Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 08:54 PM JST

PDB ID	:	8IR7 / pdb_00008ir7
Title	:	XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 200-nanosecond delay
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.25 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:

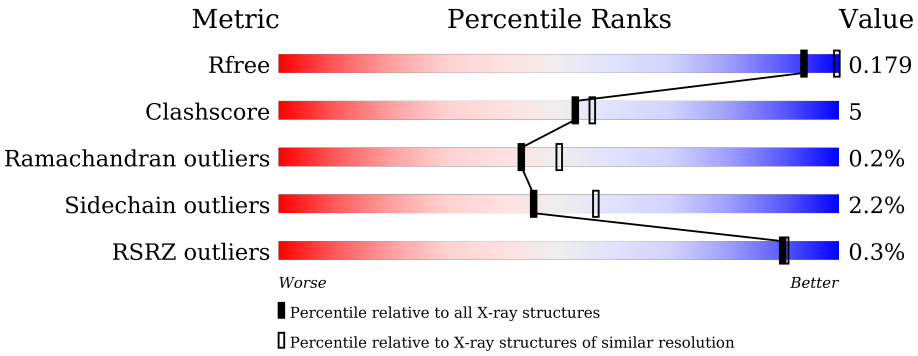
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	90% 7% .
1	a	344	87% 10% .
2	B	505	93% 7%
2	b	505	91% 9% .
3	C	455	91% 7% .
3	c	455	92% 7% .

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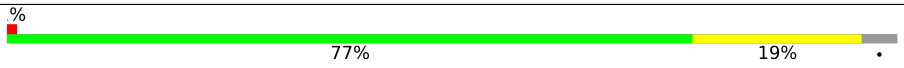
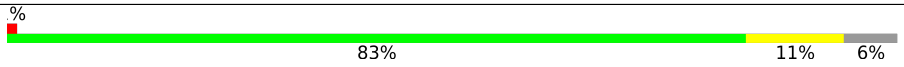
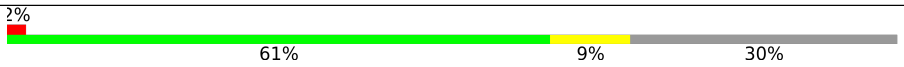
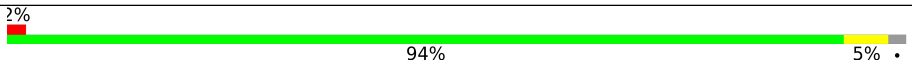
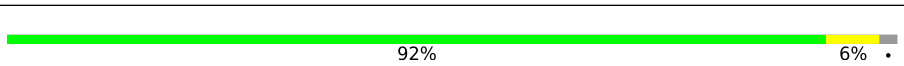
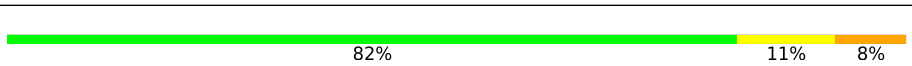
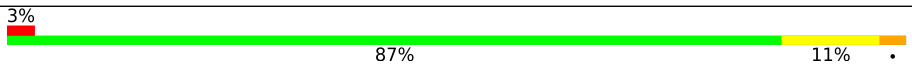
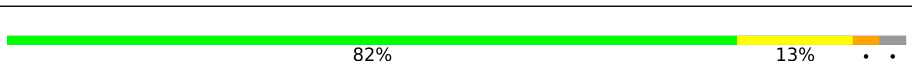
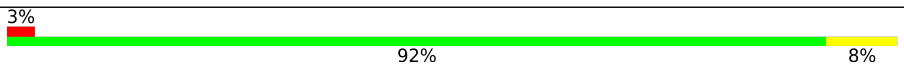
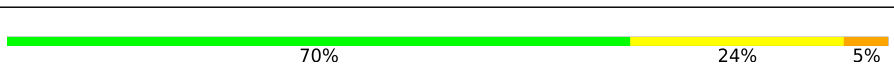
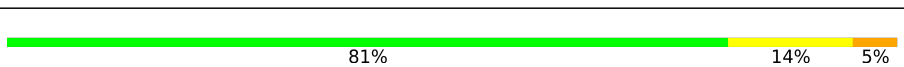
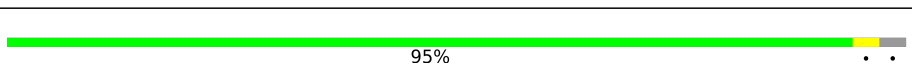
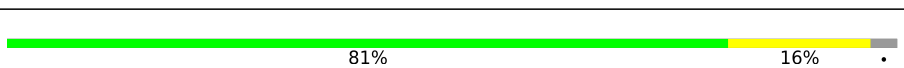
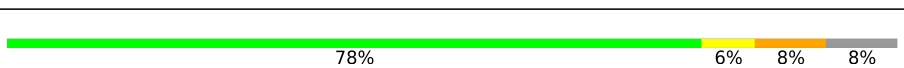
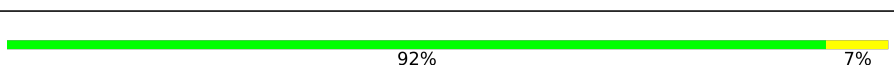
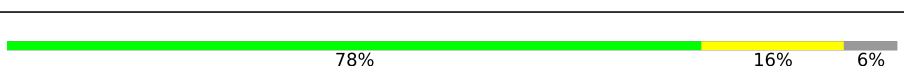
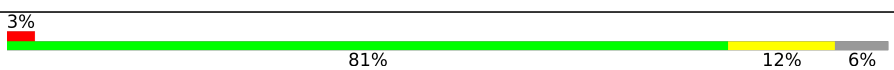
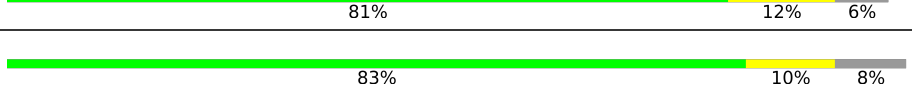
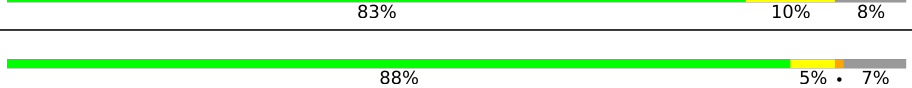
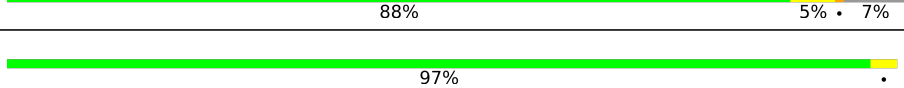
Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	91% 8%
17	X	40	85% 10% 5%
17	x	40	90% 5% 5%
18	Y	30	3% 87% 10%
18	y	30	67% 30%
19	Z	62	90% 8%
19	z	62	74% 24%
20	R	34	9% 74% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	GOL	D	402	-	-	X	-
27	GOL	D	413	-	X	-	-
27	GOL	a	417	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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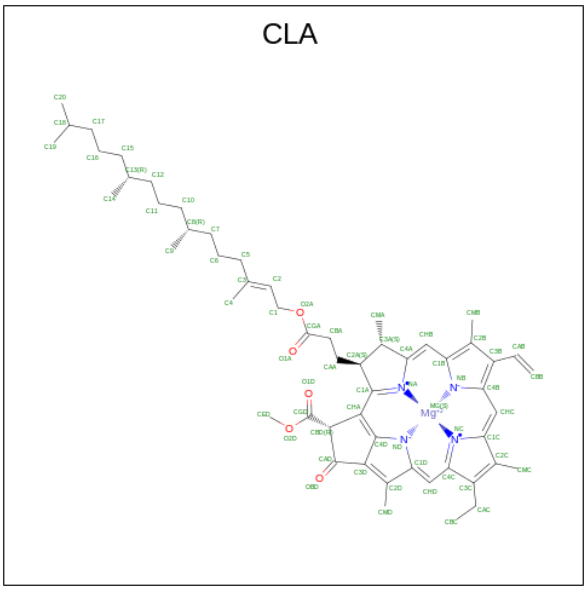
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2

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



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

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

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

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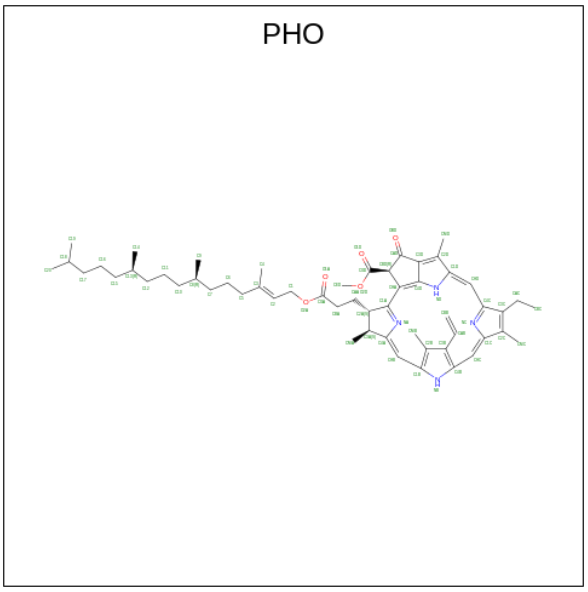
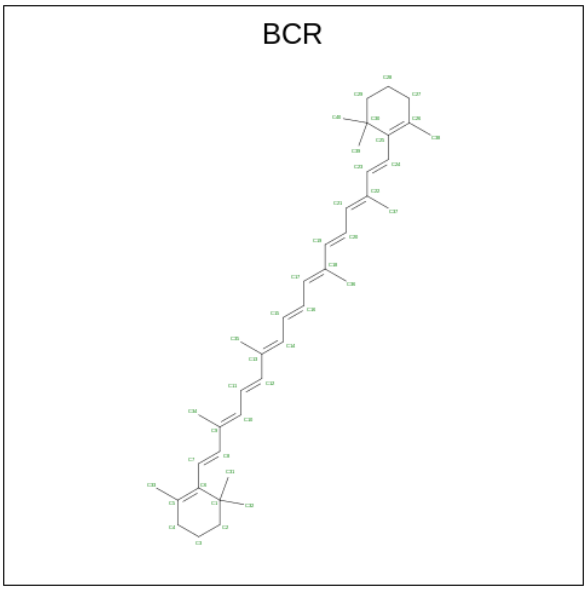
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



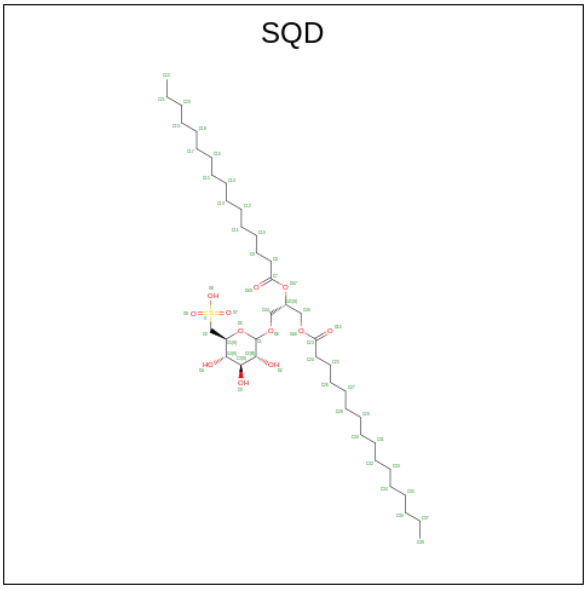
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



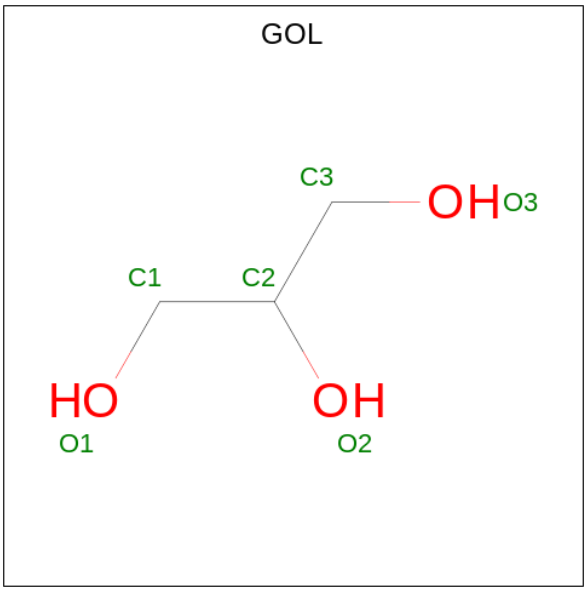
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



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

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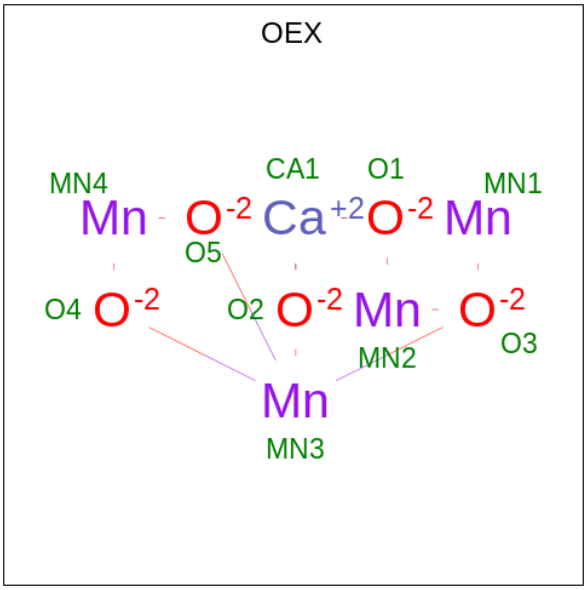
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 12 6 6	0	1
27	c	1	Total C O 6 3 3	0	0
27	d	1	Total C O 6 3 3	0	0
27	l	1	Total C O 12 6 6	0	1
27	o	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	v	1	Total C O 12 6 6	0	1

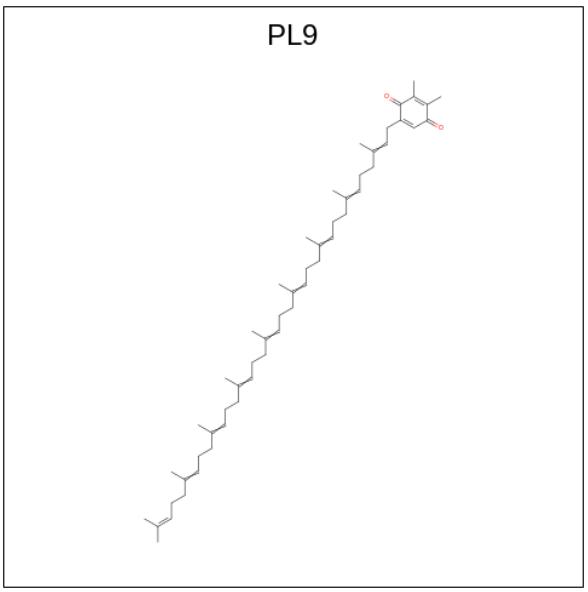
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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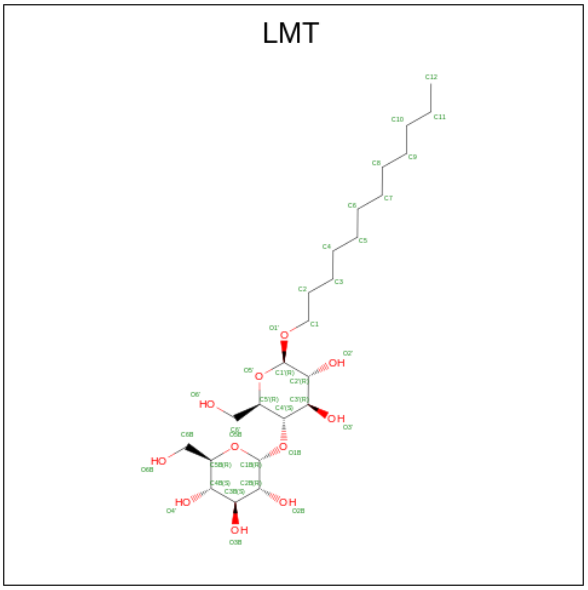
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 64 54 10	0	1
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	l	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- 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	A	1	Total C O 35 24 11	0	0

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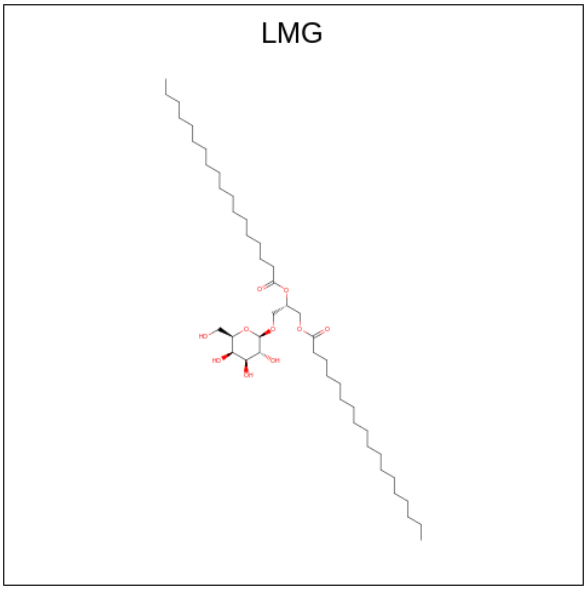
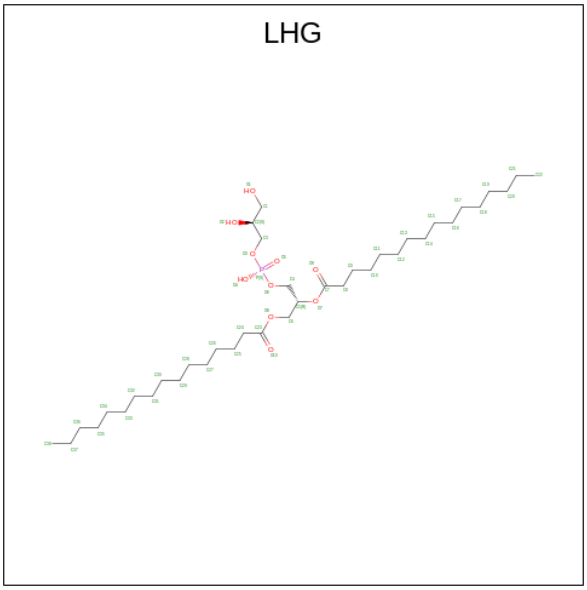
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 25 19 6	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	a	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 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-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



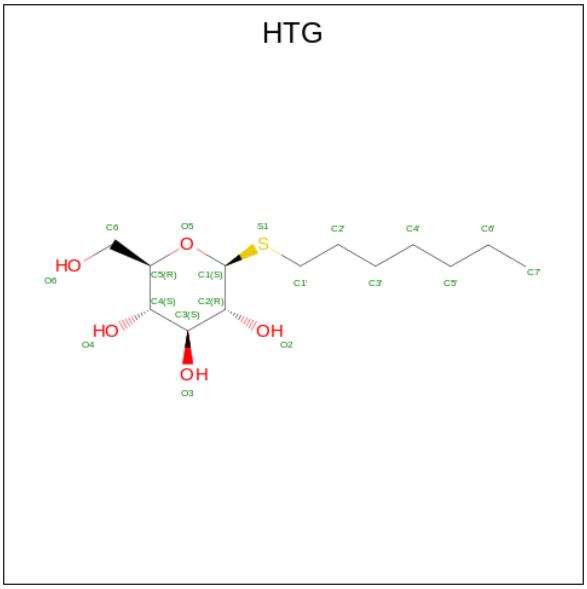
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			51	41	10		
32	B	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	C	1	Total	C	O	0	0
			51	41	10		
32	D	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total	C	O	0	0
			51	41	10		
32	c	1	Total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

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



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

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



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

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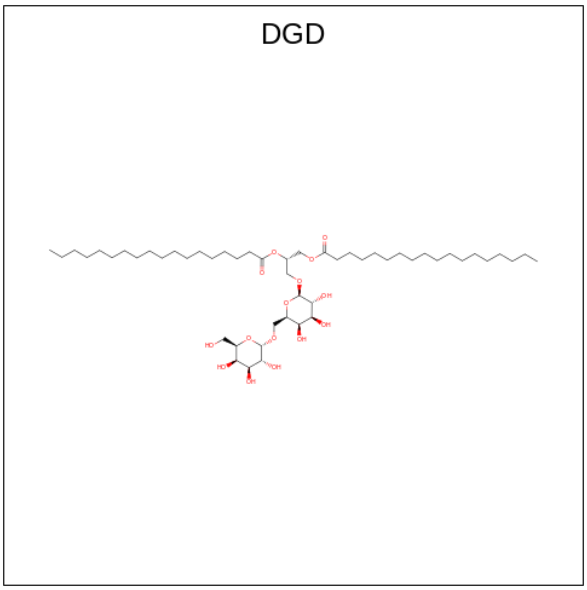
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	c	1	Total C O S 19 13 5 1	0	0
34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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1

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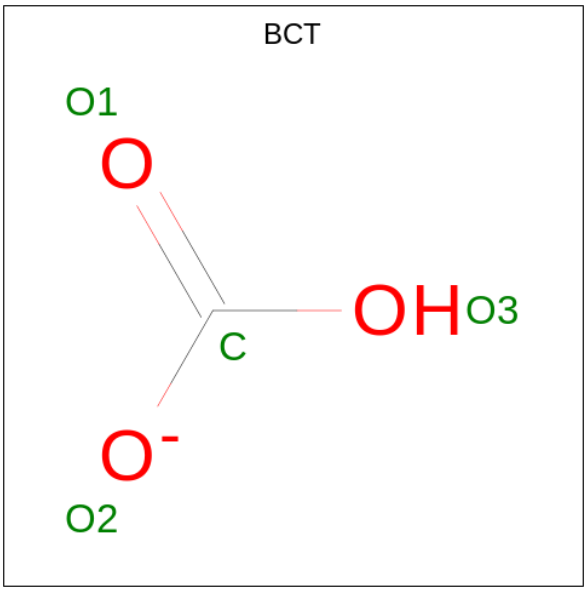
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

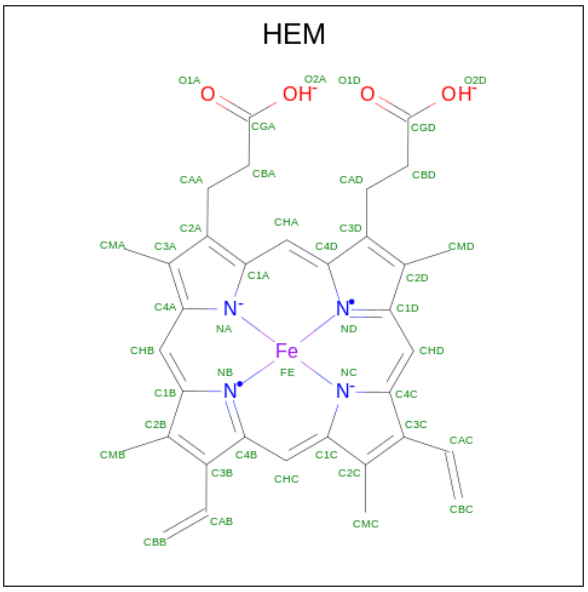
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

- 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	F	1	Total C Fe N O 43 34 1 4 4	0	0

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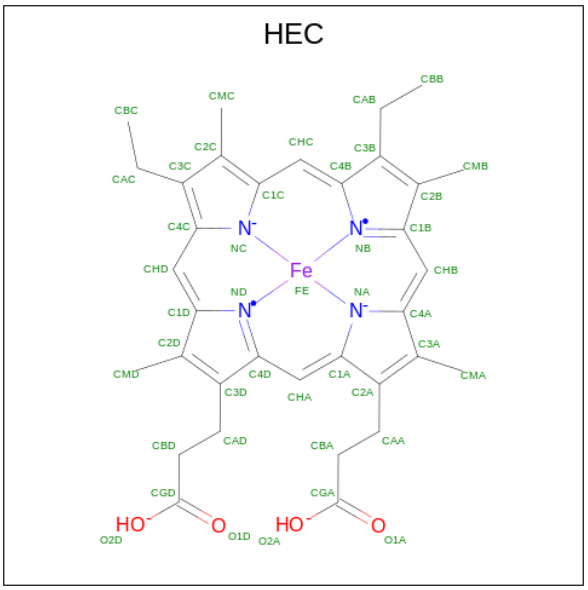
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	136	Total	O	0	86
			221	221		
41	B	189	Total	O	0	2
			191	191		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	169	Total O 206 206	0	38
41	D	123	Total O 157 157	0	34
41	E	15	Total O 15 15	0	0
41	F	6	Total O 6 6	0	0
41	H	23	Total O 23 23	0	0
41	I	4	Total O 4 4	0	0
41	J	7	Total O 7 7	0	0
41	K	6	Total O 6 6	0	0
41	L	9	Total O 10 10	0	1
41	M	5	Total O 5 5	0	0
41	O	106	Total O 111 111	0	5
41	T	11	Total O 14 14	0	3
41	U	42	Total O 44 44	0	2
41	V	80	Total O 81 81	0	1
41	X	7	Total O 7 7	0	0
41	a	129	Total O 209 209	0	81
41	b	199	Total O 202 202	0	3
41	c	158	Total O 191 191	0	34
41	d	121	Total O 153 153	0	32
41	e	9	Total O 9 9	0	0
41	f	3	Total O 3 3	0	0

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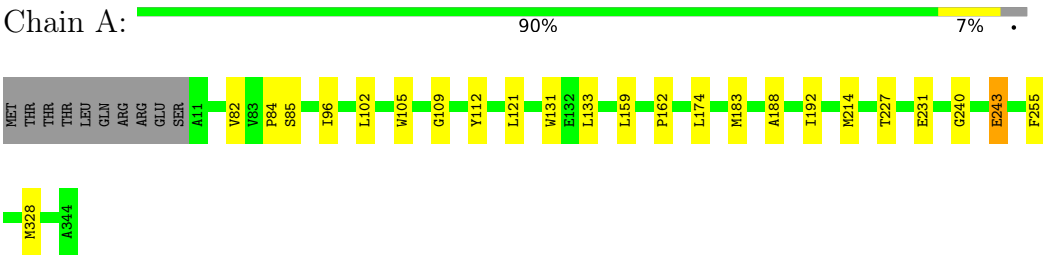
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	16	Total O 16 16	0	0
41	i	2	Total O 2 2	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	100	Total O 104 104	0	4
41	t	7	Total O 10 10	0	3
41	u	49	Total O 50 50	0	1
41	v	59	Total O 61 61	0	2
41	x	7	Total 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.

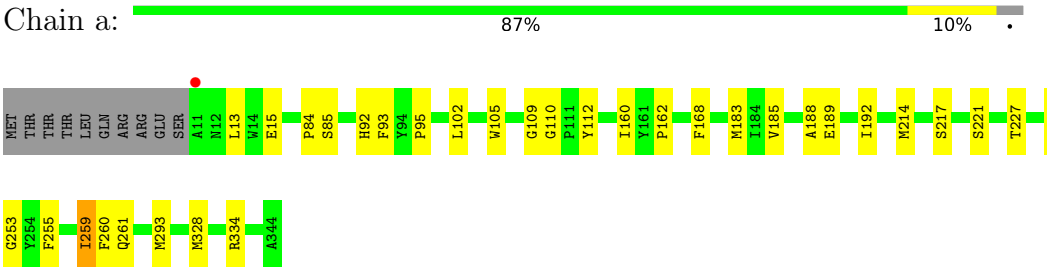
• Molecule 1: Photosystem II protein D1

Chain A:



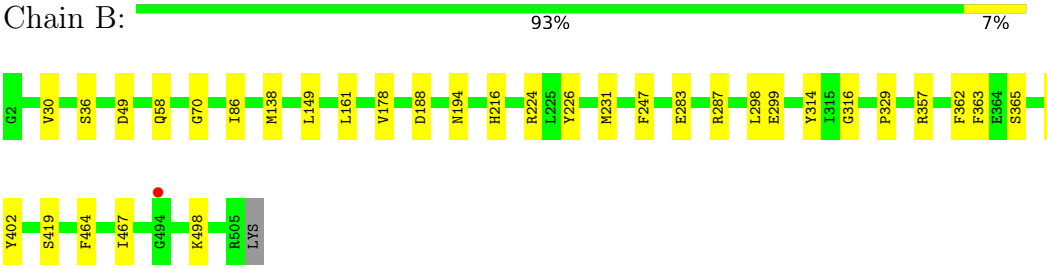
• Molecule 1: Photosystem II protein D1

Chain a:



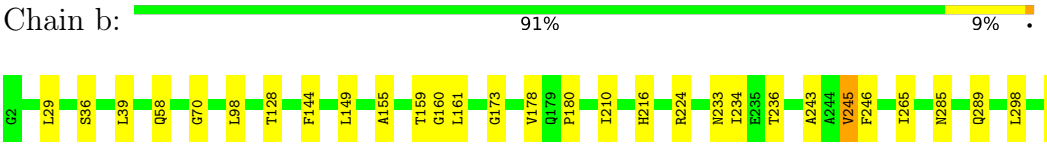
• Molecule 2: Photosystem II CP47 reaction center protein

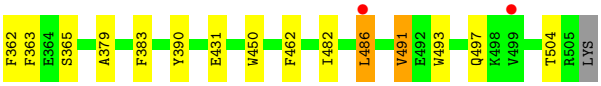
Chain B:



• Molecule 2: Photosystem II CP47 reaction center protein

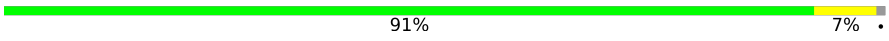
Chain b:

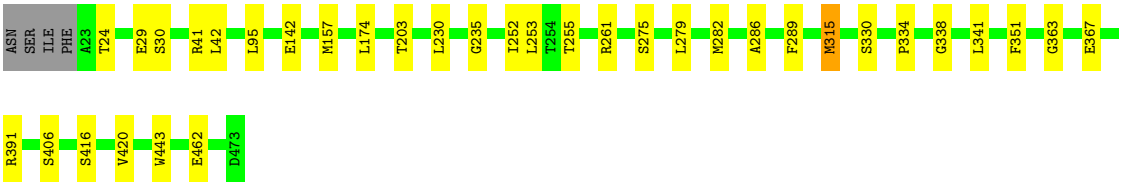




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

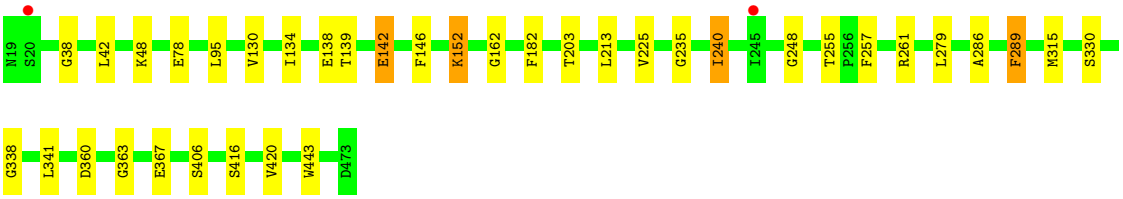




• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:





• Molecule 4: Photosystem II D2 protein

Chain D:

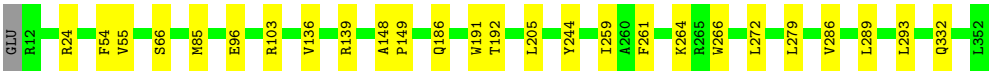




• Molecule 4: Photosystem II D2 protein

Chain d:

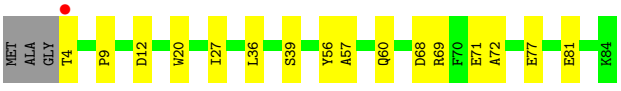




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

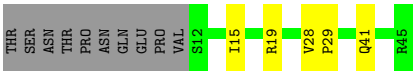




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

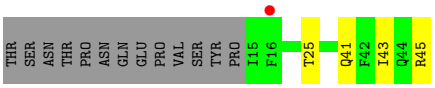




• Molecule 6: Cytochrome b559 subunit beta

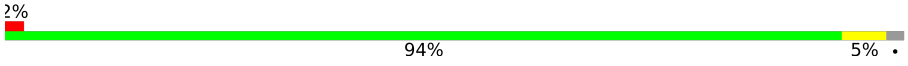
Chain f:

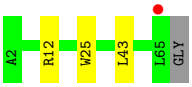




• Molecule 7: Photosystem II reaction center protein H

Chain H:





• Molecule 7: Photosystem II reaction center protein H

Chain h:

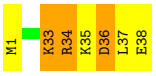




• Molecule 8: Photosystem II reaction center protein I

Chain I:

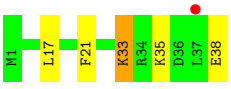




• Molecule 8: Photosystem II reaction center protein I

Chain i:

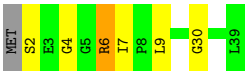




• Molecule 9: Photosystem II reaction center protein J

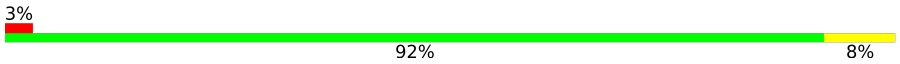
Chain J:

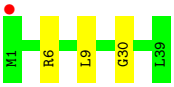




• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

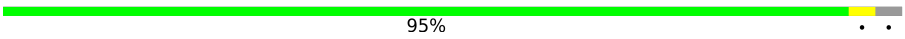
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

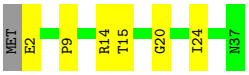




• Molecule 11: Photosystem II reaction center protein L

Chain l:

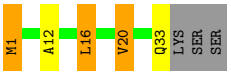




• Molecule 12: Photosystem II reaction center protein M

Chain M:

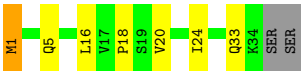




• Molecule 12: Photosystem II reaction center protein M

Chain m:

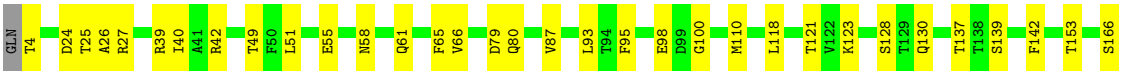


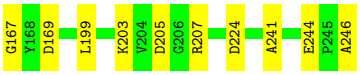


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

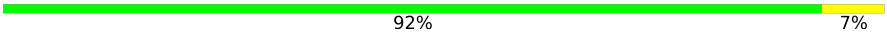


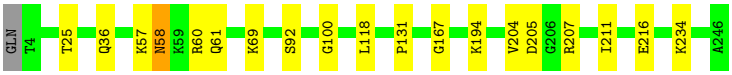




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

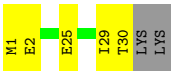




• Molecule 14: Photosystem II reaction center protein T

Chain T:

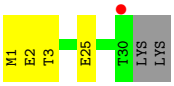




• Molecule 14: Photosystem II reaction center protein T

Chain t:

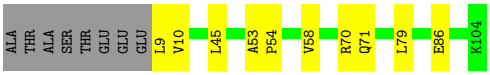




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

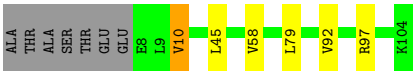




• Molecule 15: Photosystem II 12 kDa extrinsic protein

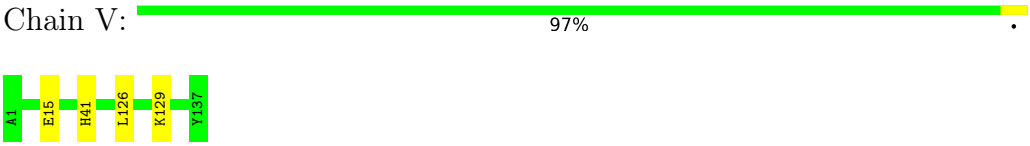
Chain u:





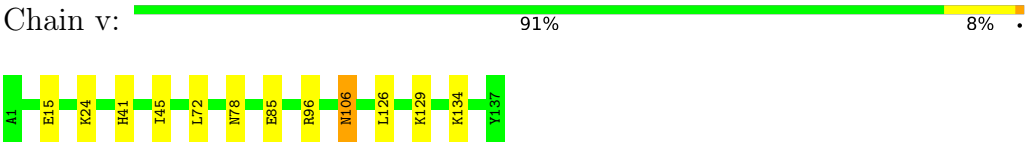
• Molecule 16: Cytochrome c-550

Chain V:



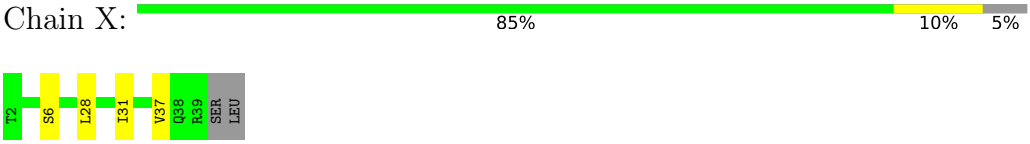
• Molecule 16: Cytochrome c-550

Chain v:



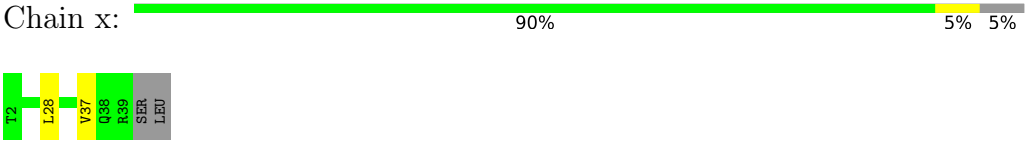
• Molecule 17: Photosystem II reaction center protein X

Chain X:



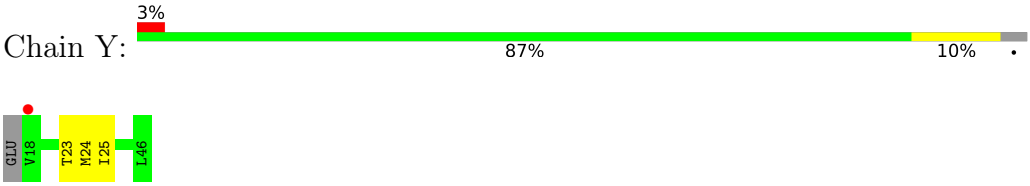
• Molecule 17: Photosystem II reaction center protein X

Chain x:



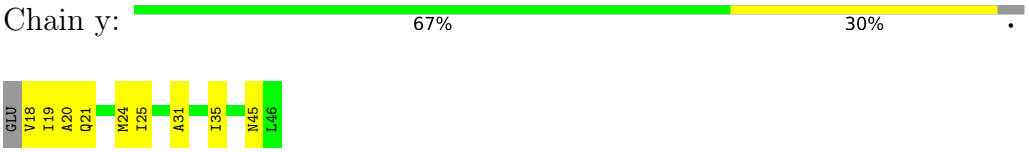
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



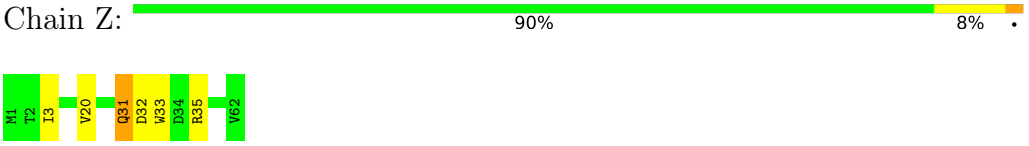
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



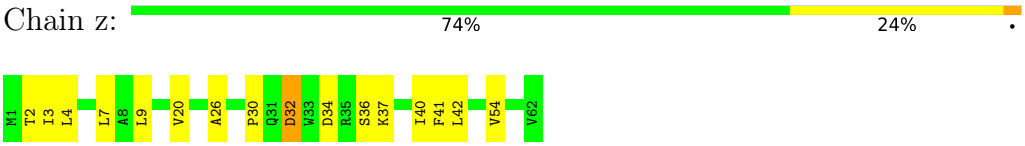
• Molecule 19: Photosystem II reaction center protein Z

Chain Z:



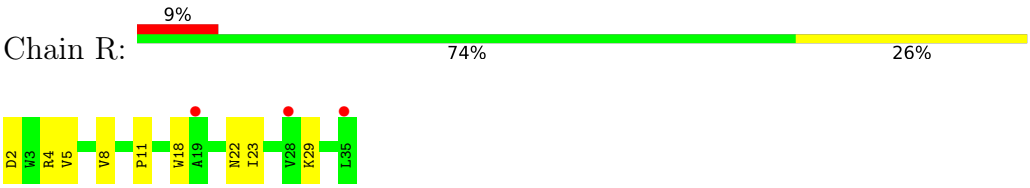
• Molecule 19: Photosystem II reaction center protein Z

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 – 2.25 19.98 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.98-2.25) 99.7 (19.98-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.140 , 0.177 0.141 , 0.179	Depositor DCC
R_{free} test set	19865 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.516	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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 1.71% 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: GOL, FE2, OEX, LMT, HTG, SQD, HEC, LMG, LHG, PHO, FME, BCR, CLA, DGD, CA, UNL, PL9, MG, CL, BCT, HEM

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	0.44	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	0.43	0/6013
3	c	0.27	0/4467	0.42	0/6082
4	D	0.31	0/3746	0.47	0/5102
4	d	0.30	0/3780	0.44	0/5147
5	E	0.31	0/681	0.48	0/928
5	e	0.28	0/690	0.46	0/939
6	F	0.28	0/284	0.45	0/387
6	f	0.26	0/269	0.38	0/365
7	H	0.30	0/519	0.49	0/708
7	h	0.28	0/530	0.46	0/722
8	I	0.26	0/311	0.42	0/419
8	i	0.32	0/311	0.43	0/419
9	J	0.28	0/278	0.38	0/376
9	j	0.28	0/283	0.40	0/383
10	K	0.32	0/303	0.47	0/416
10	k	0.33	0/303	0.45	0/416
11	L	0.34	0/318	0.47	0/433
11	l	0.35	0/318	0.47	0/433
12	M	0.39	0/261	0.55	0/357
12	m	0.32	0/279	0.48	0/380
13	O	0.33	0/1991	0.50	0/2698
13	o	0.30	0/1966	0.49	0/2665
14	T	0.32	0/310	0.41	0/419
14	t	0.31	0/301	0.43	0/406
15	U	0.35	0/811	0.55	0/1095
15	u	0.35	0/826	0.54	0/1116
16	V	0.34	0/1142	0.49	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	0.35	0/384
18	Y	0.23	0/216	0.43	0/289
18	y	0.23	0/216	0.38	0/289
19	Z	0.21	0/490	0.35	0/669
19	z	0.23	0/490	0.41	0/669
20	R	0.26	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	20	0
1	a	4318	0	4124	34	0
2	B	4166	0	3999	26	0
2	b	4134	0	3976	41	0
3	C	4272	0	4138	23	0
3	c	4316	0	4184	30	0
4	D	3625	0	3489	31	0
4	d	3658	0	3522	24	0
5	E	662	0	648	11	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	3	0
8	I	314	0	328	5	0
8	i	314	0	328	3	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	7	0
10	k	293	0	305	6	0
11	L	311	0	320	1	0
11	l	311	0	320	5	0
12	M	268	0	285	6	0
12	m	286	0	305	9	0
13	O	1958	0	1920	25	0
13	o	1933	0	1900	11	0
14	T	311	0	318	3	0
14	t	302	0	311	5	0
15	U	800	0	796	5	0
15	u	815	0	817	4	0
16	V	1120	0	1122	2	0
16	v	1117	0	1131	8	0
17	X	289	0	322	4	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	5	0
19	Z	479	0	516	2	0
19	z	479	0	516	5	0
20	R	273	0	305	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	20	0
23	B	1040	0	1152	28	0
23	C	845	0	936	37	0
23	D	195	0	216	6	0
23	a	325	0	360	17	0
23	b	1040	0	1152	28	0
23	c	845	0	936	37	0
23	d	325	0	360	15	0
24	A	256	0	296	7	0
24	a	256	0	296	3	0
25	A	40	0	56	2	0
25	B	120	0	168	8	0
25	C	80	0	112	2	0
25	D	40	0	56	1	0
25	H	40	0	56	1	0
25	K	40	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	6	0
25	Y	40	0	56	2	0
25	a	40	0	56	1	0
25	b	120	0	168	9	0
25	c	80	0	112	3	0
25	d	40	0	56	2	0
25	h	40	0	56	3	0
25	k	40	0	56	2	0
25	t	40	0	56	6	0
25	y	40	0	56	2	0
26	A	162	0	232	4	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	162	0	232	9	0
26	b	54	0	78	4	0
26	f	43	0	53	0	0
27	A	6	0	8	0	0
27	B	18	0	24	1	0
27	C	12	0	16	0	0
27	D	12	0	15	8	0
27	O	12	0	16	4	0
27	V	12	0	16	0	0
27	a	12	0	16	6	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	2	0
27	o	12	0	16	0	0
27	v	12	0	16	3	0
28	A	20	0	0	0	0
28	a	20	0	0	0	0
29	A	110	0	160	19	0
29	D	110	0	160	0	0
29	a	110	0	160	8	0
29	d	110	0	160	0	0
30	A	28	0	0	0	0
30	B	33	0	0	0	0
30	D	57	0	0	0	0
30	I	40	0	0	0	0
30	J	10	0	0	0	0
30	K	68	0	0	0	0
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	70	0	92	2	0
31	B	95	0	126	2	0
31	F	35	0	46	0	0
31	M	70	0	91	3	0
31	a	35	0	46	1	0
31	b	50	0	70	1	0
31	e	35	0	46	1	0
31	m	35	0	46	0	0
31	t	26	0	34	2	0
32	A	51	0	72	0	0
32	B	51	0	72	1	0
32	C	102	0	144	2	0
32	D	51	0	72	0	0
32	Z	37	0	44	1	0
32	c	153	0	216	2	0
32	d	51	0	72	3	0
32	m	51	0	72	0	0
32	z	39	0	48	2	0
33	A	98	0	148	3	0
33	D	196	0	296	12	0
33	E	84	0	114	8	0
33	L	98	0	148	0	0
33	a	84	0	114	8	0
33	b	98	0	148	0	0
33	d	294	0	444	23	0
34	B	57	0	78	3	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	4	0
34	c	19	0	26	1	0
34	d	16	0	17	0	0
35	C	310	0	410	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	H	62	0	82	1	0
35	c	310	0	410	7	0
35	h	62	0	82	0	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	F	43	0	30	1	0
38	f	43	0	30	1	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	1	0
40	v	43	0	30	0	0
41	A	221	0	0	0	0
41	B	191	0	0	0	0
41	C	206	0	0	3	0
41	D	157	0	0	5	0
41	E	15	0	0	0	0
41	F	6	0	0	0	0
41	H	23	0	0	0	0
41	I	4	0	0	0	0
41	J	7	0	0	2	0
41	K	6	0	0	1	0
41	L	10	0	0	0	0
41	M	5	0	0	0	0
41	O	111	0	0	2	0
41	T	14	0	0	0	0
41	U	44	0	0	0	0
41	V	81	0	0	0	0
41	X	7	0	0	0	0
41	a	209	0	0	3	0
41	b	202	0	0	0	0
41	c	191	0	0	3	0
41	d	153	0	0	1	0
41	e	9	0	0	0	0
41	f	3	0	0	1	0
41	h	16	0	0	0	0
41	i	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	10	0	0	0	0
41	m	13	0	0	0	0
41	o	104	0	0	0	0
41	t	10	0	0	1	0
41	u	50	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	61525	606	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 (606) 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:D:402:GOL:H11	12:M:1:FME:HG2	1.44	1.00
23:B:604:CLA:H42	23:B:605:CLA:H2	1.45	0.98
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.53	0.91
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.61	0.83
23:B:601:CLA:H12	23:B:601:CLA:H71	1.61	0.80
4:d:192[B]:THR:HG23	23:d:403[B]:CLA:HBC2	1.64	0.80
4:d:192[A]:THR:HG23	23:d:403[A]:CLA:HBC2	1.64	0.80
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:HBB1	1.69	0.75
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.68	0.75
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.71	0.72
23:a:407:CLA:H192	23:c:506:CLA:H142	1.73	0.71
23:C:501:CLA:H193	23:C:507:CLA:HBB1	1.72	0.71
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.73	0.70
33:D:408[A]:LHG:H382	33:D:408[A]:LHG:H112	1.74	0.70
27:a:417:GOL:O2	41:a:501:HOH:O	2.09	0.70
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.74	0.69
23:C:513:CLA:H202	32:C:520:LMG:H402	1.76	0.68
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.75	0.68
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.75	0.68
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.74	0.68
33:D:408[B]:LHG:H112	33:D:408[B]:LHG:H382	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.75	0.68
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.76	0.67
23:A:408:CLA:H193	23:C:506:CLA:H101	1.77	0.67
35:C:516[B]:DGD:O1A	41:C:601[B]:HOH:O	2.12	0.66
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.27	0.66
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.77	0.66
27:D:402:GOL:O2	41:D:501:HOH:O	2.12	0.66
23:C:505:CLA:CMD	23:C:507:CLA:HAB	2.25	0.66
29:A:414[B]:PL9:H262	33:E:101[B]:LHG:H223	1.79	0.65
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.80	0.64
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.79	0.64
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.80	0.64
29:A:414[A]:PL9:H262	33:E:101[A]:LHG:H223	1.80	0.64
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.30	0.64
23:a:407:CLA:H152	23:c:507:CLA:H142	1.80	0.64
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.81	0.63
23:c:512:CLA:H191	32:z:101:LMG:H241	1.80	0.63
23:C:505:CLA:HBB1	23:C:505:CLA:HHC	1.81	0.63
23:b:601:CLA:H72	23:b:601:CLA:H2	1.81	0.63
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.29	0.62
27:a:416:GOL:H32	12:m:1:FME:HG3	1.81	0.62
27:a:417:GOL:O3	14:t:2:GLU:OE1	2.17	0.62
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.81	0.62
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.82	0.62
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	1.80	0.62
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.32	0.62
23:C:506:CLA:H142	35:C:516[B]:DGD:HAF2	1.80	0.62
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.82	0.62
23:C:508:CLA:HBC3	23:C:510:CLA:H71	1.82	0.61
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.65	0.61
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.82	0.61
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	1.82	0.61
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.82	0.60
2:B:226:TYR:HA	2:B:231:MET:HG3	1.81	0.60
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.83	0.60
26:a:409[B]:SQD:H141	33:d:408[B]:LHG:H152	1.82	0.60
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.83	0.60
23:A:405[B]:CLA:HHC	23:A:405[B]:CLA:HBB1	1.84	0.60
27:D:402:GOL:H31	12:M:1:FME:HE3	1.82	0.60
23:C:506:CLA:H142	35:C:516[A]:DGD:HAF2	1.82	0.59
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.84	0.58
23:d:402[A]:CLA:HHC	23:d:402[A]:CLA:HBB1	1.85	0.58
26:a:409[A]:SQD:H152	33:d:408[A]:LHG:H172	1.86	0.58
34:B:622:HTG:H4'1	31:B:630:LMT:H52	1.84	0.58
10:K:17:ILE:H	10:K:17:ILE:HD13	1.67	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.69	0.57
23:C:510:CLA:HBC3	23:C:510:CLA:H192	1.85	0.57
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.37	0.57
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.04	0.57
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.13	0.57
26:F:103:SQD:H102	17:X:31:ILE:HD11	1.87	0.57
2:b:285:ASN:O	2:b:289:GLN:HG2	2.04	0.57
31:A:417:LMT:H71	2:b:39:LEU:HD13	1.86	0.57
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.40	0.56
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.87	0.56
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.36	0.56
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.06	0.56
27:O:303:GOL:O1	41:O:401:HOH:O	2.18	0.56
26:a:409[A]:SQD:H141	33:d:408[A]:LHG:H152	1.86	0.56
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.87	0.56
23:a:405[B]:CLA:H191	33:a:418[B]:LHG:H111	1.87	0.56
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.88	0.55
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.88	0.55
5:E:77:GLU:O	5:E:81:GLU:HG2	2.07	0.55
24:A:416[B]:PHO:H3A	23:D:403[B]:CLA:H142	1.88	0.55
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.88	0.55
23:c:503:CLA:H61	23:c:513:CLA:H42	1.89	0.55
32:z:101:LMG:H302	32:z:101:LMG:H141	1.88	0.55
23:B:606:CLA:H202	26:a:410:SQD:H302	1.89	0.55
23:C:503:CLA:HBB1	23:C:512:CLA:H41	1.88	0.55
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.89	0.55
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.08	0.54
27:l:102[A]:GOL:H32	14:t:25:GLU:HB2	1.88	0.54
25:t:102:BCR:H382	25:t:102:BCR:H23C	1.90	0.54
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.89	0.54
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.20	0.54
23:a:405[A]:CLA:H191	33:a:418[A]:LHG:H111	1.88	0.54
27:a:417:GOL:H31	12:m:1:FME:HG2	1.89	0.54
23:c:506:CLA:HMD1	23:c:508:CLA:HAB	1.88	0.54
23:b:604:CLA:H42	23:b:605:CLA:H2	1.89	0.54
5:E:57:ALA:HB3	5:E:60:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.41	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.90	0.54
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.90	0.53
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.08	0.53
4:D:261[B]:PHE:CZ	33:D:407[B]:LHG:HC81	2.43	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.43	0.53
29:A:414[A]:PL9:H503	26:F:103:SQD:H341	1.90	0.53
4:D:192[A]:THR:HG23	23:D:403[A]:CLA:HBC2	1.90	0.53
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.44	0.53
25:b:619:BCR:H331	25:b:619:BCR:C8	2.39	0.53
23:c:505:CLA:H62	35:c:519:DGD:HB62	1.90	0.53
16:v:45[B]:ILE:HD13	27:v:202[B]:GOL:H11	1.91	0.53
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.09	0.53
33:A:419[B]:LHG:H361	23:B:613:CLA:H51	1.91	0.53
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.91	0.52
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	1.90	0.52
23:a:404[B]:CLA:H201	33:d:407[B]:LHG:H161	1.92	0.52
23:a:407:CLA:H203	23:c:507:CLA:H101	1.92	0.52
29:a:412[B]:PL9:H28	33:a:418[B]:LHG:H222	1.92	0.52
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.22	0.52
3:c:182:PHE:HA	34:c:522:HTG:H61	1.92	0.52
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.91	0.52
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.09	0.52
15:u:10[A]:VAL:HG12	41:u:243:HOH:O	2.09	0.52
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.74	0.52
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.92	0.52
33:d:407[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.92	0.52
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.38	0.52
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.92	0.52
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.91	0.51
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.45	0.51
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.92	0.51
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.45	0.51
1:a:15:GLU:HB2	31:a:415:LMT:H6'2	1.92	0.51
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.93	0.51
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.93	0.51
26:a:409[B]:SQD:H152	33:d:408[B]:LHG:H172	1.93	0.51
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	1.91	0.51
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.91	0.51
3:C:174:LEU:HB3	23:C:502:CLA:H152	1.92	0.51
31:M:101:LMT:H72	12:m:24:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:A:414[B]:PL9:H253	23:D:403[B]:CLA:H141	1.91	0.51
32:c:520:LMG:H181	10:k:27:VAL:HG11	1.91	0.51
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.92	0.51
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.46	0.51
29:a:412[A]:PL9:H28	33:a:418[A]:LHG:H222	1.92	0.51
10:K:23:ASP:OD2	41:K:201:HOH:O	2.19	0.51
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.93	0.51
1:a:214[B]:MET:HB3	29:a:412[B]:PL9:H103	1.93	0.51
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.93	0.51
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.94	0.50
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.46	0.50
29:A:414[A]:PL9:H253	23:D:403[A]:CLA:H141	1.92	0.50
23:C:501:CLA:C3D	23:C:503:CLA:H2	2.42	0.50
33:d:407[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.94	0.50
33:a:418[B]:LHG:HC31	5:e:9:PRO:HA	1.93	0.50
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.93	0.50
4:D:85:MET:CE	4:D:96:GLU:HG2	2.42	0.50
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.41	0.50
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.47	0.50
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.18	0.50
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.12	0.50
27:D:402:GOL:H11	12:M:1:FME:CG	2.31	0.49
33:a:418[A]:LHG:HC31	5:e:9:PRO:HA	1.93	0.49
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.43	0.49
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.94	0.49
2:b:233:ASN:O	2:b:236:THR:HG22	2.13	0.49
3:C:157:MET:HE2	3:C:157:MET:HA	1.95	0.49
23:C:509:CLA:HBB1	23:C:509:CLA:HMB1	1.93	0.49
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.94	0.49
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.46	0.49
2:b:98:LEU:HD13	34:b:622:HTG:H7'1	1.94	0.49
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.93	0.49
2:B:383[B]:PHE:CZ	13:O:167:GLY:HA2	2.48	0.49
23:a:404[A]:CLA:H201	33:d:407[A]:LHG:H161	1.95	0.49
4:D:323[A]:GLU:O	27:D:413:GOL:O2	2.30	0.49
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	1.95	0.49
2:B:363:PHE:HB3	2:B:365:SER:O	2.12	0.48
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.48
19:z:32:ASP:O	19:z:36:SER:OG	2.17	0.48
29:a:412[A]:PL9:H351	6:f:25:THR:OG1	2.13	0.48
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:408[A]:LHG:H331	33:d:408[A]:LHG:H361	1.55	0.48
4:d:85:MET:CE	4:d:96:GLU:HG2	2.41	0.48
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.78	0.48
18:y:20:ALA:O	18:y:24:MET:HG2	2.14	0.48
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.95	0.48
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.96	0.48
4:D:323[B]:GLU:O	27:D:413:GOL:O2	2.31	0.48
33:D:408[A]:LHG:H382	33:D:408[A]:LHG:H132	1.96	0.48
1:a:334[B]:ARG:NH2	41:a:507[B]:HOH:O	2.47	0.48
33:d:408[B]:LHG:H342	33:d:408[B]:LHG:H151	1.96	0.48
26:A:410[B]:SQD:H152	26:A:410[B]:SQD:H122	1.58	0.48
32:c:521:LMG:H232	32:c:521:LMG:H391	1.96	0.48
33:d:408[A]:LHG:C38	33:d:408[A]:LHG:H122	2.44	0.48
27:l:102[B]:GOL:H32	14:t:25:GLU:HB2	1.95	0.48
35:c:517[B]:DGD:HG11	41:c:604[B]:HOH:O	2.14	0.48
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.96	0.48
34:B:625:HTG:H61	1:a:102:LEU:HD12	1.96	0.47
2:b:36:SER:OG	25:b:618:BCR:H362	2.13	0.47
23:c:509:CLA:HBC3	23:c:511:CLA:H71	1.96	0.47
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.74	0.47
4:D:327:ALA:HB2	27:D:413:GOL:H2	1.96	0.47
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.96	0.47
5:E:9:PRO:HA	33:E:101[B]:LHG:HC31	1.96	0.47
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.12	0.47
1:A:240[A]:GLY:HA3	14:T:29[A]:ILE:HG23	1.96	0.47
23:A:408:CLA:H18	23:C:505:CLA:H142	1.97	0.47
25:t:102:BCR:H23C	25:t:102:BCR:C38	2.44	0.47
23:A:404[B]:CLA:HBB1	23:A:404[B]:CLA:HMB3	1.96	0.47
24:A:407[B]:PHO:HAB	4:D:205[B]:LEU:HD13	1.96	0.47
25:B:618:BCR:H363	25:t:102:BCR:H19C	1.96	0.47
1:a:160[A]:ILE:HD11	35:c:517[A]:DGD:HBT1	1.96	0.47
19:Z:33:TRP:HZ2	32:Z:101:LMG:HC61	1.79	0.47
2:B:49:ASP:OD2	13:o:57:LYS:NZ	2.46	0.47
2:B:383[A]:PHE:CZ	13:O:167:GLY:HA2	2.50	0.47
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.97	0.47
26:A:410[A]:SQD:H152	26:A:410[A]:SQD:H122	1.54	0.47
23:B:614:CLA:H71	23:B:614:CLA:H112	1.57	0.47
31:B:631:LMT:H6E	31:t:101:LMT:H6D	1.97	0.47
3:C:95:LEU:HD21	23:C:501:CLA:OBD	2.14	0.47
3:C:286:ALA:HB2	23:C:502:CLA:HMD2	1.96	0.47
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:a:412[B]:PL9:H351	6:f:25:THR:OG1	2.15	0.47
27:a:416:GOL:H12	41:t:201:HOH:O	2.14	0.47
2:b:497:GLN:HB2	2:b:504:THR:HB	1.96	0.47
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.44	0.47
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.97	0.47
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.96	0.47
23:d:402[B]:CLA:HBA1	23:d:402[B]:CLA:C4A	2.45	0.47
5:e:68:ASP:O	5:e:72:ALA:HB2	2.15	0.47
1:A:214[A]:MET:HE2	1:A:255[A]:PHE:CE1	2.49	0.47
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.95	0.47
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.15	0.47
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.78	0.47
33:d:408[A]:LHG:H332	33:d:408[A]:LHG:H302	1.77	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.40	0.46
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.30	0.46
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.50	0.46
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.97	0.46
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.79	0.46
2:B:247:PHE:CE2	23:B:602:CLA:H102	2.51	0.46
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.96	0.46
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.15	0.46
9:J:6:ARG:HG3	41:J:201:HOH:O	2.15	0.46
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.96	0.46
23:C:504:CLA:H62	23:C:504:CLA:H41	1.72	0.46
29:a:412[A]:PL9:H151	29:a:412[A]:PL9:H171	1.57	0.46
27:a:417:GOL:H11	12:m:1:FME:HE3	1.97	0.46
23:b:614:CLA:H112	23:b:614:CLA:H72	1.62	0.46
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.15	0.46
13:o:58:ASN:C	13:o:60:ARG:H	2.23	0.46
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.15	0.46
5:E:27:ILE:HD11	38:F:102:HEM:HBC2	1.97	0.46
13:O:25:THR:O	13:O:27:ARG:N	2.48	0.46
23:b:614:CLA:H62	23:b:614:CLA:H41	1.64	0.46
8:i:33:LYS:O	8:i:35:LYS:HG3	2.15	0.46
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.51	0.46
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.51	0.46
26:a:409[A]:SQD:H321	23:c:509:CLA:H102	1.98	0.46
10:k:19:ASP:HB3	10:k:20:PRO:HD3	1.98	0.46
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.39	0.46
23:c:513:CLA:HMB2	23:c:513:CLA:H192	1.98	0.46
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:101:BCR:H24C	25:k:101:BCR:H371	1.75	0.46
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	1.98	0.46
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.45	0.46
33:D:408[B]:LHG:H382	33:D:408[B]:LHG:H132	1.98	0.46
23:c:510:CLA:H91	23:c:510:CLA:H111	1.80	0.46
29:A:414[B]:PL9:H121	29:A:414[B]:PL9:HC8	1.78	0.45
33:A:419[A]:LHG:H361	23:B:613:CLA:H51	1.97	0.45
4:d:332[A]:GLN:NE2	41:d:504:HOH:O	2.49	0.45
23:d:402[A]:CLA:HBA1	23:d:402[A]:CLA:C4A	2.45	0.45
33:d:408[B]:LHG:H331	33:d:408[B]:LHG:H361	1.62	0.45
26:A:410[A]:SQD:H361	10:K:34:ALA:HA	1.99	0.45
8:I:35:LYS:O	8:I:37:LEU:N	2.49	0.45
3:C:275:SER:HB3	23:C:509:CLA:HED3	1.99	0.45
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.98	0.45
3:c:443[B]:TRP:CE2	23:c:509:CLA:HMD2	2.52	0.45
23:B:615:CLA:H71	23:B:616:CLA:H172	1.98	0.45
23:C:503:CLA:CBB	23:C:512:CLA:H41	2.47	0.45
8:I:36:ASP:OD1	8:I:36:ASP:N	2.49	0.45
23:b:605:CLA:H62	23:b:605:CLA:H41	1.67	0.45
2:B:357[A]:ARG:HH12	27:B:624:GOL:H32	1.81	0.45
1:a:85[B]:SER:HA	1:a:109[B]:GLY:HA3	1.99	0.45
23:A:408:CLA:H61	23:A:408:CLA:H41	1.53	0.45
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.45
10:K:26:PRO:O	10:K:29:PRO:HD2	2.17	0.45
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.97	0.45
18:y:31:ALA:O	18:y:35:ILE:HG13	2.16	0.45
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	1.99	0.45
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.17	0.45
9:J:2:SER:N	41:J:201:HOH:O	2.50	0.45
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.52	0.45
1:a:162[B]:PRO:HB3	1:a:168[B]:PHE:HA	1.98	0.45
26:a:409[A]:SQD:H271	33:d:408[A]:LHG:H141	1.98	0.45
23:d:402[B]:CLA:H203	23:d:402[B]:CLA:H162	1.81	0.45
33:d:408[A]:LHG:H342	33:d:408[A]:LHG:H151	1.99	0.45
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.98	0.45
13:O:39[A]:ARG:HB2	13:O:246:ALA:HB2	1.99	0.45
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.98	0.45
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.83	0.45
13:O:42:ARG:O	13:O:241:ALA:HA	2.17	0.45
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.59	0.45
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:505:CLA:H93	23:C:505:CLA:H111	1.75	0.44
27:D:402:GOL:H12	14:T:2:GLU:OE1	2.16	0.44
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.17	0.44
33:d:414[B]:LHG:H211	12:m:18:PRO:HG3	1.99	0.44
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.99	0.44
29:a:412[B]:PL9:H171	29:a:412[B]:PL9:H151	1.56	0.44
26:A:412:SQD:H301	23:b:606:CLA:H202	1.99	0.44
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.51	0.44
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.82	0.44
8:I:33:LYS:HB3	8:I:34:ARG:H	1.60	0.44
23:a:404[A]:CLA:H203	23:a:404[A]:CLA:H162	1.80	0.44
23:a:405[A]:CLA:H203	32:d:412:LMG:H412	1.99	0.44
26:b:620:SQD:H462	26:b:620:SQD:H1	1.99	0.44
3:c:48:LYS:HG3	3:c:138:GLU:HG3	1.99	0.44
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.87	0.44
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.70	0.44
4:D:261[A]:PHE:CZ	33:D:407[A]:LHG:HC81	2.52	0.44
4:D:317[B]:LYS:NZ	41:D:513[B]:HOH:O	2.47	0.44
23:a:407:CLA:H172	23:c:507:CLA:H91	2.00	0.44
4:d:266[A]:TRP:CD1	33:d:407[A]:LHG:HC31	2.52	0.44
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.97	0.44
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.48	0.44
23:C:502:CLA:H151	23:C:503:CLA:HMB2	1.99	0.44
4:D:192[B]:THR:HG23	23:D:403[B]:CLA:HBC2	1.99	0.44
31:M:102:LMT:H112	31:M:102:LMT:H81	1.82	0.44
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.52	0.44
35:c:519:DGD:HBH2	33:d:408[B]:LHG:H211	2.00	0.44
23:d:404:CLA:H61	23:d:404:CLA:H41	1.65	0.44
3:C:443[B]:TRP:CE2	23:C:508:CLA:HMD2	2.53	0.44
35:C:516[B]:DGD:HG11	41:C:601[B]:HOH:O	2.18	0.44
33:E:101[A]:LHG:H241	33:E:101[A]:LHG:HC61	1.85	0.44
31:M:101:LMT:H6D	11:l:9:PRO:HA	2.00	0.44
2:b:58:GLN:C	2:b:329:PRO:HB3	2.42	0.44
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	1.99	0.44
3:c:130:VAL:O	3:c:134[A]:ILE:HG12	2.18	0.44
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	2.00	0.44
29:A:414[A]:PL9:H322	29:A:414[A]:PL9:H301	1.77	0.44
2:B:58:GLN:C	2:B:329:PRO:HB3	2.43	0.44
23:B:605:CLA:HAA1	23:B:605:CLA:HBD	2.00	0.44
33:E:101[B]:LHG:H241	33:E:101[B]:LHG:HC61	1.83	0.44
26:a:409[B]:SQD:H321	23:c:509:CLA:H102	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:d:408[B]:LHG:H122	33:d:408[B]:LHG:C38	2.48	0.44
20:R:18:TRP:O	20:R:22:ASN:ND2	2.43	0.44
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.48	0.44
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	1.99	0.44
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.75	0.44
23:d:403[A]:CLA:HAA2	23:d:403[A]:CLA:HBD	2.00	0.44
26:B:620:SQD:H1	26:B:620:SQD:H462	2.00	0.43
5:E:36:LEU:HA	5:E:39:SER:OG	2.18	0.43
13:O:58:ASN:HD21	13:O:61:GLN:HG3	1.82	0.43
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.00	0.43
23:c:509:CLA:H18	35:c:518[B]:DGD:HAT2	2.01	0.43
35:c:517[A]:DGD:HG11	41:c:604[A]:HOH:O	2.18	0.43
13:o:58:ASN:HB2	13:o:61:GLN:HG2	2.00	0.43
20:R:8:VAL:O	20:R:11:PRO:HD2	2.18	0.43
3:C:42:LEU:HD21	23:C:511:CLA:H2A	2.00	0.43
23:C:506:CLA:H18	23:C:506:CLA:H152	1.47	0.43
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.52	0.43
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CH2	2.54	0.43
33:a:418[B]:LHG:H241	33:a:418[B]:LHG:HC61	1.88	0.43
3:c:152:LYS:HD2	41:c:741:HOH:O	2.16	0.43
4:d:186[B]:GLN:HB2	23:d:403[B]:CLA:HBC1	2.00	0.43
20:R:2:ASP:HB3	20:R:5:VAL:HG23	2.00	0.43
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.73	0.43
29:A:414[B]:PL9:H171	29:A:414[B]:PL9:H151	1.55	0.43
3:C:334[A]:PRO:HA	13:O:153:THR:OG1	2.18	0.43
35:C:517[A]:DGD:HAT1	35:C:518:DGD:HBE1	1.99	0.43
33:E:101[A]:LHG:O2	6:F:19:ARG:NH1	2.51	0.43
3:c:146:PHE:HZ	23:c:513:CLA:HBB2	1.83	0.43
23:B:614:CLA:H8	25:B:617:BCR:H362	2.00	0.43
23:C:506:CLA:HBA1	23:C:506:CLA:H3A	1.79	0.43
2:b:29:LEU:HD23	26:b:620:SQD:H201	2.00	0.43
11:l:20:GLY:O	11:l:24:ILE:HG12	2.17	0.43
23:A:404[A]:CLA:H143	24:A:407[A]:PHO:H61	2.01	0.43
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.00	0.43
23:b:613:CLA:H72	23:b:613:CLA:H111	1.87	0.43
33:d:408[A]:LHG:H242	33:d:408[A]:LHG:H272	1.86	0.43
32:d:412:LMG:H221	32:d:412:LMG:H191	1.63	0.43
31:A:420:LMT:O3'	31:A:420:LMT:H6'2	2.19	0.43
3:C:330:SER:HB3	13:O:100:GLY:O	2.18	0.43
33:D:407[A]:LHG:HC62	11:L:15[A]:THR:HG23	2.00	0.43
23:b:604:CLA:HBB1	23:b:607:CLA:HAB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:279:LEU:HA	3:C:282:MET:HE3	2.01	0.43
35:C:516[A]:DGD:HG11	41:C:601[A]:HOH:O	2.18	0.43
4:D:230[B]:SER:HB2	41:D:542:HOH:O	2.18	0.43
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.54	0.43
4:d:55:VAL:O	4:d:66:SER:HB3	2.19	0.43
25:h:101:BCR:C8	25:h:101:BCR:H331	2.49	0.43
19:z:26:ALA:HB1	19:z:36:SER:HB3	2.00	0.43
23:B:613:CLA:H162	23:B:613:CLA:H121	1.59	0.43
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.86	0.43
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.43
1:a:185[B]:VAL:O	1:a:189[B]:GLU:HG3	2.18	0.43
24:a:406[B]:PHO:HAB	4:d:205[B]:LEU:HD13	2.00	0.43
23:c:509:CLA:H18	35:c:518[A]:DGD:HAT2	2.01	0.43
23:A:405[A]:CLA:HHC	23:A:405[A]:CLA:HBB1	2.01	0.43
24:A:416[A]:PHO:H3A	23:D:403[A]:CLA:H142	1.99	0.43
23:B:613:CLA:H143	23:B:613:CLA:H111	1.81	0.43
10:K:16:ALA:O	10:K:19:ASP:HB2	2.18	0.43
25:d:405:BCR:C8	25:d:405:BCR:H331	2.49	0.43
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.99	0.43
23:C:510:CLA:H112	23:C:510:CLA:H152	1.50	0.43
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.01	0.43
6:f:45:ARG:HG2	41:f:201:HOH:O	2.18	0.43
23:C:508:CLA:H142	23:C:508:CLA:H111	1.80	0.42
24:a:414[A]:PHO:HBC3	4:d:279:LEU:HD22	2.00	0.42
23:b:615:CLA:H92	23:b:615:CLA:H61	1.76	0.42
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.71	0.42
3:C:41:ARG:NH1	23:C:511:CLA:HMD1	2.34	0.42
23:C:501:CLA:HHC	23:C:501:CLA:HBB1	2.01	0.42
23:C:503:CLA:HBB1	23:C:503:CLA:HHC	2.02	0.42
25:H:101:BCR:H331	25:H:101:BCR:C8	2.49	0.42
13:O:137:THR:C	13:O:139:SER:H	2.27	0.42
23:a:405[B]:CLA:H203	32:d:412:LMG:H412	2.00	0.42
26:a:410:SQD:H1	41:a:617:HOH:O	2.19	0.42
2:b:491[A]:VAL:HG13	4:d:136[A]:VAL:HG13	2.02	0.42
24:A:416[B]:PHO:NC	24:A:416[B]:PHO:ND	2.67	0.42
3:C:252:ILE:HG22	3:C:253:LEU:HD23	2.02	0.42
23:C:505:CLA:HAA1	23:C:505:CLA:HBD	2.01	0.42
13:O:130:GLN:H	13:O:130:GLN:CD	2.25	0.42
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.86	0.42
33:a:418[A]:LHG:H241	33:a:418[A]:LHG:HC61	1.89	0.42
25:b:619:BCR:H11C	25:b:619:BCR:H341	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.23	0.42
3:c:257:PHE:O	3:c:261:ARG:HG3	2.19	0.42
23:d:403[B]:CLA:H3A	23:d:403[B]:CLA:HBA2	1.87	0.42
25:d:405:BCR:H11C	25:d:405:BCR:H341	1.96	0.42
10:k:24:VAL:HG21	18:y:25:ILE:HB	2.01	0.42
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.81	0.42
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.90	0.42
4:D:230[A]:SER:HB2	41:D:542:HOH:O	2.18	0.42
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.54	0.42
3:c:443[A]:TRP:CE2	23:c:509:CLA:HMD2	2.53	0.42
33:d:408[B]:LHG:H302	33:d:408[B]:LHG:H332	1.79	0.42
13:o:92:SER:HB3	13:o:131:PRO:HA	2.00	0.42
23:A:404[B]:CLA:HBD	23:A:405[B]:CLA:HAC2	2.02	0.42
29:A:414[A]:PL9:H171	29:A:414[A]:PL9:H151	1.53	0.42
32:B:621:LMG:H112	32:B:621:LMG:H141	1.76	0.42
5:E:9:PRO:HA	33:E:101[A]:LHG:HC31	2.01	0.42
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.02	0.42
13:O:121:THR:OG1	13:O:123:LYS:HG3	2.19	0.42
25:T:101:BCR:HC8	25:T:101:BCR:H311	2.01	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.02	0.42
3:c:95:LEU:HD21	23:c:502:CLA:OBD	2.20	0.42
31:t:101:LMT:H81	31:t:101:LMT:H112	1.61	0.42
15:u:92:VAL:HG12	15:u:97:ARG:HD2	2.01	0.42
3:C:338[A]:GLY:HA3	3:C:341[A]:LEU:O	2.20	0.42
3:C:338[B]:GLY:HA3	3:C:341[B]:LEU:O	2.20	0.42
25:T:101:BCR:H351	26:b:620:SQD:H211	2.02	0.42
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.53	0.42
23:b:607:CLA:H91	23:b:607:CLA:H112	1.70	0.42
23:c:509:CLA:H162	23:c:509:CLA:H122	1.72	0.42
23:d:403[B]:CLA:HAA2	23:d:403[B]:CLA:HBD	2.02	0.42
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.45	0.42
3:C:315[B]:MET:HE3	3:C:351[B]:PHE:HZ	1.84	0.42
33:D:408[A]:LHG:H332	33:D:408[A]:LHG:H302	1.85	0.42
33:D:408[B]:LHG:H332	33:D:408[B]:LHG:H302	1.86	0.42
1:a:259[B]:ILE:HG22	1:a:260[B]:PHE:CD1	2.54	0.42
23:b:605:CLA:H192	23:b:609:CLA:HBB2	1.99	0.42
4:d:103:ARG:HG3	5:e:73:LYS:HG3	2.02	0.42
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.83	0.42
19:z:26:ALA:HB3	19:z:40:ILE:HD11	2.01	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
23:B:602:CLA:H203	23:B:602:CLA:H162	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.76	0.42
25:C:514:BCR:H15C	25:C:514:BCR:H351	1.81	0.42
23:a:407:CLA:H41	23:a:407:CLA:H61	1.91	0.42
25:a:408:BCR:H24C	25:a:408:BCR:H371	1.79	0.42
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	2.02	0.42
29:A:414[B]:PL9:H322	29:A:414[B]:PL9:H301	1.80	0.42
2:B:188:ASP:OD2	2:B:194:ASN:ND2	2.44	0.42
13:O:79:ASP:OD1	13:O:80:GLN:N	2.47	0.42
25:b:618:BCR:H15C	25:b:618:BCR:H351	1.81	0.42
23:A:405[A]:CLA:HBA1	23:A:405[A]:CLA:C4A	2.50	0.42
23:B:615:CLA:H172	23:B:615:CLA:H13	1.91	0.42
33:D:408[A]:LHG:H382	33:D:408[A]:LHG:C11	2.45	0.42
13:O:93:LEU:O	13:O:128:SER:HA	2.20	0.42
23:a:405[B]:CLA:HHC	23:a:405[B]:CLA:HBB1	2.02	0.42
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.01	0.42
5:e:26:THR:HB	38:f:101:HEM:HAB	2.02	0.42
35:C:517[B]:DGD:HAT1	35:C:518:DGD:HBE1	2.02	0.41
32:C:520:LMG:H331	32:C:520:LMG:H362	1.93	0.41
13:O:224:ASP:OD2	41:O:403:HOH:O	2.22	0.41
2:b:341:LYS:HE3	2:b:431:GLU:OE1	2.20	0.41
3:c:330:SER:HB3	13:o:100:GLY:O	2.20	0.41
23:A:404[A]:CLA:H192	23:A:404[A]:CLA:H161	1.80	0.41
33:D:408[A]:LHG:H362	33:D:408[A]:LHG:H331	1.86	0.41
2:b:363:PHE:HB3	2:b:365:SER:O	2.20	0.41
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.02	0.41
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	2.01	0.41
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.85	0.41
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.55	0.41
33:A:419[A]:LHG:H252	2:B:464:PHE:CZ	2.55	0.41
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.56	0.41
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.55	0.41
23:b:604:CLA:H92	23:b:604:CLA:H61	1.74	0.41
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	2.02	0.41
23:B:615:CLA:H92	23:B:615:CLA:H61	1.85	0.41
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	2.02	0.41
1:a:214[A]:MET:HB3	29:a:412[A]:PL9:H103	2.01	0.41
24:a:414[A]:PHO:H42	24:a:414[A]:PHO:H11	1.92	0.41
23:b:601:CLA:H92	25:h:101:BCR:H403	2.02	0.41
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	2.02	0.41
23:b:613:CLA:H203	23:b:613:CLA:H161	1.87	0.41
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:A:416[B]:PHO:HBC3	4:D:279:LEU:HD22	2.01	0.41
23:C:508:CLA:H122	23:C:508:CLA:H162	1.87	0.41
15:U:45:LEU:HD21	15:U:71:GLN:HB3	2.01	0.41
2:b:155:ALA:O	2:b:159:THR:OG1	2.35	0.41
2:b:234:ILE:HB	27:b:624:GOL:H31	2.03	0.41
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	2.02	0.41
23:b:613:CLA:H172	25:b:618:BCR:H312	2.02	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.74	0.41
23:c:505:CLA:H151	23:c:509:CLA:H143	2.03	0.41
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.79	0.41
4:d:148[A]:ALA:HB3	4:d:149[A]:PRO:HD3	2.03	0.41
33:d:408[A]:LHG:H142	33:d:408[A]:LHG:H372	2.03	0.41
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.87	0.41
2:b:70:GLY:HA2	2:b:178:VAL:HG21	2.02	0.41
23:c:510:CLA:H112	23:c:510:CLA:H142	1.76	0.41
14:t:2:GLU:HG2	14:t:3:THR:N	2.34	0.41
16:v:72:LEU:HD23	16:v:72:LEU:HA	1.94	0.41
1:A:85[A]:SER:HA	1:A:109[A]:GLY:HA3	2.03	0.41
23:B:601:CLA:HAA1	23:B:601:CLA:HBD	2.02	0.41
3:C:363:GLY:O	3:C:367:GLU:HG2	2.21	0.41
25:C:515:BCR:H371	25:C:515:BCR:H24C	1.77	0.41
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.02	0.41
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CZ3	2.55	0.41
23:a:404[B]:CLA:H203	23:a:404[B]:CLA:H162	1.83	0.41
2:b:450:TRP:HB3	23:b:607:CLA:HMB1	2.03	0.41
23:b:606:CLA:H122	23:b:606:CLA:H162	1.76	0.41
26:b:620:SQD:H311	26:b:620:SQD:H341	1.74	0.41
33:E:101[A]:LHG:H291	33:E:101[A]:LHG:H261	1.75	0.41
23:b:616:CLA:H102	23:b:616:CLA:H13	1.87	0.41
23:c:513:CLA:H121	23:c:514:CLA:H142	2.03	0.41
25:k:101:BCR:H11C	25:k:101:BCR:H341	1.91	0.41
1:A:131:TRP:CD2	1:A:131:TRP:C	2.97	0.41
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB1	2.03	0.41
2:B:86:ILE:H	2:B:86:ILE:HG13	1.72	0.41
2:B:149:LEU:HG	23:B:606:CLA:HBB2	2.03	0.41
2:B:383[A]:PHE:O	13:O:166:SER:HA	2.21	0.41
34:B:622:HTG:H6'2	34:B:622:HTG:H3'1	1.91	0.41
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.46	0.41
41:D:549:HOH:O	17:X:6:SER:HA	2.21	0.41
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.03	0.41
23:b:614:CLA:H162	23:b:614:CLA:H122	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:203:THR:O	3:c:235:GLY:HA3	2.21	0.41
25:c:515:BCR:H351	25:c:515:BCR:H15C	1.77	0.41
25:t:102:BCR:H11C	25:t:102:BCR:H341	1.90	0.41
2:B:467:ILE:HD13	2:B:467:ILE:HA	1.87	0.41
23:B:612:CLA:H61	23:B:612:CLA:H102	1.98	0.41
23:C:511:CLA:HBA2	10:K:39:TRP:CH2	2.56	0.41
16:V:41:HIS:CD2	40:V:201:HEC:NB	2.89	0.41
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.51	0.41
4:d:261[B]:PHE:CZ	33:d:407[B]:LHG:HC81	2.55	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
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.81	0.40
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.72	0.40
4:d:148[B]:ALA:HB3	4:d:149[B]:PRO:HD3	2.03	0.40
17:x:28:LEU:HD23	17:x:28:LEU:HA	1.83	0.40
1:A:159[B]:LEU:C	1:A:162[B]:PRO:HD2	2.46	0.40
29:A:414[A]:PL9:H121	29:A:414[A]:PL9:HC8	1.78	0.40
25:B:619:BCR:H15C	25:B:619:BCR:H351	1.95	0.40
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.21	0.40
1:a:227[A]:THR:HB	1:a:231:GLU:HG3	2.01	0.40
23:d:404:CLA:HHC	23:d:404:CLA:HBB1	2.03	0.40
11:l:14:ARG:HB3	14:t:25:GLU:HG3	2.04	0.40
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.56	0.40
25:B:618:BCR:C8	25:B:618:BCR:H331	2.50	0.40
23:C:505:CLA:H61	23:C:505:CLA:H101	1.90	0.40
25:D:405:BCR:H11C	25:D:405:BCR:H341	1.99	0.40
5:E:68:ASP:O	5:E:72:ALA:HB2	2.22	0.40
13:O:169:ASP:H	27:O:303:GOL:H12	1.86	0.40
15:U:9:LEU:HA	15:U:9:LEU:HD23	1.89	0.40
1:a:92[B]:HIS:HE2	3:c:360[B]:ASP:CG	2.29	0.40
3:c:363:GLY:O	3:c:367:GLU:HG2	2.21	0.40
4:d:286:VAL:HG21	23:d:403[B]:CLA:HED2	2.03	0.40
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.22	0.40
23:A:404[B]:CLA:CAD	23:A:405[B]:CLA:HAC2	2.52	0.40
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:HC2	1.71	0.40
29:A:414[B]:PL9:H221	29:A:414[B]:PL9:H201	1.84	0.40
29:A:414[B]:PL9:H451	17:X:28:LEU:HD11	2.03	0.40
23:a:404[B]:CLA:CBD	23:d:402[B]:CLA:HAC2	2.51	0.40
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.03	0.40
2:b:462:PHE:CE2	23:b:613:CLA:HMB2	2.56	0.40
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.90	0.40
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.86	0.40
2:B:283:GLU:O	2:B:287:ARG:HG3	2.21	0.40
3:C:443[B]:TRP:CD2	23:C:508:CLA:HMD2	2.56	0.40
35:C:517[A]:DGD:HAE2	35:C:517[A]:DGD:HA81	1.86	0.40
35:C:518:DGD:HBF1	33:D:408[A]:LHG:H221	2.03	0.40
4:D:209[B]:LEU:C	4:D:209[B]:LEU:HD23	2.47	0.40
18:Y:23:THR:HB	18:Y:24:MET:HE2	2.04	0.40
23:c:510:CLA:H43	23:c:510:CLA:H12	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	31
1	a	551/344 (160%)	539 (98%)	10 (2%)	2 (0%)	30	31
2	B	524/505 (104%)	516 (98%)	8 (2%)	0	100	100
2	b	521/505 (103%)	510 (98%)	11 (2%)	0	100	100
3	C	548/455 (120%)	537 (98%)	10 (2%)	1 (0%)	43	50
3	c	554/455 (122%)	543 (98%)	10 (2%)	1 (0%)	43	50
4	D	454/342 (133%)	440 (97%)	14 (3%)	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%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	7 4
8	I	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	4 2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100 100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100 100
9	j	37/39 (95%)	37 (100%)	0	0	100 100
10	K	35/37 (95%)	35 (100%)	0	0	100 100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100 100
11	L	36/37 (97%)	36 (100%)	0	0	100 100
11	l	36/37 (97%)	36 (100%)	0	0	100 100
12	M	32/36 (89%)	32 (100%)	0	0	100 100
12	m	34/36 (94%)	34 (100%)	0	0	100 100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30 31
13	o	249/244 (102%)	243 (98%)	6 (2%)	0	100 100
14	T	33/32 (103%)	33 (100%)	0	0	100 100
14	t	32/32 (100%)	32 (100%)	0	0	100 100
15	U	97/104 (93%)	93 (96%)	4 (4%)	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%)	24 (89%)	3 (11%)	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 3
19	z	60/62 (97%)	59 (98%)	0	1 (2%)	7 3
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100 100
All	All	6180/5384 (115%)	6036 (98%)	133 (2%)	11 (0%)	43 50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	444/279 (159%)	441 (99%)	3 (1%)	76 82
1	a	442/279 (158%)	441 (100%)	1 (0%)	87 92
2	B	423/403 (105%)	418 (99%)	5 (1%)	63 74
2	b	420/403 (104%)	411 (98%)	9 (2%)	47 58
3	C	431/356 (121%)	422 (98%)	9 (2%)	47 58
3	c	437/356 (123%)	430 (98%)	7 (2%)	55 66
4	D	368/277 (133%)	365 (99%)	3 (1%)	73 80
4	d	372/277 (134%)	368 (99%)	4 (1%)	65 75
5	E	72/73 (99%)	70 (97%)	2 (3%)	38 48
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 70
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 37
7	h	55/54 (102%)	55 (100%)	0	100 100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18 18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 47
9	J	26/27 (96%)	24 (92%)	2 (8%)	12 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	j	26/27 (96%)	25 (96%)	1 (4%)	29 36
10	K	30/30 (100%)	26 (87%)	4 (13%)	4 2
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 5
11	L	36/35 (103%)	36 (100%)	0	100 100
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 48
12	M	30/32 (94%)	27 (90%)	3 (10%)	7 5
12	m	32/32 (100%)	30 (94%)	2 (6%)	16 16
13	O	216/207 (104%)	209 (97%)	7 (3%)	34 43
13	o	213/207 (103%)	207 (97%)	6 (3%)	38 48
14	T	32/28 (114%)	28 (88%)	4 (12%)	4 3
14	t	31/28 (111%)	31 (100%)	0	100 100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44 55
15	u	88/89 (99%)	86 (98%)	2 (2%)	44 55
16	V	123/117 (105%)	122 (99%)	1 (1%)	73 80
16	v	123/117 (105%)	119 (97%)	4 (3%)	33 42
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3 2
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 19
19	z	52/52 (100%)	44 (85%)	8 (15%)	2 1
20	R	29/29 (100%)	27 (93%)	2 (7%)	14 13
All	All	5110/4403 (116%)	5003 (98%)	107 (2%)	45 58

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	A	243[A]	GLU
1	A	243[B]	GLU
2	B	161	LEU
2	B	298	LEU
2	B	362	PHE
2	B	389	LYS

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Mol	Chain	Res	Type
2	B	419	SER
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	462	GLU
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	4	THR
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
9	J	9	LEU
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	87	VAL
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU

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Mol	Chain	Res	Type
1	a	13	LEU
2	b	128	THR
2	b	161	LEU
2	b	245	VAL
2	b	298	LEU
2	b	362	PHE
2	b	486[A]	LEU
2	b	486[B]	LEU
2	b	491[A]	VAL
2	b	491[B]	VAL
3	c	142	GLU
3	c	152	LYS
3	c	240	ILE
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	71	GLU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	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	106	ASN

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Mol	Chain	Res	Type
18	y	18	VAL
18	y	19	ILE
18	y	45	ASN
19	Z	3	ILE
19	Z	20	VAL
19	Z	31	GLN
20	R	4	ARG
20	R	29	LYS
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	20	VAL
19	z	32	ASP
19	z	34	ASP
19	z	42	LEU

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

Mol	Chain	Res	Type
5	E	60	GLN
11	L	8	GLN
13	O	231	HIS
17	X	38	GLN
2	b	53	ASN
2	b	331	ASN
3	c	201	ASN
3	c	415	ASN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN
18	y	45	ASN
19	Z	31	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.53	0	7,9,11	1.44	2 (28%)
12	FME	M	1	12	8,9,10	0.61	0	7,9,11	1.13	1 (14%)
8	FME	i	1	8	8,9,10	0.65	0	7,9,11	1.24	0
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.32	2 (28%)
14	FME	t	1	14	8,9,10	0.73	0	7,9,11	1.39	1 (14%)
14	FME	T	1	14	8,9,10	0.72	0	7,9,11	1.64	1 (14%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	O-C-CA	-2.74	117.60	124.78
14	T	1	FME	CG-CB-CA	2.53	119.98	112.95
12	m	1	FME	O1-CN-N	-2.45	118.81	125.27
8	I	1	FME	O-C-CA	-2.28	118.80	124.78
12	M	1	FME	O-C-CA	-2.19	119.05	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	1	FME	O-C-CA	-2.10	119.28	124.78
8	I	1	FME	CA-N-CN	-2.04	119.69	122.82

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	B	612	2	69,73,73	1.98	19 (27%)	83,113,113	2.89	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	d	403[B]	4	69,73,73	1.95	20 (28%)	83,113,113	2.82	30 (36%)
32	LMG	D	412	39	51,51,55	0.84	2 (3%)	59,59,63	1.11	4 (6%)
24	PHO	a	414[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
23	CLA	B	603	2	69,73,73	2.03	19 (27%)	83,113,113	2.94	31 (37%)
23	CLA	b	603	2	69,73,73	1.99	20 (28%)	83,113,113	2.88	33 (39%)
35	DGD	C	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.96	5 (6%)
23	CLA	C	510	3	69,73,73	2.03	20 (28%)	83,113,113	2.99	33 (39%)
23	CLA	A	404[B]	1	69,73,73	2.04	20 (28%)	83,113,113	2.83	29 (34%)
23	CLA	c	513	3	69,73,73	2.07	19 (27%)	83,113,113	2.85	31 (37%)
29	PL9	a	412[B]	-	55,55,55	0.64	2 (3%)	68,69,69	1.97	22 (32%)
23	CLA	d	404	4	69,73,73	2.03	20 (28%)	83,113,113	2.92	30 (36%)
27	GOL	o	302	-	5,5,5	0.95	0	5,5,5	0.99	0
25	BCR	c	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.44	12 (21%)
32	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.11	4 (6%)
38	HEM	f	101	6,5	50,50,50	1.48	6 (12%)	66,82,82	1.75	13 (19%)
23	CLA	b	615	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	33 (39%)
23	CLA	B	604	2	69,73,73	2.00	21 (30%)	83,113,113	2.71	30 (36%)
24	PHO	a	414[B]	-	58,69,69	2.78	13 (22%)	56,99,99	2.91	16 (28%)
33	LHG	a	418[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
32	LMG	c	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.17	4 (6%)
33	LHG	A	419[B]	-	48,48,48	0.86	2 (4%)	51,54,54	1.22	6 (11%)
23	CLA	C	504	41	69,73,73	1.96	19 (27%)	83,113,113	2.79	29 (34%)
23	CLA	B	608	2	69,73,73	1.91	21 (30%)	83,113,113	2.91	33 (39%)
27	GOL	c	527	-	5,5,5	1.12	0	5,5,5	0.97	0
28	OEX	a	411[A]	41,3,1	0,14,14	-	-	-		
23	CLA	c	508	41	69,73,73	2.03	19 (27%)	83,113,113	2.88	29 (34%)
24	PHO	A	416[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
31	LMT	M	101	-	36,36,36	1.13	4 (11%)	47,47,47	1.22	4 (8%)
33	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	609	2	69,73,73	2.01	18 (26%)	83,113,113	2.80	29 (34%)
34	HTG	B	623	-	19,19,19	0.83	2 (10%)	23,24,24	1.46	1 (4%)
31	LMT	B	630	-	36,36,36	1.04	3 (8%)	47,47,47	1.14	4 (8%)
32	LMG	Z	101	-	37,37,55	1.00	2 (5%)	45,45,63	1.46	8 (17%)
27	GOL	A	411	-	5,5,5	1.09	0	5,5,5	0.77	0
33	LHG	a	418[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.93	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	A	409	-	41,41,41	1.04	1 (2%)	56,56,56	1.29	7 (12%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.46	12 (21%)
31	LMT	t	101	-	26,26,36	0.94	2 (7%)	31,31,47	1.30	2 (6%)
23	CLA	B	610	41	69,73,73	2.06	19 (27%)	83,113,113	2.88	33 (39%)
27	GOL	d	413	-	5,5,5	1.07	0	5,5,5	0.92	0
35	DGD	C	517[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
35	DGD	c	519	-	63,63,67	0.89	4 (6%)	77,77,81	1.06	4 (5%)
32	LMG	A	418	-	51,51,55	0.91	2 (3%)	59,59,63	1.49	8 (13%)
23	CLA	b	611	2	69,73,73	1.95	21 (30%)	83,113,113	2.94	29 (34%)
24	PHO	A	407[B]	-	58,69,69	2.72	14 (24%)	56,99,99	2.68	16 (28%)
31	LMT	A	417	-	36,36,36	0.93	2 (5%)	47,47,47	1.01	1 (2%)
24	PHO	A	416[B]	-	58,69,69	2.74	15 (25%)	56,99,99	2.88	16 (28%)
31	LMT	b	627	-	25,25,36	0.88	1 (4%)	30,30,47	1.13	1 (3%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.08	5 (6%)
23	CLA	c	510	3	69,73,73	2.05	20 (28%)	83,113,113	2.84	31 (37%)
23	CLA	C	513	3	69,73,73	2.04	19 (27%)	83,113,113	2.85	31 (37%)
40	HEC	V	201	16	50,50,50	1.77	6 (12%)	68,82,82	1.47	9 (13%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
26	SQD	a	410	-	53,54,54	1.07	4 (7%)	62,65,65	1.25	8 (12%)
27	GOL	a	417	-	5,5,5	1.08	0	5,5,5	0.95	0
27	GOL	B	624	-	5,5,5	0.95	0	5,5,5	1.17	1 (20%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)
25	BCR	T	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.64	15 (26%)
28	OEX	A	413[A]	41,3,1	0,14,14	-	-	-		
33	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
35	DGD	H	102	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	6 (7%)
23	CLA	D	403[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
29	PL9	D	406[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)
29	PL9	d	406[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
31	LMT	B	631	-	25,25,36	0.88	1 (4%)	30,30,47	1.19	3 (10%)
23	CLA	C	505	3	69,73,73	1.99	19 (27%)	83,113,113	2.81	31 (37%)
23	CLA	A	406[B]	41	69,73,73	2.08	19 (27%)	83,113,113	2.84	32 (38%)
23	CLA	C	501	3	69,73,73	1.96	20 (28%)	83,113,113	2.87	32 (38%)
25	BCR	b	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.27	7 (12%)
26	SQD	F	103	-	42,43,54	1.22	4 (9%)	51,54,65	2.18	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	HTG	c	522	-	19,19,19	0.98	1 (5%)	23,24,24	1.54	1 (4%)
31	LMT	M	102	-	36,36,36	1.09	3 (8%)	47,47,47	1.07	2 (4%)
33	LHG	D	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	c	507	3	69,73,73	2.02	20 (28%)	83,113,113	2.83	31 (37%)
25	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.39	9 (16%)
23	CLA	a	404[B]	1	69,73,73	2.02	20 (28%)	83,113,113	2.91	32 (38%)
23	CLA	b	608	2	69,73,73	2.00	20 (28%)	83,113,113	2.82	33 (39%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
28	OEX	A	413[B]	41,3,1	0,14,14	-	-	-		
32	LMG	m	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.23	4 (6%)
23	CLA	C	506	3	69,73,73	2.03	21 (30%)	83,113,113	2.84	31 (37%)
33	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
23	CLA	D	403[B]	4	69,73,73	2.01	19 (27%)	83,113,113	2.83	31 (37%)
29	PL9	D	406[B]	-	55,55,55	0.61	1 (1%)	68,69,69	1.68	15 (22%)
29	PL9	d	406[B]	-	55,55,55	0.68	1 (1%)	68,69,69	1.60	19 (27%)
23	CLA	b	604	2	69,73,73	1.99	20 (28%)	83,113,113	2.83	30 (36%)
37	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
40	HEC	v	201	16	50,50,50	1.77	6 (12%)	68,82,82	1.35	5 (7%)
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
23	CLA	B	616	2	69,73,73	1.98	20 (28%)	83,113,113	2.92	27 (32%)
23	CLA	c	503	3	69,73,73	2.00	18 (26%)	83,113,113	2.69	28 (33%)
25	BCR	Y	101	-	41,41,41	0.99	1 (2%)	56,56,56	1.66	10 (17%)
33	LHG	D	407[B]	-	48,48,48	0.89	2 (4%)	51,54,54	0.98	3 (5%)
34	HTG	B	622	-	19,19,19	1.05	2 (10%)	23,24,24	1.56	5 (21%)
31	LMT	F	101	-	36,36,36	1.07	1 (2%)	47,47,47	1.05	2 (4%)
34	HTG	b	622	-	19,19,19	1.22	2 (10%)	23,24,24	1.98	7 (30%)
23	CLA	B	614	2	69,73,73	2.05	20 (28%)	83,113,113	3.01	31 (37%)
23	CLA	a	407	1	69,73,73	1.96	20 (28%)	83,113,113	2.89	31 (37%)
27	GOL	B	629	-	5,5,5	0.99	0	5,5,5	0.96	0
26	SQD	a	409[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
23	CLA	c	505	41	69,73,73	2.07	20 (28%)	83,113,113	2.80	30 (36%)
23	CLA	B	605	2	69,73,73	2.03	19 (27%)	83,113,113	2.90	30 (36%)
27	GOL	O	303	-	5,5,5	0.82	0	5,5,5	1.14	1 (20%)
29	PL9	A	414[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.98	24 (35%)
33	LHG	b	629[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.03	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	BCR	B	619	-	41,41,41	1.11	2 (4%)	56,56,56	1.37	12 (21%)
33	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.42	8 (14%)
23	CLA	C	503	3	69,73,73	2.00	19 (27%)	83,113,113	2.85	29 (34%)
33	LHG	D	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
33	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
34	HTG	C	521	-	19,19,19	0.86	1 (5%)	23,24,24	1.37	2 (8%)
31	LMT	A	420	-	36,36,36	1.06	2 (5%)	47,47,47	1.15	4 (8%)
23	CLA	B	602	2	69,73,73	2.00	20 (28%)	83,113,113	2.84	28 (33%)
34	HTG	b	625	-	19,19,19	0.97	2 (10%)	23,24,24	1.50	3 (13%)
37	BCT	D	401[B]	21	2,3,3	0.65	0	2,3,3	1.24	0
23	CLA	C	508	3	69,73,73	2.05	21 (30%)	83,113,113	2.81	26 (31%)
37	BCT	d	401[B]	21	2,3,3	0.64	0	2,3,3	1.22	0
38	HEM	F	102	6,5	50,50,50	1.54	7 (14%)	66,82,82	1.91	15 (22%)
23	CLA	b	612	2	69,73,73	2.01	20 (28%)	83,113,113	2.75	29 (34%)
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
25	BCR	D	405	-	41,41,41	1.10	1 (2%)	56,56,56	1.84	16 (28%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
23	CLA	b	616	2	69,73,73	2.00	19 (27%)	83,113,113	2.96	33 (39%)
31	LMT	a	415	-	36,36,36	1.01	1 (2%)	47,47,47	1.04	2 (4%)
26	SQD	a	409[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.64	11 (17%)
26	SQD	f	102	-	42,43,54	1.19	3 (7%)	51,54,65	1.52	11 (21%)
23	CLA	b	614	2	69,73,73	1.99	20 (28%)	83,113,113	2.95	31 (37%)
34	HTG	d	411	-	16,16,19	0.96	1 (6%)	20,21,24	1.64	1 (5%)
23	CLA	c	502	3	69,73,73	2.02	21 (30%)	83,113,113	2.87	29 (34%)
33	LHG	L	101[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.04	2 (3%)
23	CLA	B	613	2	69,73,73	2.02	20 (28%)	83,113,113	2.73	30 (36%)
33	LHG	D	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.98	3 (5%)
33	LHG	d	408[B]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	2 (3%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.71	15 (26%)
23	CLA	c	504	3	69,73,73	2.05	19 (27%)	83,113,113	2.85	30 (36%)
35	DGD	C	518	-	63,63,67	0.88	3 (4%)	77,77,81	0.99	4 (5%)
23	CLA	c	512	3	69,73,73	2.05	21 (30%)	83,113,113	2.84	32 (38%)
23	CLA	A	405[B]	41	69,73,73	2.01	20 (28%)	83,113,113	2.88	32 (38%)
26	SQD	A	412	-	53,54,54	1.01	3 (5%)	62,65,65	1.21	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	a	416	-	5,5,5	1.03	0	5,5,5	1.02	0
23	CLA	C	509	3	69,73,73	2.06	20 (28%)	83,113,113	2.89	32 (38%)
27	GOL	v	202[B]	-	5,5,5	1.05	0	5,5,5	0.88	0
23	CLA	C	502	3	69,73,73	2.03	20 (28%)	83,113,113	2.71	29 (34%)
27	GOL	l	102[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
23	CLA	B	611	2	69,73,73	2.49	19 (27%)	83,113,113	4.11	32 (38%)
25	BCR	y	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.60	11 (19%)
25	BCR	h	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.46	10 (17%)
33	LHG	d	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
23	CLA	A	408	1	69,73,73	1.93	19 (27%)	83,113,113	3.03	36 (43%)
25	BCR	H	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.49	9 (16%)
23	CLA	b	609	2	69,73,73	2.02	18 (26%)	83,113,113	2.84	31 (37%)
34	HTG	b	623	-	19,19,19	1.07	1 (5%)	23,24,24	1.87	2 (8%)
27	GOL	o	303	-	5,5,5	1.00	0	5,5,5	1.07	0
23	CLA	B	607	41	69,73,73	1.94	19 (27%)	83,113,113	2.88	30 (36%)
23	CLA	b	607	41	69,73,73	1.94	20 (28%)	83,113,113	2.77	28 (33%)
37	BCT	D	401[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	B	601	41	69,73,73	2.10	21 (30%)	83,113,113	2.89	30 (36%)
26	SQD	b	620	-	53,54,54	1.05	3 (5%)	62,65,65	1.69	12 (19%)
23	CLA	b	601	41	69,73,73	2.10	19 (27%)	83,113,113	2.82	29 (34%)
27	GOL	l	102[B]	-	5,5,5	0.84	0	5,5,5	1.02	0
27	GOL	C	522[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
27	GOL	D	402	-	5,5,5	1.64	2 (40%)	5,5,5	1.01	1 (20%)
23	CLA	c	511	3	69,73,73	1.99	20 (28%)	83,113,113	2.84	34 (40%)
23	CLA	c	509	3	69,73,73	2.09	20 (28%)	83,113,113	2.80	26 (31%)
32	LMG	B	621	-	51,51,55	0.93	2 (3%)	59,59,63	1.31	4 (6%)
23	CLA	b	610	41	69,73,73	2.03	20 (28%)	83,113,113	2.91	32 (38%)
23	CLA	a	405[B]	41	69,73,73	2.02	19 (27%)	83,113,113	2.90	31 (37%)
33	LHG	d	407[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	4 (7%)
23	CLA	b	613	2	69,73,73	1.95	19 (27%)	83,113,113	2.79	29 (34%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
25	BCR	t	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	D	404	4	69,73,73	2.11	18 (26%)	83,113,113	2.74	30 (36%)
34	HTG	D	411	-	16,16,19	1.04	1 (6%)	20,21,24	1.54	1 (5%)
32	LMG	C	519	-	51,51,55	0.94	2 (3%)	59,59,63	1.11	4 (6%)
27	GOL	C	522[B]	-	5,5,5	1.08	0	5,5,5	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
32	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.12	6 (10%)
23	CLA	C	511	3	69,73,73	2.03	20 (28%)	83,113,113	2.80	29 (34%)
27	GOL	b	624	-	5,5,5	1.20	1 (20%)	5,5,5	0.79	0
23	CLA	b	602	2	69,73,73	2.09	19 (27%)	83,113,113	2.99	36 (43%)
31	LMT	m	103	-	36,36,36	1.08	3 (8%)	47,47,47	1.08	3 (6%)
33	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
32	LMG	C	520	-	51,51,55	1.06	3 (5%)	59,59,63	1.34	6 (10%)
23	CLA	B	615	2	69,73,73	2.03	18 (26%)	83,113,113	2.88	30 (36%)
27	GOL	B	627	-	5,5,5	0.89	0	5,5,5	1.04	1 (20%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.28	7 (12%)
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
27	GOL	c	526[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.34	6 (10%)
27	GOL	V	203[B]	-	5,5,5	1.06	0	5,5,5	0.85	0
23	CLA	C	507	41	69,73,73	1.98	19 (27%)	83,113,113	2.78	27 (32%)
25	BCR	B	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.40	7 (12%)
23	CLA	b	606	2	69,73,73	1.98	19 (27%)	83,113,113	2.87	31 (37%)
23	CLA	B	606	2	69,73,73	1.95	19 (27%)	83,113,113	2.98	29 (34%)
23	CLA	C	512	3	69,73,73	2.04	19 (27%)	83,113,113	2.87	34 (40%)
27	GOL	O	302	-	5,5,5	0.96	0	5,5,5	0.89	0
33	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.10	4 (9%)
31	LMT	b	621	-	25,25,36	0.96	2 (8%)	30,30,47	1.19	3 (10%)
23	CLA	c	514	3	69,73,73	2.12	21 (30%)	83,113,113	2.87	31 (37%)
27	GOL	D	413	-	5,5,5	1.45	2 (40%)	5,5,5	0.81	0
27	GOL	c	526[B]	-	5,5,5	0.84	0	5,5,5	0.97	0
25	BCR	d	405	-	41,41,41	1.11	2 (4%)	56,56,56	2.03	17 (30%)
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.76	11 (17%)
32	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.36	7 (11%)
23	CLA	a	405[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
23	CLA	d	402[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
24	PHO	a	406[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
31	LMT	B	628	-	36,36,36	1.17	4 (11%)	47,47,47	1.37	6 (12%)
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)
35	DGD	c	518[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
35	DGD	C	516[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	d	403[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
26	SQD	B	620	-	53,54,54	1.07	4 (7%)	62,65,65	1.74	12 (19%)
34	HTG	V	202	-	11,11,19	0.26	0	15,15,24	1.20	1 (6%)
25	BCR	C	514	-	41,41,41	1.04	1 (2%)	56,56,56	1.46	6 (10%)
25	BCR	a	408	-	41,41,41	1.05	1 (2%)	56,56,56	1.40	6 (10%)
23	CLA	b	605	2	69,73,73	1.95	18 (26%)	83,113,113	2.97	31 (37%)
32	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.06	3 (6%)
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
29	PL9	a	412[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
28	OEX	a	411[B]	41,3,1	0,14,14	-	-	-		
23	CLA	d	402[B]	41	69,73,73	2.06	18 (26%)	83,113,113	2.93	32 (38%)
24	PHO	a	406[B]	-	58,69,69	2.75	13 (22%)	56,99,99	2.77	16 (28%)
27	GOL	b	628	-	5,5,5	0.50	0	5,5,5	1.34	1 (20%)
23	CLA	c	506	3	69,73,73	2.03	18 (26%)	83,113,113	2.80	29 (34%)
33	LHG	d	414[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.06	4 (7%)
25	BCR	K	102	-	41,41,41	1.04	1 (2%)	56,56,56	1.40	10 (17%)
34	HTG	B	625	-	19,19,19	1.06	2 (10%)	23,24,24	1.21	3 (13%)
35	DGD	c	517[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.10	5 (6%)
35	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.95	5 (6%)
31	LMT	e	101	-	36,36,36	1.02	4 (11%)	47,47,47	1.02	1 (2%)
35	DGD	C	516[B]	-	63,63,67	0.84	2 (3%)	77,77,81	1.10	7 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	2	-	4/39/115/115	-
23	CLA	d	403[B]	4	-	4/39/115/115	-
32	LMG	D	412	39	-	8/46/66/70	0/1/1/1
24	PHO	a	414[A]	-	-	1/37/103/103	0/5/6/6
23	CLA	B	603	2	-	6/39/115/115	-
23	CLA	b	603	2	-	6/39/115/115	-
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	C	510	3	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	404[B]	1	-	7/39/115/115	-
23	CLA	c	513	3	-	14/39/115/115	-
29	PL9	a	412[B]	-	-	15/53/73/73	0/1/1/1
23	CLA	d	404	4	-	8/39/115/115	-
27	GOL	o	302	-	-	2/4/4/4	-
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
32	LMG	d	412	39	-	10/46/66/70	0/1/1/1
38	HEM	f	101	6,5	-	6/14/54/54	-
23	CLA	b	615	2	-	7/39/115/115	-
23	CLA	B	604	2	-	1/39/115/115	-
24	PHO	a	414[B]	-	-	1/37/103/103	0/5/6/6
33	LHG	a	418[A]	-	-	16/46/46/53	-
32	LMG	c	501	-	-	13/46/66/70	0/1/1/1
33	LHG	A	419[B]	-	-	14/53/53/53	-
23	CLA	C	504	41	-	8/39/115/115	-
23	CLA	B	608	2	-	3/39/115/115	-
27	GOL	c	527	-	-	3/4/4/4	-
23	CLA	c	508	41	-	9/39/115/115	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
33	LHG	d	414[A]	-	-	13/53/53/53	-
23	CLA	B	609	2	-	1/39/115/115	-
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
31	LMT	B	630	-	-	10/21/61/61	0/2/2/2
32	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
27	GOL	A	411	-	-	2/4/4/4	-
33	LHG	a	418[B]	-	-	16/46/46/53	-
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LMT	t	101	-	-	10/17/38/61	0/1/1/2
23	CLA	B	610	41	-	9/39/115/115	-
27	GOL	d	413	-	-	4/4/4/4	-
35	DGD	C	517[A]	-	-	15/51/91/95	0/2/2/2
35	DGD	c	519	-	-	12/51/91/95	0/2/2/2
32	LMG	A	418	-	-	14/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	611	2	-	3/39/115/115	-
24	PHO	A	407[B]	-	-	2/37/103/103	0/5/6/6
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
24	PHO	A	416[B]	-	-	3/37/103/103	0/5/6/6
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
35	DGD	h	102	-	-	15/51/91/95	0/2/2/2
23	CLA	c	510	3	-	15/39/115/115	-
23	CLA	C	513	3	-	7/39/115/115	-
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
23	CLA	A	406[A]	41	-	7/39/115/115	-
26	SQD	a	410	-	-	13/49/69/69	0/1/1/1
27	GOL	a	417	-	-	0/4/4/4	-
27	GOL	B	624	-	-	3/4/4/4	-
23	CLA	a	404[A]	1	-	3/39/115/115	-
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
33	LHG	A	419[A]	-	-	10/53/53/53	-
35	DGD	H	102	-	-	9/51/91/95	0/2/2/2
23	CLA	D	403[A]	4	-	0/39/115/115	-
29	PL9	D	406[A]	-	-	8/53/73/73	0/1/1/1
29	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
31	LMT	B	631	-	-	11/17/37/61	0/1/1/2
23	CLA	C	505	3	-	6/39/115/115	-
23	CLA	A	406[B]	41	-	4/39/115/115	-
23	CLA	C	501	3	-	5/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	SQD	F	103	-	-	14/38/58/69	0/1/1/1
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
31	LMT	M	102	-	-	6/21/61/61	0/2/2/2
33	LHG	D	407[A]	-	-	16/53/53/53	-
23	CLA	c	507	3	-	6/39/115/115	-
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
23	CLA	a	404[B]	1	-	5/39/115/115	-
23	CLA	b	608	2	-	5/39/115/115	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
32	LMG	m	101	-	-	11/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	506	3	-	12/39/115/115	-
33	LHG	b	629[A]	-	-	20/53/53/53	-
23	CLA	D	403[B]	4	-	4/39/115/115	-
29	PL9	D	406[B]	-	-	9/53/73/73	0/1/1/1
29	PL9	d	406[B]	-	-	6/53/73/73	0/1/1/1
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
23	CLA	b	604	2	-	10/39/115/115	-
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
23	CLA	B	616	2	-	5/39/115/115	-
23	CLA	c	503	3	-	7/39/115/115	-
25	BCR	Y	101	-	-	2/29/63/63	0/2/2/2
33	LHG	D	407[B]	-	-	16/53/53/53	-
34	HTG	B	622	-	-	3/10/30/30	0/1/1/1
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	B	614	2	-	14/39/115/115	-
23	CLA	a	407	1	-	9/39/115/115	-
27	GOL	B	629	-	-	4/4/4/4	-
26	SQD	a	409[A]	-	-	10/49/69/69	0/1/1/1
23	CLA	c	505	41	-	6/39/115/115	-
23	CLA	B	605	2	-	5/39/115/115	-
27	GOL	O	303	-	-	2/4/4/4	-
29	PL9	A	414[B]	-	-	15/53/73/73	0/1/1/1
33	LHG	b	629[B]	-	-	19/53/53/53	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
33	LHG	L	101[A]	-	-	19/53/53/53	-
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2
23	CLA	C	503	3	-	2/39/115/115	-
33	LHG	D	408[A]	-	-	14/53/53/53	-
33	LHG	d	408[A]	-	-	11/53/53/53	-
34	HTG	C	521	-	-	0/10/30/30	0/1/1/1
31	LMT	A	420	-	-	16/21/61/61	0/2/2/2
23	CLA	B	602	2	-	9/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	C	508	3	-	3/39/115/115	-
38	HEM	F	102	6,5	-	6/14/54/54	-
23	CLA	b	612	2	-	3/39/115/115	-
23	CLA	A	405[A]	41	-	4/39/115/115	-
25	BCR	D	405	-	-	4/29/63/63	0/2/2/2
27	GOL	v	202[A]	-	-	1/4/4/4	-
23	CLA	b	616	2	-	9/39/115/115	-
31	LMT	a	415	-	-	10/21/61/61	0/2/2/2
26	SQD	a	409[B]	-	-	10/49/69/69	0/1/1/1
26	SQD	f	102	-	-	13/38/58/69	0/1/1/1
23	CLA	b	614	2	-	15/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	c	502	3	-	2/39/115/115	-
33	LHG	L	101[B]	-	-	17/53/53/53	-
23	CLA	B	613	2	-	9/39/115/115	-
33	LHG	D	408[B]	-	-	13/53/53/53	-
33	LHG	d	408[B]	-	-	14/53/53/53	-
25	BCR	c	515	-	-	0/29/63/63	0/2/2/2
23	CLA	c	504	3	-	1/39/115/115	-
35	DGD	C	518	-	-	19/51/91/95	0/2/2/2
23	CLA	c	512	3	-	6/39/115/115	-
23	CLA	A	405[B]	41	-	3/39/115/115	-
26	SQD	A	412	-	-	16/49/69/69	0/1/1/1
27	GOL	a	416	-	-	2/4/4/4	-
23	CLA	C	509	3	-	9/39/115/115	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
23	CLA	C	502	3	-	11/39/115/115	-
27	GOL	l	102[A]	-	-	2/4/4/4	-
23	CLA	B	611	2	-	1/39/115/115	-
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
25	BCR	h	101	-	-	1/29/63/63	0/2/2/2
33	LHG	d	407[A]	-	-	13/53/53/53	-
23	CLA	A	408	1	-	8/39/115/115	-
25	BCR	H	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	609	2	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	HTG	b	623	-	-	4/10/30/30	0/1/1/1
27	GOL	o	303	-	-	3/4/4/4	-
23	CLA	B	607	41	-	3/39/115/115	-
23	CLA	b	607	41	-	4/39/115/115	-
23	CLA	B	601	41	-	11/39/115/115	-
26	SQD	b	620	-	-	16/49/69/69	0/1/1/1
23	CLA	b	601	41	-	18/39/115/115	-
27	GOL	l	102[B]	-	-	1/4/4/4	-
27	GOL	C	522[A]	-	-	0/4/4/4	-
27	GOL	D	402	-	-	2/4/4/4	-
23	CLA	c	511	3	-	10/39/115/115	-
23	CLA	c	509	3	-	5/39/115/115	-
32	LMG	B	621	-	-	18/46/66/70	0/1/1/1
23	CLA	b	610	41	-	5/39/115/115	-
23	CLA	a	405[B]	41	-	5/39/115/115	-
33	LHG	d	407[B]	-	-	15/53/53/53	-
23	CLA	b	613	2	-	3/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
25	BCR	t	102	-	-	5/29/63/63	0/2/2/2
23	CLA	D	404	4	-	12/39/115/115	-
34	HTG	D	411	-	-	3/7/27/30	0/1/1/1
32	LMG	C	519	-	-	10/46/66/70	0/1/1/1
27	GOL	C	522[B]	-	-	0/4/4/4	-
32	LMG	c	520	-	-	12/46/66/70	0/1/1/1
23	CLA	C	511	3	-	4/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	b	602	2	-	5/39/115/115	-
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2
33	LHG	E	101[A]	-	-	22/46/46/53	-
32	LMG	C	520	-	-	13/46/66/70	0/1/1/1
23	CLA	B	615	2	-	8/39/115/115	-
27	GOL	B	627	-	-	0/4/4/4	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
27	GOL	c	526[A]	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	GOL	V	203[B]	-	-	2/4/4/4	-
23	CLA	C	507	41	-	7/39/115/115	-
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	b	606	2	-	13/39/115/115	-
23	CLA	B	606	2	-	9/39/115/115	-
23	CLA	C	512	3	-	11/39/115/115	-
27	GOL	O	302	-	-	2/4/4/4	-
33	LHG	E	101[B]	-	-	22/46/46/53	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	c	514	3	-	12/39/115/115	-
27	GOL	D	413	-	-	4/4/4/4	-
27	GOL	c	526[B]	-	-	0/4/4/4	-
25	BCR	d	405	-	-	5/29/63/63	0/2/2/2
26	SQD	A	410[B]	-	-	12/49/69/69	0/1/1/1
32	LMG	c	521	-	-	12/46/66/70	0/1/1/1
23	CLA	a	405[A]	41	-	7/39/115/115	-
23	CLA	d	402[A]	41	-	8/39/115/115	-
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
31	LMT	B	628	-	-	12/21/61/61	0/2/2/2
35	DGD	c	517[A]	-	-	20/51/91/95	0/2/2/2
35	DGD	c	518[A]	-	-	17/51/91/95	0/2/2/2
35	DGD	C	516[A]	-	-	11/51/91/95	0/2/2/2
23	CLA	d	403[A]	4	-	2/39/115/115	-
26	SQD	B	620	-	-	14/49/69/69	0/1/1/1
34	HTG	V	202	-	-	0/2/19/30	0/1/1/1
25	BCR	C	514	-	-	1/29/63/63	0/2/2/2
25	BCR	a	408	-	-	2/29/63/63	0/2/2/2
23	CLA	b	605	2	-	7/39/115/115	-
32	LMG	z	101	-	-	9/34/54/70	0/1/1/1
23	CLA	A	404[A]	1	-	5/39/115/115	-
29	PL9	a	412[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	d	402[B]	41	-	3/39/115/115	-
24	PHO	a	406[B]	-	-	5/37/103/103	0/5/6/6
27	GOL	b	628	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	506	3	-	7/39/115/115	-
33	LHG	d	414[B]	-	-	12/53/53/53	-
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
34	HTG	B	625	-	-	4/10/30/30	0/1/1/1
35	DGD	c	517[B]	-	-	19/51/91/95	0/2/2/2
35	DGD	c	518[B]	-	-	17/51/91/95	0/2/2/2
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
35	DGD	C	516[B]	-	-	14/51/91/95	0/2/2/2

