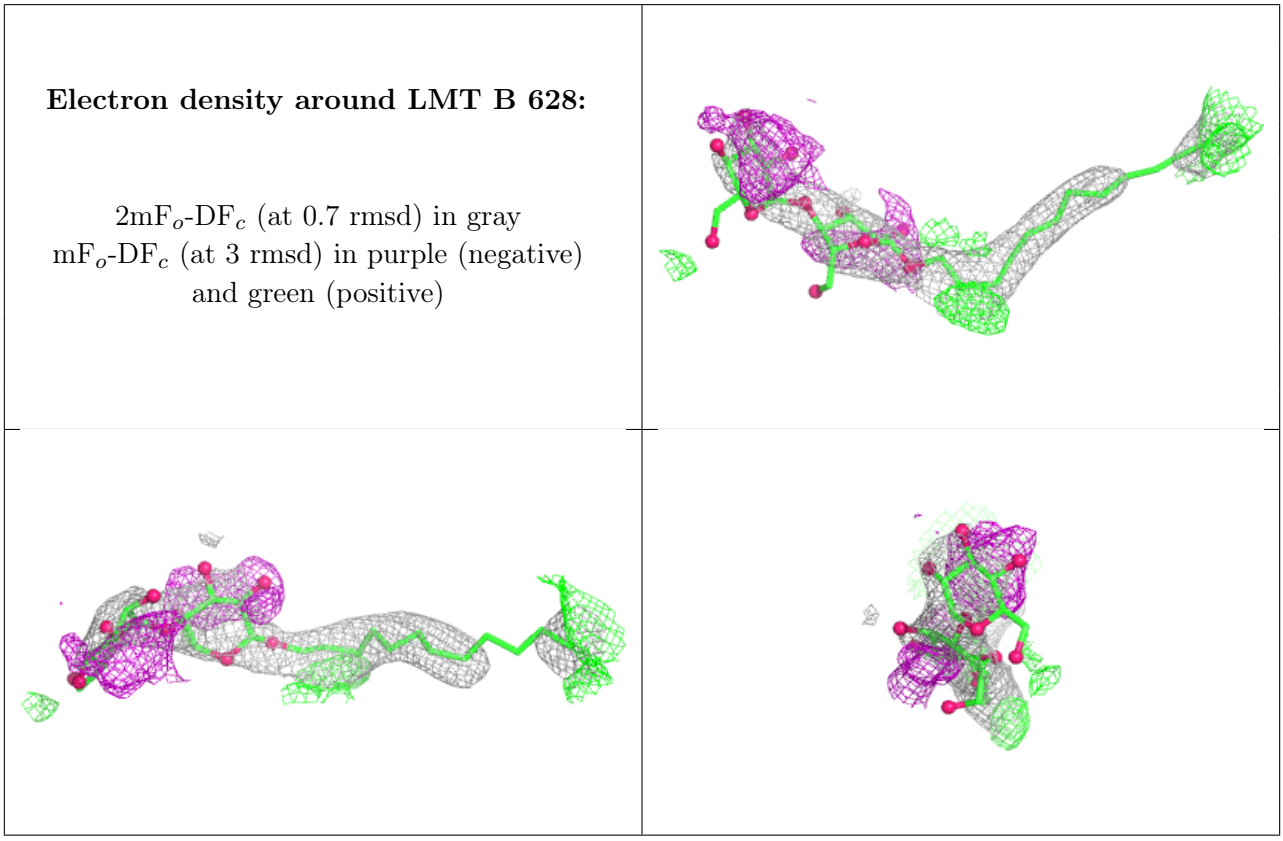
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	a	401[B]	1/1	0.99	0.02	54,54,54,54	1
28	OEX	a	412[B]	10/10	1.00	0.02	47,49,51,55	10
21	FE2	A	401[A]	1/1	1.00	0.01	51,51,51,51	1
36	CA	c	523	1/1	1.00	0.03	78,78,78,78	0
21	FE2	A	401[B]	1/1	1.00	0.01	52,52,52,52	1
28	OEX	a	412[A]	10/10	1.00	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.

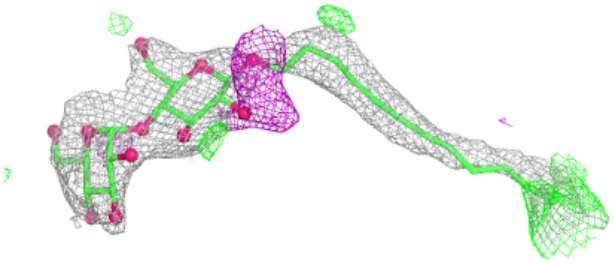
Electron density around LMT B 628:

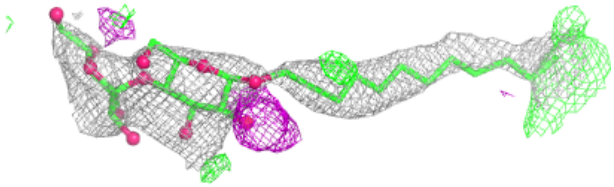
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

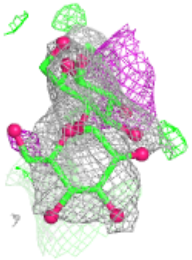


Electron density around LMT A 417:

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

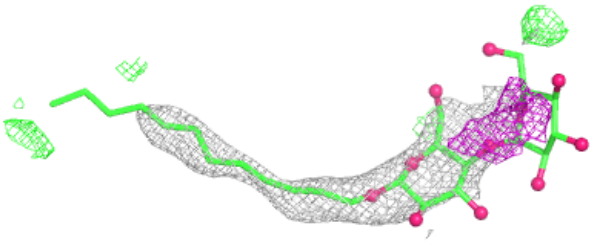


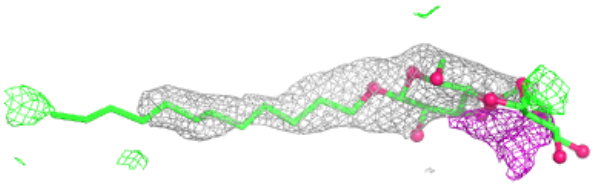


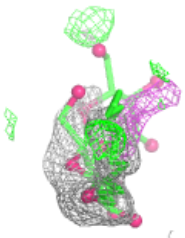


Electron density around LMT F 101:

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

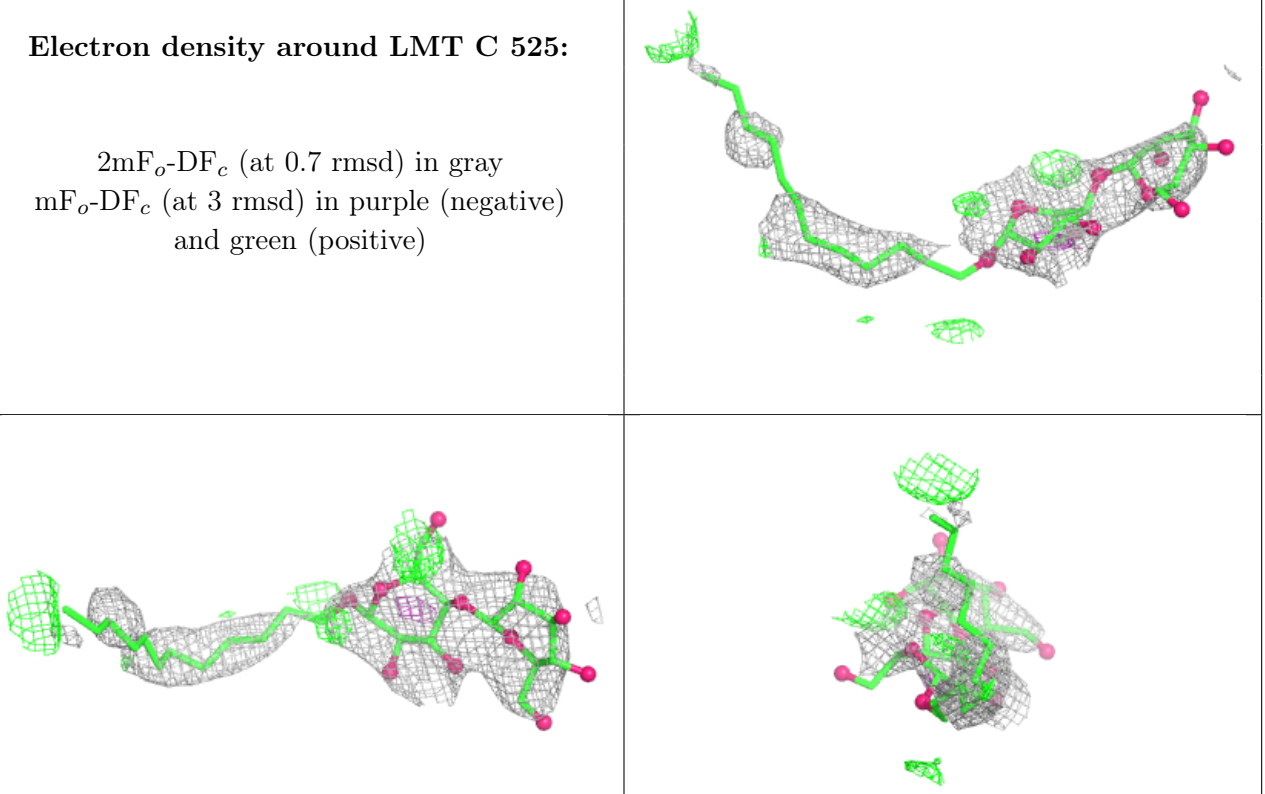






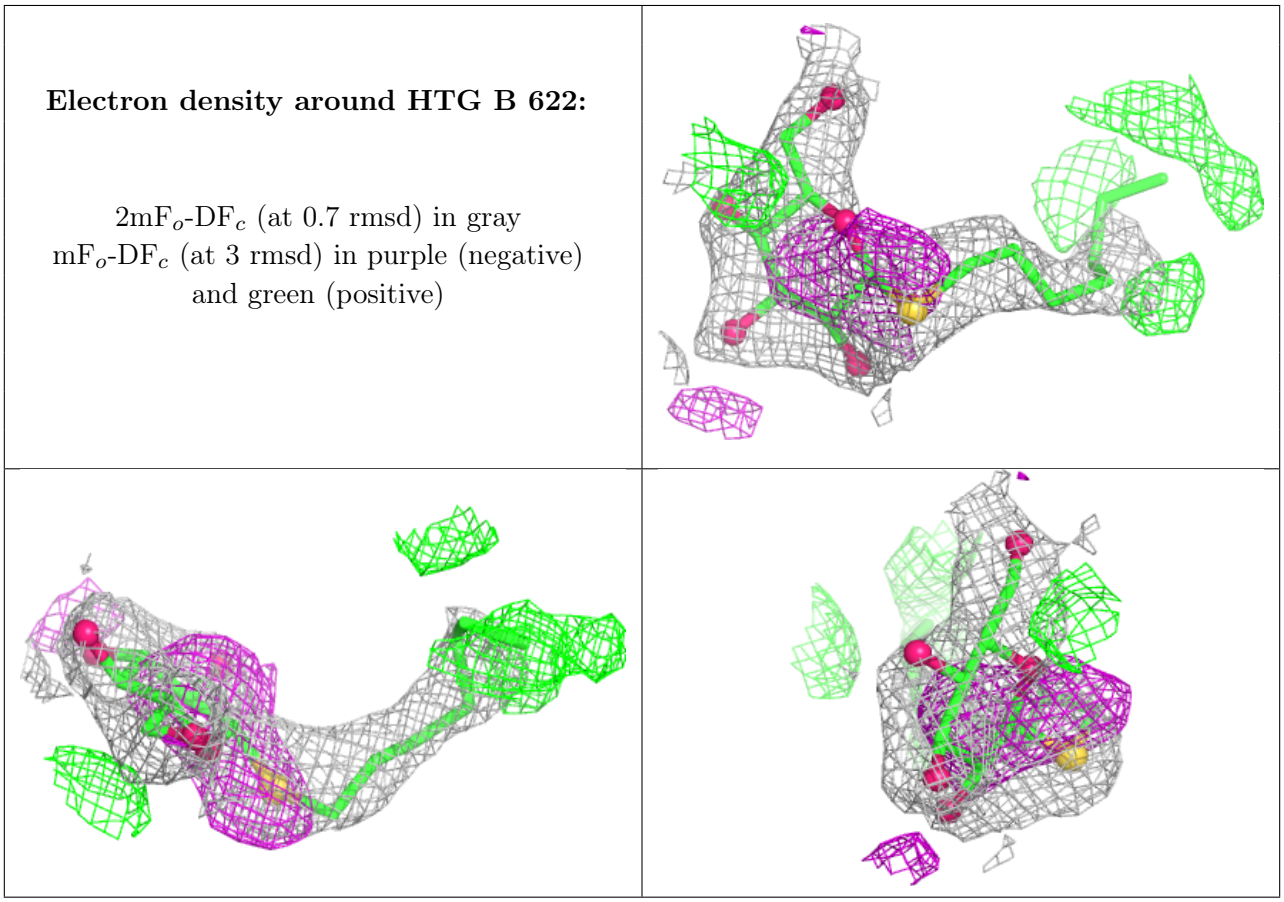
Electron density around LMT C 525:

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



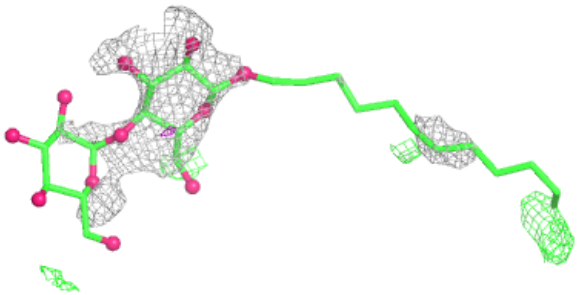
Electron density around HTG B 622:

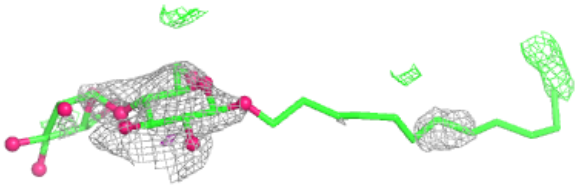
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

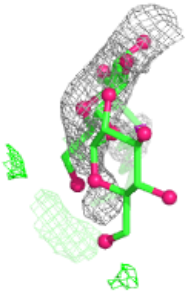


Electron density around LMT e 101:

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

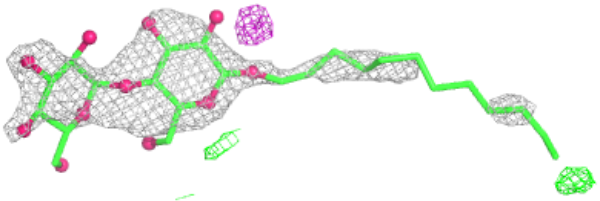


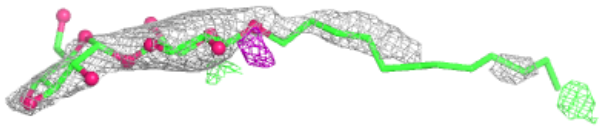




Electron density around LMT a 416:

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

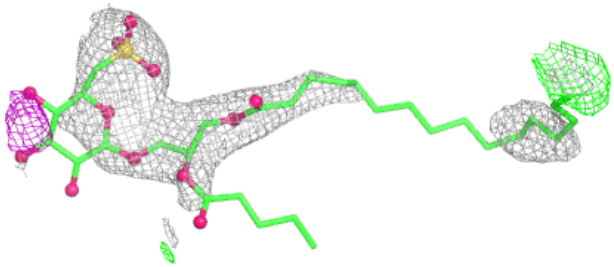


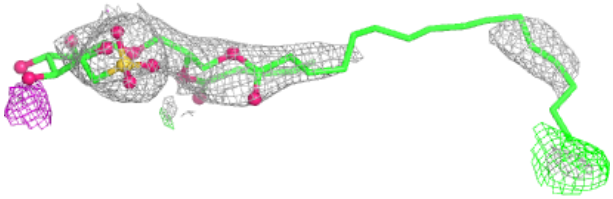


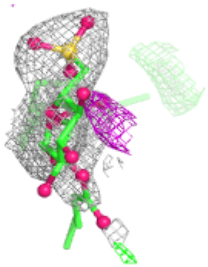


Electron density around SQD f 102:

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

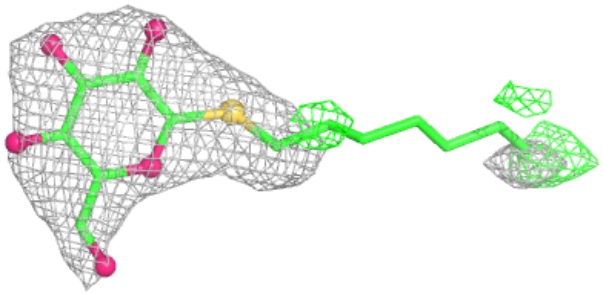


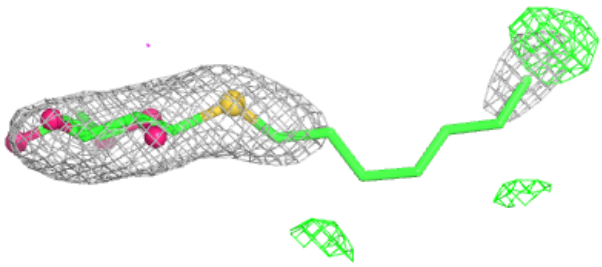


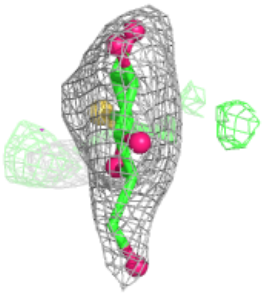


Electron density around HTG C 522:

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

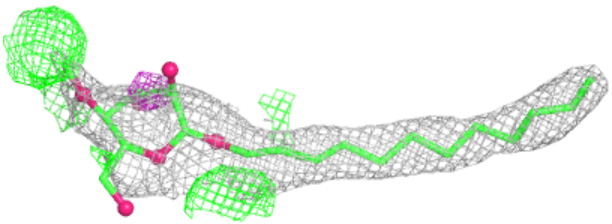


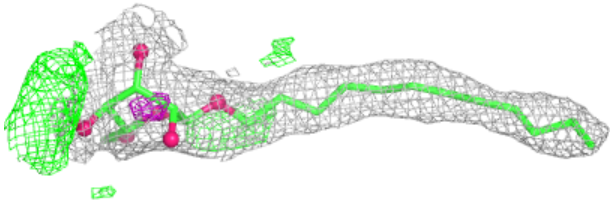


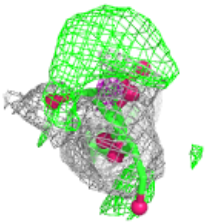


Electron density around LMT b 621:

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

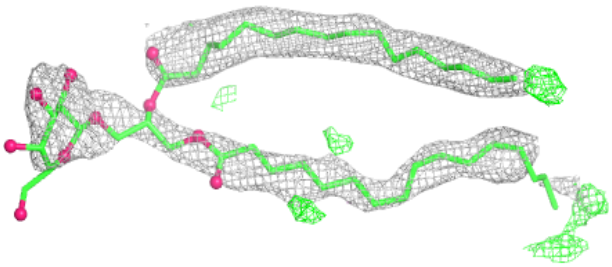


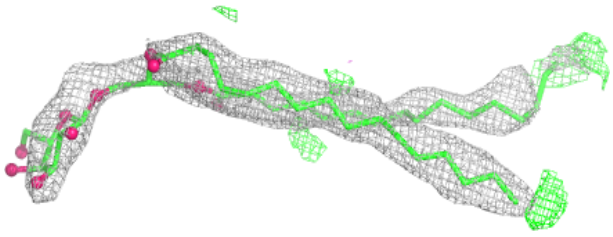


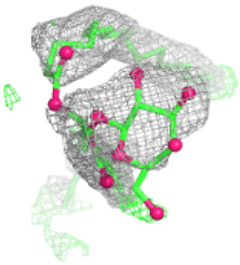


Electron density around LMG C 521:

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

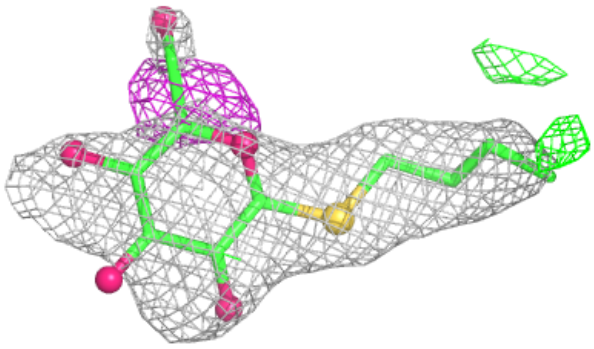


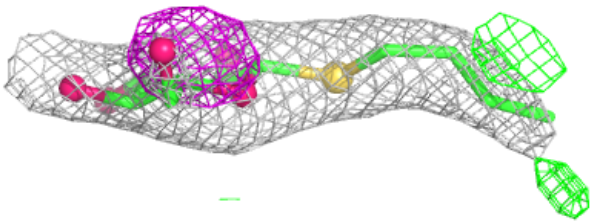


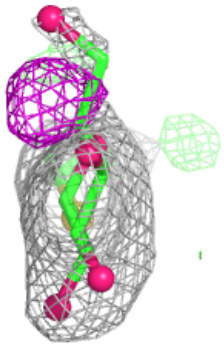


Electron density around HTG D 410:

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

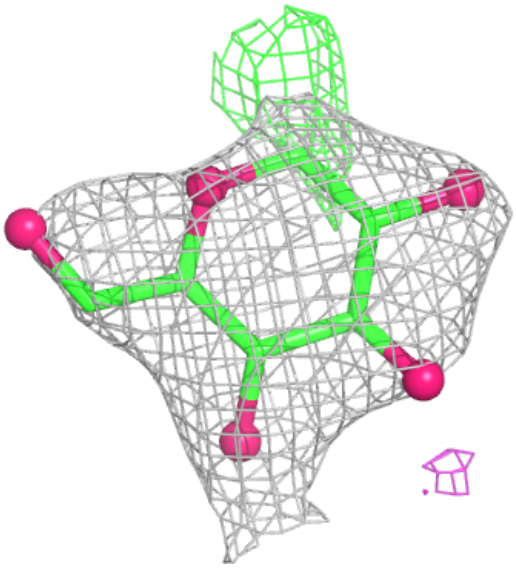


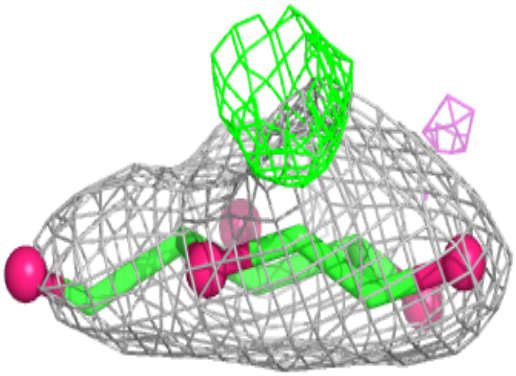


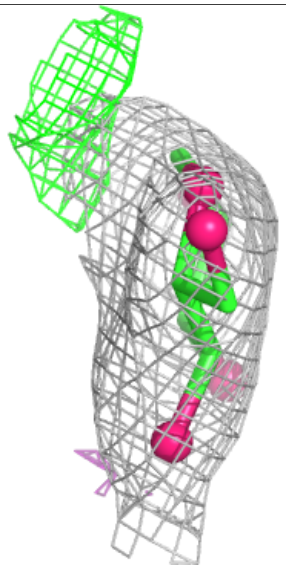


Electron density around HTG V 202:

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

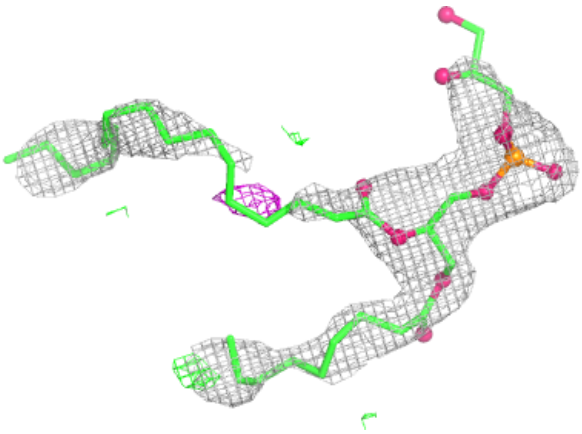


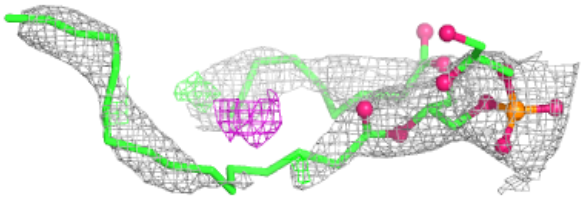


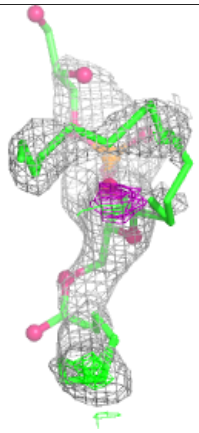


Electron density around LHG a 419 (A):

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

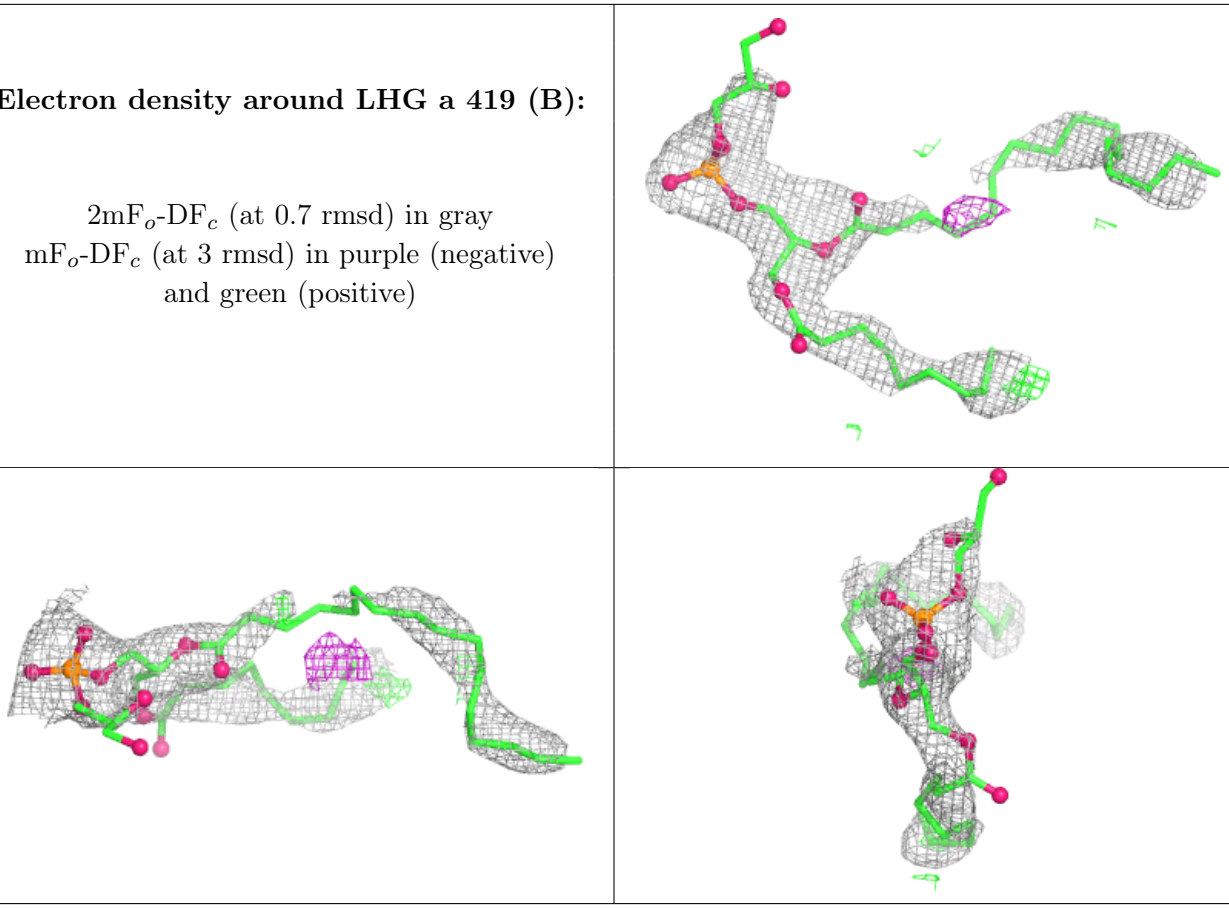






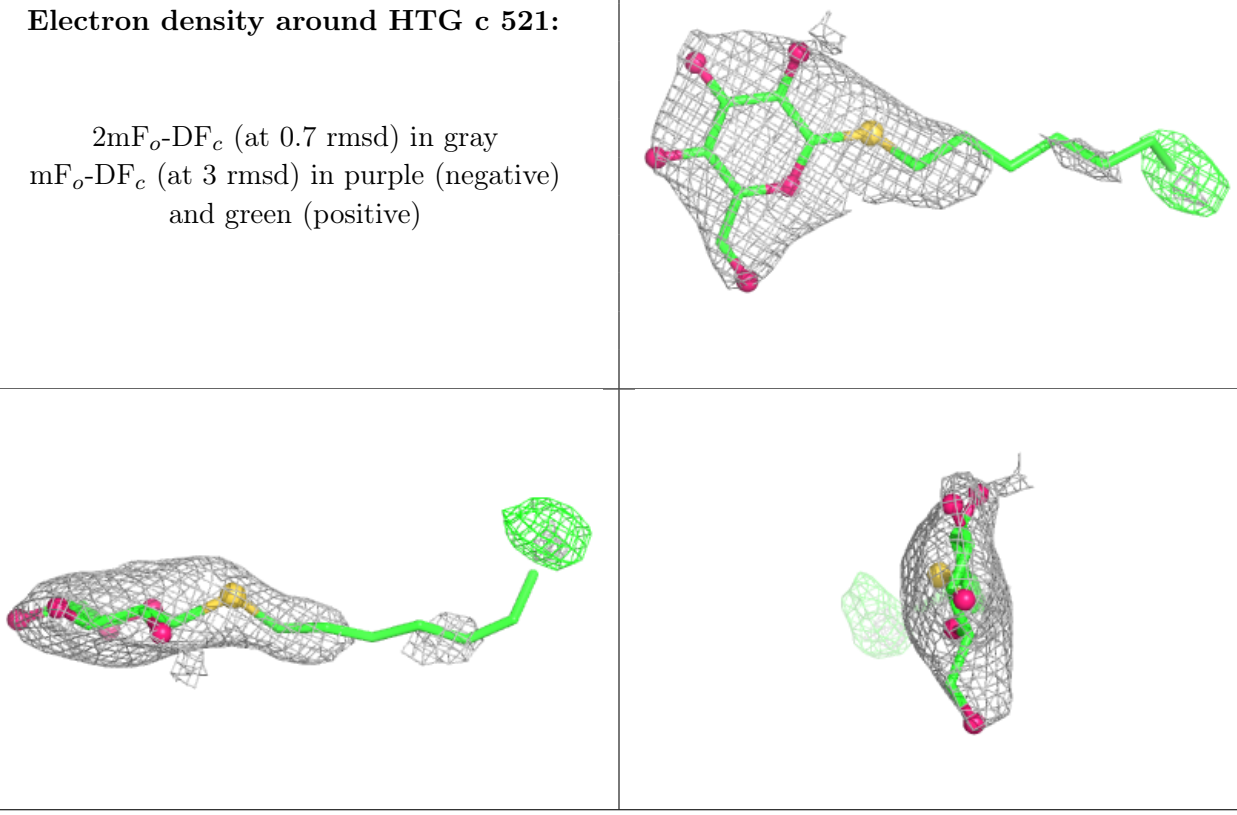
Electron density around LHG a 419 (B):

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



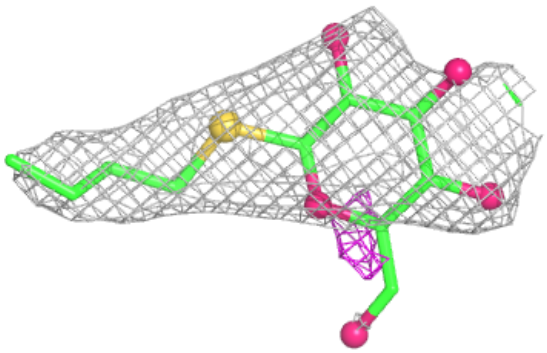
Electron density around HTG c 521:

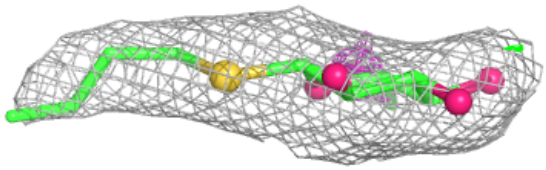
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

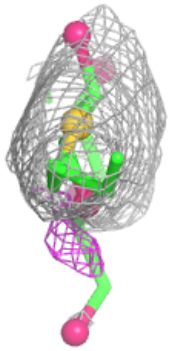


Electron density around HTG d 412:

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

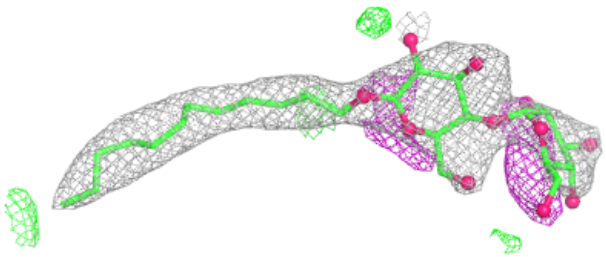


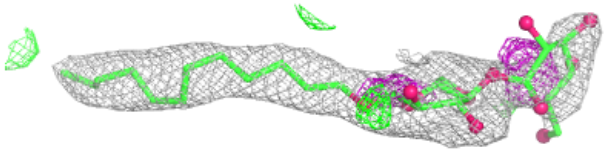


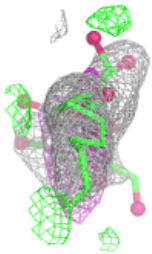


Electron density around LMT B 627:

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

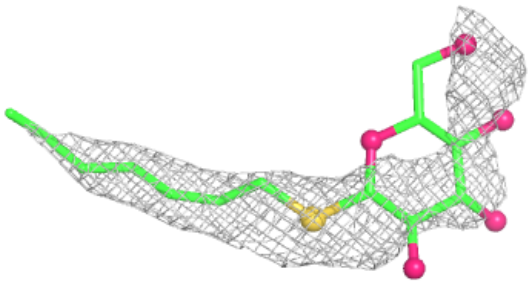


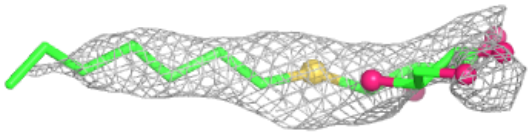


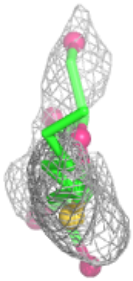


Electron density around HTG b 623:

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

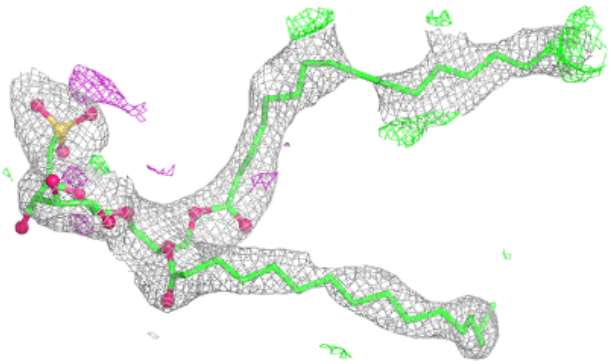


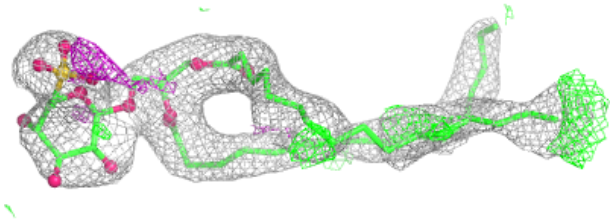


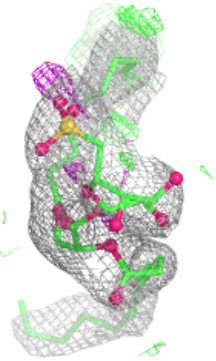


Electron density around SQD a 411:

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

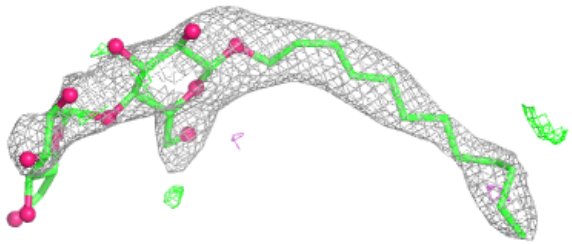


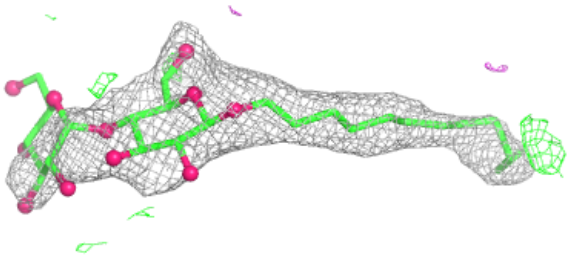


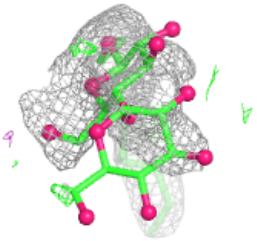


Electron density around LMT T 101:

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

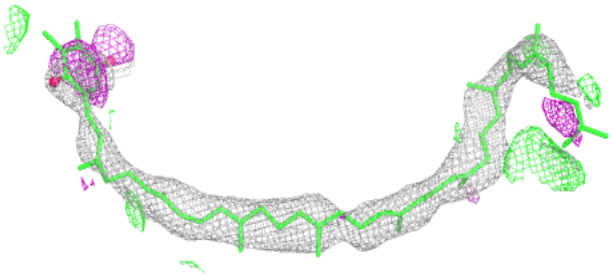


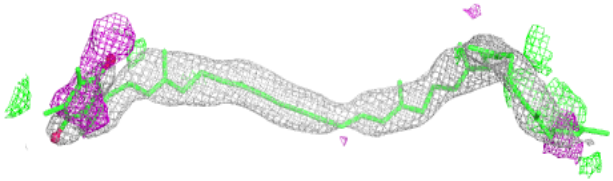


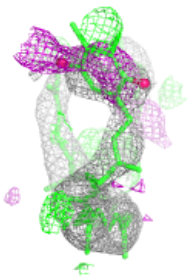


Electron density around PL9 A 414 (B):

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

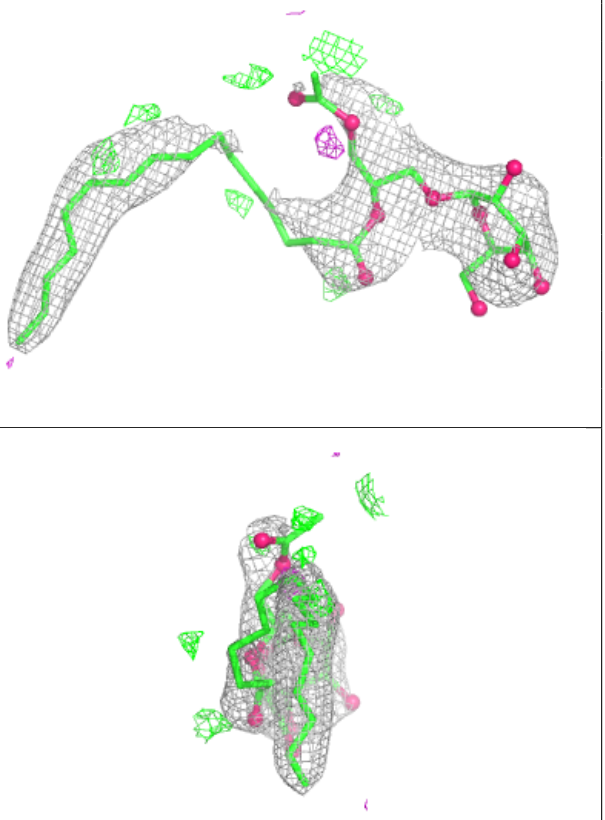






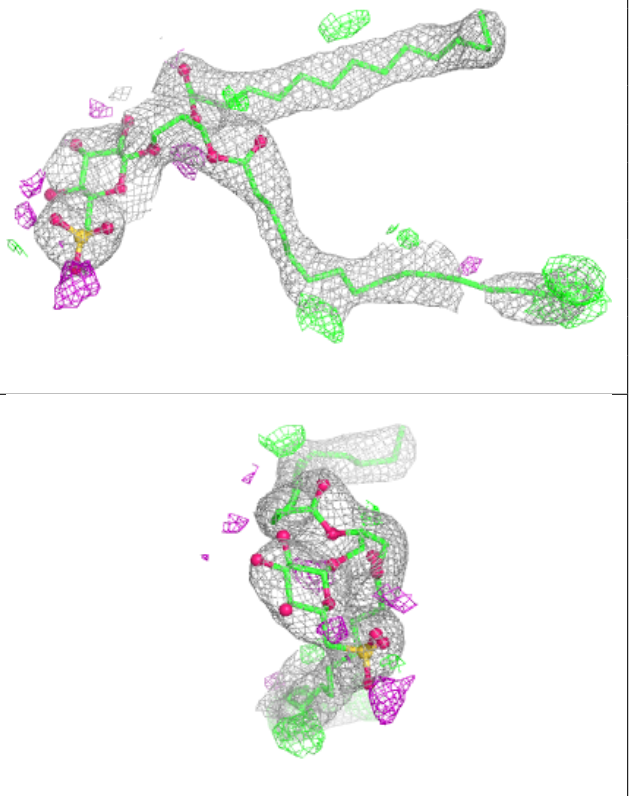
Electron density around LMG Z 101:

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



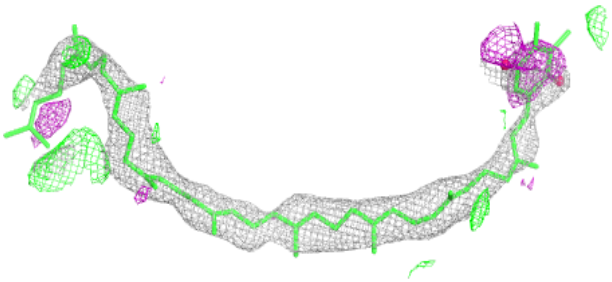
Electron density around SQD A 412:

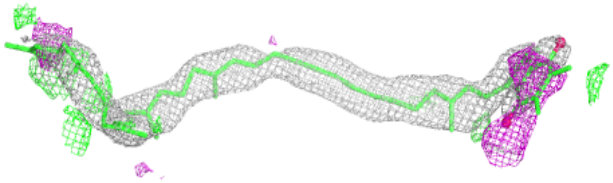
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

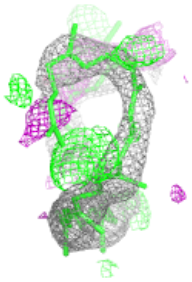


Electron density around PL9 A 414 (A):

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

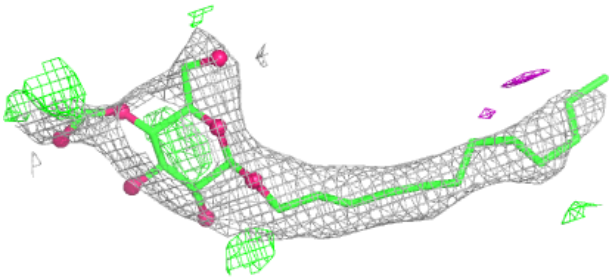


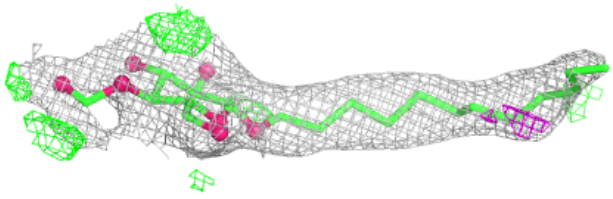


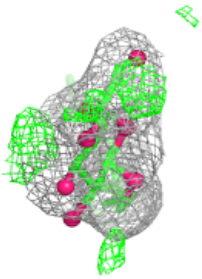


Electron density around LMT t 101:

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

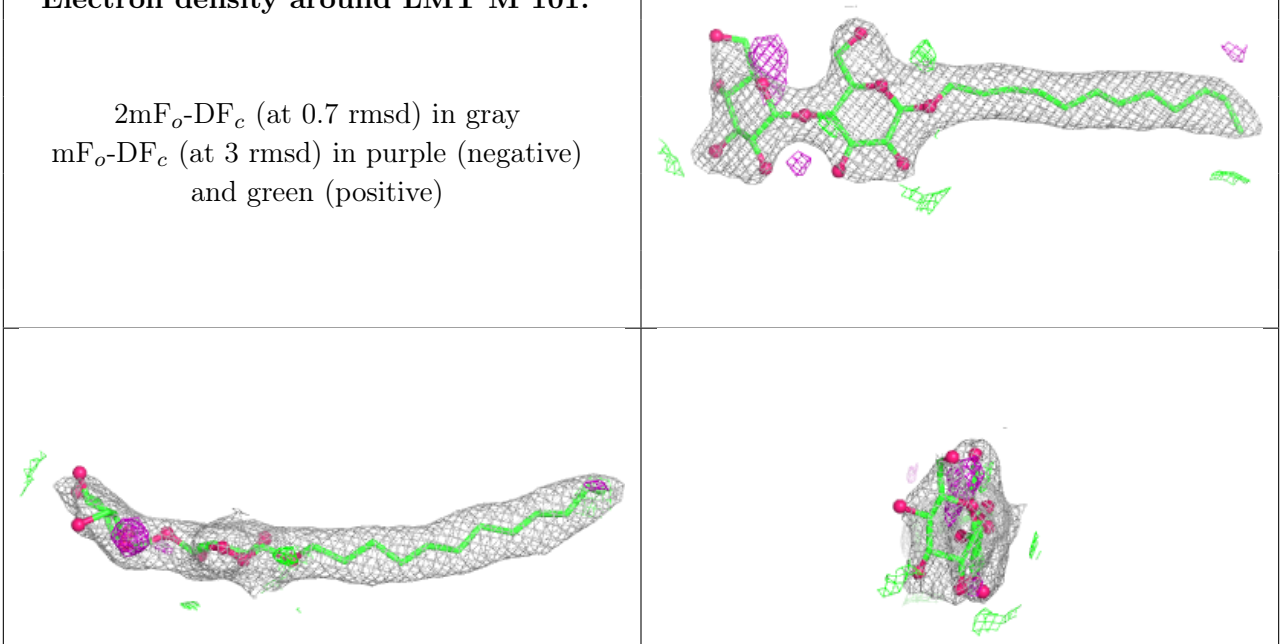






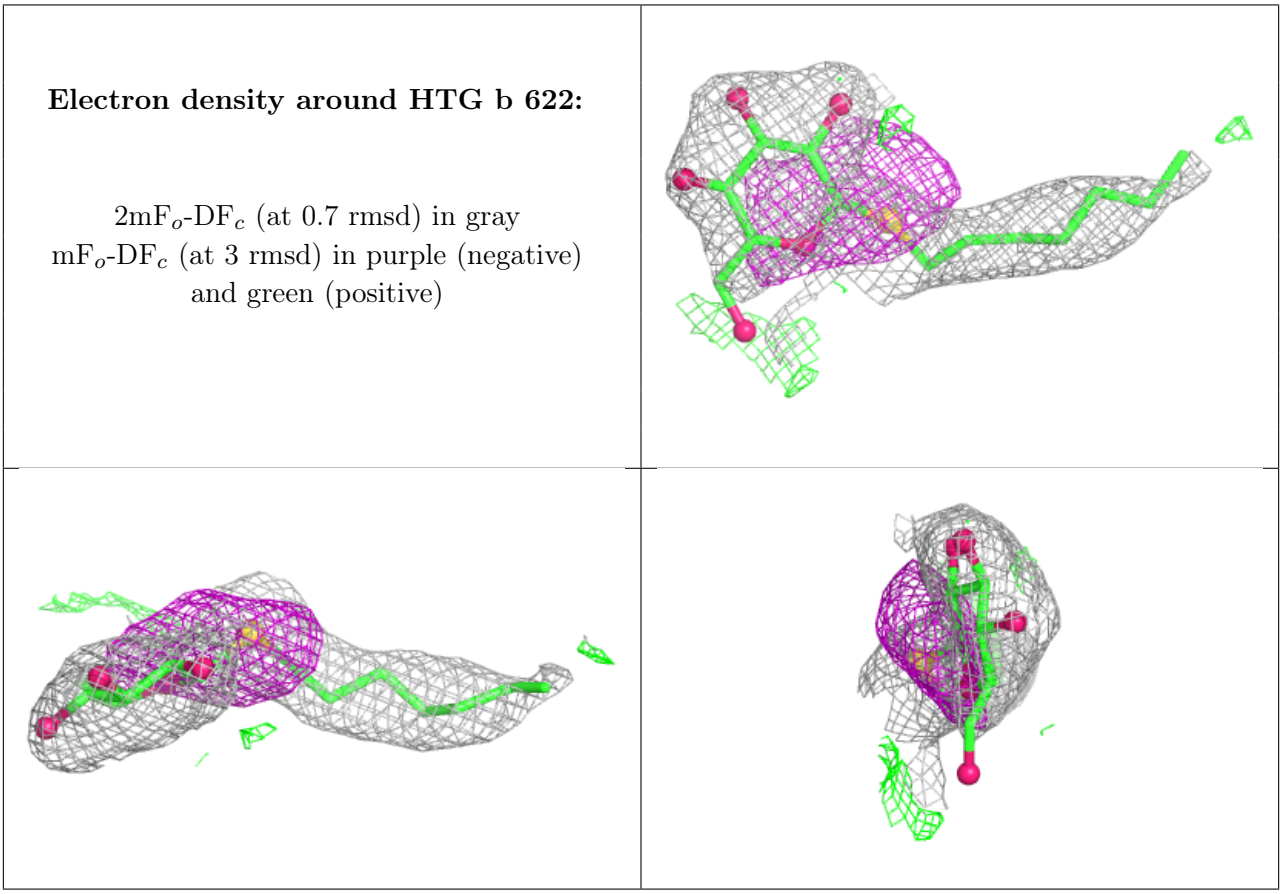
Electron density around LMT M 101:

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



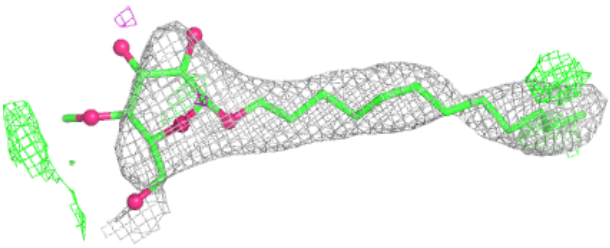
Electron density around HTG b 622:

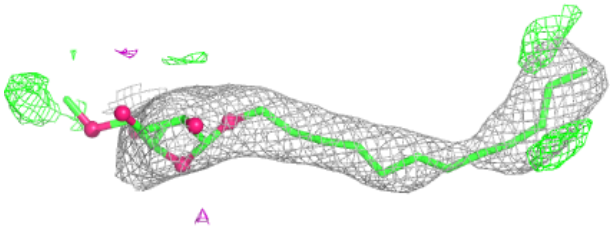
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

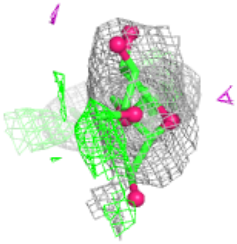


Electron density around LMT B 629:

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

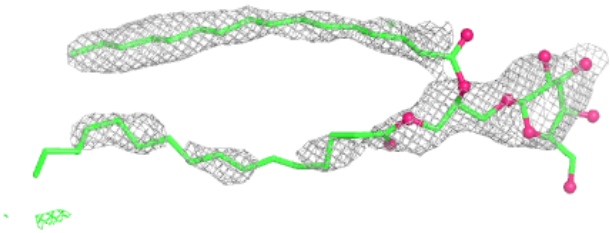


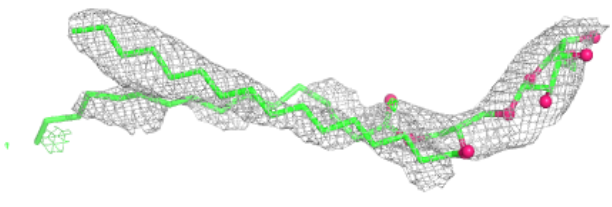


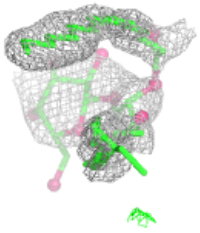


Electron density around LMG c 520:

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

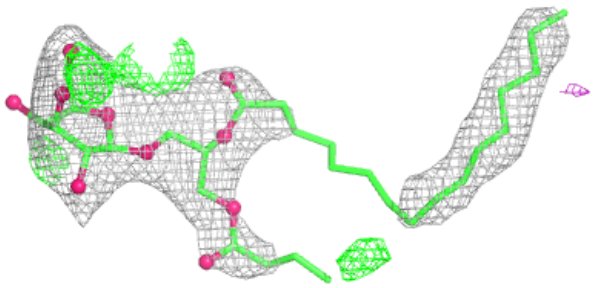


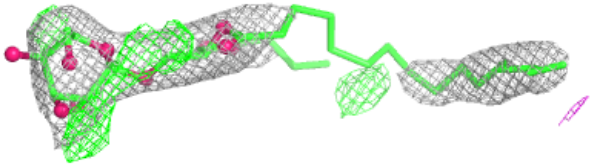


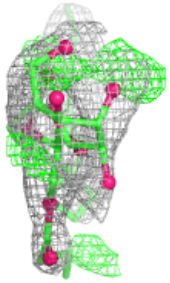


Electron density around LMG z 101:

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

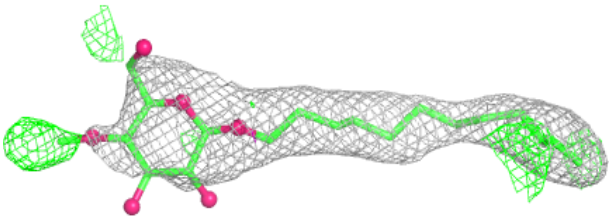


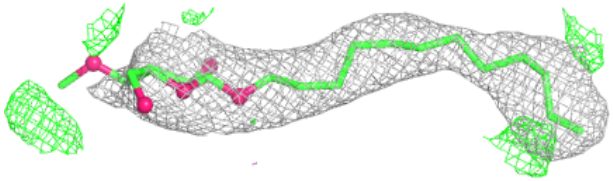


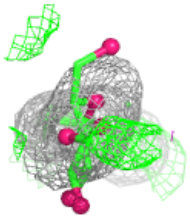


Electron density around LMT b 627:

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

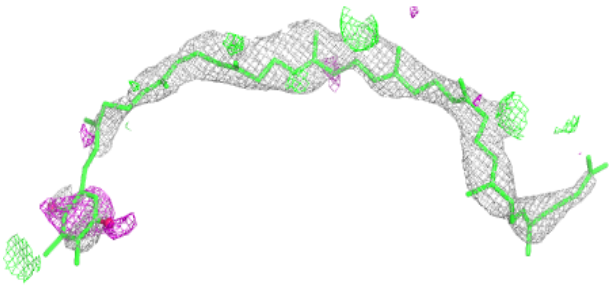


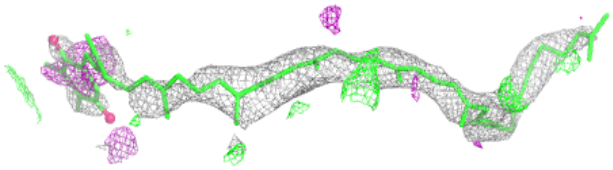


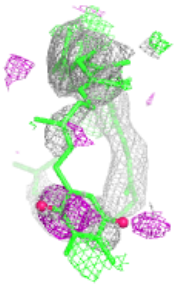


Electron density around PL9 a 413 (A):

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

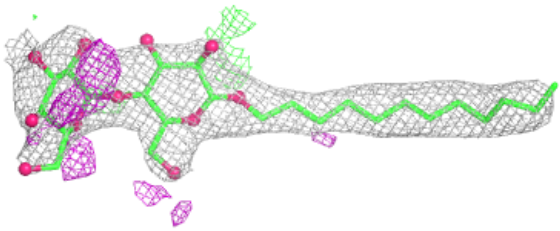


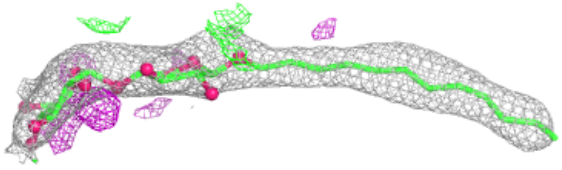


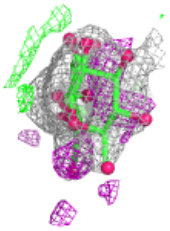


Electron density around LMT m 103:

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

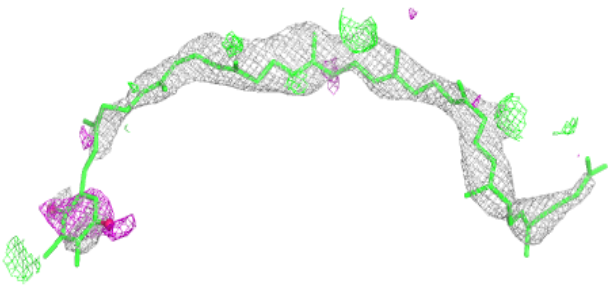


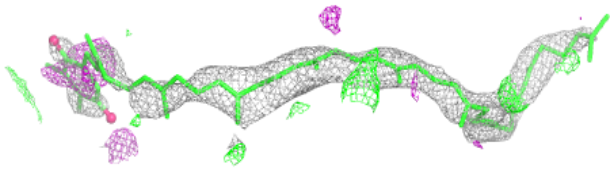


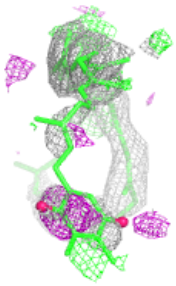


Electron density around PL9 a 413 (B):

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

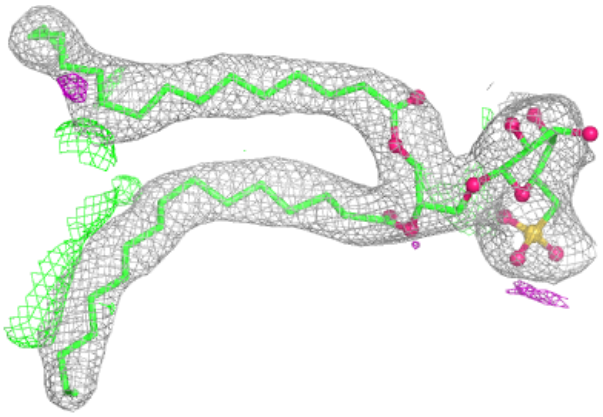


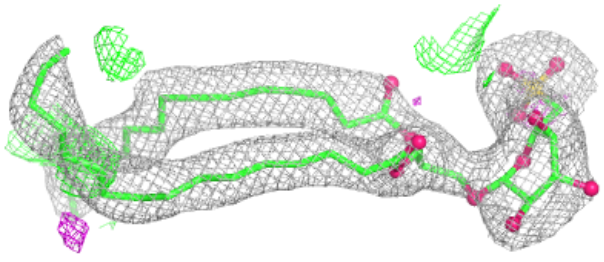


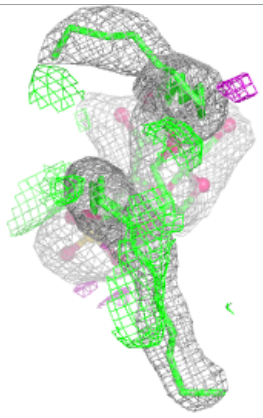


Electron density around SQD l 101:

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

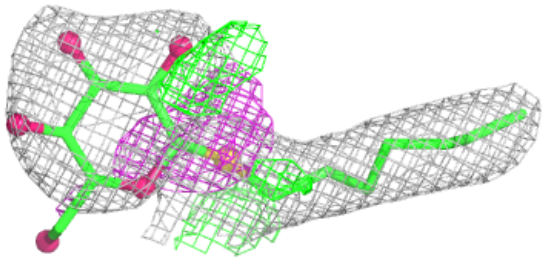


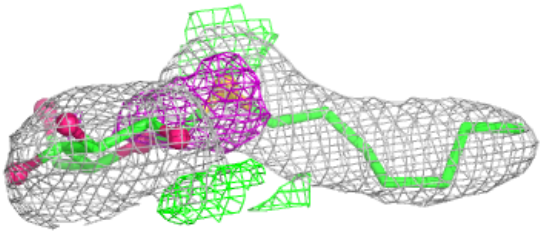


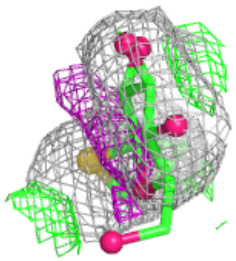


Electron density around HTG B 621:

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

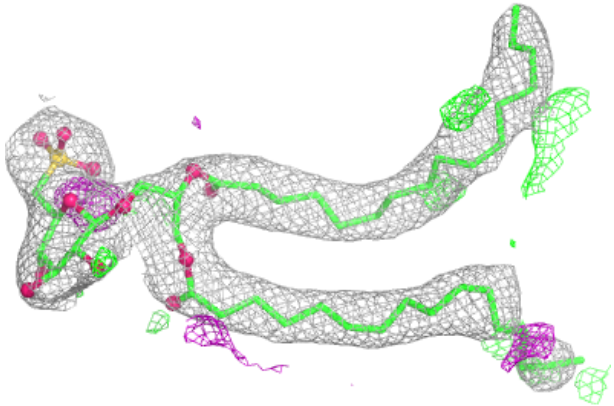


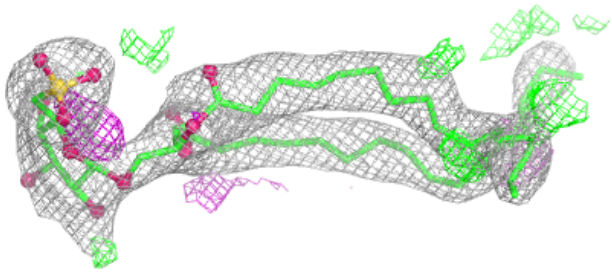


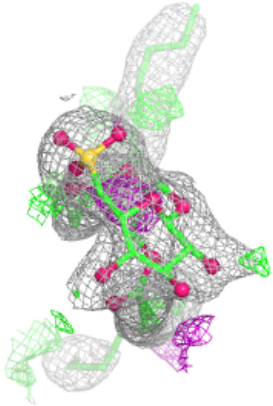


Electron density around SQD b 620:

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

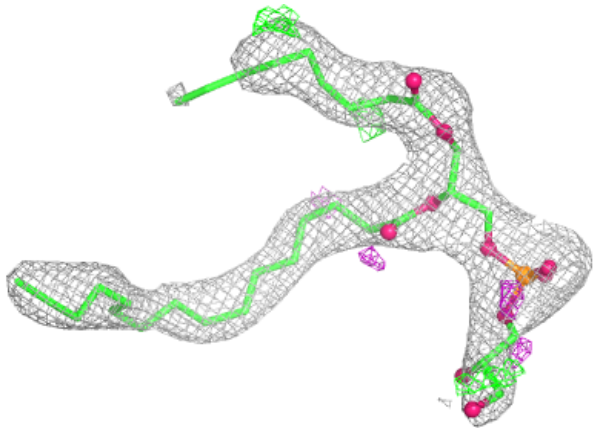


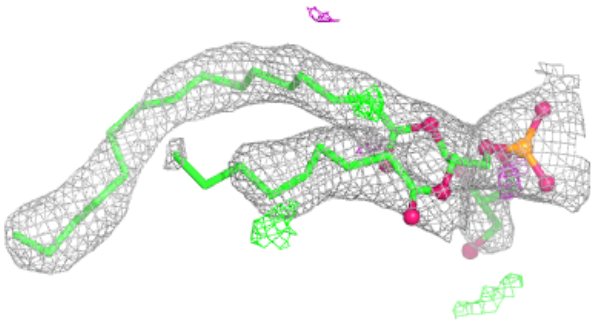


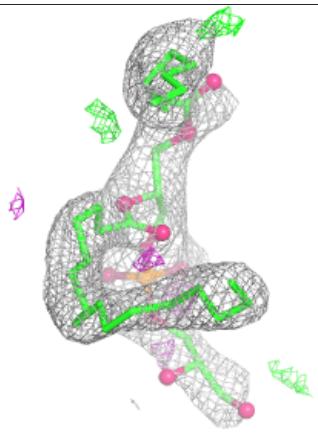


Electron density around LHG E 101 (A):

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

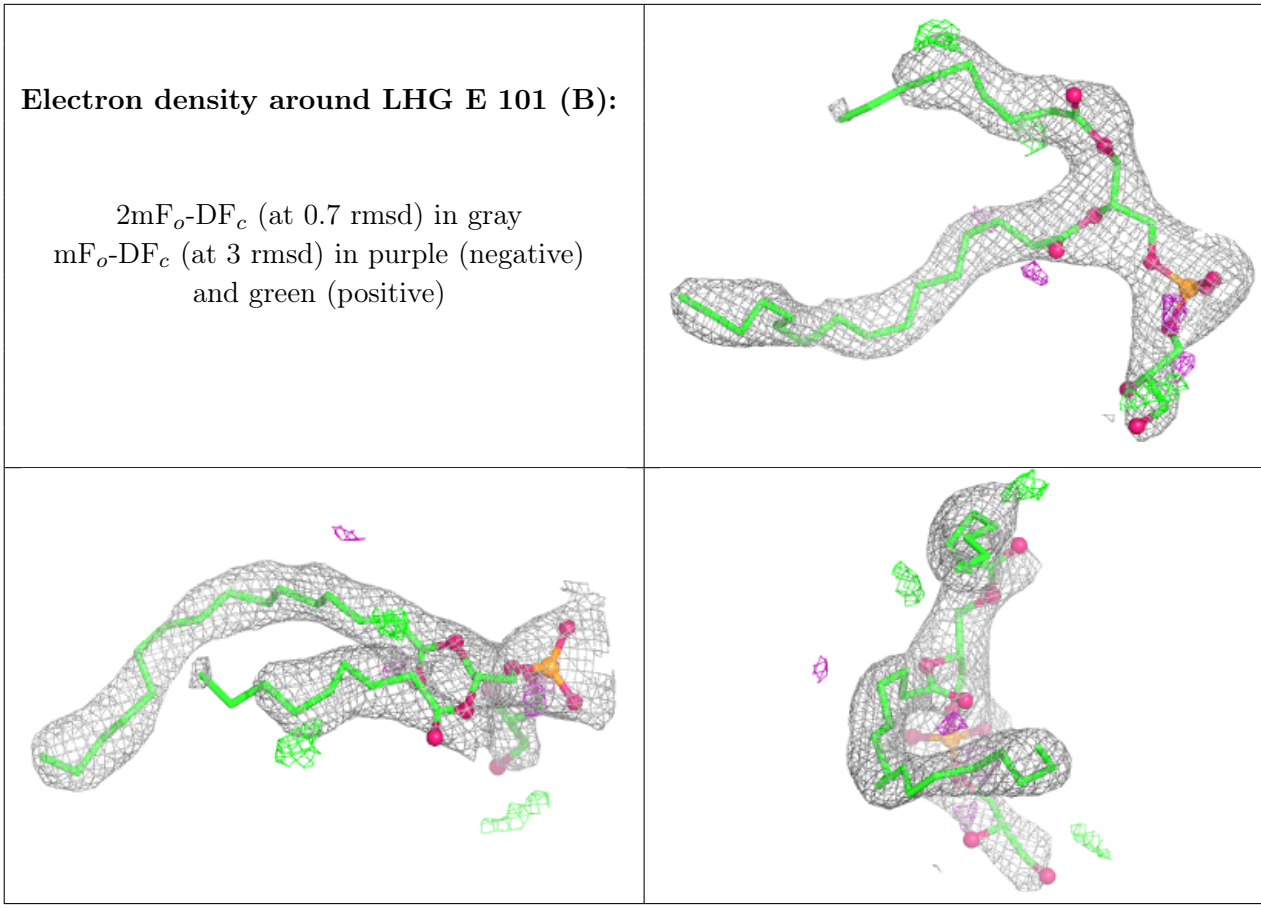






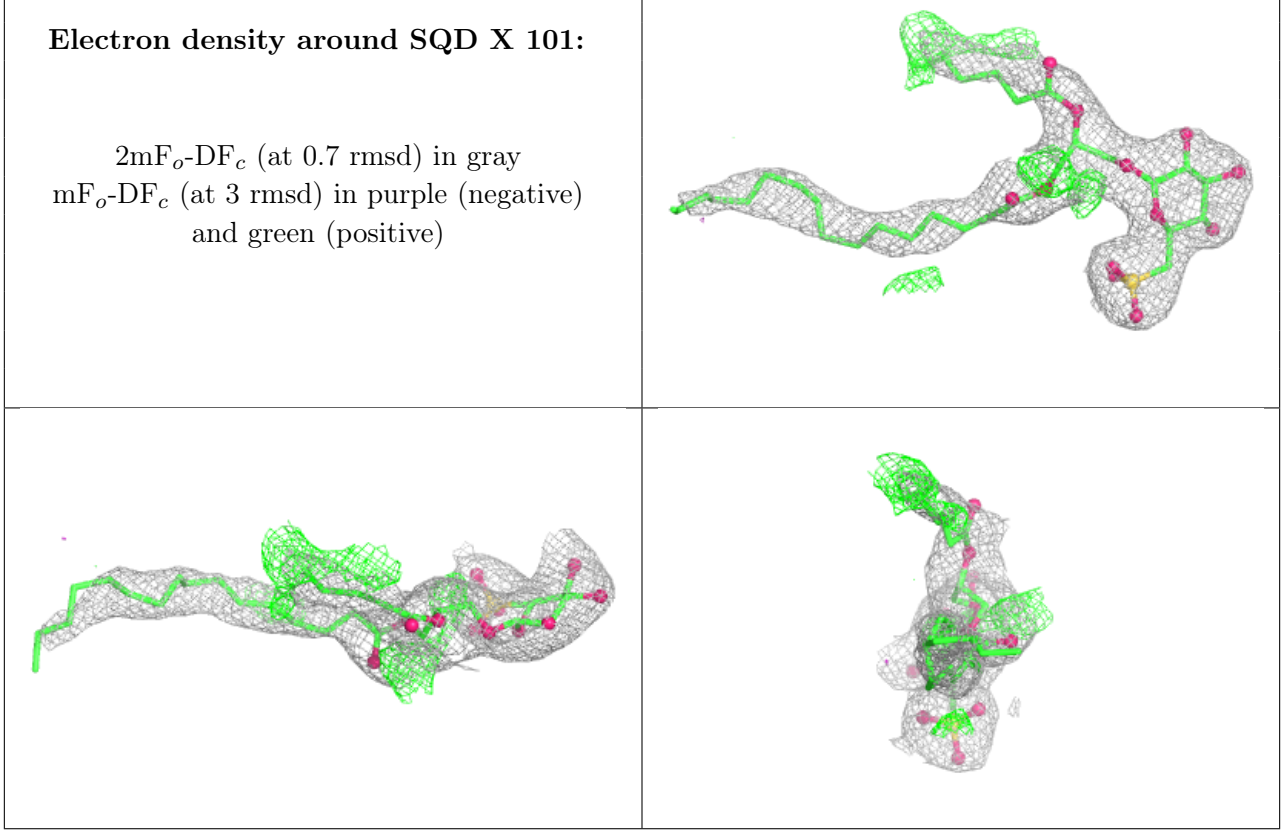
Electron density around LHG E 101 (B):

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



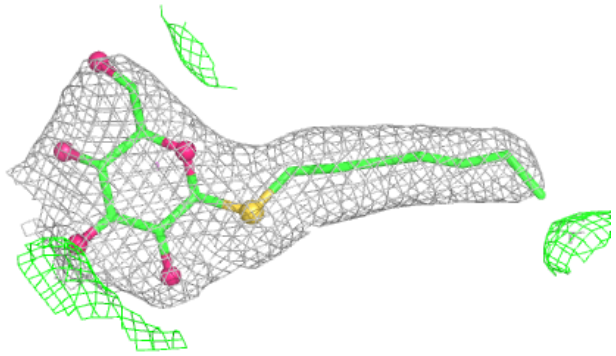
Electron density around SQD X 101:

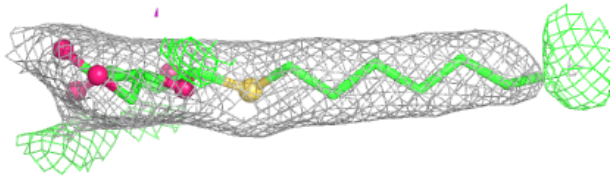
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

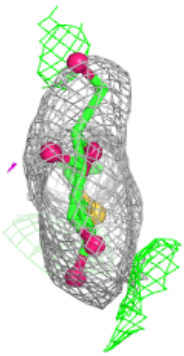


Electron density around HTG B 624:

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

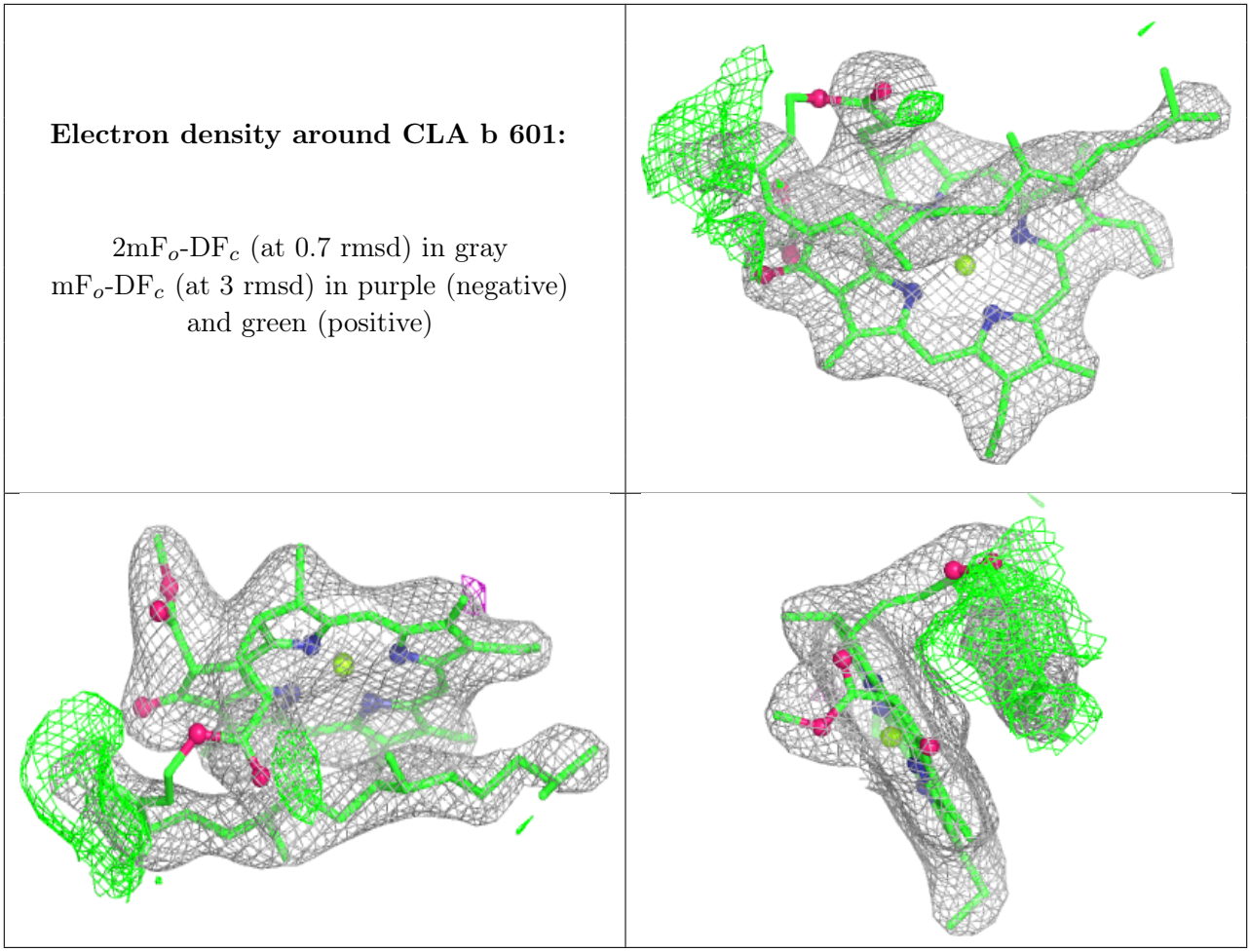






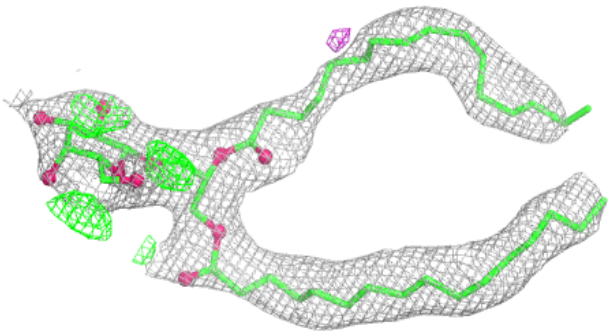
Electron density around CLA b 601:

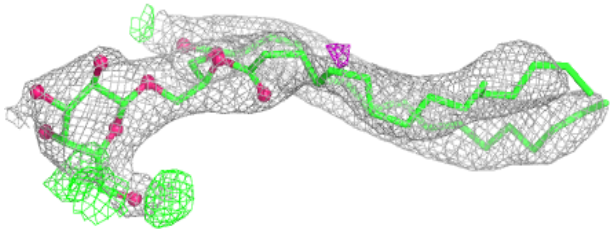
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

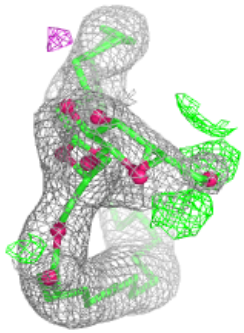


Electron density around LMG C 501:

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

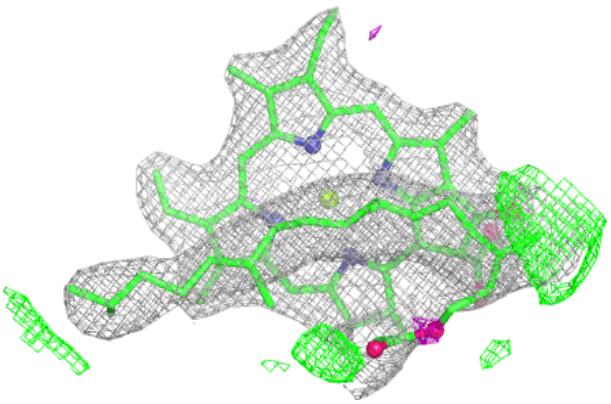


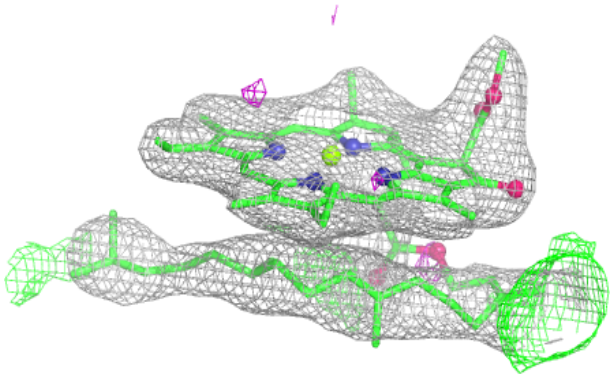


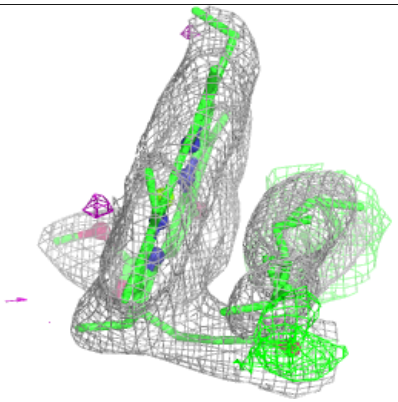


Electron density around CLA B 601:

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

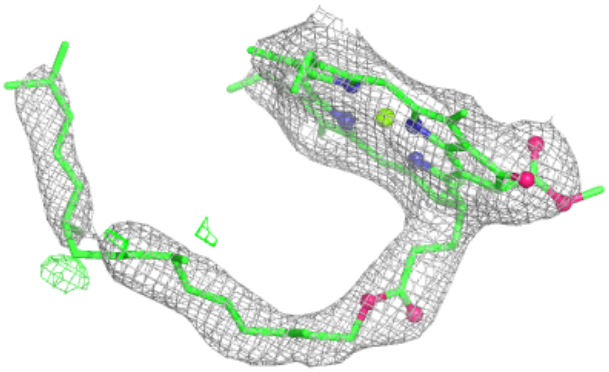


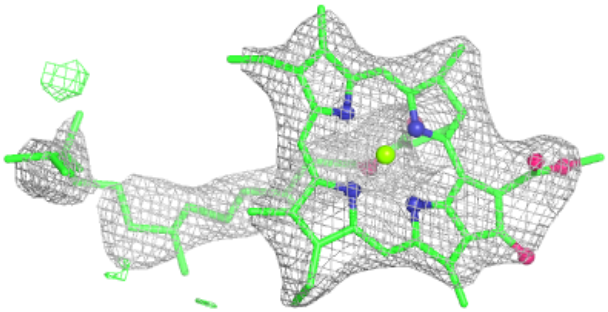


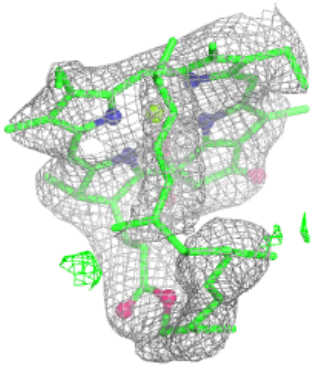


Electron density around CLA c 513:

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

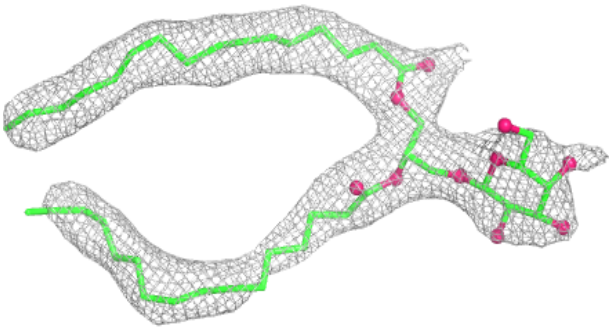


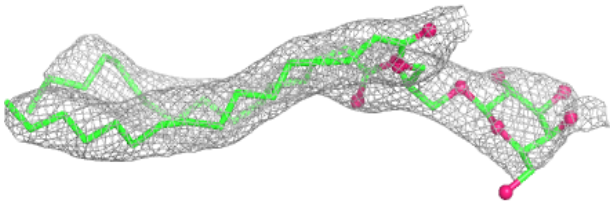


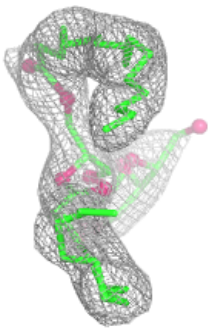


Electron density around LMG a 415:

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

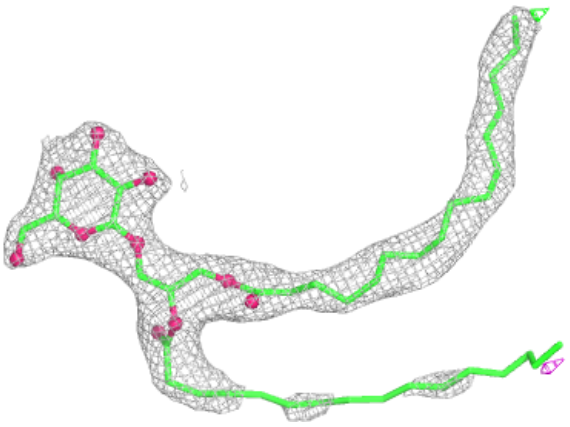


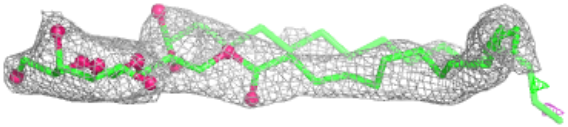


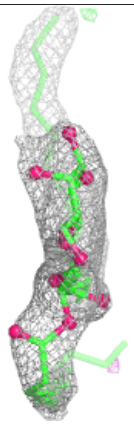


Electron density around LMG c 519:

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

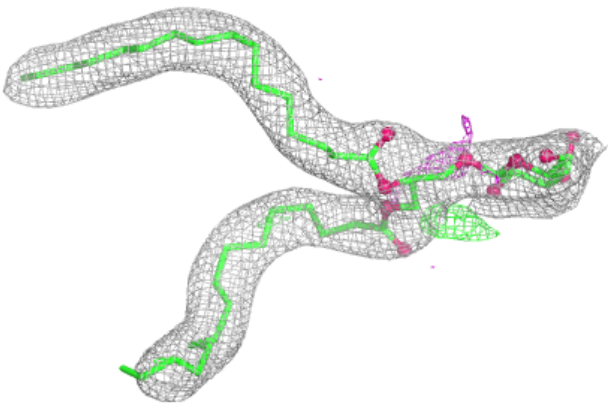


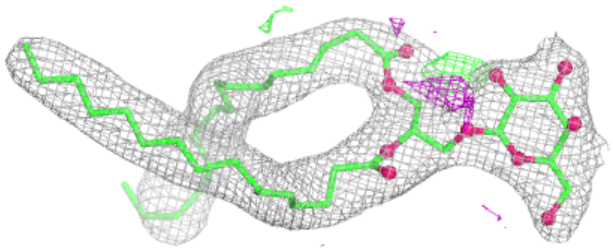


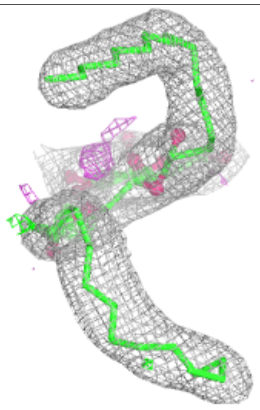


Electron density around LMG m 101:

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

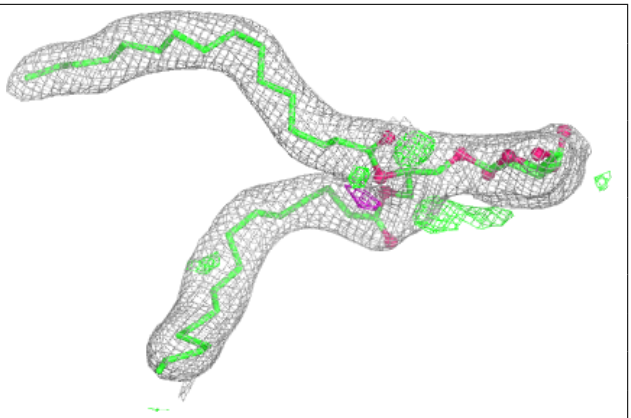


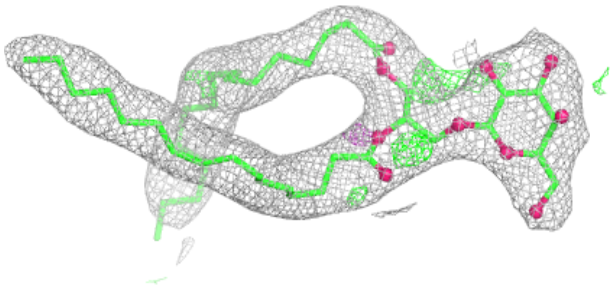


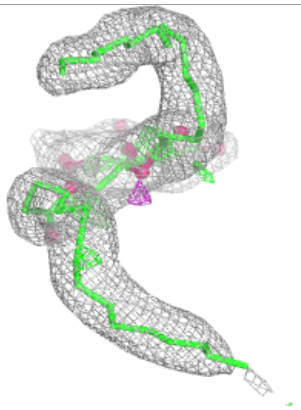


Electron density around LMG B 620:

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

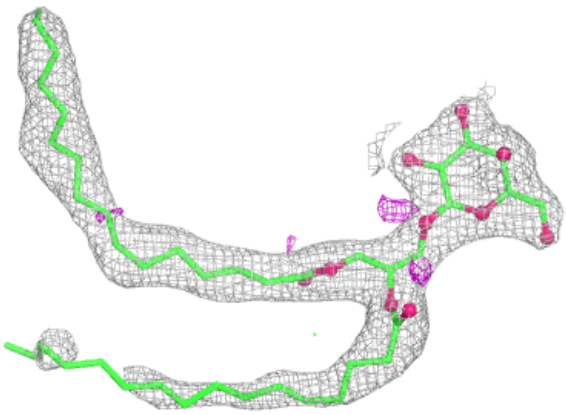


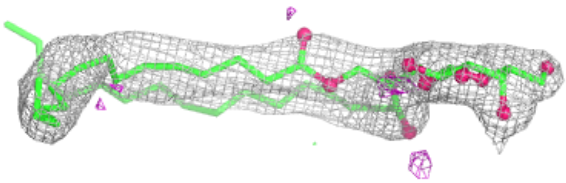


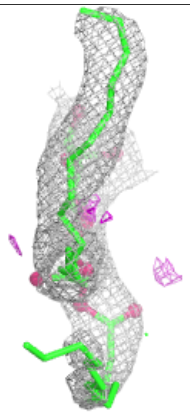


Electron density around LMG C 520:

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

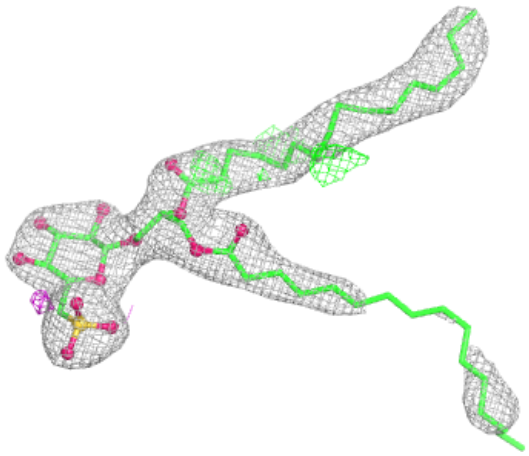


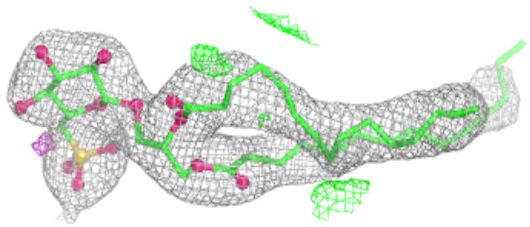


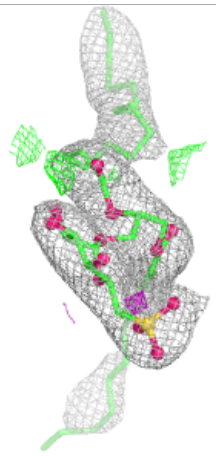


Electron density around SQD A 410 (B):

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

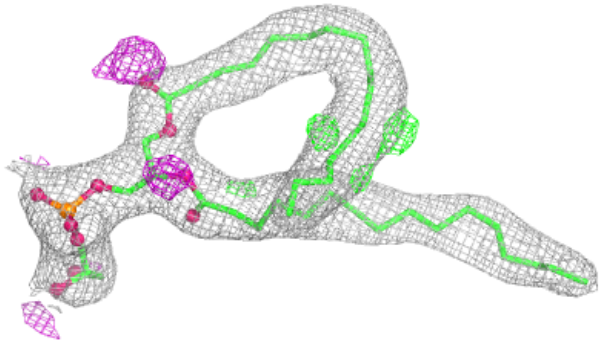


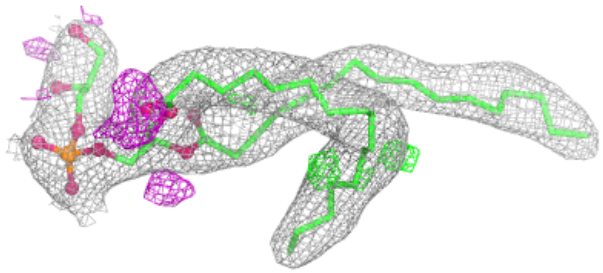


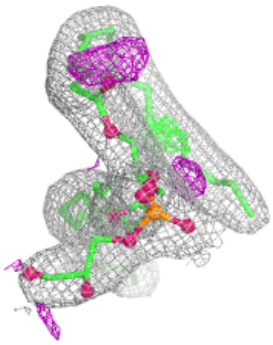


Electron density around LHG A 419 (A):

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

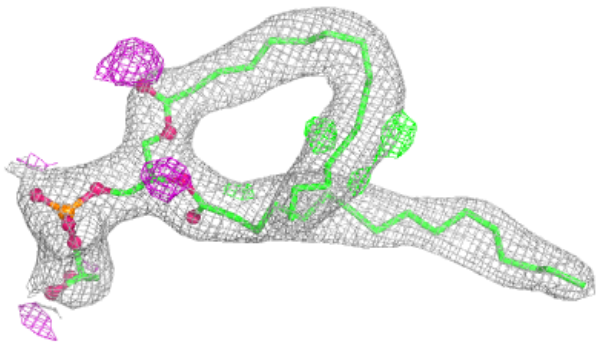


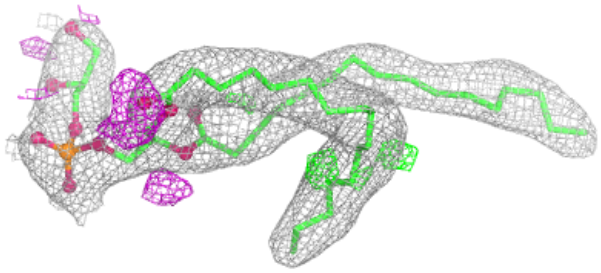




Electron density around LHG A 419 (B):

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

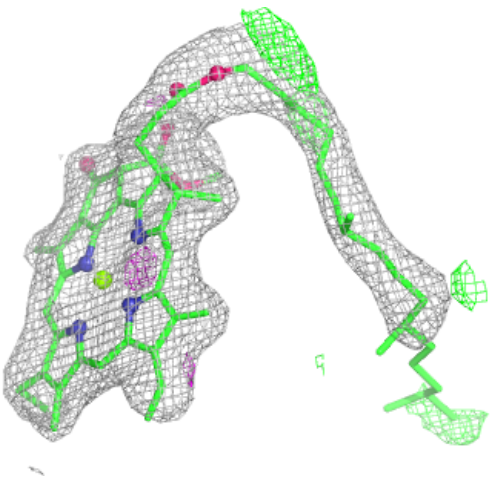


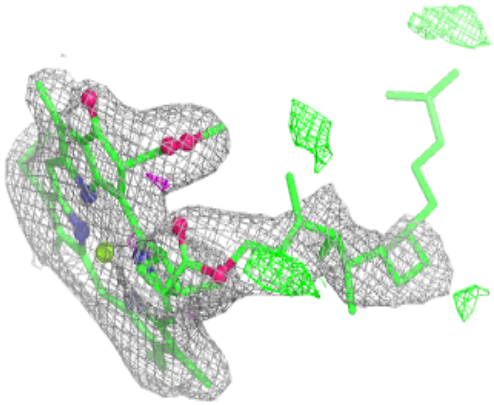


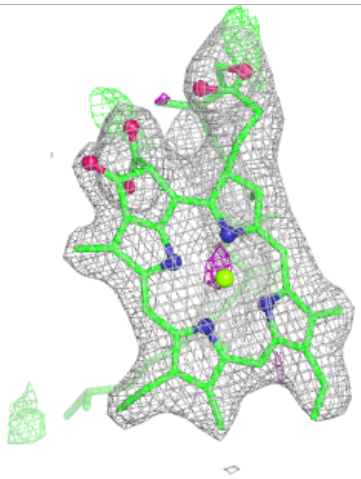


Electron density around CLA b 616:

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

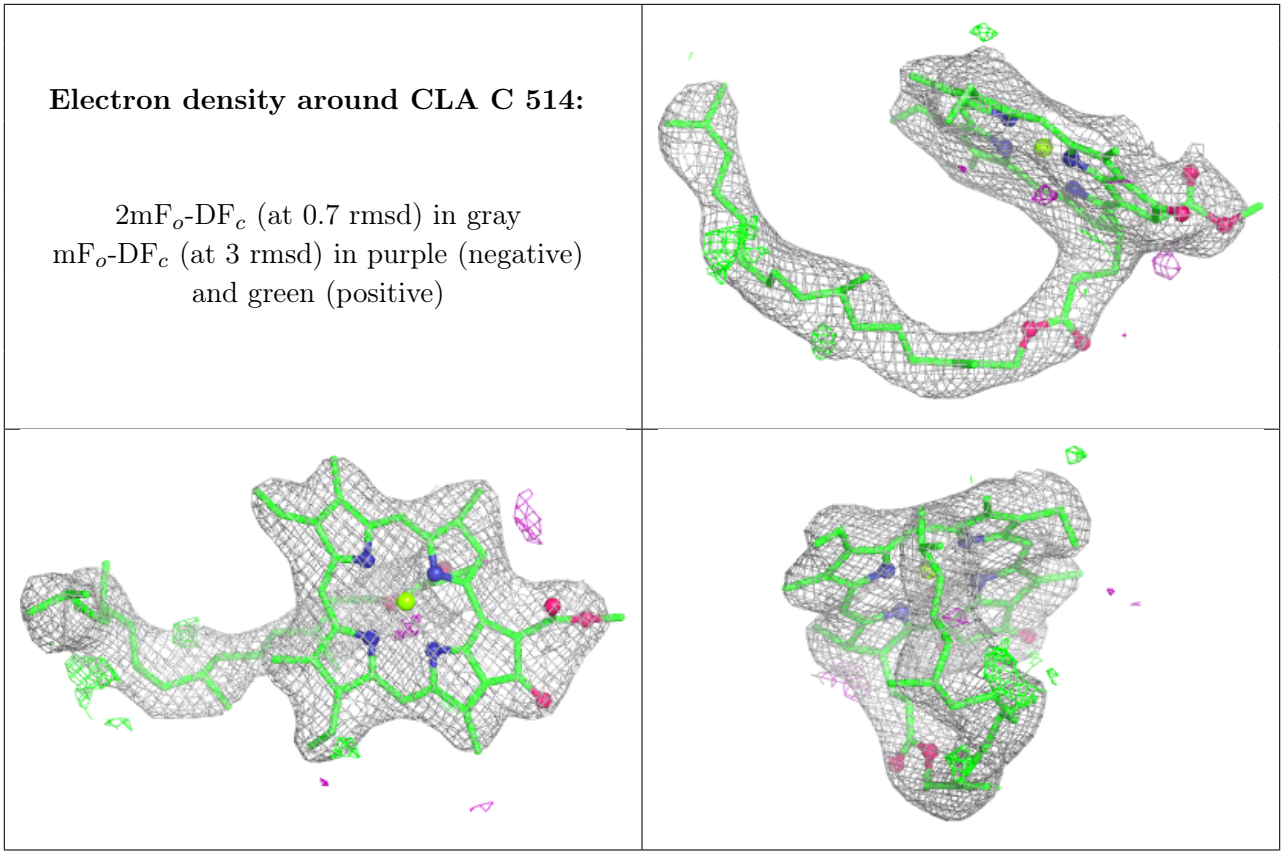






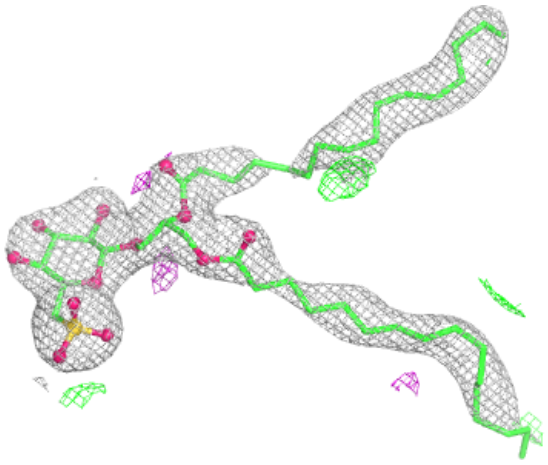
Electron density around CLA C 514:

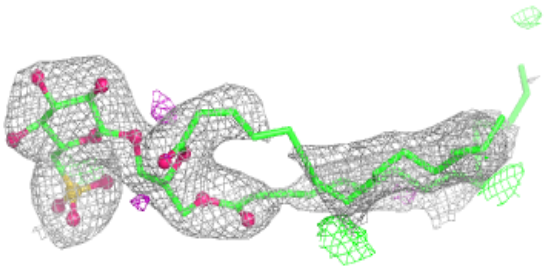
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

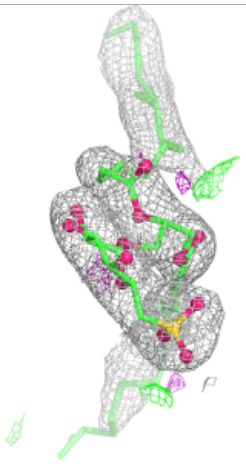


Electron density around SQD a 409 (A):

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

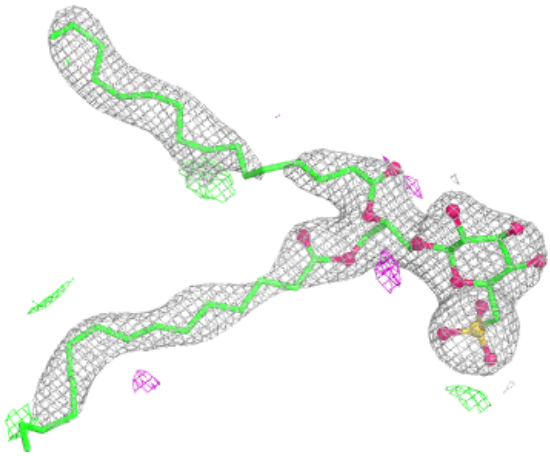


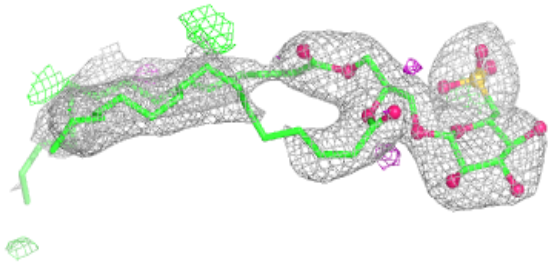


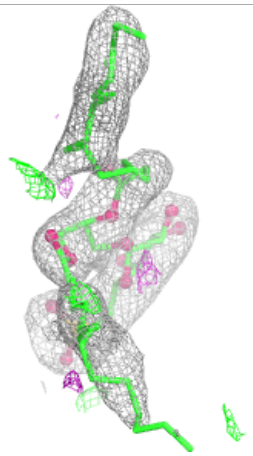


Electron density around SQD a 409 (B):

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

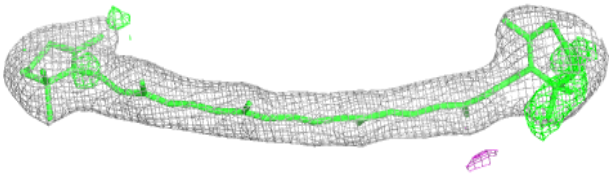


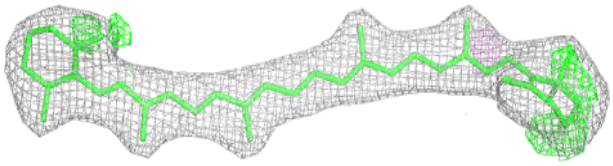


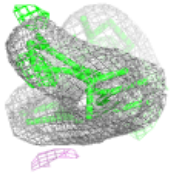


Electron density around BCR D 404:

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

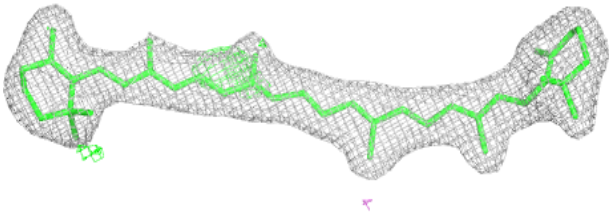


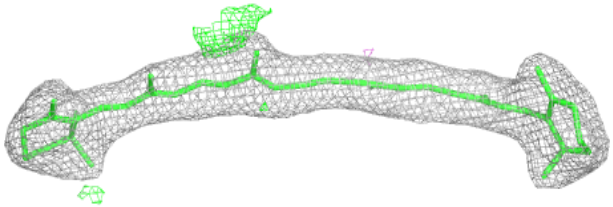


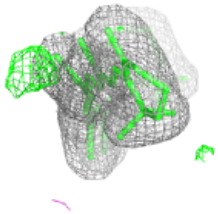


Electron density around BCR T 102:

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

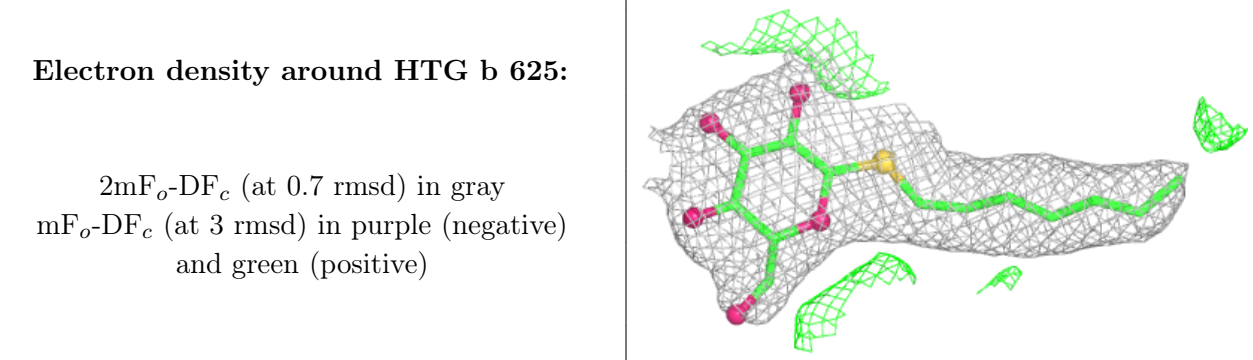


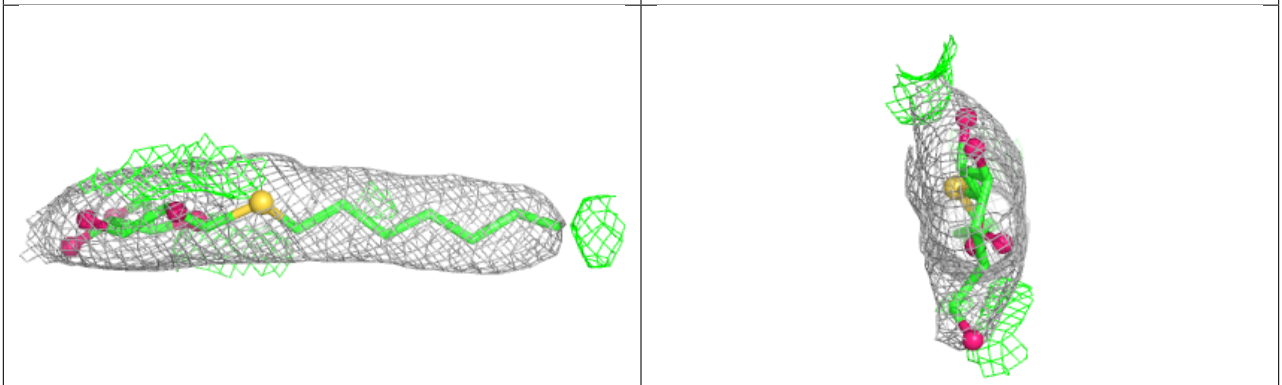




Electron density around HTG b 625:

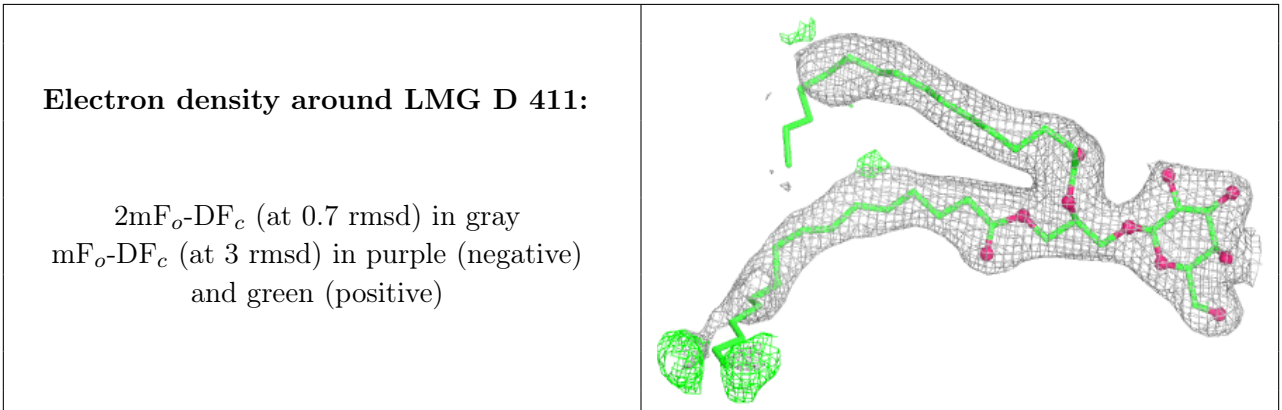
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

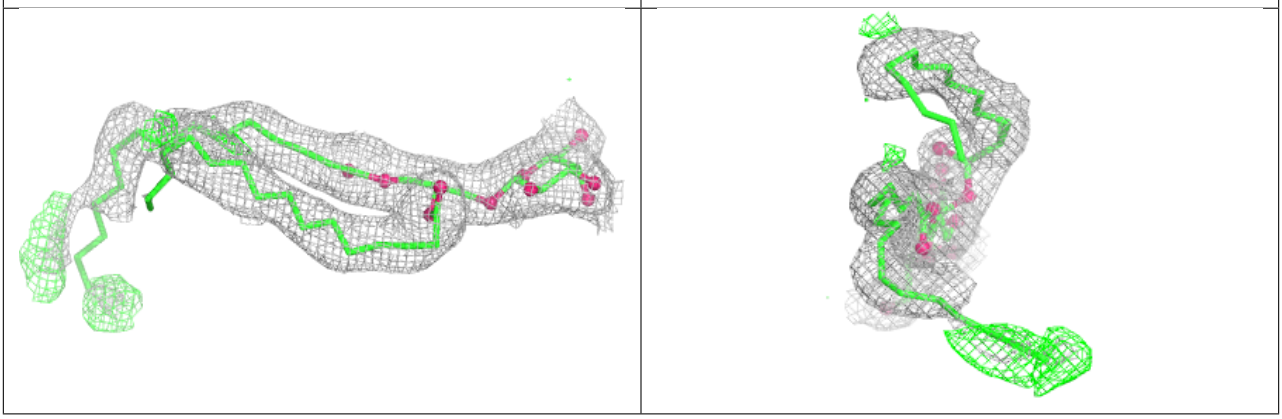




Electron density around LMG D 411:

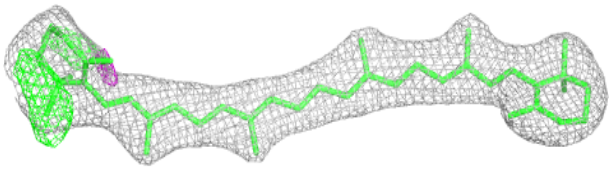
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

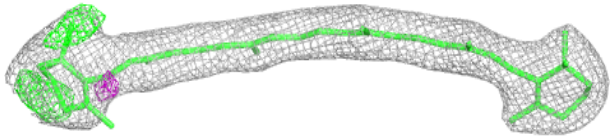


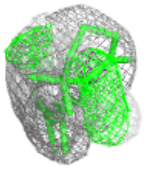


Electron density around BCR d 406:

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

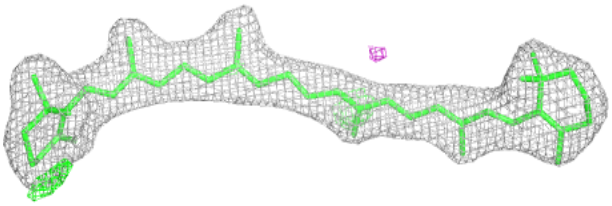


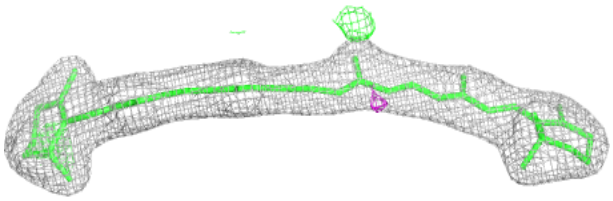


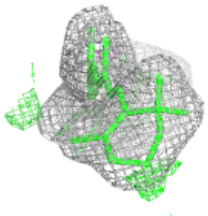


Electron density around BCR t 102:

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

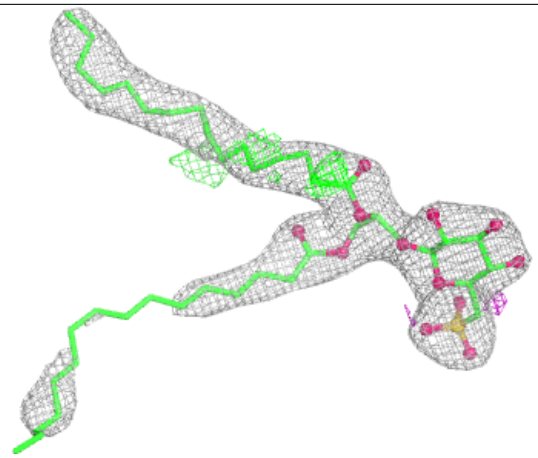


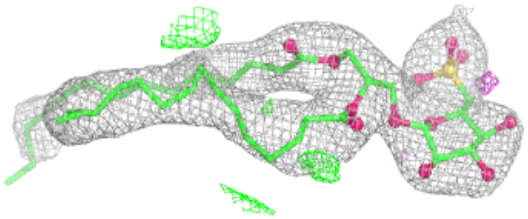


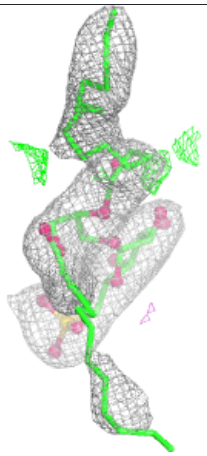


Electron density around SQD A 410 (A):

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

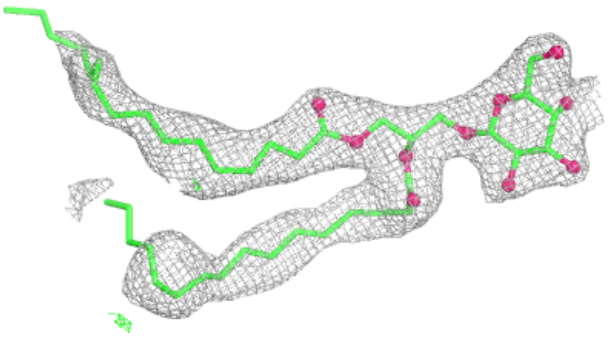


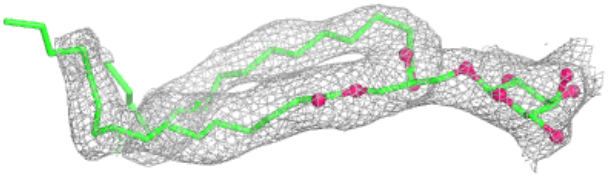


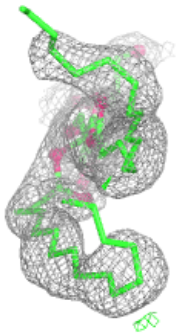


Electron density around LMG d 413:

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

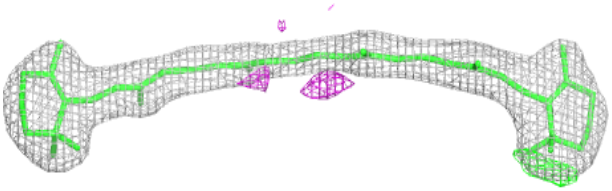


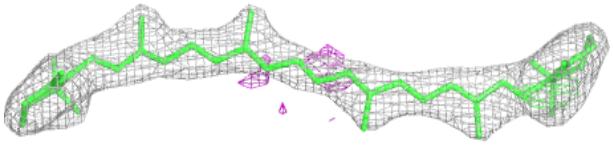


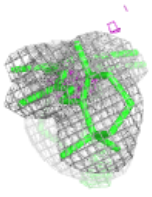


Electron density around BCR K 102:

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

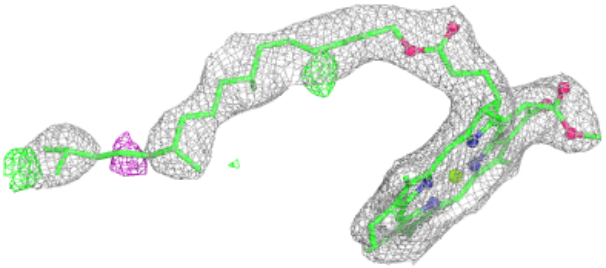


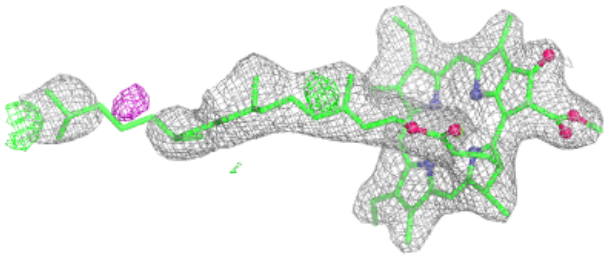


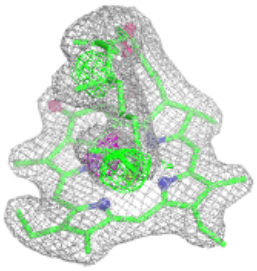


Electron density around CLA c 504:

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

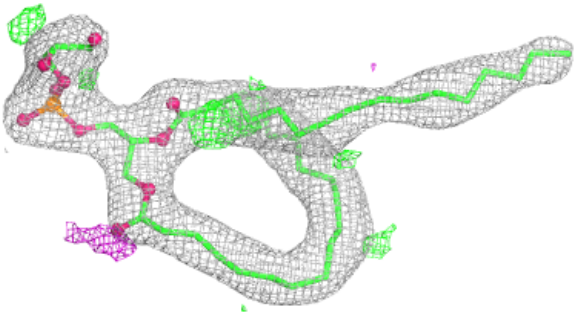


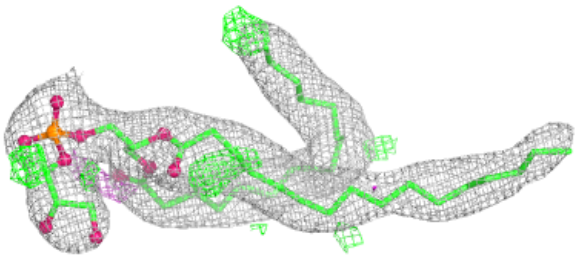


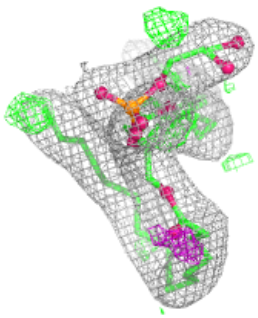


Electron density around LHG d 415 (A):

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

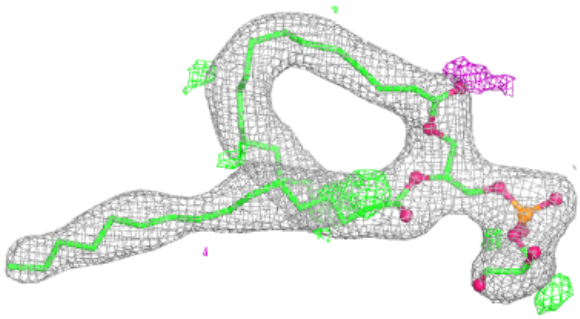


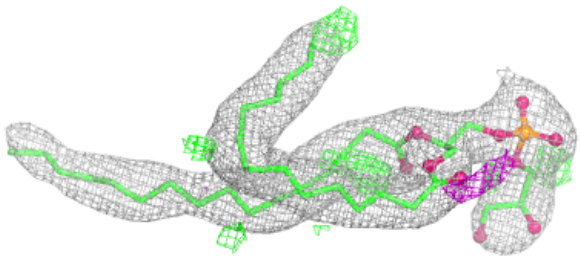


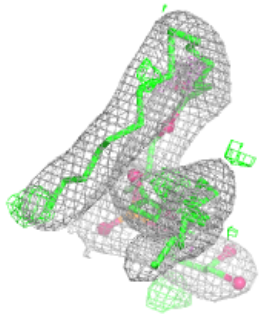


Electron density around LHG d 415 (B):

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

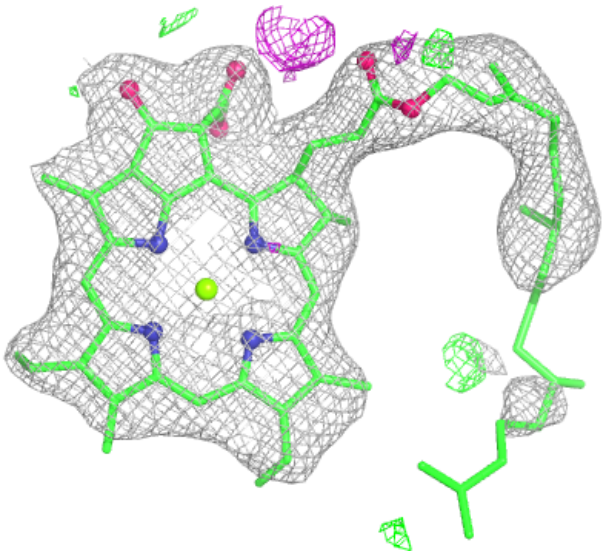


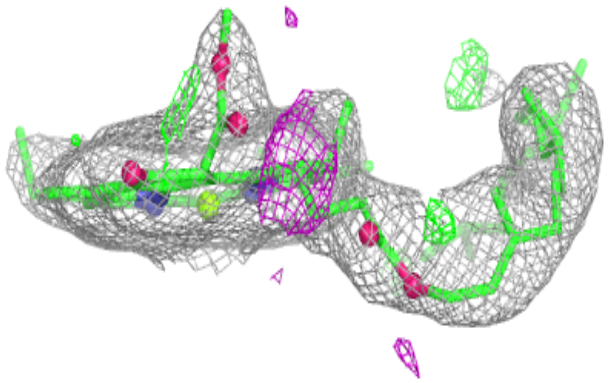


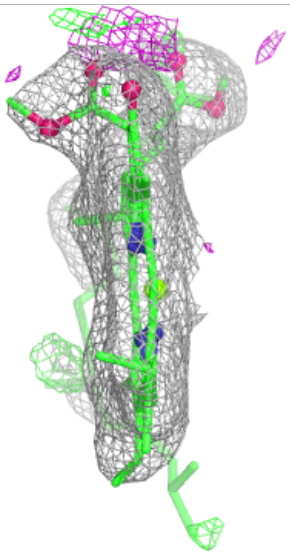


Electron density around CLA c 512:

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

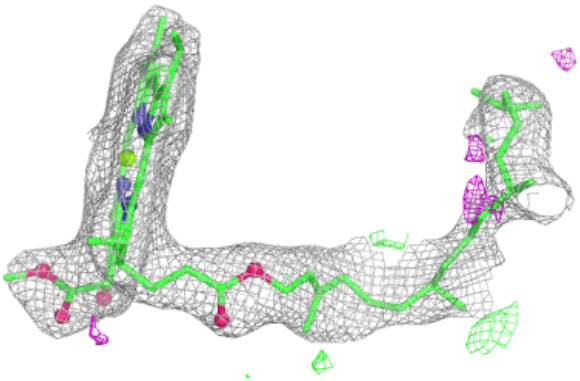


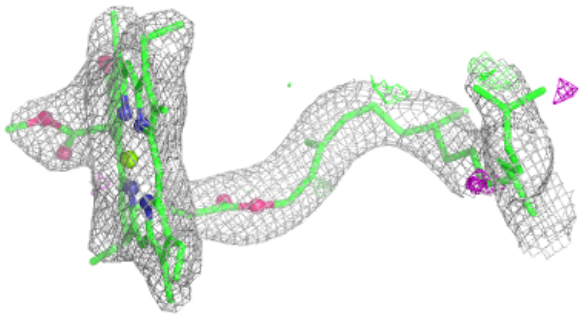


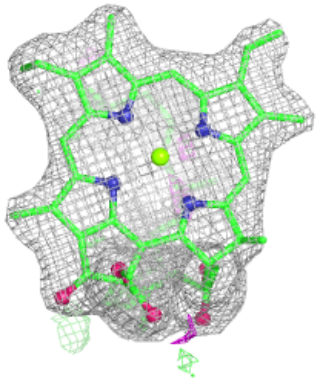


Electron density around CLA C 507:

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

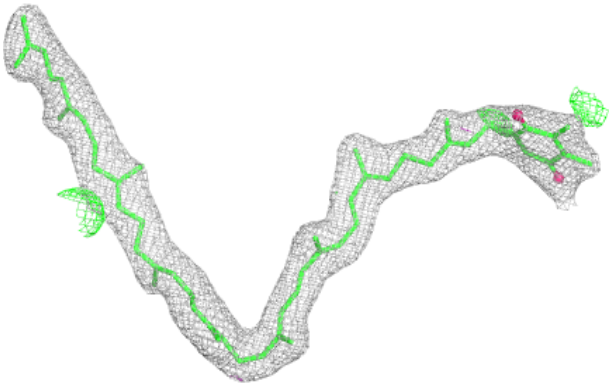


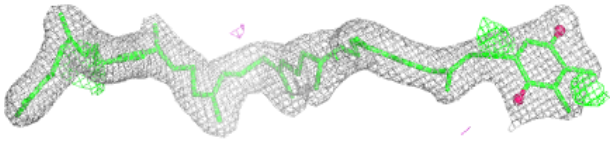


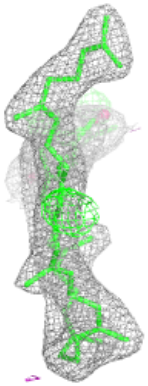


Electron density around PL9 D 405 (A):

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

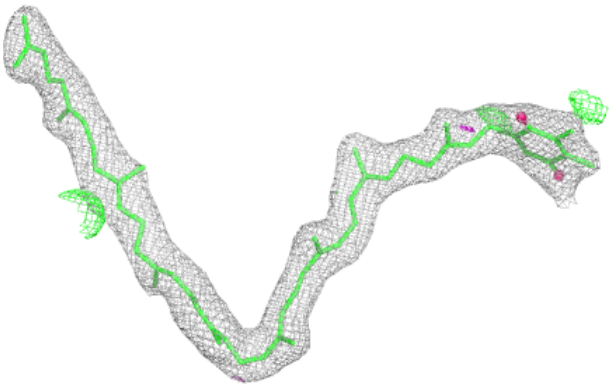


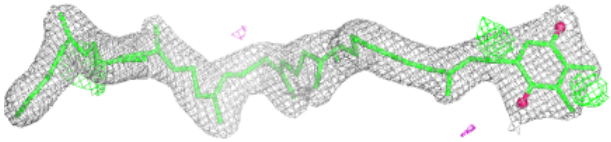


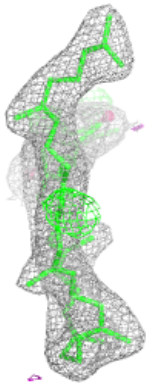


Electron density around PL9 D 405 (B):

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

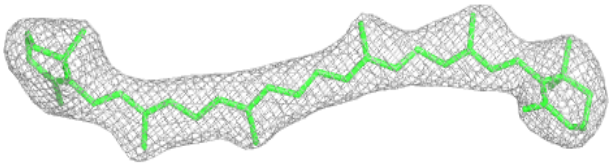


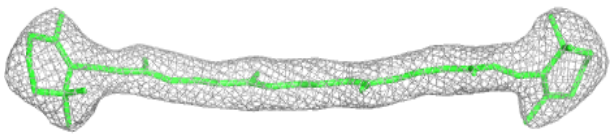


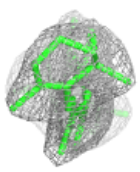


Electron density around BCR y 101:

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

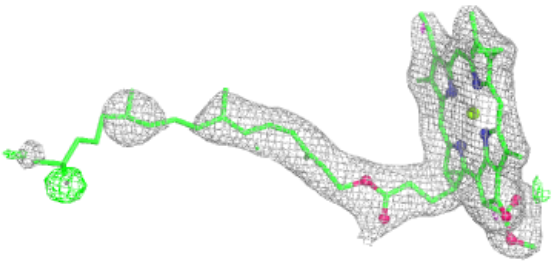


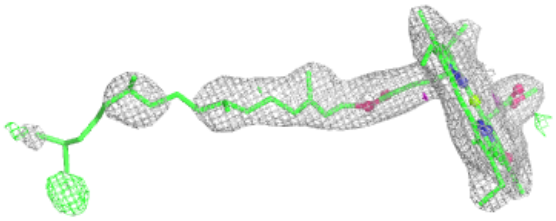


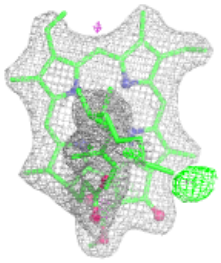


Electron density around CLA d 405:

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

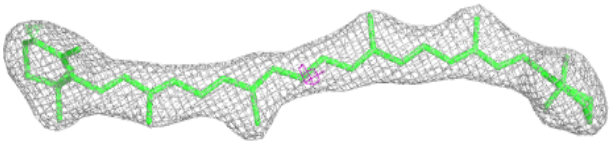


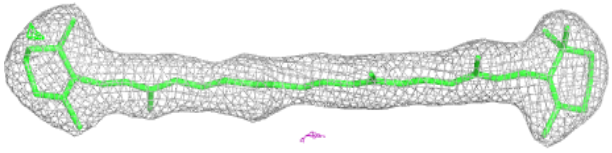


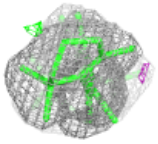


Electron density around BCR C 515:

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

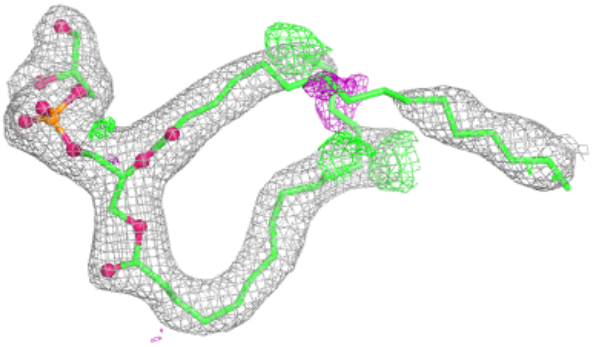


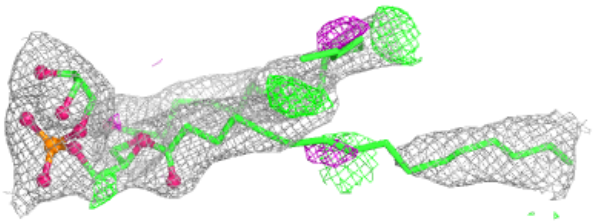


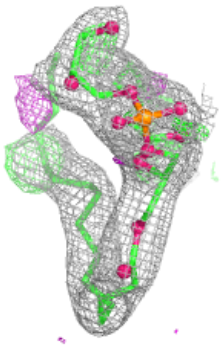


Electron density around LHG D 407 (A):

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



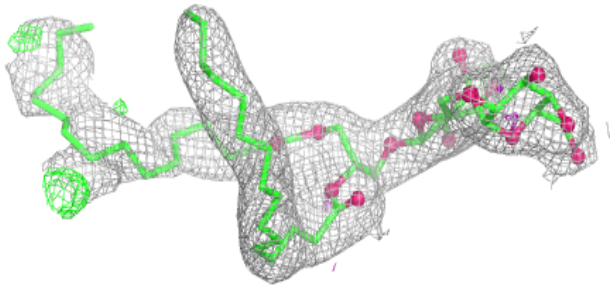


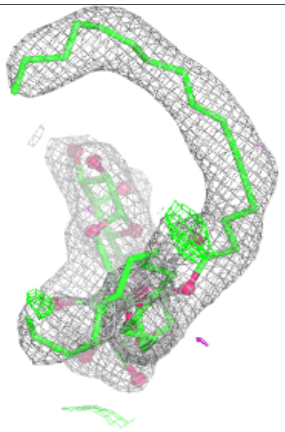


Electron density around DGD C 518 (A):

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

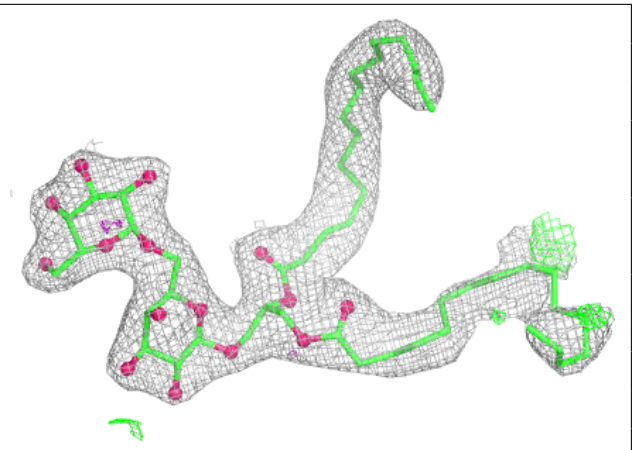


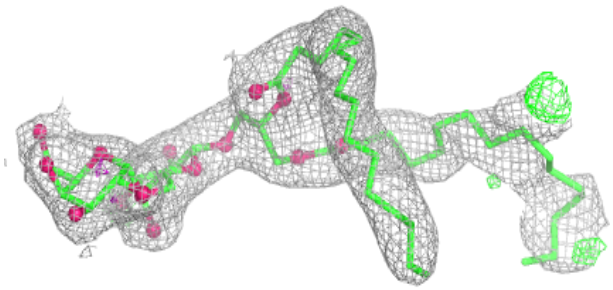


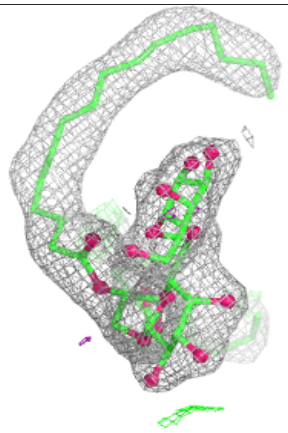


Electron density around DGD C 518 (B):

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

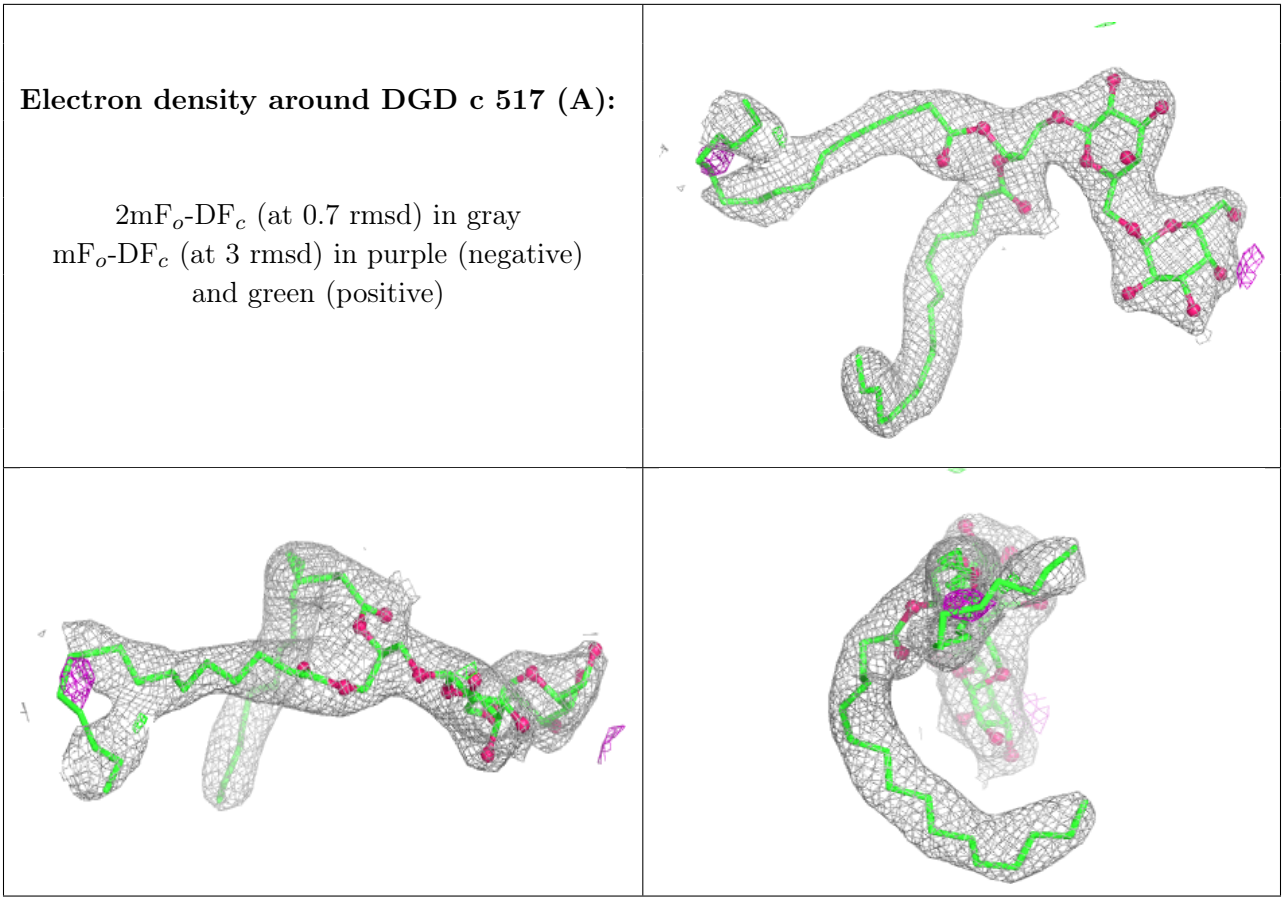






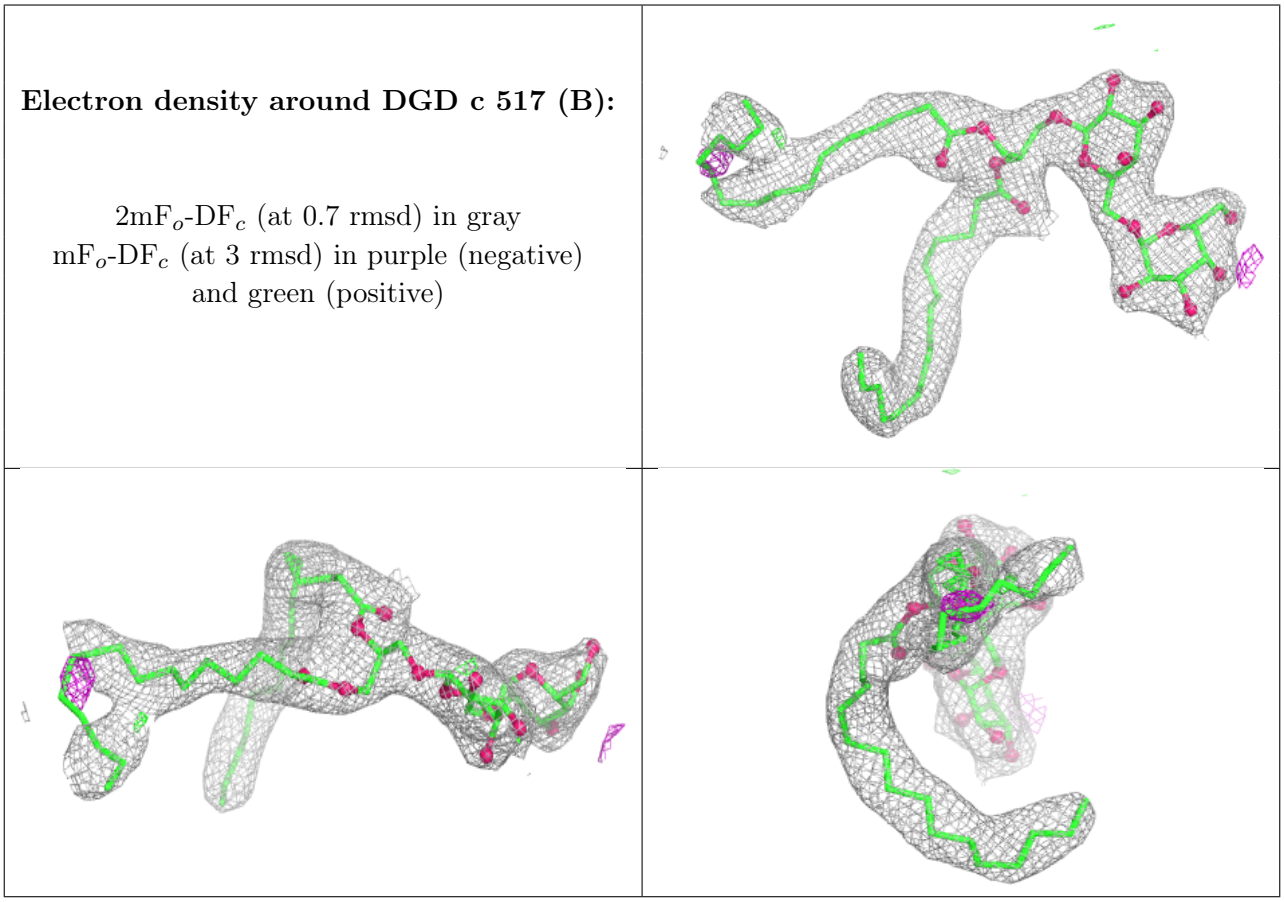
Electron density around DGD c 517 (A):

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



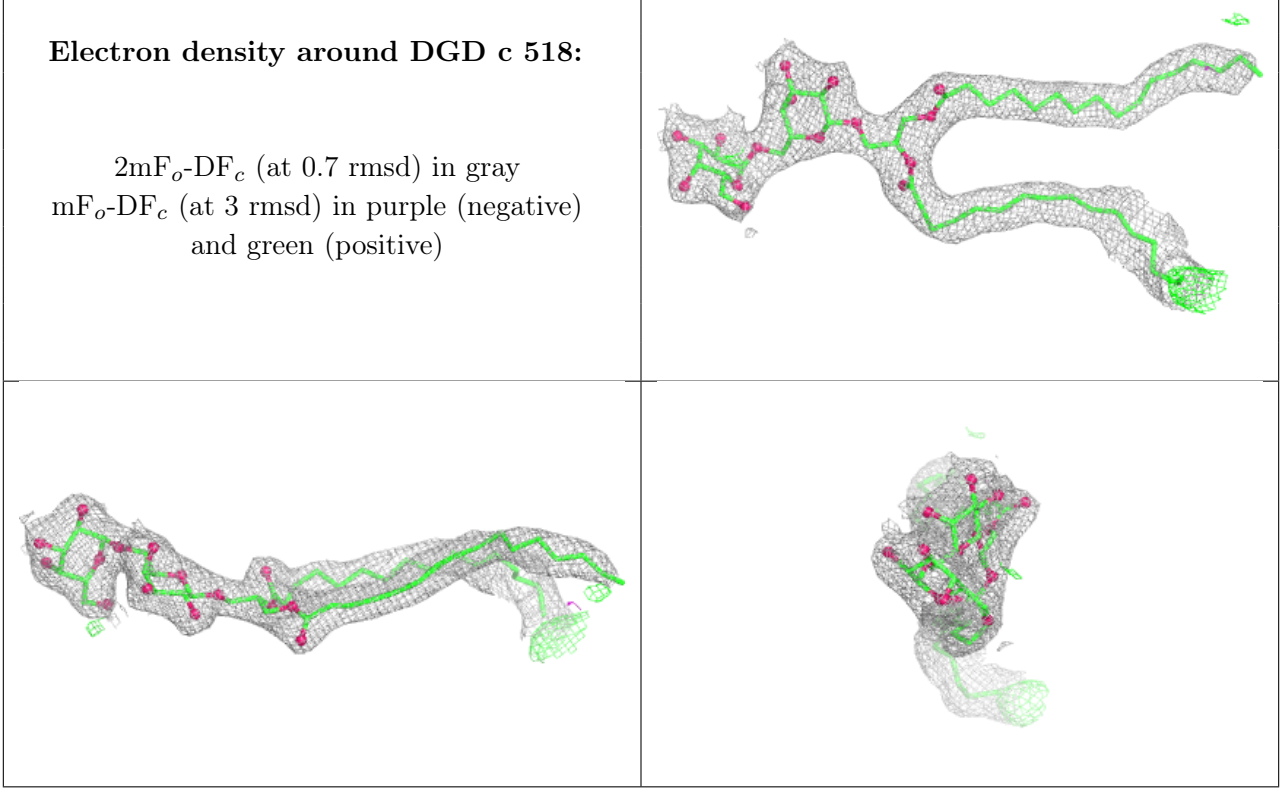
Electron density around DGD c 517 (B):

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



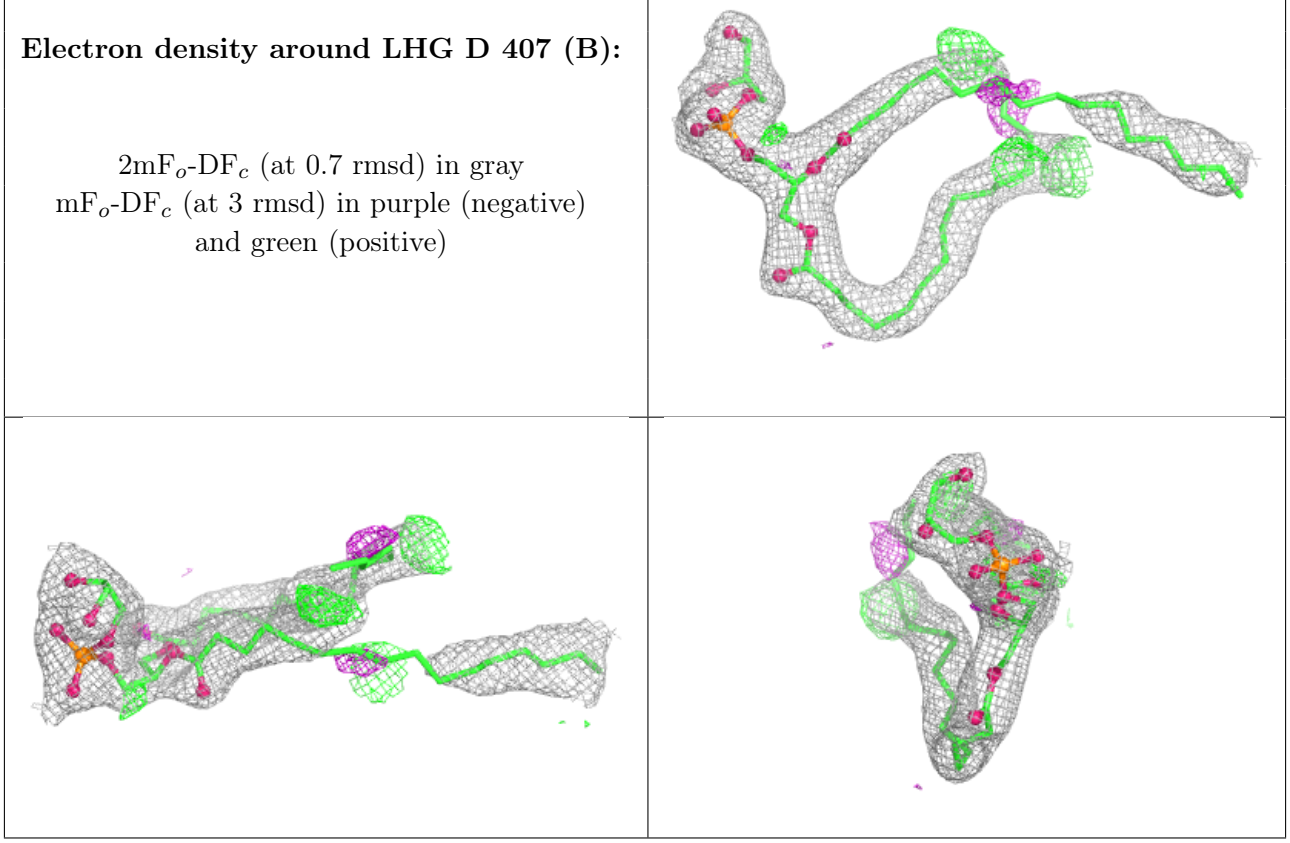
Electron density around DGD c 518:

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



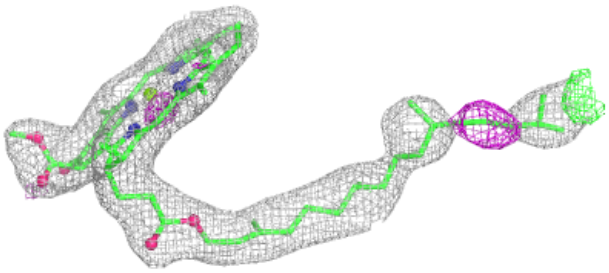
Electron density around LHG D 407 (B):

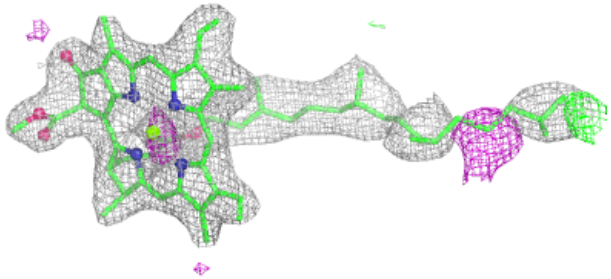
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

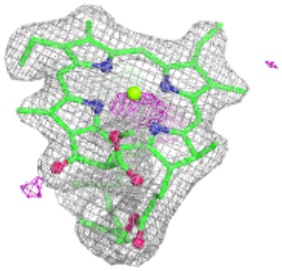


Electron density around CLA C 505:

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

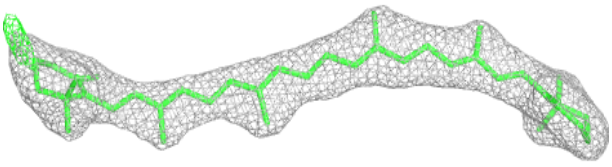


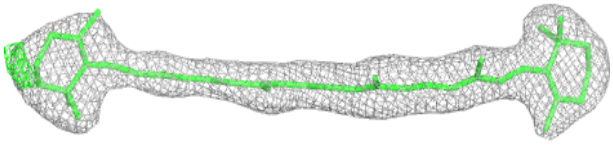


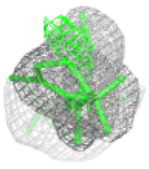


Electron density around BCR H 101:

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

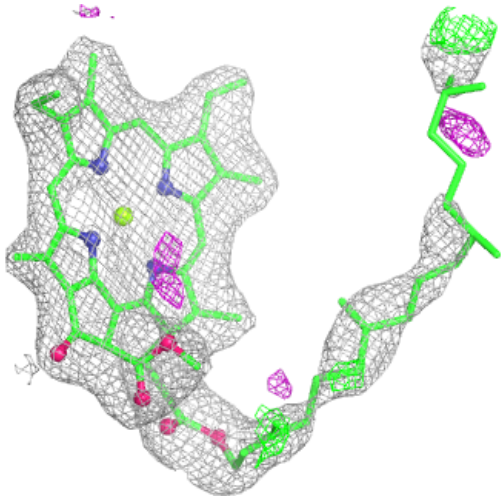


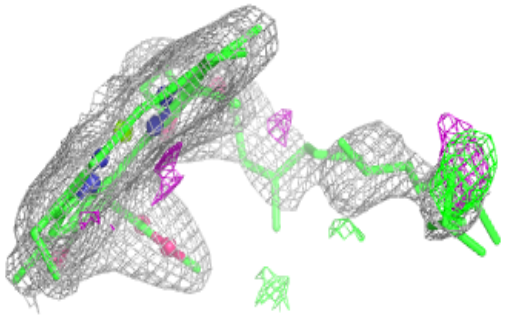


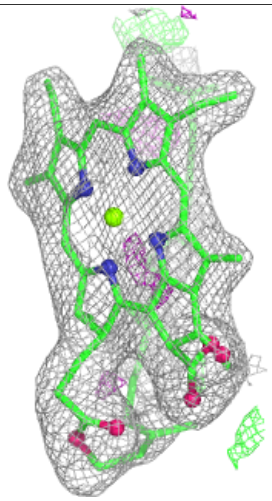


Electron density around CLA B 616:

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

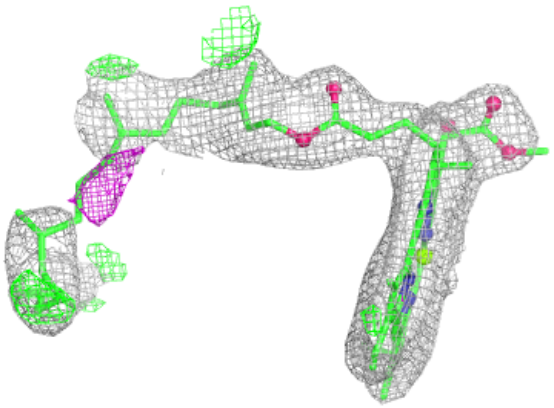


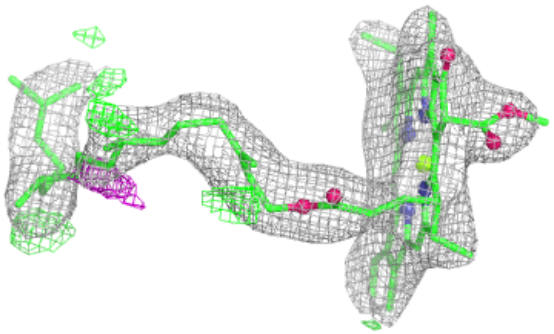


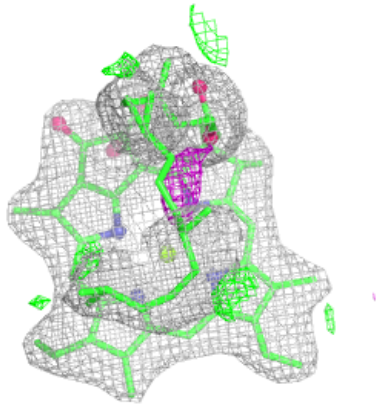


Electron density around CLA c 506:

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

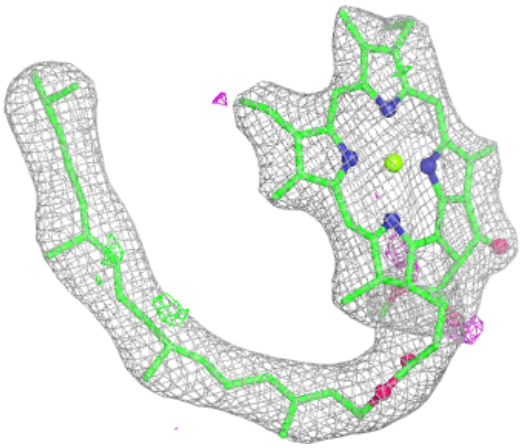


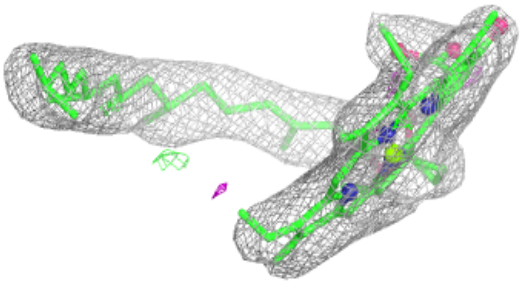


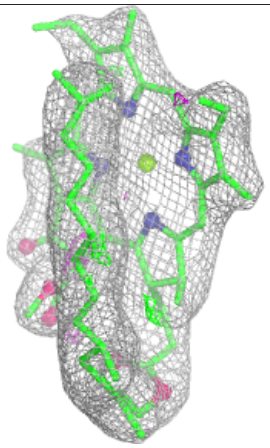


Electron density around CLA c 507:

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

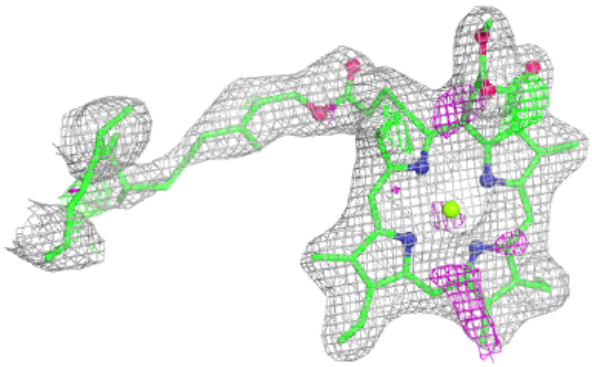


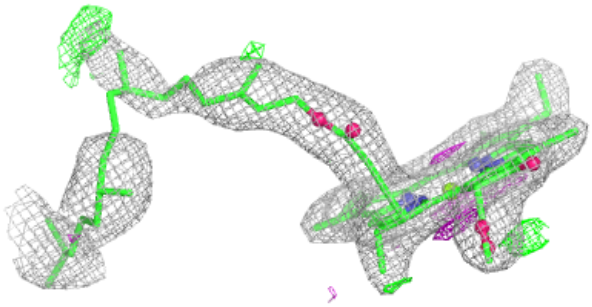


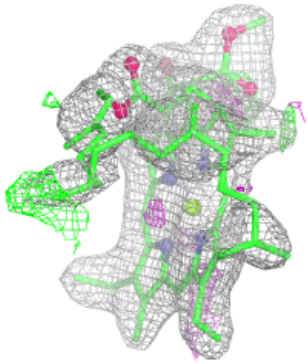


Electron density around CLA A 408:

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

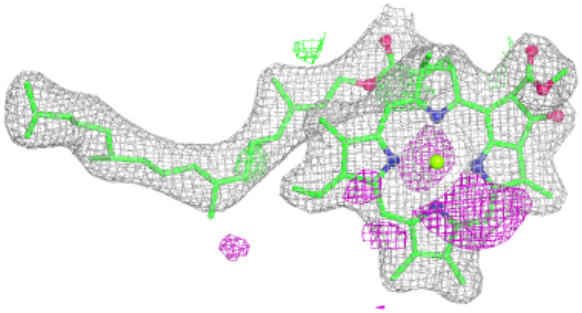


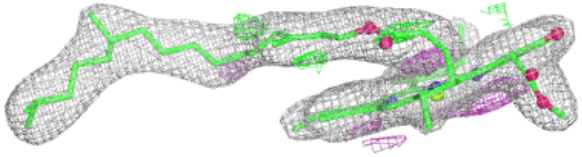


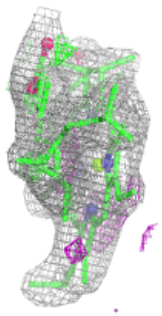


Electron density around CLA B 603:

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

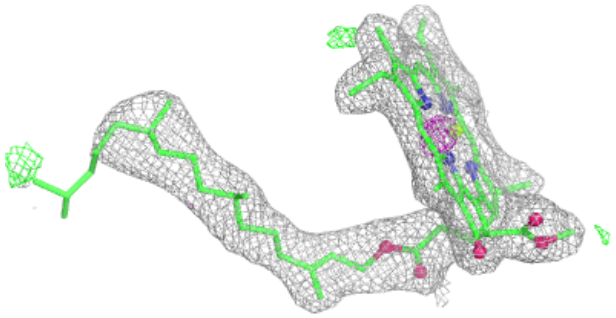


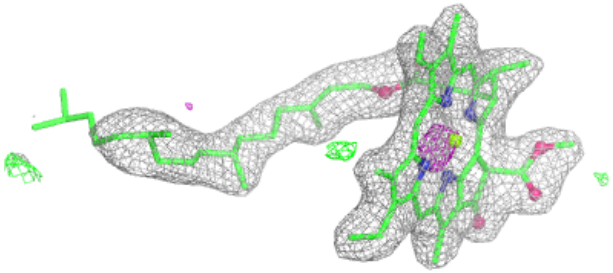


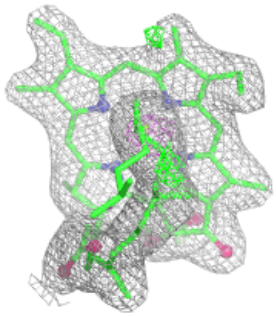


Electron density around CLA C 509:

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

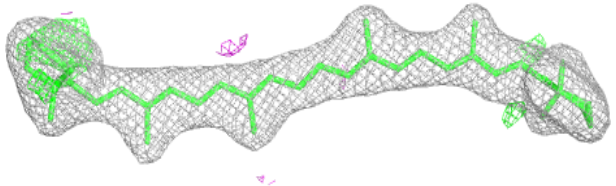


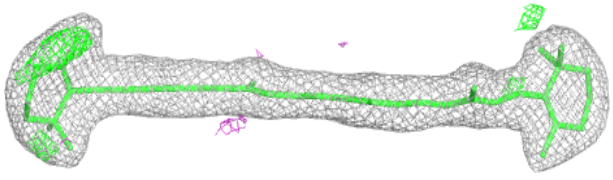


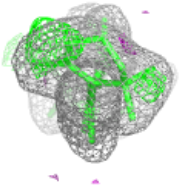


Electron density around BCR A 409:

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

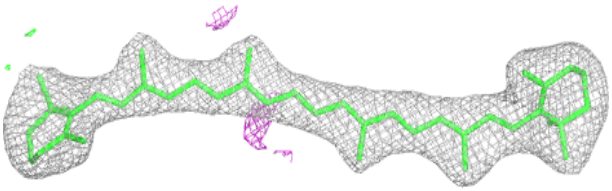


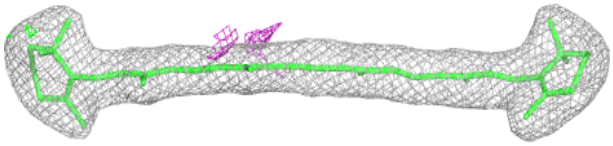


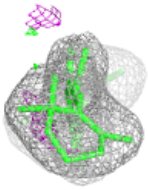


Electron density around BCR B 618:

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

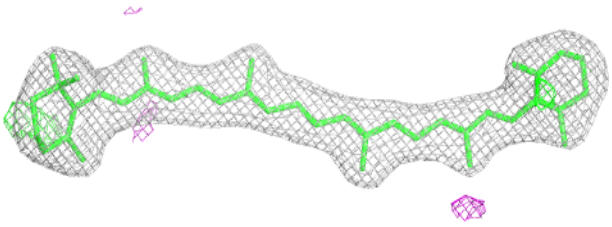


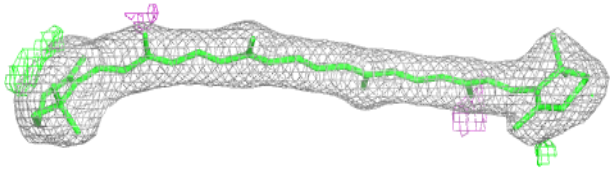


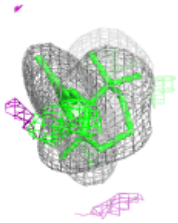


Electron density around BCR B 619:

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

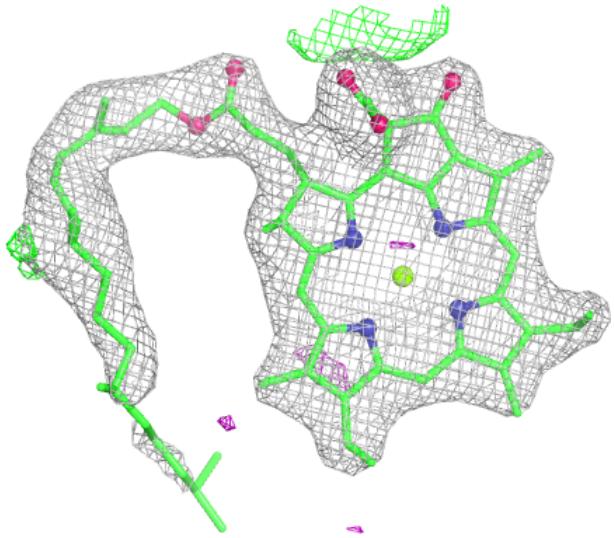


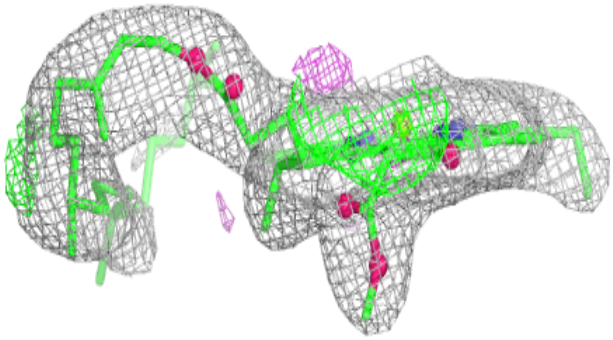


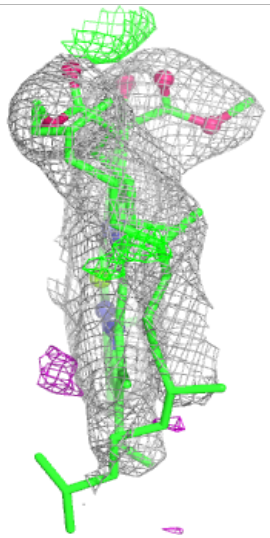


Electron density around CLA C 513:

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

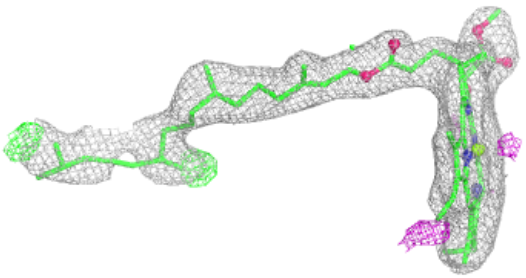


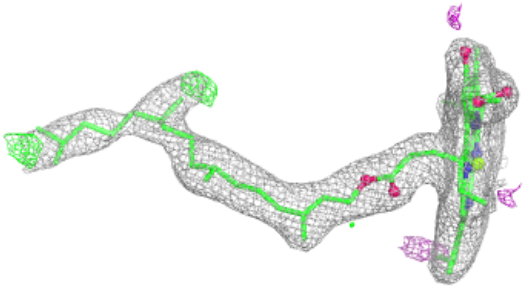


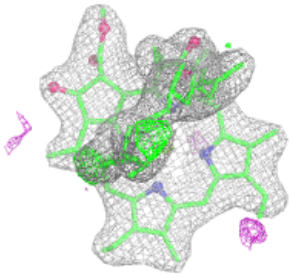


Electron density around CLA B 606:

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

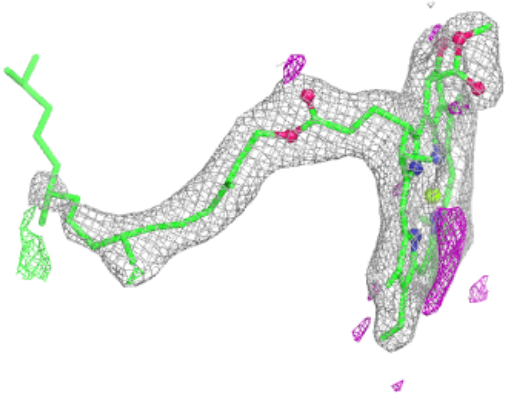


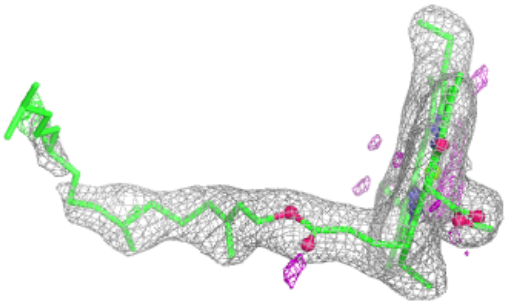


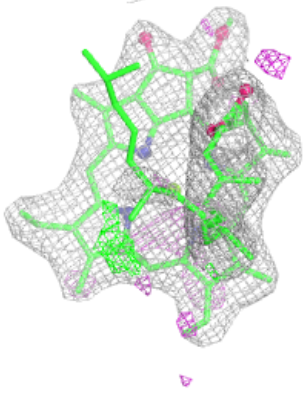


Electron density around CLA D 403:

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

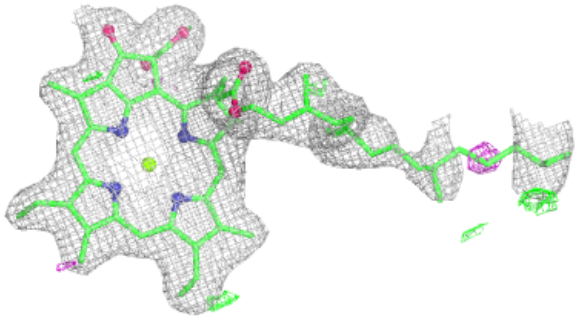


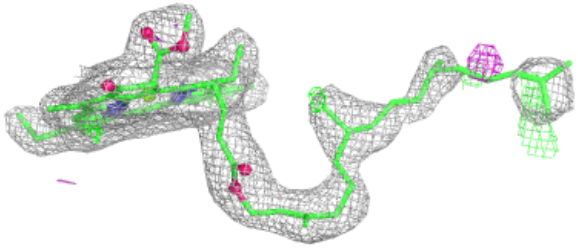


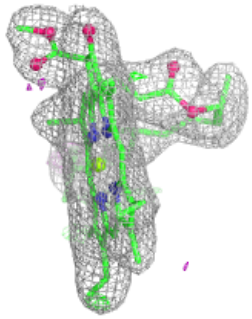


Electron density around CLA a 405 (A):

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

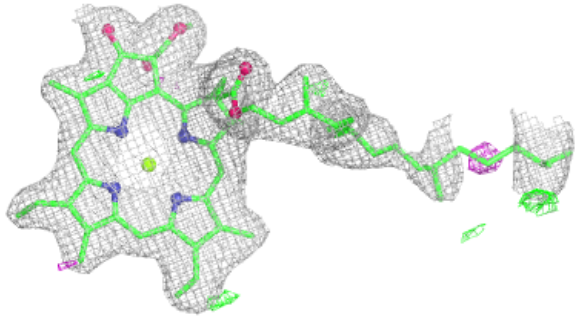


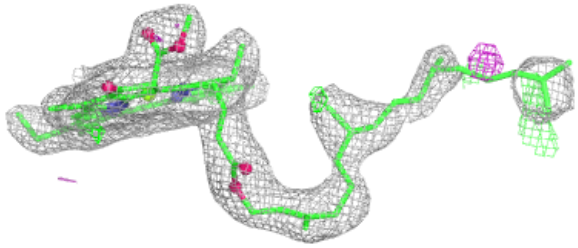




Electron density around CLA a 405 (B):

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

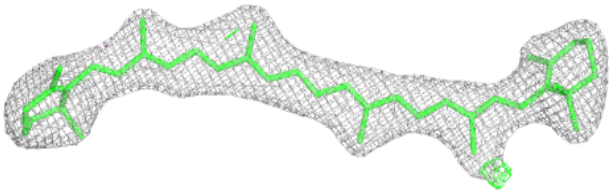


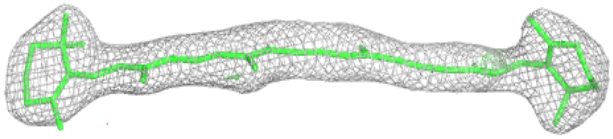


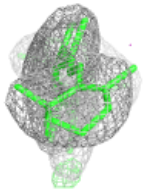


Electron density around BCR Y 101:

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

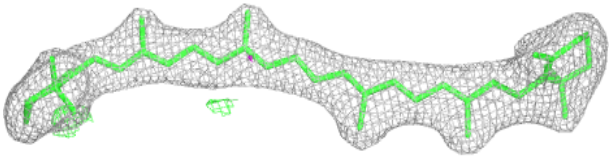


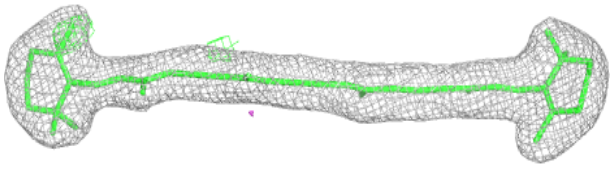


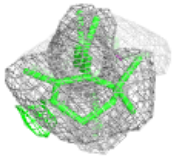


Electron density around BCR a 408:

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

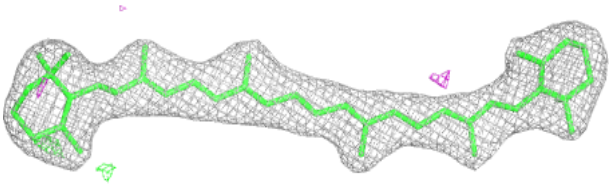


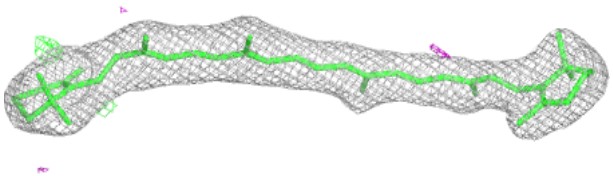


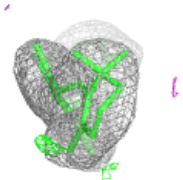


Electron density around BCR b 619:

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

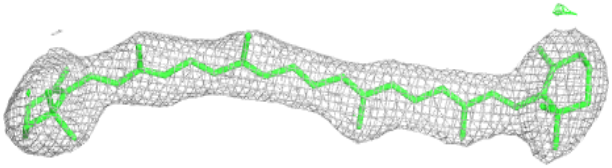


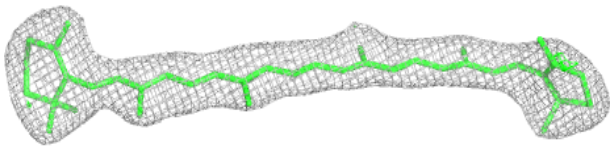


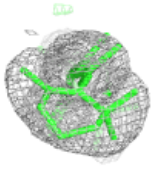


Electron density around BCR c 514:

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

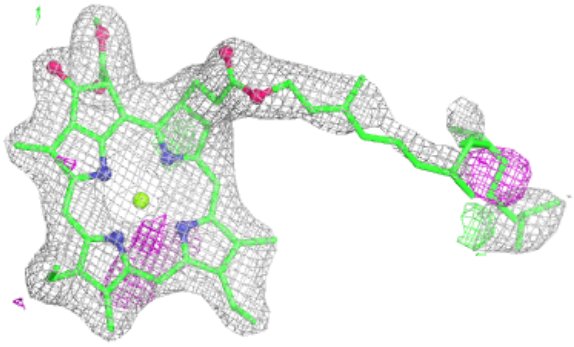


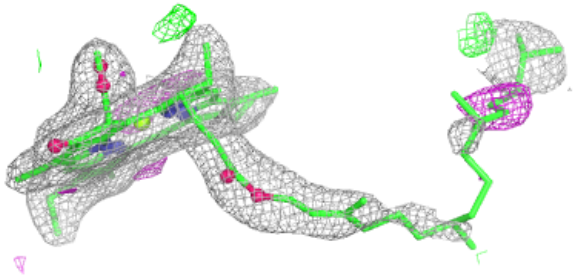


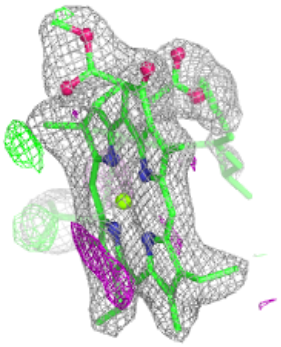


Electron density around CLA a 407:

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

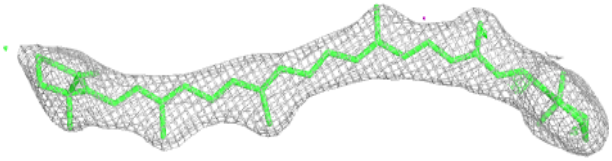


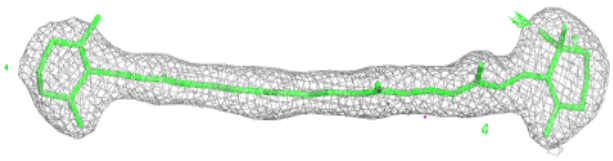


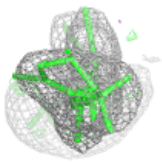


Electron density around BCR h 101:

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

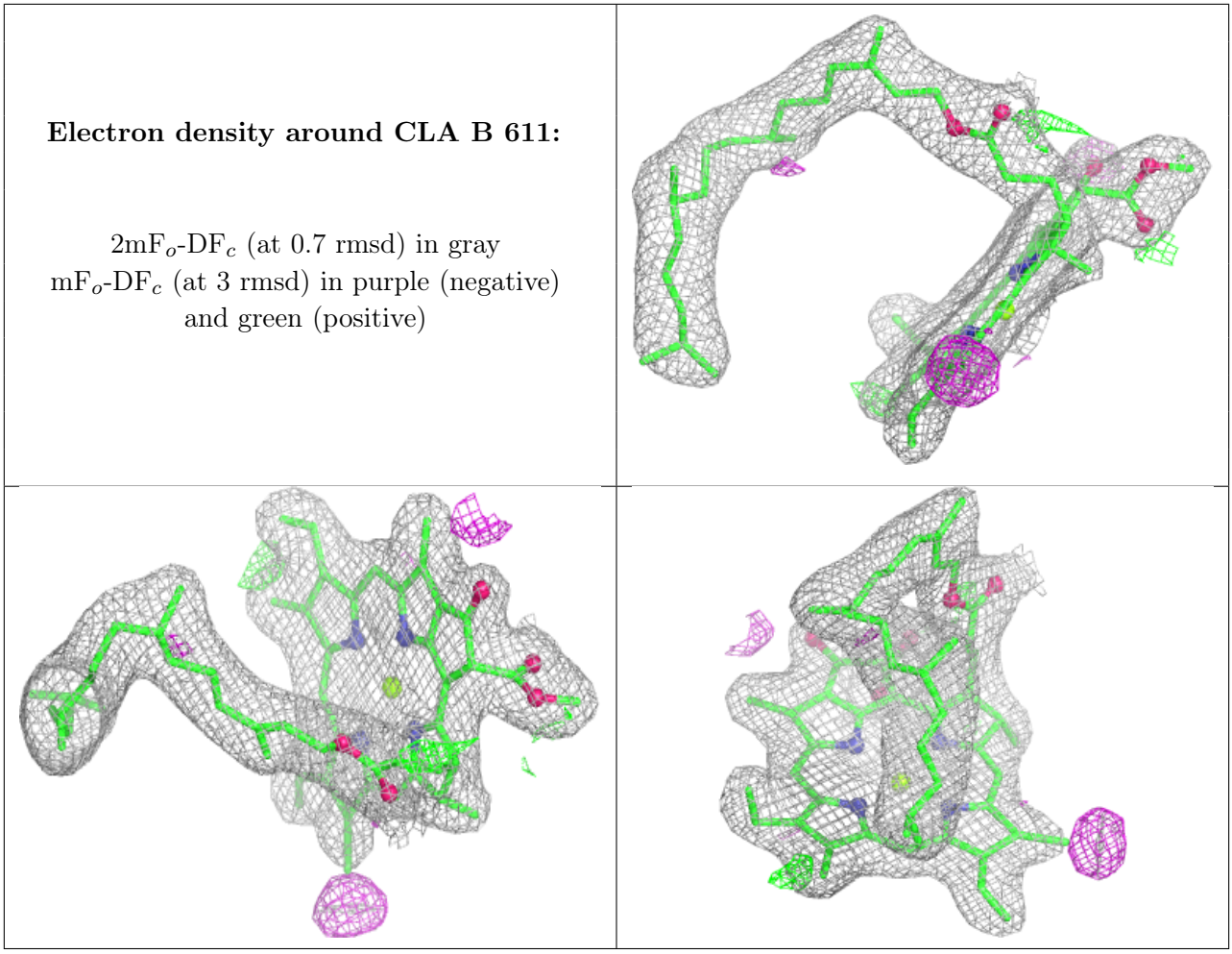






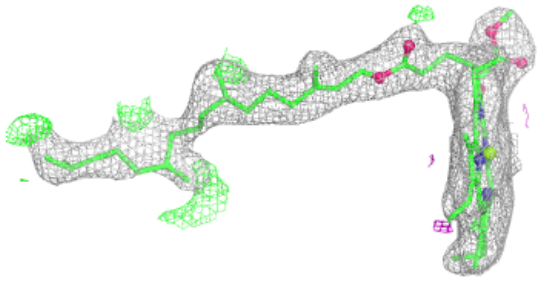
Electron density around CLA B 611:

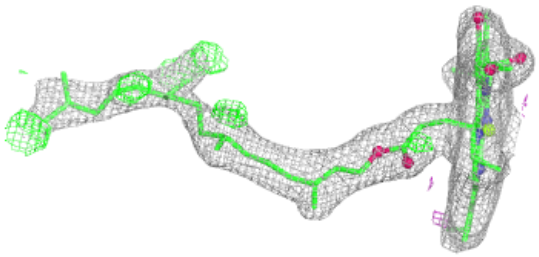
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

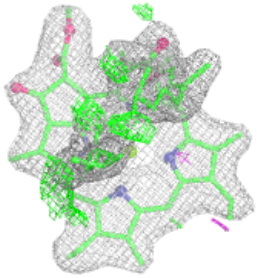


Electron density around CLA b 606:

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

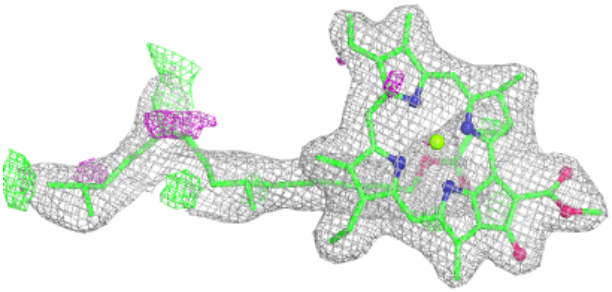


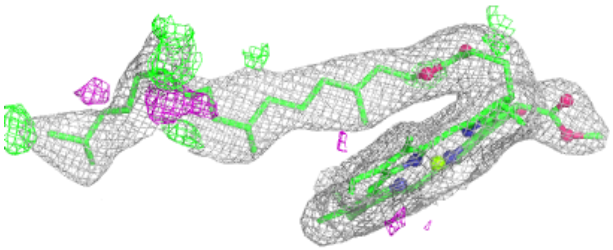




Electron density around CLA b 614:

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

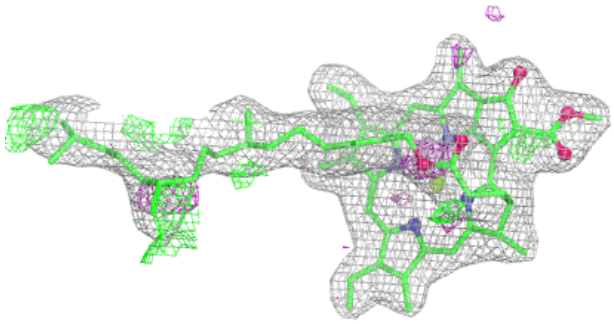


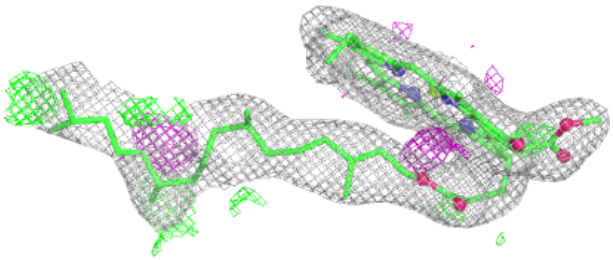


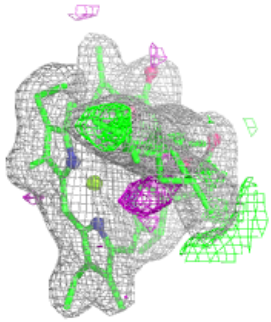


Electron density around CLA B 614:

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

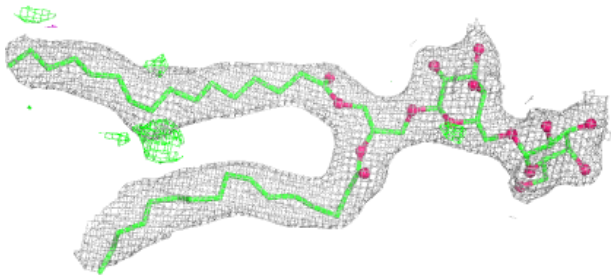


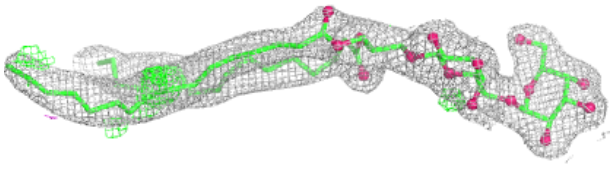


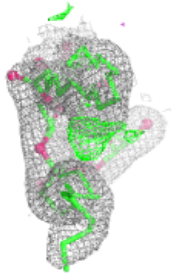


Electron density around DGD C 519:

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

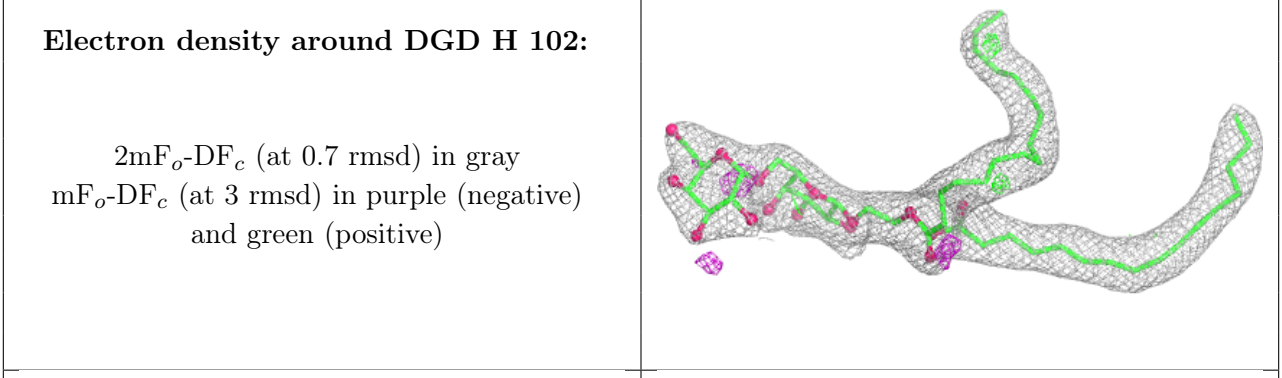


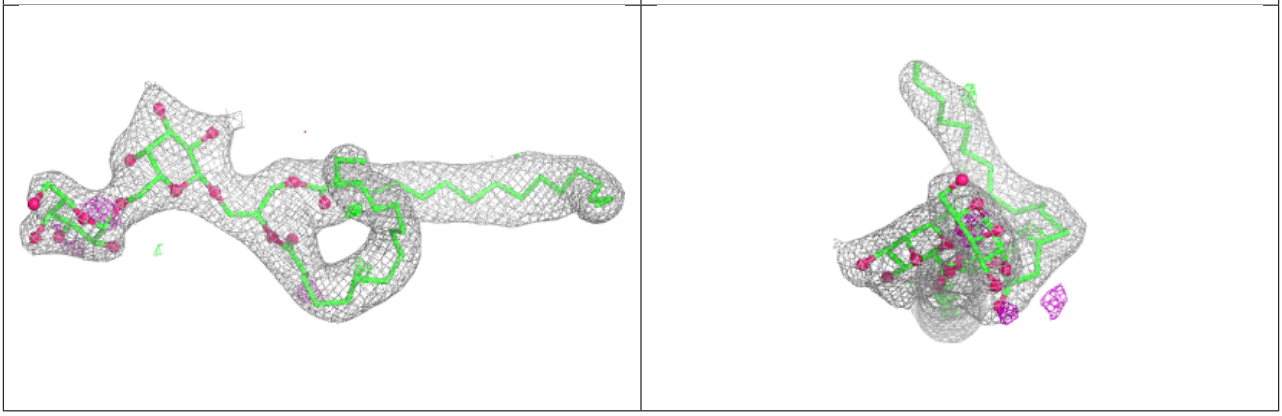




Electron density around DGD H 102:

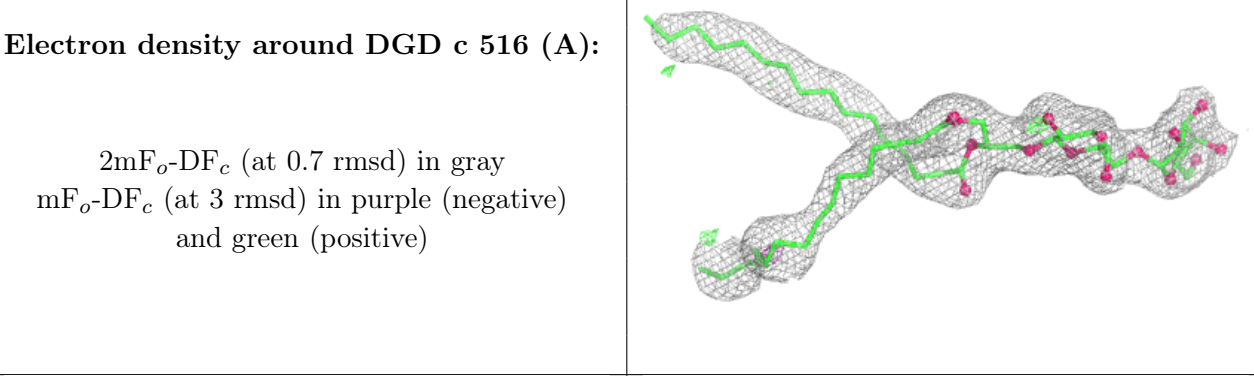
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

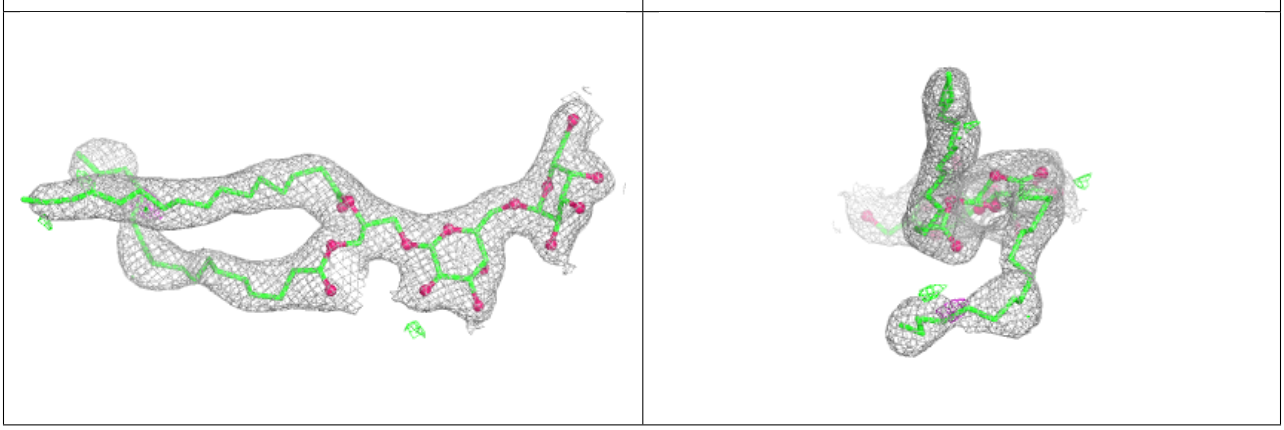




Electron density around DGD c 516 (A):

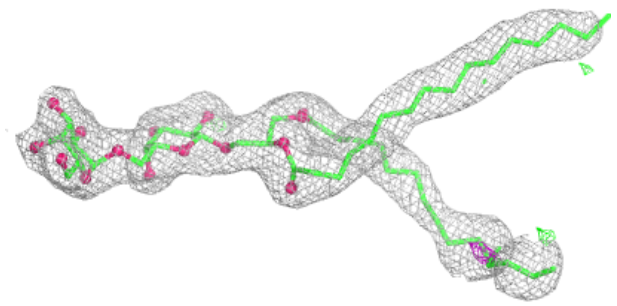
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

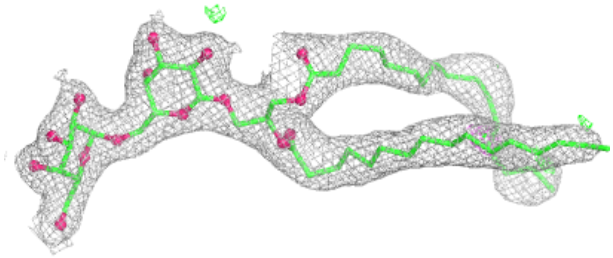


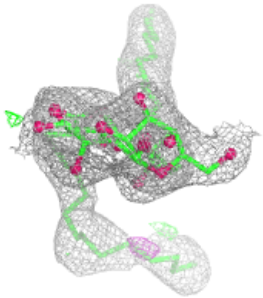


Electron density around DGD c 516 (B):

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

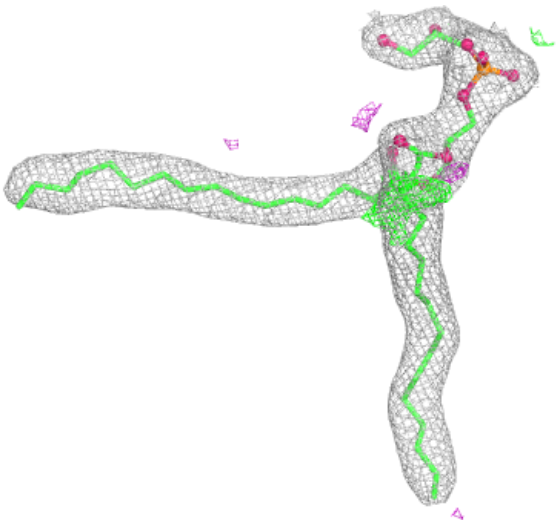


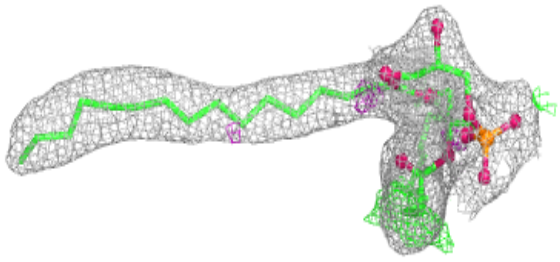


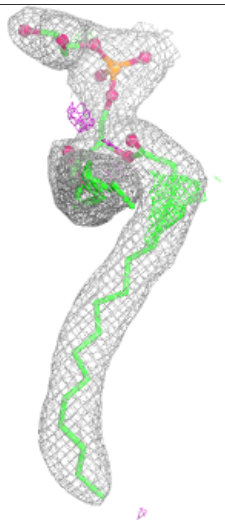


Electron density around LHG b 629 (A):

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

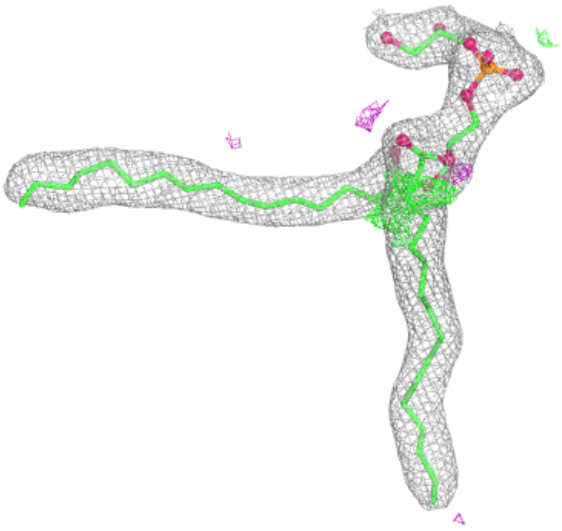


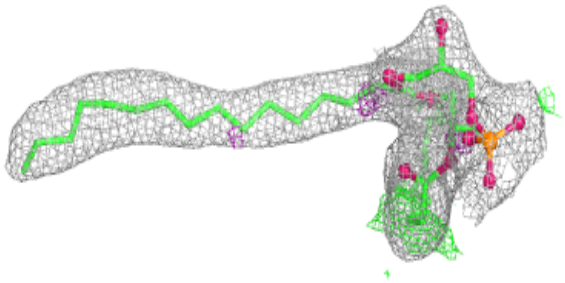


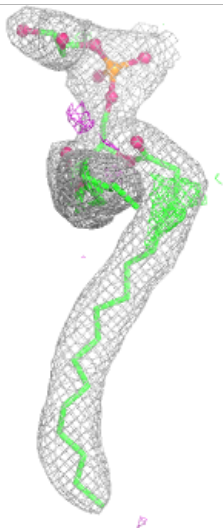


Electron density around LHG b 629 (B):

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

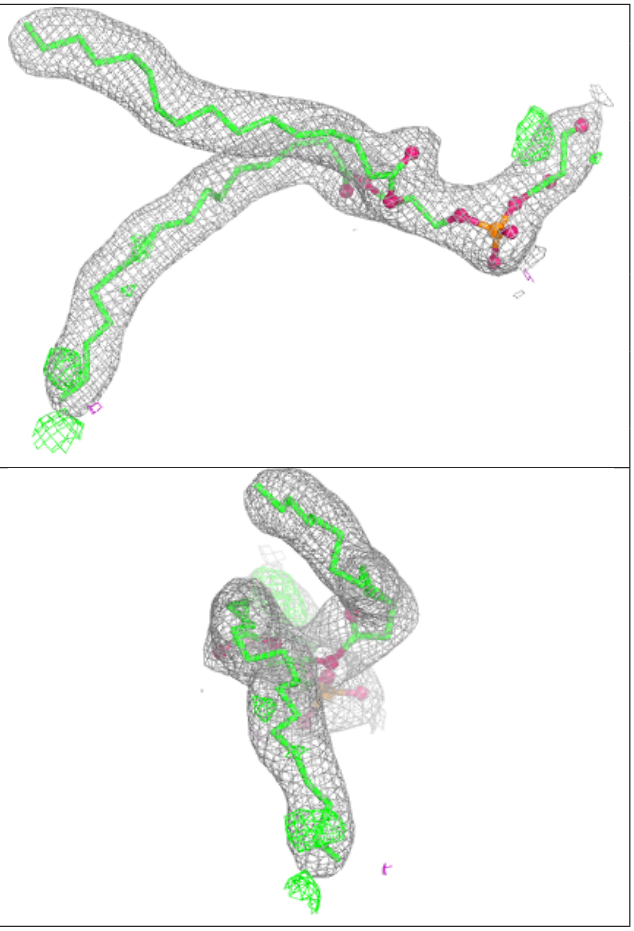






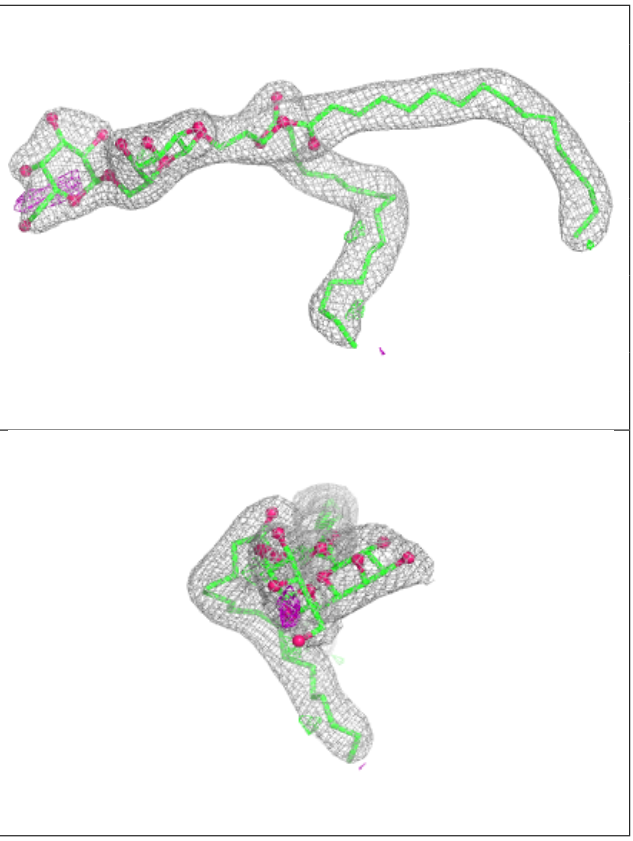
Electron density around LHG d 408 (A):

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



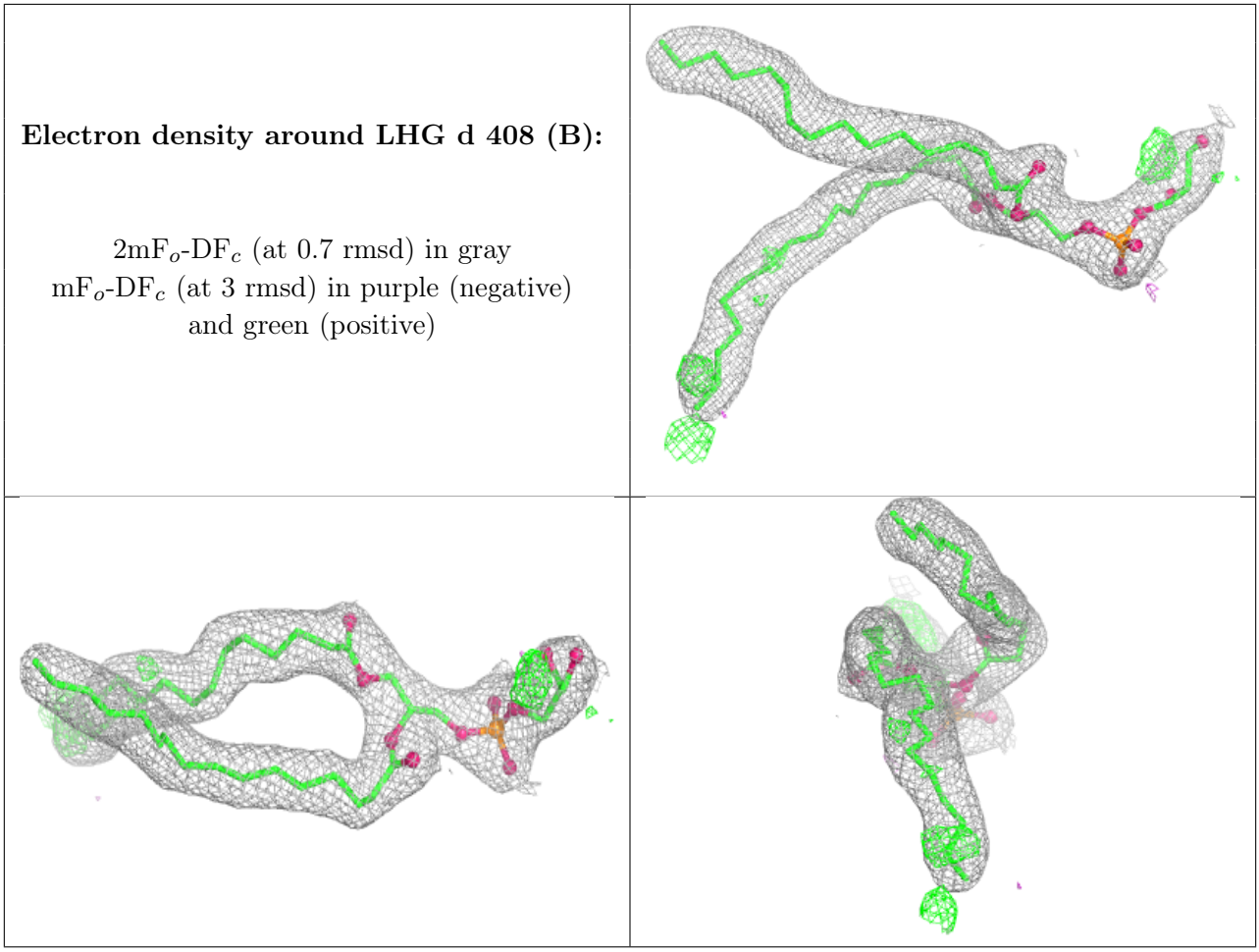
Electron density around DGD h 102:

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



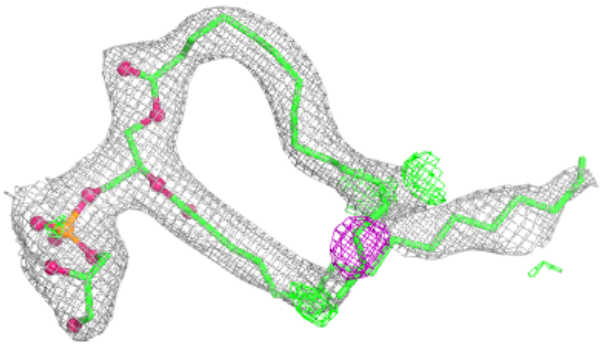
Electron density around LHG d 408 (B):

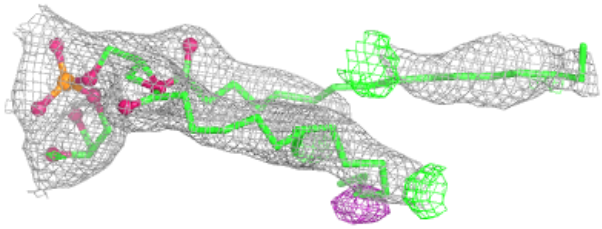
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

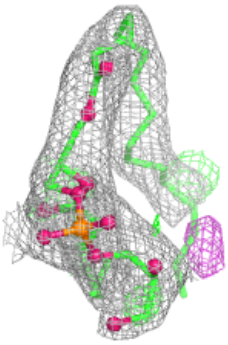


Electron density around LHG d 409 (A):

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

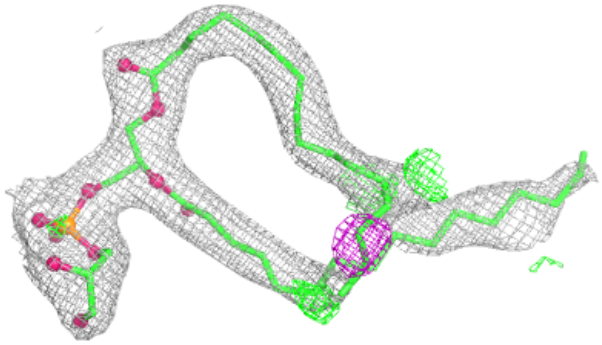


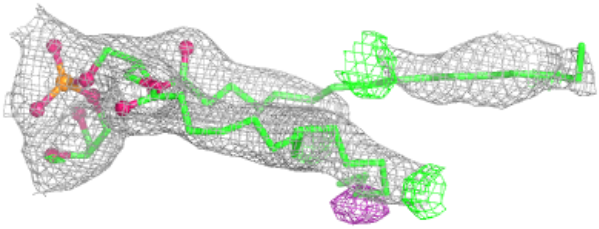


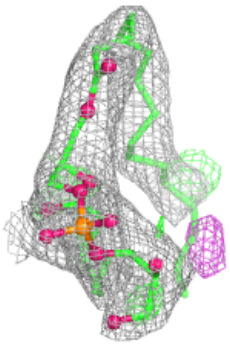


Electron density around LHG d 409 (B):

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

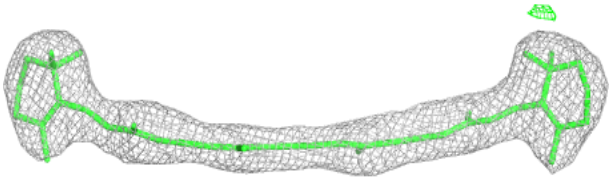


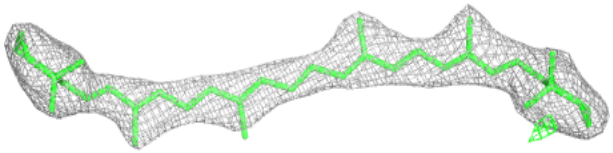


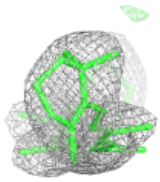


Electron density around BCR k 101:

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

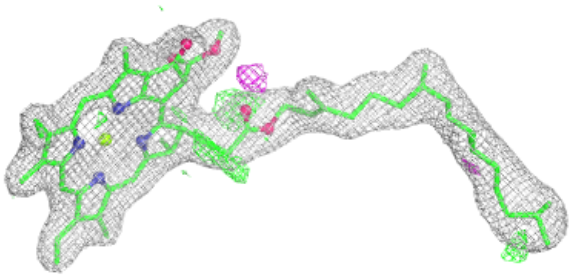


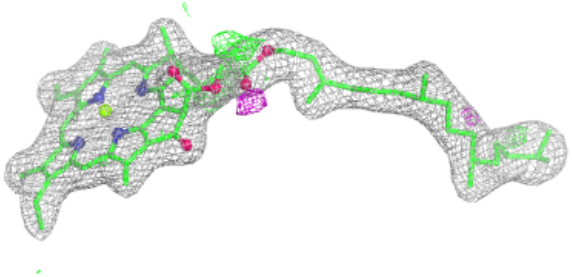


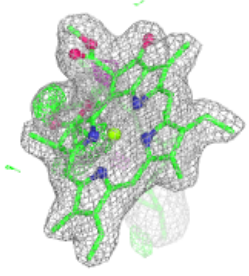


Electron density around CLA A 404 (A):

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

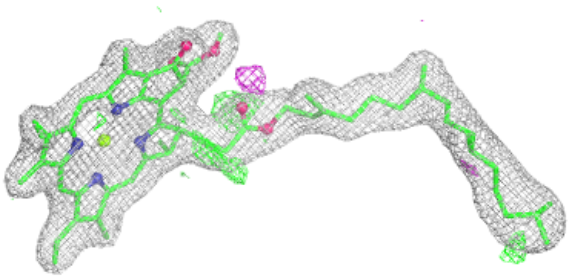


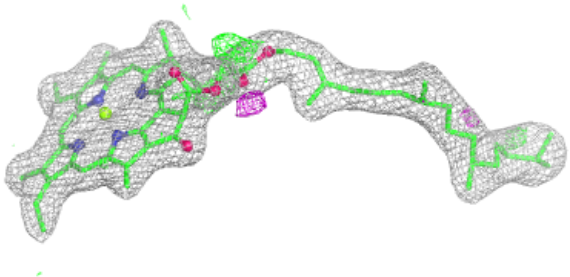


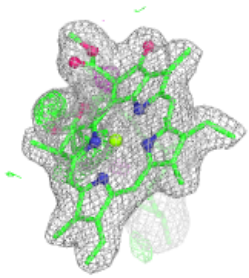


Electron density around CLA A 404 (B):

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

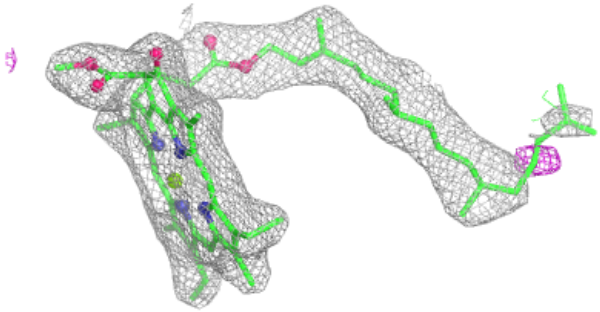


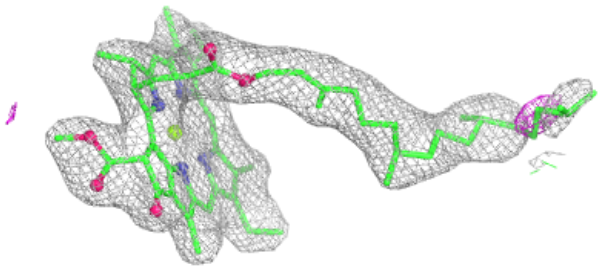


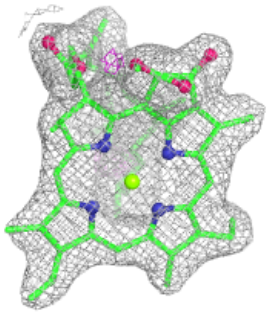


Electron density around CLA c 508:

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

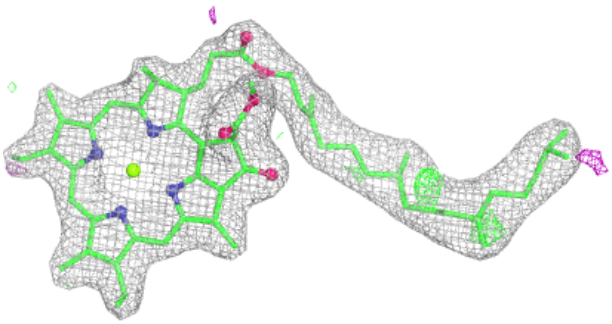


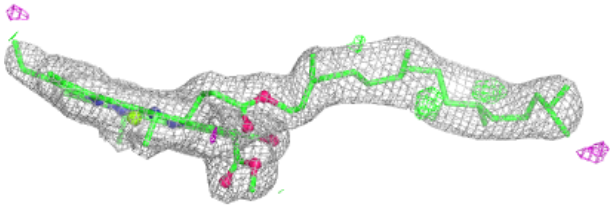


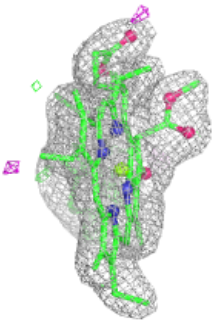


Electron density around CLA B 602:

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

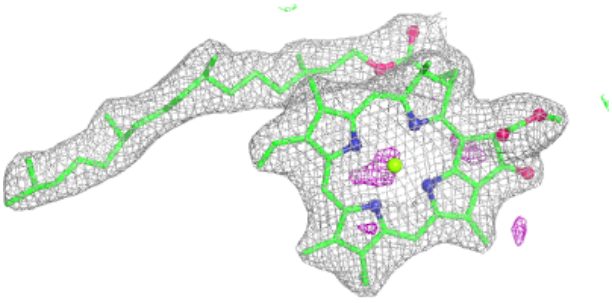


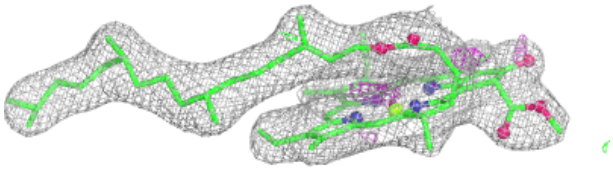


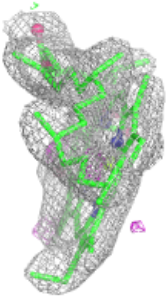


Electron density around CLA C 502:

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

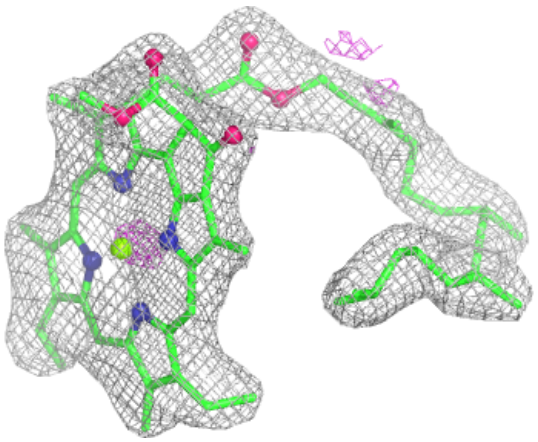


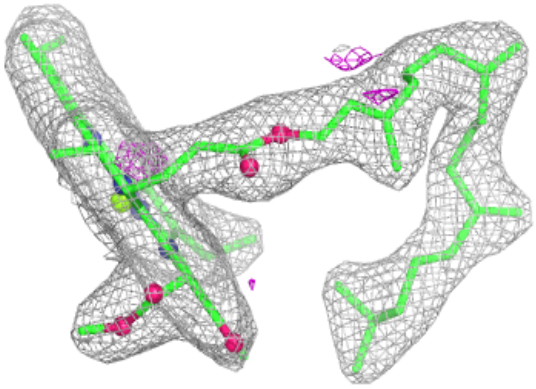


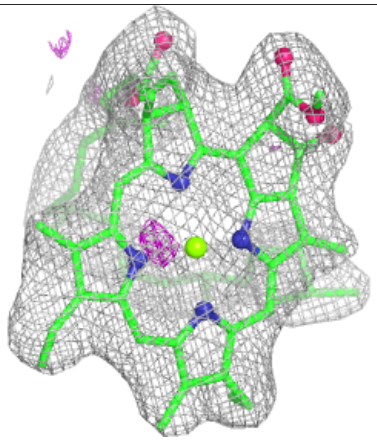


Electron density around CLA C 504:

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

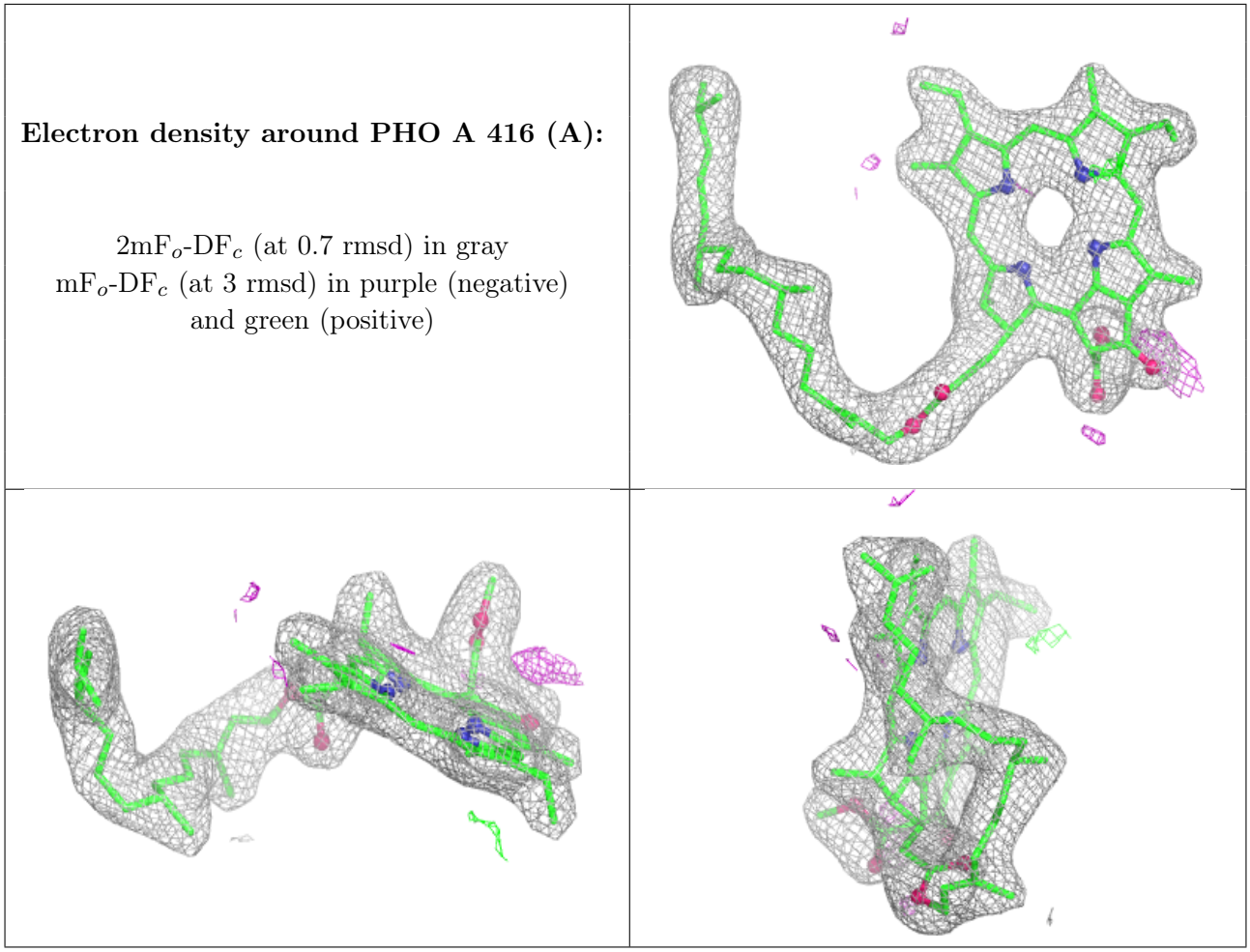






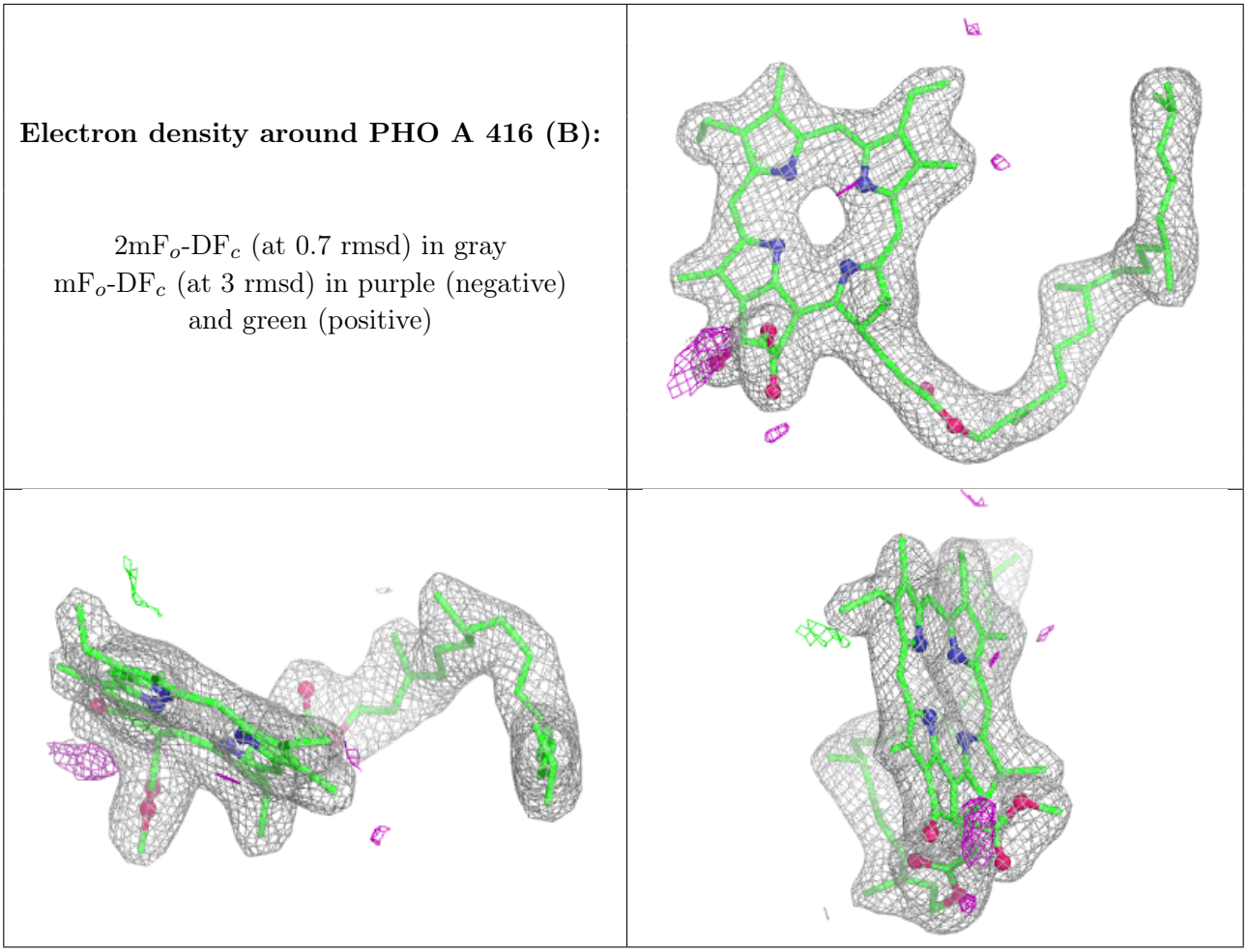
Electron density around PHO A 416 (A):

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



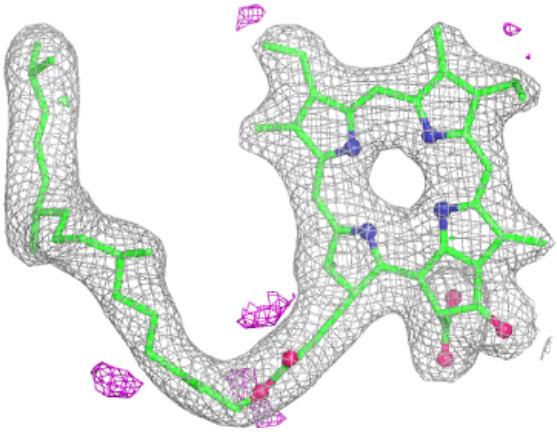
Electron density around PHO A 416 (B):

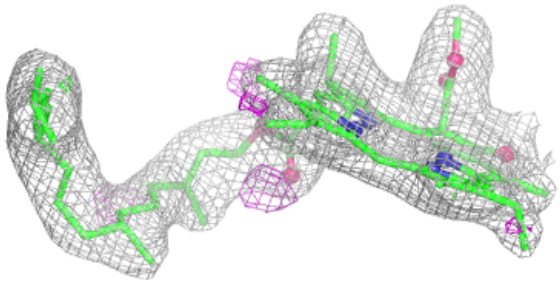
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

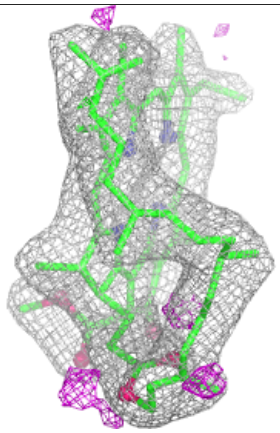


Electron density around PHO d 403 (A):

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

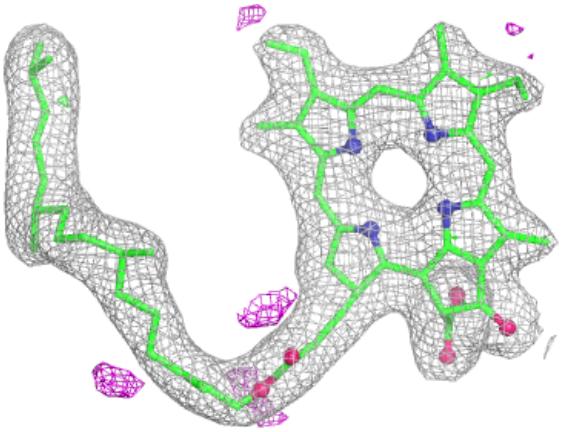


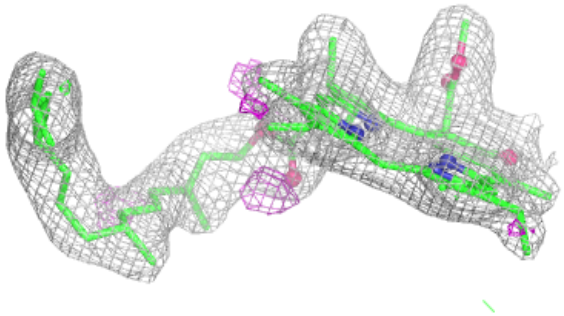


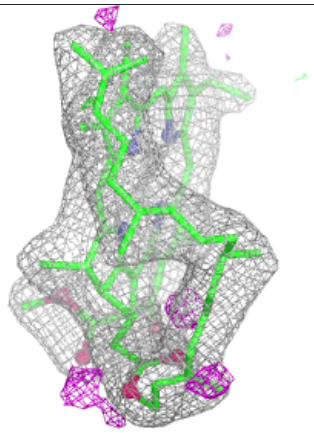


Electron density around PHO d 403 (B):

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

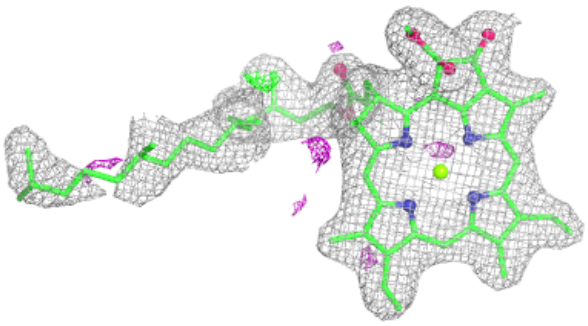


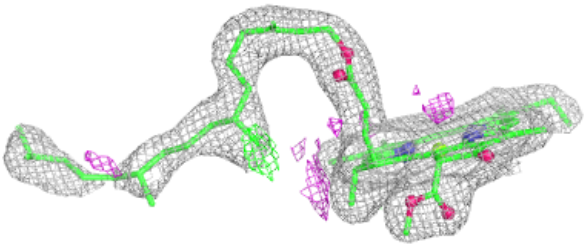


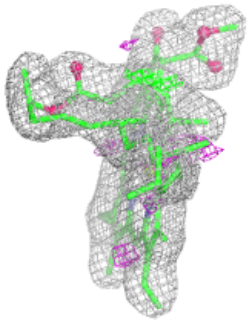


Electron density around CLA A 406 (A):

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

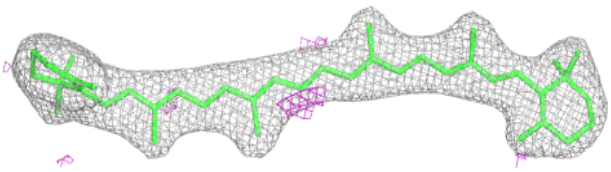


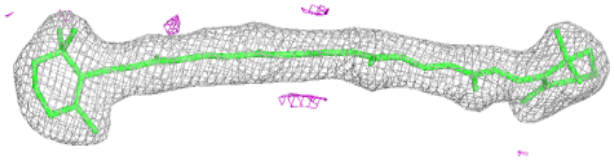


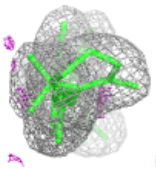


Electron density around BCR B 617:

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

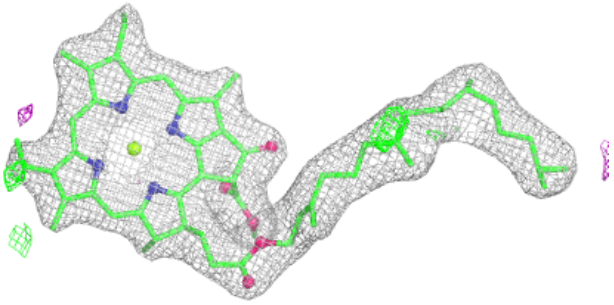


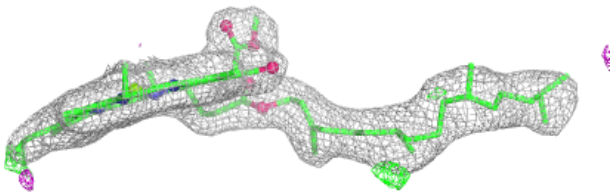


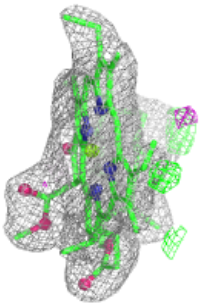


Electron density around CLA b 602:

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

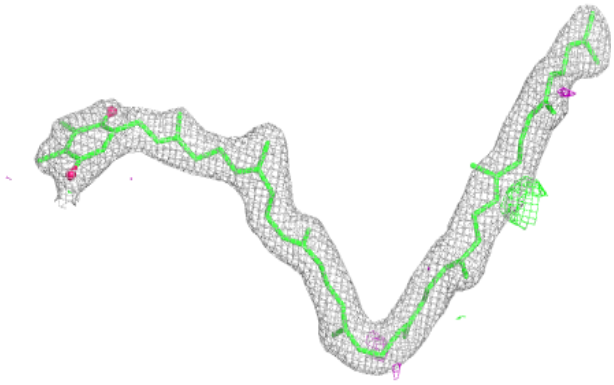


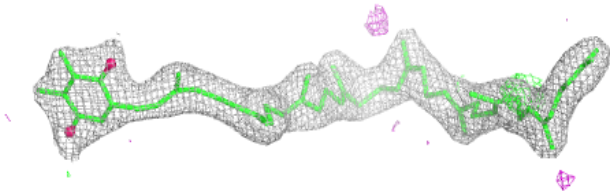


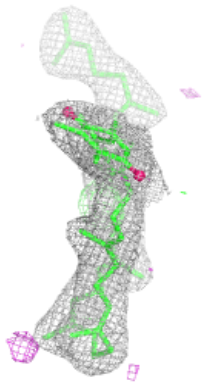


Electron density around PL9 d 407 (A):

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

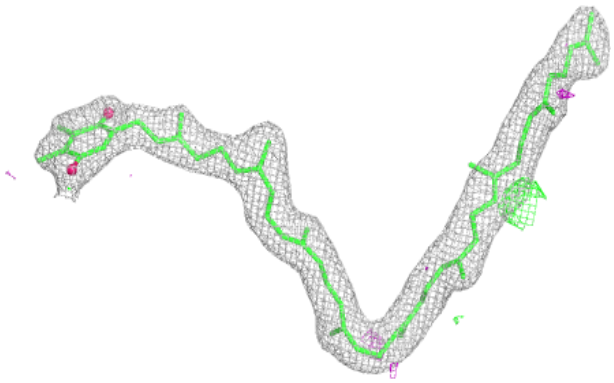


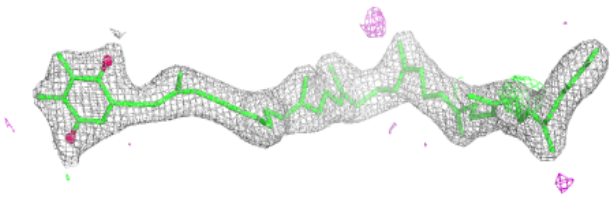




Electron density around PL9 d 407 (B):

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

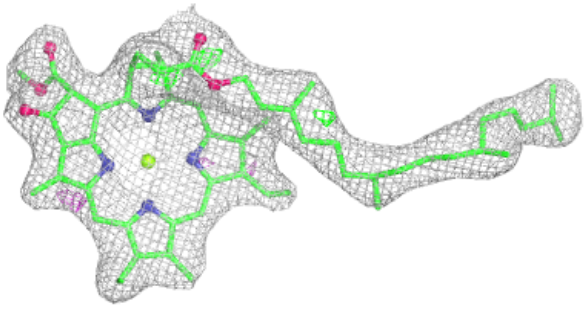


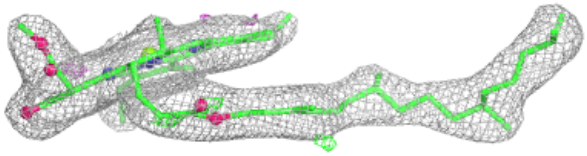


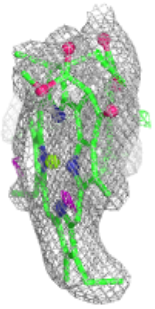


Electron density around CLA b 603:

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

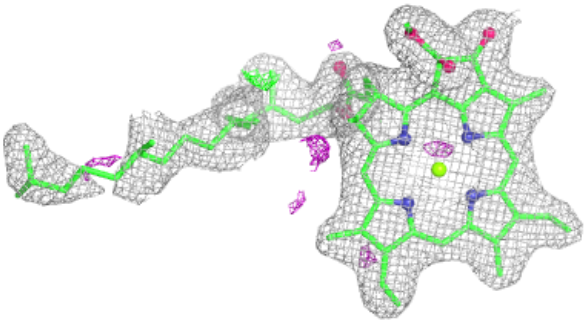


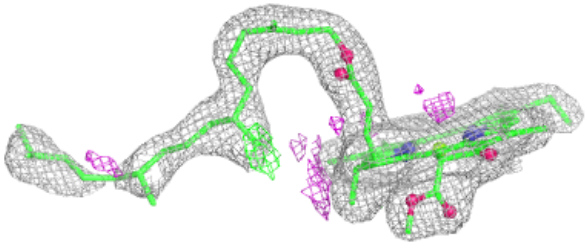


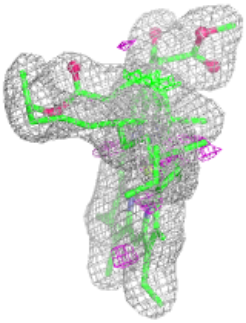


Electron density around CLA A 406 (B):

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

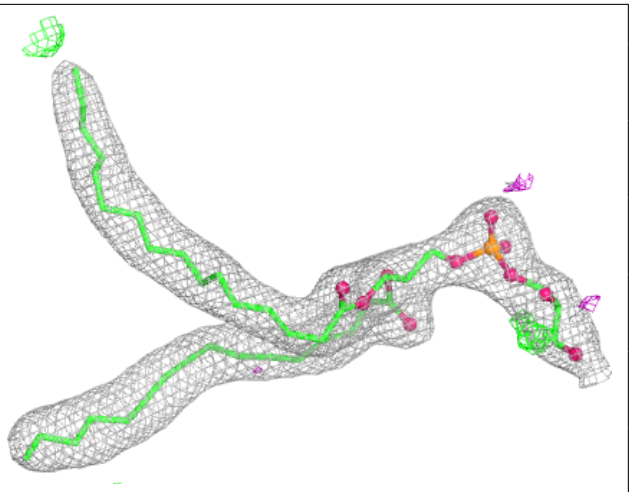


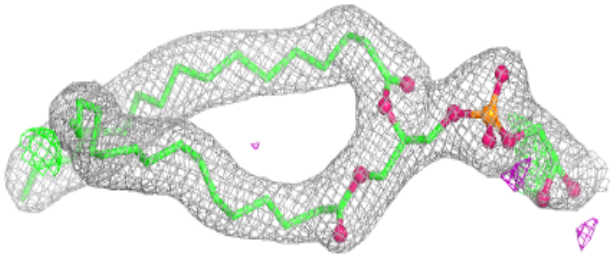


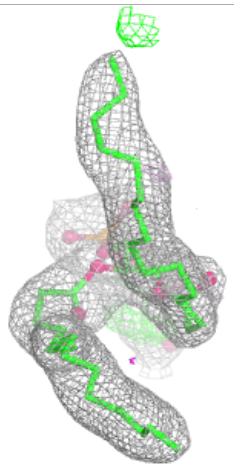


Electron density around LHG D 406 (A):

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

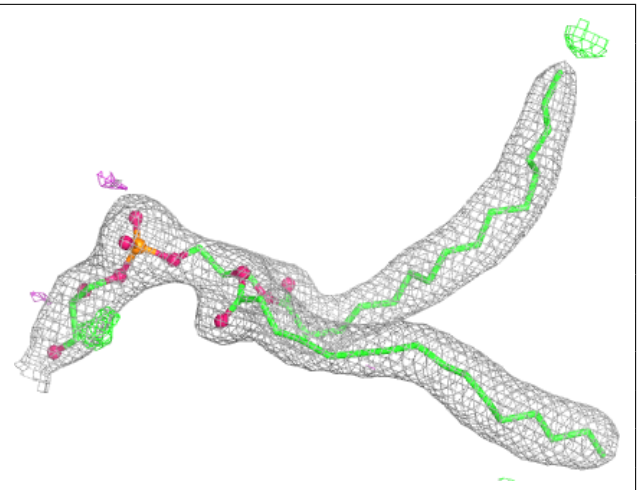


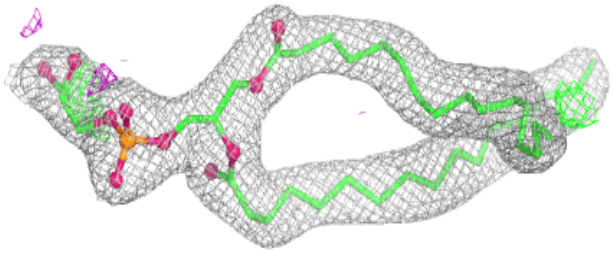


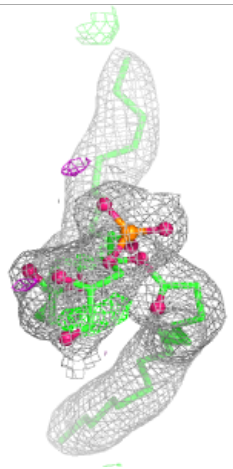


Electron density around LHG D 406 (B):

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

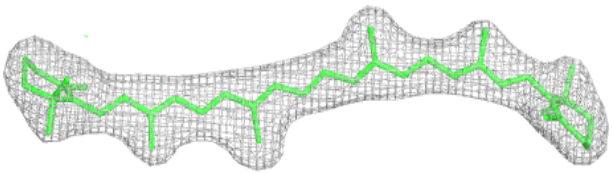


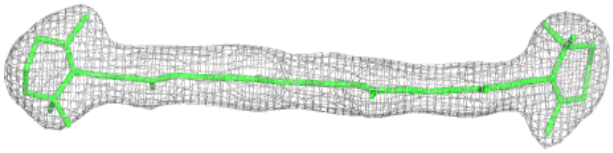


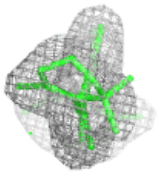


Electron density around BCR C 516:

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

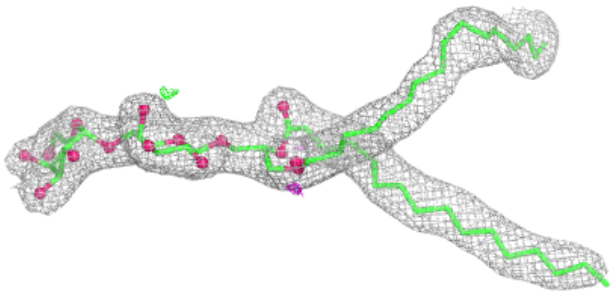


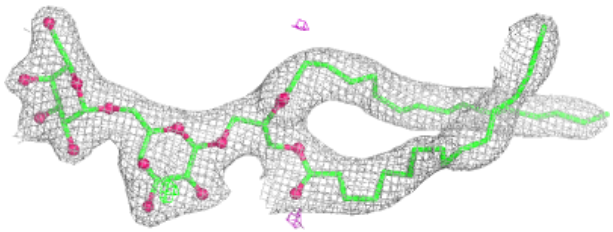


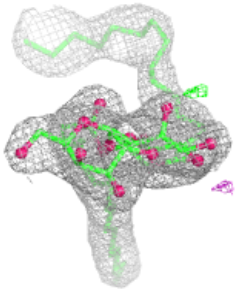


Electron density around DGD C 517 (A):

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

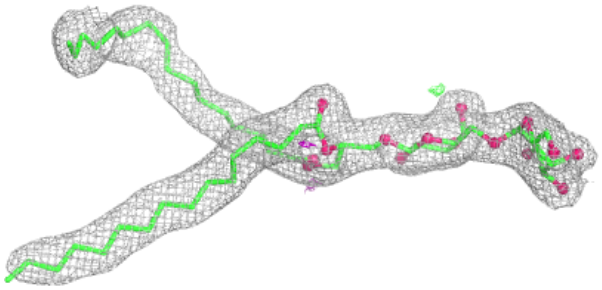


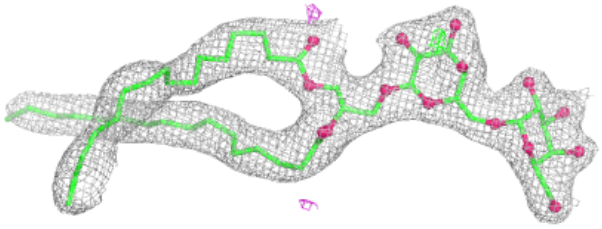


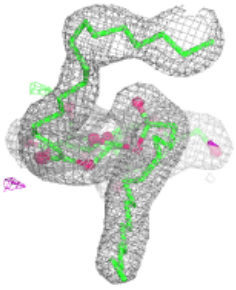


Electron density around DGD C 517 (B):

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

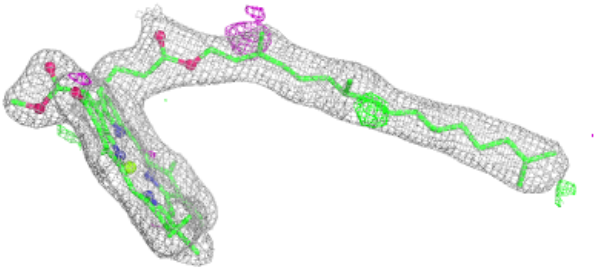


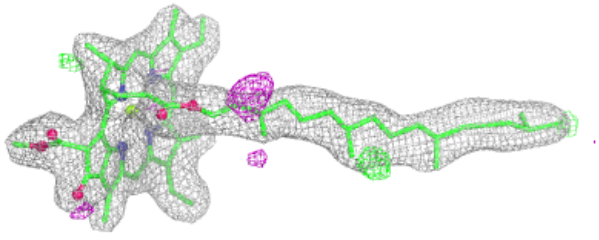


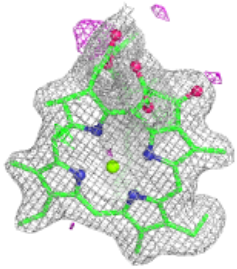


Electron density around CLA b 607:

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

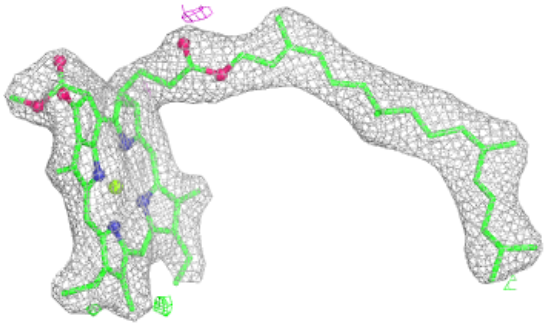


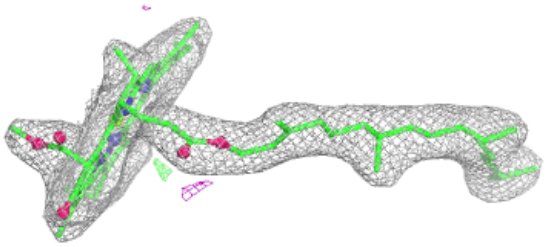


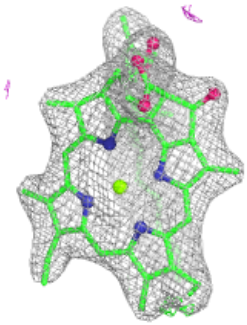


Electron density around CLA b 609:

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

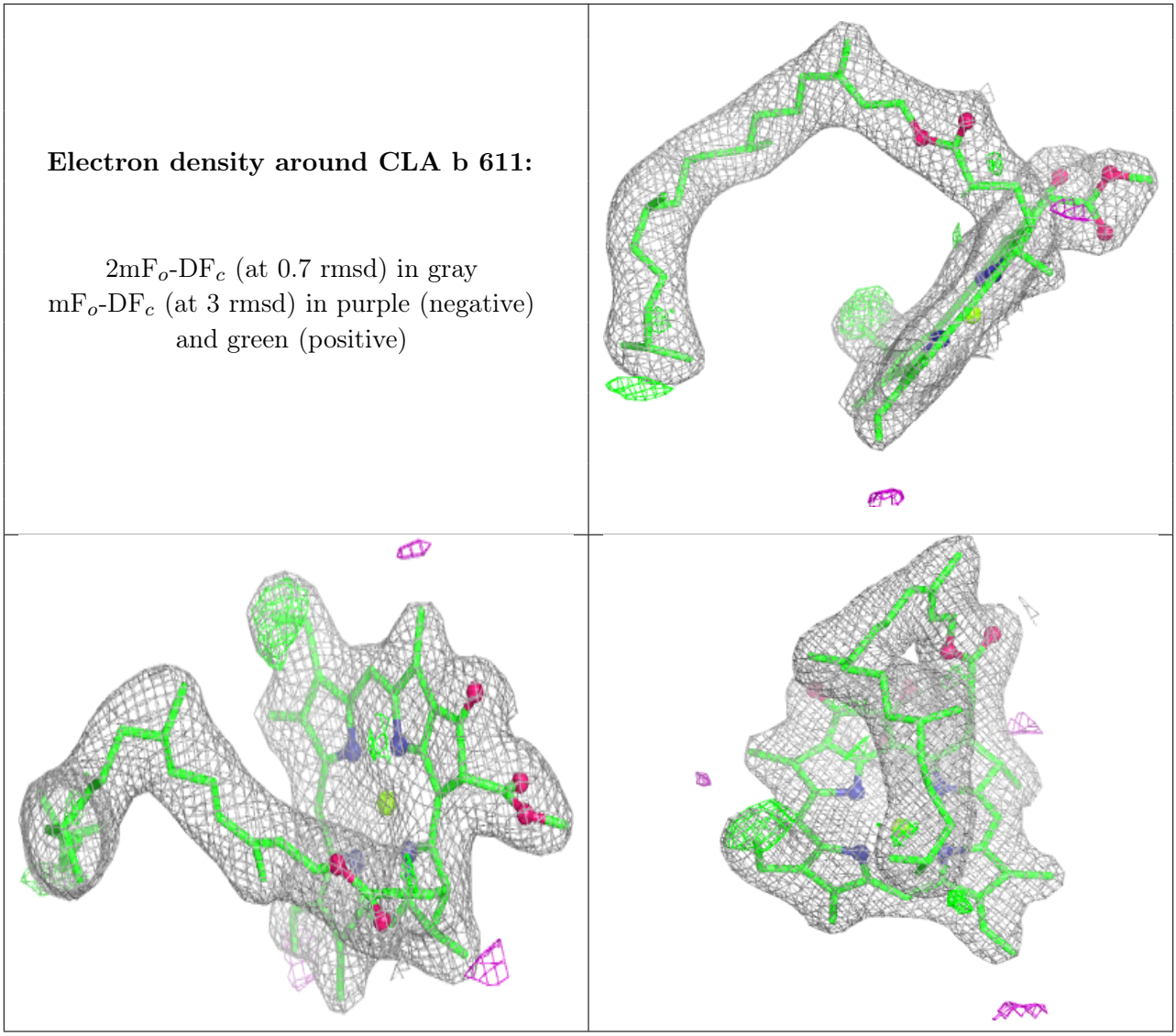






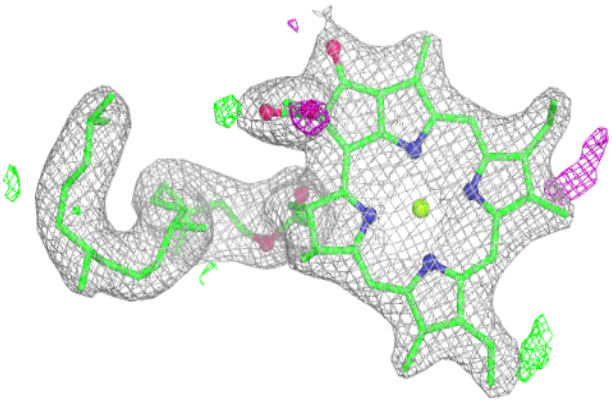
Electron density around CLA b 611:

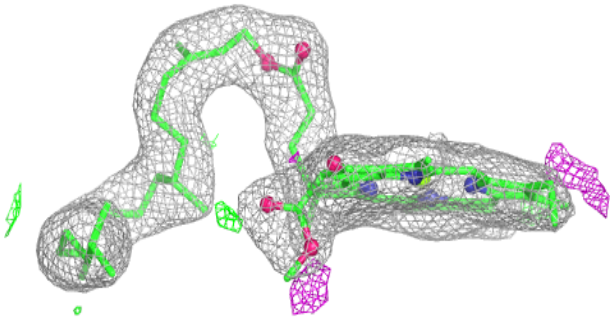
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

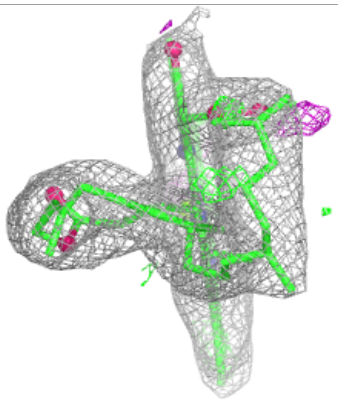


Electron density around CLA b 612:

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

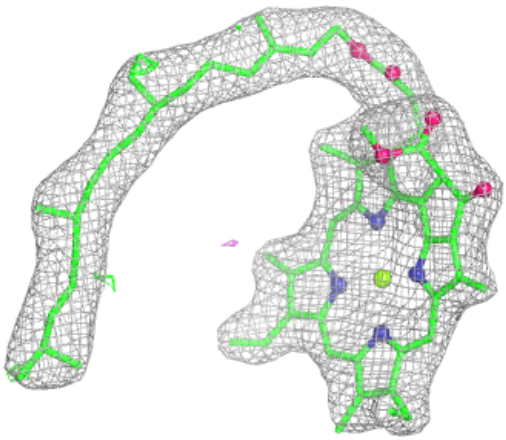


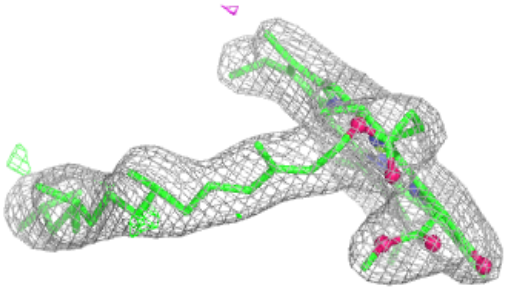


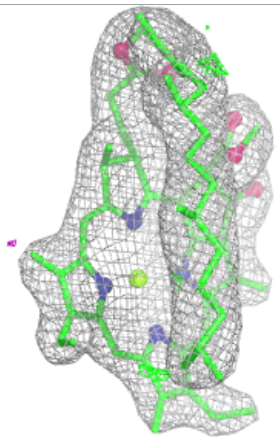


Electron density around CLA C 508:

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

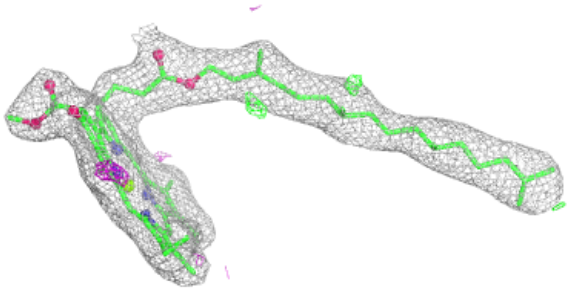


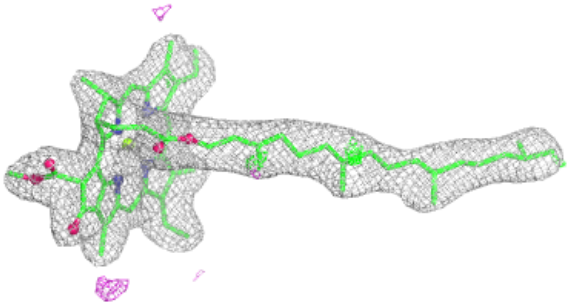


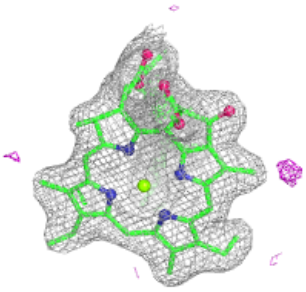


Electron density around CLA B 607:

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

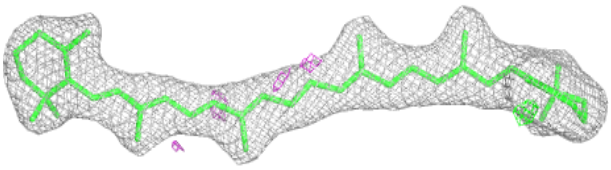


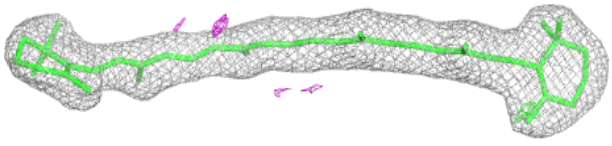


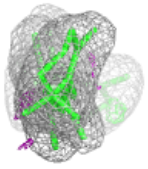


Electron density around BCR b 617:

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

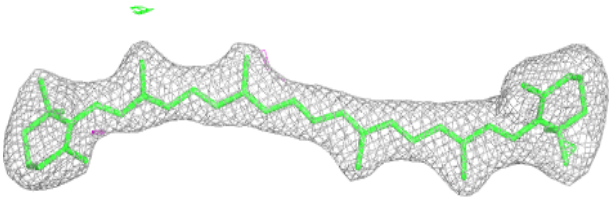


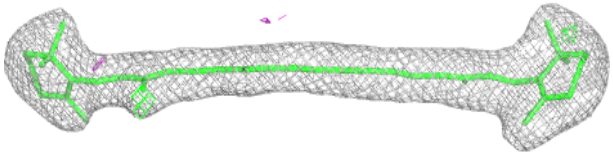


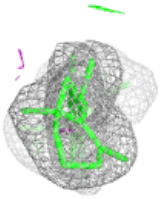


Electron density around BCR b 618:

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

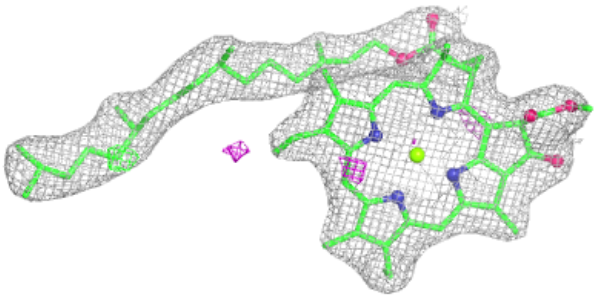


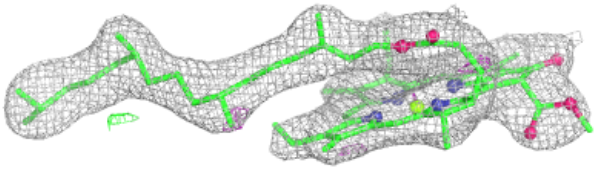


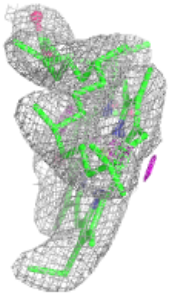


Electron density around CLA c 501:

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

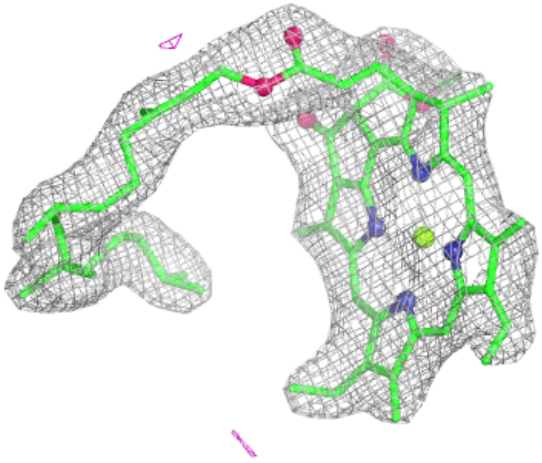


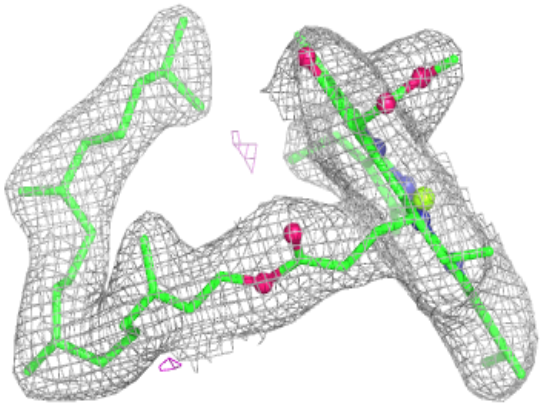


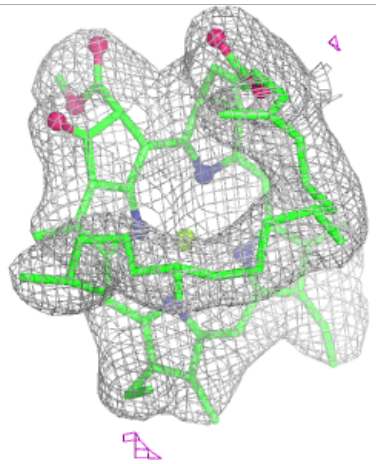


Electron density around CLA c 503:

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

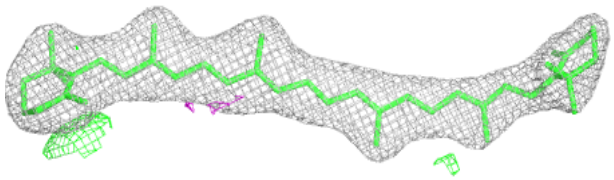


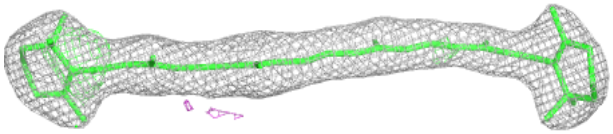


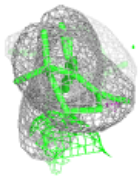


Electron density around BCR c 515:

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

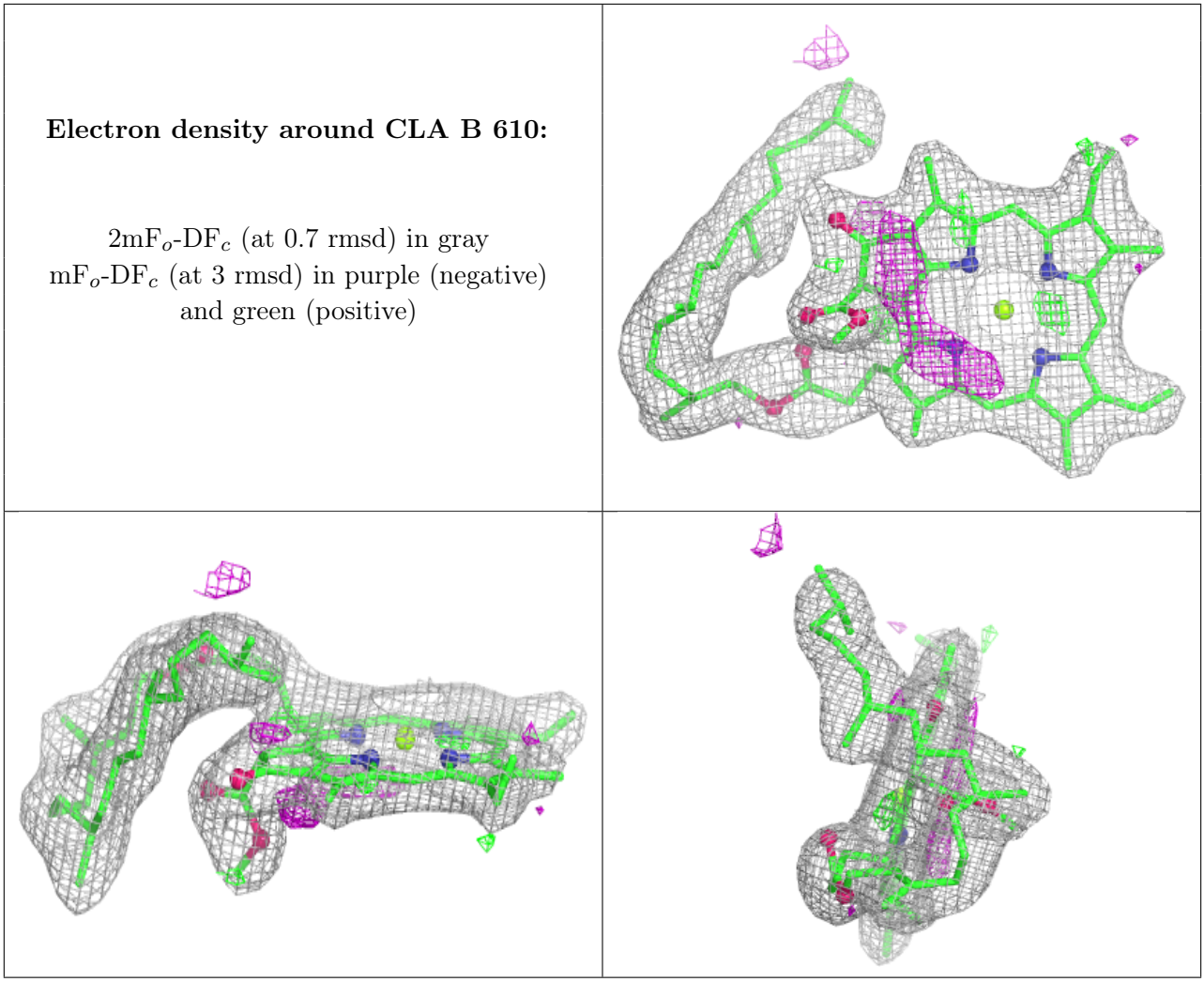






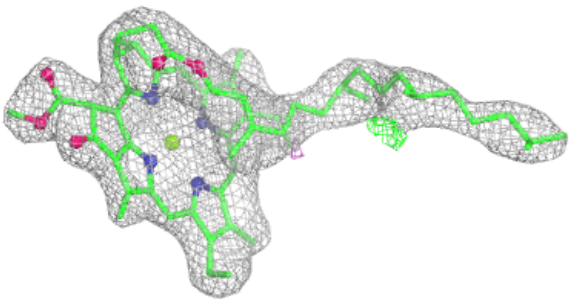
Electron density around CLA B 610:

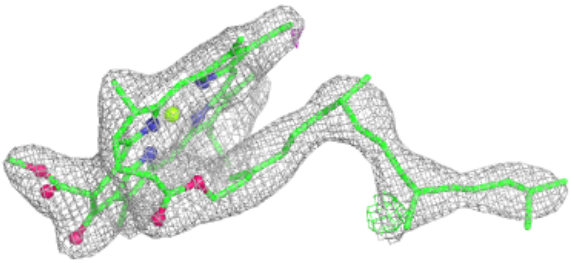
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

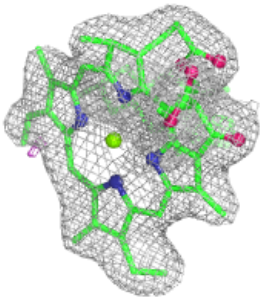


Electron density around CLA c 505:

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

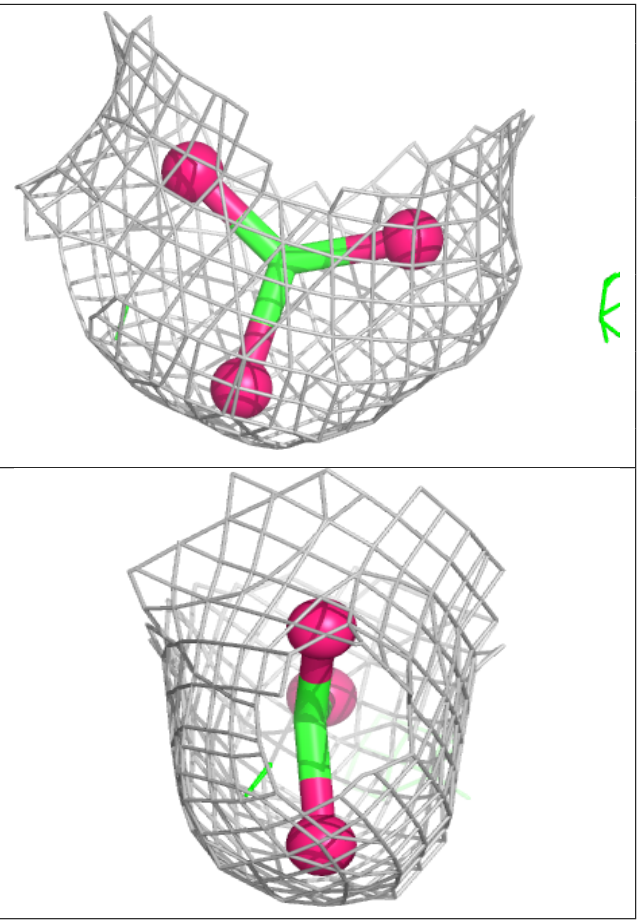






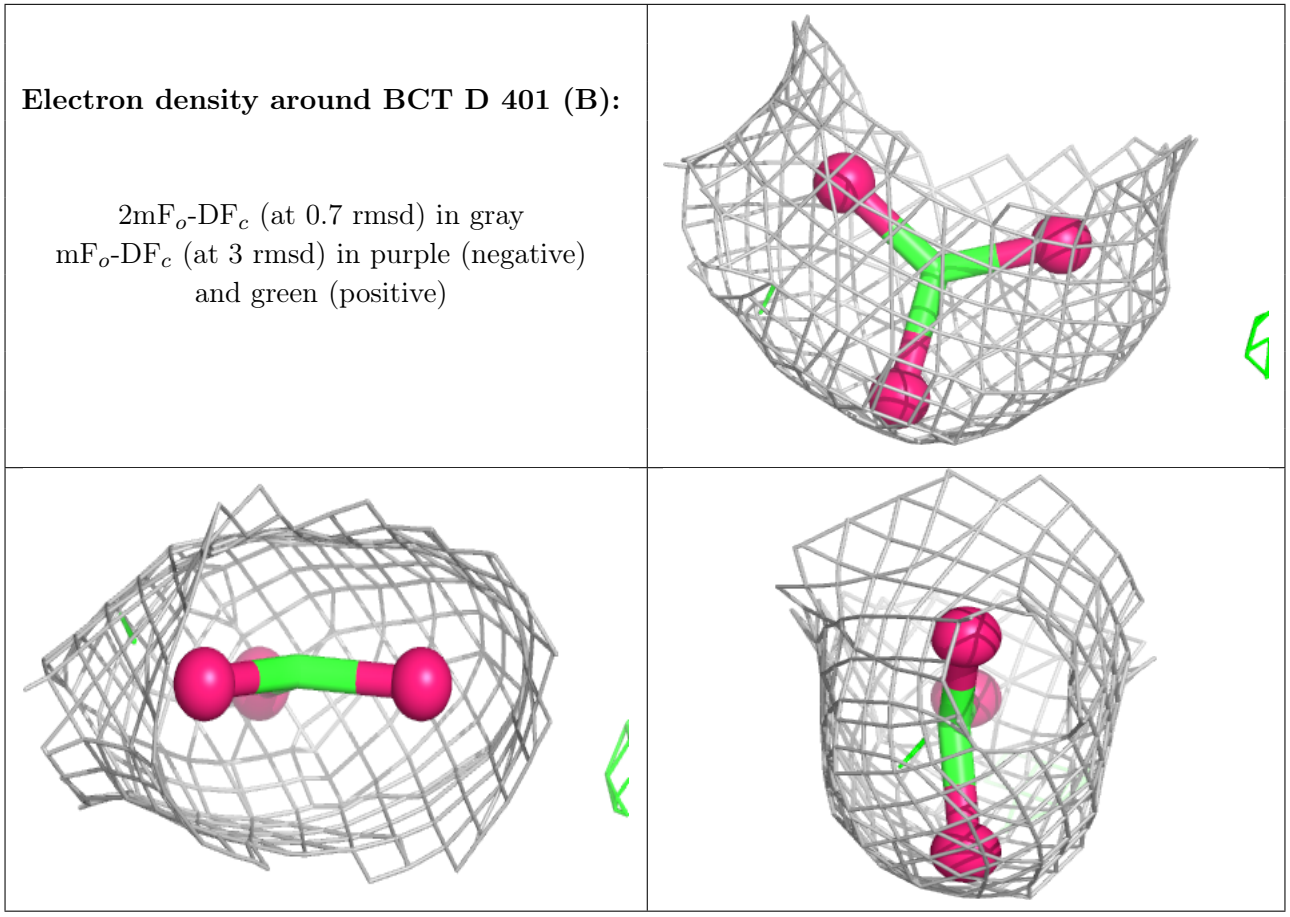
Electron density around BCT D 401 (A):

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



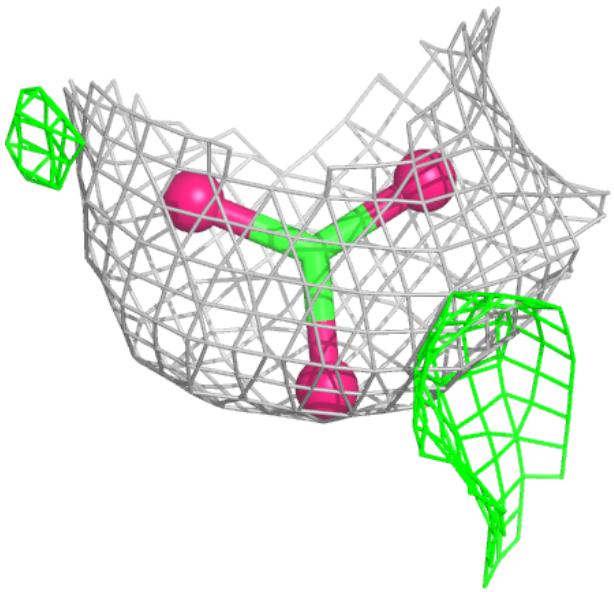
Electron density around BCT D 401 (B):

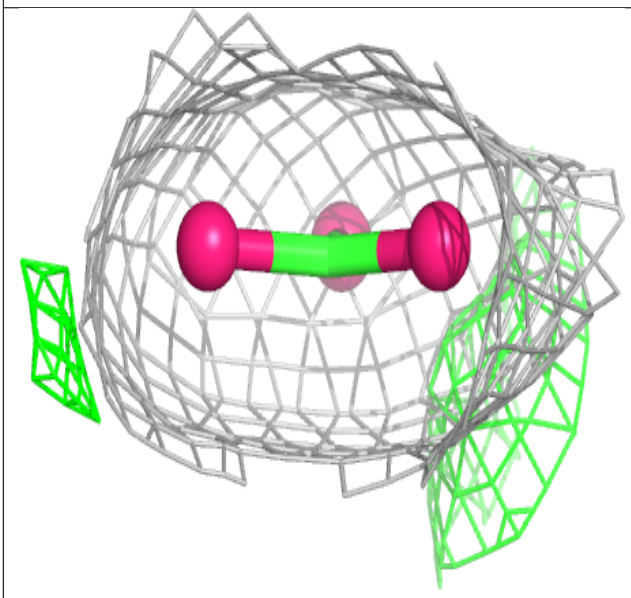
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

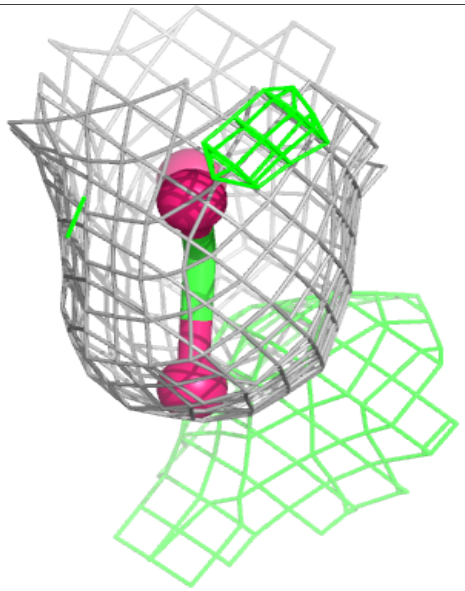


Electron density around BCT d 401 (A):

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

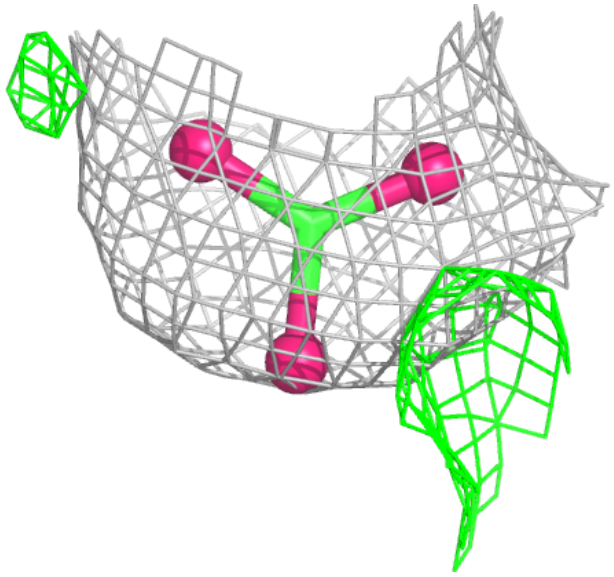


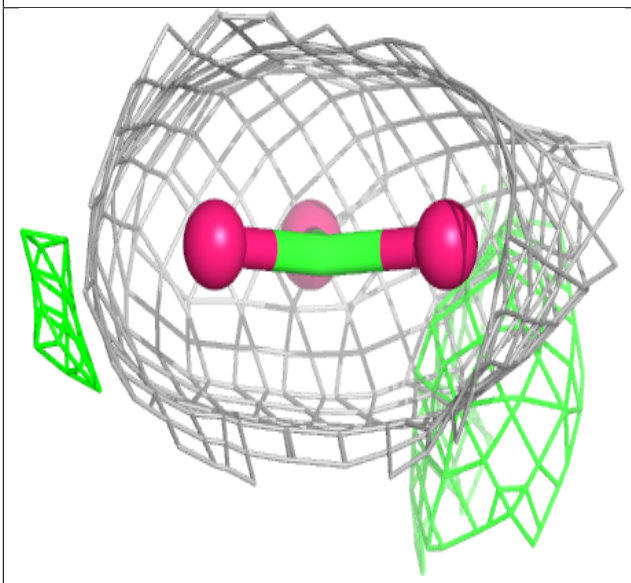


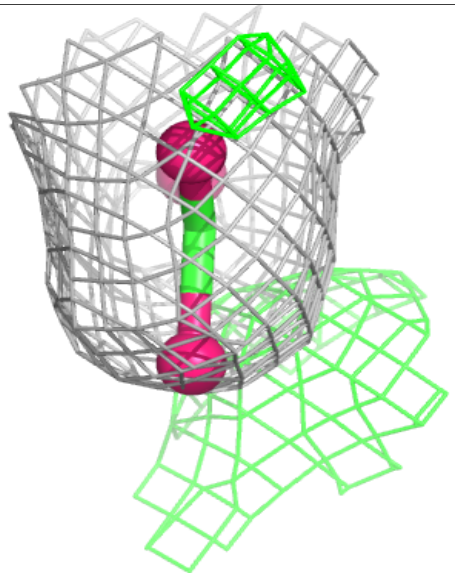


Electron density around BCT d 401 (B):

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

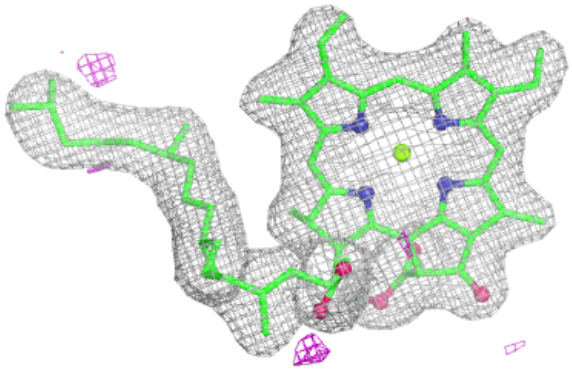


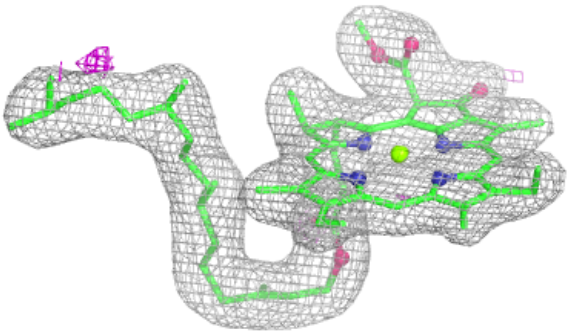


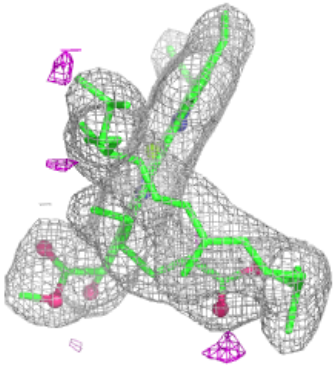


Electron density around CLA d 402 (B):

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

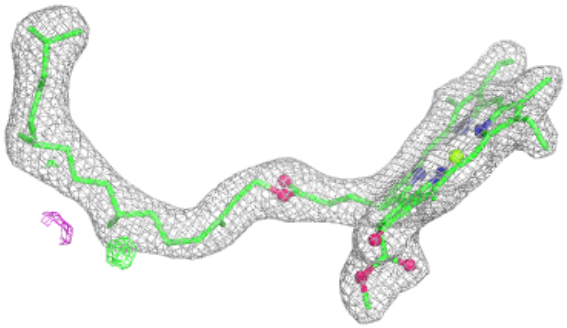


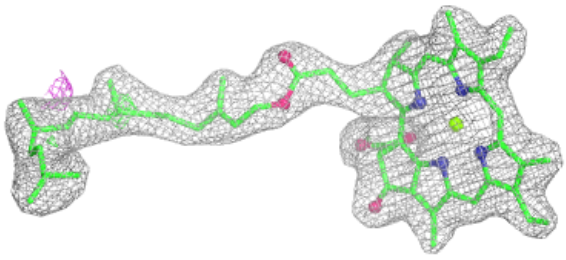


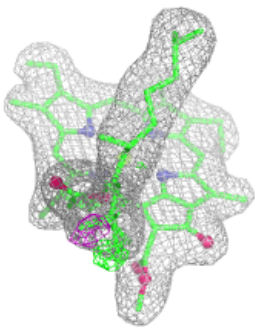


Electron density around CLA d 404 (A):

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

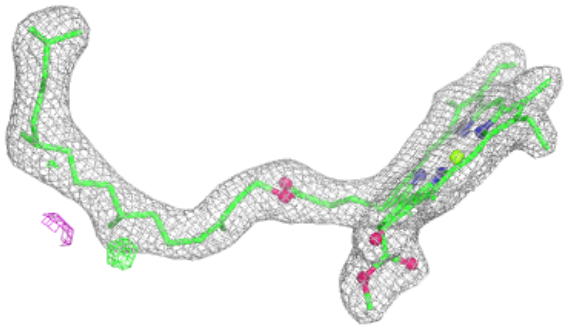


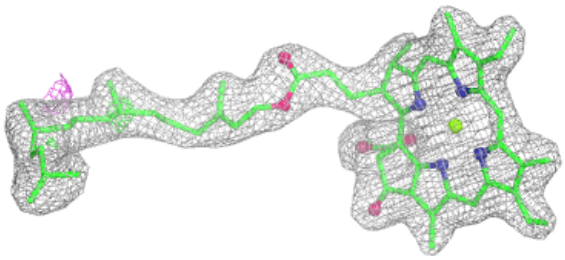


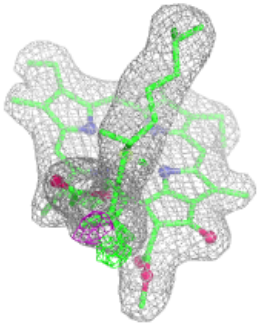


Electron density around CLA d 404 (B):

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

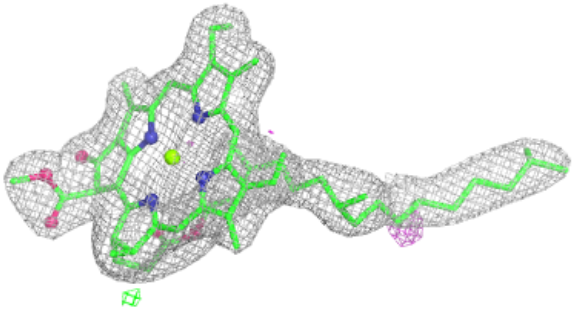


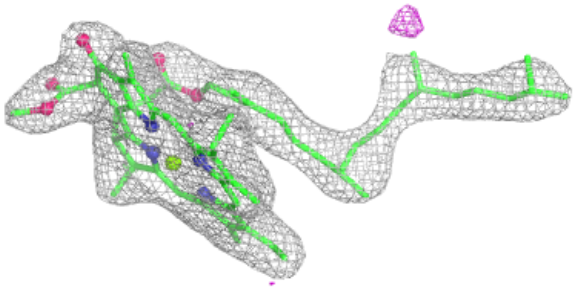


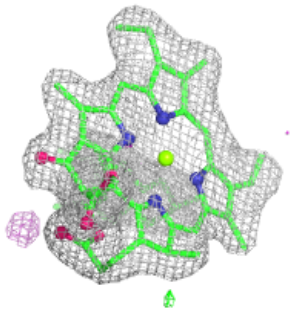


Electron density around CLA C 506:

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

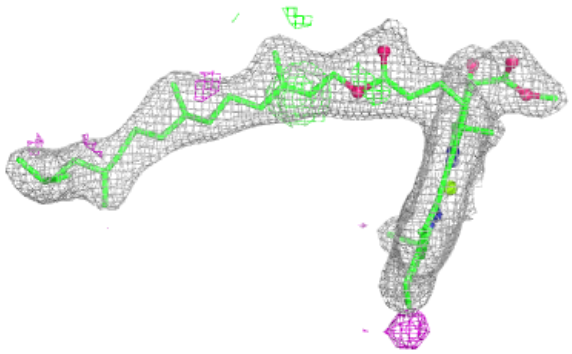


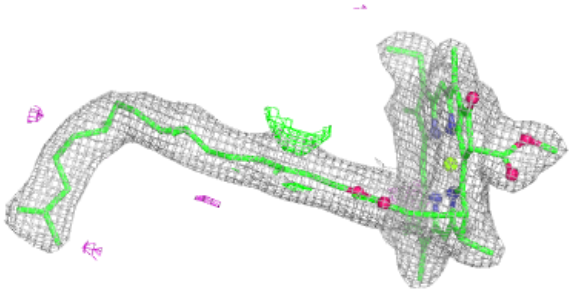


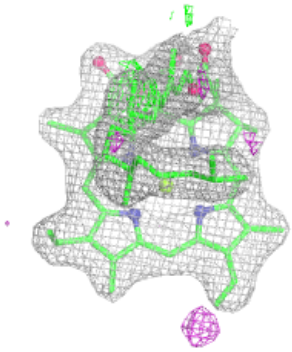


Electron density around CLA B 605:

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

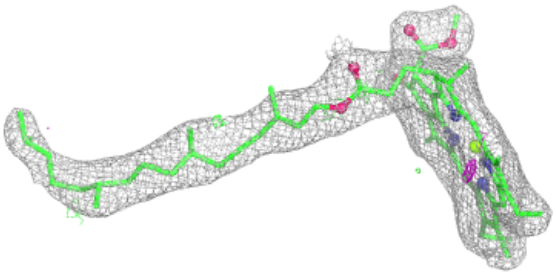


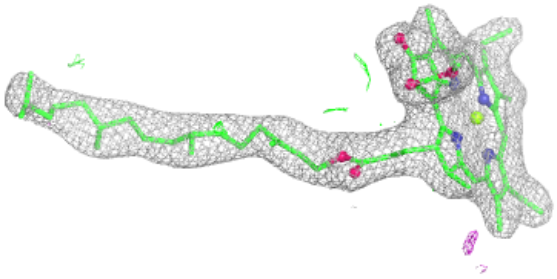


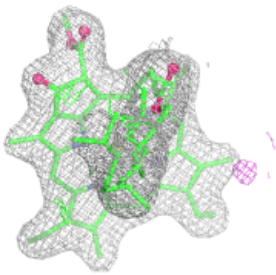


Electron density around CLA b 604:

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

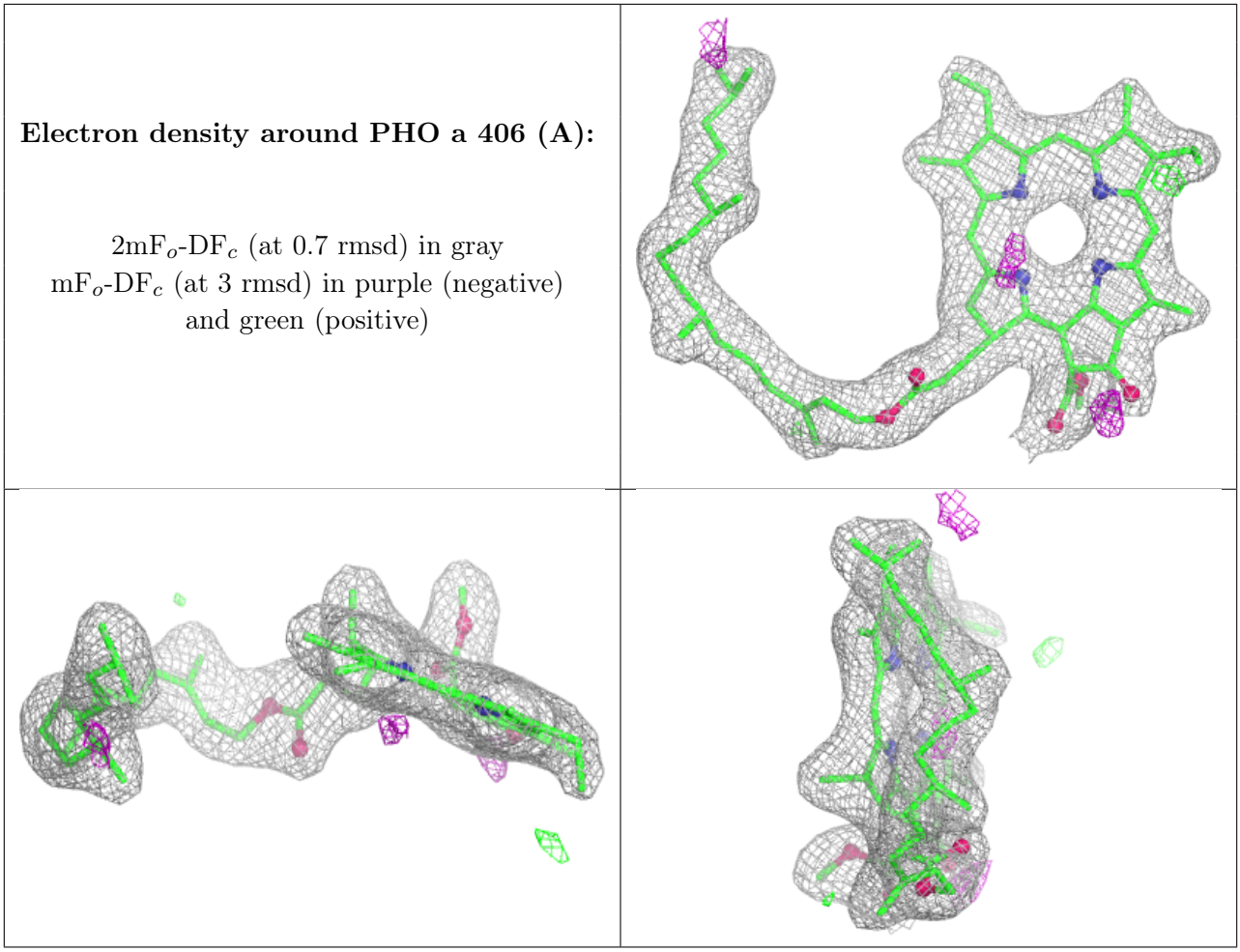






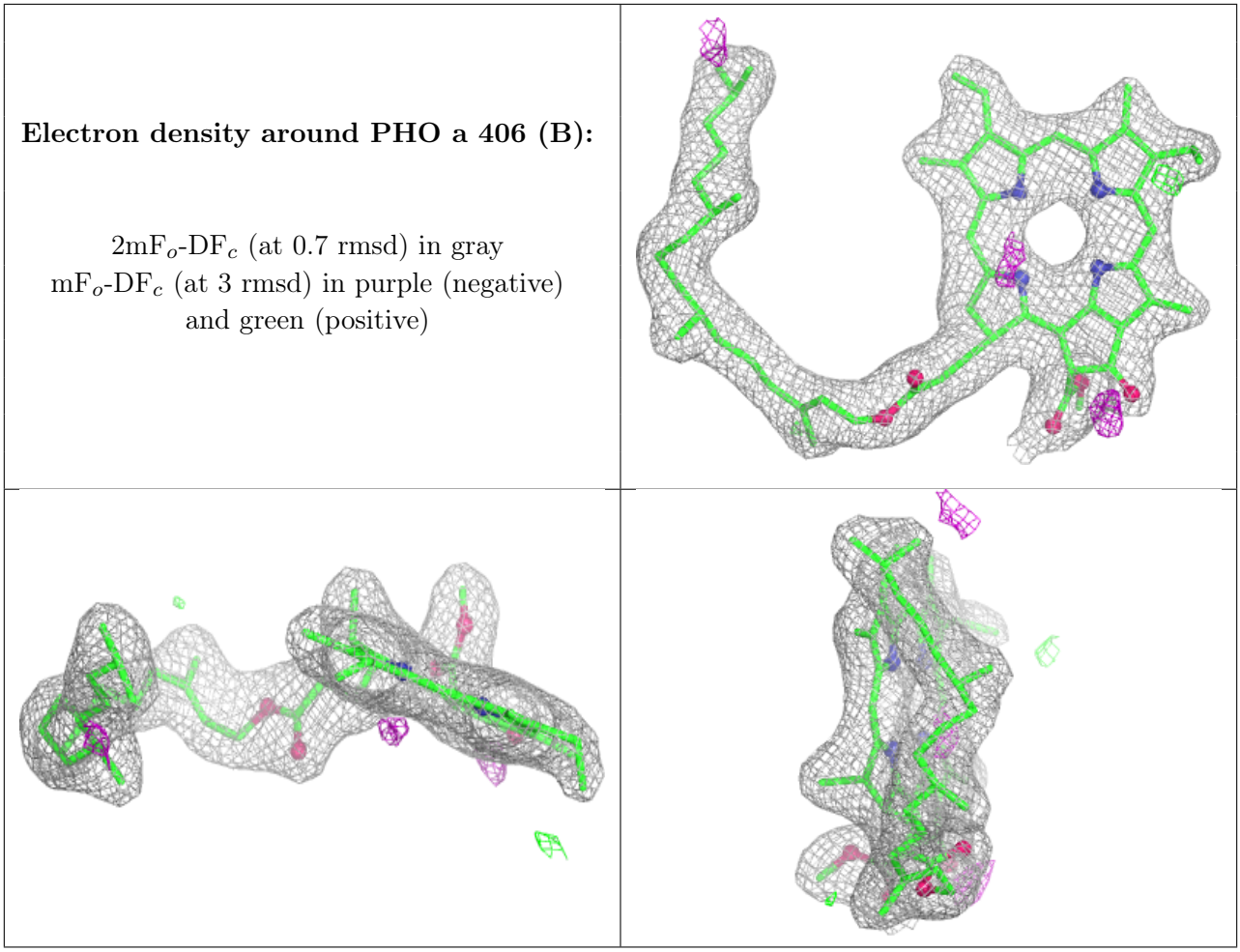
Electron density around PHO a 406 (A):

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



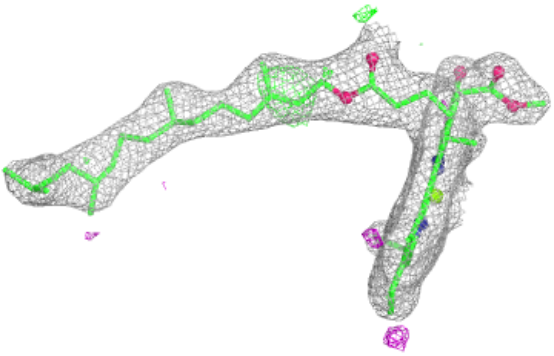
Electron density around PHO a 406 (B):

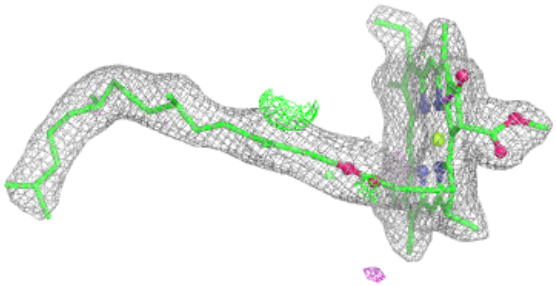
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

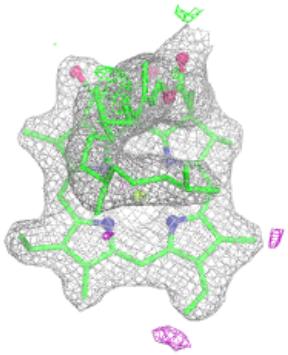


Electron density around CLA b 605:

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

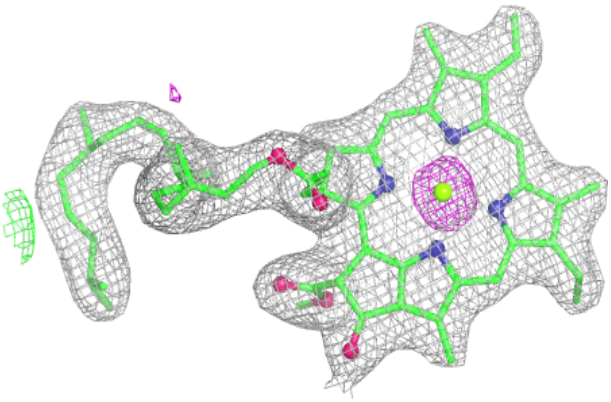


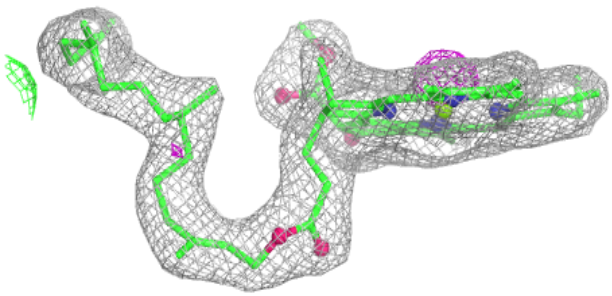


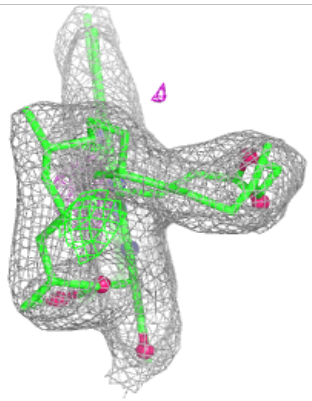


Electron density around CLA B 612:

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

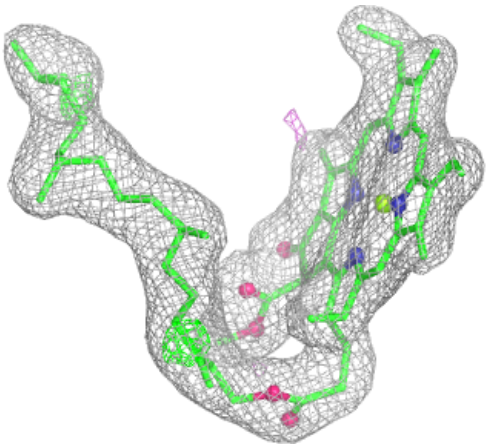


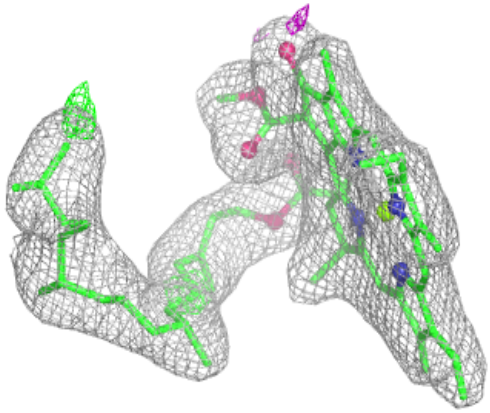


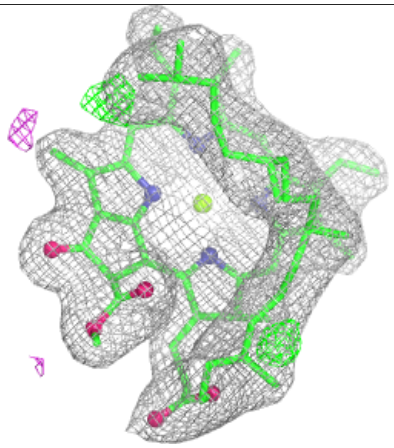


Electron density around CLA B 613:

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

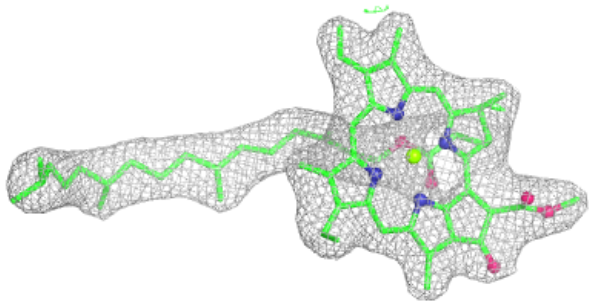


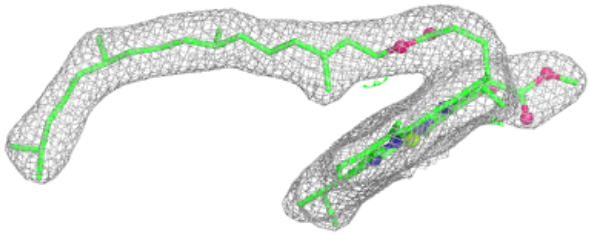


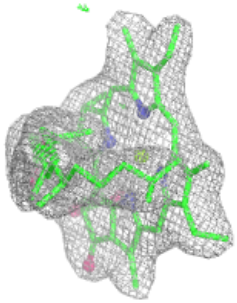


Electron density around CLA b 608:

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

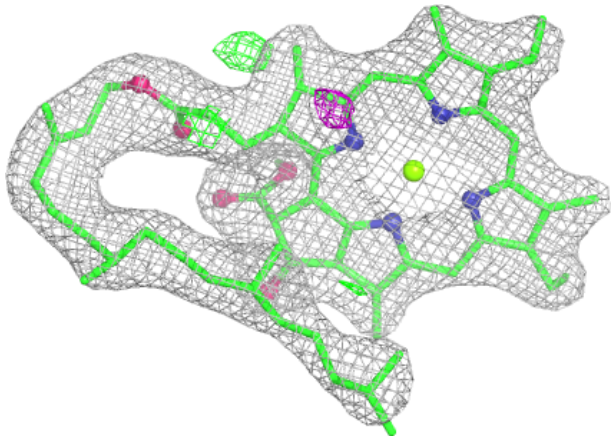


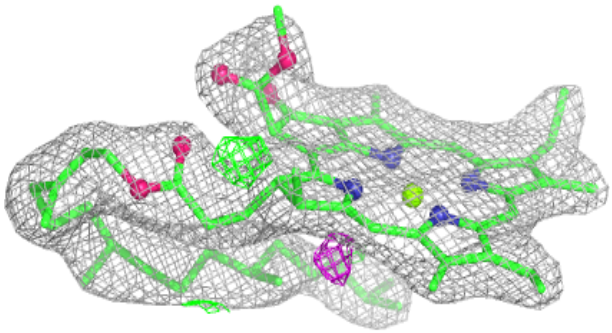


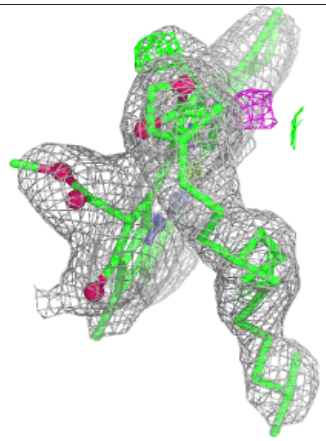


Electron density around CLA C 510:

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

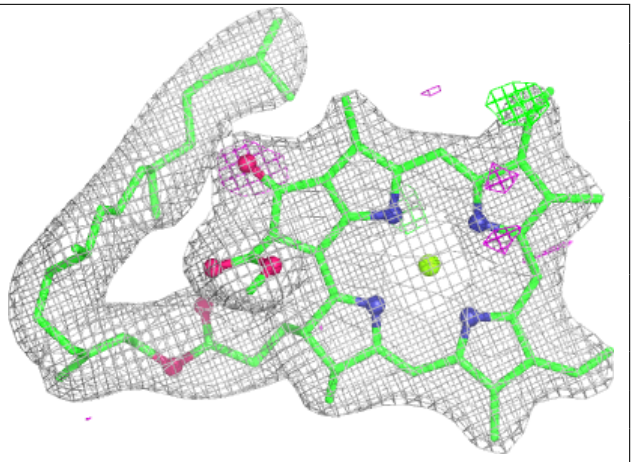


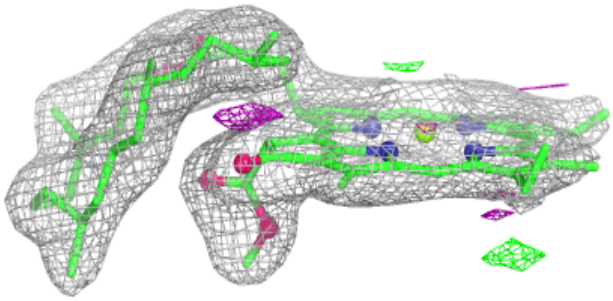


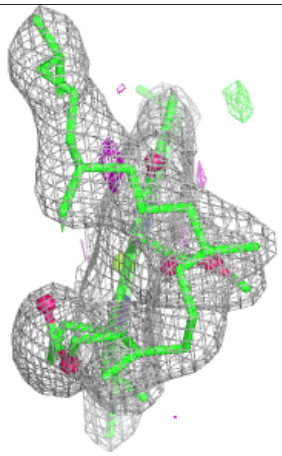


Electron density around CLA b 610:

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

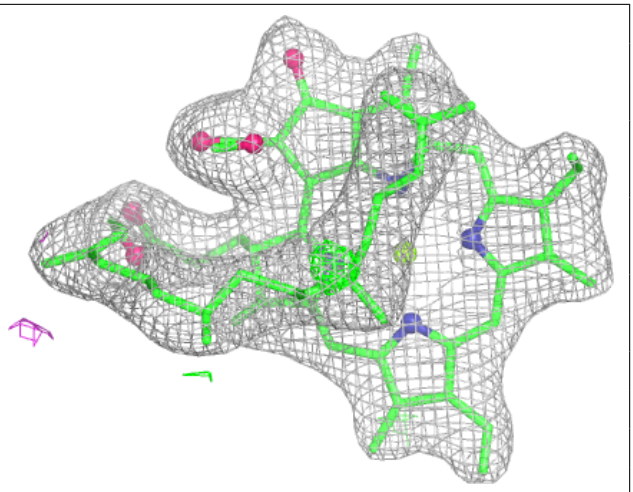


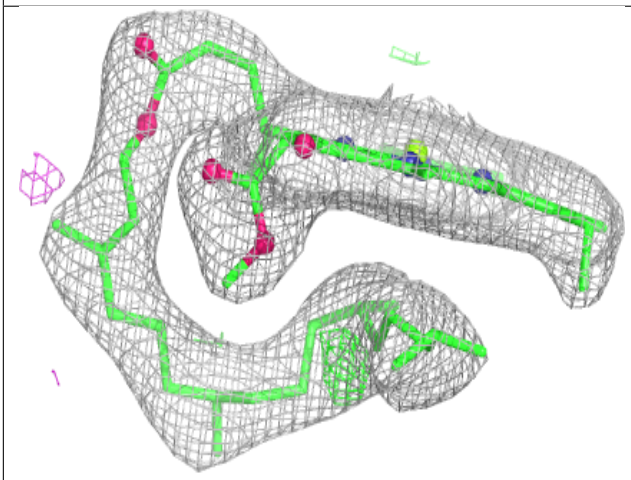


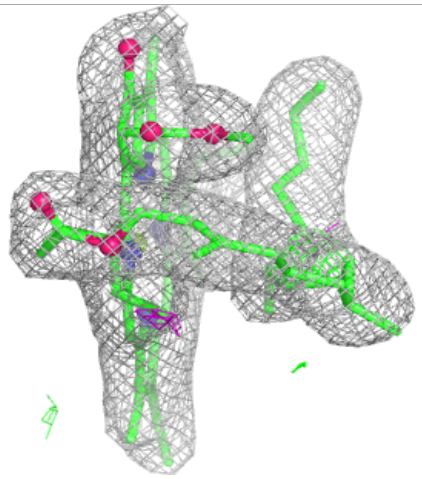


Electron density around CLA C 511:

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

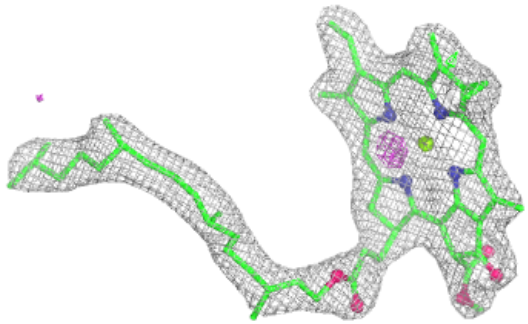


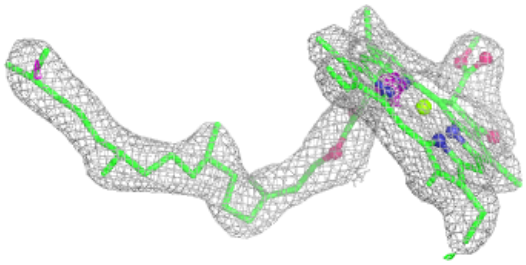


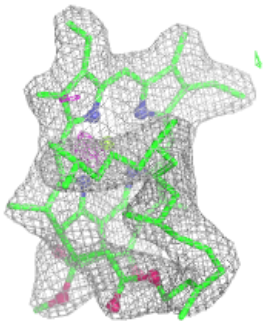


Electron density around CLA C 512:

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



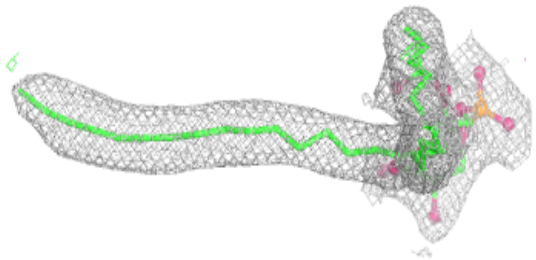


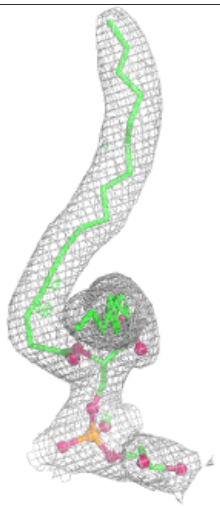


Electron density around LHG L 101 (A):

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



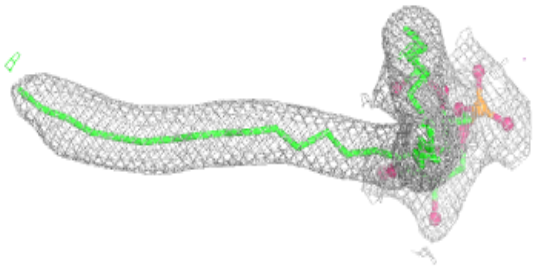


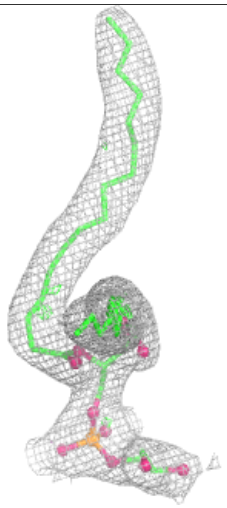


Electron density around LHG L 101 (B):