All (1871) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C1D-C2D	9.33	1.49	1.39
24	a	406[B]	PHO	C1B-C2B	9.13	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	8.96	1.49	1.39
24	a	414[B]	PHO	C1D-C2D	8.78	1.49	1.39
24	a	414[A]	PHO	C1B-C2B	8.77	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	8.76	1.49	1.39
24	A	416[A]	PHO	C1D-C2D	8.71	1.49	1.39
24	a	414[B]	PHO	C1B-C2B	8.67	1.49	1.39
24	a	414[A]	PHO	C1D-C2D	8.58	1.49	1.39
24	a	406[B]	PHO	C1D-C2D	8.56	1.49	1.39
24	a	406[A]	PHO	C1D-C2D	8.45	1.48	1.39
24	A	416[B]	PHO	C1B-C2B	8.40	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	C1D-C2D	8.16	1.48	1.39
40	v	201	HEC	C3D-C2D	8.02	1.53	1.36
40	V	201	HEC	C3D-C2D	7.48	1.52	1.36
24	a	414[A]	PHO	C3B-C4B	7.11	1.49	1.41
24	A	416[B]	PHO	C3B-C4B	7.06	1.49	1.41
24	a	414[B]	PHO	C3B-C4B	6.97	1.49	1.41
23	B	611	CLA	C1B-C2B	6.81	1.59	1.43
24	a	406[B]	PHO	C3B-C4B	6.72	1.49	1.41
23	B	611	CLA	CMB-C2B	6.65	1.64	1.50
24	A	416[A]	PHO	C3B-C4B	6.61	1.49	1.41
24	A	416[B]	PHO	C4D-CHA	6.57	1.50	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	C1D-ND	6.40	1.45	1.37
24	a	406[B]	PHO	C4D-CHA	6.39	1.49	1.39
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	414[B]	PHO	C3B-C2B	6.35	1.49	1.40
24	a	406[A]	PHO	C4D-CHA	6.34	1.49	1.39
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
24	A	407[B]	PHO	C4D-CHA	6.18	1.49	1.39
24	A	416[B]	PHO	C3B-C2B	6.15	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	6.12	1.48	1.40
24	A	407[B]	PHO	C3B-C4B	6.12	1.48	1.41
24	a	414[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	414[B]	PHO	C4D-CHA	6.05	1.49	1.39
24	A	407[B]	PHO	C3B-C2B	6.03	1.48	1.40
24	a	406[B]	PHO	C3B-C2B	6.00	1.48	1.40
24	a	414[A]	PHO	C3C-C2C	5.98	1.49	1.36
24	a	414[A]	PHO	C3B-C2B	5.90	1.48	1.40
24	a	414[B]	PHO	C3C-C2C	5.77	1.49	1.36
23	c	514	CLA	C1D-ND	5.77	1.44	1.37
24	A	416[B]	PHO	C3C-C2C	5.75	1.49	1.36
24	a	406[B]	PHO	C3D-C2D	5.73	1.49	1.39
23	c	509	CLA	C3C-C2C	5.71	1.48	1.36
23	C	510	CLA	C1D-ND	5.59	1.44	1.37
23	D	404	CLA	C3C-C2C	5.58	1.48	1.36
24	A	407[A]	PHO	C3C-C2C	5.58	1.48	1.36
23	B	610	CLA	C3C-C2C	5.58	1.48	1.36
24	A	407[B]	PHO	C3C-C2C	5.57	1.48	1.36
23	C	512	CLA	C3C-C2C	5.55	1.48	1.36
23	B	611	CLA	C3C-C2C	5.55	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.52	1.48	1.36
23	C	503	CLA	C3C-C2C	5.52	1.48	1.36
23	a	404[B]	CLA	C3C-C2C	5.52	1.48	1.36
23	d	402[B]	CLA	C3C-C2C	5.52	1.48	1.36
24	a	406[B]	PHO	C3C-C2C	5.51	1.48	1.36
24	a	406[A]	PHO	C3C-C2C	5.49	1.48	1.36
23	b	605	CLA	C3C-C2C	5.49	1.48	1.36
23	C	507	CLA	C3C-C2C	5.49	1.48	1.36
23	c	513	CLA	C3C-C2C	5.49	1.48	1.36
40	V	201	HEC	FE-ND	5.46	2.11	1.94
24	a	414[B]	PHO	C3D-C2D	5.45	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
23	C	508	CLA	C3C-C2C	5.44	1.48	1.36
23	B	601	CLA	C3C-C2C	5.44	1.48	1.36
23	B	605	CLA	C3C-C2C	5.43	1.48	1.36
23	b	606	CLA	C3C-C2C	5.42	1.48	1.36
23	c	505	CLA	O2D-CGD	5.42	1.46	1.33
23	C	502	CLA	C1D-ND	5.41	1.44	1.37
24	a	406[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	d	404	CLA	C3C-C2C	5.41	1.48	1.36
23	B	601	CLA	C1D-ND	5.40	1.44	1.37
23	B	603	CLA	C3C-C2C	5.39	1.48	1.36
23	c	506	CLA	C3C-C2C	5.39	1.48	1.36
23	B	614	CLA	C3C-C2C	5.38	1.48	1.36
23	C	509	CLA	C3C-C2C	5.38	1.48	1.36
23	d	402[B]	CLA	C1D-ND	5.36	1.44	1.37
23	b	601	CLA	C3C-C2C	5.36	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.35	1.48	1.36
23	d	402[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	b	601	CLA	C1D-ND	5.35	1.44	1.37
23	a	405[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	c	503	CLA	C3C-C2C	5.33	1.48	1.36
23	B	603	CLA	C1D-ND	5.33	1.44	1.37
23	d	404	CLA	C1D-ND	5.33	1.44	1.37
23	c	504	CLA	C3C-C2C	5.32	1.48	1.36
23	c	510	CLA	O2D-CGD	5.32	1.46	1.33
23	b	603	CLA	C3C-C2C	5.32	1.48	1.36
23	B	611	CLA	CHC-C1C	5.30	1.49	1.38
23	b	614	CLA	C3C-C2C	5.30	1.48	1.36
23	b	602	CLA	C3C-C2C	5.29	1.48	1.36
23	c	512	CLA	C1D-ND	5.29	1.44	1.37
23	D	403[B]	CLA	C3C-C2C	5.28	1.48	1.36
23	b	615	CLA	C3C-C2C	5.28	1.48	1.36
24	a	414[A]	PHO	C3D-C2D	5.28	1.48	1.39
23	b	610	CLA	C3C-C2C	5.28	1.48	1.36
23	b	602	CLA	O2D-CGD	5.27	1.46	1.33
23	b	607	CLA	C3C-C2C	5.26	1.47	1.36
23	C	508	CLA	C1D-ND	5.26	1.44	1.37
23	C	510	CLA	C3C-C2C	5.25	1.47	1.36
24	A	416[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	A	408	CLA	C3C-C2C	5.25	1.47	1.36
23	B	613	CLA	C1D-ND	5.25	1.44	1.37
23	B	605	CLA	C1D-ND	5.24	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	C1D-ND	5.23	1.44	1.37
23	d	403[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	a	405[B]	CLA	C3C-C2C	5.23	1.47	1.36
23	B	604	CLA	C3C-C2C	5.23	1.47	1.36
23	d	402[B]	CLA	O2D-CGD	5.22	1.45	1.33
23	D	403[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	B	614	CLA	C1D-ND	5.21	1.44	1.37
23	b	603	CLA	O2D-CGD	5.21	1.45	1.33
23	b	616	CLA	C3C-C2C	5.20	1.47	1.36
23	c	510	CLA	C3C-C2C	5.20	1.47	1.36
23	b	609	CLA	O2D-CGD	5.20	1.45	1.33
23	c	503	CLA	C1D-ND	5.20	1.44	1.37
23	c	514	CLA	C3C-C2C	5.20	1.47	1.36
23	c	509	CLA	O2D-CGD	5.20	1.45	1.33
23	c	513	CLA	C1D-ND	5.19	1.44	1.37
23	b	612	CLA	C3C-C2C	5.19	1.47	1.36
23	D	404	CLA	C1D-ND	5.17	1.44	1.37
24	A	416[B]	PHO	O2D-CGD	5.17	1.45	1.33
23	d	402[A]	CLA	C1D-ND	5.16	1.44	1.37
23	B	606	CLA	C3C-C2C	5.15	1.47	1.36
23	C	502	CLA	C3C-C2C	5.15	1.47	1.36
24	a	414[B]	PHO	OBD-CAD	5.14	1.29	1.22
23	C	513	CLA	C3C-C2C	5.13	1.47	1.36
23	c	505	CLA	C1D-ND	5.13	1.44	1.37
23	A	404[B]	CLA	C1D-ND	5.12	1.44	1.37
23	c	509	CLA	C1D-ND	5.12	1.44	1.37
23	C	512	CLA	CHC-C1C	5.12	1.48	1.38
24	a	414[B]	PHO	O2D-CGD	5.11	1.45	1.33
23	C	506	CLA	O2D-CGD	5.11	1.45	1.33
23	c	505	CLA	C3C-C2C	5.11	1.47	1.36
23	A	405[B]	CLA	O2D-CGD	5.11	1.45	1.33
23	c	511	CLA	C3C-C2C	5.11	1.47	1.36
24	A	416[B]	PHO	C3D-C2D	5.11	1.48	1.39
23	C	509	CLA	O2D-CGD	5.11	1.45	1.33
23	B	615	CLA	O2D-CGD	5.10	1.45	1.33
23	B	613	CLA	CHC-C1C	5.10	1.48	1.38
23	d	403[B]	CLA	C3C-C2C	5.10	1.47	1.36
23	c	510	CLA	C1D-ND	5.10	1.44	1.37
23	C	509	CLA	C1D-ND	5.09	1.44	1.37
23	C	508	CLA	O2D-CGD	5.08	1.45	1.33
23	c	502	CLA	C3C-C2C	5.08	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	601	CLA	O2D-CGD	5.08	1.45	1.33
25	k	101	BCR	C23-C22	-5.07	1.35	1.45
23	B	616	CLA	C3C-C2C	5.07	1.47	1.36
23	B	609	CLA	C3C-C2C	5.07	1.47	1.36
23	a	407	CLA	C3C-C2C	5.07	1.47	1.36
23	c	511	CLA	O2D-CGD	5.06	1.45	1.33
23	c	507	CLA	C1D-ND	5.06	1.44	1.37
23	B	615	CLA	C1D-ND	5.06	1.44	1.37
23	C	513	CLA	C1D-ND	5.06	1.44	1.37
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
25	C	515	BCR	C23-C22	-5.05	1.35	1.45
23	c	502	CLA	C1D-ND	5.05	1.44	1.37
23	B	605	CLA	O2D-CGD	5.05	1.45	1.33
23	B	610	CLA	C1D-ND	5.04	1.44	1.37
23	C	504	CLA	C3C-C2C	5.04	1.47	1.36
23	B	612	CLA	CHC-C1C	5.04	1.48	1.38
25	d	405	BCR	C23-C22	-5.03	1.35	1.45
24	a	406[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	b	610	CLA	O2D-CGD	5.02	1.45	1.33
23	C	501	CLA	C3C-C2C	5.02	1.47	1.36
23	B	601	CLA	O2A-CGA	5.02	1.48	1.33
23	c	514	CLA	O2D-CGD	5.02	1.45	1.33
23	b	611	CLA	C3C-C2C	5.01	1.47	1.36
24	a	406[B]	PHO	O2D-CGD	5.01	1.45	1.33
38	f	101	HEM	FE-NB	5.01	2.10	1.94
23	a	405[B]	CLA	CHC-C1C	5.00	1.48	1.38
25	T	101	BCR	C23-C22	-5.00	1.35	1.45
23	c	512	CLA	C3C-C2C	5.00	1.47	1.36
23	b	608	CLA	C3C-C2C	4.99	1.47	1.36
23	c	507	CLA	C3C-C2C	4.99	1.47	1.36
25	C	514	BCR	C23-C22	-4.98	1.35	1.45
23	d	402[A]	CLA	O2D-CGD	4.98	1.45	1.33
23	D	403[B]	CLA	O2D-CGD	4.98	1.45	1.33
23	b	613	CLA	C3C-C2C	4.97	1.47	1.36
23	C	511	CLA	O2D-CGD	4.97	1.45	1.33
23	A	405[B]	CLA	C3C-C2C	4.96	1.47	1.36
25	A	409	BCR	C23-C22	-4.96	1.35	1.45
23	a	404[B]	CLA	C1D-ND	4.96	1.43	1.37
23	c	513	CLA	CHC-C1C	4.95	1.48	1.38
23	B	609	CLA	O2D-CGD	4.95	1.45	1.33
24	a	414[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	B	612	CLA	C3C-C2C	4.95	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	O2D-CGD	4.95	1.45	1.33
23	A	406[B]	CLA	O2D-CGD	4.94	1.45	1.33
23	B	607	CLA	C3C-C2C	4.94	1.47	1.36
23	b	616	CLA	CHC-C1C	4.94	1.48	1.38
24	A	407[B]	PHO	C3D-C2D	4.94	1.48	1.39
23	B	602	CLA	C3C-C2C	4.94	1.47	1.36
24	A	407[B]	PHO	O2D-CGD	4.94	1.45	1.33
23	C	506	CLA	C3C-C2C	4.93	1.47	1.36
23	B	613	CLA	O2D-CGD	4.92	1.45	1.33
23	C	513	CLA	O2D-CGD	4.92	1.45	1.33
23	A	406[B]	CLA	C1D-ND	4.92	1.43	1.37
23	C	504	CLA	O2D-CGD	4.91	1.45	1.33
23	a	407	CLA	CHC-C1C	4.91	1.48	1.38
23	c	502	CLA	CHC-C1C	4.91	1.48	1.38
23	b	602	CLA	CHC-C1C	4.91	1.48	1.38
23	b	606	CLA	C1D-ND	4.91	1.43	1.37
24	A	416[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	B	615	CLA	C3C-C2C	4.90	1.47	1.36
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	c	508	CLA	C1D-ND	4.90	1.43	1.37
23	B	601	CLA	CHC-C1C	4.90	1.48	1.38
23	b	613	CLA	O2D-CGD	4.89	1.45	1.33
23	c	511	CLA	C1D-ND	4.89	1.43	1.37
23	A	404[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	C	501	CLA	CHC-C1C	4.89	1.48	1.38
23	c	506	CLA	CHC-C1C	4.89	1.48	1.38
23	b	609	CLA	C3C-C2C	4.88	1.47	1.36
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
23	c	508	CLA	O2D-CGD	4.88	1.45	1.33
23	c	508	CLA	C3C-C2C	4.88	1.47	1.36
23	b	601	CLA	CHC-C1C	4.87	1.48	1.38
23	B	602	CLA	C1D-ND	4.87	1.43	1.37
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	C	505	CLA	CHC-C1C	4.86	1.48	1.38
23	b	614	CLA	O2D-CGD	4.86	1.45	1.33
23	C	505	CLA	O2D-CGD	4.86	1.45	1.33
23	a	407	CLA	O2D-CGD	4.86	1.45	1.33
23	c	507	CLA	O2D-CGD	4.86	1.45	1.33
23	d	404	CLA	CHC-C1C	4.85	1.48	1.38
23	b	605	CLA	O2D-CGD	4.85	1.45	1.33
23	C	511	CLA	C3C-C2C	4.85	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	C3C-C2C	4.85	1.47	1.36
26	F	103	SQD	O47-C7	4.84	1.48	1.34
23	c	509	CLA	CHC-C1C	4.84	1.48	1.38
23	b	601	CLA	O2D-CGD	4.84	1.45	1.33
24	a	414[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	c	503	CLA	O2D-CGD	4.84	1.45	1.33
25	B	619	BCR	C23-C22	-4.83	1.35	1.45
23	b	610	CLA	CHC-C1C	4.83	1.48	1.38
23	b	615	CLA	O2D-CGD	4.83	1.45	1.33
24	A	416[B]	PHO	OBD-CAD	4.83	1.29	1.22
23	b	601	CLA	O2A-CGA	4.83	1.47	1.33
23	D	404	CLA	CHC-C1C	4.82	1.48	1.38
23	B	608	CLA	C3C-C2C	4.82	1.47	1.36
23	C	512	CLA	C1D-ND	4.82	1.43	1.37
23	B	606	CLA	CHC-C1C	4.81	1.48	1.38
23	c	513	CLA	O2D-CGD	4.81	1.44	1.33
23	B	606	CLA	C1D-ND	4.81	1.43	1.37
23	b	613	CLA	CHC-C1C	4.80	1.48	1.38
23	B	609	CLA	CHC-C1C	4.80	1.48	1.38
23	D	403[A]	CLA	O2D-CGD	4.80	1.44	1.33
23	a	405[B]	CLA	O2D-CGD	4.80	1.44	1.33
23	B	615	CLA	CHC-C1C	4.80	1.48	1.38
25	K	102	BCR	C23-C22	-4.80	1.35	1.45
38	F	102	HEM	FE-NB	4.80	2.09	1.94
23	C	512	CLA	O2D-CGD	4.78	1.44	1.33
25	b	617	BCR	C23-C22	-4.77	1.35	1.45
23	c	504	CLA	CHC-C1C	4.76	1.48	1.38
24	A	407[B]	PHO	OBD-CAD	4.76	1.29	1.22
23	b	609	CLA	CHC-C1C	4.76	1.48	1.38
23	B	603	CLA	O2D-CGD	4.76	1.44	1.33
23	C	510	CLA	O2D-CGD	4.76	1.44	1.33
23	C	505	CLA	C3C-C2C	4.75	1.46	1.36
23	C	502	CLA	O2D-CGD	4.75	1.44	1.33
23	b	604	CLA	C3C-C2C	4.75	1.46	1.36
23	b	614	CLA	CHC-C1C	4.75	1.48	1.38
23	b	604	CLA	C1D-ND	4.74	1.43	1.37
23	C	503	CLA	CHC-C1C	4.74	1.48	1.38
23	A	405[B]	CLA	C1D-ND	4.74	1.43	1.37
23	b	613	CLA	C1D-ND	4.73	1.43	1.37
23	d	403[B]	CLA	O2D-CGD	4.73	1.44	1.33
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
25	D	405	BCR	C23-C22	-4.73	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHC-C1C	4.72	1.48	1.38
23	b	609	CLA	C1D-ND	4.72	1.43	1.37
23	C	501	CLA	C1D-ND	4.72	1.43	1.37
23	A	406[A]	CLA	CHC-C1C	4.72	1.48	1.38
23	C	507	CLA	O2D-CGD	4.71	1.44	1.33
23	b	616	CLA	C1D-ND	4.71	1.43	1.37
23	b	611	CLA	CHC-C1C	4.70	1.48	1.38
23	D	404	CLA	O2D-CGD	4.70	1.44	1.33
25	c	516	BCR	C23-C22	-4.69	1.35	1.45
25	b	619	BCR	C23-C22	-4.69	1.35	1.45
23	C	510	CLA	CHC-C1C	4.69	1.48	1.38
23	a	405[B]	CLA	C1D-ND	4.68	1.43	1.37
23	B	611	CLA	CHC-C4B	4.68	1.49	1.39
23	A	406[B]	CLA	CHC-C1C	4.68	1.48	1.38
23	b	612	CLA	C1D-ND	4.68	1.43	1.37
23	c	514	CLA	CHC-C1C	4.68	1.48	1.38
23	A	408	CLA	O2D-CGD	4.67	1.44	1.33
23	d	403[A]	CLA	O2D-CGD	4.66	1.44	1.33
23	d	402[B]	CLA	CHC-C1C	4.66	1.48	1.38
32	c	521	LMG	O7-C10	4.66	1.47	1.34
23	B	614	CLA	O2D-CGD	4.65	1.44	1.33
23	b	608	CLA	O2D-CGD	4.64	1.44	1.33
23	C	511	CLA	CHC-C1C	4.63	1.47	1.38
32	C	520	LMG	O7-C10	4.62	1.47	1.34
25	B	617	BCR	C23-C22	-4.62	1.36	1.45
23	b	615	CLA	CHC-C1C	4.62	1.47	1.38
23	B	616	CLA	CHC-C1C	4.62	1.47	1.38
23	b	606	CLA	O2D-CGD	4.62	1.44	1.33
23	b	604	CLA	CHC-C1C	4.62	1.47	1.38
23	B	611	CLA	O2D-CGD	4.62	1.44	1.33
23	c	512	CLA	O2D-CGD	4.62	1.44	1.33
23	a	404[A]	CLA	C1D-ND	4.62	1.43	1.37
23	B	616	CLA	O2D-CGD	4.62	1.44	1.33
23	C	506	CLA	CHD-C1D	4.61	1.47	1.38
23	A	404[B]	CLA	CHC-C1C	4.60	1.47	1.38
23	A	405[B]	CLA	CHC-C1C	4.60	1.47	1.38
23	b	603	CLA	CHC-C1C	4.60	1.47	1.38
25	t	102	BCR	C23-C22	-4.60	1.36	1.45
23	b	605	CLA	C1D-ND	4.60	1.43	1.37
23	b	606	CLA	CHC-C1C	4.59	1.47	1.38
23	c	506	CLA	O2D-CGD	4.59	1.44	1.33
25	y	101	BCR	C23-C22	-4.59	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	CHC-C1C	4.59	1.47	1.38
23	C	507	CLA	CHC-C1C	4.58	1.47	1.38
23	c	504	CLA	CHD-C1D	4.58	1.47	1.38
23	b	602	CLA	CHD-C1D	4.58	1.47	1.38
23	a	405[A]	CLA	CHC-C1C	4.58	1.47	1.38
23	b	607	CLA	CHC-C1C	4.58	1.47	1.38
23	C	505	CLA	C1D-ND	4.58	1.43	1.37
23	B	610	CLA	OBD-CAD	4.58	1.30	1.22
23	B	605	CLA	CHC-C1C	4.58	1.47	1.38
23	b	612	CLA	O2D-CGD	4.57	1.44	1.33
23	c	514	CLA	O2A-CGA	4.56	1.46	1.33
23	b	602	CLA	C1D-ND	4.56	1.43	1.37
23	C	503	CLA	O2D-CGD	4.55	1.44	1.33
23	b	603	CLA	C1D-ND	4.55	1.43	1.37
23	b	610	CLA	C1D-ND	4.55	1.43	1.37
23	B	604	CLA	O2D-CGD	4.55	1.44	1.33
23	A	405[A]	CLA	CHC-C1C	4.55	1.47	1.38
25	c	515	BCR	C23-C22	-4.55	1.36	1.45
26	f	102	SQD	O47-C7	4.54	1.47	1.34
23	a	404[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	c	512	CLA	CHC-C1C	4.53	1.47	1.38
23	B	615	CLA	CHD-C1D	4.52	1.47	1.38
23	a	404[B]	CLA	O2D-CGD	4.52	1.44	1.33
23	b	615	CLA	C1D-ND	4.51	1.43	1.37
23	B	608	CLA	C1D-ND	4.51	1.43	1.37
26	a	410	SQD	O48-C23	4.51	1.46	1.33
23	B	604	CLA	CHD-C1D	4.51	1.47	1.38
23	C	504	CLA	C1D-ND	4.51	1.43	1.37
26	B	620	SQD	O47-C7	4.50	1.47	1.34
23	a	405[A]	CLA	O2D-CGD	4.50	1.44	1.33
32	C	520	LMG	O8-C28	4.49	1.46	1.33
23	b	607	CLA	C1B-NB	-4.49	1.32	1.37
23	B	614	CLA	CHC-C1C	4.49	1.47	1.38
25	a	408	BCR	C23-C22	-4.48	1.36	1.45
33	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
23	c	514	CLA	CHD-C1D	4.47	1.47	1.38
23	B	607	CLA	CHC-C1C	4.47	1.47	1.38
23	D	403[B]	CLA	C1D-ND	4.46	1.43	1.37
23	D	404	CLA	CHD-C1D	4.46	1.47	1.38
23	C	503	CLA	C1D-ND	4.46	1.43	1.37
32	z	101	LMG	O8-C28	4.46	1.46	1.33
32	B	621	LMG	O8-C28	4.45	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	CHC-C1C	4.45	1.47	1.38
33	E	101[B]	LHG	O8-C23	4.45	1.46	1.33
23	C	504	CLA	CHC-C1C	4.44	1.47	1.38
25	Y	101	BCR	C23-C22	-4.43	1.36	1.45
24	a	406[B]	PHO	OBD-CAD	4.43	1.28	1.22
23	B	611	CLA	C4B-NB	-4.42	1.32	1.37
23	C	513	CLA	CHC-C1C	4.42	1.47	1.38
23	B	609	CLA	C1D-ND	4.42	1.43	1.37
23	B	604	CLA	CHC-C1C	4.42	1.47	1.38
26	A	412	SQD	O48-C23	4.42	1.46	1.33
23	b	608	CLA	CHC-C1C	4.42	1.47	1.38
23	B	609	CLA	CHD-C1D	4.41	1.47	1.38
23	B	602	CLA	O2D-CGD	4.41	1.44	1.33
23	d	402[A]	CLA	CHC-C1C	4.40	1.47	1.38
23	b	611	CLA	O2D-CGD	4.40	1.43	1.33
25	H	101	BCR	C23-C22	-4.40	1.36	1.45
25	h	101	BCR	C23-C22	-4.40	1.36	1.45
33	a	418[A]	LHG	O8-C23	4.39	1.46	1.33
23	B	606	CLA	O2D-CGD	4.39	1.43	1.33
23	B	610	CLA	O2D-CGD	4.39	1.43	1.33
23	c	513	CLA	O2A-CGA	4.39	1.46	1.33
23	B	612	CLA	CHB-C1B	4.39	1.49	1.39
23	b	602	CLA	CHC-C4B	4.39	1.49	1.39
23	B	612	CLA	O2D-CGD	4.39	1.43	1.33
23	C	509	CLA	CHD-C1D	4.38	1.46	1.38
35	c	519	DGD	O1G-C1A	4.38	1.46	1.33
23	d	402[A]	CLA	C3D-C2D	4.38	1.51	1.39
23	c	513	CLA	CHD-C1D	4.37	1.46	1.38
33	a	418[B]	LHG	O8-C23	4.37	1.46	1.33
23	b	614	CLA	C1D-ND	4.37	1.43	1.37
23	D	403[B]	CLA	O2A-CGA	4.37	1.46	1.33
23	a	404[A]	CLA	CHC-C1C	4.36	1.47	1.38
23	c	512	CLA	CHD-C1D	4.36	1.46	1.38
26	b	620	SQD	O48-C23	4.36	1.46	1.33
23	B	602	CLA	CHD-C1D	4.36	1.46	1.38
24	a	406[A]	PHO	OBD-CAD	4.36	1.28	1.22
23	c	503	CLA	CHC-C1C	4.35	1.47	1.38
23	C	510	CLA	CHD-C4C	4.35	1.49	1.39
23	C	502	CLA	CHC-C1C	4.35	1.47	1.38
38	F	102	HEM	FE-NC	4.35	2.09	1.95
26	b	620	SQD	O47-C7	4.35	1.46	1.34
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C1D-ND	4.34	1.43	1.37
23	C	506	CLA	C1D-ND	4.34	1.43	1.37
23	c	508	CLA	CHD-C1D	4.34	1.46	1.38
33	d	408[B]	LHG	O8-C23	4.33	1.46	1.33
23	c	503	CLA	O2A-CGA	4.33	1.46	1.33
23	b	601	CLA	CHD-C1D	4.33	1.46	1.38
23	b	607	CLA	CHD-C1D	4.33	1.46	1.38
23	C	502	CLA	C3D-C2D	4.33	1.50	1.39
23	c	505	CLA	CHC-C1C	4.33	1.47	1.38
23	D	403[B]	CLA	CHC-C1C	4.32	1.47	1.38
23	c	506	CLA	C1D-ND	4.32	1.43	1.37
23	B	605	CLA	CHC-C4B	4.32	1.49	1.39
25	b	618	BCR	C23-C22	-4.32	1.36	1.45
23	b	604	CLA	O2D-CGD	4.32	1.43	1.33
24	A	416[A]	PHO	OBD-CAD	4.31	1.28	1.22
23	C	508	CLA	CHC-C1C	4.31	1.47	1.38
23	a	404[B]	CLA	CHD-C1D	4.31	1.46	1.38
23	c	502	CLA	CHD-C1D	4.31	1.46	1.38
23	b	608	CLA	CHD-C1D	4.31	1.46	1.38
23	A	404[A]	CLA	CHC-C1C	4.31	1.47	1.38
33	d	408[A]	LHG	O8-C23	4.31	1.45	1.33
23	d	403[B]	CLA	CHC-C1C	4.30	1.47	1.38
32	m	101	LMG	O8-C28	4.30	1.45	1.33
23	c	511	CLA	CHC-C1C	4.30	1.47	1.38
23	b	605	CLA	CHC-C1C	4.30	1.47	1.38
23	b	612	CLA	CHC-C1C	4.30	1.47	1.38
23	C	508	CLA	O2A-CGA	4.30	1.45	1.33
23	b	611	CLA	O2A-CGA	4.30	1.45	1.33
23	A	408	CLA	O2A-CGA	4.28	1.45	1.33
23	d	404	CLA	O2A-CGA	4.28	1.45	1.33
23	A	408	CLA	CHC-C1C	4.28	1.47	1.38
23	D	403[A]	CLA	C1D-ND	4.27	1.43	1.37
23	c	512	CLA	O2A-CGA	4.27	1.45	1.33
23	A	406[B]	CLA	CHD-C1D	4.26	1.46	1.38
23	B	604	CLA	C1D-ND	4.26	1.43	1.37
23	B	607	CLA	C1B-NB	-4.26	1.32	1.37
23	C	502	CLA	CHD-C1D	4.26	1.46	1.38
23	C	501	CLA	CHD-C1D	4.25	1.46	1.38
23	a	407	CLA	O2A-CGA	4.25	1.45	1.33
32	c	521	LMG	O8-C28	4.25	1.45	1.33
23	D	403[A]	CLA	CHC-C1C	4.25	1.47	1.38
23	a	404[B]	CLA	CHC-C1C	4.25	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	508	CLA	O2A-CGA	4.24	1.45	1.33
23	C	513	CLA	CHD-C1D	4.24	1.46	1.38
23	c	509	CLA	CHD-C1D	4.24	1.46	1.38
23	c	505	CLA	C3D-C2D	4.24	1.50	1.39
23	d	404	CLA	O2D-CGD	4.23	1.43	1.33
23	B	609	CLA	O2A-CGA	4.23	1.45	1.33
23	C	513	CLA	O2A-CGA	4.23	1.45	1.33
23	b	601	CLA	C3D-C2D	4.22	1.50	1.39
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
23	b	616	CLA	O2A-CGA	4.22	1.45	1.33
23	D	403[A]	CLA	O2A-CGA	4.22	1.45	1.33
32	C	519	LMG	O8-C28	4.22	1.45	1.33
23	c	507	CLA	CHC-C1C	4.22	1.47	1.38
23	C	511	CLA	CHD-C1D	4.21	1.46	1.38
23	B	611	CLA	CHB-C1B	4.21	1.48	1.39
23	A	408	CLA	C1D-ND	4.21	1.43	1.37
23	C	508	CLA	C3D-C2D	4.21	1.50	1.39
26	f	102	SQD	O48-C23	4.20	1.45	1.33
35	C	518	DGD	O1G-C1A	4.20	1.45	1.33
23	D	403[B]	CLA	CHD-C1D	4.20	1.46	1.38
23	b	607	CLA	O2D-CGD	4.20	1.43	1.33
23	d	404	CLA	CHD-C1D	4.20	1.46	1.38
23	B	614	CLA	CHD-C4C	4.20	1.48	1.39
23	b	610	CLA	CHB-C1B	4.19	1.48	1.39
23	d	402[B]	CLA	O2A-CGA	4.19	1.45	1.33
23	b	611	CLA	C1D-ND	4.19	1.42	1.37
23	B	601	CLA	CHD-C1D	4.19	1.46	1.38
33	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	C	507	CLA	O2A-CGA	4.19	1.45	1.33
23	c	510	CLA	C1B-NB	-4.19	1.32	1.37
26	B	620	SQD	O48-C23	4.18	1.45	1.33
35	C	516[B]	DGD	O2G-C1B	4.18	1.46	1.34
23	B	608	CLA	CHD-C1D	4.18	1.46	1.38
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
23	b	604	CLA	CHC-C4B	4.18	1.48	1.39
23	B	603	CLA	CHC-C1C	4.18	1.47	1.38
23	B	614	CLA	CHB-C1B	4.18	1.48	1.39
23	c	504	CLA	CHD-C4C	4.18	1.48	1.39
33	E	101[B]	LHG	O7-C7	4.18	1.46	1.34
23	b	609	CLA	CHB-C1B	4.18	1.48	1.39
23	b	611	CLA	CHB-C1B	4.17	1.48	1.39
23	C	509	CLA	CHC-C1C	4.17	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	C3D-C2D	4.17	1.50	1.39
23	C	512	CLA	O2A-CGA	4.17	1.45	1.33
23	b	602	CLA	CHD-C4C	4.16	1.48	1.39
23	B	616	CLA	C1D-ND	4.16	1.42	1.37
23	c	507	CLA	CHD-C1D	4.16	1.46	1.38
32	Z	101	LMG	O7-C10	4.16	1.46	1.34
23	a	404[B]	CLA	CHD-C4C	4.16	1.48	1.39
23	B	611	CLA	O2A-CGA	4.16	1.45	1.33
23	d	403[B]	CLA	CHB-C1B	4.16	1.48	1.39
33	a	418[B]	LHG	O7-C7	4.16	1.46	1.34
23	c	512	CLA	CHB-C1B	4.15	1.48	1.39
23	B	608	CLA	O2D-CGD	4.15	1.43	1.33
23	a	405[A]	CLA	C1D-ND	4.15	1.42	1.37
33	L	101[B]	LHG	O8-C23	4.15	1.45	1.33
23	b	609	CLA	CHD-C1D	4.14	1.46	1.38
24	A	407[A]	PHO	OBD-CAD	4.14	1.28	1.22
23	b	601	CLA	CHD-C4C	4.14	1.48	1.39
23	d	402[B]	CLA	C3D-C2D	4.14	1.50	1.39
23	b	612	CLA	CHD-C1D	4.13	1.46	1.38
33	a	418[A]	LHG	O7-C7	4.13	1.46	1.34
23	A	406[B]	CLA	CHD-C4C	4.13	1.48	1.39
26	a	409[B]	SQD	O47-C7	4.13	1.46	1.34
23	C	501	CLA	O2A-CGA	4.13	1.45	1.33
23	d	403[A]	CLA	CHC-C1C	4.13	1.46	1.38
23	b	603	CLA	CHD-C1D	4.13	1.46	1.38
26	a	410	SQD	O47-C7	4.13	1.45	1.34
23	c	514	CLA	CHD-C4C	4.12	1.48	1.39
32	C	519	LMG	O7-C10	4.12	1.45	1.34
23	A	404[B]	CLA	CHD-C1D	4.12	1.46	1.38
23	a	405[A]	CLA	O2A-CGA	4.12	1.45	1.33
23	c	503	CLA	C3D-C2D	4.12	1.50	1.39
23	c	510	CLA	CHC-C1C	4.12	1.46	1.38
23	B	610	CLA	CHB-C1B	4.12	1.48	1.39
23	b	604	CLA	CHD-C1D	4.12	1.46	1.38
23	C	512	CLA	CHD-C1D	4.11	1.46	1.38
23	d	403[A]	CLA	CHB-C1B	4.11	1.48	1.39
23	A	405[B]	CLA	O2A-CGA	4.11	1.45	1.33
35	c	517[B]	DGD	O2G-C1B	4.11	1.45	1.34
23	C	507	CLA	C1D-ND	4.11	1.42	1.37
23	A	405[B]	CLA	CHD-C1D	4.11	1.46	1.38
23	C	507	CLA	CHD-C1D	4.10	1.46	1.38
32	c	501	LMG	O7-C10	4.10	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	CHD-C1D	4.10	1.46	1.38
23	c	506	CLA	CHD-C1D	4.10	1.46	1.38
35	c	518[B]	DGD	O1G-C1A	4.10	1.45	1.33
23	B	614	CLA	C4B-NB	-4.09	1.32	1.37
23	C	503	CLA	CHC-C4B	4.09	1.48	1.39
23	B	616	CLA	CHB-C1B	4.09	1.48	1.39
32	z	101	LMG	O7-C10	4.09	1.45	1.34
23	C	508	CLA	OBD-CAD	4.09	1.29	1.22
23	c	509	CLA	C3D-C2D	4.09	1.50	1.39
23	A	406[B]	CLA	C3D-C2D	4.09	1.50	1.39
35	c	517[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	d	403[B]	CLA	O2A-CGA	4.09	1.45	1.33
23	c	510	CLA	CHD-C1D	4.09	1.46	1.38
23	c	508	CLA	CHD-C4C	4.08	1.48	1.39
23	d	402[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	C	511	CLA	O2A-CGA	4.08	1.45	1.33
23	b	610	CLA	OBD-CAD	4.08	1.29	1.22
23	B	611	CLA	C1C-C2C	4.07	1.52	1.44
23	b	610	CLA	CHD-C1D	4.07	1.46	1.38
26	a	409[A]	SQD	O47-C7	4.07	1.45	1.34
23	B	601	CLA	CHC-C4B	4.07	1.48	1.39
23	C	502	CLA	O2A-CGA	4.07	1.45	1.33
23	c	507	CLA	O2A-CGA	4.06	1.45	1.33
26	F	103	SQD	O48-C23	4.06	1.45	1.33
35	h	102	DGD	O2G-C1B	4.06	1.45	1.34
23	c	502	CLA	CHB-C1B	4.06	1.48	1.39
23	D	404	CLA	CHB-C1B	4.06	1.48	1.39
23	C	504	CLA	C3D-C2D	4.06	1.50	1.39
32	c	520	LMG	O7-C10	4.06	1.45	1.34
35	C	516[A]	DGD	O2G-C1B	4.06	1.45	1.34
23	B	607	CLA	O2D-CGD	4.06	1.43	1.33
23	D	403[A]	CLA	CHB-C1B	4.06	1.48	1.39
23	C	513	CLA	CHD-C4C	4.05	1.48	1.39
23	A	405[A]	CLA	C3D-C2D	4.05	1.50	1.39
23	d	403[A]	CLA	O2A-CGA	4.05	1.45	1.33
38	f	101	HEM	FE-NC	4.05	2.08	1.95
23	D	403[B]	CLA	CHD-C4C	4.05	1.48	1.39
23	C	506	CLA	CHC-C1C	4.05	1.46	1.38
32	c	520	LMG	O8-C28	4.05	1.45	1.33
32	c	501	LMG	O8-C28	4.04	1.45	1.33
23	B	611	CLA	C3B-C2B	4.04	1.54	1.41
23	c	505	CLA	CHD-C1D	4.04	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	CHB-C1B	4.04	1.48	1.39
35	H	102	DGD	O1G-C1A	4.04	1.45	1.33
23	A	404[B]	CLA	CHD-C4C	4.04	1.48	1.39
23	C	512	CLA	CHC-C4B	4.04	1.48	1.39
23	B	612	CLA	C1B-NB	-4.04	1.32	1.37
23	c	509	CLA	O2A-CGA	4.04	1.45	1.33
23	A	404[A]	CLA	CHD-C1D	4.03	1.46	1.38
23	B	606	CLA	CHB-C1B	4.03	1.48	1.39
23	c	502	CLA	O2D-CGD	4.03	1.43	1.33
23	c	504	CLA	CHC-C4B	4.03	1.48	1.39
23	A	408	CLA	CHD-C1D	4.02	1.46	1.38
23	B	610	CLA	CHD-C1D	4.02	1.46	1.38
23	A	406[B]	CLA	O2A-CGA	4.02	1.45	1.33
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
23	C	505	CLA	CHC-C4B	4.02	1.48	1.39
32	A	418	LMG	O8-C28	4.02	1.45	1.33
23	b	612	CLA	C3D-C2D	4.02	1.50	1.39
23	B	603	CLA	CHB-C1B	4.02	1.48	1.39
26	a	409[B]	SQD	O48-C23	4.01	1.45	1.33
23	c	504	CLA	O2A-CGA	4.01	1.45	1.33
23	C	503	CLA	CHD-C1D	4.01	1.46	1.38
23	b	615	CLA	O2A-CGA	4.01	1.45	1.33
23	B	602	CLA	CHD-C4C	4.01	1.48	1.39
23	a	405[B]	CLA	O2A-CGA	4.00	1.45	1.33
23	b	614	CLA	C3D-C2D	4.00	1.50	1.39
23	B	615	CLA	C3D-C2D	4.00	1.50	1.39
32	B	621	LMG	O7-C10	4.00	1.45	1.34
23	c	505	CLA	O2A-CGA	4.00	1.45	1.33
34	b	622	HTG	C1'-S1	-4.00	1.76	1.81
23	c	502	CLA	CHD-C4C	3.99	1.48	1.39
23	C	506	CLA	O2A-CGA	3.99	1.45	1.33
23	b	608	CLA	C1D-ND	3.99	1.42	1.37
23	c	504	CLA	CHB-C1B	3.99	1.48	1.39
26	A	410[B]	SQD	O48-C23	3.99	1.45	1.33
23	a	404[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	c	511	CLA	O2A-CGA	3.99	1.45	1.33
23	b	604	CLA	CHB-C1B	3.99	1.48	1.39
33	D	408[B]	LHG	O8-C23	3.99	1.45	1.33
23	c	506	CLA	CHC-C4B	3.99	1.48	1.39
23	B	616	CLA	O2A-CGA	3.99	1.45	1.33
23	b	616	CLA	C3D-C2D	3.98	1.50	1.39
23	C	505	CLA	CHD-C1D	3.98	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	D	408[A]	LHG	O7-C7	3.98	1.45	1.34
24	A	416[B]	PHO	O2A-CGA	3.98	1.45	1.33
26	a	409[A]	SQD	O48-C23	3.98	1.45	1.33
26	A	412	SQD	O47-C7	3.98	1.45	1.34
23	B	610	CLA	CHD-C4C	3.98	1.48	1.39
23	c	508	CLA	C3D-C2D	3.98	1.50	1.39
23	B	607	CLA	OBD-CAD	3.98	1.29	1.22
23	d	402[B]	CLA	CHD-C1D	3.98	1.46	1.38
23	c	502	CLA	O2A-CGA	3.97	1.44	1.33
23	B	616	CLA	C3D-C2D	3.97	1.50	1.39
23	c	513	CLA	CHD-C4C	3.97	1.48	1.39
23	B	604	CLA	CHB-C1B	3.97	1.48	1.39
23	C	509	CLA	CHD-C4C	3.97	1.48	1.39
23	c	510	CLA	O2A-CGA	3.96	1.44	1.33
23	B	608	CLA	C3D-C2D	3.96	1.49	1.39
23	b	612	CLA	CHB-C1B	3.96	1.48	1.39
23	B	610	CLA	C3D-C2D	3.96	1.49	1.39
23	B	615	CLA	OBD-CAD	3.96	1.29	1.22
23	a	404[A]	CLA	CHD-C4C	3.96	1.48	1.39
23	B	614	CLA	CHC-C4B	3.95	1.48	1.39
23	C	511	CLA	CHB-C1B	3.94	1.48	1.39
23	B	605	CLA	CHB-C1B	3.94	1.48	1.39
25	B	618	BCR	C23-C22	-3.94	1.37	1.45
23	C	509	CLA	C3D-C2D	3.94	1.49	1.39
23	B	614	CLA	O2A-CGA	3.94	1.44	1.33
23	B	613	CLA	C3D-C2D	3.94	1.49	1.39
35	C	517[B]	DGD	O1G-C1A	3.94	1.44	1.33
23	c	507	CLA	CHD-C4C	3.94	1.48	1.39
23	d	403[B]	CLA	C1D-ND	3.94	1.42	1.37
32	d	412	LMG	O8-C28	3.94	1.44	1.33
23	D	404	CLA	OBD-CAD	3.93	1.29	1.22
23	d	404	CLA	CHB-C1B	3.93	1.48	1.39
23	b	608	CLA	C3D-C2D	3.93	1.49	1.39
23	b	607	CLA	CHB-C1B	3.93	1.48	1.39
23	B	607	CLA	CHD-C1D	3.92	1.46	1.38
23	B	609	CLA	C3D-C2D	3.92	1.49	1.39
23	c	509	CLA	CHD-C4C	3.92	1.48	1.39
23	b	609	CLA	O2A-CGA	3.92	1.44	1.33
23	B	613	CLA	CHB-C1B	3.92	1.48	1.39
23	c	504	CLA	O2D-CGD	3.92	1.42	1.33
23	D	403[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	C	506	CLA	CHD-C4C	3.92	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	404	CLA	CHC-C4B	3.92	1.48	1.39
23	B	605	CLA	O2A-CGA	3.92	1.44	1.33
23	B	611	CLA	OBD-CAD	3.92	1.29	1.22
23	C	513	CLA	C3D-C2D	3.91	1.49	1.39
23	C	501	CLA	CHC-C4B	3.91	1.48	1.39
23	C	511	CLA	C3D-C2D	3.91	1.49	1.39
23	B	613	CLA	CHD-C1D	3.91	1.46	1.38
23	C	503	CLA	CHD-C4C	3.91	1.48	1.39
23	B	601	CLA	CHD-C4C	3.91	1.48	1.39
23	b	608	CLA	OBD-CAD	3.91	1.29	1.22
23	b	610	CLA	CHC-C4B	3.91	1.48	1.39
33	d	407[B]	LHG	O7-C7	3.91	1.45	1.34
23	b	610	CLA	CHD-C4C	3.91	1.48	1.39
23	b	613	CLA	C1B-NB	-3.91	1.33	1.37
33	D	408[A]	LHG	O8-C23	3.90	1.44	1.33
32	A	418	LMG	O7-C10	3.90	1.45	1.34
23	C	508	CLA	CHD-C1D	3.90	1.46	1.38
23	b	616	CLA	CHD-C1D	3.90	1.46	1.38
23	c	510	CLA	CHB-C1B	3.90	1.48	1.39
23	c	506	CLA	CHD-C4C	3.90	1.48	1.39
23	c	513	CLA	CHB-C1B	3.90	1.48	1.39
23	b	613	CLA	C3D-C2D	3.90	1.49	1.39
23	a	405[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	B	612	CLA	CHD-C1D	3.90	1.46	1.38
24	a	414[B]	PHO	O2A-CGA	3.90	1.44	1.33
23	D	403[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	C	510	CLA	CHD-C1D	3.89	1.45	1.38
23	b	606	CLA	CHD-C1D	3.89	1.45	1.38
23	c	502	CLA	C3D-C2D	3.89	1.49	1.39
23	B	609	CLA	CHC-C4B	3.89	1.48	1.39
35	h	102	DGD	O1G-C1A	3.89	1.44	1.33
23	B	607	CLA	CHB-C1B	3.89	1.48	1.39
23	C	504	CLA	CHB-C1B	3.89	1.48	1.39
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
23	C	505	CLA	CHD-C4C	3.89	1.48	1.39
23	c	513	CLA	CHC-C4B	3.89	1.48	1.39
23	A	406[B]	CLA	OBD-CAD	3.89	1.29	1.22
23	B	615	CLA	O2A-CGA	3.89	1.44	1.33
23	c	506	CLA	CHB-C1B	3.89	1.48	1.39
23	a	405[B]	CLA	CHC-C4B	3.88	1.48	1.39
23	B	612	CLA	C4B-NB	-3.88	1.33	1.37
23	C	509	CLA	C4B-NB	-3.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	CHB-C1B	3.87	1.48	1.39
23	c	512	CLA	CHD-C4C	3.87	1.48	1.39
23	d	403[A]	CLA	C1B-NB	-3.87	1.33	1.37
23	B	604	CLA	CHD-C4C	3.87	1.48	1.39
33	b	629[B]	LHG	O7-C7	3.87	1.45	1.34
23	b	615	CLA	CHC-C4B	3.87	1.48	1.39
23	C	512	CLA	C3D-C2D	3.87	1.49	1.39
33	L	101[B]	LHG	O7-C7	3.87	1.45	1.34
23	c	503	CLA	CHD-C1D	3.86	1.45	1.38
23	B	609	CLA	CHD-C4C	3.86	1.48	1.39
23	A	405[B]	CLA	C3D-C2D	3.86	1.49	1.39
33	D	407[B]	LHG	O8-C23	3.86	1.44	1.33
23	d	402[B]	CLA	C1B-NB	-3.86	1.33	1.37
23	d	404	CLA	C3D-C2D	3.86	1.49	1.39
24	A	416[A]	PHO	O2A-CGA	3.86	1.44	1.33
32	d	412	LMG	O7-C10	3.86	1.45	1.34
23	c	503	CLA	CHB-C1B	3.85	1.48	1.39
23	C	509	CLA	O2A-CGA	3.85	1.44	1.33
35	C	517[A]	DGD	O2G-C1B	3.85	1.45	1.34
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	b	614	CLA	O2A-CGA	3.84	1.44	1.33
40	v	201	HEC	FE-NB	3.84	2.06	1.94
23	C	505	CLA	CHB-C1B	3.84	1.48	1.39
23	D	404	CLA	CHD-C4C	3.84	1.48	1.39
33	L	101[A]	LHG	O8-C23	3.84	1.44	1.33
23	c	511	CLA	CHD-C4C	3.84	1.48	1.39
33	D	408[B]	LHG	O7-C7	3.84	1.45	1.34
23	b	606	CLA	CHB-C1B	3.84	1.48	1.39
23	b	611	CLA	CHC-C4B	3.84	1.48	1.39
23	b	614	CLA	CHD-C1D	3.84	1.45	1.38
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
23	C	507	CLA	CHC-C4B	3.84	1.48	1.39
23	b	605	CLA	CHD-C4C	3.84	1.48	1.39
23	b	611	CLA	CHD-C4C	3.84	1.48	1.39
23	d	403[B]	CLA	CHD-C1D	3.84	1.45	1.38
35	c	518[A]	DGD	O1G-C1A	3.83	1.44	1.33
23	a	404[B]	CLA	C3D-C2D	3.83	1.49	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	C	510	CLA	O2A-CGA	3.83	1.44	1.33
23	C	512	CLA	CHD-C4C	3.83	1.48	1.39
23	c	510	CLA	C3D-C2D	3.83	1.49	1.39
24	a	414[A]	PHO	O2A-CGA	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	CHD-C4C	3.82	1.48	1.39
23	B	608	CLA	CHC-C1C	3.82	1.46	1.38
23	b	608	CLA	O2A-CGA	3.82	1.44	1.33
23	a	404[B]	CLA	O2A-CGA	3.82	1.44	1.33
23	b	615	CLA	CHB-C1B	3.82	1.48	1.39
23	c	514	CLA	C3D-C2D	3.82	1.49	1.39
23	A	408	CLA	CHD-C4C	3.82	1.48	1.39
23	c	511	CLA	C3D-C2D	3.82	1.49	1.39
33	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
24	A	407[B]	PHO	O2A-CGA	3.82	1.44	1.33
23	C	513	CLA	CHB-C1B	3.82	1.48	1.39
23	B	604	CLA	OBD-CAD	3.81	1.29	1.22
23	C	506	CLA	C4B-NB	-3.81	1.33	1.37
23	b	608	CLA	CHD-C4C	3.81	1.47	1.39
23	b	603	CLA	CHC-C4B	3.81	1.48	1.39
23	C	501	CLA	O2D-CGD	3.81	1.42	1.33
23	b	605	CLA	CHB-C1B	3.81	1.48	1.39
23	B	603	CLA	CHD-C1D	3.81	1.45	1.38
23	B	602	CLA	C3D-C2D	3.81	1.49	1.39
34	b	623	HTG	C1'-S1	-3.81	1.76	1.81
40	v	201	HEC	FE-ND	3.81	2.06	1.94
23	b	611	CLA	CHD-C1D	3.81	1.45	1.38
23	d	403[A]	CLA	CHD-C1D	3.81	1.45	1.38
23	B	605	CLA	CHD-C1D	3.81	1.45	1.38
23	b	605	CLA	CHD-C1D	3.81	1.45	1.38
23	c	509	CLA	OBD-CAD	3.81	1.29	1.22
23	b	602	CLA	O2A-CGA	3.80	1.44	1.33
23	B	603	CLA	C1B-NB	-3.80	1.33	1.37
35	C	516[B]	DGD	O1G-C1A	3.80	1.44	1.33
33	b	629[B]	LHG	O8-C23	3.80	1.44	1.33
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
33	d	414[B]	LHG	O8-C23	3.80	1.44	1.33
23	b	604	CLA	OBD-CAD	3.80	1.29	1.22
35	c	517[B]	DGD	O1G-C1A	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
23	A	406[B]	CLA	CHC-C4B	3.80	1.47	1.39
35	c	518[B]	DGD	O2G-C1B	3.79	1.45	1.34
23	b	613	CLA	CHC-C4B	3.79	1.47	1.39
23	b	609	CLA	CHC-C4B	3.79	1.47	1.39
23	c	506	CLA	O2A-CGA	3.79	1.44	1.33
23	c	503	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	603	CLA	O2A-CGA	3.78	1.44	1.33
23	A	405[A]	CLA	CHB-C1B	3.78	1.47	1.39
23	b	607	CLA	C3D-C2D	3.78	1.49	1.39
23	c	507	CLA	CHB-C1B	3.78	1.47	1.39
23	C	505	CLA	O2A-CGA	3.78	1.44	1.33
23	A	404[B]	CLA	CHB-C1B	3.78	1.47	1.39
23	B	605	CLA	CHD-C4C	3.78	1.47	1.39
23	c	507	CLA	C3D-C2D	3.78	1.49	1.39
23	b	615	CLA	C1B-NB	-3.78	1.33	1.37
23	c	508	CLA	CHC-C4B	3.78	1.47	1.39
23	c	513	CLA	C3D-C2D	3.78	1.49	1.39
23	d	404	CLA	CHC-C4B	3.77	1.47	1.39
35	C	517[B]	DGD	O2G-C1B	3.77	1.44	1.34
23	b	615	CLA	CHD-C4C	3.77	1.47	1.39
23	c	512	CLA	OBD-CAD	3.77	1.29	1.22
23	d	402[A]	CLA	OBD-CAD	3.77	1.29	1.22
23	a	405[B]	CLA	CHD-C1D	3.77	1.45	1.38
33	D	407[B]	LHG	O7-C7	3.77	1.44	1.34
23	b	615	CLA	C3D-C2D	3.77	1.49	1.39
23	C	511	CLA	CHD-C4C	3.77	1.47	1.39
23	B	603	CLA	C3D-C2D	3.77	1.49	1.39
23	b	603	CLA	C3D-C2D	3.76	1.49	1.39
23	a	405[B]	CLA	CHD-C4C	3.76	1.47	1.39
23	B	615	CLA	CHB-C1B	3.76	1.47	1.39
23	B	605	CLA	C3D-C2D	3.76	1.49	1.39
23	C	513	CLA	OBD-CAD	3.76	1.29	1.22
23	b	603	CLA	CHD-C4C	3.76	1.47	1.39
23	a	407	CLA	C1B-NB	-3.76	1.33	1.37
23	C	501	CLA	CHB-C1B	3.76	1.47	1.39
23	C	506	CLA	C3D-C2D	3.76	1.49	1.39
23	a	407	CLA	CHB-C1B	3.75	1.47	1.39
23	b	602	CLA	C1B-NB	-3.75	1.33	1.37
23	a	405[A]	CLA	CHB-C1B	3.75	1.47	1.39
23	c	502	CLA	CHC-C4B	3.75	1.47	1.39
23	c	511	CLA	CHD-C1D	3.75	1.45	1.38
23	c	508	CLA	OBD-CAD	3.75	1.28	1.22
23	c	510	CLA	CHD-C4C	3.75	1.47	1.39
23	b	608	CLA	CHB-C1B	3.75	1.47	1.39
33	d	414[A]	LHG	O8-C23	3.75	1.44	1.33
23	B	607	CLA	CHC-C4B	3.74	1.47	1.39
23	b	609	CLA	OBD-CAD	3.74	1.28	1.22
23	C	504	CLA	C1B-NB	-3.74	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	505	CLA	C1B-NB	-3.74	1.33	1.37
33	A	419[B]	LHG	O8-C23	3.74	1.44	1.33
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	A	405[B]	CLA	CHC-C4B	3.74	1.47	1.39
23	a	405[B]	CLA	C3D-C2D	3.73	1.49	1.39
23	d	402[B]	CLA	CHC-C4B	3.73	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	c	513	CLA	OBD-CAD	3.73	1.28	1.22
23	b	606	CLA	O2A-CGA	3.73	1.44	1.33
23	B	611	CLA	CHD-C1D	3.73	1.45	1.38
23	C	507	CLA	CHB-C1B	3.73	1.47	1.39
23	a	404[B]	CLA	OBD-CAD	3.73	1.28	1.22
23	D	403[A]	CLA	C1B-NB	-3.72	1.33	1.37
33	d	407[A]	LHG	O7-C7	3.72	1.44	1.34
23	A	405[A]	CLA	CHD-C1D	3.72	1.45	1.38
23	b	616	CLA	CHC-C4B	3.72	1.47	1.39
23	A	405[B]	CLA	CHD-C4C	3.72	1.47	1.39
23	c	506	CLA	OBD-CAD	3.72	1.28	1.22
23	c	509	CLA	CHB-C1B	3.72	1.47	1.39
32	m	101	LMG	O7-C10	3.72	1.44	1.34
33	d	408[B]	LHG	O7-C7	3.71	1.44	1.34
23	B	601	CLA	C3D-C2D	3.71	1.49	1.39
23	B	604	CLA	CHC-C4B	3.71	1.47	1.39
23	C	510	CLA	OBD-CAD	3.71	1.28	1.22
35	C	517[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	b	602	CLA	C3D-C2D	3.71	1.49	1.39
33	d	414[B]	LHG	O7-C7	3.71	1.44	1.34
23	c	508	CLA	CHB-C1B	3.71	1.47	1.39
23	b	614	CLA	CHC-C4B	3.71	1.47	1.39
23	b	614	CLA	CHD-C4C	3.71	1.47	1.39
23	C	510	CLA	C3D-C2D	3.71	1.49	1.39
23	d	404	CLA	CHD-C4C	3.70	1.47	1.39
23	d	402[B]	CLA	CHD-C4C	3.70	1.47	1.39
23	B	606	CLA	CHC-C4B	3.70	1.47	1.39
23	c	503	CLA	OBD-CAD	3.70	1.28	1.22
23	b	614	CLA	CHB-C1B	3.70	1.47	1.39
23	c	506	CLA	C3D-C2D	3.70	1.49	1.39
23	c	512	CLA	C3D-C2D	3.69	1.49	1.39
23	a	404[A]	CLA	CHB-C1B	3.69	1.47	1.39
23	a	405[B]	CLA	OBD-CAD	3.69	1.28	1.22
23	C	503	CLA	O2A-CGA	3.69	1.44	1.33
23	C	506	CLA	CHB-C1B	3.69	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	613	CLA	CHD-C4C	3.69	1.47	1.39
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	A	405[B]	CLA	CHB-C1B	3.68	1.47	1.39
23	B	607	CLA	CHD-C4C	3.68	1.47	1.39
23	a	405[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	a	407	CLA	CHC-C4B	3.68	1.47	1.39
23	b	601	CLA	CHC-C4B	3.68	1.47	1.39
23	a	407	CLA	C1D-ND	3.68	1.42	1.37
23	A	404[A]	CLA	C4B-NB	-3.68	1.33	1.37
35	C	518	DGD	O2G-C1B	3.68	1.44	1.34
23	A	406[A]	CLA	C1B-NB	-3.67	1.33	1.37
23	B	602	CLA	O2A-CGA	3.67	1.44	1.33
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	C	510	CLA	CHB-C1B	3.67	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.66	1.49	1.39
23	d	403[B]	CLA	CHD-C4C	3.66	1.47	1.39
23	a	404[A]	CLA	C3D-C2D	3.66	1.49	1.39
33	d	408[A]	LHG	O7-C7	3.66	1.44	1.34
23	A	405[A]	CLA	C1B-NB	-3.66	1.33	1.37
23	a	407	CLA	CHD-C1D	3.66	1.45	1.38
23	B	603	CLA	CHC-C4B	3.65	1.47	1.39
23	B	615	CLA	CHD-C4C	3.65	1.47	1.39
23	b	604	CLA	CHD-C4C	3.65	1.47	1.39
23	b	612	CLA	CHC-C4B	3.65	1.47	1.39
23	D	403[B]	CLA	C3D-C2D	3.65	1.49	1.39
23	C	503	CLA	OBD-CAD	3.65	1.28	1.22
23	b	604	CLA	C3D-C2D	3.65	1.49	1.39
23	c	509	CLA	CHC-C4B	3.65	1.47	1.39
26	A	410[B]	SQD	O47-C7	3.64	1.44	1.34
23	D	403[B]	CLA	CHB-C1B	3.64	1.47	1.39
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
23	c	511	CLA	CHC-C4B	3.64	1.47	1.39
23	C	502	CLA	CHD-C4C	3.64	1.47	1.39
23	B	606	CLA	CHD-C4C	3.64	1.47	1.39
23	B	616	CLA	CHC-C4B	3.64	1.47	1.39
23	C	503	CLA	C3D-C2D	3.63	1.49	1.39
23	C	504	CLA	CHD-C1D	3.63	1.45	1.38
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	C	502	CLA	CHC-C4B	3.63	1.47	1.39
23	b	606	CLA	CHD-C4C	3.63	1.47	1.39
23	B	602	CLA	CHB-C1B	3.63	1.47	1.39
23	C	509	CLA	CHB-C1B	3.63	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	CHC-C4B	3.63	1.47	1.39
23	B	610	CLA	CHC-C4B	3.62	1.47	1.39
23	D	404	CLA	O2A-CGA	3.62	1.43	1.33
35	c	517[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	d	402[A]	CLA	CHD-C4C	3.62	1.47	1.39
33	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	a	404[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	b	609	CLA	CHD-C4C	3.61	1.47	1.39
23	B	606	CLA	CHD-C1D	3.61	1.45	1.38
23	C	507	CLA	C3D-C2D	3.61	1.49	1.39
23	C	509	CLA	OBD-CAD	3.61	1.28	1.22
23	C	501	CLA	C3D-C2D	3.61	1.49	1.39
23	C	506	CLA	OBD-CAD	3.61	1.28	1.22
23	B	613	CLA	OBD-CAD	3.60	1.28	1.22
23	B	616	CLA	C1B-NB	-3.60	1.33	1.37
23	B	603	CLA	OBD-CAD	3.60	1.28	1.22
33	D	407[A]	LHG	O7-C7	3.60	1.44	1.34
23	B	614	CLA	C3D-C2D	3.60	1.48	1.39
23	b	613	CLA	O2A-CGA	3.60	1.43	1.33
40	V	201	HEC	FE-NC	3.60	2.07	1.95
34	B	625	HTG	C1'-S1	-3.59	1.76	1.81
23	C	502	CLA	CHB-C1B	3.59	1.47	1.39
23	B	610	CLA	O2A-CGA	3.59	1.43	1.33
23	A	406[B]	CLA	CHB-C1B	3.59	1.47	1.39
24	a	406[B]	PHO	O2A-CGA	3.59	1.43	1.33
23	B	602	CLA	CHC-C4B	3.58	1.47	1.39
23	a	405[B]	CLA	CHB-C1B	3.58	1.47	1.39
23	B	613	CLA	C1B-NB	-3.58	1.33	1.37
23	b	601	CLA	OBD-CAD	3.58	1.28	1.22
23	a	405[A]	CLA	CHD-C4C	3.58	1.47	1.39
23	b	609	CLA	C3D-C2D	3.58	1.48	1.39
38	f	101	HEM	C4D-ND	-3.58	1.34	1.40
23	C	511	CLA	C4B-NB	-3.58	1.33	1.37
23	B	601	CLA	CHB-C1B	3.58	1.47	1.39
23	B	603	CLA	CHD-C4C	3.58	1.47	1.39
23	C	502	CLA	OBD-CAD	3.57	1.28	1.22
23	b	612	CLA	OBD-CAD	3.57	1.28	1.22
23	d	403[A]	CLA	CHD-C4C	3.57	1.47	1.39
23	B	608	CLA	CHB-C1B	3.57	1.47	1.39
23	b	606	CLA	CHC-C4B	3.57	1.47	1.39
23	D	404	CLA	C1B-NB	-3.57	1.33	1.37
23	A	408	CLA	C3D-C2D	3.57	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4B-NB	-3.56	1.33	1.37
35	c	519	DGD	O2G-C1B	3.56	1.44	1.34
23	C	504	CLA	O2A-CGA	3.56	1.43	1.33
33	A	419[B]	LHG	O7-C7	3.56	1.44	1.34
23	B	607	CLA	O2A-CGA	3.56	1.43	1.33
23	b	603	CLA	O2A-CGA	3.56	1.43	1.33
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	c	507	CLA	OBD-CAD	3.56	1.28	1.22
23	b	606	CLA	C3D-C2D	3.56	1.48	1.39
23	A	404[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	B	609	CLA	C3B-C4B	3.55	1.51	1.42
35	C	516[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	d	403[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	601	CLA	OBD-CAD	3.54	1.28	1.22
34	B	622	HTG	C1'-S1	-3.54	1.76	1.81
23	a	405[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	b	604	CLA	C1B-NB	-3.54	1.33	1.37
23	b	605	CLA	OBD-CAD	3.54	1.28	1.22
23	a	404[B]	CLA	CHB-C1B	3.54	1.47	1.39
23	b	602	CLA	OBD-CAD	3.54	1.28	1.22
35	c	518[A]	DGD	O2G-C1B	3.53	1.44	1.34
23	B	611	CLA	CHD-C4C	3.53	1.47	1.39
33	d	407[A]	LHG	O8-C23	3.53	1.43	1.33
33	D	407[A]	LHG	O8-C23	3.53	1.43	1.33
23	c	505	CLA	CHD-C4C	3.52	1.47	1.39
23	B	612	CLA	O2A-CGA	3.52	1.43	1.33
33	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
23	A	405[B]	CLA	OBD-CAD	3.52	1.28	1.22
33	d	407[B]	LHG	O8-C23	3.52	1.43	1.33
23	c	514	CLA	C4B-NB	-3.52	1.33	1.37
23	C	503	CLA	CHB-C1B	3.52	1.47	1.39
23	b	612	CLA	O2A-CGA	3.52	1.43	1.33
23	d	404	CLA	OBD-CAD	3.52	1.28	1.22
23	D	403[B]	CLA	CHC-C4B	3.51	1.47	1.39
23	b	608	CLA	CHC-C4B	3.51	1.47	1.39
23	b	610	CLA	C3D-C2D	3.51	1.48	1.39
23	d	402[B]	CLA	OBD-CAD	3.51	1.28	1.22
23	d	402[B]	CLA	CHB-C1B	3.51	1.47	1.39
23	B	606	CLA	C3D-C2D	3.51	1.48	1.39
23	b	601	CLA	CHB-C1B	3.51	1.47	1.39
35	H	102	DGD	O2G-C1B	3.51	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	C3D-C2D	3.51	1.48	1.39
23	C	504	CLA	CHD-C4C	3.51	1.47	1.39
23	b	606	CLA	OBD-CAD	3.50	1.28	1.22
33	d	414[A]	LHG	O7-C7	3.50	1.44	1.34
23	B	607	CLA	C1D-ND	3.50	1.42	1.37
23	b	613	CLA	CHD-C1D	3.50	1.45	1.38
23	C	506	CLA	C1B-NB	-3.50	1.33	1.37
23	B	616	CLA	CHD-C1D	3.50	1.45	1.38
23	B	609	CLA	CHB-C1B	3.49	1.47	1.39
33	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
33	b	629[A]	LHG	O8-C23	3.49	1.43	1.33
23	C	509	CLA	CHC-C4B	3.49	1.47	1.39
23	C	501	CLA	CHD-C4C	3.49	1.47	1.39
23	c	507	CLA	CHC-C4B	3.48	1.47	1.39
23	c	514	CLA	CHB-C1B	3.48	1.47	1.39
23	B	606	CLA	O2A-CGA	3.48	1.43	1.33
32	D	412	LMG	O7-C10	3.48	1.44	1.34
23	A	404[B]	CLA	O2A-CGA	3.48	1.43	1.33
23	d	402[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	B	611	CLA	C3B-C4B	3.48	1.50	1.42
23	c	514	CLA	C1B-NB	-3.47	1.33	1.37
23	D	403[B]	CLA	OBD-CAD	3.47	1.28	1.22
23	C	512	CLA	OBD-CAD	3.47	1.28	1.22
23	d	402[A]	CLA	CHC-C4B	3.47	1.47	1.39
23	c	514	CLA	CHC-C4B	3.47	1.47	1.39
23	c	508	CLA	C1B-NB	-3.46	1.33	1.37
23	B	612	CLA	C1D-ND	3.46	1.42	1.37
23	c	505	CLA	OBD-CAD	3.45	1.28	1.22
23	d	403[B]	CLA	C3D-C2D	3.45	1.48	1.39
23	b	616	CLA	OBD-CAD	3.45	1.28	1.22
23	c	511	CLA	OBD-CAD	3.45	1.28	1.22
23	c	512	CLA	CHC-C4B	3.44	1.47	1.39
23	C	504	CLA	CHC-C4B	3.44	1.47	1.39
23	b	613	CLA	CHB-C1B	3.44	1.47	1.39
38	F	102	HEM	C4D-ND	-3.44	1.34	1.40
23	d	403[B]	CLA	OBD-CAD	3.44	1.28	1.22
23	B	602	CLA	C1B-NB	-3.44	1.33	1.37
23	c	514	CLA	OBD-CAD	3.43	1.28	1.22
23	c	507	CLA	C1B-NB	-3.43	1.33	1.37
23	D	403[A]	CLA	C3D-C2D	3.43	1.48	1.39
32	D	412	LMG	O8-C28	3.43	1.43	1.33
23	A	406[A]	CLA	CHB-C1B	3.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[B]	CLA	C4B-NB	-3.43	1.33	1.37
23	b	605	CLA	CHC-C4B	3.43	1.47	1.39
23	B	608	CLA	CHD-C4C	3.42	1.47	1.39
23	D	403[B]	CLA	C1B-NB	-3.42	1.33	1.37
23	d	403[A]	CLA	CHC-C4B	3.42	1.47	1.39
23	b	607	CLA	C1D-ND	3.42	1.42	1.37
23	b	603	CLA	OBD-CAD	3.42	1.28	1.22
23	B	612	CLA	CHD-C4C	3.42	1.47	1.39
23	B	611	CLA	C3D-C2D	3.41	1.48	1.39
23	A	404[B]	CLA	CHC-C4B	3.41	1.47	1.39
23	d	403[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	B	604	CLA	O2A-CGA	3.41	1.43	1.33
23	C	507	CLA	CHD-C4C	3.40	1.47	1.39
23	C	508	CLA	CHD-C4C	3.40	1.47	1.39
23	b	612	CLA	C1B-NB	-3.40	1.33	1.37
23	C	510	CLA	CHC-C4B	3.40	1.47	1.39
23	B	613	CLA	CHC-C4B	3.40	1.47	1.39
23	b	605	CLA	O2A-CGA	3.40	1.43	1.33
24	a	406[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	b	601	CLA	C3B-C4B	3.39	1.50	1.42
23	c	505	CLA	CHB-C1B	3.38	1.47	1.39
23	C	501	CLA	C1B-NB	-3.38	1.33	1.37
23	C	506	CLA	CHC-C4B	3.38	1.47	1.39
23	b	615	CLA	OBD-CAD	3.38	1.28	1.22
38	F	102	HEM	C1B-NB	-3.38	1.34	1.40
23	b	603	CLA	CHB-C1B	3.37	1.47	1.39
23	b	605	CLA	C1B-NB	-3.37	1.33	1.37
23	c	510	CLA	OBD-CAD	3.37	1.28	1.22
23	B	615	CLA	CHC-C4B	3.36	1.47	1.39
23	D	404	CLA	C3B-C4B	3.36	1.50	1.42
23	b	602	CLA	C3B-C4B	3.36	1.50	1.42
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	d	403[B]	CLA	CHC-C4B	3.36	1.46	1.39
23	b	612	CLA	CHD-C4C	3.36	1.46	1.39
23	B	614	CLA	CHD-C1D	3.35	1.44	1.38
23	A	404[B]	CLA	OBD-CAD	3.35	1.28	1.22
34	c	522	HTG	C1'-S1	-3.35	1.77	1.81
23	C	505	CLA	C3D-C2D	3.35	1.48	1.39
23	c	504	CLA	C3D-C2D	3.34	1.48	1.39
23	B	607	CLA	C3D-C2D	3.34	1.48	1.39
23	d	403[B]	CLA	C4B-NB	-3.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	C	510	CLA	C1B-NB	-3.34	1.33	1.37
23	D	403[A]	CLA	CHC-C4B	3.33	1.46	1.39
23	B	612	CLA	C3D-C2D	3.33	1.48	1.39
23	C	512	CLA	CHB-C1B	3.33	1.46	1.39
23	c	507	CLA	C4B-NB	-3.33	1.33	1.37
23	a	404[B]	CLA	CHC-C4B	3.33	1.46	1.39
23	b	616	CLA	C3B-C4B	3.32	1.50	1.42
23	b	614	CLA	OBD-CAD	3.32	1.28	1.22
23	A	406[B]	CLA	C3B-C4B	3.32	1.50	1.42
23	C	509	CLA	C1B-NB	-3.31	1.33	1.37
23	C	505	CLA	OBD-CAD	3.31	1.28	1.22
23	c	504	CLA	C3B-C4B	3.31	1.50	1.42
23	C	513	CLA	CHC-C4B	3.31	1.46	1.39
23	c	505	CLA	C4B-NB	-3.30	1.33	1.37
23	B	612	CLA	CHC-C4B	3.30	1.46	1.39
23	b	607	CLA	CHD-C4C	3.30	1.46	1.39
23	a	404[A]	CLA	C1B-NB	-3.30	1.33	1.37
40	v	201	HEC	FE-NC	3.30	2.06	1.95
23	b	610	CLA	C1B-NB	-3.29	1.33	1.37
23	a	405[B]	CLA	C3B-C4B	3.29	1.50	1.42
23	B	608	CLA	O2A-CGA	3.29	1.43	1.33
23	c	510	CLA	C4B-NB	-3.29	1.33	1.37
23	c	505	CLA	CHC-C4B	3.29	1.46	1.39
23	B	610	CLA	C1B-NB	-3.28	1.33	1.37
23	A	404[B]	CLA	C1B-NB	-3.28	1.33	1.37
23	b	602	CLA	CHB-C1B	3.28	1.46	1.39
23	c	502	CLA	OBD-CAD	3.28	1.28	1.22
23	B	603	CLA	C4B-NB	-3.28	1.33	1.37
23	C	513	CLA	C1B-NB	-3.28	1.33	1.37
23	B	604	CLA	C3D-C2D	3.28	1.48	1.39
23	d	403[A]	CLA	C1D-ND	3.27	1.41	1.37
34	D	411	HTG	C1'-S1	-3.27	1.77	1.81
23	B	602	CLA	OBD-CAD	3.27	1.28	1.22
23	B	613	CLA	O2A-CGA	3.27	1.42	1.33
23	D	403[A]	CLA	OBD-CAD	3.26	1.28	1.22
23	C	503	CLA	C1B-NB	-3.26	1.33	1.37
23	b	610	CLA	O2A-CGA	3.26	1.42	1.33
23	C	507	CLA	OBD-CAD	3.25	1.28	1.22
23	b	604	CLA	O2A-CGA	3.25	1.42	1.33
23	b	608	CLA	C1B-NB	-3.25	1.33	1.37
23	C	508	CLA	CHC-C4B	3.24	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	C1B-NB	-3.24	1.33	1.37
23	a	405[A]	CLA	CHC-C4B	3.24	1.46	1.39
23	a	407	CLA	C3D-C2D	3.24	1.48	1.39
23	b	612	CLA	C4B-NB	-3.23	1.33	1.37
23	B	615	CLA	C1C-C2C	3.23	1.50	1.44
23	B	612	CLA	OBD-CAD	3.23	1.28	1.22
23	c	506	CLA	C3B-C4B	3.23	1.50	1.42
23	b	616	CLA	CHB-C1B	3.23	1.46	1.39
23	a	407	CLA	CHD-C4C	3.23	1.46	1.39
23	C	512	CLA	C3B-C4B	3.22	1.50	1.42
23	A	408	CLA	CHC-C4B	3.21	1.46	1.39
23	b	611	CLA	C3D-C2D	3.21	1.47	1.39
23	B	616	CLA	CHD-C4C	3.21	1.46	1.39
38	f	101	HEM	C1B-NB	-3.21	1.34	1.40
23	B	608	CLA	C4B-NB	-3.20	1.33	1.37
23	b	611	CLA	C1B-NB	-3.20	1.33	1.37
23	C	513	CLA	C4B-NB	-3.20	1.33	1.37
23	B	608	CLA	CHC-C4B	3.20	1.46	1.39
23	A	405[A]	CLA	C3B-C4B	3.20	1.50	1.42
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	c	508	CLA	C4B-NB	-3.19	1.33	1.37
23	b	607	CLA	CHC-C4B	3.19	1.46	1.39
23	B	604	CLA	C1B-C2B	3.19	1.50	1.43
23	D	404	CLA	C1C-C2C	3.19	1.50	1.44
23	b	613	CLA	CHD-C4C	3.19	1.46	1.39
23	D	403[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	C	511	CLA	OBD-CAD	3.17	1.27	1.22
23	a	404[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	B	609	CLA	OBD-CAD	3.17	1.27	1.22
23	A	404[A]	CLA	CHC-C4B	3.15	1.46	1.39
23	B	605	CLA	C3B-C4B	3.15	1.50	1.42
23	C	507	CLA	C1B-NB	-3.14	1.33	1.37
23	C	505	CLA	C1B-NB	-3.14	1.33	1.37
23	C	501	CLA	C3B-C4B	3.14	1.50	1.42
23	b	603	CLA	C3B-C4B	3.13	1.50	1.42
23	b	602	CLA	C1C-C2C	3.13	1.50	1.44
23	A	406[A]	CLA	C3B-C4B	3.13	1.50	1.42
23	A	405[B]	CLA	C3B-C4B	3.12	1.50	1.42
23	b	613	CLA	C4B-NB	-3.12	1.33	1.37
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
23	d	403[B]	CLA	C1B-NB	-3.12	1.34	1.37
23	a	407	CLA	C1B-C2B	3.12	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	408	CLA	CHB-C1B	3.12	1.46	1.39
23	A	408	CLA	C1B-NB	-3.11	1.34	1.37
23	c	510	CLA	CHC-C4B	3.10	1.46	1.39
23	c	503	CLA	CHC-C4B	3.10	1.46	1.39
24	A	416[A]	PHO	CHA-CBD	-3.10	1.47	1.51
34	d	411	HTG	C1'-S1	-3.10	1.77	1.81
23	B	604	CLA	C1B-NB	-3.10	1.34	1.37
23	A	404[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	a	405[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	C	502	CLA	C4B-NB	-3.09	1.34	1.37
23	b	606	CLA	C1B-NB	-3.09	1.34	1.37
23	C	504	CLA	OBD-CAD	3.08	1.27	1.22
23	b	607	CLA	C1B-C2B	3.08	1.50	1.43
23	C	503	CLA	C3B-C4B	3.08	1.50	1.42
23	B	608	CLA	C1B-NB	-3.07	1.34	1.37
23	a	404[A]	CLA	O2A-CGA	3.07	1.42	1.33
23	C	507	CLA	C4B-NB	-3.07	1.34	1.37
23	b	607	CLA	O2A-CGA	3.07	1.42	1.33
23	c	506	CLA	C1B-NB	-3.07	1.34	1.37
23	a	404[B]	CLA	C4B-NB	-3.07	1.34	1.37
34	b	625	HTG	C1'-S1	-3.07	1.77	1.81
23	A	406[B]	CLA	C1B-NB	-3.06	1.34	1.37
23	b	601	CLA	C1B-NB	-3.06	1.34	1.37
23	C	505	CLA	C3B-C4B	3.06	1.49	1.42
23	c	513	CLA	C3B-C4B	3.06	1.49	1.42
23	c	511	CLA	C1B-NB	-3.06	1.34	1.37
23	A	405[B]	CLA	C1B-NB	-3.05	1.34	1.37
23	a	405[A]	CLA	C3B-C4B	3.05	1.49	1.42
23	c	512	CLA	C1B-C2B	3.04	1.50	1.43
23	B	601	CLA	C3B-C4B	3.04	1.49	1.42
23	b	608	CLA	C3B-C4B	3.04	1.49	1.42
23	a	404[B]	CLA	C1B-NB	-3.04	1.34	1.37
23	a	407	CLA	OBD-CAD	3.04	1.27	1.22
23	B	616	CLA	C1C-C2C	3.03	1.50	1.44
23	B	614	CLA	OBD-CAD	3.03	1.27	1.22
23	B	607	CLA	C1B-C2B	3.02	1.50	1.43
23	d	402[B]	CLA	C3B-C4B	3.02	1.49	1.42
23	c	504	CLA	OBD-CAD	3.01	1.27	1.22
23	a	405[B]	CLA	C1B-NB	-3.00	1.34	1.37
23	C	505	CLA	C1B-C2B	2.99	1.50	1.43
23	B	615	CLA	C1B-C2B	2.99	1.50	1.43
23	d	403[A]	CLA	C4B-NB	-2.99	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	C1C-C2C	2.99	1.50	1.44
23	B	607	CLA	C4D-CHA	2.98	1.49	1.38
23	b	609	CLA	C1B-NB	-2.98	1.34	1.37
23	B	606	CLA	C1C-C2C	2.98	1.50	1.44
23	c	506	CLA	C1B-C2B	2.97	1.50	1.43
23	b	609	CLA	C3B-C4B	2.97	1.49	1.42
23	d	404	CLA	C3B-C4B	2.96	1.49	1.42
23	B	606	CLA	OBD-CAD	2.96	1.27	1.22
23	C	511	CLA	C4D-CHA	2.96	1.48	1.38
23	B	609	CLA	C1B-NB	-2.96	1.34	1.37
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	d	402[A]	CLA	C3B-C4B	2.96	1.49	1.42
23	B	606	CLA	C1B-NB	-2.95	1.34	1.37
23	c	505	CLA	C1B-C2B	2.95	1.50	1.43
23	c	504	CLA	C4B-NB	-2.95	1.34	1.37
23	b	612	CLA	C1B-C2B	2.94	1.50	1.43
23	C	502	CLA	C1B-NB	-2.94	1.34	1.37
23	B	616	CLA	C1B-C2B	2.94	1.50	1.43
23	C	504	CLA	C4D-CHA	2.94	1.48	1.38
23	c	514	CLA	C3B-C4B	2.93	1.49	1.42
23	B	614	CLA	C1B-C2B	2.93	1.50	1.43
23	D	403[B]	CLA	C4B-NB	-2.92	1.34	1.37
23	b	601	CLA	C4B-NB	-2.92	1.34	1.37
23	b	604	CLA	C1B-C2B	2.92	1.50	1.43
23	B	602	CLA	C4B-NB	-2.92	1.34	1.37
23	B	615	CLA	C3B-C4B	2.92	1.49	1.42
23	B	613	CLA	C1B-C2B	2.91	1.50	1.43
23	C	511	CLA	C1C-C2C	2.91	1.50	1.44
34	C	521	HTG	C1'-S1	-2.91	1.77	1.81
23	c	511	CLA	C1B-C2B	2.90	1.50	1.43
23	b	611	CLA	C1B-C2B	2.90	1.50	1.43
23	C	510	CLA	C4B-NB	-2.90	1.34	1.37
23	D	404	CLA	C4C-C3C	2.90	1.50	1.45
23	C	512	CLA	C1B-NB	-2.89	1.34	1.37
23	c	512	CLA	C1B-NB	-2.89	1.34	1.37
23	a	405[B]	CLA	C4B-NB	-2.89	1.34	1.37
23	b	610	CLA	C1B-C2B	2.89	1.50	1.43
23	a	404[B]	CLA	C4C-C3C	2.89	1.50	1.45
23	c	506	CLA	C4C-C3C	2.89	1.50	1.45
23	C	504	CLA	C4B-NB	-2.88	1.34	1.37
23	B	610	CLA	C3B-C4B	2.88	1.49	1.42
23	c	504	CLA	C1B-NB	-2.88	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C4B-NB	-2.87	1.34	1.37
23	A	406[A]	CLA	C4B-NB	-2.87	1.34	1.37
23	B	604	CLA	C4D-CHA	2.87	1.48	1.38
23	A	404[B]	CLA	C4C-C3C	2.86	1.50	1.45
23	c	512	CLA	C4B-NB	-2.86	1.34	1.37
23	B	614	CLA	C4D-CHA	2.86	1.48	1.38
23	C	508	CLA	C4B-NB	-2.85	1.34	1.37
24	a	414[B]	PHO	C3A-C2A	-2.85	1.52	1.54
23	d	403[B]	CLA	C1B-C2B	2.84	1.50	1.43
23	b	614	CLA	C3B-C4B	2.84	1.49	1.42
23	c	504	CLA	C1C-C2C	2.84	1.50	1.44
23	c	502	CLA	C3B-C4B	2.84	1.49	1.42
23	A	408	CLA	C1B-C2B	2.84	1.49	1.43
23	B	605	CLA	C1B-C2B	2.84	1.49	1.43
23	b	613	CLA	C1B-C2B	2.83	1.49	1.43
23	D	403[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	612	CLA	C1C-C2C	2.83	1.50	1.44
23	b	611	CLA	OBD-CAD	2.82	1.27	1.22
23	C	513	CLA	C1B-C2B	2.82	1.49	1.43
23	B	602	CLA	C1C-C2C	2.82	1.50	1.44
23	B	606	CLA	C3B-C4B	2.82	1.49	1.42
23	c	509	CLA	C3B-C4B	2.82	1.49	1.42
23	B	604	CLA	C1C-C2C	2.82	1.50	1.44
23	c	510	CLA	C4D-CHA	2.82	1.48	1.38
23	B	616	CLA	C4D-CHA	2.81	1.48	1.38
23	A	406[B]	CLA	C4B-NB	-2.81	1.34	1.37
23	B	608	CLA	OBD-CAD	2.81	1.27	1.22
23	c	503	CLA	C1B-C2B	2.81	1.49	1.43
23	b	614	CLA	C1B-C2B	2.80	1.49	1.43
27	D	402	GOL	O2-C2	-2.80	1.35	1.43
26	a	409[B]	SQD	C6-S	-2.80	1.67	1.77
23	A	405[B]	CLA	C4B-NB	-2.80	1.34	1.37
23	B	616	CLA	OBD-CAD	2.80	1.27	1.22
23	c	503	CLA	C3B-C4B	2.79	1.49	1.42
31	t	101	LMT	O3'-C3'	-2.79	1.36	1.43
23	B	615	CLA	C1B-NB	-2.79	1.34	1.37
23	b	606	CLA	C3B-C4B	2.79	1.49	1.42
23	b	605	CLA	C4B-NB	-2.78	1.34	1.37
23	b	607	CLA	C1C-C2C	2.78	1.50	1.44
23	c	504	CLA	C1B-C2B	2.78	1.49	1.43
23	B	605	CLA	C1B-NB	-2.78	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	V	201	HEC	CAC-C3C	2.78	1.58	1.51
23	C	512	CLA	C1C-C2C	2.78	1.49	1.44
23	B	601	CLA	C1B-NB	-2.78	1.34	1.37
23	A	408	CLA	OBD-CAD	2.78	1.27	1.22
31	M	101	LMT	O2'-C2'	-2.77	1.36	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	b	615	CLA	C4D-CHA	2.76	1.48	1.38
23	b	605	CLA	C3B-C4B	2.76	1.49	1.42
23	c	509	CLA	C4B-NB	-2.76	1.34	1.37
23	A	408	CLA	C4B-NB	-2.75	1.34	1.37
29	a	412[A]	PL9	C6-C5	2.75	1.49	1.35
23	A	404[A]	CLA	C1B-C2B	2.75	1.49	1.43
23	c	511	CLA	C3B-C4B	2.75	1.49	1.42
23	a	407	CLA	C3B-C4B	2.75	1.49	1.42
23	B	612	CLA	C1C-C2C	2.75	1.49	1.44
23	C	507	CLA	C4D-CHA	2.75	1.48	1.38
23	b	609	CLA	C1C-C2C	2.74	1.49	1.44
23	C	501	CLA	C4D-CHA	2.74	1.48	1.38
23	c	514	CLA	C1B-C2B	2.74	1.49	1.43
23	c	509	CLA	C4D-CHA	2.74	1.48	1.38
23	A	408	CLA	C3B-C4B	2.74	1.49	1.42
23	C	506	CLA	C4C-C3C	2.74	1.49	1.45
23	C	511	CLA	C1B-C2B	2.74	1.49	1.43
23	b	604	CLA	C4B-NB	-2.73	1.34	1.37
23	B	610	CLA	C1B-C2B	2.73	1.49	1.43
26	a	409[A]	SQD	C6-S	-2.73	1.67	1.77
23	B	610	CLA	C4D-CHA	2.73	1.48	1.38
23	B	613	CLA	C4D-CHA	2.73	1.48	1.38
23	A	405[A]	CLA	C4B-NB	-2.73	1.34	1.37
26	A	410[A]	SQD	C6-S	-2.73	1.67	1.77
23	B	604	CLA	C4C-C3C	2.73	1.49	1.45
23	c	503	CLA	C4B-NB	-2.73	1.34	1.37
23	B	608	CLA	C1B-C2B	2.73	1.49	1.43
23	b	610	CLA	C3B-C4B	2.73	1.49	1.42
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	c	510	CLA	C1B-C2B	2.72	1.49	1.43
23	d	402[A]	CLA	C1B-C2B	2.72	1.49	1.43
26	A	410[B]	SQD	C6-S	-2.72	1.67	1.77
23	d	404	CLA	C4B-NB	-2.72	1.34	1.37
23	A	404[B]	CLA	C1B-C2B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C1B-NB	-2.72	1.34	1.37
23	B	605	CLA	OBD-CAD	2.72	1.27	1.22
23	c	508	CLA	C1B-C2B	2.72	1.49	1.43
23	D	403[A]	CLA	C4D-CHA	2.71	1.48	1.38
23	a	407	CLA	C4B-NB	-2.71	1.34	1.37
23	B	612	CLA	C1B-C2B	2.71	1.49	1.43
23	B	612	CLA	C3B-C2B	2.71	1.50	1.41
23	B	612	CLA	C4D-CHA	2.71	1.48	1.38
23	C	501	CLA	C1C-C2C	2.71	1.49	1.44
23	c	514	CLA	C1C-C2C	2.71	1.49	1.44
23	c	509	CLA	C1B-C2B	2.71	1.49	1.43
23	C	502	CLA	C1B-C2B	2.70	1.49	1.43
23	a	405[B]	CLA	C1C-C2C	2.70	1.49	1.44
32	Z	101	LMG	O8-C28	2.70	1.46	1.33
23	c	502	CLA	C1C-C2C	2.70	1.49	1.44
23	c	512	CLA	C4D-CHA	2.70	1.48	1.38
23	b	609	CLA	C4D-CHA	2.69	1.48	1.38
29	a	412[B]	PL9	C6-C5	2.69	1.49	1.35
23	b	607	CLA	OBD-CAD	2.69	1.27	1.22
23	c	505	CLA	C4C-C3C	2.69	1.49	1.45
26	f	102	SQD	C6-S	-2.69	1.67	1.77
23	b	616	CLA	C1C-C2C	2.69	1.49	1.44
23	B	614	CLA	C3B-C4B	2.69	1.49	1.42
29	A	414[B]	PL9	C6-C5	2.68	1.49	1.35
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
23	c	513	CLA	C1B-NB	-2.68	1.34	1.37
23	C	508	CLA	C1B-C2B	2.68	1.49	1.43
34	b	622	HTG	O5-C1	2.68	1.46	1.42
23	a	405[A]	CLA	C1B-C2B	2.68	1.49	1.43
23	b	604	CLA	C4D-CHA	2.68	1.47	1.38
26	A	412	SQD	C6-S	-2.67	1.67	1.77
23	B	601	CLA	C4B-NB	-2.67	1.34	1.37
23	C	511	CLA	C1B-NB	-2.67	1.34	1.37
23	b	613	CLA	OBD-CAD	2.67	1.27	1.22
23	C	504	CLA	C1C-C2C	2.67	1.49	1.44
23	C	501	CLA	OBD-CAD	2.66	1.27	1.22
23	c	505	CLA	C1C-C2C	2.66	1.49	1.44
23	C	502	CLA	C1C-C2C	2.66	1.49	1.44
35	H	102	DGD	O5D-C1E	2.66	1.44	1.40
23	C	507	CLA	C1B-C2B	2.66	1.49	1.43
23	C	505	CLA	C1C-C2C	2.66	1.49	1.44
23	b	613	CLA	C1C-C2C	2.66	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	616	CLA	C1B-C2B	2.66	1.49	1.43
23	a	404[A]	CLA	C1B-C2B	2.66	1.49	1.43
23	b	606	CLA	C1B-C2B	2.66	1.49	1.43
31	B	630	LMT	O2'-C2'	-2.65	1.36	1.43
23	b	612	CLA	C4D-CHA	2.65	1.47	1.38
23	d	403[A]	CLA	C1B-C2B	2.65	1.49	1.43
23	C	503	CLA	C4B-NB	-2.65	1.34	1.37
23	c	506	CLA	C4D-CHA	2.65	1.47	1.38
23	B	608	CLA	C4D-CHA	2.65	1.47	1.38
23	c	508	CLA	C4D-CHA	2.65	1.47	1.38
23	A	408	CLA	C4D-CHA	2.65	1.47	1.38
23	b	615	CLA	C1B-C2B	2.64	1.49	1.43
23	C	509	CLA	C4D-CHA	2.64	1.47	1.38
23	b	603	CLA	C1B-C2B	2.64	1.49	1.43
23	c	504	CLA	C3D-C4D	-2.64	1.38	1.44
24	A	416[B]	PHO	CHA-CBD	-2.64	1.48	1.51
23	A	404[B]	CLA	C4D-CHA	2.63	1.47	1.38
23	D	404	CLA	C1B-C2B	2.63	1.49	1.43
23	b	613	CLA	C4D-CHA	2.63	1.47	1.38
23	B	601	CLA	C1C-C2C	2.63	1.49	1.44
23	C	502	CLA	C3B-C4B	2.63	1.48	1.42
23	B	602	CLA	C1B-C2B	2.63	1.49	1.43
23	B	609	CLA	C4D-CHA	2.63	1.47	1.38
23	C	506	CLA	C4D-CHA	2.63	1.47	1.38
23	a	405[A]	CLA	C4B-NB	-2.63	1.34	1.37
23	b	612	CLA	C3B-C4B	2.62	1.48	1.42
23	c	505	CLA	C4D-CHA	2.62	1.47	1.38
23	B	615	CLA	C4D-CHA	2.62	1.47	1.38
23	a	405[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	b	610	CLA	C1C-C2C	2.62	1.49	1.44
23	c	506	CLA	C1C-C2C	2.62	1.49	1.44
23	A	405[A]	CLA	C1B-C2B	2.62	1.49	1.43
23	C	508	CLA	C3B-C2B	2.62	1.50	1.41
23	c	508	CLA	C1C-C2C	2.61	1.49	1.44
23	c	509	CLA	C4C-C3C	2.61	1.49	1.45
23	c	511	CLA	C1C-C2C	2.61	1.49	1.44
34	b	625	HTG	C1-S1	-2.61	1.76	1.80
23	d	404	CLA	C1B-NB	-2.61	1.34	1.37
23	B	605	CLA	C1C-C2C	2.61	1.49	1.44
23	B	614	CLA	C1B-NB	-2.60	1.34	1.37
23	b	605	CLA	C1B-C2B	2.60	1.49	1.43
23	A	405[B]	CLA	C4D-CHA	2.60	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C4D-CHA	2.60	1.47	1.38
23	b	601	CLA	C1C-C2C	2.59	1.49	1.44
23	C	505	CLA	C4D-CHA	2.59	1.47	1.38
23	C	509	CLA	C1B-C2B	2.59	1.49	1.43
23	c	513	CLA	C4B-NB	-2.59	1.34	1.37
23	a	404[B]	CLA	C1B-C2B	2.59	1.49	1.43
23	C	508	CLA	C4D-CHA	2.59	1.47	1.38
23	c	512	CLA	C1C-C2C	2.59	1.49	1.44
23	C	501	CLA	C3D-C4D	-2.58	1.38	1.44
23	c	507	CLA	C1B-C2B	2.58	1.49	1.43
23	c	513	CLA	C1B-C2B	2.58	1.49	1.43
23	B	609	CLA	C1B-C2B	2.58	1.49	1.43
35	c	519	DGD	O2G-C2G	-2.58	1.40	1.46
26	a	410	SQD	C6-S	-2.58	1.67	1.77
23	C	513	CLA	C4D-CHA	2.58	1.47	1.38
23	B	602	CLA	C3D-C4D	-2.58	1.38	1.44
23	a	404[A]	CLA	C3B-C4B	2.57	1.48	1.42
23	b	611	CLA	C1C-C2C	2.57	1.49	1.44
23	C	512	CLA	C4D-CHA	2.57	1.47	1.38
23	c	502	CLA	C4D-CHA	2.57	1.47	1.38
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	c	513	CLA	C4D-CHA	2.57	1.47	1.38
34	B	625	HTG	C1-S1	-2.57	1.76	1.80
23	B	603	CLA	C1B-C2B	2.57	1.49	1.43
23	C	504	CLA	C1B-C2B	2.57	1.49	1.43
23	B	613	CLA	C4B-NB	-2.57	1.34	1.37
23	b	616	CLA	C3D-C4D	-2.57	1.38	1.44
23	b	604	CLA	C3B-C4B	2.57	1.48	1.42
23	c	504	CLA	C4D-CHA	2.56	1.47	1.38
23	b	606	CLA	C4B-NB	-2.56	1.34	1.37
23	b	609	CLA	C4B-NB	-2.56	1.34	1.37
23	C	510	CLA	C1C-C2C	2.56	1.49	1.44
23	b	607	CLA	C3D-C4D	-2.56	1.38	1.44
23	B	608	CLA	C4C-C3C	2.56	1.49	1.45
23	c	507	CLA	C3B-C4B	2.56	1.48	1.42
23	d	404	CLA	C4D-CHA	2.56	1.47	1.38
23	d	403[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	b	614	CLA	C4D-CHA	2.55	1.47	1.38
23	C	511	CLA	C3B-C4B	2.55	1.48	1.42
23	B	607	CLA	C1C-C2C	2.55	1.49	1.44
23	b	614	CLA	C4B-NB	-2.55	1.34	1.37
24	a	414[A]	PHO	C3A-C2A	-2.55	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	512	CLA	C3B-C4B	2.55	1.48	1.42
23	C	501	CLA	C1B-C2B	2.54	1.49	1.43
23	b	616	CLA	C4D-CHA	2.54	1.47	1.38
23	b	615	CLA	C3B-C4B	2.54	1.48	1.42
26	b	620	SQD	C6-S	-2.54	1.68	1.77
23	b	601	CLA	C4D-CHA	2.54	1.47	1.38
23	C	508	CLA	C4C-C3C	2.54	1.49	1.45
23	c	510	CLA	C4C-C3C	2.53	1.49	1.45
23	b	607	CLA	C4D-CHA	2.53	1.47	1.38
23	b	608	CLA	C4D-CHA	2.53	1.47	1.38
23	C	509	CLA	C1C-C2C	2.53	1.49	1.44
23	D	403[B]	CLA	C1B-C2B	2.53	1.49	1.43
23	c	510	CLA	C3B-C4B	2.53	1.48	1.42
23	C	508	CLA	C1B-NB	-2.53	1.34	1.37
23	C	509	CLA	C3B-C4B	2.53	1.48	1.42
23	A	405[B]	CLA	C1B-C2B	2.52	1.49	1.43
23	d	403[B]	CLA	C4C-C3C	2.51	1.49	1.45
23	C	503	CLA	C1C-C2C	2.51	1.49	1.44
23	B	604	CLA	C3B-C4B	2.51	1.48	1.42
31	B	628	LMT	C3'-C2'	2.51	1.58	1.52
29	d	406[B]	PL9	C6-C5	2.51	1.48	1.35
31	e	101	LMT	O3'-C3'	-2.51	1.37	1.43
29	D	406[B]	PL9	C6-C5	2.51	1.48	1.35
23	c	503	CLA	C4D-CHA	2.51	1.47	1.38
26	F	103	SQD	O6-C1	2.51	1.44	1.40
23	B	603	CLA	C4D-CHA	2.51	1.47	1.38
23	B	610	CLA	C1C-C2C	2.51	1.49	1.44
23	b	611	CLA	C4B-NB	-2.51	1.34	1.37
23	B	605	CLA	C4D-CHA	2.50	1.47	1.38
23	B	602	CLA	C3B-C4B	2.50	1.48	1.42
23	B	616	CLA	C4B-NB	-2.50	1.34	1.37
31	B	631	LMT	O3'-C3'	-2.50	1.37	1.43
23	b	615	CLA	C3D-C4D	-2.50	1.38	1.44
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	A	405[B]	CLA	C1C-C2C	2.49	1.49	1.44
31	A	420	LMT	O3'-C3'	-2.49	1.37	1.43
23	a	404[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	b	602	CLA	C4B-NB	-2.49	1.34	1.37
23	b	602	CLA	C4C-C3C	2.49	1.49	1.45
23	a	404[B]	CLA	C4D-CHA	2.49	1.47	1.38
23	b	607	CLA	C4B-NB	-2.49	1.34	1.37
23	a	405[B]	CLA	C4D-CHA	2.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C4B-NB	-2.49	1.34	1.37
23	c	502	CLA	C1B-C2B	2.49	1.49	1.43
23	C	511	CLA	C3B-C2B	2.48	1.49	1.41
23	b	603	CLA	C4D-CHA	2.48	1.47	1.38
23	C	506	CLA	C1B-C2B	2.48	1.49	1.43
23	C	510	CLA	C3B-C4B	2.48	1.48	1.42
23	B	607	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	507	CLA	C1C-C2C	2.48	1.49	1.44
23	d	404	CLA	C1C-C2C	2.48	1.49	1.44
23	C	507	CLA	C4C-C3C	2.48	1.49	1.45
23	a	404[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	b	615	CLA	C4B-NB	-2.48	1.34	1.37
23	b	606	CLA	C1C-C2C	2.48	1.49	1.44
23	d	402[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	C	505	CLA	C4B-NB	-2.48	1.34	1.37
23	D	403[B]	CLA	C4D-CHA	2.47	1.47	1.38
23	C	509	CLA	C3B-C2B	2.47	1.49	1.41
24	A	416[B]	PHO	C4B-NB	-2.47	1.34	1.38
26	F	103	SQD	C6-S	-2.47	1.68	1.77
23	C	506	CLA	C3B-C4B	2.47	1.48	1.42
23	A	406[B]	CLA	C1C-C2C	2.47	1.49	1.44
23	c	514	CLA	C4D-CHA	2.47	1.47	1.38
23	A	406[B]	CLA	C1B-C2B	2.46	1.49	1.43
23	c	502	CLA	C4B-NB	-2.46	1.34	1.37
23	d	403[B]	CLA	C4D-CHA	2.46	1.47	1.38
23	C	510	CLA	C1B-C2B	2.46	1.49	1.43
23	b	606	CLA	C4D-CHA	2.46	1.47	1.38
23	b	610	CLA	C4D-CHA	2.46	1.47	1.38
23	C	505	CLA	C4C-C3C	2.46	1.49	1.45
23	c	509	CLA	C1C-C2C	2.46	1.49	1.44
23	d	402[B]	CLA	C4D-CHA	2.46	1.47	1.38
23	b	614	CLA	C1C-C2C	2.46	1.49	1.44
23	c	505	CLA	C1C-NC	-2.46	1.34	1.37
23	B	616	CLA	C3B-C2B	2.45	1.49	1.41
23	B	614	CLA	C3D-C4D	-2.45	1.38	1.44
31	b	621	LMT	C3'-C2'	2.45	1.58	1.52
23	b	611	CLA	C3B-C4B	2.45	1.48	1.42
23	b	610	CLA	C3D-C4D	-2.45	1.38	1.44
23	C	513	CLA	C1C-C2C	2.45	1.49	1.44
31	M	102	LMT	O2'-C2'	-2.44	1.37	1.43
23	a	405[A]	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	602	CLA	C4D-CHA	2.44	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	606	CLA	C4D-CHA	2.44	1.47	1.38
23	A	406[A]	CLA	C1B-C2B	2.44	1.49	1.43
23	B	602	CLA	C4D-CHA	2.44	1.47	1.38
23	b	611	CLA	C4C-C3C	2.44	1.49	1.45
26	B	620	SQD	C6-S	-2.44	1.68	1.77
23	C	509	CLA	C4C-C3C	2.43	1.49	1.45
23	B	616	CLA	C1C-NC	-2.43	1.34	1.37
40	v	201	HEC	CAC-C3C	2.43	1.57	1.51
23	C	503	CLA	C4D-CHA	2.43	1.47	1.38
23	B	614	CLA	C1C-C2C	2.43	1.49	1.44
23	C	503	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	606	CLA	C3D-C4D	-2.43	1.38	1.44
38	F	102	HEM	C1C-C2C	-2.43	1.40	1.45
23	b	606	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	601	CLA	C4D-CHA	2.43	1.47	1.38
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42
23	a	405[B]	CLA	C1B-C2B	2.42	1.49	1.43
23	B	605	CLA	C3D-C4D	-2.42	1.38	1.44
23	C	511	CLA	C4C-C3C	2.42	1.49	1.45
23	C	510	CLA	C4D-CHA	2.42	1.47	1.38
23	b	615	CLA	C4C-C3C	2.42	1.49	1.45
31	F	101	LMT	O3'-C3'	-2.41	1.37	1.43
23	C	506	CLA	C1C-C2C	2.41	1.49	1.44
23	c	502	CLA	C1B-NB	-2.41	1.34	1.37
23	A	405[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	A	406[A]	CLA	C1C-C2C	2.41	1.49	1.44
23	A	408	CLA	C3D-C4D	-2.41	1.38	1.44
23	c	507	CLA	C4D-CHA	2.41	1.47	1.38
23	b	612	CLA	C3B-C2B	2.41	1.49	1.41
23	b	603	CLA	C3D-C4D	-2.41	1.38	1.44
23	a	404[B]	CLA	C3B-C4B	2.40	1.48	1.42
23	A	404[B]	CLA	C3B-C2B	2.40	1.49	1.41
23	B	608	CLA	C1C-NC	-2.40	1.34	1.37
31	M	101	LMT	O2B-C2B	-2.40	1.37	1.43
23	b	611	CLA	C4D-CHA	2.40	1.46	1.38
23	b	603	CLA	C1B-NB	-2.40	1.34	1.37
23	B	613	CLA	C4C-C3C	2.40	1.49	1.45
23	A	406[B]	CLA	C4D-CHA	2.40	1.46	1.38
23	D	403[A]	CLA	C3D-C4D	-2.39	1.38	1.44
23	C	506	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	610	CLA	C3D-C4D	-2.39	1.38	1.44
23	B	614	CLA	C4C-C3C	2.39	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	611	CLA	MG-NB	2.39	2.10	2.05
23	c	507	CLA	C4C-C3C	2.39	1.49	1.45
23	b	609	CLA	C1B-C2B	2.39	1.48	1.43
23	D	403[B]	CLA	C3D-C4D	-2.39	1.38	1.44
23	c	509	CLA	C1B-NB	-2.38	1.34	1.37
23	A	404[B]	CLA	C1C-C2C	2.38	1.49	1.44
23	C	510	CLA	C4C-C3C	2.38	1.49	1.45
23	c	503	CLA	C3B-C2B	2.38	1.49	1.41
24	A	416[B]	PHO	C3A-C2A	-2.38	1.52	1.54
23	d	403[A]	CLA	C4D-CHA	2.38	1.46	1.38
31	A	420	LMT	O2'-C2'	-2.38	1.37	1.43
23	C	513	CLA	C3B-C4B	2.38	1.48	1.42
35	C	518	DGD	O2G-C2G	-2.37	1.40	1.46
34	B	623	HTG	C1'-S1	-2.37	1.78	1.81
23	c	511	CLA	C4B-NB	-2.37	1.34	1.37
23	b	604	CLA	C1C-C2C	2.37	1.49	1.44
23	c	502	CLA	C4C-C3C	2.37	1.49	1.45
23	B	602	CLA	C4C-C3C	2.37	1.49	1.45
25	B	619	BCR	C30-C25	-2.37	1.50	1.53
23	b	605	CLA	C4D-CHA	2.37	1.46	1.38
23	B	603	CLA	C3B-C4B	2.37	1.48	1.42
23	b	608	CLA	C1B-C2B	2.37	1.48	1.43
23	b	603	CLA	C3B-C2B	2.37	1.49	1.41
23	C	502	CLA	C4D-CHA	2.37	1.46	1.38
23	b	609	CLA	C3D-C4D	-2.37	1.38	1.44
31	a	415	LMT	O3'-C3'	-2.37	1.37	1.43
23	b	612	CLA	C3D-C4D	-2.36	1.38	1.44
23	B	603	CLA	C1C-C2C	2.36	1.49	1.44
23	b	608	CLA	C1C-C2C	2.36	1.49	1.44
23	c	504	CLA	C4C-C3C	2.36	1.49	1.45
23	c	512	CLA	C3B-C2B	2.36	1.49	1.41
23	C	513	CLA	C3B-C2B	2.36	1.49	1.41
23	B	610	CLA	C4C-C3C	2.36	1.49	1.45
23	C	502	CLA	C4C-C3C	2.35	1.49	1.45
29	d	406[A]	PL9	C6-C5	2.35	1.47	1.35
23	c	513	CLA	C4C-C3C	2.35	1.49	1.45
23	B	613	CLA	C3B-C4B	2.35	1.48	1.42
31	B	628	LMT	O3'-C3'	-2.35	1.37	1.43
23	d	403[B]	CLA	C3D-C4D	-2.35	1.38	1.44
31	B	630	LMT	O2B-C2B	-2.35	1.37	1.43
23	c	507	CLA	C3D-C4D	-2.35	1.38	1.44
23	a	404[B]	CLA	C1C-C2C	2.35	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	416[A]	PHO	C3D-C4D	-2.35	1.37	1.41
23	C	507	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	416[A]	PHO	C3A-C2A	-2.34	1.52	1.54
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
23	c	502	CLA	C3D-C4D	-2.34	1.38	1.44
24	A	416[B]	PHO	C3D-C4D	-2.34	1.37	1.41
32	C	520	LMG	O1-C1	2.34	1.44	1.40
23	A	406[B]	CLA	C3D-C4D	-2.34	1.38	1.44
23	B	613	CLA	C1C-C2C	2.34	1.49	1.44
23	c	513	CLA	C1C-C2C	2.34	1.49	1.44
23	c	514	CLA	C3D-C4D	-2.34	1.38	1.44
29	D	406[A]	PL9	C6-C5	2.34	1.47	1.35
23	B	601	CLA	C1B-C2B	2.34	1.48	1.43
24	a	406[B]	PHO	C4B-NB	-2.34	1.34	1.38
23	A	408	CLA	C3B-C2B	2.34	1.49	1.41
23	C	512	CLA	C1B-C2B	2.33	1.48	1.43
23	b	611	CLA	C3D-C4D	-2.33	1.38	1.44
23	b	616	CLA	C4B-NB	-2.33	1.34	1.37
23	b	614	CLA	C3D-C4D	-2.33	1.38	1.44
23	B	612	CLA	C3B-C4B	2.33	1.48	1.42
24	a	406[A]	PHO	CBD-CGD	-2.33	1.49	1.52
23	C	510	CLA	C3D-C4D	-2.33	1.38	1.44
23	C	513	CLA	C3D-C4D	-2.33	1.38	1.44
23	b	603	CLA	C1C-C2C	2.33	1.49	1.44
38	f	101	HEM	C1C-C2C	-2.33	1.40	1.45
31	M	102	LMT	O3'-C3'	-2.33	1.37	1.43
23	b	602	CLA	C3D-C4D	-2.32	1.38	1.44
23	a	404[A]	CLA	C3B-C2B	2.32	1.49	1.41
23	A	404[A]	CLA	C3B-C2B	2.32	1.49	1.41
23	D	403[B]	CLA	C1C-C2C	2.32	1.49	1.44
31	M	101	LMT	O3'-C3'	-2.32	1.37	1.43
31	m	103	LMT	O2B-C2B	-2.32	1.37	1.43
23	C	512	CLA	C3D-C4D	-2.32	1.38	1.44
23	b	615	CLA	C1C-C2C	2.32	1.49	1.44
38	f	101	HEM	C1D-ND	-2.32	1.34	1.38
23	B	603	CLA	C3B-C2B	2.31	1.49	1.41
23	B	606	CLA	C1B-C2B	2.31	1.48	1.43
23	B	609	CLA	C1C-C2C	2.31	1.49	1.44
23	c	505	CLA	C3B-C4B	2.31	1.48	1.42
23	C	511	CLA	C3D-C4D	-2.31	1.39	1.44
23	D	403[B]	CLA	C4C-C3C	2.31	1.49	1.45
23	c	514	CLA	C4C-C3C	2.31	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C3B-C2B	2.31	1.49	1.41
23	B	606	CLA	C4B-NB	-2.31	1.34	1.37
23	C	503	CLA	C1B-C2B	2.31	1.48	1.43
24	A	407[B]	PHO	CBD-CGD	-2.31	1.49	1.52
23	b	610	CLA	C4C-C3C	2.31	1.49	1.45
23	B	608	CLA	C3B-C4B	2.31	1.48	1.42
23	d	403[A]	CLA	C1C-C2C	2.30	1.49	1.44
23	d	403[A]	CLA	C3D-C4D	-2.30	1.39	1.44
35	c	519	DGD	O5D-C1E	2.30	1.44	1.40
23	b	613	CLA	C3B-C2B	2.30	1.49	1.41
23	d	403[B]	CLA	C3B-C4B	2.30	1.48	1.42
23	b	608	CLA	C3B-C2B	2.30	1.49	1.41
23	D	404	CLA	C4D-CHA	2.30	1.46	1.38
23	c	508	CLA	C4C-C3C	2.30	1.49	1.45
23	C	508	CLA	C3B-C4B	2.30	1.48	1.42
23	B	616	CLA	C3D-C4D	-2.29	1.39	1.44
23	c	513	CLA	C3D-C4D	-2.29	1.39	1.44
23	d	402[B]	CLA	C1C-C2C	2.29	1.49	1.44
23	b	601	CLA	C3B-C2B	2.28	1.48	1.41
23	c	509	CLA	C3B-C2B	2.28	1.48	1.41
23	c	509	CLA	C3D-C4D	-2.28	1.39	1.44
31	m	103	LMT	C3'-C2'	2.27	1.58	1.52
23	B	605	CLA	C4B-NB	-2.27	1.35	1.37
23	B	616	CLA	C3B-C4B	2.27	1.48	1.42
23	B	607	CLA	C4B-NB	-2.27	1.35	1.37
23	c	502	CLA	C1C-NC	-2.26	1.34	1.37
24	A	416[A]	PHO	C4B-NB	-2.26	1.34	1.38
23	a	404[B]	CLA	C3B-C2B	2.26	1.48	1.41
23	b	614	CLA	C3B-C2B	2.26	1.48	1.41
23	B	611	CLA	C4D-CHA	2.25	1.46	1.38
23	c	512	CLA	C4C-C3C	2.25	1.48	1.45
23	a	404[A]	CLA	C1C-C2C	2.25	1.48	1.44
23	a	407	CLA	C4D-CHA	2.25	1.46	1.38
23	C	504	CLA	C3B-C2B	2.25	1.48	1.41
23	c	511	CLA	C3B-C2B	2.25	1.48	1.41
23	c	510	CLA	C3B-C2B	2.25	1.48	1.41
23	c	503	CLA	C1B-NB	-2.25	1.35	1.37
23	B	604	CLA	C4B-NB	-2.24	1.35	1.37
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
40	V	201	HEC	FE-NB	2.24	2.01	1.94
23	B	610	CLA	C4B-NB	-2.24	1.35	1.37
23	c	505	CLA	C3B-C2B	2.24	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	403[A]	CLA	C3B-C4B	2.24	1.48	1.42
23	d	404	CLA	C1B-C2B	2.24	1.48	1.43
23	c	507	CLA	C3B-C2B	2.24	1.48	1.41
31	t	101	LMT	O2'-C2'	-2.24	1.37	1.43
27	b	624	GOL	C3-C2	2.24	1.60	1.51
23	B	609	CLA	C4B-NB	-2.23	1.35	1.37
24	A	407[B]	PHO	C1B-NB	-2.23	1.34	1.38
23	B	609	CLA	C3D-C4D	-2.23	1.39	1.44
27	D	402	GOL	C3-C2	2.23	1.60	1.51
23	C	502	CLA	C3D-C4D	-2.23	1.39	1.44
23	a	405[B]	CLA	C3D-C4D	-2.22	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.22	1.39	1.44
23	b	610	CLA	C3B-C2B	2.22	1.48	1.41
23	d	403[B]	CLA	C1C-C2C	2.22	1.48	1.44
23	B	608	CLA	C3B-C2B	2.22	1.48	1.41
23	d	404	CLA	C3D-C4D	-2.21	1.39	1.44
23	A	406[B]	CLA	C4C-C3C	2.21	1.48	1.45
35	C	517[A]	DGD	O5D-C1E	2.21	1.44	1.40
23	B	604	CLA	C1A-CHA	2.21	1.52	1.43
23	D	403[A]	CLA	C4C-C3C	2.21	1.48	1.45
35	h	102	DGD	O5D-C1E	2.21	1.44	1.40
31	A	417	LMT	O3'-C3'	-2.21	1.37	1.43
23	B	601	CLA	C3B-C2B	2.20	1.48	1.41
23	d	402[A]	CLA	C4B-NB	-2.20	1.35	1.37
23	B	601	CLA	C4C-C3C	2.20	1.48	1.45
23	b	607	CLA	C3B-C4B	2.20	1.47	1.42
24	A	416[A]	PHO	C1D-ND	-2.20	1.34	1.38
23	C	501	CLA	C4C-C3C	2.20	1.48	1.45
23	b	612	CLA	C4C-C3C	2.19	1.48	1.45
23	D	403[A]	CLA	C3B-C2B	2.19	1.48	1.41
24	a	414[B]	PHO	C4B-NB	-2.19	1.34	1.38
29	a	412[A]	PL9	C2-C3	2.19	1.40	1.34
23	d	404	CLA	C4C-C3C	2.19	1.48	1.45
23	b	605	CLA	C3D-C4D	-2.19	1.39	1.44
23	D	403[B]	CLA	C3B-C2B	2.19	1.48	1.41
24	a	406[B]	PHO	C3A-C2A	-2.18	1.52	1.54
23	A	404[B]	CLA	C3D-C4D	-2.18	1.39	1.44
31	m	103	LMT	O3'-C3'	-2.18	1.37	1.43
23	B	601	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	505	CLA	C3D-C4D	-2.18	1.39	1.44
23	B	606	CLA	C3B-C2B	2.18	1.48	1.41
23	c	510	CLA	C1C-C2C	2.18	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	C3B-C2B	2.18	1.48	1.41
23	B	613	CLA	C3B-C2B	2.18	1.48	1.41
23	c	511	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	506	CLA	C1D-C2D	2.17	1.49	1.45
23	A	404[B]	CLA	C3B-C4B	2.17	1.47	1.42
34	B	622	HTG	O5-C1	2.17	1.45	1.42
40	V	201	HEC	CMB-C2B	2.17	1.55	1.50
23	a	405[B]	CLA	C4C-C3C	2.17	1.48	1.45
23	c	508	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	608	CLA	C3D-C4D	-2.17	1.39	1.44
23	C	501	CLA	C4B-NB	-2.17	1.35	1.37
23	a	407	CLA	C4C-C3C	2.17	1.48	1.45
23	C	502	CLA	C3B-C2B	2.17	1.48	1.41
23	d	403[B]	CLA	C3B-C2B	2.16	1.48	1.41
31	B	630	LMT	O3'-C3'	-2.16	1.37	1.43
23	C	504	CLA	C3B-C4B	2.16	1.47	1.42
23	b	605	CLA	C1D-C2D	2.16	1.49	1.45
23	b	607	CLA	C4C-C3C	2.16	1.48	1.45
23	D	403[A]	CLA	C3B-C4B	2.16	1.47	1.42
25	d	405	BCR	C30-C25	-2.16	1.50	1.53
23	b	614	CLA	C4C-C3C	2.16	1.48	1.45
31	M	102	LMT	O3B-C3B	-2.16	1.37	1.43
23	c	508	CLA	C3B-C4B	2.16	1.47	1.42
23	B	608	CLA	C1C-C2C	2.16	1.48	1.44
23	B	601	CLA	C1C-NC	-2.16	1.34	1.37
23	c	511	CLA	C4C-C3C	2.16	1.48	1.45
23	b	607	CLA	C3B-C2B	2.15	1.48	1.41
23	a	407	CLA	C3B-C2B	2.15	1.48	1.41
23	C	504	CLA	C3D-C4D	-2.15	1.39	1.44
23	b	613	CLA	C3B-C4B	2.15	1.47	1.42
24	a	406[A]	PHO	C4B-NB	-2.14	1.34	1.38
23	A	405[B]	CLA	C3D-C4D	-2.14	1.39	1.44
23	d	402[B]	CLA	C4B-NB	-2.14	1.35	1.37
23	B	604	CLA	C3B-C2B	2.13	1.48	1.41
23	b	604	CLA	C3B-C2B	2.13	1.48	1.41
23	c	514	CLA	C3B-C2B	2.13	1.48	1.41
24	a	414[A]	PHO	C4B-NB	-2.13	1.34	1.38
23	A	405[B]	CLA	C4C-C3C	2.13	1.48	1.45
23	a	404[B]	CLA	C3D-C4D	-2.13	1.39	1.44
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
40	v	201	HEC	CMC-C2C	2.12	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C3B-C2B	2.12	1.48	1.41
23	c	506	CLA	C3D-C4D	-2.12	1.39	1.44
24	a	406[B]	PHO	C1B-NB	-2.12	1.34	1.38
31	A	417	LMT	O2'-C2'	-2.12	1.38	1.43
23	b	601	CLA	C1B-C2B	2.12	1.48	1.43
23	B	615	CLA	MG-NA	2.12	2.11	2.06
23	B	615	CLA	C4B-NB	-2.12	1.35	1.37
23	d	402[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	B	612	CLA	C4C-C3C	2.12	1.48	1.45
23	b	606	CLA	C3B-C2B	2.12	1.48	1.41
23	d	404	CLA	C3B-C2B	2.11	1.48	1.41
23	C	508	CLA	C3D-C4D	-2.11	1.39	1.44
23	D	404	CLA	C3D-C4D	-2.11	1.39	1.44
23	C	503	CLA	C4C-C3C	2.11	1.48	1.45
23	C	512	CLA	C3B-C2B	2.11	1.48	1.41
23	b	608	CLA	C3D-C4D	-2.10	1.39	1.44
23	b	610	CLA	C4B-NB	-2.10	1.35	1.37
29	a	412[B]	PL9	C2-C3	2.10	1.40	1.34
24	A	407[A]	PHO	C1B-NB	-2.09	1.34	1.38
23	a	405[A]	CLA	C4C-C3C	2.08	1.48	1.45
31	b	627	LMT	O3'-C3'	-2.08	1.38	1.43
23	c	510	CLA	C3D-C4D	-2.08	1.39	1.44
23	C	510	CLA	C3B-C2B	2.08	1.48	1.41
23	b	602	CLA	C1B-C2B	2.07	1.48	1.43
23	d	403[A]	CLA	C3B-C2B	2.07	1.48	1.41
23	c	512	CLA	MG-NA	2.07	2.11	2.06
23	b	613	CLA	C3D-C4D	-2.07	1.39	1.44
24	A	407[A]	PHO	C1D-ND	-2.07	1.34	1.38
23	c	502	CLA	C3B-C2B	2.06	1.48	1.41
23	B	613	CLA	C3D-C4D	-2.06	1.39	1.44
29	A	414[B]	PL9	C2-C3	2.06	1.40	1.34
38	F	102	HEM	C3C-C4C	-2.06	1.42	1.46
26	B	620	SQD	O6-C1	2.06	1.43	1.40
23	b	608	CLA	C4C-C3C	2.06	1.48	1.45
31	M	101	LMT	O1'-C1'	-2.06	1.36	1.40
23	C	506	CLA	C3B-C2B	2.05	1.48	1.41
23	B	614	CLA	C3B-C2B	2.05	1.48	1.41
23	c	514	CLA	C1D-C2D	2.05	1.49	1.45
24	A	407[B]	PHO	C4B-NB	-2.05	1.34	1.38
23	b	604	CLA	C4C-C3C	2.05	1.48	1.45
23	c	503	CLA	C3D-C4D	-2.05	1.39	1.44
31	e	101	LMT	O2'-C2'	-2.05	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	611	CLA	C1D-C2D	2.05	1.49	1.45
27	D	413	GOL	O2-C2	-2.05	1.37	1.43
26	a	410	SQD	O6-C1	2.05	1.43	1.40
23	d	402[B]	CLA	C3D-C4D	-2.05	1.39	1.44
23	b	604	CLA	C1A-CHA	2.04	1.51	1.43
23	C	501	CLA	C3B-C2B	2.04	1.48	1.41
24	A	407[B]	PHO	C1D-ND	-2.04	1.34	1.38
23	b	603	CLA	C4C-C3C	2.04	1.48	1.45
29	D	406[A]	PL9	C2-C3	2.04	1.40	1.34
23	B	605	CLA	C4C-C3C	2.04	1.48	1.45
31	B	628	LMT	O5'-C5'	-2.04	1.39	1.44
23	a	407	CLA	C3D-C4D	-2.04	1.39	1.44
24	a	414[A]	PHO	C1B-NB	-2.03	1.34	1.38
23	C	509	CLA	C3D-C4D	-2.03	1.39	1.44
31	b	621	LMT	O3'-C3'	-2.03	1.38	1.43
31	B	628	LMT	O4'-C4B	-2.03	1.38	1.43
23	A	408	CLA	C1C-C2C	2.03	1.48	1.44
31	e	101	LMT	O2B-C2B	-2.03	1.38	1.43
33	b	629[A]	LHG	O7-C5	-2.02	1.41	1.46
23	c	507	CLA	C1C-C2C	2.02	1.48	1.44
23	b	616	CLA	C3B-C2B	2.02	1.48	1.41
23	B	607	CLA	C3B-C2B	2.02	1.48	1.41
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
23	C	508	CLA	C1C-NC	-2.01	1.34	1.37
23	C	507	CLA	C3B-C2B	2.01	1.48	1.41
23	C	508	CLA	C1A-CHA	2.01	1.51	1.43
24	a	414[B]	PHO	C1B-NB	-2.01	1.34	1.38
24	A	416[B]	PHO	C1D-ND	-2.01	1.34	1.38
27	D	413	GOL	C3-C2	2.01	1.60	1.51
34	B	623	HTG	C1-S1	-2.01	1.77	1.80
23	B	607	CLA	C3B-C4B	2.01	1.47	1.42
31	e	101	LMT	O3B-C3B	-2.01	1.38	1.43
23	c	512	CLA	C1D-C2D	2.01	1.49	1.45
23	B	603	CLA	C4C-C3C	2.01	1.48	1.45
23	b	601	CLA	C1D-C2D	2.00	1.49	1.45
24	a	414[A]	PHO	CBD-CGD	-2.00	1.49	1.52
38	F	102	HEM	C1D-ND	-2.00	1.34	1.38