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

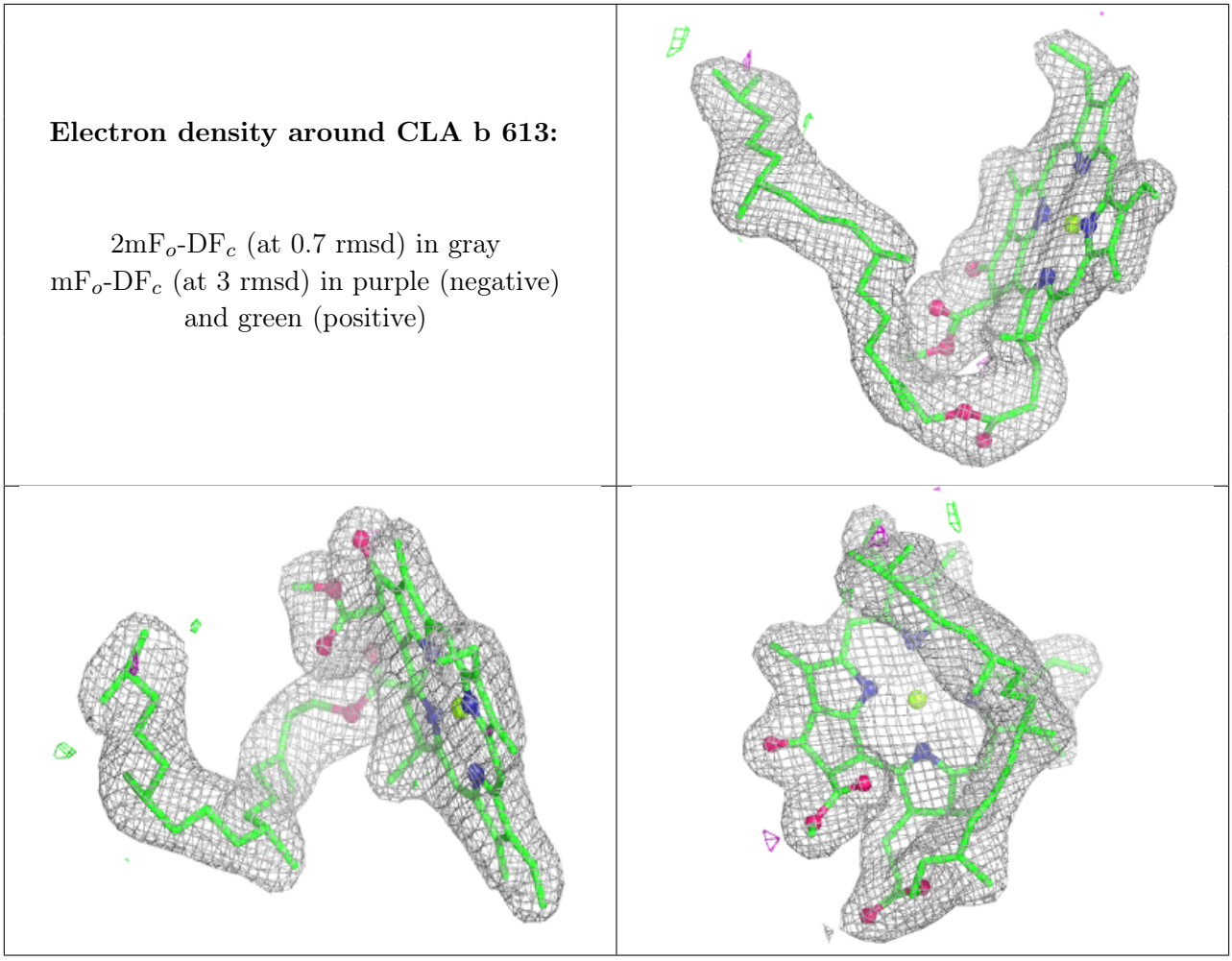






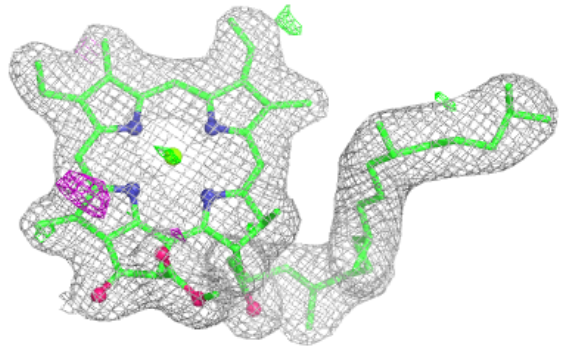
Electron density around CLA b 613:

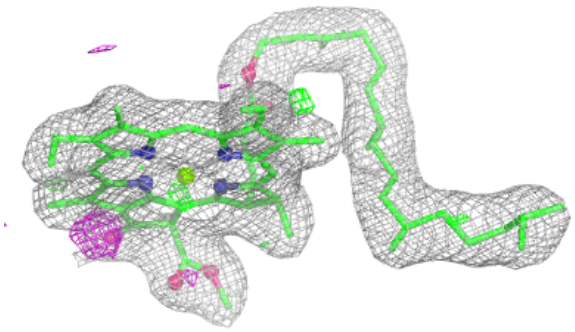
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

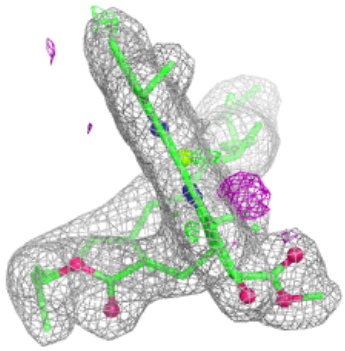


Electron density around CLA A 405 (A):

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

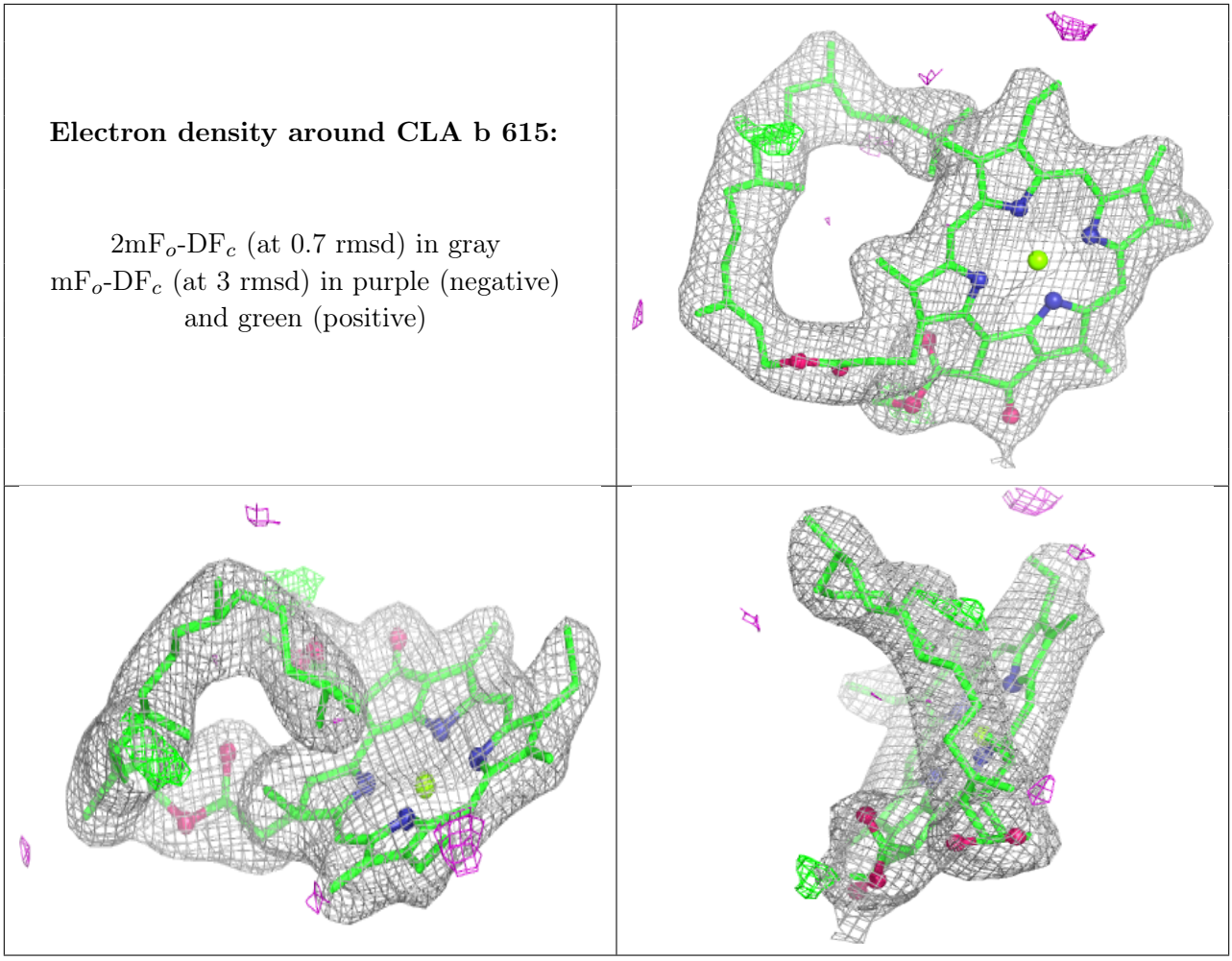






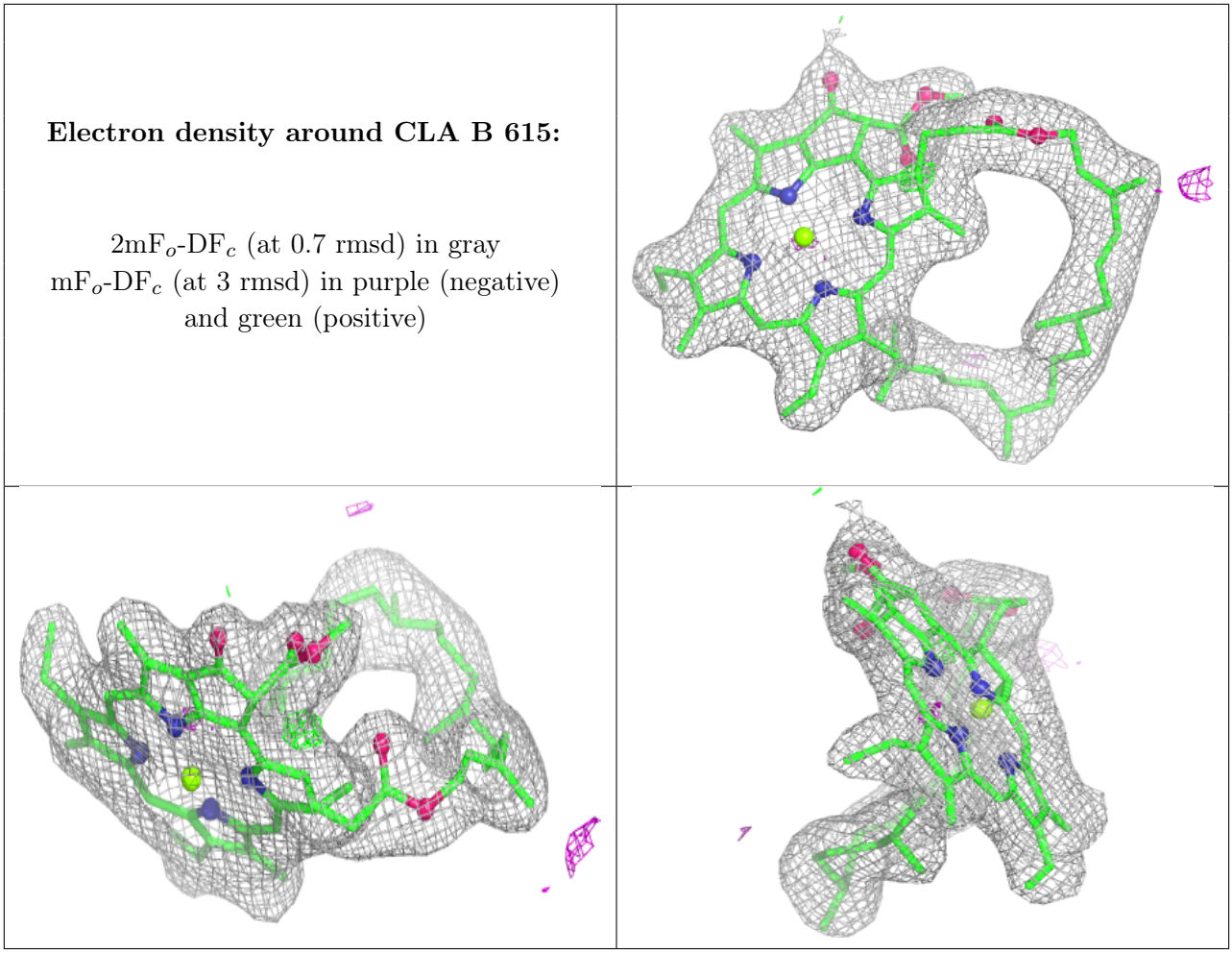
Electron density around CLA b 615:

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



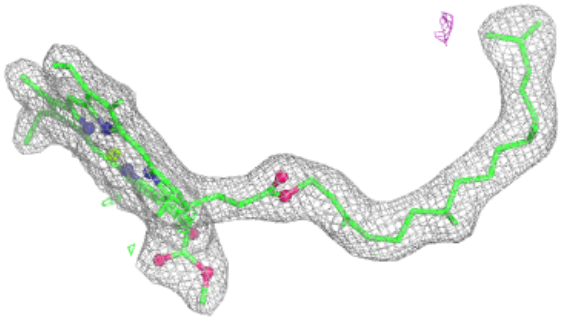
Electron density around CLA B 615:

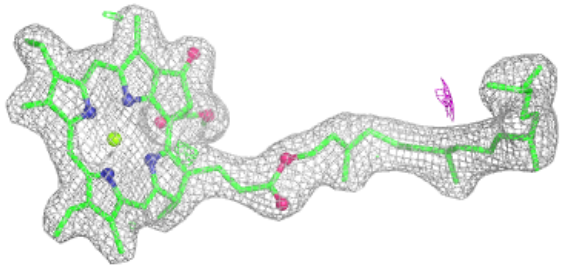
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

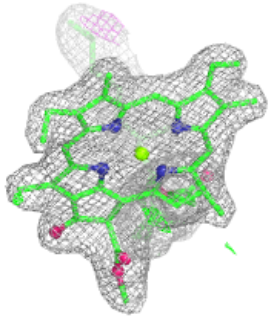


Electron density around CLA D 402 (A):

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

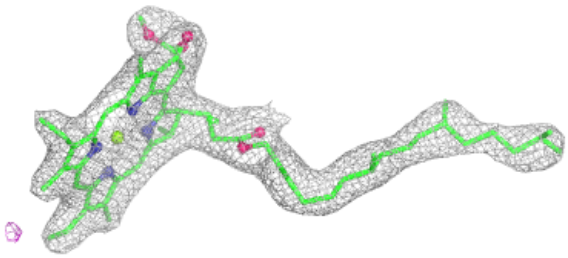


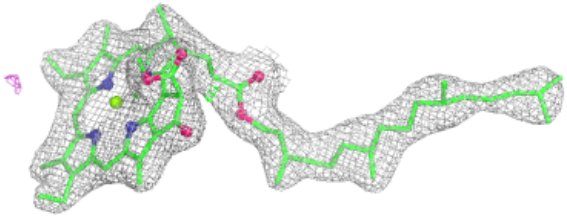


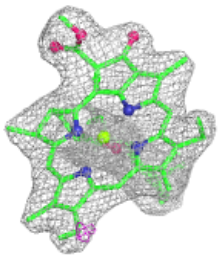


Electron density around CLA c 502:

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

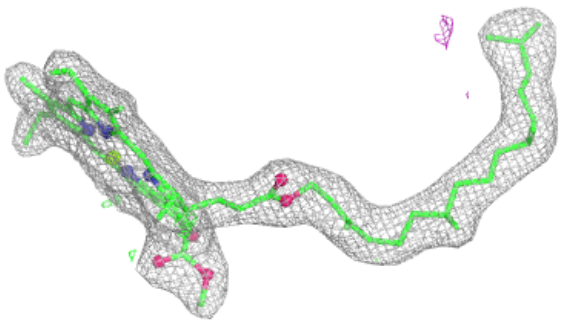


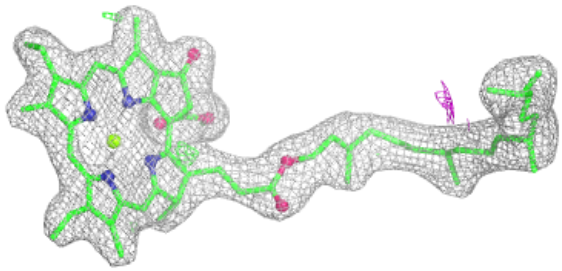


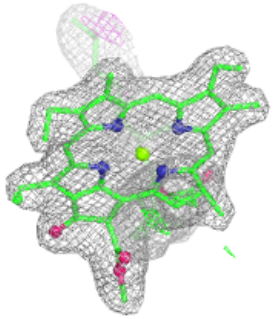


Electron density around CLA D 402 (B):

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

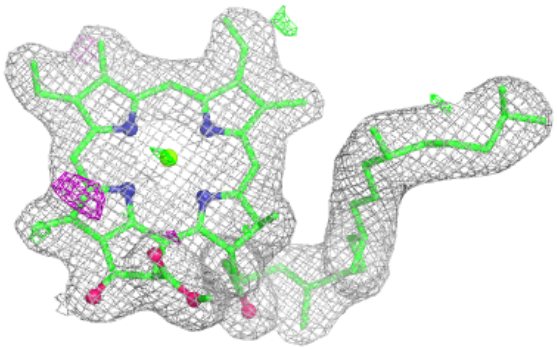


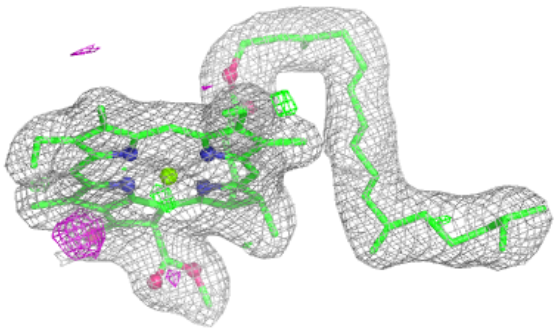


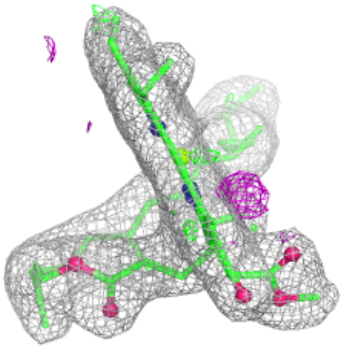


Electron density around CLA A 405 (B):

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

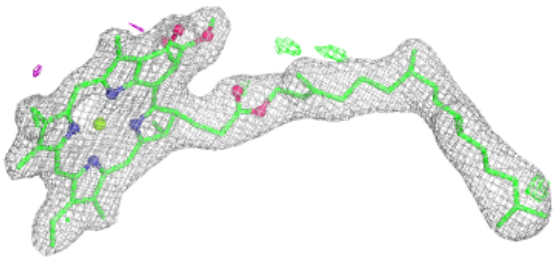


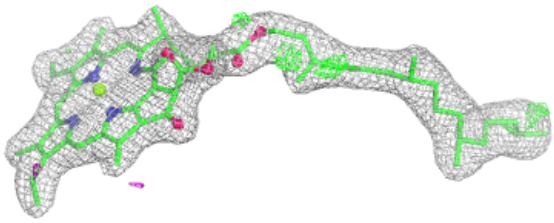


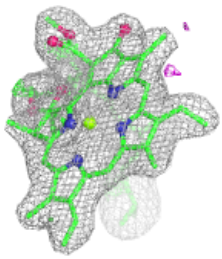


Electron density around CLA a 404 (A):

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

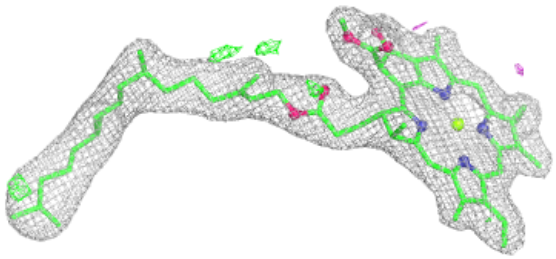


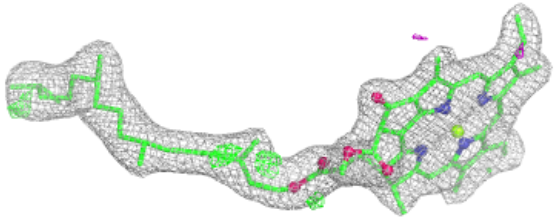


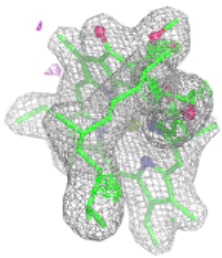


Electron density around CLA a 404 (B):

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

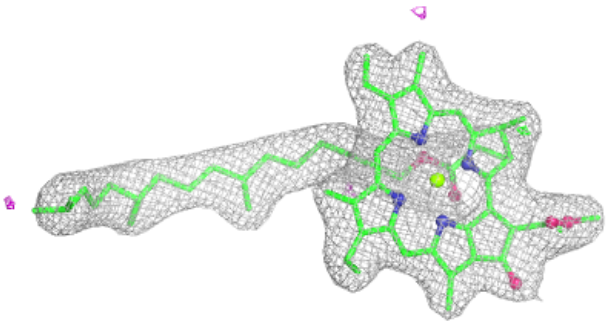


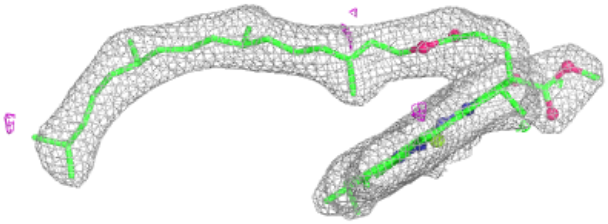




Electron density around CLA B 608:

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

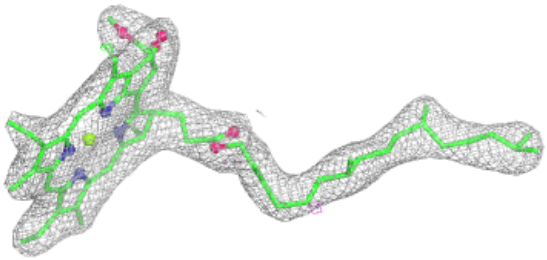


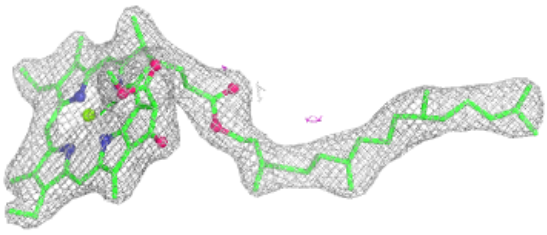


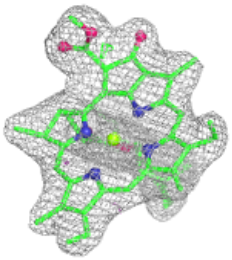


Electron density around CLA C 503:

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

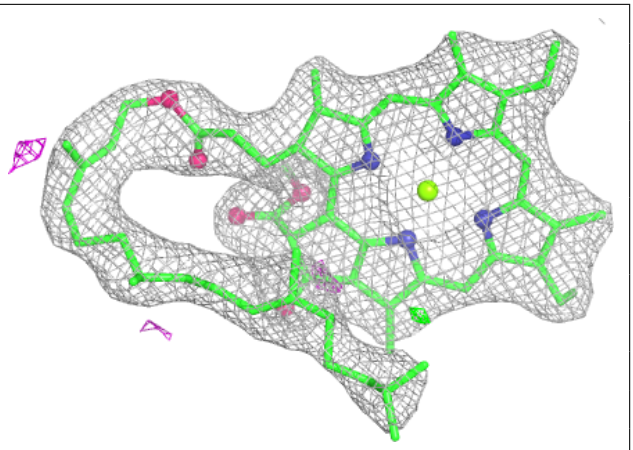


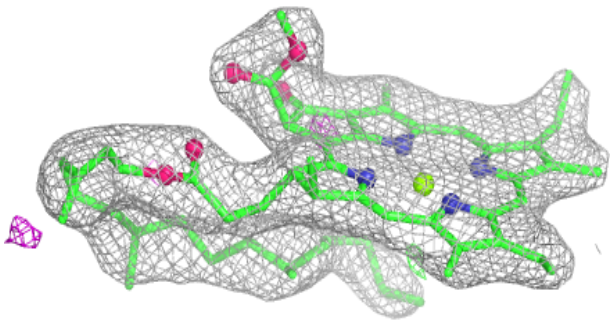


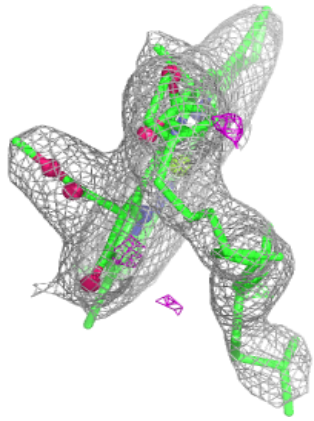


Electron density around CLA c 509:

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

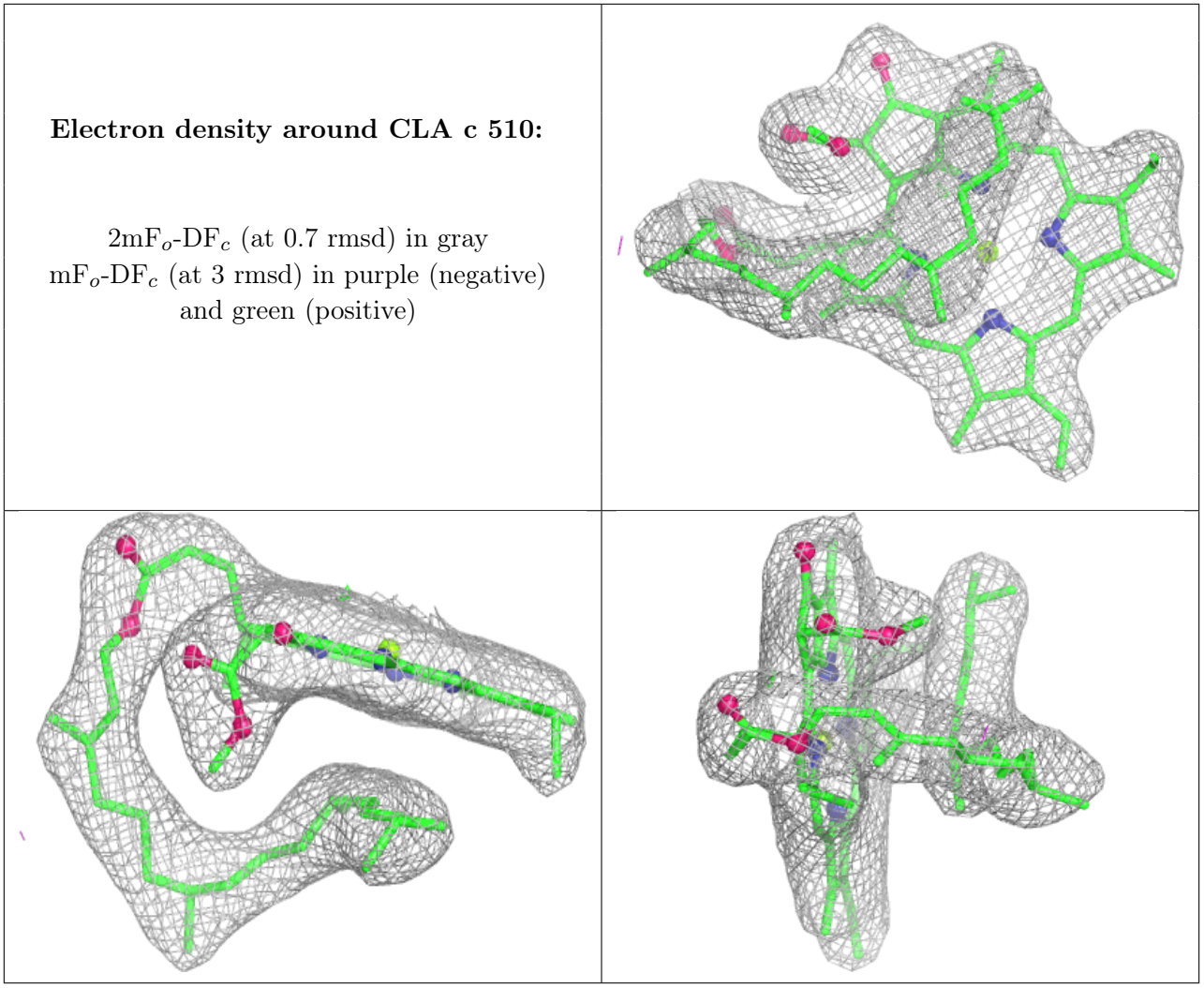






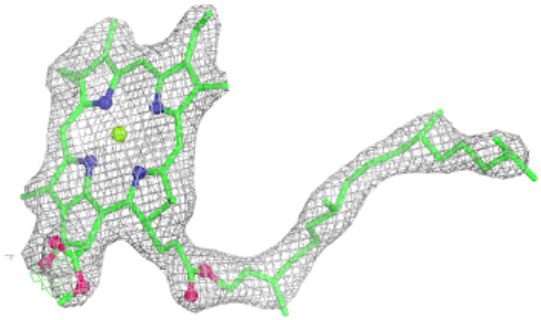
Electron density around CLA c 510:

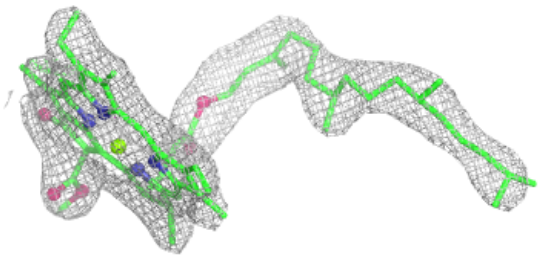
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

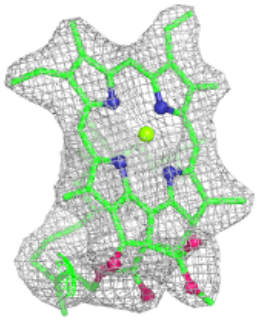


Electron density around CLA c 511:

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

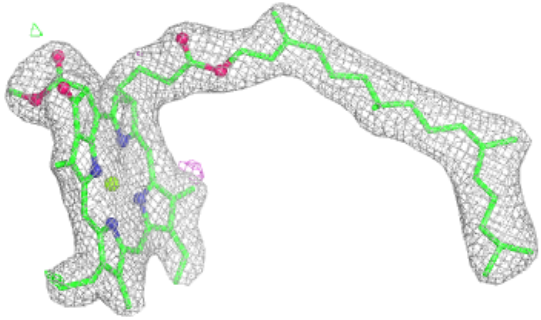


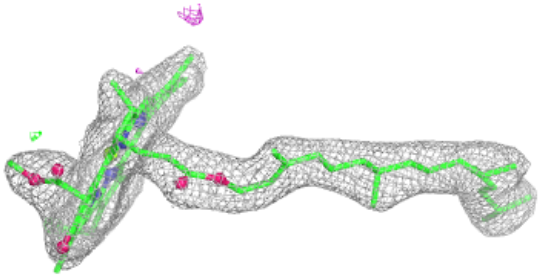


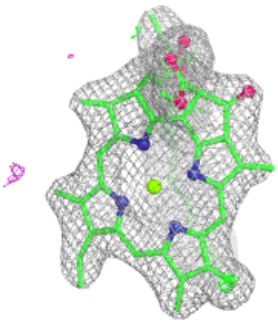


Electron density around CLA B 609:

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

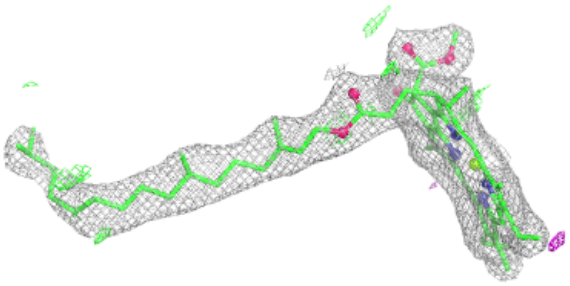


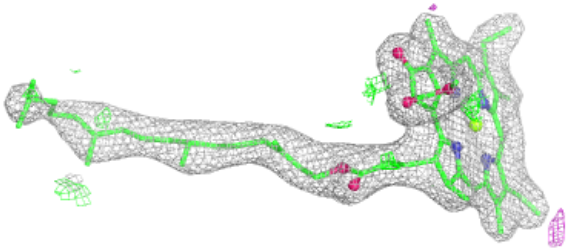


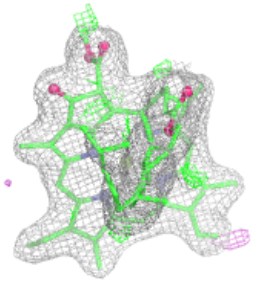


Electron density around CLA B 604:

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

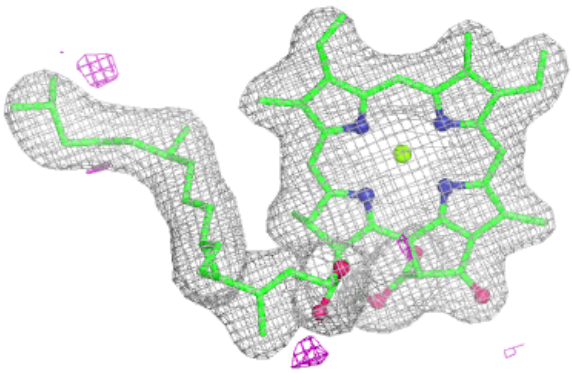


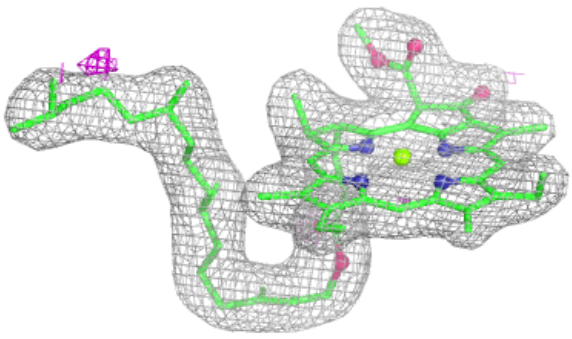


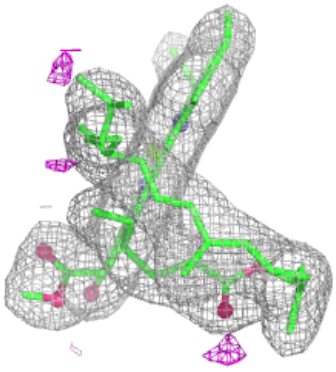


Electron density around CLA d 402 (A):

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

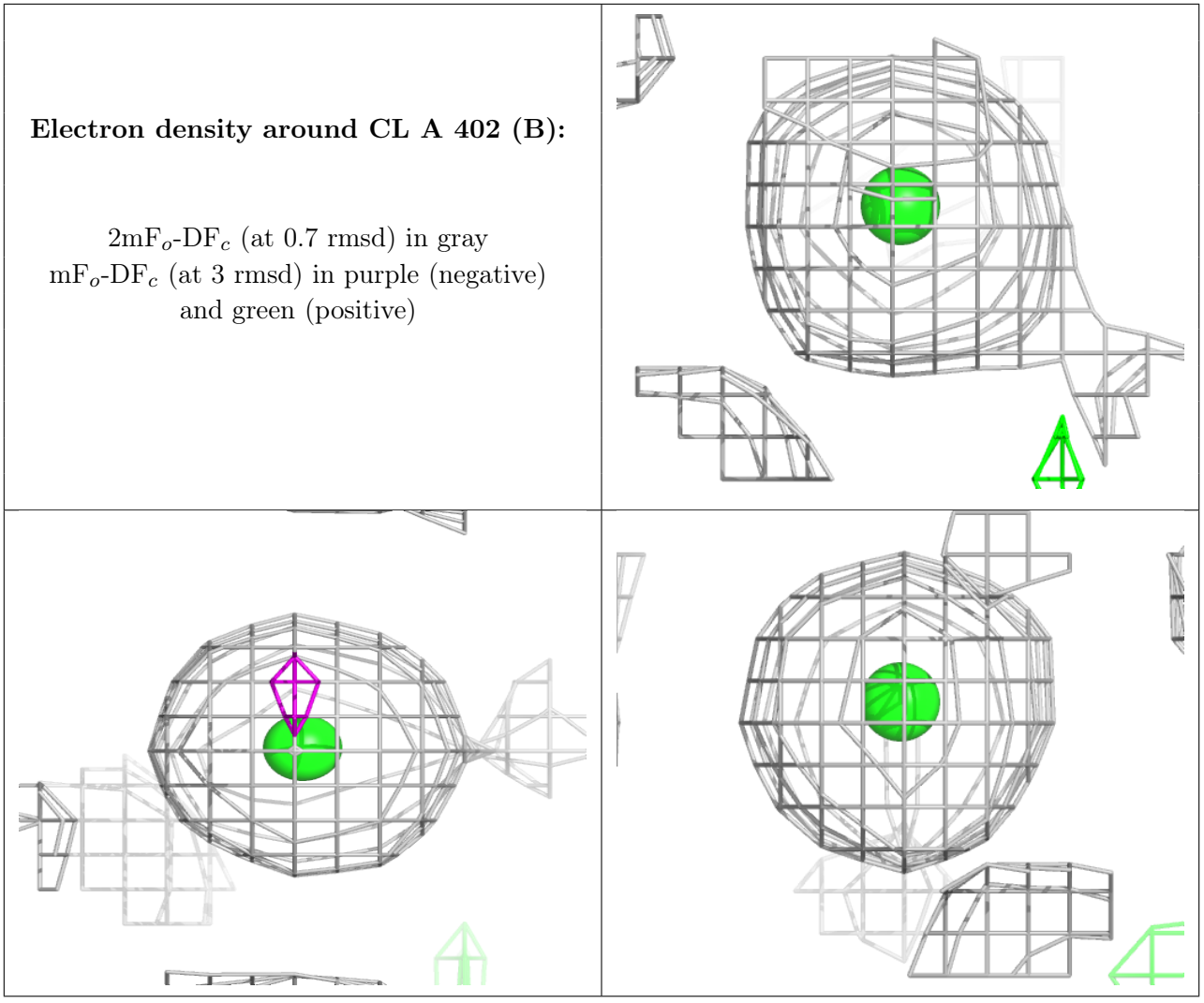






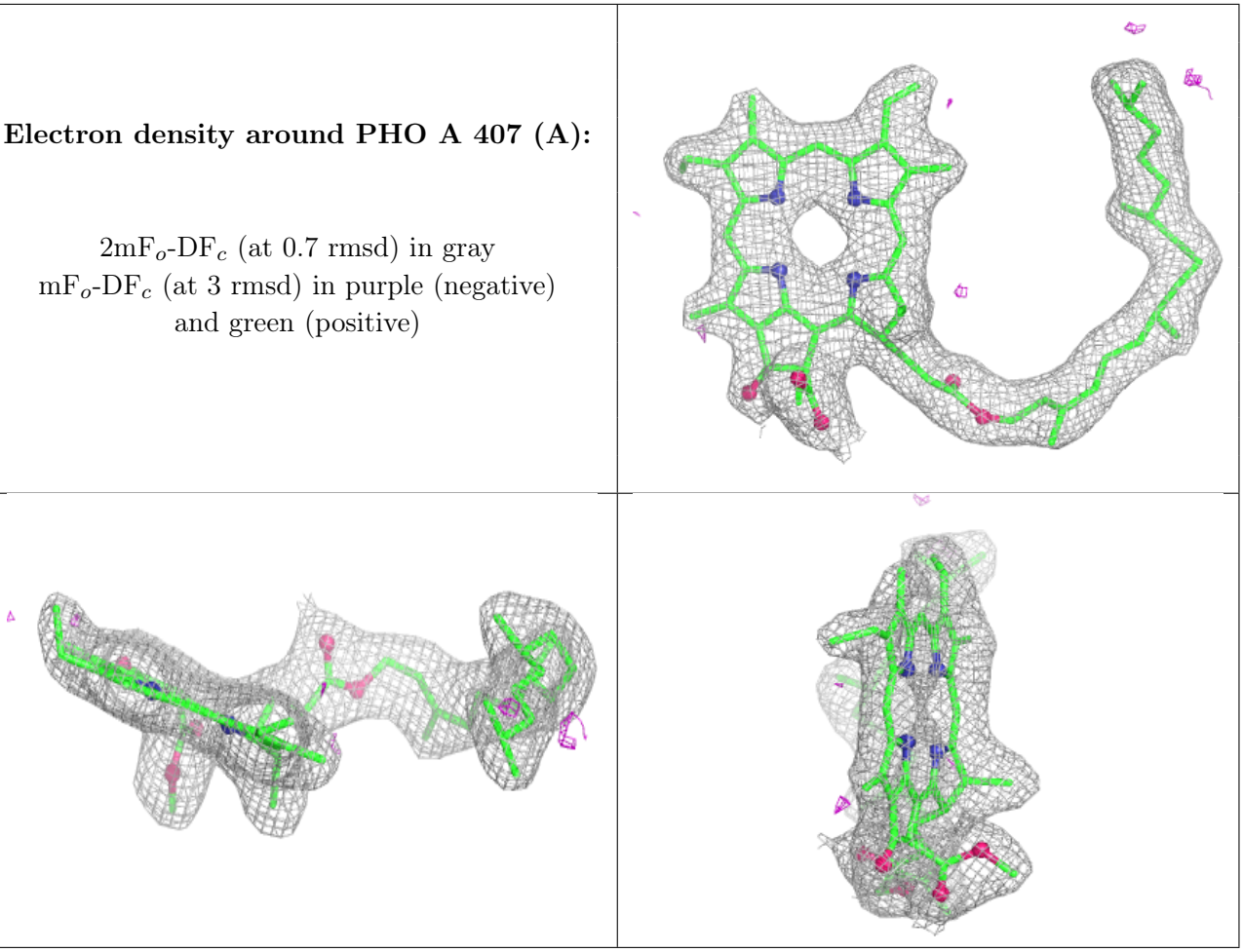
Electron density around CL A 402 (B):

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



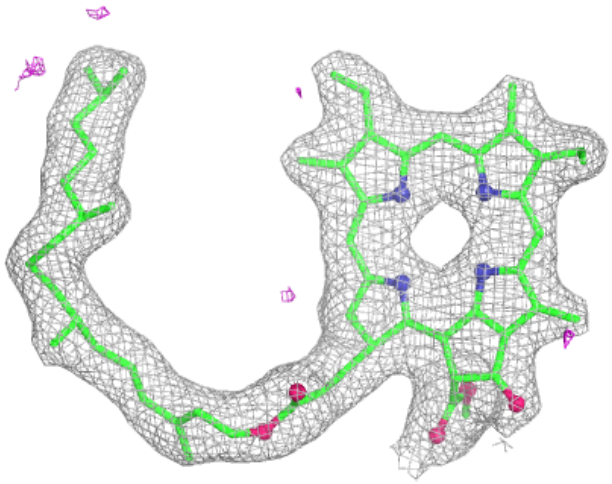
Electron density around PHO A 407 (A):

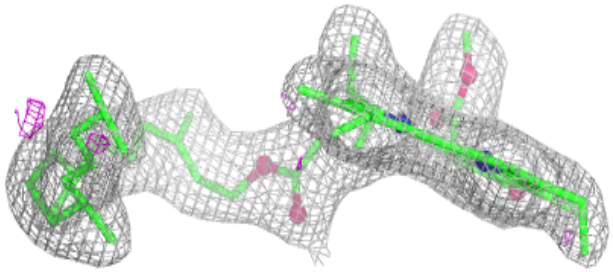
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

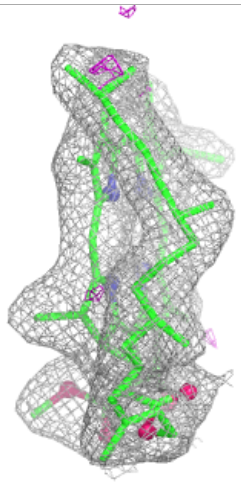


Electron density around PHO A 407 (B):

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

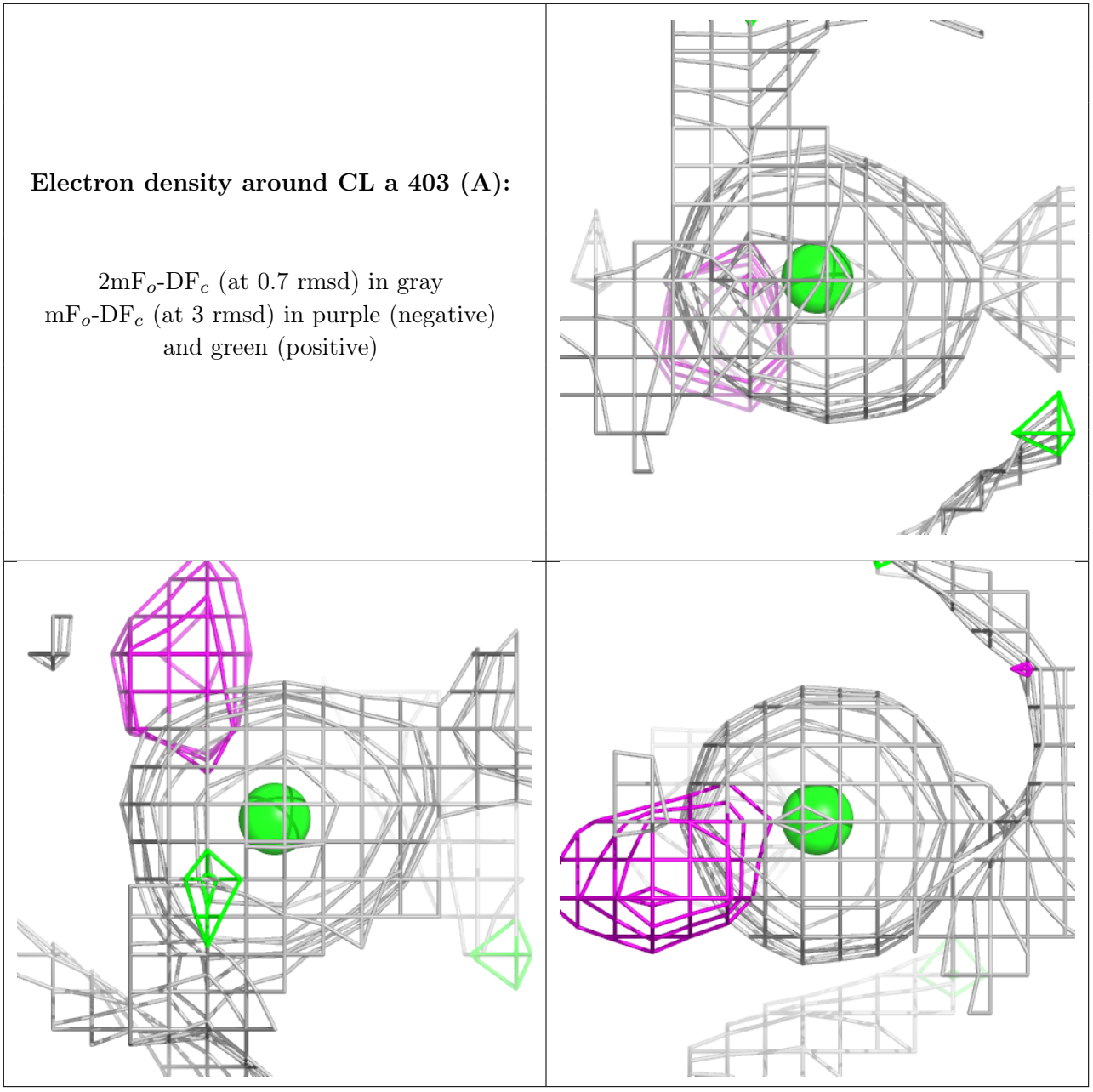






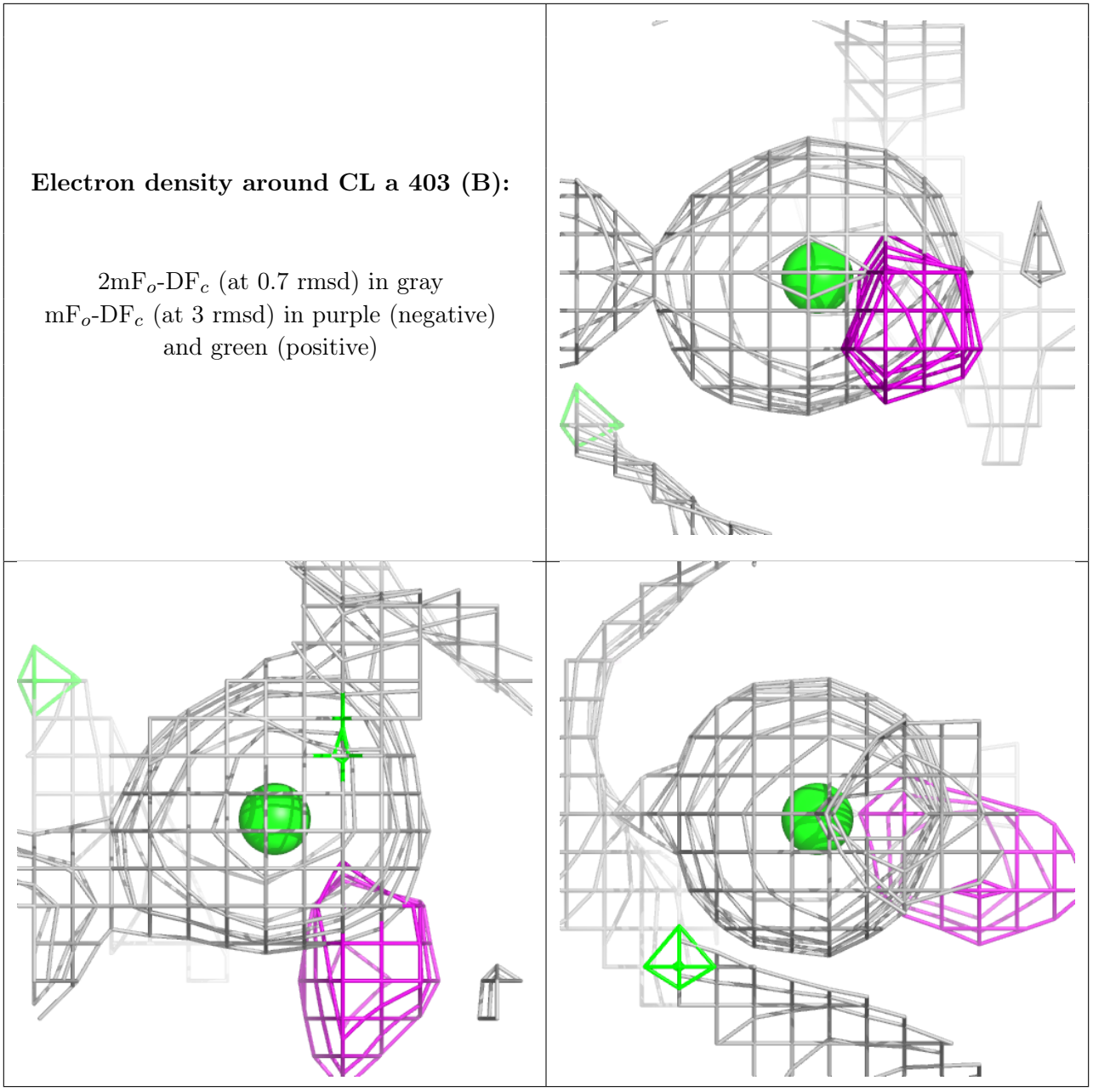
Electron density around CL a 403 (A):

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



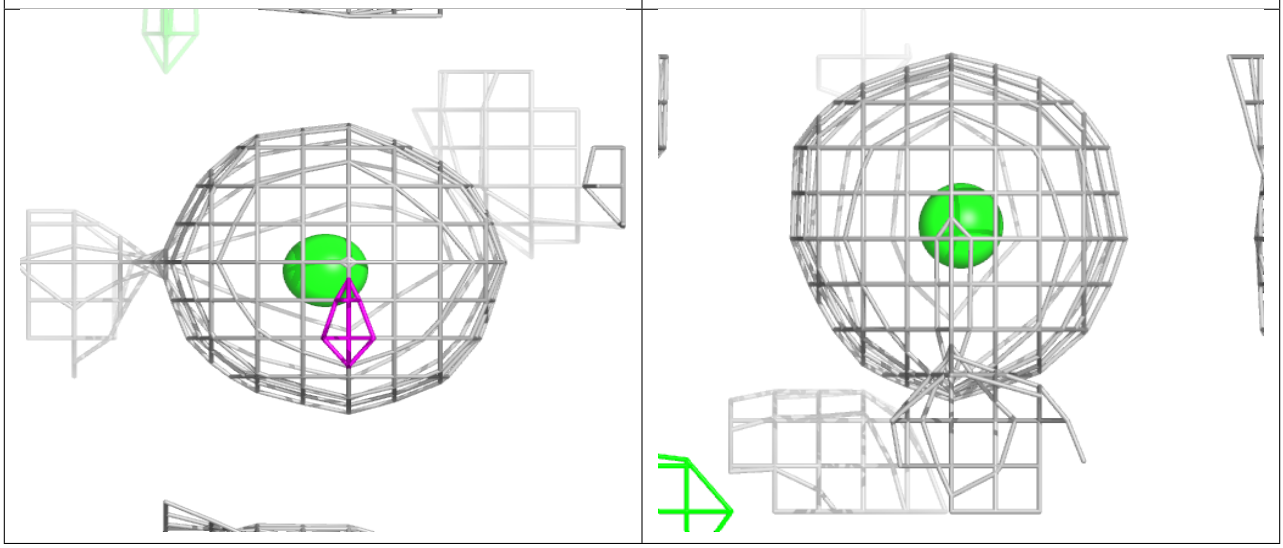
Electron density around CL a 403 (B):