All (3321) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	16.86	121.53	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C3B-C2B-C1B	-13.43	90.94	107.16
23	B	611	CLA	C1D-ND-C4D	-12.14	97.71	106.33
24	a	414[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	A	407[A]	PHO	C2D-C1D-ND	11.43	117.42	109.53
24	a	414[B]	PHO	C2D-C1D-ND	11.39	117.39	109.53
24	a	406[A]	PHO	C2D-C1D-ND	11.21	117.26	109.53
24	A	416[B]	PHO	C2D-C1D-ND	11.13	117.21	109.53
23	B	611	CLA	CHB-C1B-NB	-11.00	112.62	124.26
23	B	612	CLA	C1D-ND-C4D	-10.81	98.65	106.33
24	a	406[B]	PHO	C2D-C1D-ND	10.74	116.94	109.53
24	A	416[A]	PHO	C2D-C1D-ND	10.73	116.93	109.53
24	A	407[B]	PHO	C2D-C1D-ND	10.68	116.90	109.53
23	b	605	CLA	C1D-ND-C4D	-10.51	98.87	106.33
23	B	611	CLA	C2D-C1D-ND	10.51	117.85	110.10
23	a	405[B]	CLA	C1D-ND-C4D	-10.23	99.07	106.33
23	b	611	CLA	C1D-ND-C4D	-10.06	99.19	106.33
23	A	408	CLA	C1D-ND-C4D	-10.01	99.22	106.33
23	B	601	CLA	C1D-ND-C4D	-10.00	99.23	106.33
23	a	407	CLA	C1D-ND-C4D	-10.00	99.23	106.33
23	c	502	CLA	C1D-ND-C4D	-9.94	99.27	106.33
23	B	607	CLA	C1D-ND-C4D	-9.94	99.28	106.33
23	C	503	CLA	C1D-ND-C4D	-9.93	99.28	106.33
23	B	612	CLA	C2D-C1D-ND	9.80	117.32	110.10
23	d	402[B]	CLA	C1D-ND-C4D	-9.73	99.42	106.33
23	B	606	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	B	614	CLA	C1D-ND-C4D	-9.70	99.45	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	c	512	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	d	404	CLA	C1D-ND-C4D	-9.65	99.48	106.33
23	B	615	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	C	510	CLA	C1D-ND-C4D	-9.59	99.53	106.33
23	d	403[B]	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	b	610	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	B	616	CLA	C2D-C1D-ND	9.52	117.12	110.10
23	A	406[B]	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	c	506	CLA	C1D-ND-C4D	-9.46	99.62	106.33
23	B	603	CLA	C1D-ND-C4D	-9.44	99.63	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	B	605	CLA	C1D-ND-C4D	-9.39	99.67	106.33
23	C	501	CLA	C1D-ND-C4D	-9.38	99.67	106.33
23	b	609	CLA	C1D-ND-C4D	-9.37	99.68	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	C1D-ND-C4D	-9.36	99.69	106.33
23	b	614	CLA	C2D-C1D-ND	9.34	116.99	110.10
23	A	408	CLA	C2D-C1D-ND	9.32	116.97	110.10
23	b	608	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	C	505	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	b	614	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	B	608	CLA	C1D-ND-C4D	-9.25	99.76	106.33
23	B	616	CLA	C1D-ND-C4D	-9.22	99.78	106.33
23	c	504	CLA	C1D-ND-C4D	-9.21	99.79	106.33
23	B	607	CLA	C2D-C1D-ND	9.21	116.89	110.10
23	b	615	CLA	C1D-ND-C4D	-9.20	99.80	106.33
23	b	606	CLA	C1D-ND-C4D	-9.18	99.81	106.33
23	b	602	CLA	C1D-ND-C4D	-9.18	99.81	106.33
23	B	615	CLA	C2D-C1D-ND	9.15	116.85	110.10
23	B	608	CLA	C2D-C1D-ND	9.15	116.85	110.10
23	a	404[B]	CLA	C1D-ND-C4D	-9.15	99.84	106.33
23	c	514	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	D	403[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	601	CLA	C1D-ND-C4D	-9.12	99.86	106.33
23	B	606	CLA	C2D-C1D-ND	9.10	116.81	110.10
23	c	507	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	A	405[A]	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	a	407	CLA	C2D-C1D-ND	9.06	116.78	110.10
23	A	405[A]	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	B	614	CLA	C2D-C1D-ND	9.05	116.77	110.10
23	B	610	CLA	C1D-ND-C4D	-9.04	99.92	106.33
23	d	403[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	b	611	CLA	C2D-C1D-ND	8.97	116.72	110.10
23	c	510	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	a	404[A]	CLA	C1D-ND-C4D	-8.97	99.96	106.33
23	b	603	CLA	C1D-ND-C4D	-8.90	100.02	106.33
23	b	616	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	c	503	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	B	609	CLA	C1D-ND-C4D	-8.89	100.02	106.33
23	a	405[B]	CLA	C2D-C1D-ND	8.87	116.64	110.10
23	b	605	CLA	C2D-C1D-ND	8.86	116.64	110.10
23	c	511	CLA	C1D-ND-C4D	-8.86	100.04	106.33
23	b	613	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	d	404	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	d	402[B]	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	C	504	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	c	513	CLA	C1D-ND-C4D	-8.84	100.06	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	a	405[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	D	403[B]	CLA	C1D-ND-C4D	-8.80	100.09	106.33
23	B	603	CLA	C2D-C1D-ND	8.79	116.58	110.10
23	b	607	CLA	C1D-ND-C4D	-8.77	100.11	106.33
23	A	405[B]	CLA	C2D-C1D-ND	8.73	116.54	110.10
23	C	506	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	B	602	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	C	512	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	d	402[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	C	507	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-8.64	100.19	106.33
23	C	504	CLA	C1D-ND-C4D	-8.63	100.20	106.33
23	C	508	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	604	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	C	503	CLA	C2D-C1D-ND	8.57	116.42	110.10
23	D	404	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	b	616	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	c	502	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	c	512	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	C	511	CLA	C1D-ND-C4D	-8.49	100.30	106.33
23	D	403[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	505	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	b	607	CLA	C2D-C1D-ND	8.44	116.32	110.10
23	C	508	CLA	C2D-C1D-ND	8.42	116.31	110.10
23	c	509	CLA	C2D-C1D-ND	8.38	116.28	110.10
23	b	610	CLA	C2D-C1D-ND	8.38	116.28	110.10
23	b	609	CLA	C2D-C1D-ND	8.37	116.28	110.10
23	B	601	CLA	C2D-C1D-ND	8.37	116.27	110.10
23	B	610	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	b	613	CLA	C1D-ND-C4D	-8.34	100.41	106.33
23	B	613	CLA	C1D-ND-C4D	-8.30	100.44	106.33
23	b	615	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	c	503	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	C	501	CLA	C2D-C1D-ND	8.24	116.18	110.10
23	B	605	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	b	602	CLA	C2B-C1B-NB	8.17	115.71	110.23
23	C	511	CLA	C2D-C1D-ND	8.14	116.10	110.10
23	c	509	CLA	C1D-ND-C4D	-8.14	100.56	106.33
24	a	406[B]	PHO	O2D-CGD-CBD	8.14	121.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C2D-C1D-ND	8.12	116.09	110.10
23	c	508	CLA	C1D-ND-C4D	-8.10	100.58	106.33
23	b	614	CLA	C2B-C1B-NB	8.10	115.66	110.23
23	A	408	CLA	C2B-C1B-NB	8.09	115.65	110.23
23	C	512	CLA	C2B-C1B-NB	8.09	115.65	110.23
23	b	604	CLA	C2D-C1D-ND	8.09	116.06	110.10
23	C	513	CLA	C2D-C1D-ND	8.08	116.06	110.10
23	c	514	CLA	C2B-C1B-NB	8.07	115.64	110.23
23	A	406[B]	CLA	C2D-C1D-ND	8.06	116.04	110.10
23	C	509	CLA	C2D-C1D-ND	8.05	116.04	110.10
23	a	404[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	C	507	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	c	506	CLA	C2D-C1D-ND	8.01	116.01	110.10
23	b	612	CLA	C1D-ND-C4D	-8.00	100.65	106.33
23	c	510	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	B	609	CLA	C2D-C1D-ND	7.98	115.99	110.10
23	c	511	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	b	601	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	c	505	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	B	604	CLA	C1D-ND-C4D	-7.95	100.68	106.33
23	d	403[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	c	507	CLA	C2D-C1D-ND	7.91	115.93	110.10
23	c	513	CLA	C2B-C1B-NB	7.90	115.53	110.23
23	C	505	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	b	601	CLA	C2B-C1B-NB	7.87	115.51	110.23
23	d	403[B]	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	C	502	CLA	C1D-ND-C4D	-7.83	100.77	106.33
23	B	613	CLA	C2D-C1D-ND	7.78	115.83	110.10
23	B	611	CLA	CMB-C2B-C1B	7.78	137.21	125.37
23	B	601	CLA	C2B-C1B-NB	7.76	115.43	110.23
23	a	404[B]	CLA	C2B-C1B-NB	7.76	115.43	110.23
23	b	606	CLA	C2D-C1D-ND	7.73	115.80	110.10
23	b	602	CLA	C4A-NA-C1A	-7.72	103.23	106.71
23	a	404[B]	CLA	C2D-C1D-ND	7.70	115.78	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	C	512	CLA	C2D-C1D-ND	7.69	115.77	110.10
23	c	508	CLA	C2D-C1D-ND	7.69	115.77	110.10
23	c	513	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	b	603	CLA	C2D-C1D-ND	7.65	115.74	110.10
23	b	616	CLA	C2B-C1B-NB	7.64	115.36	110.23
23	C	510	CLA	C2B-C1B-NB	7.63	115.35	110.23
23	d	404	CLA	C2B-C1B-NB	7.63	115.35	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	C2B-C1B-NB	7.63	115.34	110.23
23	D	404	CLA	C2D-C1D-ND	7.63	115.72	110.10
23	b	608	CLA	C2B-C1B-NB	7.62	115.34	110.23
23	B	602	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	C	506	CLA	C2D-C1D-ND	7.59	115.70	110.10
23	C	510	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	a	405[B]	CLA	C2B-C1B-NB	7.57	115.31	110.23
23	C	510	CLA	CMD-C2D-C1D	7.55	138.02	124.71
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	C	509	CLA	C2B-C1B-NB	7.52	115.28	110.23
23	D	403[B]	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	c	508	CLA	O2D-CGD-CBD	7.50	124.59	111.27
23	c	504	CLA	C2D-C1D-ND	7.49	115.62	110.10
24	a	414[B]	PHO	O2D-CGD-CBD	7.47	120.46	111.00
23	c	505	CLA	C2B-C1B-NB	7.46	115.24	110.23
23	b	602	CLA	C2D-C1D-ND	7.46	115.60	110.10
23	c	514	CLA	C2D-C1D-ND	7.45	115.59	110.10
23	c	504	CLA	C4A-NA-C1A	-7.45	103.36	106.71
23	B	611	CLA	CHD-C4C-C3C	-7.44	113.91	124.84
26	F	103	SQD	O6-C1-C2	7.44	119.91	108.30
23	B	606	CLA	C4A-NA-C1A	-7.40	103.38	106.71
23	C	513	CLA	C2B-C1B-NB	7.40	115.19	110.23
24	A	416[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
34	b	623	HTG	C1'-S1-C1	7.36	113.86	100.09
23	C	511	CLA	C2B-C1B-NB	7.36	115.17	110.23
23	A	404[B]	CLA	C2D-C1D-ND	7.33	115.51	110.10
23	C	502	CLA	C2D-C1D-ND	7.30	115.48	110.10
23	d	402[B]	CLA	C2B-C1B-NB	7.26	115.10	110.23
23	B	606	CLA	CMD-C2D-C1D	7.25	137.50	124.71
23	B	616	CLA	O2D-CGD-CBD	7.25	124.16	111.27
23	B	602	CLA	C2B-C1B-NB	7.23	115.08	110.23
24	A	416[B]	PHO	O2D-CGD-CBD	7.22	120.14	111.00
23	b	611	CLA	CMD-C2D-C1D	7.21	137.42	124.71
24	a	414[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
23	A	404[A]	CLA	C2B-C1B-NB	7.20	115.06	110.23
23	C	503	CLA	C4A-NA-C1A	-7.17	103.48	106.71
24	a	406[A]	PHO	O2D-CGD-CBD	7.16	120.07	111.00
24	a	406[A]	PHO	C1C-C2C-C3C	-7.15	102.67	108.61
23	c	504	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	A	406[B]	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	C	503	CLA	C2B-C1B-NB	7.12	115.01	110.23
24	A	416[A]	PHO	C2B-C1B-NB	7.12	114.44	109.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	414[A]	PHO	C2B-C1B-NB	7.11	114.44	109.53
23	A	406[A]	CLA	C2B-C1B-NB	7.10	114.99	110.23
24	a	414[A]	PHO	C4D-ND-C1D	-7.08	101.62	108.83
23	B	605	CLA	CHD-C4C-C3C	-7.05	114.47	124.84
23	b	616	CLA	C4A-NA-C1A	-7.04	103.54	106.71
23	B	616	CLA	CHD-C4C-C3C	-7.03	114.50	124.84
23	C	502	CLA	C2B-C1B-NB	7.01	114.93	110.23
23	B	611	CLA	CMD-C2D-C1D	7.01	137.07	124.71
24	A	416[B]	PHO	C2B-C1B-NB	7.00	114.36	109.53
23	b	606	CLA	C2B-C1B-NB	7.00	114.93	110.23
23	D	404	CLA	C2B-C1B-NB	7.00	114.92	110.23
23	a	404[A]	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	B	609	CLA	C2B-C1B-NB	6.98	114.91	110.23
24	A	407[B]	PHO	O2D-CGD-CBD	6.96	119.81	111.00
23	A	405[B]	CLA	C2B-C1B-NB	6.94	114.89	110.23
23	B	603	CLA	C2B-C1B-NB	6.93	114.88	110.23
23	c	502	CLA	CHD-C1D-ND	-6.92	118.10	124.45
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	C	508	CLA	C2C-C1C-NC	6.90	116.44	109.97
24	a	414[B]	PHO	C4D-ND-C1D	-6.90	101.81	108.83
24	a	414[A]	PHO	C1C-C2C-C3C	-6.90	102.87	108.61
23	c	509	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	b	610	CLA	CMD-C2D-C1D	6.89	136.85	124.71
23	B	608	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	a	405[B]	CLA	CHD-C1D-ND	-6.88	118.13	124.45
23	c	504	CLA	CMD-C2D-C1D	6.88	136.84	124.71
23	B	604	CLA	C2D-C1D-ND	6.86	115.16	110.10
23	a	405[A]	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	C	512	CLA	C4A-NA-C1A	-6.86	103.62	106.71
23	b	612	CLA	C2D-C1D-ND	6.85	115.15	110.10
23	B	606	CLA	CHD-C1D-ND	-6.85	118.16	124.45
24	A	407[A]	PHO	C4D-ND-C1D	-6.85	101.86	108.83
23	C	506	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	B	614	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	c	511	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	D	403[B]	CLA	C4A-NA-C1A	-6.83	103.64	106.71
23	b	605	CLA	C2B-C1B-NB	6.82	114.81	110.23
23	A	408	CLA	CHD-C1D-ND	-6.81	118.20	124.45
23	a	407	CLA	C2B-C1B-NB	6.80	114.79	110.23
23	b	609	CLA	CHD-C4C-C3C	-6.80	114.85	124.84
23	B	609	CLA	C4A-NA-C1A	-6.79	103.65	106.71
23	A	404[B]	CLA	C2B-C1B-NB	6.79	114.78	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	507	CLA	C2B-C1B-NB	6.79	114.78	110.23
23	B	603	CLA	O2D-CGD-CBD	6.78	123.32	111.27
23	c	514	CLA	CMD-C2D-C1D	6.78	136.67	124.71
23	b	616	CLA	O2D-CGD-CBD	6.77	123.30	111.27
23	C	505	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	c	510	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	B	615	CLA	C4A-NA-C1A	-6.74	103.68	106.71
23	c	508	CLA	CMD-C2D-C1D	6.73	136.58	124.71
23	C	501	CLA	C2B-C1B-NB	6.72	114.74	110.23
23	A	404[B]	CLA	CMD-C2D-C1D	6.71	136.55	124.71
23	b	606	CLA	CMD-C2D-C1D	6.70	136.52	124.71
23	B	613	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	A	405[A]	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	b	603	CLA	C4A-NA-C1A	-6.70	103.69	106.71
23	b	601	CLA	O2D-CGD-CBD	6.70	123.17	111.27
23	b	616	CLA	CHD-C4C-C3C	-6.69	115.01	124.84
23	d	402[A]	CLA	C2B-C1B-NB	6.67	114.71	110.23
23	a	407	CLA	CHD-C4C-C3C	-6.66	115.06	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.65	115.07	124.84
23	A	408	CLA	CMD-C2D-C1D	6.65	136.43	124.71
23	b	615	CLA	C2B-C1B-NB	6.64	114.69	110.23
23	c	506	CLA	C2B-C1B-NB	6.64	114.69	110.23
23	d	402[B]	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
23	C	510	CLA	CHD-C1D-ND	-6.64	118.35	124.45
23	B	615	CLA	CHD-C4C-C3C	-6.64	115.08	124.84
23	b	612	CLA	C2B-C1B-NB	6.64	114.68	110.23
23	c	503	CLA	C2B-C1B-NB	6.64	114.68	110.23
23	B	614	CLA	CMD-C2D-C1D	6.63	136.40	124.71
23	b	606	CLA	CHD-C4C-C3C	-6.63	115.09	124.84
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	B	604	CLA	C2C-C1C-NC	6.61	116.17	109.97
23	b	605	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	d	403[B]	CLA	C2C-C1C-NC	6.59	116.14	109.97
24	A	416[A]	PHO	C1C-C2C-C3C	-6.58	103.14	108.61
23	b	611	CLA	CHD-C1D-ND	-6.58	118.41	124.45
23	c	502	CLA	CMD-C2D-C1D	6.57	136.29	124.71
23	d	404	CLA	CMD-C2D-C1D	6.56	136.28	124.71
23	C	512	CLA	CHD-C4C-C3C	-6.55	115.22	124.84
23	C	501	CLA	C4A-NA-C1A	-6.54	103.77	106.71
23	c	505	CLA	CHD-C1D-ND	-6.54	118.45	124.45
23	a	404[B]	CLA	C2C-C1C-NC	6.53	116.09	109.97
23	b	610	CLA	CHD-C4C-C3C	-6.53	115.24	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C2C-C1C-NC	6.53	116.09	109.97
23	D	403[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
24	a	406[B]	PHO	C2B-C1B-NB	6.52	114.03	109.53
23	D	403[B]	CLA	CHD-C1D-ND	-6.52	118.47	124.45
23	d	403[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
24	A	407[B]	PHO	C4D-ND-C1D	-6.51	102.20	108.83
23	b	615	CLA	C4A-NA-C1A	-6.50	103.78	106.71
23	C	507	CLA	CMD-C2D-C1D	6.50	136.16	124.71
23	c	508	CLA	CHD-C1D-ND	-6.50	118.48	124.45
23	b	605	CLA	CMD-C2D-C1D	6.50	136.16	124.71
24	a	414[B]	PHO	C2B-C1B-NB	6.48	114.00	109.53
23	C	506	CLA	CMD-C2D-C1D	6.48	136.14	124.71
23	C	503	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
34	c	522	HTG	C1'-S1-C1	6.48	112.21	100.09
23	c	502	CLA	C2B-C1B-NB	6.48	114.58	110.23
23	B	610	CLA	C2B-C1B-NB	6.46	114.57	110.23
23	C	506	CLA	CHD-C1D-ND	-6.46	118.51	124.45
24	A	416[B]	PHO	C4D-ND-C1D	-6.46	102.25	108.83
23	D	403[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	b	602	CLA	O2D-CGD-CBD	6.44	122.72	111.27
24	a	406[B]	PHO	C1C-C2C-C3C	-6.43	103.27	108.61
23	B	601	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	B	611	CLA	O2D-CGD-CBD	6.42	122.69	111.27
23	C	501	CLA	CHD-C4C-C3C	-6.42	115.41	124.84
24	A	416[A]	PHO	C4D-ND-C1D	-6.42	102.30	108.83
23	B	605	CLA	CMD-C2D-C1D	6.42	136.02	124.71
24	a	406[A]	PHO	C2B-C1B-NB	6.41	113.95	109.53
24	A	416[B]	PHO	C1C-C2C-C3C	-6.41	103.28	108.61
23	b	613	CLA	C2B-C1B-NB	6.41	114.53	110.23
23	B	611	CLA	CHD-C1D-ND	-6.41	118.57	124.45
23	A	406[B]	CLA	CHD-C1D-ND	-6.40	118.57	124.45
23	D	404	CLA	C4A-NA-C1A	-6.39	103.83	106.71
23	C	511	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	b	613	CLA	CHD-C4C-C3C	-6.37	115.47	124.84
23	b	605	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	c	507	CLA	CMD-C2D-C1D	6.37	135.94	124.71
23	c	511	CLA	CHD-C4C-C3C	-6.37	115.48	124.84
23	c	512	CLA	C2B-C1B-NB	6.36	114.50	110.23
23	b	606	CLA	C4A-NA-C1A	-6.36	103.85	106.71
34	D	411	HTG	C1'-S1-C1	6.35	111.97	100.09
23	b	604	CLA	O2D-CGD-CBD	6.35	122.55	111.27
24	a	406[A]	PHO	C4D-ND-C1D	-6.34	102.38	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	O2D-CGD-CBD	6.34	122.54	111.27
23	d	404	CLA	CHD-C1D-ND	-6.34	118.63	124.45
23	a	405[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	B	603	CLA	CHD-C4C-C3C	-6.34	115.53	124.84
23	b	610	CLA	C2B-C1B-NB	6.33	114.48	110.23
23	D	403[B]	CLA	CMD-C2D-C1D	6.33	135.87	124.71
23	a	405[B]	CLA	CMD-C2D-C1D	6.33	135.87	124.71
23	C	504	CLA	C2C-C1C-NC	6.31	115.89	109.97
24	A	407[B]	PHO	C1C-C2C-C3C	-6.31	103.36	108.61
23	b	614	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
23	a	405[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	B	612	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
23	b	612	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
23	c	509	CLA	C2C-C1C-NC	6.29	115.87	109.97
23	B	607	CLA	CHD-C4C-C3C	-6.29	115.59	124.84
23	c	513	CLA	CMD-C2D-C1D	6.28	135.79	124.71
23	C	503	CLA	CMD-C2D-C1D	6.28	135.79	124.71
23	b	609	CLA	C2B-C1B-NB	6.28	114.44	110.23
23	b	611	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	B	601	CLA	CHD-C4C-C3C	-6.28	115.61	124.84
23	B	616	CLA	C3C-C4C-NC	6.27	117.60	110.57
23	C	508	CLA	C2B-C1B-NB	6.27	114.44	110.23
23	b	611	CLA	C2B-C1B-NB	6.27	114.43	110.23
23	D	403[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	d	402[B]	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	a	404[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	A	405[B]	CLA	CHD-C1D-ND	-6.25	118.71	124.45
24	A	407[A]	PHO	C2B-C1B-NB	6.25	113.84	109.53
25	D	405	BCR	C7-C8-C9	-6.23	116.82	126.23
24	a	406[B]	PHO	C4D-ND-C1D	-6.22	102.50	108.83
23	d	402[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	A	408	CLA	CHD-C4C-C3C	-6.21	115.72	124.84
23	b	602	CLA	CHD-C1D-ND	-6.20	118.76	124.45
23	a	404[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	b	601	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	c	514	CLA	CHD-C1D-ND	-6.19	118.77	124.45
23	c	512	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	B	604	CLA	C2B-C1B-NB	6.18	114.38	110.23
23	A	406[B]	CLA	CMD-C2D-C1D	6.18	135.60	124.71
23	a	404[B]	CLA	CMD-C2D-C1D	6.18	135.60	124.71
23	B	615	CLA	C2B-C1B-NB	6.18	114.37	110.23
23	B	602	CLA	CMD-C2D-C1D	6.16	135.58	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	403[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	C	508	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
23	a	405[B]	CLA	CHD-C4C-C3C	-6.16	115.79	124.84
23	A	404[B]	CLA	C2C-C1C-NC	6.16	115.74	109.97
24	A	407[A]	PHO	C1C-C2C-C3C	-6.15	103.49	108.61
23	c	503	CLA	C2C-C1C-NC	6.14	115.72	109.97
26	F	103	SQD	O47-C7-C8	6.12	124.70	111.50
23	C	509	CLA	CMD-C2D-C1D	6.12	135.50	124.71
23	B	605	CLA	C2B-C1B-NB	6.12	114.33	110.23
23	b	607	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	b	606	CLA	CHD-C1D-ND	-6.10	118.85	124.45
23	b	607	CLA	C2C-C1C-NC	6.09	115.68	109.97
23	C	501	CLA	CMD-C2D-C1D	6.09	135.45	124.71
23	B	609	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
23	c	508	CLA	C2B-C1B-NB	6.09	114.31	110.23
23	b	601	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	d	403[B]	CLA	CMD-C2D-C1D	6.08	135.43	124.71
23	c	508	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	b	616	CLA	CMD-C2D-C1D	6.07	135.40	124.71
23	B	608	CLA	CHD-C1D-ND	-6.06	118.88	124.45
23	B	614	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	B	608	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
23	D	403[B]	CLA	C2B-C1B-NB	6.05	114.29	110.23
23	B	608	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	b	604	CLA	C2B-C1B-NB	6.04	114.28	110.23
23	C	505	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
23	A	404[B]	CLA	CHD-C1D-ND	-6.04	118.91	124.45
23	B	601	CLA	CHD-C1D-ND	-6.04	118.91	124.45
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	b	604	CLA	C2C-C1C-NC	6.03	115.62	109.97
23	c	507	CLA	CHD-C1D-ND	-6.03	118.91	124.45
23	d	403[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	B	605	CLA	C4A-NA-C1A	-6.02	104.00	106.71
24	a	414[B]	PHO	C1C-C2C-C3C	-6.02	103.61	108.61
23	d	403[B]	CLA	C2B-C1B-NB	6.01	114.26	110.23
23	C	504	CLA	C2B-C1B-NB	6.01	114.26	110.23
23	C	509	CLA	C2C-C1C-NC	6.01	115.60	109.97
23	c	507	CLA	C2C-C1C-NC	6.01	115.60	109.97
23	b	609	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	d	404	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	B	612	CLA	O2D-CGD-CBD	6.00	121.92	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	603	CLA	CHD-C4C-C3C	-6.00	116.03	124.84
23	B	601	CLA	O2D-CGD-CBD	5.99	121.91	111.27
23	C	507	CLA	CHD-C4C-C3C	-5.99	116.04	124.84
23	C	502	CLA	C2C-C1C-NC	5.99	115.58	109.97
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	d	402[B]	CLA	CMD-C2D-C1D	5.98	135.24	124.71
23	a	404[B]	CLA	CHD-C1D-ND	-5.98	118.96	124.45
23	A	406[B]	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	b	615	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	D	403[B]	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	C	502	CLA	CHD-C4C-C3C	-5.96	116.09	124.84
23	B	614	CLA	CHD-C1D-ND	-5.95	118.99	124.45
23	C	509	CLA	CHD-C1D-ND	-5.94	118.99	124.45
23	b	602	CLA	CMD-C2D-C1D	5.94	135.19	124.71
23	C	510	CLA	O2D-CGD-CBD	5.94	121.82	111.27
23	b	615	CLA	CMD-C2D-C1D	5.94	135.18	124.71
23	c	511	CLA	CMD-C2D-C1D	5.94	135.17	124.71
23	c	509	CLA	CHD-C4C-C3C	-5.93	116.12	124.84
23	C	505	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	B	616	CLA	C2B-C1B-NB	5.92	114.20	110.23
23	C	503	CLA	CHD-C1D-ND	-5.91	119.02	124.45
23	a	404[B]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
34	d	411	HTG	C1'-S1-C1	5.91	111.14	100.09
23	C	513	CLA	CHD-C1D-ND	-5.90	119.03	124.45
23	C	507	CLA	O2D-CGD-CBD	5.90	121.75	111.27
40	V	201	HEC	C1D-ND-C4D	5.89	111.16	105.07
23	b	601	CLA	CHD-C1D-ND	-5.89	119.04	124.45
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
29	A	414[A]	PL9	C7-C8-C9	-5.89	116.99	126.79
23	B	606	CLA	O2D-CGD-CBD	5.89	121.73	111.27
23	B	614	CLA	O2D-CGD-CBD	5.89	121.73	111.27
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	614	CLA	C2C-C1C-NC	5.88	115.48	109.97
23	B	610	CLA	CMD-C2D-C1D	5.87	135.05	124.71
23	D	403[A]	CLA	C2B-C1B-NB	5.87	114.17	110.23
23	B	609	CLA	CHD-C1D-ND	-5.86	119.06	124.45
23	c	504	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	b	604	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.84	116.25	124.84
23	c	502	CLA	CHD-C4C-C3C	-5.84	116.26	124.84
23	c	508	CLA	CHD-C4C-C3C	-5.84	116.26	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
23	b	601	CLA	CMD-C2D-C1D	5.83	134.99	124.71
23	b	614	CLA	O2D-CGD-CBD	5.83	121.63	111.27
23	C	509	CLA	CHD-C4C-C3C	-5.83	116.27	124.84
23	B	612	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	c	514	CLA	C4A-NA-C1A	-5.82	104.09	106.71
23	C	509	CLA	C4A-NA-C1A	-5.82	104.09	106.71
23	b	607	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	c	503	CLA	CHD-C4C-C3C	-5.81	116.30	124.84
23	A	404[A]	CLA	CHD-C1D-ND	-5.81	119.11	124.45
23	b	608	CLA	CHD-C1D-ND	-5.81	119.11	124.45
24	A	407[B]	PHO	C2B-C1B-NB	5.81	113.54	109.53
23	b	607	CLA	CHD-C4C-C3C	-5.81	116.31	124.84
25	t	102	BCR	C33-C5-C6	-5.80	118.01	124.53
34	B	623	HTG	C1'-S1-C1	5.80	110.94	100.09
23	b	602	CLA	CHD-C4C-C3C	-5.79	116.32	124.84
23	B	609	CLA	CMD-C2D-C1D	5.79	134.92	124.71
26	A	410[B]	SQD	O6-C1-C2	5.79	117.34	108.30
23	A	405[B]	CLA	CHD-C4C-C3C	-5.78	116.35	124.84
23	c	504	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	B	613	CLA	CMD-C2D-C1D	5.77	134.87	124.71
23	c	510	CLA	C1-C2-C3	-5.76	116.08	126.04
23	c	510	CLA	CHD-C4C-C3C	-5.75	116.38	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	610	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	c	506	CLA	O2D-CGD-CBD	5.75	121.48	111.27
23	C	504	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
23	B	603	CLA	CMD-C2D-C1D	5.73	134.82	124.71
23	b	613	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	C	507	CLA	CHD-C1D-ND	-5.73	119.19	124.45
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	C	510	CLA	CHD-C4C-C3C	-5.72	116.43	124.84
23	c	512	CLA	CMD-C2D-C1D	5.72	134.79	124.71
23	B	606	CLA	C2B-C1B-NB	5.72	114.07	110.23
23	c	506	CLA	CMD-C2D-C1D	5.72	134.79	124.71
23	c	514	CLA	CHD-C4C-C3C	-5.72	116.44	124.84
23	C	513	CLA	CHD-C4C-C3C	-5.71	116.44	124.84
23	c	512	CLA	CHD-C1D-ND	-5.71	119.21	124.45
23	B	607	CLA	CHD-C1D-ND	-5.70	119.21	124.45
23	C	513	CLA	CMD-C2D-C1D	5.70	134.76	124.71
23	c	513	CLA	C4A-NA-C1A	-5.70	104.14	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	501	CLA	O2D-CGD-CBD	5.70	121.40	111.27
23	b	612	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	d	403[B]	CLA	CHD-C4C-C3C	-5.70	116.47	124.84
23	B	611	CLA	C3D-C2D-C1D	-5.69	98.06	105.83
23	b	611	CLA	O2D-CGD-CBD	5.68	121.36	111.27
23	c	513	CLA	O2D-CGD-CBD	5.68	121.36	111.27
23	D	404	CLA	CHD-C4C-C3C	-5.67	116.50	124.84
23	B	604	CLA	CMD-C2D-C1D	5.67	134.71	124.71
23	d	404	CLA	O2D-CGD-CBD	5.67	121.34	111.27
23	d	403[A]	CLA	C2B-C1B-NB	5.67	114.03	110.23
23	B	603	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	B	615	CLA	CHD-C1D-ND	-5.66	119.25	124.45
23	b	608	CLA	C2C-C1C-NC	5.66	115.27	109.97
23	C	505	CLA	O2D-CGD-CBD	5.65	121.31	111.27
23	c	505	CLA	CMD-C2D-C1D	5.65	134.68	124.71
24	a	414[B]	PHO	C1-C2-C3	-5.65	116.27	126.04
23	C	507	CLA	C2C-C1C-NC	5.65	115.27	109.97
23	d	403[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	B	602	CLA	C4A-NA-C1A	-5.64	104.17	106.71
40	v	201	HEC	C1D-ND-C4D	5.64	110.89	105.07
23	c	507	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
23	A	405[B]	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	A	408	CLA	C2C-C1C-NC	5.63	115.24	109.97
23	b	603	CLA	O2D-CGD-CBD	5.62	121.26	111.27
23	b	603	CLA	CMD-C2D-C1D	5.62	134.61	124.71
23	B	602	CLA	O2D-CGD-CBD	5.61	121.24	111.27
23	d	402[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	b	604	CLA	C1-C2-C3	-5.61	116.35	126.04
23	c	502	CLA	O2D-CGD-CBD	5.60	121.22	111.27
23	A	405[B]	CLA	CMD-C2D-C1D	5.60	134.58	124.71
23	b	609	CLA	C4A-NA-C1A	-5.59	104.19	106.71
23	b	605	CLA	C2C-C1C-NC	5.59	115.20	109.97
23	d	403[B]	CLA	CHD-C1D-ND	-5.58	119.32	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	B	604	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	c	510	CLA	C2C-C1C-NC	5.57	115.19	109.97
23	c	513	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	c	510	CLA	CMD-C2D-C1D	5.56	134.52	124.71
23	B	613	CLA	C2C-C1C-NC	5.56	115.18	109.97
23	B	616	CLA	C4A-NA-C1A	-5.56	104.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403[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
25	d	405	BCR	C7-C8-C9	-5.55	117.84	126.23
23	d	403[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
26	B	620	SQD	O6-C1-C2	5.55	116.96	108.30
23	c	505	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	B	611	CLA	CMC-C2C-C1C	5.54	133.48	125.04
23	b	611	CLA	C2C-C1C-NC	5.54	115.17	109.97
23	C	502	CLA	CMD-C2D-C1D	5.54	134.48	124.71
23	c	513	CLA	CHD-C1D-ND	-5.54	119.36	124.45
23	B	613	CLA	C1-C2-C3	-5.54	116.47	126.04
23	C	512	CLA	CMD-C2D-C1D	5.53	134.47	124.71
23	D	403[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	B	609	CLA	C2C-C1C-NC	5.53	115.15	109.97
23	b	608	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
23	B	604	CLA	C3C-C4C-NC	5.52	116.77	110.57
23	C	505	CLA	C2C-C1C-NC	5.52	115.15	109.97
26	B	620	SQD	O47-C7-C8	5.51	123.37	111.50
23	b	613	CLA	CMD-C2D-C1D	5.50	134.41	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-5.50	104.23	106.71
23	A	406[B]	CLA	C4A-NA-C1A	-5.50	104.23	106.71
23	c	506	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	B	603	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	b	608	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	a	405[B]	CLA	C4A-NA-C1A	-5.49	104.24	106.71
23	c	511	CLA	CHD-C1D-ND	-5.48	119.42	124.45
26	b	620	SQD	O6-C1-C2	5.47	116.85	108.30
23	B	615	CLA	CMD-C2D-C1D	5.47	134.35	124.71
23	b	607	CLA	C2B-C1B-NB	5.47	113.90	110.23
23	b	610	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	c	508	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	B	613	CLA	CHD-C4C-C3C	-5.46	116.81	124.84
23	c	511	CLA	C2C-C1C-NC	5.45	115.08	109.97
23	b	610	CLA	O2D-CGD-CBD	5.45	120.95	111.27
23	C	507	CLA	C2B-C1B-NB	5.45	113.88	110.23
23	c	509	CLA	C4A-NA-C1A	-5.45	104.26	106.71
23	C	510	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	B	614	CLA	C3D-C2D-C1D	-5.44	98.40	105.83
23	C	511	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	B	607	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	d	402[A]	CLA	CHD-C1D-ND	-5.44	119.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	CHD-C1D-ND	-5.43	119.46	124.45
23	B	610	CLA	C4A-NA-C1A	-5.43	104.26	106.71
23	B	606	CLA	C3D-C2D-C1D	-5.43	98.42	105.83
23	C	513	CLA	C2C-C1C-NC	5.43	115.06	109.97
23	C	504	CLA	CHD-C1D-ND	-5.42	119.47	124.45
23	C	511	CLA	CMD-C2D-C1D	5.42	134.26	124.71
23	b	614	CLA	CHD-C1D-ND	-5.42	119.47	124.45
23	b	616	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	B	616	CLA	C3D-C2D-C1D	-5.40	98.46	105.83
23	b	609	CLA	CHD-C1D-ND	-5.39	119.50	124.45
23	a	404[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	C	502	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	A	408	CLA	C3D-C2D-C1D	-5.38	98.49	105.83
23	A	404[B]	CLA	CHD-C4C-C3C	-5.37	116.94	124.84
23	B	610	CLA	CHD-C1D-ND	-5.37	119.52	124.45
23	B	602	CLA	C2C-C1C-NC	5.37	115.00	109.97
24	a	414[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	C	511	CLA	O2D-CGD-CBD	5.36	120.80	111.27
23	d	402[B]	CLA	C2C-C1C-NC	5.36	115.00	109.97
23	B	605	CLA	CHD-C1D-ND	-5.36	119.53	124.45
23	c	507	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	c	505	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	c	509	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
23	a	405[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	c	509	CLA	CMD-C2D-C1D	5.33	134.11	124.71
23	A	406[A]	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	b	603	CLA	C2C-C1C-NC	5.32	114.96	109.97
23	B	605	CLA	C2C-C1C-NC	5.32	114.96	109.97
23	c	506	CLA	C4A-NA-C1A	-5.32	104.31	106.71
23	B	602	CLA	CHD-C1D-ND	-5.32	119.56	124.45
23	B	607	CLA	O2D-CGD-CBD	5.32	120.72	111.27
23	b	611	CLA	C3D-C2D-C1D	-5.32	98.58	105.83
23	a	404[B]	CLA	CHD-C4C-C3C	-5.31	117.03	124.84
23	C	512	CLA	CHD-C1D-ND	-5.31	119.58	124.45
23	b	615	CLA	C2C-C1C-NC	5.30	114.94	109.97
23	C	501	CLA	CHD-C1D-ND	-5.30	119.58	124.45
23	a	404[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45
23	B	608	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
23	C	502	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	C	506	CLA	C4A-NA-C1A	-5.28	104.33	106.71
23	c	512	CLA	C2C-C1C-NC	5.28	114.92	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	CHD-C1D-ND	-5.28	119.61	124.45
23	C	504	CLA	CMD-C2D-C1D	5.28	134.01	124.71
23	C	511	CLA	C3B-C2B-C1B	-5.27	100.80	107.16
23	b	613	CLA	C3D-C2D-C1D	-5.26	98.65	105.83
23	C	508	CLA	O2D-CGD-CBD	5.25	120.60	111.27
23	c	505	CLA	C2C-C1C-NC	5.25	114.89	109.97
23	b	614	CLA	C3D-C2D-C1D	-5.25	98.67	105.83
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	D	403[B]	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
23	B	612	CLA	CMD-C2D-C1D	5.25	133.96	124.71
23	C	509	CLA	C3B-C2B-C1B	-5.24	100.84	107.16
23	c	511	CLA	C4A-NA-C1A	-5.23	104.35	106.71
23	c	509	CLA	O2D-CGD-CBD	5.23	120.56	111.27
24	a	414[B]	PHO	C3D-C4D-ND	5.23	114.85	107.72
23	C	504	CLA	C3D-C2D-C1D	-5.23	98.70	105.83
34	C	521	HTG	C1'-S1-C1	5.22	109.86	100.09
23	b	616	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
26	a	409[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	C	504	CLA	O2D-CGD-CBD	5.21	120.52	111.27
23	B	614	CLA	C3B-C2B-C1B	-5.21	100.88	107.16
23	C	507	CLA	C4A-NA-C1A	-5.20	104.37	106.71
23	C	508	CLA	CMD-C2D-C1D	5.20	133.87	124.71
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
24	A	407[A]	PHO	C3D-C4D-ND	5.17	114.77	107.72
23	a	407	CLA	O2D-CGD-CBD	5.17	120.46	111.27
23	b	614	CLA	C2C-C1C-NC	5.17	114.82	109.97
23	b	613	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	d	404	CLA	C3D-C2D-C1D	-5.17	98.77	105.83
23	C	513	CLA	O2D-CGD-CBD	5.17	120.45	111.27
38	F	102	HEM	CAD-CBD-CGD	5.17	124.73	113.60
25	d	405	BCR	C15-C14-C13	-5.17	119.93	127.31
23	C	508	CLA	C3C-C4C-NC	5.16	116.36	110.57
23	b	613	CLA	CHD-C1D-ND	-5.16	119.71	124.45
23	b	607	CLA	C3C-C4C-NC	5.15	116.35	110.57
23	B	608	CLA	CMD-C2D-C1D	5.15	133.79	124.71
23	B	610	CLA	C2C-C1C-NC	5.15	114.80	109.97
23	D	404	CLA	O2D-CGD-CBD	5.15	120.41	111.27
23	c	504	CLA	C2C-C1C-NC	5.14	114.79	109.97
23	B	615	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
32	A	418	LMG	C7-O1-C1	-5.14	103.71	113.74
23	C	512	CLA	O2D-CGD-CBD	5.13	120.39	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	O2D-CGD-CBD	5.12	120.37	111.27
23	D	403[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	A	406[A]	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	c	502	CLA	O2D-CGD-O1D	-5.11	113.84	123.84
23	C	506	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
23	B	614	CLA	C4A-NA-C1A	-5.11	104.41	106.71
23	b	606	CLA	O2D-CGD-CBD	5.11	120.35	111.27
23	B	604	CLA	C1-C2-C3	-5.11	117.21	126.04
23	c	514	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	c	510	CLA	O2D-CGD-CBD	5.10	120.33	111.27
23	c	510	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	B	616	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	c	505	CLA	C3B-C2B-C1B	-5.09	101.01	107.16
23	a	407	CLA	CHD-C1D-ND	-5.09	119.77	124.45
26	b	620	SQD	O47-C7-C8	5.09	122.47	111.50
23	A	406[B]	CLA	C2C-C1C-NC	5.09	114.74	109.97
24	a	414[A]	PHO	C3D-C4D-ND	5.09	114.66	107.72
23	a	407	CLA	C3C-C4C-NC	5.09	116.28	110.57
24	A	407[B]	PHO	C3D-C4D-ND	5.08	114.64	107.72
23	B	612	CLA	C3C-C4C-NC	5.08	116.27	110.57
32	B	621	LMG	O7-C10-C11	5.08	122.44	111.50
23	b	612	CLA	C4A-NA-C1A	-5.07	104.42	106.71
23	C	505	CLA	CHD-C1D-ND	-5.07	119.80	124.45
23	b	607	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	A	405[B]	CLA	C3D-C2D-C1D	-5.06	98.93	105.83
23	B	605	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	B	608	CLA	O2D-CGD-CBD	5.05	120.24	111.27
23	B	607	CLA	C2B-C1B-NB	5.05	113.62	110.23
23	d	404	CLA	C2C-C1C-NC	5.05	114.70	109.97
23	c	502	CLA	C2C-C1C-NC	5.04	114.69	109.97
23	b	604	CLA	CMD-C2D-C1D	5.04	133.59	124.71
23	b	614	CLA	CMD-C2D-C1D	5.04	133.59	124.71
23	d	402[B]	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	C	513	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
23	C	510	CLA	C4A-NA-C1A	-5.04	104.44	106.71
38	F	102	HEM	CHC-C4B-NB	5.03	129.88	124.42
23	a	407	CLA	C2C-C1C-NC	5.03	114.68	109.97
23	b	612	CLA	C3C-C4C-NC	5.02	116.20	110.57
23	b	603	CLA	CHD-C1D-ND	-5.02	119.84	124.45
23	C	505	CLA	C3C-C4C-NC	5.01	116.19	110.57
23	C	510	CLA	C1-C2-C3	-5.01	117.38	126.04
23	d	404	CLA	C4A-NA-C1A	-5.01	104.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CMD-C2D-C1D	5.01	133.54	124.71
23	c	513	CLA	C3B-C2B-C1B	-5.00	101.12	107.16
23	b	605	CLA	C4A-NA-C1A	-5.00	104.46	106.71
23	c	506	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	c	503	CLA	O2D-CGD-CBD	5.00	120.14	111.27
23	B	604	CLA	O2D-CGD-CBD	4.99	120.14	111.27
23	B	606	CLA	C2C-C1C-NC	4.99	114.65	109.97
23	D	404	CLA	CHD-C1D-ND	-4.99	119.87	124.45
23	B	603	CLA	C4A-NA-C1A	-4.99	104.46	106.71
23	B	606	CLA	C3C-C4C-NC	4.98	116.16	110.57
23	b	605	CLA	O2D-CGD-CBD	4.98	120.11	111.27
23	b	610	CLA	C2C-C1C-NC	4.97	114.63	109.97
23	D	404	CLA	CMD-C2D-C1D	4.96	133.46	124.71
26	a	409[B]	SQD	O47-C7-C8	4.96	122.19	111.50
23	c	514	CLA	C3B-C2B-C1B	-4.96	101.17	107.16
23	B	607	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
23	b	606	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	b	609	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	b	605	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
23	b	614	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
23	d	402[B]	CLA	O2D-CGD-CBD	4.94	120.05	111.27
25	Y	101	BCR	C33-C5-C6	-4.94	118.98	124.53
23	B	603	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
23	a	405[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	B	610	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
26	A	410[B]	SQD	C1-O5-C5	-4.92	104.03	113.69
23	b	613	CLA	C4A-NA-C1A	-4.92	104.49	106.71
23	B	605	CLA	C3C-C4C-NC	4.92	116.09	110.57
23	a	404[B]	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
23	b	605	CLA	C3D-C4D-ND	4.92	118.19	110.24
23	a	405[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
23	B	608	CLA	C3C-C4C-NC	4.91	116.08	110.57
24	A	416[A]	PHO	C3D-C4D-ND	4.91	114.42	107.72
23	b	604	CLA	CHD-C1D-ND	-4.90	119.95	124.45
23	C	508	CLA	C3D-C2D-C1D	-4.90	99.14	105.83
23	C	512	CLA	C3B-C2B-C1B	-4.90	101.25	107.16
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	A	408	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
23	C	501	CLA	C2C-C1C-NC	4.88	114.55	109.97
23	B	615	CLA	C2C-C1C-NC	4.88	114.54	109.97
23	b	609	CLA	C3C-C4C-NC	4.88	116.04	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	C2B-C1B-NB	4.88	113.50	110.23
23	b	615	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
23	C	509	CLA	O2D-CGD-CBD	4.87	119.92	111.27
23	a	405[B]	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
23	d	403[B]	CLA	C4A-NA-C1A	-4.85	104.52	106.71
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	B	612	CLA	C2C-C1C-NC	4.85	114.51	109.97
23	d	403[B]	CLA	O2D-CGD-CBD	4.84	119.87	111.27
26	a	409[B]	SQD	O6-C1-C2	4.84	115.86	108.30
23	B	613	CLA	CHD-C1D-ND	-4.84	120.01	124.45
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	c	505	CLA	O2D-CGD-CBD	4.84	119.86	111.27
23	b	612	CLA	CMD-C2D-C1D	4.83	133.22	124.71
23	A	404[B]	CLA	C3B-C2B-C1B	-4.83	101.34	107.16
23	A	405[B]	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	b	604	CLA	C3C-C4C-NC	4.82	115.98	110.57
23	b	609	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	B	605	CLA	O2D-CGD-CBD	4.82	119.83	111.27
23	b	610	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
23	B	608	CLA	C4A-NA-C1A	-4.81	104.54	106.71
23	B	608	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
23	c	502	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	C	502	CLA	C3B-C2B-C1B	-4.81	101.36	107.16
26	f	102	SQD	O47-C7-C8	4.80	121.85	111.50
23	C	501	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	C	504	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
23	c	510	CLA	CHD-C1D-ND	-4.80	120.04	124.45
23	c	504	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
23	C	502	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	C	505	CLA	C4A-NA-C1A	-4.78	104.56	106.71
24	a	406[B]	PHO	C3D-C4D-ND	4.78	114.24	107.72
23	c	502	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	c	507	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
29	a	412[B]	PL9	C7-C3-C4	4.78	120.76	116.88
23	b	602	CLA	C3B-C2B-C1B	-4.77	101.40	107.16
23	b	610	CLA	C1-C2-C3	-4.77	117.79	126.04
38	f	101	HEM	CHC-C4B-NB	4.77	129.60	124.42
23	B	602	CLA	C3B-C2B-C1B	-4.76	101.41	107.16
23	c	505	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	c	508	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
23	a	405[B]	CLA	C3D-C4D-ND	4.76	117.93	110.24
23	c	508	CLA	C3B-C2B-C1B	-4.75	101.43	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	CHD-C1D-ND	-4.75	120.09	124.45
23	C	503	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	B	601	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	C	507	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	c	503	CLA	C1C-C2C-C3C	-4.74	101.97	106.96
23	c	504	CLA	O2D-CGD-CBD	4.74	119.70	111.27
23	b	608	CLA	CMD-C2D-C1D	4.74	133.07	124.71
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	A	406[B]	CLA	C3D-C4D-ND	4.74	117.90	110.24
23	b	610	CLA	C3C-C4C-NC	4.73	115.88	110.57
23	a	407	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
23	a	407	CLA	CMD-C2D-C1D	4.73	133.05	124.71
23	C	510	CLA	C3B-C2B-C1B	-4.72	101.46	107.16
23	D	404	CLA	C2C-C1C-NC	4.72	114.39	109.97
23	C	506	CLA	C1C-C2C-C3C	-4.72	101.99	106.96
23	B	601	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
23	C	511	CLA	C3C-C4C-NC	4.72	115.86	110.57
23	a	405[B]	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	B	611	CLA	C3D-C4D-ND	4.71	117.86	110.24
23	A	405[A]	CLA	C1C-C2C-C3C	-4.71	102.00	106.96
23	d	404	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
26	F	103	SQD	C1-O5-C5	-4.70	104.46	113.69
23	C	507	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	B	616	CLA	CMD-C2D-C1D	4.70	133.00	124.71
23	C	509	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	B	601	CLA	C4A-NA-C1A	-4.69	104.60	106.71
23	a	407	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	C	506	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	C	504	CLA	C3C-C4C-NC	4.68	115.83	110.57
23	c	509	CLA	CHD-C1D-ND	-4.68	120.15	124.45
23	a	405[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
23	b	604	CLA	C4A-NA-C1A	-4.68	104.60	106.71
23	A	405[B]	CLA	C1C-C2C-C3C	-4.68	102.04	106.96
23	c	512	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
23	B	611	CLA	C3C-C4C-NC	4.68	115.81	110.57
23	B	601	CLA	C2C-C1C-NC	4.67	114.35	109.97
23	B	613	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
24	a	406[A]	PHO	C3D-C4D-ND	4.67	114.08	107.72
23	B	609	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	C	507	CLA	C3C-C4C-NC	4.67	115.81	110.57
23	d	403[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	513	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
23	c	503	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
23	c	508	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
23	C	508	CLA	C4A-NA-C1A	-4.66	104.61	106.71
29	A	414[B]	PL9	C7-C8-C9	-4.66	119.04	126.79
26	F	103	SQD	O8-S-C6	4.65	113.15	105.74
23	d	403[B]	CLA	C3D-C4D-ND	4.65	117.76	110.24
23	b	603	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
23	c	509	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
23	c	503	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	b	613	CLA	C3B-C2B-C1B	-4.64	101.57	107.16
23	C	511	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	b	611	CLA	C3C-C4C-NC	4.63	115.77	110.57
34	b	622	HTG	C1-O5-C5	4.63	121.11	112.58
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
25	H	101	BCR	C38-C26-C25	-4.62	119.34	124.53
23	b	602	CLA	C3D-C4D-ND	4.62	117.70	110.24
24	A	416[B]	PHO	C1-C2-C3	-4.61	118.06	126.04
23	d	403[B]	CLA	C1C-C2C-C3C	-4.61	102.11	106.96
23	c	502	CLA	C3D-C4D-ND	4.61	117.70	110.24
23	b	608	CLA	C3D-C4D-ND	4.61	117.69	110.24
23	B	603	CLA	C3C-C4C-NC	4.61	115.74	110.57
23	C	506	CLA	C3B-C2B-C1B	-4.61	101.60	107.16
29	a	412[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	c	514	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	B	603	CLA	C3B-C2B-C1B	-4.60	101.61	107.16
23	b	608	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
23	B	609	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	A	406[B]	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	B	602	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
26	b	620	SQD	C1-O5-C5	-4.58	104.70	113.69
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	B	615	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	c	511	CLA	C1-C2-C3	-4.58	118.12	126.04
23	C	504	CLA	C4A-NA-C1A	-4.58	104.65	106.71
24	A	416[B]	PHO	C3D-C4D-ND	4.58	113.96	107.72
23	a	405[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27
23	b	601	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	C	513	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	C	510	CLA	C3D-C4D-ND	4.57	117.64	110.24
23	c	506	CLA	C3D-C4D-ND	4.57	117.64	110.24
23	b	601	CLA	C3D-C2D-C1D	-4.57	99.59	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
23	B	612	CLA	C3B-C2B-C1B	-4.56	101.65	107.16
23	c	513	CLA	C2C-C1C-NC	4.56	114.25	109.97
23	b	603	CLA	C1D-CHD-C4C	-4.56	116.22	126.06
23	D	403[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	B	601	CLA	C3D-C4D-ND	4.55	117.60	110.24
23	d	402[B]	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	B	615	CLA	CMB-C2B-C1B	4.55	132.30	125.37
23	C	503	CLA	C3D-C4D-ND	4.55	117.59	110.24
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	b	612	CLA	C3B-C2B-C1B	-4.55	101.67	107.16
23	C	502	CLA	C3D-C2D-C1D	-4.55	99.63	105.83
23	b	602	CLA	C2C-C1C-NC	4.54	114.23	109.97
23	b	606	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
23	C	505	CLA	C3B-C2B-C1B	-4.54	101.68	107.16
23	b	607	CLA	C1C-C2C-C3C	-4.54	102.19	106.96
38	F	102	HEM	C1B-NB-C4B	4.53	109.75	105.07
23	B	610	CLA	O2A-CGA-CBA	4.53	126.13	111.91
23	C	503	CLA	O2D-CGD-CBD	4.53	119.31	111.27
24	A	416[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
23	C	503	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
23	B	616	CLA	CHD-C1D-ND	-4.52	120.30	124.45
23	B	612	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	b	601	CLA	C3D-C4D-ND	4.51	117.53	110.24
23	A	408	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	B	612	CLA	C3D-C4D-ND	4.50	117.52	110.24
23	b	605	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
23	C	513	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	D	404	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	A	405[B]	CLA	O2D-CGD-CBD	4.50	119.26	111.27
23	d	402[B]	CLA	C3D-C4D-ND	4.50	117.51	110.24
23	b	616	CLA	C3B-C2B-C1B	-4.49	101.74	107.16
23	d	402[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	B	612	CLA	O2D-CGD-O1D	-4.49	115.06	123.84
23	c	514	CLA	O2D-CGD-CBD	4.49	119.24	111.27
23	B	613	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	c	504	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	a	405[B]	CLA	O2D-CGD-CBD	4.48	119.23	111.27
23	a	404[A]	CLA	C3B-C2B-C1B	-4.48	101.75	107.16
23	b	608	CLA	O2D-CGD-CBD	4.48	119.23	111.27
23	c	509	CLA	C3C-C4C-NC	4.48	115.59	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
23	C	512	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	C	503	CLA	C2C-C1C-NC	4.47	114.16	109.97
23	b	608	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	C	511	CLA	C4A-NA-C1A	-4.46	104.70	106.71
23	c	510	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	c	510	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	C	506	CLA	O2D-CGD-CBD	4.46	119.19	111.27
23	C	508	CLA	CHD-C1D-ND	-4.45	120.36	124.45
23	c	503	CLA	CHD-C1D-ND	-4.45	120.36	124.45
23	C	510	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	b	611	CLA	C3D-C4D-ND	4.45	117.43	110.24
23	d	403[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	b	611	CLA	C4A-NA-C1A	-4.44	104.71	106.71
23	A	404[B]	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	A	406[B]	CLA	O2D-CGD-CBD	4.44	119.16	111.27
23	b	604	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
23	d	403[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	a	404[B]	CLA	C3D-C4D-ND	4.43	117.41	110.24
23	d	403[B]	CLA	C3B-C2B-C1B	-4.43	101.81	107.16
23	B	616	CLA	O2D-CGD-O1D	-4.43	115.17	123.84
23	b	612	CLA	O2D-CGD-CBD	4.43	119.14	111.27
23	c	511	CLA	C3C-C4C-NC	4.42	115.53	110.57
32	d	412	LMG	O7-C10-C11	4.42	121.03	111.50
23	b	603	CLA	C3D-C2D-C1D	-4.42	99.80	105.83
23	b	605	CLA	C3C-C4C-NC	4.42	115.52	110.57
23	D	403[B]	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
23	b	610	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	c	511	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	D	403[B]	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
23	C	502	CLA	C1C-C2C-C3C	-4.41	102.32	106.96
23	c	503	CLA	C4A-NA-C1A	-4.41	104.72	106.71
23	C	505	CLA	CMB-C2B-C1B	4.41	132.08	125.37
23	c	507	CLA	C3B-C2B-C1B	-4.40	101.85	107.16
23	D	404	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	D	403[A]	CLA	C3B-C2B-C1B	-4.39	101.86	107.16
23	d	402[A]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	b	612	CLA	CMC-C2C-C1C	4.39	131.72	125.04
23	a	407	CLA	C4A-NA-C1A	-4.39	104.73	106.71
23	B	607	CLA	C3C-C4C-NC	4.39	115.49	110.57
23	b	609	CLA	O2D-CGD-CBD	4.38	119.06	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[B]	CLA	C1C-C2C-C3C	-4.38	102.35	106.96
23	A	408	CLA	C3D-C4D-ND	4.38	117.33	110.24
23	B	607	CLA	C3D-C4D-ND	4.38	117.33	110.24
29	a	412[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	B	613	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	b	607	CLA	O2D-CGD-CBD	4.38	119.05	111.27
23	a	407	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	C	501	CLA	C1D-CHD-C4C	-4.37	116.63	126.06
23	B	609	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	C	513	CLA	C3D-C4D-ND	4.36	117.30	110.24
29	A	414[B]	PL9	C7-C3-C4	4.36	120.42	116.88
32	c	521	LMG	O6-C5-C4	4.36	117.61	109.69
23	b	615	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	A	405[B]	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	b	614	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	c	514	CLA	C1D-CHD-C4C	-4.35	116.67	126.06
23	b	603	CLA	C3D-C4D-ND	4.35	117.28	110.24
23	b	612	CLA	CAC-C3C-C4C	4.35	130.45	124.81
23	a	404[B]	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
23	b	601	CLA	C2C-C1C-NC	4.35	114.05	109.97
23	C	506	CLA	C3D-C4D-ND	4.35	117.27	110.24
26	A	410[B]	SQD	C1-C2-C3	-4.34	100.97	110.00
23	C	503	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	b	616	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	C	508	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
23	C	512	CLA	C3C-C4C-NC	4.33	115.42	110.57
33	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
23	B	605	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	b	616	CLA	C1D-CHD-C4C	-4.32	116.73	126.06
23	B	607	CLA	C4A-NA-C1A	-4.32	104.76	106.71
38	f	101	HEM	C4C-NC-C1C	4.32	109.58	105.35
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.52	110.52
23	D	403[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	C	512	CLA	C2C-C1C-NC	4.31	114.01	109.97
23	a	404[B]	CLA	O2D-CGD-CBD	4.31	118.93	111.27
25	d	405	BCR	C40-C30-C25	-4.31	103.30	110.30
23	B	616	CLA	C4C-C3C-C2C	-4.31	100.61	106.90
23	b	602	CLA	O2D-CGD-O1D	-4.31	115.41	123.84
23	C	510	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
23	b	610	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	c	509	CLA	C1C-C2C-C3C	-4.31	102.43	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[B]	CLA	C1C-C2C-C3C	-4.30	102.43	106.96
23	B	610	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	B	613	CLA	C3B-C4B-NB	4.30	114.50	110.52
23	c	507	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	B	607	CLA	C1C-C2C-C3C	-4.30	102.44	106.96
29	A	414[B]	PL9	C32-C33-C34	-4.30	117.31	127.66
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	b	615	CLA	C3B-C2B-C1B	-4.30	101.97	107.16
23	b	603	CLA	C3C-C4C-NC	4.29	115.38	110.57
23	B	613	CLA	O2D-CGD-CBD	4.29	118.89	111.27
23	D	404	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	a	404[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
25	y	101	BCR	C33-C5-C6	-4.29	119.72	124.53
23	B	613	CLA	C3B-C2B-C1B	-4.29	101.99	107.16
23	c	514	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	b	615	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	C	501	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	b	607	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	a	405[B]	CLA	C2C-C1C-NC	4.28	113.98	109.97
23	B	615	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	C	505	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
23	c	513	CLA	C1-C2-C3	-4.28	118.64	126.04
23	B	616	CLA	C3B-C4B-NB	4.28	114.48	110.52
25	C	515	BCR	C7-C8-C9	-4.28	119.77	126.23
23	b	606	CLA	C3C-C4C-NC	4.27	115.36	110.57
26	A	410[B]	SQD	C44-O6-C1	-4.27	105.40	113.74
31	t	101	LMT	C3'-C4'-C5'	-4.27	101.14	110.93
23	A	404[B]	CLA	O2D-CGD-CBD	4.27	118.85	111.27
23	c	507	CLA	O2D-CGD-CBD	4.27	118.85	111.27
23	B	601	CLA	C3C-C4C-NC	4.26	115.35	110.57
25	b	617	BCR	C33-C5-C6	-4.26	119.75	124.53
23	b	612	CLA	CHD-C1D-ND	-4.25	120.54	124.45
23	a	405[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
26	f	102	SQD	C1-O5-C5	4.25	122.03	113.69
23	c	503	CLA	C3D-C4D-ND	4.25	117.12	110.24
23	C	501	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
23	D	403[B]	CLA	C3C-C4C-NC	4.25	115.33	110.57
23	b	612	CLA	C1-C2-C3	-4.24	118.70	126.04
33	E	101[B]	LHG	O7-C7-C8	4.24	120.65	111.50
23	b	608	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	c	504	CLA	C1D-CHD-C4C	-4.24	116.91	126.06
23	c	504	CLA	C3C-C4C-NC	4.24	115.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C1D-CHD-C4C	-4.24	116.92	126.06
23	b	611	CLA	C3B-C2B-C1B	-4.24	102.05	107.16
23	A	408	CLA	C3C-C4C-NC	4.24	115.32	110.57
23	C	508	CLA	C3B-C4B-NB	4.23	114.44	110.52
23	A	404[B]	CLA	C1D-CHD-C4C	-4.23	116.93	126.06
23	c	506	CLA	C3D-C2D-C1D	-4.23	100.06	105.83
23	B	610	CLA	C3D-C4D-ND	4.23	117.08	110.24
25	c	515	BCR	C11-C10-C9	-4.22	121.28	127.31
23	d	404	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	b	606	CLA	C1D-CHD-C4C	-4.22	116.95	126.06
23	C	505	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	A	405[B]	CLA	C3B-C2B-C1B	-4.22	102.07	107.16
38	F	102	HEM	C4C-NC-C1C	4.22	109.48	105.35
23	a	404[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	405[A]	CLA	C3B-C2B-C1B	-4.21	102.07	107.16
23	B	604	CLA	C3B-C4B-NB	4.21	114.42	110.52
23	c	502	CLA	C3B-C2B-C1B	-4.21	102.08	107.16
29	a	412[B]	PL9	C7-C8-C9	-4.21	119.78	126.79
23	a	404[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	D	403[B]	CLA	O2D-CGD-CBD	4.20	118.73	111.27
23	c	507	CLA	C1-C2-C3	-4.20	118.78	126.04
23	A	406[B]	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
23	D	403[B]	CLA	C3D-C4D-ND	4.20	117.03	110.24
23	c	503	CLA	CMD-C2D-C1D	4.20	132.11	124.71
23	C	501	CLA	C3D-C4D-ND	4.19	117.02	110.24
26	F	103	SQD	C44-O6-C1	-4.19	105.55	113.74
23	b	602	CLA	C3D-C2D-C1D	-4.19	100.11	105.83
26	a	409[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	c	508	CLA	CMC-C2C-C1C	4.19	131.42	125.04
23	B	615	CLA	CMC-C2C-C1C	4.19	131.42	125.04
32	A	418	LMG	O7-C10-C11	4.19	120.52	111.50
23	A	404[B]	CLA	CAA-C2A-C3A	-4.18	101.32	112.78
23	d	403[B]	CLA	C3C-C4C-NC	4.18	115.26	110.57
23	b	609	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	B	603	CLA	C3D-C4D-ND	4.18	116.99	110.24
23	C	509	CLA	C3C-C4C-NC	4.18	115.25	110.57
23	a	404[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
23	b	606	CLA	C3D-C4D-ND	4.17	116.99	110.24
23	C	512	CLA	C3D-C4D-ND	4.17	116.99	110.24
23	C	509	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	B	615	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
23	c	505	CLA	C3D-C4D-ND	4.17	116.98	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	A	408	CLA	C3B-C4B-NB	4.16	114.37	110.52
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	c	502	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	b	613	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	A	404[B]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	c	505	CLA	C1-O2A-CGA	4.14	127.31	116.44
23	D	403[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	B	605	CLA	C1D-CHD-C4C	-4.14	117.13	126.06
23	c	504	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	B	602	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	d	402[B]	CLA	C3C-C4C-NC	4.14	115.21	110.57
23	d	403[B]	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
23	b	602	CLA	C3C-C4C-NC	4.13	115.20	110.57
23	C	509	CLA	C3D-C4D-ND	4.13	116.91	110.24
32	A	418	LMG	O1-C1-C2	4.13	114.75	108.30
23	C	502	CLA	C3C-C4C-NC	4.12	115.20	110.57
23	d	402[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
32	C	520	LMG	O7-C10-C11	4.12	120.38	111.50
23	B	608	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	b	604	CLA	CAC-C3C-C4C	4.11	130.15	124.81
23	d	403[A]	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	d	403[A]	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
32	c	501	LMG	O7-C10-C11	4.11	120.36	111.50
23	b	609	CLA	C1-C2-C3	-4.11	118.94	126.04
23	c	512	CLA	O2D-CGD-O1D	-4.11	115.81	123.84
23	B	604	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
23	C	512	CLA	C1D-CHD-C4C	-4.11	117.20	126.06
23	c	510	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	B	614	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	C	513	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	D	403[B]	CLA	C1-C2-C3	-4.10	118.95	126.04
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
32	Z	101	LMG	O7-C10-C11	4.10	120.33	111.50
23	d	402[B]	CLA	C3B-C2B-C1B	-4.10	102.22	107.16
23	c	510	CLA	C1D-CHD-C4C	-4.10	117.22	126.06
23	b	614	CLA	O2D-CGD-O1D	-4.10	115.83	123.84
23	a	404[A]	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	A	408	CLA	C1C-C2C-C3C	-4.09	102.65	106.96
23	B	615	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	A	404[B]	CLA	C3D-C4D-ND	4.09	116.85	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
23	c	513	CLA	C3D-C4D-ND	4.09	116.85	110.24
23	C	508	CLA	C1-C2-C3	-4.09	118.97	126.04
23	b	604	CLA	C3B-C2B-C1B	-4.08	102.23	107.16
23	b	616	CLA	C2C-C1C-NC	4.08	113.80	109.97
23	b	614	CLA	C3D-C4D-ND	4.08	116.84	110.24
23	A	404[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
23	A	405[A]	CLA	CAA-C2A-C3A	-4.08	101.61	112.78
35	C	516[A]	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	c	512	CLA	C4A-NA-C1A	-4.07	104.87	106.71
23	c	505	CLA	C3C-C4C-NC	4.07	115.14	110.57
26	a	409[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
23	C	504	CLA	C3B-C2B-C1B	-4.07	102.25	107.16
25	h	101	BCR	C7-C8-C9	-4.07	120.09	126.23
23	D	403[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	b	616	CLA	C3D-C4D-ND	4.06	116.81	110.24
23	B	607	CLA	C3B-C4B-NB	4.06	114.28	110.52
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
26	B	620	SQD	C3-C4-C5	4.06	117.48	110.24
23	c	512	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	b	607	CLA	C3B-C4B-NB	4.06	114.28	110.52
23	d	402[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	c	514	CLA	C3C-C4C-NC	4.05	115.11	110.57
23	A	404[B]	CLA	C3C-C4C-NC	4.05	115.11	110.57
32	c	521	LMG	O7-C10-C11	4.05	120.22	111.50
23	B	616	CLA	C3B-C2B-C1B	-4.04	102.28	107.16
23	B	605	CLA	CMB-C2B-C1B	4.04	131.53	125.37
23	B	604	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
23	C	503	CLA	C1D-CHD-C4C	-4.04	117.34	126.06
23	A	404[B]	CLA	C3B-C4B-NB	4.04	114.27	110.52
23	b	604	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	a	404[B]	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
29	a	412[B]	PL9	C32-C33-C34	-4.03	117.95	127.66
23	B	614	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	c	508	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	b	610	CLA	C4A-NA-C1A	-4.03	104.89	106.71
32	C	519	LMG	O7-C10-C11	4.03	120.18	111.50
23	b	614	CLA	C4A-NA-C1A	-4.02	104.90	106.71
23	d	404	CLA	C3C-C4C-NC	4.02	115.08	110.57
23	a	407	CLA	CMC-C2C-C1C	4.01	131.15	125.04
23	c	510	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	d	402[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	520	LMG	O6-C5-C4	4.01	116.97	109.69
23	c	504	CLA	CMB-C2B-C1B	4.01	131.47	125.37
23	b	604	CLA	CMC-C2C-C1C	4.01	131.14	125.04
23	c	505	CLA	C3B-C4B-NB	4.01	114.23	110.52
23	b	601	CLA	C3C-C4C-NC	4.01	115.06	110.57
23	B	601	CLA	C1D-CHD-C4C	-4.01	117.42	126.06
23	c	511	CLA	C3D-C4D-ND	4.00	116.72	110.24
25	c	515	BCR	C15-C14-C13	-4.00	121.60	127.31
23	B	616	CLA	C3D-C4D-ND	4.00	116.71	110.24
23	B	602	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
23	C	508	CLA	C1C-C2C-C3C	-4.00	102.75	106.96
23	B	610	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
23	d	403[A]	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
23	b	613	CLA	C1-C2-C3	-4.00	119.13	126.04
23	d	402[A]	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
23	c	508	CLA	O2D-CGD-O1D	-3.99	116.04	123.84
23	A	408	CLA	O2D-CGD-CBD	3.98	118.35	111.27
23	C	501	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
23	c	506	CLA	C3B-C2B-C1B	-3.98	102.35	107.16
25	Y	101	BCR	C15-C14-C13	-3.98	121.63	127.31
23	b	612	CLA	C3B-C4B-NB	3.98	114.21	110.52
23	B	606	CLA	C3D-C4D-ND	3.98	116.67	110.24
23	a	404[B]	CLA	C3B-C4B-NB	3.98	114.20	110.52
23	b	616	CLA	O2A-CGA-CBA	3.98	124.38	111.91
23	c	511	CLA	O2D-CGD-CBD	3.97	118.33	111.27
23	b	615	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
29	A	414[B]	PL9	C7-C3-C2	-3.97	118.08	123.30
23	B	602	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	c	512	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
23	b	607	CLA	C4A-NA-C1A	-3.97	104.92	106.71
23	c	507	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
23	b	612	CLA	C3D-C4D-ND	3.96	116.64	110.24
23	D	403[B]	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
26	B	620	SQD	O7-S-C6	3.96	111.64	106.94
23	b	606	CLA	C4-C3-C5	3.96	121.93	115.27
23	B	614	CLA	C3D-C4D-ND	3.96	116.64	110.24
23	c	503	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	a	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	C	504	CLA	C3D-C4D-ND	3.95	116.63	110.24
29	D	406[B]	PL9	C42-C43-C44	-3.95	118.15	127.66
29	a	412[B]	PL9	C7-C3-C2	-3.95	118.11	123.30
23	b	603	CLA	O2D-CGD-O1D	-3.95	116.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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	c	512	CLA	C3B-C4B-NB	3.95	114.18	110.52
23	b	610	CLA	O2A-CGA-CBA	3.95	124.29	111.91
26	A	412	SQD	O47-C7-C8	3.95	120.00	111.50
23	B	611	CLA	O2D-CGD-O1D	-3.94	116.13	123.84
23	C	502	CLA	C3D-C4D-ND	3.94	116.61	110.24
29	d	406[A]	PL9	C42-C43-C44	-3.93	118.19	127.66
23	a	404[B]	CLA	C3C-C4C-NC	3.93	114.98	110.57
23	c	511	CLA	C1C-C2C-C3C	-3.93	102.82	106.96
23	B	603	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
23	D	403[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
25	T	101	BCR	C15-C16-C17	-3.92	115.44	123.47
23	d	404	CLA	O2D-CGD-O1D	-3.92	116.17	123.84
23	B	615	CLA	C1C-C2C-C3C	-3.91	102.84	106.96
26	a	409[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
23	C	511	CLA	C3D-C4D-ND	3.91	116.56	110.24
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	b	614	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	C	504	CLA	C3B-C4B-NB	3.90	114.14	110.52
23	B	605	CLA	C4-C3-C5	3.90	121.83	115.27
23	A	406[B]	CLA	C3C-C4C-NC	3.90	114.95	110.57
23	c	509	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
29	a	412[A]	PL9	C32-C33-C34	-3.89	118.28	127.66
32	c	521	LMG	C3-C4-C5	3.89	117.18	110.24
23	C	508	CLA	C3D-C4D-ND	3.89	116.54	110.24
23	B	603	CLA	C1D-CHD-C4C	-3.89	117.66	126.06
34	b	625	HTG	C1-O5-C5	3.89	119.76	112.58
23	B	610	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	B	608	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
23	B	614	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	d	402[B]	CLA	C1D-CHD-C4C	-3.89	117.67	126.06
23	B	609	CLA	CMB-C2B-C1B	3.89	131.29	125.37
34	b	622	HTG	C1'-S1-C1	3.89	107.36	100.09
23	B	602	CLA	O2D-CGD-O1D	-3.89	116.24	123.84
33	A	419[A]	LHG	O8-C23-O10	-3.88	113.79	123.59
35	c	517[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	B	606	CLA	C1D-CHD-C4C	-3.88	117.68	126.06
23	A	405[A]	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	c	507	CLA	C3B-C4B-NB	3.88	114.11	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
23	b	608	CLA	CMC-C2C-C1C	3.88	130.94	125.04
23	b	607	CLA	C3B-C2B-C1B	-3.88	102.48	107.16
23	C	513	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	c	508	CLA	CMB-C2B-C1B	3.87	131.27	125.37
23	a	405[B]	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	d	402[A]	CLA	CAA-C2A-C3A	-3.87	102.19	112.78
23	b	601	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	b	609	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
25	a	408	BCR	C38-C26-C25	-3.86	120.19	124.53
23	c	507	CLA	C3C-C4C-NC	3.86	114.91	110.57
23	C	507	CLA	C3D-C4D-ND	3.86	116.49	110.24
23	C	509	CLA	C1-C2-C3	-3.86	119.37	126.04
23	B	611	CLA	CHD-C4C-NC	3.86	130.28	124.20
23	B	604	CLA	C3D-C2D-C1D	-3.86	100.57	105.83
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
23	A	406[B]	CLA	C1C-C2C-C3C	-3.85	102.91	106.96
32	Z	101	LMG	C1-C2-C3	3.85	118.00	110.00
23	b	604	CLA	C3D-C4D-ND	3.84	116.45	110.24
25	C	514	BCR	C15-C14-C13	-3.84	121.83	127.31
23	b	612	CLA	C1D-CHD-C4C	-3.84	117.77	126.06
23	C	513	CLA	C3B-C4B-NB	3.84	114.08	110.52
23	B	602	CLA	C1C-C2C-C3C	-3.84	102.92	106.96
29	a	412[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
23	B	613	CLA	C4-C3-C5	3.84	121.72	115.27
38	F	102	HEM	CHD-C4C-NC	3.83	128.59	124.44
23	B	610	CLA	CAA-C2A-C3A	-3.83	102.28	112.78
23	C	507	CLA	CMB-C2B-C1B	3.83	131.21	125.37
23	B	606	CLA	C3B-C2B-C1B	-3.83	102.54	107.16
29	A	414[B]	PL9	C37-C38-C39	-3.83	118.44	127.66
23	b	602	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
23	A	408	CLA	C1-C2-C3	-3.83	119.43	126.04
23	D	404	CLA	C3B-C2B-C1B	-3.82	102.55	107.16
23	B	606	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
23	b	612	CLA	C3D-C2D-C1D	-3.82	100.62	105.83
25	B	618	BCR	C29-C30-C25	3.82	116.36	110.48
23	b	608	CLA	C3B-C4B-NB	3.82	114.06	110.52
23	d	403[B]	CLA	C3B-C4B-NB	3.82	114.06	110.52
23	B	606	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	B	604	CLA	C1C-C2C-C3C	-3.81	102.95	106.96
23	b	603	CLA	CAA-C2A-C3A	-3.81	102.34	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[B]	CLA	CAA-C2A-C3A	-3.81	102.35	112.78
23	C	512	CLA	C1-C2-C3	-3.81	119.46	126.04
25	d	405	BCR	C38-C26-C25	-3.81	120.25	124.53
23	A	405[B]	CLA	CAA-C2A-C3A	-3.80	102.36	112.78
31	B	628	LMT	C1'-O5'-C5'	-3.80	106.22	113.69
25	d	405	BCR	C29-C30-C25	3.80	116.34	110.48
23	d	402[A]	CLA	CMB-C2B-C1B	3.80	131.16	125.37
23	B	609	CLA	C3B-C2B-C1B	-3.80	102.57	107.16
33	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
23	b	605	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
38	f	101	HEM	CAD-CBD-CGD	3.80	121.78	113.60
23	c	508	CLA	C3D-C4D-ND	3.80	116.38	110.24
38	F	102	HEM	CBD-CAD-C3D	-3.79	102.08	112.63
33	b	629[B]	LHG	O7-C7-C8	3.79	119.67	111.50
25	A	409	BCR	C24-C23-C22	-3.79	120.51	126.23
23	d	404	CLA	C1C-C2C-C3C	-3.79	102.97	106.96
23	c	514	CLA	C3B-C4B-NB	3.79	114.03	110.52
23	b	604	CLA	C3B-C4B-NB	3.79	114.03	110.52
23	B	607	CLA	C4-C3-C5	3.79	121.64	115.27
23	B	614	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74
26	A	410[B]	SQD	O47-C7-C8	3.78	119.64	111.50
23	b	616	CLA	O2D-CGD-O1D	-3.78	116.45	123.84
32	m	101	LMG	O7-C10-C11	3.78	119.64	111.50
23	b	615	CLA	CMB-C2B-C1B	3.77	131.12	125.37
23	a	404[B]	CLA	CAA-C2A-C3A	-3.77	102.45	112.78
23	B	604	CLA	C4A-NA-C1A	-3.77	105.01	106.71
23	b	611	CLA	O2D-CGD-O1D	-3.77	116.46	123.84
23	c	513	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
34	V	202	HTG	C1-O5-C5	3.77	117.30	112.19
23	c	503	CLA	C3C-C4C-NC	3.77	114.80	110.57
23	c	513	CLA	C3C-C4C-NC	3.77	114.80	110.57
24	a	414[A]	PHO	C4-C3-C5	3.76	121.59	115.27
23	D	404	CLA	CMB-C2B-C1B	3.76	131.09	125.37
23	B	613	CLA	C3D-C4D-ND	3.76	116.31	110.24
23	B	603	CLA	C3B-C4B-NB	3.75	114.00	110.52
23	C	506	CLA	C1-C2-C3	-3.75	119.56	126.04
23	C	510	CLA	C4-C3-C5	3.75	121.58	115.27
23	B	614	CLA	O2A-CGA-O1A	-3.75	114.13	123.59
23	c	510	CLA	C3B-C4B-NB	3.75	113.99	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
23	C	510	CLA	C1D-CHD-C4C	-3.74	117.98	126.06
35	c	518[B]	DGD	O2G-C1B-C2B	3.74	119.56	111.50
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
23	C	513	CLA	C1D-CHD-C4C	-3.74	117.99	126.06
23	b	609	CLA	C3B-C2B-C1B	-3.74	102.65	107.16
29	a	412[A]	PL9	C15-C14-C16	3.74	121.56	115.27
23	A	406[B]	CLA	C1D-CHD-C4C	-3.74	118.00	126.06
34	B	625	HTG	C1'-S1-C1	3.73	107.07	100.09
23	B	611	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
23	c	506	CLA	CAC-C3C-C4C	3.73	129.65	124.81
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
25	b	619	BCR	C11-C10-C9	-3.72	122.00	127.31
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24
35	C	517[B]	DGD	O2G-C1B-C2B	3.72	119.51	111.50
23	C	505	CLA	C1-C2-C3	-3.72	119.62	126.04
23	c	511	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	b	611	CLA	C3B-C4B-NB	3.71	113.96	110.52
23	b	613	CLA	C3B-C4B-NB	3.71	113.96	110.52
23	c	506	CLA	CMB-C2B-C1B	3.71	131.02	125.37
23	C	511	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
23	b	608	CLA	C3C-C4C-NC	3.71	114.73	110.57
23	b	605	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
23	d	403[B]	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
23	A	405[B]	CLA	CMC-C2C-C1C	3.70	130.68	125.04
23	B	609	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	b	606	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
23	C	505	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
23	d	402[B]	CLA	CMB-C2B-C1B	3.70	131.00	125.37
23	b	601	CLA	O2D-CGD-O1D	-3.70	116.61	123.84
35	C	517[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	B	607	CLA	CMC-C2C-C1C	3.69	130.66	125.04
23	b	611	CLA	C1-C2-C3	-3.69	119.66	126.04
23	c	503	CLA	O2D-CGD-O1D	-3.69	116.63	123.84
23	B	604	CLA	C3D-C4D-ND	3.69	116.20	110.24
23	B	614	CLA	C1-C2-C3	-3.68	119.67	126.04
23	c	509	CLA	C3D-C4D-ND	3.68	116.19	110.24
23	C	507	CLA	C1C-C2C-C3C	-3.68	103.09	106.96
33	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.50
23	c	504	CLA	O2D-CGD-O1D	-3.68	116.65	123.84
23	B	608	CLA	C4C-C3C-C2C	-3.68	101.54	106.90
23	A	406[A]	CLA	CMB-C2B-C1B	3.68	130.97	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
23	B	613	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
23	b	603	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
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
35	c	517[B]	DGD	O2G-C1B-C2B	3.66	119.39	111.50
23	C	506	CLA	C3C-C4C-NC	3.66	114.68	110.57
23	b	604	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
23	C	507	CLA	C1D-CHD-C4C	-3.65	118.17	126.06
29	a	412[B]	PL9	C15-C14-C16	3.65	121.42	115.27
23	A	405[B]	CLA	CBC-CAC-C3C	-3.65	102.36	112.43
26	a	409[B]	SQD	C44-O6-C1	-3.65	106.61	113.74
23	B	607	CLA	C3B-C2B-C1B	-3.65	102.76	107.16
25	K	102	BCR	C7-C8-C9	-3.65	120.72	126.23
23	C	511	CLA	C4-C3-C5	3.64	121.39	115.27
23	D	403[A]	CLA	C3B-C4B-NB	3.64	113.89	110.52
23	a	407	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
25	T	101	BCR	C11-C10-C9	-3.64	122.12	127.31
25	Y	101	BCR	C16-C17-C18	-3.64	122.12	127.31
23	D	404	CLA	O2D-CGD-O1D	-3.64	116.73	123.84
23	c	505	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	b	605	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	b	614	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	b	614	CLA	C1-C2-C3	-3.63	119.76	126.04
26	a	409[A]	SQD	O9-S-C6	3.63	111.25	106.94
23	b	611	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	C	506	CLA	C3B-C4B-NB	3.63	113.88	110.52
23	b	602	CLA	CMC-C2C-C1C	3.63	130.56	125.04
23	b	616	CLA	CMB-C2B-C1B	3.63	130.89	125.37
25	b	617	BCR	C7-C8-C9	-3.62	120.76	126.23
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	c	502	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	B	608	CLA	CAC-C3C-C4C	3.62	129.50	124.81
23	b	615	CLA	O2D-CGD-CBD	3.62	117.69	111.27
33	d	408[B]	LHG	O7-C7-C8	3.61	119.29	111.50
23	c	506	CLA	C4C-C3C-C2C	-3.61	101.63	106.90
29	D	406[B]	PL9	C10-C9-C11	3.61	121.35	115.27
23	a	407	CLA	C1D-CHD-C4C	-3.61	118.27	126.06
23	B	615	CLA	O2D-CGD-CBD	3.61	117.67	111.27
25	D	405	BCR	C28-C27-C26	-3.61	107.64	114.08
23	B	612	CLA	CMC-C2C-C1C	3.60	130.53	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
26	a	410	SQD	O47-C7-C8	3.60	119.26	111.50
25	H	101	BCR	C16-C17-C18	-3.60	122.17	127.31
23	c	512	CLA	C1C-C2C-C3C	-3.60	103.17	106.96
23	B	602	CLA	CMC-C2C-C1C	3.60	130.52	125.04
23	B	611	CLA	CHB-C4A-NA	3.60	129.49	124.51
24	A	416[A]	PHO	C4D-CHA-CBD	3.59	110.14	108.52
23	B	610	CLA	CMB-C2B-C1B	3.59	130.84	125.37
23	C	508	CLA	C4C-C3C-C2C	-3.59	101.67	106.90
40	V	201	HEC	CBD-CAD-C3D	-3.59	102.66	112.63
23	c	506	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
34	B	622	HTG	O5-C1-C2	3.58	114.82	110.31
23	d	403[A]	CLA	C3B-C4B-NB	3.58	113.84	110.52
23	D	404	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
23	B	611	CLA	C4C-C3C-C2C	-3.58	101.69	106.90
23	c	513	CLA	CMB-C2B-C1B	3.58	130.81	125.37
23	C	510	CLA	C3B-C4B-NB	3.57	113.83	110.52
23	c	511	CLA	C3B-C4B-NB	3.57	113.82	110.52
32	c	501	LMG	C7-O1-C1	-3.56	106.78	113.74
29	A	414[B]	PL9	C15-C14-C16	3.56	121.26	115.27
25	h	101	BCR	C38-C26-C25	-3.56	120.53	124.53
23	b	603	CLA	C3B-C4B-NB	3.56	113.82	110.52
23	d	403[A]	CLA	C1-C2-C3	-3.56	119.89	126.04
23	b	614	CLA	C3B-C4B-NB	3.56	113.81	110.52
23	c	507	CLA	C1D-CHD-C4C	-3.56	118.39	126.06
23	b	607	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
23	A	405[B]	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
23	B	603	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	B	612	CLA	C4C-C3C-C2C	-3.55	101.73	106.90
29	d	406[A]	PL9	C40-C39-C41	3.55	121.23	115.27
38	f	101	HEM	C1B-NB-C4B	3.54	108.73	105.07
25	k	101	BCR	C7-C8-C9	-3.54	120.88	126.23
29	a	412[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
23	c	510	CLA	C1C-C2C-C3C	-3.54	103.23	106.96
32	c	520	LMG	O7-C10-C11	3.54	119.12	111.50
24	a	414[B]	PHO	C4-C3-C5	3.54	121.22	115.27
23	A	405[B]	CLA	C3C-C4C-NC	3.53	114.53	110.57
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	A	408	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
23	B	604	CLA	CHD-C1D-ND	-3.53	121.21	124.45
23	b	612	CLA	C1C-C2C-C3C	-3.53	103.25	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	C	520	LMG	C3-C4-C5	3.52	116.52	110.24
23	C	509	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	C	505	CLA	CAC-C3C-C4C	3.52	129.38	124.81
23	B	611	CLA	C2A-C1A-CHA	-3.52	117.71	123.86
23	b	602	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
24	A	407[B]	PHO	C1A-C2A-C3A	-3.52	99.49	102.84
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66
25	D	405	BCR	C38-C26-C25	-3.51	120.58	124.53
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	502	CLA	O2D-CGD-O1D	-3.50	116.99	123.84
23	B	616	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
29	D	406[A]	PL9	C53-C6-C1	3.50	122.15	114.99
33	A	419[B]	LHG	O7-C7-C8	3.50	119.04	111.50
23	C	502	CLA	C1D-CHD-C4C	-3.50	118.52	126.06
40	V	201	HEC	CAD-CBD-CGD	-3.49	106.08	113.60
23	d	402[B]	CLA	CHD-C4C-NC	3.49	129.71	124.20
25	D	405	BCR	C10-C11-C12	-3.49	112.32	123.22
23	a	405[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	a	405[B]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
29	A	414[B]	PL9	C22-C23-C24	-3.49	119.26	127.66
23	c	514	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	c	504	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
23	C	509	CLA	C3B-C4B-NB	3.48	113.75	110.52
29	a	412[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
23	c	511	CLA	C4-C3-C5	3.48	121.12	115.27
23	b	613	CLA	C3D-C4D-ND	3.47	115.86	110.24
29	D	406[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
23	C	511	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
25	d	405	BCR	C10-C11-C12	-3.47	112.38	123.22
25	k	101	BCR	C29-C30-C25	3.47	115.82	110.48
23	b	604	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
23	a	404[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
23	D	403[B]	CLA	C3B-C4B-NB	3.47	113.73	110.52
34	B	622	HTG	C1'-S1-C1	3.46	106.57	100.09
26	b	620	SQD	O8-S-C6	3.46	111.26	105.74
23	b	609	CLA	CMC-C2C-C1C	3.46	130.31	125.04
23	B	605	CLA	C1C-C2C-C3C	-3.46	103.32	106.96
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	d	403[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
29	a	412[B]	PL9	C30-C29-C31	3.46	121.09	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	605	CLA	CMB-C2B-C1B	3.46	130.64	125.37
23	b	612	CLA	C4-C3-C5	3.45	121.08	115.27
33	L	101[B]	LHG	O7-C7-C8	3.45	118.95	111.50
23	C	509	CLA	CMC-C2C-C1C	3.45	130.30	125.04
23	B	604	CLA	C4C-C3C-C2C	-3.45	101.87	106.90
23	A	408	CLA	CAA-C2A-C3A	-3.45	103.34	112.78
23	c	509	CLA	C1-C2-C3	-3.45	120.08	126.04
26	F	103	SQD	O7-S-C6	3.44	111.03	106.94
32	C	519	LMG	O8-C28-C29	3.43	122.69	111.91
23	b	613	CLA	O2A-CGA-O1A	-3.43	114.93	123.59
23	B	602	CLA	C3B-C4B-NB	3.43	113.70	110.52
23	a	405[B]	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	b	605	CLA	O2A-CGA-O1A	-3.42	114.95	123.59
23	b	616	CLA	O2A-CGA-O1A	-3.42	114.95	123.59
25	C	514	BCR	C7-C8-C9	-3.42	121.07	126.23
23	d	403[B]	CLA	C1-C2-C3	-3.42	120.13	126.04
23	C	504	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
23	b	613	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
23	B	614	CLA	CMC-C2C-C1C	3.41	130.24	125.04
25	B	617	BCR	C33-C5-C6	-3.41	120.69	124.53
23	a	404[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
29	a	412[A]	PL9	C35-C34-C36	3.41	121.01	115.27
23	B	610	CLA	C1D-CHD-C4C	-3.41	118.70	126.06
23	C	511	CLA	C3B-C4B-NB	3.41	113.68	110.52
23	b	606	CLA	O2D-CGD-O1D	-3.41	117.18	123.84
23	B	609	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	b	616	CLA	CHD-C4C-NC	3.40	129.56	124.20
23	C	506	CLA	CBC-CAC-C3C	-3.40	103.06	112.43
23	D	404	CLA	C1C-C2C-C3C	-3.40	103.38	106.96
29	d	406[B]	PL9	C37-C38-C39	-3.40	119.48	127.66
23	c	510	CLA	CAC-C3C-C4C	3.40	129.22	124.81
23	B	609	CLA	O2D-CGD-CBD	3.40	117.30	111.27
23	b	610	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
23	B	607	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
23	B	602	CLA	CAA-C2A-C3A	-3.39	103.49	112.78
23	c	502	CLA	CMB-C2B-C1B	3.39	130.54	125.37
38	f	101	HEM	CHA-C4D-ND	3.39	128.56	124.37
23	D	404	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	B	614	CLA	CAC-C3C-C4C	3.39	129.21	124.81
23	b	606	CLA	CHD-C4C-NC	3.39	129.54	124.20
29	D	406[A]	PL9	C25-C24-C26	3.39	120.97	115.27
24	A	416[B]	PHO	C4-C3-C5	3.38	120.96	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	515	BCR	C16-C17-C18	-3.38	122.49	127.31
23	B	603	CLA	CAA-C2A-C3A	-3.38	103.52	112.78
23	B	601	CLA	C4C-C3C-C2C	-3.38	101.97	106.90
23	C	505	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	B	610	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
23	b	602	CLA	C1C-C2C-C3C	-3.38	103.41	106.96
23	c	507	CLA	CAC-C3C-C4C	3.37	129.19	124.81
33	d	414[B]	LHG	O7-C7-C8	3.37	118.77	111.50
35	c	518[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
38	F	102	HEM	CHB-C1B-NB	3.37	128.53	124.37
23	B	612	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
23	b	615	CLA	C1C-C2C-C3C	-3.37	103.42	106.96
32	B	621	LMG	O8-C28-C29	3.37	122.47	111.91
23	b	612	CLA	C4C-C3C-C2C	-3.36	101.99	106.90
26	F	103	SQD	C1-C2-C3	-3.36	102.99	110.00
34	b	622	HTG	O2-C2-C1	3.36	116.44	110.27
23	A	406[B]	CLA	CMB-C2B-C1B	3.36	130.49	125.37
23	B	610	CLA	CAA-CBA-CGA	-3.35	103.46	113.25
24	A	416[B]	PHO	C1A-C2A-C3A	-3.35	99.65	102.84
23	C	501	CLA	C1C-C2C-C3C	-3.35	103.44	106.96
23	B	613	CLA	C1D-CHD-C4C	-3.34	118.85	126.06
23	C	510	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
23	C	508	CLA	CHC-C1C-C2C	-3.34	117.46	126.73
29	d	406[B]	PL9	C10-C9-C11	3.34	120.88	115.27
23	C	501	CLA	CMC-C2C-C1C	3.33	130.12	125.04
26	A	412	SQD	O8-S-C6	3.33	111.05	105.74
32	Z	101	LMG	O6-C1-C2	3.33	117.40	110.35
23	d	403[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
26	a	409[B]	SQD	O9-S-C6	3.33	110.89	106.94
23	C	507	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
23	B	605	CLA	CHD-C4C-NC	3.32	129.44	124.20
23	C	512	CLA	C4-C3-C5	3.32	120.86	115.27
23	c	509	CLA	CMB-C2B-C1B	3.32	130.43	125.37
23	d	402[B]	CLA	C3B-C4B-NB	3.32	113.59	110.52
23	B	606	CLA	O2A-CGA-O1A	-3.32	115.22	123.59
38	F	102	HEM	CBA-CAA-C2A	-3.32	103.41	112.63
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
26	a	410	SQD	O7-S-C6	3.32	110.88	106.94
23	A	406[A]	CLA	C3B-C4B-NB	3.32	113.59	110.52
23	C	513	CLA	C1-C2-C3	-3.31	120.31	126.04
34	b	625	HTG	O5-C5-C4	3.31	115.71	109.69
23	C	508	CLA	O2D-CGD-O1D	-3.31	117.36	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
33	A	419[B]	LHG	O8-C23-O10	-3.31	115.25	123.59
23	C	506	CLA	C1D-CHD-C4C	-3.30	118.93	126.06
23	b	613	CLA	O2D-CGD-CBD	3.30	117.13	111.27
23	B	614	CLA	O2A-CGA-CBA	3.30	122.26	111.91
29	d	406[B]	PL9	C40-C39-C41	3.30	120.82	115.27
23	a	404[B]	CLA	CHC-C1C-C2C	-3.30	117.57	126.73
33	d	414[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
23	B	613	CLA	CAC-C3C-C4C	3.30	129.09	124.81
23	c	512	CLA	C4-C3-C5	3.30	120.81	115.27
35	C	516[B]	DGD	O2G-C1B-C2B	3.29	118.60	111.50
23	b	608	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
33	d	408[A]	LHG	O7-C7-C8	3.29	118.59	111.50
23	C	505	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
23	C	506	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
23	C	507	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
23	B	610	CLA	O2A-CGA-O1A	-3.29	115.29	123.59
23	b	610	CLA	O2A-CGA-O1A	-3.29	115.29	123.59
32	z	101	LMG	O7-C10-C11	3.28	118.58	111.50
25	D	405	BCR	C29-C30-C25	3.28	115.53	110.48
29	a	412[B]	PL9	C27-C28-C29	-3.28	119.76	127.66
23	B	608	CLA	C1C-C2C-C3C	-3.28	103.51	106.96
23	C	512	CLA	CHD-C4C-NC	3.27	129.36	124.20
23	C	503	CLA	C4C-C3C-C2C	-3.27	102.13	106.90
23	C	511	CLA	CMC-C2C-C1C	3.27	130.02	125.04
23	c	511	CLA	CMC-C2C-C1C	3.27	130.02	125.04
23	b	605	CLA	CHD-C4C-NC	3.27	129.35	124.20
23	b	608	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
23	C	510	CLA	C3C-C4C-NC	3.26	114.23	110.57
23	b	609	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
25	b	618	BCR	C15-C14-C13	-3.26	122.66	127.31
23	C	510	CLA	CHD-C4C-NC	3.26	129.34	124.20
23	b	610	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	C	502	CLA	CMB-C2B-C1B	3.26	130.33	125.37
33	D	407[B]	LHG	O7-C7-C8	3.25	118.51	111.50
23	B	603	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
25	K	102	BCR	C38-C26-C25	-3.25	120.88	124.53
23	c	513	CLA	O2A-CGA-CBA	3.25	122.11	111.91
33	d	414[A]	LHG	O7-C7-C8	3.25	118.50	111.50
33	A	419[B]	LHG	C5-O7-C7	-3.25	109.80	117.79
35	h	102	DGD	O2G-C1B-C2B	3.25	118.50	111.50
31	B	628	LMT	C4B-C3B-C2B	3.25	116.49	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	409[B]	SQD	C1-C2-C3	-3.24	103.24	110.00
31	b	627	LMT	C3'-C4'-C5'	-3.24	103.49	110.93
23	B	605	CLA	C4C-C3C-C2C	-3.24	102.17	106.90
29	a	412[B]	PL9	C25-C24-C26	3.24	120.73	115.27
23	b	609	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	c	506	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	B	604	CLA	CAC-C3C-C4C	3.24	129.01	124.81
23	C	509	CLA	O2A-CGA-CBA	3.24	122.06	111.91
23	a	405[B]	CLA	CHD-C4C-NC	3.23	129.30	124.20
26	a	410	SQD	O48-C23-C24	3.23	122.06	111.91
23	C	511	CLA	C4C-C3C-C2C	-3.23	102.18	106.90
29	d	406[B]	PL9	C42-C43-C44	-3.23	119.88	127.66
23	B	608	CLA	C1D-CHD-C4C	-3.23	119.09	126.06
23	A	405[A]	CLA	C3B-C4B-NB	3.23	113.51	110.52
38	F	102	HEM	CHD-C1D-ND	3.23	127.92	124.42
23	B	612	CLA	CAC-C3C-C4C	3.23	129.00	124.81
26	a	409[B]	SQD	C1-O5-C5	-3.22	107.36	113.69
23	c	505	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
24	a	414[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	c	502	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
23	b	616	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	c	508	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
23	b	614	CLA	CMB-C2B-C1B	3.22	130.27	125.37
23	C	513	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
33	d	414[A]	LHG	O8-C23-C24	3.22	122.00	111.91
25	C	514	BCR	C33-C5-C6	-3.22	120.92	124.53
23	B	616	CLA	C1-O2A-CGA	3.22	124.88	116.44
29	D	406[B]	PL9	C27-C28-C29	-3.22	119.92	127.66
23	B	607	CLA	CAA-C2A-C3A	-3.22	103.97	112.78
23	b	612	CLA	CHB-C1B-NB	-3.21	120.86	124.26
23	C	503	CLA	CHD-C4C-NC	3.21	129.26	124.20
23	B	612	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
23	B	602	CLA	CAC-C3C-C4C	3.20	128.96	124.81
23	c	513	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
38	f	101	HEM	CHD-C4C-NC	3.20	127.90	124.44
23	C	512	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
23	a	404[A]	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
23	b	616	CLA	CBC-CAC-C3C	-3.19	103.63	112.43
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	b	613	CLA	O2A-CGA-CBA	3.19	121.92	111.91
25	B	619	BCR	C24-C23-C22	-3.19	121.42	126.23
29	a	412[A]	PL9	C17-C18-C19	-3.19	119.99	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	C3B-C4B-NB	3.19	113.47	110.52
25	a	408	BCR	C29-C30-C25	3.18	115.38	110.48
23	C	501	CLA	CHD-C4C-NC	3.18	129.22	124.20
23	d	404	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
25	t	102	BCR	C28-C27-C26	-3.18	108.40	114.08
23	C	503	CLA	C4-C3-C5	3.18	120.62	115.27
32	C	520	LMG	O8-C28-C29	3.18	121.89	111.91
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	B	615	CLA	CHD-C4C-NC	3.18	129.21	124.20
23	C	505	CLA	CMC-C2C-C1C	3.18	129.88	125.04
23	b	615	CLA	C4C-C3C-C2C	-3.17	102.27	106.90
23	C	506	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
31	A	417	LMT	O5B-C5B-C4B	3.17	115.45	109.69
29	a	412[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	b	605	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	D	403[B]	CLA	CAC-C3C-C4C	3.17	128.92	124.81
23	D	403[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	c	513	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
23	C	502	CLA	C3B-C4B-NB	3.17	113.45	110.52
23	b	608	CLA	C1-C2-C3	-3.17	120.56	126.04
23	C	506	CLA	CAC-C3C-C4C	3.17	128.92	124.81
23	c	507	CLA	CHC-C1C-C2C	-3.16	117.94	126.73
23	a	407	CLA	C4C-C3C-C2C	-3.16	102.29	106.90
23	b	607	CLA	C1D-CHD-C4C	-3.16	119.24	126.06
25	y	101	BCR	C38-C26-C25	-3.16	120.98	124.53
23	A	404[B]	CLA	O2A-CGA-CBA	3.16	121.81	111.91
24	A	416[A]	PHO	C4-C3-C5	3.15	120.58	115.27
23	B	610	CLA	C3B-C4B-NB	3.15	113.44	110.52
23	b	609	CLA	CAC-C3C-C4C	3.15	128.90	124.81
32	Z	101	LMG	C4-C3-C2	3.15	116.33	110.82
26	B	620	SQD	O9-S-C6	3.15	110.69	106.94
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
23	B	611	CLA	C1-C2-C3	-3.15	120.59	126.04
33	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79
23	B	601	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
26	B	620	SQD	O48-C23-C24	3.15	121.79	111.91
33	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	406[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
23	D	404	CLA	C4C-C3C-C2C	-3.15	102.31	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	521	LMG	C9-C8-C7	-3.15	104.35	111.79
33	d	414[B]	LHG	O8-C23-O10	-3.15	115.65	123.59
23	c	509	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
23	c	509	CLA	C3B-C4B-NB	3.14	113.43	110.52
23	A	405[B]	CLA	C3B-C4B-NB	3.14	113.43	110.52
23	C	511	CLA	C1-C2-C3	-3.14	120.61	126.04
23	b	612	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
23	b	614	CLA	CBC-CAC-C3C	-3.14	103.77	112.43
23	c	505	CLA	C1D-CHD-C4C	-3.14	119.29	126.06
23	C	512	CLA	C4C-C3C-C2C	-3.14	102.33	106.90
23	B	612	CLA	C11-C12-C13	-3.14	105.78	115.92
23	A	404[B]	CLA	CHC-C1C-C2C	-3.14	118.02	126.73
23	C	504	CLA	CMC-C2C-C1C	3.14	129.81	125.04
23	C	511	CLA	CAC-C3C-C4C	3.14	128.88	124.81
23	a	405[B]	CLA	C4-C3-C5	3.13	120.54	115.27
23	B	613	CLA	O2A-CGA-O1A	-3.13	115.68	123.59
23	B	609	CLA	CBC-CAC-C3C	-3.13	103.79	112.43
25	d	405	BCR	C16-C17-C18	-3.13	122.84	127.31
23	B	604	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
23	C	510	CLA	CHC-C1C-C2C	-3.13	118.03	126.73
23	c	503	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	b	613	CLA	C4C-C3C-C2C	-3.13	102.34	106.90
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
23	b	601	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
23	a	405[A]	CLA	C1-C2-C3	-3.13	120.64	126.04
23	d	403[A]	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
33	d	414[B]	LHG	O8-C23-C24	3.13	121.72	111.91
35	C	518	DGD	O1G-C1A-C2A	3.13	121.72	111.91
23	b	611	CLA	C1D-CHD-C4C	-3.13	119.31	126.06
23	a	407	CLA	C3B-C4B-NB	3.12	113.41	110.52
23	c	512	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	b	601	CLA	C4-C3-C5	3.12	120.52	115.27
23	A	406[B]	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
25	b	618	BCR	C37-C22-C21	-3.12	118.55	122.92
23	b	602	CLA	CAC-C3C-C4C	3.12	128.86	124.81
24	a	406[B]	PHO	CMA-C3A-C4A	-3.12	107.55	114.38
23	c	510	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	c	502	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	A	405[B]	CLA	CHD-C4C-NC	3.12	129.12	124.20
25	y	101	BCR	C24-C23-C22	-3.12	121.53	126.23
29	D	406[A]	PL9	C51-C49-C50	3.12	121.49	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	CAC-C3C-C4C	3.12	128.85	124.81
23	C	504	CLA	CBC-CAC-C3C	-3.11	103.85	112.43
26	A	412	SQD	O48-C23-C24	3.11	121.68	111.91
23	b	604	CLA	CMB-C2B-C1B	3.11	130.11	125.37
26	a	409[B]	SQD	O8-S-C6	3.11	110.70	105.74
23	c	512	CLA	CMC-C2C-C1C	3.11	129.78	125.04
23	c	508	CLA	C4-C3-C5	3.11	120.51	115.27
23	c	507	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	c	513	CLA	CAC-C3C-C4C	3.11	128.84	124.81
23	B	601	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
23	b	609	CLA	C3B-C4B-NB	3.11	113.40	110.52
23	b	607	CLA	C4-C3-C5	3.11	120.50	115.27
29	D	406[A]	PL9	C10-C9-C11	3.11	120.50	115.27
23	a	407	CLA	O2A-CGA-CBA	3.11	121.66	111.91
23	B	611	CLA	C4A-NA-C1A	-3.10	105.31	106.71
23	b	610	CLA	CMB-C2B-C1B	3.10	130.09	125.37
29	D	406[B]	PL9	C53-C6-C1	3.10	121.33	114.99
23	b	609	CLA	CHD-C4C-NC	3.10	129.09	124.20
23	b	609	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	k	101	BCR	C20-C21-C22	-3.10	122.89	127.31
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
23	c	506	CLA	C1D-CHD-C4C	-3.10	119.38	126.06
23	a	407	CLA	C4-C3-C5	3.09	120.48	115.27
23	b	609	CLA	CBC-CAC-C3C	-3.09	103.90	112.43
33	D	408[B]	LHG	O7-C7-C8	3.09	118.17	111.50
23	b	601	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
33	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	A	405[B]	CLA	C4-C3-C5	3.09	120.47	115.27
23	c	513	CLA	C4-C3-C5	3.09	120.47	115.27
23	b	611	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
23	d	403[B]	CLA	O2A-CGA-CBA	3.08	121.59	111.91
23	d	403[B]	CLA	C2A-C1A-CHA	-3.08	118.47	123.86
29	D	406[B]	PL9	C25-C24-C26	3.08	120.46	115.27
24	a	414[A]	PHO	CMB-C2B-C3B	3.08	130.44	124.68
29	a	412[A]	PL9	C10-C9-C11	3.08	120.45	115.27
23	b	610	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
24	a	406[B]	PHO	C1A-C2A-C3A	-3.08	99.91	102.84
31	M	101	LMT	C1'-O5'-C5'	-3.07	107.65	113.69
23	B	612	CLA	O2A-CGA-CBA	3.07	121.55	111.91
23	a	404[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
23	c	510	CLA	O2A-CGA-CBA	3.07	121.55	111.91
23	b	614	CLA	CHC-C1C-C2C	-3.07	118.20	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	CMC-C2C-C1C	3.07	129.72	125.04
23	c	510	CLA	CHC-C1C-C2C	-3.07	118.20	126.73
29	a	412[B]	PL9	C37-C38-C39	-3.07	120.27	127.66
29	A	414[B]	PL9	C27-C28-C29	-3.07	120.27	127.66
23	B	601	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	b	601	CLA	CHD-C4C-NC	3.07	129.04	124.20
23	a	407	CLA	CAA-C2A-C3A	-3.07	104.38	112.78
26	a	409[B]	SQD	C45-O47-C7	-3.06	110.25	117.79
23	d	403[B]	CLA	C4-C3-C5	3.06	120.42	115.27
23	b	612	CLA	O2A-CGA-O1A	-3.06	115.87	123.59
34	b	622	HTG	O5-C5-C4	3.06	115.25	109.69
23	c	505	CLA	CAC-C3C-C4C	3.06	128.78	124.81
29	a	412[B]	PL9	C17-C18-C19	-3.06	120.30	127.66
23	B	607	CLA	CBC-CAC-C3C	-3.05	104.01	112.43
29	d	406[A]	PL9	C10-C9-C11	3.05	120.41	115.27
23	B	604	CLA	CMB-C2B-C1B	3.05	130.02	125.37
23	B	613	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	b	615	CLA	C4-C3-C5	3.05	120.41	115.27
23	c	509	CLA	C4C-C3C-C2C	-3.05	102.45	106.90
23	a	404[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	a	405[B]	CLA	CMC-C2C-C1C	3.05	129.69	125.04
23	D	403[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	d	403[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
26	b	620	SQD	C3-C4-C5	3.05	115.67	110.24
23	B	609	CLA	C4C-C3C-C2C	-3.05	102.46	106.90
23	B	604	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
23	B	605	CLA	O2A-CGA-O1A	-3.04	115.91	123.59
23	b	614	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	c	510	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
23	d	403[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	D	403[B]	CLA	O2A-CGA-CBA	3.04	121.46	111.91
23	C	504	CLA	C1-O2A-CGA	3.04	124.42	116.44
23	A	406[B]	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	b	603	CLA	C2A-C1A-CHA	-3.04	118.55	123.86
26	A	410[B]	SQD	O9-S-C6	3.04	110.55	106.94
23	B	603	CLA	CHC-C1C-C2C	-3.04	118.30	126.73
23	c	511	CLA	CHD-C4C-NC	3.03	128.98	124.20
23	d	403[A]	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	B	603	CLA	CAC-C3C-C4C	3.03	128.74	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	b	614	CLA	CHD-C4C-NC	3.03	128.97	124.20
23	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
23	d	403[A]	CLA	C4-C3-C5	3.02	120.36	115.27
23	b	607	CLA	C4C-C3C-C2C	-3.02	102.49	106.90
29	d	406[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
31	A	420	LMT	O5B-C5B-C4B	3.02	115.18	109.69
23	c	514	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	b	603	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	A	408	CLA	CHD-C4C-NC	3.02	128.96	124.20
23	c	504	CLA	CMC-C2C-C1C	3.02	129.63	125.04
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
23	B	605	CLA	C1-C2-C3	-3.01	120.83	126.04
23	c	509	CLA	CHC-C1C-C2C	-3.01	118.36	126.73
29	a	412[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
25	T	101	BCR	C12-C13-C14	-3.01	114.32	118.94
33	d	407[A]	LHG	O7-C7-C8	3.01	117.99	111.50
32	c	520	LMG	O1-C7-C8	-3.01	103.64	110.90
23	D	403[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	b	605	CLA	CHC-C1C-C2C	-3.01	118.38	126.73
23	C	510	CLA	O2A-CGA-O1A	-3.01	116.00	123.59
25	C	514	BCR	C16-C17-C18	-3.01	123.02	127.31
23	B	610	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
25	B	618	BCR	C37-C22-C21	-3.00	118.71	122.92
29	a	412[B]	PL9	C35-C34-C36	3.00	120.32	115.27
23	a	407	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	B	608	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
26	A	410[B]	SQD	O48-C23-C24	3.00	121.32	111.91
23	a	405[B]	CLA	C1-C2-C3	-3.00	120.86	126.04
23	B	606	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	b	603	CLA	O2A-CGA-CBA	3.00	121.31	111.91
23	b	615	CLA	C3B-C4B-NB	3.00	113.30	110.52
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
23	D	404	CLA	C4-C3-C5	2.99	120.30	115.27
23	b	615	CLA	C11-C10-C8	-2.99	106.25	115.92
23	B	607	CLA	CHD-C4C-NC	2.99	128.91	124.20
23	A	404[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	a	404[B]	CLA	O2A-CGA-CBA	2.99	121.29	111.91
23	b	611	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	C	506	CLA	CMC-C2C-C1C	2.99	129.59	125.04
23	c	503	CLA	CHD-C4C-NC	2.99	128.91	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404	CLA	CHD-C4C-NC	2.99	128.91	124.20
33	a	418[B]	LHG	O7-C7-C8	2.99	117.93	111.50
33	D	408[A]	LHG	O8-C23-C24	2.98	121.27	111.91
23	c	504	CLA	C4C-C3C-C2C	-2.98	102.55	106.90
24	A	416[B]	PHO	CED-O2D-CGD	2.98	122.68	115.94
25	c	515	BCR	C20-C21-C22	-2.98	123.05	127.31
23	B	614	CLA	CHC-C1C-C2C	-2.98	118.45	126.73
35	H	102	DGD	O1G-C1A-C2A	2.98	121.25	111.91
23	d	403[B]	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
32	D	412	LMG	O7-C10-C11	2.98	117.91	111.50
23	c	512	CLA	CAC-C3C-C4C	2.97	128.67	124.81
23	C	502	CLA	CHC-C1C-C2C	-2.97	118.47	126.73
23	B	612	CLA	C4A-NA-C1A	-2.97	105.37	106.71
23	c	504	CLA	CAC-C3C-C4C	2.97	128.67	124.81
23	B	616	CLA	CAC-C3C-C4C	2.97	128.67	124.81
33	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	C	502	CLA	CBC-CAC-C3C	-2.97	104.24	112.43
23	C	509	CLA	O2A-CGA-O1A	-2.97	116.10	123.59
25	c	515	BCR	C37-C22-C21	-2.97	118.76	122.92
23	b	606	CLA	C3B-C4B-NB	2.97	113.27	110.52
31	m	103	LMT	C3'-C4'-C5'	-2.97	104.13	110.93
23	b	610	CLA	CHD-C4C-NC	2.97	128.88	124.20
23	D	403[B]	CLA	C1D-CHD-C4C	-2.97	119.66	126.06
23	C	513	CLA	CMC-C2C-C1C	2.96	129.55	125.04
29	d	406[B]	PL9	C7-C8-C9	-2.96	121.86	126.79
29	a	412[B]	PL9	C22-C23-C24	-2.96	120.52	127.66
23	c	513	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	B	611	CLA	CAC-C3C-C4C	2.96	128.65	124.81
23	b	602	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	B	614	CLA	CHD-C4C-NC	2.96	128.87	124.20
23	B	603	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
23	B	607	CLA	O2A-CGA-O1A	-2.96	116.12	123.59
23	c	503	CLA	CHC-C1C-C2C	-2.96	118.51	126.73
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	b	610	CLA	C4-C3-C5	2.96	120.24	115.27
24	a	414[B]	PHO	CMB-C2B-C3B	2.95	130.21	124.68
23	d	402[A]	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
23	C	501	CLA	CAC-C3C-C4C	2.95	128.64	124.81
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
23	b	608	CLA	CAC-C3C-C4C	2.95	128.63	124.81
38	f	101	HEM	CHB-C1B-NB	2.95	128.01	124.37
25	y	101	BCR	C15-C14-C13	-2.94	123.11	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	501	CLA	C4C-C3C-C2C	-2.94	102.61	106.90
25	T	101	BCR	C15-C14-C13	2.94	131.51	127.31
23	c	514	CLA	CAC-C3C-C4C	2.94	128.63	124.81
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
29	A	414[B]	PL9	C17-C18-C19	-2.94	120.58	127.66
23	B	613	CLA	O2A-CGA-CBA	2.94	121.13	111.91
23	C	503	CLA	O2A-CGA-O1A	-2.94	116.18	123.59
23	D	403[B]	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
23	C	503	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
33	a	418[A]	LHG	O7-C7-C8	2.94	117.83	111.50
23	d	403[B]	CLA	CHC-C1C-C2C	-2.94	118.58	126.73
23	b	611	CLA	O2A-CGA-O1A	-2.93	116.19	123.59
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
33	D	407[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
23	c	504	CLA	C4-C3-C5	2.93	120.20	115.27
29	d	406[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
23	B	606	CLA	CMC-C2C-C1C	2.93	129.50	125.04
25	a	408	BCR	C40-C30-C25	-2.93	105.55	110.30
23	C	513	CLA	CBC-CAC-C3C	-2.93	104.35	112.43
23	c	510	CLA	C4-C3-C5	2.93	120.20	115.27
23	b	602	CLA	CMB-C2B-C1B	2.93	129.83	125.37
23	B	608	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
23	a	405[B]	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	c	516	BCR	C32-C1-C6	-2.93	105.55	110.30
29	d	406[A]	PL9	C27-C28-C29	-2.93	120.61	127.66
23	C	502	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	A	404[A]	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	a	404[B]	CLA	CAA-C2A-C1A	-2.92	102.40	111.97
25	h	101	BCR	C33-C5-C6	-2.92	121.25	124.53
23	A	408	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
23	d	402[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	A	406[A]	CLA	CAA-C2A-C3A	-2.92	104.78	112.78
23	A	408	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
29	d	406[A]	PL9	C53-C6-C1	2.92	120.95	114.99
23	A	404[B]	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
29	a	412[A]	PL9	C22-C23-C24	-2.92	120.64	127.66
33	A	419[B]	LHG	O8-C23-C24	2.91	121.06	111.91
23	b	605	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
25	T	101	BCR	C16-C17-C18	-2.91	123.15	127.31
25	b	619	BCR	C24-C23-C22	-2.91	121.83	126.23
38	f	101	HEM	C4D-ND-C1D	2.91	108.08	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	C6-C5-C3	-2.91	105.82	113.45
23	D	403[B]	CLA	CHC-C1C-C2C	-2.91	118.65	126.73
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91
23	c	509	CLA	CAA-C2A-C3A	-2.91	104.81	112.78
23	A	408	CLA	CMC-C2C-C1C	2.91	129.47	125.04
33	D	408[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
23	b	607	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
23	A	405[B]	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
23	a	404[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
29	D	406[B]	PL9	C51-C49-C50	2.90	121.02	114.60
23	a	405[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	b	616	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
23	C	509	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
29	A	414[B]	PL9	C20-C19-C21	2.90	120.15	115.27
23	C	510	CLA	O2A-CGA-CBA	2.90	121.01	111.91
23	b	611	CLA	C2A-C1A-CHA	-2.90	118.79	123.86
23	C	512	CLA	O2A-CGA-CBA	2.90	121.01	111.91
23	C	507	CLA	C4-C3-C5	2.90	120.15	115.27
23	B	606	CLA	CHD-C4C-NC	2.90	128.77	124.20
23	c	514	CLA	O2A-CGA-CBA	2.90	121.00	111.91
23	d	402[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
25	c	516	BCR	C7-C8-C9	-2.90	121.86	126.23
23	B	605	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
23	a	405[A]	CLA	CMB-C2B-C1B	2.89	129.78	125.37
23	b	608	CLA	CBC-CAC-C3C	-2.89	104.45	112.43
23	B	609	CLA	C3B-C4B-NB	2.89	113.20	110.52
25	K	102	BCR	C20-C21-C22	-2.89	123.18	127.31
23	b	615	CLA	CHC-C1C-C2C	-2.89	118.70	126.73
23	c	512	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	D	403[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
26	a	410	SQD	C3-C4-C5	2.88	115.39	110.24
23	B	609	CLA	O2A-CGA-CBA	2.88	120.96	111.91
23	B	613	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	A	405[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	D	403[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	b	603	CLA	C4-C3-C5	2.88	120.12	115.27
23	B	607	CLA	CMB-C2B-C1B	2.88	129.76	125.37
23	a	404[B]	CLA	CMA-C3A-C4A	-2.88	104.03	111.77
23	A	406[B]	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
33	E	101[B]	LHG	O8-C23-C24	2.88	120.94	111.91
25	d	405	BCR	C28-C27-C26	-2.88	108.94	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	H	102	DGD	O1G-C1A-O1A	-2.88	116.33	123.59
32	m	101	LMG	O8-C28-C29	2.88	120.93	111.91
23	B	603	CLA	CHD-C4C-NC	2.87	128.73	124.20
25	B	618	BCR	C15-C14-C13	-2.87	123.21	127.31
35	C	516[B]	DGD	C3G-C2G-C1G	-2.87	104.99	111.79
23	B	609	CLA	CHC-C1C-C2C	-2.87	118.75	126.73
23	c	506	CLA	C3B-C4B-NB	2.87	113.18	110.52
23	b	610	CLA	CMC-C2C-C1C	2.87	129.41	125.04
24	a	406[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	D	403[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
23	a	405[B]	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
23	b	614	CLA	CHB-C1B-NB	-2.87	121.22	124.26
23	A	408	CLA	O2A-CGA-CBA	2.87	120.91	111.91
26	f	102	SQD	O5-C1-C2	2.87	116.42	110.35
23	B	614	CLA	C2A-C1A-CHA	-2.87	118.85	123.86
23	c	506	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
35	c	519	DGD	O2G-C1B-C2B	2.86	117.67	111.50
29	a	412[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
23	D	404	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
25	b	619	BCR	C34-C9-C10	-2.86	118.91	122.92
23	b	608	CLA	CHC-C1C-C2C	-2.86	118.78	126.73
23	b	606	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
23	C	505	CLA	C4-C3-C5	2.86	120.08	115.27
23	b	602	CLA	C1-C2-C3	-2.86	121.09	126.04
25	a	408	BCR	C7-C8-C9	-2.86	121.91	126.23
23	C	502	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	A	406[B]	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
23	B	602	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	d	404	CLA	CBC-CAC-C3C	-2.86	104.55	112.43
23	B	611	CLA	C3B-C4B-NB	2.86	113.17	110.52
23	b	614	CLA	O2A-CGA-O1A	-2.86	116.38	123.59
23	c	510	CLA	O2A-C1-C2	2.86	116.14	108.64
33	d	407[B]	LHG	O7-C7-C8	2.85	117.65	111.50
23	d	404	CLA	C4C-C3C-C2C	-2.85	102.74	106.90
23	D	404	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	B	606	CLA	C4-C3-C5	2.85	120.07	115.27
24	a	406[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	c	513	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
23	B	615	CLA	C4-C3-C5	2.85	120.06	115.27
33	b	629[A]	LHG	O8-C23-C24	2.85	120.84	111.91
23	c	506	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	C	502	CLA	O2A-CGA-CBA	2.85	120.84	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C11-C12-C13	-2.85	106.72	115.92
31	b	621	LMT	C1'-O5'-C5'	-2.84	108.10	113.69
23	c	512	CLA	CHC-C1C-C2C	-2.84	118.83	126.73
23	b	601	CLA	C1-O2A-CGA	2.84	123.91	116.44
32	c	520	LMG	O8-C28-C29	2.84	120.83	111.91
23	b	607	CLA	CBC-CAC-C3C	-2.84	104.59	112.43
23	b	605	CLA	C4-C3-C5	2.84	120.05	115.27
24	a	406[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
23	B	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
23	c	507	CLA	CMC-C2C-C1C	2.84	129.37	125.04
23	C	503	CLA	C1-C2-C3	-2.84	121.13	126.04
26	a	410	SQD	C1-O5-C5	2.84	119.26	113.69
23	b	604	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
34	b	622	HTG	O2-C2-C3	-2.84	103.79	110.35
23	C	511	CLA	CHD-C4C-NC	2.84	128.67	124.20
23	b	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	a	405[B]	CLA	CAA-C2A-C3A	-2.83	105.02	112.78
24	a	414[B]	PHO	C4A-C3A-C2A	-2.83	100.14	102.84
23	c	505	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
23	a	407	CLA	CHD-C4C-NC	2.83	128.66	124.20
31	B	630	LMT	O1'-C1'-C2'	2.83	112.72	108.30
23	b	616	CLA	C3B-C4B-NB	2.83	113.14	110.52
32	z	101	LMG	O8-C28-C29	2.83	120.78	111.91
23	c	511	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
38	f	101	HEM	CHD-C1D-ND	2.83	127.49	124.42
24	a	414[B]	PHO	O2D-CGD-O1D	-2.83	118.31	123.84
23	c	502	CLA	C1-C2-C3	-2.83	121.16	126.04
23	A	406[B]	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
23	b	603	CLA	CHC-C1C-C2C	-2.82	118.89	126.73
23	A	406[B]	CLA	C3B-C4B-NB	2.82	113.14	110.52
23	b	615	CLA	CAC-C3C-C4C	2.82	128.47	124.81
23	B	614	CLA	C4C-C3C-C2C	-2.82	102.78	106.90
23	A	406[B]	CLA	O2A-CGA-CBA	2.82	120.77	111.91
23	B	605	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
23	B	612	CLA	C1-C2-C3	-2.82	121.17	126.04
23	d	404	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
23	b	607	CLA	CAA-C2A-C3A	-2.82	105.06	112.78
23	C	513	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
23	C	504	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	b	613	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	c	508	CLA	CHD-C4C-NC	2.82	128.64	124.20
35	c	517[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	C4C-C3C-C2C	-2.82	102.79	106.90
23	c	509	CLA	O2A-CGA-CBA	2.81	120.74	111.91
23	C	513	CLA	CAC-C3C-C4C	2.81	128.46	124.81
23	D	403[B]	CLA	C4-C3-C5	2.81	120.00	115.27
23	C	505	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
23	A	405[B]	CLA	CMB-C2B-C1B	2.81	129.65	125.37
23	D	403[B]	CLA	CMB-C2B-C1B	2.81	129.65	125.37
29	D	406[B]	PL9	C40-C39-C41	2.81	119.99	115.27
29	A	414[B]	PL9	C30-C29-C31	2.81	119.99	115.27
23	b	613	CLA	C4-C3-C5	2.81	119.99	115.27
26	f	102	SQD	C4-C3-C2	-2.81	105.93	110.82
23	c	511	CLA	O2A-CGA-CBA	2.80	120.71	111.91
26	B	620	SQD	C1-O5-C5	-2.80	108.18	113.69
23	b	604	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
23	B	601	CLA	O2A-CGA-CBA	2.80	120.71	111.91
23	b	611	CLA	CHD-C4C-NC	2.80	128.62	124.20
26	B	620	SQD	C4-C3-C2	2.80	115.72	110.82
23	D	403[B]	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	c	503	CLA	O2A-CGA-CBA	2.80	120.69	111.91
23	c	502	CLA	C3B-C4B-NB	2.80	113.11	110.52
23	d	402[B]	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
23	b	602	CLA	C2A-C1A-CHA	-2.80	118.97	123.86
23	d	402[B]	CLA	C1-C2-C3	-2.80	121.21	126.04
23	d	403[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.73
23	A	404[B]	CLA	O2A-CGA-O1A	-2.80	116.54	123.59
25	C	515	BCR	C33-C5-C6	-2.80	121.39	124.53
23	B	615	CLA	C3B-C4B-NB	2.80	113.11	110.52
23	c	511	CLA	O2A-CGA-O1A	-2.79	116.54	123.59
35	C	516[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
24	A	407[B]	PHO	CBC-CAC-C3C	-2.79	108.79	112.88
23	C	509	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
23	B	615	CLA	C11-C10-C8	-2.79	106.90	115.92
23	D	403[B]	CLA	O2A-CGA-O1A	-2.79	116.55	123.59
23	D	403[B]	CLA	CAA-C2A-C3A	-2.79	105.14	112.78
23	b	612	CLA	O2A-CGA-CBA	2.79	120.66	111.91
23	B	610	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
23	A	406[A]	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
25	c	516	BCR	C37-C22-C21	-2.79	119.02	122.92
23	d	404	CLA	CMB-C2B-C1B	2.79	129.61	125.37
33	D	408[A]	LHG	O7-C7-C8	2.79	117.50	111.50
24	a	406[B]	PHO	O2D-CGD-O1D	-2.78	118.39	123.84
25	D	405	BCR	C37-C22-C23	2.78	122.46	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	a	409[A]	SQD	O47-C7-O49	-2.78	116.98	123.70
23	b	603	CLA	CHD-C4C-NC	2.78	128.59	124.20
23	b	606	CLA	CHC-C1C-C2C	-2.78	119.01	126.73
23	A	406[B]	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
23	a	407	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
33	b	629[B]	LHG	O8-C23-C24	2.78	120.62	111.91
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
23	a	404[B]	CLA	C4C-C3C-C2C	-2.78	102.85	106.90
23	c	512	CLA	O2A-CGA-CBA	2.78	120.62	111.91
23	A	406[B]	CLA	CBC-CAC-C3C	-2.77	104.79	112.43
23	C	513	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
32	B	621	LMG	C12-C11-C10	-2.77	103.55	113.62
23	D	404	CLA	O2A-CGA-O1A	-2.77	116.60	123.59
34	b	623	HTG	O5-C1-C2	2.77	113.80	110.31
35	c	519	DGD	O1G-C1A-C2A	2.77	120.60	111.91
23	c	507	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
23	c	504	CLA	C3B-C4B-NB	2.77	113.08	110.52
23	C	501	CLA	CBC-CAC-C3C	-2.77	104.81	112.43
38	f	101	HEM	CBD-CAD-C3D	-2.77	104.94	112.63
25	T	101	BCR	C2-C1-C6	2.77	114.74	110.48
25	Y	101	BCR	C10-C11-C12	-2.76	114.59	123.22
23	A	408	CLA	CBC-CAC-C3C	-2.76	104.82	112.43
29	a	412[A]	PL9	C53-C6-C1	2.76	120.64	114.99
23	A	405[B]	CLA	CAC-C3C-C4C	2.76	128.39	124.81
35	c	517[B]	DGD	C3G-C2G-C1G	-2.76	105.26	111.79
23	b	608	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	c	513	CLA	CHD-C4C-NC	2.76	128.55	124.20
23	b	611	CLA	O2A-CGA-CBA	2.76	120.56	111.91
35	C	516[B]	DGD	O6D-C1D-O3G	-2.76	103.44	109.97
23	C	510	CLA	CMC-C2C-C1C	2.76	129.24	125.04
23	c	510	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	b	612	CLA	C2A-C1A-CHA	-2.75	119.05	123.86
23	C	506	CLA	CAA-C2A-C3A	-2.75	105.24	112.78
23	C	513	CLA	CHC-C1C-C2C	-2.75	119.09	126.73
23	b	606	CLA	CMB-C2B-C1B	2.75	129.56	125.37
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
29	a	412[B]	PL9	C42-C43-C44	-2.75	121.04	127.66
23	B	603	CLA	O2A-CGA-CBA	2.75	120.53	111.91
29	D	406[B]	PL9	C17-C18-C19	-2.75	121.04	127.66
31	M	102	LMT	C1'-O5'-C5'	-2.75	108.30	113.69
32	A	418	LMG	C8-O7-C10	-2.75	111.03	117.79
23	c	507	CLA	CHD-C4C-NC	2.75	128.53	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	CMC-C2C-C1C	2.74	129.22	125.04
23	C	512	CLA	CMB-C2B-C1B	2.74	129.55	125.37
23	c	502	CLA	CHC-C1C-C2C	-2.74	119.11	126.73
23	c	508	CLA	O2A-CGA-CBA	2.74	120.52	111.91
23	C	503	CLA	CMB-C2B-C1B	2.74	129.55	125.37
23	B	601	CLA	CAC-C3C-C4C	2.74	128.37	124.81
23	C	509	CLA	C16-C15-C13	-2.74	107.06	115.92
23	b	603	CLA	CMA-C3A-C2A	-2.74	102.78	113.83
23	c	511	CLA	C4C-C3C-C2C	-2.74	102.91	106.90
23	c	514	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
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	c	502	CLA	CHD-C4C-NC	2.73	128.51	124.20
25	B	618	BCR	C2-C1-C6	2.73	114.69	110.48
25	B	619	BCR	C21-C20-C19	-2.73	114.69	123.22
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
25	H	101	BCR	C37-C22-C21	-2.73	119.10	122.92
32	A	418	LMG	O6-C1-O1	-2.73	103.51	109.97
35	C	516[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
32	c	501	LMG	C8-O7-C10	-2.73	111.08	117.79
25	b	619	BCR	C38-C26-C25	-2.73	121.47	124.53
33	d	408[A]	LHG	O8-C23-C24	2.73	120.46	111.91
23	C	512	CLA	CMA-C3A-C4A	-2.72	104.45	111.77
33	d	407[B]	LHG	O8-C23-O10	-2.72	116.72	123.59
23	B	605	CLA	CHC-C1C-C2C	-2.72	119.16	126.73
25	k	101	BCR	C11-C10-C9	-2.72	123.42	127.31
23	A	406[B]	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
23	d	402[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
23	c	508	CLA	C3B-C4B-NB	2.72	113.04	110.52
26	B	620	SQD	O48-C23-O10	-2.72	116.72	123.59
29	D	406[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
23	B	616	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
23	D	403[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	a	404[B]	CLA	C1-C2-C3	-2.72	121.34	126.04
29	a	412[B]	PL9	C53-C6-C1	2.72	120.55	114.99
33	D	408[B]	LHG	O8-C23-C24	2.72	120.44	111.91
33	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
32	c	521	LMG	O8-C28-C29	2.72	120.43	111.91
34	b	622	HTG	O5-C1-C2	2.72	113.73	110.31
23	B	616	CLA	O2A-CGA-CBA	2.72	120.43	111.91
23	b	605	CLA	C3B-C4B-NB	2.72	113.03	110.52
29	A	414[B]	PL9	C10-C9-C11	2.71	119.84	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	406[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
23	C	507	CLA	CHC-C1C-C2C	-2.71	119.20	126.73
25	b	617	BCR	C29-C30-C25	2.71	114.66	110.48
23	d	403[B]	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
32	A	418	LMG	C6-C5-C4	2.71	119.35	113.00
23	c	503	CLA	CBC-CAC-C3C	-2.71	104.96	112.43
23	C	501	CLA	C1-O2A-CGA	2.71	123.55	116.44
23	b	602	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	a	405[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	B	606	CLA	O2A-CGA-CBA	2.71	120.40	111.91
25	h	101	BCR	C16-C17-C18	-2.71	123.45	127.31
23	C	509	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	a	404[B]	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
24	a	406[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	B	608	CLA	CMC-C2C-C1C	2.71	129.16	125.04
23	C	508	CLA	CAC-C3C-C4C	2.71	128.32	124.81
25	h	101	BCR	C10-C11-C12	-2.71	114.77	123.22
25	c	516	BCR	C15-C14-C13	-2.71	123.45	127.31
23	A	406[A]	CLA	C2A-C1A-CHA	-2.71	119.13	123.86
23	A	404[A]	CLA	C2A-C1A-CHA	-2.70	119.13	123.86
23	b	615	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	B	610	CLA	CAC-C3C-C4C	2.70	128.32	124.81
23	a	405[B]	CLA	CMB-C2B-C1B	2.70	129.49	125.37
26	b	620	SQD	O7-S-C6	2.70	110.15	106.94
23	C	512	CLA	CMC-C2C-C1C	2.70	129.15	125.04
25	K	102	BCR	C24-C23-C22	-2.70	122.16	126.23
35	C	517[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	C	511	CLA	CMB-C2B-C1B	2.70	129.48	125.37
23	C	501	CLA	C3B-C4B-NB	2.70	113.02	110.52
24	a	406[B]	PHO	O2A-CGA-O1A	-2.70	116.79	123.59
23	D	403[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	A	405[B]	CLA	C2A-C1A-CHA	-2.70	119.15	123.86
23	B	602	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
23	a	407	CLA	CAC-C3C-C4C	2.69	128.30	124.81
25	T	101	BCR	C33-C5-C6	-2.69	121.51	124.53
23	B	615	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
24	a	406[B]	PHO	O2A-CGA-CBA	2.69	120.34	111.91
23	c	514	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	B	612	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
32	D	412	LMG	O8-C28-C29	2.69	120.34	111.91
29	a	412[B]	PL9	C40-C39-C41	2.69	119.79	115.27
25	c	515	BCR	C36-C18-C17	-2.69	119.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	c	502	CLA	CAC-C3C-C4C	2.69	128.30	124.81
23	b	603	CLA	CBC-CAC-C3C	-2.69	105.03	112.43
23	c	514	CLA	CHC-C1C-C2C	-2.68	119.27	126.73
32	D	412	LMG	O8-C28-O10	-2.68	116.82	123.59
23	c	504	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	d	402[B]	CLA	C4C-C3C-C2C	-2.68	102.99	106.90
32	m	101	LMG	C8-O7-C10	-2.68	111.19	117.79
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
40	V	201	HEC	CBC-CAC-C3C	2.68	119.82	112.43
23	d	402[B]	CLA	C4-C3-C5	2.68	119.78	115.27
29	a	412[B]	PL9	C10-C9-C11	2.68	119.78	115.27
38	f	101	HEM	CMD-C2D-C1D	2.68	129.12	125.04
23	a	405[A]	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
23	C	506	CLA	C4-C3-C5	2.68	119.77	115.27
23	B	608	CLA	CHB-C4A-NA	2.68	128.21	124.51
33	a	418[A]	LHG	O8-C23-C24	2.68	120.30	111.91
24	a	414[A]	PHO	CBA-CAA-C2A	-2.68	105.99	113.81
35	c	517[A]	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	406[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
31	B	628	LMT	C2'-C3'-C4'	2.67	115.79	109.68
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
26	f	102	SQD	O48-C23-C24	2.67	120.28	111.91
24	a	406[B]	PHO	O1D-CGD-CBD	-2.67	120.30	124.74
23	b	603	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
29	d	406[B]	PL9	C36-C34-C33	-2.67	115.72	121.12
23	A	404[B]	CLA	CAC-C3C-C4C	2.66	128.27	124.81
23	B	615	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
24	A	416[B]	PHO	OBD-CAD-C3D	-2.66	123.56	127.98
23	a	405[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	C	513	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	C	504	CLA	CMB-C2B-C1B	2.66	129.41	125.37
32	C	519	LMG	O8-C28-O10	-2.66	116.89	123.59
23	C	512	CLA	CBC-CAC-C3C	-2.66	105.11	112.43
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59
23	B	609	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	a	404[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
25	B	618	BCR	C37-C22-C23	2.65	122.26	118.08
23	d	402[B]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	B	608	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
23	c	504	CLA	C1-C2-C3	-2.65	121.46	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	406[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	b	610	CLA	C3B-C4B-NB	2.65	112.97	110.52
23	c	504	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
26	A	410[B]	SQD	O7-S-C6	2.64	110.08	106.94
23	B	601	CLA	C1-O2A-CGA	2.64	123.38	116.44
29	a	412[B]	PL9	C20-C19-C21	2.64	119.71	115.27
23	C	507	CLA	O2A-CGA-CBA	2.64	120.19	111.91
23	B	615	CLA	C6-C7-C8	-2.64	107.38	115.92
23	B	602	CLA	CMA-C3A-C4A	-2.64	104.68	111.77
29	A	414[B]	PL9	C40-C39-C41	2.64	119.71	115.27
23	D	404	CLA	CHC-C1C-C2C	-2.64	119.40	126.73
23	B	605	CLA	CMC-C2C-C1C	2.64	129.06	125.04
23	C	510	CLA	C2A-C1A-CHA	-2.64	119.25	123.86
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
26	F	103	SQD	O48-C23-C24	2.64	120.18	111.91
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
33	d	407[B]	LHG	C6-C5-C4	-2.63	105.56	111.79
24	A	416[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
23	D	403[B]	CLA	C2A-C1A-CHA	-2.63	119.26	123.86
23	c	508	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
23	b	614	CLA	CMC-C2C-C1C	2.63	129.05	125.04
23	C	510	CLA	CMB-C2B-C1B	2.63	129.38	125.37
25	t	102	BCR	C11-C10-C9	-2.63	123.56	127.31
40	v	201	HEC	CHA-C4D-ND	2.63	127.27	124.42
23	C	506	CLA	O2A-CGA-CBA	2.63	120.15	111.91
26	f	102	SQD	O5-C5-C4	2.62	114.46	109.69
23	c	503	CLA	CMB-C2B-C1B	2.62	129.37	125.37
23	C	504	CLA	CHB-C1B-NB	-2.62	121.48	124.26
31	F	101	LMT	C1'-O5'-C5'	-2.62	108.54	113.69
23	B	601	CLA	CMB-C2B-C1B	2.62	129.36	125.37
23	d	403[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	B	612	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
25	D	405	BCR	C3-C4-C5	-2.62	109.40	114.08
23	C	511	CLA	C1-O2A-CGA	2.62	123.31	116.44
31	e	101	LMT	O1'-C1'-C2'	2.62	112.39	108.30
23	b	601	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
23	D	403[B]	CLA	CBC-CAC-C3C	-2.61	105.22	112.43
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
26	A	412	SQD	C4-C3-C2	-2.61	106.26	110.82
23	c	514	CLA	CMC-C2C-C1C	2.61	129.02	125.04
23	D	404	CLA	O2A-CGA-CBA	2.61	120.10	111.91
23	d	404	CLA	C4-C3-C5	2.61	119.66	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	CMC-C2C-C1C	2.61	129.01	125.04
23	B	601	CLA	C3B-C4B-NB	2.61	112.94	110.52
33	D	407[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	b	609	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
33	a	418[B]	LHG	O8-C23-C24	2.61	120.09	111.91
23	B	601	CLA	CHC-C1C-C2C	-2.61	119.49	126.73
33	D	407[A]	LHG	O7-C7-C8	2.61	117.12	111.50
23	d	402[B]	CLA	CAC-C3C-C2C	2.61	131.99	127.53
23	c	514	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
25	c	516	BCR	C37-C22-C23	2.60	122.18	118.08
23	B	602	CLA	C11-C12-C13	-2.60	107.50	115.92
23	c	507	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
31	M	101	LMT	C3'-C4'-C5'	-2.60	104.96	110.93
23	b	604	CLA	C4-C3-C5	2.60	119.65	115.27
23	C	506	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
33	L	101[A]	LHG	O8-C23-C24	2.60	120.06	111.91
23	b	610	CLA	CAA-CBA-CGA	-2.60	105.66	113.25
23	b	614	CLA	O2A-CGA-CBA	2.60	120.06	111.91
35	H	102	DGD	O2G-C1B-C2B	2.60	117.10	111.50
31	a	415	LMT	C3'-C4'-C5'	-2.60	104.97	110.93
23	B	607	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
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
33	d	407[B]	LHG	O8-C23-C24	2.59	120.04	111.91
24	a	414[B]	PHO	CBA-CAA-C2A	-2.59	106.24	113.81
23	c	504	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
23	d	402[B]	CLA	CBC-CAC-C3C	-2.59	105.29	112.43
35	h	102	DGD	O1G-C1A-C2A	2.59	120.04	111.91
25	C	514	BCR	C38-C26-C25	-2.59	121.62	124.53
23	C	513	CLA	O2A-CGA-CBA	2.59	120.03	111.91
23	c	509	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	a	404[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
23	C	506	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	D	404	CLA	C3B-C4B-NB	2.59	112.91	110.52
23	C	504	CLA	C4C-C3C-C2C	-2.58	103.13	106.90
23	B	604	CLA	C6-C7-C8	-2.58	107.57	115.92
23	A	406[B]	CLA	C4-C3-C5	2.58	119.61	115.27
35	h	102	DGD	O1G-C1A-O1A	-2.58	117.08	123.59
23	b	615	CLA	C1-C2-C3	-2.58	121.58	126.04
29	d	406[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
25	D	405	BCR	C24-C23-C22	-2.58	122.34	126.23
23	A	408	CLA	CHB-C4A-NA	2.58	128.08	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	CHB-C1B-NB	-2.58	121.53	124.26
23	d	403[B]	CLA	CHD-C4C-NC	2.58	128.27	124.20
23	c	507	CLA	C4-C3-C5	2.58	119.61	115.27
33	d	408[B]	LHG	O8-C23-C24	2.58	119.99	111.91
23	b	615	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
25	y	101	BCR	C10-C11-C12	-2.57	115.18	123.22
23	C	511	CLA	CHC-C1C-C2C	-2.57	119.58	126.73
23	c	509	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
35	c	518[B]	DGD	O1G-C1A-C2A	2.57	119.98	111.91
25	C	515	BCR	C11-C10-C9	-2.57	123.64	127.31
31	B	631	LMT	C3'-C4'-C5'	-2.57	105.03	110.93
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	c	506	CLA	C1-C2-C3	-2.57	121.60	126.04
23	C	505	CLA	C3B-C4B-NB	2.57	112.90	110.52
23	C	501	CLA	CHC-C1C-C2C	-2.57	119.60	126.73
23	D	403[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	B	612	CLA	C4-C3-C5	2.56	119.58	115.27
23	D	403[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
29	A	414[B]	PL9	C53-C6-C1	2.56	120.23	114.99
35	c	517[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
23	b	606	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
25	H	101	BCR	C10-C11-C12	-2.56	115.23	123.22
25	h	101	BCR	C36-C18-C17	-2.56	119.34	122.92
23	b	616	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
25	T	101	BCR	C7-C8-C9	-2.56	122.37	126.23
24	A	407[B]	PHO	O2A-CGA-CBA	2.56	119.94	111.91
23	b	606	CLA	CMC-C2C-C1C	2.56	128.93	125.04
23	b	610	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
23	d	402[B]	CLA	C2A-C1A-CHA	-2.56	119.39	123.86
24	A	416[B]	PHO	O2D-CGD-O1D	-2.56	118.84	123.84
23	C	502	CLA	O2A-CGA-O1A	-2.56	117.14	123.59
23	a	404[B]	CLA	C4-C3-C5	2.55	119.57	115.27
23	c	512	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
25	c	516	BCR	C21-C20-C19	-2.55	115.25	123.22
23	b	612	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
40	v	201	HEC	C4B-NB-C1B	2.55	107.71	105.07
25	D	405	BCR	C16-C17-C18	-2.55	123.67	127.31
23	C	513	CLA	C4-C3-C5	2.55	119.56	115.27
40	V	201	HEC	C4B-NB-C1B	2.55	107.71	105.07
23	c	505	CLA	CMB-C2B-C1B	2.55	129.25	125.37
23	B	614	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
23	b	612	CLA	CHD-C4C-NC	2.55	128.22	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	420	LMT	O5'-C5'-C6'	2.55	112.77	106.44
23	B	610	CLA	CHD-C4C-NC	2.54	128.21	124.20
23	A	404[B]	CLA	CAA-C2A-C1A	-2.54	103.64	111.97
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	c	514	CLA	CMB-C2B-C1B	2.54	129.24	125.37
23	A	404[B]	CLA	C2A-C1A-CHA	-2.54	119.42	123.86
23	C	503	CLA	CHC-C1C-C2C	-2.54	119.67	126.73
31	B	628	LMT	O1'-C1'-C2'	2.54	112.27	108.30
24	a	414[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
23	b	604	CLA	C6-C5-C3	-2.54	106.80	113.45
35	C	518	DGD	O2G-C1B-C2B	2.54	116.97	111.50
25	A	409	BCR	C15-C14-C13	-2.54	123.69	127.31
23	B	614	CLA	CBC-CAC-C3C	-2.53	105.44	112.43
23	B	606	CLA	C1-C2-C3	-2.53	121.66	126.04
23	c	510	CLA	C1-O2A-CGA	2.53	123.09	116.44
23	C	510	CLA	CBC-CAC-C3C	-2.53	105.45	112.43
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
25	B	619	BCR	C38-C26-C25	-2.53	121.69	124.53
25	T	101	BCR	C3-C4-C5	-2.53	109.56	114.08
23	b	602	CLA	CAA-CBA-CGA	-2.53	105.86	113.25
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	A	405[B]	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
23	B	602	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	C	501	CLA	C4-C3-C5	2.53	119.52	115.27
25	Y	101	BCR	C15-C16-C17	-2.53	118.30	123.47
25	h	101	BCR	C37-C22-C21	-2.53	119.38	122.92
23	C	502	CLA	C4C-C3C-C2C	-2.53	103.22	106.90
33	A	419[B]	LHG	O7-C7-O9	-2.53	117.60	123.70
23	B	609	CLA	O2A-CGA-O1A	-2.53	117.22	123.59
25	B	617	BCR	C7-C8-C9	-2.53	122.42	126.23
23	B	608	CLA	C1-C2-C3	-2.52	121.68	126.04
23	C	501	CLA	C1-C2-C3	-2.52	121.68	126.04
25	A	409	BCR	C33-C5-C6	-2.52	121.69	124.53
23	c	512	CLA	CMB-C2B-C1B	2.52	129.21	125.37
23	a	405[A]	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	d	404	CLA	C3B-C4B-NB	2.52	112.85	110.52
23	A	406[A]	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
23	c	505	CLA	CED-O2D-CGD	2.52	121.63	115.94
23	B	607	CLA	O2A-C1-C2	-2.52	102.02	108.64
23	b	609	CLA	C16-C15-C13	-2.52	107.78	115.92
25	H	101	BCR	C31-C1-C6	-2.52	106.22	110.30
27	b	628	GOL	C3-C2-C1	-2.52	101.92	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	F	102	HEM	C4D-ND-C1D	2.52	107.67	105.07
24	A	407[B]	PHO	O1D-CGD-CBD	-2.51	120.55	124.74
29	a	412[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
23	c	508	CLA	O1D-CGD-CBD	-2.51	119.34	124.48
29	D	406[B]	PL9	C20-C19-C21	2.51	119.50	115.27
23	d	402[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
26	F	103	SQD	O5-C1-O6	2.51	115.92	109.97
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
29	A	414[B]	PL9	C45-C44-C46	2.51	119.49	115.27
23	b	613	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	C	507	CLA	CHD-C4C-NC	2.51	128.16	124.20
25	d	405	BCR	C24-C23-C22	-2.51	122.44	126.23
23	a	405[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	B	612	CLA	CHD-C4C-NC	2.51	128.15	124.20
35	c	519	DGD	O3G-C1D-C2D	-2.51	104.39	108.30
23	C	501	CLA	CMB-C2B-C1B	2.50	129.18	125.37
26	f	102	SQD	O7-S-C6	2.50	109.91	106.94
23	D	403[B]	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
23	C	505	CLA	O2A-CGA-CBA	2.50	119.76	111.91
23	B	603	CLA	C4-C3-C5	2.50	119.48	115.27
23	C	507	CLA	C1-C2-C3	-2.50	121.72	126.04
33	D	407[B]	LHG	O8-C23-O10	-2.50	117.28	123.59
23	B	609	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
23	B	608	CLA	CMB-C2B-C1B	2.50	129.17	125.37
23	c	505	CLA	C2A-C1A-CHA	-2.50	119.49	123.86
29	A	414[B]	PL9	C42-C43-C44	-2.50	121.65	127.66
26	F	103	SQD	O47-C7-O49	-2.50	117.67	123.70
23	a	404[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
26	f	102	SQD	O47-C7-O49	-2.50	117.67	123.70
23	A	408	CLA	C4-C3-C5	2.50	119.47	115.27
23	C	512	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	B	603	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
25	A	409	BCR	C8-C7-C6	-2.49	120.20	127.20
23	C	504	CLA	C4-C3-C5	2.49	119.46	115.27
25	a	408	BCR	C37-C22-C21	-2.49	119.43	122.92
38	F	102	HEM	CHA-C4D-ND	2.49	127.45	124.37
23	b	602	CLA	CMA-C3A-C4A	-2.49	105.08	111.77
23	a	405[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
23	B	606	CLA	CHC-C1C-C2C	-2.49	119.82	126.73
24	A	416[B]	PHO	C4D-CHA-CBD	2.49	109.64	108.52
23	b	612	CLA	C11-C12-C13	-2.49	107.88	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	t	102	BCR	C1-C6-C7	2.49	122.81	115.78
24	a	406[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
23	b	610	CLA	CHC-C1C-C2C	-2.48	119.83	126.73
23	C	507	CLA	C3B-C4B-NB	2.48	112.82	110.52
25	c	516	BCR	C2-C1-C6	2.48	114.30	110.48
23	a	405[B]	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
33	D	408[B]	LHG	O8-C23-O10	-2.48	117.33	123.59
23	a	404[B]	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
23	B	616	CLA	CHC-C1C-C2C	-2.48	119.84	126.73
35	C	516[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05
29	d	406[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
23	c	511	CLA	C4-C3-C2	-2.48	117.32	123.68
25	c	516	BCR	C20-C21-C22	-2.48	123.77	127.31
25	D	405	BCR	C40-C30-C25	-2.48	106.28	110.30
23	a	405[B]	CLA	O2A-CGA-O1A	-2.48	117.34	123.59
23	C	509	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
23	c	506	CLA	O2A-CGA-CBA	2.48	119.68	111.91
23	C	513	CLA	CAA-C2A-C3A	-2.48	106.00	112.78
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
29	d	406[B]	PL9	C27-C28-C29	-2.47	121.70	127.66
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	D	404	CLA	C2A-C1A-CHA	-2.47	119.53	123.86
29	D	406[B]	PL9	C22-C23-C24	-2.47	121.71	127.66
23	C	512	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
26	F	103	SQD	C46-C45-C44	-2.47	105.94	111.79
29	D	406[B]	PL9	C37-C38-C39	-2.47	121.72	127.66
26	b	620	SQD	C1-C2-C3	-2.47	104.85	110.00
23	d	403[B]	CLA	O2A-CGA-O1A	-2.47	117.36	123.59
25	K	102	BCR	C29-C30-C25	2.47	114.28	110.48
23	c	504	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
25	k	101	BCR	C39-C30-C25	-2.47	106.30	110.30
23	b	602	CLA	C11-C10-C8	-2.47	107.95	115.92
23	B	604	CLA	CMC-C2C-C1C	2.47	128.79	125.04
23	B	615	CLA	CED-O2D-CGD	2.47	121.52	115.94
23	A	404[B]	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
23	a	407	CLA	CBC-CAC-C3C	-2.47	105.64	112.43
23	a	404[B]	CLA	O2A-CGA-O1A	-2.46	117.37	123.59
25	Y	101	BCR	C36-C18-C17	-2.46	119.47	122.92
29	d	406[B]	PL9	C7-C3-C4	2.46	118.88	116.88
33	d	407[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
23	b	607	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
23	C	503	CLA	CMC-C2C-C1C	2.46	128.79	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	404	CLA	O2A-CGA-CBA	2.46	119.63	111.91
26	a	409[A]	SQD	O7-S-C6	2.46	109.86	106.94
23	C	502	CLA	CAC-C3C-C4C	2.46	128.00	124.81
26	a	409[B]	SQD	O47-C7-O49	-2.46	117.76	123.70
23	c	514	CLA	C1-C2-C3	-2.46	121.79	126.04
38	F	102	HEM	C4A-NA-C1A	2.46	107.76	105.35
23	a	405[B]	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	d	404	CLA	C1-O2A-CGA	2.46	122.89	116.44
23	C	501	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
25	c	515	BCR	C36-C18-C19	2.46	121.95	118.08
23	C	508	CLA	C4-C3-C5	2.46	119.40	115.27
23	C	502	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
23	A	408	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
23	B	612	CLA	C3B-C4B-NB	2.45	112.79	110.52
35	C	516[B]	DGD	O3G-C3G-C2G	-2.45	104.98	110.90
23	C	510	CLA	CAC-C3C-C4C	2.45	127.99	124.81
23	d	402[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
23	A	406[B]	CLA	CMA-C3A-C2A	-2.45	103.94	113.83
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
23	d	404	CLA	C2A-C1A-CHA	-2.45	119.58	123.86
23	d	403[B]	CLA	CMC-C2C-C1C	2.45	128.77	125.04
23	B	608	CLA	C11-C12-C13	-2.45	108.00	115.92
23	b	613	CLA	CED-O2D-CGD	2.45	121.47	115.94
29	a	412[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	B	615	CLA	CAC-C3C-C4C	2.45	127.98	124.81
23	a	407	CLA	CMB-C2B-C1B	2.45	129.09	125.37
29	A	414[B]	PL9	C35-C34-C36	2.45	119.39	115.27
24	A	407[B]	PHO	C1-C2-C3	-2.45	121.81	126.04
23	c	508	CLA	O2A-CGA-O1A	-2.45	117.42	123.59
23	a	404[B]	CLA	CAC-C3C-C4C	2.45	127.98	124.81
23	c	502	CLA	CMC-C2C-C1C	2.45	128.76	125.04
29	D	406[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
29	a	412[A]	PL9	C20-C19-C21	2.44	119.38	115.27
26	B	620	SQD	C44-O6-C1	-2.44	108.96	113.74
25	H	101	BCR	C36-C18-C17	-2.44	119.50	122.92
29	D	406[B]	PL9	C7-C8-C9	-2.44	122.72	126.79
23	b	605	CLA	C1-C2-C3	-2.44	121.82	126.04
23	B	606	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
25	C	515	BCR	C3-C4-C5	-2.44	109.72	114.08
23	a	407	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
25	B	619	BCR	C29-C30-C25	2.44	114.24	110.48
23	B	607	CLA	CHC-C1C-C2C	-2.44	119.95	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	630	LMT	O5'-C5'-C6'	2.44	112.50	106.44
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
23	B	603	CLA	CMC-C2C-C1C	2.44	128.75	125.04
23	b	607	CLA	C2A-C1A-CHA	-2.44	119.60	123.86
23	c	506	CLA	C4-C3-C5	2.44	119.37	115.27
23	c	511	CLA	CMB-C2B-C1B	2.44	129.08	125.37
25	C	515	BCR	C24-C23-C22	-2.44	122.55	126.23
23	D	403[B]	CLA	CED-O2D-CGD	2.43	121.44	115.94
23	B	604	CLA	O2A-CGA-CBA	2.43	119.54	111.91
25	b	618	BCR	C29-C30-C25	2.43	114.22	110.48
23	d	403[B]	CLA	CMB-C2B-C1B	2.43	129.07	125.37
24	a	406[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
25	d	405	BCR	C37-C22-C23	2.43	121.90	118.08
23	b	608	CLA	C11-C12-C13	-2.43	108.07	115.92
23	B	601	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
23	A	408	CLA	CAC-C3C-C4C	2.43	127.96	124.81
23	C	504	CLA	CAC-C3C-C4C	2.43	127.96	124.81
29	d	406[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
23	C	501	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
23	b	615	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
23	C	505	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
25	A	409	BCR	C16-C17-C18	-2.42	123.86	127.31
25	H	101	BCR	C16-C15-C14	-2.42	118.52	123.47
26	A	412	SQD	O48-C23-O10	-2.42	117.49	123.59
29	D	406[B]	PL9	C45-C44-C46	2.42	119.33	115.27
23	b	602	CLA	C4-C3-C5	2.42	119.33	115.27
23	A	405[B]	CLA	CMA-C3A-C2A	-2.42	104.08	113.83
26	a	409[A]	SQD	O8-S-C6	2.41	109.59	105.74
23	c	507	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
25	D	405	BCR	C15-C14-C13	-2.41	123.86	127.31
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68
25	c	515	BCR	C28-C27-C26	-2.41	109.78	114.08
23	c	509	CLA	C4-C3-C5	2.41	119.32	115.27
23	D	404	CLA	CHD-C4C-NC	2.41	128.00	124.20
23	b	601	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
25	y	101	BCR	C21-C20-C19	-2.40	115.71	123.22
23	B	610	CLA	C1-C2-C3	-2.40	121.89	126.04
23	C	505	CLA	O2A-CGA-O1A	-2.40	117.53	123.59
23	B	604	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
35	c	519	DGD	O2G-C1B-O1B	-2.40	117.90	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	C2A-C1A-CHA	-2.40	119.66	123.86
26	A	410[B]	SQD	O48-C23-O10	-2.40	117.53	123.59
23	c	513	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	C	506	CLA	CHD-C4C-NC	2.40	127.99	124.20
23	b	604	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
35	H	102	DGD	O6E-C5E-C6E	2.40	112.40	106.44
25	b	618	BCR	C37-C22-C23	2.40	121.86	118.08
23	b	602	CLA	CHB-C1B-C2B	-2.40	120.47	127.24
29	D	406[B]	PL9	C36-C37-C38	-2.40	104.00	111.88
23	C	505	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
31	B	631	LMT	O5'-C5'-C4'	2.40	114.81	109.75
23	B	608	CLA	CHD-C4C-NC	2.40	127.98	124.20
23	c	512	CLA	CMA-C3A-C4A	2.39	118.21	111.77
23	b	615	CLA	O2A-CGA-CBA	2.39	119.42	111.91
23	a	407	CLA	CMA-C3A-C2A	-2.39	104.17	113.83
23	a	404[B]	CLA	CHD-C4C-NC	2.39	127.97	124.20
23	c	511	CLA	C11-C10-C8	-2.39	108.19	115.92
25	k	101	BCR	C2-C1-C6	2.39	114.16	110.48
23	c	510	CLA	CMC-C2C-C1C	2.39	128.68	125.04
29	d	406[B]	PL9	C36-C37-C38	-2.39	104.02	111.88
31	A	420	LMT	O5'-C5'-C4'	2.39	114.79	109.75
23	A	405[B]	CLA	O2A-CGA-O1A	-2.39	117.56	123.59
23	c	507	CLA	CMB-C2B-C1B	2.39	129.01	125.37
25	c	516	BCR	C11-C10-C9	-2.39	123.90	127.31
31	B	631	LMT	O1'-C1'-C2'	2.39	112.03	108.30
23	c	514	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	D	406[B]	PL9	C32-C33-C34	-2.39	121.92	127.66
23	c	513	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	C	512	CLA	CHC-C1C-C2C	-2.38	120.11	126.73
23	B	608	CLA	O2A-CGA-CBA	2.38	119.38	111.91
23	B	602	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	b	608	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
26	b	620	SQD	O48-C23-C24	2.38	119.38	111.91
23	c	505	CLA	CHB-C1B-NB	-2.38	121.74	124.26
33	L	101[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
23	b	614	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
23	A	404[B]	CLA	CHD-C4C-NC	2.38	127.95	124.20
29	a	412[A]	PL9	C10-C9-C8	-2.38	117.58	123.68
29	d	406[A]	PL9	C7-C8-C9	-2.38	122.84	126.79
23	a	405[B]	CLA	O2A-CGA-CBA	2.38	119.36	111.91
23	c	502	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
29	D	406[A]	PL9	C45-C44-C46	2.38	119.27	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	CBC-CAC-C3C	-2.38	105.88	112.43
23	C	505	CLA	CHA-C1A-NA	-2.37	120.96	126.40
23	b	601	CLA	C3B-C4B-NB	2.37	112.72	110.52
23	C	507	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
23	B	615	CLA	CHC-C1C-C2C	-2.37	120.14	126.73
23	c	513	CLA	C3B-C4B-NB	2.37	112.72	110.52
23	c	512	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
40	v	201	HEC	CBD-CAD-C3D	-2.37	106.03	112.63
23	b	605	CLA	CMC-C2C-C1C	2.37	128.65	125.04
23	C	513	CLA	CMB-C2B-C1B	2.37	128.98	125.37
23	B	613	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
33	D	407[B]	LHG	O8-C23-C24	2.37	119.35	111.91
23	B	601	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	a	406[B]	PHO	CMB-C2B-C3B	2.37	129.11	124.68
23	C	506	CLA	CGD-CBD-CAD	-2.37	103.06	110.73
35	C	518	DGD	O3G-C3G-C2G	-2.37	105.18	110.90
33	L	101[B]	LHG	O8-C23-C24	2.37	119.34	111.91
23	b	614	CLA	CAC-C3C-C4C	2.37	127.88	124.81
25	d	405	BCR	C21-C20-C19	-2.37	115.83	123.22
23	B	606	CLA	C3B-C4B-NB	2.37	112.71	110.52
23	B	613	CLA	CHB-C4A-NA	2.37	127.78	124.51
25	t	102	BCR	C21-C20-C19	-2.36	115.84	123.22
35	H	102	DGD	C1E-O6E-C5E	-2.36	109.05	113.69
23	c	512	CLA	C1-C2-C3	-2.36	121.96	126.04
29	D	406[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
25	Y	101	BCR	C36-C18-C19	2.36	121.79	118.08
23	A	406[B]	CLA	C1-C2-C3	-2.36	121.96	126.04
31	B	628	LMT	C1B-C2B-C3B	2.36	114.91	110.00
23	c	510	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
25	C	515	BCR	C32-C1-C6	-2.36	106.48	110.30
23	c	507	CLA	CAA-C2A-C3A	-2.36	106.33	112.78
23	b	608	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
23	C	512	CLA	CBA-CAA-C2A	-2.36	106.91	113.86
24	A	416[B]	PHO	CMB-C2B-C3B	2.35	129.08	124.68
35	c	517[B]	DGD	O3G-C3G-C2G	-2.35	105.22	110.90
23	B	609	CLA	C1-C2-C3	-2.35	121.97	126.04
24	A	416[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
23	B	611	CLA	C4D-CHA-C1A	-2.35	118.39	121.25
31	m	103	LMT	C3B-C4B-C5B	-2.35	106.05	110.24
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
35	C	517[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44
29	a	412[A]	PL9	C45-C44-C46	2.35	119.22	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	CMA-C3A-C4A	-2.35	105.46	111.77
26	a	410	SQD	O5-C5-C4	2.35	113.96	109.69
23	d	402[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	C	509	CLA	CHB-C1B-NB	-2.35	121.77	124.26
23	C	510	CLA	CMD-C2D-C3D	-2.34	122.22	127.61
23	b	609	CLA	O2A-CGA-CBA	2.34	119.26	111.91
25	h	101	BCR	C24-C23-C22	-2.34	122.69	126.23
23	B	614	CLA	CMB-C2B-C1B	2.34	128.94	125.37
23	C	506	CLA	C4C-C3C-C2C	-2.34	103.48	106.90
26	F	103	SQD	O8-S-O7	-2.34	105.56	111.27
26	b	620	SQD	C44-O6-C1	-2.34	109.17	113.74
29	a	412[B]	PL9	C45-C44-C46	2.34	119.20	115.27
23	B	616	CLA	CHD-C4C-NC	2.34	127.89	124.20
29	d	406[B]	PL9	C45-C44-C46	2.34	119.20	115.27
23	d	403[B]	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
23	B	603	CLA	CMA-C3A-C2A	-2.33	104.41	113.83
35	C	517[B]	DGD	C2G-O2G-C1B	-2.33	112.05	117.79
34	B	622	HTG	C1-O5-C5	2.33	116.88	112.58
23	C	501	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
23	B	613	CLA	C4-C3-C2	-2.33	117.70	123.68
23	C	509	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	D	403[A]	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	d	402[A]	CLA	C1-O2A-CGA	2.33	122.56	116.44
23	c	505	CLA	CHD-C4C-NC	2.33	127.88	124.20
23	c	507	CLA	O2A-CGA-CBA	2.33	119.22	111.91
25	K	102	BCR	C37-C22-C21	-2.33	119.66	122.92
29	a	412[A]	PL9	C35-C34-C33	-2.33	117.70	123.68
29	d	406[B]	PL9	C53-C6-C1	2.33	119.75	114.99
35	C	517[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
23	d	402[B]	CLA	C1-O2A-CGA	2.33	122.55	116.44
35	c	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
25	B	617	BCR	C31-C1-C6	-2.33	106.53	110.30
23	b	616	CLA	CMC-C2C-C1C	2.33	128.58	125.04
23	B	602	CLA	CMB-C2B-C1B	2.33	128.91	125.37
33	d	407[A]	LHG	O8-C23-C24	2.33	119.21	111.91
40	V	201	HEC	CBA-CAA-C2A	-2.33	106.17	112.63
23	c	508	CLA	CBC-CAC-C3C	-2.32	106.02	112.43
29	a	412[B]	PL9	C47-C48-C49	-2.32	119.81	127.75
25	T	101	BCR	C21-C20-C19	-2.32	115.97	123.22
26	a	410	SQD	O48-C23-O10	-2.32	117.73	123.59
23	d	402[B]	CLA	CMA-C3A-C2A	-2.32	104.46	113.83
23	c	505	CLA	O2A-CGA-CBA	2.32	119.20	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	517[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
23	B	615	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	B	601	CLA	CMC-C2C-C1C	2.32	128.57	125.04
23	B	605	CLA	CED-O2D-CGD	2.32	121.18	115.94
23	a	405[A]	CLA	C4-C3-C5	2.32	119.17	115.27
26	f	102	SQD	O8-S-C6	2.32	109.44	105.74
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
24	A	416[B]	PHO	O2A-CGA-CBA	2.32	119.18	111.91
23	b	606	CLA	O2A-CGA-CBA	2.32	119.18	111.91
26	a	409[A]	SQD	O48-C23-C24	2.32	119.17	111.91
23	B	609	CLA	CAC-C3C-C4C	2.32	127.81	124.81
23	b	611	CLA	CMB-C2B-C1B	2.31	128.89	125.37
23	C	513	CLA	CHB-C1B-NB	-2.31	121.81	124.26
23	C	508	CLA	CHD-C4C-NC	2.31	127.85	124.20
23	A	408	CLA	CMA-C3A-C2A	-2.31	104.50	113.83
23	C	511	CLA	O2A-CGA-CBA	2.31	119.17	111.91
25	H	101	BCR	C24-C23-C22	-2.31	122.74	126.23
23	c	504	CLA	O2A-CGA-CBA	2.31	119.16	111.91
29	d	406[B]	PL9	C47-C48-C49	-2.31	119.85	127.75
23	a	405[B]	CLA	CAC-C3C-C4C	2.31	127.81	124.81
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
29	A	414[B]	PL9	C37-C36-C34	-2.31	105.38	112.98
26	A	410[B]	SQD	O8-S-C6	2.31	109.42	105.74
23	C	505	CLA	CHD-C4C-NC	2.31	127.84	124.20
23	B	605	CLA	C3B-C4B-NB	2.31	112.66	110.52
23	c	510	CLA	C4-C3-C2	-2.31	117.76	123.68
32	C	520	LMG	C9-C8-C7	-2.31	106.33	111.79
32	m	101	LMG	C3-C4-C5	2.30	114.35	110.24
31	A	420	LMT	O1'-C1'-C2'	2.30	111.90	108.30
23	b	603	CLA	C7-C6-C5	-2.30	107.10	113.36
23	d	403[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
31	M	102	LMT	C3'-C4'-C5'	-2.30	105.65	110.93
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
23	C	502	CLA	C1-C2-C3	-2.30	122.06	126.04
29	d	406[B]	PL9	C22-C23-C24	-2.30	122.12	127.66
23	c	502	CLA	O2A-CGA-CBA	2.30	119.13	111.91
26	a	409[B]	SQD	C3-C4-C5	2.30	114.34	110.24
23	c	502	CLA	O2A-CGA-O1A	-2.30	117.79	123.59
35	c	518[B]	DGD	C2G-O2G-C1B	-2.30	112.13	117.79
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
23	d	404	CLA	CMC-C2C-C1C	2.30	128.54	125.04
25	d	405	BCR	C39-C30-C25	-2.30	106.57	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	CHB-C1B-NB	-2.30	121.83	124.26
23	b	604	CLA	O2A-CGA-CBA	2.30	119.11	111.91
23	A	408	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	B	619	BCR	C7-C8-C9	-2.29	122.77	126.23
23	b	601	CLA	O2A-CGA-CBA	2.29	119.10	111.91
25	B	617	BCR	C16-C17-C18	-2.29	124.04	127.31
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
23	b	608	CLA	C4C-C3C-C2C	-2.29	103.56	106.90
24	a	414[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
24	A	407[B]	PHO	CMB-C2B-C3B	2.29	128.96	124.68
33	d	408[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
23	A	404[B]	CLA	C1-C2-C3	-2.29	122.09	126.04
23	a	405[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	C	501	CLA	O2A-CGA-CBA	2.29	119.08	111.91
35	H	102	DGD	C3E-C4E-C5E	-2.29	106.16	110.24
32	c	521	LMG	O8-C28-O10	-2.29	117.82	123.59
23	C	503	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
25	K	102	BCR	C2-C1-C6	2.28	114.00	110.48
25	T	101	BCR	C35-C13-C12	2.28	121.67	118.08
23	C	509	CLA	CMB-C2B-C1B	2.28	128.85	125.37
25	B	617	BCR	C15-C14-C13	-2.28	124.05	127.31
23	b	606	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
25	Y	101	BCR	C28-C27-C26	-2.28	110.00	114.08
23	c	513	CLA	CBA-CAA-C2A	-2.28	107.13	113.86
23	B	614	CLA	CMA-C3A-C2A	-2.28	104.63	113.83
23	C	503	CLA	C2A-C1A-CHA	-2.28	119.87	123.86
23	A	404[B]	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
23	C	510	CLA	C4-C3-C2	-2.28	117.83	123.68
23	b	616	CLA	C4-C3-C5	2.28	119.10	115.27
38	F	102	HEM	O2A-CGA-CBA	2.28	121.35	114.03
34	b	622	HTG	C6-C5-C4	-2.28	107.67	113.00
23	b	609	CLA	C7-C6-C5	-2.28	107.18	113.36
23	B	613	CLA	CMC-C2C-C1C	2.27	128.50	125.04
23	c	508	CLA	C4C-C3C-C2C	-2.27	103.58	106.90
23	a	404[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	B	610	CLA	CMA-C3A-C2A	-2.27	104.67	113.83
29	d	406[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
31	t	101	LMT	C1-O1'-C1'	2.27	117.60	113.84
23	C	508	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
23	c	503	CLA	C2A-C1A-CHA	-2.27	119.89	123.86
23	A	406[B]	CLA	CMC-C2C-C1C	2.27	128.49	125.04
24	A	416[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	C2A-C1A-CHA	-2.27	119.90	123.86
23	A	408	CLA	C11-C12-C13	-2.27	108.60	115.92
23	c	504	CLA	O2A-CGA-O1A	-2.27	117.88	123.59
26	b	620	SQD	O47-C7-O49	-2.26	118.23	123.70
29	A	414[B]	PL9	C10-C9-C8	-2.26	117.87	123.68
23	B	604	CLA	C11-C12-C13	-2.26	108.60	115.92
23	c	503	CLA	C1-C2-C3	-2.26	122.13	126.04
23	C	506	CLA	CMB-C2B-C1B	2.26	128.81	125.37
33	d	414[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
25	k	101	BCR	C10-C11-C12	-2.26	116.16	123.22
23	b	605	CLA	O2A-CGA-CBA	2.26	119.00	111.91
23	D	403[A]	CLA	C4-C3-C5	2.26	119.07	115.27
23	b	604	CLA	CHD-C4C-NC	2.26	127.77	124.20
33	d	407[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
23	c	508	CLA	CAC-C3C-C4C	2.26	127.74	124.81
23	C	504	CLA	CHD-C4C-NC	2.26	127.76	124.20
26	a	409[B]	SQD	O48-C23-C24	2.26	119.00	111.91
23	C	501	CLA	OBD-CAD-C3D	-2.26	123.09	128.52
23	B	607	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
33	b	629[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
24	a	414[A]	PHO	C4-C3-C2	-2.26	117.89	123.68
25	t	102	BCR	C36-C18-C19	2.26	121.63	118.08
29	A	414[B]	PL9	C12-C13-C14	-2.26	122.23	127.66
23	d	403[B]	CLA	CBC-CAC-C3C	-2.25	106.22	112.43
23	c	511	CLA	CAC-C3C-C4C	2.25	127.73	124.81
25	c	515	BCR	C33-C5-C6	-2.25	122.00	124.53
23	d	403[B]	CLA	CAC-C3C-C4C	2.25	127.73	124.81
23	c	505	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
23	C	510	CLA	C4C-C3C-C2C	-2.25	103.61	106.90
23	C	503	CLA	O2A-CGA-CBA	2.25	118.97	111.91
23	C	508	CLA	O2A-CGA-CBA	2.25	118.97	111.91
25	c	515	BCR	C38-C26-C25	-2.25	122.00	124.53
29	D	406[A]	PL9	C20-C19-C21	2.25	119.05	115.27
23	c	514	CLA	CHB-C1B-NB	-2.25	121.88	124.26
23	c	511	CLA	C2A-C1A-CHA	-2.25	119.93	123.86
24	A	416[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68
25	D	405	BCR	C11-C10-C9	-2.25	124.10	127.31
23	c	513	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
23	c	503	CLA	C4C-C3C-C2C	-2.25	103.62	106.90
23	b	602	CLA	CHC-C1C-C2C	-2.24	120.50	126.73
25	Y	101	BCR	C37-C22-C23	2.24	121.61	118.08
25	b	618	BCR	C8-C7-C6	-2.24	120.91	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	414[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
35	h	102	DGD	O3G-C1D-C2D	2.24	111.80	108.30
25	D	405	BCR	C15-C16-C17	-2.24	118.89	123.47
25	b	619	BCR	C16-C15-C14	-2.24	118.89	123.47
23	b	615	CLA	CMC-C2C-C1C	2.24	128.45	125.04
35	h	102	DGD	C6D-C5D-C4D	2.24	116.77	112.09
23	C	510	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	C	503	CLA	CAC-C3C-C4C	2.24	127.71	124.81
25	d	405	BCR	C40-C30-C39	2.24	115.39	108.53
25	b	619	BCR	C15-C14-C13	-2.24	124.12	127.31
24	A	416[B]	PHO	O1D-CGD-CBD	-2.23	121.02	124.74
23	c	512	CLA	CHB-C1B-NB	-2.23	121.89	124.26
26	b	620	SQD	O9-S-C6	2.23	109.59	106.94
29	d	406[B]	PL9	C17-C18-C19	-2.23	122.28	127.66
23	B	603	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
23	b	606	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
25	y	101	BCR	C1-C6-C7	2.23	122.10	115.78
29	D	406[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
34	B	625	HTG	C3-C4-C5	2.23	114.22	110.24
23	c	512	CLA	C1-O2A-CGA	2.23	122.30	116.44
25	Y	101	BCR	C38-C26-C25	-2.23	122.02	124.53
23	B	612	CLA	CHC-C1C-C2C	-2.23	120.54	126.73
25	A	409	BCR	C11-C10-C9	-2.23	124.13	127.31
25	d	405	BCR	C11-C10-C9	-2.23	124.13	127.31
25	d	405	BCR	C33-C5-C6	-2.23	122.03	124.53
23	c	502	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
23	c	512	CLA	C2A-C1A-CHA	-2.23	119.97	123.86
38	F	102	HEM	O2D-CGD-CBD	2.22	121.18	114.03
23	a	404[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
26	A	410[A]	SQD	O8-S-C6	2.22	109.28	105.74
23	c	502	CLA	C4-C3-C5	2.22	119.01	115.27
23	C	505	CLA	CBC-CAC-C3C	-2.22	106.31	112.43
23	D	404	CLA	CMA-C3A-C4A	-2.22	105.81	111.77
26	f	102	SQD	O48-C23-O10	-2.22	117.99	123.59
23	d	402[B]	CLA	O2A-CGA-CBA	2.22	118.87	111.91
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
35	C	516[B]	DGD	O5D-C6D-C5D	-2.22	104.94	109.05
23	C	509	CLA	C11-C12-C13	-2.22	108.75	115.92
23	C	509	CLA	C4-C3-C5	2.22	119.00	115.27
35	C	516[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
23	b	601	CLA	CHB-C1B-C2B	-2.22	120.98	127.24
23	d	402[B]	CLA	CHB-C1B-NB	-2.22	121.91	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	518[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
25	t	102	BCR	C35-C13-C12	2.22	121.57	118.08
25	A	409	BCR	C40-C30-C25	-2.21	106.71	110.30
23	c	514	CLA	C1-O2A-CGA	2.21	122.24	116.44
23	C	512	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
25	t	102	BCR	C7-C6-C5	-2.21	116.11	121.46
35	C	517[B]	DGD	O1G-C1A-C2A	2.21	118.84	111.91
25	B	618	BCR	C38-C26-C25	-2.21	122.05	124.53
23	b	602	CLA	C7-C6-C5	-2.21	107.37	113.36
23	b	605	CLA	C1-O2A-CGA	2.21	122.23	116.44
34	B	622	HTG	C2'-C1'-S1	-2.21	105.27	112.40
23	d	402[B]	CLA	CHB-C4A-NA	2.20	127.56	124.51
23	c	514	CLA	C4-C3-C5	2.20	118.98	115.27
23	C	512	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
23	b	614	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
24	a	414[B]	PHO	C4-C3-C2	-2.20	118.03	123.68
23	c	505	CLA	CMC-C2C-C1C	2.20	128.39	125.04
23	b	602	CLA	O2A-CGA-CBA	2.20	118.82	111.91
23	b	608	CLA	O2A-CGA-CBA	2.20	118.81	111.91
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
29	A	414[B]	PL9	C47-C48-C49	-2.20	120.23	127.75
25	b	618	BCR	C35-C13-C14	-2.20	119.84	122.92
25	k	101	BCR	C36-C18-C19	2.20	121.54	118.08
23	b	603	CLA	CMC-C2C-C1C	2.20	128.39	125.04
23	A	406[B]	CLA	CAC-C3C-C4C	2.20	127.66	124.81
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
24	A	416[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
23	B	614	CLA	OBD-CAD-C3D	-2.20	123.24	128.52
29	d	406[B]	PL9	C35-C34-C36	2.19	118.96	115.27
24	A	407[B]	PHO	O2A-CGA-O1A	-2.19	118.06	123.59
31	m	103	LMT	C1'-O5'-C5'	-2.19	109.39	113.69
23	b	603	CLA	CMB-C2B-C1B	2.19	128.71	125.37
25	k	101	BCR	C24-C23-C22	-2.19	122.92	126.23
29	a	412[B]	PL9	C51-C49-C50	2.19	119.44	114.60
23	b	616	CLA	C2A-C1A-CHA	-2.19	120.03	123.86
32	c	520	LMG	O6-C5-C4	2.19	113.67	109.69
24	a	406[B]	PHO	C1-C2-C3	-2.19	122.26	126.04
29	A	414[B]	PL9	C35-C34-C33	-2.19	118.07	123.68
25	B	618	BCR	C16-C17-C18	-2.19	124.19	127.31
23	D	403[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
25	T	101	BCR	C1-C6-C7	2.18	121.96	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	OBD-CAD-C3D	-2.18	123.26	128.52
26	a	409[A]	SQD	O9-S-O7	-2.18	106.39	113.95
23	c	514	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	b	605	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	b	613	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	a	405[B]	CLA	CBC-CAC-C3C	-2.18	106.41	112.43
23	B	611	CLA	C4-C3-C5	2.18	118.94	115.27
23	c	504	CLA	OBD-CAD-C3D	-2.18	123.27	128.52
24	a	414[B]	PHO	C7-C6-C5	-2.18	107.44	113.36
29	d	406[A]	PL9	C51-C49-C50	2.18	119.42	114.60
23	C	511	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	a	407	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
23	d	403[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	b	607	CLA	CMB-C2B-C1B	2.18	128.68	125.37
40	v	201	HEC	C4A-NA-C1A	2.18	107.48	105.35
35	c	518[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
31	B	630	LMT	O5'-C5'-C4'	2.18	114.34	109.75
23	b	603	CLA	C5-C3-C2	-2.17	116.72	121.12
25	d	405	BCR	C38-C26-C27	2.17	117.79	113.62
32	d	412	LMG	O8-C28-C29	2.17	118.73	111.91
23	c	503	CLA	O2A-CGA-O1A	-2.17	118.11	123.59
23	B	611	CLA	OBD-CAD-C3D	-2.17	123.29	128.52
32	d	412	LMG	O8-C28-O10	-2.17	118.11	123.59
25	t	102	BCR	C29-C28-C27	-2.17	106.52	111.38
23	c	505	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	d	405	BCR	C3-C4-C5	-2.17	110.20	114.08
23	C	512	CLA	CHB-C1B-C2B	-2.17	121.11	127.24
26	a	410	SQD	O8-S-C6	2.17	109.20	105.74
24	a	406[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
23	c	511	CLA	CED-O2D-CGD	2.17	120.84	115.94
23	B	610	CLA	CMA-C3A-C4A	-2.17	105.95	111.77
23	C	505	CLA	CHB-C1B-NB	-2.17	121.96	124.26
25	D	405	BCR	C30-C25-C24	2.17	121.91	115.78
33	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24
23	c	510	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	C	502	CLA	C4-C3-C5	2.17	118.92	115.27
23	B	606	CLA	CHB-C1B-C2B	-2.17	121.12	127.24
25	K	102	BCR	C32-C1-C6	-2.16	106.79	110.30
25	y	101	BCR	C34-C9-C10	-2.16	119.89	122.92
23	B	610	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
25	b	618	BCR	C33-C5-C6	-2.16	122.10	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	CAC-C3C-C4C	2.16	127.61	124.81
25	C	515	BCR	C39-C30-C25	-2.16	106.80	110.30
23	C	507	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
23	b	606	CLA	C1-O2A-CGA	2.16	122.11	116.44
23	b	611	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
25	h	101	BCR	C16-C15-C14	-2.16	119.05	123.47
25	y	101	BCR	C34-C9-C8	2.16	121.48	118.08
29	A	414[B]	PL9	C51-C49-C50	2.16	119.37	114.60
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	B	602	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	b	602	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
23	b	601	CLA	CMC-C2C-C1C	2.16	128.32	125.04
23	A	404[B]	CLA	CMA-C3A-C2A	-2.16	105.13	113.83
24	A	407[B]	PHO	O2D-CGD-O1D	-2.15	119.63	123.84
25	c	515	BCR	C37-C22-C23	2.15	121.47	118.08
33	E	101[B]	LHG	O7-C7-O9	-2.15	118.50	123.70
23	B	611	CLA	CMB-C2B-C3B	2.15	131.80	126.59
23	b	606	CLA	C1-C2-C3	-2.15	122.32	126.04
23	a	405[B]	CLA	C3B-C4B-NB	2.15	112.51	110.52
26	A	412	SQD	C1-C2-C3	-2.15	105.51	110.00
25	C	515	BCR	C15-C16-C17	-2.15	119.07	123.47
29	A	414[B]	PL9	C25-C24-C26	2.15	118.89	115.27
23	a	405[B]	CLA	CHB-C1B-C2B	-2.15	121.17	127.24
23	A	408	CLA	C2A-C1A-CHA	-2.15	120.10	123.86
35	C	517[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
27	B	624	GOL	C3-C2-C1	-2.15	103.35	111.70
23	B	613	CLA	CHD-C4C-NC	2.15	127.59	124.20
25	c	516	BCR	C28-C27-C26	-2.15	110.24	114.08
35	c	517[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
23	D	404	CLA	CMA-C3A-C2A	-2.15	105.17	113.83
29	d	406[A]	PL9	C35-C34-C36	2.15	118.88	115.27
23	C	512	CLA	O2D-CGD-O1D	-2.14	119.64	123.84
23	A	405[B]	CLA	C4C-C3C-C2C	-2.14	103.77	106.90
23	b	608	CLA	CMB-C2B-C3B	2.14	131.78	126.59
23	a	404[B]	CLA	CMA-C3A-C2A	-2.14	105.19	113.83
26	A	412	SQD	O6-C44-C45	-2.14	105.73	110.90
25	D	405	BCR	C37-C22-C21	-2.14	119.92	122.92
24	A	407[B]	PHO	CBA-CAA-C2A	-2.14	107.55	113.81
23	B	608	CLA	CAA-C2A-C3A	-2.14	106.92	112.78
23	c	503	CLA	C1-O2A-CGA	2.14	122.06	116.44
25	k	101	BCR	C3-C4-C5	-2.14	110.25	114.08
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	101	BCR	C36-C18-C19	2.14	121.45	118.08
25	T	101	BCR	C7-C6-C5	-2.14	116.28	121.46
23	A	408	CLA	CHB-C1B-NB	-2.14	122.00	124.26
23	b	606	CLA	CHB-C1B-C2B	-2.14	121.20	127.24
23	c	506	CLA	CHD-C4C-NC	2.14	127.57	124.20
23	C	504	CLA	CAA-C2A-C3A	-2.14	106.93	112.78
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
34	B	625	HTG	O5-C5-C4	2.13	113.57	109.69
23	B	605	CLA	CAC-C3C-C4C	2.13	127.58	124.81
23	B	616	CLA	CMC-C2C-C1C	2.13	128.29	125.04
23	B	611	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	b	610	CLA	C4-C3-C2	-2.13	118.21	123.68
23	b	603	CLA	CAC-C3C-C4C	2.13	127.58	124.81
35	C	517[B]	DGD	O1G-C1A-O1A	-2.13	118.21	123.59
23	C	503	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
31	b	621	LMT	C2'-C3'-C4'	2.13	114.54	109.68
32	A	418	LMG	C12-C11-C10	-2.13	105.88	113.62
33	b	629[B]	LHG	O8-C23-O10	-2.13	118.22	123.59
23	b	609	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
27	O	303	GOL	C3-C2-C1	-2.13	103.44	111.70
35	C	516[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
23	B	606	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
23	b	613	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
35	c	518[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
25	b	619	BCR	C21-C20-C19	-2.13	116.58	123.22
23	b	609	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
23	B	604	CLA	C4-C3-C5	2.12	118.84	115.27
33	d	414[B]	LHG	O7-C7-O9	-2.12	118.57	123.70
24	a	414[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
23	C	503	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
32	Z	101	LMG	C1-O6-C5	2.12	117.85	113.69
35	C	516[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
25	B	617	BCR	C11-C10-C9	-2.12	124.28	127.31
23	b	615	CLA	CHA-C1A-NA	-2.12	121.54	126.40
25	c	515	BCR	C29-C30-C25	2.12	113.74	110.48
25	t	102	BCR	C33-C5-C4	2.12	117.69	113.62
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
26	F	103	SQD	O9-S-C6	-2.12	104.42	106.94
24	a	414[B]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
32	d	412	LMG	O7-C10-O9	-2.12	118.59	123.70
23	D	403[B]	CLA	CHD-C4C-NC	2.12	127.54	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	c	515	BCR	C31-C1-C6	-2.11	106.87	110.30
25	K	102	BCR	C3-C4-C5	-2.11	110.30	114.08
23	b	604	CLA	C4-C3-C2	-2.11	118.26	123.68
32	c	520	LMG	C8-O7-C10	-2.11	112.59	117.79
24	a	414[B]	PHO	O1D-CGD-CBD	-2.11	121.22	124.74
23	C	511	CLA	CHB-C1B-NB	-2.11	122.02	124.26
23	A	405[B]	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	B	619	BCR	C2-C1-C6	2.11	113.73	110.48
23	B	613	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
32	A	418	LMG	O8-C28-C29	2.11	118.53	111.91
23	C	512	CLA	C3B-C4B-NB	2.11	112.47	110.52
23	B	615	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
23	B	615	CLA	CHA-C1A-NA	-2.11	121.57	126.40
35	c	518[B]	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
25	b	617	BCR	C21-C20-C19	-2.11	116.64	123.22
23	b	615	CLA	C11-C12-C13	-2.11	109.10	115.92
23	b	614	CLA	CED-O2D-CGD	2.11	120.71	115.94
23	d	404	CLA	CAC-C3C-C4C	2.11	127.55	124.81
26	F	103	SQD	O48-C23-O10	-2.11	118.28	123.59
31	b	621	LMT	C1-O1'-C1'	2.11	117.33	113.84
29	a	412[B]	PL9	C35-C34-C33	-2.11	118.28	123.68
24	A	416[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
23	C	508	CLA	CAA-C2A-C3A	-2.10	107.02	112.78
23	b	607	CLA	CMC-C2C-C1C	2.10	128.24	125.04
23	A	408	CLA	C1-O2A-CGA	2.10	121.96	116.44
25	k	101	BCR	C15-C14-C13	-2.10	124.31	127.31
29	d	406[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
25	b	617	BCR	C24-C23-C22	-2.10	123.06	126.23
38	F	102	HEM	CHA-C1A-NA	2.10	127.71	123.85
31	B	628	LMT	O1B-C4'-C5'	-2.10	103.69	109.45
23	B	605	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
33	b	629[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
23	B	606	CLA	CMB-C2B-C1B	2.10	128.56	125.37
23	b	615	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
23	B	616	CLA	C2A-C1A-CHA	-2.10	120.19	123.86
25	h	101	BCR	C20-C21-C22	-2.10	124.32	127.31
23	b	605	CLA	CED-O2D-CGD	2.10	120.68	115.94
23	b	610	CLA	CAC-C3C-C4C	2.09	127.53	124.81
33	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
23	B	603	CLA	C7-C6-C5	-2.09	107.67	113.36
25	c	516	BCR	C15-C16-C17	-2.09	119.19	123.47
23	D	403[A]	CLA	CMB-C2B-C1B	2.09	128.56	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	615	CLA	C6-C7-C8	-2.09	109.16	115.92
32	c	501	LMG	O6-C5-C4	2.09	113.49	109.69
23	c	506	CLA	CHB-C1B-NB	-2.09	122.04	124.26
23	b	607	CLA	CAC-C3C-C4C	2.09	127.52	124.81
32	D	412	LMG	C7-O1-C1	-2.09	109.66	113.74
23	b	601	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
26	B	620	SQD	O47-C7-O49	-2.09	118.65	123.70
40	V	201	HEC	CHA-C1A-NA	2.09	126.70	124.44
25	K	102	BCR	C33-C5-C6	-2.09	122.18	124.53
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36
23	c	510	CLA	CHB-C1B-NB	-2.09	122.05	124.26
23	c	511	CLA	CMA-C3A-C4A	-2.09	106.17	111.77
23	C	510	CLA	CHB-C1B-NB	-2.08	122.05	124.26
23	B	605	CLA	O2A-CGA-CBA	2.08	118.45	111.91
23	d	403[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
23	A	405[B]	CLA	O2A-CGA-CBA	2.08	118.44	111.91
25	B	617	BCR	C34-C9-C8	2.08	121.36	118.08
31	F	101	LMT	O1'-C1'-C2'	2.08	111.55	108.30
25	T	101	BCR	C39-C30-C25	-2.08	106.93	110.30
23	B	610	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
38	f	101	HEM	CHA-C4D-C3D	-2.08	121.43	125.33
23	c	513	CLA	C2A-C1A-CHA	-2.08	120.23	123.86
23	b	602	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
23	d	404	CLA	C6-C7-C8	-2.08	109.21	115.92
23	B	607	CLA	C11-C10-C8	-2.08	109.21	115.92
32	B	621	LMG	O8-C28-O10	-2.08	118.35	123.59
29	d	406[B]	PL9	C51-C49-C50	2.08	119.19	114.60
23	b	609	CLA	CMB-C2B-C1B	2.08	128.53	125.37
24	a	406[B]	PHO	CBA-CAA-C2A	-2.08	107.75	113.81
35	C	517[B]	DGD	O2G-C1B-O1B	-2.07	118.69	123.70
27	D	402	GOL	C3-C2-C1	-2.07	103.64	111.70
25	B	619	BCR	C3-C4-C5	-2.07	110.37	114.08
35	c	517[B]	DGD	C2G-O2G-C1B	-2.07	112.68	117.79
25	y	101	BCR	C37-C22-C23	2.07	121.34	118.08
23	B	609	CLA	C2A-C1A-CHA	-2.07	120.23	123.86
26	b	620	SQD	O5-C1-C2	-2.07	105.96	110.35
29	d	406[B]	PL9	C12-C13-C14	-2.07	122.67	127.66
23	b	608	CLA	CAA-C2A-C3A	-2.07	107.10	112.78
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	406[A]	PL9	C12-C13-C14	-2.07	122.68	127.66
23	b	608	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
23	b	616	CLA	O1D-CGD-CBD	-2.07	120.25	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	c	517[B]	DGD	O6D-C1D-O3G	-2.07	105.08	109.97
23	B	609	CLA	C16-C15-C13	-2.07	109.24	115.92
29	d	406[B]	PL9	C20-C19-C21	2.07	118.75	115.27
29	D	406[A]	PL9	C30-C29-C31	2.07	118.75	115.27
29	a	412[A]	PL9	C51-C49-C50	2.07	119.17	114.60
23	b	601	CLA	CAC-C3C-C4C	2.07	127.49	124.81
29	D	406[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
23	C	512	CLA	C4-C3-C2	-2.06	118.38	123.68
23	B	607	CLA	O2A-CGA-CBA	2.06	118.38	111.91
23	B	608	CLA	C4-C3-C5	2.06	118.74	115.27
29	a	412[B]	PL9	C10-C9-C8	-2.06	118.39	123.68
25	c	515	BCR	C34-C9-C10	-2.06	120.04	122.92
23	b	607	CLA	C1-O2A-CGA	2.06	121.85	116.44
23	B	608	CLA	CMA-C3A-C2A	-2.06	105.52	113.83
25	a	408	BCR	C8-C7-C6	-2.06	121.42	127.20
23	b	603	CLA	CHB-C1B-C2B	-2.06	121.42	127.24
23	b	608	CLA	CMA-C3A-C4A	-2.06	106.24	111.77
31	B	630	LMT	O5B-C5B-C6B	2.06	111.56	106.44
34	B	622	HTG	O2-C2-C3	-2.06	105.59	110.35
32	z	101	LMG	C7-O1-C1	-2.06	109.72	113.74
35	C	516[B]	DGD	O1G-C1A-C2A	2.06	118.36	111.91
24	A	407[B]	PHO	CMA-C3A-C4A	-2.06	109.87	114.38
25	c	516	BCR	C16-C17-C18	-2.06	124.38	127.31
23	b	605	CLA	CHB-C4A-NA	2.06	127.35	124.51
23	c	513	CLA	OBD-CAD-C3D	-2.05	123.58	128.52
25	B	619	BCR	C34-C9-C8	2.05	121.31	118.08
25	y	101	BCR	C40-C30-C25	-2.05	106.97	110.30
23	A	406[B]	CLA	CHB-C1B-C2B	-2.05	121.44	127.24
23	b	608	CLA	C11-C10-C8	-2.05	109.28	115.92
35	C	516[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
31	M	101	LMT	O5B-C5B-C6B	2.05	111.54	106.44
23	a	407	CLA	CHB-C4A-NA	2.05	127.35	124.51
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
34	C	521	HTG	C1-O5-C5	2.05	116.36	112.58
25	c	515	BCR	C35-C13-C14	-2.05	120.05	122.92
23	A	404[A]	CLA	CHB-C4A-NA	2.05	127.34	124.51
40	V	201	HEC	C1D-C2D-C3D	-2.05	104.80	106.96
32	C	519	LMG	C8-O7-C10	-2.04	112.76	117.79
32	Z	101	LMG	C9-C8-C7	-2.04	106.95	111.79
26	A	410[B]	SQD	O9-S-O7	-2.04	106.88	113.95
33	D	408[A]	LHG	O4-P-O5	2.04	122.34	112.24
23	b	601	CLA	CAA-C2A-C3A	-2.04	107.18	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
23	b	616	CLA	CHB-C1B-C2B	-2.04	121.47	127.24
23	b	613	CLA	CHB-C4A-NA	2.04	127.34	124.51
33	A	419[B]	LHG	O4-P-O5	2.04	122.33	112.24
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27
24	a	406[B]	PHO	C4-C3-C5	2.04	118.70	115.27
25	B	619	BCR	C39-C30-C25	-2.04	106.99	110.30
25	C	514	BCR	C40-C30-C25	-2.04	106.99	110.30
23	b	613	CLA	C16-C15-C13	-2.04	109.33	115.92
23	c	507	CLA	CAA-CBA-CGA	2.04	119.21	113.25
25	H	101	BCR	C7-C8-C9	-2.04	123.16	126.23
23	b	602	CLA	CHB-C4A-NA	2.04	127.33	124.51
23	b	611	CLA	CMC-C2C-C1C	2.03	128.14	125.04
23	c	506	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	B	616	CLA	C4-C3-C2	-2.03	118.46	123.68
23	C	507	CLA	C6-C7-C8	-2.03	109.34	115.92
33	E	101[B]	LHG	C5-O7-C7	-2.03	112.78	117.79
23	B	601	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
23	B	601	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
23	b	616	CLA	C11-C12-C13	-2.03	109.35	115.92
23	A	405[B]	CLA	CED-O2D-CGD	2.03	120.53	115.94
23	B	603	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
23	C	504	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	a	404[A]	CLA	CMB-C2B-C3B	2.03	131.51	126.59
25	B	619	BCR	C16-C15-C14	-2.03	119.31	123.47
35	C	518	DGD	O1G-C1A-O1A	-2.03	118.47	123.59
32	C	520	LMG	O1-C1-C2	2.03	111.47	108.30
23	b	615	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
23	b	616	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
23	B	611	CLA	C2C-C1C-NC	2.03	111.87	109.97
23	c	507	CLA	CBC-CAC-C3C	-2.03	106.83	112.43
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
33	b	629[B]	LHG	O7-C7-O9	-2.03	118.80	123.70
25	b	617	BCR	C20-C21-C22	-2.03	124.42	127.31
24	a	406[A]	PHO	CBC-CAC-C3C	-2.03	109.91	112.88
31	M	101	LMT	C3B-C4B-C5B	-2.03	106.62	110.24
23	b	610	CLA	CHB-C4A-NA	2.03	127.31	124.51
32	c	520	LMG	O8-C28-O10	-2.03	118.48	123.59
29	d	406[A]	PL9	C45-C44-C46	2.03	118.68	115.27
26	B	620	SQD	O5-C1-C2	-2.03	106.06	110.35
23	c	511	CLA	C7-C6-C5	-2.02	107.86	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	c	521	LMG	C1-C2-C3	-2.02	105.78	110.00
23	B	611	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
27	B	627	GOL	C3-C2-C1	-2.02	103.84	111.70
24	a	414[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91
25	B	619	BCR	C15-C14-C13	-2.02	124.43	127.31
25	D	405	BCR	C38-C26-C27	2.02	117.50	113.62
35	c	518[B]	DGD	O2G-C1B-O1B	-2.02	118.82	123.70
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
23	c	506	CLA	C1-O2A-CGA	2.02	121.74	116.44
23	B	616	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	d	406[B]	PL9	C40-C39-C38	-2.02	118.50	123.68
25	B	619	BCR	C10-C11-C12	-2.02	116.92	123.22
38	f	101	HEM	CHA-C1A-NA	2.02	127.56	123.85
23	a	404[B]	CLA	CMC-C2C-C1C	2.02	128.11	125.04
23	B	611	CLA	C11-C12-C13	-2.02	109.40	115.92
24	A	416[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	d	403[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
32	Z	101	LMG	C3-C4-C5	2.01	113.83	110.24
23	b	613	CLA	OBD-CAD-C3D	-2.01	123.67	128.52
24	a	406[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
25	b	619	BCR	C7-C8-C9	-2.01	123.19	126.23
40	V	201	HEC	C2A-C1A-NA	-2.01	108.37	110.32
37	D	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
35	C	516[B]	DGD	O1G-C1A-O1A	-2.01	118.52	123.59
32	Z	101	LMG	C7-O1-C1	-2.01	109.81	113.74
23	B	601	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
23	D	403[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
34	b	625	HTG	C1-C2-C3	-2.01	106.62	110.59
23	B	612	CLA	CMB-C2B-C3B	2.01	131.46	126.59
25	k	101	BCR	C34-C9-C8	2.01	121.24	118.08
29	D	406[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
23	c	511	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
23	a	404[B]	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	b	604	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
23	b	616	CLA	CHA-C1A-NA	-2.01	121.80	126.40
23	c	508	CLA	C1-O2A-CGA	2.01	121.71	116.44
23	b	611	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
23	A	408	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
26	f	102	SQD	C44-O6-C1	-2.00	109.82	113.74
25	C	515	BCR	C2-C1-C6	2.00	113.56	110.48
23	b	611	CLA	CAC-C3C-C4C	2.00	127.41	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	415	LMT	C1'-O5'-C5'	-2.00	109.76	113.69
23	C	509	CLA	C11-C10-C8	-2.00	109.45	115.92

All (2) chirality outliers are listed below:

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

All (1656) 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	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	507	CLA	C2B-C3B-CAB-CBB
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
23	d	404	CLA	C2-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
25	D	405	BCR	C21-C22-C23-C24
25	D	405	BCR	C37-C22-C23-C24
25	D	405	BCR	C23-C24-C25-C30
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	d	405	BCR	C21-C22-C23-C24
25	d	405	BCR	C37-C22-C23-C24
25	y	101	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	y	101	BCR	C5-C6-C7-C8
26	A	410[A]	SQD	O49-C7-O47-C45
26	A	410[B]	SQD	C8-C7-O47-C45
26	A	412	SQD	O6-C44-C45-O47
26	B	620	SQD	O5-C1-O6-C44
26	B	620	SQD	O49-C7-O47-C45
26	F	103	SQD	C2-C1-O6-C44
26	F	103	SQD	O49-C7-O47-C45
26	F	103	SQD	C8-C7-O47-C45
26	a	410	SQD	O6-C44-C45-O47
26	a	410	SQD	C5-C6-S-O7
26	a	410	SQD	C5-C6-S-O8
26	a	410	SQD	C5-C6-S-O9
26	b	620	SQD	O49-C7-O47-C45
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	A	411	GOL	O1-C1-C2-C3
27	B	624	GOL	C1-C2-C3-O3
27	B	629	GOL	O1-C1-C2-C3
27	D	402	GOL	O1-C1-C2-C3
27	D	413	GOL	C1-C2-C3-O3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	527	GOL	C1-C2-C3-O3
27	c	527	GOL	O2-C2-C3-O3
27	o	302	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	C18-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	412[A]	PL9	C9-C11-C12-C13
29	a	412[A]	PL9	C14-C16-C17-C18
29	a	412[A]	PL9	C25-C24-C26-C27
29	a	412[B]	PL9	C9-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	a	412[B]	PL9	C14-C16-C17-C18
29	a	412[B]	PL9	C25-C24-C26-C27
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	420	LMT	C2'-C1'-O1'-C1
31	A	420	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2'-C1'-O1'-C1
31	B	631	LMT	O5'-C1'-O1'-C1
31	B	631	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	M	102	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	b	627	LMT	C2-C1-O1'-C1'
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
32	C	520	LMG	C11-C10-O7-C8
32	c	521	LMG	O9-C10-O7-C8
32	Z	101	LMG	O9-C10-O7-C8
32	Z	101	LMG	C11-C10-O7-C8
32	z	101	LMG	O6-C1-O1-C7
32	z	101	LMG	O9-C10-O7-C8
33	A	419[B]	LHG	O2-C2-C3-O3
33	D	407[A]	LHG	O2-C2-C3-O3
33	D	407[A]	LHG	C3-O3-P-O4
33	D	407[A]	LHG	C3-O3-P-O5
33	D	407[A]	LHG	C3-O3-P-O6
33	D	407[A]	LHG	C4-O6-P-O4
33	D	407[B]	LHG	O2-C2-C3-O3
33	D	407[B]	LHG	C3-O3-P-O4
33	D	407[B]	LHG	C4-O6-P-O4
33	D	407[B]	LHG	C4-O6-P-O5
33	E	101[A]	LHG	C3-O3-P-O4
33	E	101[A]	LHG	C3-O3-P-O5
33	E	101[A]	LHG	O10-C23-O8-C6
33	E	101[A]	LHG	C24-C23-O8-C6
33	E	101[B]	LHG	C3-O3-P-O4
33	E	101[B]	LHG	C3-O3-P-O5
33	E	101[B]	LHG	C3-O3-P-O6
33	E	101[B]	LHG	O10-C23-O8-C6
33	E	101[B]	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
33	L	101[A]	LHG	C4-O6-P-O4
33	L	101[A]	LHG	C4-O6-P-O5
33	L	101[B]	LHG	C4-O6-P-O3
33	L	101[B]	LHG	C4-O6-P-O4
33	L	101[B]	LHG	C4-O6-P-O5
33	a	418[A]	LHG	C3-O3-P-O4
33	a	418[A]	LHG	C4-O6-P-O5
33	a	418[A]	LHG	O10-C23-O8-C6
33	a	418[A]	LHG	C24-C23-O8-C6
33	a	418[B]	LHG	C3-O3-P-O4
33	a	418[B]	LHG	C4-O6-P-O5
33	a	418[B]	LHG	O10-C23-O8-C6
33	a	418[B]	LHG	C24-C23-O8-C6
33	b	629[A]	LHG	C4-O6-P-O3
33	b	629[A]	LHG	C4-O6-P-O4
33	b	629[A]	LHG	C4-O6-P-O5
33	b	629[B]	LHG	C4-O6-P-O3
33	b	629[B]	LHG	C4-O6-P-O4
33	b	629[B]	LHG	C4-O6-P-O5
33	d	407[A]	LHG	C3-O3-P-O5
33	d	407[A]	LHG	C4-O6-P-O4
33	d	407[B]	LHG	O2-C2-C3-O3
33	d	407[B]	LHG	C3-O3-P-O4
33	d	407[B]	LHG	C3-O3-P-O6
33	d	407[B]	LHG	C4-O6-P-O4
33	d	414[A]	LHG	C3-O3-P-O5
34	B	622	HTG	C2'-C1'-S1-C1
38	F	102	HEM	C2C-C3C-CAC-CBC
38	F	102	HEM	C4C-C3C-CAC-CBC
31	A	420	LMT	O5B-C1B-O1B-C4'
31	a	415	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	C4'-C5'-C6'-O6'
26	A	410[B]	SQD	O49-C7-O47-C45
32	C	520	LMG	O9-C10-O7-C8
23	D	404	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	404	CLA	C3-C5-C6-C7
31	B	630	LMT	O5B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
32	c	521	LMG	C11-C10-O7-C8
32	z	101	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
31	M	102	LMT	C4B-C5B-C6B-O6B
23	C	504	CLA	C4-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
23	A	408	CLA	C2-C3-C5-C6
23	a	407	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22
29	a	412[B]	PL9	C23-C24-C26-C27
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
31	M	102	LMT	O5'-C5'-C6'-O6'
31	m	103	LMT	O5B-C5B-C6B-O6B
34	D	411	HTG	O5-C5-C6-O6
31	m	103	LMT	C4B-C5B-C6B-O6B
31	B	628	LMT	C6-C7-C8-C9
34	b	625	HTG	S1-C1'-C2'-C3'
31	B	628	LMT	C4'-C5'-C6'-O6'
34	b	625	HTG	O5-C5-C6-O6
23	C	501	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	D	404	CLA	CBD-CGD-O2D-CED
23	c	514	CLA	CBD-CGD-O2D-CED
33	E	101[A]	LHG	O2-C2-C3-O3
33	d	407[A]	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
31	B	628	LMT	O5B-C5B-C6B-O6B
23	C	503	CLA	CBD-CGD-O2D-CED
31	a	415	LMT	C4B-C5B-C6B-O6B
32	C	520	LMG	O6-C5-C6-O5
31	B	630	LMT	C4B-C5B-C6B-O6B
32	c	521	LMG	C4-C5-C6-O5
34	D	411	HTG	C4-C5-C6-O6
34	D	411	HTG	S1-C1'-C2'-C3'
31	A	420	LMT	O5'-C5'-C6'-O6'
31	B	628	LMT	O5'-C5'-C6'-O6'
31	F	101	LMT	C4'-C5'-C6'-O6'
31	A	420	LMT	O5B-C5B-C6B-O6B
31	B	630	LMT	O5'-C5'-C6'-O6'
31	B	631	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
31	b	621	LMT	O5'-C5'-C6'-O6'
23	B	605	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	D	404	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
23	c	508	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	a	412[A]	PL9	C15-C14-C16-C17
29	a	412[A]	PL9	C30-C29-C31-C32
29	a	412[B]	PL9	C15-C14-C16-C17
29	a	412[B]	PL9	C30-C29-C31-C32
23	B	605	CLA	C2-C3-C5-C6
23	C	507	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C13-C14-C16-C17
29	A	414[B]	PL9	C13-C14-C16-C17
29	a	412[A]	PL9	C13-C14-C16-C17
29	a	412[A]	PL9	C28-C29-C31-C32
29	a	412[B]	PL9	C13-C14-C16-C17
29	a	412[B]	PL9	C28-C29-C31-C32
31	M	102	LMT	O5B-C5B-C6B-O6B
34	B	625	HTG	O5-C5-C6-O6
31	M	102	LMT	C4'-C5'-C6'-O6'
31	e	101	LMT	O5'-C1'-O1'-C1
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	406[A]	PL9	C39-C41-C42-C43
29	D	406[B]	PL9	C39-C41-C42-C43
29	d	406[B]	PL9	C39-C41-C42-C43
23	c	510	CLA	C3-C5-C6-C7
40	v	201	HEC	C2C-C3C-CAC-CBC
31	b	627	LMT	O5'-C5'-C6'-O6'
31	e	101	LMT	C4'-C5'-C6'-O6'
32	c	521	LMG	O6-C5-C6-O5
33	A	419[B]	LHG	C1-C2-C3-O3
33	D	407[B]	LHG	C1-C2-C3-O3
33	d	407[A]	LHG	C1-C2-C3-O3
31	b	627	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
23	a	407	CLA	CBA-CGA-O2A-C1
23	c	510	CLA	CBA-CGA-O2A-C1
35	C	518	DGD	C6B-C7B-C8B-C9B
31	A	420	LMT	C4B-C5B-C6B-O6B
33	D	408[A]	LHG	C33-C34-C35-C36
23	b	606	CLA	C10-C11-C12-C13
26	F	103	SQD	C23-C24-C25-C26
31	B	631	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	O5'-C5'-C6'-O6'
23	C	504	CLA	C2-C3-C5-C6
29	a	412[A]	PL9	C23-C24-C26-C27
23	B	602	CLA	C6-C7-C8-C9
23	C	502	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C9
23	b	604	CLA	C6-C7-C8-C9
23	b	616	CLA	C6-C7-C8-C9
23	c	505	CLA	C11-C12-C13-C14
23	c	510	CLA	C11-C10-C8-C9
25	K	102	BCR	C7-C8-C9-C34
25	b	619	BCR	C7-C8-C9-C34
25	t	102	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
26	b	620	SQD	C18-C19-C20-C21
32	B	621	LMG	C39-C40-C41-C42
26	A	410[B]	SQD	C7-C8-C9-C10
23	a	407	CLA	O1A-CGA-O2A-C1
31	e	101	LMT	O5B-C5B-C6B-O6B
31	b	621	LMT	C4'-C5'-C6'-O6'
23	B	601	CLA	C10-C11-C12-C13
23	B	602	CLA	C13-C15-C16-C17
23	B	606	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	b	604	CLA	C8-C10-C11-C12
23	b	614	CLA	C8-C10-C11-C12
35	h	102	DGD	C6B-C7B-C8B-C9B
35	C	518	DGD	C2B-C3B-C4B-C5B
23	A	408	CLA	C5-C6-C7-C8
23	B	601	CLA	C5-C6-C7-C8
23	C	508	CLA	C10-C11-C12-C13
23	c	513	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
27	V	203[A]	GOL	O2-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
35	c	518[B]	DGD	C1B-C2B-C3B-C4B
31	a	415	LMT	O1'-C1-C2-C3
31	B	628	LMT	C5'-C4'-O1B-C1B
33	D	408[B]	LHG	C33-C34-C35-C36
31	A	420	LMT	C4'-C5'-C6'-O6'
31	A	420	LMT	O1'-C1-C2-C3
23	C	507	CLA	C5-C6-C7-C8
32	Z	101	LMG	C10-C11-C12-C13
33	E	101[A]	LHG	C23-C24-C25-C26
35	c	518[A]	DGD	C1B-C2B-C3B-C4B
23	c	513	CLA	CBD-CGD-O2D-CED
31	A	417	LMT	O5B-C5B-C6B-O6B
23	a	404[B]	CLA	C15-C16-C17-C18
23	C	510	CLA	C11-C12-C13-C15
23	D	404	CLA	C11-C10-C8-C7
25	T	101	BCR	C13-C14-C15-C16
23	B	603	CLA	C13-C15-C16-C17
23	B	614	CLA	C8-C10-C11-C12
23	D	404	CLA	C10-C11-C12-C13
23	b	605	CLA	C8-C10-C11-C12
34	b	623	HTG	C1'-C2'-C3'-C4'
23	c	512	CLA	CBD-CGD-O2D-CED
31	B	630	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
23	b	604	CLA	C5-C6-C7-C8
23	b	604	CLA	C15-C16-C17-C18
29	A	414[A]	PL9	C44-C46-C47-C48
29	d	406[A]	PL9	C39-C41-C42-C43
34	B	625	HTG	S1-C1'-C2'-C3'
23	C	512	CLA	C10-C11-C12-C13
23	b	611	CLA	C15-C16-C17-C18
31	A	420	LMT	C5'-C4'-O1B-C1B
23	c	510	CLA	O1A-CGA-O2A-C1
40	V	201	HEC	C4C-C3C-CAC-CBC
31	B	628	LMT	C4B-C5B-C6B-O6B
31	B	631	LMT	C4'-C5'-C6'-O6'
23	B	614	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	611	CLA	C8-C10-C11-C12
23	c	514	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	a	404[A]	CLA	C15-C16-C17-C18
23	b	606	CLA	C15-C16-C17-C18
33	D	407[B]	LHG	C3-O3-P-O6
33	D	407[B]	LHG	C4-O6-P-O3
33	E	101[A]	LHG	C3-O3-P-O6
33	E	101[A]	LHG	C4-O6-P-O3
33	E	101[B]	LHG	C4-O6-P-O3
33	L	101[A]	LHG	C4-O6-P-O3
33	a	418[A]	LHG	C3-O3-P-O6
33	a	418[A]	LHG	C4-O6-P-O3
33	a	418[B]	LHG	C3-O3-P-O6
33	a	418[B]	LHG	C4-O6-P-O3
33	d	407[A]	LHG	C3-O3-P-O6
26	B	620	SQD	C7-C8-C9-C10
31	A	417	LMT	O1'-C1-C2-C3
34	B	622	HTG	C1'-C2'-C3'-C4'
34	b	625	HTG	C4-C5-C6-O6
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
40	V	201	HEC	C2C-C3C-CAC-CBC
34	b	622	HTG	S1-C1'-C2'-C3'
34	d	411	HTG	S1-C1'-C2'-C3'
26	A	410[A]	SQD	C7-C8-C9-C10
33	D	407[A]	LHG	C1-C2-C3-O3
33	d	407[B]	LHG	C1-C2-C3-O3
32	B	621	LMG	O9-C10-O7-C8
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	b	615	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C20
35	C	516[B]	DGD	O6D-C5D-C6D-O5D
26	A	410[A]	SQD	C15-C16-C17-C18
26	A	410[B]	SQD	C15-C16-C17-C18
32	D	412	LMG	C19-C20-C21-C22
33	D	407[B]	LHG	C16-C17-C18-C19
33	L	101[A]	LHG	C12-C13-C14-C15
33	L	101[B]	LHG	C12-C13-C14-C15
33	L	101[B]	LHG	C15-C16-C17-C18
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
32	B	621	LMG	C11-C10-O7-C8
23	C	502	CLA	C15-C16-C17-C18
26	F	103	SQD	C30-C31-C32-C33
26	f	102	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	b	627	LMT	C7-C8-C9-C10
33	L	101[A]	LHG	C17-C18-C19-C20
33	b	629[B]	LHG	C14-C15-C16-C17
33	d	414[A]	LHG	C16-C17-C18-C19
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
23	B	615	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C19
23	b	606	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
23	c	509	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C20
31	t	101	LMT	C4-C5-C6-C7
32	C	520	LMG	C18-C19-C20-C21
32	m	101	LMG	C35-C36-C37-C38
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
35	h	102	DGD	C9A-CAA-CBA-CCA
31	e	101	LMT	O5'-C5'-C6'-O6'
33	d	414[B]	LHG	C16-C17-C18-C19
35	C	517[A]	DGD	CCB-CDB-CEB-CFB
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
23	c	507	CLA	C15-C16-C17-C18
33	E	101[B]	LHG	O2-C2-C3-O3
31	A	420	LMT	C3-C4-C5-C6
32	D	412	LMG	C35-C36-C37-C38
33	D	408[B]	LHG	C32-C33-C34-C35
35	C	516[A]	DGD	C4B-C5B-C6B-C7B
23	C	511	CLA	C3-C5-C6-C7
32	c	520	LMG	C10-C11-C12-C13
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
35	C	517[A]	DGD	C2E-C1E-O5D-C6D
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
26	F	103	SQD	C24-C25-C26-C27
32	c	501	LMG	C30-C31-C32-C33
33	L	101[B]	LHG	C13-C14-C15-C16
33	a	418[B]	LHG	C26-C27-C28-C29
35	C	516[A]	DGD	C5B-C6B-C7B-C8B
35	C	516[B]	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
23	B	603	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
24	a	406[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C45-C44-C46-C47
33	D	407[A]	LHG	C16-C17-C18-C19
33	a	418[A]	LHG	C26-C27-C28-C29
33	b	629[A]	LHG	C14-C15-C16-C17
35	C	517[B]	DGD	CCB-CDB-CEB-CFB
29	d	406[A]	PL9	C13-C14-C16-C17
23	B	613	CLA	C11-C12-C13-C14
23	a	405[A]	CLA	C11-C12-C13-C14
23	a	405[B]	CLA	C11-C12-C13-C14
23	b	610	CLA	C11-C12-C13-C14
23	c	505	CLA	C14-C13-C15-C16
40	v	201	HEC	C4C-C3C-CAC-CBC
32	A	418	LMG	C10-C11-C12-C13
33	E	101[B]	LHG	C23-C24-C25-C26
26	A	412	SQD	C17-C18-C19-C20
32	A	418	LMG	C12-C13-C14-C15
32	B	621	LMG	C17-C18-C19-C20
33	D	408[A]	LHG	C32-C33-C34-C35
33	L	101[A]	LHG	C15-C16-C17-C18
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
23	c	508	CLA	C2A-CAA-CBA-CGA
31	B	630	LMT	C2-C3-C4-C5
32	c	501	LMG	C34-C35-C36-C37
33	d	407[B]	LHG	C34-C35-C36-C37
33	d	414[A]	LHG	C32-C33-C34-C35
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
27	B	624	GOL	O1-C1-C2-C3
27	B	629	GOL	C1-C2-C3-O3
27	D	413	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	O	303	GOL	O1-C1-C2-C3
27	a	416	GOL	O1-C1-C2-C3
27	d	413	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
31	A	420	LMT	C1-C2-C3-C4
32	Z	101	LMG	O6-C5-C6-O5
23	C	502	CLA	C13-C15-C16-C17
32	A	418	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	L	101[A]	LHG	C25-C26-C27-C28
33	d	408[B]	LHG	C27-C28-C29-C30
32	c	501	LMG	C10-C11-C12-C13
31	B	631	LMT	C3-C4-C5-C6
31	e	101	LMT	C4-C5-C6-C7
32	C	520	LMG	C13-C14-C15-C16
32	C	520	LMG	C17-C18-C19-C20
33	A	419[A]	LHG	C34-C35-C36-C37
33	A	419[B]	LHG	C34-C35-C36-C37
33	L	101[B]	LHG	C17-C18-C19-C20
33	d	407[A]	LHG	C11-C10-C9-C8
35	H	102	DGD	C5B-C6B-C7B-C8B
35	h	102	DGD	C7B-C8B-C9B-CAB
40	V	201	HEC	C2B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
23	B	603	CLA	C16-C17-C18-C19
23	B	615	CLA	C16-C17-C18-C20
23	a	407	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C19
26	F	103	SQD	O5-C1-O6-C44
26	A	410[A]	SQD	C12-C13-C14-C15
31	e	101	LMT	C5-C6-C7-C8
32	c	520	LMG	C34-C35-C36-C37
33	L	101[A]	LHG	C13-C14-C15-C16
33	L	101[B]	LHG	C25-C26-C27-C28
33	d	407[A]	LHG	C34-C35-C36-C37
35	C	516[B]	DGD	C4B-C5B-C6B-C7B
26	B	620	SQD	C11-C10-C9-C8
26	B	620	SQD	C30-C31-C32-C33
32	m	101	LMG	C39-C40-C41-C42
33	d	408[A]	LHG	C27-C28-C29-C30
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	519	DGD	CBB-CCB-CDB-CEB
26	a	410	SQD	C31-C32-C33-C34
35	H	102	DGD	CCB-CDB-CEB-CFB
23	C	513	CLA	O1D-CGD-O2D-CED
23	A	404[B]	CLA	C13-C15-C16-C17
35	C	516[B]	DGD	C4D-C5D-C6D-O5D
31	A	420	LMT	C2-C1-O1'-C1'
31	B	628	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
31	m	103	LMT	C2-C1-O1'-C1'
26	F	103	SQD	C29-C30-C31-C32
26	a	410	SQD	C16-C17-C18-C19
26	b	620	SQD	C27-C28-C29-C30
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
32	c	520	LMG	C33-C34-C35-C36
33	A	419[A]	LHG	C12-C13-C14-C15
33	b	629[A]	LHG	C16-C17-C18-C19
33	A	419[B]	LHG	C12-C13-C14-C15
33	E	101[A]	LHG	C24-C25-C26-C27
35	H	102	DGD	C9B-CAB-CBB-CCB
35	c	517[A]	DGD	O6D-C5D-C6D-O5D
31	B	631	LMT	C4-C5-C6-C7
32	B	621	LMG	C34-C35-C36-C37
23	A	406[B]	CLA	C13-C15-C16-C17
23	b	614	CLA	C10-C11-C12-C13
29	D	406[B]	PL9	C15-C14-C16-C17
29	d	406[A]	PL9	C15-C14-C16-C17
29	d	406[B]	PL9	C15-C14-C16-C17
35	c	517[A]	DGD	C2A-C1A-O1G-C1G
35	c	517[B]	DGD	C2A-C1A-O1G-C1G
23	D	404	CLA	C2-C3-C5-C6
23	c	506	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	D	406[A]	PL9	C13-C14-C16-C17
29	d	406[B]	PL9	C13-C14-C16-C17
23	c	514	CLA	O1D-CGD-O2D-CED
26	B	620	SQD	C34-C35-C36-C37
27	A	411	GOL	O1-C1-C2-O2
27	B	624	GOL	O2-C2-C3-O3
27	B	629	GOL	O1-C1-C2-O2
27	B	629	GOL	O2-C2-C3-O3
27	D	402	GOL	O1-C1-C2-O2
27	O	302	GOL	O1-C1-C2-O2
27	V	203[B]	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
31	B	630	LMT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	D	412	LMG	C30-C31-C32-C33
32	c	520	LMG	C31-C32-C33-C34
33	d	414[B]	LHG	C32-C33-C34-C35
35	c	518[A]	DGD	CBB-CCB-CDB-CEB
32	A	418	LMG	C19-C20-C21-C22
23	a	405[A]	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C2B-C3B-CAB-CBB
32	D	412	LMG	C12-C13-C14-C15
33	D	408[A]	LHG	C15-C16-C17-C18
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
35	c	517[B]	DGD	C4D-C5D-C6D-O5D
35	H	102	DGD	C7A-C8A-C9A-CAA
31	b	627	LMT	C5-C6-C7-C8
32	C	520	LMG	C19-C20-C21-C22
33	D	407[B]	LHG	C12-C13-C14-C15
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
32	C	519	LMG	C16-C17-C18-C19
33	D	408[B]	LHG	C29-C30-C31-C32
33	d	414[A]	LHG	C29-C30-C31-C32
31	a	415	LMT	C1-C2-C3-C4
31	B	628	LMT	C5-C6-C7-C8
35	c	517[A]	DGD	C7A-C8A-C9A-CAA
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
35	c	518[B]	DGD	CBB-CCB-CDB-CEB
25	D	405	BCR	C23-C24-C25-C26
25	b	617	BCR	C5-C6-C7-C8
25	t	102	BCR	C23-C24-C25-C26
33	E	101[B]	LHG	C24-C25-C26-C27
33	D	408[B]	LHG	C24-C23-O8-C6
26	A	410[B]	SQD	C12-C13-C14-C15
31	M	102	LMT	C7-C8-C9-C10
35	c	518[A]	DGD	C6A-C7A-C8A-C9A
31	b	621	LMT	C3'-C4'-O1B-C1B
33	b	629[B]	LHG	C16-C17-C18-C19
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	406[A]	PL9	C15-C14-C16-C17
23	C	503	CLA	O1D-CGD-O2D-CED
23	D	404	CLA	O1D-CGD-O2D-CED
23	A	408	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C11-C10-C8-C7
23	C	510	CLA	C2-C3-C5-C6
23	a	405[A]	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
23	c	505	CLA	C12-C13-C15-C16
23	c	511	CLA	C12-C13-C15-C16
29	A	414[B]	PL9	C12-C11-C9-C8
35	c	517[B]	DGD	O1A-C1A-O1G-C1G
31	M	101	LMT	O1'-C1-C2-C3
23	c	509	CLA	C16-C17-C18-C20
23	C	501	CLA	O1D-CGD-O2D-CED
26	b	620	SQD	C24-C23-O48-C46
33	D	408[A]	LHG	C29-C30-C31-C32
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
23	C	510	CLA	C10-C11-C12-C13
33	D	407[A]	LHG	C13-C14-C15-C16
32	A	418	LMG	C36-C37-C38-C39
26	F	103	SQD	C7-C8-C9-C10
23	B	615	CLA	C10-C11-C12-C13
26	a	410	SQD	C25-C26-C27-C28
31	B	631	LMT	O1'-C1-C2-C3
33	D	408[B]	LHG	C15-C16-C17-C18
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
32	A	418	LMG	C29-C30-C31-C32
35	C	516[A]	DGD	C8A-C9A-CAA-CBA
35	h	102	DGD	CAA-CBA-CCA-CDA
33	D	408[B]	LHG	O10-C23-O8-C6
35	c	517[A]	DGD	O1A-C1A-O1G-C1G
35	C	517[A]	DGD	O6E-C1E-O5D-C6D
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
23	C	506	CLA	C5-C6-C7-C8
26	a	409[A]	SQD	C9-C10-C11-C12
26	b	620	SQD	C26-C27-C28-C29
32	c	501	LMG	C35-C36-C37-C38
33	b	629[B]	LHG	C27-C28-C29-C30
33	d	414[B]	LHG	C25-C26-C27-C28
32	m	101	LMG	C11-C10-O7-C8
26	A	412	SQD	C26-C27-C28-C29
31	b	621	LMT	C3-C4-C5-C6
32	c	501	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	d	414[B]	LHG	C29-C30-C31-C32
35	C	516[B]	DGD	C9A-CAA-CBA-CCA
31	B	628	LMT	C1-C2-C3-C4
23	C	509	CLA	CBD-CGD-O2D-CED
32	m	101	LMG	O9-C10-O7-C8
26	f	102	SQD	C25-C26-C27-C28
32	D	412	LMG	C36-C37-C38-C39
26	A	412	SQD	C2-C1-O6-C44
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
26	b	620	SQD	C14-C15-C16-C17
35	C	516[A]	DGD	C9A-CAA-CBA-CCA
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
34	b	623	HTG	O5-C5-C6-O6
23	c	508	CLA	C5-C6-C7-C8
23	C	510	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C45-C44-C46-C47
23	B	606	CLA	C11-C10-C8-C9
23	C	513	CLA	C6-C7-C8-C9
23	D	404	CLA	C11-C10-C8-C9
23	D	404	CLA	C14-C13-C15-C16
23	c	506	CLA	C11-C12-C13-C14
31	M	101	LMT	O5'-C5'-C6'-O6'
35	C	516[A]	DGD	O6E-C5E-C6E-O5E
31	B	628	LMT	C3'-C4'-O1B-C1B
31	M	101	LMT	C3-C4-C5-C6
32	C	519	LMG	C17-C18-C19-C20
33	b	629[A]	LHG	C13-C14-C15-C16
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
32	A	418	LMG	C39-C40-C41-C42
32	C	519	LMG	C37-C38-C39-C40
23	B	614	CLA	C5-C6-C7-C8
25	t	102	BCR	C21-C22-C23-C24
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
31	A	420	LMT	C3'-C4'-O1B-C1B
31	A	420	LMT	C5-C6-C7-C8
31	B	630	LMT	C6-C7-C8-C9
33	D	408[A]	LHG	C17-C18-C19-C20
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	608	CLA	C13-C15-C16-C17
23	b	601	CLA	C8-C10-C11-C12
23	b	610	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	d	407[B]	LHG	C4-O6-P-O3
34	b	622	HTG	C3'-C4'-C5'-C6'
35	C	516[B]	DGD	C8A-C9A-CAA-CBA
33	D	408[B]	LHG	C17-C18-C19-C20
23	c	513	CLA	C10-C11-C12-C13
23	C	512	CLA	CBA-CGA-O2A-C1
31	t	101	LMT	O1'-C1-C2-C3
32	d	412	LMG	C29-C30-C31-C32
23	A	404[A]	CLA	C13-C15-C16-C17
23	b	615	CLA	C16-C17-C18-C20
23	d	403[A]	CLA	C16-C17-C18-C20
33	d	408[A]	LHG	C25-C26-C27-C28
31	e	101	LMT	C1-C2-C3-C4
31	b	621	LMT	C11-C10-C9-C8
35	c	518[B]	DGD	C6A-C7A-C8A-C9A
32	A	418	LMG	C11-C12-C13-C14
23	c	506	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C30-C29-C31-C32
31	b	627	LMT	C3-C4-C5-C6
33	d	408[B]	LHG	C9-C10-C11-C12
26	a	409[B]	SQD	C12-C13-C14-C15
26	b	620	SQD	C11-C10-C9-C8
32	A	418	LMG	C13-C14-C15-C16
33	d	414[B]	LHG	C24-C25-C26-C27
35	c	518[A]	DGD	C4A-C5A-C6A-C7A
23	d	403[B]	CLA	C16-C17-C18-C20
32	d	412	LMG	O6-C5-C6-O5
35	C	516[B]	DGD	O6E-C5E-C6E-O5E
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	410[B]	SQD	O6-C44-C45-C46
26	A	412	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
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
31	B	631	LMT	C11-C10-C9-C8
33	E	101[B]	LHG	C4-C5-C6-O8
33	d	408[B]	LHG	C25-C26-C27-C28
23	B	613	CLA	C13-C15-C16-C17
31	a	415	LMT	C3-C4-C5-C6
33	D	407[B]	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
33	E	101[A]	LHG	C25-C26-C27-C28
31	t	101	LMT	C4'-C5'-C6'-O6'
35	C	517[A]	DGD	C2G-C3G-O3G-C1D
35	C	517[A]	DGD	C5D-C6D-O5D-C1E
35	C	517[B]	DGD	C5D-C6D-O5D-C1E
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
26	F	103	SQD	C34-C35-C36-C37
35	C	517[A]	DGD	CDA-CEA-CFA-CGA
26	b	620	SQD	C13-C14-C15-C16
35	h	102	DGD	C2B-C3B-C4B-C5B
35	c	517[A]	DGD	C4D-C5D-C6D-O5D
31	a	415	LMT	C9-C10-C11-C12
34	B	622	HTG	C2'-C3'-C4'-C5'
35	C	516[A]	DGD	C3B-C4B-C5B-C6B
23	C	506	CLA	C15-C16-C17-C18
27	D	413	GOL	O2-C2-C3-O3
27	O	303	GOL	O1-C1-C2-O2
27	o	302	GOL	O2-C2-C3-O3
32	m	101	LMG	C38-C39-C40-C41
35	C	517[B]	DGD	CDA-CEA-CFA-CGA
26	b	620	SQD	O10-C23-O48-C46
35	c	518[B]	DGD	C4A-C5A-C6A-C7A
23	A	405[A]	CLA	C15-C16-C17-C18
32	D	412	LMG	O6-C5-C6-O5
35	c	517[A]	DGD	O6E-C5E-C6E-O5E
23	C	505	CLA	C4-C3-C5-C6
29	a	412[A]	PL9	C12-C11-C9-C10
29	a	412[B]	PL9	C12-C11-C9-C10
33	b	629[B]	LHG	C12-C13-C14-C15
23	B	608	CLA	C16-C17-C18-C20
23	B	610	CLA	C16-C17-C18-C19
23	c	513	CLA	CBA-CGA-O2A-C1
23	d	404	CLA	CBA-CGA-O2A-C1
23	B	615	CLA	C5-C6-C7-C8
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
33	d	414[A]	LHG	C33-C34-C35-C36
34	c	522	HTG	C4'-C5'-C6'-C7'
35	h	102	DGD	CDB-CEB-CFB-CGB
26	b	620	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
35	c	517[B]	DGD	O6E-C5E-C6E-O5E
23	B	601	CLA	C13-C15-C16-C17
23	A	408	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
31	A	420	LMT	C4-C5-C6-C7
33	d	408[A]	LHG	C34-C35-C36-C37
26	a	409[A]	SQD	C12-C13-C14-C15
32	C	519	LMG	C31-C32-C33-C34
32	Z	101	LMG	C11-C12-C13-C14
33	D	407[A]	LHG	C12-C13-C14-C15
40	v	201	HEC	C2B-C3B-CAB-CBB
23	B	612	CLA	C10-C11-C12-C13
32	B	621	LMG	C29-C30-C31-C32
32	d	412	LMG	C16-C17-C18-C19
33	L	101[B]	LHG	C27-C28-C29-C30
33	d	414[B]	LHG	C33-C34-C35-C36
23	b	601	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	C16-C17-C18-C20
33	D	408[B]	LHG	C13-C14-C15-C16
33	d	408[B]	LHG	C28-C29-C30-C31
23	C	512	CLA	O1A-CGA-O2A-C1
23	d	404	CLA	O1A-CGA-O2A-C1
35	c	519	DGD	CBA-CCA-CDA-CEA
32	d	412	LMG	C10-C11-C12-C13
31	t	101	LMT	C7-C8-C9-C10
35	C	516[A]	DGD	O6D-C5D-C6D-O5D
23	d	403[A]	CLA	C16-C17-C18-C19
32	B	621	LMG	C15-C16-C17-C18
33	d	408[A]	LHG	C29-C30-C31-C32
35	C	517[B]	DGD	C8B-C9B-CAB-CBB
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	B	602	CLA	C11-C12-C13-C15
23	B	614	CLA	C11-C10-C8-C7
23	C	513	CLA	C11-C10-C8-C7
23	D	404	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	505	CLA	C11-C12-C13-C15
23	c	506	CLA	C11-C12-C13-C15
23	c	513	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	D	406[B]	PL9	C13-C14-C16-C17
23	B	602	CLA	C11-C12-C13-C14
23	C	504	CLA	C14-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C14
23	C	510	CLA	C14-C13-C15-C16
23	C	513	CLA	C11-C10-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
32	z	101	LMG	C14-C15-C16-C17
33	E	101[B]	LHG	C25-C26-C27-C28
33	d	408[A]	LHG	C28-C29-C30-C31
35	C	516[B]	DGD	C7A-C8A-C9A-CAA
26	F	103	SQD	C24-C23-O48-C46
32	m	101	LMG	C37-C38-C39-C40
35	h	102	DGD	C6A-C7A-C8A-C9A
32	C	520	LMG	C35-C36-C37-C38
33	d	408[B]	LHG	C29-C30-C31-C32
35	h	102	DGD	CDA-CEA-CFA-CGA
31	a	415	LMT	C2-C3-C4-C5
33	b	629[A]	LHG	C27-C28-C29-C30
34	B	625	HTG	C4'-C5'-C6'-C7'
31	e	101	LMT	C9-C10-C11-C12
32	B	621	LMG	O6-C5-C6-O5
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
23	A	406[A]	CLA	C4B-C3B-CAB-CBB
23	B	602	CLA	C4B-C3B-CAB-CBB
23	D	403[B]	CLA	C4B-C3B-CAB-CBB
23	a	405[A]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
33	E	101[A]	LHG	O6-C4-C5-C6
33	L	101[B]	LHG	O6-C4-C5-C6
33	b	629[A]	LHG	O6-C4-C5-C6
33	D	407[A]	LHG	C10-C11-C12-C13
33	D	408[A]	LHG	C13-C14-C15-C16
33	d	408[A]	LHG	C9-C10-C11-C12
23	b	602	CLA	C10-C11-C12-C13
29	d	406[A]	PL9	C45-C44-C46-C47
23	C	505	CLA	C2-C3-C5-C6
32	d	412	LMG	C28-C29-C30-C31
23	A	405[B]	CLA	C15-C16-C17-C18
26	A	412	SQD	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	a	409[B]	SQD	C9-C10-C11-C12
33	A	419[A]	LHG	C26-C27-C28-C29
33	d	407[A]	LHG	C13-C14-C15-C16
23	d	403[B]	CLA	C16-C17-C18-C19
32	C	519	LMG	C36-C37-C38-C39
35	C	518	DGD	CDB-CEB-CFB-CGB
23	B	601	CLA	CBA-CGA-O2A-C1
35	C	516[A]	DGD	C7A-C8A-C9A-CAA
23	c	513	CLA	O1D-CGD-O2D-CED
35	c	519	DGD	C2B-C3B-C4B-C5B
31	e	101	LMT	C2-C1-O1'-C1'
26	A	412	SQD	C7-C8-C9-C10
23	C	510	CLA	CBA-CGA-O2A-C1
32	c	521	LMG	C29-C28-O8-C9
35	c	518[A]	DGD	CDA-CEA-CFA-CGA
26	a	409[B]	SQD	O6-C44-C45-C46
33	a	418[A]	LHG	C4-C5-C6-O8
33	a	418[B]	LHG	C4-C5-C6-O8
33	L	101[A]	LHG	C24-C25-C26-C27
33	a	418[A]	LHG	C10-C11-C12-C13
33	b	629[A]	LHG	C12-C13-C14-C15
24	a	406[A]	PHO	O2A-C1-C2-C3
23	B	615	CLA	C13-C15-C16-C17
26	a	410	SQD	C18-C19-C20-C21
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
23	c	514	CLA	C4-C3-C5-C6
24	a	406[A]	PHO	C4-C3-C5-C6
23	B	608	CLA	C16-C17-C18-C19
29	D	406[A]	PL9	C43-C44-C46-C47
33	L	101[A]	LHG	C11-C12-C13-C14
31	F	101	LMT	C4-C5-C6-C7
33	a	418[A]	LHG	C7-C8-C9-C10
23	b	601	CLA	O1A-CGA-O2A-C1
31	m	103	LMT	O5'-C5'-C6'-O6'
27	c	527	GOL	O1-C1-C2-O2
33	E	101[A]	LHG	O6-C4-C5-O7
33	E	101[B]	LHG	O6-C4-C5-O7
33	d	407[B]	LHG	C24-C23-O8-C6
35	c	517[B]	DGD	C7A-C8A-C9A-CAA
32	C	520	LMG	C10-C11-C12-C13
35	c	518[B]	DGD	C1A-C2A-C3A-C4A
23	A	406[A]	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C16-C17-C18-C19
32	C	519	LMG	C34-C35-C36-C37
33	b	629[A]	LHG	C31-C32-C33-C34
23	B	602	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
31	F	101	LMT	C2-C3-C4-C5
26	a	409[A]	SQD	C34-C35-C36-C37
26	a	409[A]	SQD	O6-C44-C45-O47
26	a	409[B]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
35	C	517[A]	DGD	C8B-C9B-CAB-CBB
35	C	518	DGD	CAB-CBB-CCB-CDB
33	E	101[A]	LHG	C17-C18-C19-C20
31	a	415	LMT	O5'-C1'-O1'-C1
23	d	402[B]	CLA	C15-C16-C17-C18
29	a	412[A]	PL9	C24-C26-C27-C28
33	D	408[A]	LHG	C10-C11-C12-C13
33	d	407[B]	LHG	C13-C14-C15-C16
23	b	608	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
26	b	620	SQD	C31-C32-C33-C34
23	B	601	CLA	C15-C16-C17-C18
23	B	610	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	c	513	CLA	C6-C7-C8-C9
33	D	408[B]	LHG	C2-C3-O3-P
23	c	513	CLA	O1A-CGA-O2A-C1
33	a	418[B]	LHG	C10-C11-C12-C13
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
23	B	601	CLA	C2A-CAA-CBA-CGA
25	B	617	BCR	C1-C6-C7-C8
25	B	617	BCR	C5-C6-C7-C8
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	d	405	BCR	C23-C24-C25-C26
25	d	405	BCR	C23-C24-C25-C30
25	t	102	BCR	C23-C24-C25-C30
23	C	510	CLA	C13-C15-C16-C17
23	b	605	CLA	C5-C6-C7-C8
32	A	418	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
35	H	102	DGD	CAB-CBB-CCB-CDB
35	h	102	DGD	C9B-CAB-CBB-CCB
33	d	414[A]	LHG	C25-C26-C27-C28
25	K	102	BCR	C7-C8-C9-C10
32	c	501	LMG	C21-C22-C23-C24
33	E	101[B]	LHG	C17-C18-C19-C20
23	B	602	CLA	C15-C16-C17-C18
32	d	412	LMG	C18-C19-C20-C21
23	C	502	CLA	C16-C17-C18-C19
23	c	512	CLA	O1D-CGD-O2D-CED
23	c	510	CLA	C10-C11-C12-C13
34	B	625	HTG	C4-C5-C6-O6
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	502	CLA	C12-C13-C15-C16
23	C	504	CLA	C12-C13-C15-C16
23	C	505	CLA	C11-C12-C13-C15
23	C	506	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	c	507	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
24	a	406[A]	PHO	C2-C3-C5-C6
23	b	615	CLA	C10-C11-C12-C13
33	L	101[A]	LHG	C11-C10-C9-C8
33	b	629[B]	LHG	C13-C14-C15-C16
33	d	414[A]	LHG	C24-C25-C26-C27
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
24	a	414[B]	PHO	C2C-C3C-CAC-CBC
33	b	629[A]	LHG	C34-C35-C36-C37
23	C	511	CLA	C8-C10-C11-C12
26	A	412	SQD	C30-C31-C32-C33
26	a	409[B]	SQD	C34-C35-C36-C37
35	C	516[A]	DGD	CCA-CDA-CEA-CFA
33	b	629[A]	LHG	C9-C10-C11-C12
34	c	522	HTG	C2'-C1'-S1-C1
33	a	418[B]	LHG	C23-C24-C25-C26
23	b	607	CLA	C3-C5-C6-C7
32	c	520	LMG	C29-C30-C31-C32
32	m	101	LMG	C14-C15-C16-C17
32	C	519	LMG	C30-C31-C32-C33
26	F	103	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
23	c	513	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	406[A]	PHO	CAD-CBD-CGD-O2D
26	B	620	SQD	C46-C45-O47-C7
38	f	101	HEM	C2B-C3B-CAB-CBB
31	e	101	LMT	C3-C4-C5-C6
33	E	101[A]	LHG	C13-C14-C15-C16
23	c	513	CLA	C13-C15-C16-C17
26	a	409[A]	SQD	C27-C28-C29-C30
33	d	408[B]	LHG	C24-C23-O8-C6
23	c	511	CLA	C4-C3-C5-C6
33	D	407[A]	LHG	C34-C35-C36-C37
31	e	101	LMT	C4B-C5B-C6B-O6B
32	c	520	LMG	C4-C5-C6-O5
26	A	412	SQD	O5-C1-O6-C44
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
29	a	412[B]	PL9	C24-C26-C27-C28
26	a	410	SQD	O6-C44-C45-C46
32	c	501	LMG	C7-C8-C9-O8
33	E	101[A]	LHG	C4-C5-C6-O8
33	L	101[B]	LHG	O6-C4-C5-O7
33	b	629[A]	LHG	O6-C4-C5-O7
23	b	601	CLA	C13-C15-C16-C17
34	b	623	HTG	C4'-C5'-C6'-C7'
31	F	101	LMT	C6-C7-C8-C9
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
31	B	630	LMT	C3-C4-C5-C6
33	D	407[B]	LHG	C13-C14-C15-C16
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O1D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	O1A-CGA-O2A-C1
32	c	521	LMG	O10-C28-O8-C9
33	d	407[B]	LHG	O10-C23-O8-C6
33	d	407[B]	LHG	C11-C10-C9-C8
32	z	101	LMG	C19-C20-C21-C22
33	L	101[B]	LHG	C11-C10-C9-C8
33	a	418[A]	LHG	O7-C5-C6-O8
33	a	418[B]	LHG	O7-C5-C6-O8
26	F	103	SQD	C32-C33-C34-C35
29	D	406[A]	PL9	C45-C44-C46-C47
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
29	A	414[B]	PL9	C43-C44-C46-C47
23	C	506	CLA	C6-C7-C8-C9
23	a	405[B]	CLA	C6-C7-C8-C9
23	c	511	CLA	C11-C10-C8-C9
35	C	516[A]	DGD	C4D-C5D-C6D-O5D
23	C	511	CLA	O1A-CGA-O2A-C1
33	d	408[B]	LHG	O10-C23-O8-C6
23	b	612	CLA	C8-C10-C11-C12
23	C	506	CLA	C16-C17-C18-C20
23	C	501	CLA	C2A-CAA-CBA-CGA
35	h	102	DGD	CAB-CBB-CCB-CDB
27	d	413	GOL	C1-C2-C3-O3
27	l	102[B]	GOL	O1-C1-C2-C3
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
31	B	628	LMT	C9-C10-C11-C12
35	c	518[B]	DGD	C7B-C8B-C9B-CAB
25	y	101	BCR	C21-C22-C23-C24
33	L	101[B]	LHG	C26-C27-C28-C29
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	C	501	CLA	C1A-C2A-CAA-CBA
23	d	402[A]	CLA	C1A-C2A-CAA-CBA
23	A	406[B]	CLA	C16-C17-C18-C20
33	d	408[A]	LHG	C24-C23-O8-C6
33	A	419[A]	LHG	C32-C33-C34-C35
31	b	627	LMT	C1-C2-C3-C4
33	D	407[A]	LHG	C4-O6-P-O3
33	d	414[A]	LHG	C3-O3-P-O6
32	A	418	LMG	C18-C19-C20-C21
32	d	412	LMG	C11-C12-C13-C14
33	a	418[A]	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	a	409[A]	SQD	C35-C36-C37-C38
33	E	101[B]	LHG	C13-C14-C15-C16
33	D	408[A]	LHG	C2-C3-O3-P
33	d	408[A]	LHG	C2-C3-O3-P
33	d	408[B]	LHG	C2-C3-O3-P
29	a	412[B]	PL9	C12-C11-C9-C8
33	D	407[A]	LHG	C4-O6-P-O5
33	E	101[A]	LHG	C4-O6-P-O5
33	E	101[B]	LHG	C4-O6-P-O5
33	a	418[A]	LHG	C4-O6-P-O4
33	a	418[B]	LHG	C4-O6-P-O4
33	d	407[A]	LHG	C3-O3-P-O4
33	d	407[B]	LHG	C3-O3-P-O5
33	d	407[B]	LHG	C4-O6-P-O5
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
23	c	510	CLA	C15-C16-C17-C18
33	D	407[B]	LHG	O6-C4-C5-C6
33	E	101[B]	LHG	O6-C4-C5-C6
33	L	101[A]	LHG	O6-C4-C5-C6
33	b	629[B]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
31	B	631	LMT	C6-C7-C8-C9
35	C	516[B]	DGD	CDB-CEB-CFB-CGB
32	c	501	LMG	C31-C32-C33-C34
33	D	408[B]	LHG	C10-C11-C12-C13
32	B	621	LMG	C18-C19-C20-C21
33	d	414[A]	LHG	C27-C28-C29-C30
35	c	517[A]	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	C	502	CLA	CAD-CBD-CGD-O1D
23	C	504	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
32	c	520	LMG	C28-C29-C30-C31
35	H	102	DGD	O2G-C1B-C2B-C3B
33	d	408[B]	LHG	C34-C35-C36-C37
32	C	520	LMG	C12-C13-C14-C15
35	h	102	DGD	C3B-C4B-C5B-C6B
23	c	507	CLA	C10-C11-C12-C13
26	a	410	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	C24-C23-O48-C46
33	D	408[A]	LHG	C24-C23-O8-C6
33	E	101[A]	LHG	C1-C2-C3-O3
23	c	512	CLA	C8-C10-C11-C12
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C6-C7-C8-C10
23	C	510	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	c	510	CLA	C11-C10-C8-C7
23	d	403[B]	CLA	C11-C12-C13-C15
33	d	408[A]	LHG	O10-C23-O8-C6
35	c	519	DGD	O6D-C5D-C6D-O5D
23	B	601	CLA	CAA-CBA-CGA-O2A
23	b	601	CLA	CAA-CBA-CGA-O2A
31	e	101	LMT	C2-C3-C4-C5
35	C	518	DGD	C7A-C8A-C9A-CAA
23	c	510	CLA	C8-C10-C11-C12
26	f	102	SQD	C23-C24-C25-C26
35	C	517[A]	DGD	C1A-C2A-C3A-C4A
33	D	407[B]	LHG	C11-C10-C9-C8
33	D	408[A]	LHG	O10-C23-O8-C6
31	b	627	LMT	C6-C7-C8-C9
33	A	419[B]	LHG	C26-C27-C28-C29
35	c	517[A]	DGD	C8B-C9B-CAB-CBB
23	C	512	CLA	CBD-CGD-O2D-CED
26	A	410[A]	SQD	C34-C35-C36-C37
35	C	516[B]	DGD	CCA-CDA-CEA-CFA
40	V	201	HEC	C4B-C3B-CAB-CBB
23	B	607	CLA	C3-C5-C6-C7
26	B	620	SQD	O47-C45-C46-O48
33	E	101[A]	LHG	O7-C5-C6-O8
33	E	101[B]	LHG	O7-C5-C6-O8
35	H	102	DGD	O1G-C1G-C2G-O2G
26	b	620	SQD	C28-C29-C30-C31
32	B	621	LMG	C37-C38-C39-C40
23	C	511	CLA	CBA-CGA-O2A-C1
33	b	629[B]	LHG	C25-C26-C27-C28
33	d	407[B]	LHG	C9-C10-C11-C12
26	a	409[A]	SQD	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
35	C	517[B]	DGD	C2G-C3G-O3G-C1D
35	c	518[B]	DGD	C2G-C3G-O3G-C1D
23	C	502	CLA	C16-C17-C18-C20
23	b	612	CLA	C10-C11-C12-C13
31	b	627	LMT	O1'-C1-C2-C3
31	m	103	LMT	C7-C8-C9-C10
35	c	519	DGD	C2A-C1A-O1G-C1G
32	C	519	LMG	C29-C30-C31-C32
33	b	629[B]	LHG	C28-C29-C30-C31
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	c	510	CLA	C6-C7-C8-C9
26	A	412	SQD	O10-C23-O48-C46
35	C	518	DGD	O1A-C1A-O1G-C1G
24	a	406[A]	PHO	C8-C10-C11-C12
33	A	419[B]	LHG	C18-C19-C20-C21
35	C	518	DGD	CAA-CBA-CCA-CDA
32	c	501	LMG	C33-C34-C35-C36
35	c	519	DGD	O1A-C1A-O1G-C1G
26	A	410[B]	SQD	C11-C10-C9-C8
26	B	620	SQD	C24-C25-C26-C27
26	a	409[B]	SQD	C27-C28-C29-C30
26	b	620	SQD	C33-C34-C35-C36
23	A	406[A]	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C2B-C3B-CAB-CBB
23	C	504	CLA	C2B-C3B-CAB-CBB
23	D	403[B]	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
31	B	631	LMT	C1-C2-C3-C4
34	b	622	HTG	C1'-C2'-C3'-C4'
23	b	601	CLA	C4-C3-C5-C6
32	B	621	LMG	C32-C33-C34-C35
23	c	511	CLA	C2-C3-C5-C6
29	a	412[A]	PL9	C12-C11-C9-C8
33	d	414[A]	LHG	C34-C35-C36-C37
34	b	623	HTG	S1-C1'-C2'-C3'
33	d	408[A]	LHG	C32-C33-C34-C35
32	m	101	LMG	C11-C12-C13-C14
33	L	101[B]	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
35	c	519	DGD	CDA-CEA-CFA-CGA
23	c	512	CLA	O1A-CGA-O2A-C1
23	B	613	CLA	C2-C1-O2A-CGA
23	C	506	CLA	C2-C1-O2A-CGA
23	C	509	CLA	C2-C1-O2A-CGA
26	A	410[A]	SQD	C16-C17-C18-C19
31	b	621	LMT	C7-C8-C9-C10
35	C	518	DGD	CBA-CCA-CDA-CEA
35	C	518	DGD	C9A-CAA-CBA-CCA
23	c	504	CLA	C8-C10-C11-C12
23	C	509	CLA	O1D-CGD-O2D-CED
33	d	407[A]	LHG	O10-C23-O8-C6
33	L	101[A]	LHG	O6-C4-C5-O7
32	z	101	LMG	C20-C21-C22-C23
29	A	414[A]	PL9	C28-C29-C31-C32
32	B	621	LMG	C14-C15-C16-C17
32	B	621	LMG	C36-C37-C38-C39
33	d	407[A]	LHG	C24-C23-O8-C6
35	C	518	DGD	C2A-C1A-O1G-C1G
23	d	402[A]	CLA	C4C-C3C-CAC-CBC
35	C	518	DGD	C8A-C9A-CAA-CBA
35	h	102	DGD	CBA-CCA-CDA-CEA
35	C	516[B]	DGD	O6E-C1E-O5D-C6D
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
35	C	516[A]	DGD	C6A-C7A-C8A-C9A
31	a	415	LMT	C2'-C1'-O1'-C1
35	C	516[B]	DGD	C2E-C1E-O5D-C6D
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
33	L	101[A]	LHG	C26-C27-C28-C29
35	C	518	DGD	C7B-C8B-C9B-CAB
35	c	517[B]	DGD	C4B-C5B-C6B-C7B
33	d	414[B]	LHG	C3-O3-P-O6
33	A	419[B]	LHG	C23-C24-C25-C26
35	c	517[B]	DGD	C1A-C2A-C3A-C4A
32	z	101	LMG	C13-C14-C15-C16
33	D	407[B]	LHG	C26-C27-C28-C29
33	L	101[A]	LHG	C27-C28-C29-C30
35	C	518	DGD	CDA-CEA-CFA-CGA
35	H	102	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
29	D	406[B]	PL9	C45-C44-C46-C47
23	B	613	CLA	C11-C12-C13-C15
23	C	509	CLA	C6-C7-C8-C9
23	C	510	CLA	C11-C12-C13-C14
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
26	a	410	SQD	C26-C27-C28-C29
35	c	519	DGD	C7B-C8B-C9B-CAB
23	b	614	CLA	CBD-CGD-O2D-CED
33	D	408[A]	LHG	C27-C28-C29-C30
33	b	629[B]	LHG	C9-C10-C11-C12
23	a	404[B]	CLA	C2C-C3C-CAC-CBC
23	B	606	CLA	C15-C16-C17-C18
26	a	409[B]	SQD	C11-C12-C13-C14
31	A	417	LMT	C7-C8-C9-C10
35	H	102	DGD	CCA-CDA-CEA-CFA
35	c	517[A]	DGD	C4B-C5B-C6B-C7B
33	d	414[A]	LHG	C1-C2-C3-O3
27	d	413	GOL	O1-C1-C2-O2
23	d	402[B]	CLA	C4C-C3C-CAC-CBC
23	c	512	CLA	CBA-CGA-O2A-C1
33	d	408[A]	LHG	C33-C34-C35-C36
23	C	502	CLA	C4B-C3B-CAB-CBB
23	C	504	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
38	F	102	HEM	CAD-CBD-CGD-O1D
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
23	B	606	CLA	C8-C10-C11-C12
33	a	418[B]	LHG	C24-C25-C26-C27
33	b	629[B]	LHG	C10-C11-C12-C13
29	D	406[B]	PL9	C28-C29-C31-C32
26	A	410[A]	SQD	C11-C10-C9-C8
23	B	613	CLA	C15-C16-C17-C18
33	b	629[A]	LHG	C25-C26-C27-C28
32	Z	101	LMG	C29-C28-O8-C9
26	B	620	SQD	C29-C30-C31-C32
35	c	518[B]	DGD	C9B-CAB-CBB-CCB
23	B	611	CLA	C8-C10-C11-C12
23	C	506	CLA	C16-C17-C18-C19
31	M	101	LMT	C2-C3-C4-C5
33	D	407[A]	LHG	C11-C10-C9-C8
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
32	c	521	LMG	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
33	D	408[B]	LHG	C28-C29-C30-C31
33	a	418[A]	LHG	C24-C25-C26-C27
35	C	516[B]	DGD	C6A-C7A-C8A-C9A
35	c	518[B]	DGD	CDA-CEA-CFA-CGA
23	C	506	CLA	C3A-C2A-CAA-CBA
40	v	201	HEC	C4B-C3B-CAB-CBB
35	h	102	DGD	O2G-C1B-C2B-C3B
29	A	414[B]	PL9	C12-C11-C9-C10
29	d	406[B]	PL9	C45-C44-C46-C47
34	b	622	HTG	O5-C5-C6-O6
29	A	414[B]	PL9	C4-C3-C7-C8
29	a	412[A]	PL9	C4-C3-C7-C8
29	a	412[B]	PL9	C4-C3-C7-C8
23	B	610	CLA	C11-C12-C13-C14
23	a	405[A]	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
23	A	408	CLA	C16-C17-C18-C19
23	c	507	CLA	C13-C15-C16-C17
32	z	101	LMG	C10-C11-C12-C13
32	Z	101	LMG	C21-C22-C23-C24
33	b	629[B]	LHG	C34-C35-C36-C37
35	c	518[A]	DGD	C7B-C8B-C9B-CAB
33	L	101[A]	LHG	C23-C24-C25-C26
24	a	406[B]	PHO	C2C-C3C-CAC-CBC
24	A	407[B]	PHO	O2A-C1-C2-C3
32	B	621	LMG	O6-C1-O1-C7
29	A	414[B]	PL9	C39-C41-C42-C43
33	A	419[B]	LHG	C17-C18-C19-C20
23	b	601	CLA	C3-C5-C6-C7
23	b	610	CLA	C13-C15-C16-C17
23	d	402[A]	CLA	C15-C16-C17-C18
33	a	418[B]	LHG	C7-C8-C9-C10
26	A	410[A]	SQD	C13-C14-C15-C16
23	c	509	CLA	C1A-C2A-CAA-CBA
32	d	412	LMG	C13-C14-C15-C16
23	B	613	CLA	C11-C10-C8-C7
23	B	613	CLA	C12-C13-C15-C16
23	C	513	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C6-C7-C8-C10
23	b	607	CLA	C12-C13-C15-C16
23	b	608	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a	412[B]	PL9	C43-C44-C46-C47
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
23	c	511	CLA	O1A-CGA-O2A-C1
33	A	419[A]	LHG	C18-C19-C20-C21
33	b	629[A]	LHG	C17-C18-C19-C20
38	F	102	HEM	CAD-CBD-CGD-O2D
23	b	608	CLA	C16-C17-C18-C20
32	B	621	LMG	O8-C28-C29-C30
32	c	501	LMG	O8-C28-C29-C30
38	f	101	HEM	CAD-CBD-CGD-O1D
33	A	419[B]	LHG	C35-C36-C37-C38
33	D	407[A]	LHG	C26-C27-C28-C29
32	d	412	LMG	C35-C36-C37-C38
33	d	407[A]	LHG	C16-C17-C18-C19
29	a	412[B]	PL9	C45-C44-C46-C47
29	d	406[A]	PL9	C43-C44-C46-C47
23	C	512	CLA	C2B-C3B-CAB-CBB
26	a	409[B]	SQD	C35-C36-C37-C38
33	A	419[B]	LHG	C29-C30-C31-C32
33	A	419[B]	LHG	C32-C33-C34-C35
35	C	517[B]	DGD	C1A-C2A-C3A-C4A
23	a	404[B]	CLA	C4C-C3C-CAC-CBC
32	c	501	LMG	O7-C8-C9-O8
33	b	629[B]	LHG	C31-C32-C33-C34
35	h	102	DGD	C7A-C8A-C9A-CAA
31	B	628	LMT	C4-C5-C6-C7
23	A	406[A]	CLA	C16-C17-C18-C19
32	C	520	LMG	C38-C39-C40-C41
35	C	518	DGD	C6A-C7A-C8A-C9A
29	A	414[A]	PL9	C39-C41-C42-C43
33	d	414[B]	LHG	C1-C2-C3-O3
23	C	512	CLA	O1D-CGD-O2D-CED
29	D	406[B]	PL9	C35-C34-C36-C37
29	a	412[A]	PL9	C45-C44-C46-C47
23	a	404[B]	CLA	C2-C1-O2A-CGA
23	c	513	CLA	C2-C1-O2A-CGA
29	D	406[B]	PL9	C43-C44-C46-C47
23	D	404	CLA	C8-C10-C11-C12
23	b	605	CLA	C13-C15-C16-C17
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
23	D	403[B]	CLA	C16-C17-C18-C20
23	B	603	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	C	512	CLA	C6-C7-C8-C9
23	b	605	CLA	C6-C7-C8-C9
23	b	614	CLA	C11-C12-C13-C14
23	C	509	CLA	C3-C5-C6-C7
40	V	201	HEC	CAD-CBD-CGD-O1D
32	z	101	LMG	O7-C10-C11-C12
33	A	419[A]	LHG	C29-C30-C31-C32
33	E	101[B]	LHG	C11-C10-C9-C8
35	c	517[A]	DGD	CAB-CBB-CCB-CDB
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
25	C	514	BCR	C23-C24-C25-C30
25	a	408	BCR	C1-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C30
25	t	102	BCR	C5-C6-C7-C8
25	y	101	BCR	C23-C24-C25-C30
26	A	410[B]	SQD	C16-C17-C18-C19
32	A	418	LMG	O1-C7-C8-C9
40	V	201	HEC	CAD-CBD-CGD-O2D
27	l	102[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
31	e	101	LMT	C2B-C1B-O1B-C4'
29	D	406[A]	PL9	C35-C34-C36-C37
29	a	412[B]	PL9	C35-C34-C36-C37
25	d	405	BCR	C7-C8-C9-C10
23	b	601	CLA	C2-C3-C5-C6
29	a	412[A]	PL9	C43-C44-C46-C47
23	C	510	CLA	C8-C10-C11-C12
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
31	e	101	LMT	O1'-C1-C2-C3
33	L	101[B]	LHG	C11-C12-C13-C14
23	A	404[A]	CLA	C16-C17-C18-C19
33	A	419[A]	LHG	C35-C36-C37-C38
33	D	407[B]	LHG	C32-C33-C34-C35
33	d	414[B]	LHG	C18-C19-C20-C21
33	b	629[A]	LHG	C10-C11-C12-C13
33	d	414[B]	LHG	C34-C35-C36-C37
32	C	520	LMG	C4-C5-C6-O5
23	C	506	CLA	C4-C3-C5-C6
23	B	603	CLA	C11-C12-C13-C15
23	a	405[A]	CLA	C6-C7-C8-C10
23	b	615	CLA	C11-C12-C13-C15
23	c	503	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
38	f	101	HEM	CAA-CBA-CGA-O2A
33	L	101[A]	LHG	C16-C17-C18-C19
35	c	519	DGD	C9B-CAB-CBB-CCB
27	D	413	GOL	O1-C1-C2-O2
27	a	416	GOL	O1-C1-C2-O2
27	d	413	GOL	O2-C2-C3-O3
25	a	408	BCR	C19-C20-C21-C22
32	B	621	LMG	C2-C1-O1-C7
32	Z	101	LMG	C2-C1-O1-C7
32	A	418	LMG	O1-C7-C8-O7
23	b	616	CLA	C5-C6-C7-C8
26	a	410	SQD	C24-C25-C26-C27
35	C	518	DGD	C4A-C5A-C6A-C7A
33	A	419[A]	LHG	O8-C23-C24-C25
23	b	616	CLA	C4-C3-C5-C6
23	c	505	CLA	C4-C3-C5-C6
29	D	406[B]	PL9	C20-C19-C21-C22
23	B	610	CLA	C13-C15-C16-C17
23	b	608	CLA	C13-C15-C16-C17
31	A	417	LMT	C9-C10-C11-C12
23	c	514	CLA	C2-C3-C5-C6
29	d	406[B]	PL9	C43-C44-C46-C47
35	c	518[A]	DGD	C9B-CAB-CBB-CCB
32	Z	101	LMG	O7-C10-C11-C12
33	d	414[B]	LHG	C13-C14-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	B	615	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	a	405[A]	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
23	b	608	CLA	C14-C13-C15-C16
23	c	503	CLA	C11-C12-C13-C14
23	c	506	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C14
40	v	201	HEC	CAD-CBD-CGD-O2D
31	t	101	LMT	C2-C3-C4-C5
23	C	510	CLA	CAA-CBA-CGA-O2A
23	C	512	CLA	CAA-CBA-CGA-O2A
23	c	511	CLA	CAA-CBA-CGA-O2A
23	A	404[B]	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	B	612	CLA	CAD-CBD-CGD-O2D
23	C	512	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	c	502	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
24	a	406[B]	PHO	CAD-CBD-CGD-O2D
24	a	414[A]	PHO	CAD-CBD-CGD-O2D
38	F	102	HEM	C2B-C3B-CAB-CBB
23	D	403[B]	CLA	C16-C17-C18-C19
33	D	408[A]	LHG	C28-C29-C30-C31
23	B	605	CLA	C8-C10-C11-C12
31	t	101	LMT	C11-C10-C9-C8
33	b	629[A]	LHG	C30-C31-C32-C33
33	b	629[B]	LHG	C17-C18-C19-C20
23	B	613	CLA	CAA-CBA-CGA-O2A
33	L	101[A]	LHG	O7-C7-C8-C9
33	a	418[A]	LHG	O8-C23-C24-C25
33	a	418[B]	LHG	O8-C23-C24-C25
26	f	102	SQD	C34-C35-C36-C37
29	A	414[A]	PL9	C25-C24-C26-C27
38	f	101	HEM	CAA-CBA-CGA-O1A
38	f	101	HEM	CAD-CBD-CGD-O2D
26	A	412	SQD	C9-C10-C11-C12
23	b	616	CLA	C2-C3-C5-C6
33	b	629[B]	LHG	O7-C7-C8-C9
32	B	621	LMG	O1-C7-C8-C9
33	D	407[B]	LHG	C34-C35-C36-C37
35	C	518	DGD	O6D-C5D-C6D-O5D
33	E	101[B]	LHG	O7-C7-C8-C9
33	L	101[B]	LHG	O7-C7-C8-C9
33	b	629[A]	LHG	O7-C7-C8-C9
33	d	408[B]	LHG	C32-C33-C34-C35
33	d	408[B]	LHG	C33-C34-C35-C36
23	A	404[A]	CLA	C15-C16-C17-C18
23	B	602	CLA	O2A-C1-C2-C3
23	C	509	CLA	O2A-C1-C2-C3
24	A	407[A]	PHO	O2A-C1-C2-C3
24	a	406[B]	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	D	404	CLA	O1A-CGA-O2A-C1
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
32	B	621	LMG	C20-C21-C22-C23
38	F	102	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4B-C3B-CAB-CBB
32	c	520	LMG	O7-C10-C11-C12
40	v	201	HEC	CAD-CBD-CGD-O1D
26	A	410[B]	SQD	C13-C14-C15-C16
32	c	520	LMG	C35-C36-C37-C38
26	B	620	SQD	C31-C32-C33-C34
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-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	C	504	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
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
31	A	420	LMT	C7-C8-C9-C10
23	b	613	CLA	CAA-CBA-CGA-O2A
35	C	518	DGD	O1G-C1A-C2A-C3A
33	A	419[A]	LHG	C17-C18-C19-C20
33	d	414[A]	LHG	C13-C14-C15-C16
26	F	103	SQD	O47-C45-C46-O48
35	C	517[A]	DGD	CAB-CBB-CCB-CDB
26	B	620	SQD	C12-C13-C14-C15
23	c	513	CLA	CAA-CBA-CGA-O2A
33	A	419[B]	LHG	O8-C23-C24-C25
33	d	408[B]	LHG	C30-C31-C32-C33
35	c	517[B]	DGD	C7B-C8B-C9B-CAB
23	B	606	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
24	A	416[B]	PHO	CHA-CBD-CGD-O1D
24	A	416[B]	PHO	CHA-CBD-CGD-O2D
23	b	604	CLA	C10-C11-C12-C13
23	c	511	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C31-C32-C33-C34
23	B	602	CLA	C6-C7-C8-C10
23	B	615	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
23	d	402[A]	CLA	C11-C12-C13-C15
29	A	414[B]	PL9	C28-C29-C31-C32
29	A	414[A]	PL9	C4-C3-C7-C8
32	c	521	LMG	C32-C33-C34-C35
33	A	419[B]	LHG	C9-C10-C11-C12
23	A	408	CLA	C14-C13-C15-C16
23	B	614	CLA	C6-C7-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C14
23	b	614	CLA	C14-C13-C15-C16
29	d	406[B]	PL9	C34-C36-C37-C38
35	C	518	DGD	C2A-C3A-C4A-C5A
23	b	615	CLA	C5-C6-C7-C8
26	a	409[B]	SQD	C10-C11-C12-C13
33	d	414[A]	LHG	C18-C19-C20-C21
29	D	406[B]	PL9	C36-C37-C38-C39
32	Z	101	LMG	O9-C10-C11-C12
33	b	629[A]	LHG	C24-C25-C26-C27
35	C	517[B]	DGD	C3A-C4A-C5A-C6A
23	c	508	CLA	C8-C10-C11-C12
23	C	501	CLA	C16-C17-C18-C20
33	d	407[B]	LHG	C25-C26-C27-C28
27	l	102[A]	GOL	C1-C2-C3-O3
27	o	303	GOL	O1-C1-C2-C3
29	D	406[A]	PL9	C28-C29-C31-C32
33	E	101[B]	LHG	O8-C23-C24-C25
35	c	519	DGD	C6B-C7B-C8B-C9B
33	b	629[B]	LHG	O6-C4-C5-O7
23	b	604	CLA	C13-C15-C16-C17
33	D	408[B]	LHG	C27-C28-C29-C30
35	h	102	DGD	CCB-CDB-CEB-CFB
23	c	512	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	A	410[B]	SQD	C18-C19-C20-C21
33	A	419[A]	LHG	O10-C23-C24-C25
32	d	412	LMG	C19-C20-C21-C22
33	d	408[B]	LHG	C11-C10-C9-C8
23	C	513	CLA	C2-C1-O2A-CGA
23	C	512	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
33	L	101[B]	LHG	O9-C7-C8-C9
33	a	418[A]	LHG	O10-C23-C24-C25
33	b	629[A]	LHG	O9-C7-C8-C9
32	C	519	LMG	O1-C7-C8-C9
35	c	517[A]	DGD	O2G-C1B-C2B-C3B
32	C	519	LMG	C12-C13-C14-C15
23	B	614	CLA	C2A-CAA-CBA-CGA
23	a	404[B]	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
23	A	404[B]	CLA	C16-C17-C18-C19
23	C	510	CLA	CAA-CBA-CGA-O1A
33	a	418[B]	LHG	O10-C23-C24-C25
23	A	404[B]	CLA	C4C-C3C-CAC-CBC
32	m	101	LMG	C32-C33-C34-C35
33	E	101[A]	LHG	O7-C7-C8-C9
23	A	404[B]	CLA	C15-C16-C17-C18
23	B	612	CLA	O1A-CGA-O2A-C1
23	a	407	CLA	C15-C16-C17-C18
23	B	610	CLA	C4B-C3B-CAB-CBB
23	C	512	CLA	C4B-C3B-CAB-CBB
33	d	407[A]	LHG	C4-O6-P-O5
33	d	414[B]	LHG	C3-O3-P-O5
32	m	101	LMG	C30-C31-C32-C33
35	c	519	DGD	CDB-CEB-CFB-CGB
23	A	404[B]	CLA	C2C-C3C-CAC-CBC
26	A	412	SQD	C15-C16-C17-C18
32	c	521	LMG	C28-C29-C30-C31
32	c	520	LMG	O9-C10-C11-C12
33	E	101[B]	LHG	O9-C7-C8-C9
33	L	101[A]	LHG	O9-C7-C8-C9
33	b	629[B]	LHG	O9-C7-C8-C9
23	b	616	CLA	O1A-CGA-O2A-C1
33	D	408[B]	LHG	O8-C23-C24-C25
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
35	c	517[A]	DGD	C1A-C2A-C3A-C4A

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	CAA-CBA-CGA-O1A
35	C	517[B]	DGD	O2G-C1B-C2B-C3B
32	C	520	LMG	C11-C12-C13-C14
35	C	516[B]	DGD	C1B-C2B-C3B-C4B
35	C	518	DGD	O1A-C1A-C2A-C3A
29	d	406[A]	PL9	C11-C12-C13-C14
32	c	501	LMG	C4-C5-C6-O5
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	C7-C8-C9-C10
26	a	409[A]	SQD	C10-C11-C12-C13
35	c	519	DGD	C6A-C7A-C8A-C9A
23	B	605	CLA	C5-C6-C7-C8
31	A	417	LMT	C2B-C1B-O1B-C4'
23	a	405[B]	CLA	C14-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C14
32	c	501	LMG	C14-C15-C16-C17
23	c	513	CLA	CAA-CBA-CGA-O1A
31	a	415	LMT	C7-C8-C9-C10
23	B	612	CLA	CBA-CGA-O2A-C1
33	D	408[A]	LHG	O8-C23-C24-C25
35	c	517[B]	DGD	O2G-C1B-C2B-C3B
32	c	520	LMG	C30-C31-C32-C33
23	b	611	CLA	C13-C15-C16-C17
32	c	521	LMG	C16-C17-C18-C19
26	f	102	SQD	C28-C29-C30-C31
23	b	602	CLA	C2A-CAA-CBA-CGA
32	D	412	LMG	O7-C10-C11-C12
26	a	409[B]	SQD	C18-C19-C20-C21
26	a	409[A]	SQD	C19-C20-C21-C22
29	D	406[A]	PL9	C40-C39-C41-C42
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
23	B	615	CLA	C11-C12-C13-C15
23	C	505	CLA	C12-C13-C15-C16
23	C	509	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C10-C8-C7
33	A	419[B]	LHG	O10-C23-C24-C25
35	c	517[B]	DGD	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
26	A	412	SQD	O48-C23-C24-C25
33	E	101[A]	LHG	O8-C23-C24-C25
35	C	517[A]	DGD	O2G-C1B-C2B-C3B
26	f	102	SQD	C26-C27-C28-C29
32	D	412	LMG	C16-C17-C18-C19
33	D	407[A]	LHG	C28-C29-C30-C31
33	D	408[A]	LHG	O10-C23-C24-C25
33	E	101[B]	LHG	O10-C23-C24-C25
35	c	517[A]	DGD	O1B-C1B-C2B-C3B
25	H	101	BCR	C9-C10-C11-C12
32	A	418	LMG	C31-C32-C33-C34
35	C	517[A]	DGD	C3A-C4A-C5A-C6A
23	c	502	CLA	CAA-CBA-CGA-O2A
26	a	410	SQD	O48-C23-C24-C25
32	c	521	LMG	O7-C10-C11-C12
33	d	408[B]	LHG	O8-C23-C24-C25
32	c	520	LMG	C32-C33-C34-C35
23	b	602	CLA	C8-C10-C11-C12
23	b	613	CLA	CAA-CBA-CGA-O1A
34	B	623	HTG	C2'-C3'-C4'-C5'
26	A	412	SQD	O10-C23-C24-C25
33	E	101[A]	LHG	O9-C7-C8-C9
33	E	101[A]	LHG	O10-C23-C24-C25
23	B	603	CLA	C2A-CAA-CBA-CGA
23	C	509	CLA	C8-C10-C11-C12
23	b	616	CLA	CBA-CGA-O2A-C1
32	c	521	LMG	O9-C10-C11-C12
35	C	517[A]	DGD	O1B-C1B-C2B-C3B
35	C	517[B]	DGD	O1B-C1B-C2B-C3B
32	m	101	LMG	C40-C41-C42-C43

There are no ring outliers.

170 monomers are involved in 371 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	612	CLA	1	0
23	d	403[B]	CLA	5	0
24	a	414[A]	PHO	2	0
35	C	517[B]	DGD	1	0
23	C	510	CLA	4	0
23	A	404[B]	CLA	4	0
23	c	513	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	412[B]	PL9	4	0
23	d	404	CLA	2	0
32	d	412	LMG	3	0
38	f	101	HEM	1	0
23	b	615	CLA	1	0
23	B	604	CLA	1	0
33	a	418[A]	LHG	4	0
33	A	419[B]	LHG	1	0
23	C	504	CLA	1	0
23	c	508	CLA	2	0
24	A	416[A]	PHO	1	0
31	M	101	LMT	2	0
23	B	609	CLA	2	0
31	B	630	LMT	1	0
32	Z	101	LMG	1	0
33	a	418[B]	LHG	4	0
25	A	409	BCR	2	0
25	k	101	BCR	2	0
31	t	101	LMT	2	0
35	C	517[A]	DGD	2	0
35	c	519	DGD	2	0
24	A	407[B]	PHO	1	0
31	A	417	LMT	1	0
24	A	416[B]	PHO	3	0
23	c	510	CLA	4	0
23	C	513	CLA	1	0
40	V	201	HEC	1	0
23	A	406[A]	CLA	1	0
26	a	410	SQD	2	0
27	a	417	GOL	4	0
27	B	624	GOL	1	0
23	a	404[A]	CLA	3	0
25	T	101	BCR	6	0
33	A	419[A]	LHG	2	0
35	H	102	DGD	1	0
23	D	403[A]	CLA	3	0
31	B	631	LMT	1	0
23	C	505	CLA	6	0
23	A	406[B]	CLA	1	0
23	C	501	CLA	5	0
25	b	618	BCR	4	0
26	F	103	SQD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	c	522	HTG	1	0
31	M	102	LMT	1	0
33	D	407[A]	LHG	2	0
23	c	507	CLA	4	0
25	C	515	BCR	1	0
23	a	404[B]	CLA	4	0
29	A	414[A]	PL9	10	0
23	C	506	CLA	5	0
23	D	403[B]	CLA	3	0
23	b	604	CLA	4	0
24	A	407[A]	PHO	2	0
23	B	616	CLA	4	0
23	c	503	CLA	2	0
25	Y	101	BCR	2	0
33	D	407[B]	LHG	1	0
34	B	622	HTG	2	0
34	b	622	HTG	3	0
23	B	614	CLA	2	0
23	a	407	CLA	5	0
26	a	409[A]	SQD	4	0
23	c	505	CLA	2	0
23	B	605	CLA	4	0
27	O	303	GOL	3	0
29	A	414[B]	PL9	9	0
25	B	619	BCR	2	0
25	b	619	BCR	4	0
23	C	503	CLA	6	0
33	D	408[A]	LHG	6	0
33	d	408[A]	LHG	9	0
31	A	420	LMT	1	0
23	B	602	CLA	2	0
34	b	625	HTG	1	0
23	C	508	CLA	5	0
38	F	102	HEM	1	0
23	b	612	CLA	1	0
23	A	405[A]	CLA	4	0
25	D	405	BCR	1	0
27	v	202[A]	GOL	1	0
23	b	616	CLA	1	0
31	a	415	LMT	1	0
26	a	409[B]	SQD	3	0
23	b	614	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	502	CLA	3	0
23	B	613	CLA	5	0
33	D	408[B]	LHG	3	0
33	d	408[B]	LHG	7	0
25	c	515	BCR	3	0
23	c	504	CLA	3	0
35	C	518	DGD	3	0
23	c	512	CLA	5	0
23	A	405[B]	CLA	6	0
26	A	412	SQD	1	0
27	a	416	GOL	2	0
23	C	509	CLA	2	0
27	v	202[B]	GOL	2	0
23	C	502	CLA	3	0
27	l	102[A]	GOL	1	0
25	y	101	BCR	2	0
25	h	101	BCR	3	0
33	d	407[A]	LHG	3	0
23	A	408	CLA	3	0
25	H	101	BCR	1	0
23	b	609	CLA	4	0
23	b	607	CLA	3	0
23	B	601	CLA	3	0
26	b	620	SQD	4	0
23	b	601	CLA	2	0
27	l	102[B]	GOL	1	0
27	D	402	GOL	5	0
23	c	511	CLA	1	0
23	c	509	CLA	9	0
32	B	621	LMG	1	0
23	a	405[B]	CLA	3	0
33	d	407[B]	LHG	3	0
23	b	613	CLA	4	0
25	t	102	BCR	6	0
32	c	520	LMG	1	0
23	C	511	CLA	3	0
27	b	624	GOL	1	0
33	E	101[A]	LHG	5	0
32	C	520	LMG	2	0
23	B	615	CLA	6	0
25	B	617	BCR	2	0
26	A	410[A]	SQD	2	0

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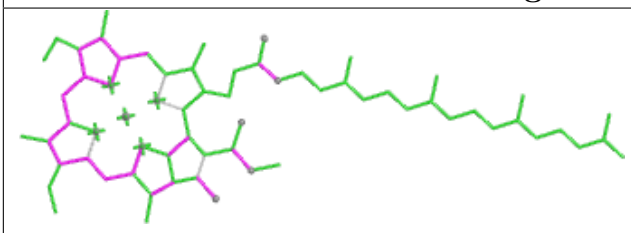
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	b	617	BCR	1	0
23	C	507	CLA	2	0
25	B	618	BCR	4	0
23	b	606	CLA	3	0
23	B	606	CLA	2	0
23	C	512	CLA	2	0
27	O	302	GOL	1	0
33	E	101[B]	LHG	3	0
31	b	621	LMT	1	0
23	c	514	CLA	2	0
27	D	413	GOL	3	0
25	d	405	BCR	2	0
26	A	410[B]	SQD	1	0
32	c	521	LMG	1	0
23	a	405[A]	CLA	2	0
23	d	402[A]	CLA	2	0
35	c	517[A]	DGD	2	0
35	c	518[A]	DGD	1	0
35	C	516[A]	DGD	2	0
23	d	403[A]	CLA	2	0
26	B	620	SQD	1	0
25	C	514	BCR	1	0
25	a	408	BCR	1	0
23	b	605	CLA	5	0
32	z	101	LMG	2	0
23	A	404[A]	CLA	5	0
29	a	412[A]	PL9	4	0
23	d	402[B]	CLA	4	0
24	a	406[B]	PHO	1	0
23	c	506	CLA	4	0
33	d	414[B]	LHG	1	0
25	K	102	BCR	1	0
34	B	625	HTG	1	0
35	c	517[B]	DGD	1	0
35	c	518[B]	DGD	1	0
31	e	101	LMT	1	0
35	C	516[B]	DGD	3	0

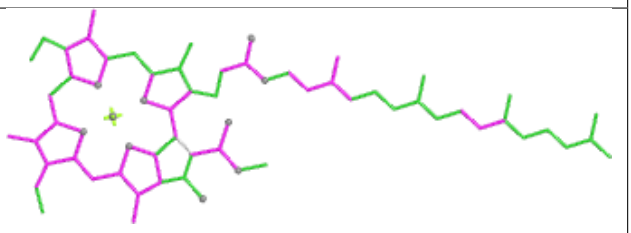
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

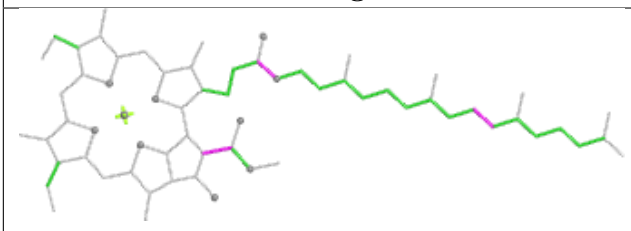
Ligand CLA B 612



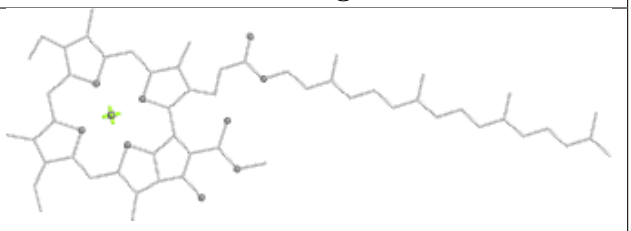
Bond lengths



Bond angles

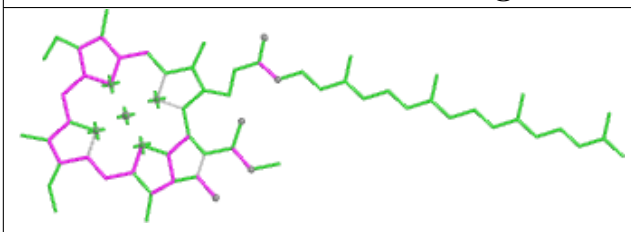


Torsions

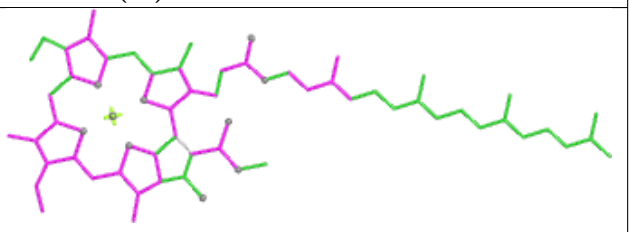


Rings

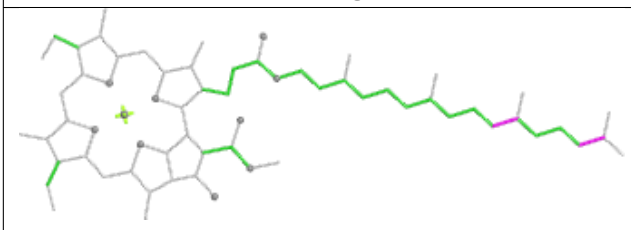
Ligand CLA d 403 (B)



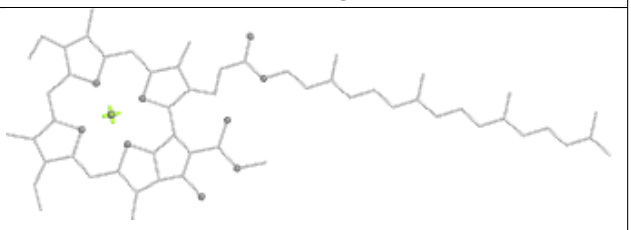
Bond lengths



Bond angles

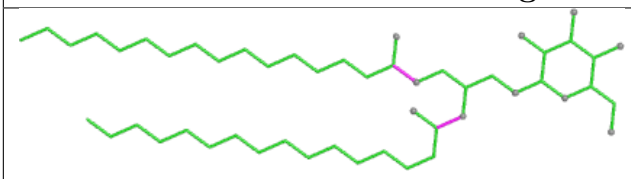


Torsions

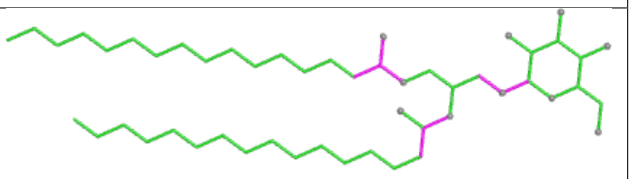


Rings

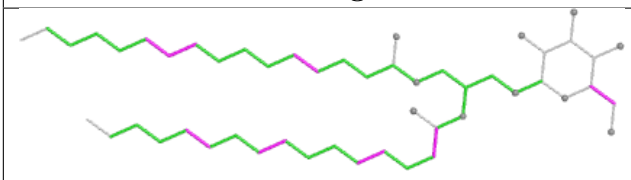
Ligand LMG D 412



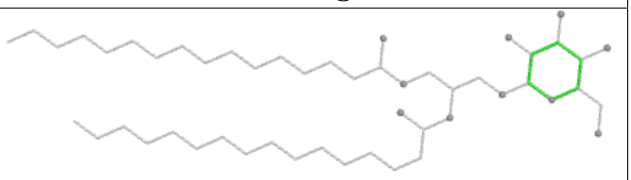
Bond lengths



Bond angles

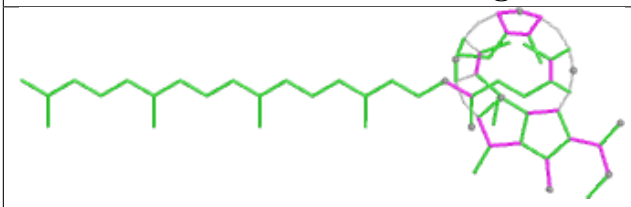


Torsions

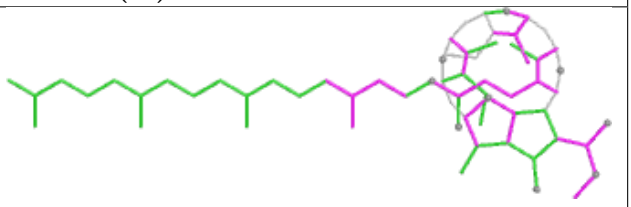


Rings

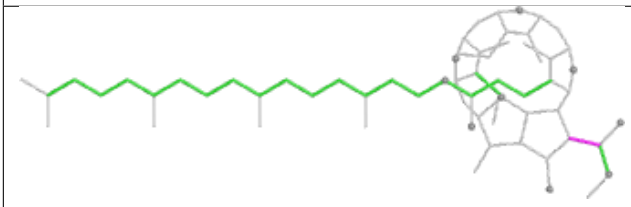
Ligand PHO a 414 (A)



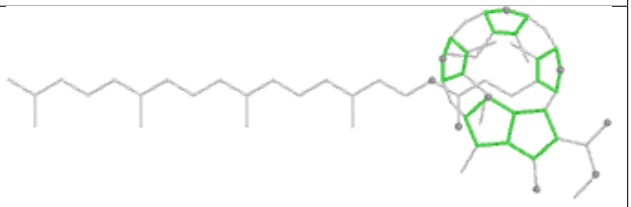
Bond lengths



Bond angles

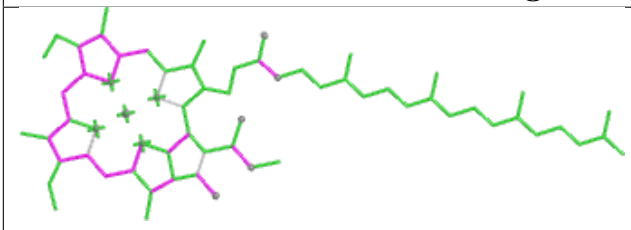


Torsions



Rings

Ligand CLA B 603



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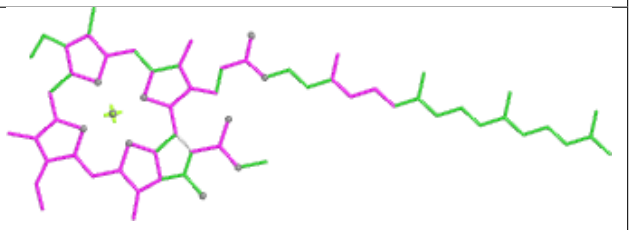

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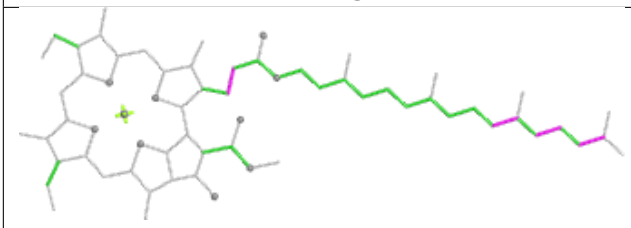

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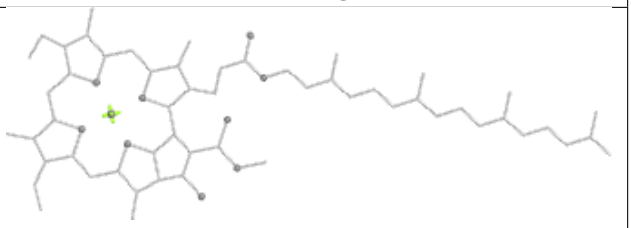
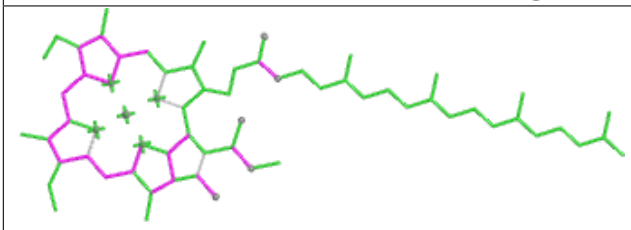


Rings

Ligand CLA b 603



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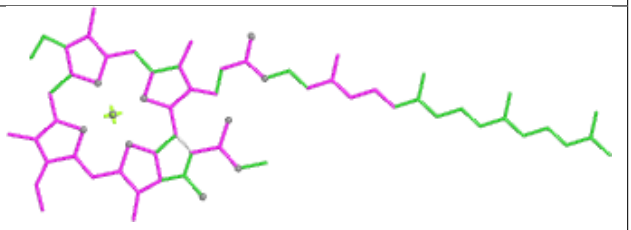

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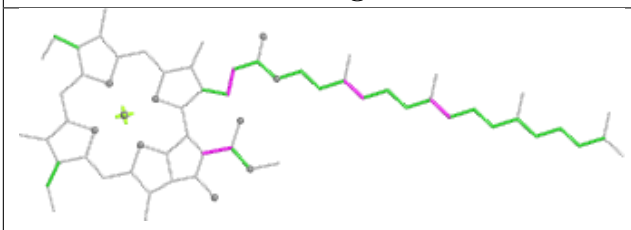

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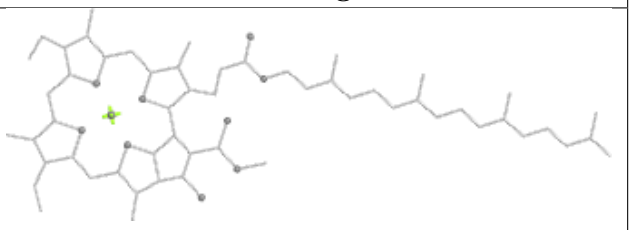
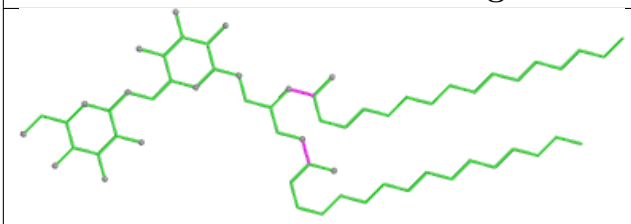


Rings

Ligand DGD C 517 (B)



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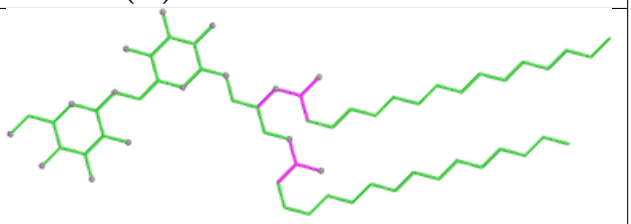
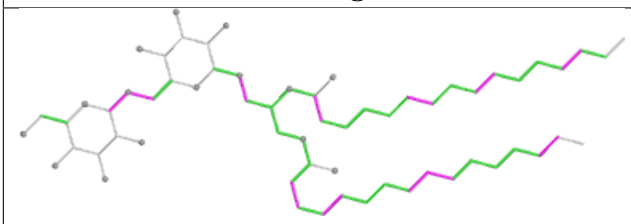


Bond angles



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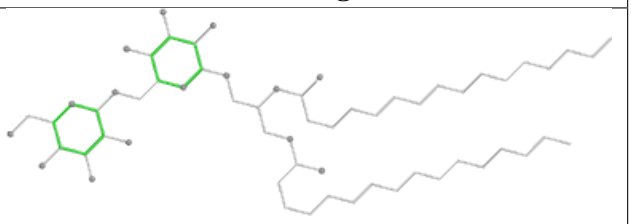
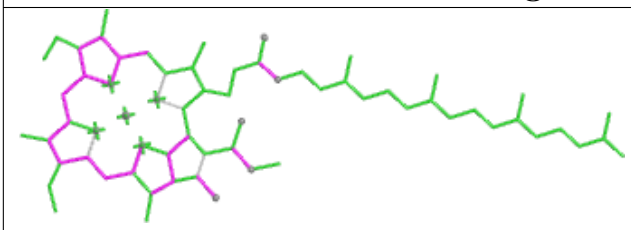


Rings

Ligand CLA C 510



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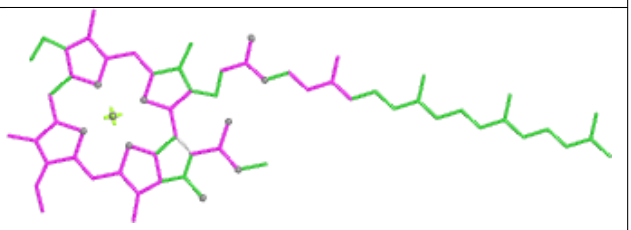
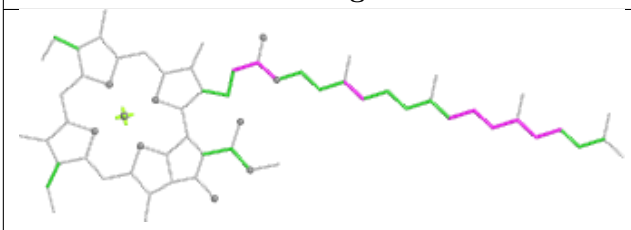


Bond angles



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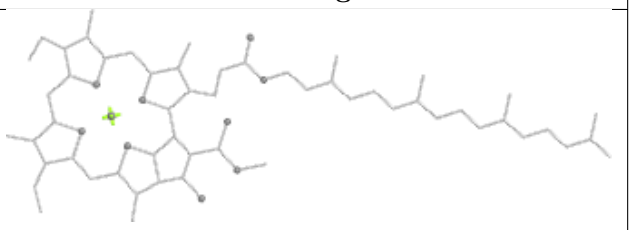
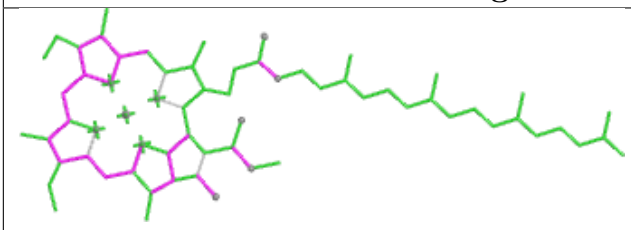


Rings

Ligand CLA A 404 (B)



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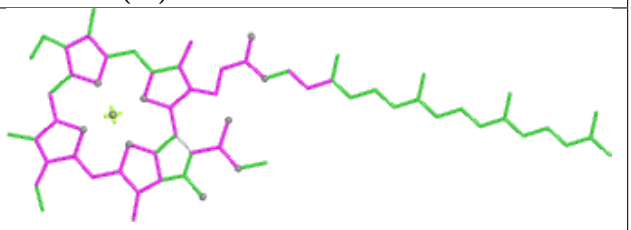
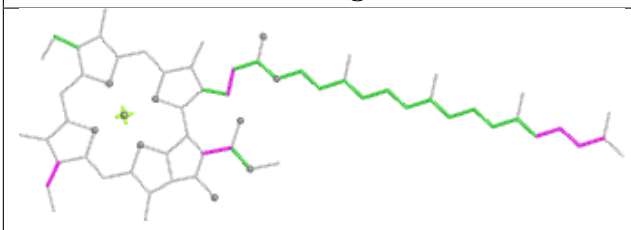


Bond angles



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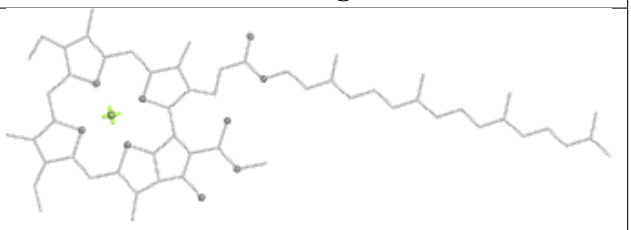
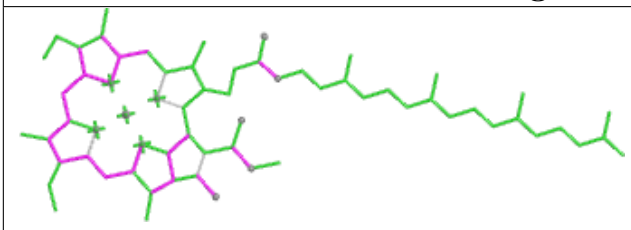


Rings

Ligand CLA c 513



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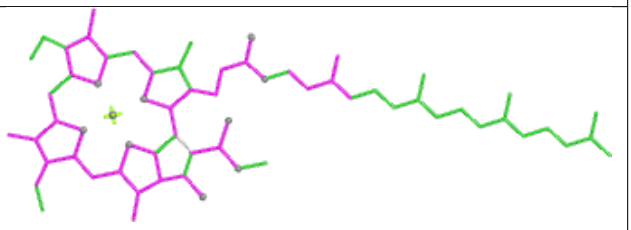
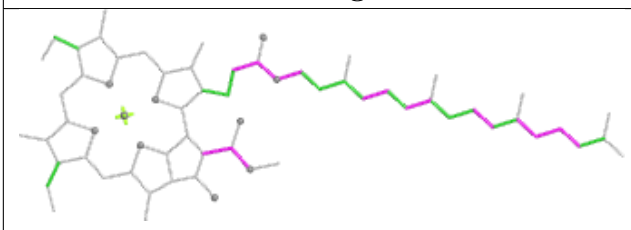


Bond angles



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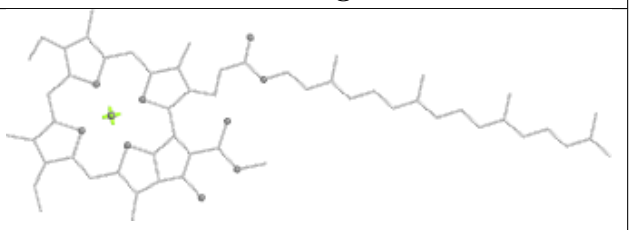
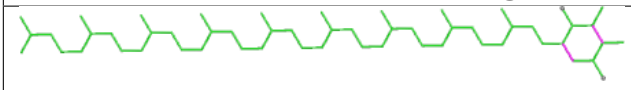


Rings

Ligand PL9 a 412 (B)



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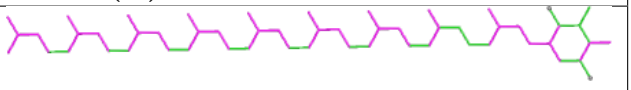
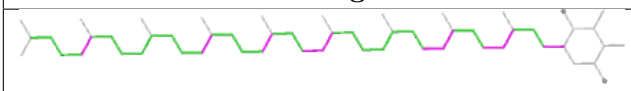


Bond angles



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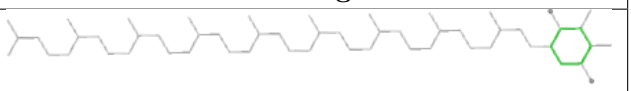
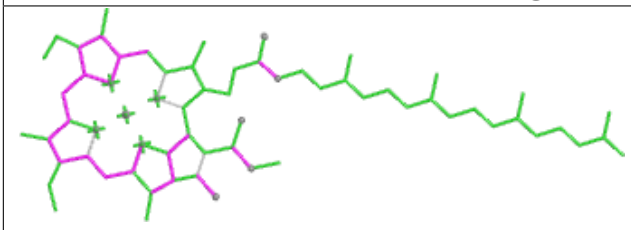


Rings

Ligand CLA d 404



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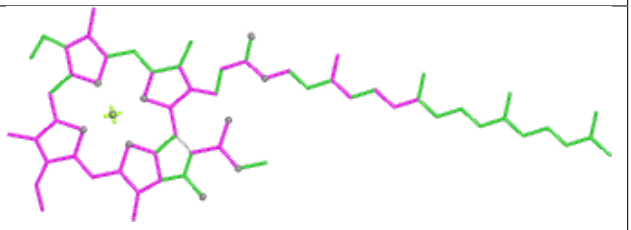
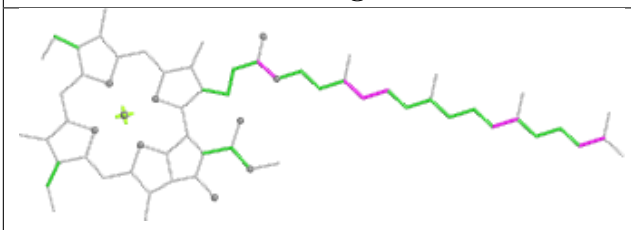


Bond angles



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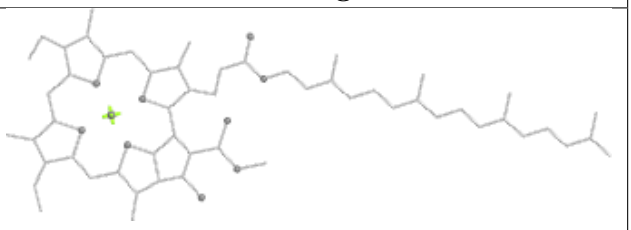
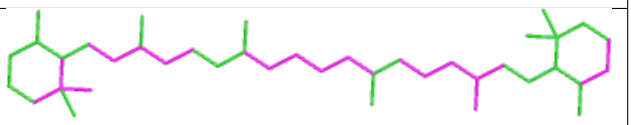


Rings

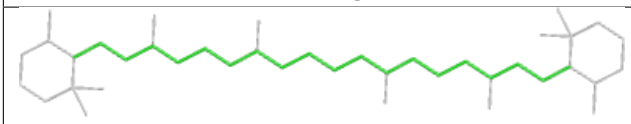
Ligand BCR c 516



Bond lengths



Bond angles



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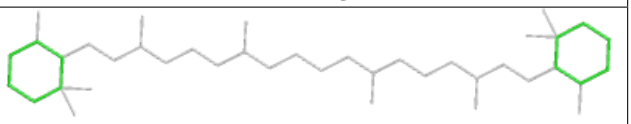
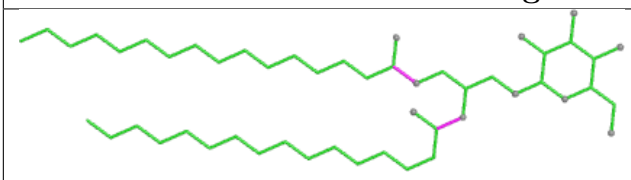


Rings

Ligand LMG d 412



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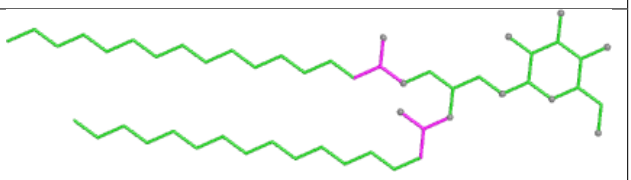
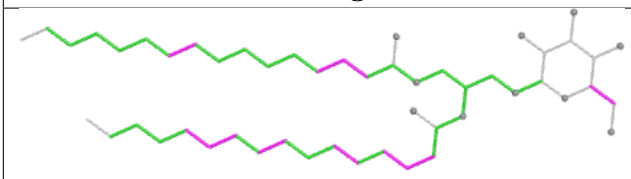


Bond angles



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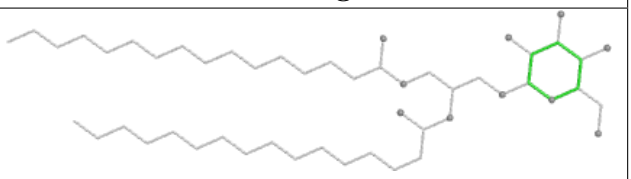
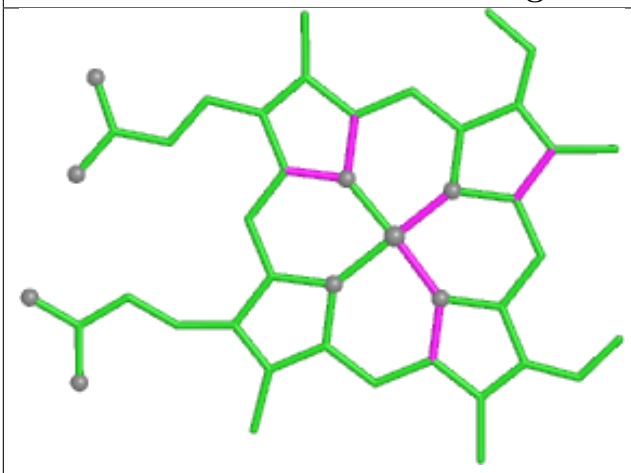
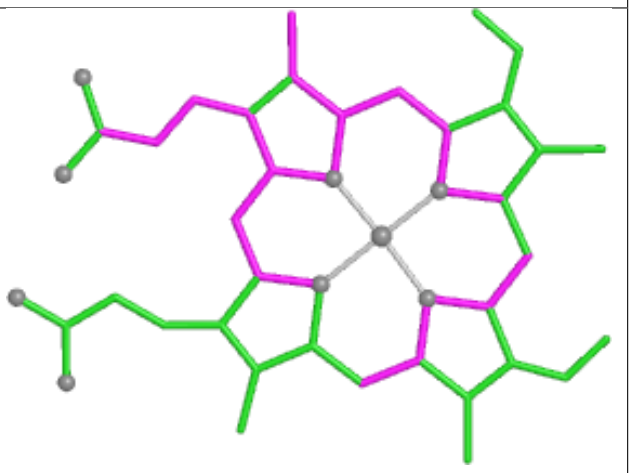


Rings

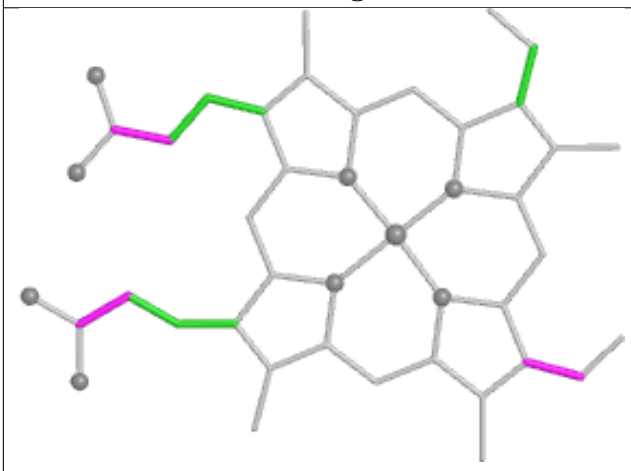
Ligand HEM f 101



Bond lengths



Bond angles



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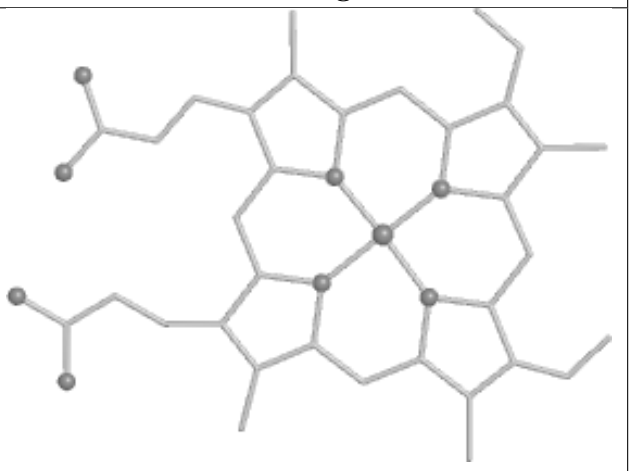
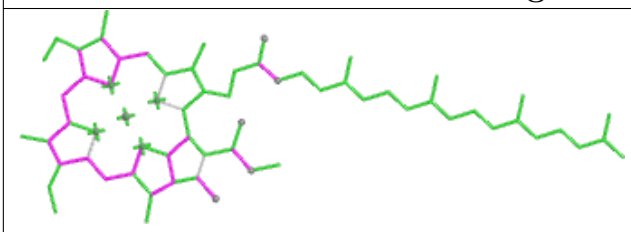
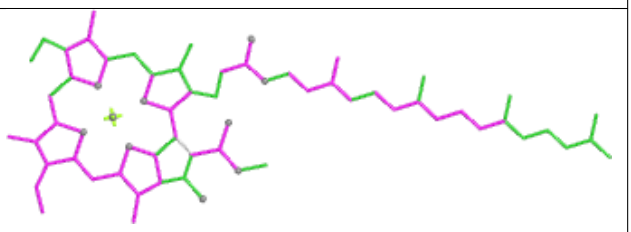


Rings

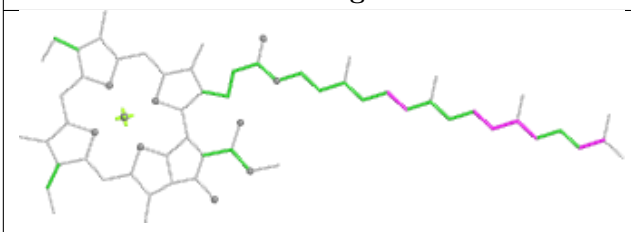
Ligand CLA b 615



Bond lengths



Bond angles



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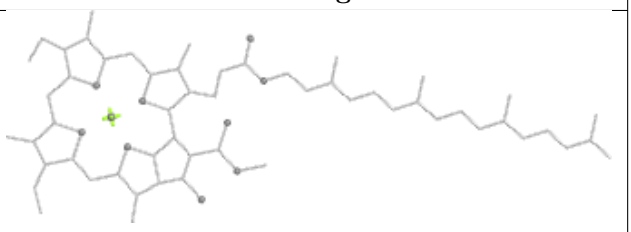
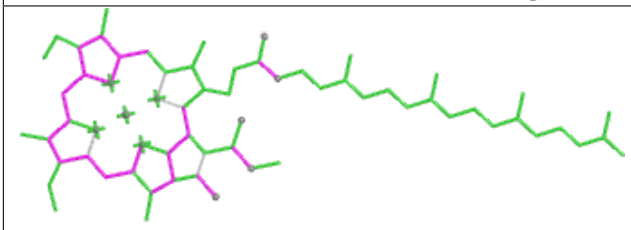
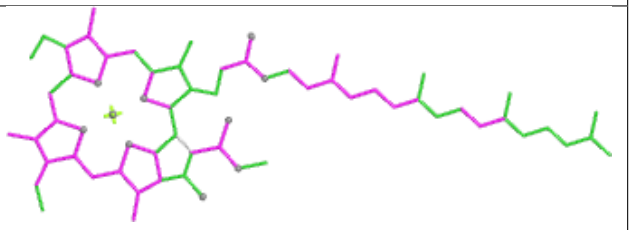


Rings

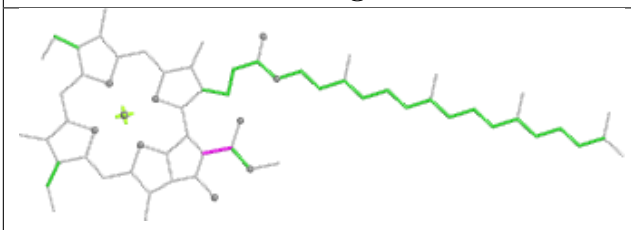
Ligand CLA B 604



Bond lengths



Bond angles



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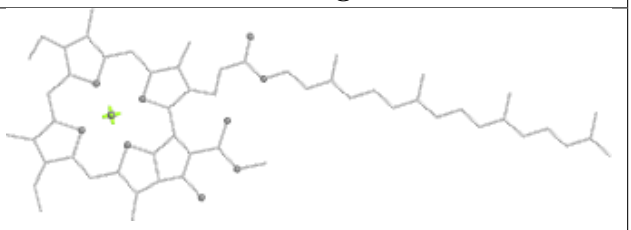


Rings

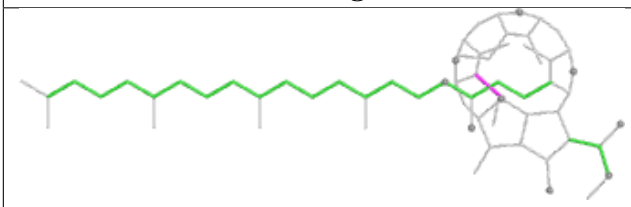
Ligand PHO a 414 (B)



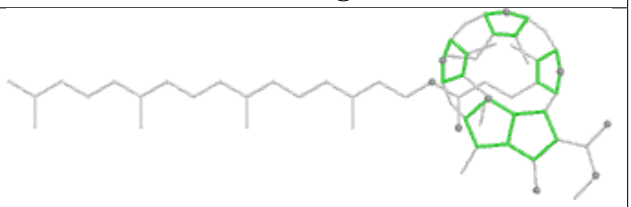
Bond lengths



Bond angles

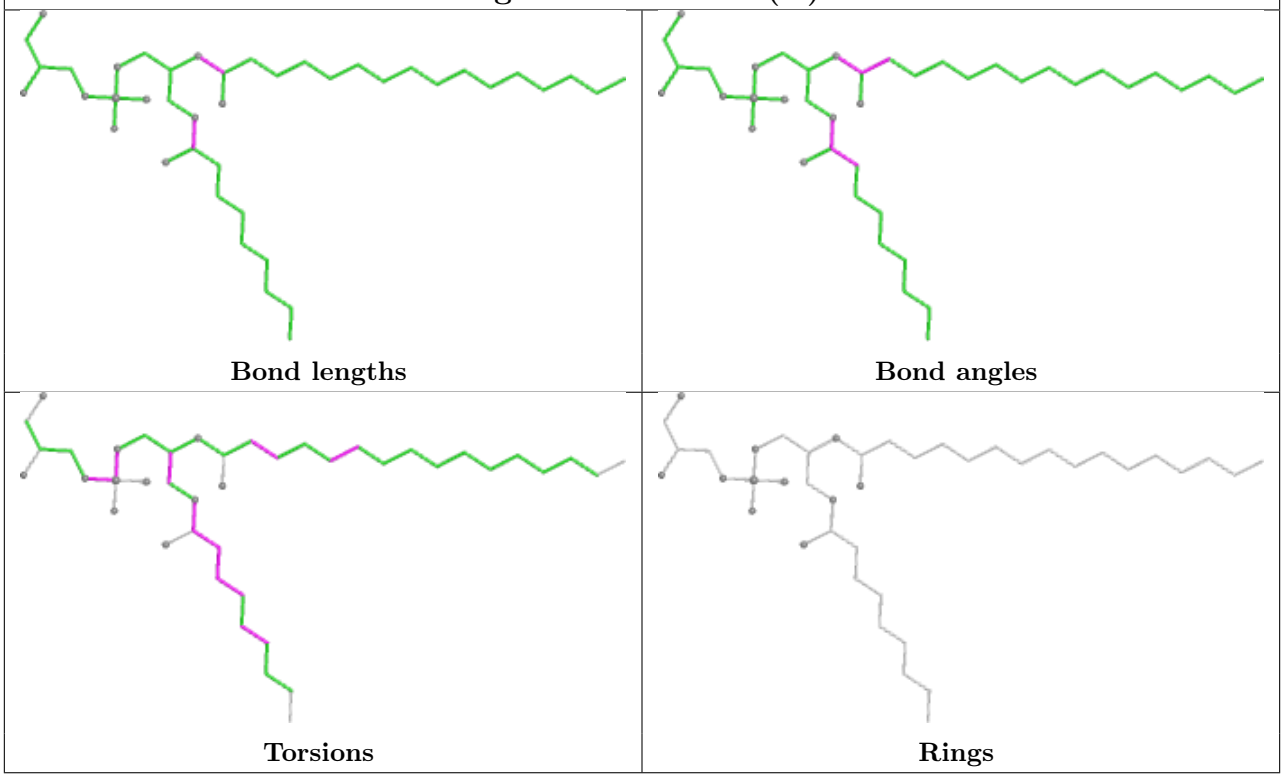


Torsions

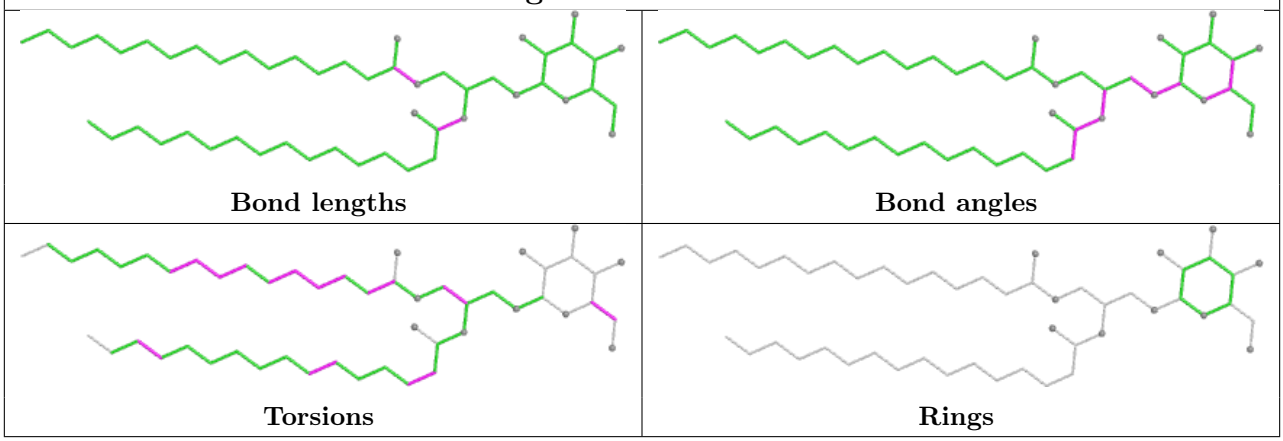


Rings

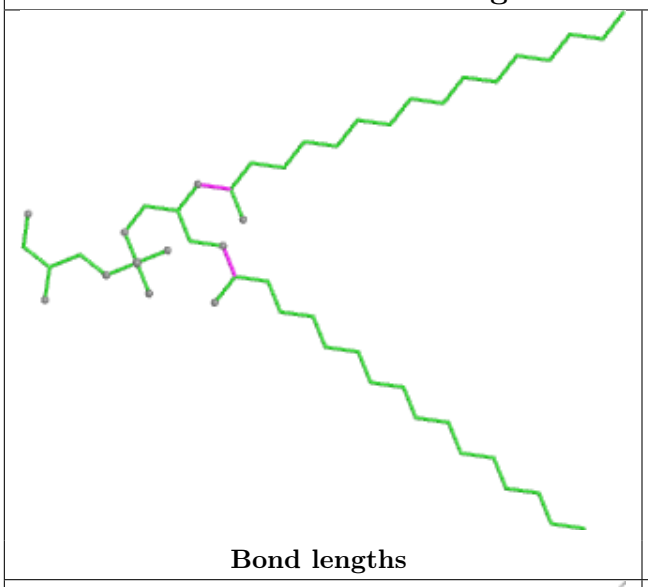
Ligand LHG a 418 (A)



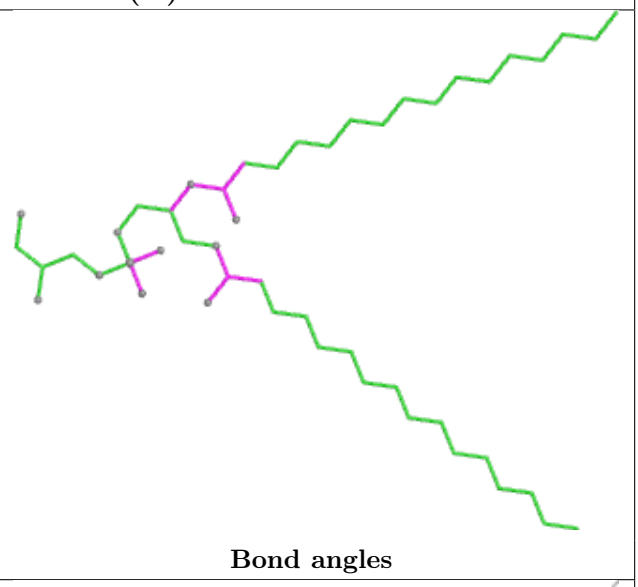
Ligand LMG c 501



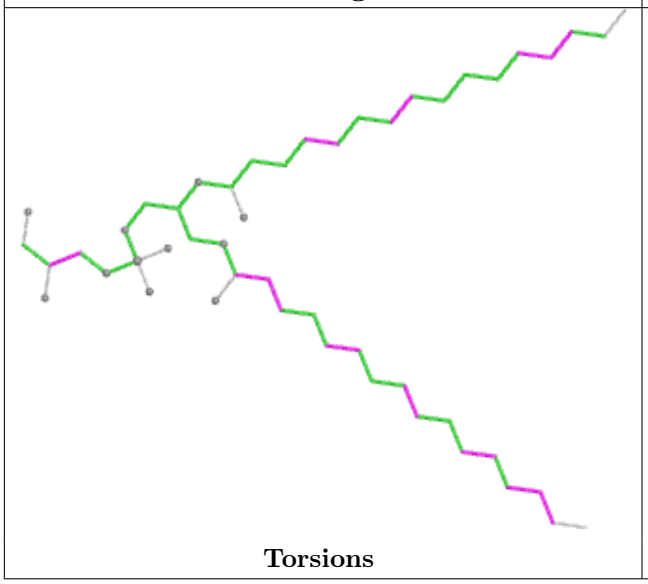
Ligand LHG A 419 (B)



Bond lengths



Bond angles



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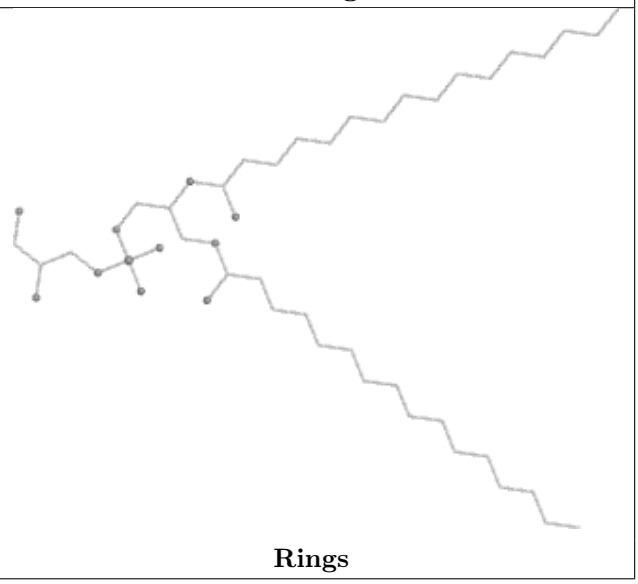
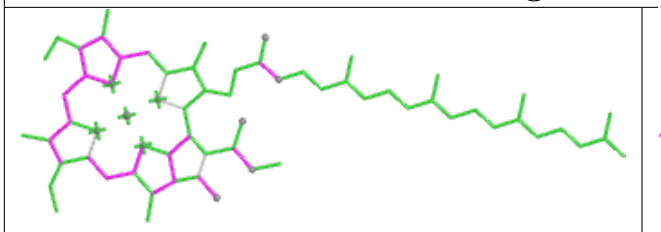
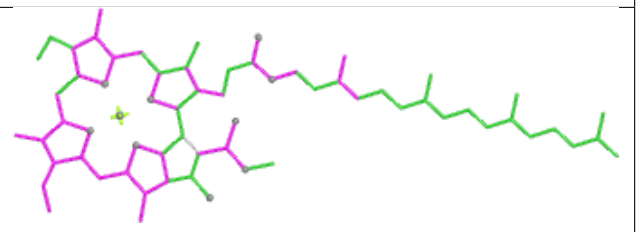


Rings

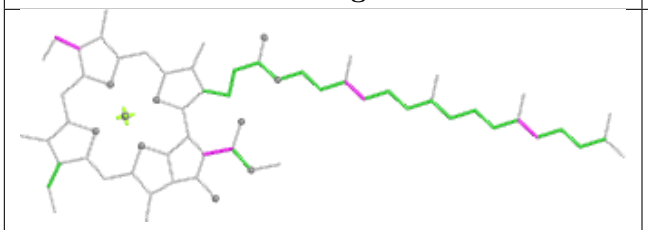
Ligand CLA C 504



Bond lengths



Bond angles



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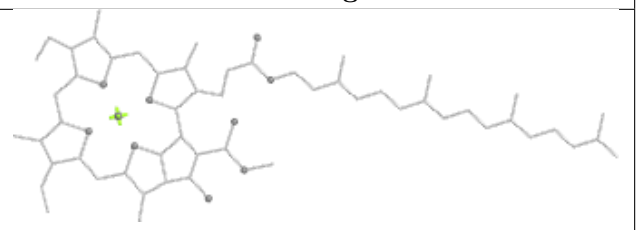
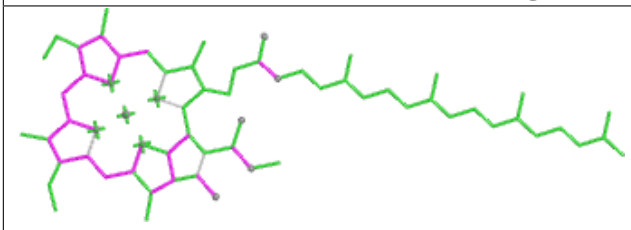


Rings

Ligand CLA B 608



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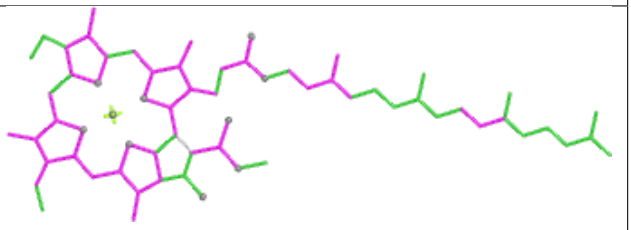
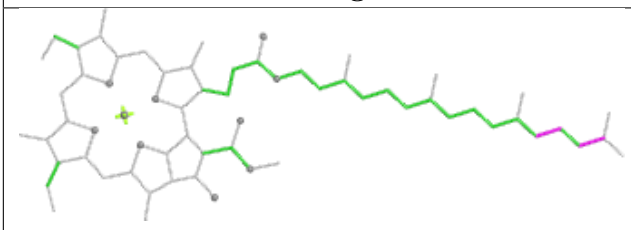


Bond angles



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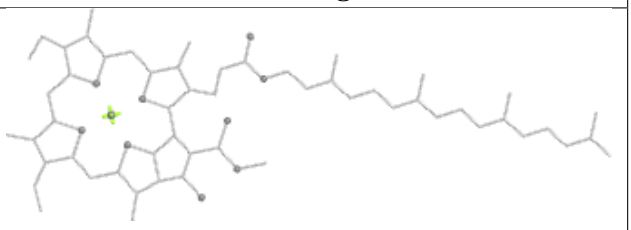
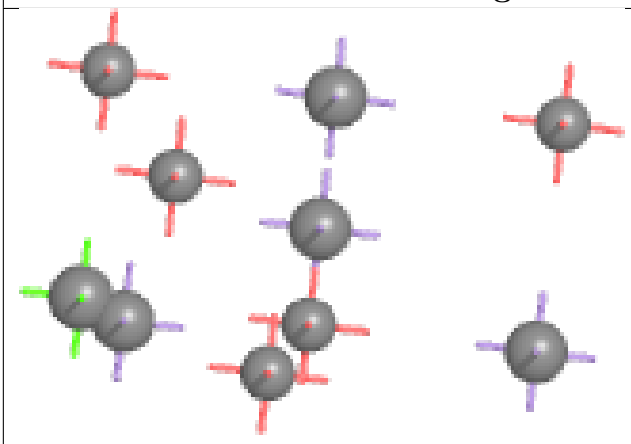


Rings

Ligand OEX a 411 (A)



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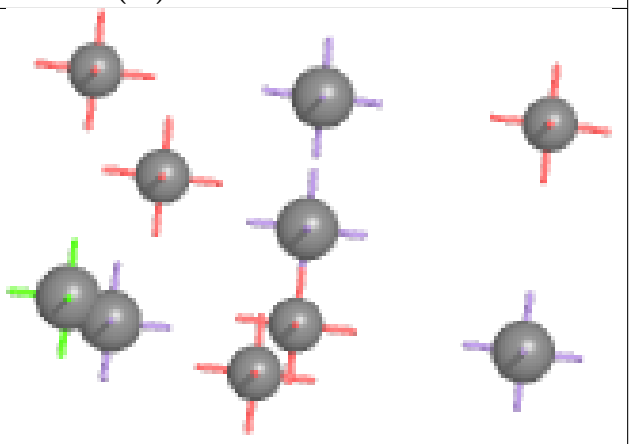
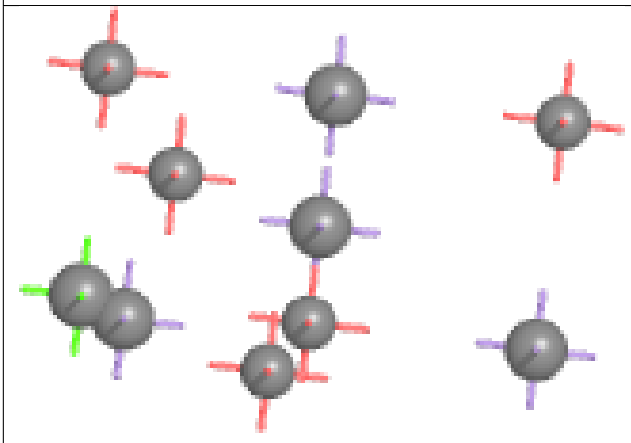


Bond angles



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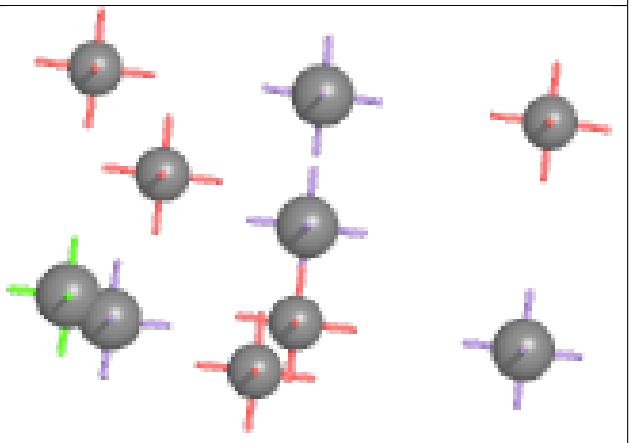
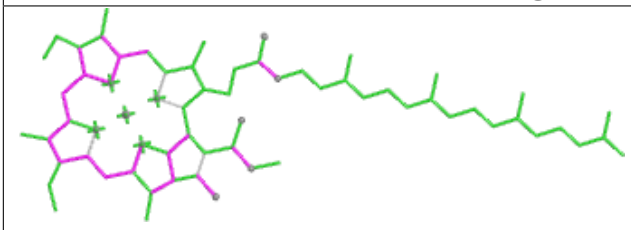


Rings

Ligand CLA c 508



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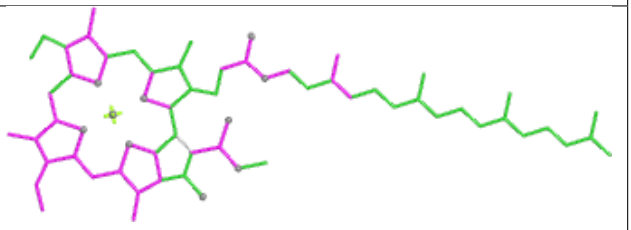
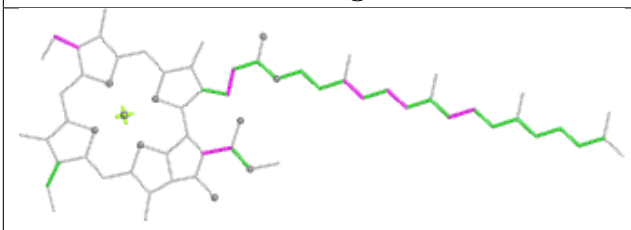
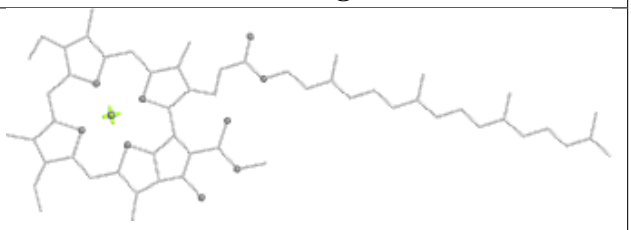


Bond angles



Torsions



Rings

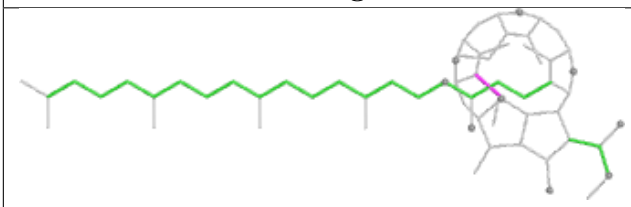
Ligand PHO A 416 (A)



Bond lengths



Bond angles



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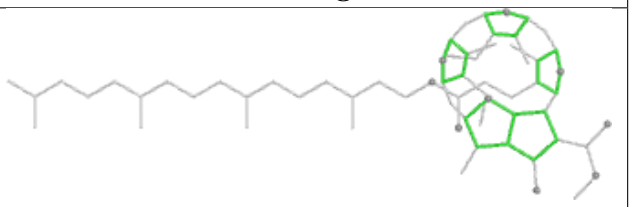
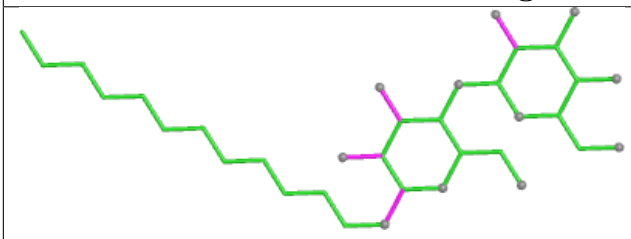
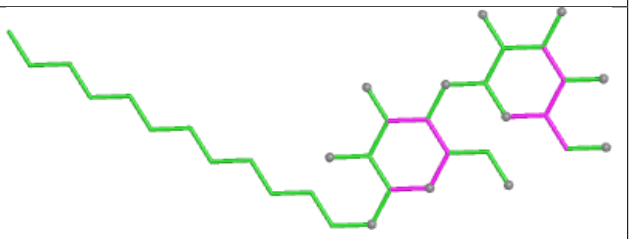


Rings

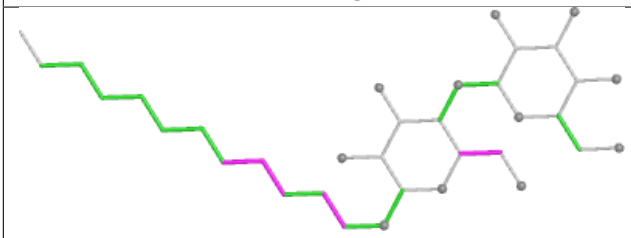
Ligand LMT M 101



Bond lengths



Bond angles



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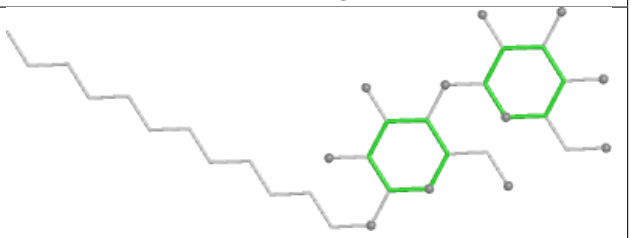
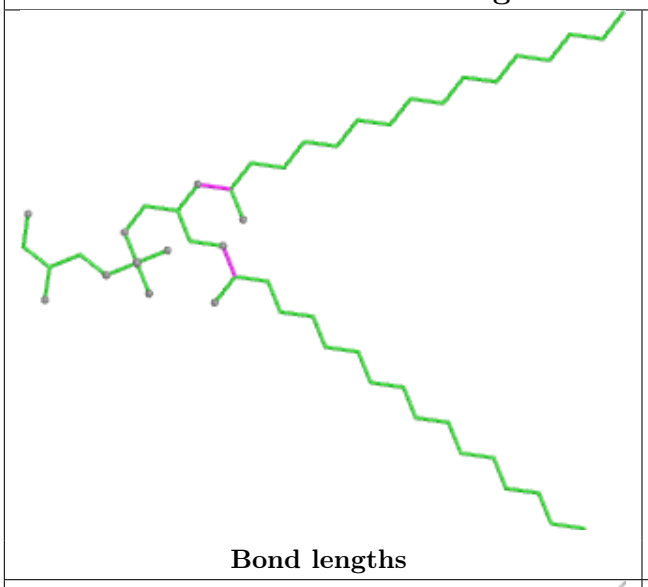


Rings

Ligand LHG d 414 (A)



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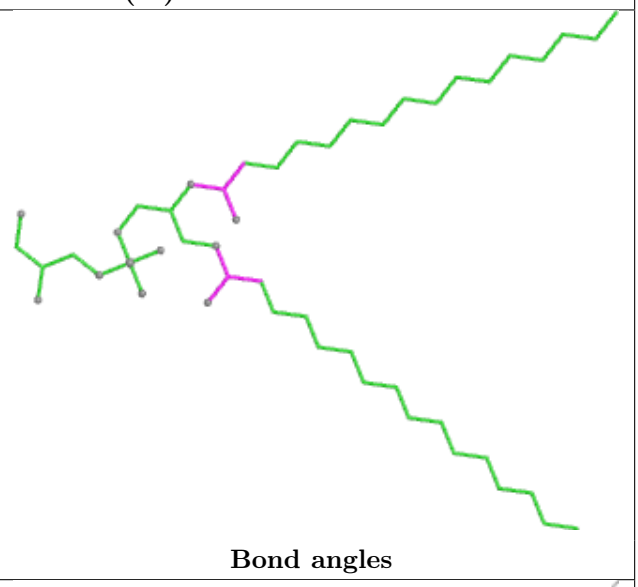
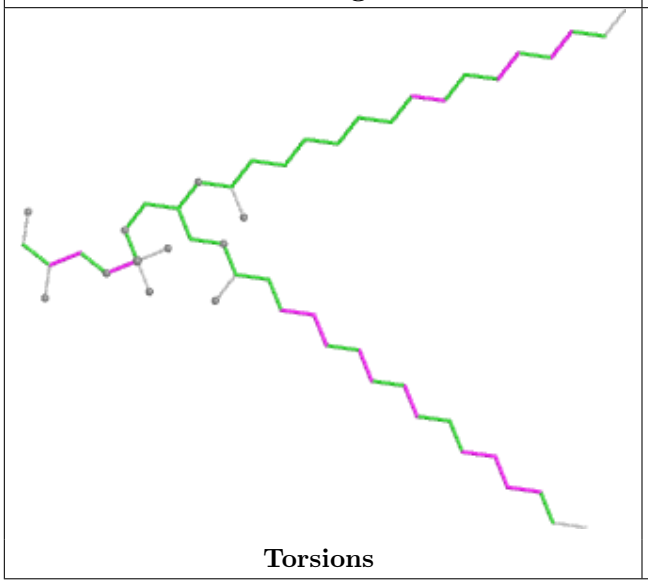


Bond angles



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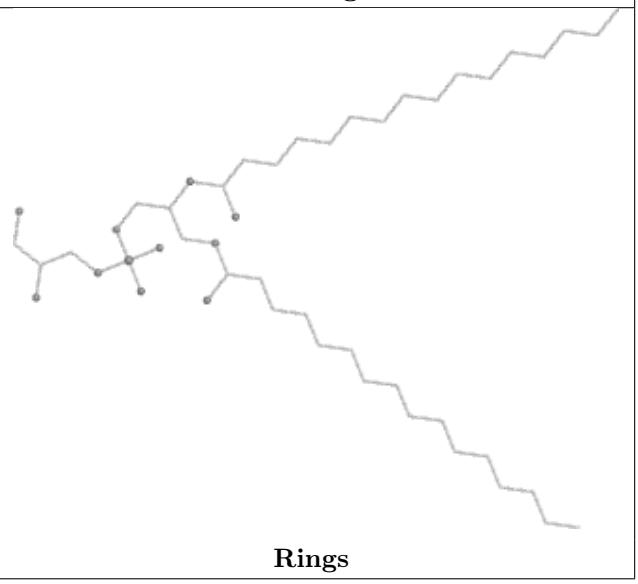
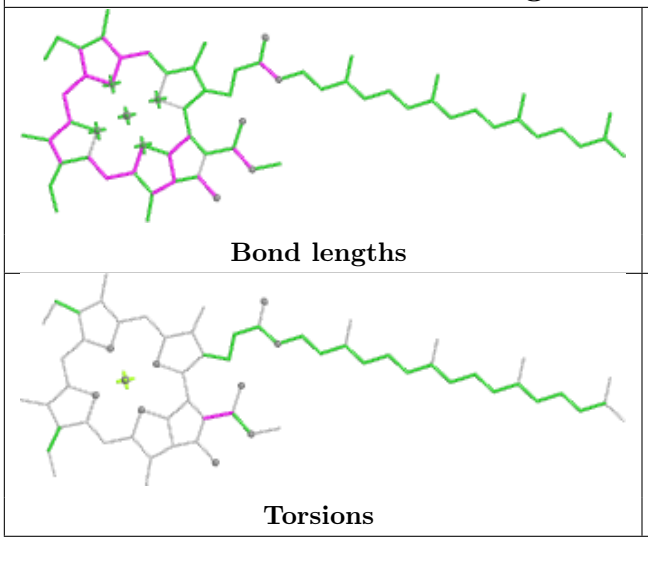
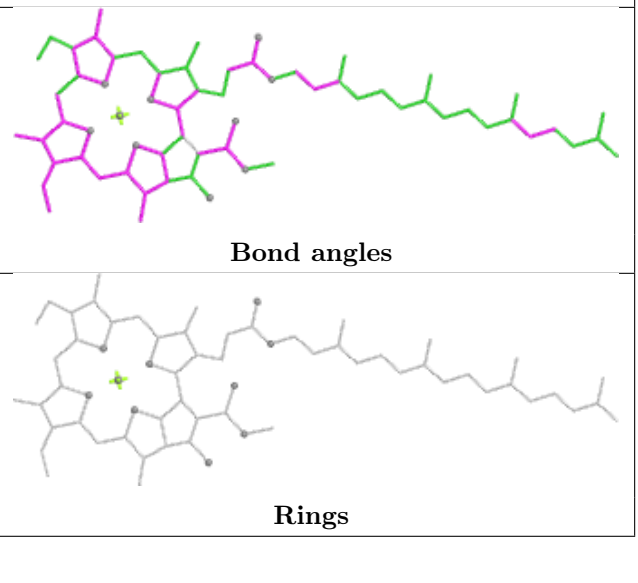


Rings

Ligand CLA B 609



Bond lengths

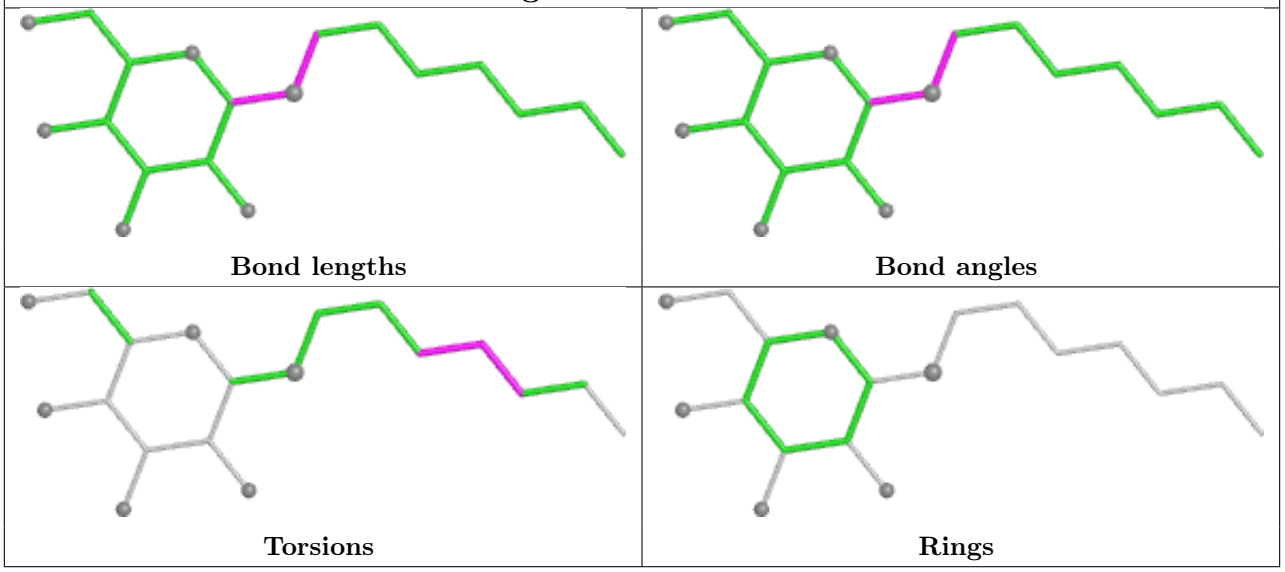


Bond angles

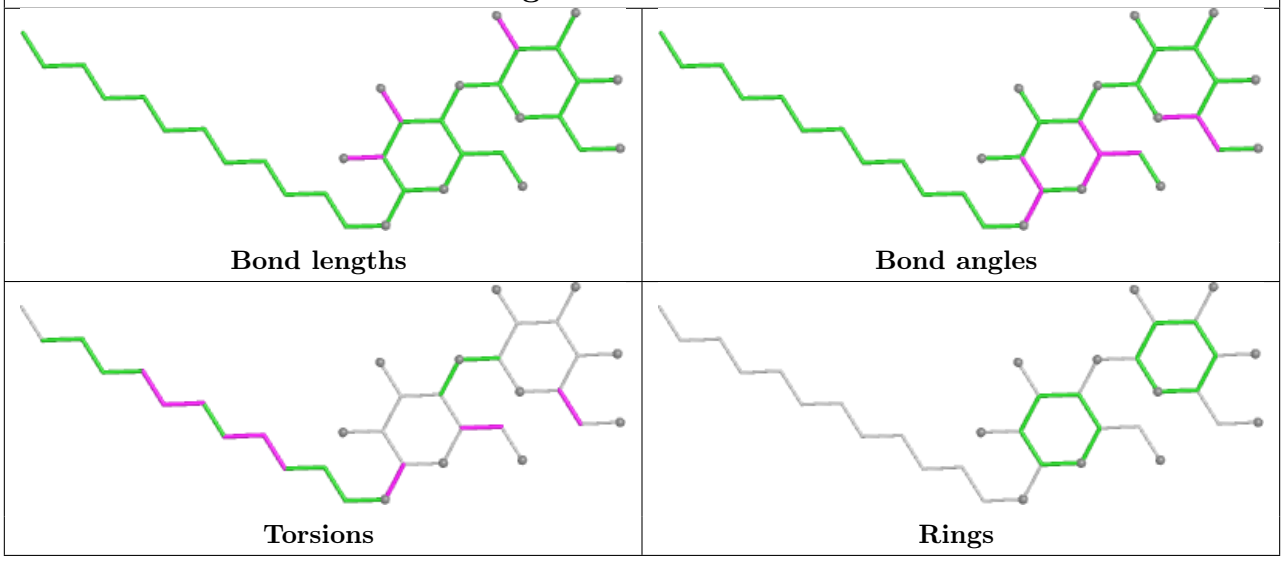
Torsions

Rings

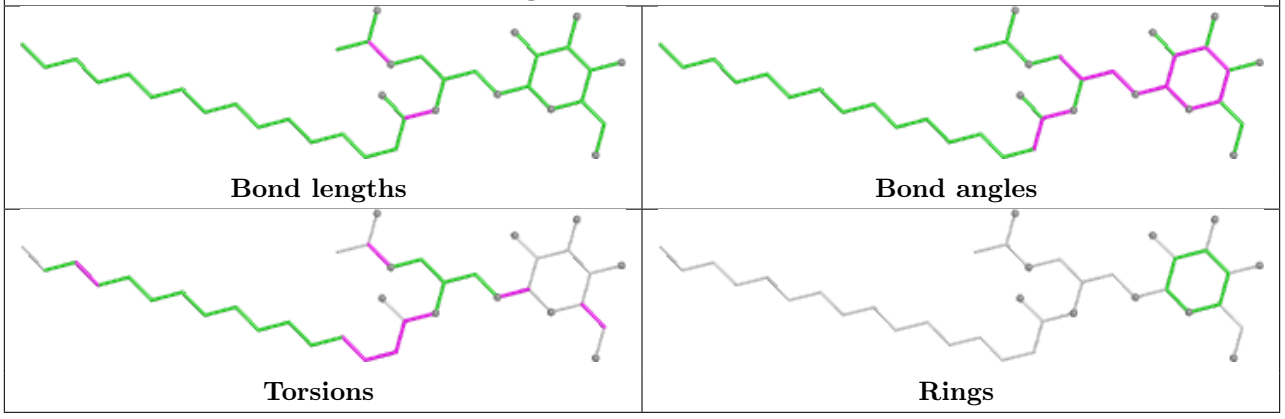
Ligand HTG B 623



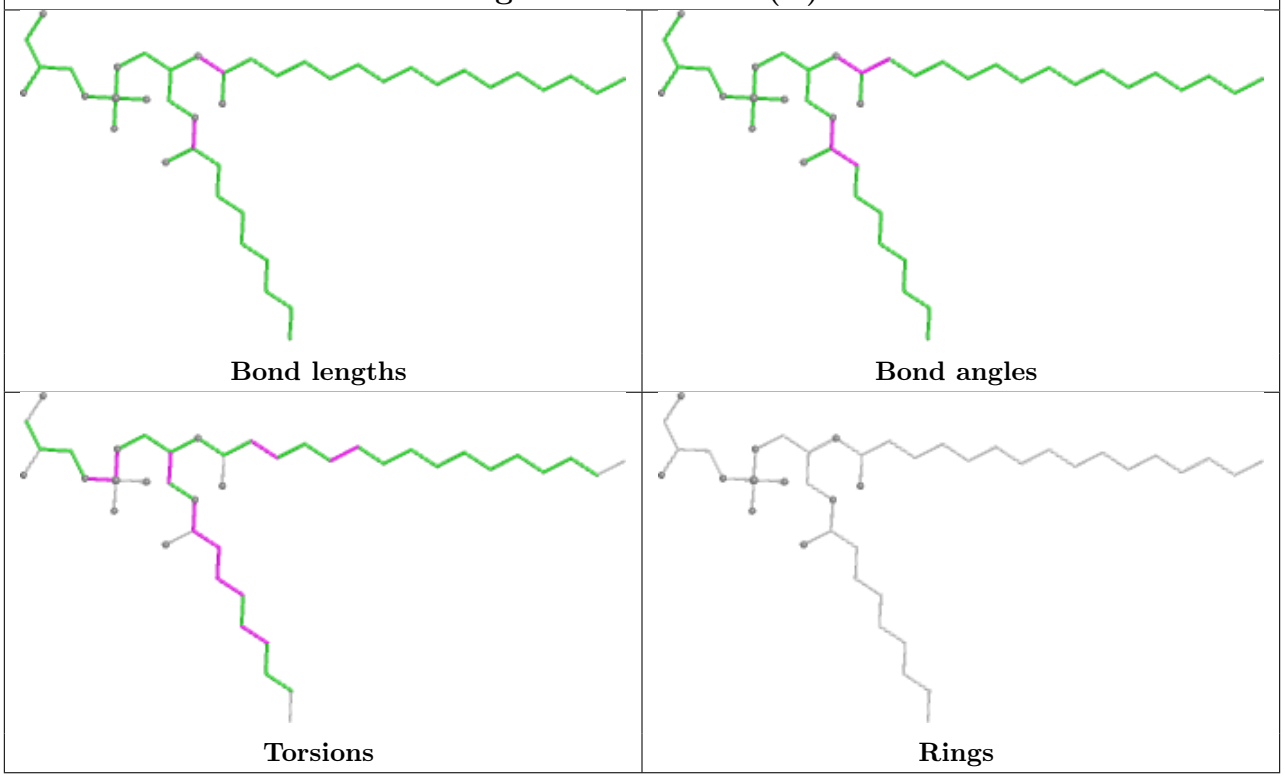
Ligand LMT B 630



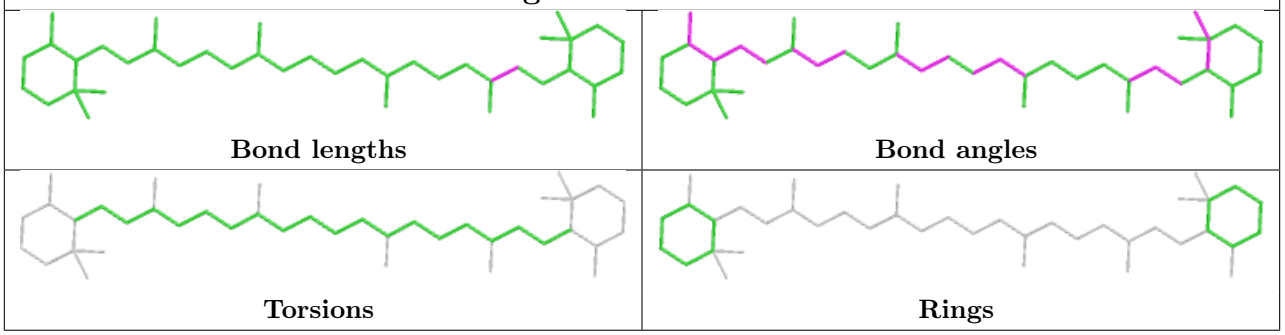
Ligand LMG Z 101



Ligand LHG a 418 (B)



Ligand BCR A 409



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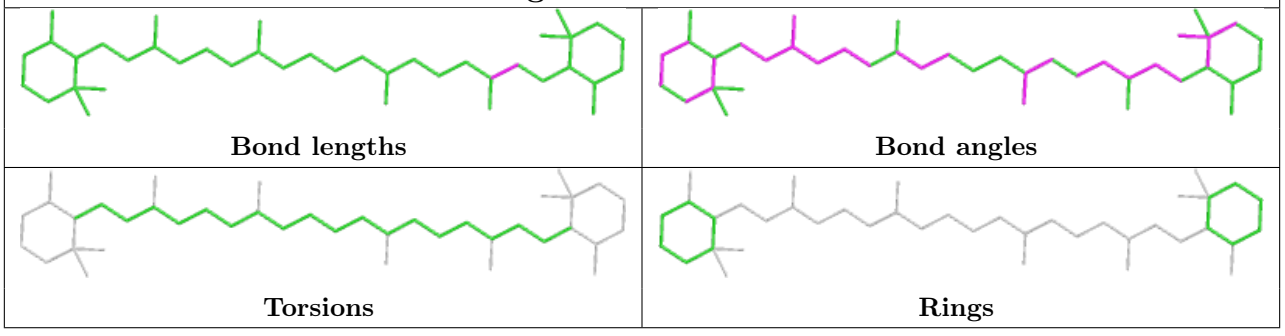
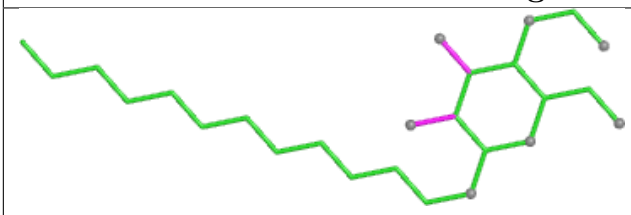
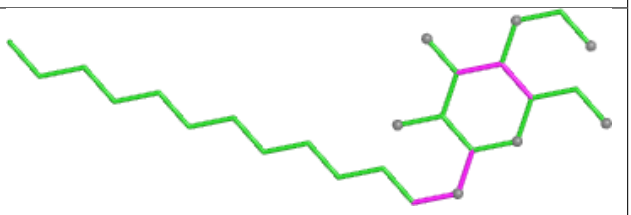


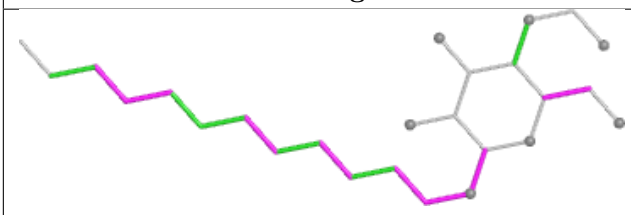
Ligand LMT t 101



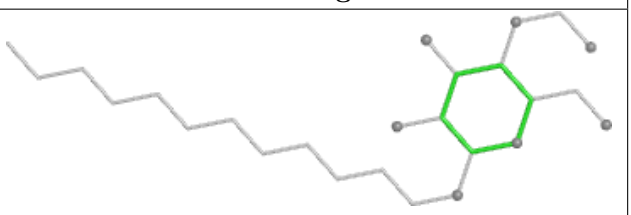
Bond lengths



Bond angles

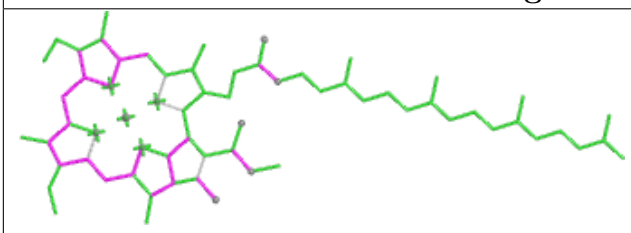


Torsions



Rings

Ligand CLA B 610



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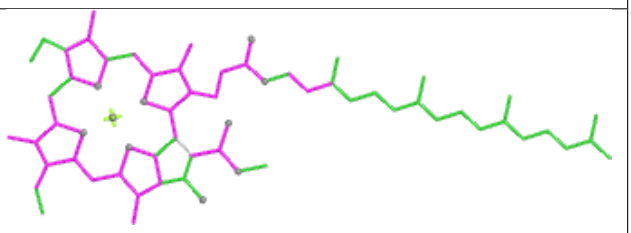
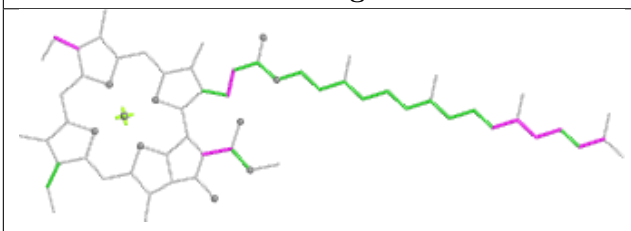


Bond angles



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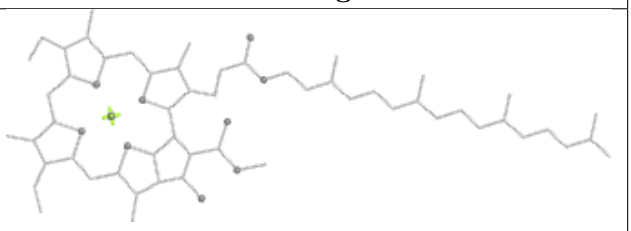
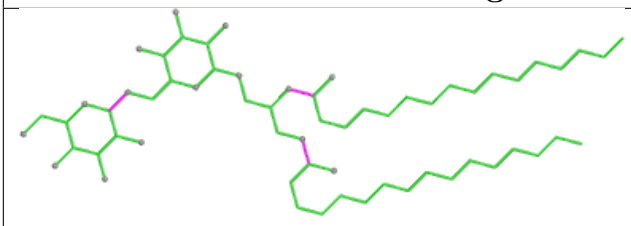
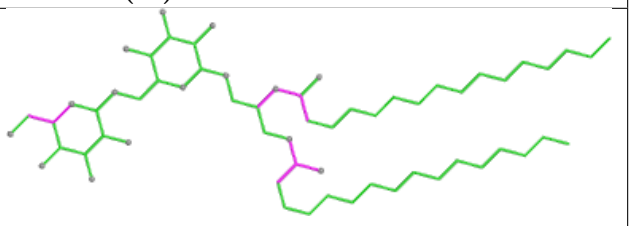


Rings

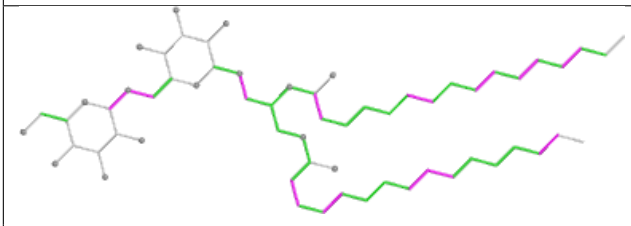
Ligand DGD C 517 (A)



Bond lengths



Bond angles



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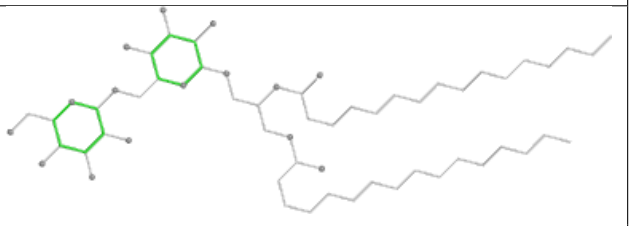
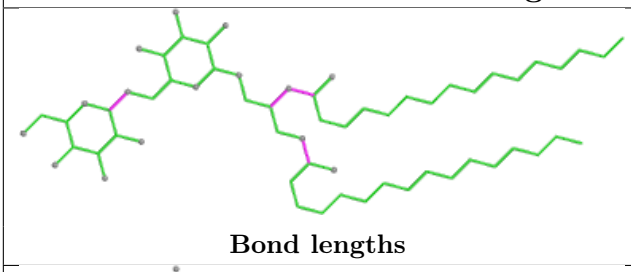
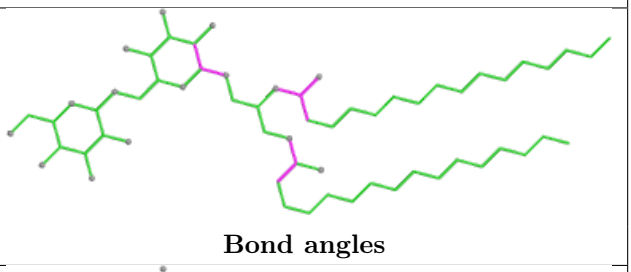


Rings

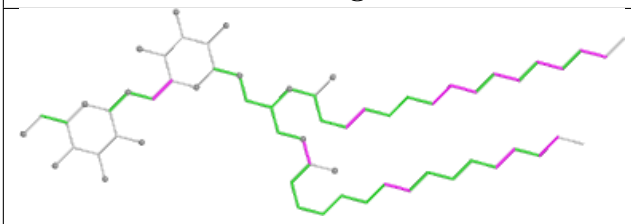
Ligand DGD c 519



Bond lengths



Bond angles



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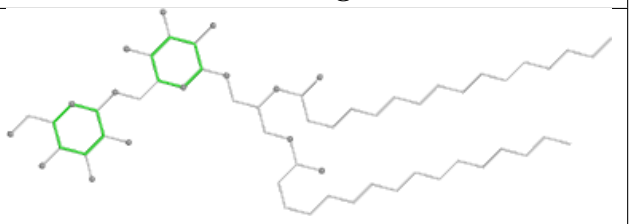
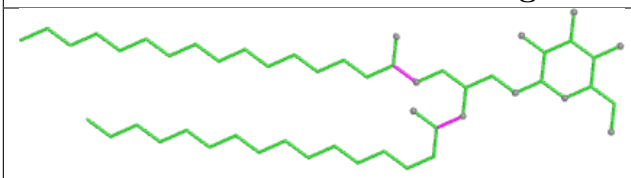
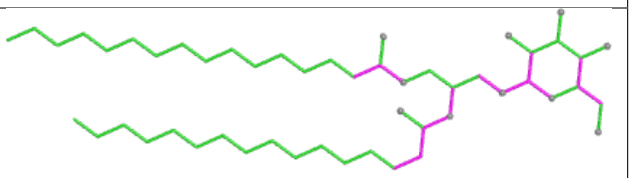


Rings

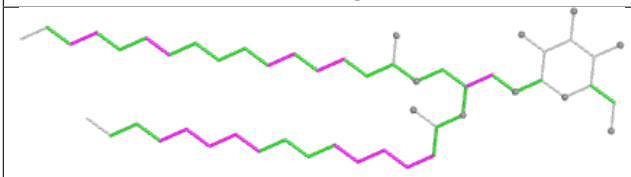
Ligand LMG A 418



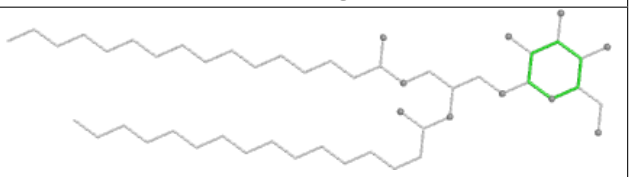
Bond lengths



Bond angles

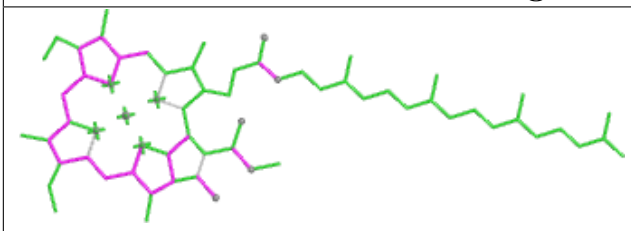


Torsions



Rings

Ligand CLA b 611



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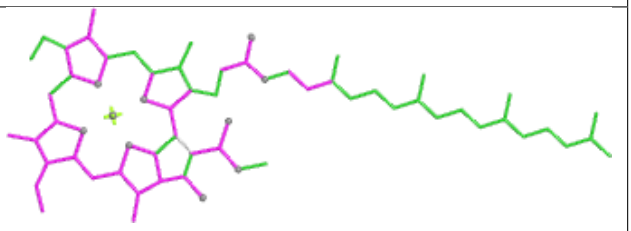
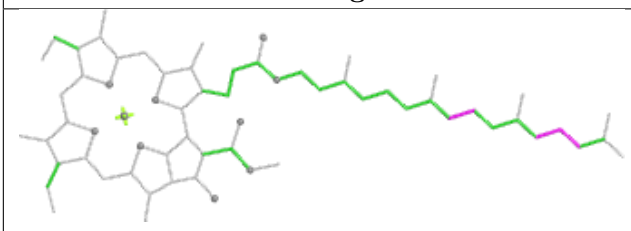
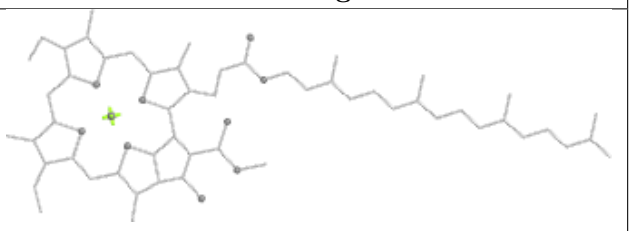


Bond angles

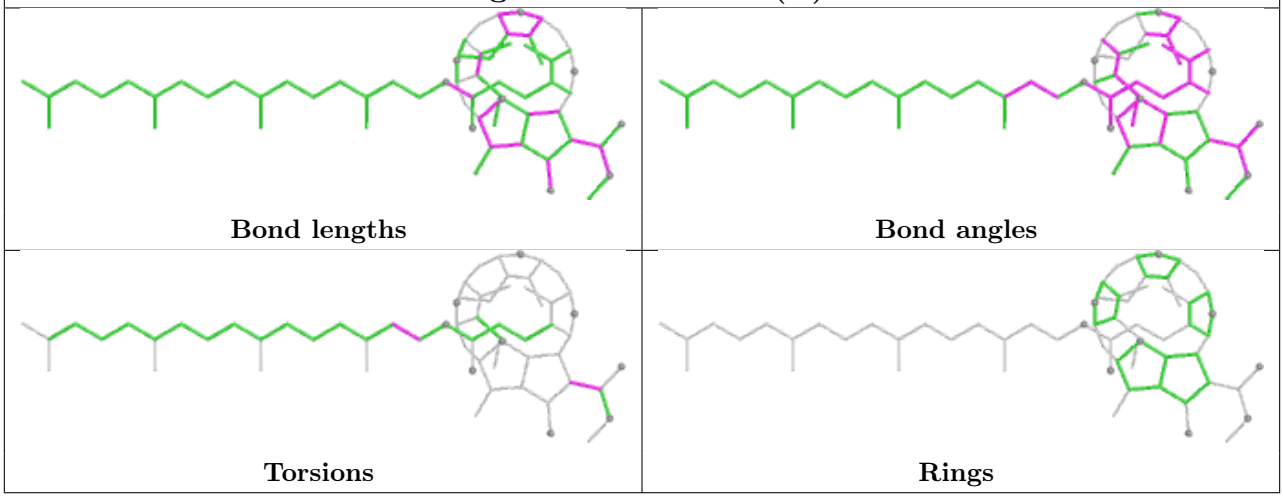


Torsions

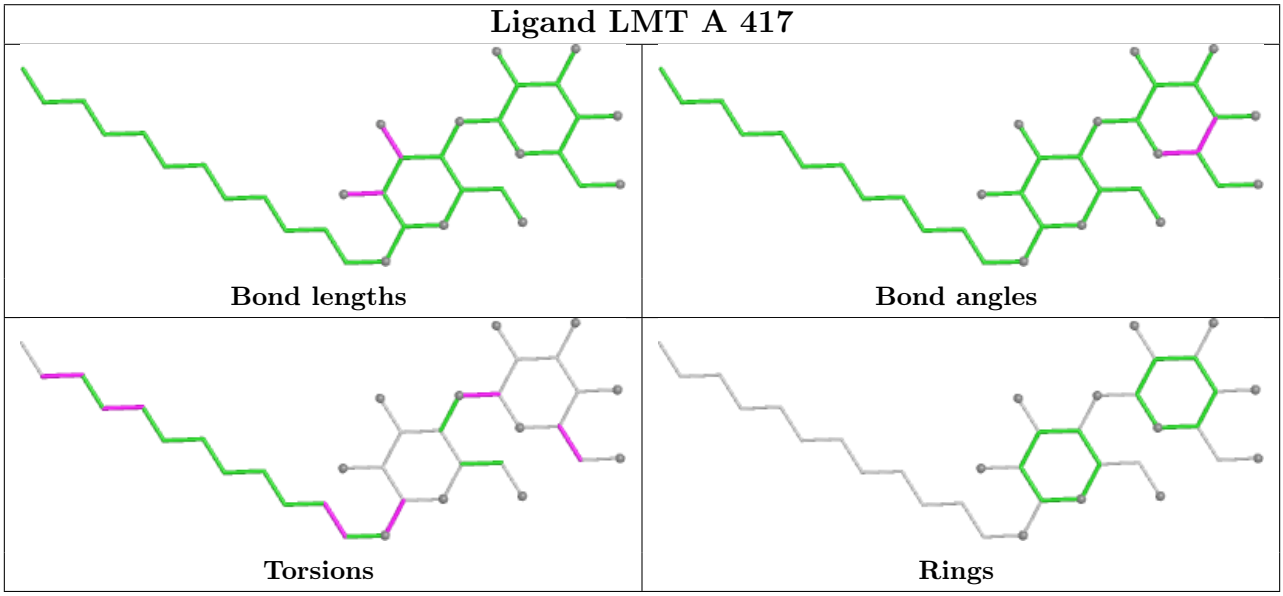


Rings

Ligand PHO A 407 (B)



Ligand LMT A 417



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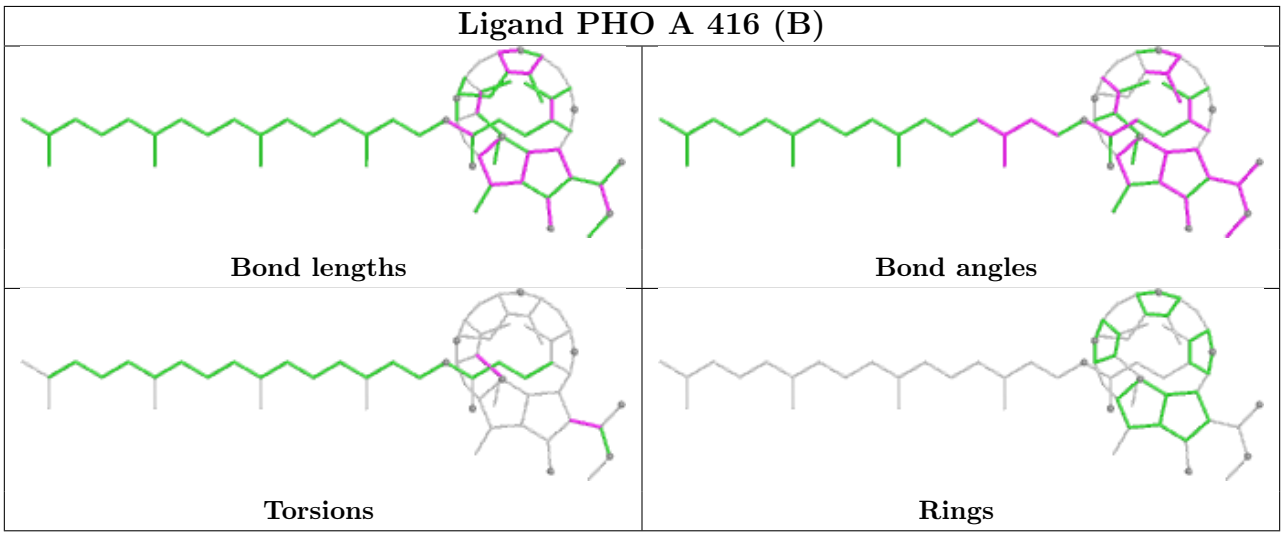
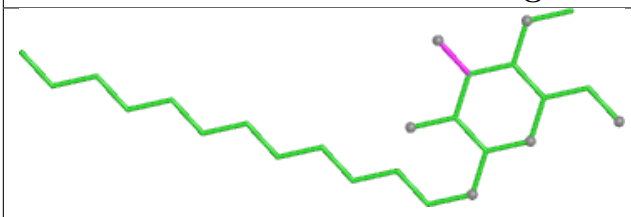
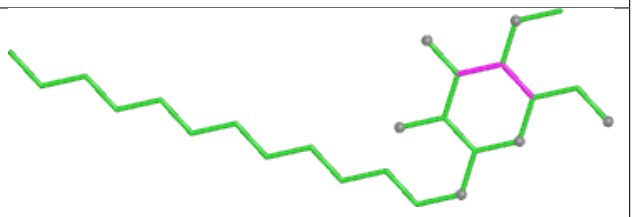


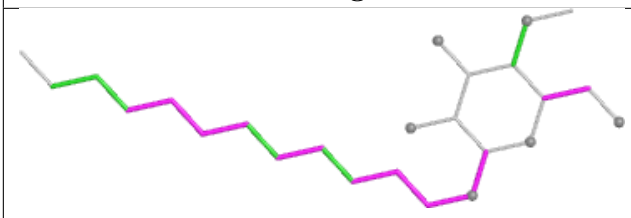
Ligand LMT b 627



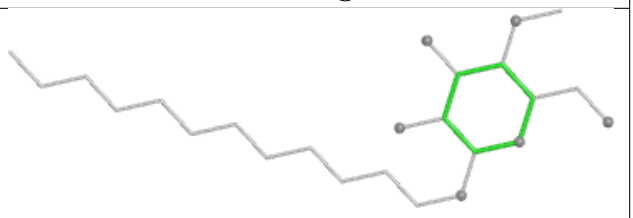
Bond lengths



Bond angles

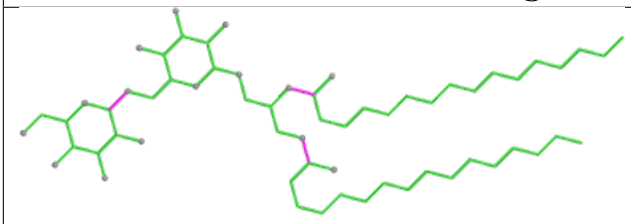


Torsions



Rings

Ligand DGD h 102



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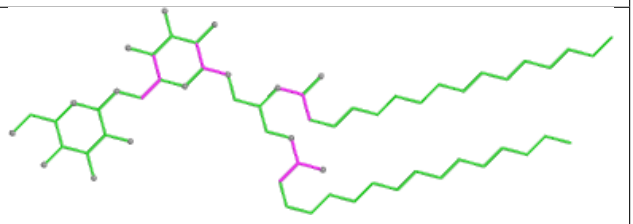
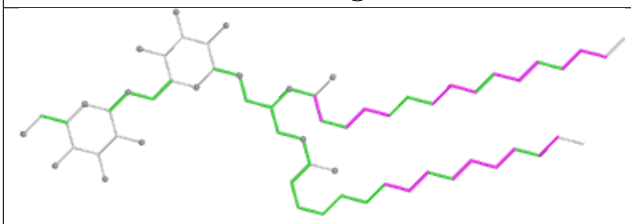


Bond angles



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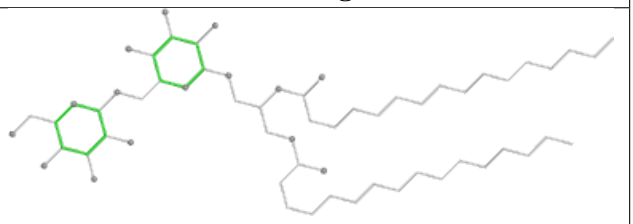
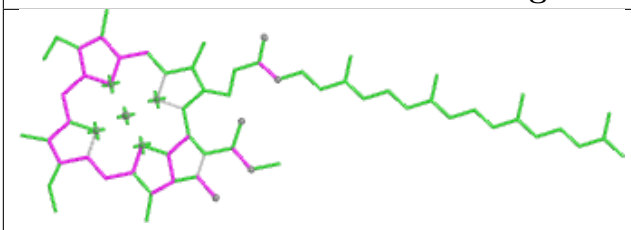


Rings

Ligand CLA c 510



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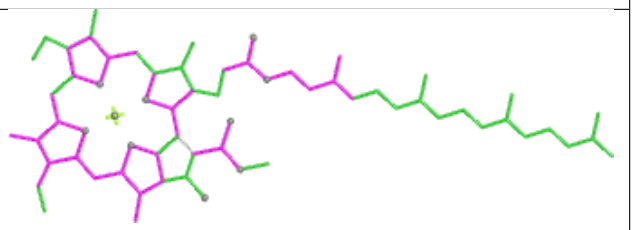
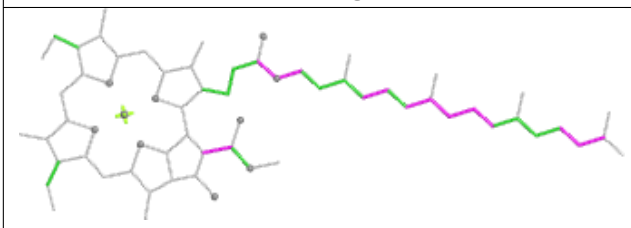


Bond angles



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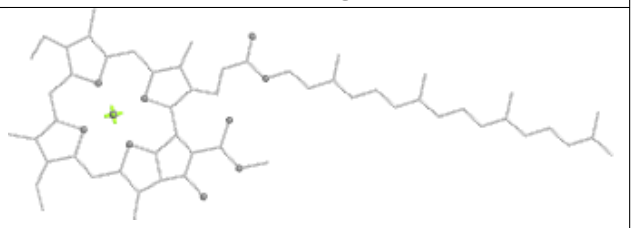
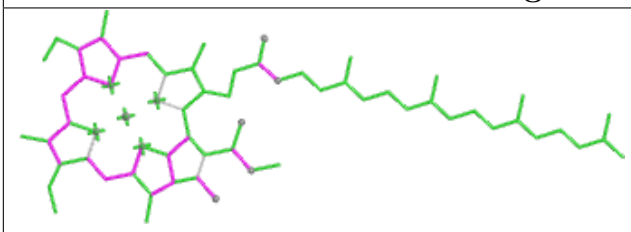


Rings

Ligand CLA C 513



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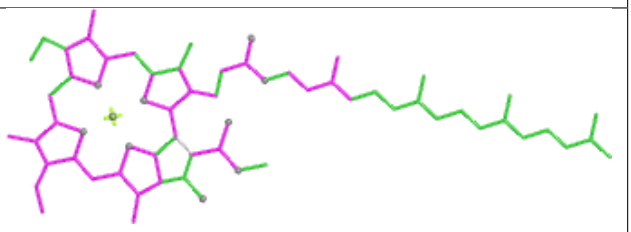
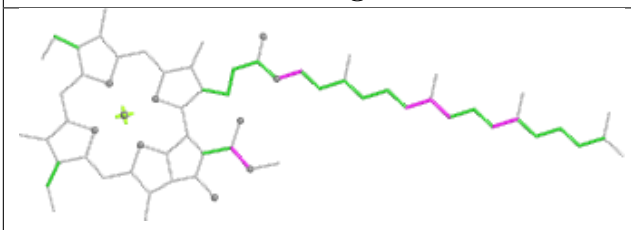


Bond angles



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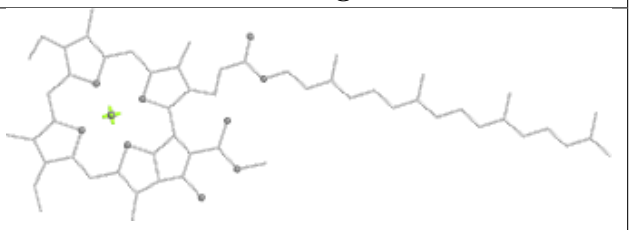
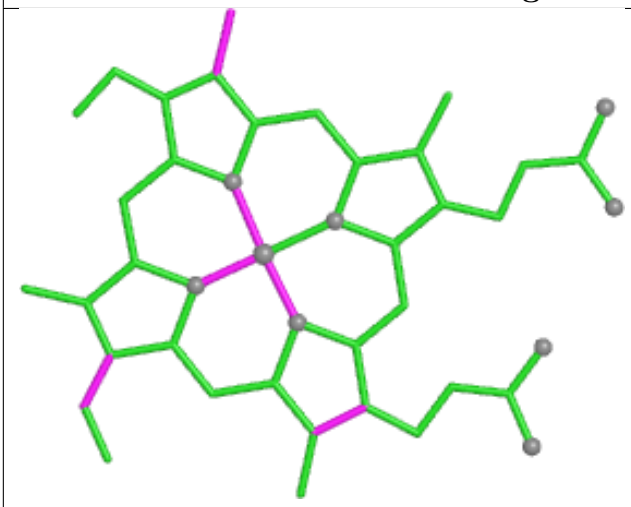


Rings

Ligand HEC V 201



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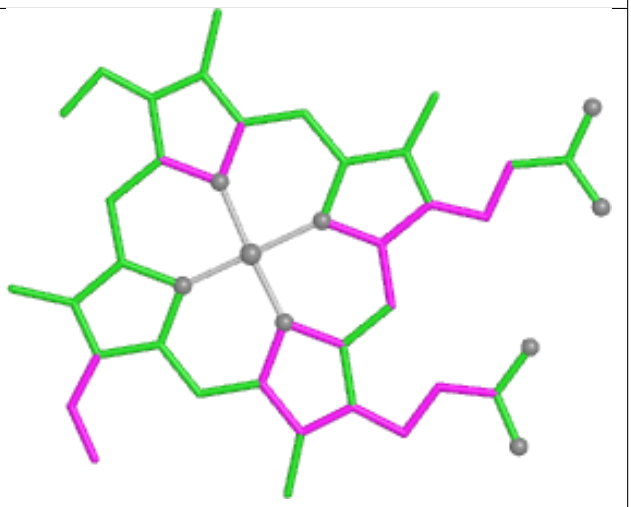
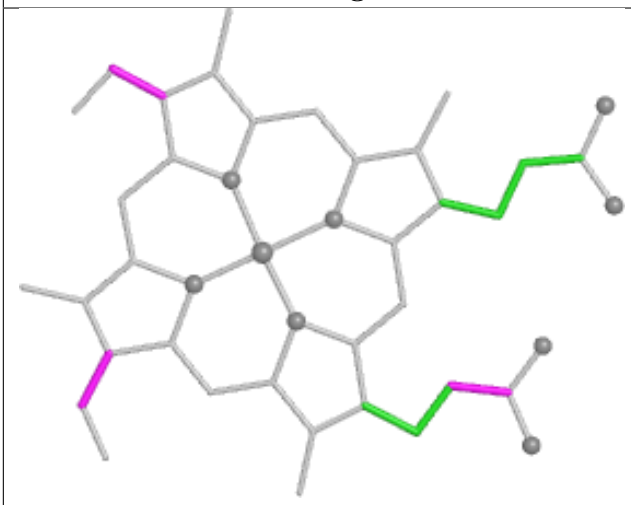


Bond angles



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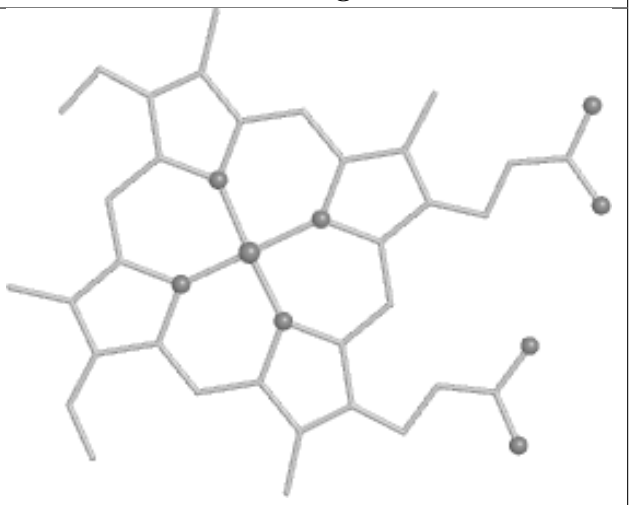
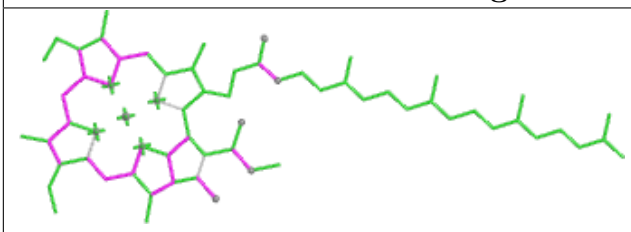


Rings

Ligand CLA A 406 (A)



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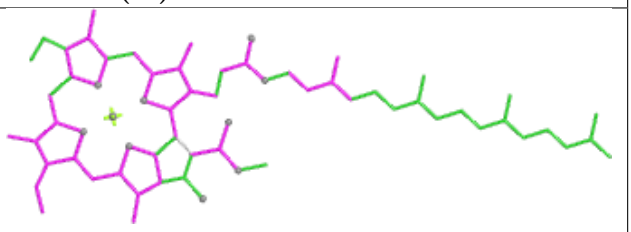
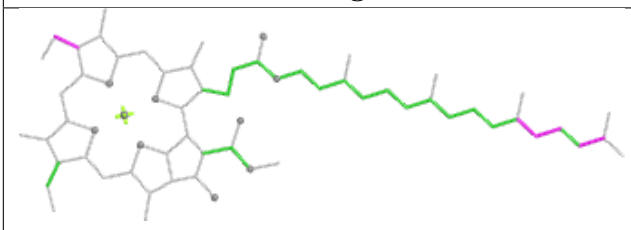


Bond angles



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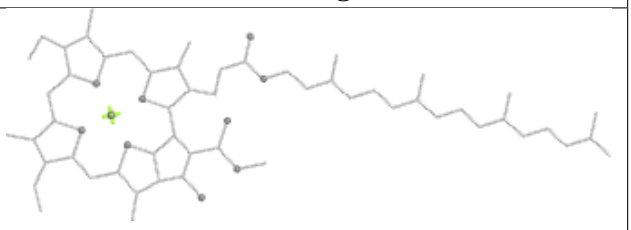
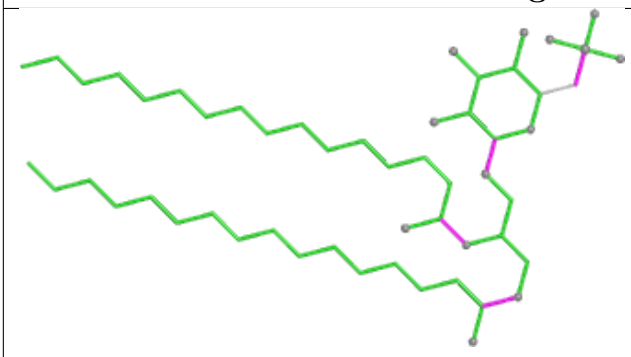


Rings

Ligand SQD a 410



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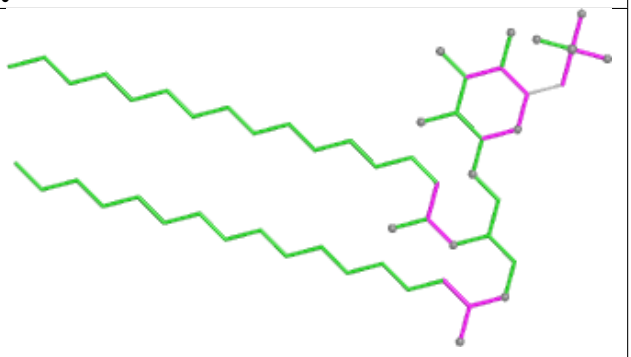
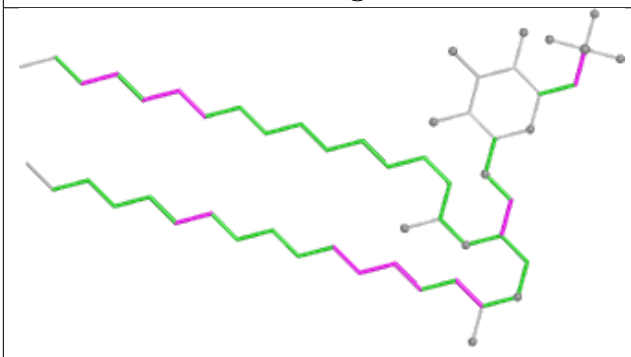


Bond angles



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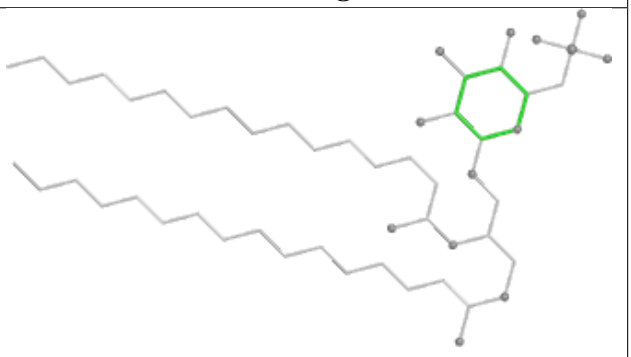
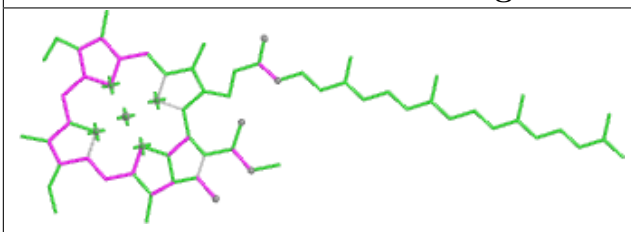


Rings

Ligand CLA a 404 (A)



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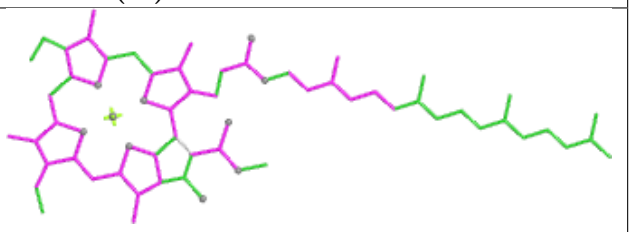
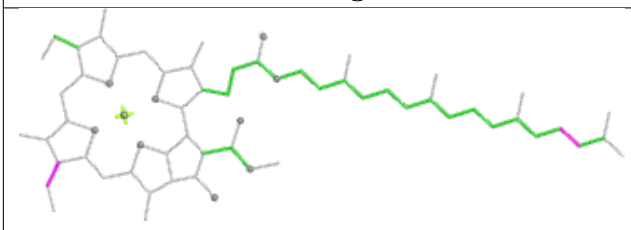


Bond angles



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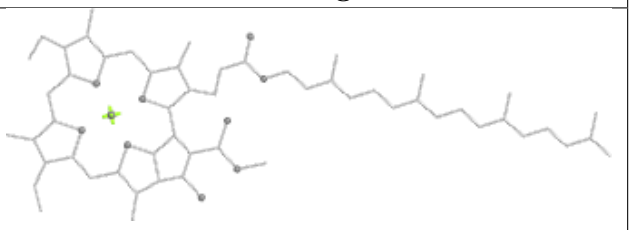


Rings

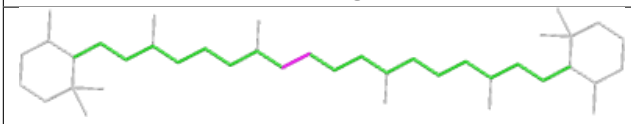
Ligand BCR T 101



Bond lengths



Bond angles



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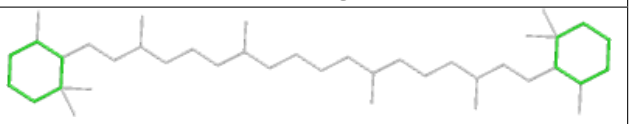
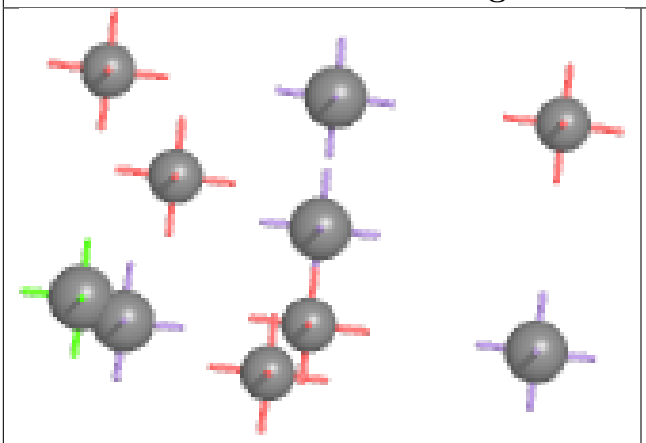


Rings

Ligand OEX A 413 (A)



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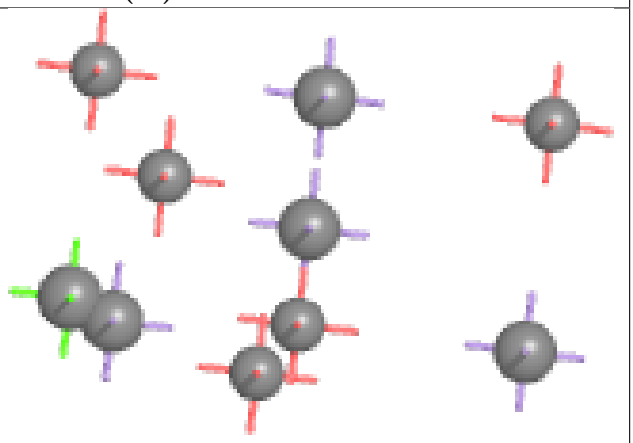
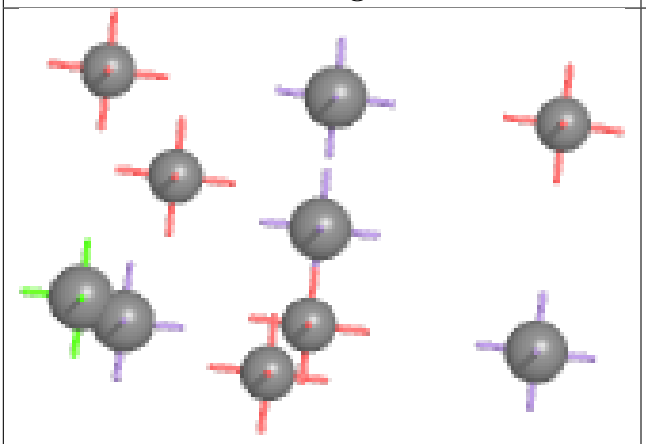


Bond angles



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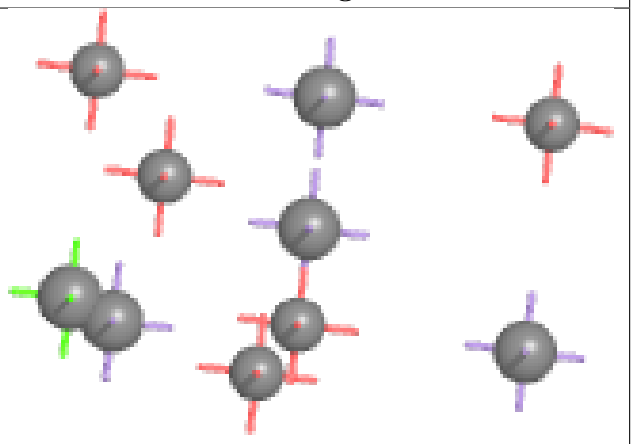
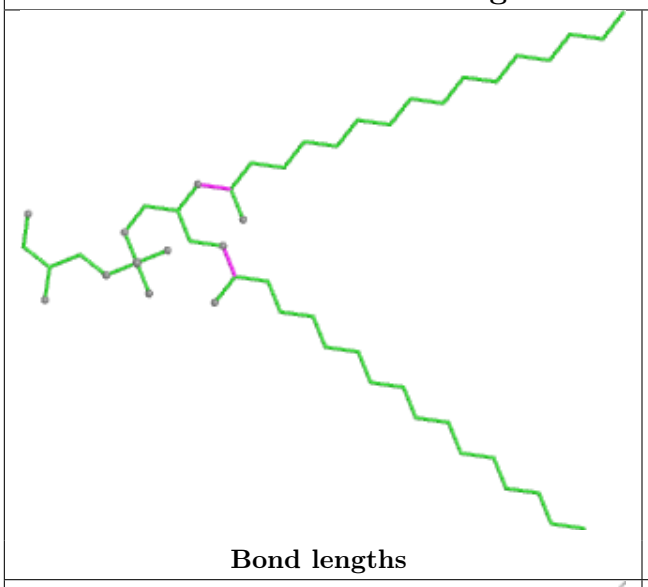


Rings

Ligand LHG A 419 (A)



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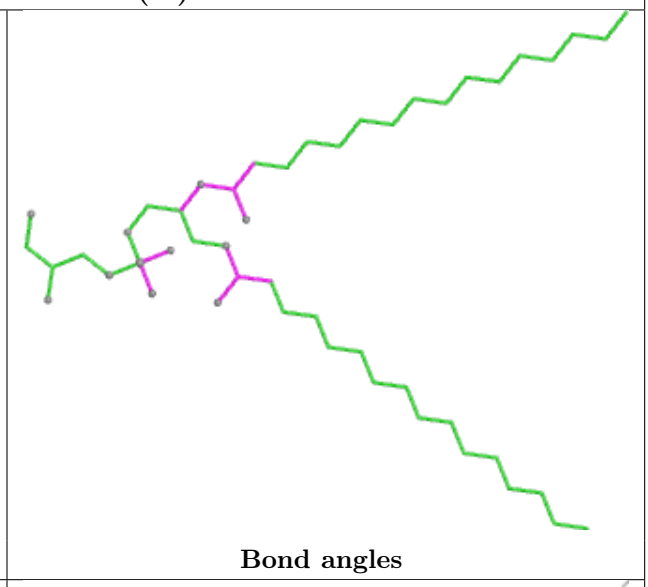
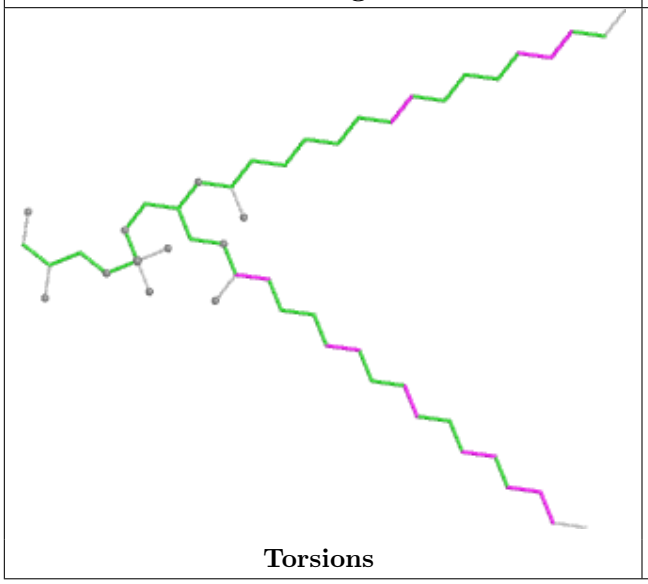


Bond angles



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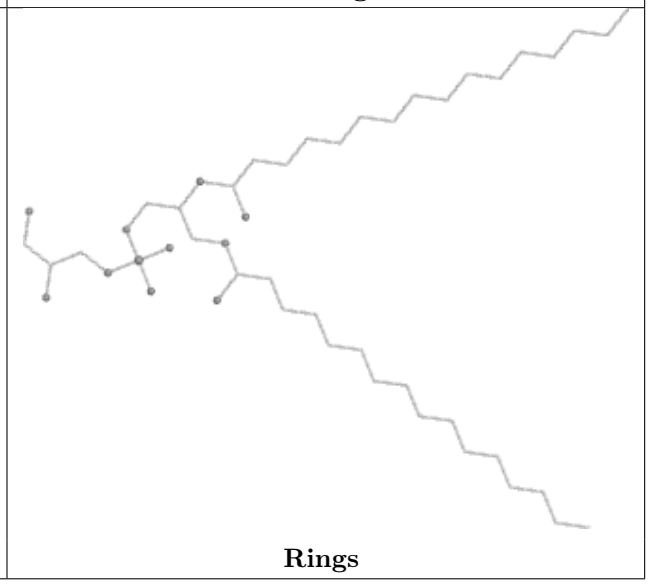
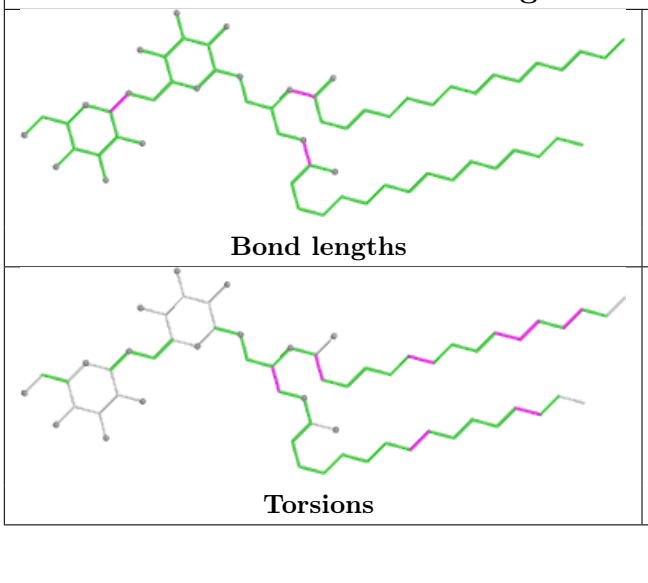


Rings

Ligand DGD H 102



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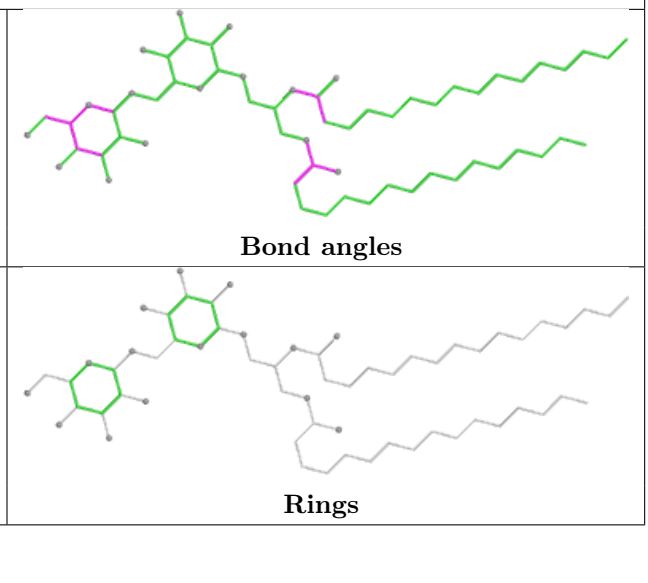
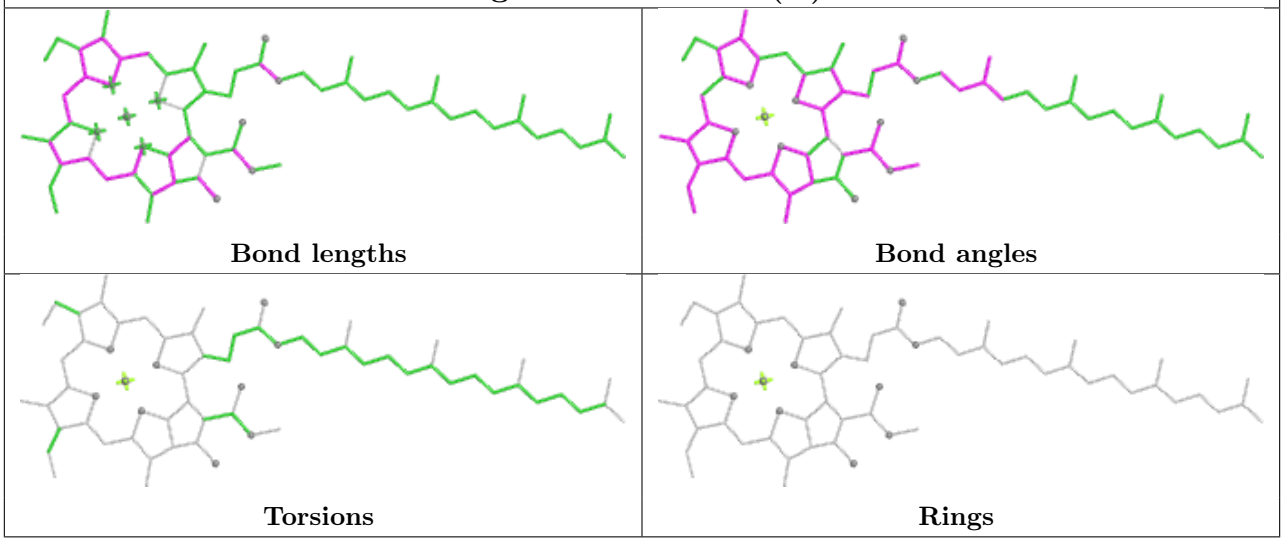


Bond angles

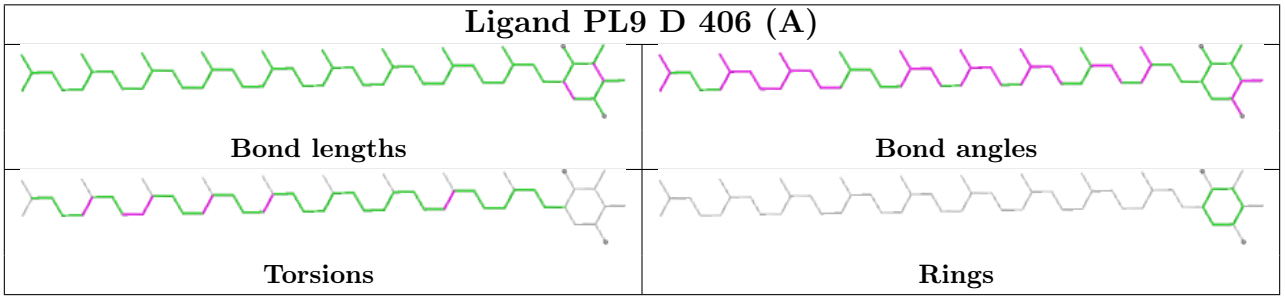
Torsions

Rings

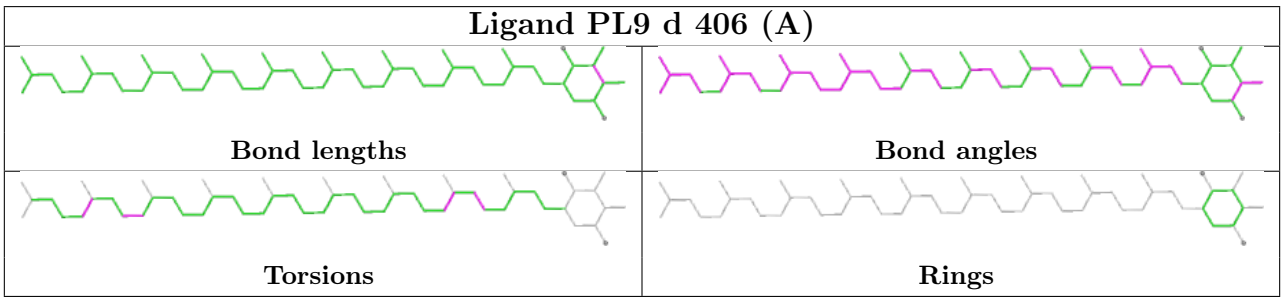
Ligand CLA D 403 (A)



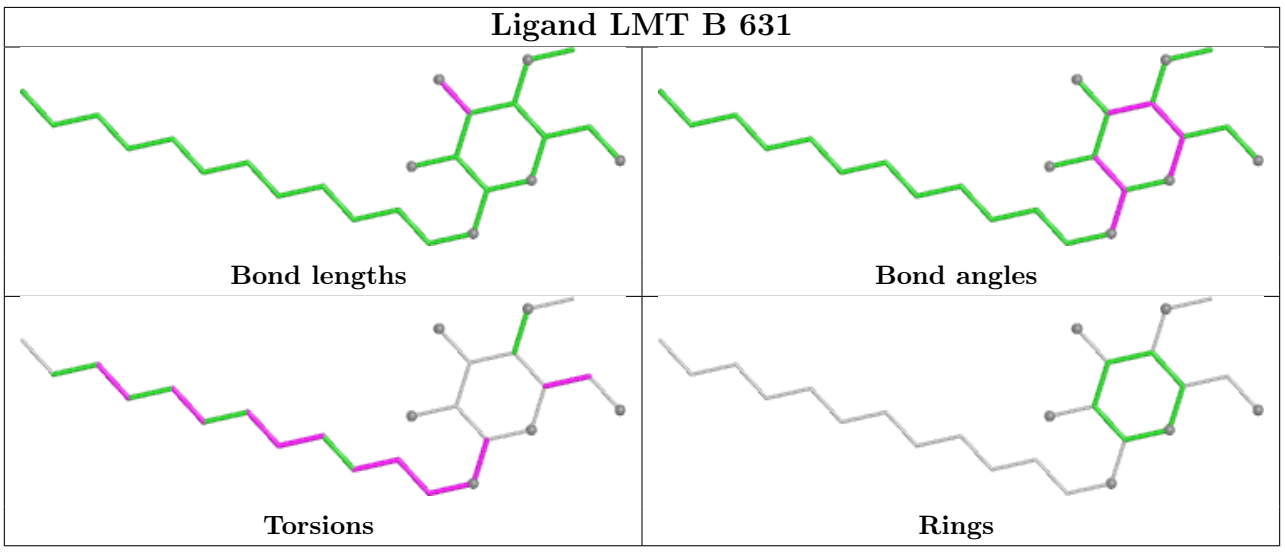
Ligand PL9 D 406 (A)



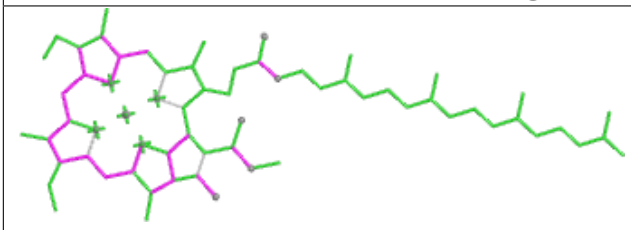
Ligand PL9 d 406 (A)



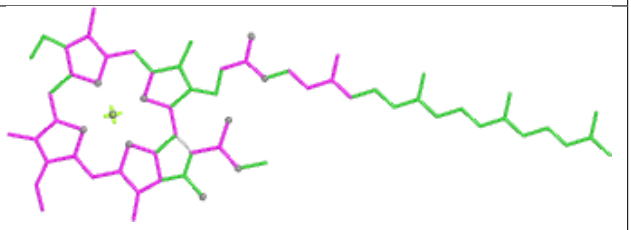
Ligand LMT B 631



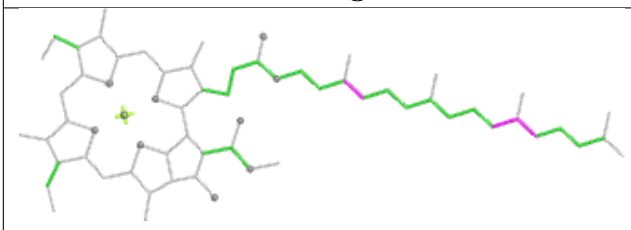
Ligand CLA C 505



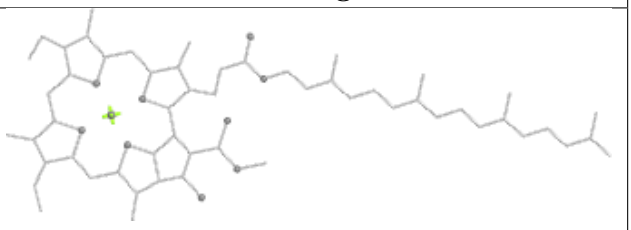
Bond lengths



Bond angles

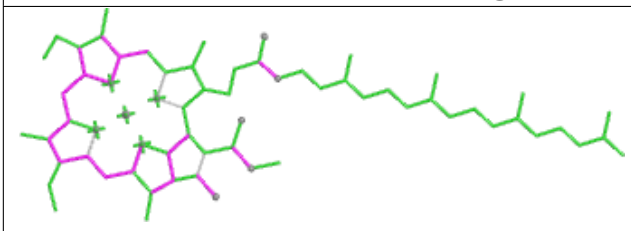


Torsions

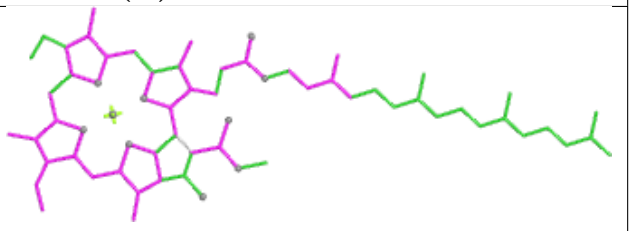


Rings

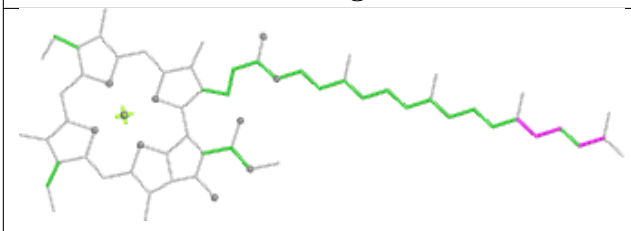
Ligand CLA A 406 (B)



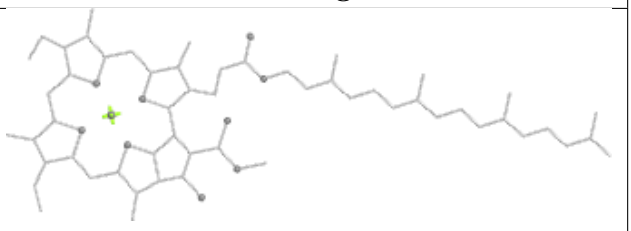
Bond lengths



Bond angles

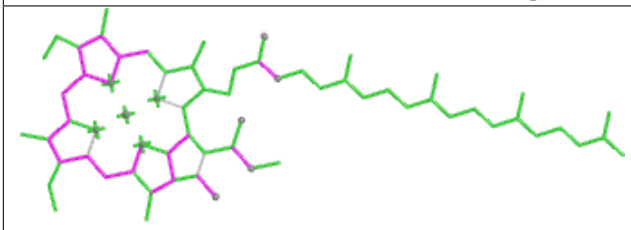


Torsions

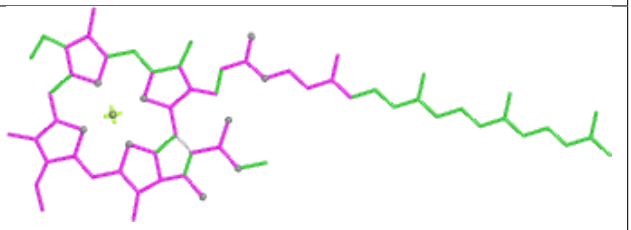


Rings

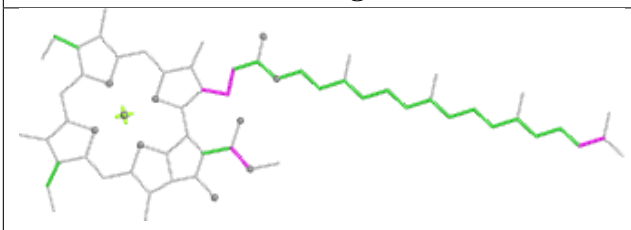
Ligand CLA C 501



Bond lengths



Bond angles



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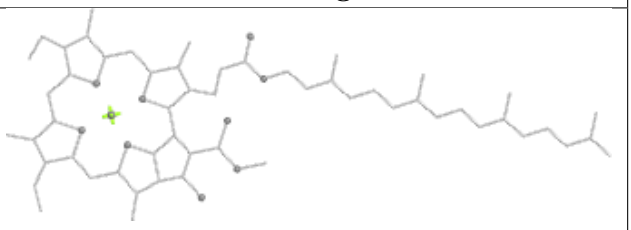
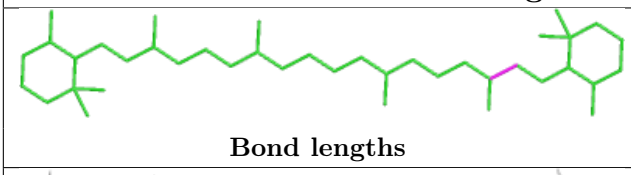
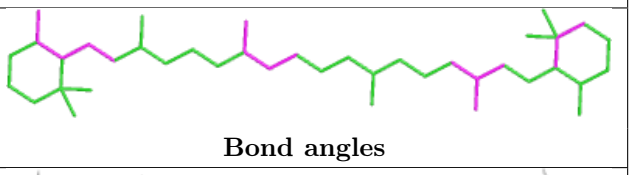


Rings

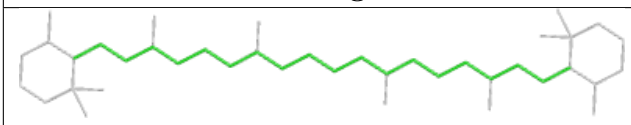
Ligand BCR b 618



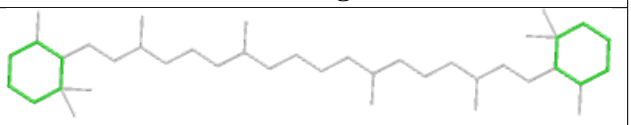
Bond lengths



Bond angles

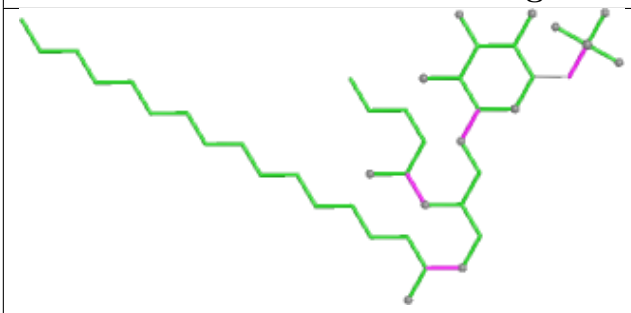


Torsions



Rings

Ligand SQD F 103



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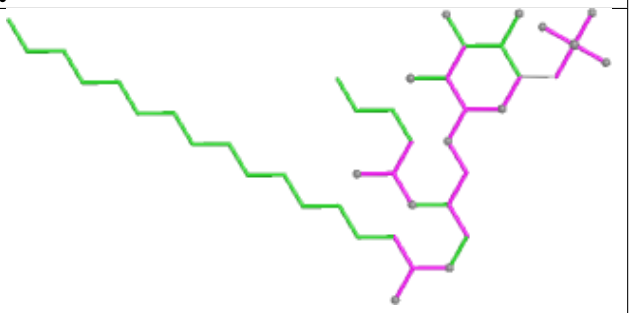
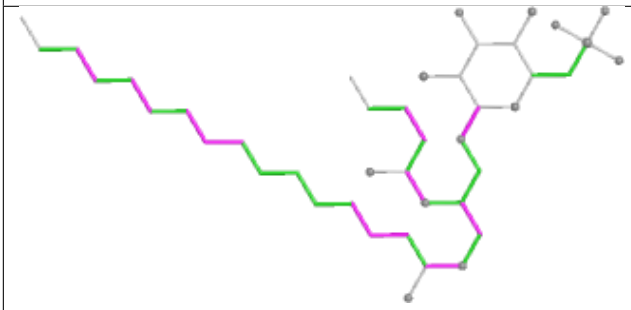


Bond angles



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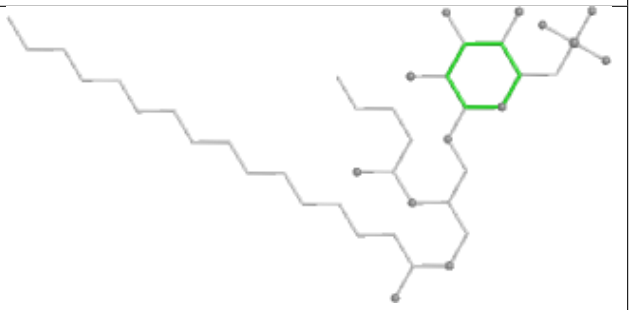
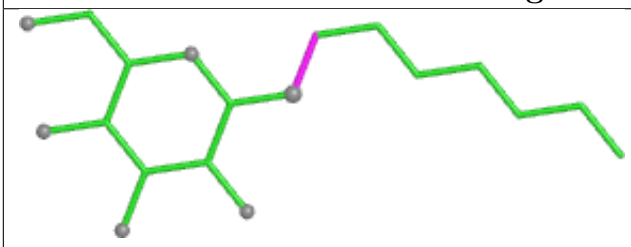
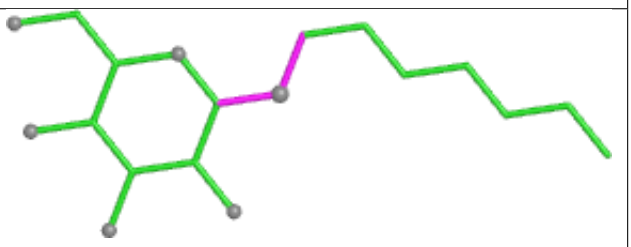


Rings

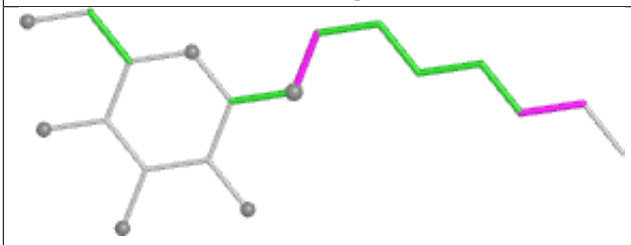
Ligand HTG c 522



Bond lengths



Bond angles



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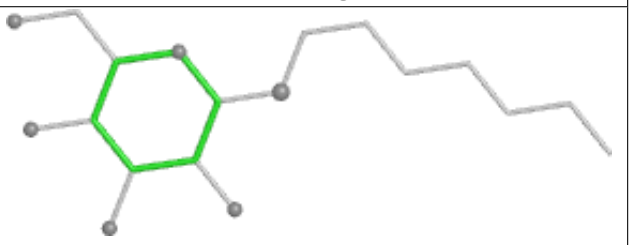
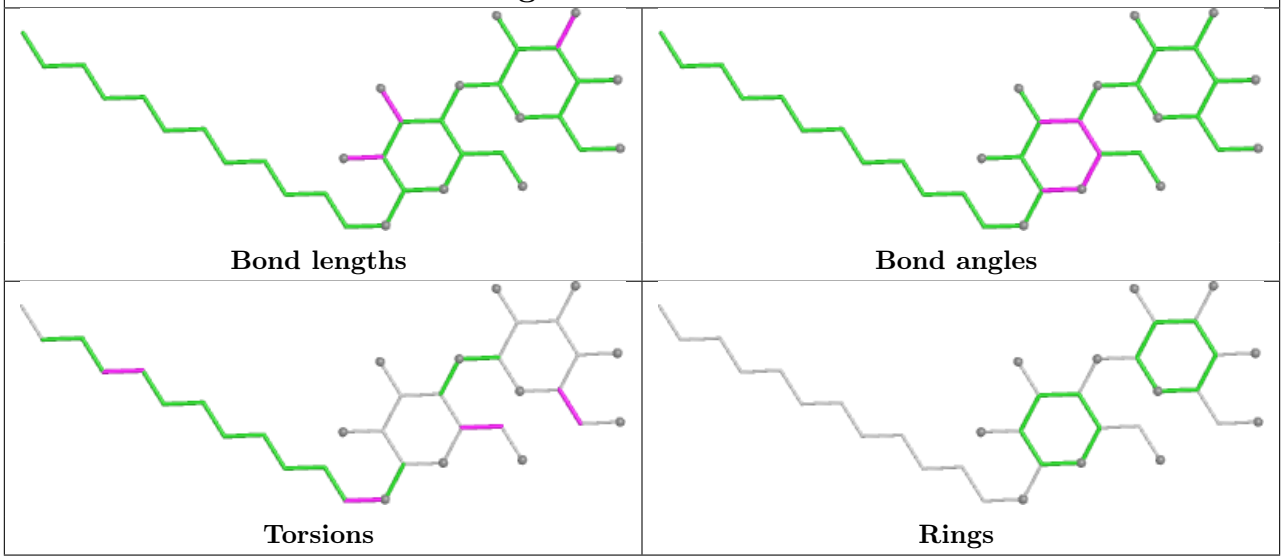
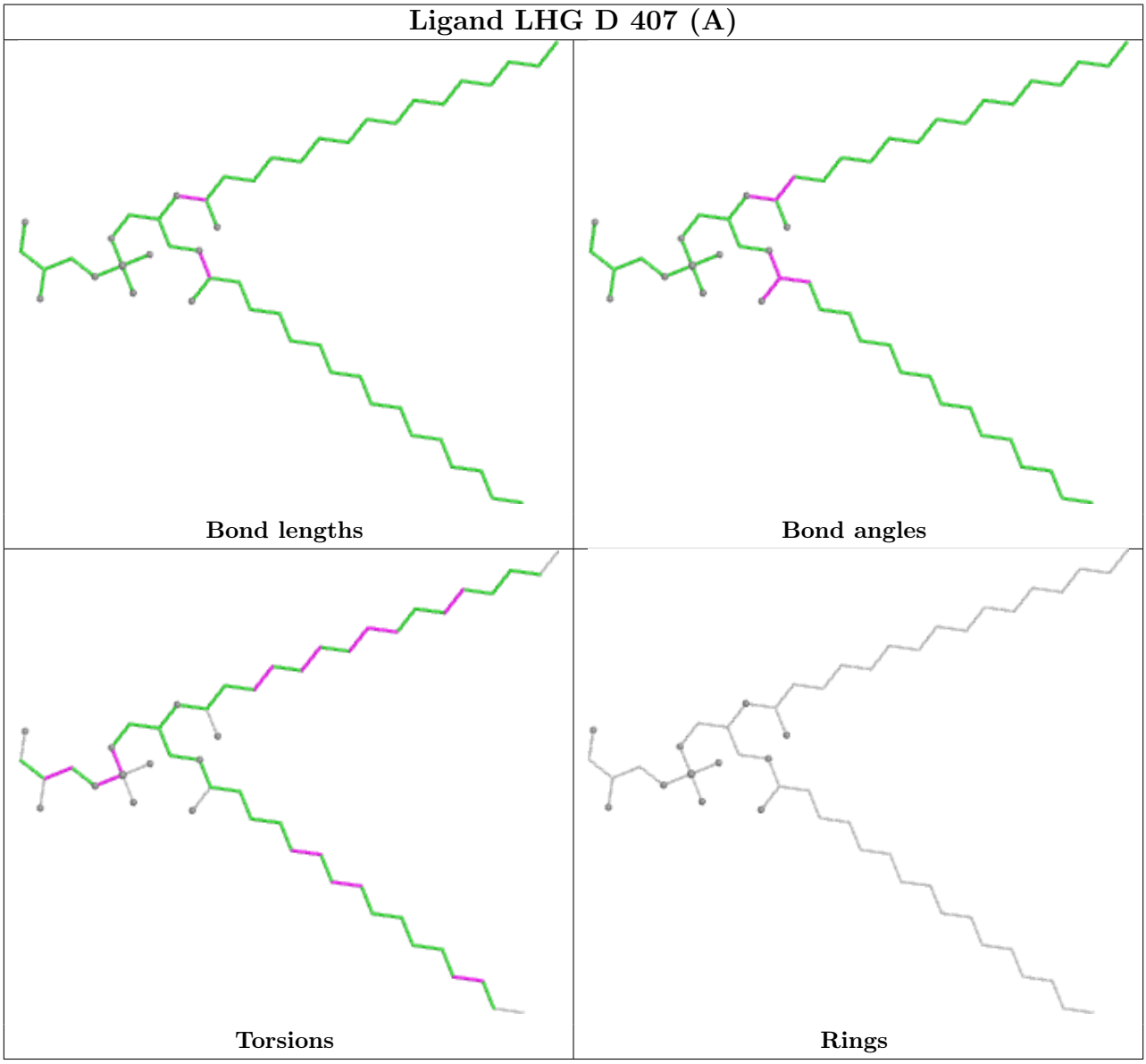


Rings

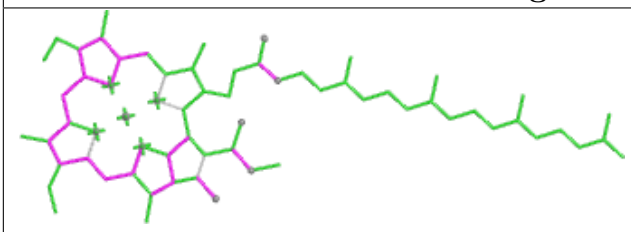
Ligand LMT M 102



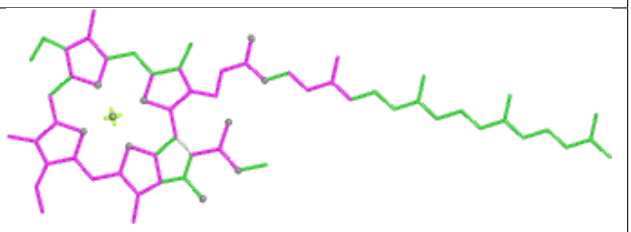
Ligand LHG D 407 (A)



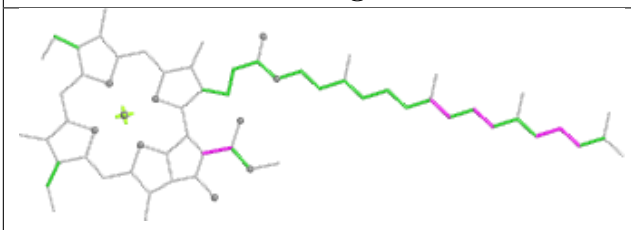
Ligand CLA c 507



Bond lengths



Bond angles



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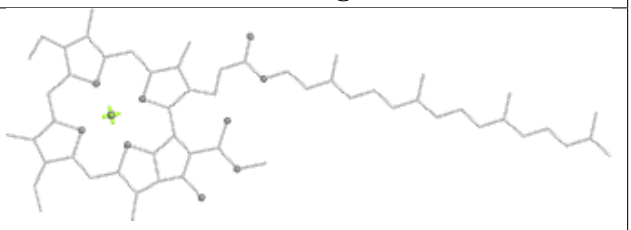
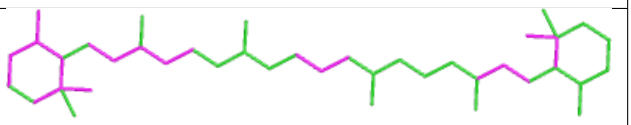


Rings

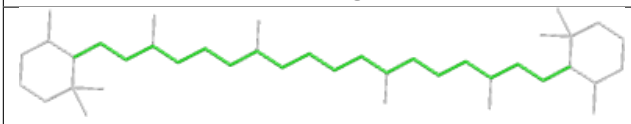
Ligand BCR C 515



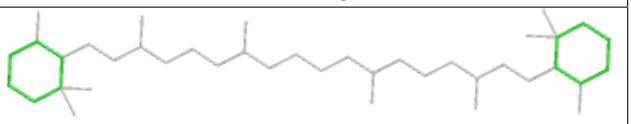
Bond lengths



Bond angles

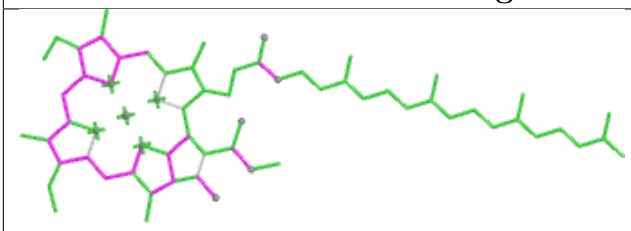


Torsions

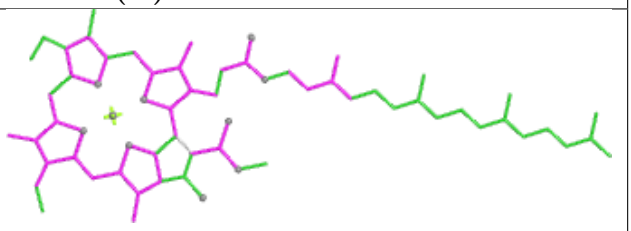


Rings

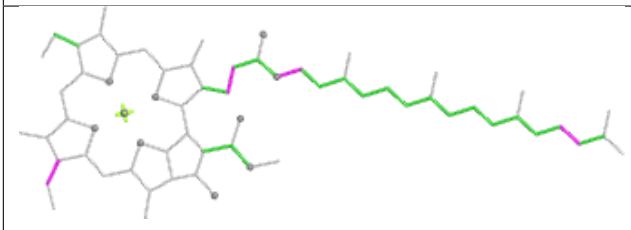
Ligand CLA a 404 (B)



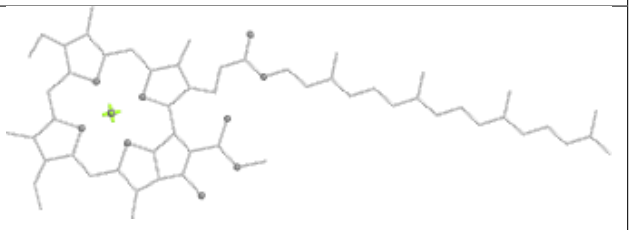
Bond lengths



Bond angles

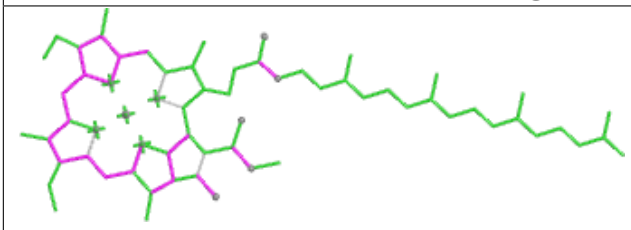


Torsions

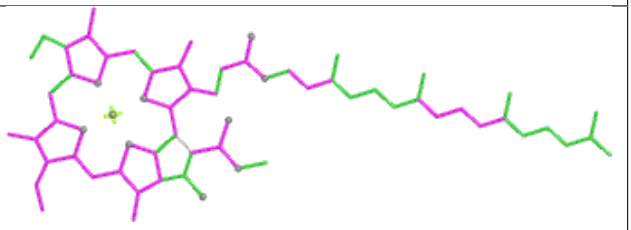


Rings

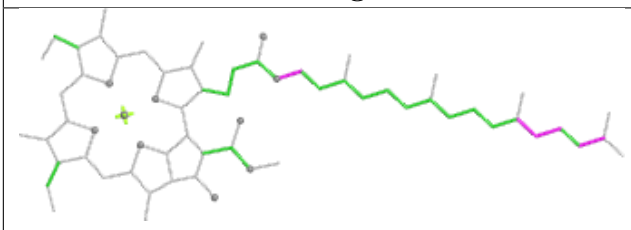
Ligand CLA b 608



Bond lengths



Bond angles



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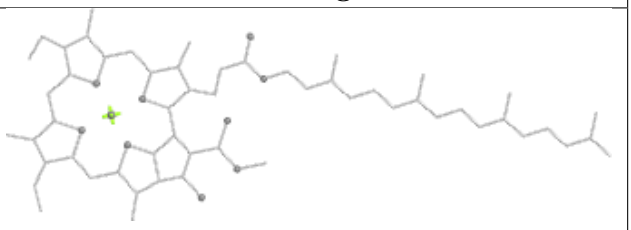
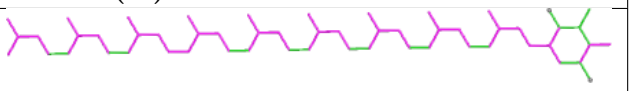


Rings

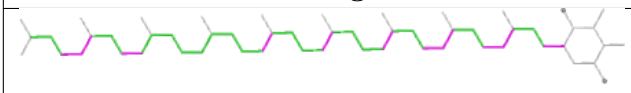
Ligand PL9 A 414 (A)



Bond lengths



Bond angles



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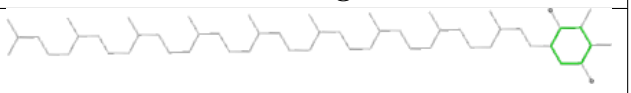
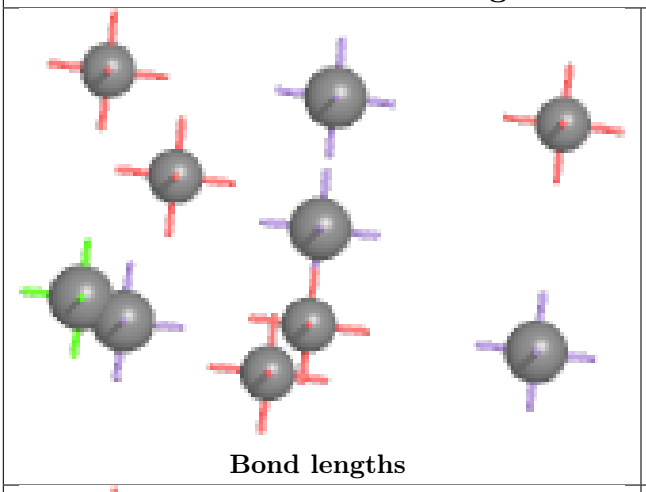
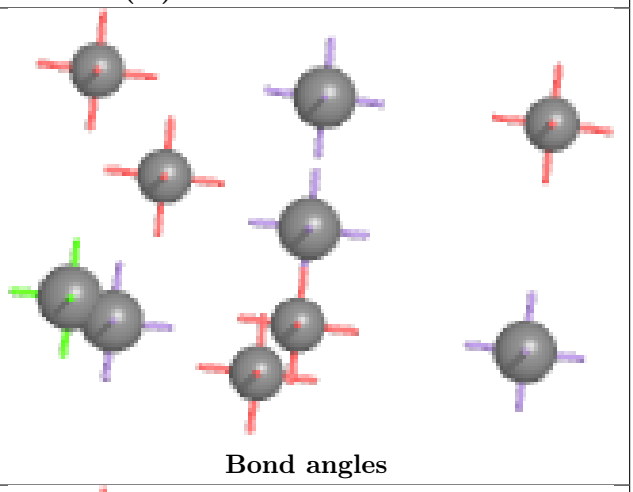


Rings

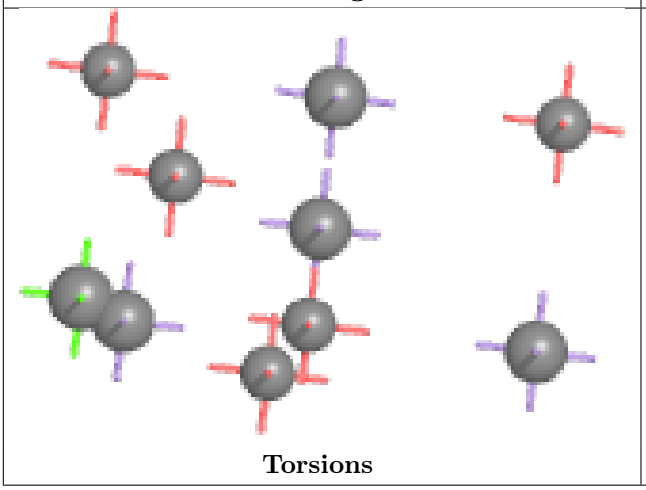
Ligand OEX A 413 (B)



Bond lengths



Bond angles



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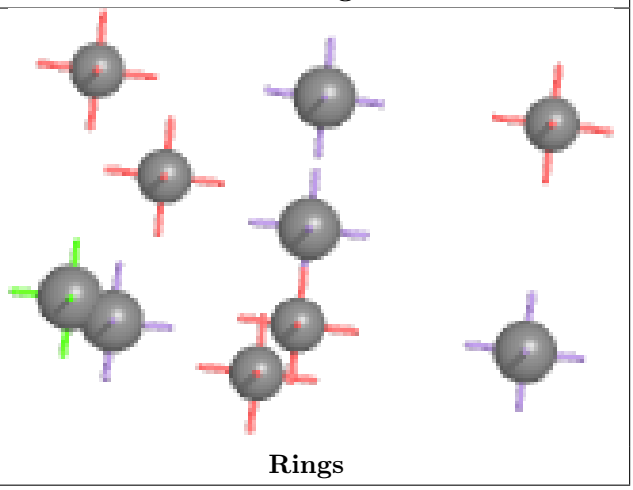
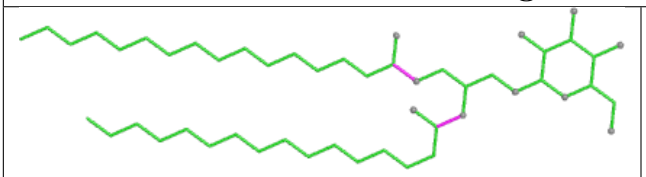
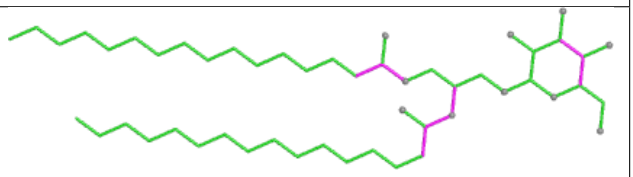


Rings

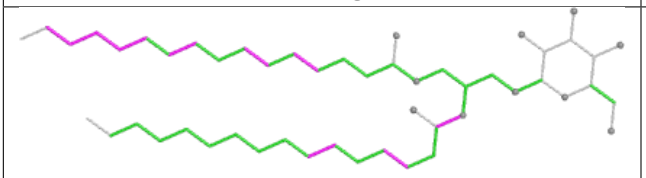
Ligand LMG m 101



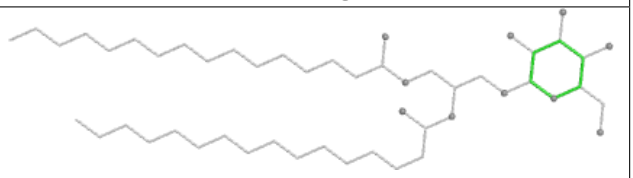
Bond lengths



Bond angles

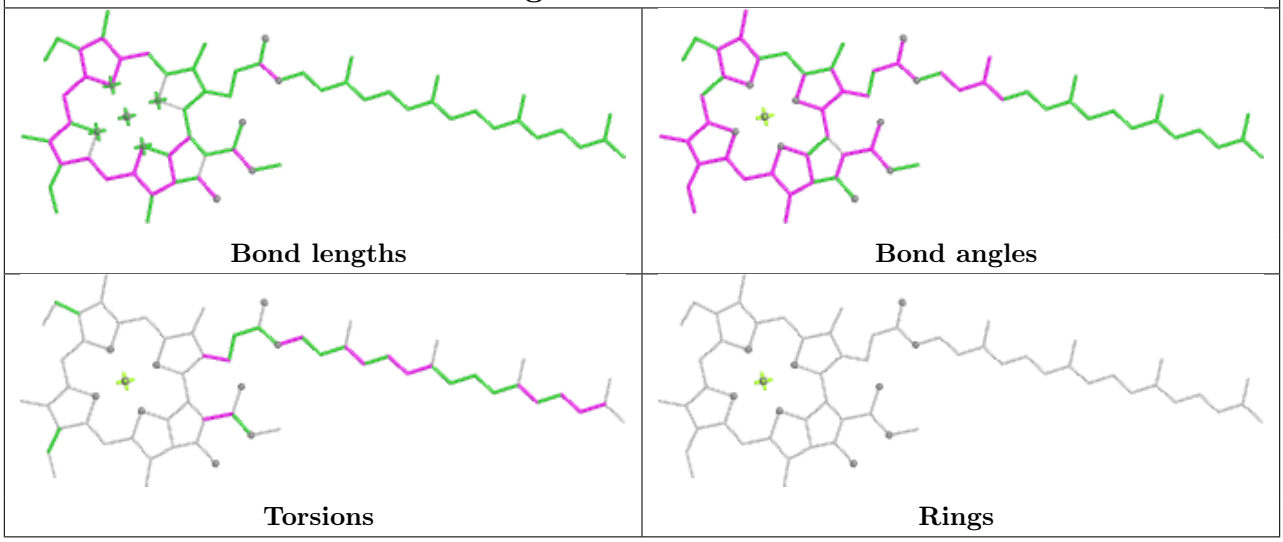


Torsions

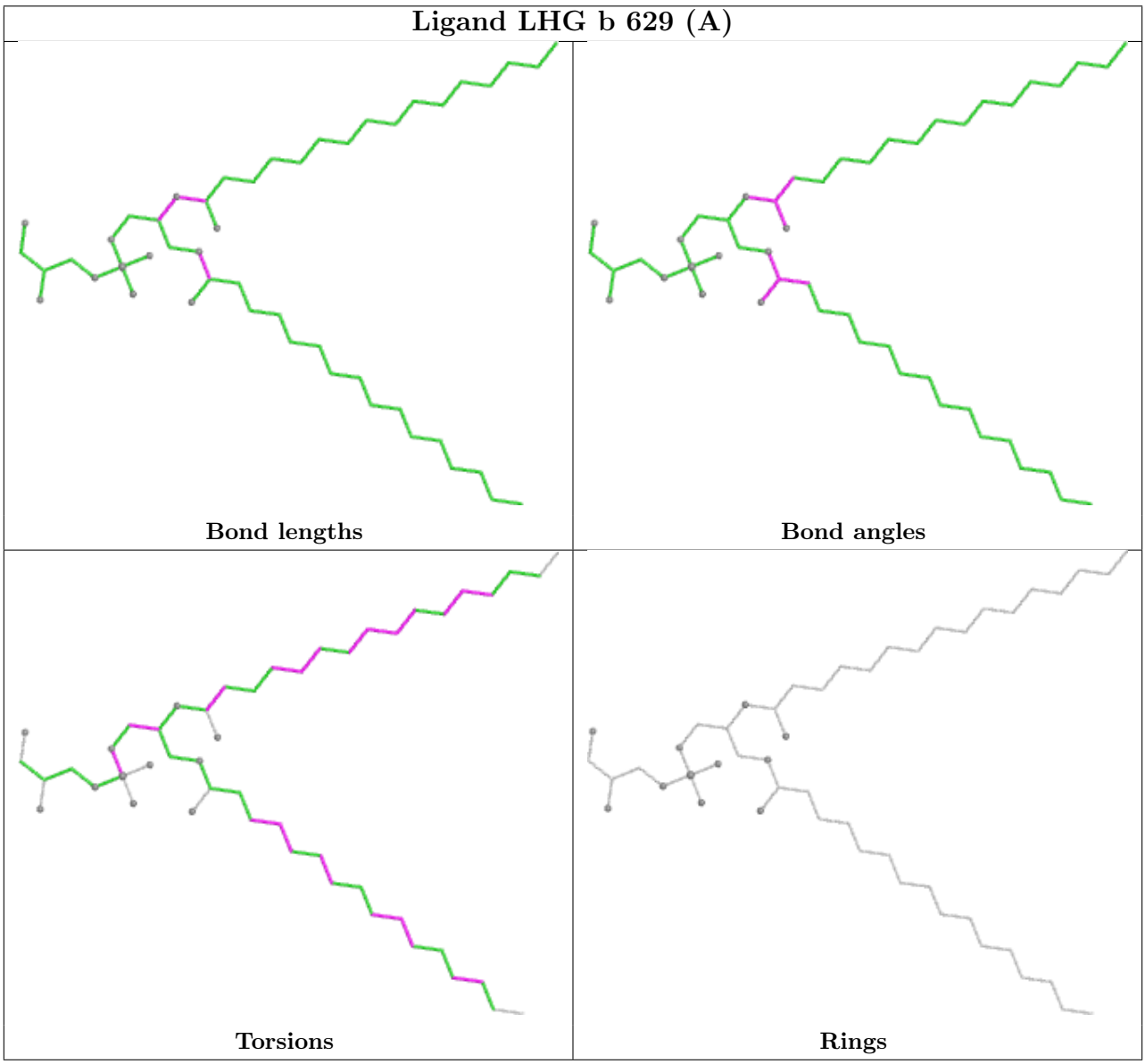


Rings

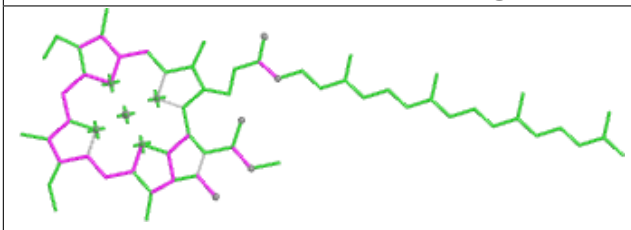
Ligand CLA C 506



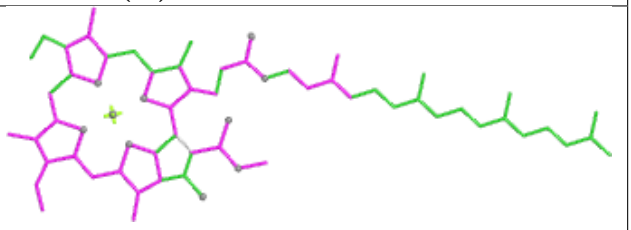
Ligand LHG b 629 (A)



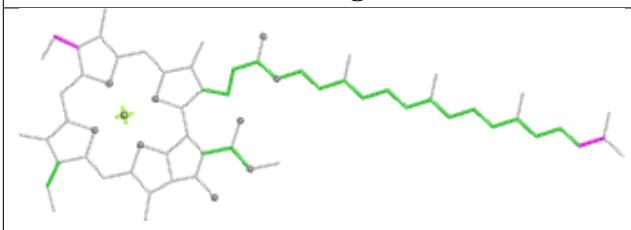
Ligand CLA D 403 (B)



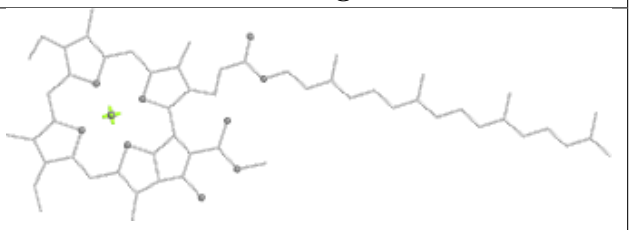
Bond lengths



Bond angles



Torsions

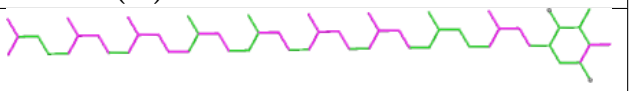


Rings

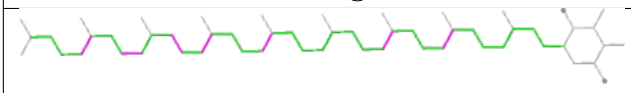
Ligand PL9 D 406 (B)



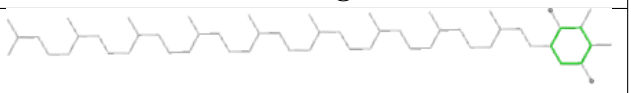
Bond lengths



Bond angles



Torsions



Rings

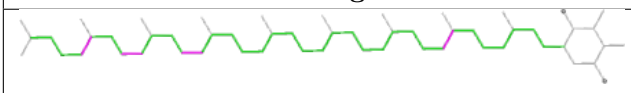
Ligand PL9 d 406 (B)



Bond lengths



Bond angles



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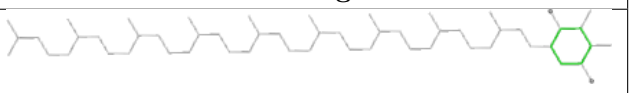
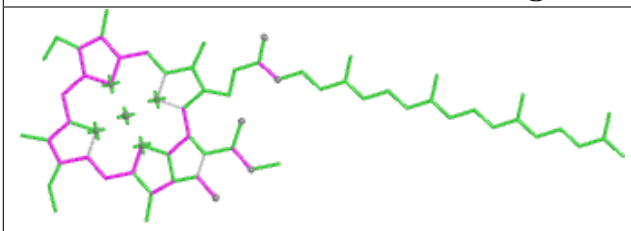
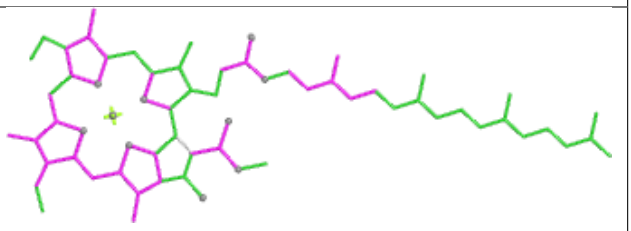


Rings

Ligand CLA b 604



Bond lengths



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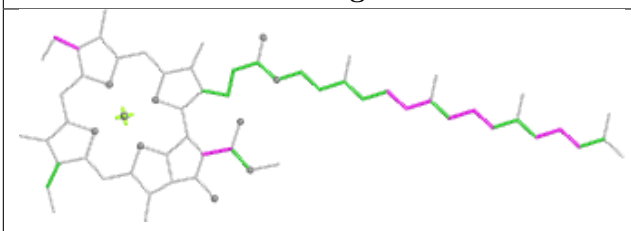

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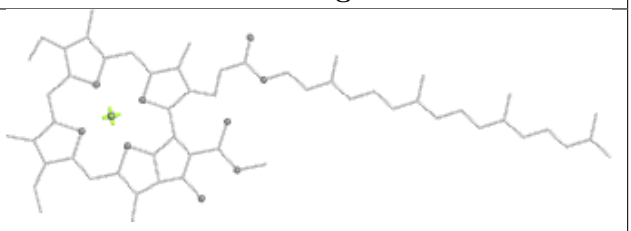
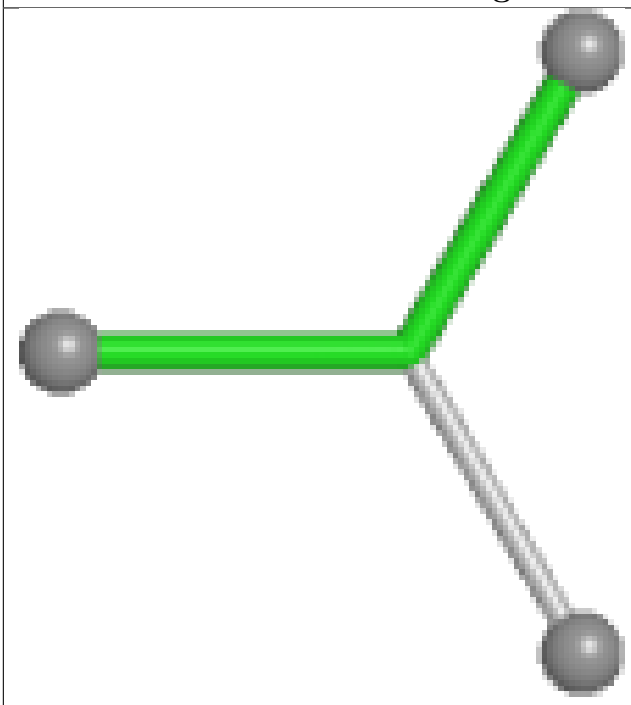
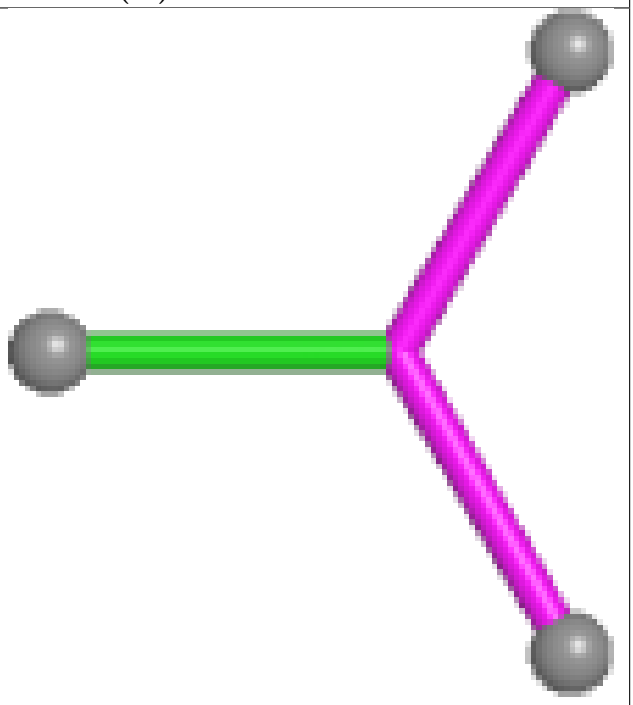


Rings

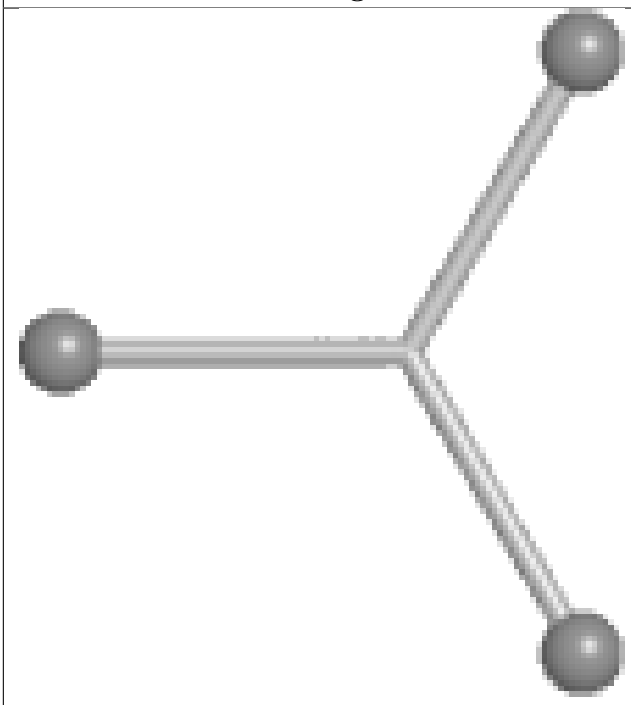
Ligand BCT d 401 (A)



Bond lengths



Bond angles



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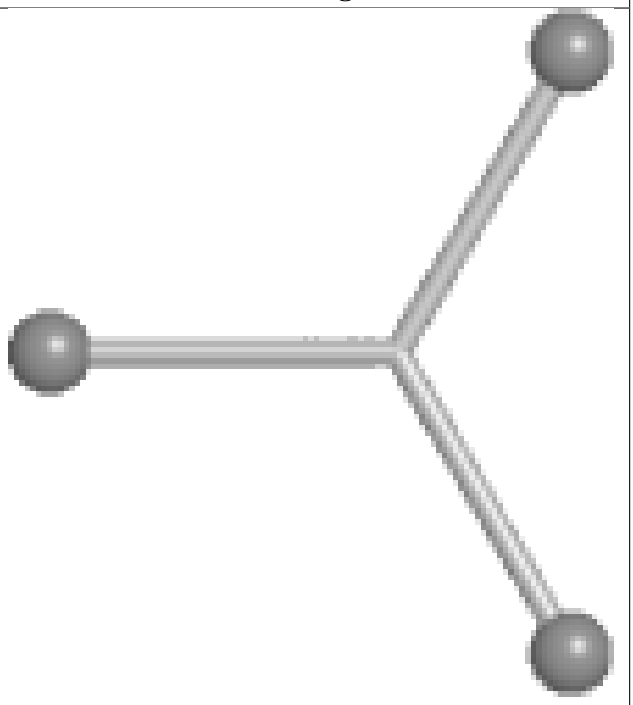
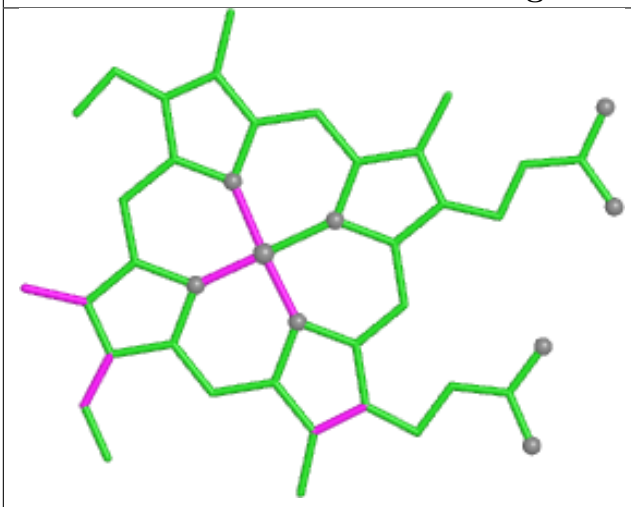


Rings

Ligand HEC v 201



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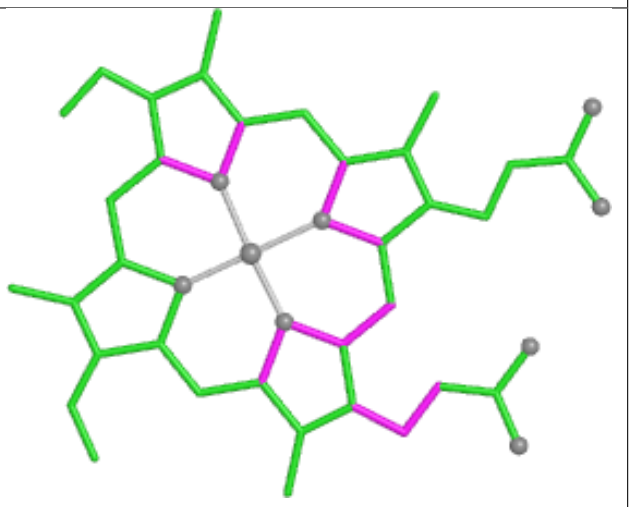
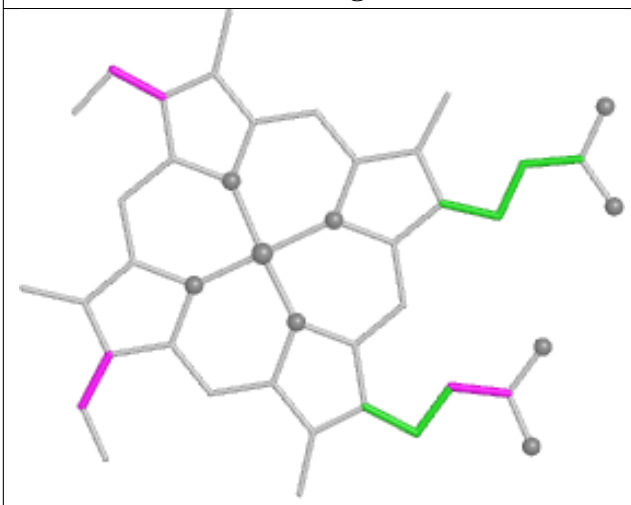


Bond angles



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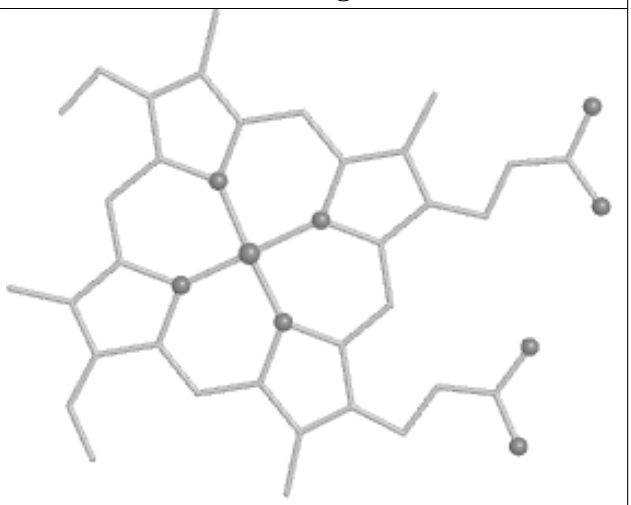
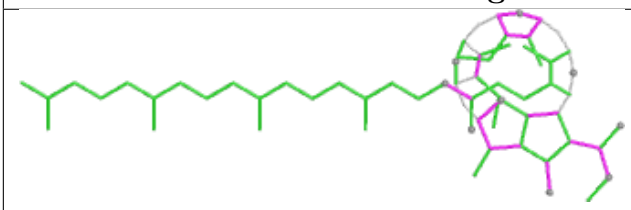


Rings

Ligand PHO A 407 (A)



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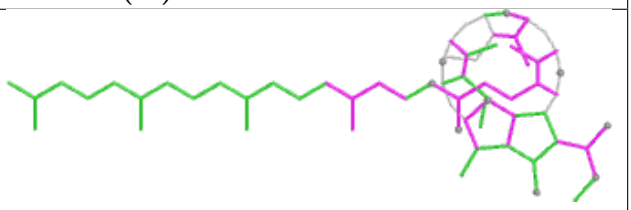
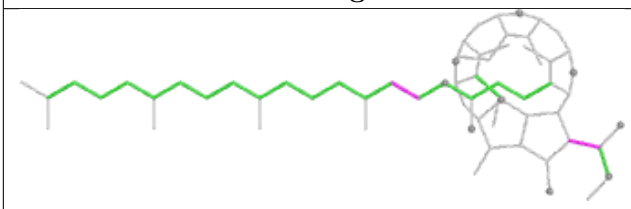


Bond angles



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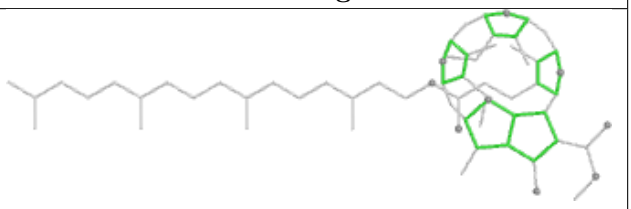
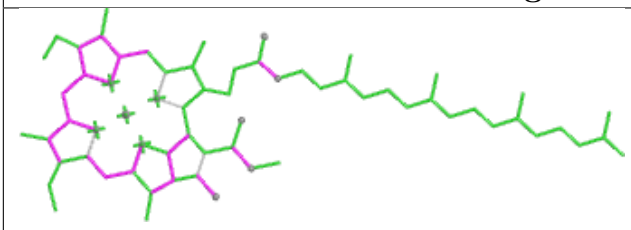


Rings

Ligand CLA B 616



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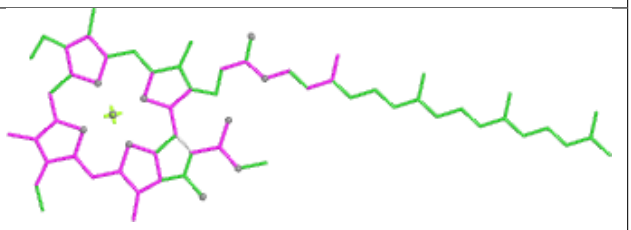
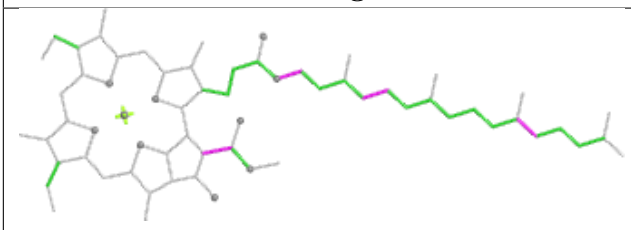


Bond angles



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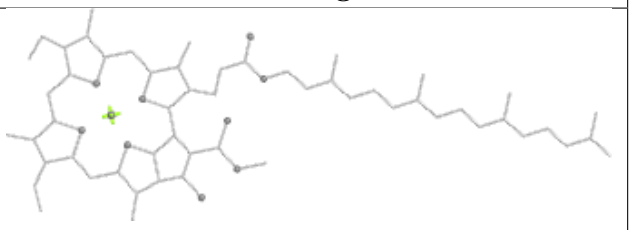
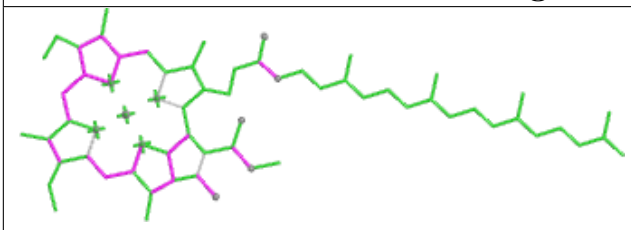


Rings

Ligand CLA c 503



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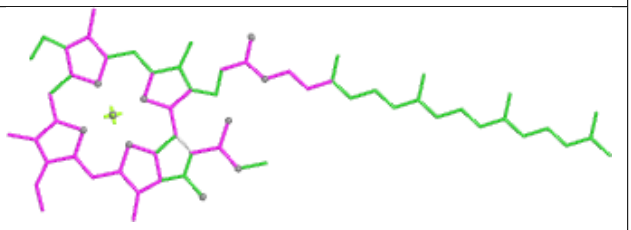
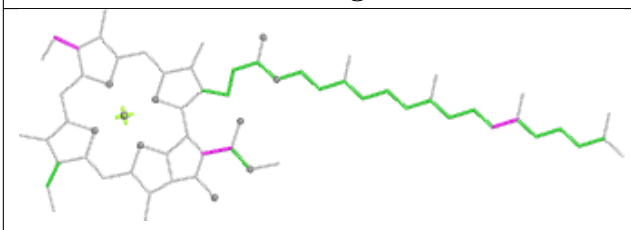


Bond angles



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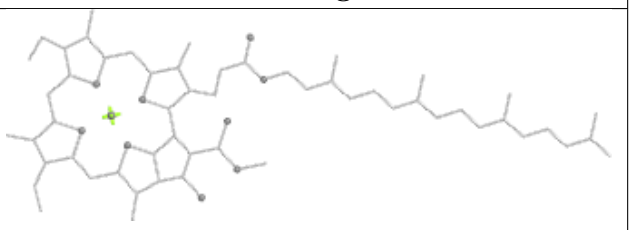
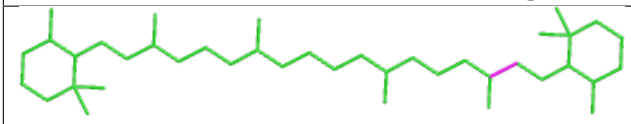


Rings

Ligand BCR Y 101



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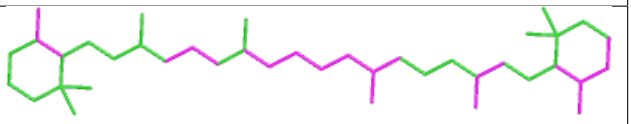
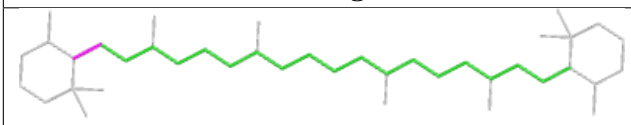


Bond angles



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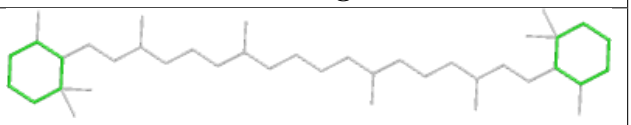
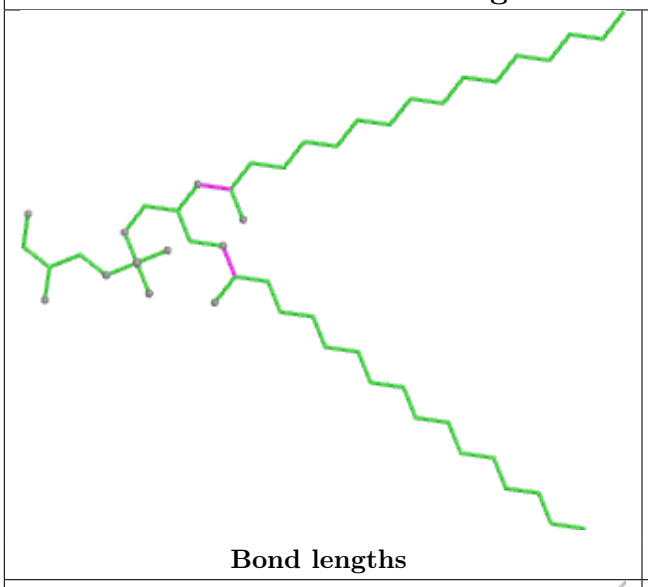


Rings

Ligand LHG D 407 (B)



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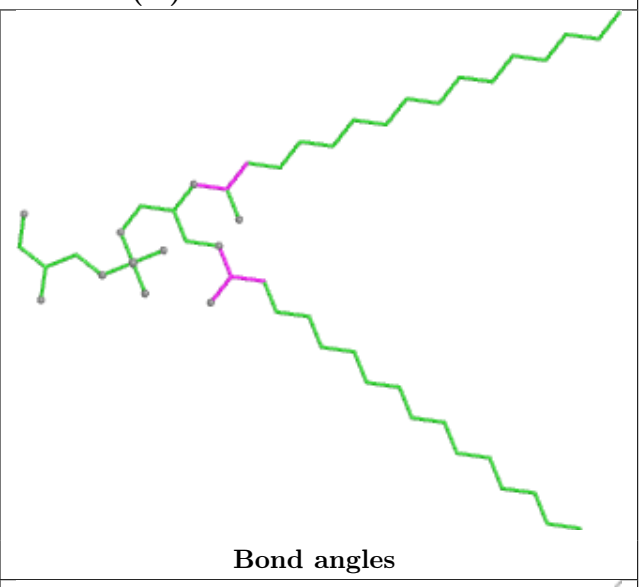
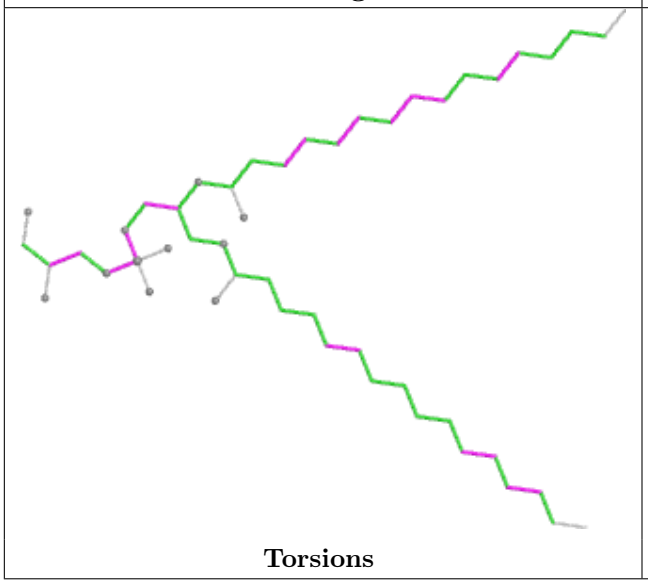


Bond angles



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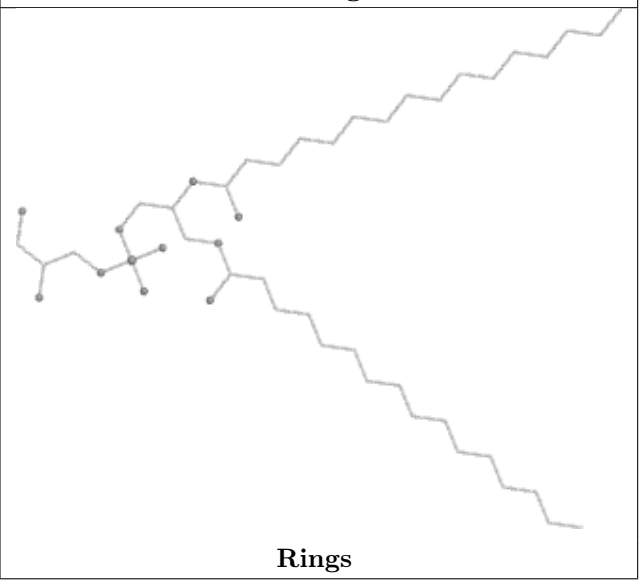
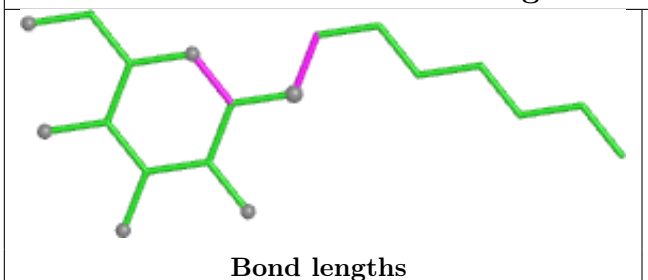


Rings

Ligand HTG B 622



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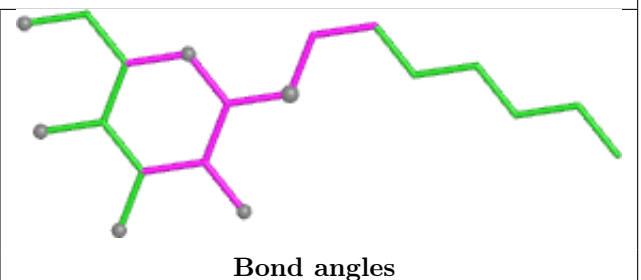
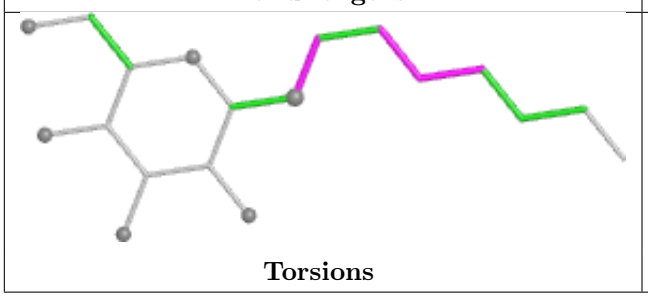


Bond angles



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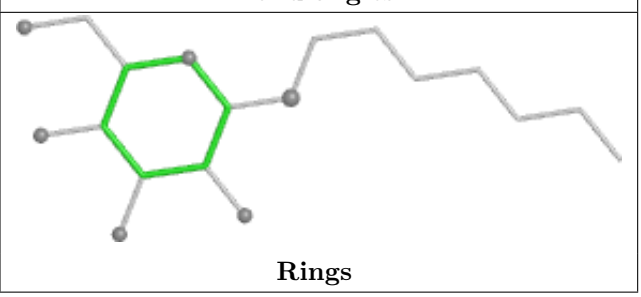
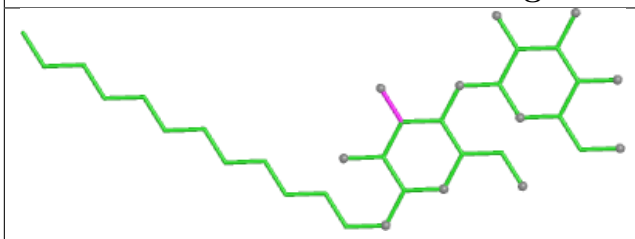


Rings

Ligand LMT F 101



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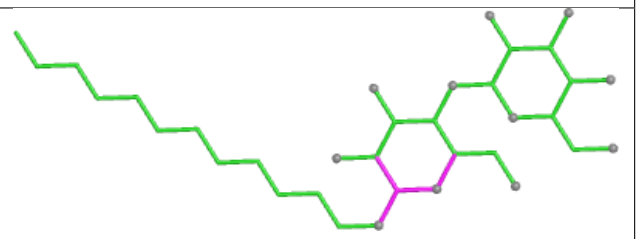
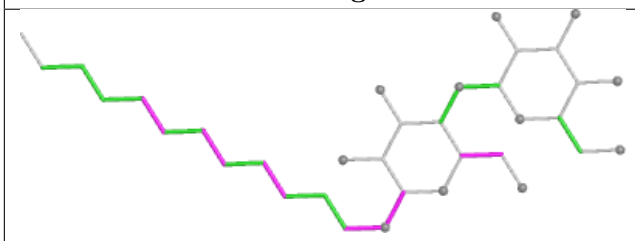


Bond angles



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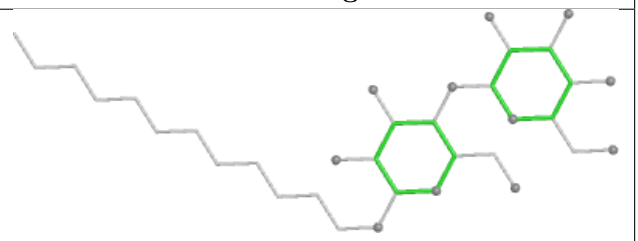
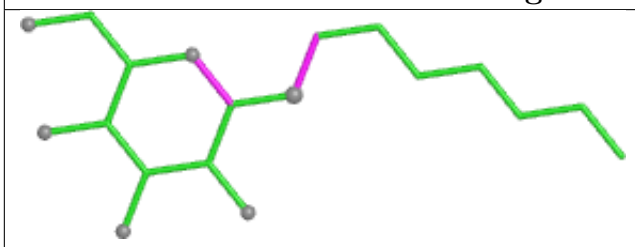


Rings

Ligand HTG b 622



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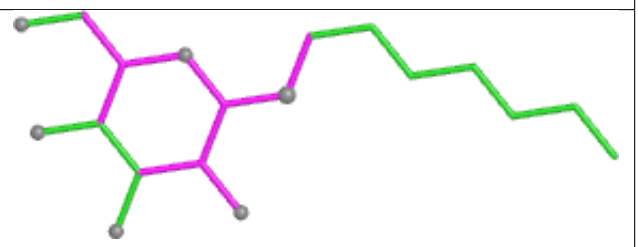
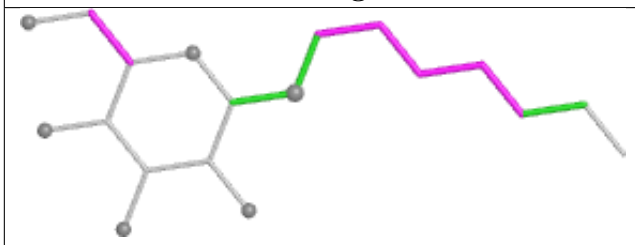


Bond angles



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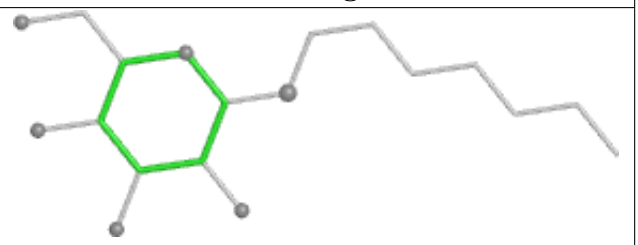
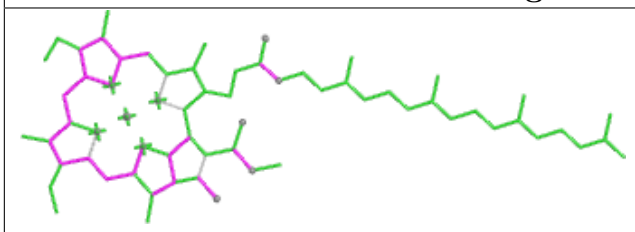
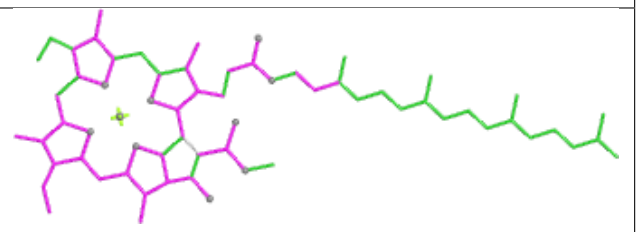


Rings

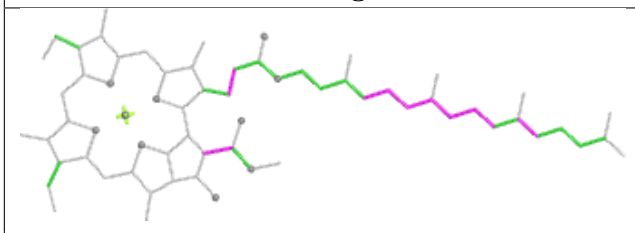
Ligand CLA B 614



Bond lengths



Bond angles



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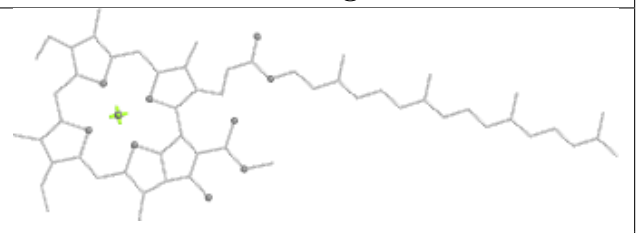
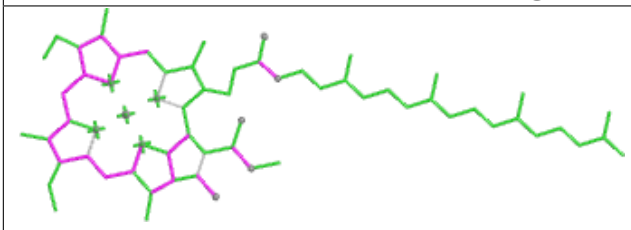
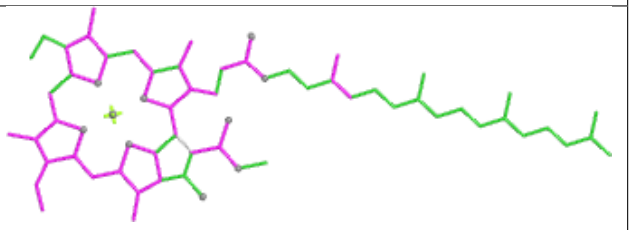


Rings

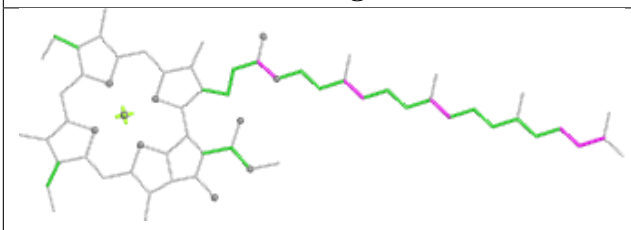
Ligand CLA a 407



Bond lengths



Bond angles



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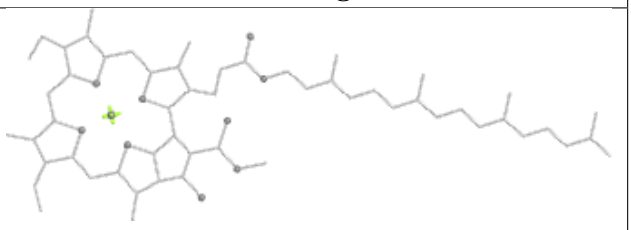
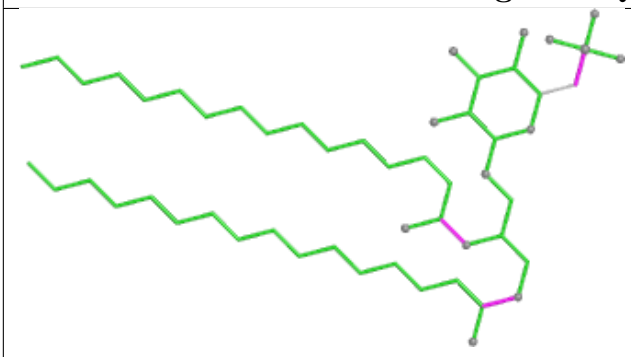
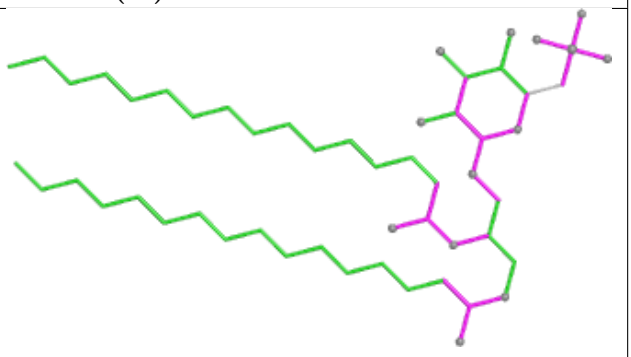


Rings

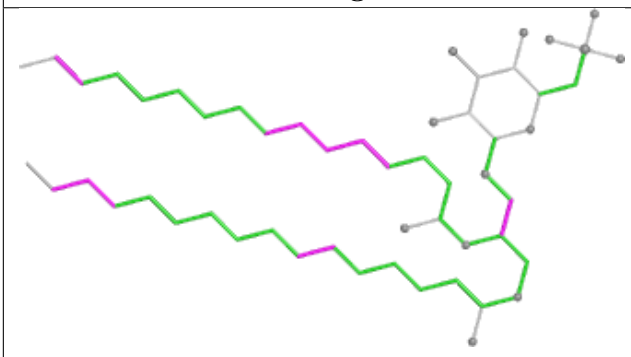
Ligand SQD a 409 (A)



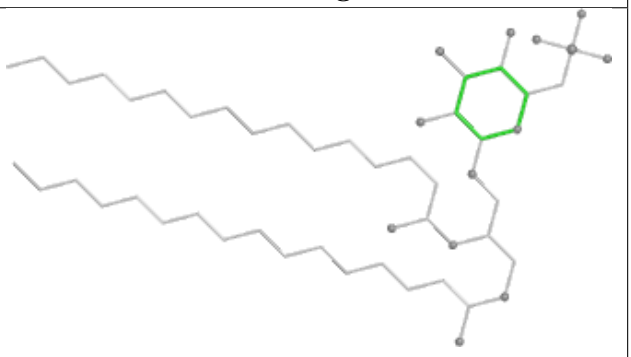
Bond lengths



Bond angles

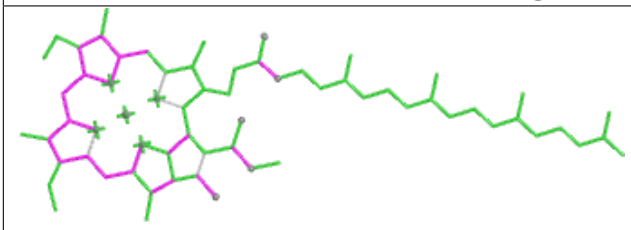


Torsions

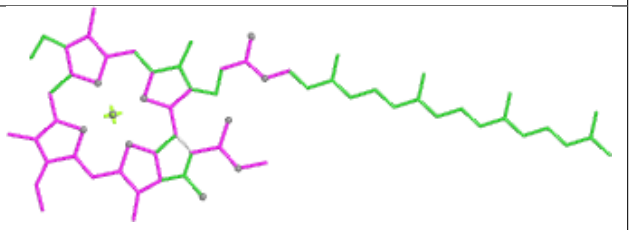


Rings

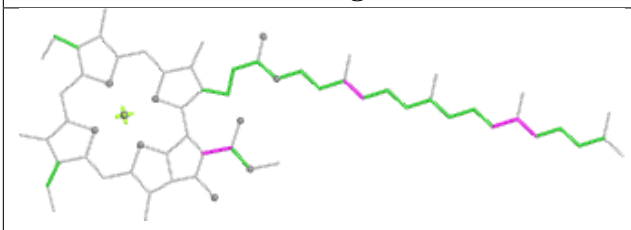
Ligand CLA c 505



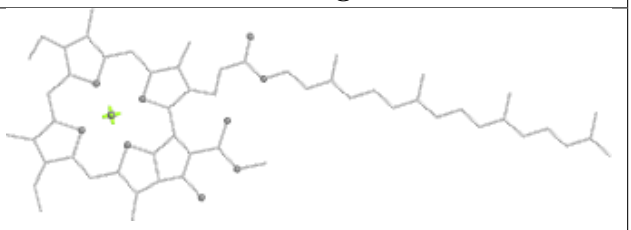
Bond lengths



Bond angles

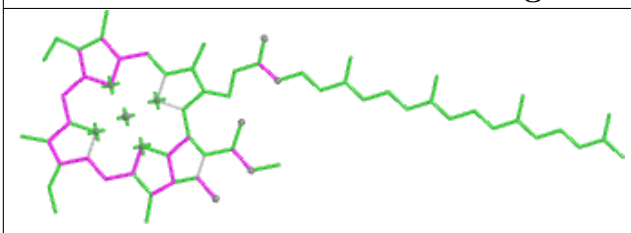


Torsions

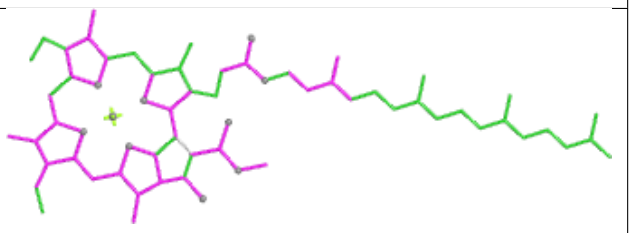


Rings

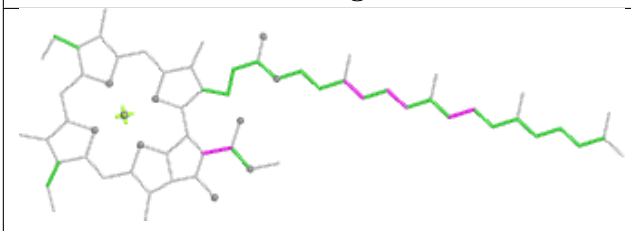
Ligand CLA B 605



Bond lengths



Bond angles



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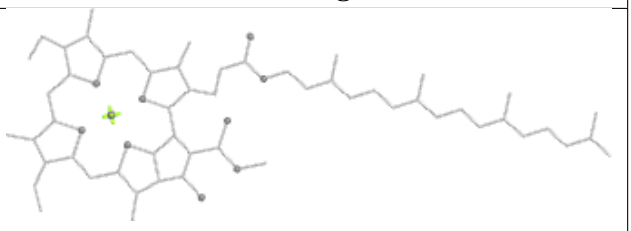
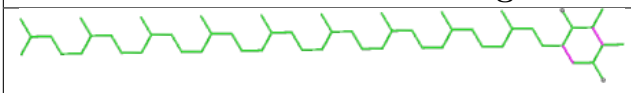


Rings

Ligand PL9 A 414 (B)



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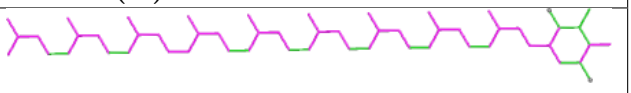
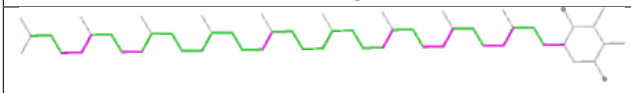


Bond angles



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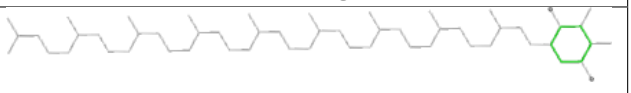
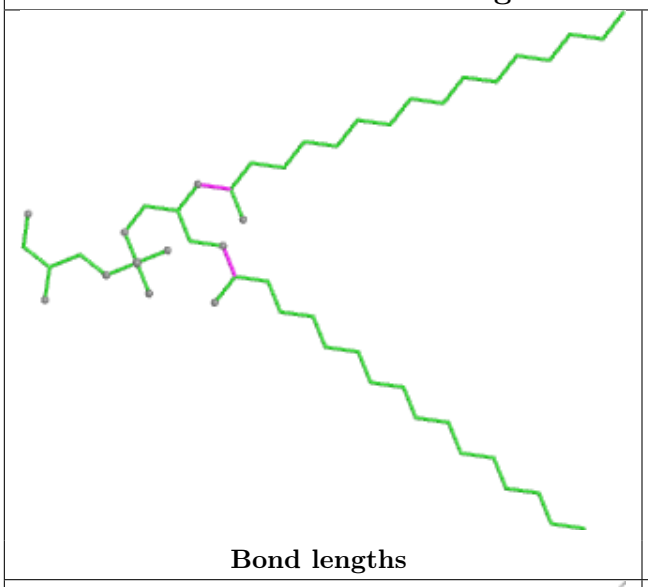


Rings

Ligand LHG b 629 (B)



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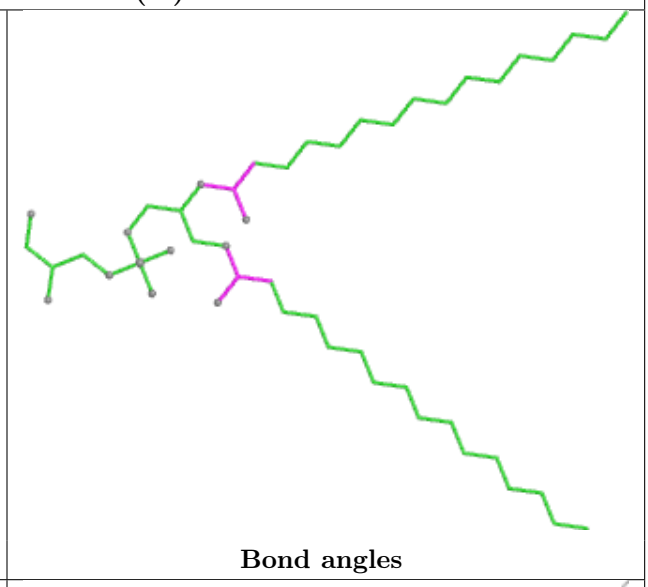
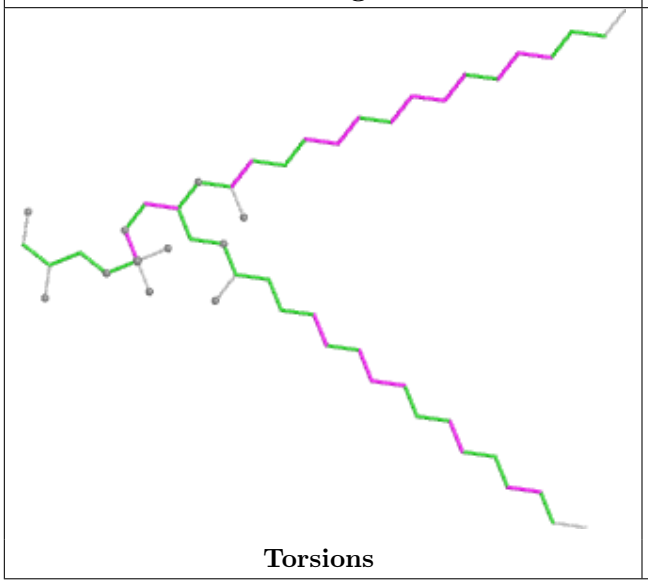


Bond angles



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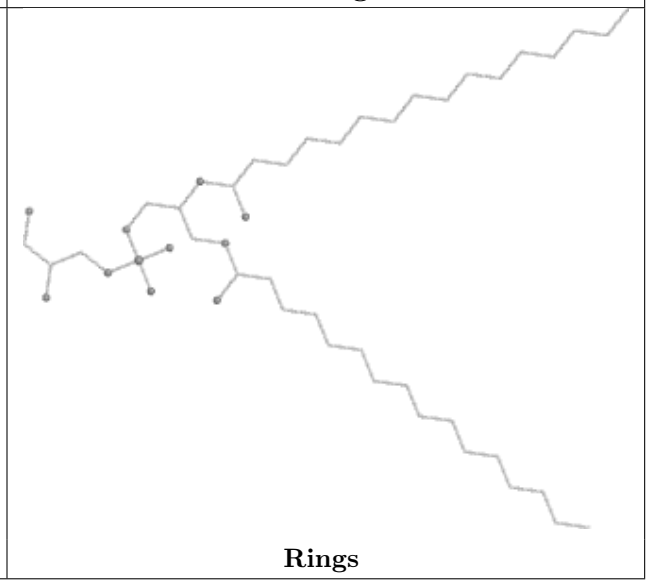
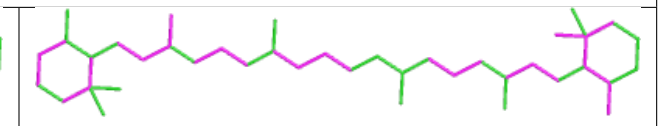


Rings

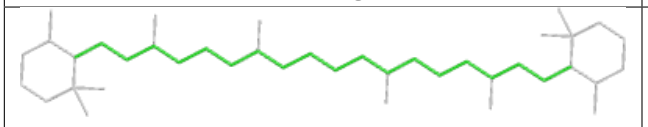
Ligand BCR B 619



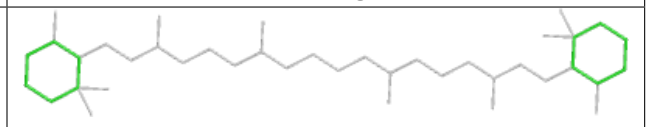
Bond lengths



Bond angles

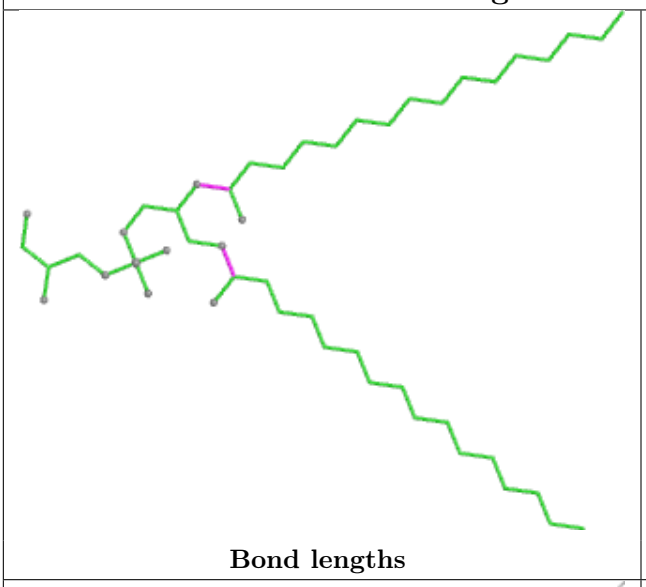


Torsions

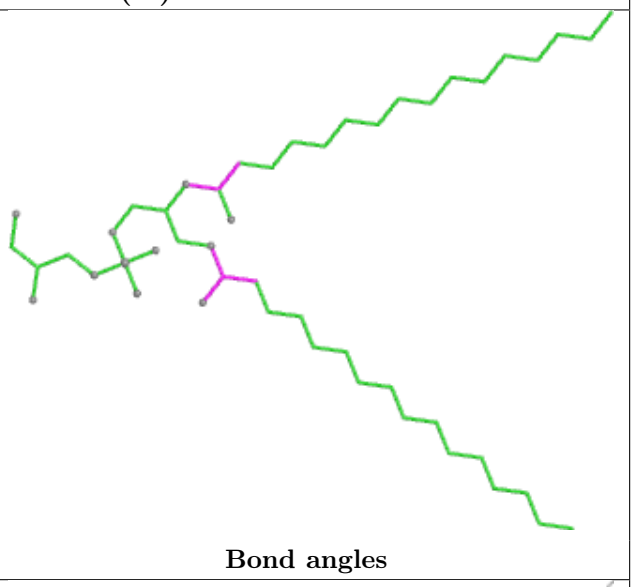


Rings

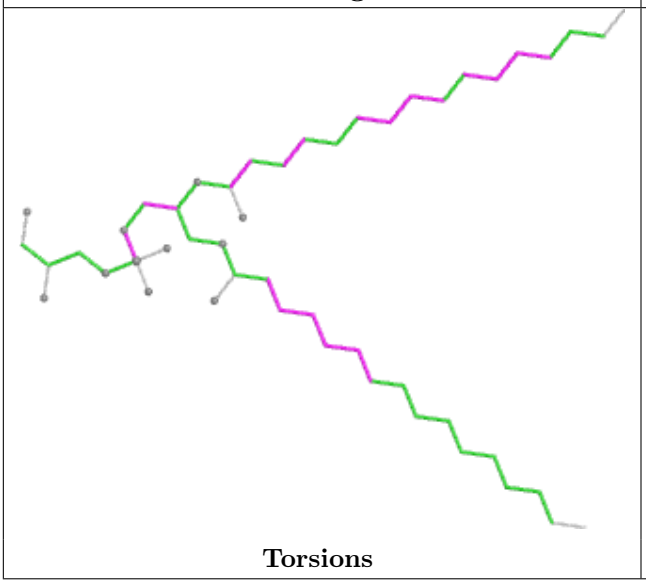
Ligand LHG L 101 (A)



Bond lengths



Bond angles



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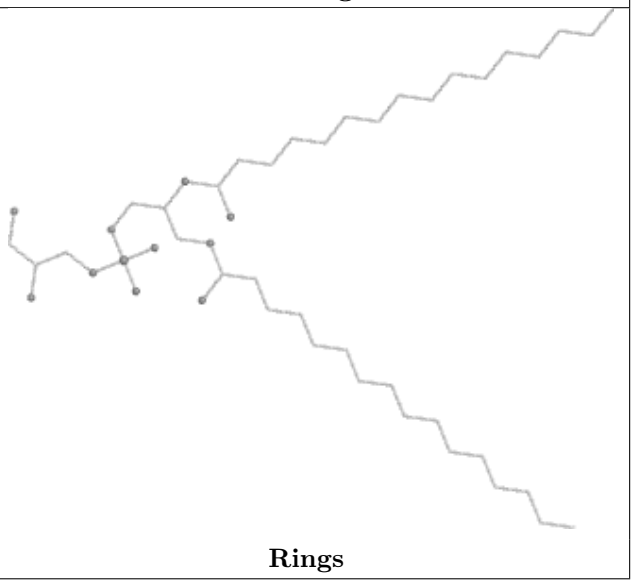
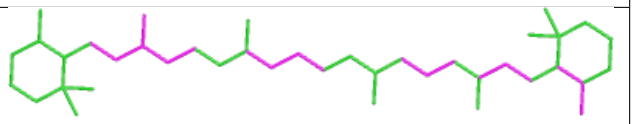


Rings

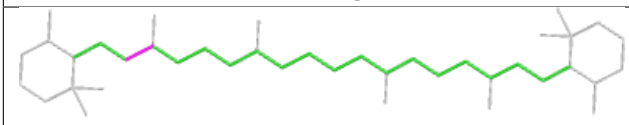
Ligand BCR b 619



Bond lengths



Bond angles



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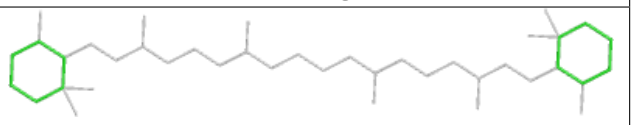
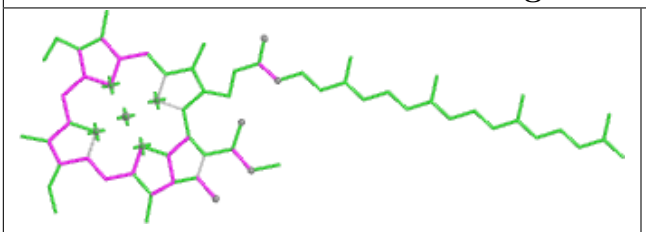


Rings

Ligand CLA C 503



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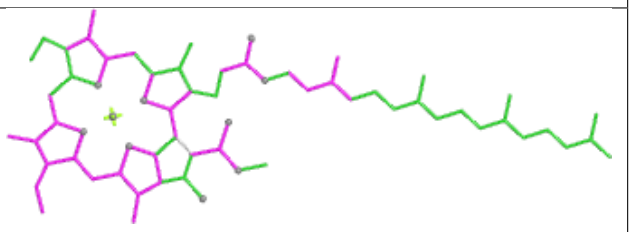
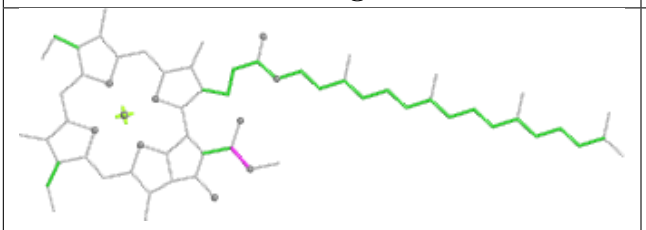


Bond angles



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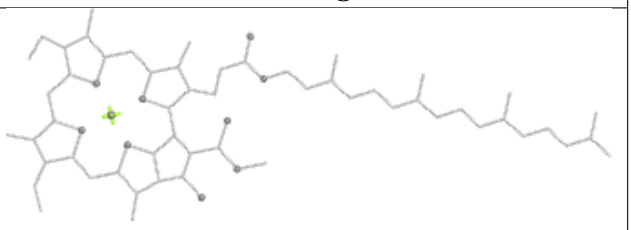
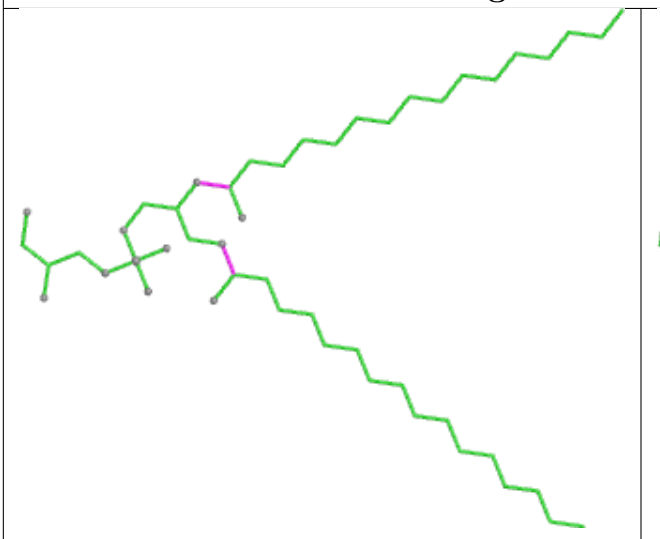


Rings

Ligand LHG D 408 (A)



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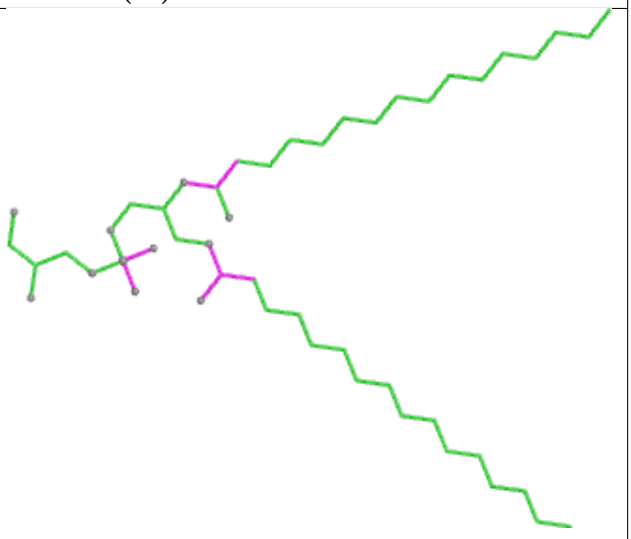
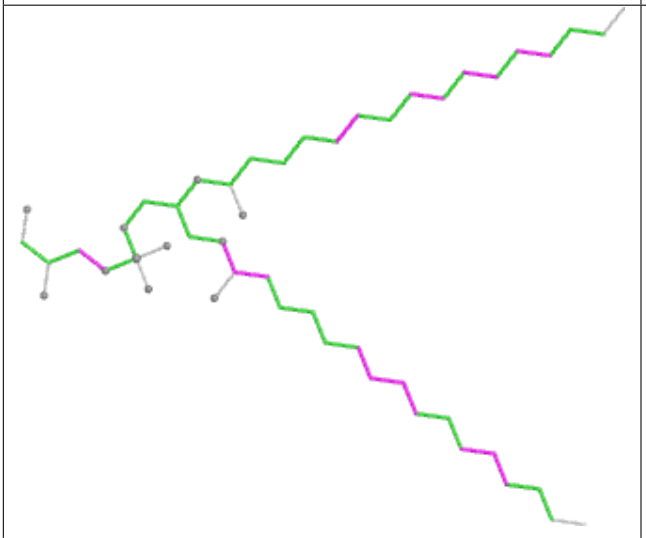
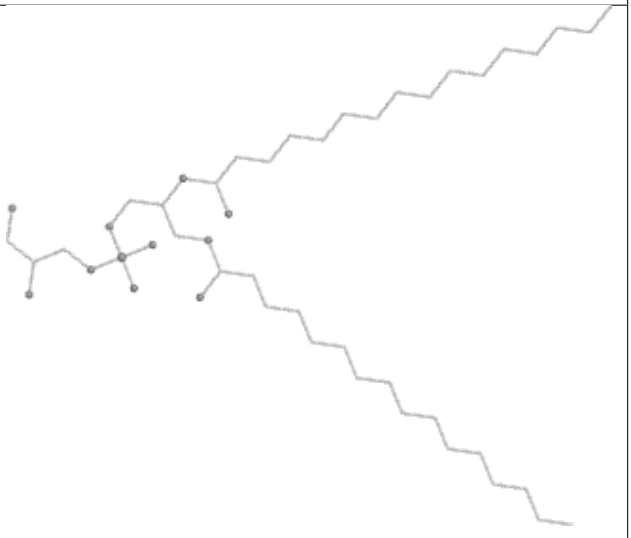


Bond angles

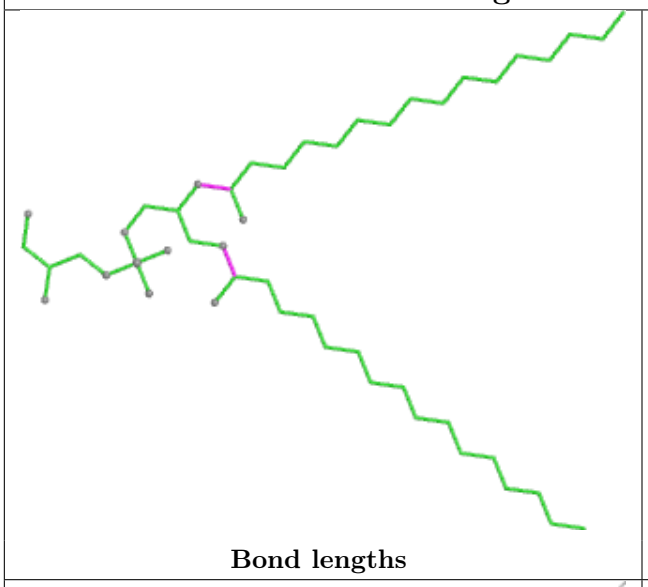


Torsions



Rings

Ligand LHG d 408 (A)



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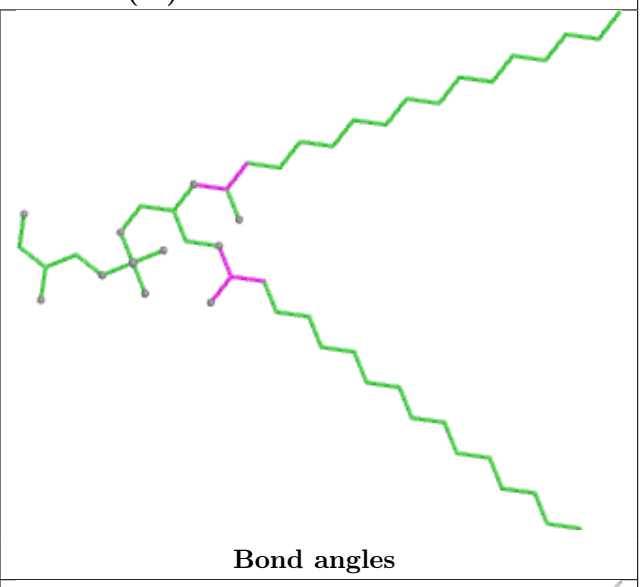
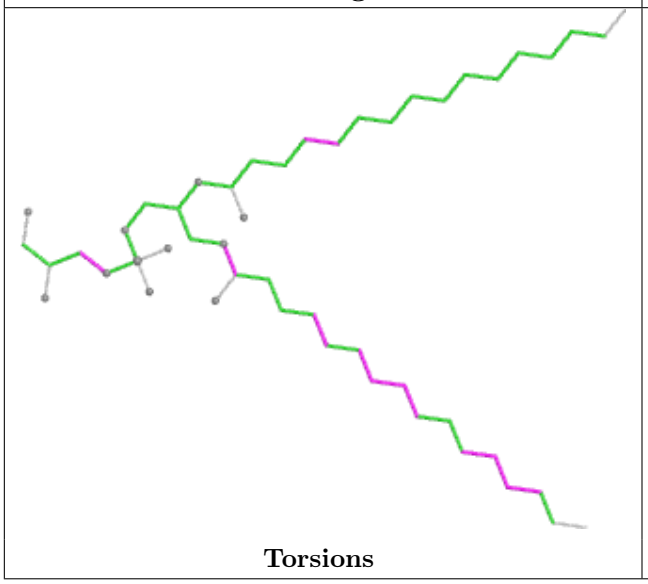


Bond angles



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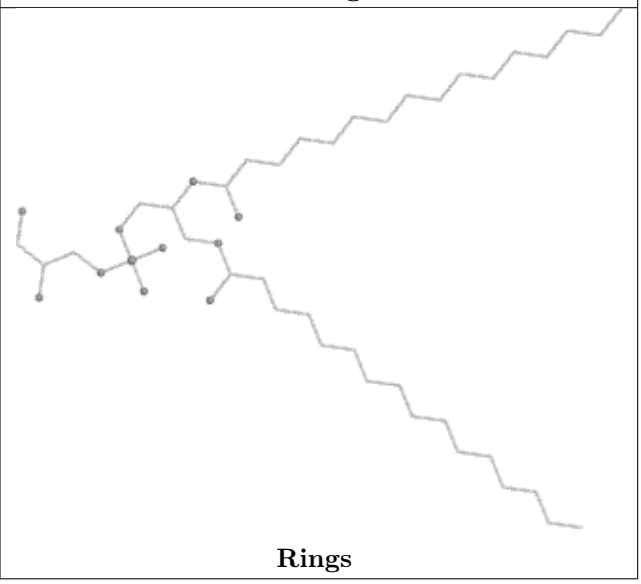
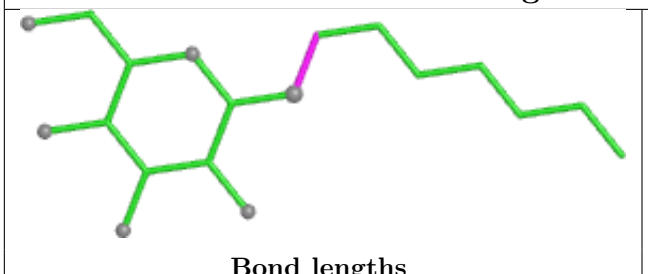


Rings

Ligand HTG C 521



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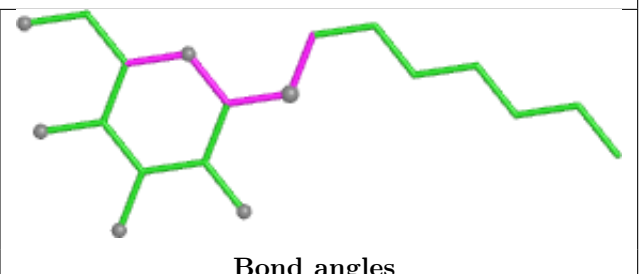
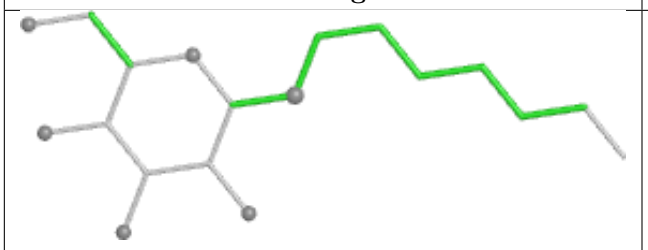


Bond angles



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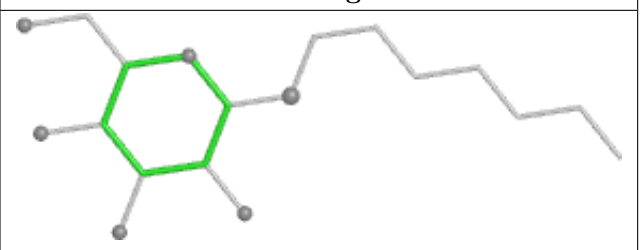
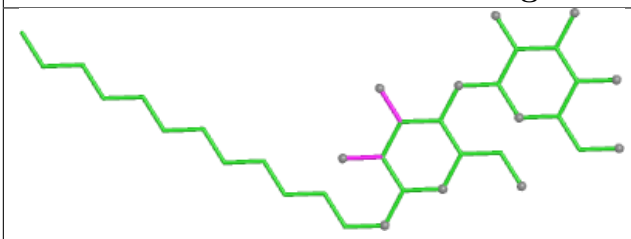


Rings

Ligand LMT A 420



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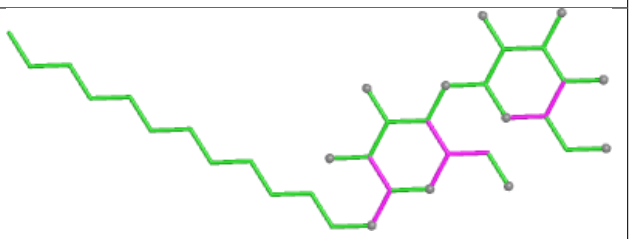
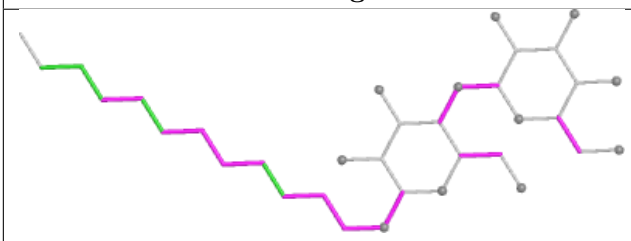


Bond angles



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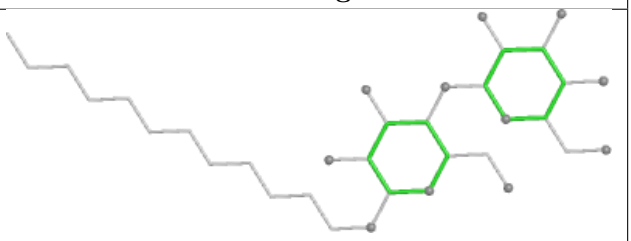
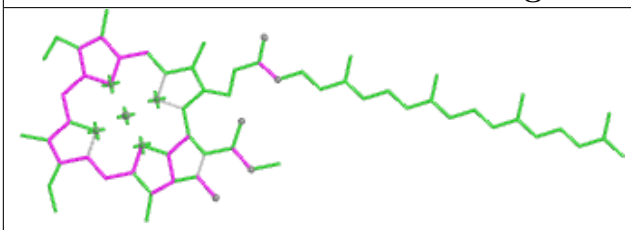


Rings

Ligand CLA B 602



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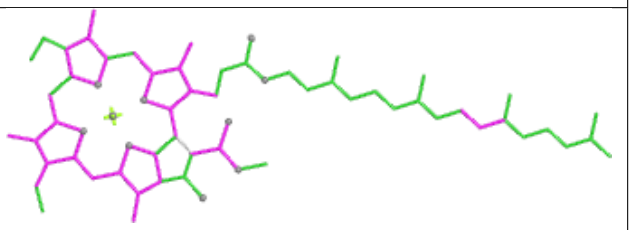
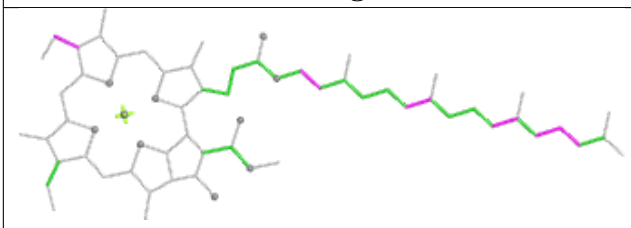


Bond angles



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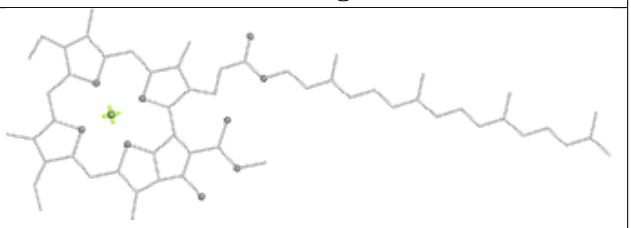
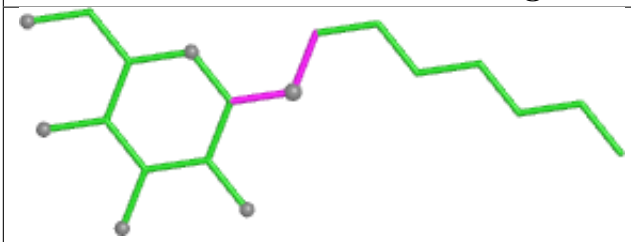
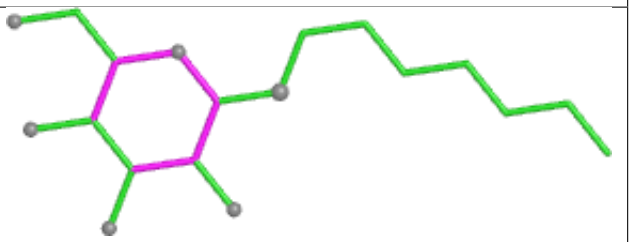


Rings

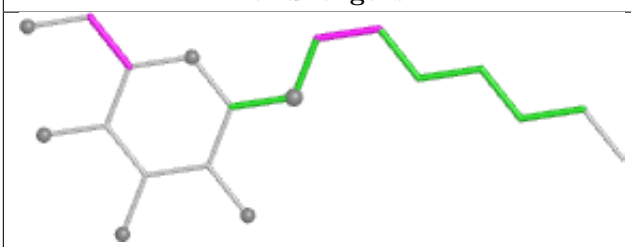
Ligand HTG b 625



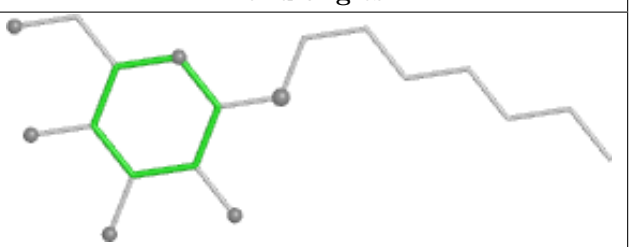
Bond lengths



Bond angles

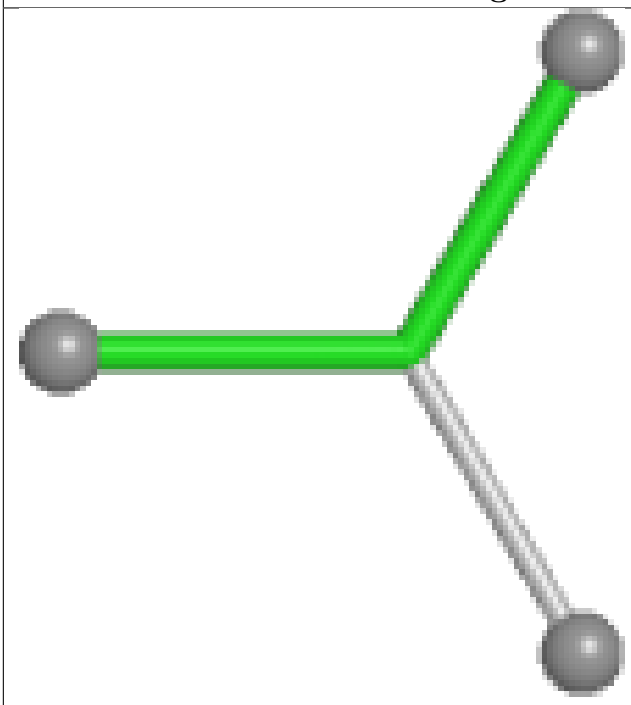


Torsions

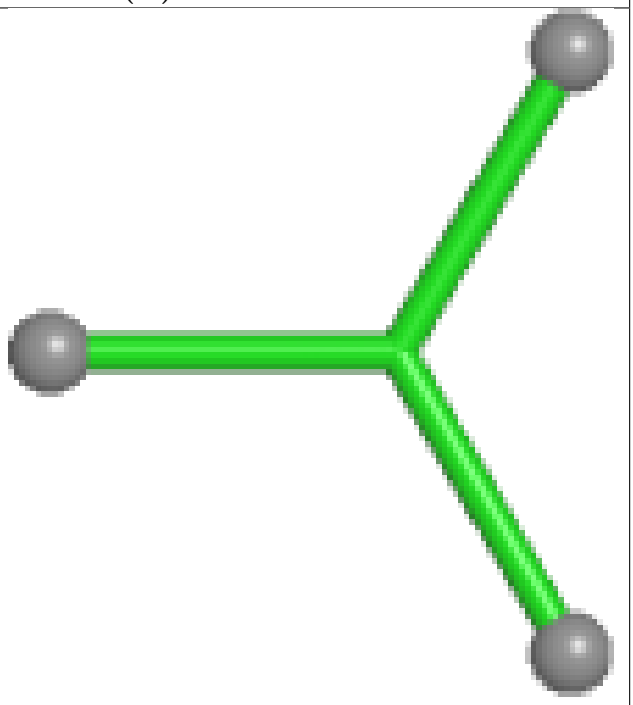


Rings

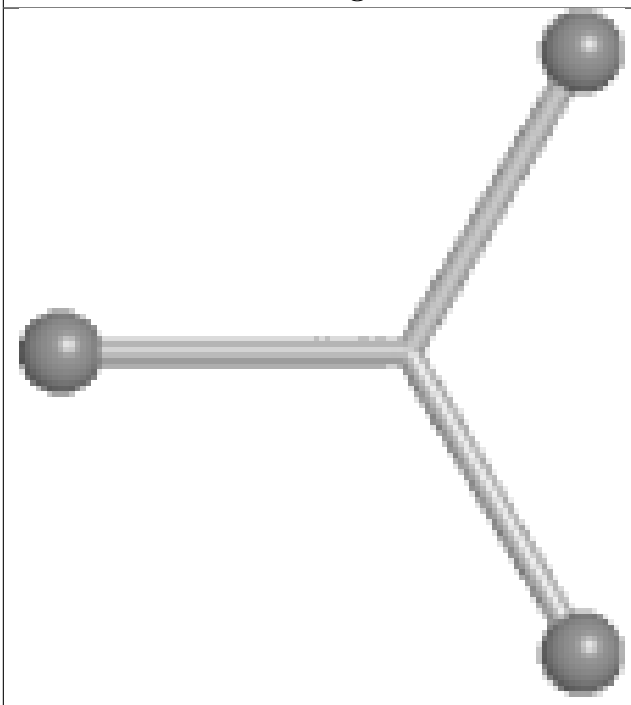
Ligand BCT D 401 (B)