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



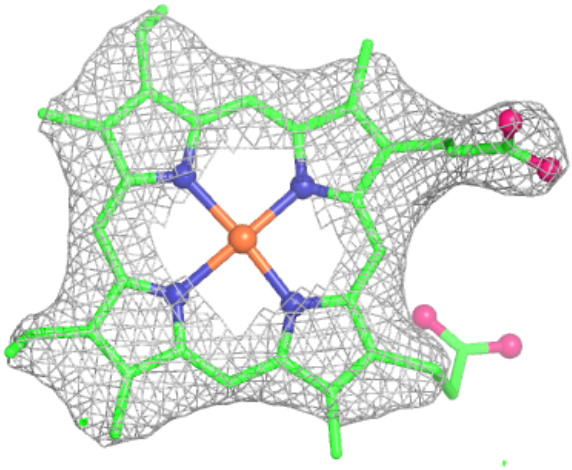
Electron density around CL A 402 (A):

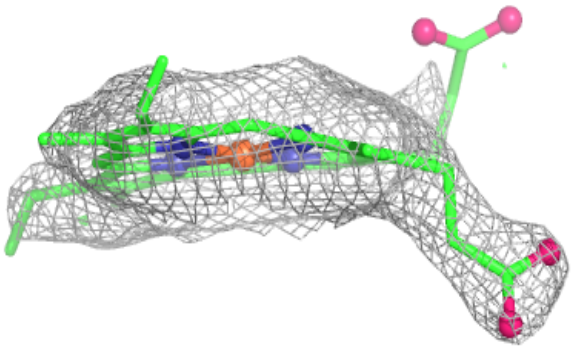
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

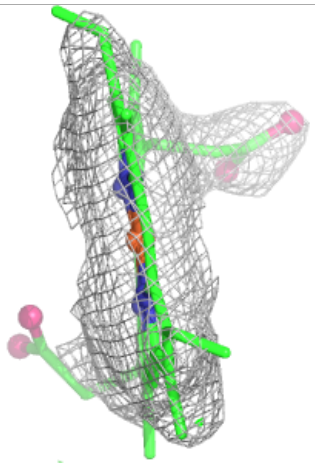


Electron density around HEM f 101:

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

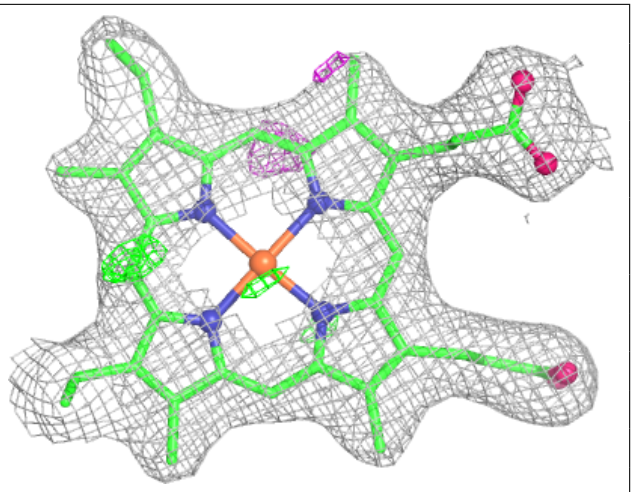


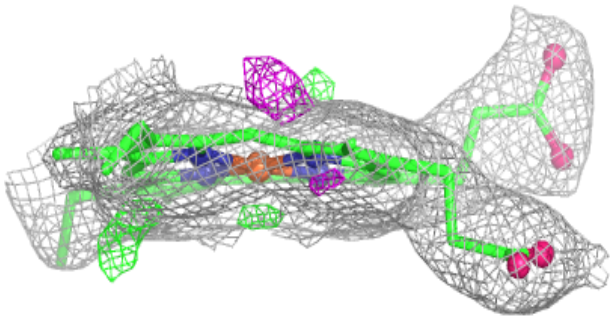




Electron density around HEC V 201:

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

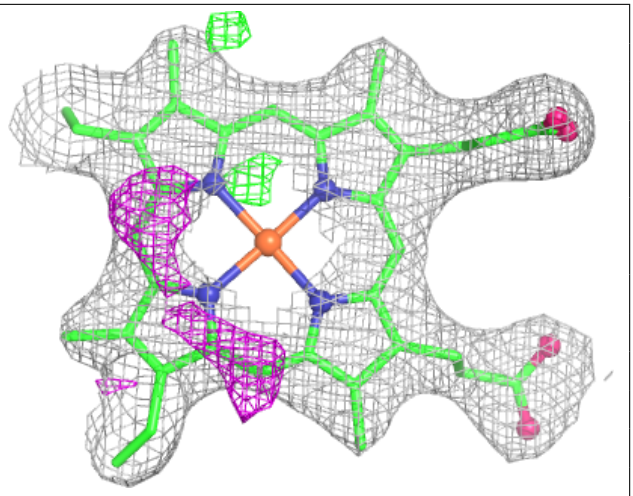


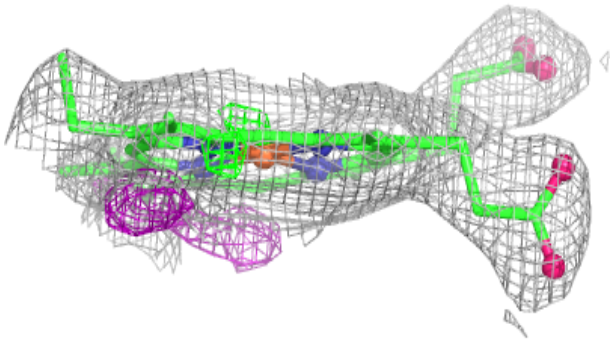


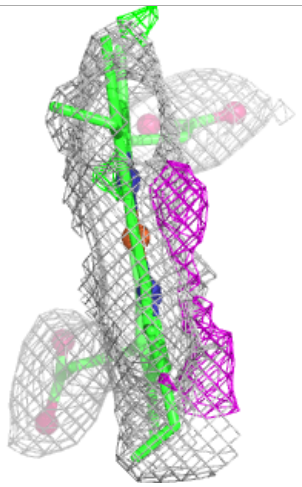


Electron density around HEC v 201:

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

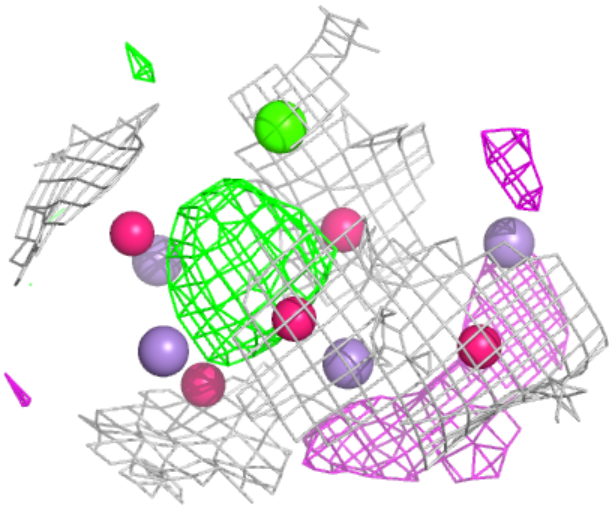


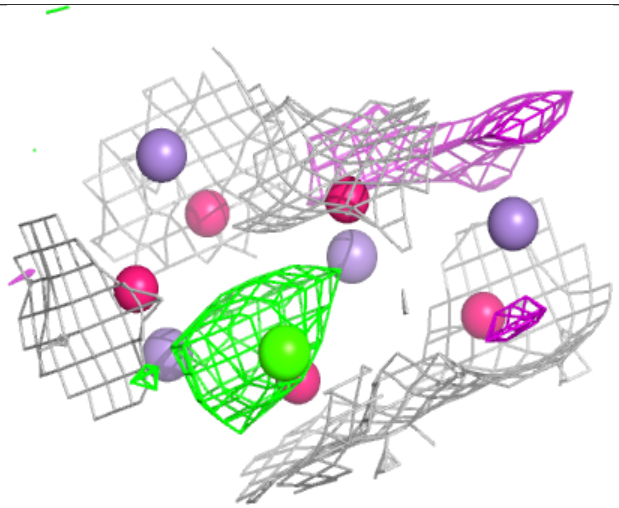


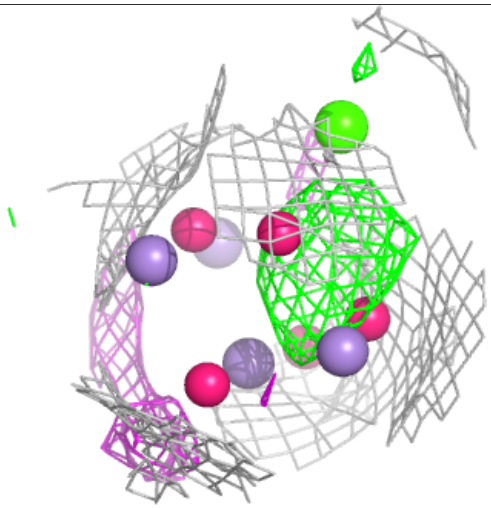


Electron density around OEX A 413 (A):

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

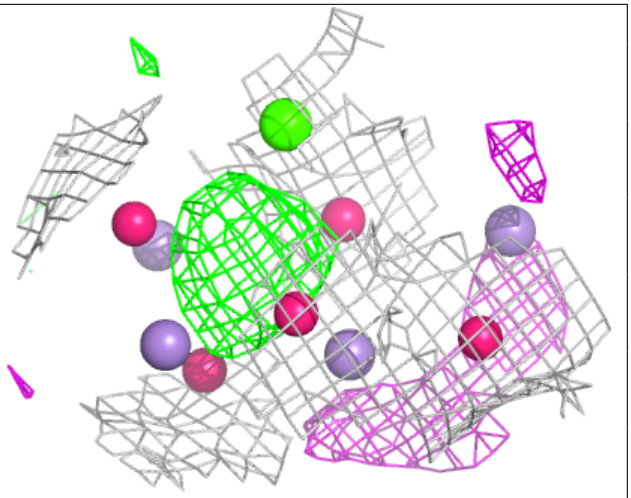


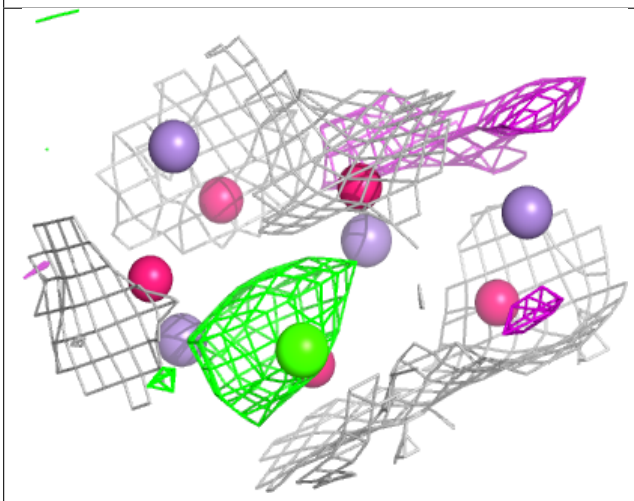


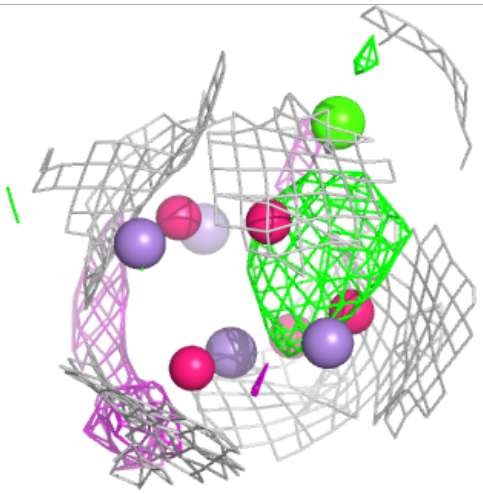


Electron density around OEX A 413 (B):

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

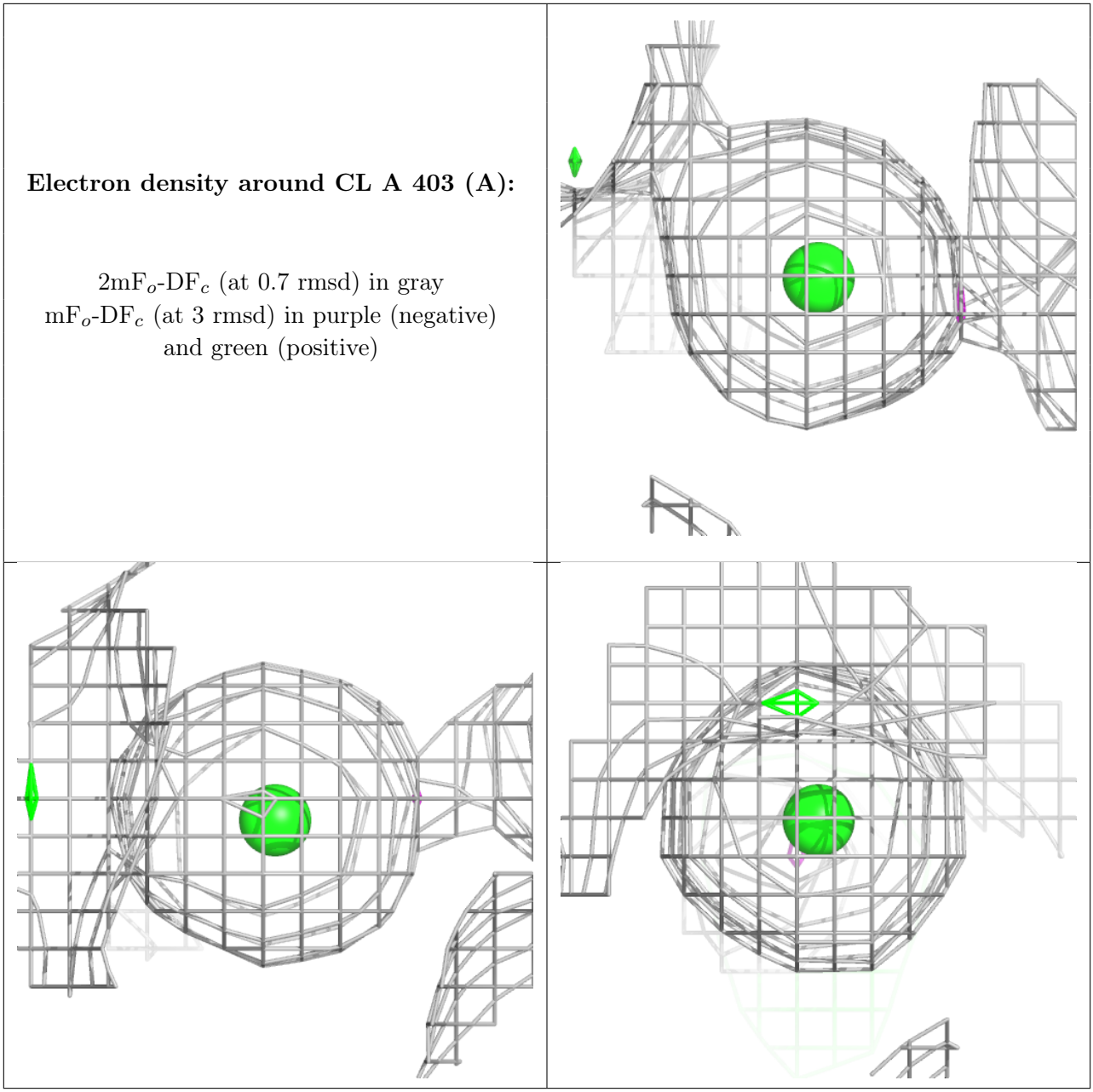






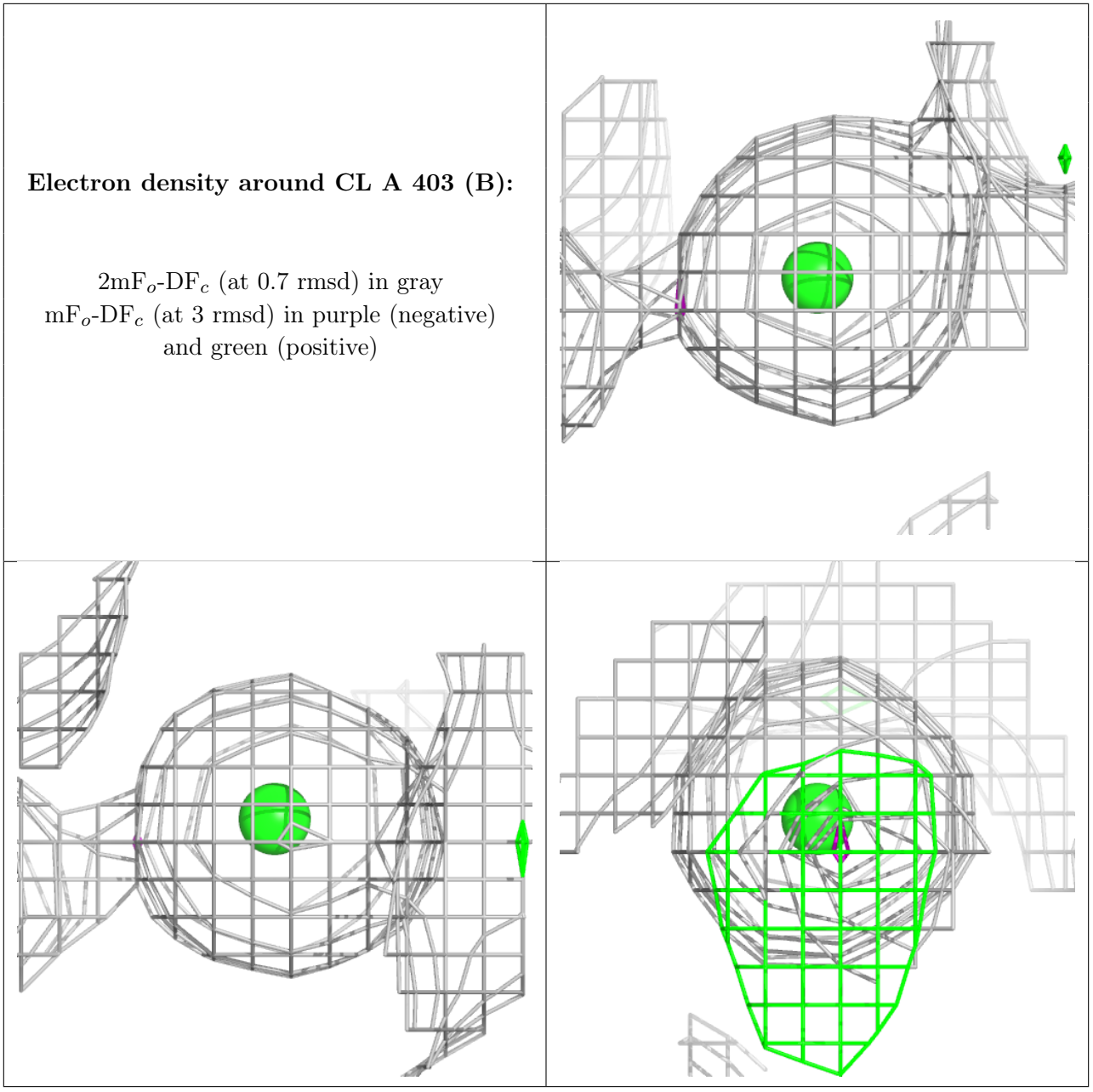
Electron density around CL A 403 (A):

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



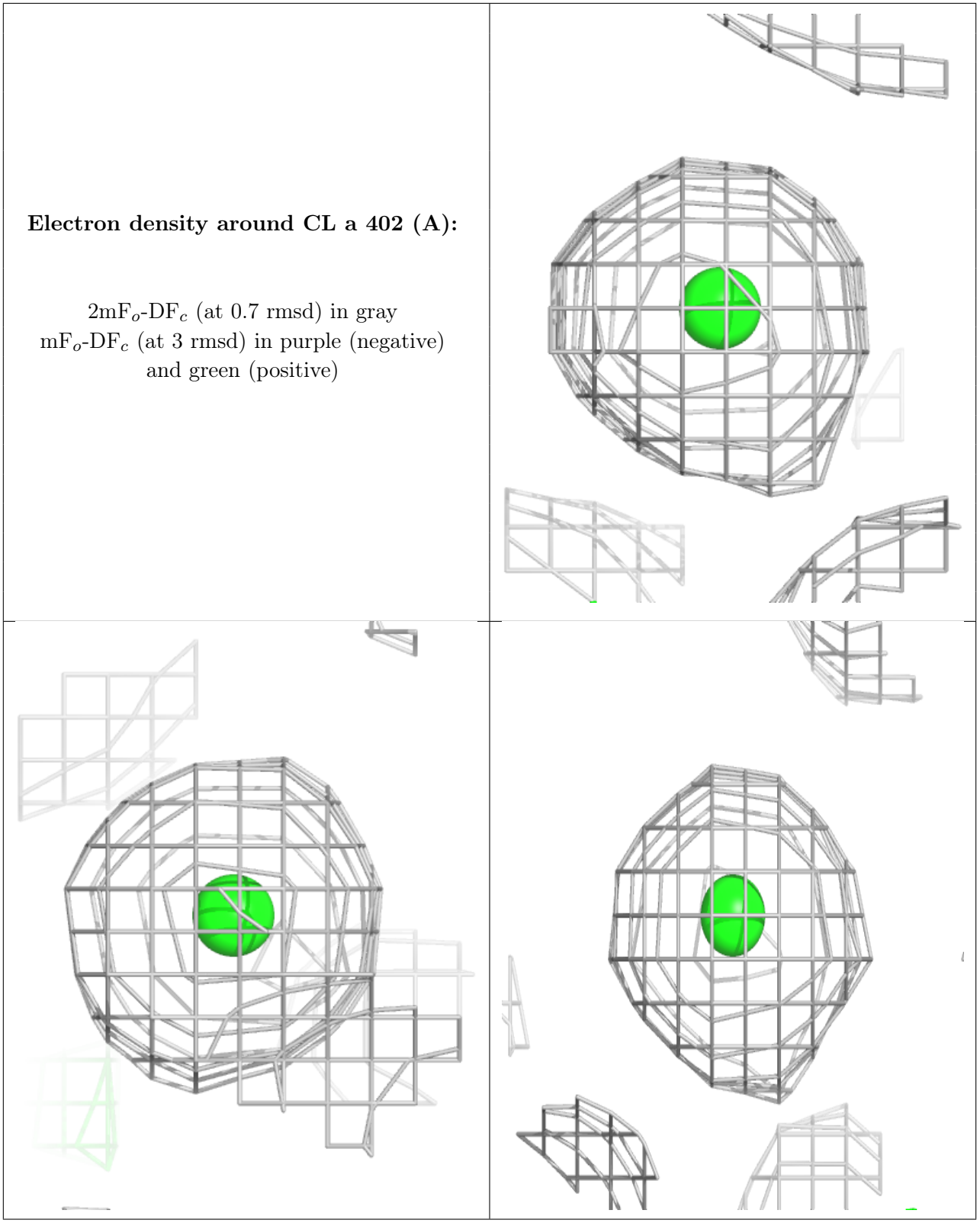
Electron density around CL A 403 (B):

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



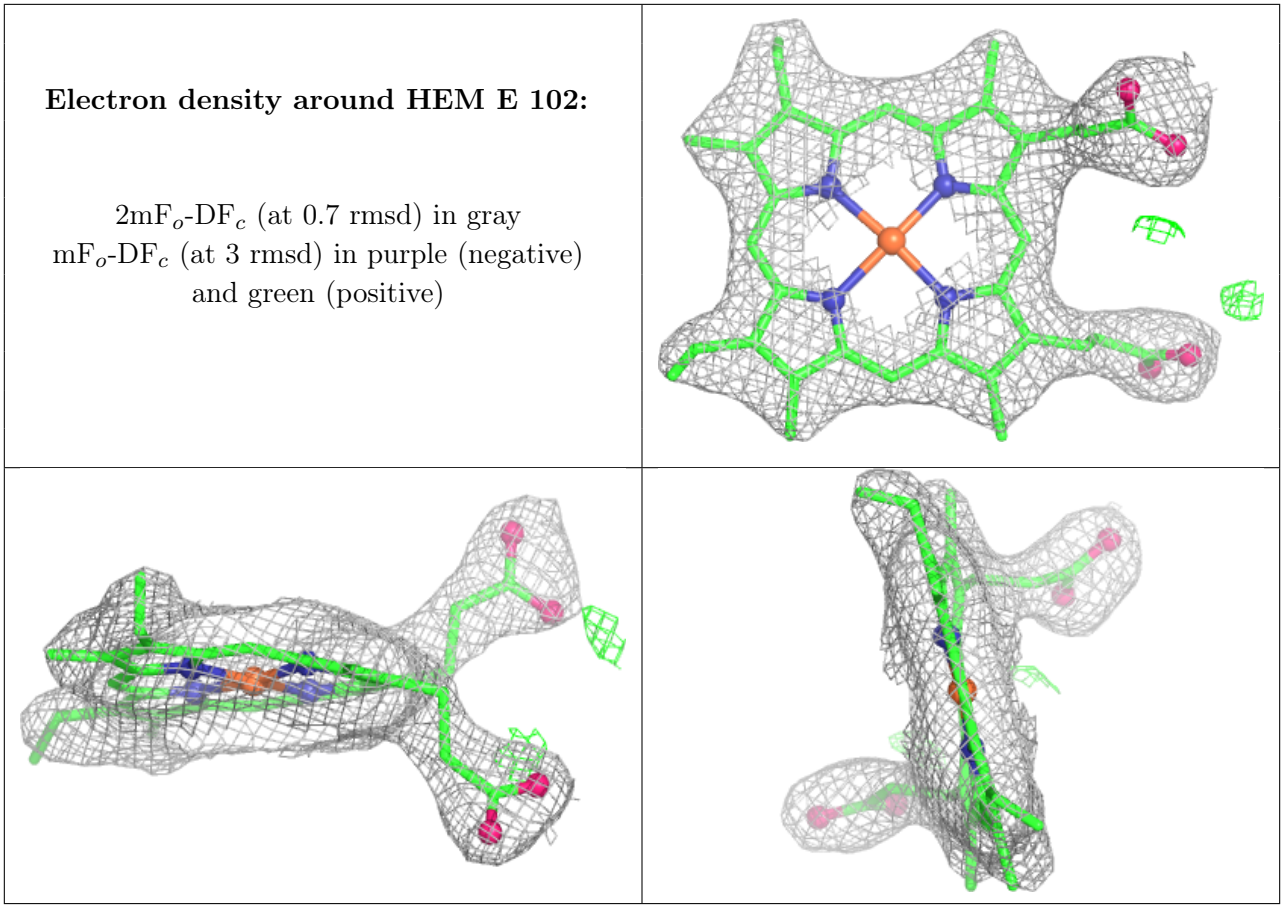
Electron density around CL a 402 (A):

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



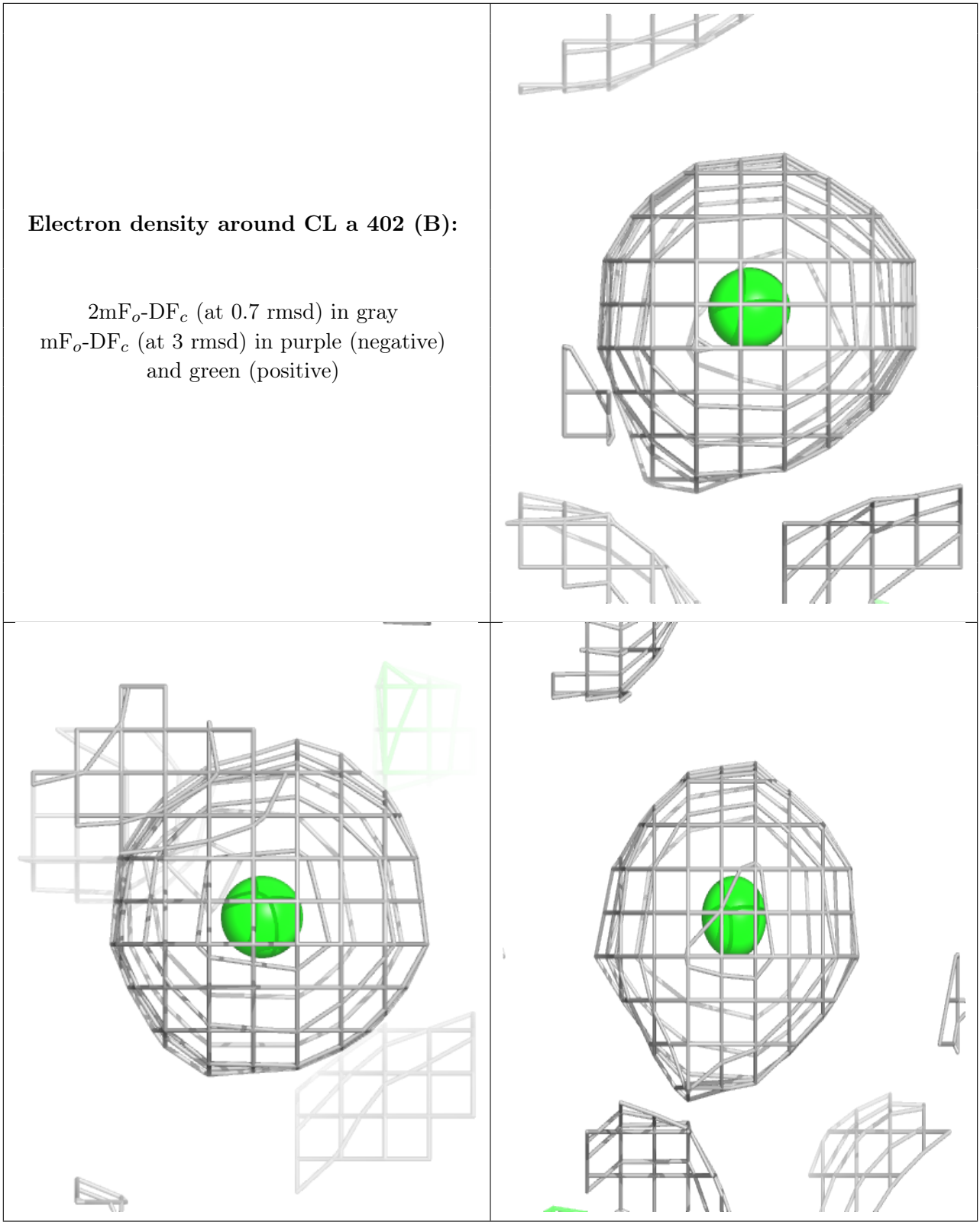
Electron density around HEM E 102:

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



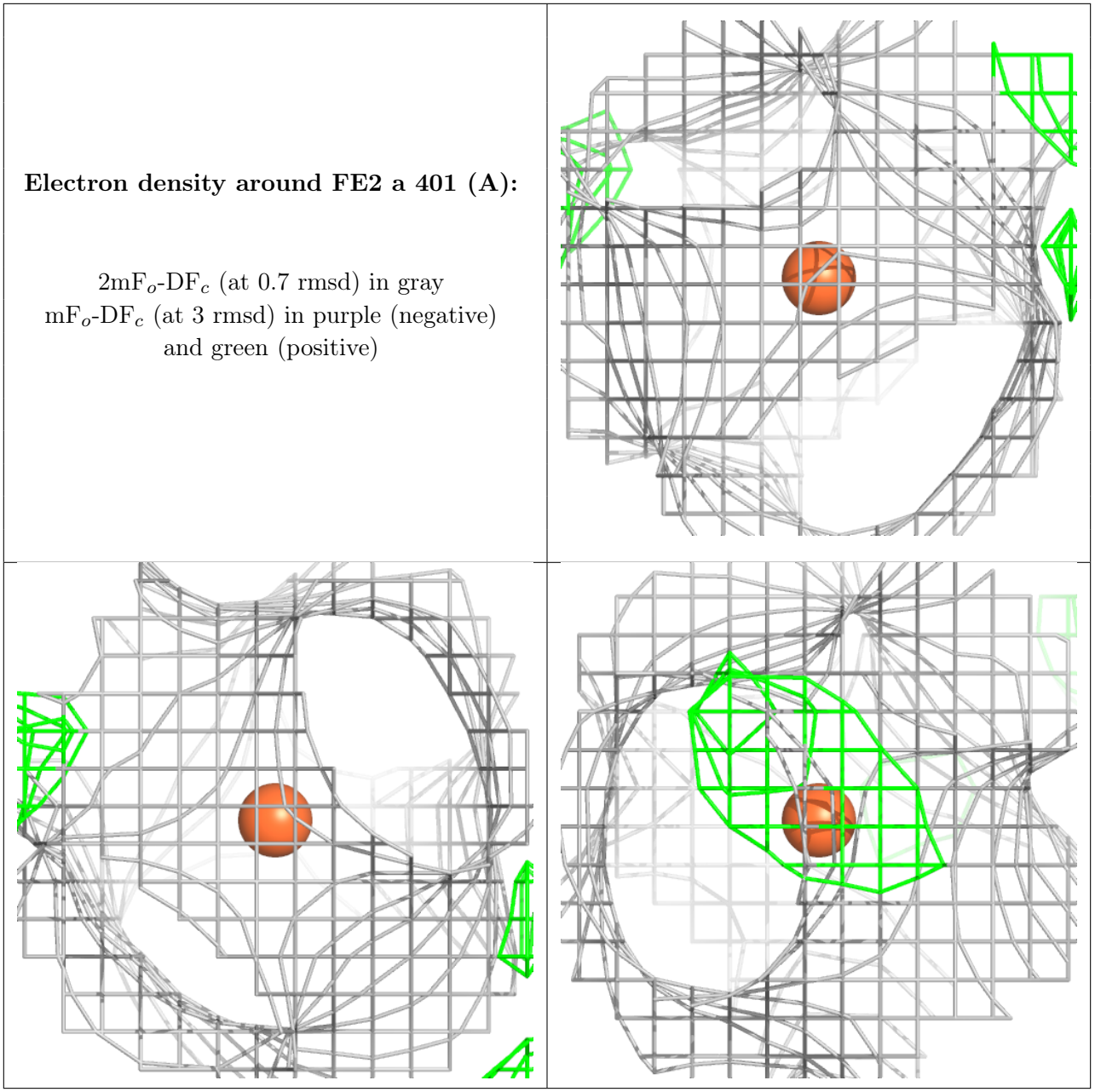
Electron density around CL a 402 (B):

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



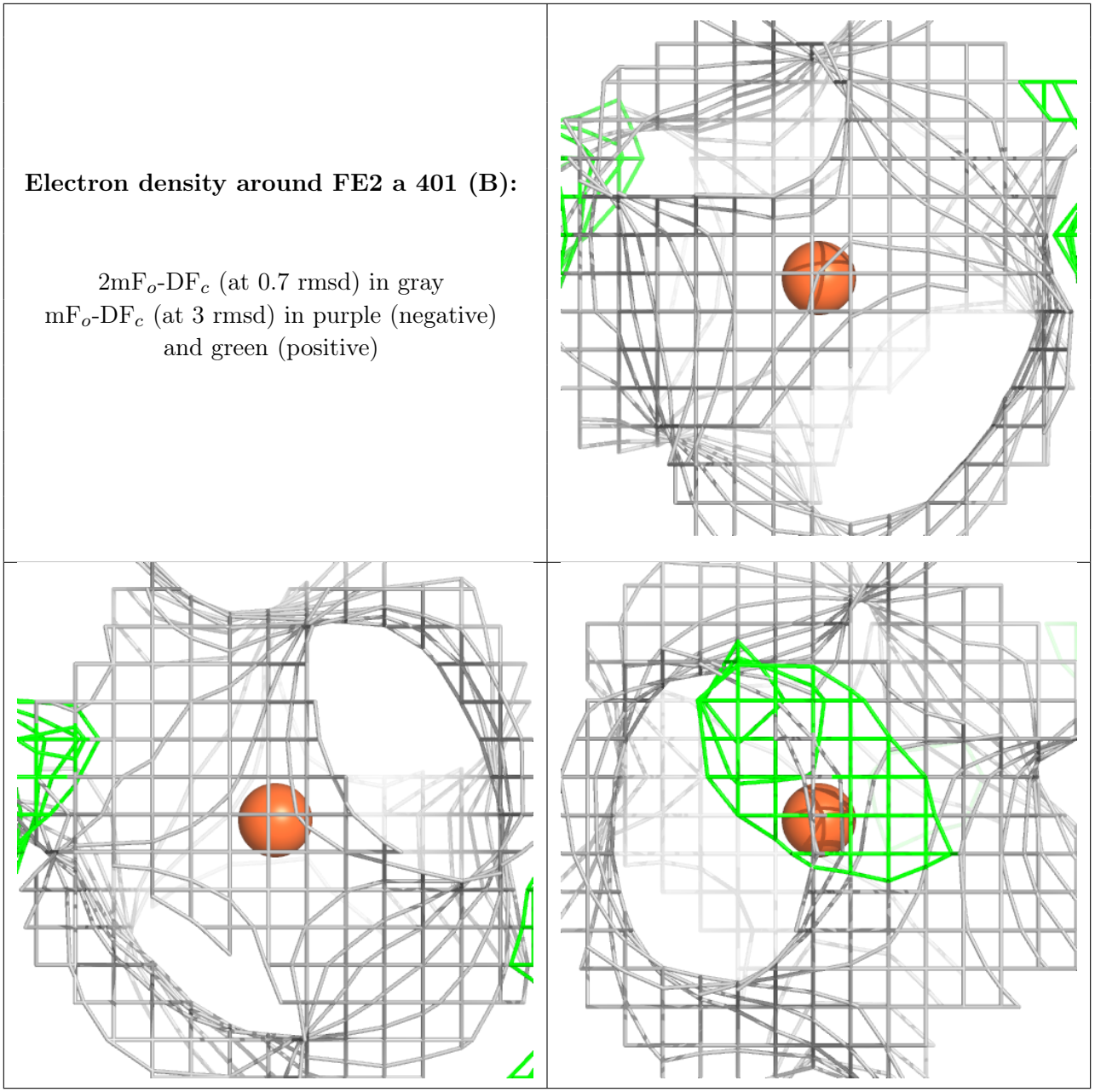
Electron density around FE2 a 401 (A):

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



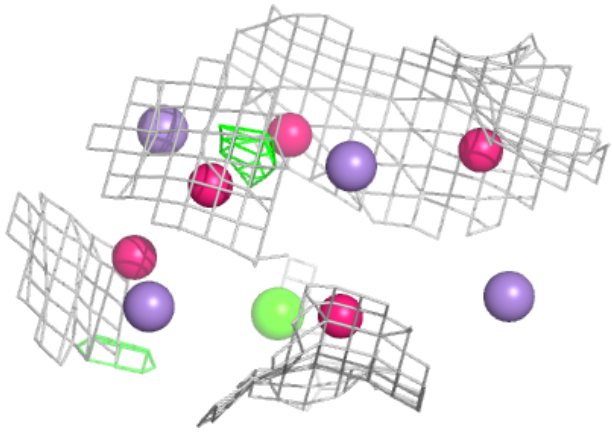
Electron density around FE2 a 401 (B):

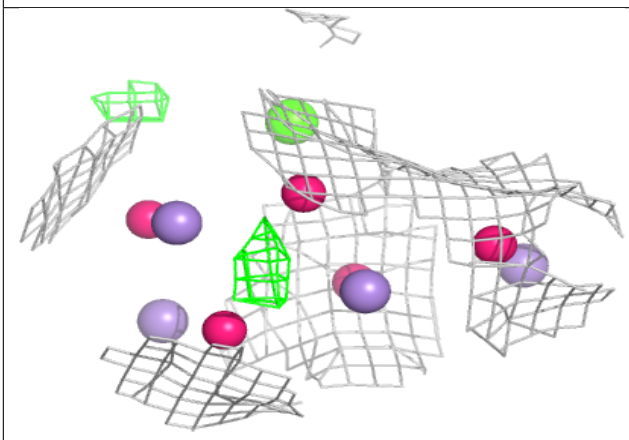
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

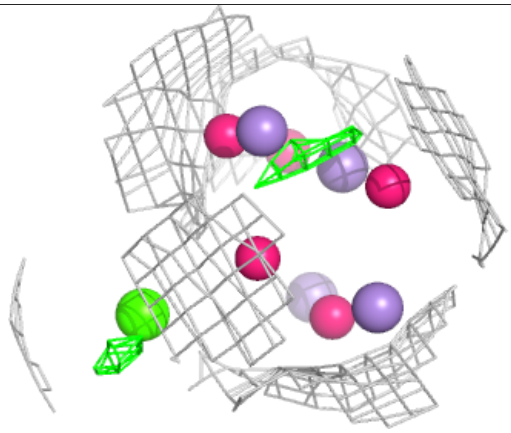


Electron density around OEX a 412 (B):

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

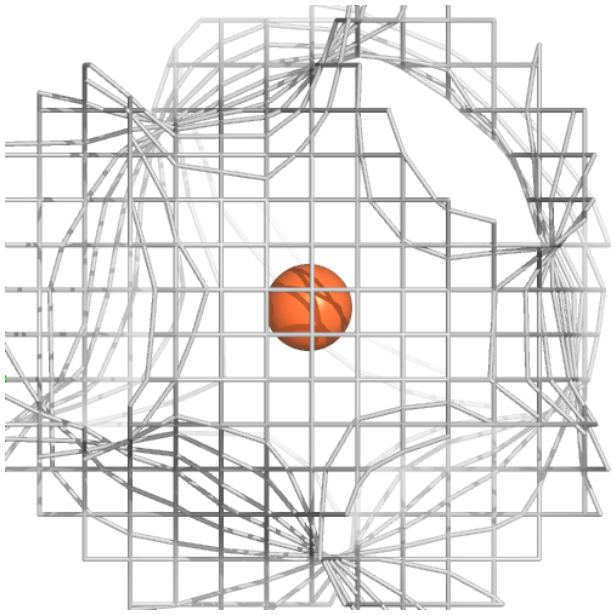


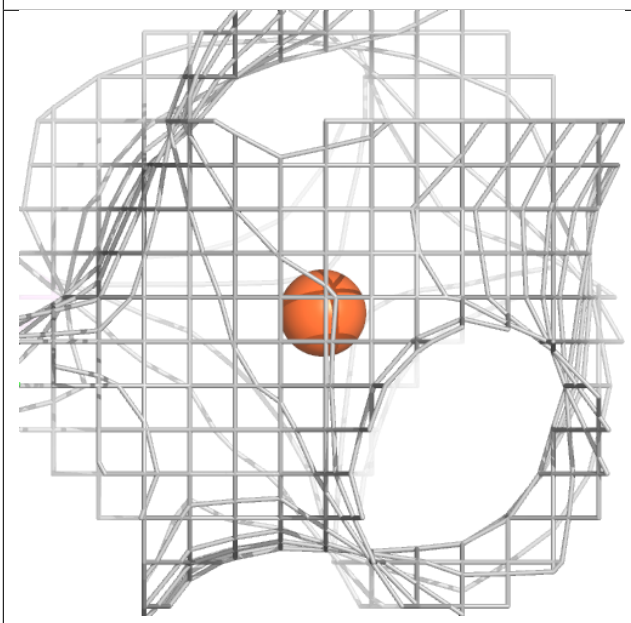


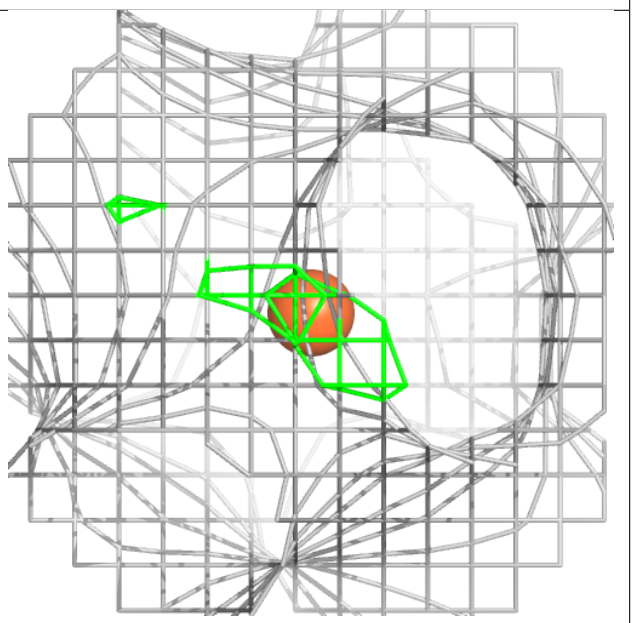


Electron density around FE2 A 401 (A):

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

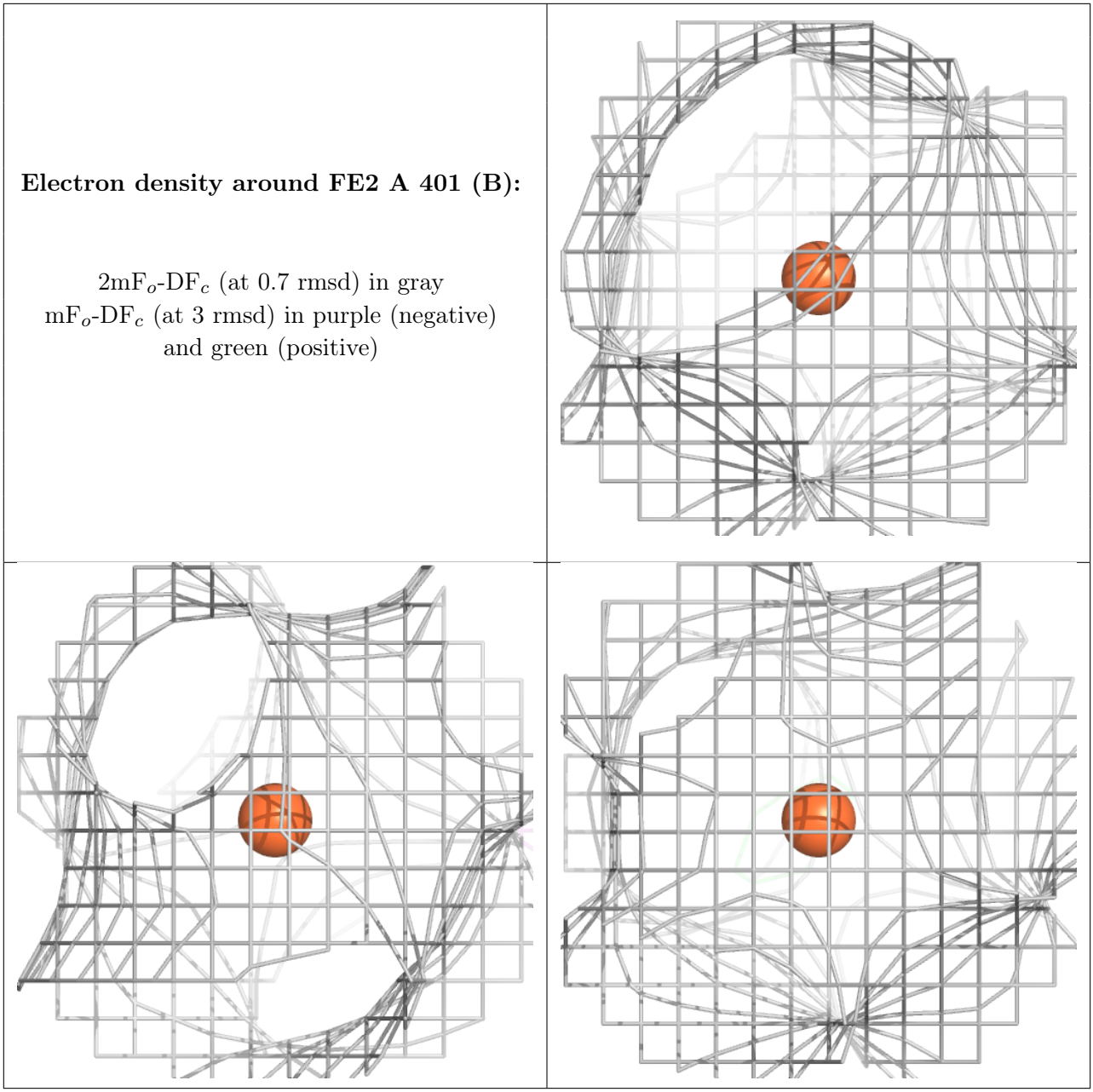






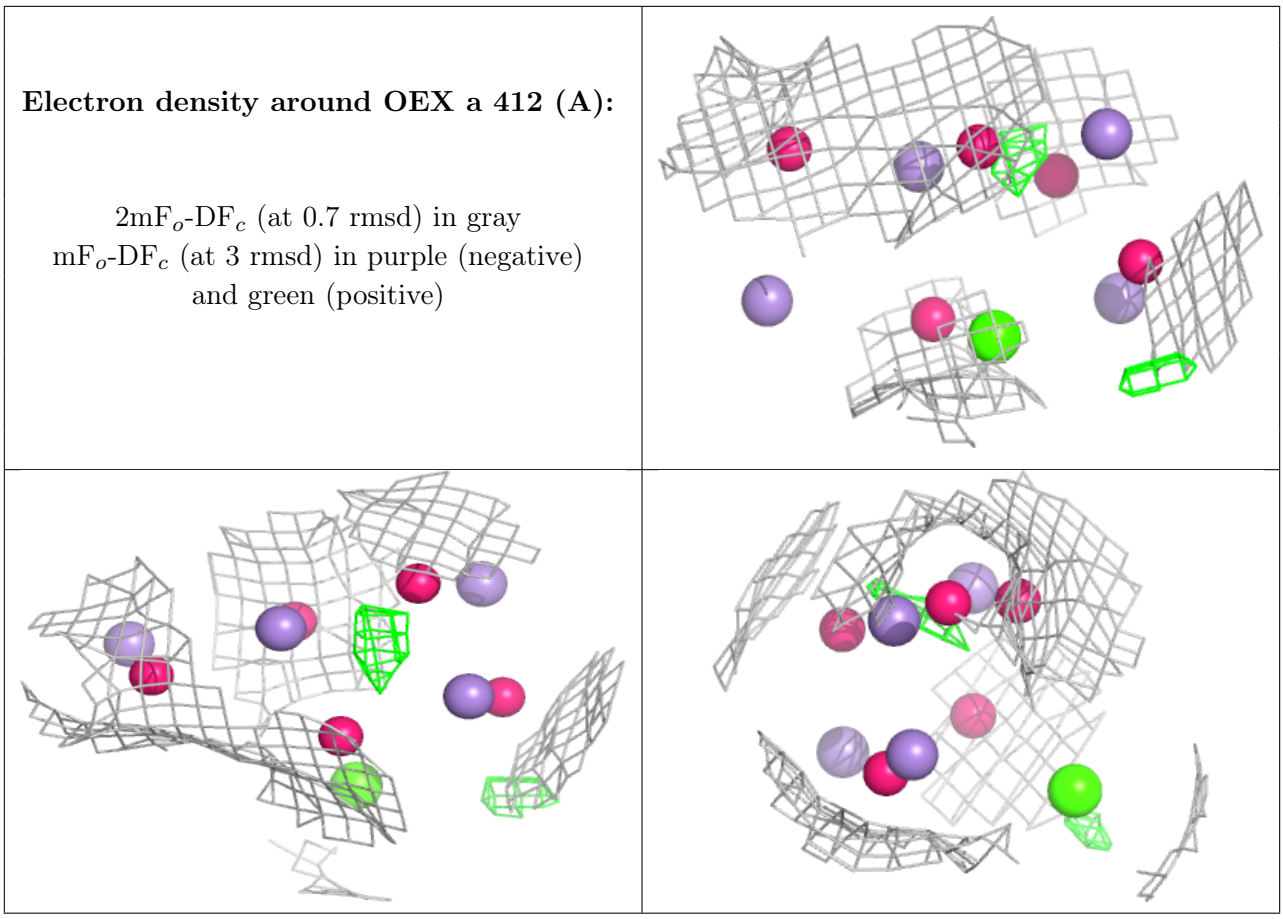
Electron density around FE2 A 401 (B):

$2mF_o$-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.