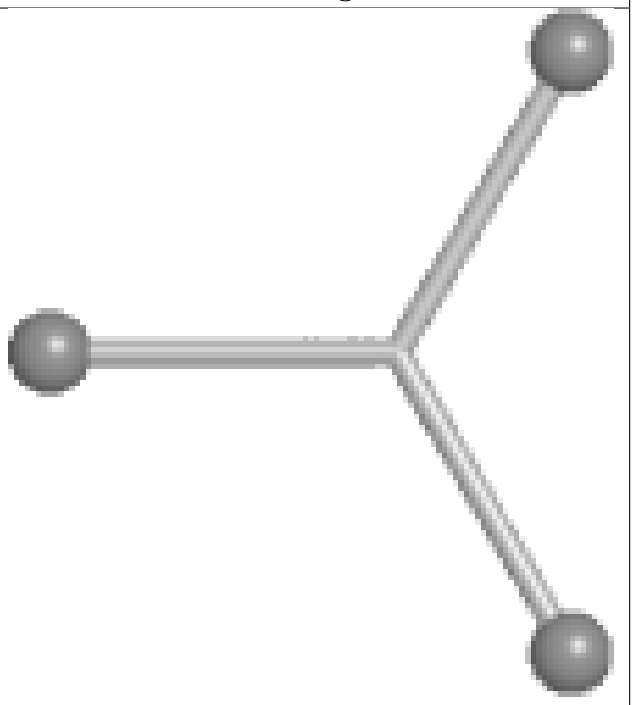
Bond lengths



Bond angles

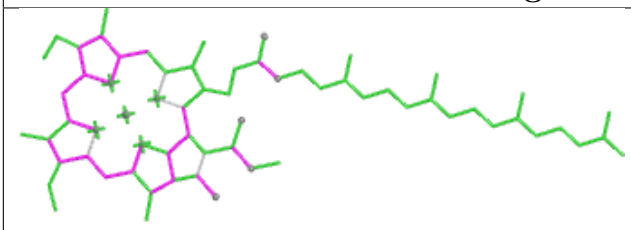


Torsions

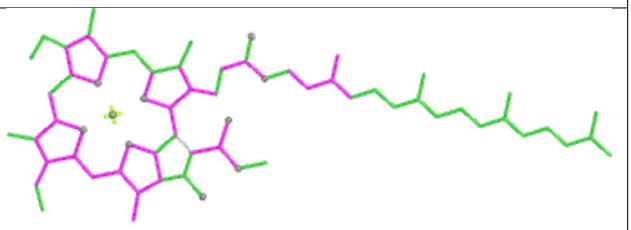


Rings

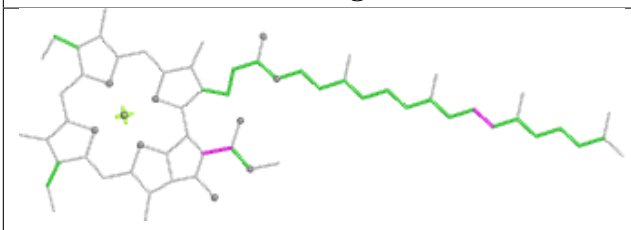
Ligand CLA C 508



Bond lengths



Bond angles



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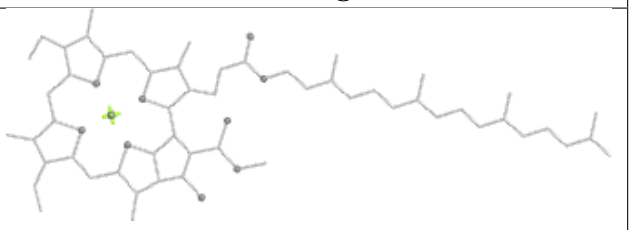
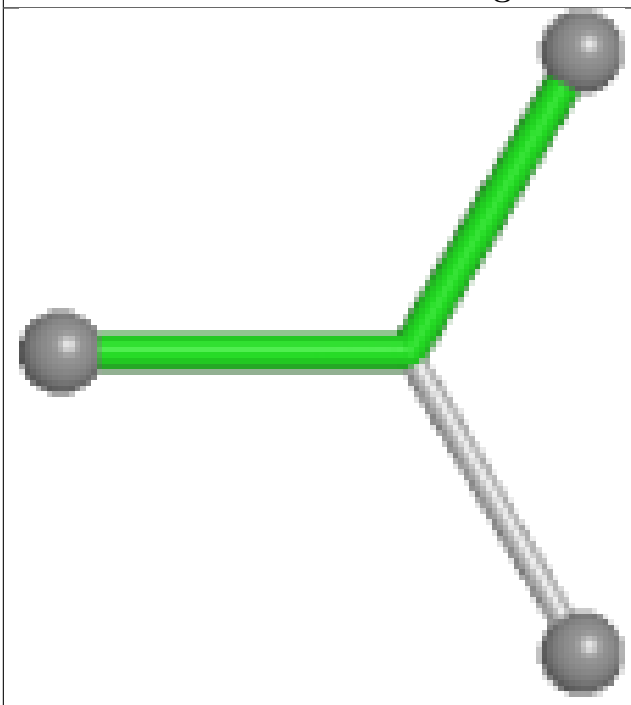


Rings

Ligand BCT d 401 (B)



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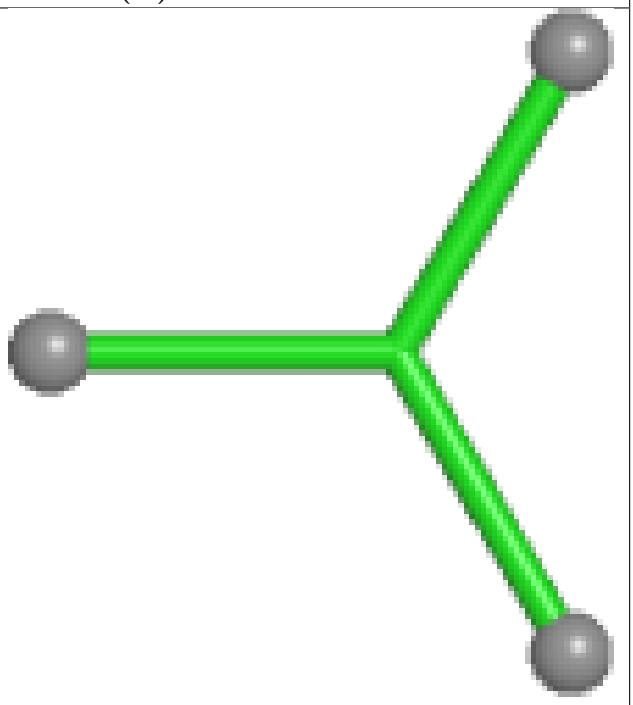
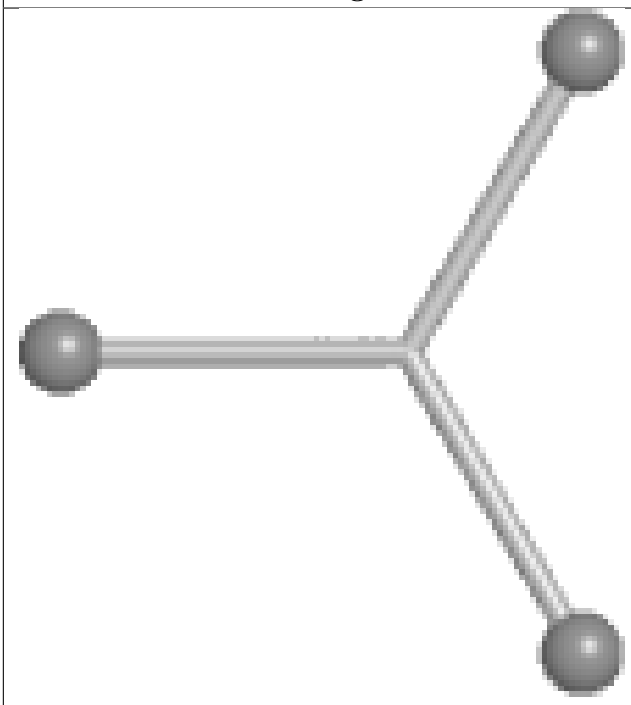


Bond angles



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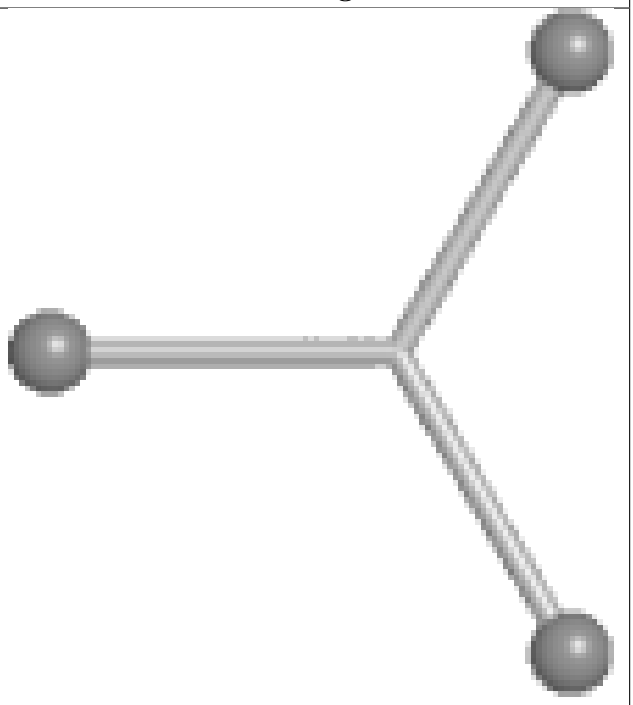
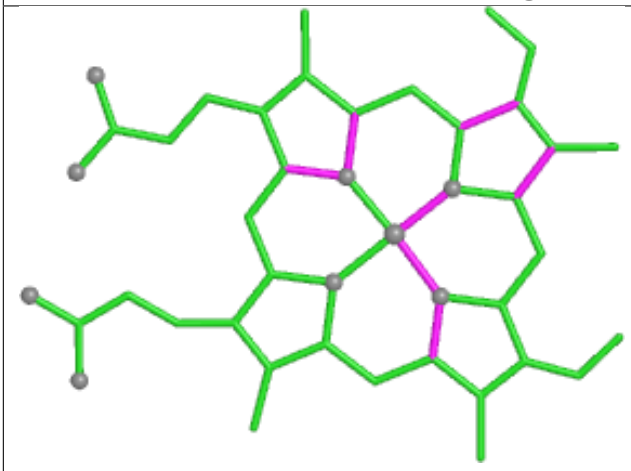


Rings

Ligand HEM F 102



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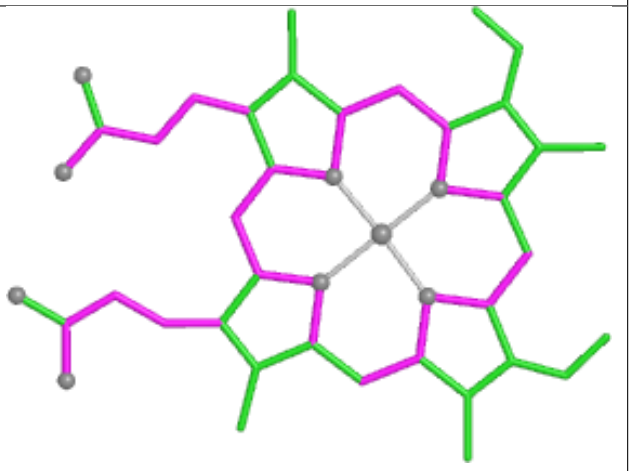
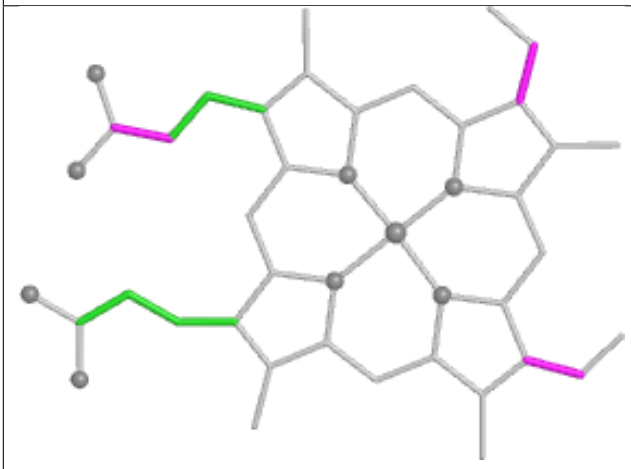


Bond angles



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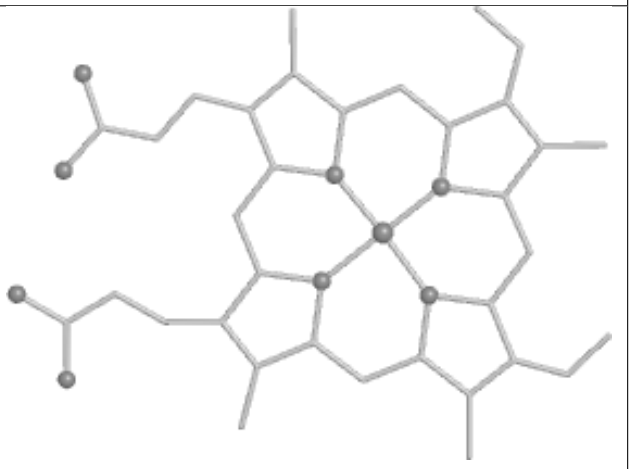
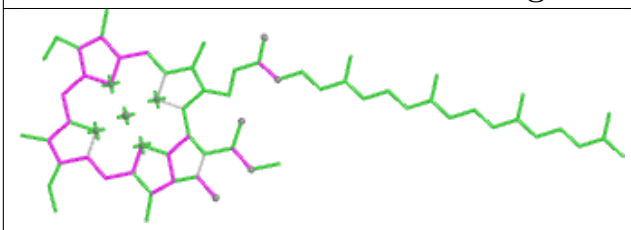
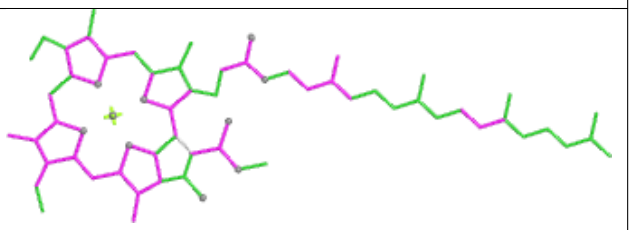


Rings

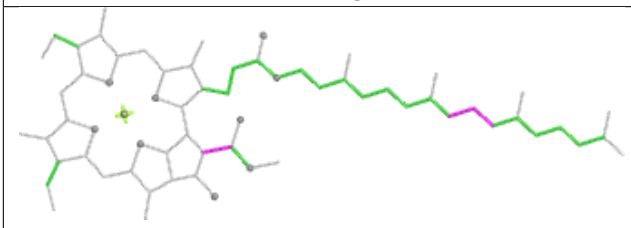
Ligand CLA b 612



Bond lengths



Bond angles



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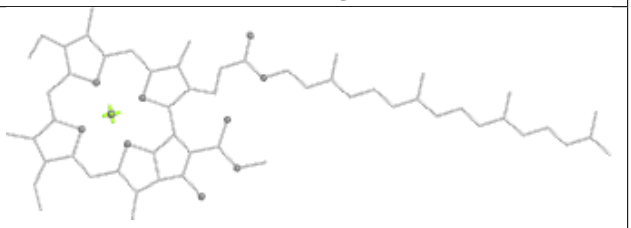
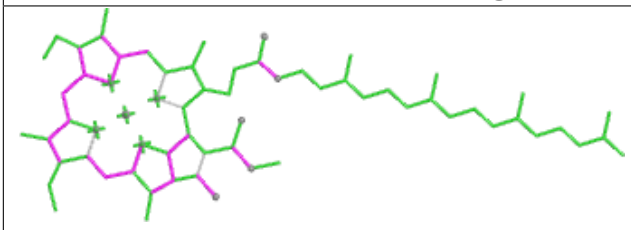


Rings

Ligand CLA A 405 (A)



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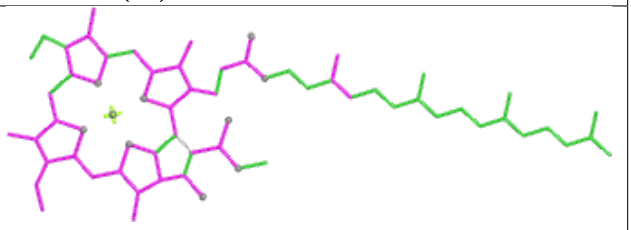

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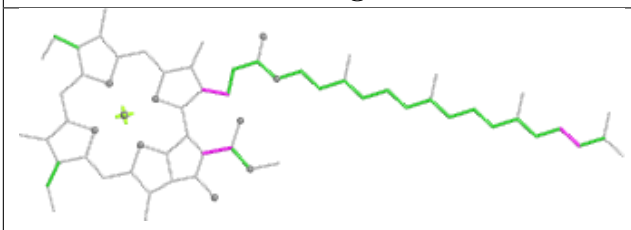

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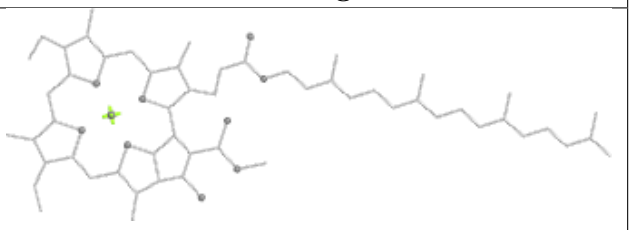
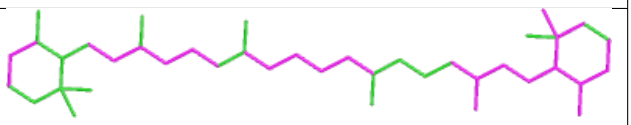


Rings

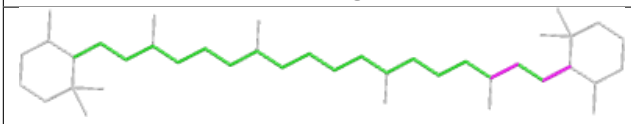
Ligand BCR D 405



Bond lengths



Bond angles



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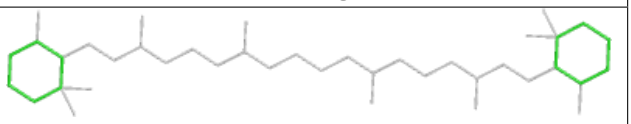
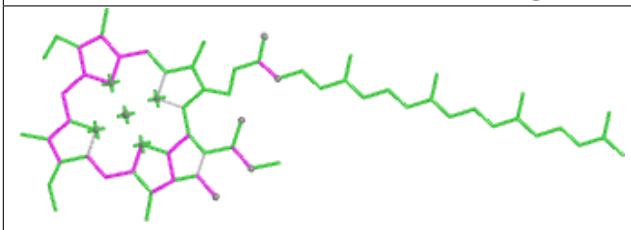


Rings

Ligand CLA b 616



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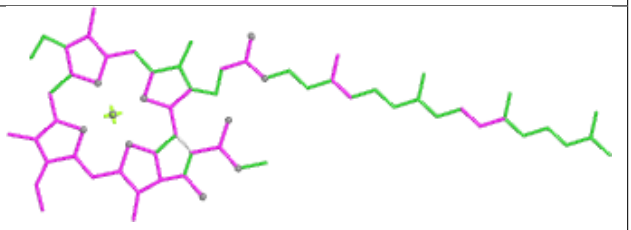
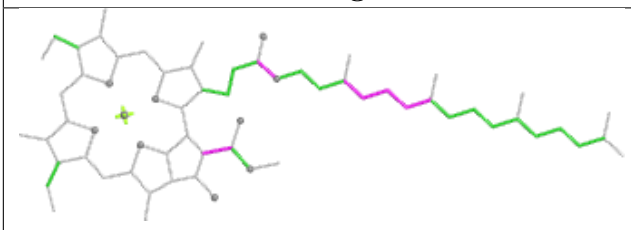


Bond angles



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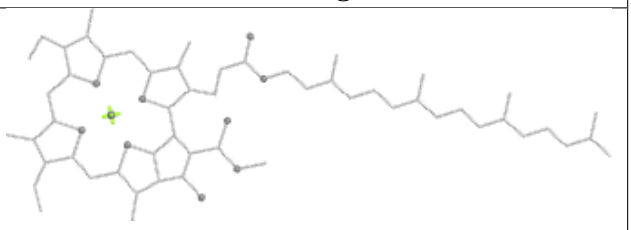
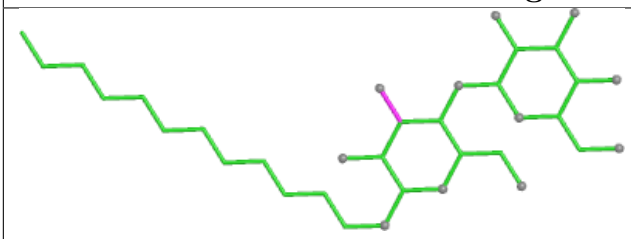


Rings

Ligand LMT a 415



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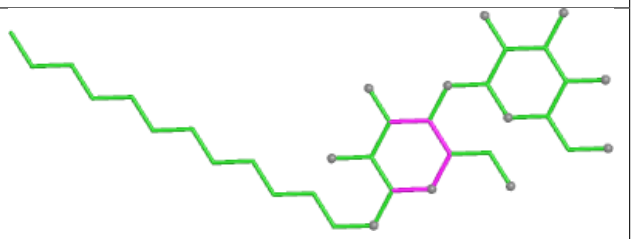
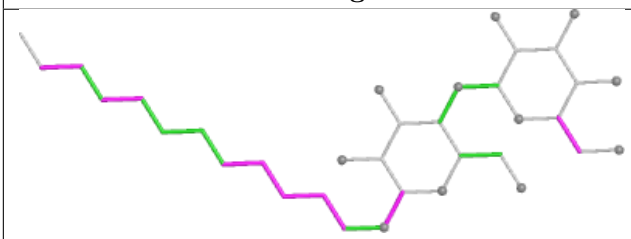


Bond angles



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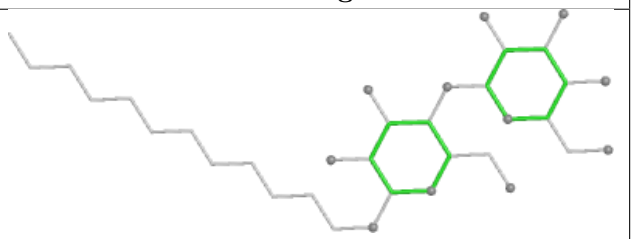
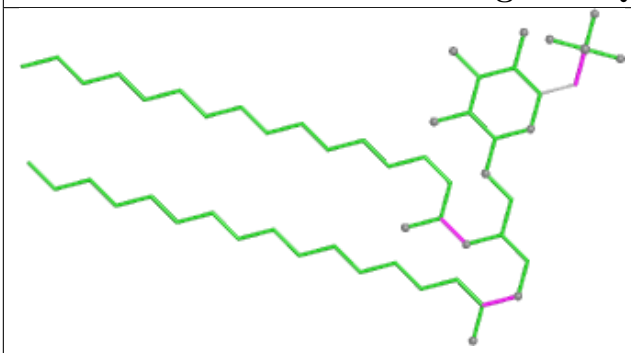


Rings

Ligand SQD a 409 (B)



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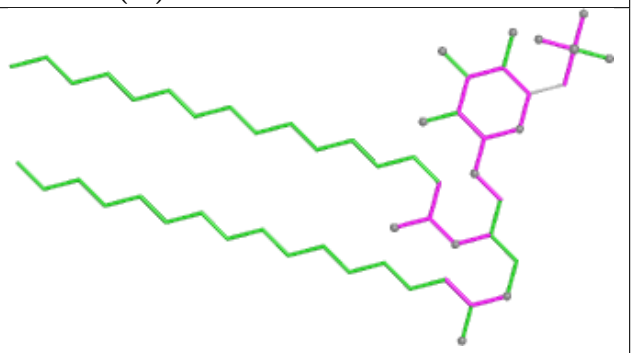
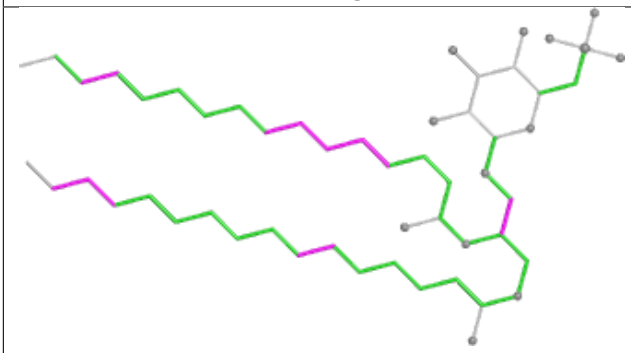


Bond angles



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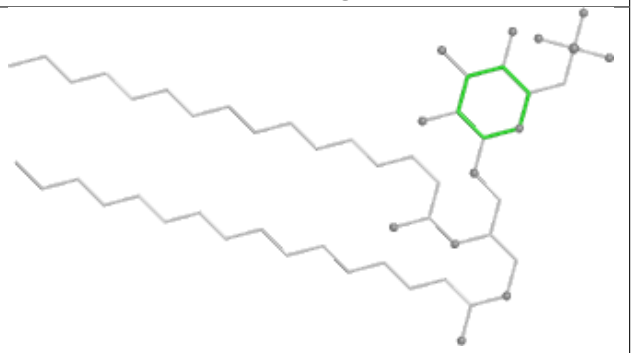
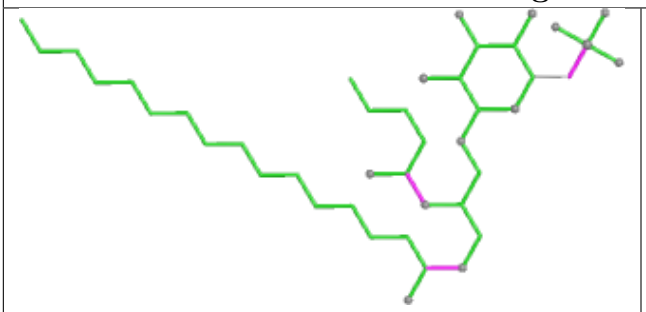


Rings

Ligand SQD f 102



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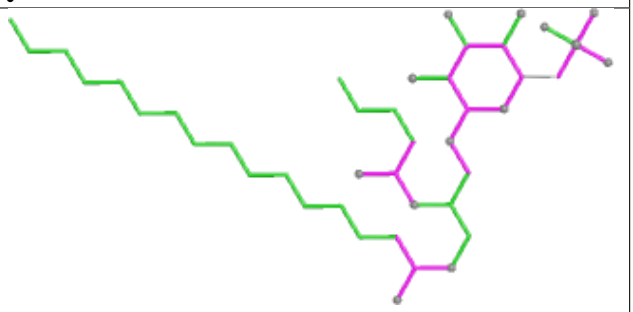
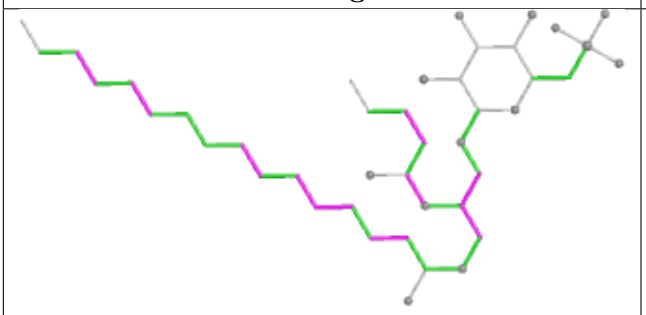


Bond angles



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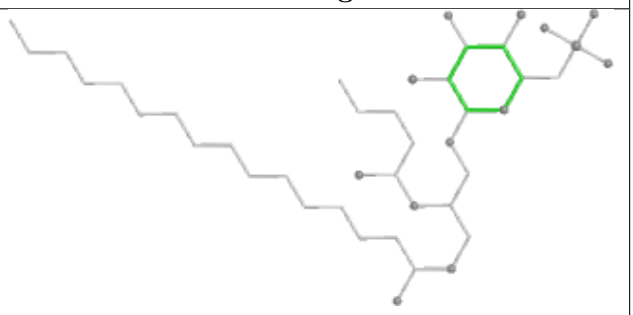
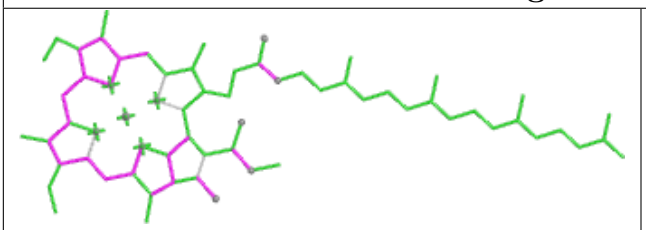


Rings

Ligand CLA b 614



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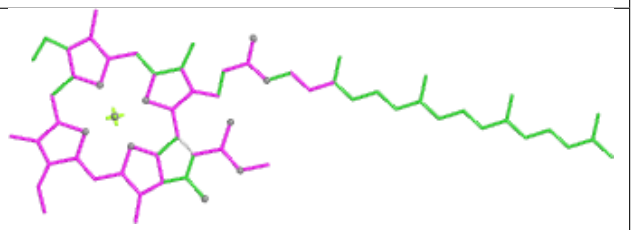
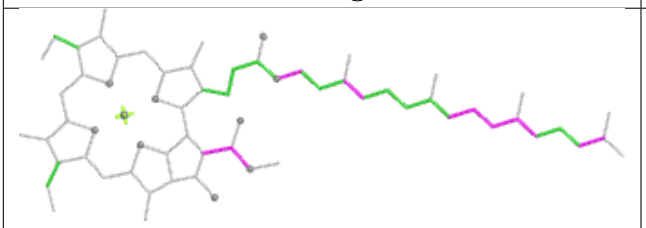


Bond angles



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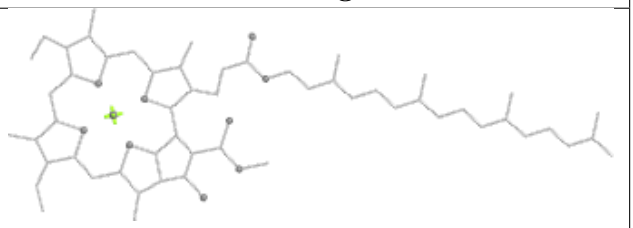
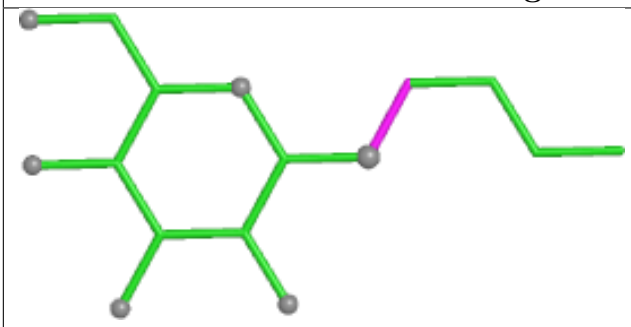
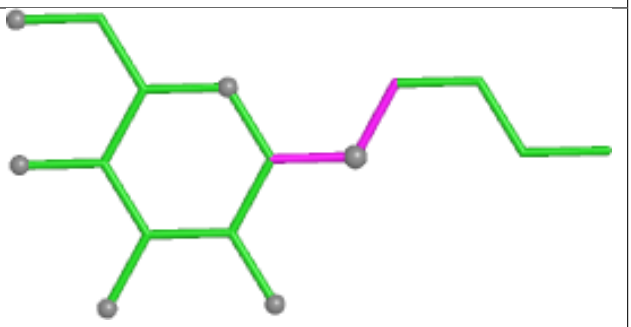
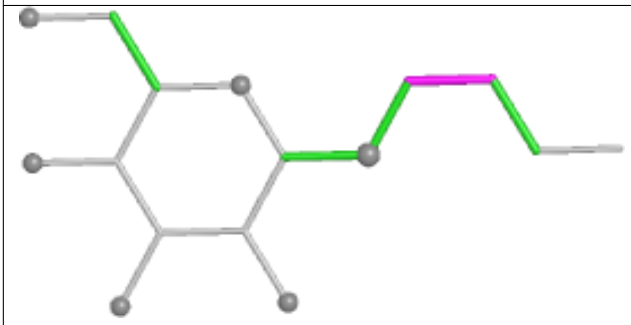
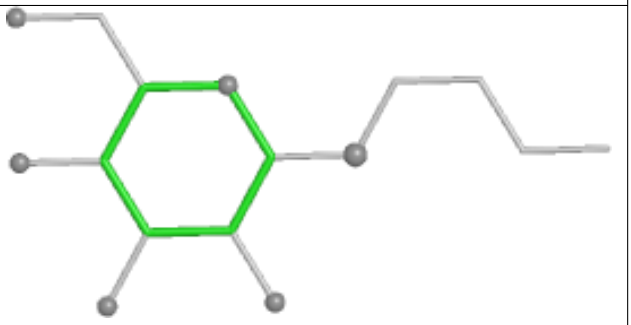
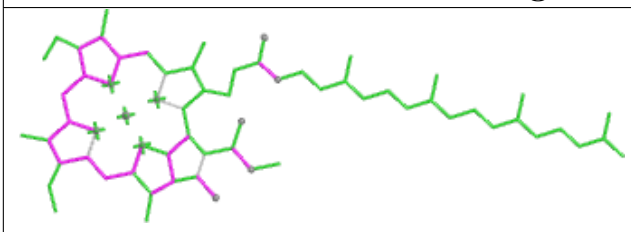
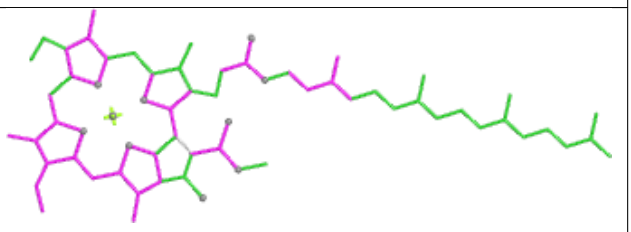
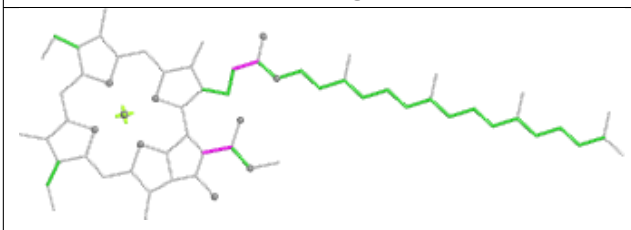
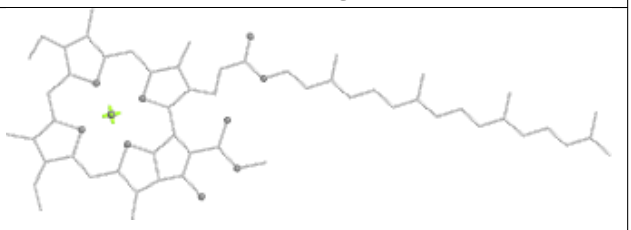
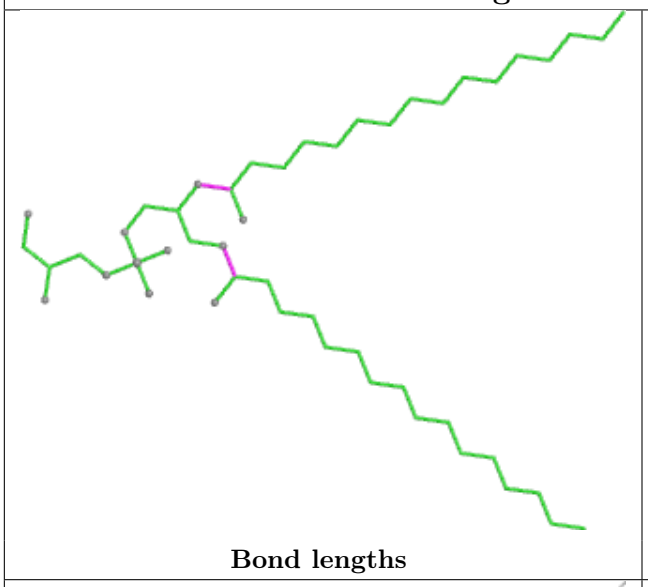


Rings

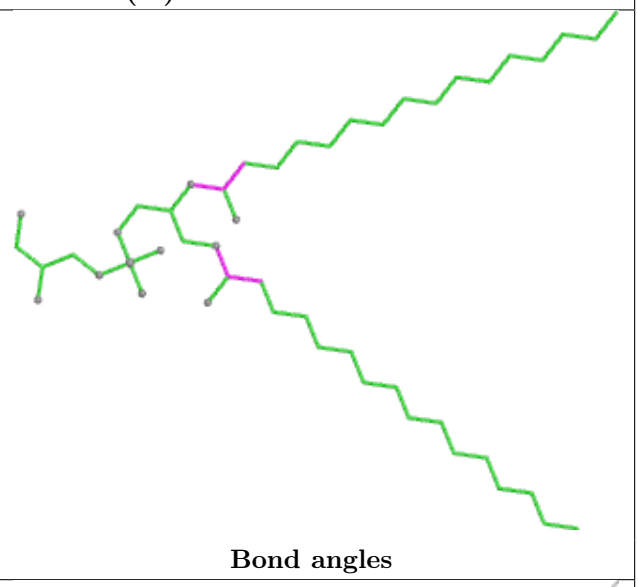
Ligand HTG d 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

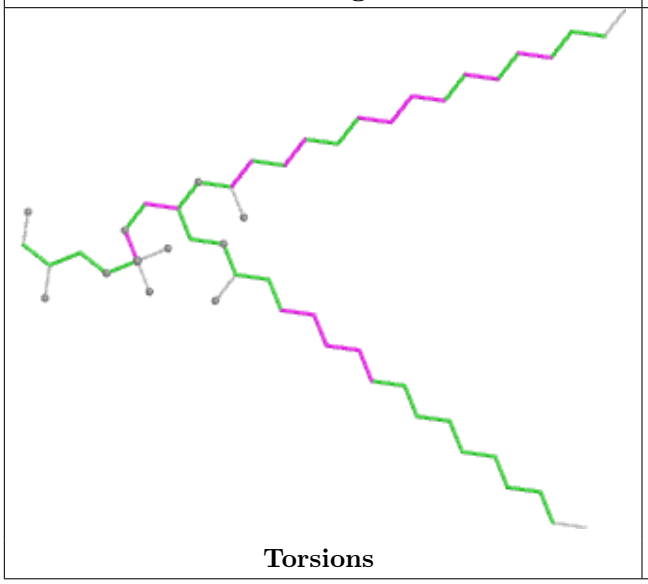
Ligand LHG L 101 (B)



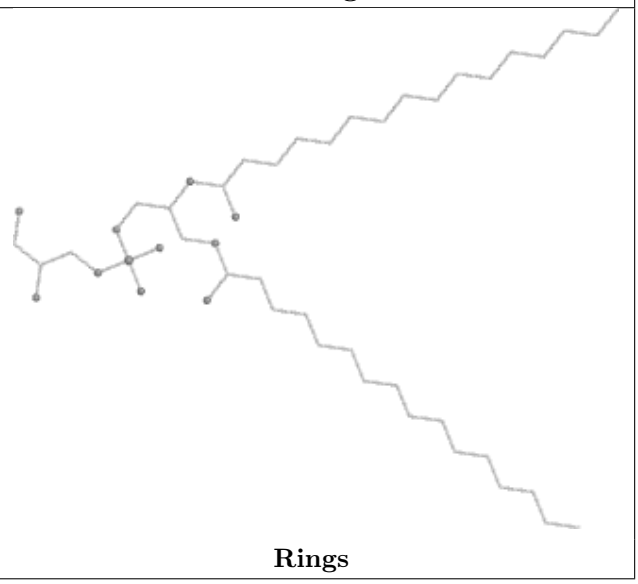
Bond lengths



Bond angles

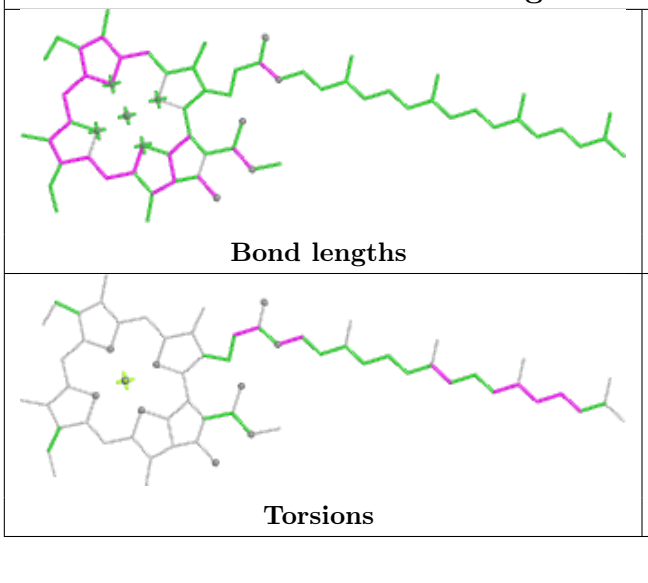


Torsions

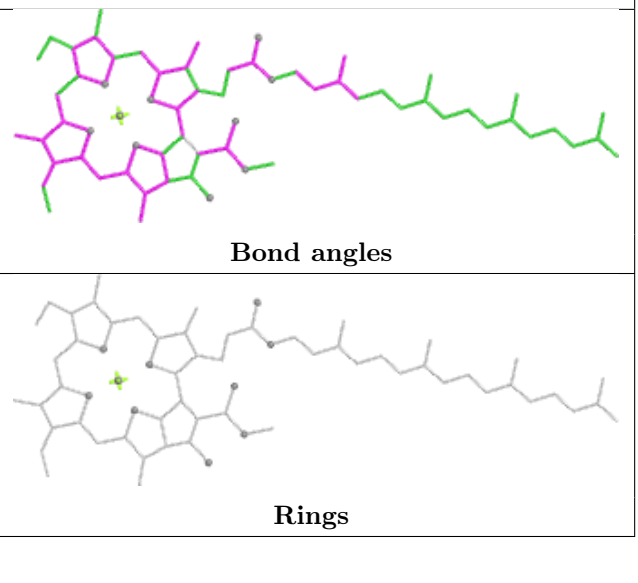


Rings

Ligand CLA B 613



Bond lengths

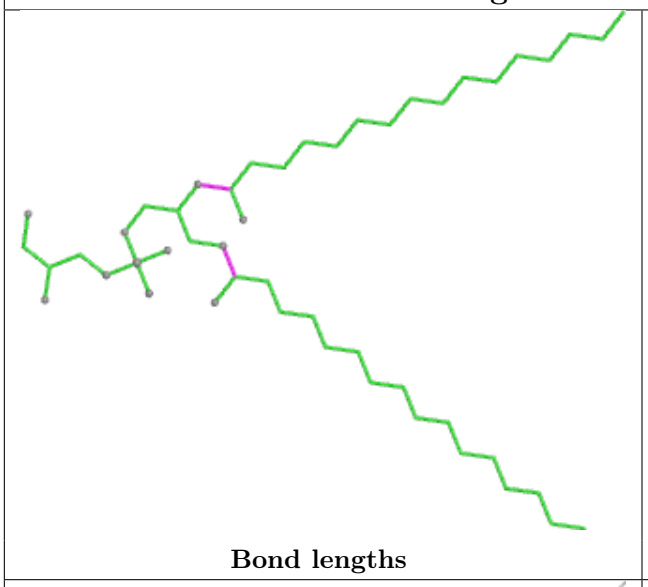


Bond angles

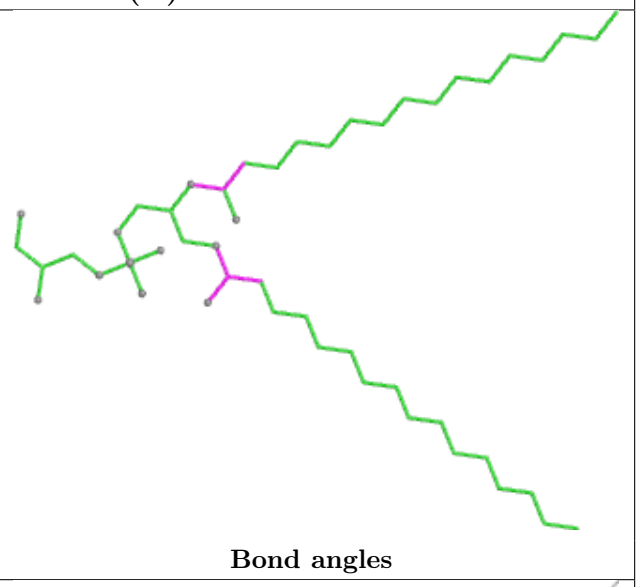
Torsions

Rings

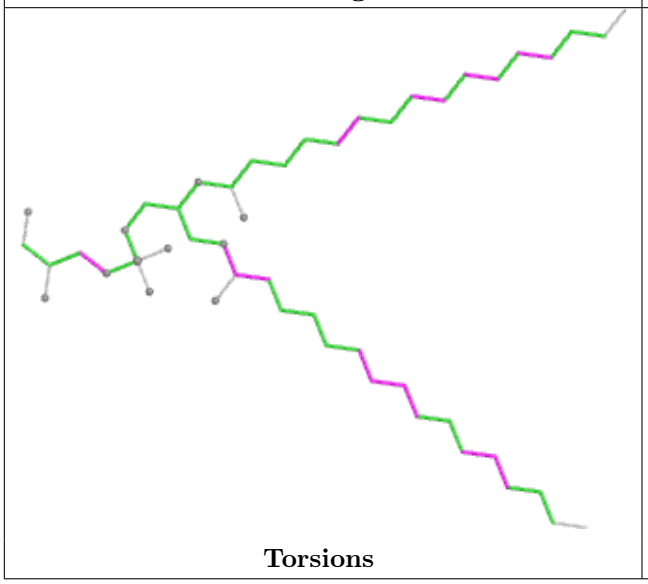
Ligand LHG D 408 (B)



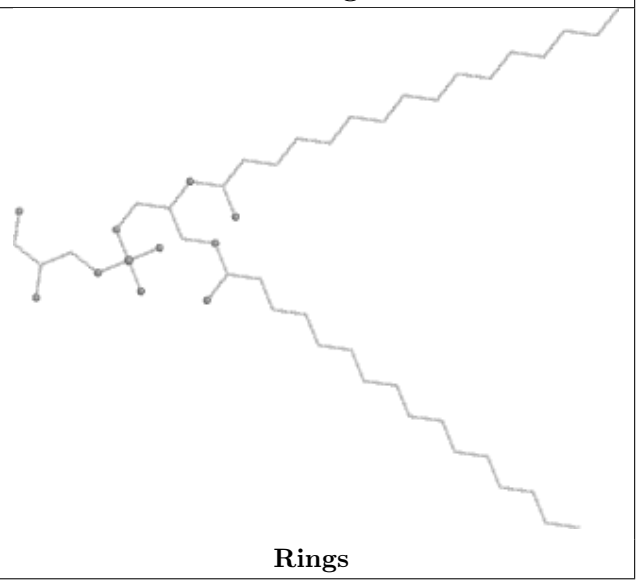
Bond lengths



Bond angles

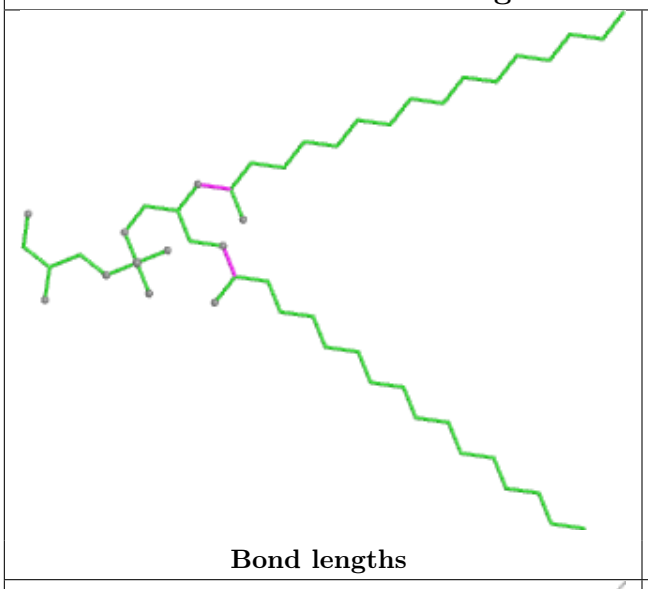


Torsions



Rings

Ligand LHG d 408 (B)



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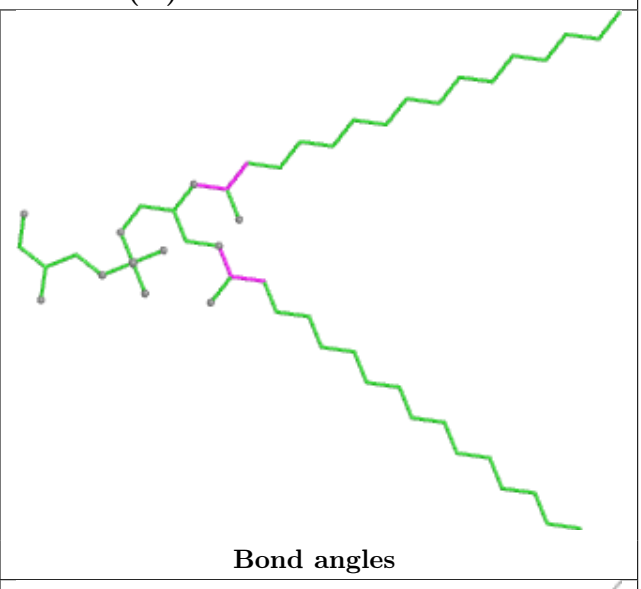
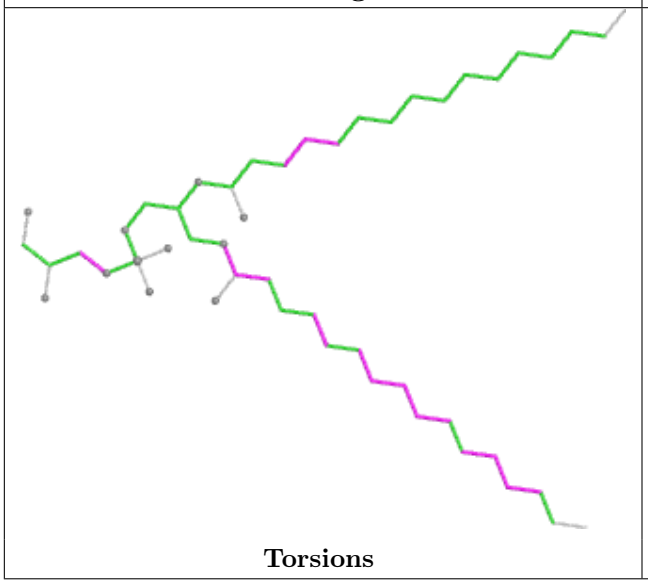


Bond angles



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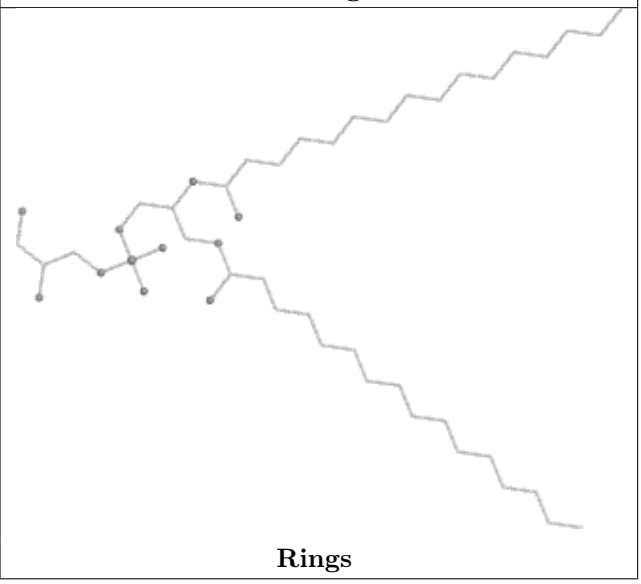
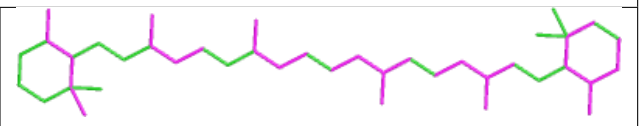


Rings

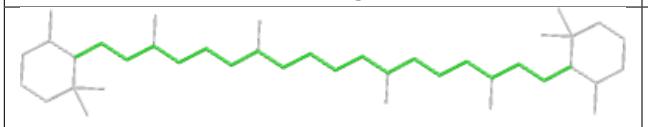
Ligand BCR c 515



Bond lengths



Bond angles



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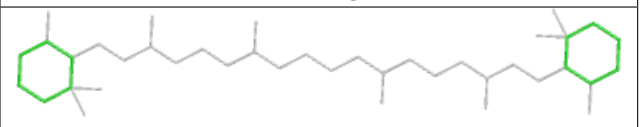
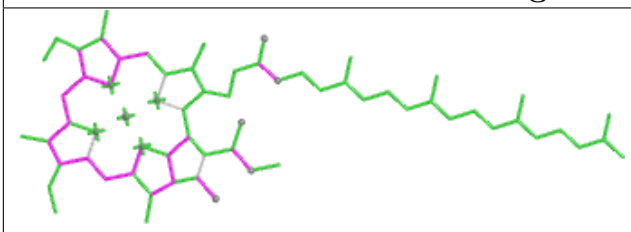


Rings

Ligand CLA c 504



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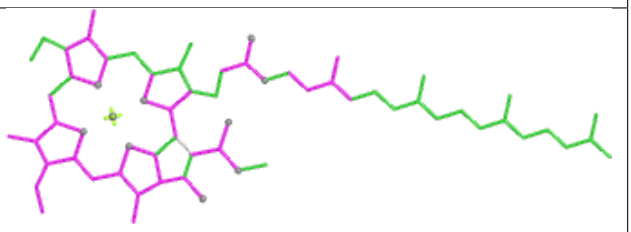

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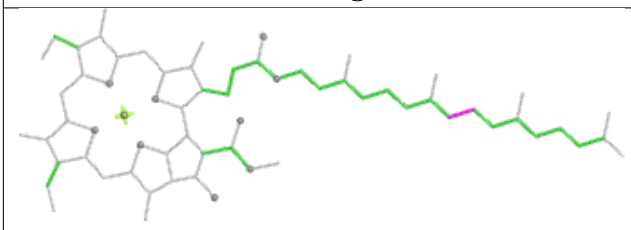

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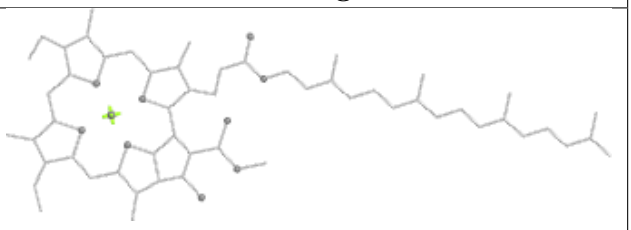
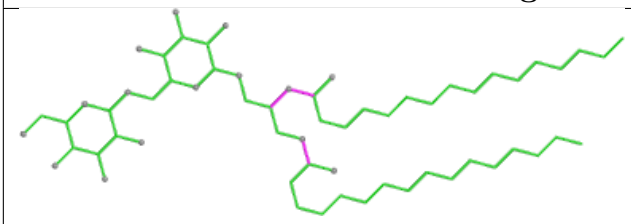


Rings

Ligand DGD C 518



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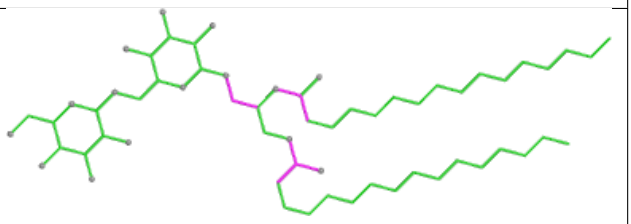
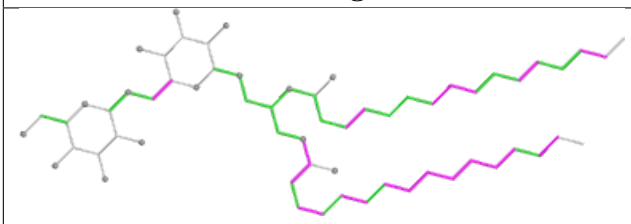


Bond angles



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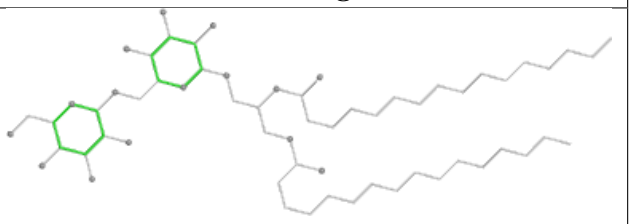
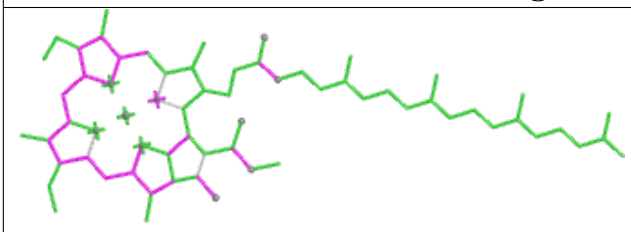


Rings

Ligand CLA c 512



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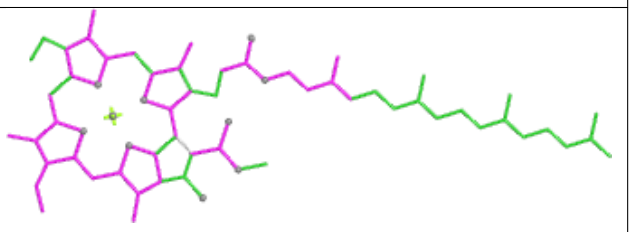
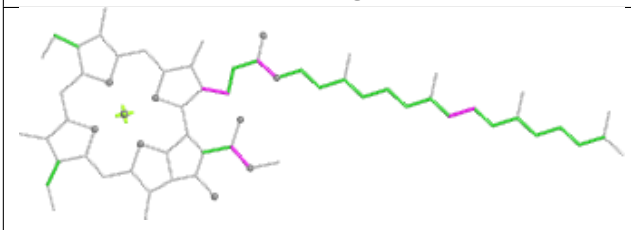


Bond angles



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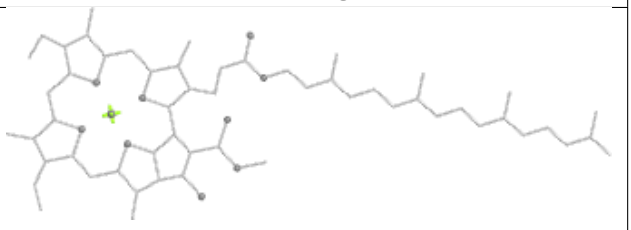
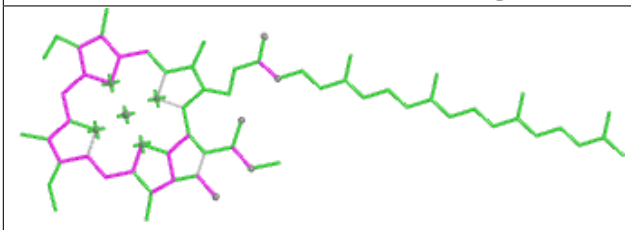


Rings

Ligand CLA A 405 (B)



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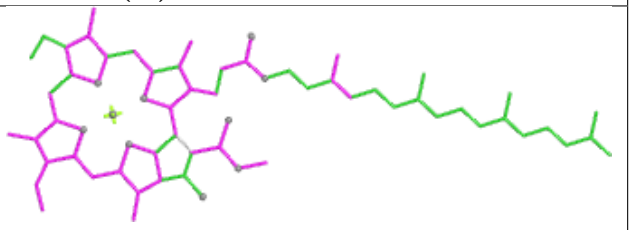
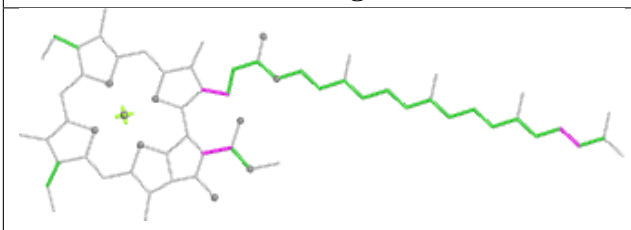


Bond angles



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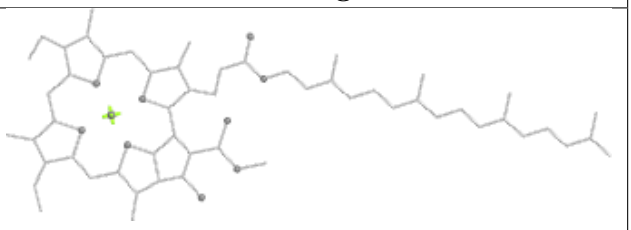
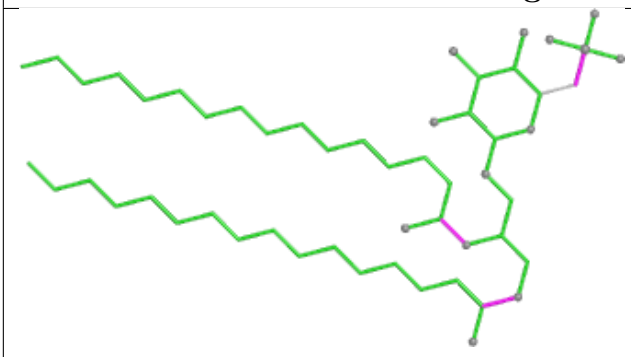


Rings

Ligand SQD A 412



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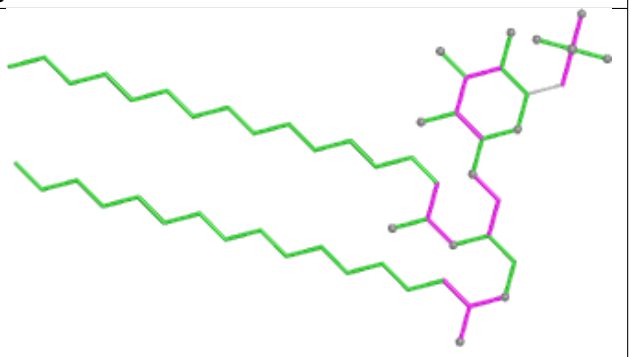
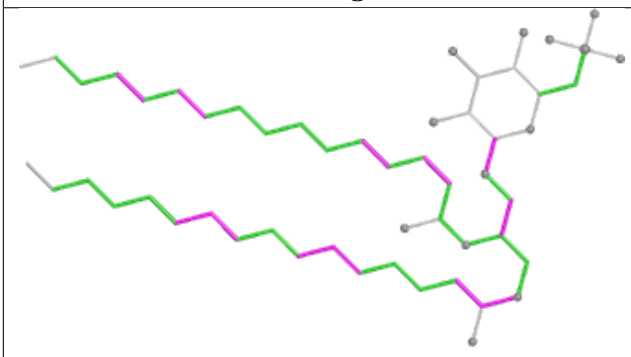


Bond angles



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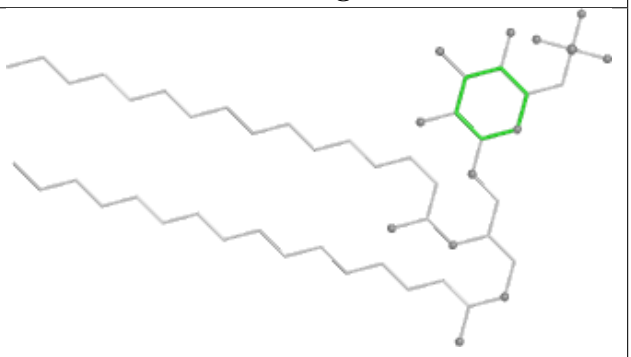
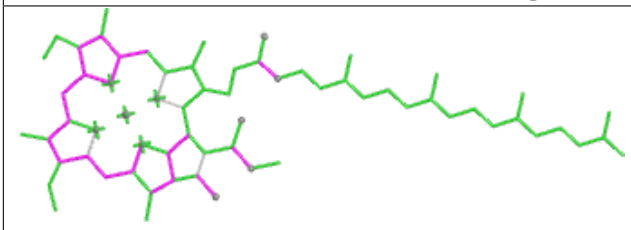


Rings

Ligand CLA C 509



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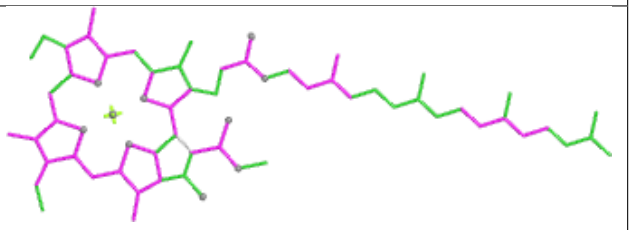
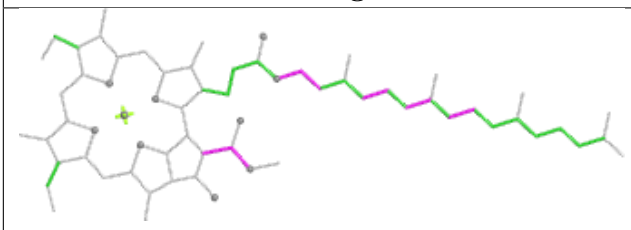


Bond angles



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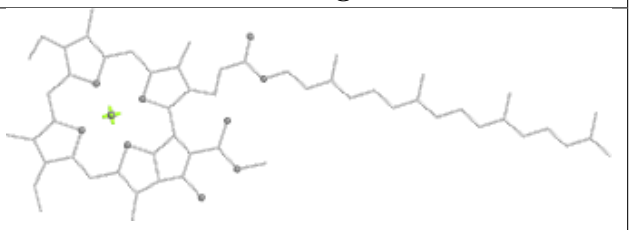
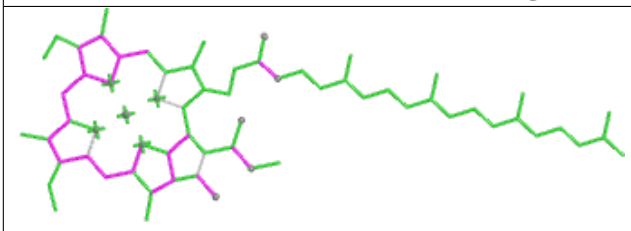


Rings

Ligand CLA C 502



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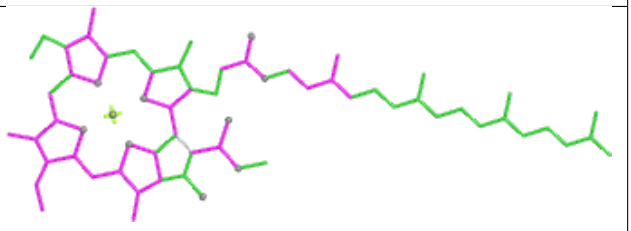
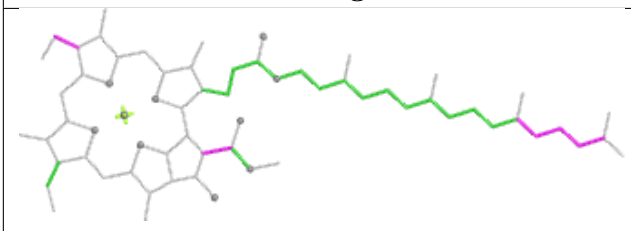


Bond angles



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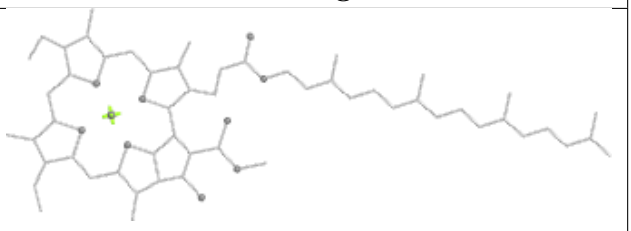
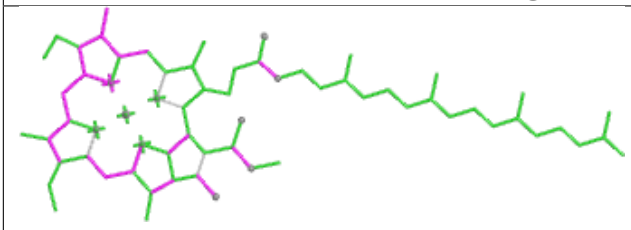
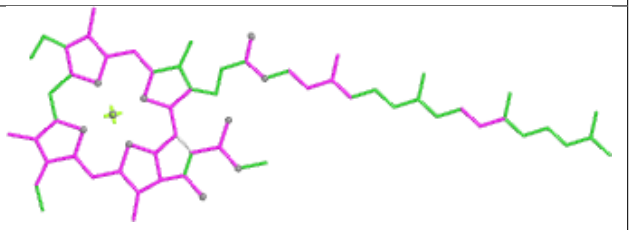


Rings

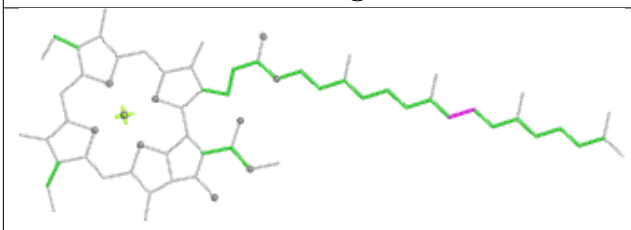
Ligand CLA B 611



Bond lengths



Bond angles



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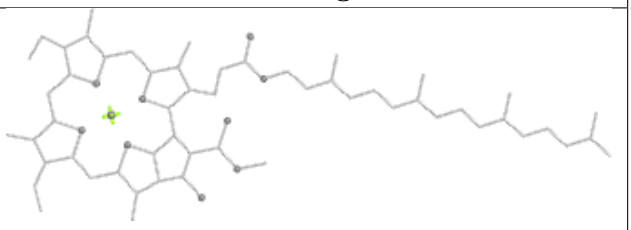
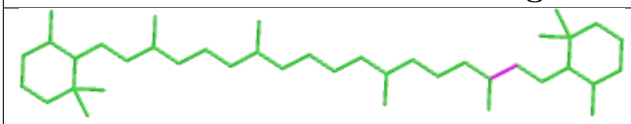
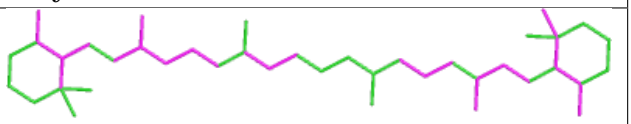
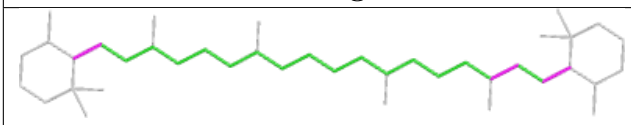
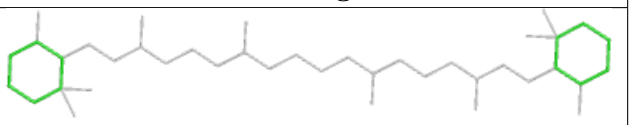
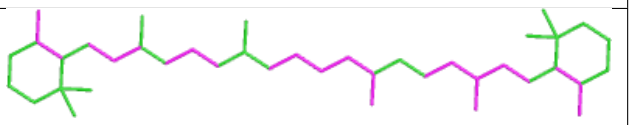
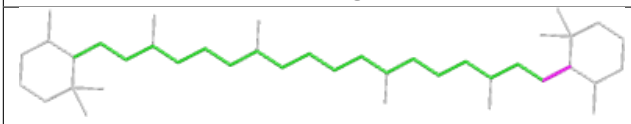
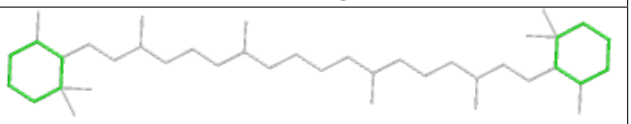
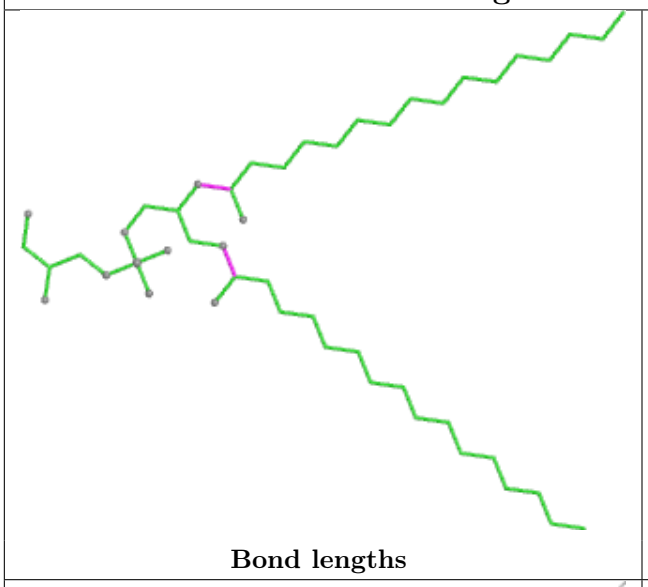


Rings

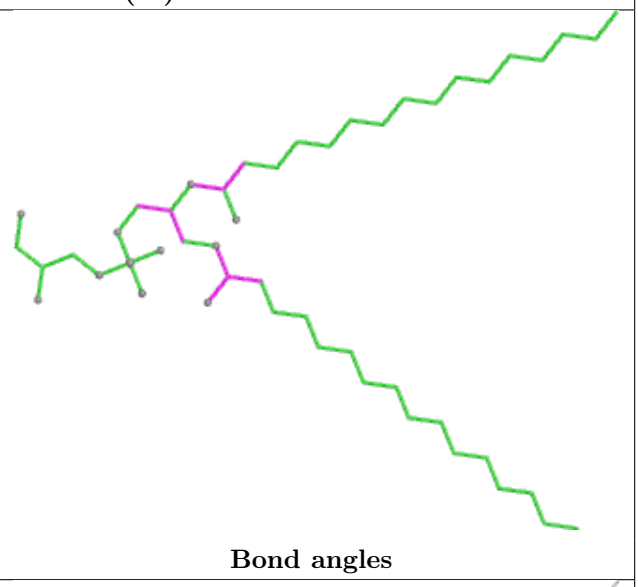
Ligand BCR y 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR h 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

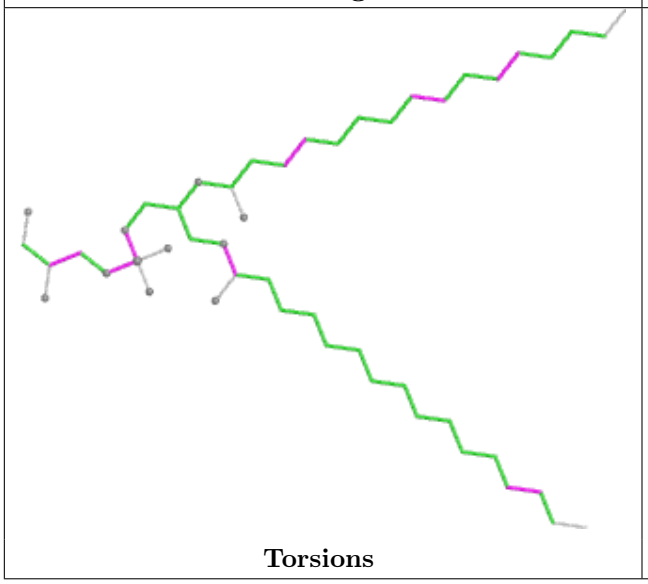
Ligand LHG d 407 (A)



Bond lengths



Bond angles



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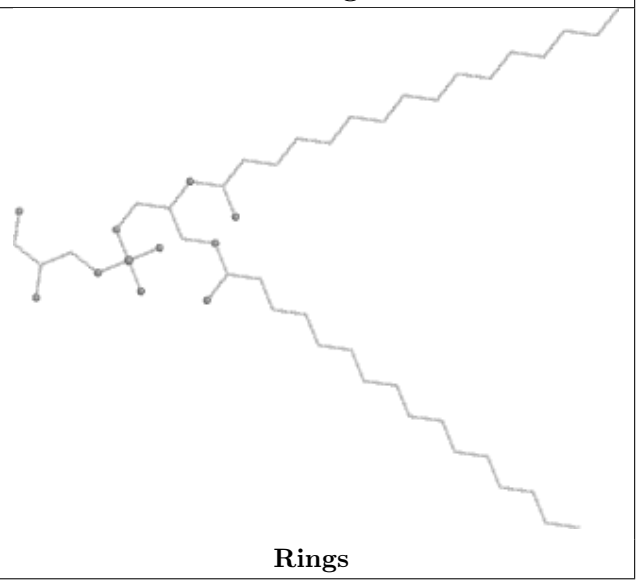
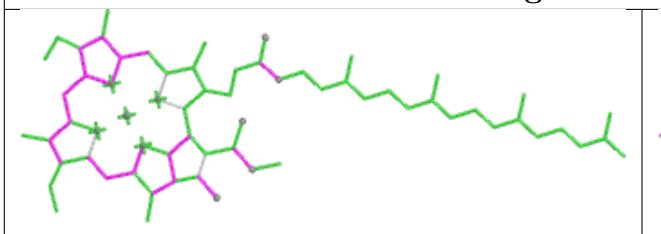


Rings

Ligand CLA A 408



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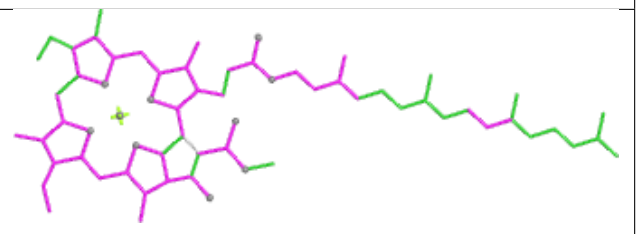
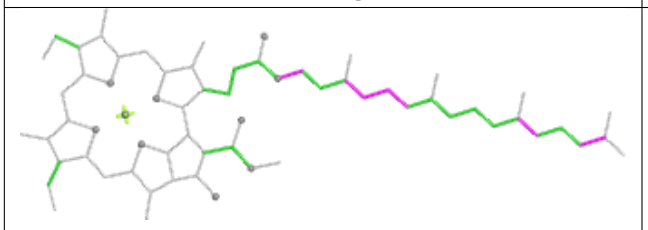
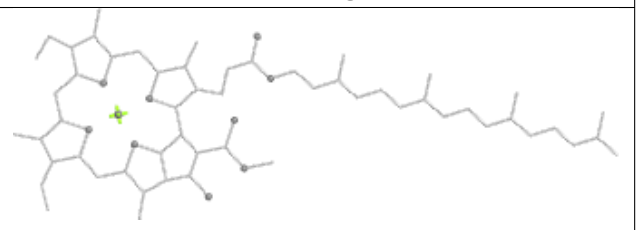


Bond angles

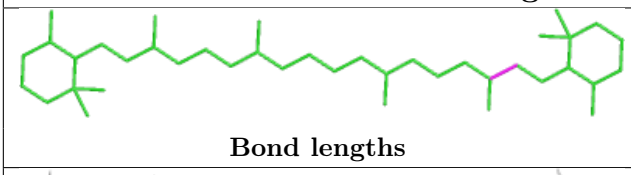


Torsions



Rings

Ligand BCR H 101



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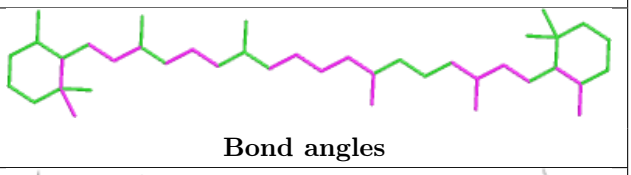
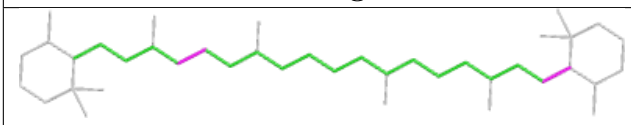


Bond angles



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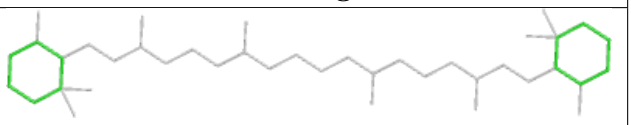
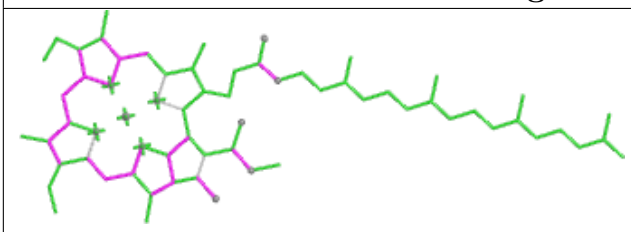


Rings

Ligand CLA b 609



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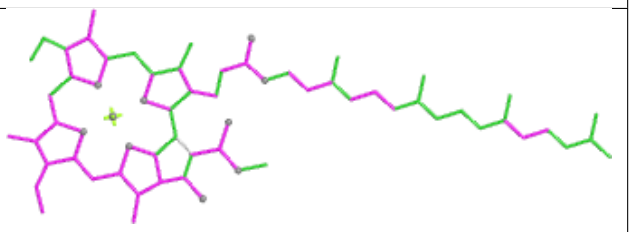
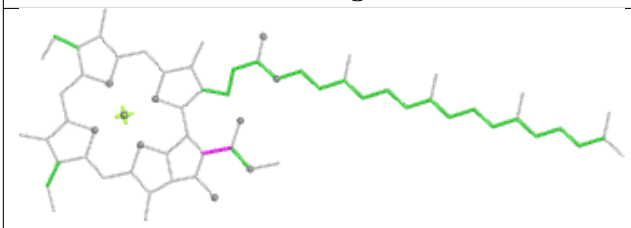


Bond angles



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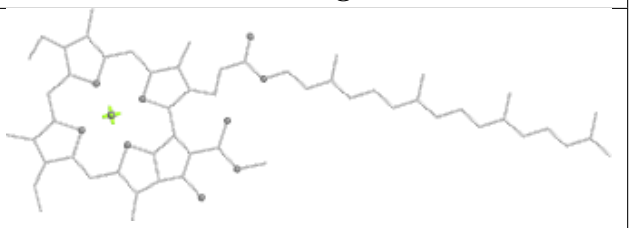
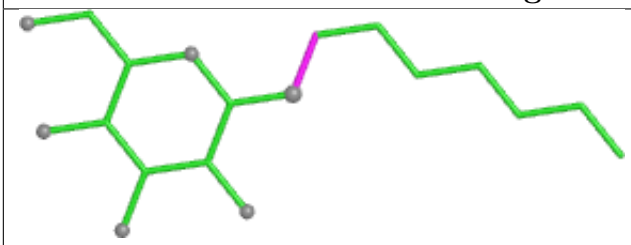


Rings

Ligand HTG b 623



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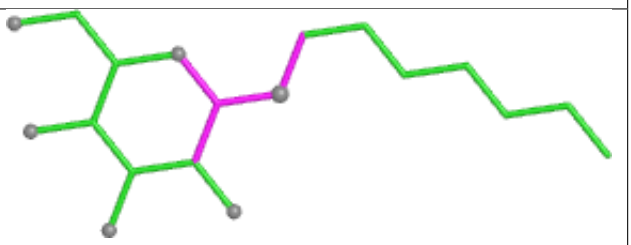
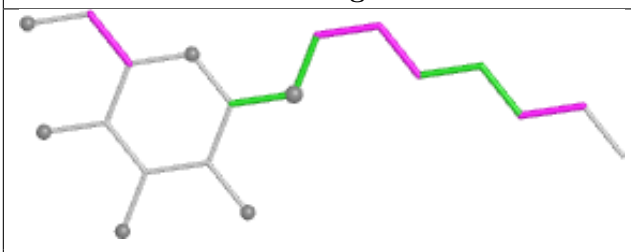


Bond angles



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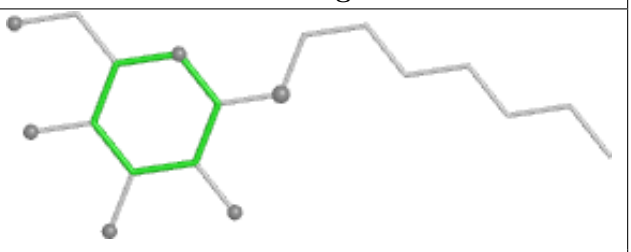
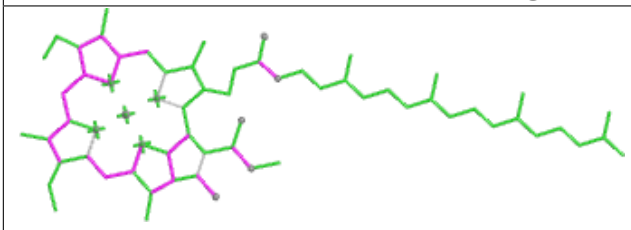


Rings

Ligand CLA B 607



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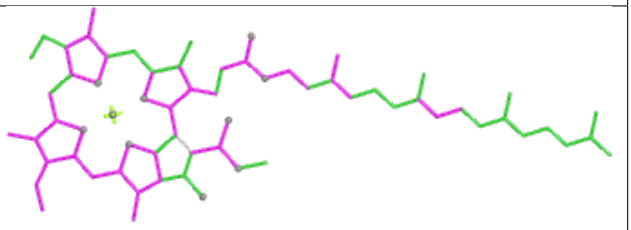
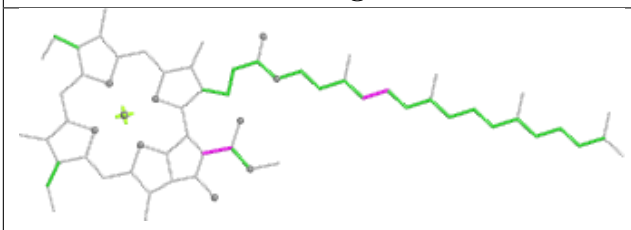


Bond angles



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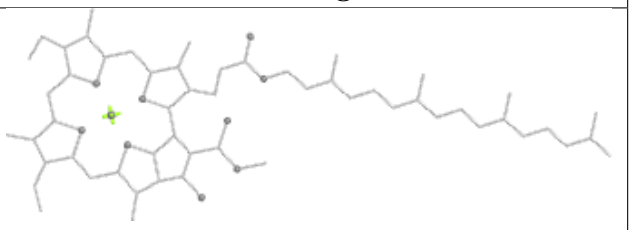
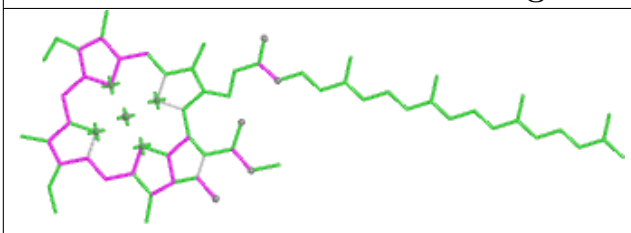


Rings

Ligand CLA b 607



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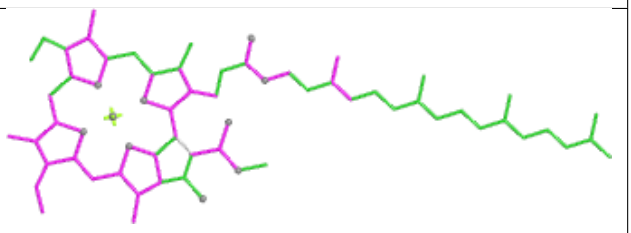
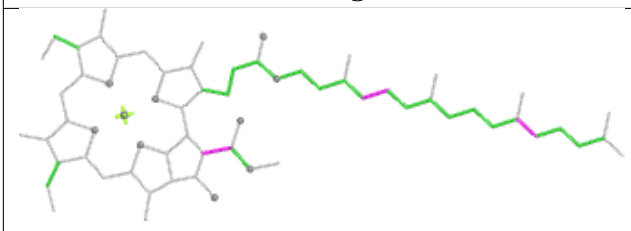


Bond angles



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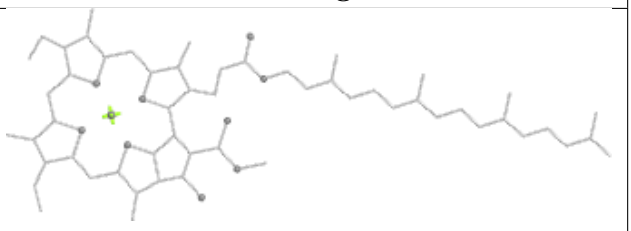
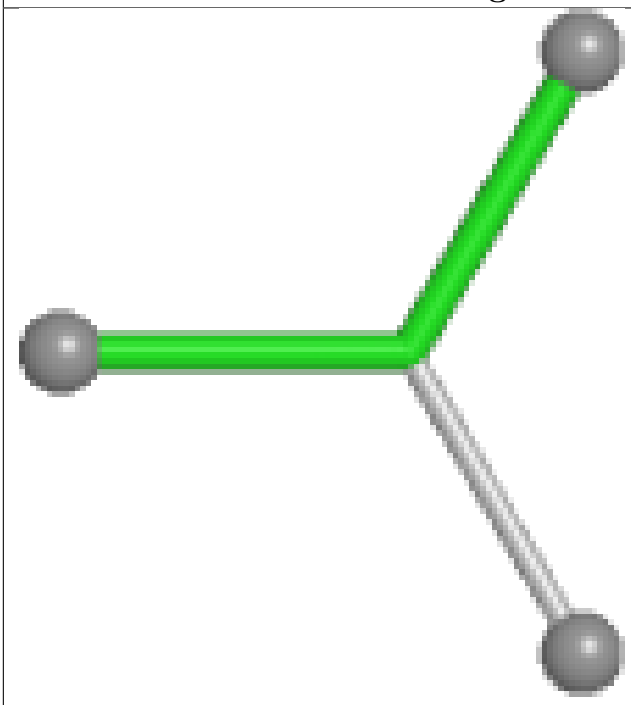


Rings

Ligand BCT D 401 (A)



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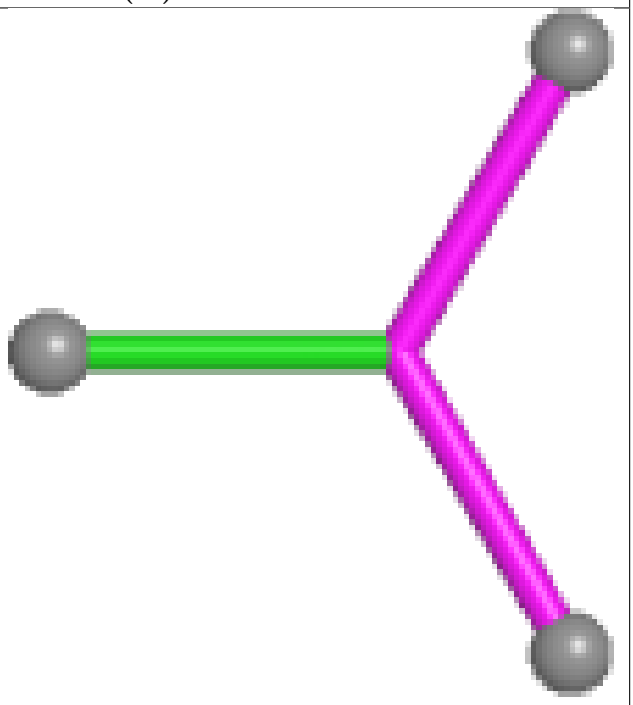
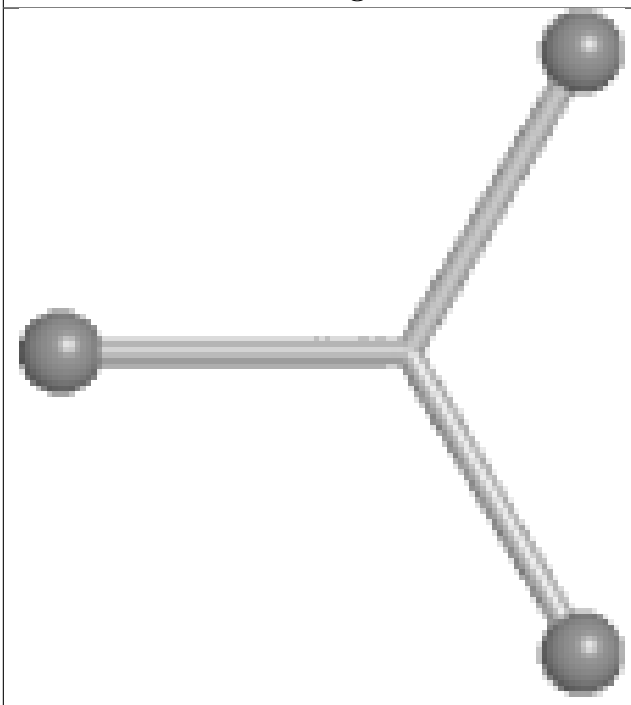


Bond angles



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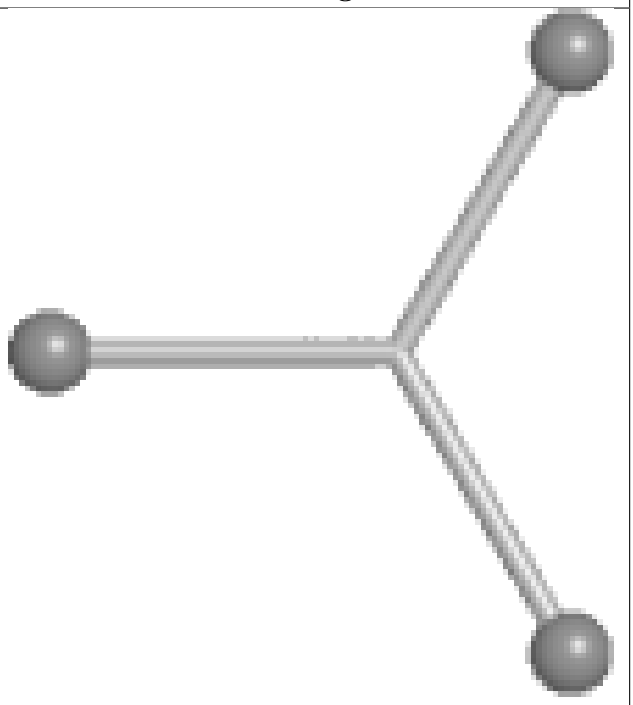
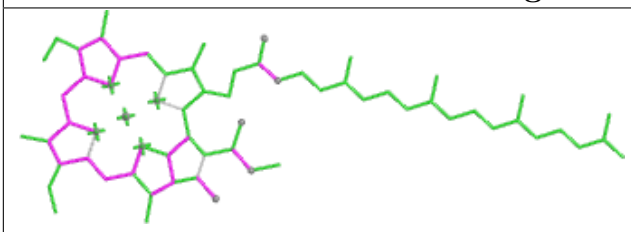


Rings

Ligand CLA B 601



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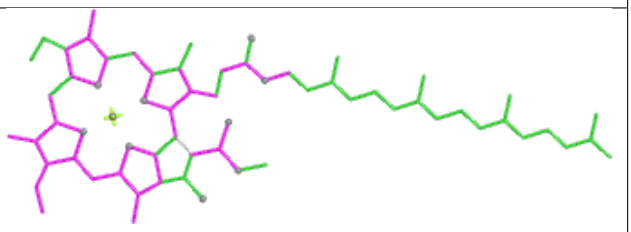
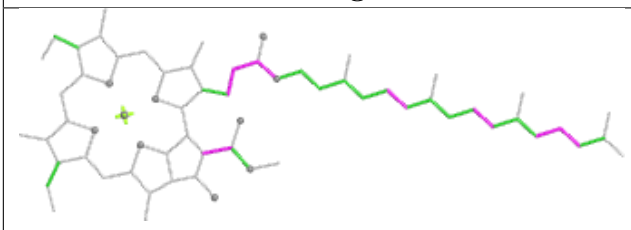


Bond angles



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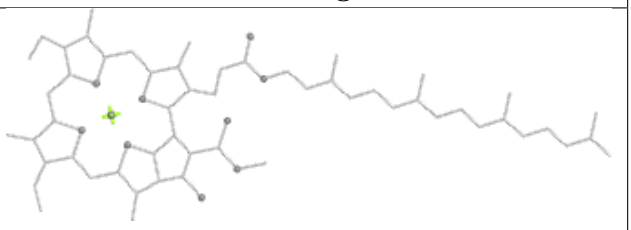
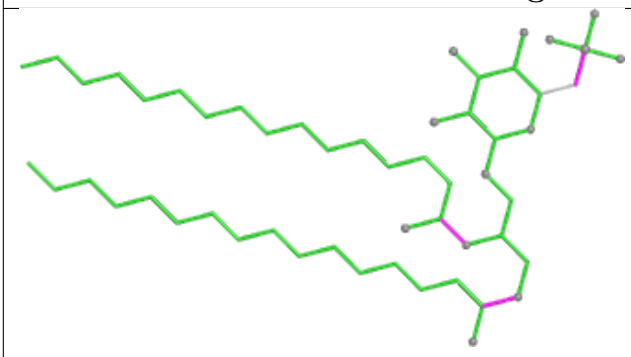


Rings

Ligand SQD b 620



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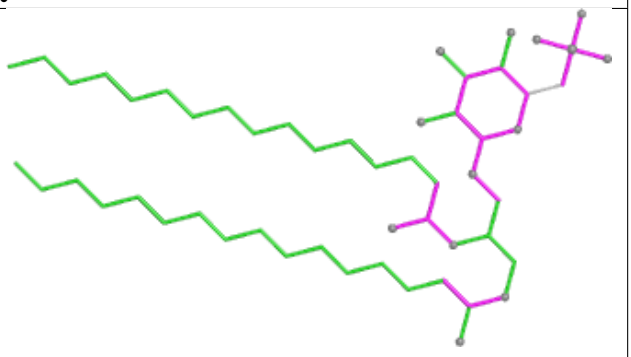
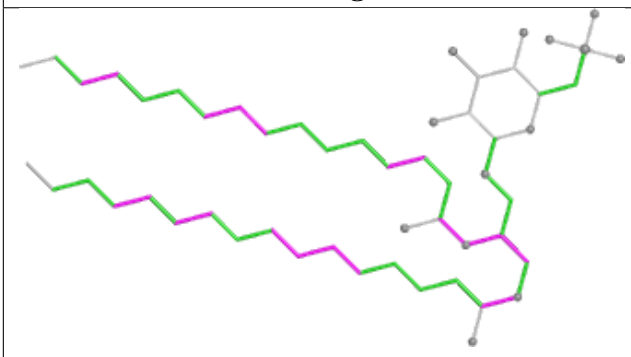


Bond angles



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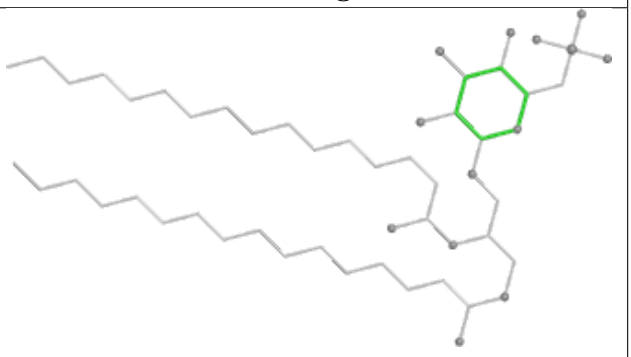
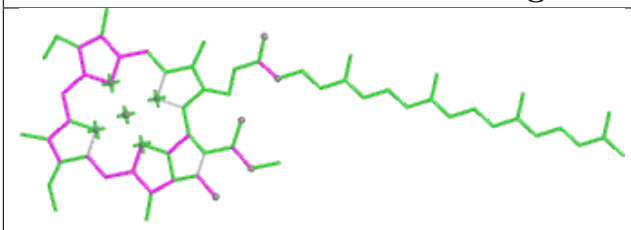


Rings

Ligand CLA b 601



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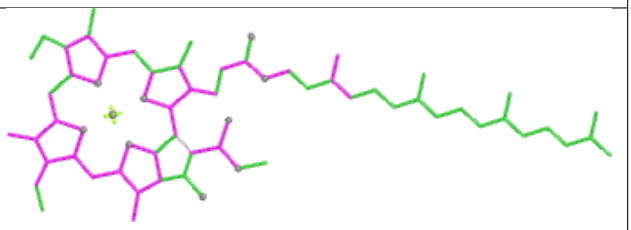
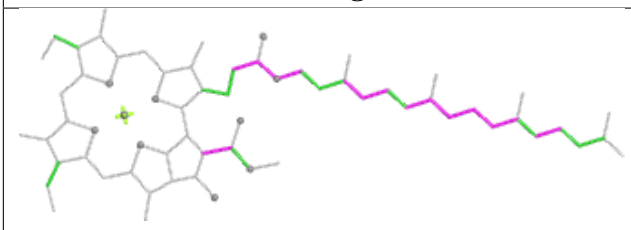


Bond angles



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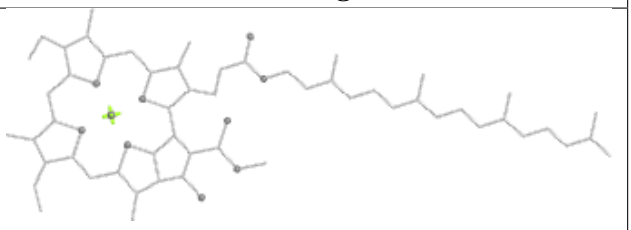
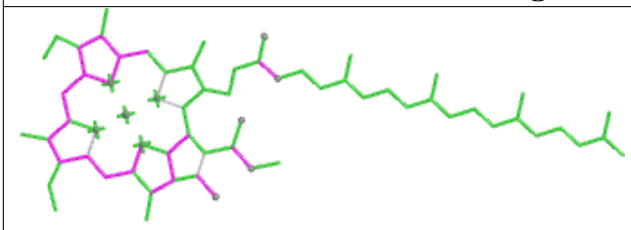


Rings

Ligand CLA c 511



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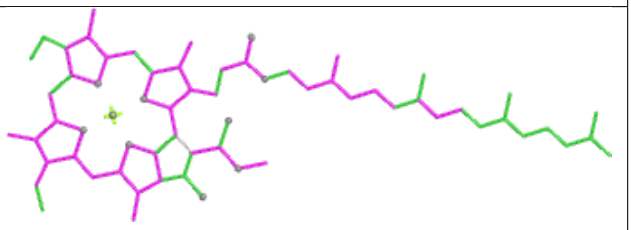

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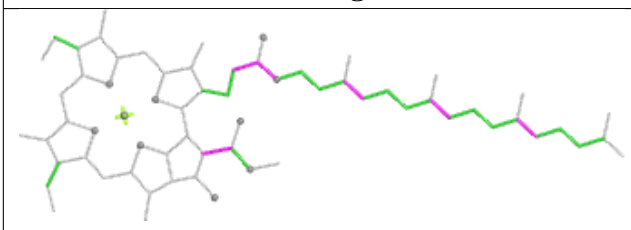

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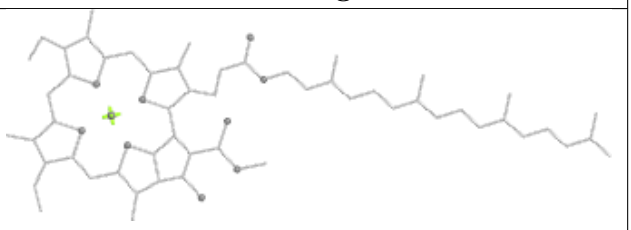
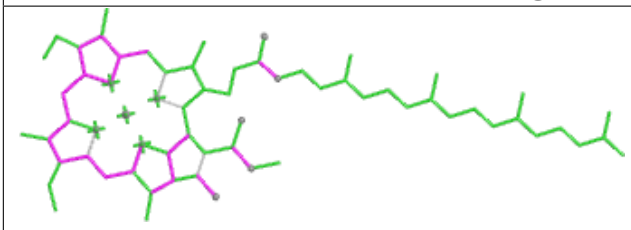


Rings

Ligand CLA c 509



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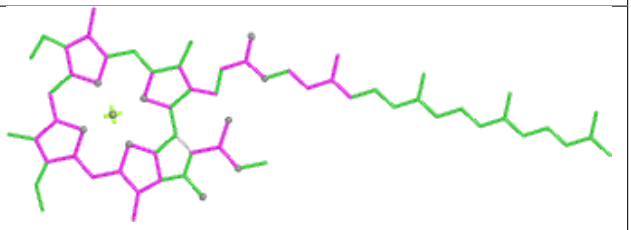
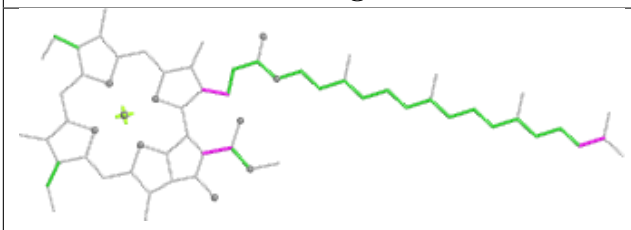


Bond angles



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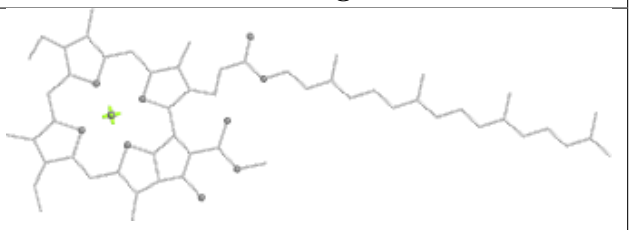
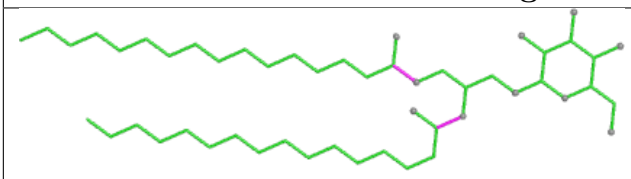


Rings

Ligand LMG B 621



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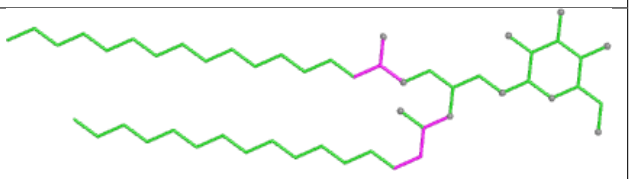
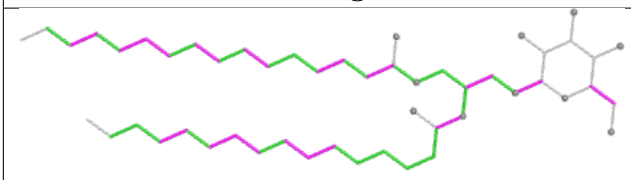


Bond angles



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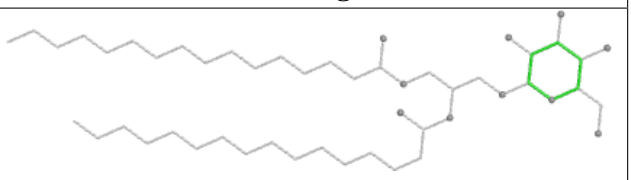
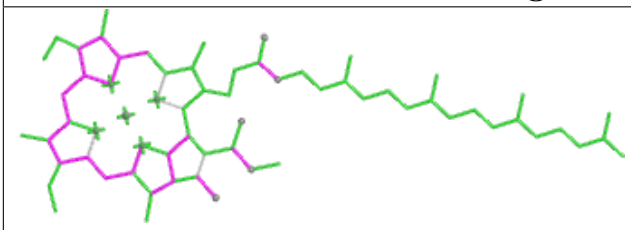


Rings

Ligand CLA b 610



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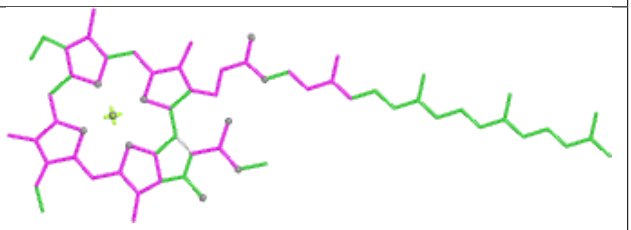
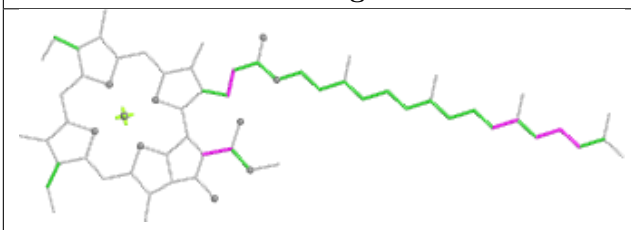


Bond angles



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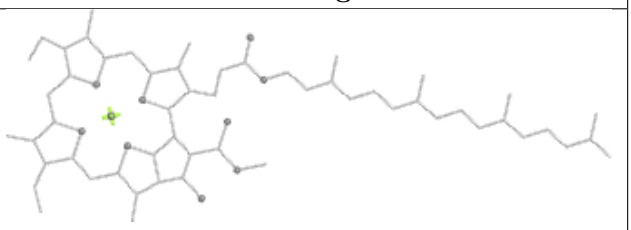
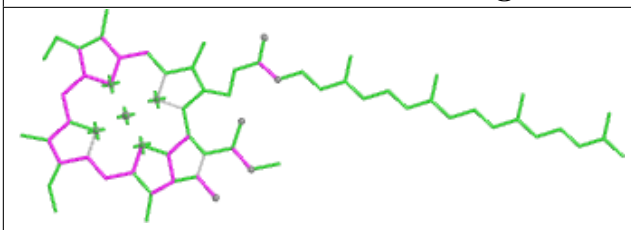


Rings

Ligand CLA a 405 (B)



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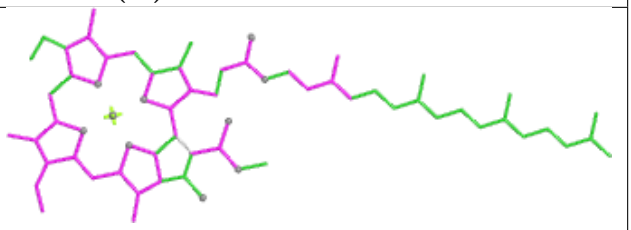
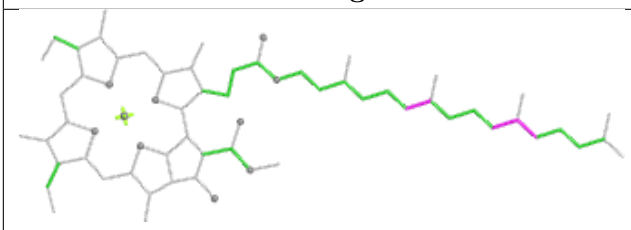


Bond angles



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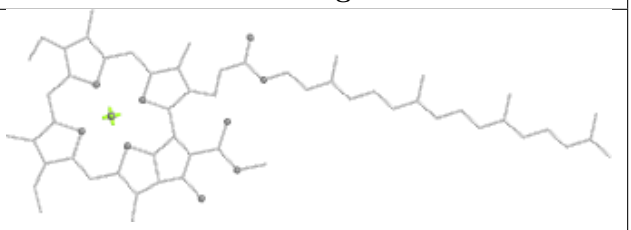
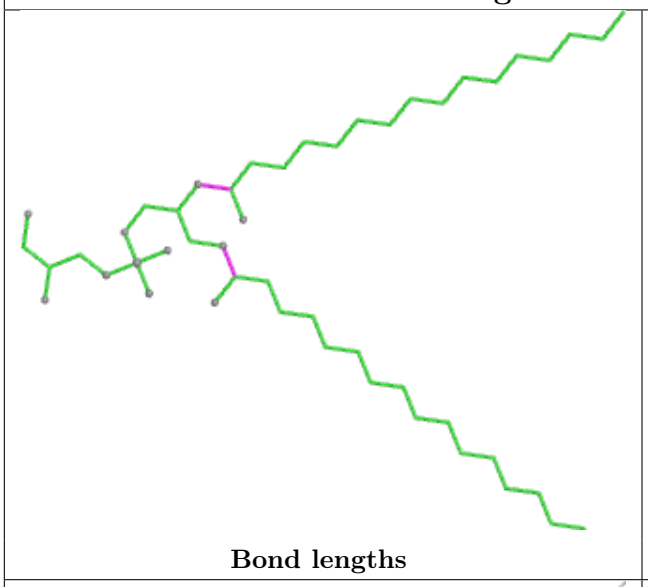
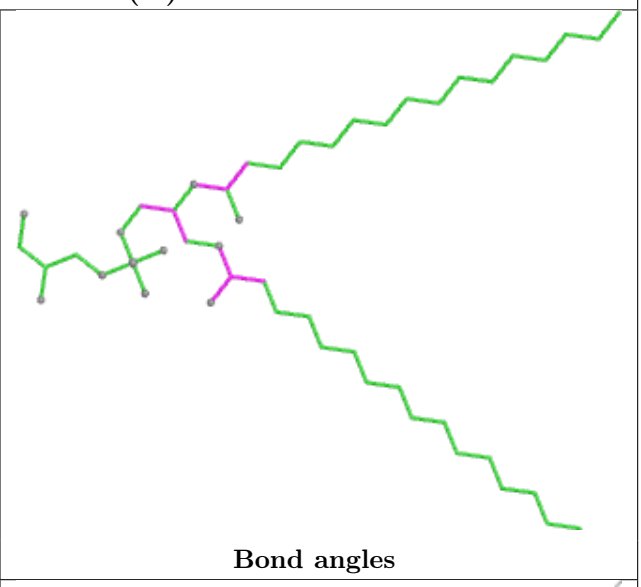


Rings

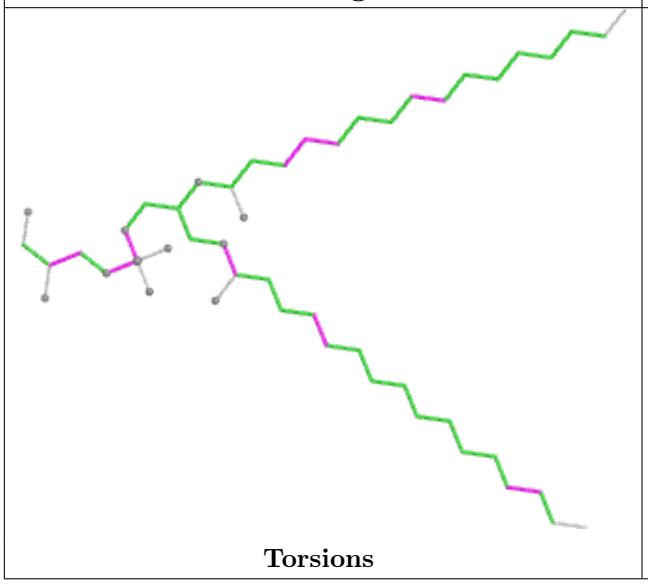
Ligand LHG d 407 (B)



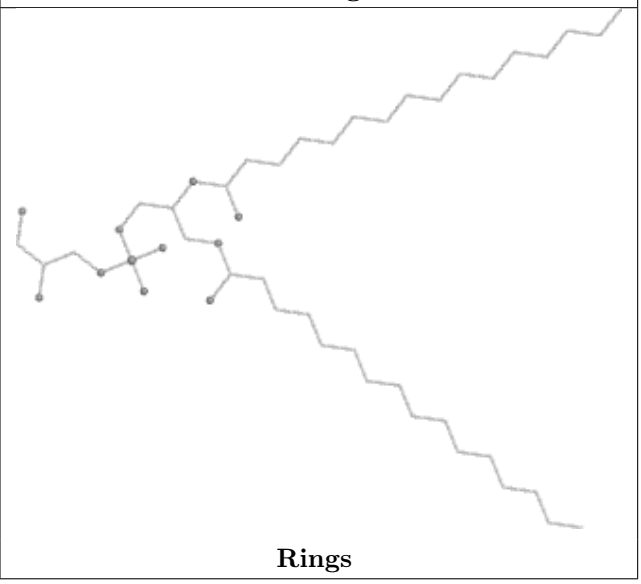
Bond lengths



Bond angles

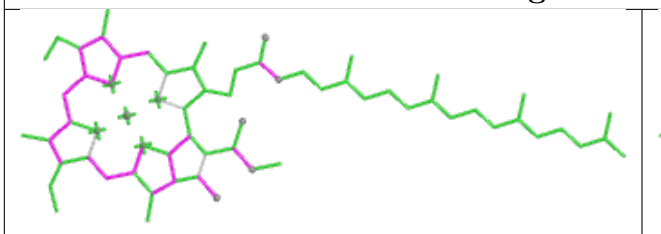


Torsions



Rings

Ligand CLA b 613



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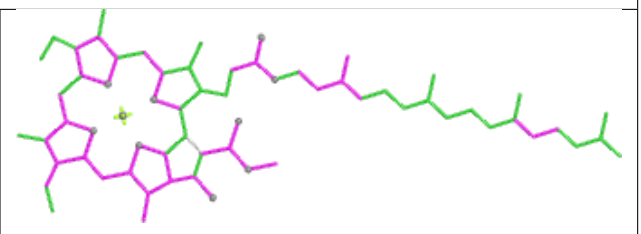
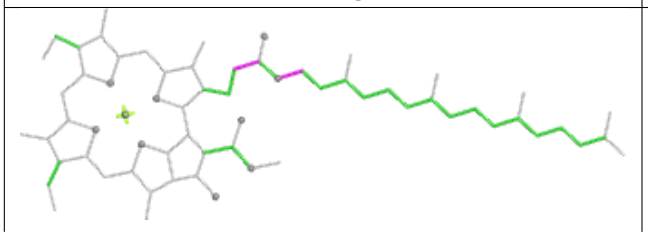


Bond angles



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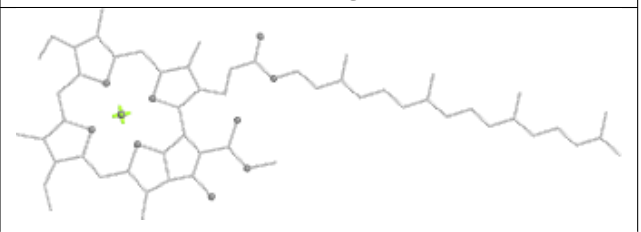
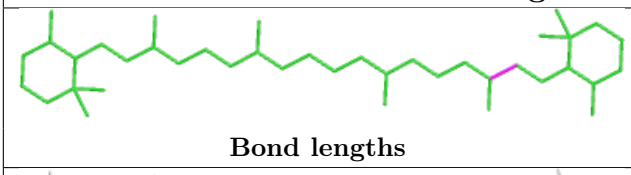


Rings

Ligand BCR t 102



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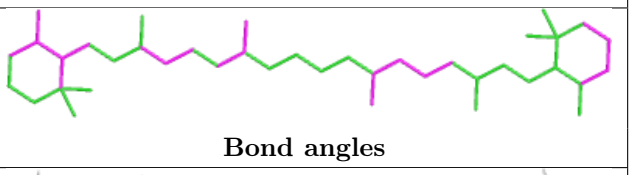

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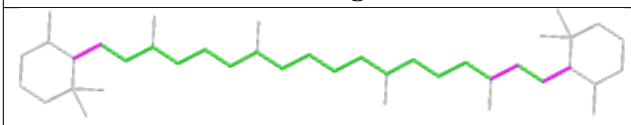

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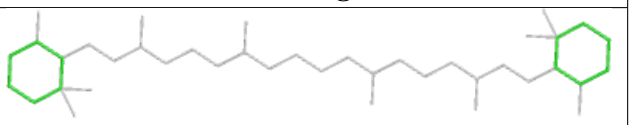
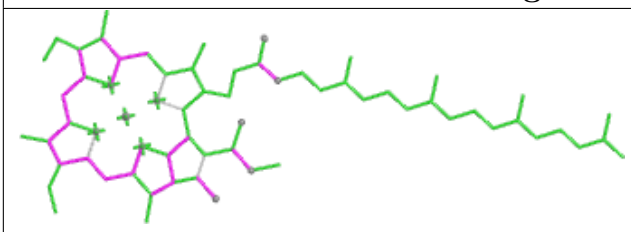


Rings

Ligand CLA D 404



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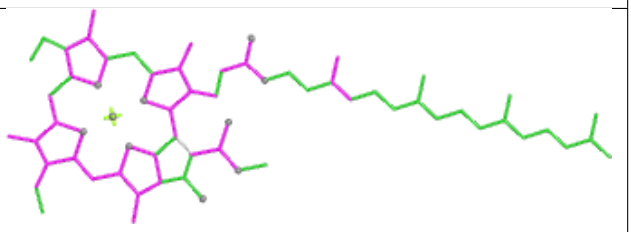
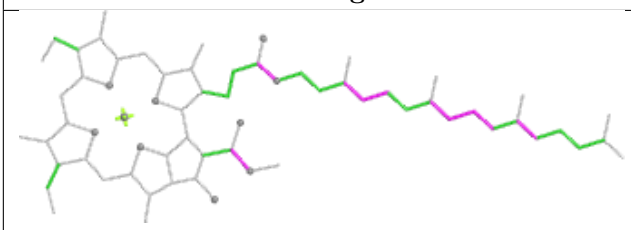


Bond angles



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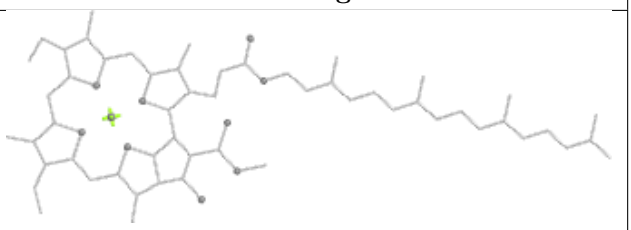
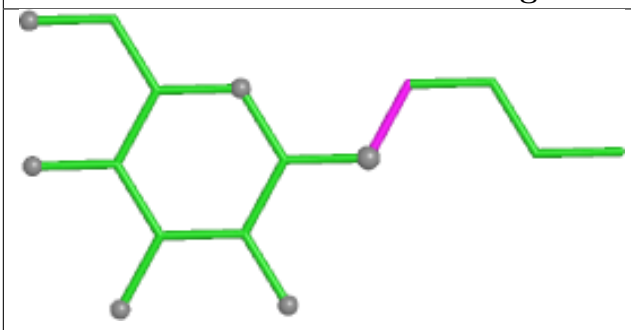


Rings

Ligand HTG D 411



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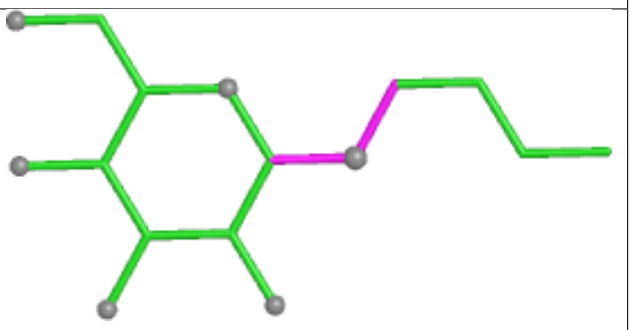

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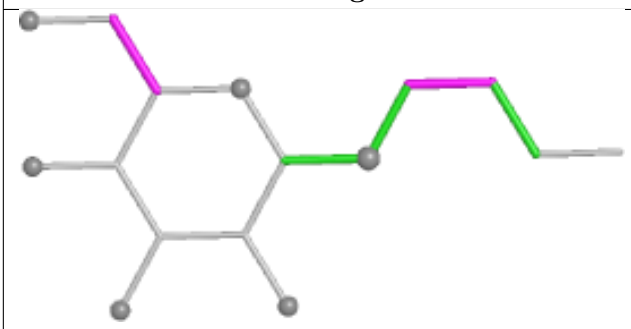

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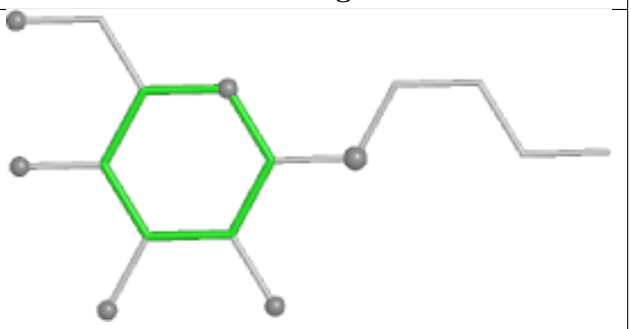
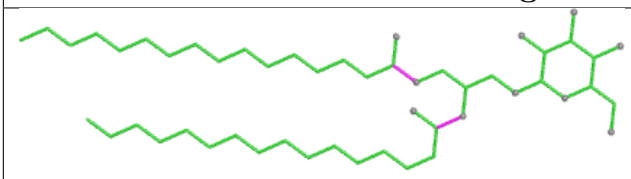


Rings

Ligand LMG C 519



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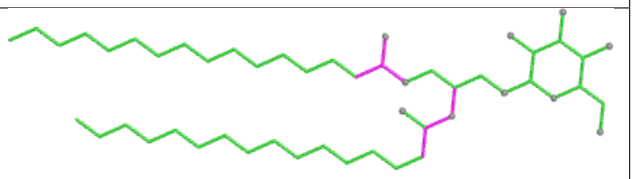
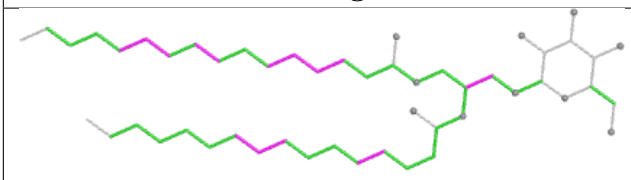


Bond angles



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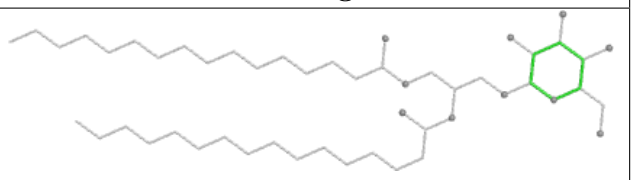
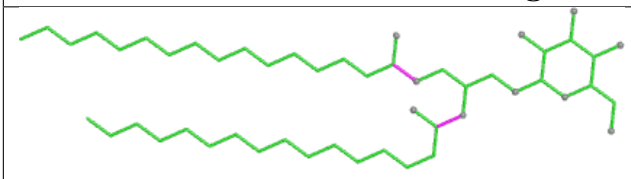


Rings

Ligand LMG c 520



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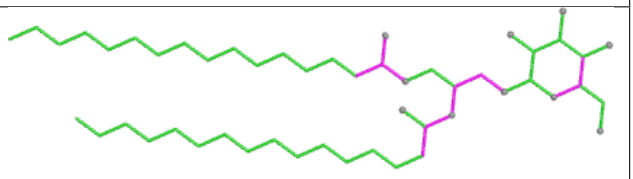
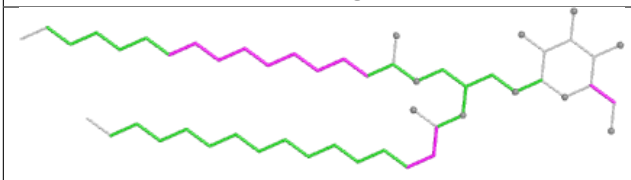


Bond angles



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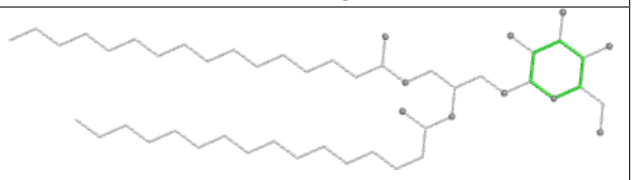
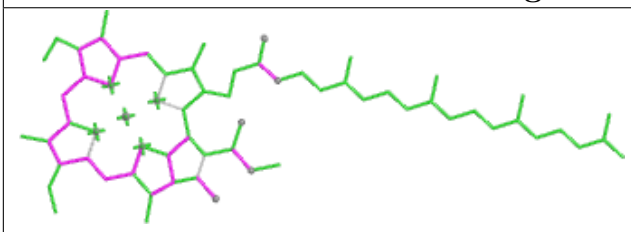


Rings

Ligand CLA C 511



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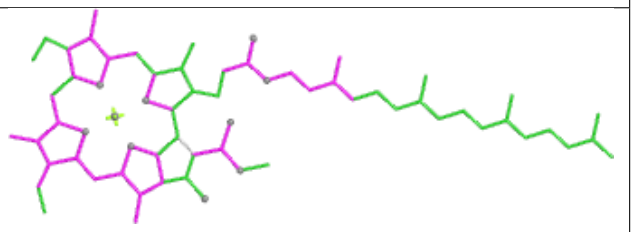
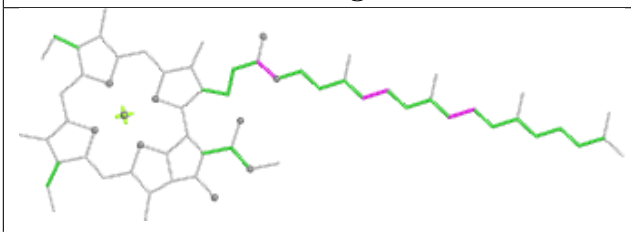


Bond angles



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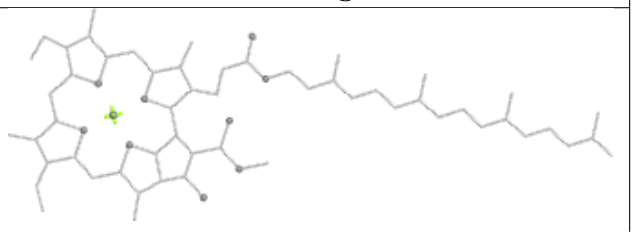
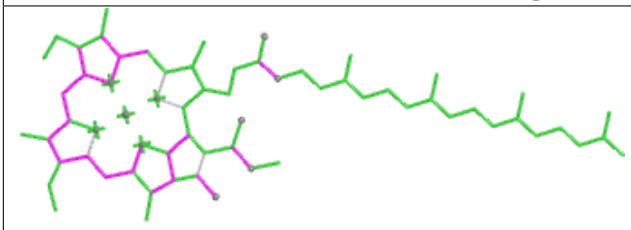


Rings

Ligand CLA b 602



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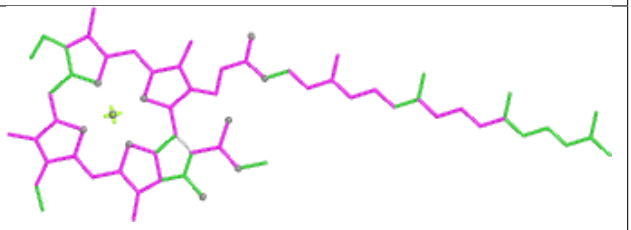
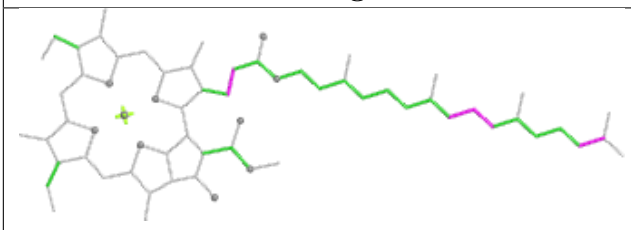


Bond angles



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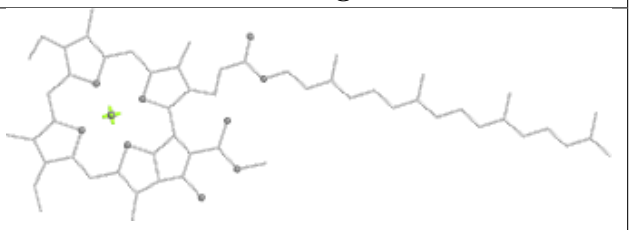
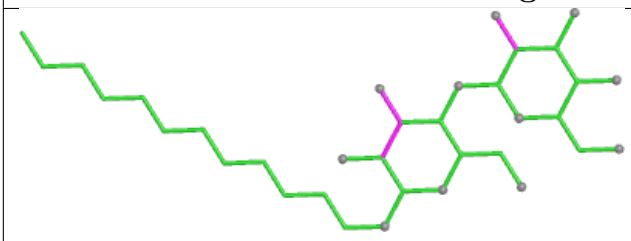


Rings

Ligand LMT m 103



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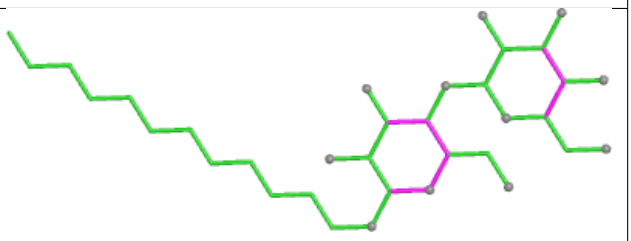
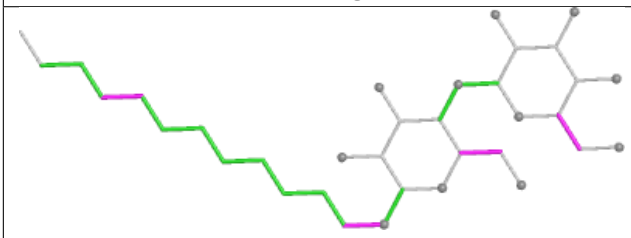


Bond angles



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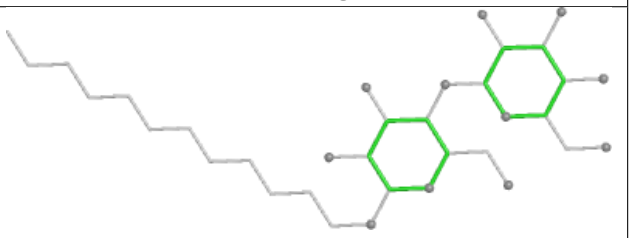
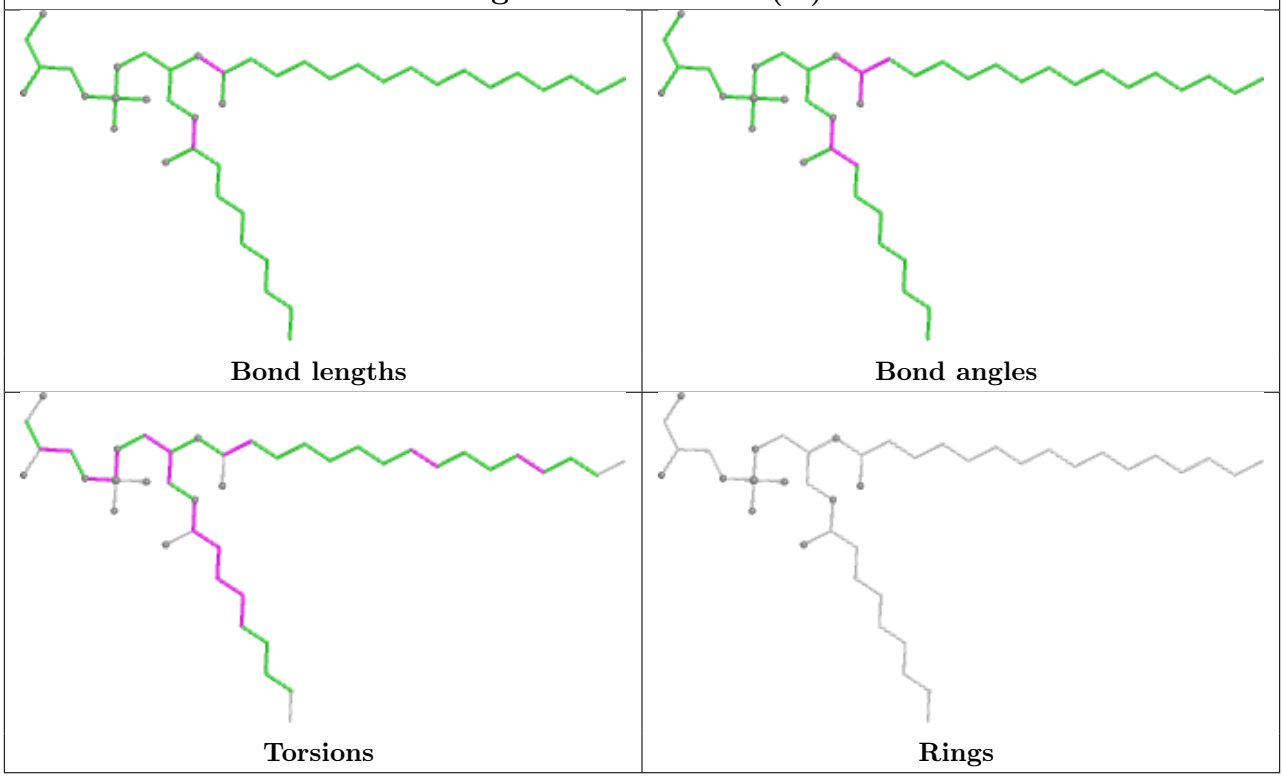
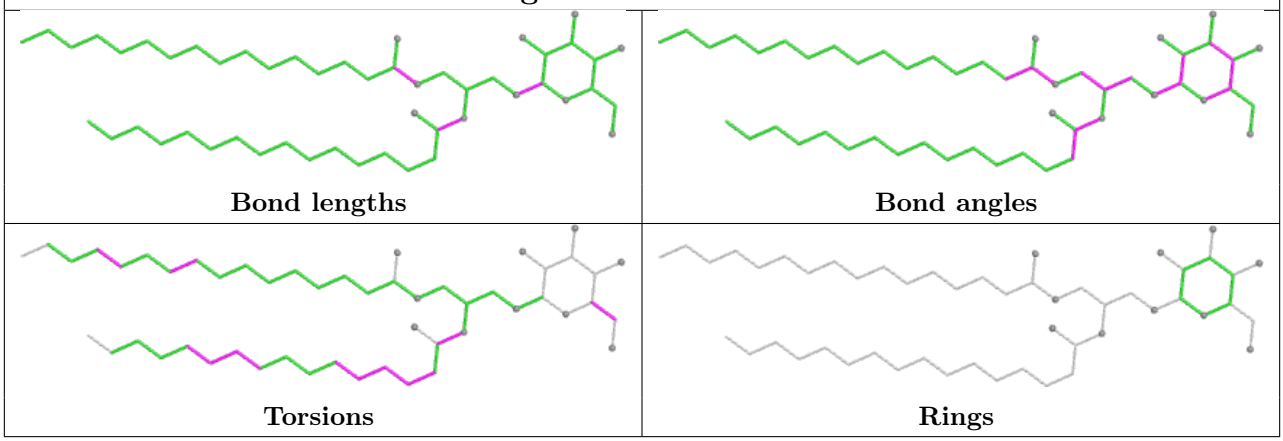


Rings

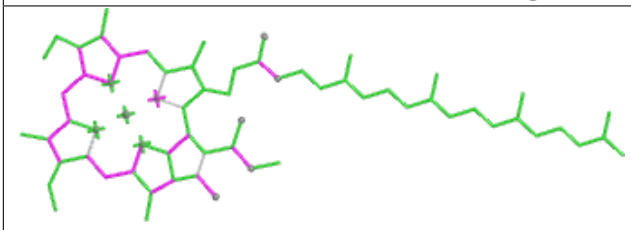
Ligand LHG E 101 (A)



Ligand LMG C 520



Ligand CLA B 615



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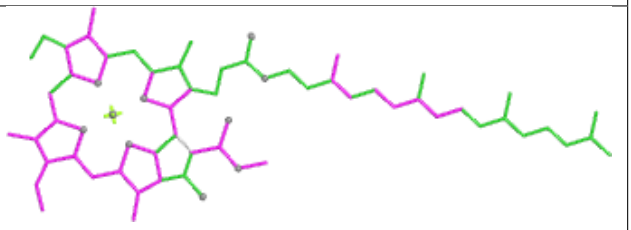
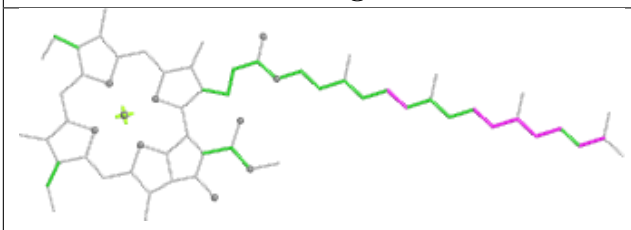


Bond angles



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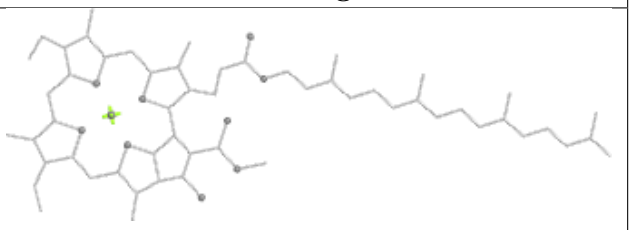
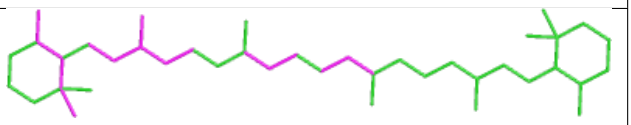


Rings

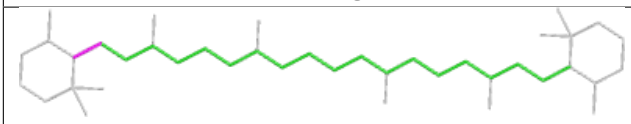
Ligand BCR B 617



Bond lengths



Bond angles



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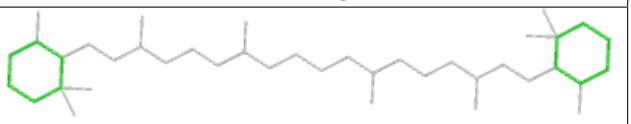
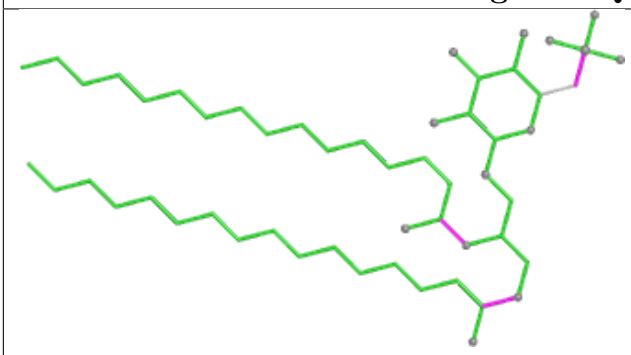


Rings

Ligand SQD A 410 (A)



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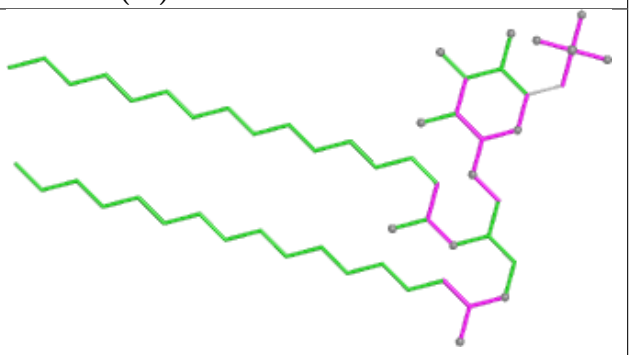
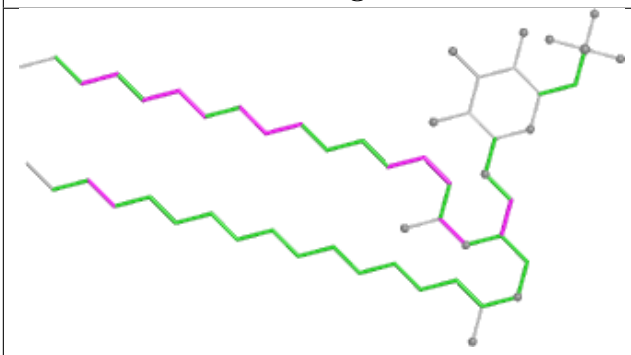


Bond angles



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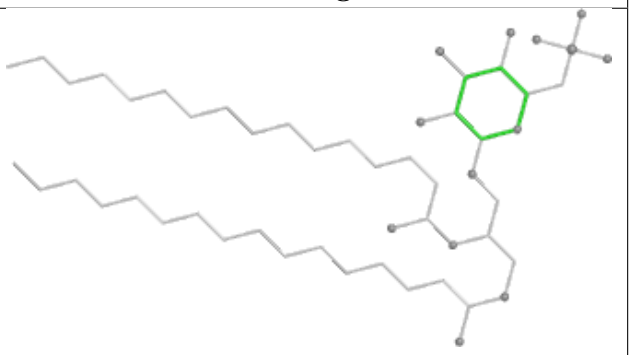
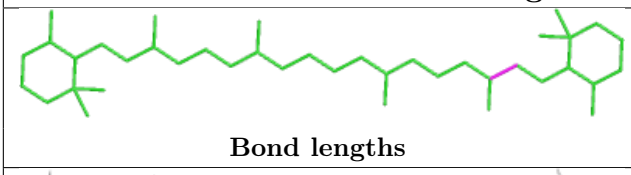
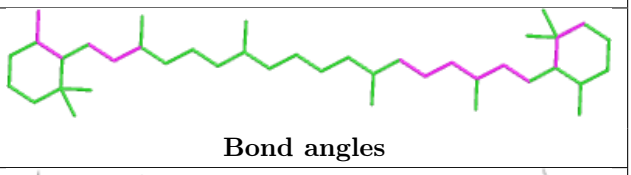


Rings

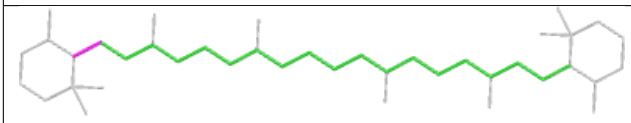
Ligand BCR b 617



Bond lengths



Bond angles



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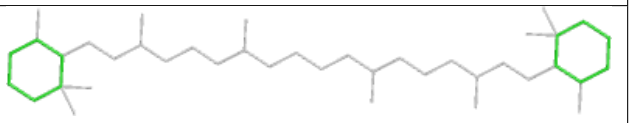
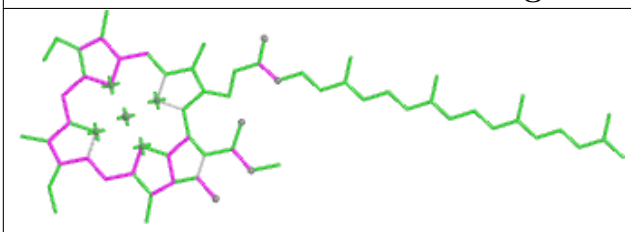
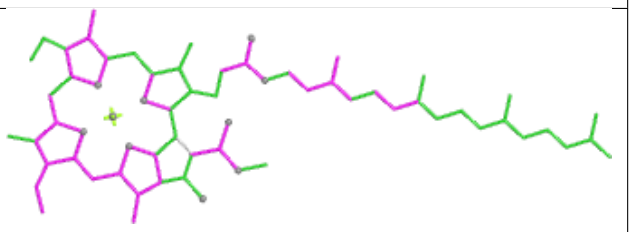


Rings

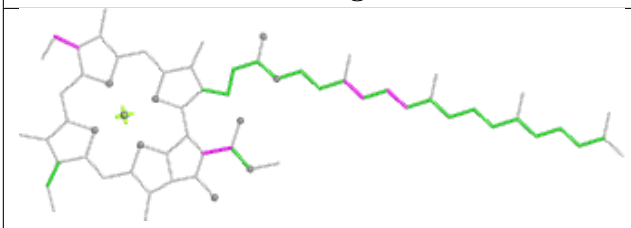
Ligand CLA C 507



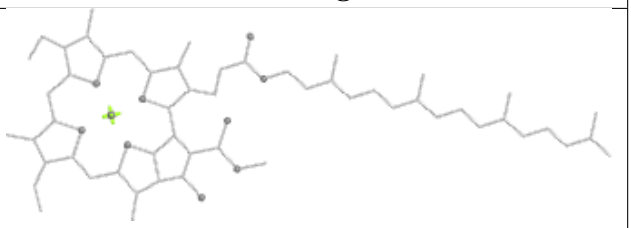
Bond lengths



Bond angles

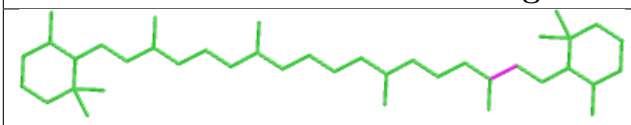


Torsions

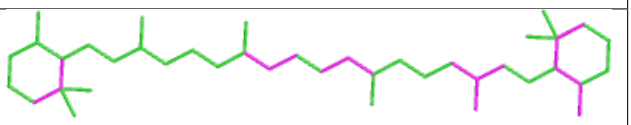


Rings

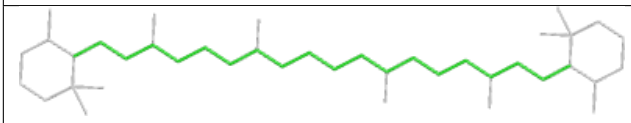
Ligand BCR B 618



Bond lengths



Bond angles



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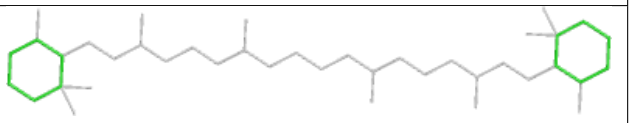
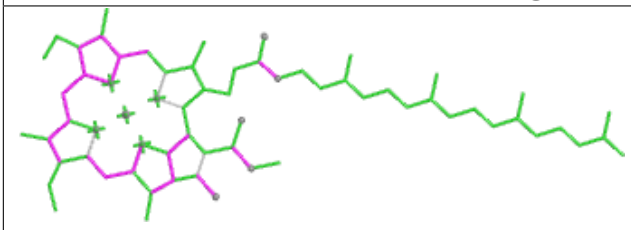


Rings

Ligand CLA b 606



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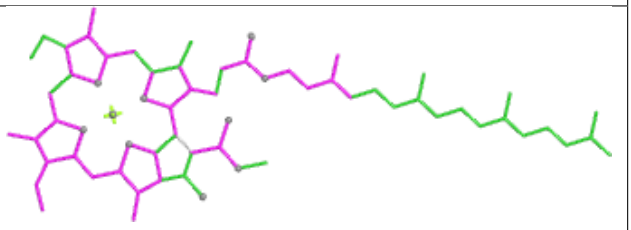
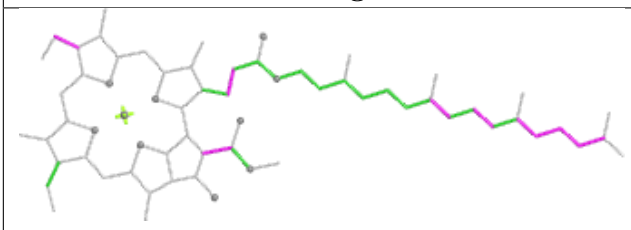
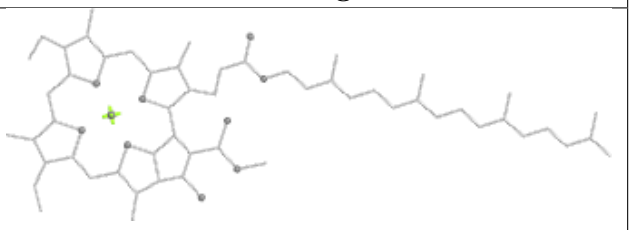


Bond angles

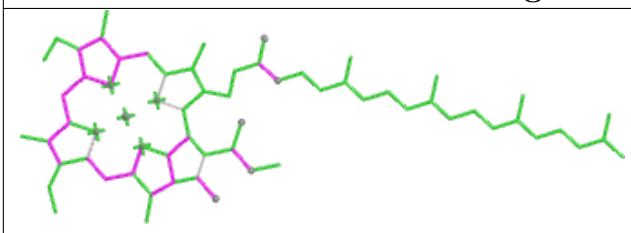


Torsions



Rings

Ligand CLA B 606



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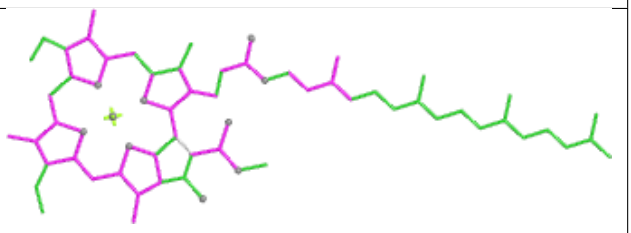
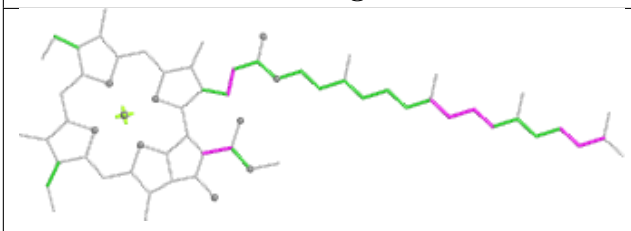
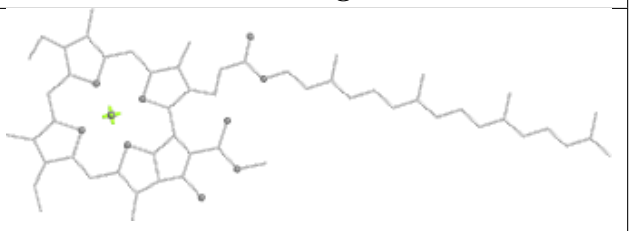


Bond angles

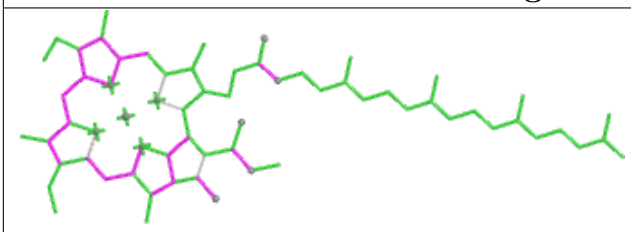


Torsions



Rings

Ligand CLA C 512



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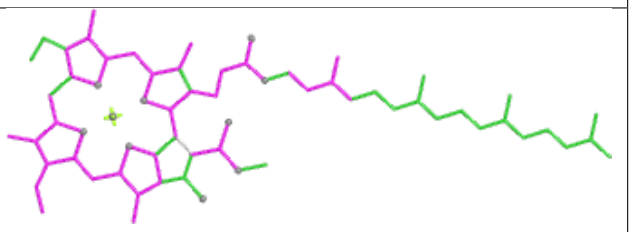
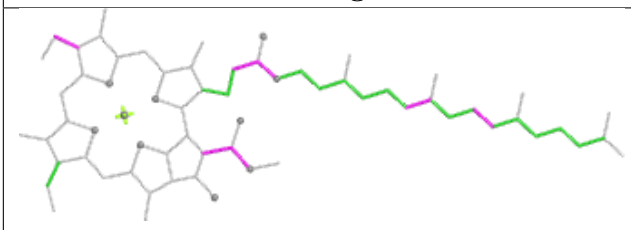


Bond angles



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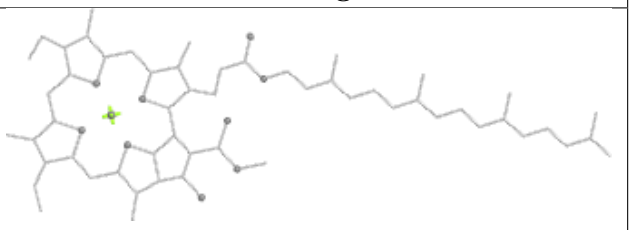
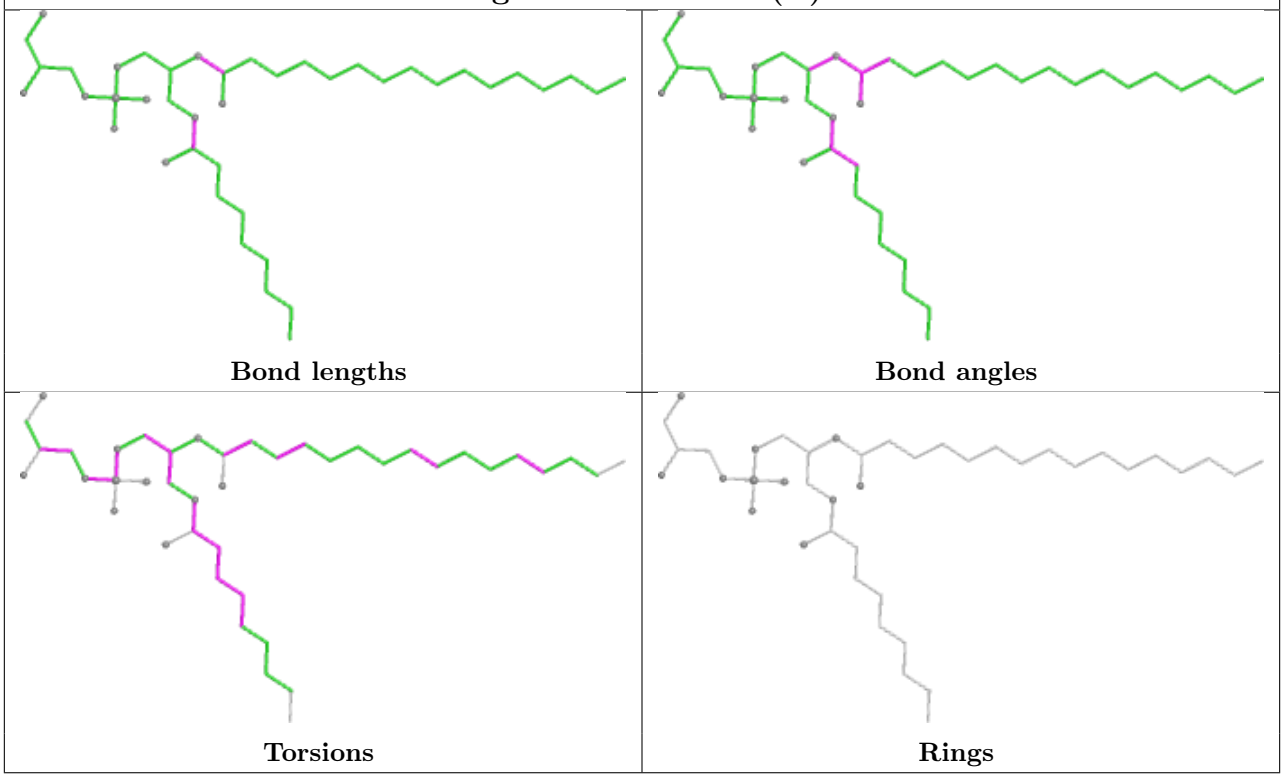
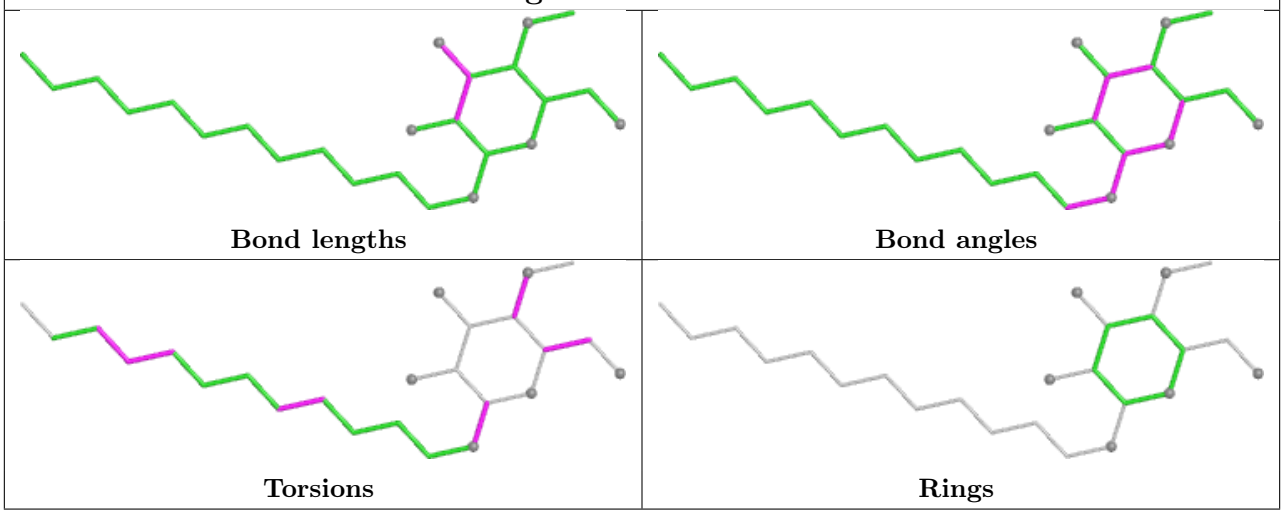


Rings

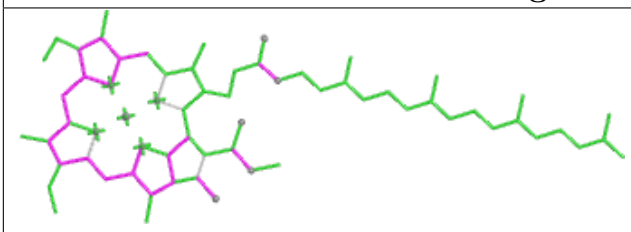
Ligand LHG E 101 (B)



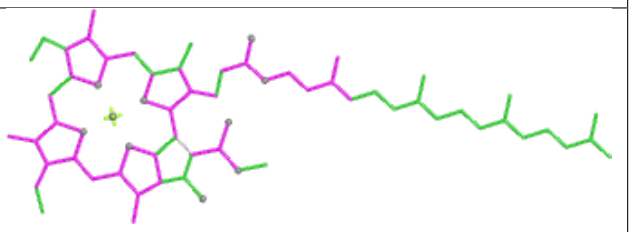
Ligand LMT b 621



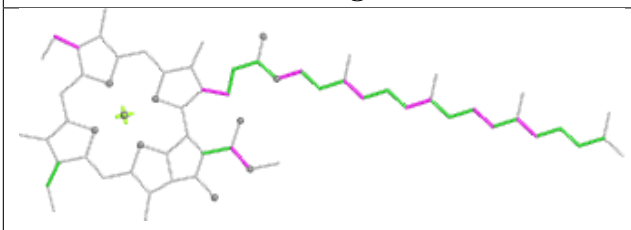
Ligand CLA c 514



Bond lengths



Bond angles



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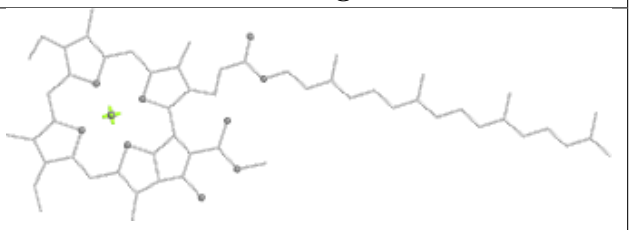
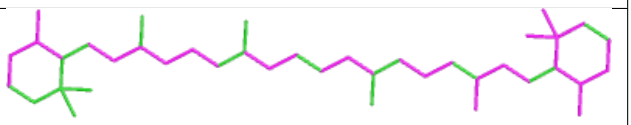


Rings

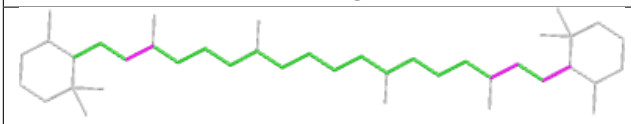
Ligand BCR d 405



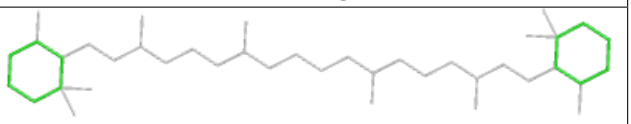
Bond lengths



Bond angles

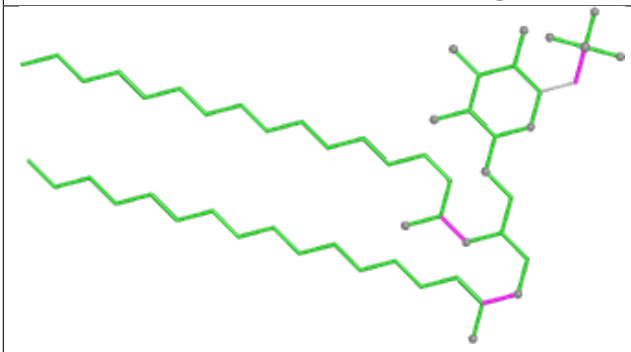


Torsions

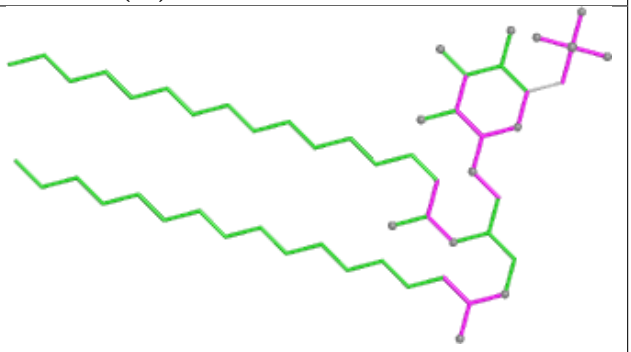


Rings

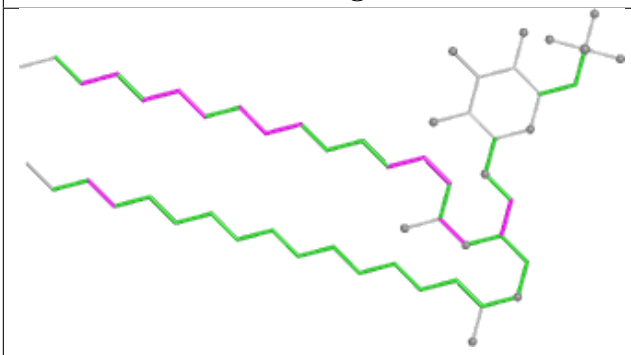
Ligand SQD A 410 (B)



Bond lengths



Bond angles



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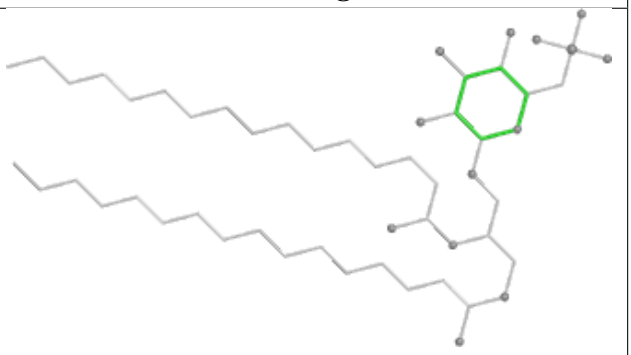
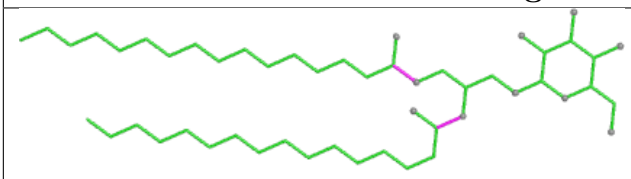
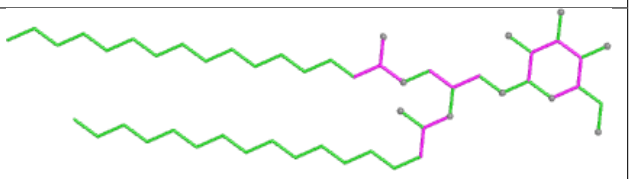


Rings

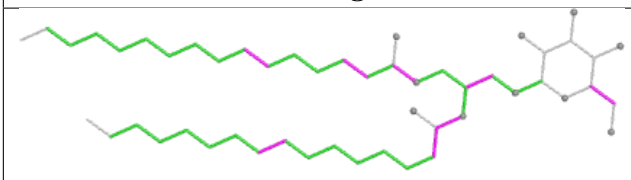
Ligand LMG c 521



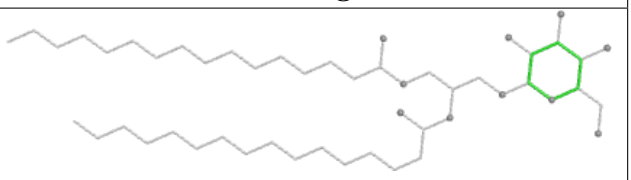
Bond lengths



Bond angles

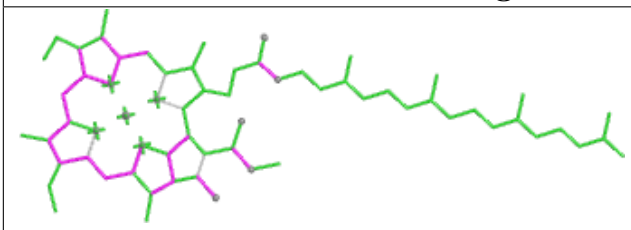


Torsions



Rings

Ligand CLA a 405 (A)



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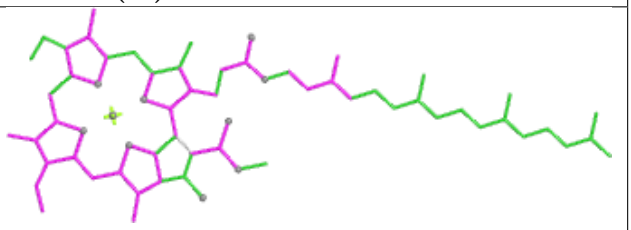
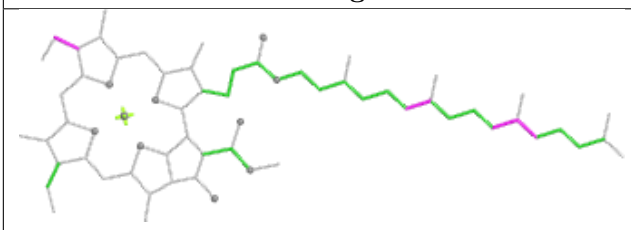
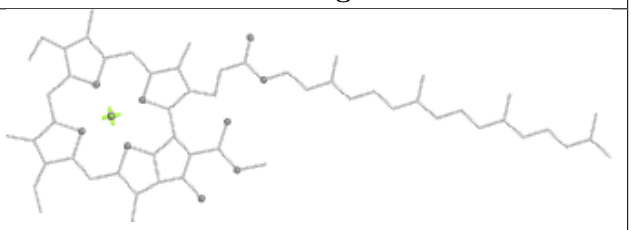


Bond angles

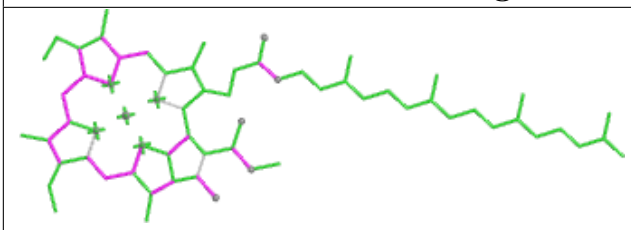


Torsions

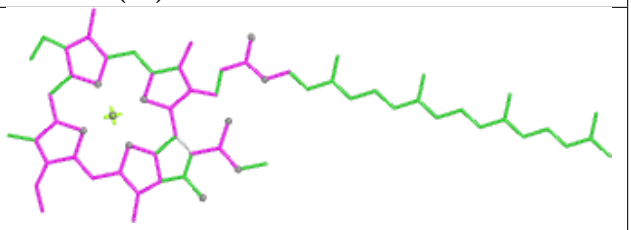


Rings

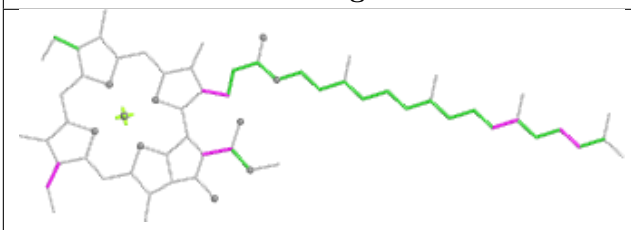
Ligand CLA d 402 (A)



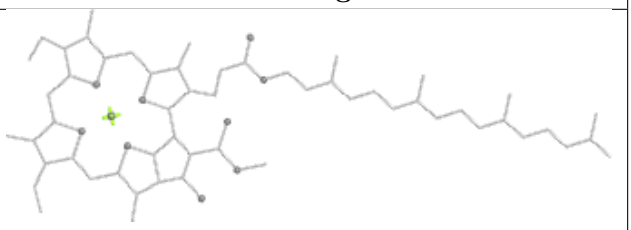
Bond lengths



Bond angles

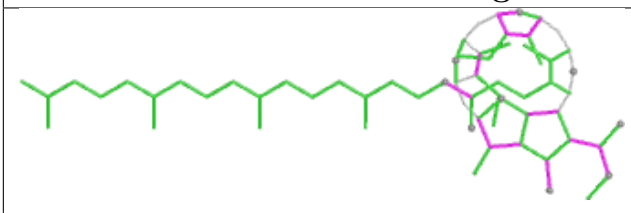


Torsions



Rings

Ligand PHO a 406 (A)



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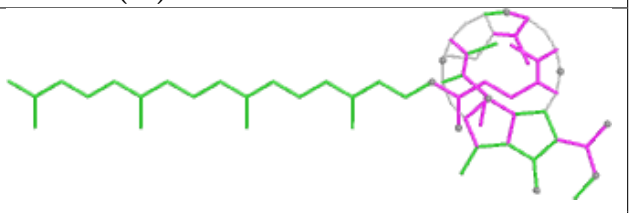
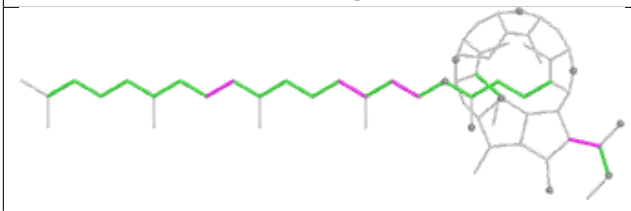


Bond angles



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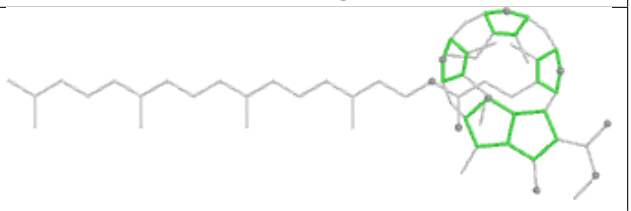
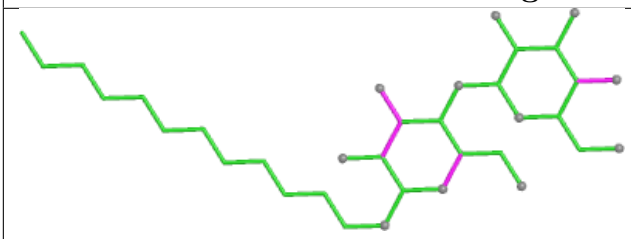


Rings

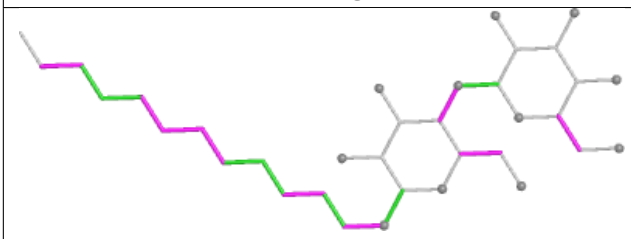
Ligand LMT B 628



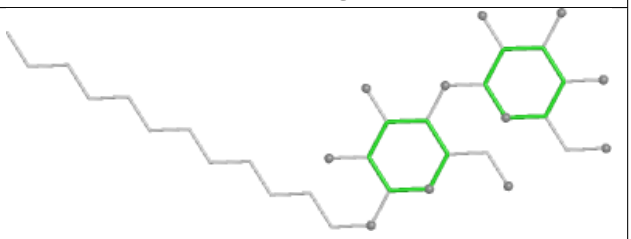
Bond lengths



Bond angles

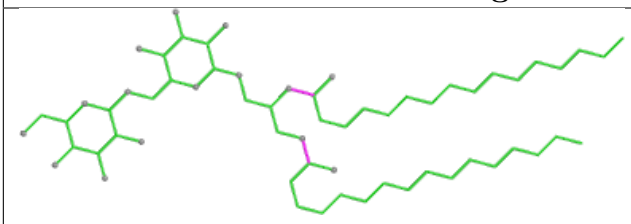


Torsions

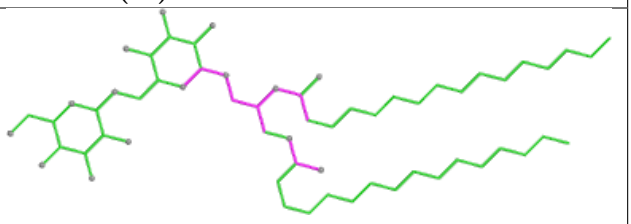


Rings

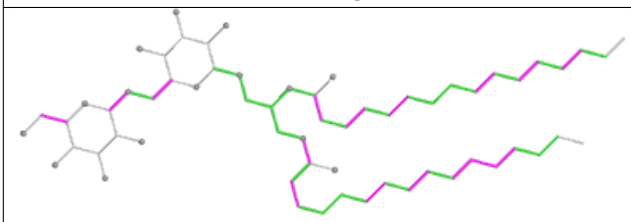
Ligand DGD c 517 (A)



Bond lengths



Bond angles



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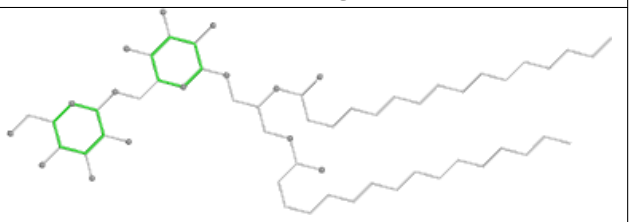
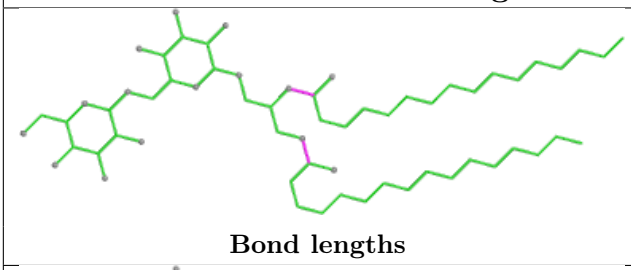
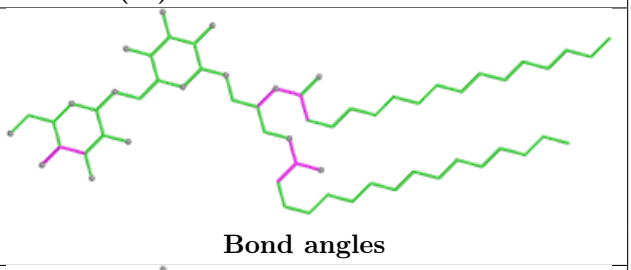


Rings

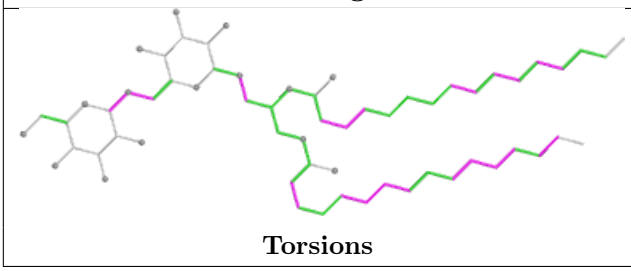
Ligand DGD c 518 (A)



Bond lengths



Bond angles



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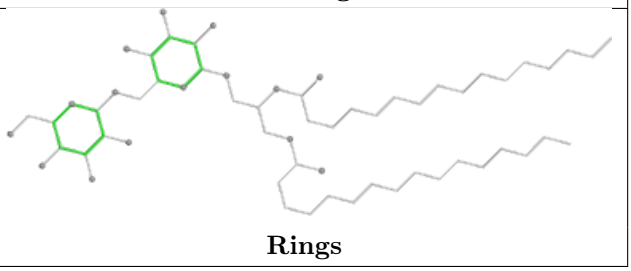
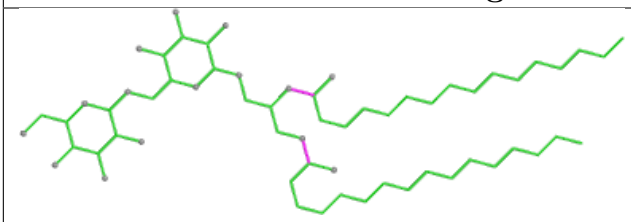
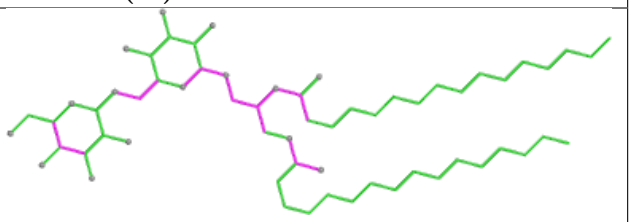


Rings

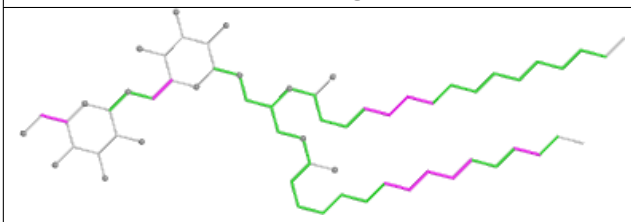
Ligand DGD C 516 (A)



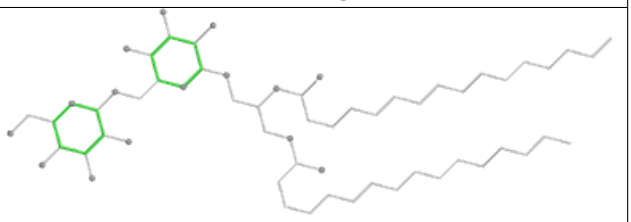
Bond lengths



Bond angles

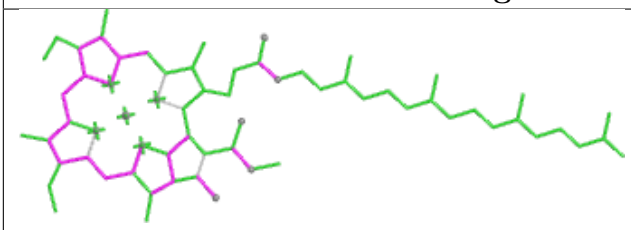


Torsions



Rings

Ligand CLA d 403 (A)



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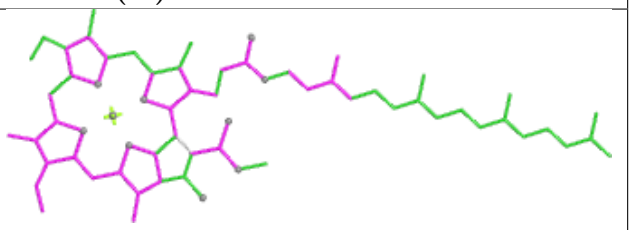

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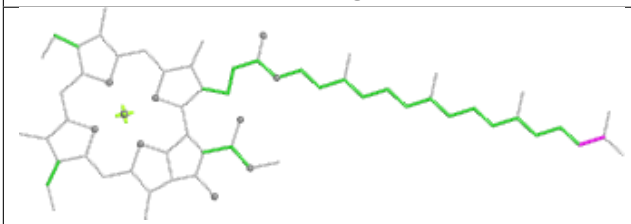

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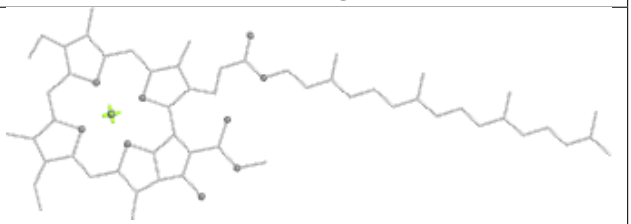
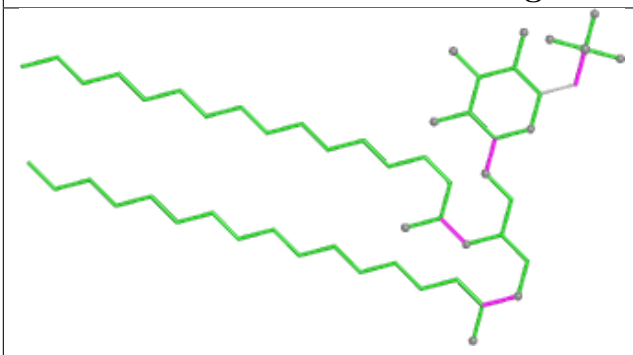


Rings

Ligand SQD B 620



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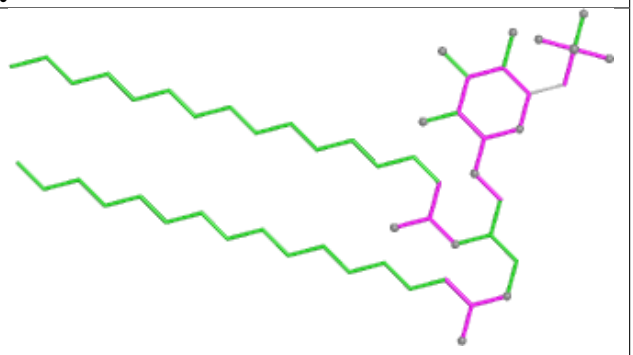
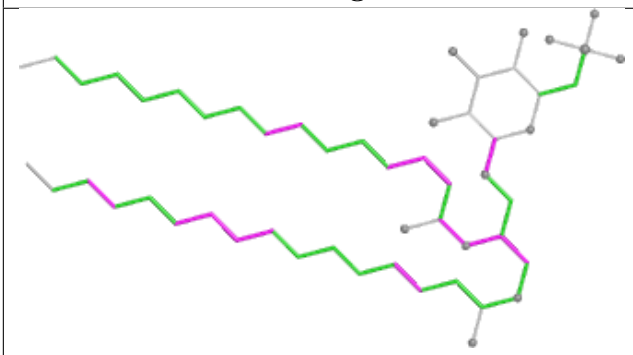


Bond angles



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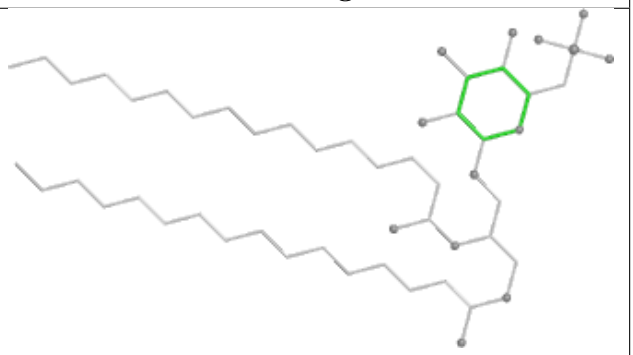
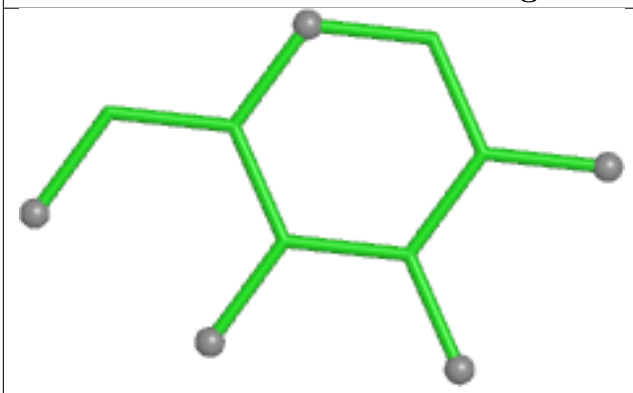


Rings

Ligand HTG V 202



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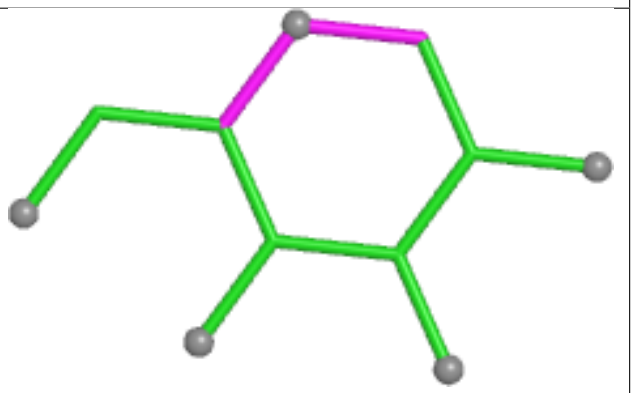
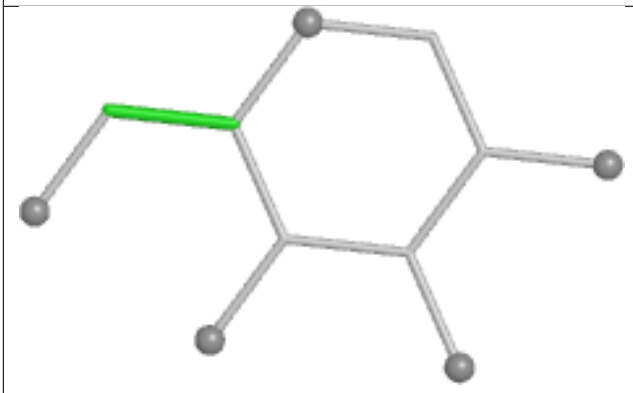


Bond angles



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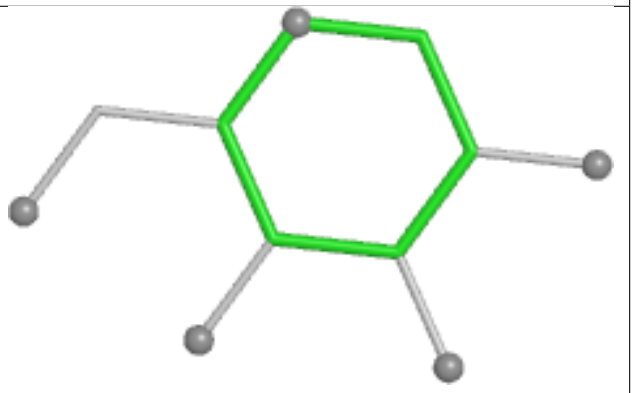
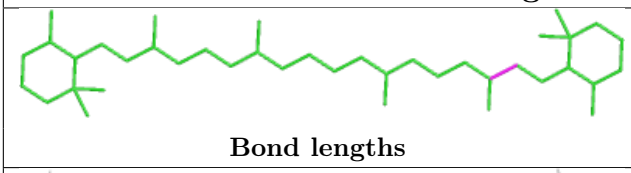


Rings

Ligand BCR C 514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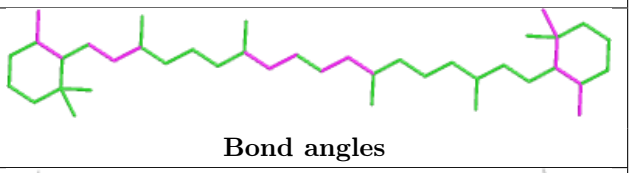
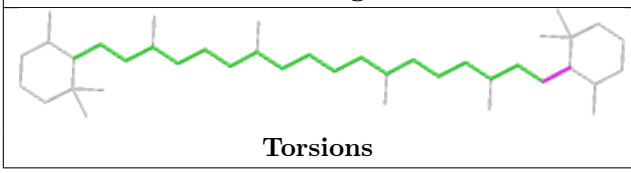

Bond angles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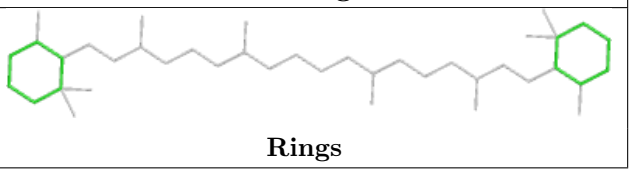
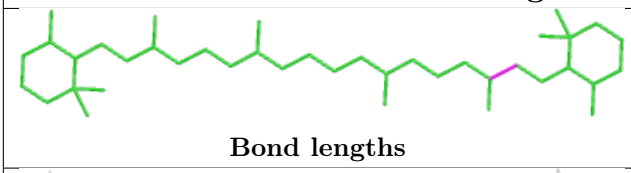

Rings

Ligand BCR a 408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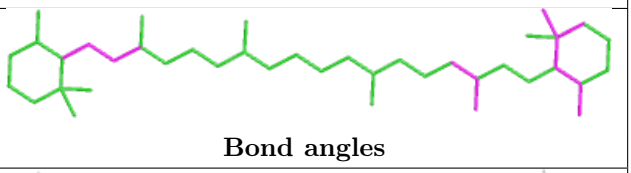
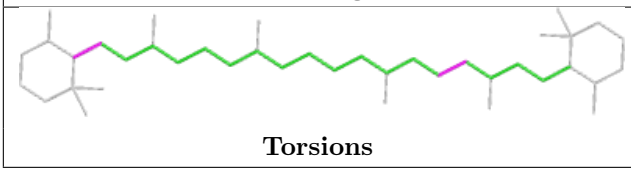

Bond angles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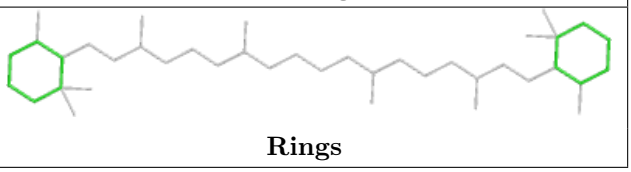
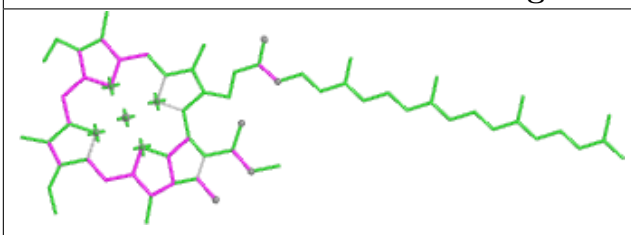

Rings

Ligand CLA b 605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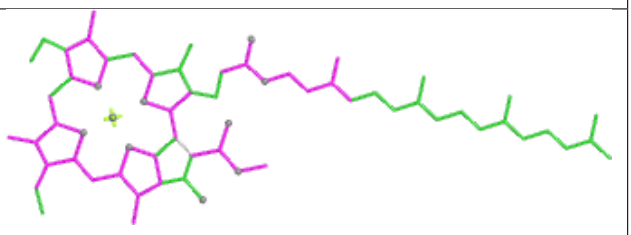
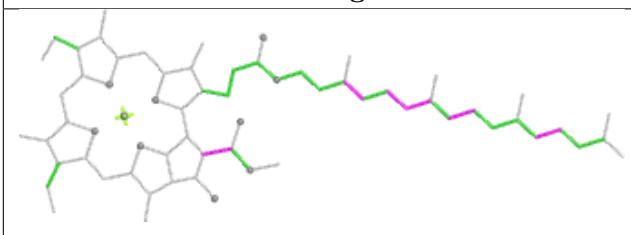

Bond angles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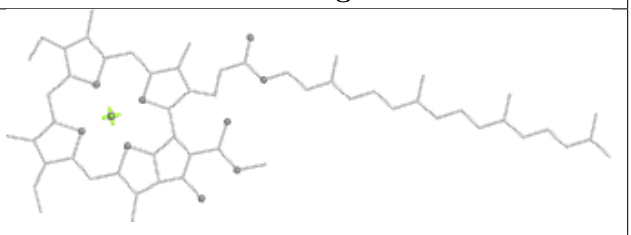
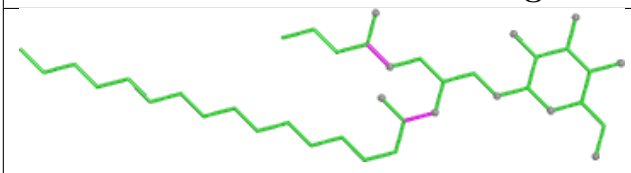
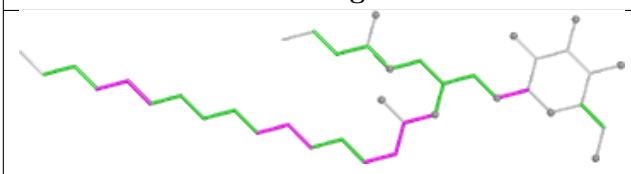

Rings

Ligand LMG z 101


Bond lengths


Bond angles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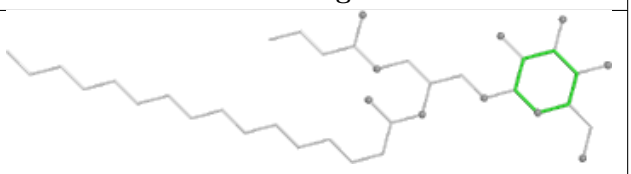
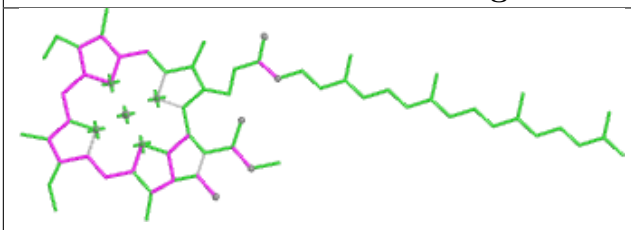

Rings

Ligand CLA A 404 (A)



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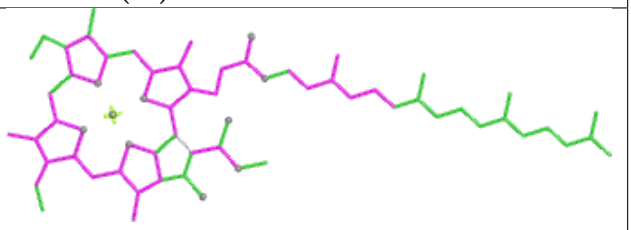
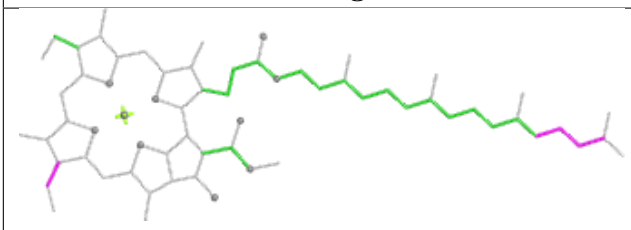
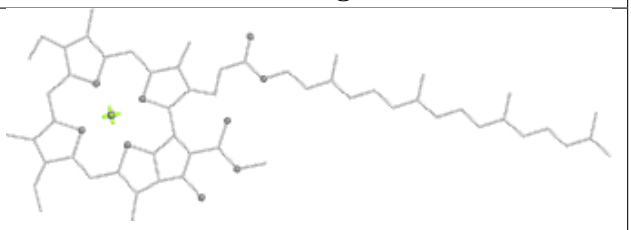


Bond angles

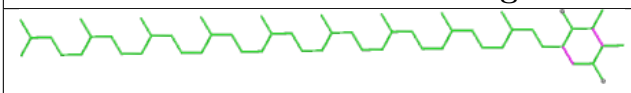


Torsions



Rings

Ligand PL9 a 412 (A)



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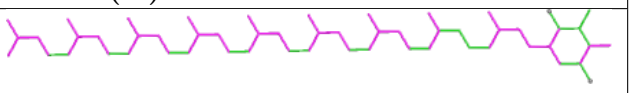
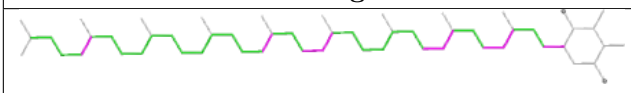


Bond angles



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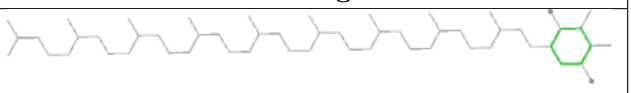
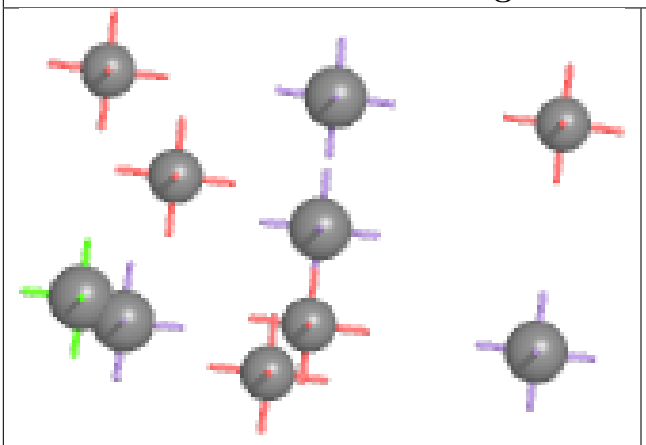


Rings

Ligand OEX a 411 (B)



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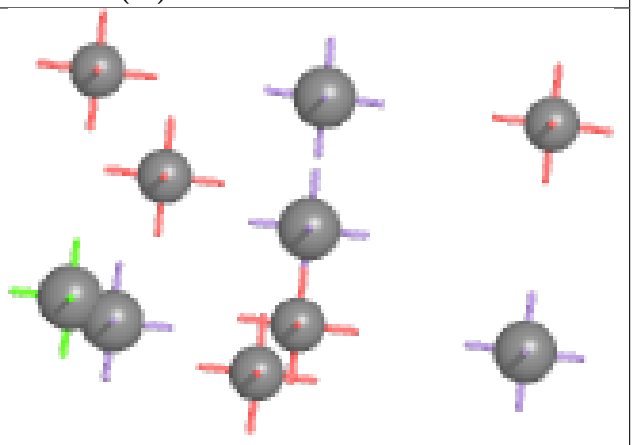
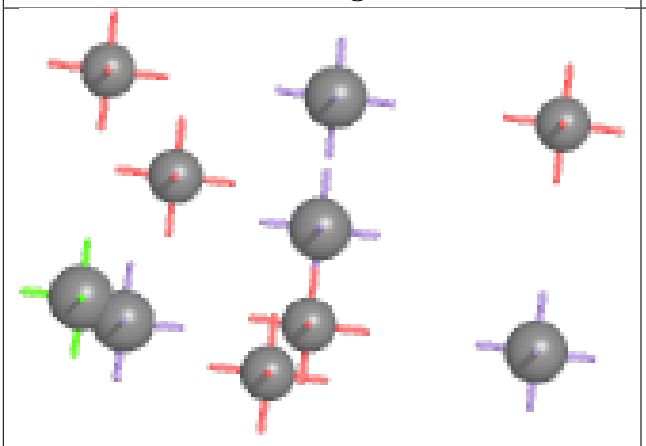


Bond angles



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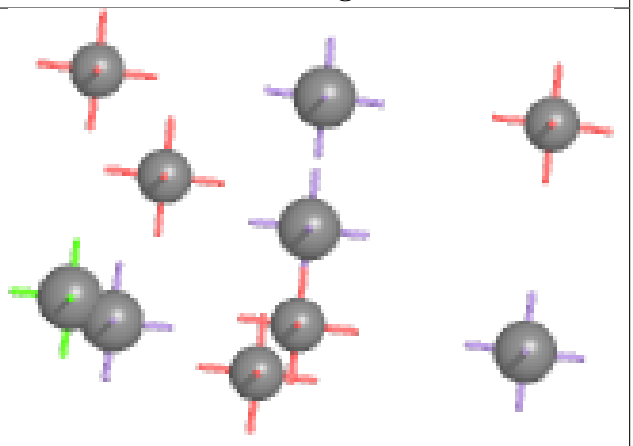
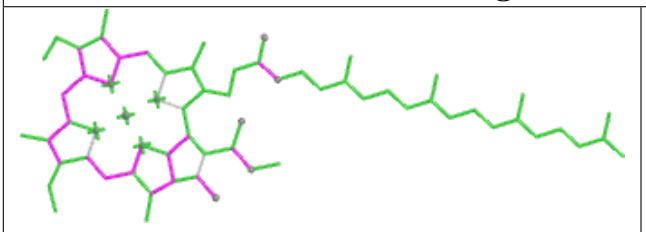


Rings

Ligand CLA d 402 (B)



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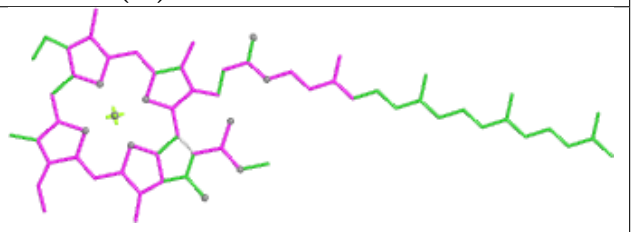
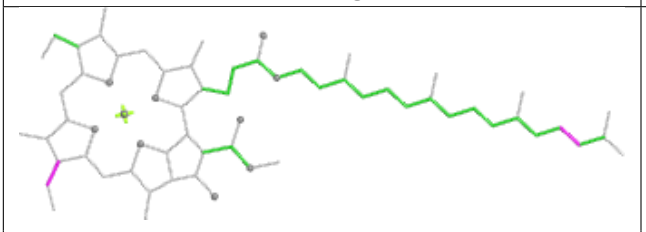


Bond angles



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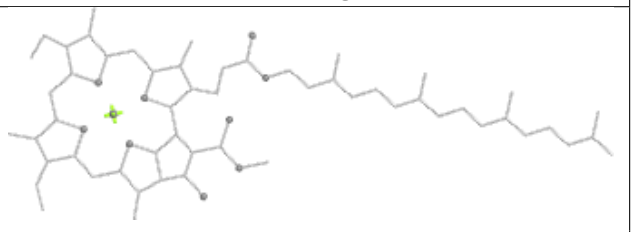
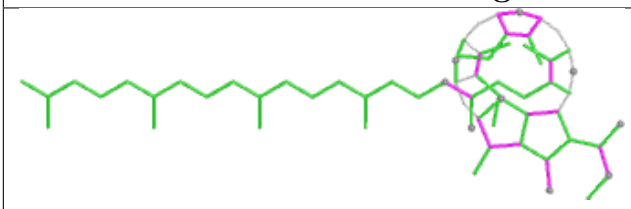
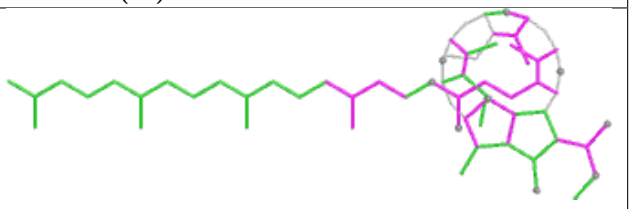


Rings

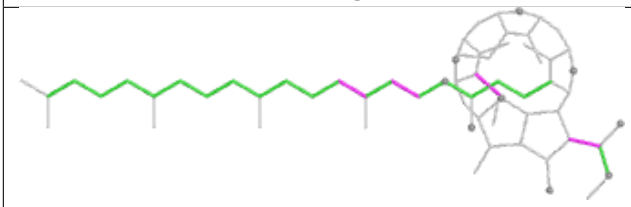
Ligand PHO a 406 (B)



Bond lengths



Bond angles



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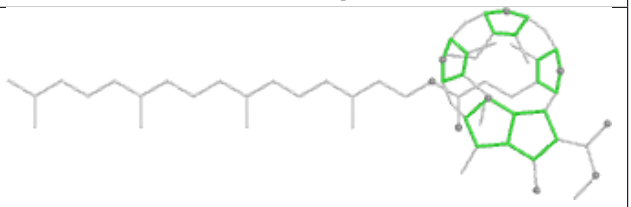
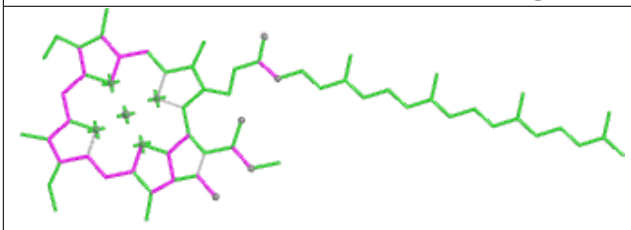


Rings

Ligand CLA c 506



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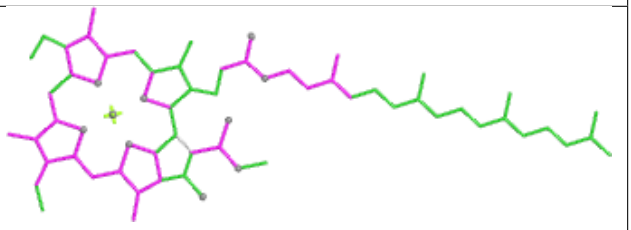
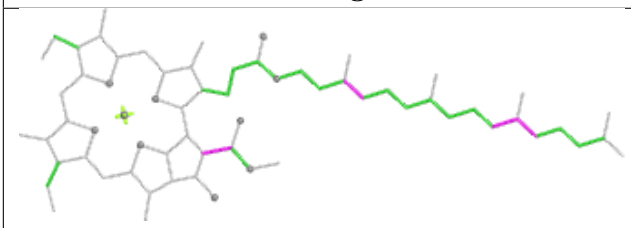


Bond angles



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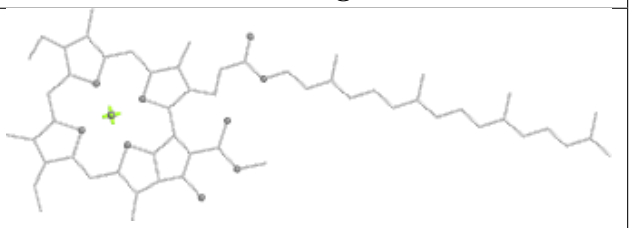
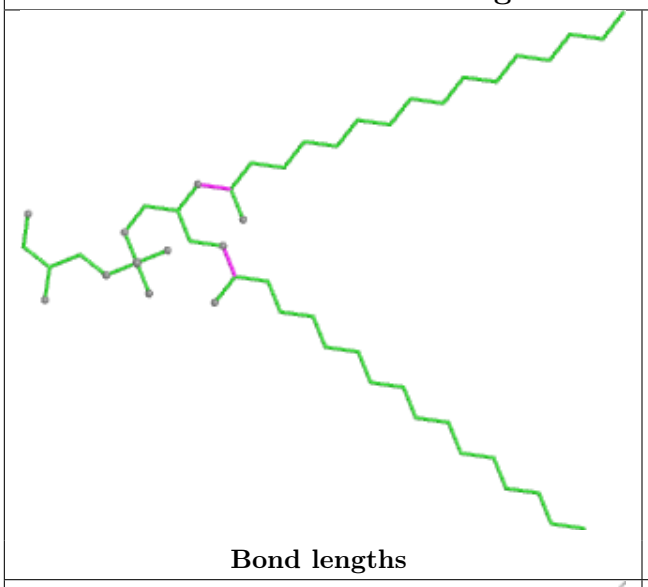
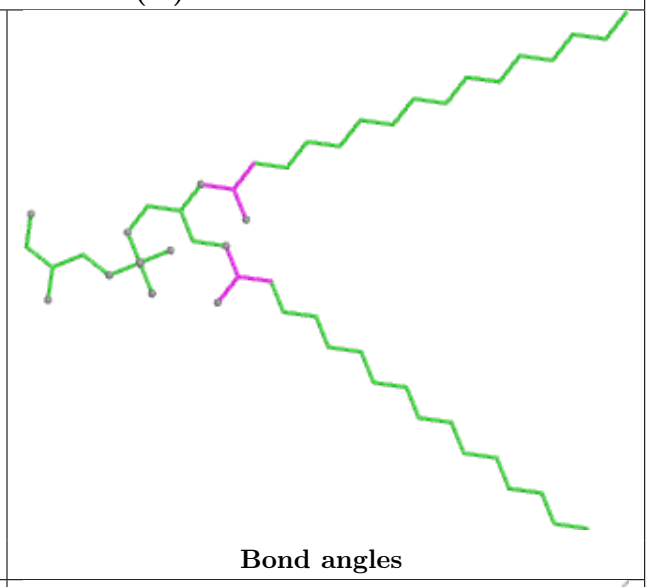


Rings

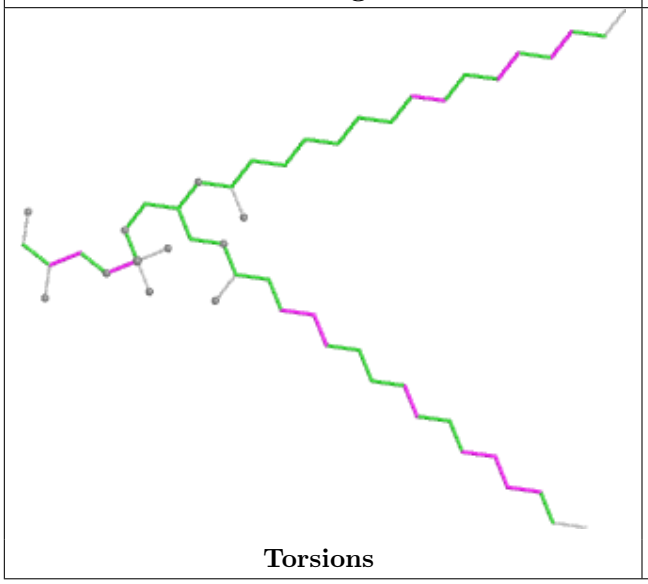
Ligand LHG d 414 (B)



Bond lengths



Bond angles



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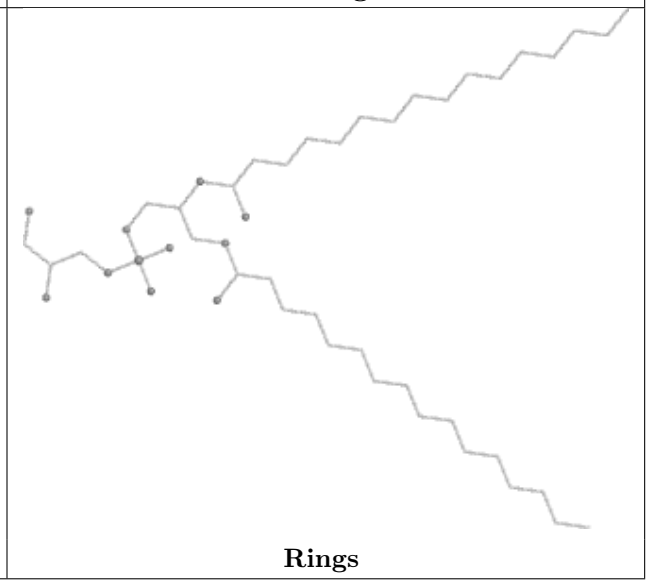


Rings

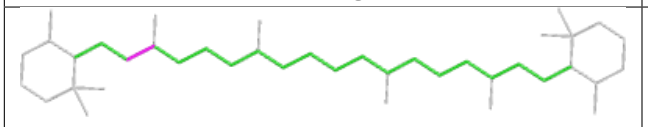
Ligand BCR K 102



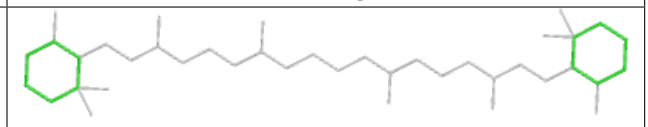
Bond lengths



Bond angles

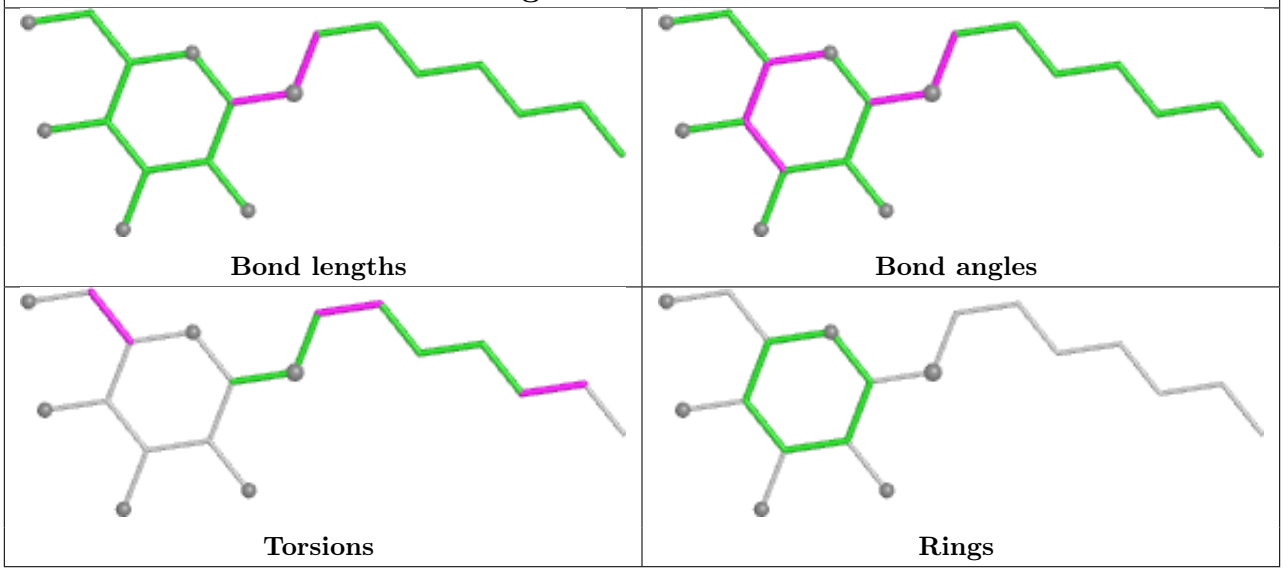


Torsions

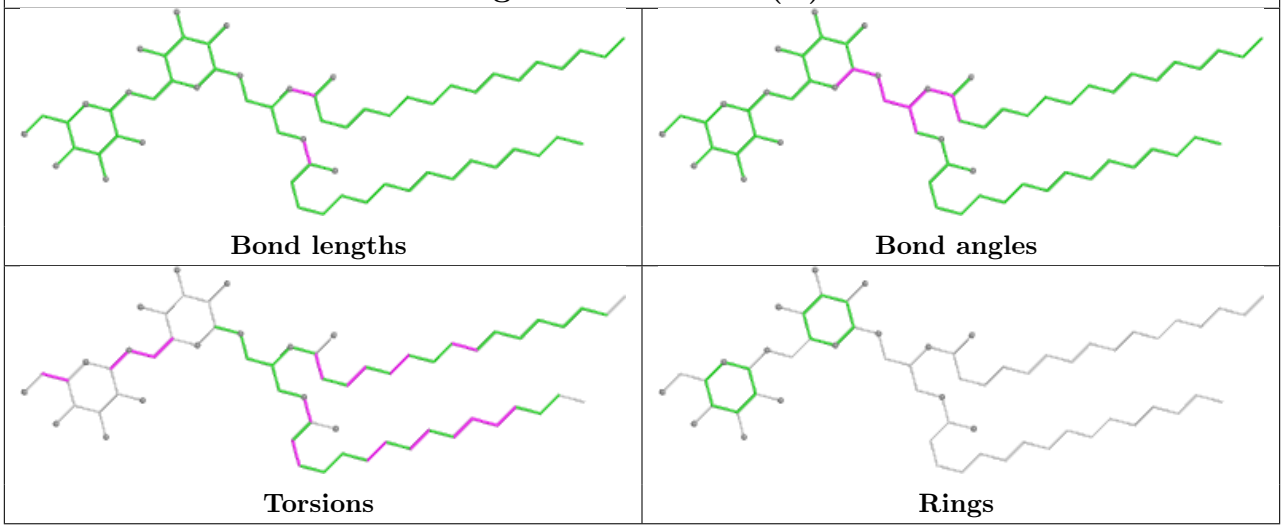


Rings

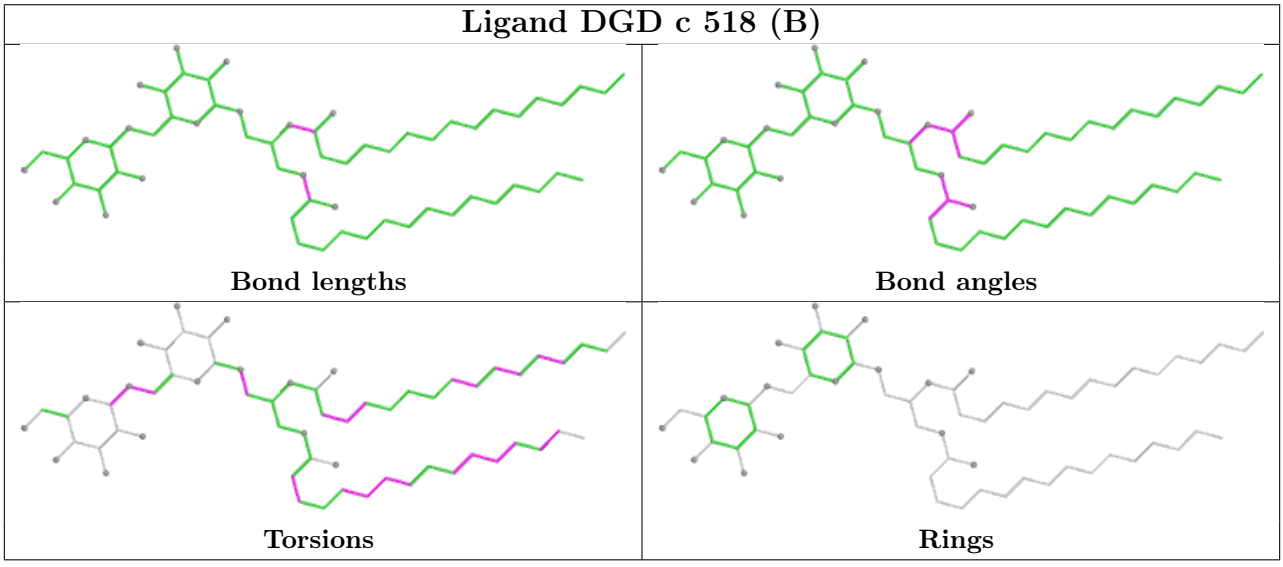
Ligand HTG B 625



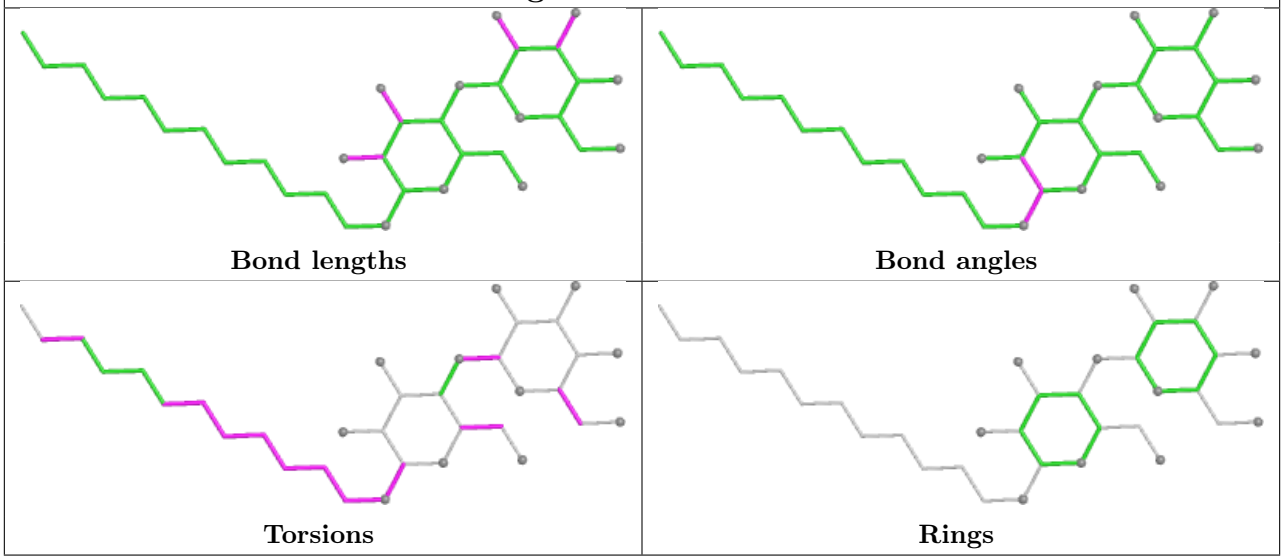
Ligand DGD c 517 (B)



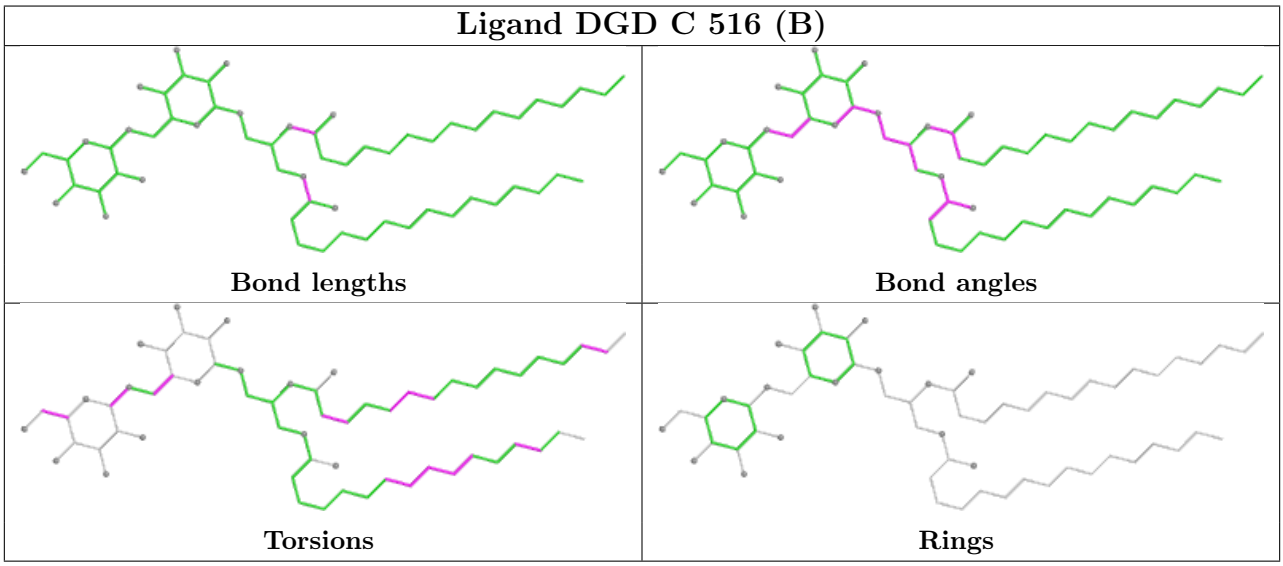
Ligand DGD c 518 (B)



Ligand LMT e 101



Ligand DGD C 516 (B)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.58	0 100 100	21, 27, 60, 127	222 (66%)
1	a	334/344 (97%)	-0.56	1 (0%) 90 90	21, 29, 65, 127	220 (65%)
2	B	504/505 (99%)	-0.54	1 (0%) 91 92	22, 54, 83, 117	22 (4%)
2	b	504/505 (99%)	-0.46	2 (0%) 88 89	24, 58, 95, 162	19 (3%)
3	C	451/455 (99%)	-0.52	0 100 100	22, 59, 81, 158	99 (21%)
3	c	455/455 (100%)	-0.50	2 (0%) 88 89	24, 65, 86, 124	101 (22%)
4	D	342/342 (100%)	-0.60	0 100 100	21, 47, 65, 138	115 (33%)
4	d	341/342 (99%)	-0.60	0 100 100	22, 50, 72, 134	119 (34%)
5	E	81/84 (96%)	-0.38	1 (1%) 76 77	52, 71, 98, 166	0
5	e	79/84 (94%)	-0.38	1 (1%) 75 76	32, 76, 119, 150	2 (2%)
6	F	34/44 (77%)	-0.60	0 100 100	54, 62, 88, 115	0
6	f	31/44 (70%)	-0.39	1 (3%) 50 50	56, 67, 96, 152	1 (3%)
7	H	64/65 (98%)	-0.31	1 (1%) 70 71	51, 63, 84, 112	0
7	h	64/65 (98%)	-0.43	0 100 100	39, 69, 94, 111	1 (1%)
8	I	37/38 (97%)	-0.20	0 100 100	56, 63, 127, 163	0
8	i	37/38 (97%)	-0.34	1 (2%) 56 57	56, 63, 124, 148	0
9	J	38/39 (97%)	-0.33	0 100 100	53, 71, 122, 182	0
9	j	39/39 (100%)	-0.36	1 (2%) 57 58	60, 75, 131, 175	0
10	K	37/37 (100%)	-0.69	0 100 100	59, 69, 88, 110	0
10	k	37/37 (100%)	-0.55	0 100 100	69, 75, 98, 113	0
11	L	36/37 (97%)	-0.60	0 100 100	23, 47, 105, 144	2 (5%)
11	l	36/37 (97%)	-0.55	0 100 100	25, 48, 97, 125	2 (5%)
12	M	32/36 (88%)	-0.58	0 100 100	27, 49, 77, 140	1 (3%)
12	m	33/36 (91%)	-0.50	0 100 100	24, 50, 72, 153	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.54	0 100 100	22, 64, 119, 185	10 (4%)
13	o	243/244 (99%)	-0.50	0 100 100	23, 67, 128, 169	8 (3%)
14	T	29/32 (90%)	-0.56	0 100 100	27, 48, 58, 66	6 (20%)
14	t	29/32 (90%)	-0.56	1 (3%) 48 48	28, 49, 64, 75	5 (17%)
15	U	96/104 (92%)	-0.59	0 100 100	26, 59, 92, 101	4 (4%)
15	u	97/104 (93%)	-0.63	0 100 100	29, 62, 83, 135	5 (5%)
16	V	137/137 (100%)	-0.67	0 100 100	24, 58, 82, 105	6 (4%)
16	v	137/137 (100%)	-0.60	0 100 100	27, 71, 104, 138	6 (4%)
17	X	38/40 (95%)	-0.31	0 100 100	35, 72, 94, 115	1 (2%)
17	x	38/40 (95%)	-0.14	0 100 100	65, 78, 119, 163	0
18	Y	29/30 (96%)	-0.06	1 (3%) 48 48	69, 85, 126, 135	0
18	y	29/30 (96%)	-0.34	0 100 100	77, 90, 111, 120	0
19	Z	62/62 (100%)	-0.33	0 100 100	67, 80, 140, 163	0
19	z	62/62 (100%)	0.05	0 100 100	80, 95, 144, 189	0
20	R	34/34 (100%)	0.56	3 (8%) 15 14	85, 109, 136, 155	0
All	All	5283/5384 (98%)	-0.51	17 (0%) 90 90	21, 58, 100, 189	979 (18%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.0
5	e	79[A]	PHE	3.6
6	f	16[A]	PHE	2.9
2	b	499	VAL	2.8
14	t	30[A]	THR	2.6
3	c	245[A]	ILE	2.4
20	R	28	VAL	2.4
5	E	4	THR	2.3
8	i	37	LEU	2.2
1	a	11	ALA	2.2
20	R	19	ALA	2.2
18	Y	18	VAL	2.1
2	B	494	GLY	2.1
3	c	20	SER	2.1
2	b	486[A]	LEU	2.0
20	R	35	LEU	2.0
9	j	1	MET	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.94	0.07	43,57,72,74	0
8	FME	I	1	10/11	0.96	0.07	61,69,76,80	0
8	FME	i	1	10/11	0.96	0.07	53,71,78,80	0
14	FME	t	1	10/11	0.96	0.07	46,50,59,77	0
12	FME	m	1	10/11	0.97	0.07	50,64,86,115	0
12	FME	M	1	10/11	0.97	0.06	48,60,93,98	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	416	6/6	0.61	0.15	77,99,109,115	0
31	LMT	F	101	35/35	0.69	0.15	101,134,184,188	0
30	UNL	j	101	10/-	0.70	0.19	75,91,107,111	0
30	UNL	A	415	28/-	0.71	0.14	89,114,133,157	0
31	LMT	B	630	35/35	0.71	0.14	65,119,149,170	0
30	UNL	a	413	30/-	0.71	0.12	91,122,144,152	0
30	UNL	J	101	10/-	0.72	0.26	74,84,93,99	0
30	UNL	m	102	10/-	0.72	0.20	72,78,95,98	0
30	UNL	I	101	40/-	0.73	0.15	72,105,157,164	0
31	LMT	A	417	35/35	0.74	0.13	67,117,141,143	0
30	UNL	K	101[A]	34/-	0.75	0.14	89,111,127,127	34
30	UNL	K	101[B]	34/-	0.75	0.14	89,111,127,127	34
31	LMT	a	415	35/35	0.75	0.13	108,136,150,161	0
30	UNL	l	101	10/-	0.76	0.17	72,84,95,97	0
36	CA	F	104	1/1	0.76	0.24	128,128,128,128	0
27	GOL	o	302	6/6	0.77	0.18	89,105,115,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	LMT	e	101	35/35	0.77	0.13	103,152,193,201	0
34	HTG	C	521	19/19	0.77	0.12	105,130,146,146	0
31	LMT	A	420	35/35	0.77	0.12	98,138,160,173	0
26	SQD	f	102	43/54	0.78	0.12	98,128,180,194	0
34	HTG	B	623	19/19	0.78	0.15	65,97,115,117	0
30	UNL	i	101	40/-	0.79	0.13	78,107,158,162	0
30	UNL	D	410	40/-	0.79	0.13	66,93,138,147	0
34	HTG	D	411	16/19	0.79	0.12	85,109,138,155	0
32	LMG	C	520	51/55	0.79	0.11	63,120,162,184	0
27	GOL	d	413	6/6	0.80	0.25	56,70,85,97	0
33	LHG	a	418[A]	42/49	0.80	0.11	99,142,159,169	42
33	LHG	a	418[B]	42/49	0.80	0.11	99,142,160,170	42
27	GOL	B	627	6/6	0.80	0.14	67,92,106,120	0
27	GOL	b	624	6/6	0.80	0.18	87,102,106,114	0
30	UNL	b	626	33/-	0.80	0.12	72,98,155,160	0
30	UNL	d	410	36/-	0.80	0.12	72,94,131,144	0
27	GOL	O	302	6/6	0.81	0.10	76,91,103,107	0
30	UNL	c	525[A]	32/-	0.81	0.14	97,116,129,140	32
30	UNL	c	525[B]	32/-	0.81	0.14	97,116,129,141	32
31	LMT	b	621	25/35	0.81	0.12	80,113,162,172	0
27	GOL	o	303	6/6	0.81	0.15	84,94,101,105	0
34	HTG	V	202	11/19	0.81	0.09	77,111,125,125	0
27	GOL	A	411	6/6	0.81	0.13	65,81,86,86	0
27	GOL	l	102[A]	6/6	0.82	0.18	70,103,107,112	6
34	HTG	c	522	19/19	0.82	0.09	111,129,143,150	0
27	GOL	l	102[B]	6/6	0.82	0.18	69,103,108,112	6
31	LMT	B	628	35/35	0.83	0.11	65,105,146,152	0
27	GOL	O	303	6/6	0.83	0.13	85,103,105,108	0
30	UNL	B	626	33/-	0.83	0.14	52,106,144,150	0
34	HTG	b	622	19/19	0.84	0.12	58,88,121,122	0
26	SQD	a	410	54/54	0.84	0.10	63,99,137,154	0
34	HTG	d	411	16/19	0.84	0.10	84,123,143,152	0
31	LMT	M	102	35/35	0.84	0.11	74,127,183,188	0
36	CA	f	103	1/1	0.84	0.13	124,124,124,124	0
31	LMT	B	631	25/35	0.85	0.12	62,89,154,167	0
34	HTG	b	623	19/19	0.85	0.10	86,126,163,167	0
29	PL9	A	414[B]	55/55	0.85	0.14	73,99,113,115	55
31	LMT	m	103	35/35	0.85	0.11	59,91,108,120	0
26	SQD	A	412	54/54	0.85	0.11	68,93,134,159	0
29	PL9	A	414[A]	55/55	0.85	0.14	73,99,113,114	55
31	LMT	b	627	25/35	0.86	0.12	60,99,146,162	0
31	LMT	t	101	26/35	0.86	0.11	72,104,148,156	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	c	527	6/6	0.86	0.18	106,114,129,130	0
32	LMG	Z	101	37/55	0.86	0.13	70,121,155,172	0
27	GOL	v	202[B]	6/6	0.87	0.13	67,80,85,87	6
32	LMG	z	101	39/55	0.87	0.12	76,128,154,167	0
27	GOL	B	629	6/6	0.87	0.13	75,77,89,98	0
27	GOL	v	202[A]	6/6	0.87	0.13	67,80,85,87	6
29	PL9	a	412[A]	55/55	0.87	0.15	89,110,123,125	55
29	PL9	a	412[B]	55/55	0.87	0.15	90,110,123,126	55
32	LMG	c	521	51/55	0.87	0.10	74,136,164,192	0
26	SQD	b	620	54/54	0.88	0.10	66,95,127,132	0
27	GOL	V	203[A]	6/6	0.88	0.12	56,66,76,77	6
27	GOL	V	203[B]	6/6	0.88	0.12	56,66,76,77	6
27	GOL	D	413	6/6	0.88	0.16	50,65,76,97	0
31	LMT	M	101	35/35	0.88	0.10	60,98,124,133	0
27	GOL	a	417	6/6	0.88	0.13	59,81,81,85	0
26	SQD	F	103	43/54	0.88	0.11	70,104,133,142	0
23	CLA	b	601	65/65	0.89	0.10	59,84,124,161	0
27	GOL	D	402	6/6	0.89	0.28	53,80,82,89	0
26	SQD	B	620	54/54	0.89	0.10	64,93,135,152	0
30	UNL	D	409	17/-	0.89	0.11	59,77,102,118	0
33	LHG	E	101[A]	42/49	0.90	0.11	76,106,119,123	42
33	LHG	E	101[B]	42/49	0.90	0.11	76,106,119,124	42
27	GOL	B	624	6/6	0.90	0.09	73,81,88,89	0
32	LMG	A	418	51/55	0.90	0.09	67,91,119,134	0
34	HTG	B	622	19/19	0.90	0.11	60,87,119,127	0
34	HTG	B	625	19/19	0.91	0.08	68,82,99,100	0
27	GOL	C	522[A]	6/6	0.91	0.09	58,61,63,72	6
27	GOL	C	522[B]	6/6	0.91	0.09	58,62,63,72	6
23	CLA	B	601	65/65	0.91	0.09	53,79,109,156	0
32	LMG	m	101	51/55	0.91	0.09	57,77,101,118	0
32	LMG	C	519	51/55	0.92	0.09	59,83,120,134	0
23	CLA	c	514	65/65	0.92	0.09	62,95,121,145	0
32	LMG	c	501	51/55	0.92	0.08	65,96,111,119	0
32	LMG	c	520	51/55	0.92	0.09	60,90,133,162	0
25	BCR	T	101	40/40	0.92	0.07	45,60,73,80	0
25	BCR	t	102	40/40	0.92	0.07	43,60,79,87	0
30	UNL	d	409	17/-	0.92	0.09	67,83,114,117	0
32	LMG	B	621	51/55	0.92	0.08	55,73,94,118	0
33	LHG	A	419[A]	49/49	0.93	0.09	50,65,85,89	49
33	LHG	A	419[B]	49/49	0.93	0.09	50,65,85,90	49
34	HTG	b	625	19/19	0.93	0.07	65,80,96,103	0
32	LMG	d	412	51/55	0.93	0.08	55,71,117,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	513	65/65	0.93	0.08	60,86,109,119	0
35	DGD	C	517[A]	62/66	0.93	0.08	51,65,110,116	62
35	DGD	C	517[B]	62/66	0.93	0.08	51,65,110,116	62
25	BCR	d	405	40/40	0.93	0.08	51,65,107,114	0
32	LMG	D	412	51/55	0.93	0.09	51,66,122,146	0
23	CLA	b	616	65/65	0.94	0.08	48,64,125,141	0
26	SQD	A	410[A]	54/54	0.94	0.08	56,80,112,118	54
26	SQD	A	410[B]	54/54	0.94	0.08	56,80,112,119	54
33	LHG	D	408[A]	49/49	0.94	0.09	49,62,111,112	49
33	LHG	D	408[B]	49/49	0.94	0.09	49,62,111,113	49
23	CLA	c	505	65/65	0.94	0.07	50,65,107,140	0
23	CLA	c	507	65/65	0.94	0.08	55,72,124,142	0
23	CLA	c	513	65/65	0.94	0.09	62,82,129,135	0
26	SQD	a	409[A]	54/54	0.94	0.09	58,83,118,125	54
26	SQD	a	409[B]	54/54	0.94	0.09	58,83,119,125	54
30	UNL	X	101	18/-	0.94	0.11	63,74,107,110	0
23	CLA	C	504	65/65	0.94	0.08	39,58,107,136	0
23	CLA	d	404	65/65	0.94	0.09	50,67,120,154	0
25	BCR	B	619	40/40	0.94	0.08	48,60,92,98	0
25	BCR	C	514	40/40	0.94	0.07	55,76,88,94	0
25	BCR	D	405	40/40	0.94	0.08	46,62,103,107	0
25	BCR	H	101	40/40	0.94	0.08	49,66,82,87	0
25	BCR	K	102	40/40	0.94	0.09	58,67,79,84	0
23	CLA	C	506	65/65	0.94	0.08	57,71,122,143	0
25	BCR	Y	101	40/40	0.94	0.08	53,66,81,88	0
29	PL9	D	406[A]	55/55	0.94	0.07	39,50,60,73	55
29	PL9	D	406[B]	55/55	0.94	0.07	39,50,60,73	55
35	DGD	c	517[A]	62/66	0.94	0.07	50,65,99,107	62
35	DGD	c	517[B]	62/66	0.94	0.07	50,65,100,107	62
35	DGD	c	518[A]	62/66	0.94	0.07	53,68,119,132	62
35	DGD	c	518[B]	62/66	0.94	0.07	53,68,119,133	62
35	DGD	c	519	62/66	0.94	0.07	51,68,101,132	0
25	BCR	c	515	40/40	0.94	0.08	68,80,93,96	0
23	CLA	b	614	65/65	0.94	0.07	42,51,101,119	0
36	CA	o	301	1/1	0.94	0.05	104,104,104,104	0
25	BCR	A	409	40/40	0.95	0.07	40,52,65,71	0
25	BCR	B	618	40/40	0.95	0.06	44,57,74,83	0
23	CLA	B	606	65/65	0.95	0.08	44,59,106,130	0
23	CLA	D	404	65/65	0.95	0.08	48,60,122,143	0
23	CLA	a	405[A]	65/65	0.95	0.07	42,54,121,135	65
23	CLA	a	405[B]	65/65	0.95	0.07	42,54,121,135	65
23	CLA	a	407	65/65	0.95	0.10	45,58,147,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	LHG	b	629[A]	49/49	0.95	0.08	50,59,71,93	49
33	LHG	b	629[B]	49/49	0.95	0.08	50,59,71,94	49
33	LHG	d	408[A]	49/49	0.95	0.08	52,65,110,124	49
33	LHG	d	408[B]	49/49	0.95	0.08	52,65,110,124	49
33	LHG	d	414[A]	49/49	0.95	0.09	55,68,80,91	49
33	LHG	d	414[B]	49/49	0.95	0.09	55,69,80,91	49
23	CLA	B	611	65/65	0.95	0.07	38,47,67,77	0
29	PL9	d	406[A]	55/55	0.95	0.07	42,52,62,71	55
29	PL9	d	406[B]	55/55	0.95	0.07	42,53,62,71	55
23	CLA	b	606	65/65	0.95	0.07	45,60,112,121	0
25	BCR	a	408	40/40	0.95	0.06	46,55,66,71	0
25	BCR	b	618	40/40	0.95	0.06	45,58,78,85	0
25	BCR	b	619	40/40	0.95	0.07	50,66,88,92	0
23	CLA	b	612	65/65	0.95	0.08	42,54,66,75	0
23	CLA	B	614	65/65	0.95	0.07	41,50,106,118	0
25	BCR	h	101	40/40	0.95	0.08	57,70,91,98	0
23	CLA	B	616	65/65	0.95	0.09	46,60,132,143	0
35	DGD	C	516[A]	62/66	0.95	0.07	48,59,99,107	62
35	DGD	C	516[B]	62/66	0.95	0.07	48,59,99,107	62
25	BCR	y	101	40/40	0.95	0.07	59,71,85,102	0
23	CLA	C	501	65/65	0.95	0.07	49,61,72,80	0
35	DGD	C	518	62/66	0.95	0.07	46,62,94,114	0
35	DGD	H	102	62/66	0.95	0.09	46,61,80,94	0
27	GOL	c	526[A]	6/6	0.95	0.08	66,69,73,74	6
27	GOL	c	526[B]	6/6	0.95	0.08	66,69,73,74	6
23	CLA	A	408	65/65	0.95	0.08	43,53,132,147	0
23	CLA	c	508	65/65	0.95	0.08	54,69,86,92	0
23	CLA	c	509	65/65	0.95	0.07	47,63,123,148	0
35	DGD	h	102	62/66	0.95	0.08	52,66,82,87	0
23	CLA	B	603	65/65	0.95	0.08	45,53,72,83	0
23	CLA	C	508	65/65	0.95	0.07	47,56,111,146	0
23	CLA	C	512	65/65	0.95	0.08	57,74,115,133	0
37	BCT	d	401[A]	4/4	0.95	0.07	59,63,67,79	4
37	BCT	d	401[B]	4/4	0.95	0.07	59,64,67,80	4
33	LHG	L	101[A]	49/49	0.96	0.07	50,58,71,92	49
33	LHG	L	101[B]	49/49	0.96	0.07	49,58,71,92	49
27	GOL	b	628	6/6	0.96	0.07	78,86,89,89	0
23	CLA	b	611	65/65	0.96	0.06	39,50,72,82	0
23	CLA	C	503	65/65	0.96	0.06	51,61,72,78	0
30	UNL	x	101	18/-	0.96	0.10	72,82,136,137	0
33	LHG	d	407[A]	49/49	0.96	0.07	49,57,71,77	49
33	LHG	d	407[B]	49/49	0.96	0.07	49,57,72,78	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	602	65/65	0.96	0.07	45,57,73,89	0
25	BCR	c	516	40/40	0.96	0.07	55,67,77,93	0
23	CLA	C	505	65/65	0.96	0.07	48,60,89,106	0
23	CLA	c	502	65/65	0.96	0.07	56,68,81,89	0
25	BCR	k	101	40/40	0.96	0.08	56,74,87,91	0
23	CLA	c	504	65/65	0.96	0.06	51,71,84,98	0
23	CLA	A	405[A]	65/65	0.96	0.06	38,45,56,70	65
23	CLA	c	506	65/65	0.96	0.07	49,65,91,99	0
23	CLA	C	507	65/65	0.96	0.07	49,64,82,96	0
23	CLA	A	405[B]	65/65	0.96	0.06	37,45,56,70	65
23	CLA	C	509	65/65	0.96	0.08	46,60,85,93	0
23	CLA	c	512	65/65	0.96	0.07	57,68,88,104	0
23	CLA	B	607	65/65	0.96	0.06	36,49,73,84	0
23	CLA	B	609	65/65	0.96	0.07	43,59,71,80	0
23	CLA	B	610	65/65	0.96	0.08	43,56,67,85	0
24	PHO	A	416[A]	64/64	0.96	0.06	39,51,57,64	64
24	PHO	A	416[B]	64/64	0.96	0.06	38,51,57,65	64
24	PHO	a	414[A]	64/64	0.96	0.06	45,55,62,67	64
24	PHO	a	414[B]	64/64	0.96	0.06	45,55,62,67	64
23	CLA	A	406[A]	65/65	0.96	0.06	41,48,114,126	65
25	BCR	B	617	40/40	0.96	0.06	42,53,64,66	0
23	CLA	B	613	65/65	0.96	0.06	40,47,94,117	0
23	CLA	A	406[B]	65/65	0.96	0.06	41,48,114,126	65
23	CLA	A	404[A]	65/65	0.96	0.06	37,44,62,70	65
25	BCR	C	515	40/40	0.96	0.06	50,65,76,85	0
23	CLA	b	602	65/65	0.96	0.07	48,60,80,86	0
23	CLA	b	603	65/65	0.96	0.06	45,57,81,98	0
23	CLA	b	604	65/65	0.96	0.07	39,52,101,120	0
36	CA	c	523	1/1	0.96	0.07	75,75,75,75	0
23	CLA	A	404[B]	65/65	0.96	0.06	37,44,63,70	65
23	CLA	b	607	65/65	0.96	0.07	38,49,81,92	0
23	CLA	b	609	65/65	0.96	0.06	47,65,78,89	0
25	BCR	b	617	40/40	0.96	0.06	46,55,65,68	0
23	CLA	d	402[A]	65/65	0.97	0.05	40,45,63,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	40,45,64,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	39,47,77,91	65
23	CLA	d	403[B]	65/65	0.97	0.06	39,47,77,91	65
22	CL	A	403[A]	1/1	0.97	0.03	47,47,47,47	1
24	PHO	A	407[A]	64/64	0.97	0.05	38,47,55,57	64
24	PHO	A	407[B]	64/64	0.97	0.05	38,47,55,57	64
23	CLA	b	605	65/65	0.97	0.07	39,51,72,81	0
23	CLA	B	612	65/65	0.97	0.06	37,50,64,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PHO	a	406[A]	64/64	0.97	0.05	44,50,54,57	64
24	PHO	a	406[B]	64/64	0.97	0.05	44,50,54,58	64
22	CL	A	403[B]	1/1	0.97	0.03	47,47,47,47	1
23	CLA	b	608	65/65	0.97	0.05	43,57,78,91	0
23	CLA	C	510	65/65	0.97	0.06	46,60,82,88	0
23	CLA	b	610	65/65	0.97	0.07	49,58,69,74	0
23	CLA	C	511	65/65	0.97	0.07	49,65,83,87	0
23	CLA	B	604	65/65	0.97	0.06	38,48,111,141	0
23	CLA	b	613	65/65	0.97	0.06	42,50,90,102	0
23	CLA	B	615	65/65	0.97	0.06	43,54,80,90	0
23	CLA	b	615	65/65	0.97	0.06	46,59,79,92	0
23	CLA	D	403[A]	65/65	0.97	0.06	34,44,71,78	65
23	CLA	D	403[B]	65/65	0.97	0.06	34,44,72,79	65
23	CLA	c	503	65/65	0.97	0.06	44,59,89,106	0
23	CLA	B	605	65/65	0.97	0.06	40,49,66,84	0
23	CLA	a	404[A]	65/65	0.97	0.06	39,48,64,75	65
33	LHG	D	407[A]	49/49	0.97	0.07	48,56,68,81	49
33	LHG	D	407[B]	49/49	0.97	0.07	47,56,68,81	49
23	CLA	a	404[B]	65/65	0.97	0.06	39,48,65,75	65
22	CL	a	403[A]	1/1	0.97	0.08	52,52,52,52	1
23	CLA	C	502	65/65	0.97	0.06	45,56,83,92	0
36	CA	C	523	1/1	0.97	0.06	75,75,75,75	0
22	CL	a	403[B]	1/1	0.97	0.08	52,52,52,52	1
36	CA	O	301	1/1	0.97	0.04	105,105,105,105	0
23	CLA	c	510	65/65	0.97	0.07	47,63,88,100	0
23	CLA	c	511	65/65	0.97	0.06	51,65,80,93	0
23	CLA	B	608	65/65	0.97	0.05	43,51,71,83	0
37	BCT	D	401[A]	4/4	0.97	0.06	55,60,61,68	4
37	BCT	D	401[B]	4/4	0.97	0.06	55,57,62,72	4
22	CL	A	402[A]	1/1	0.97	0.06	44,44,44,44	1
22	CL	A	402[B]	1/1	0.97	0.06	44,44,44,44	1
22	CL	a	402[B]	1/1	0.98	0.05	50,50,50,50	1
22	CL	a	402[A]	1/1	0.98	0.05	50,50,50,50	1
38	HEM	f	101	43/43	0.98	0.08	61,82,118,133	0
39	MG	J	102	1/1	0.98	0.04	59,59,59,59	0
40	HEC	V	201	43/43	0.98	0.06	39,50,58,63	0
40	HEC	v	201	43/43	0.98	0.07	52,63,72,74	0
21	FE2	a	401[B]	1/1	0.99	0.02	55,55,55,55	1
38	HEM	F	102	43/43	0.99	0.06	55,69,84,89	0
28	OEX	A	413[A]	10/10	0.99	0.03	40,44,50,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	40,44,50,51	10
39	MG	j	102	1/1	0.99	0.07	63,63,63,63	0

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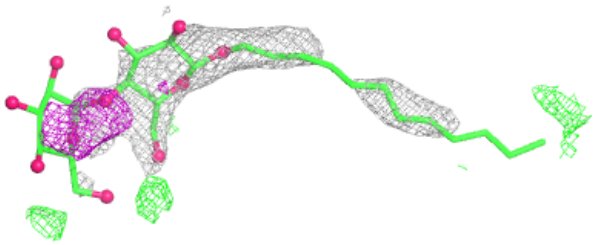
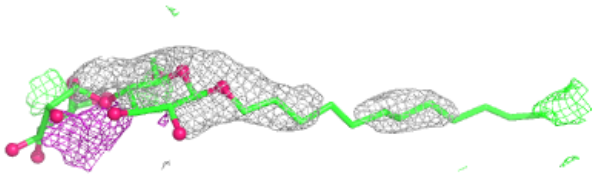
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	a	401[A]	1/1	0.99	0.02	55,55,55,55	1
36	CA	c	524	1/1	0.99	0.04	77,77,77,77	0
28	OEX	a	411[A]	10/10	1.00	0.02	46,49,51,56	10
28	OEX	a	411[B]	10/10	1.00	0.02	46,50,54,56	10
21	FE2	A	401[A]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	A	401[B]	1/1	1.00	0.01	52,52,52,52	1

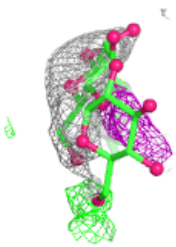
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

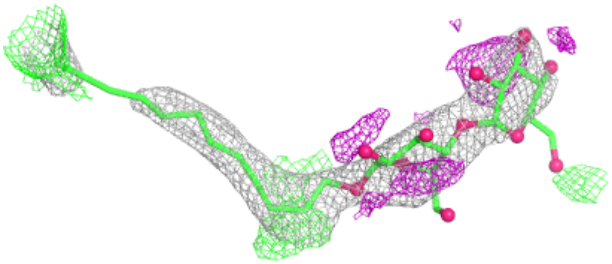


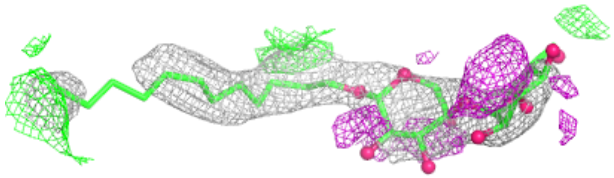


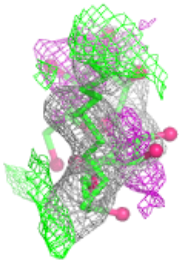


Electron density around LMT B 630:

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

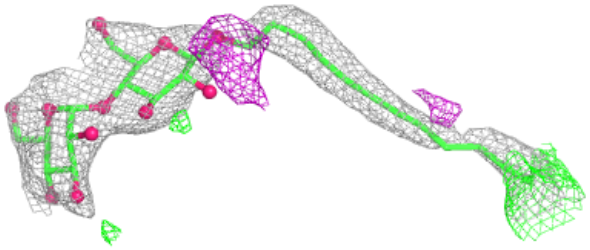


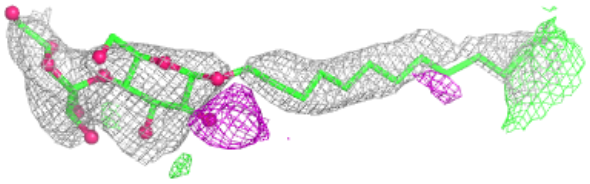


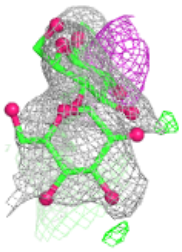


Electron density around LMT A 417:

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

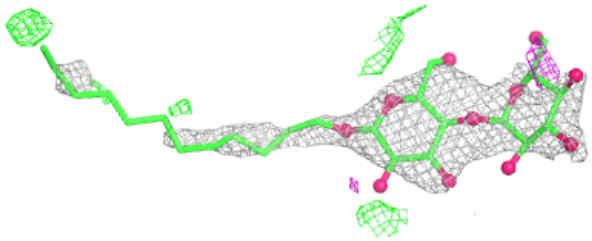


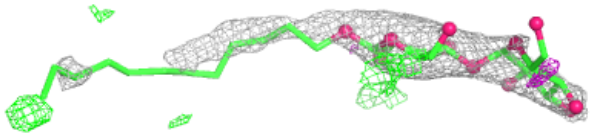


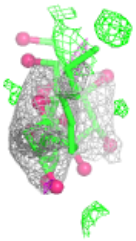


Electron density around LMT a 415:

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

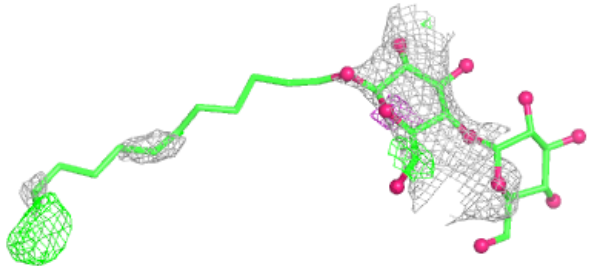


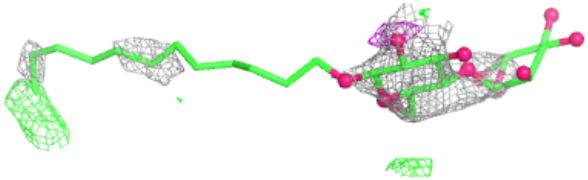


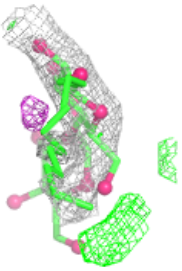


Electron density around LMT e 101:

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

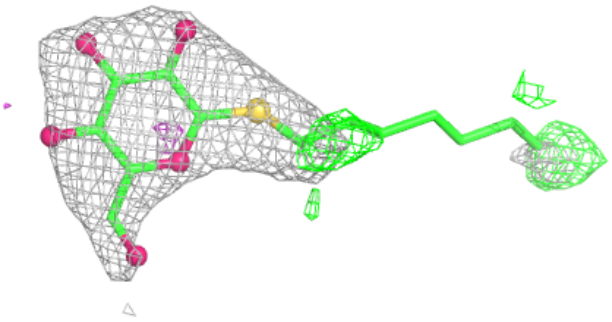


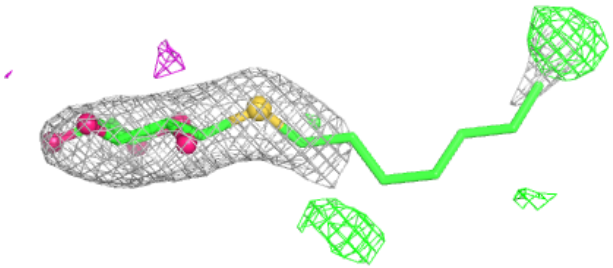


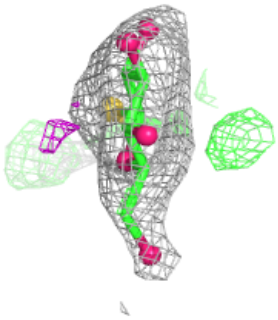


Electron density around HTG C 521:

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

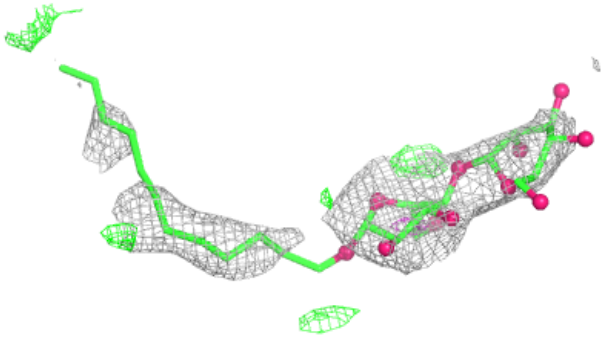


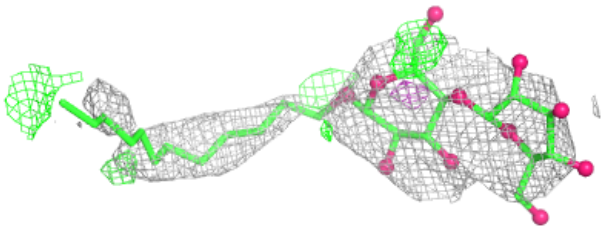


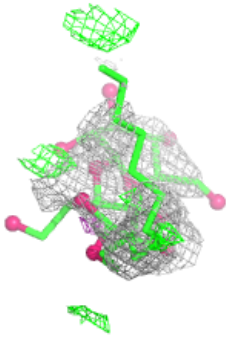


Electron density around LMT A 420:

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

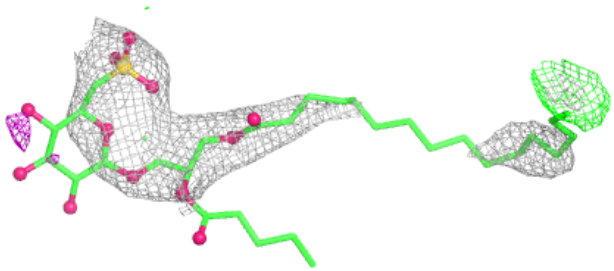


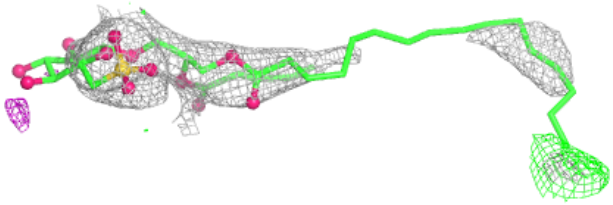


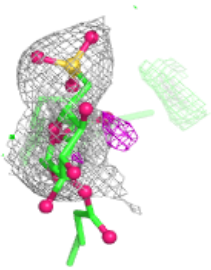


Electron density around SQD f 102:

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

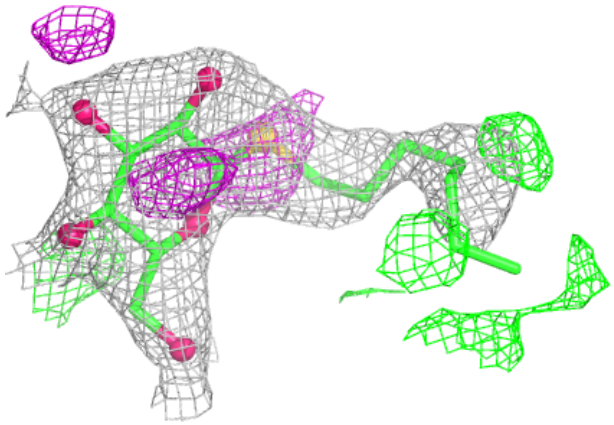


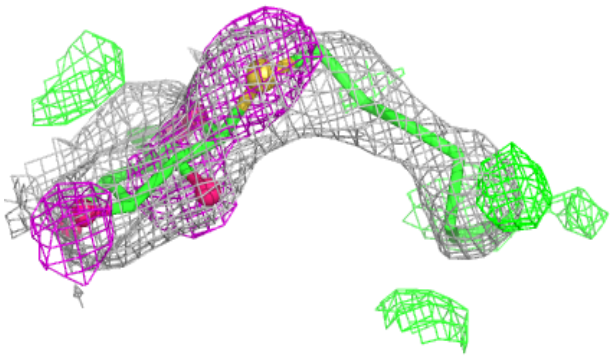


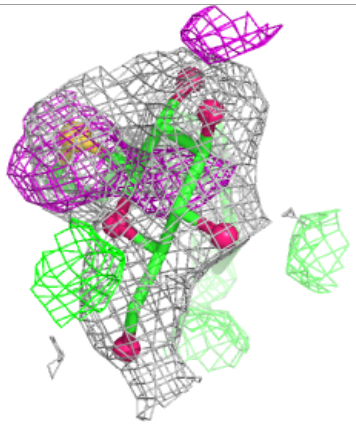


Electron density around HTG B 623:

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

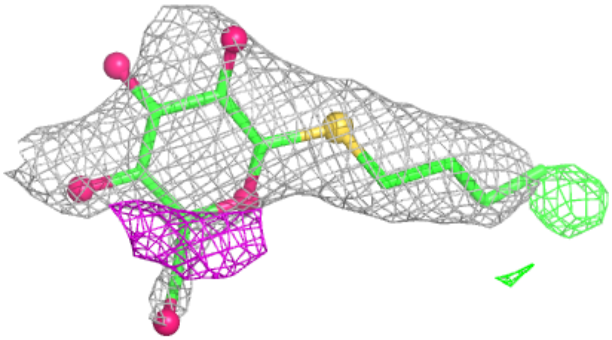


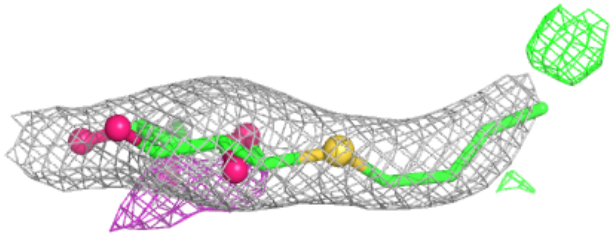


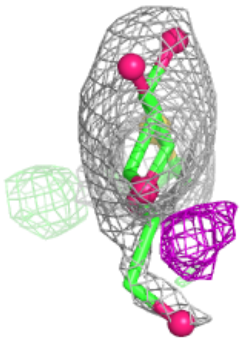


Electron density around HTG D 411:

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

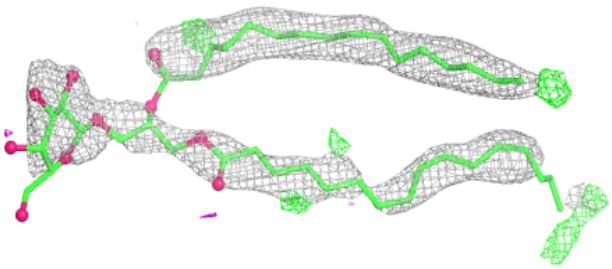


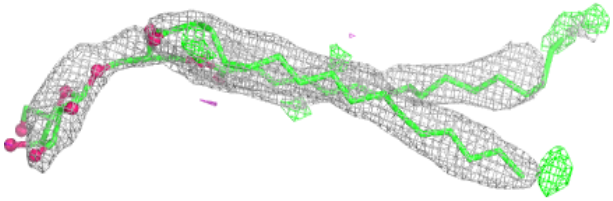


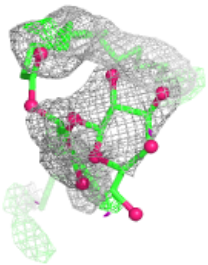


Electron density around LMG C 520:

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

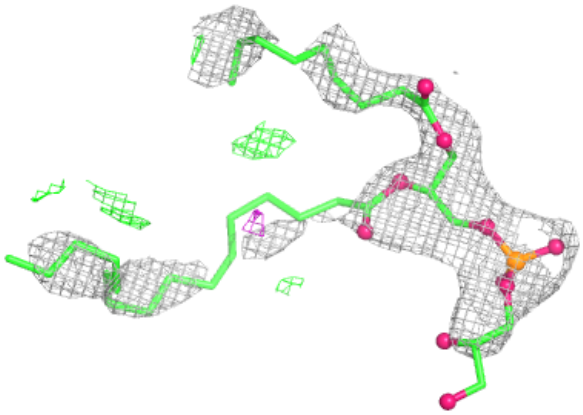


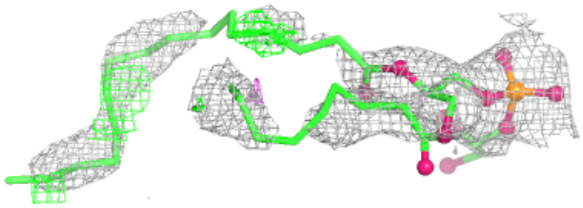


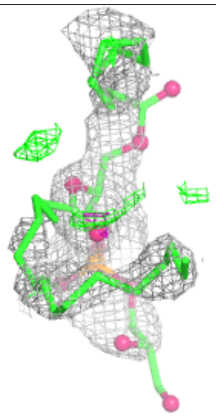


Electron density around LHG a 418 (A):

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

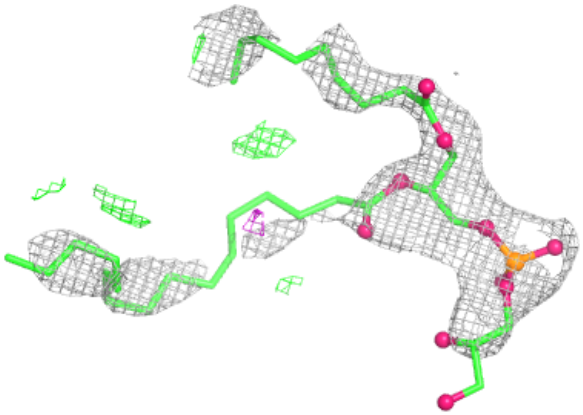


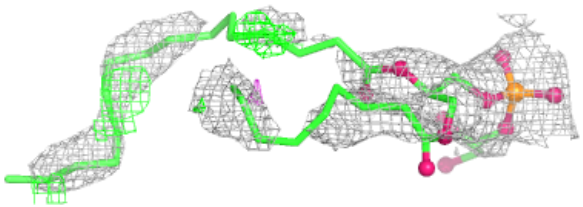


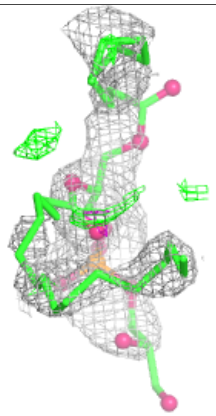


Electron density around LHG a 418 (B):

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

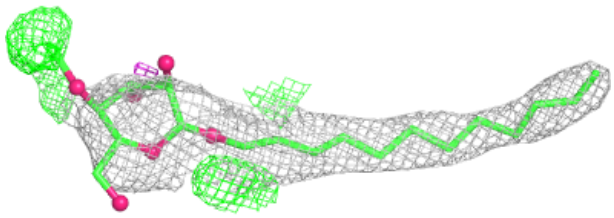


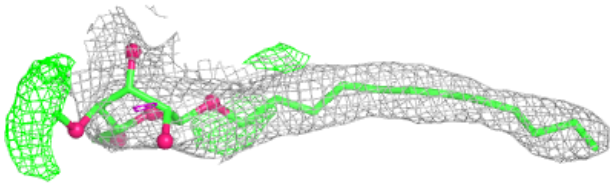


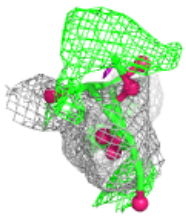


Electron density around LMT b 621:

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

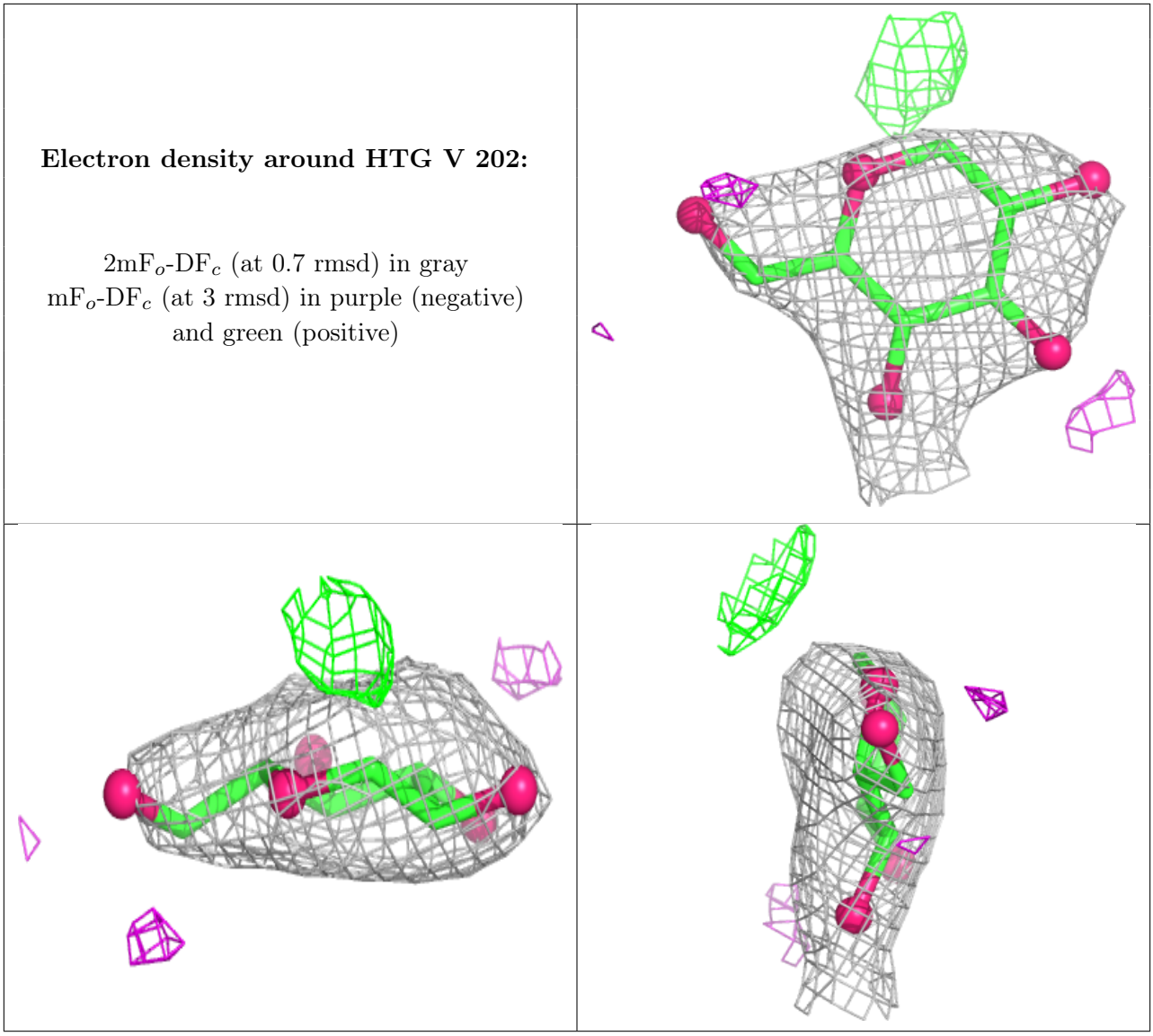






Electron density around HTG V 202:

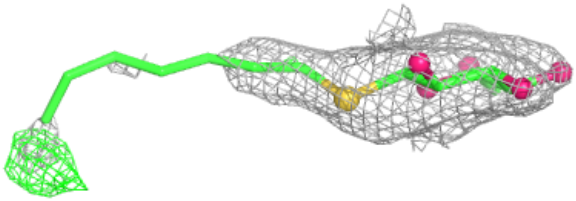
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

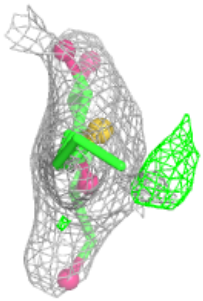


Electron density around HTG c 522:

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

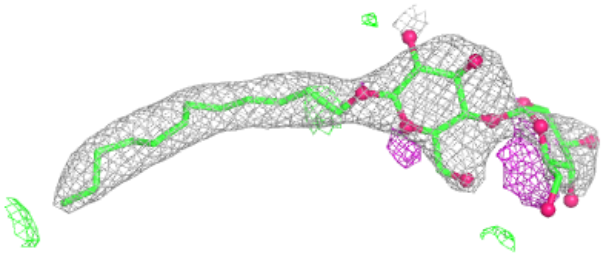


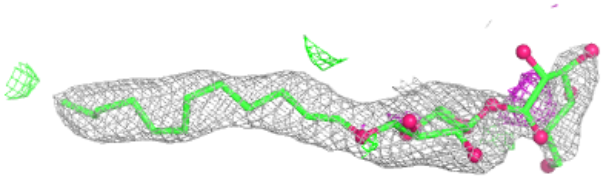


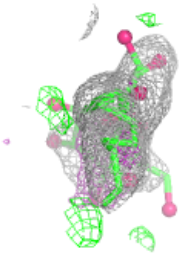


Electron density around LMT B 628:

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

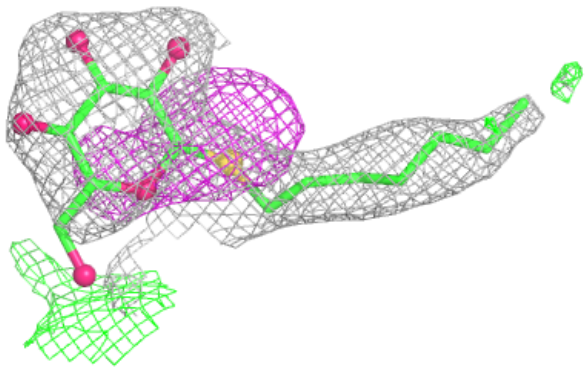


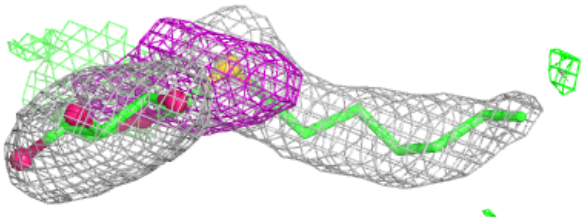


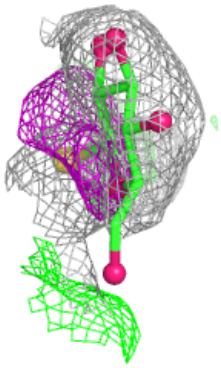


Electron density around HTG b 622:

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

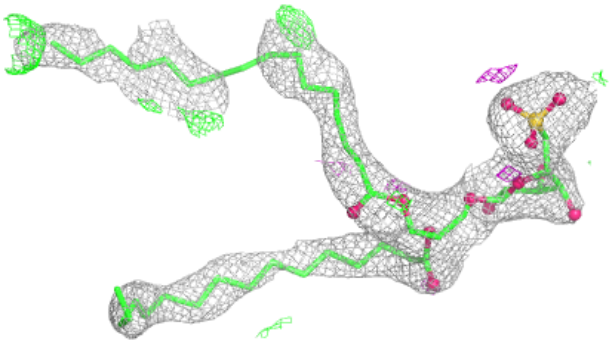


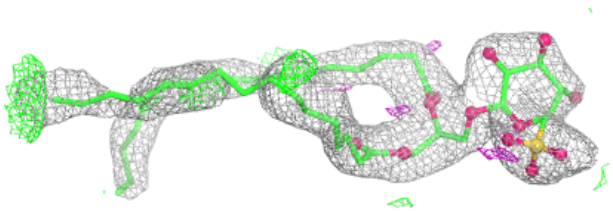


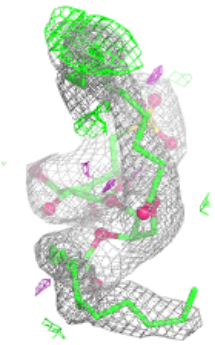


Electron density around SQD a 410:

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

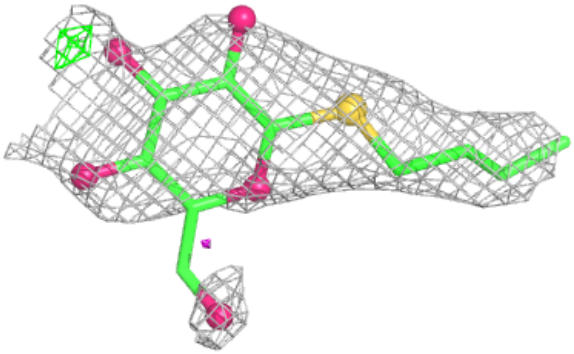


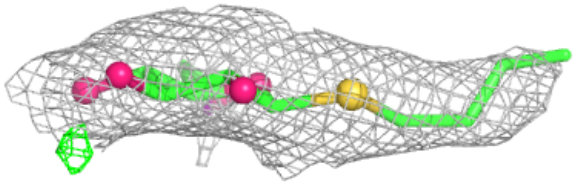


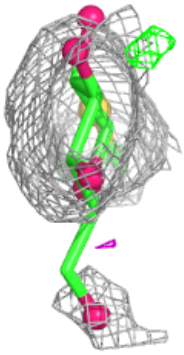


Electron density around HTG d 411:

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

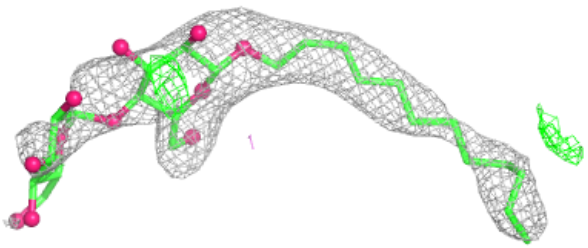


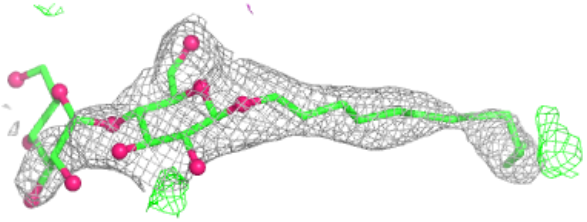


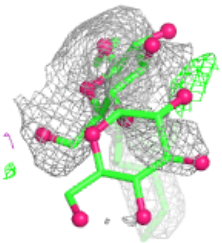


Electron density around LMT M 102:

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

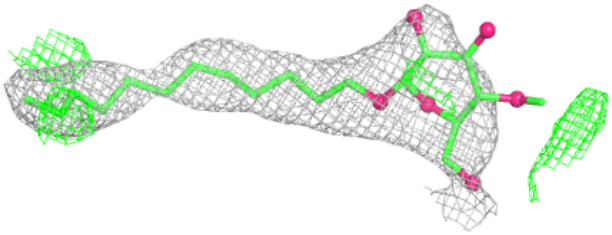


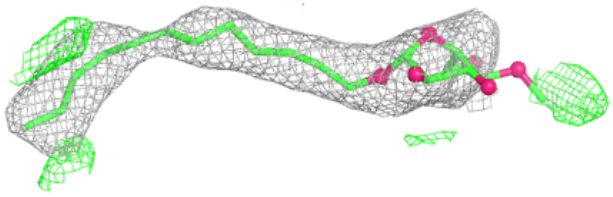


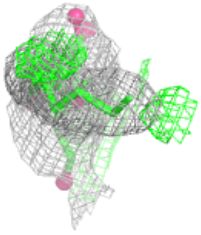


Electron density around LMT B 631:

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

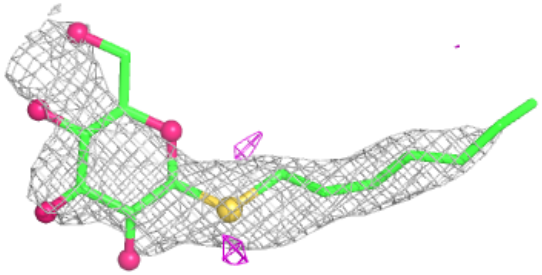


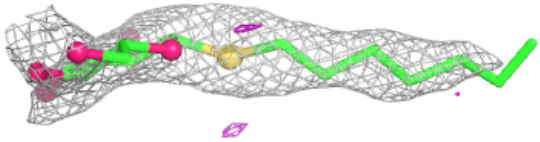


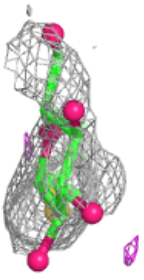


Electron density around HTG b 623:

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

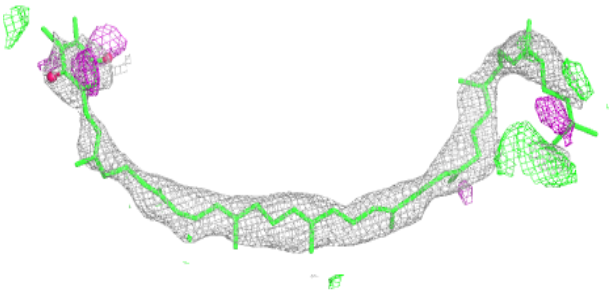


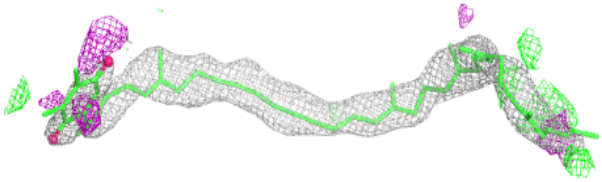


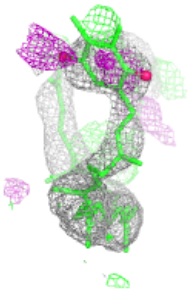


Electron density around PL9 A 414 (B):

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

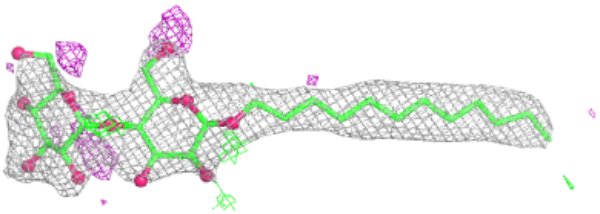


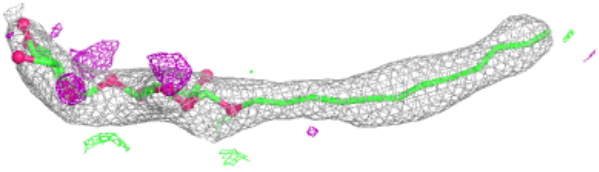


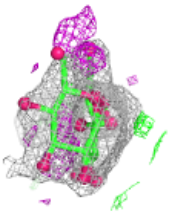


Electron density around LMT m 103:

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

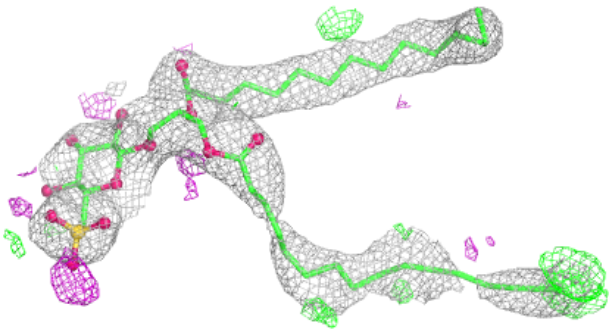


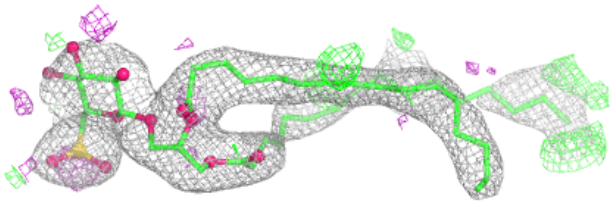


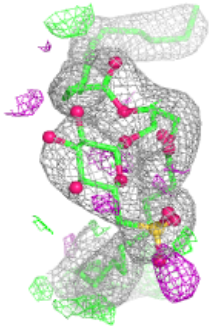


Electron density around SQD A 412:

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

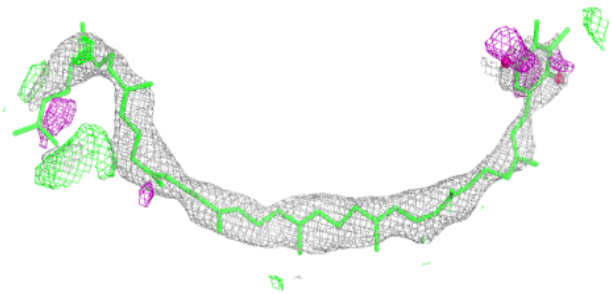


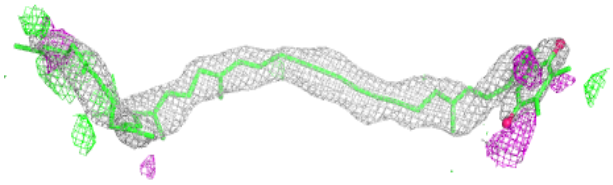


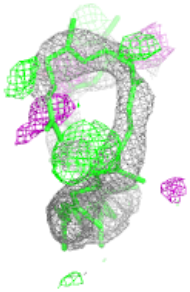


Electron density around PL9 A 414 (A):

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

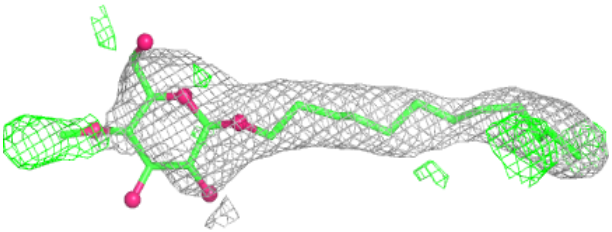


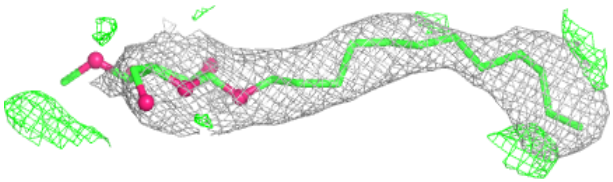


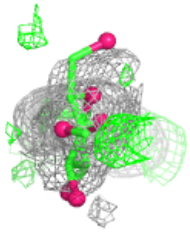


Electron density around LMT b 627:

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

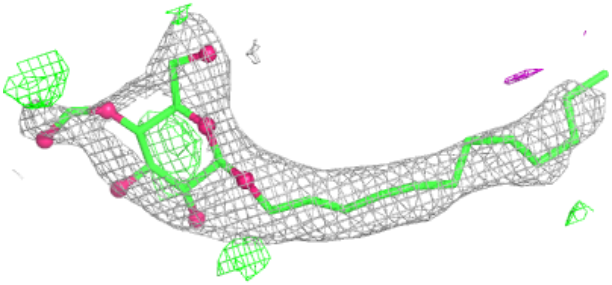


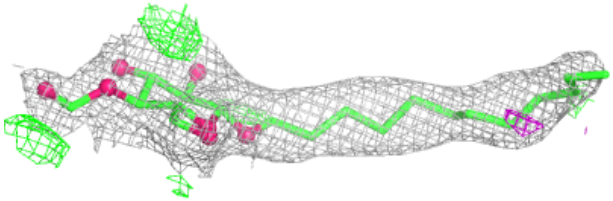


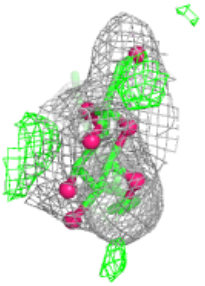


Electron density around LMT t 101:

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

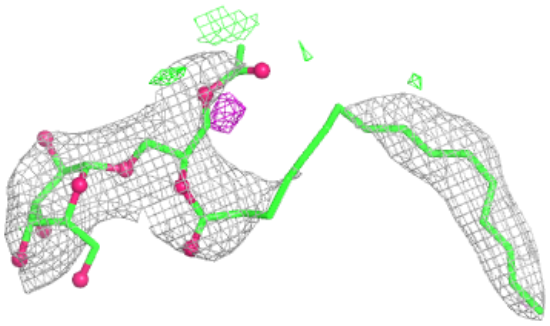


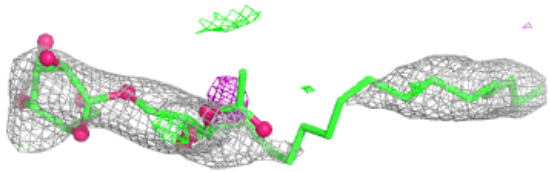


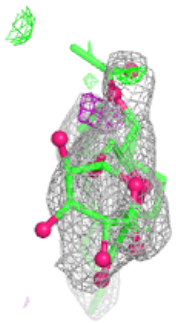


Electron density around LMG Z 101:

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

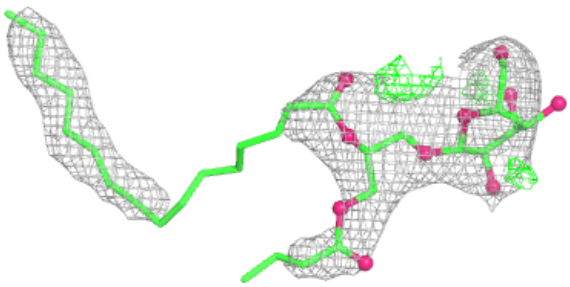


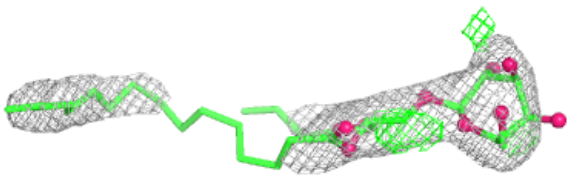


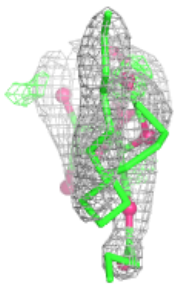


Electron density around LMG z 101:

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

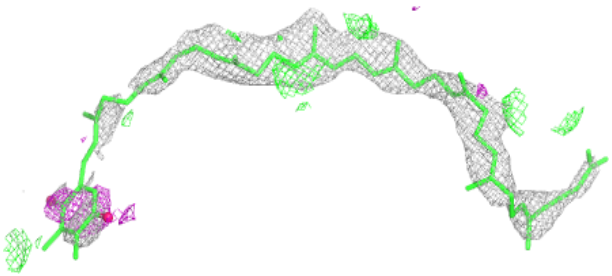


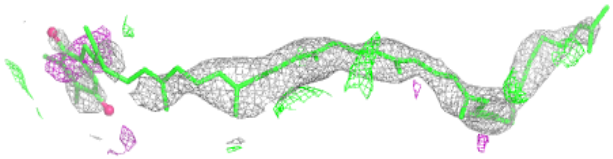


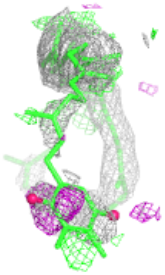


Electron density around PL9 a 412 (A):

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

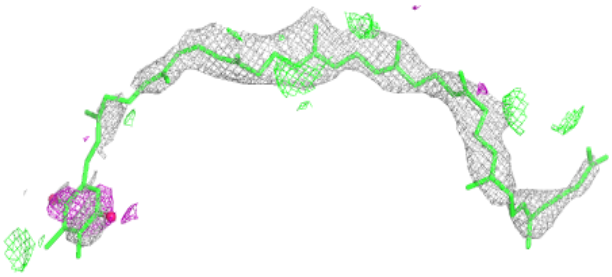


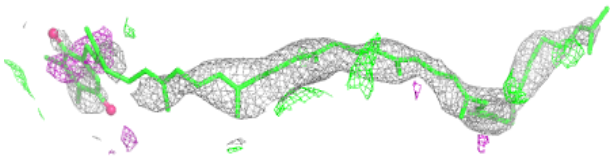


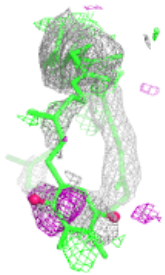


Electron density around PL9 a 412 (B):

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

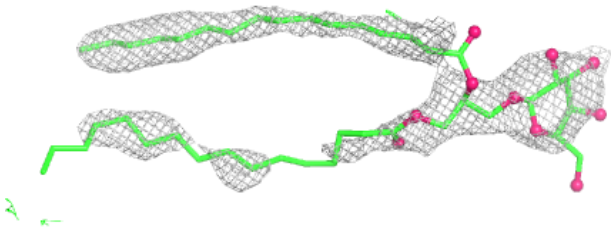


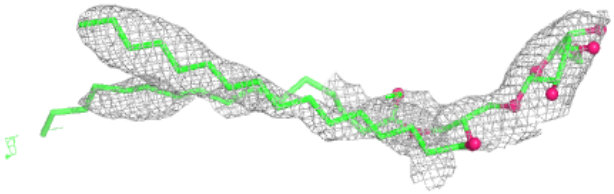


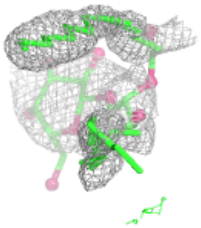


Electron density around LMG c 521:

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

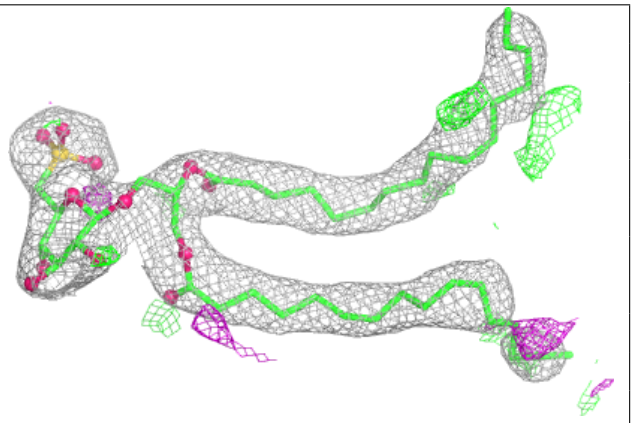


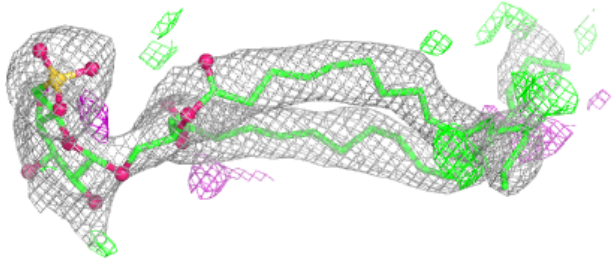


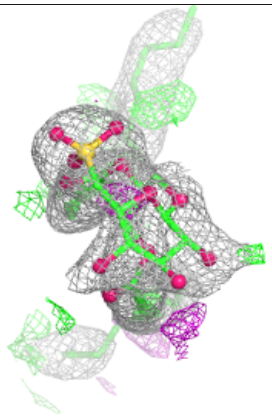


Electron density around SQD b 620:

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

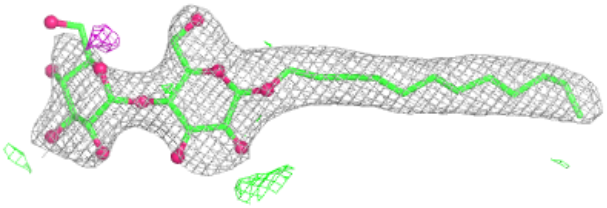


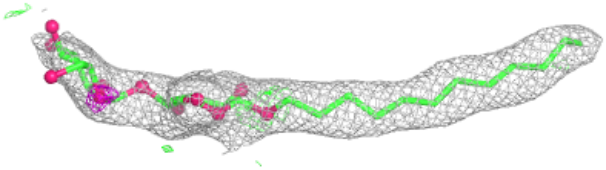




Electron density around LMT M 101:

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

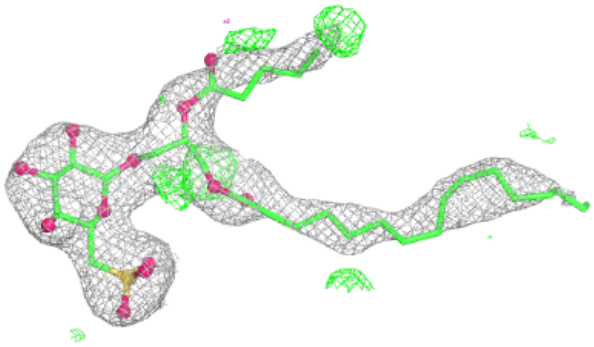


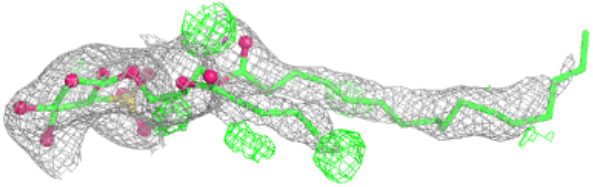


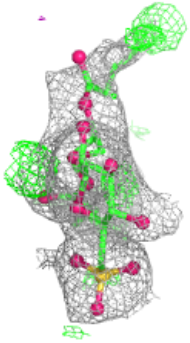


Electron density around SQD F 103:

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

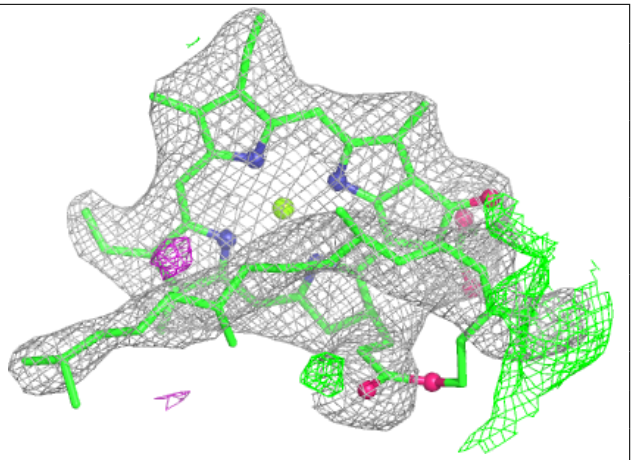


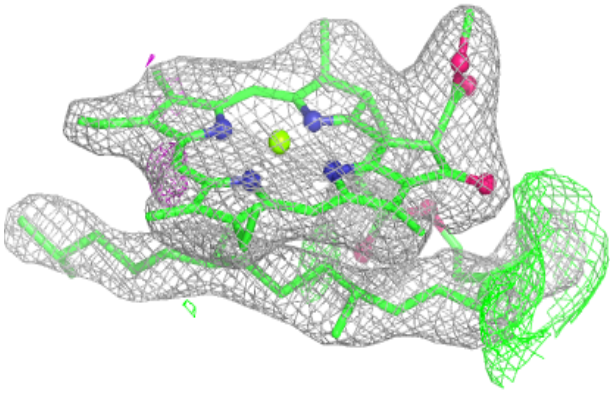


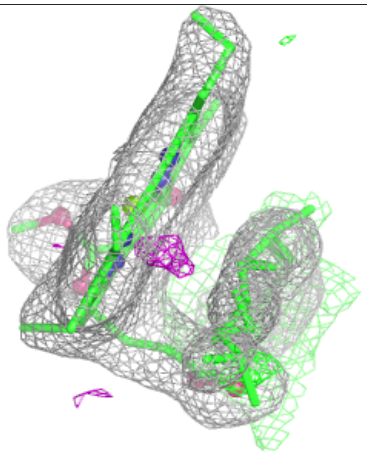


Electron density around CLA b 601:

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

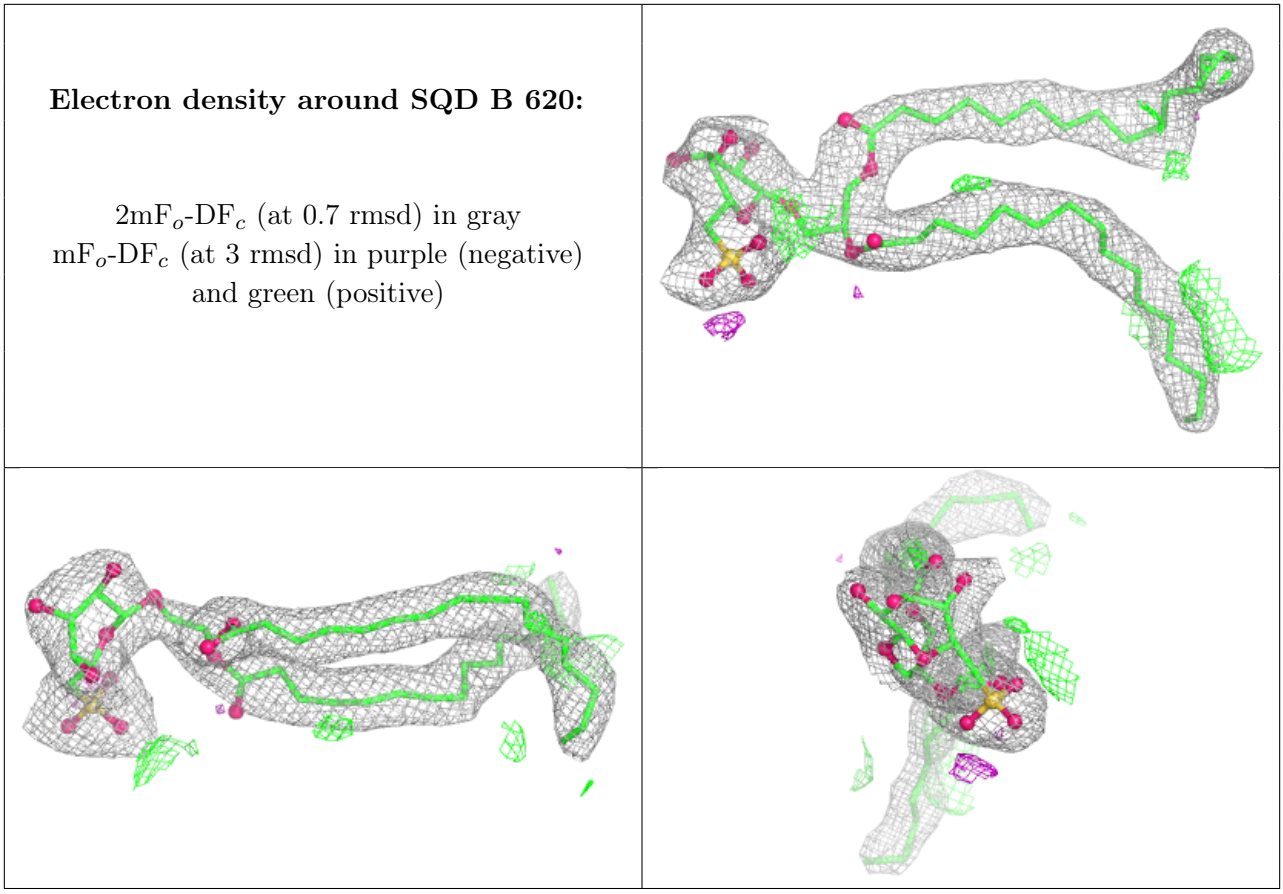






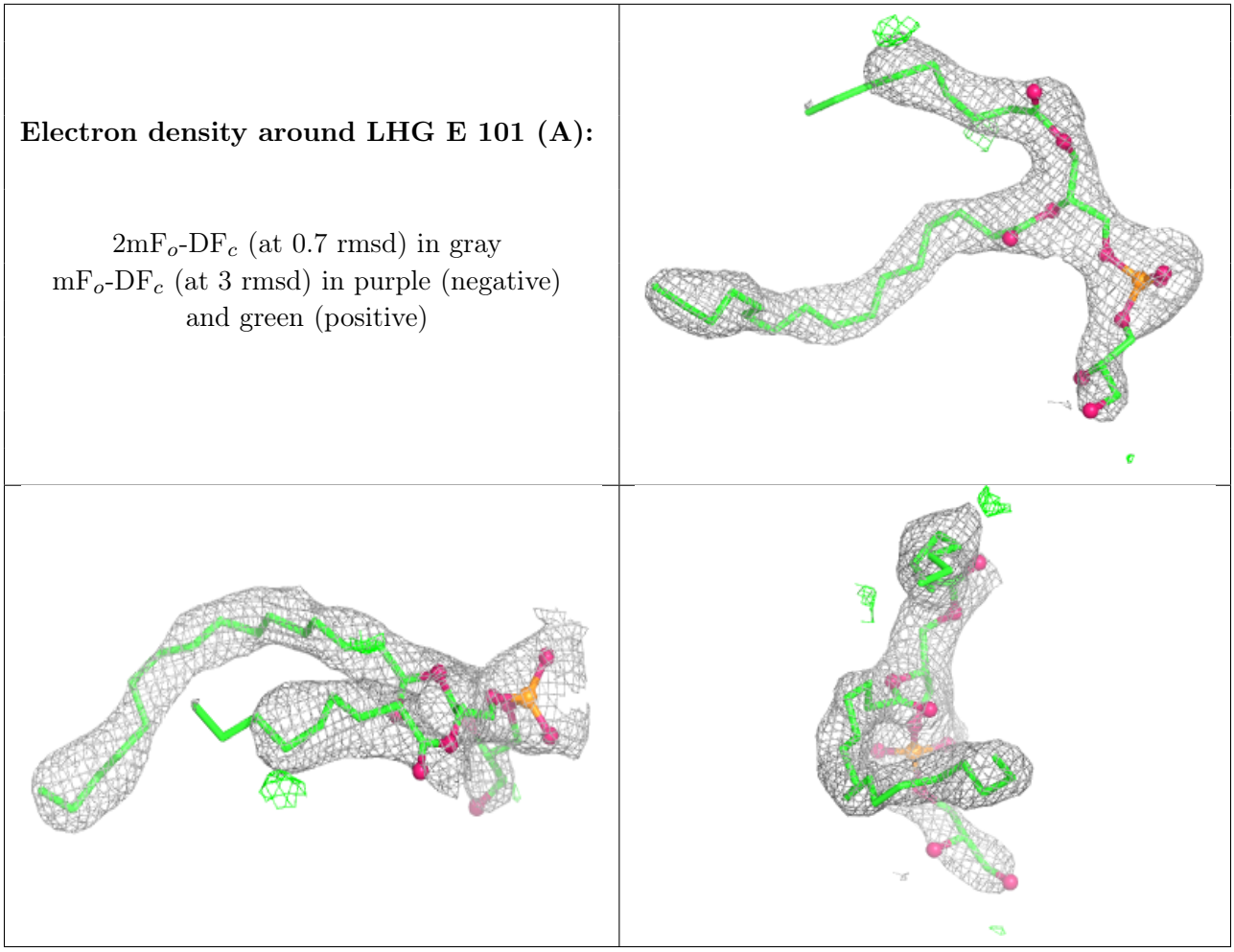
Electron density around SQD B 620:

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



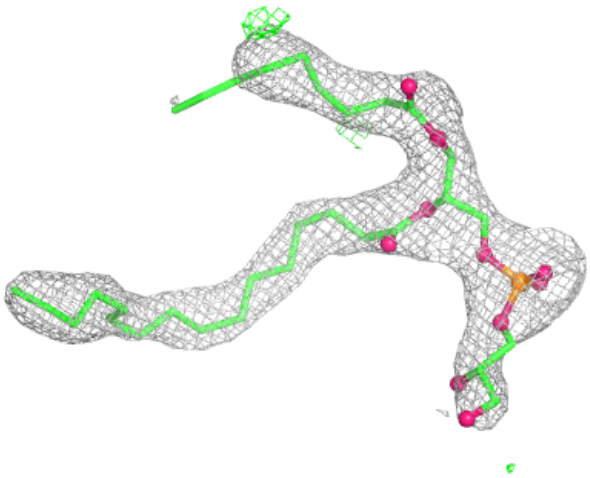
Electron density around LHG E 101 (A):

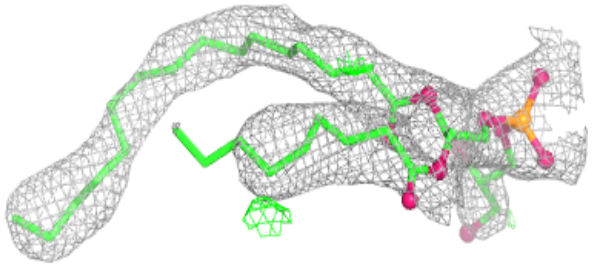
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

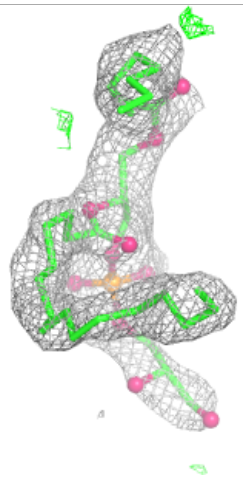


Electron density around LHG E 101 (B):

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

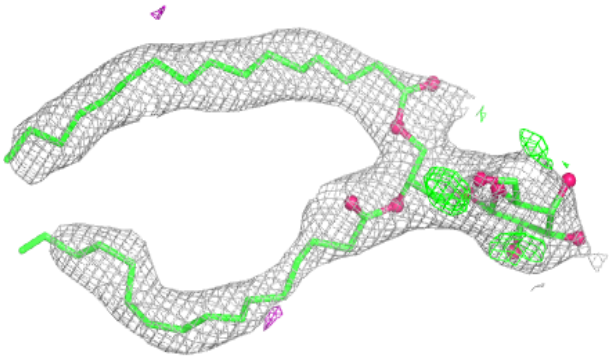


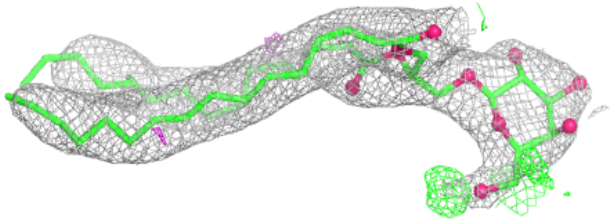


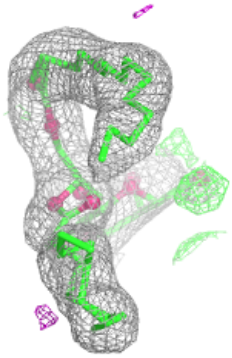


Electron density around LMG A 418:

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

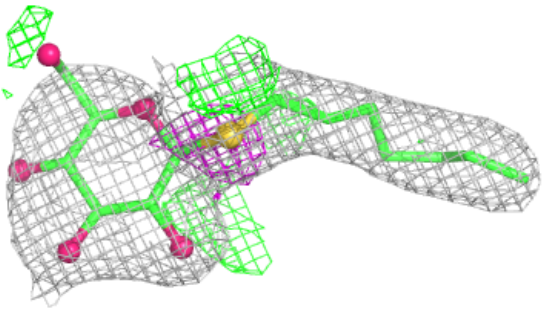


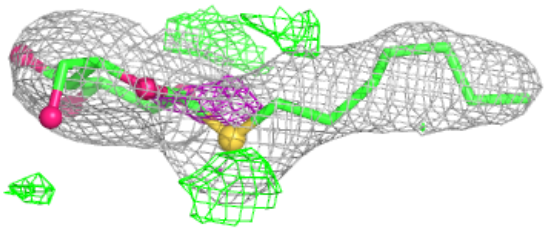


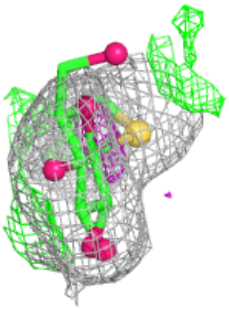


Electron density around HTG B 622:

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

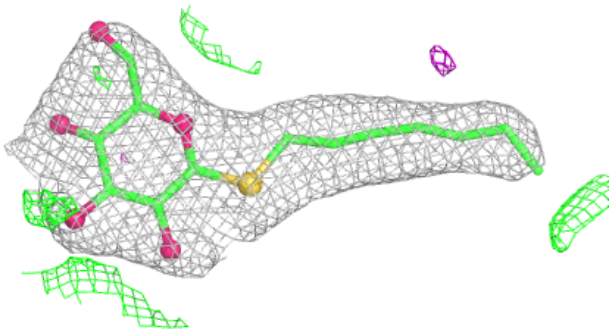


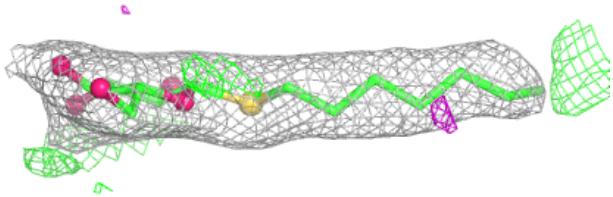


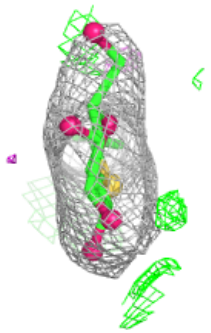


Electron density around HTG B 625:

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

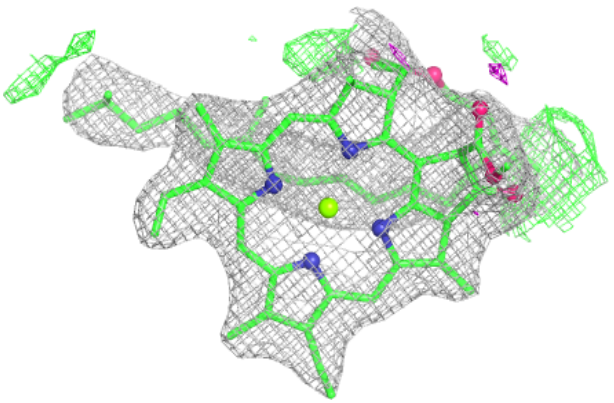


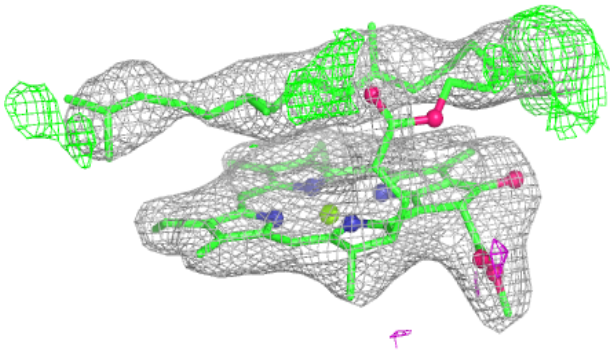


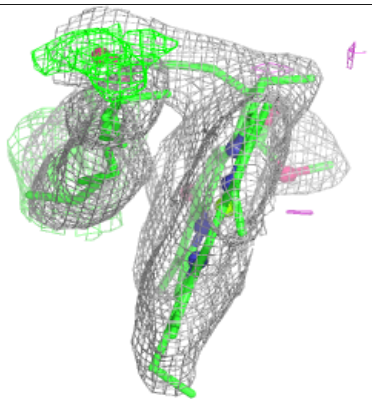


Electron density around CLA B 601:

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

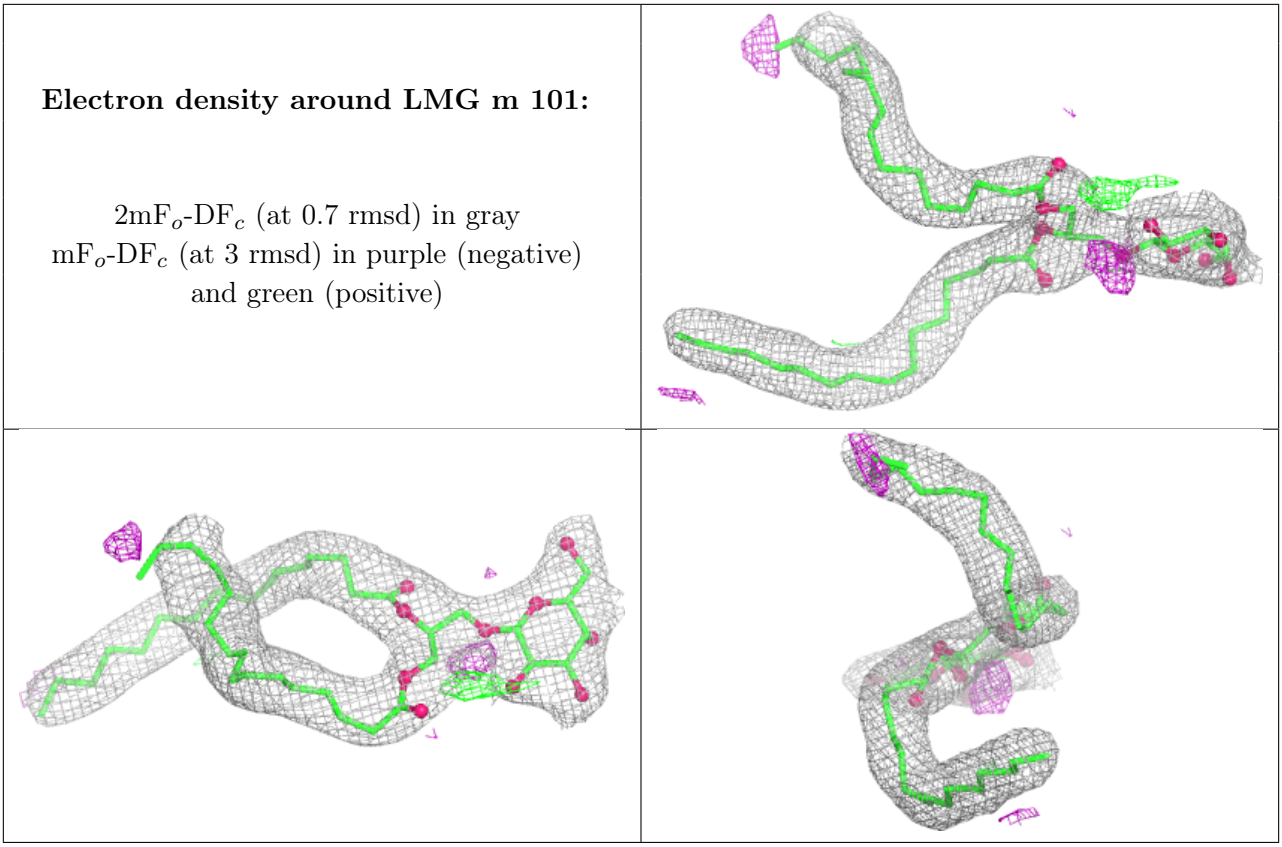






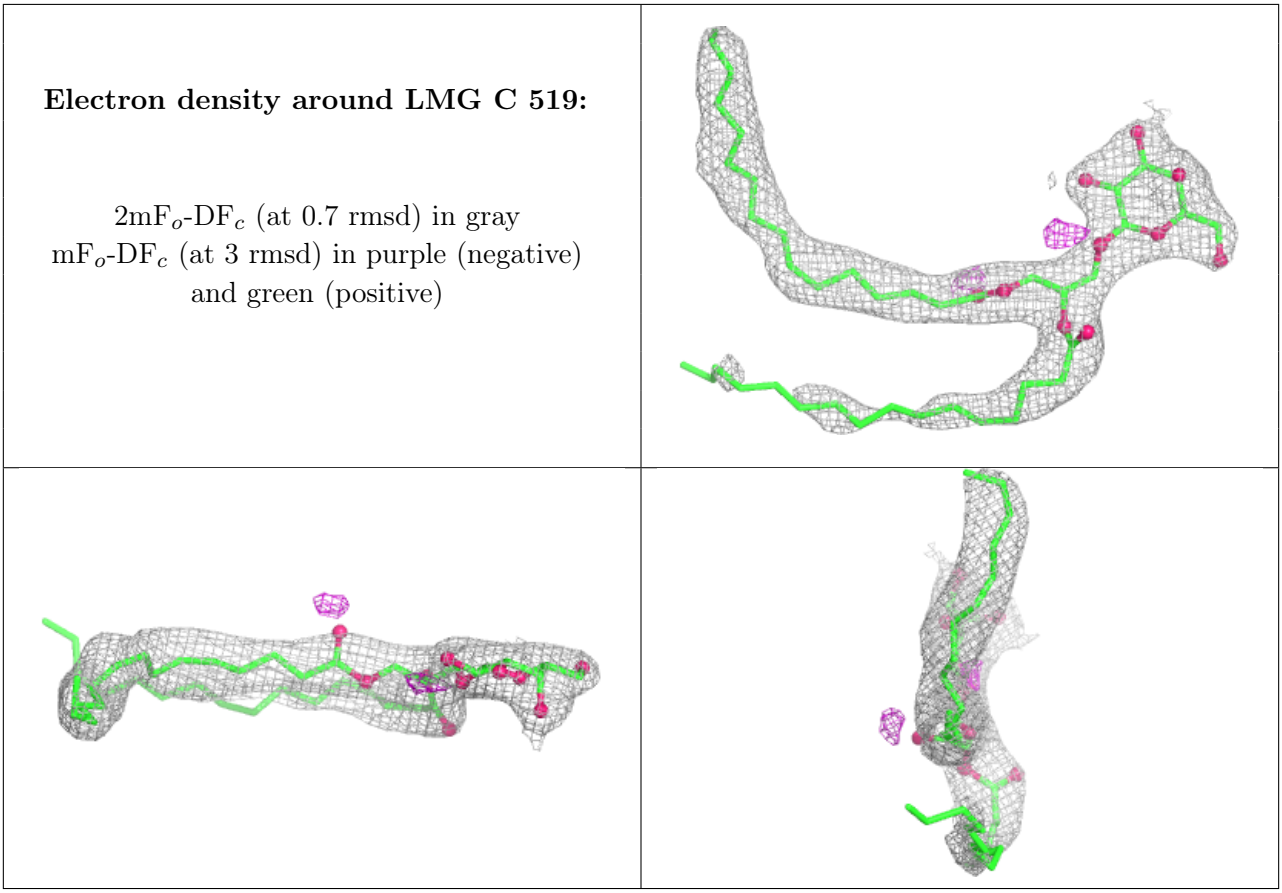
Electron density around LMG m 101:

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



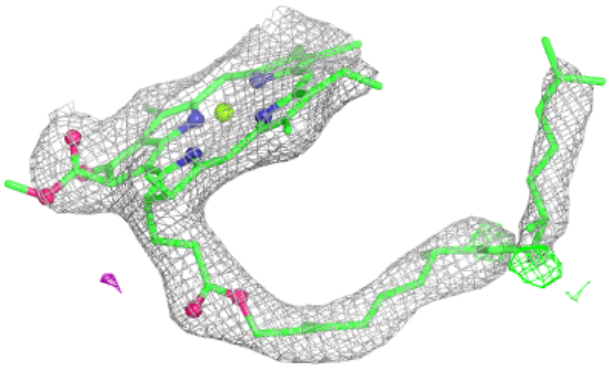
Electron density around LMG C 519:

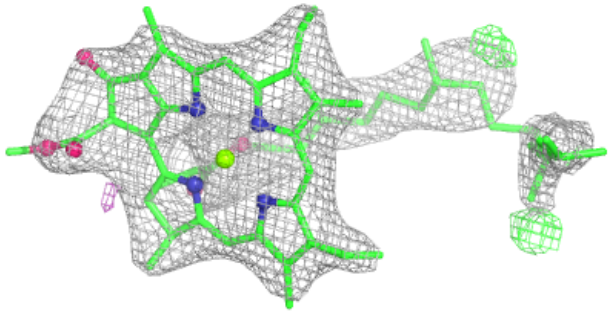
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

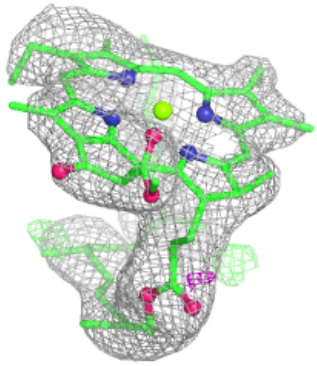


Electron density around CLA c 514:

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

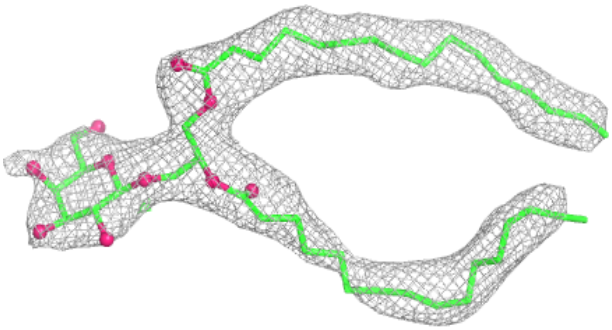


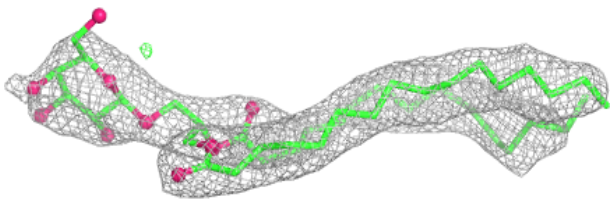


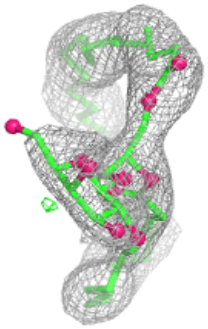


Electron density around LMG c 501:

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

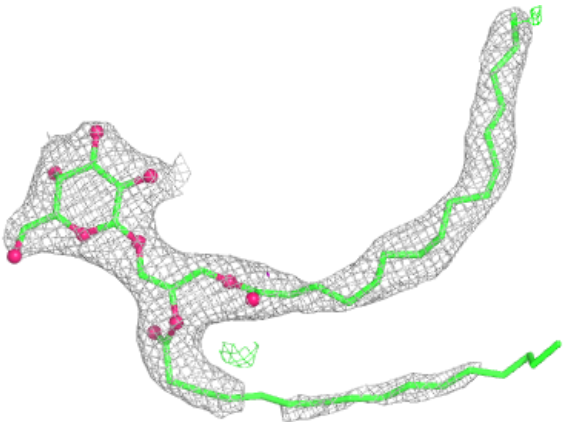


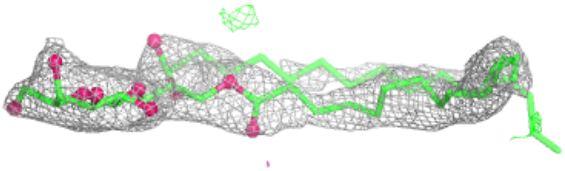


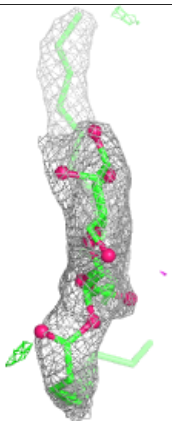


Electron density around LMG c 520:

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

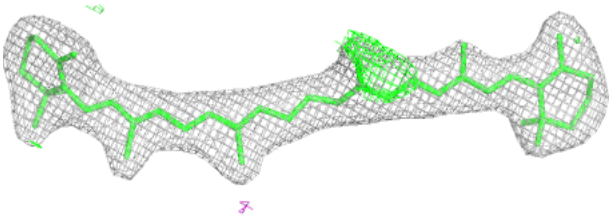


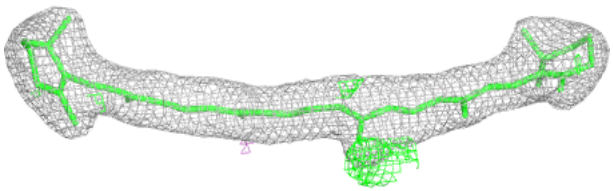


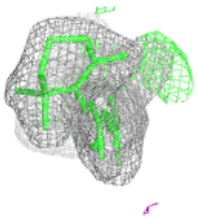


Electron density around BCR T 101:

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

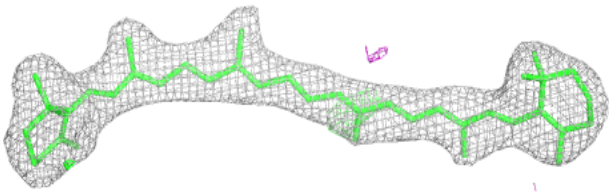


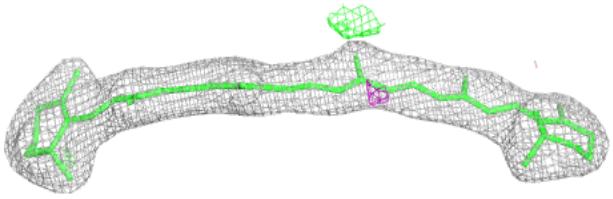


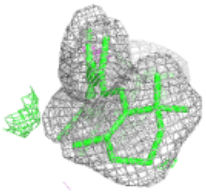


Electron density around BCR t 102:

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

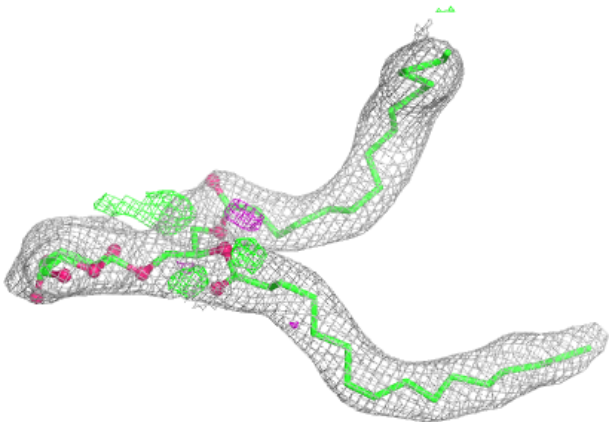


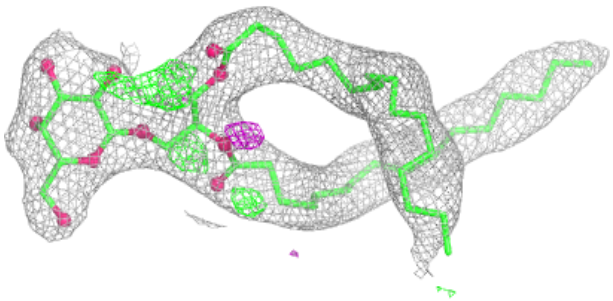




Electron density around LMG B 621:

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

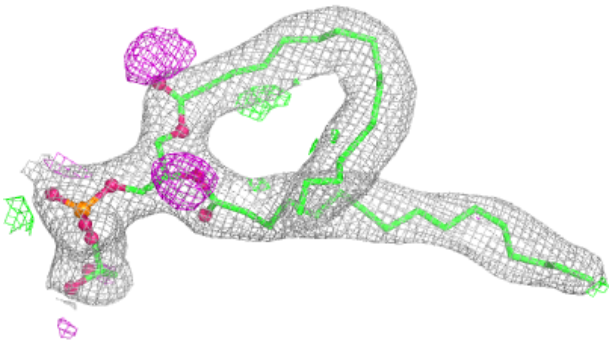


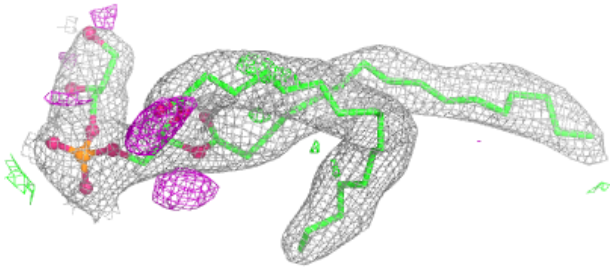


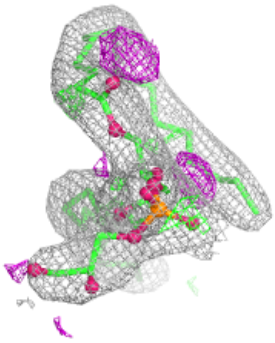


Electron density around LHG A 419 (A):

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

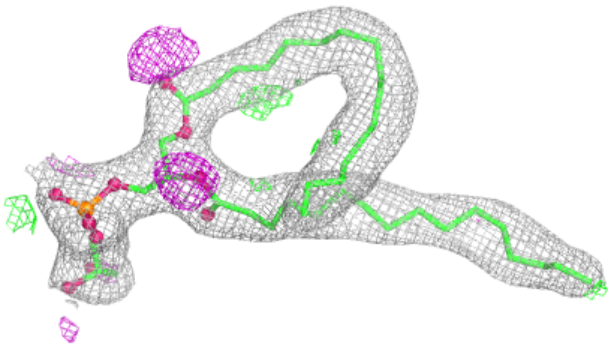


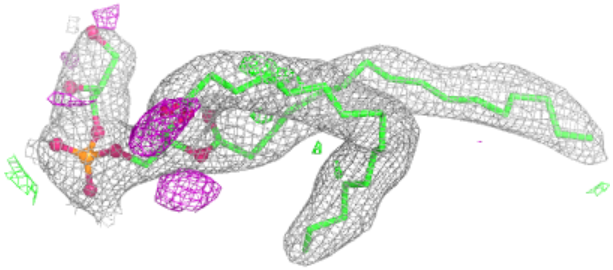




Electron density around LHG A 419 (B):

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

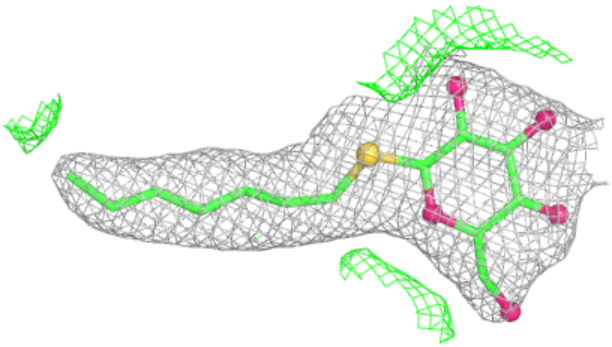


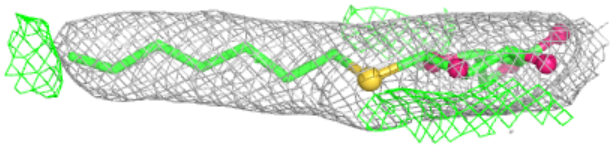


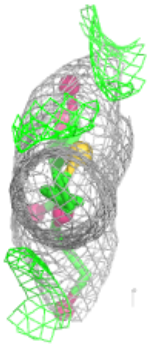


Electron density around HTG b 625:

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

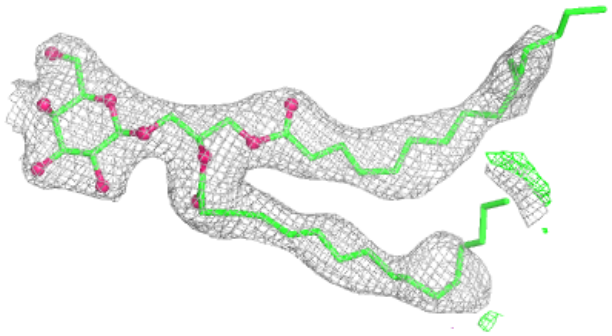


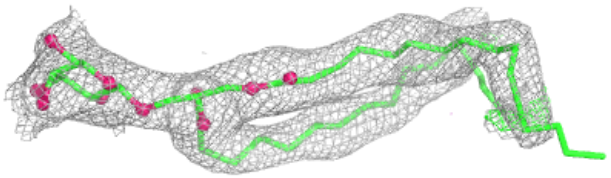




Electron density around LMG d 412:

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

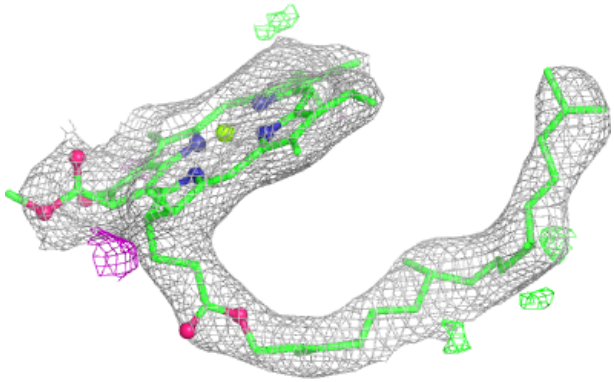


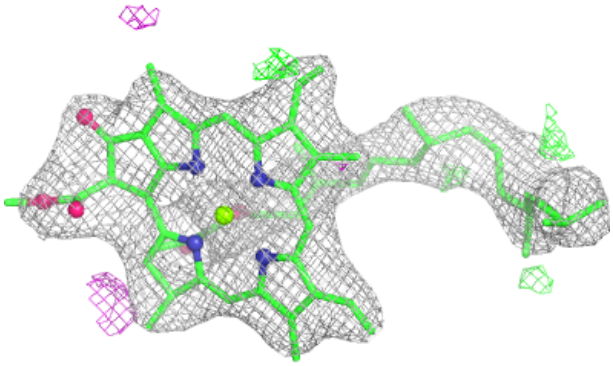


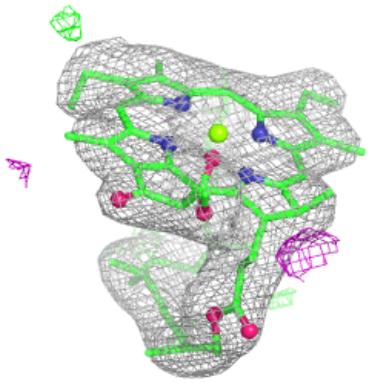


Electron density around CLA C 513:

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

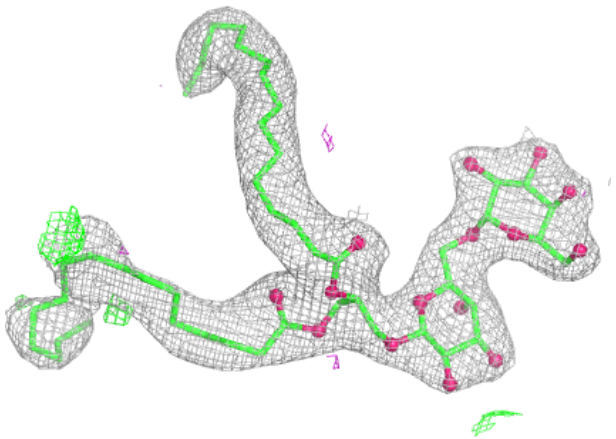


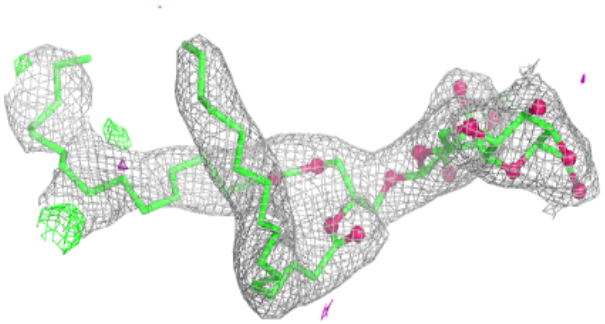


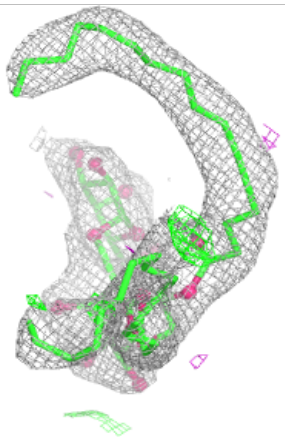


Electron density around DGD C 517 (A):

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

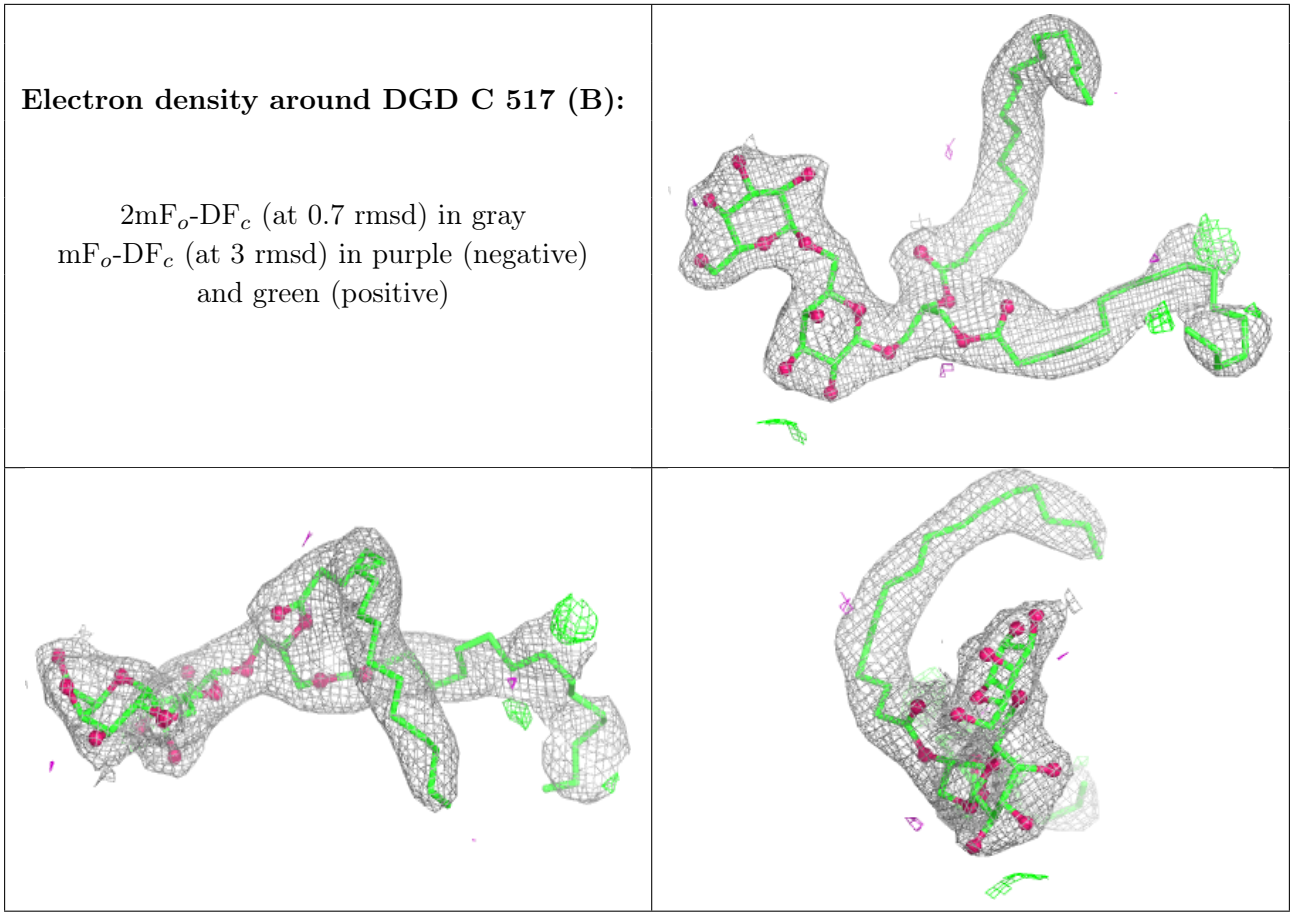






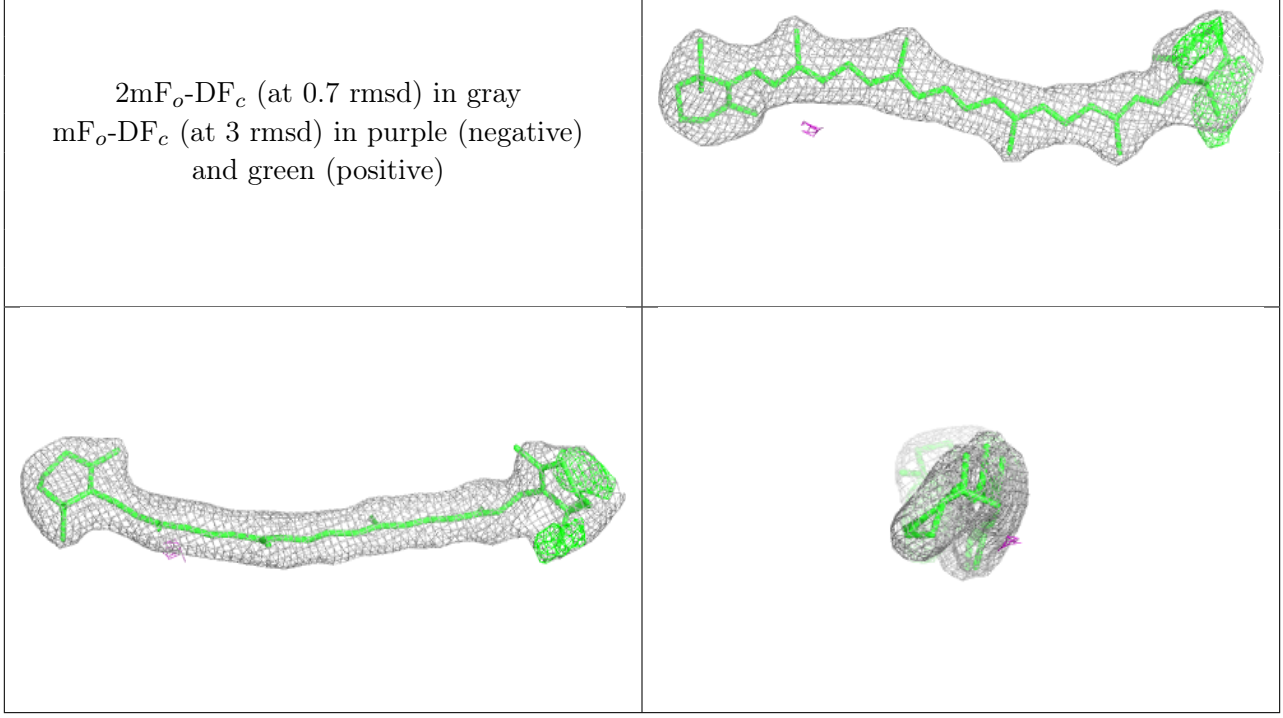
Electron density around DGD C 517 (B):

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



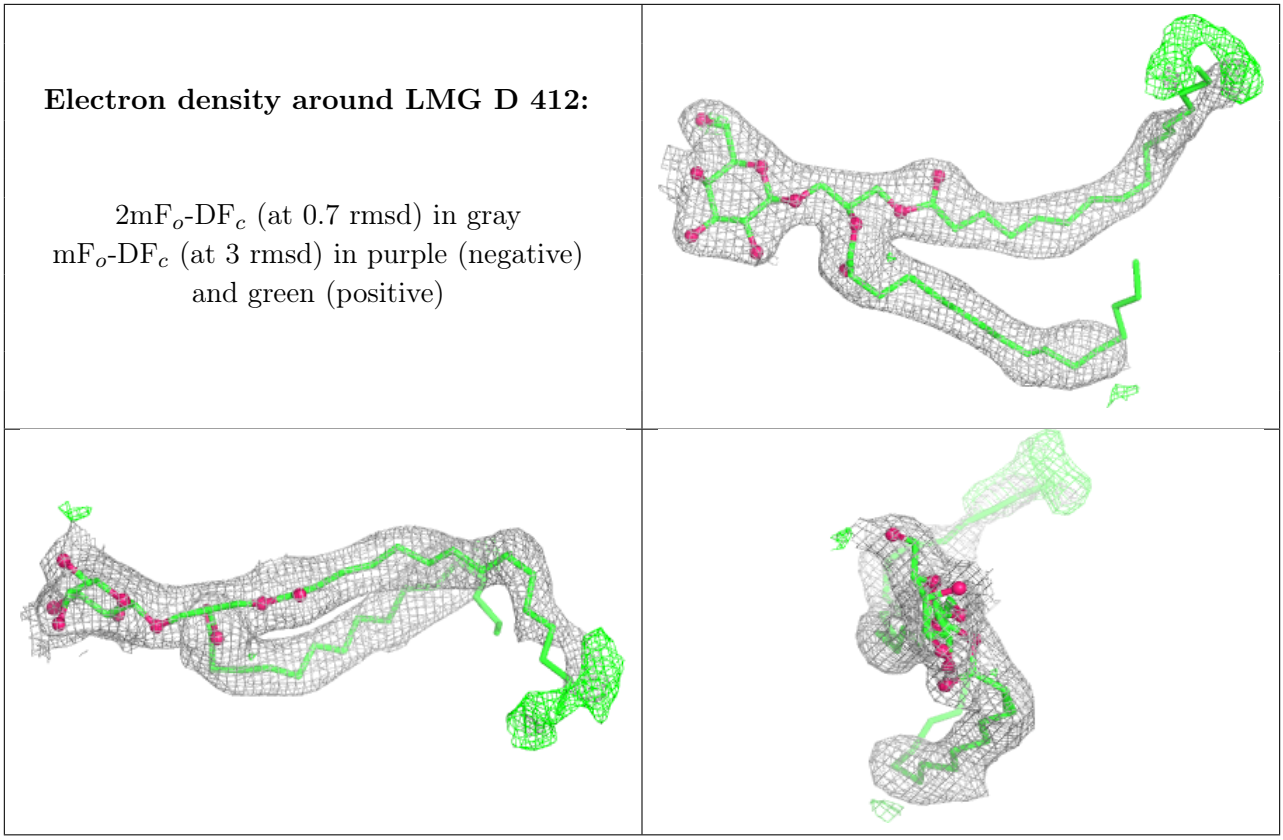
Electron density around BCR d 405:

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



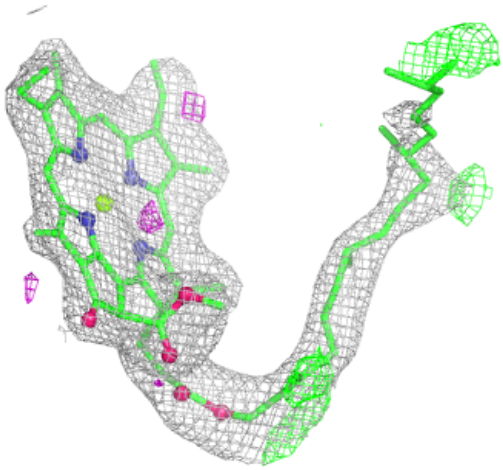
Electron density around LMG D 412:

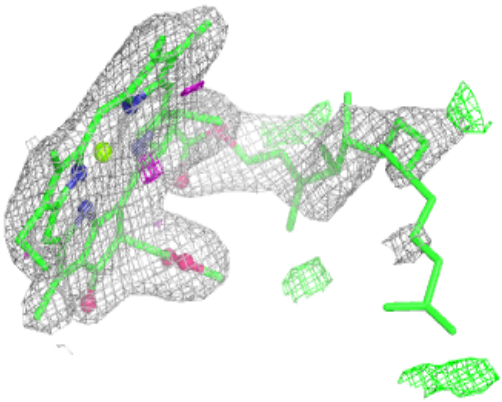
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

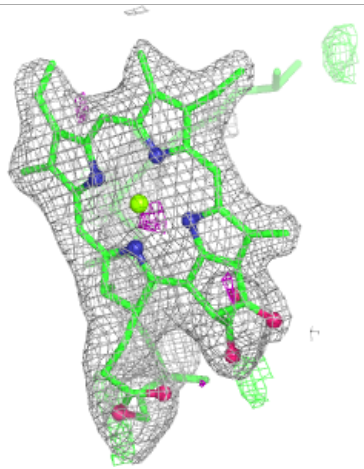


Electron density around CLA b 616:

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

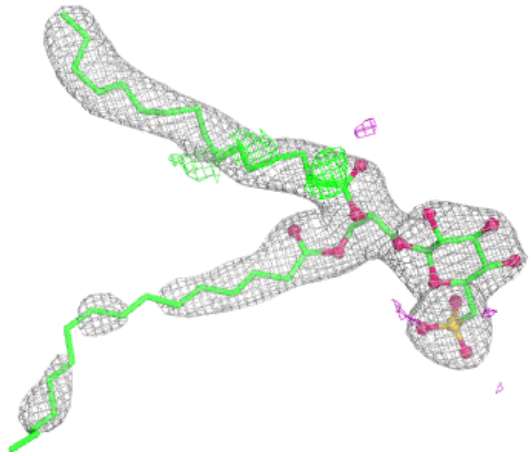


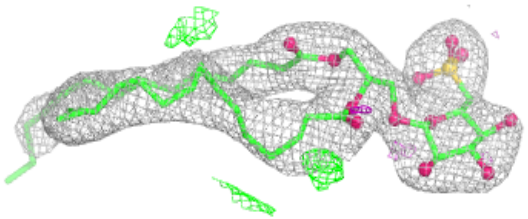


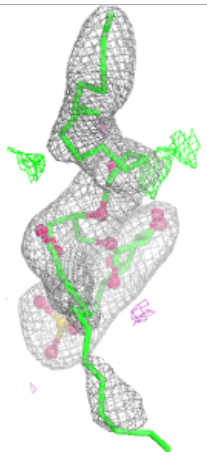


Electron density around SQD A 410 (A):

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

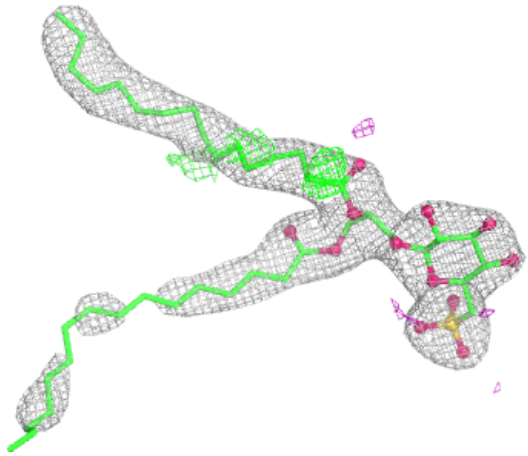


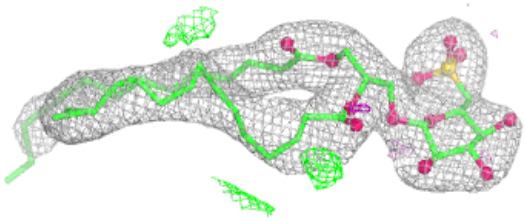


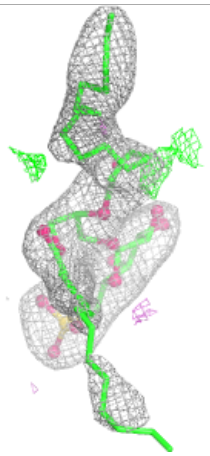


Electron density around SQD A 410 (B):

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

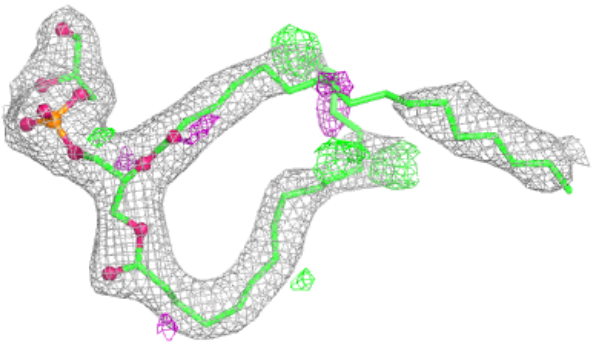


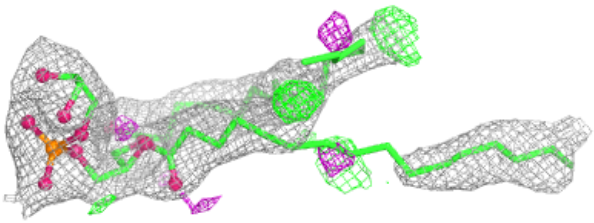


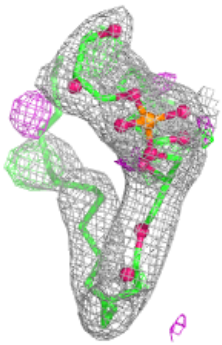


Electron density around LHG D 408 (A):

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

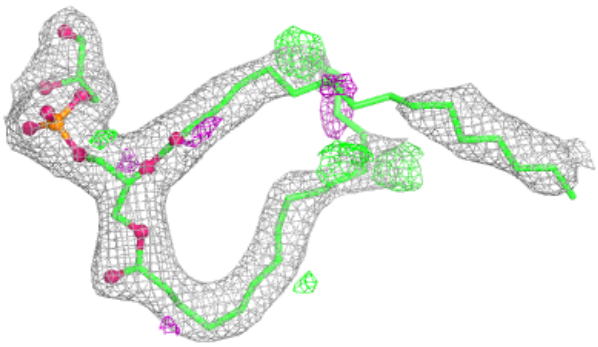


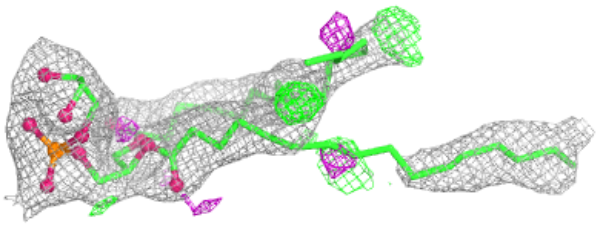




Electron density around LHG D 408 (B):

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

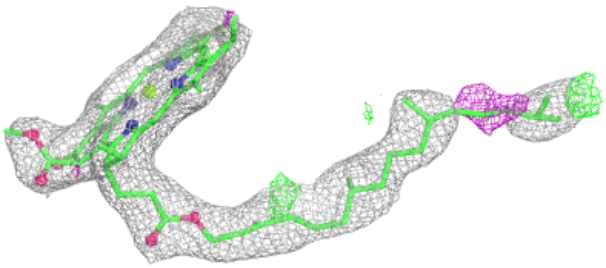


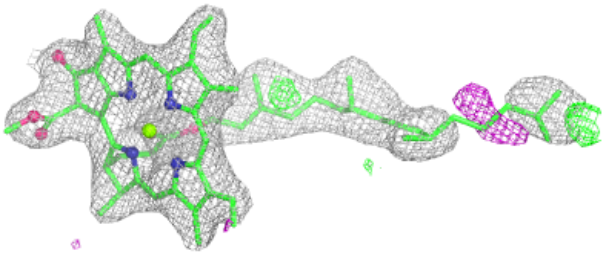


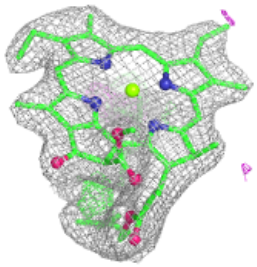


Electron density around CLA c 505:

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

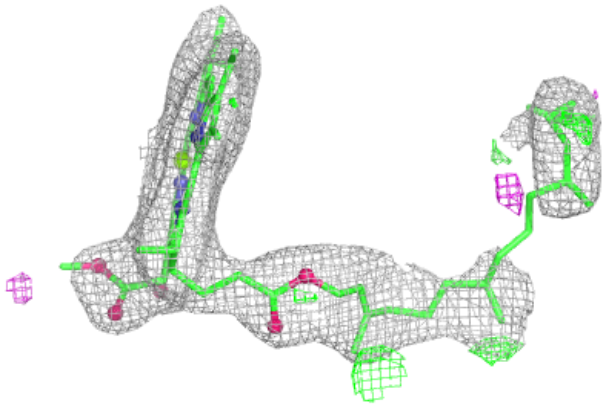


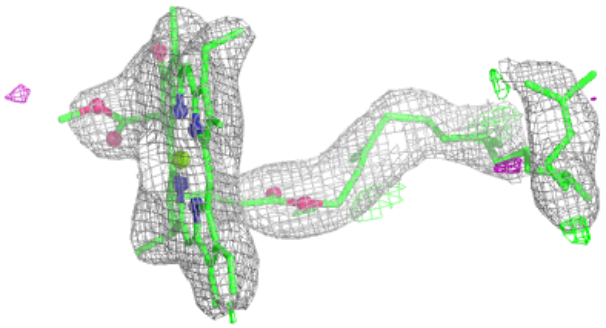


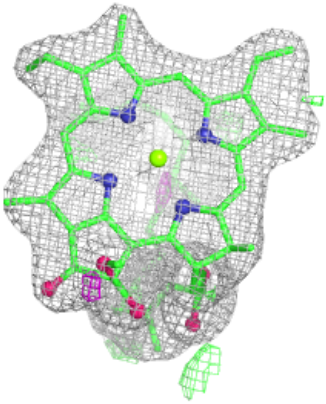


Electron density around CLA c 507:

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

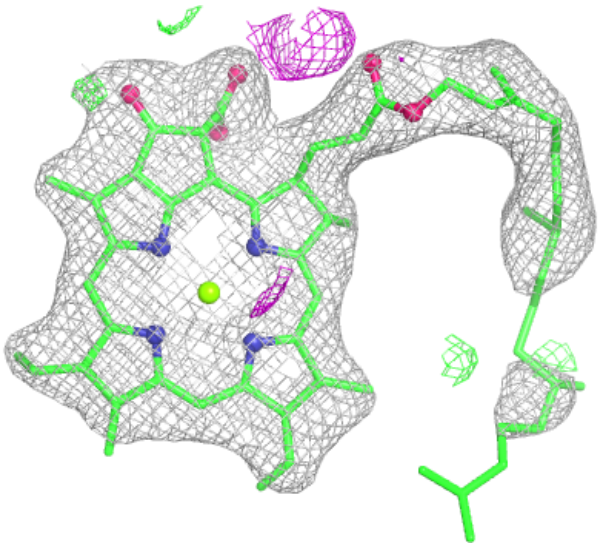


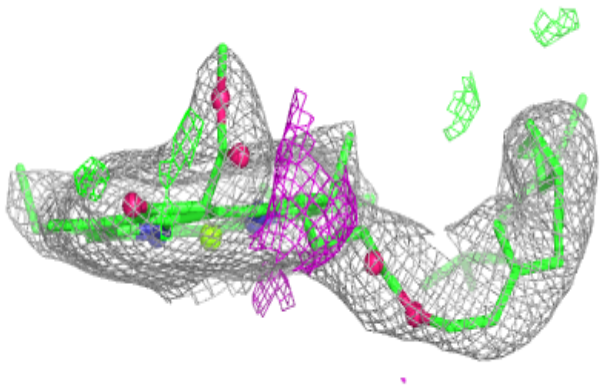


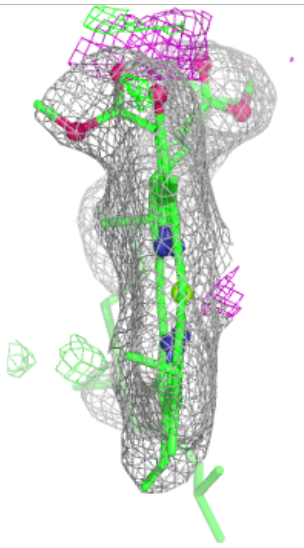


Electron density around CLA c 513:

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

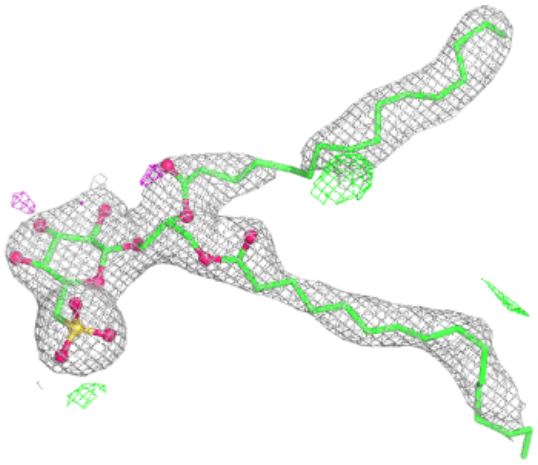


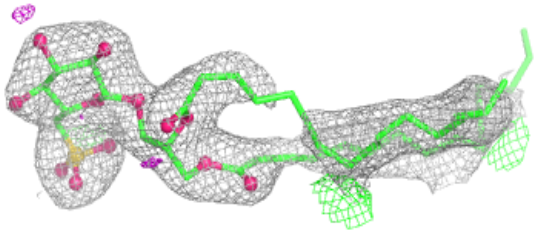




Electron density around SQD a 409 (A):

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

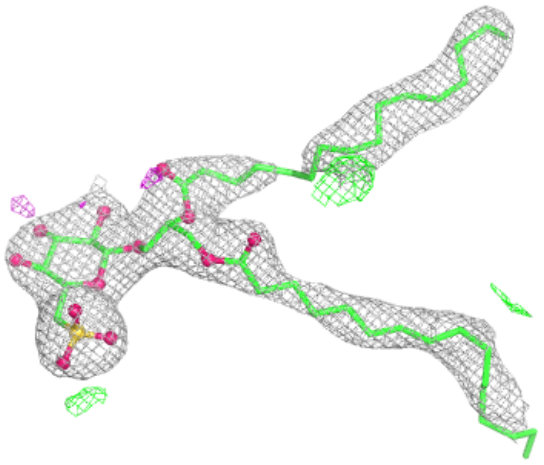


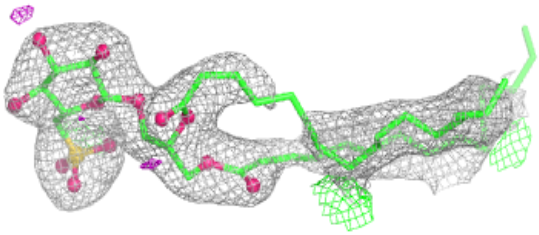


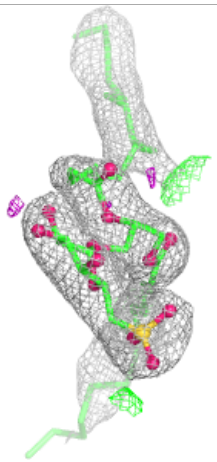


Electron density around SQD a 409 (B):

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

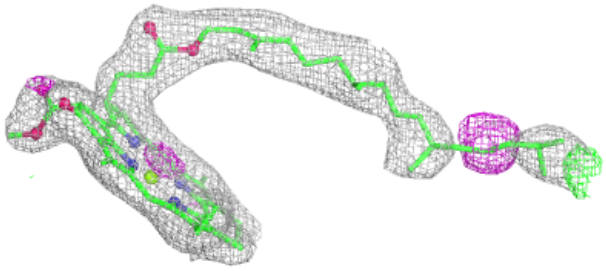


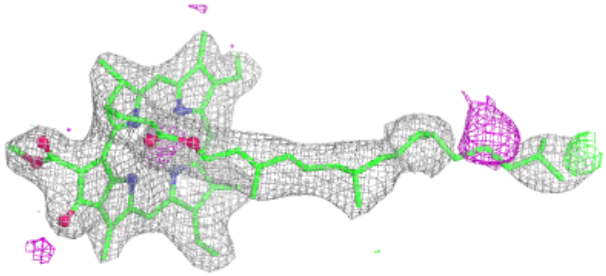


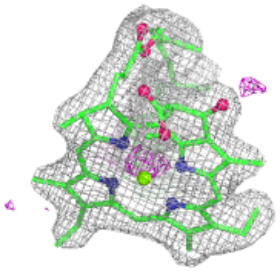


Electron density around CLA C 504:

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

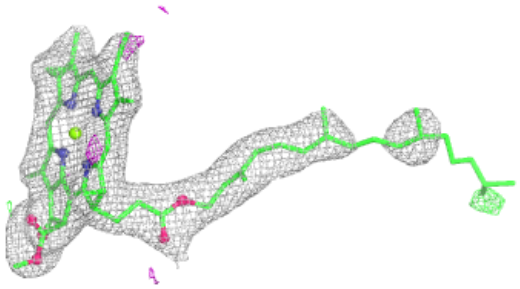


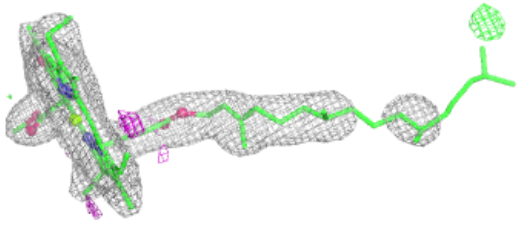


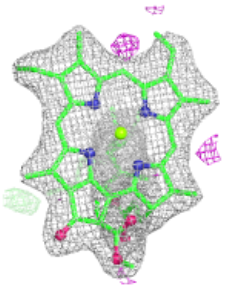


Electron density around CLA d 404:

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

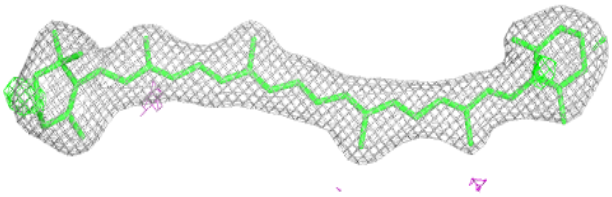


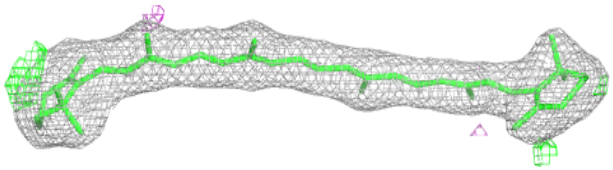


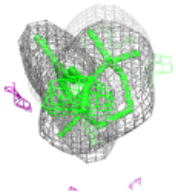


Electron density around BCR B 619:

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



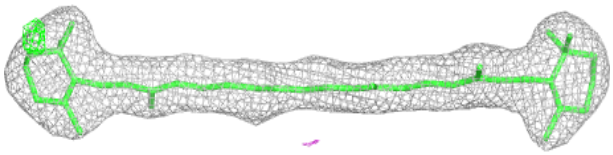


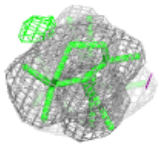


Electron density around BCR C 514:

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

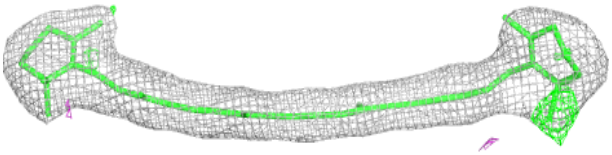


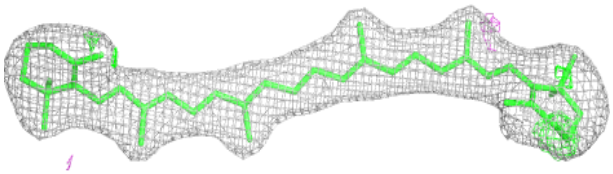


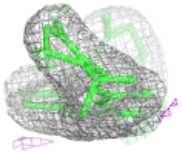


Electron density around BCR D 405:

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

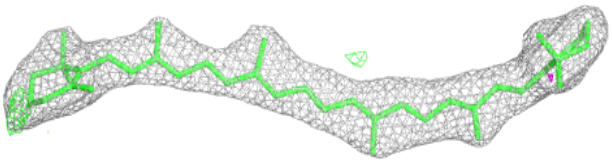


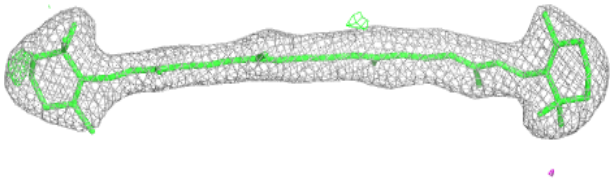


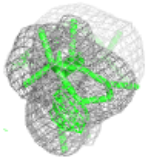


Electron density around BCR H 101:

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

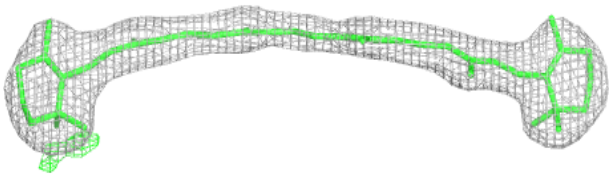


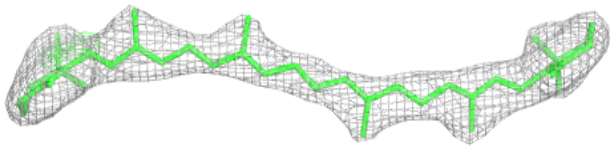


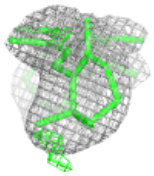


Electron density around BCR K 102:

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

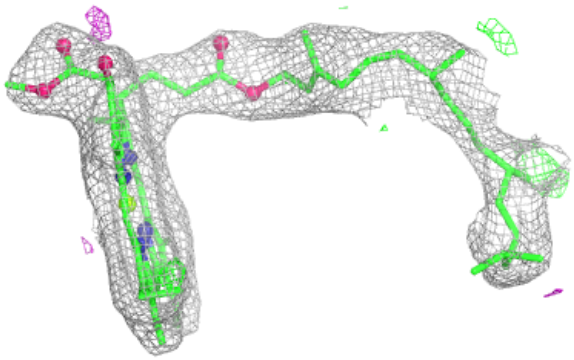


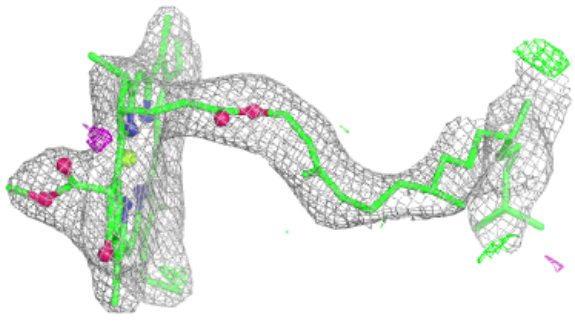


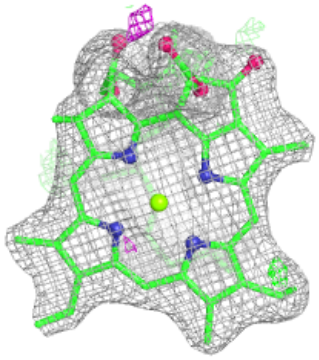


Electron density around CLA C 506:

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

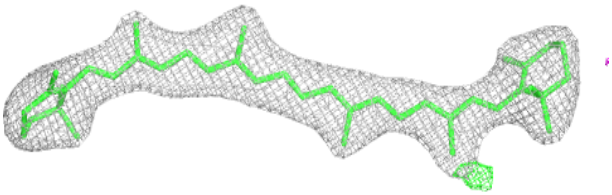


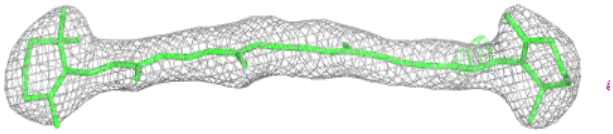


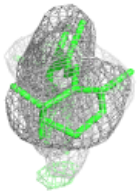


Electron density around BCR Y 101:

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

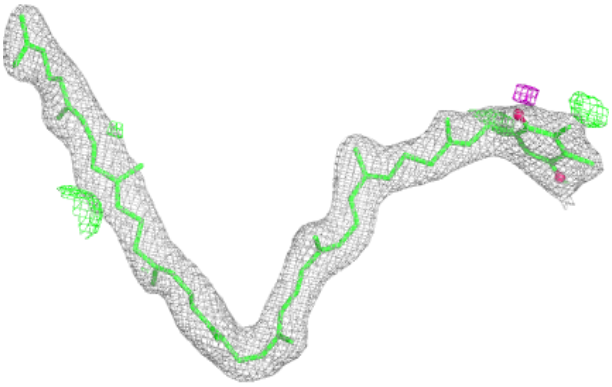


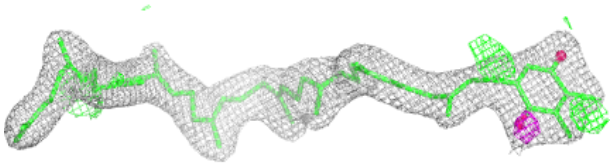


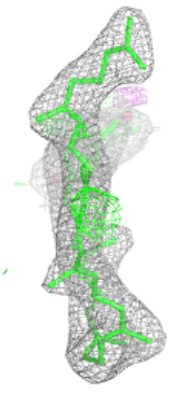


Electron density around PL9 D 406 (A):

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

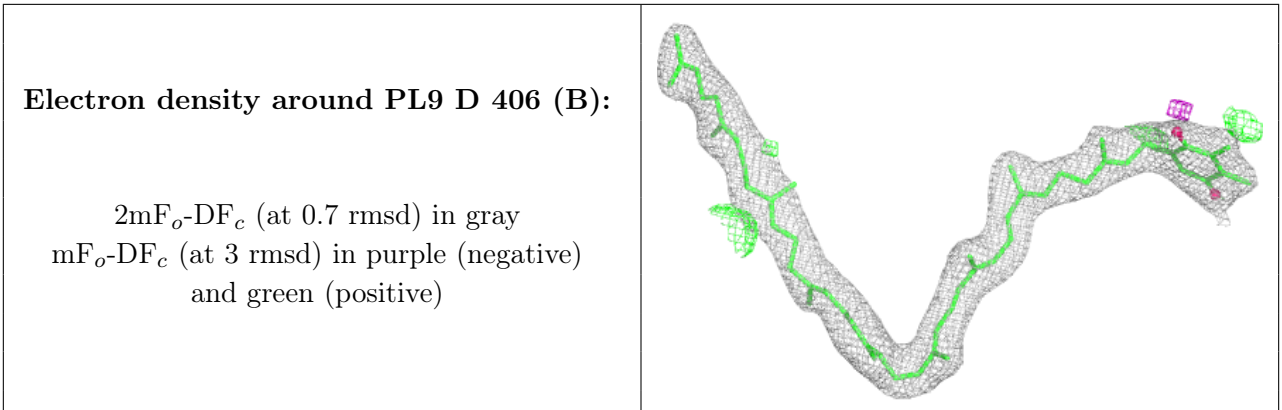


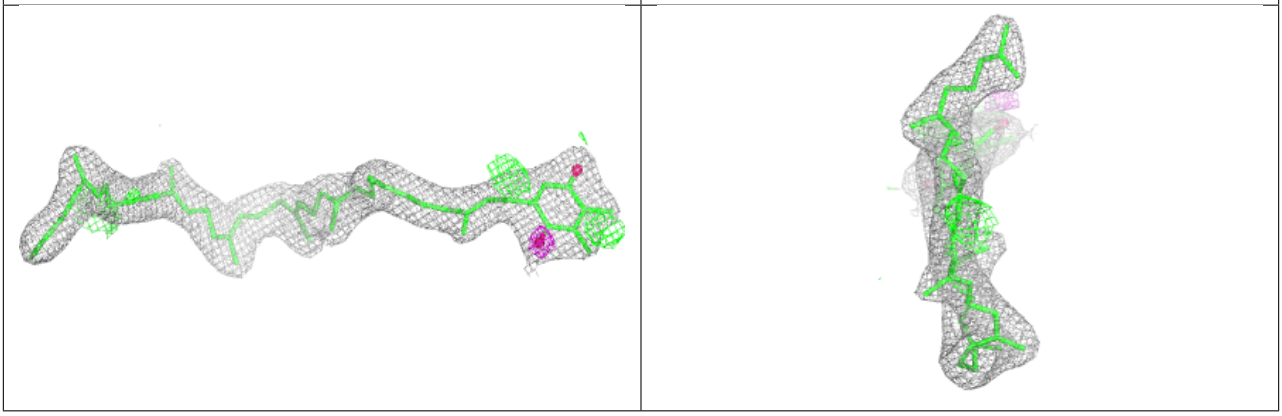




Electron density around PL9 D 406 (B):

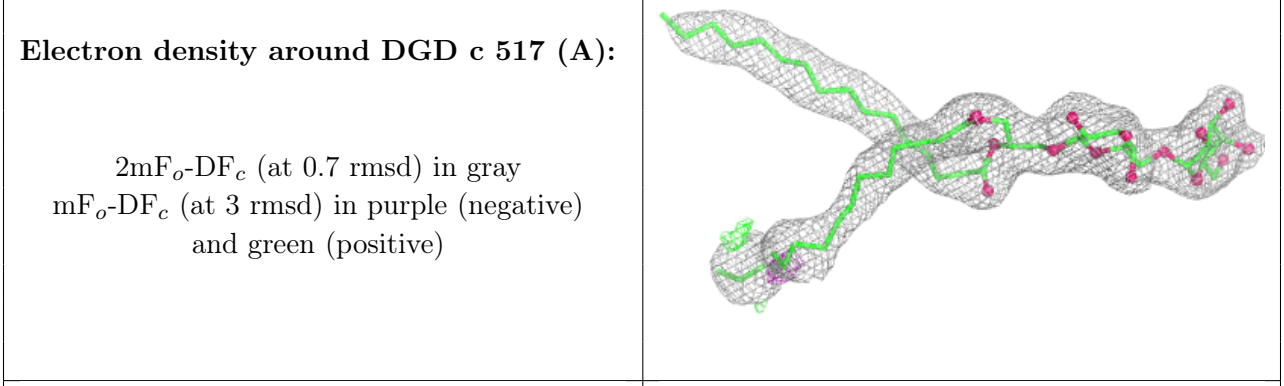
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

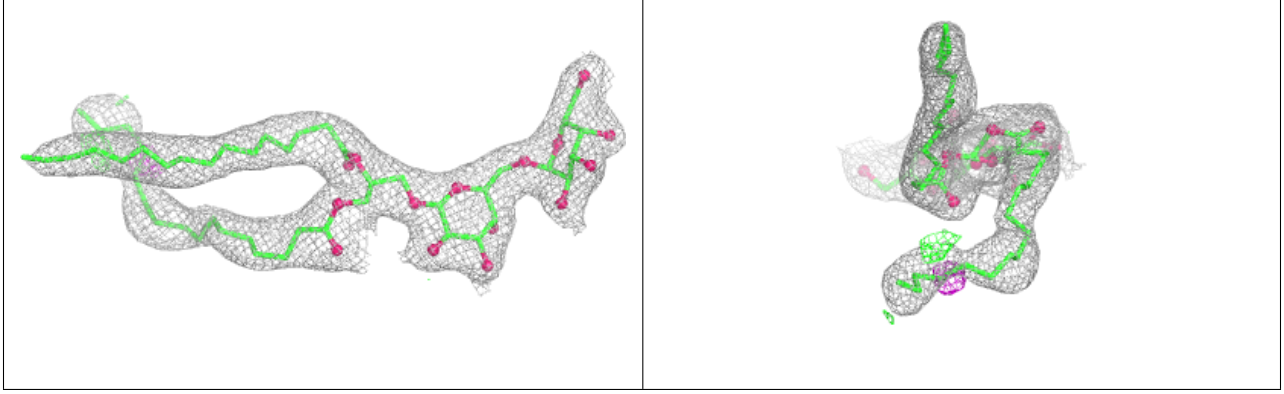




Electron density around DGD c 517 (A):

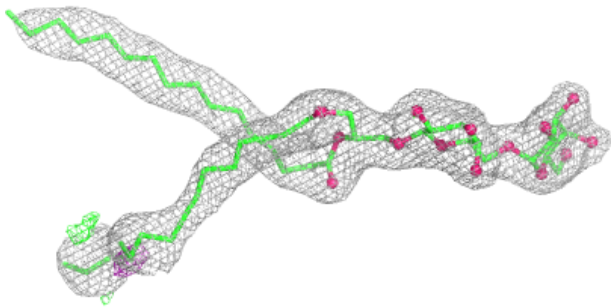
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

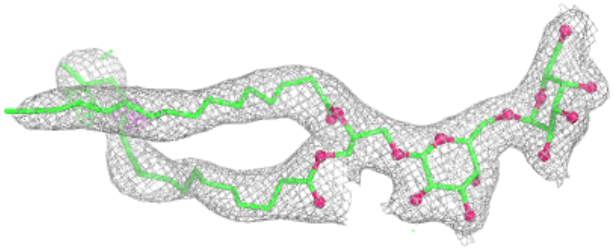


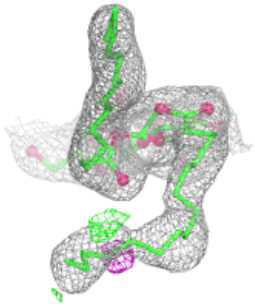


Electron density around DGD c 517 (B):

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

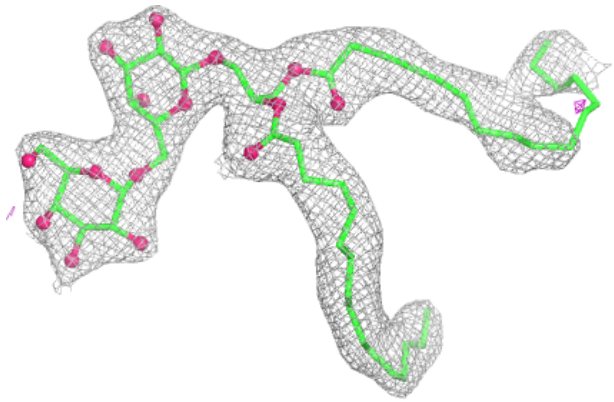


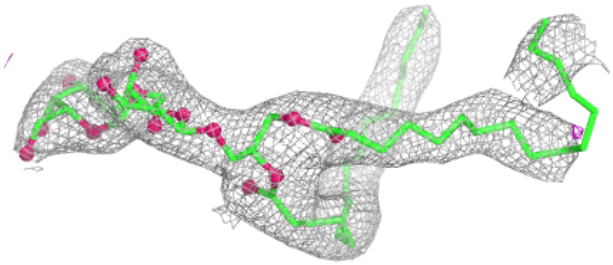


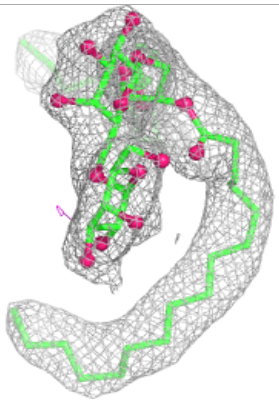


Electron density around DGD c 518 (A):

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

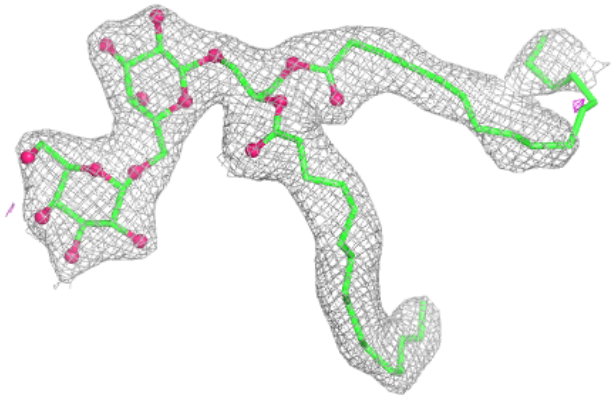


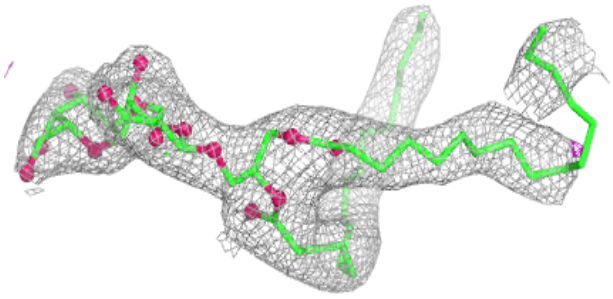


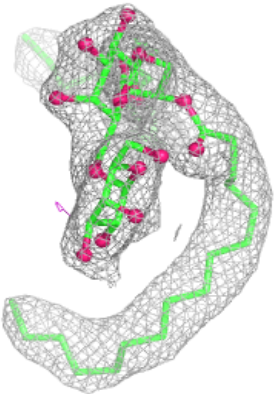


Electron density around DGD c 518 (B):

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

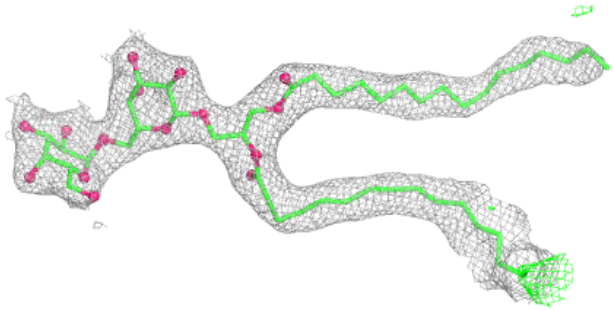


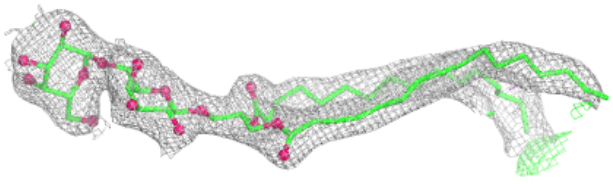


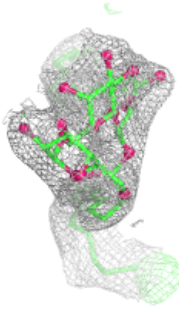


Electron density around DGD c 519:

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

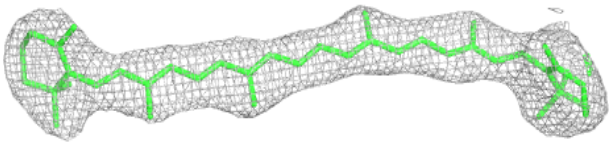


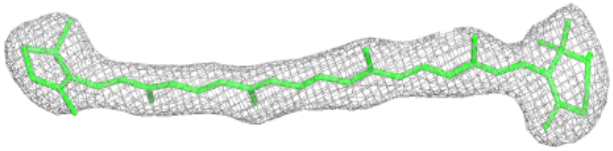


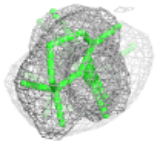


Electron density around BCR c 515:

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

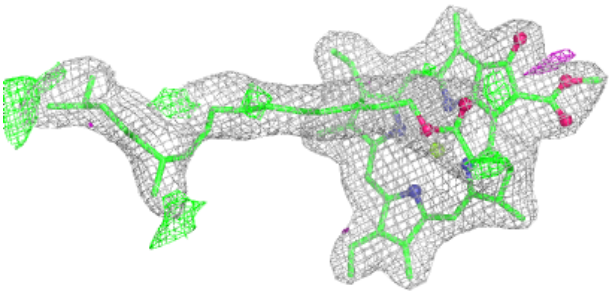


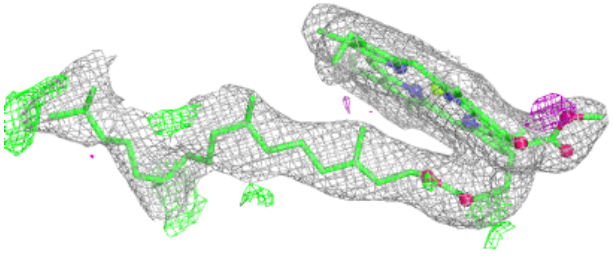


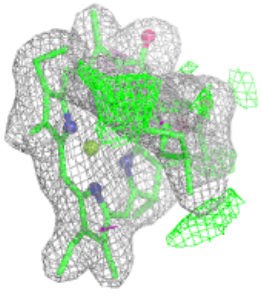


Electron density around CLA b 614:

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

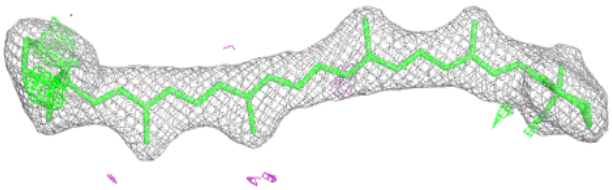


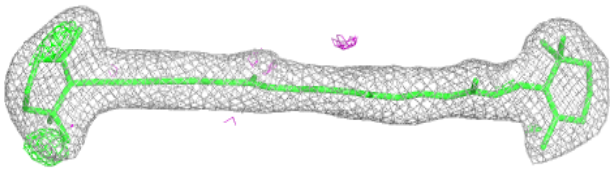


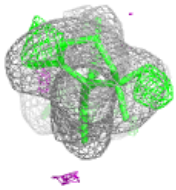


Electron density around BCR A 409:

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

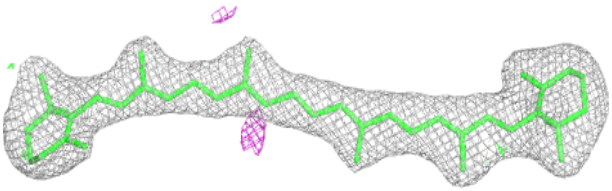


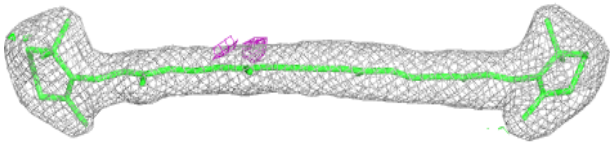


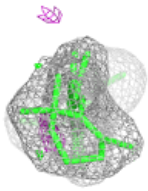


Electron density around BCR B 618:

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

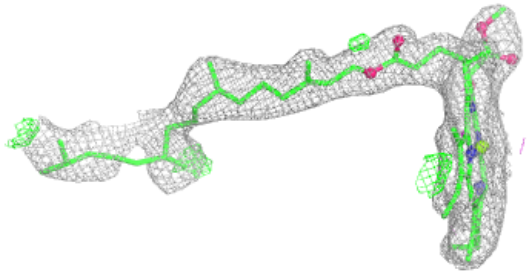


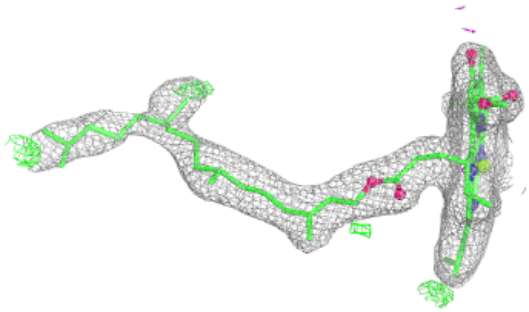


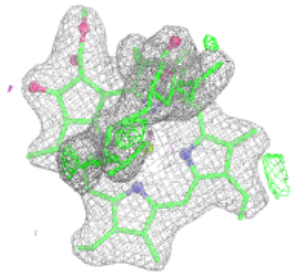


Electron density around CLA B 606:

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

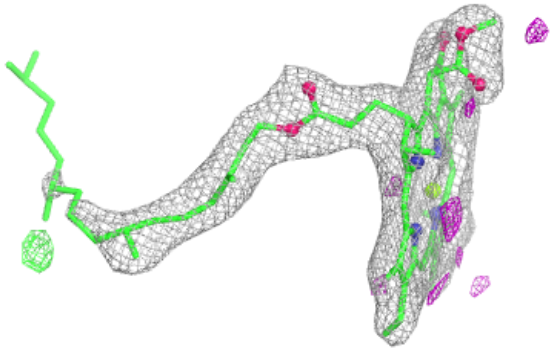


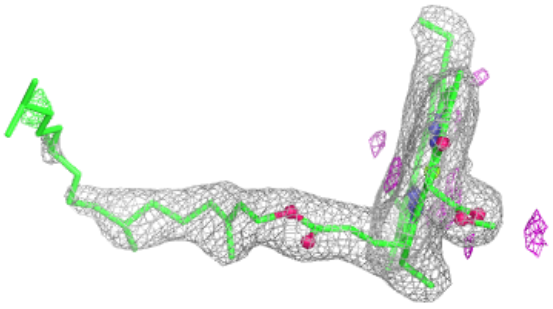


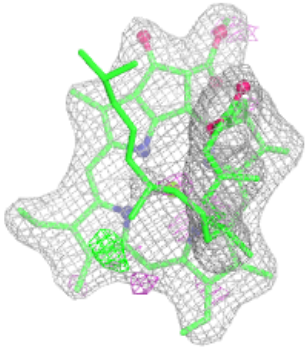


Electron density around CLA D 404:

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

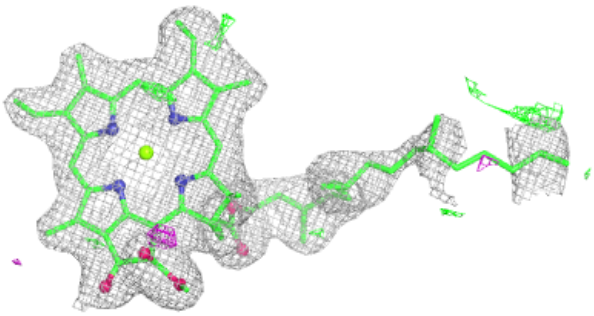


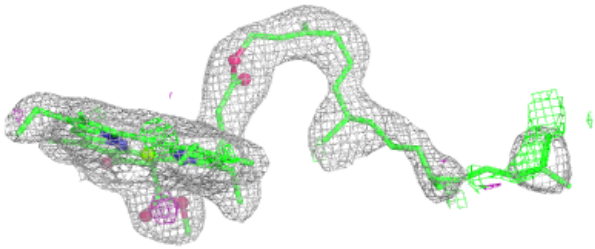


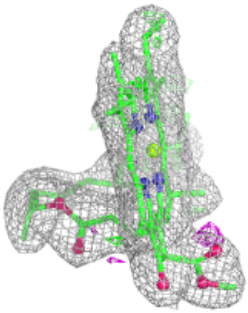


Electron density around CLA a 405 (A):

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

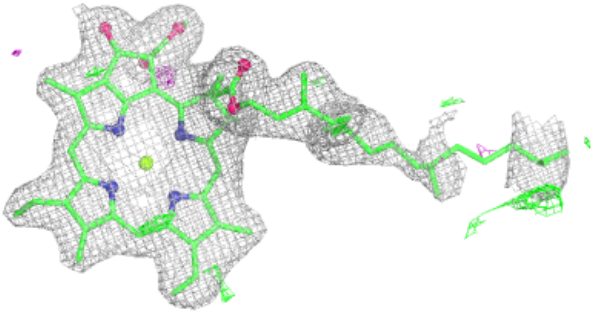


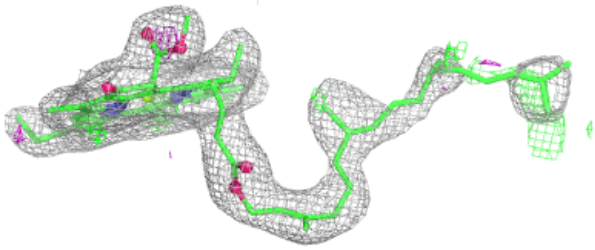


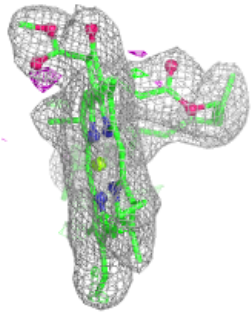


Electron density around CLA a 405 (B):

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

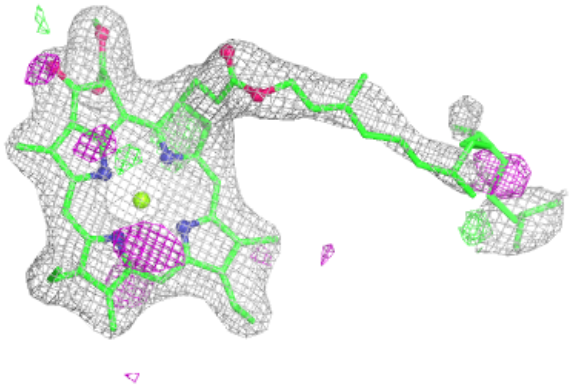


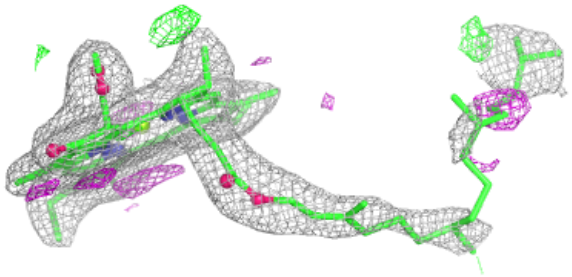


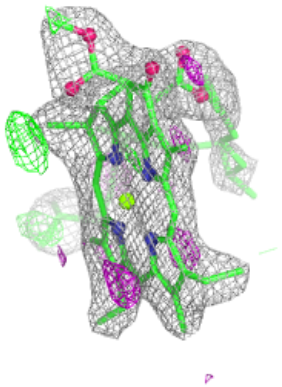


Electron density around CLA a 407:

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

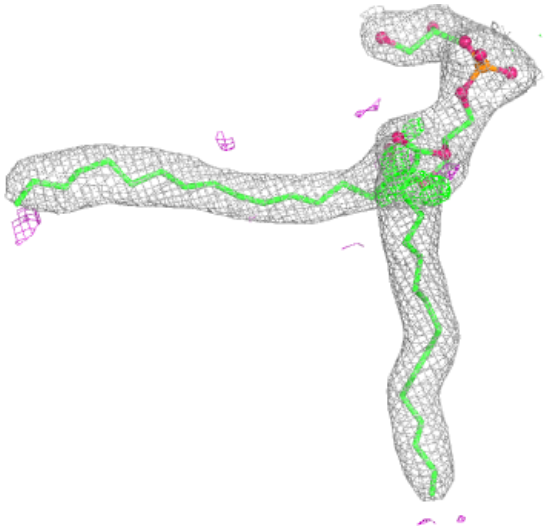


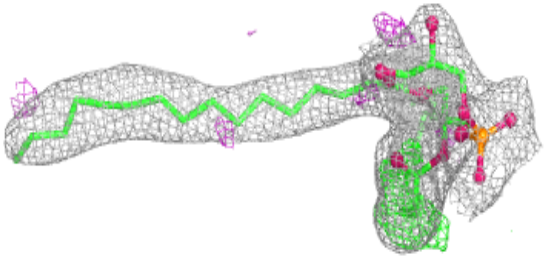


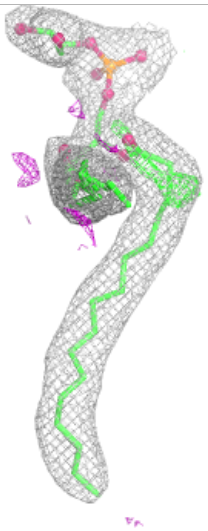


Electron density around LHG b 629 (A):

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

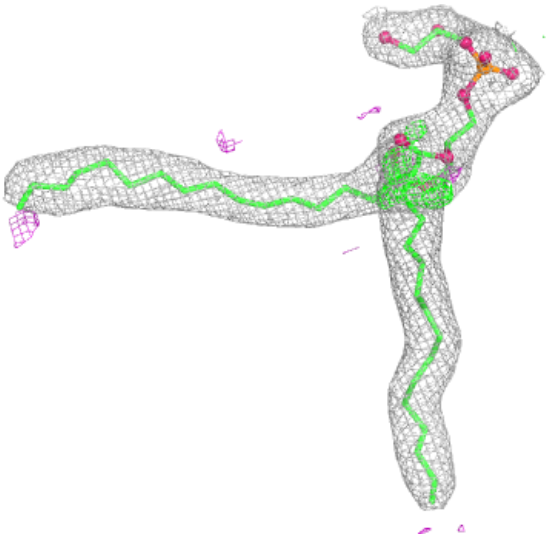


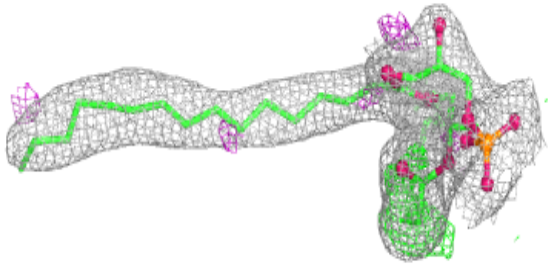


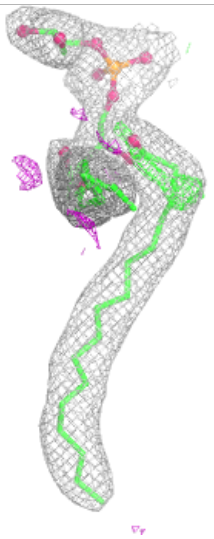


Electron density around LHG b 629 (B):

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

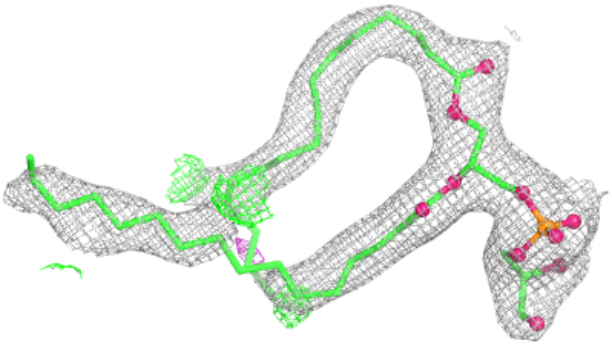


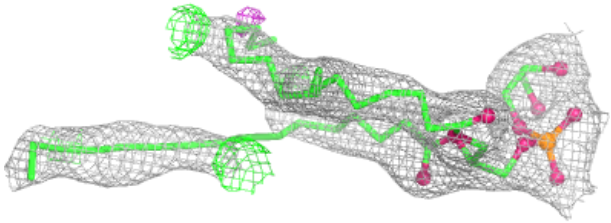


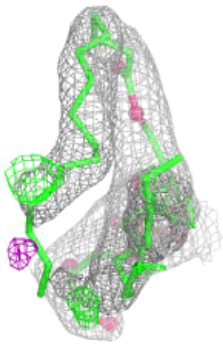


Electron density around LHG d 408 (A):

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

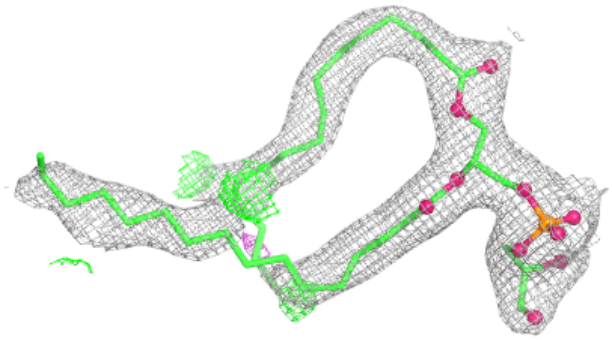


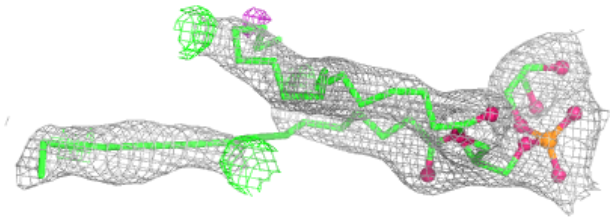


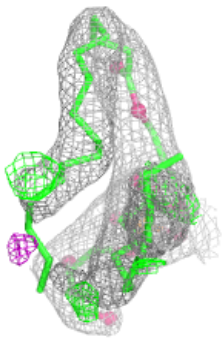


Electron density around LHG d 408 (B):

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

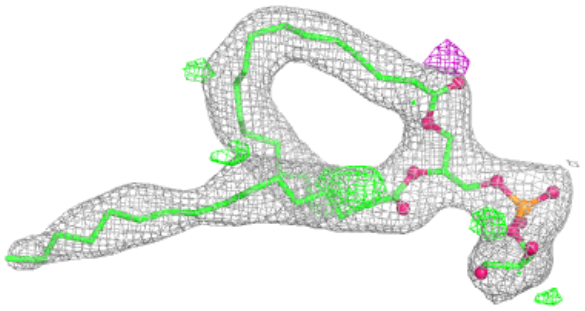


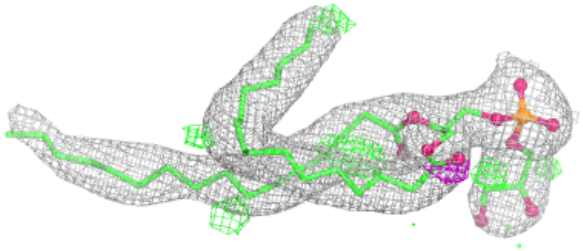


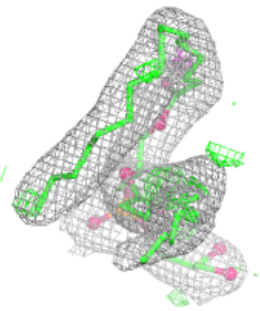


Electron density around LHG d 414 (A):

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

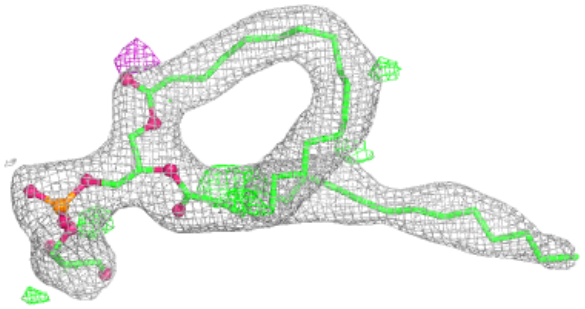


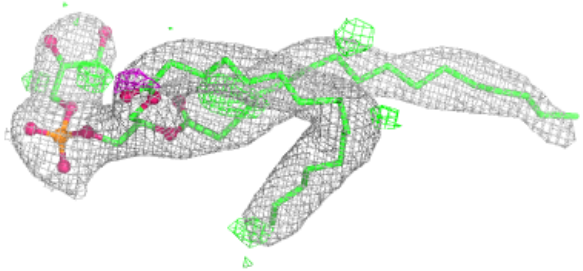


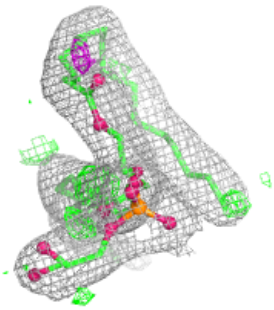


Electron density around LHG d 414 (B):

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

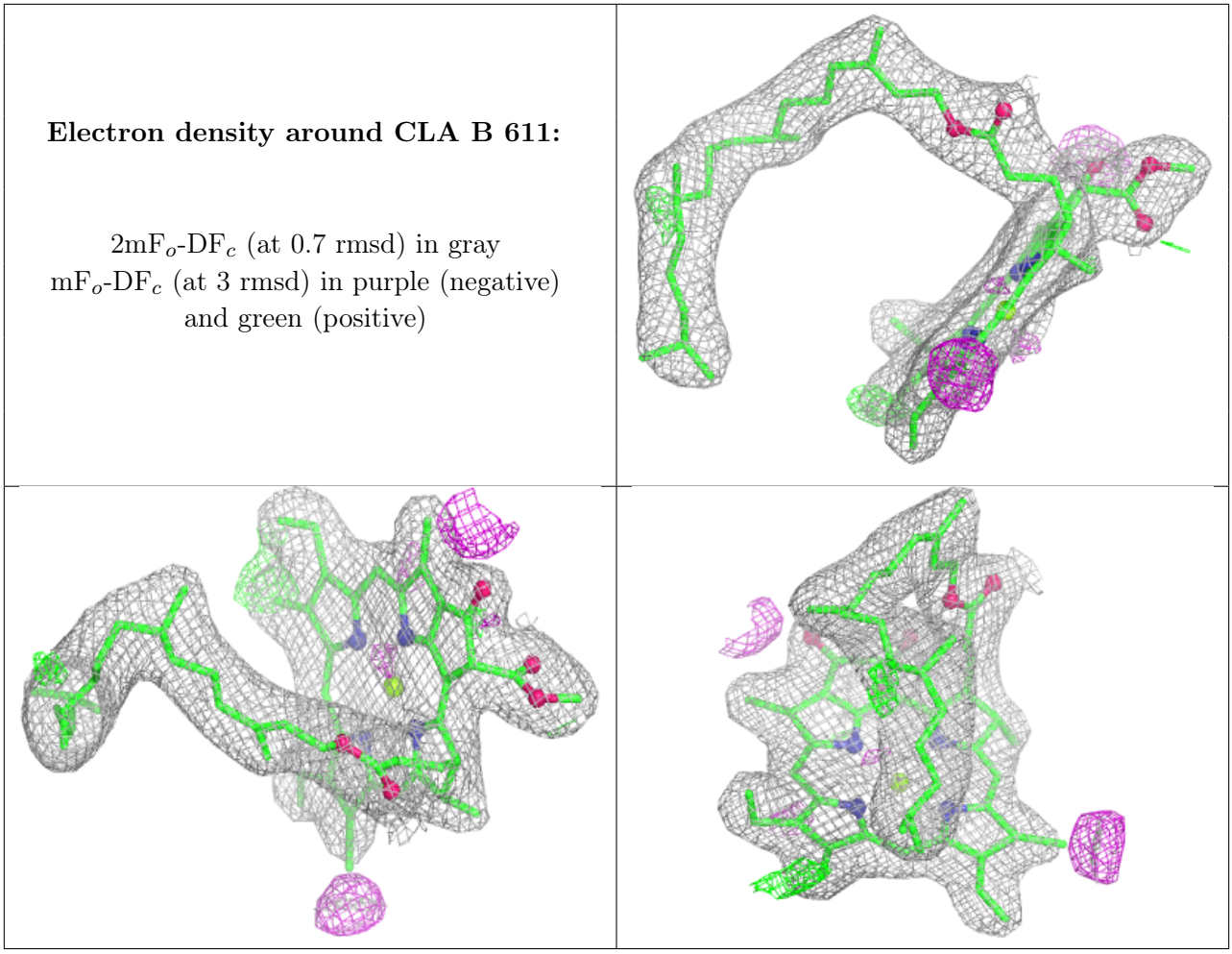






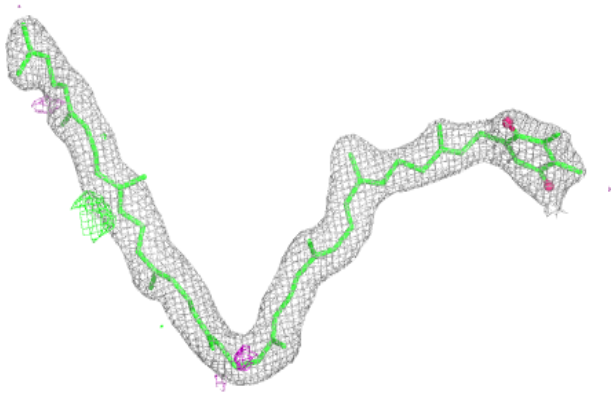
Electron density around CLA B 611:

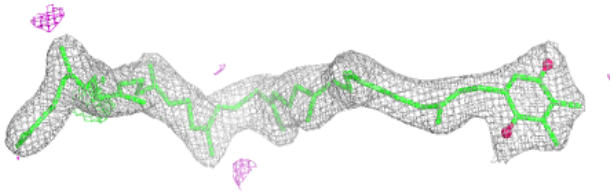
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

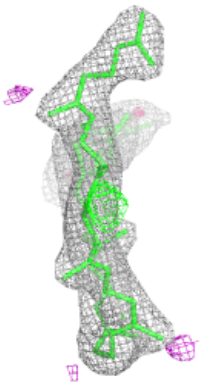


Electron density around PL9 d 406 (A):

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

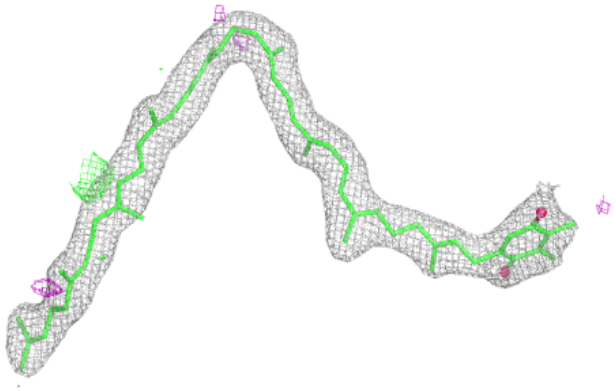


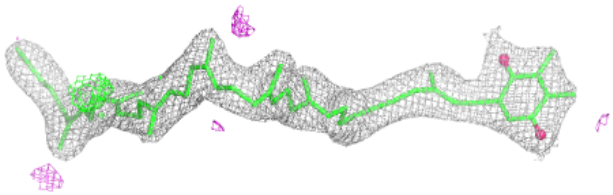


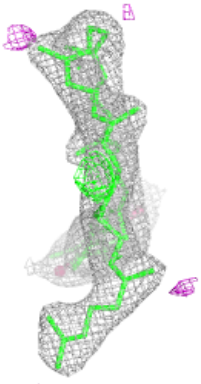


Electron density around PL9 d 406 (B):

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

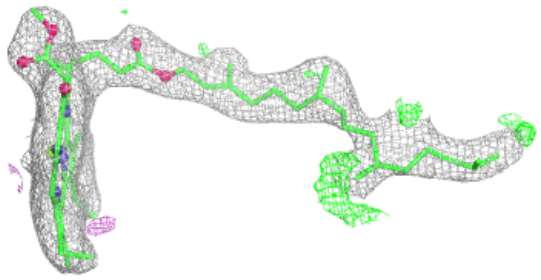


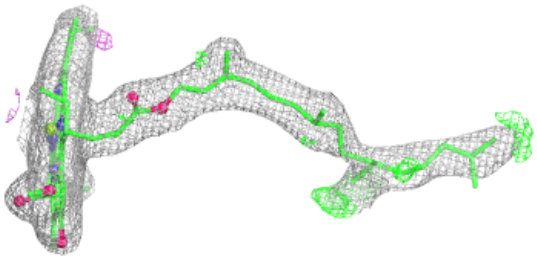


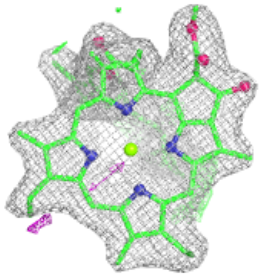


Electron density around CLA b 606:

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

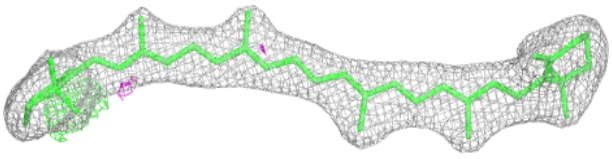


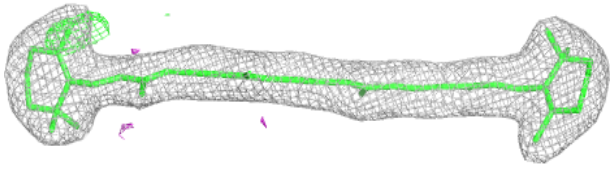


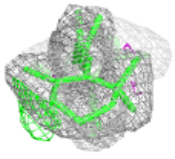


Electron density around BCR a 408:

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

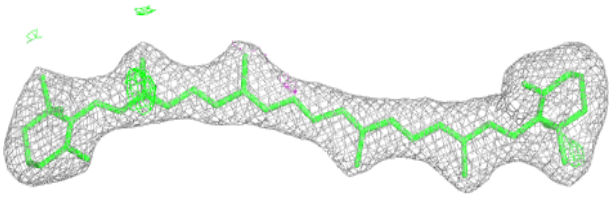


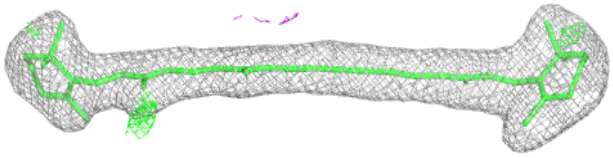


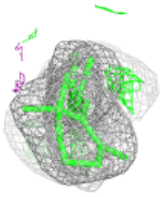


Electron density around BCR b 618:

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

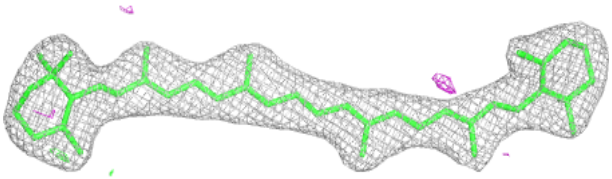


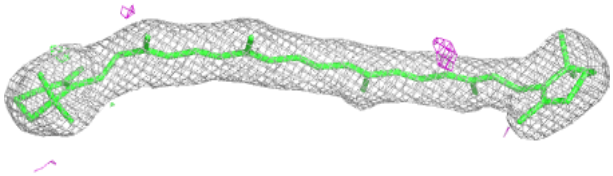


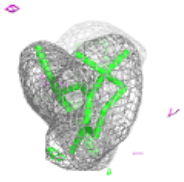


Electron density around BCR b 619:

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

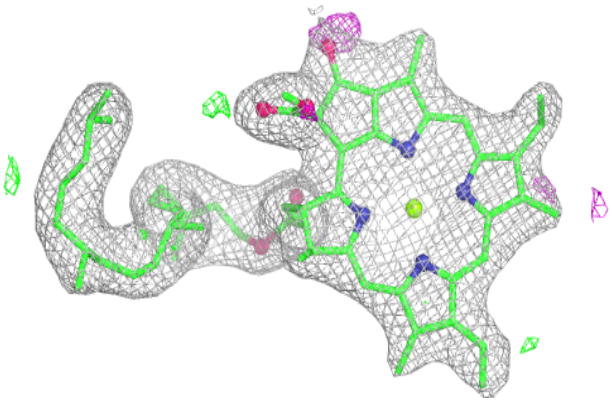


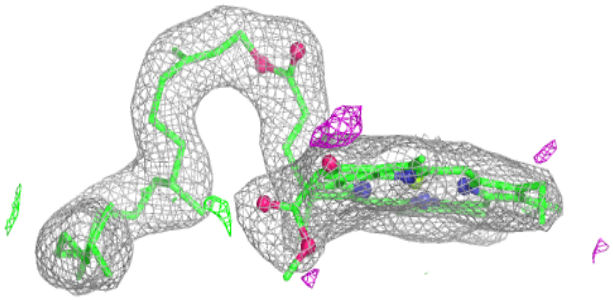


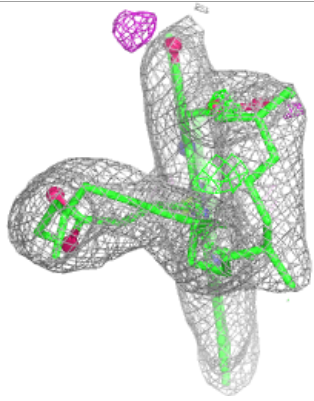


Electron density around CLA b 612:

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

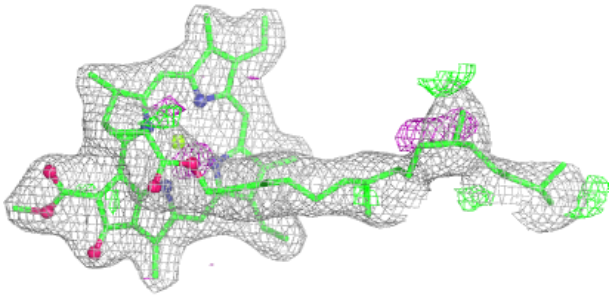


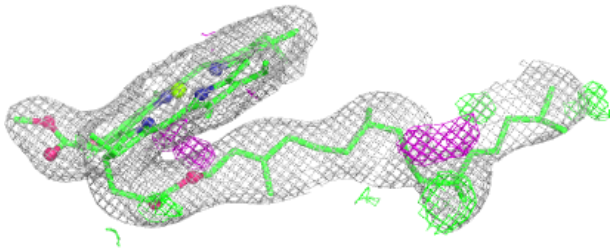


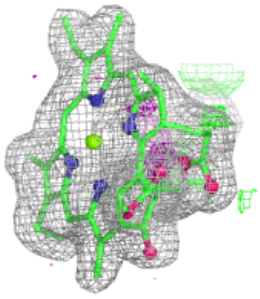


Electron density around CLA B 614:

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

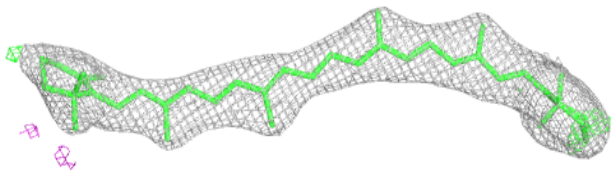


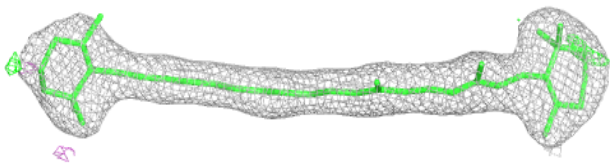


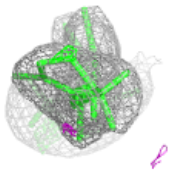


Electron density around BCR h 101:

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

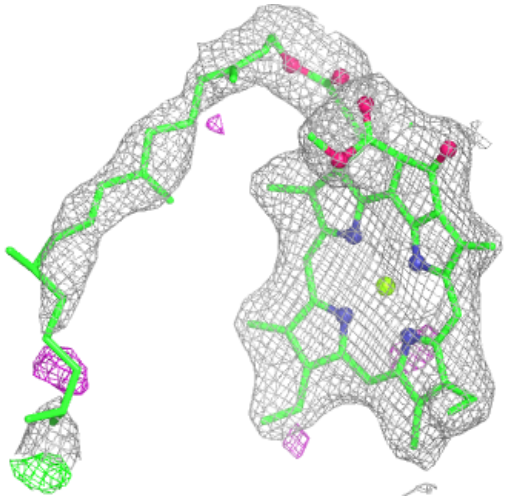


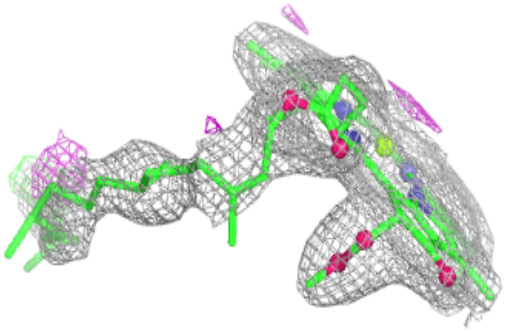


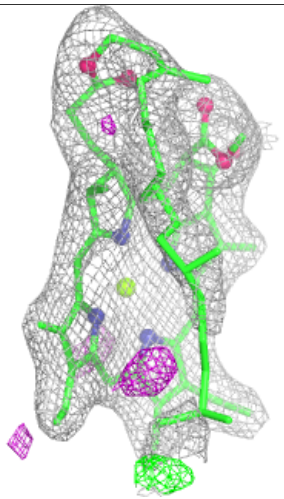


Electron density around CLA B 616:

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

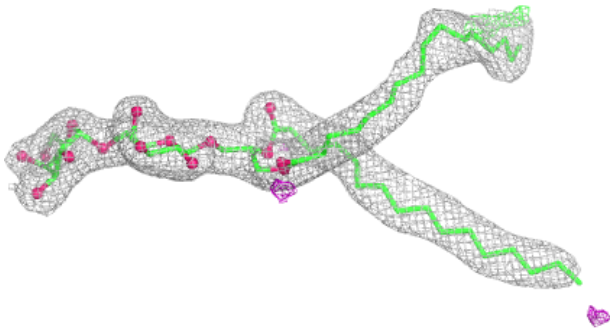


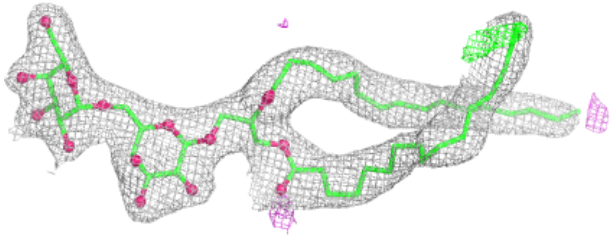


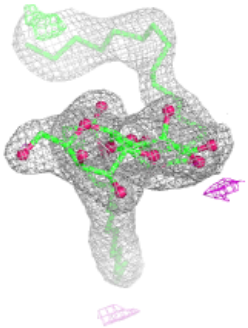


Electron density around DGD C 516 (A):

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

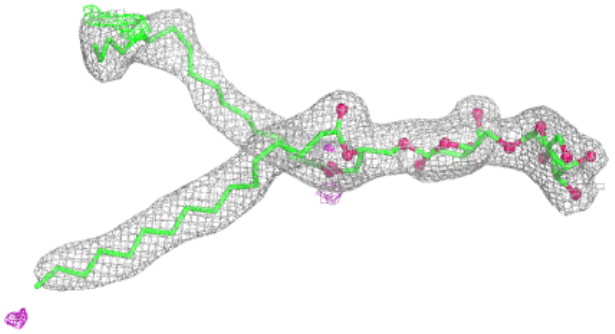


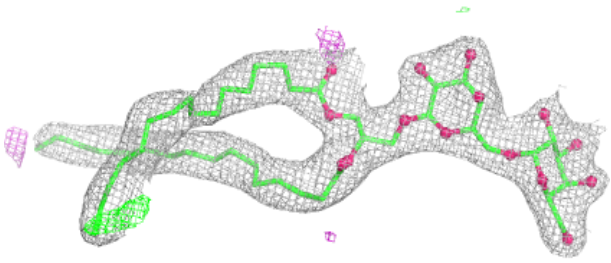


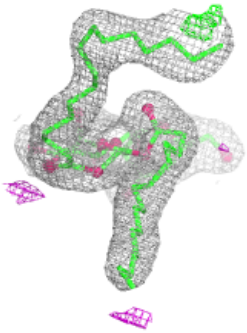


Electron density around DGD C 516 (B):

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

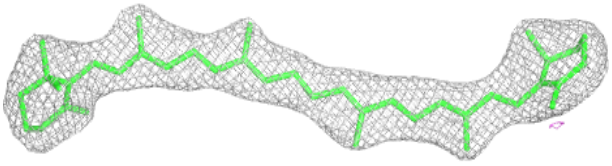


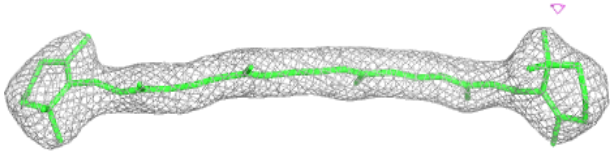


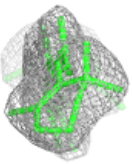


Electron density around BCR y 101:

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

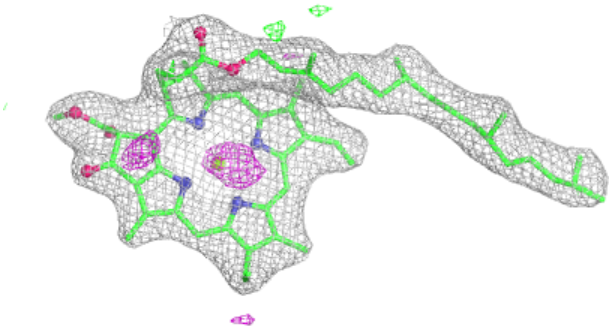


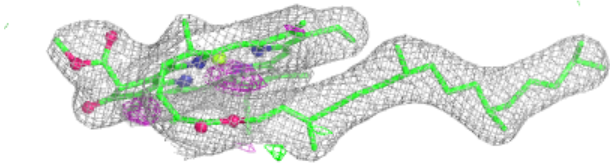


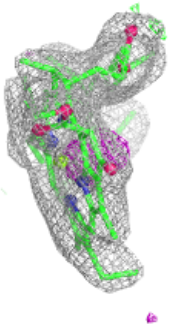


Electron density around CLA C 501:

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

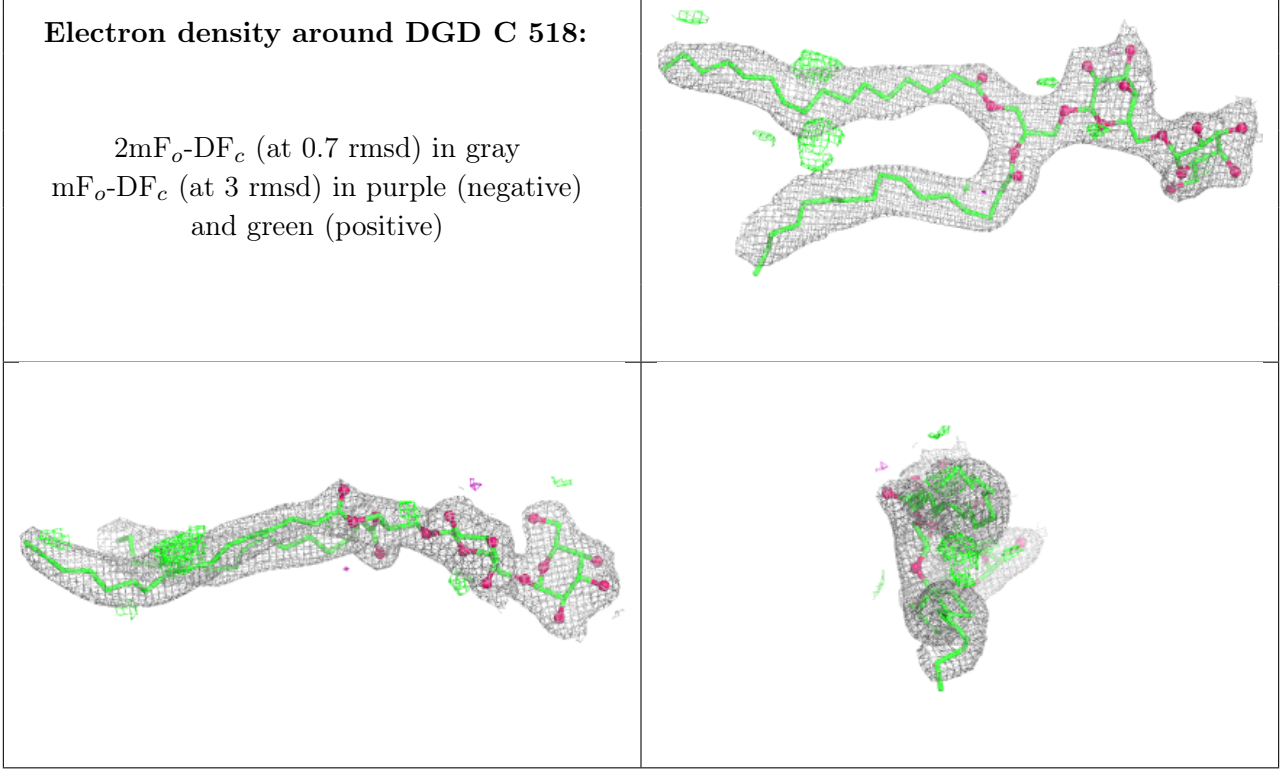






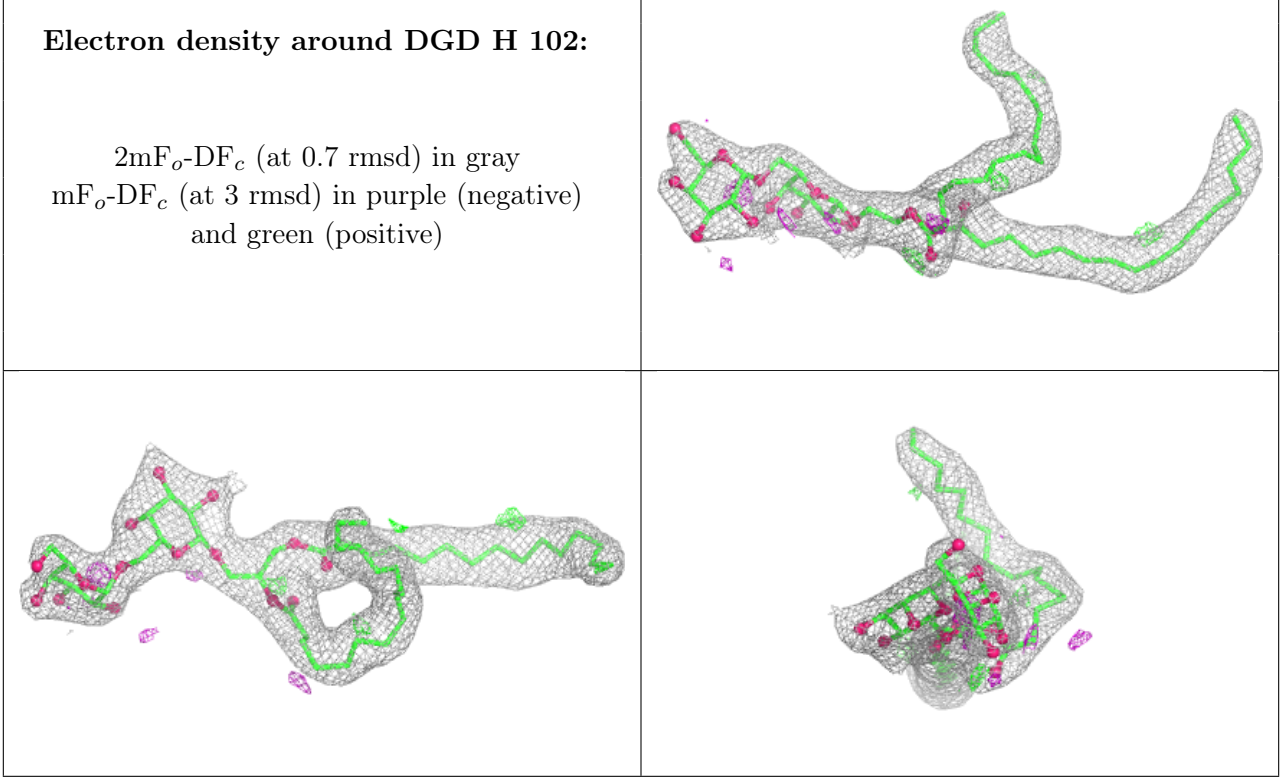
Electron density around DGD C 518:

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



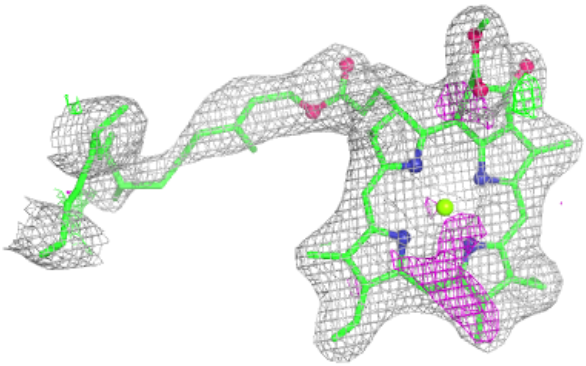
Electron density around DGD H 102:

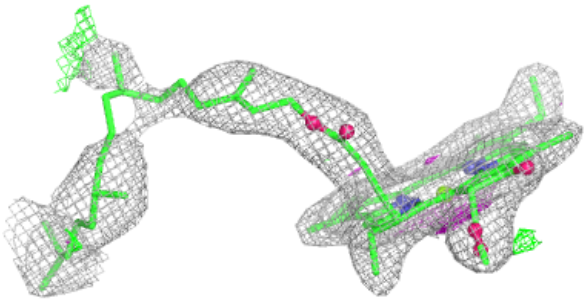
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

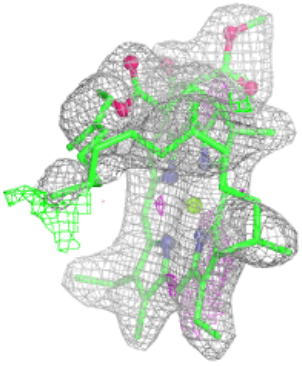


Electron density around CLA A 408:

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

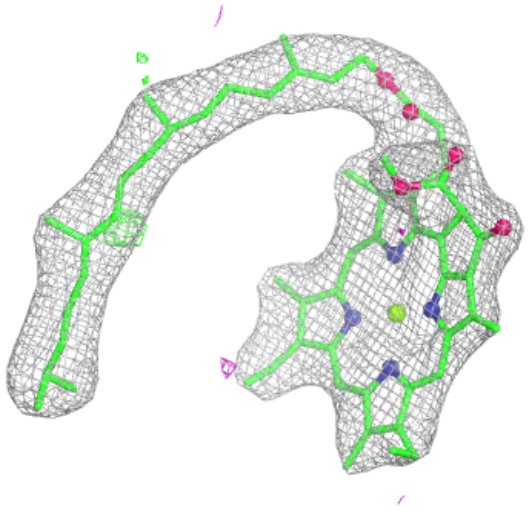


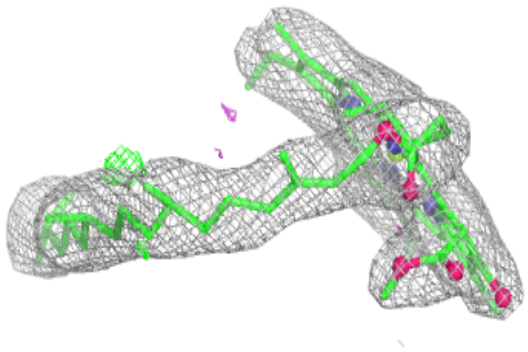


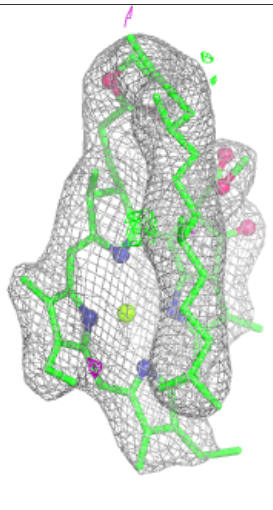


Electron density around CLA c 508:

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

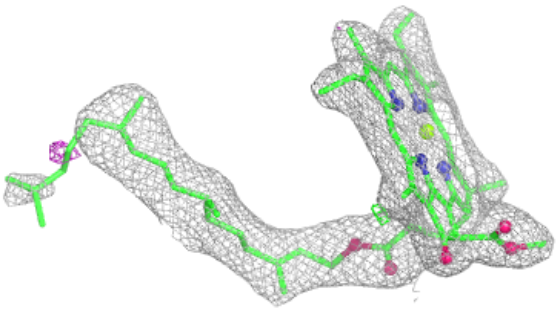


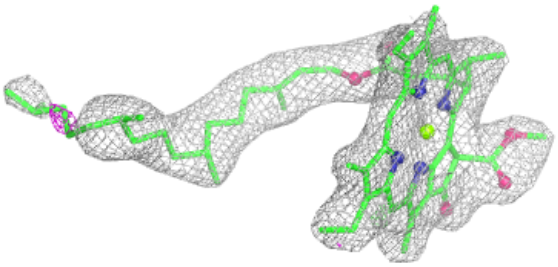


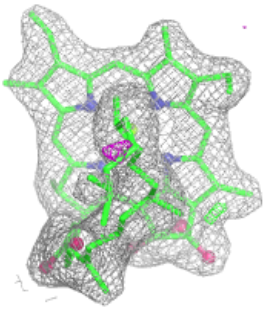


Electron density around CLA c 509:

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

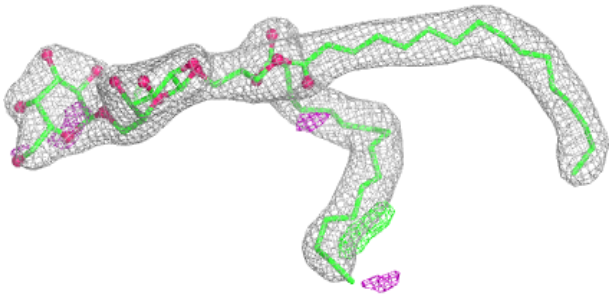


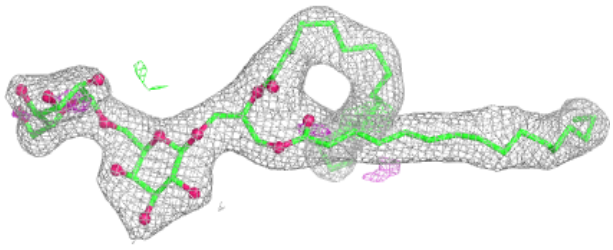




Electron density around DGD h 102:

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

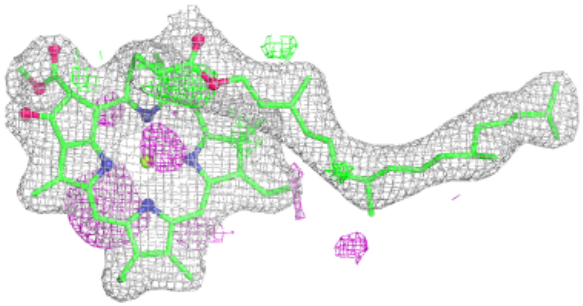


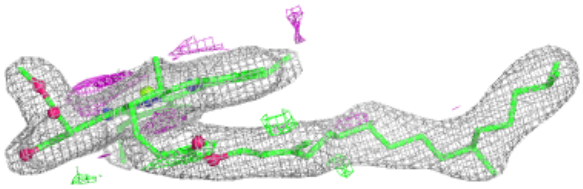


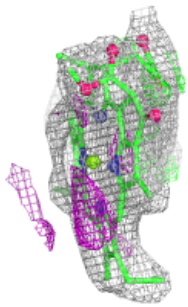


Electron density around CLA B 603:

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

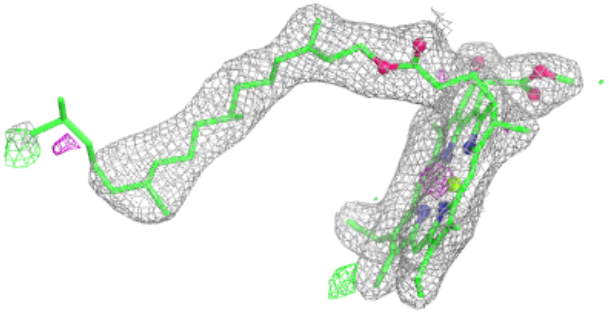


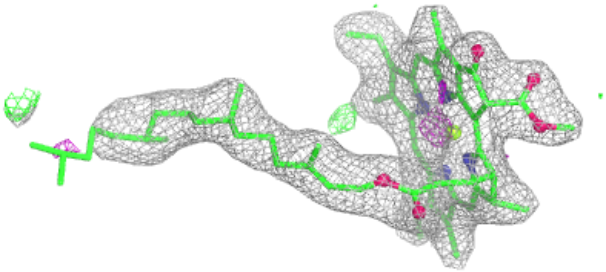


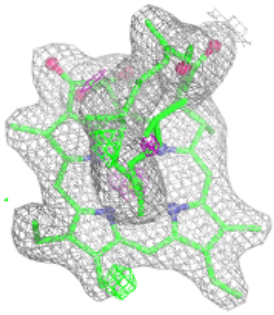


Electron density around CLA C 508:

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

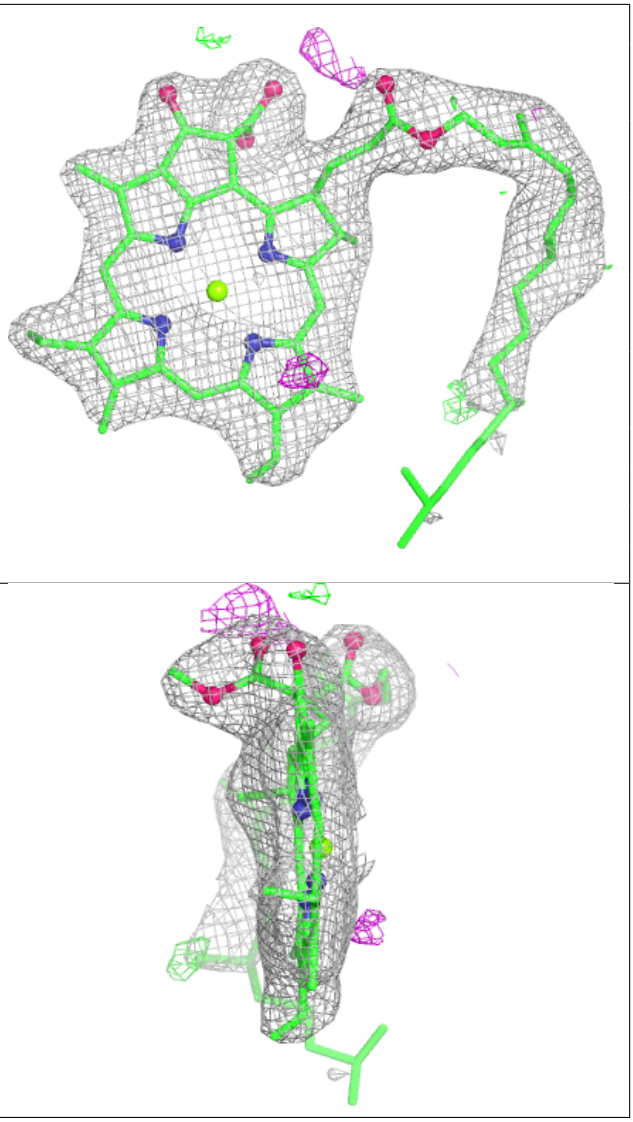


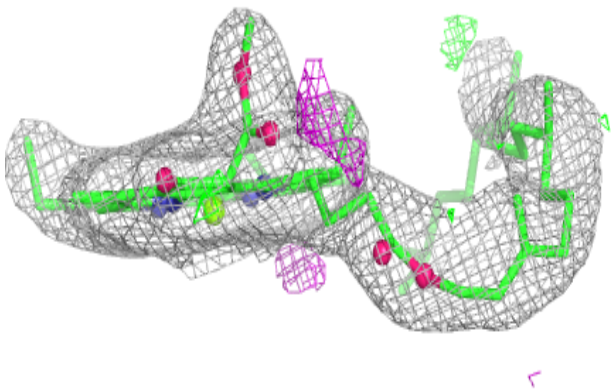




Electron density around CLA C 512:

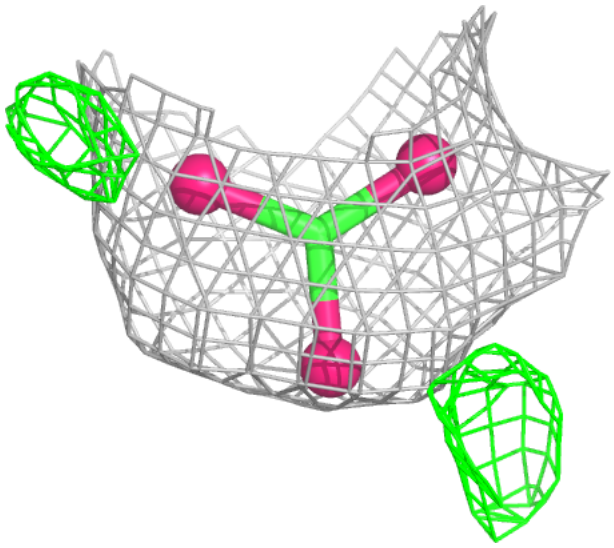
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

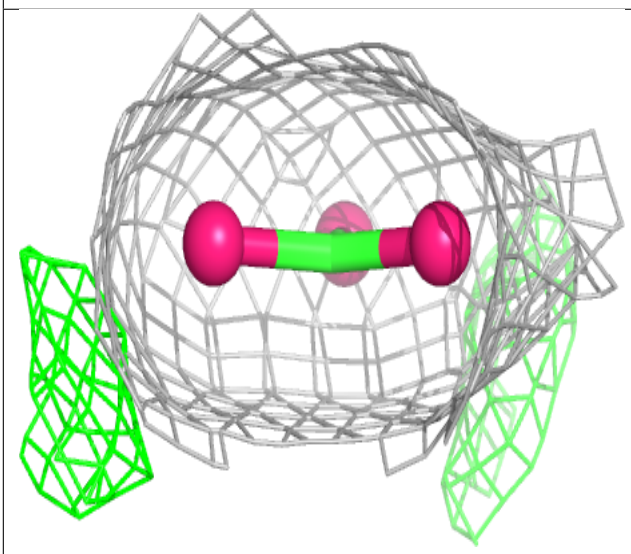


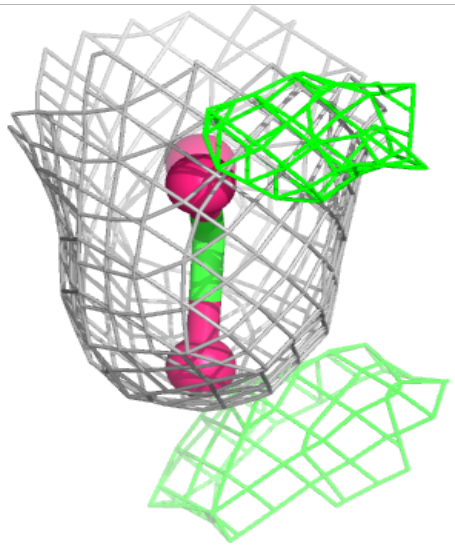


Electron density around BCT d 401 (A):

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

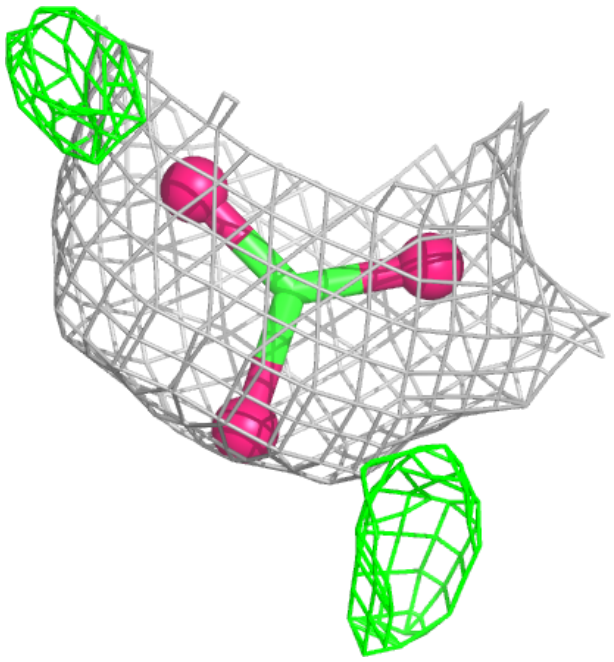


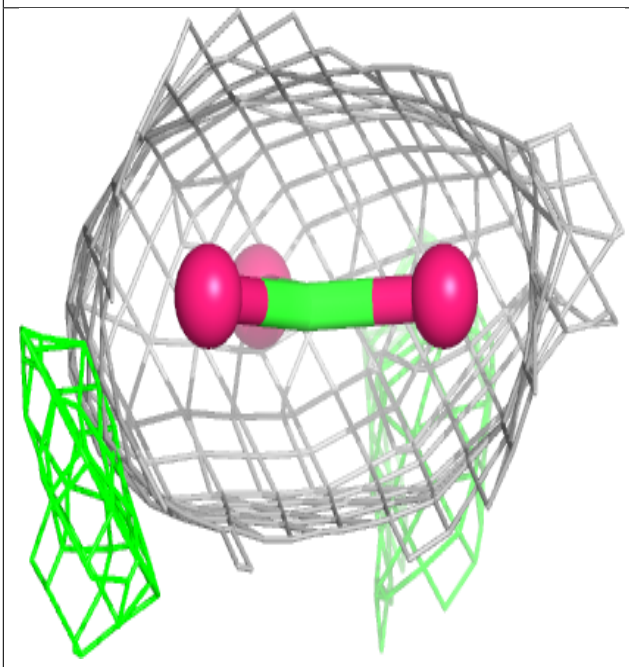


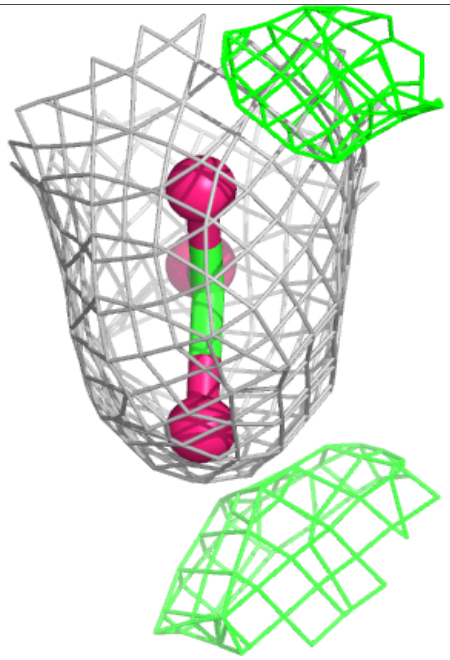


Electron density around BCT d 401 (B):

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

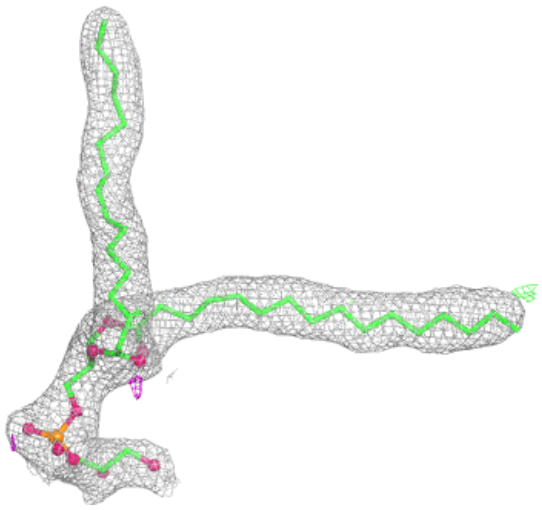


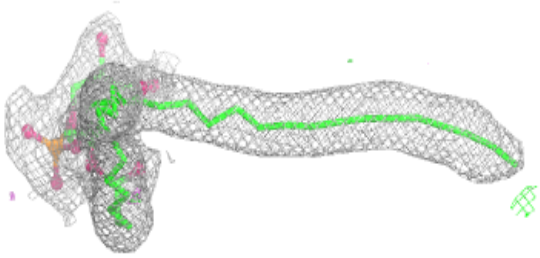


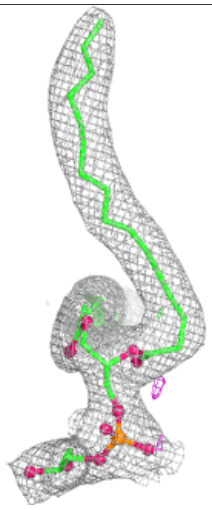


Electron density around LHG L 101 (A):

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

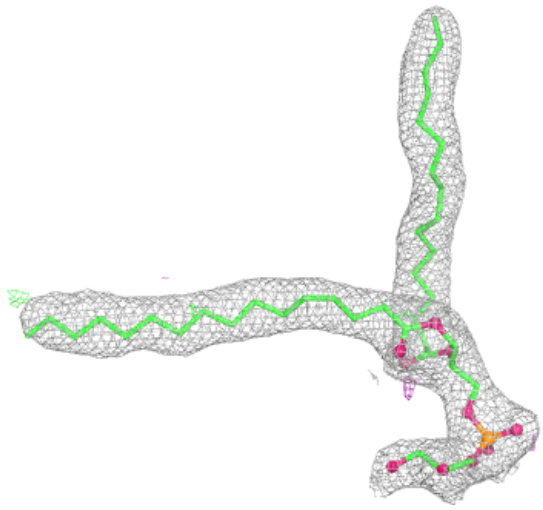


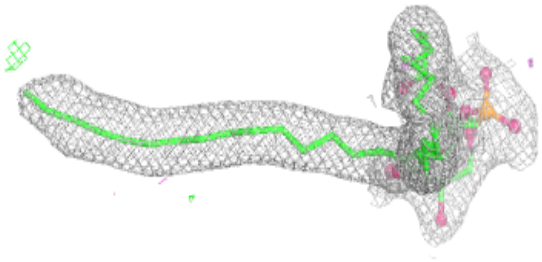


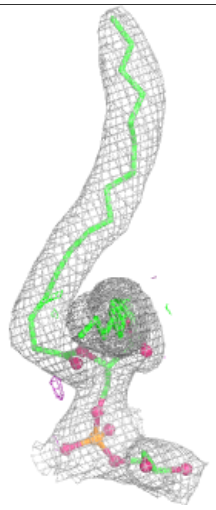


Electron density around LHG L 101 (B):

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

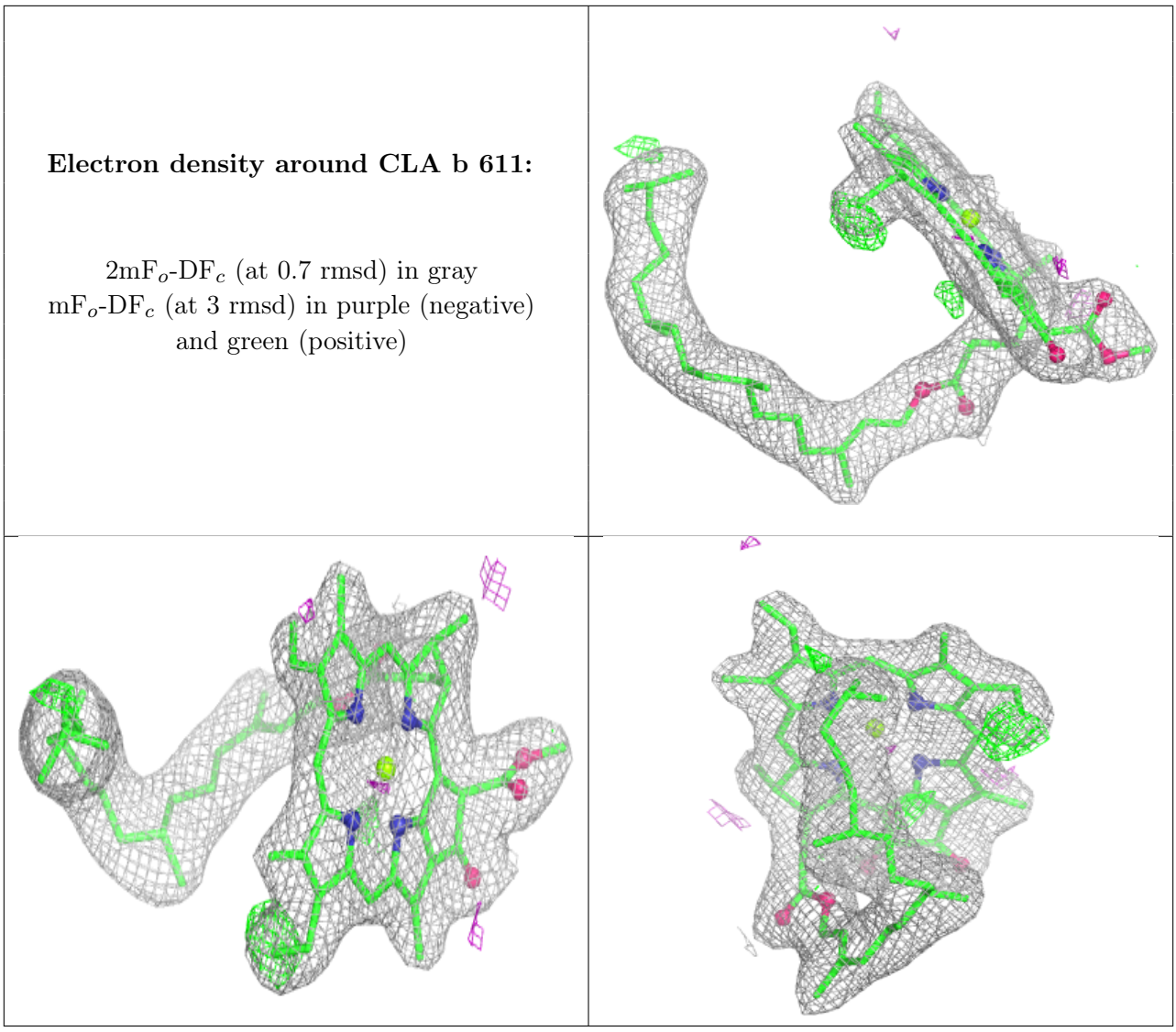






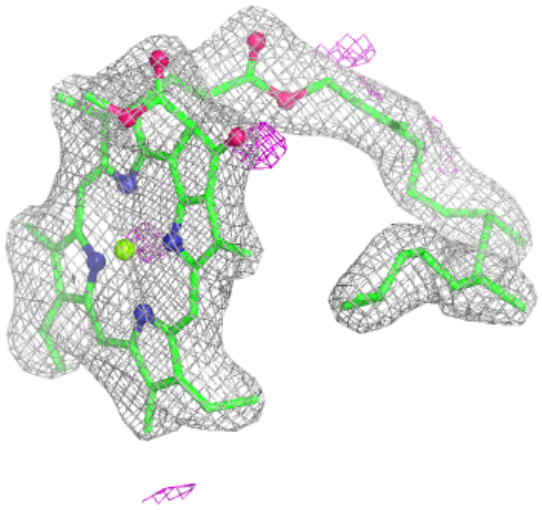
Electron density around CLA b 611:

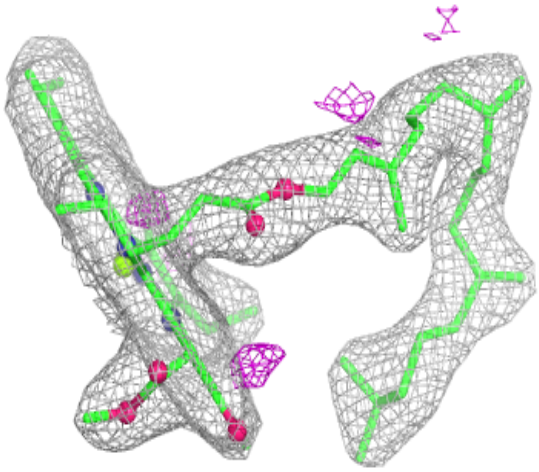
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

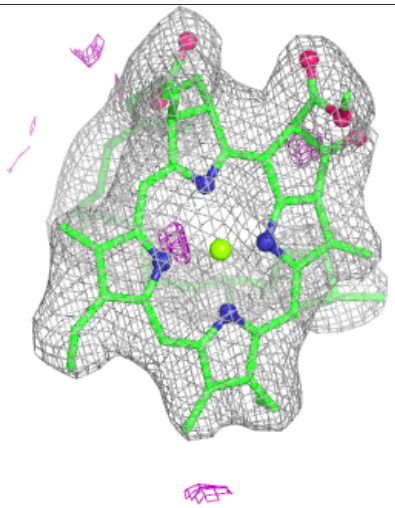


Electron density around CLA C 503:

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

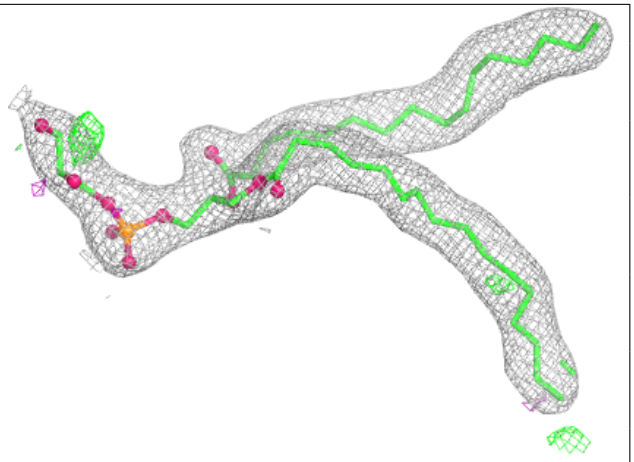


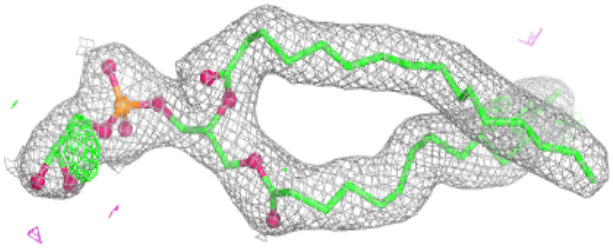




Electron density around LHG d 407 (A):

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

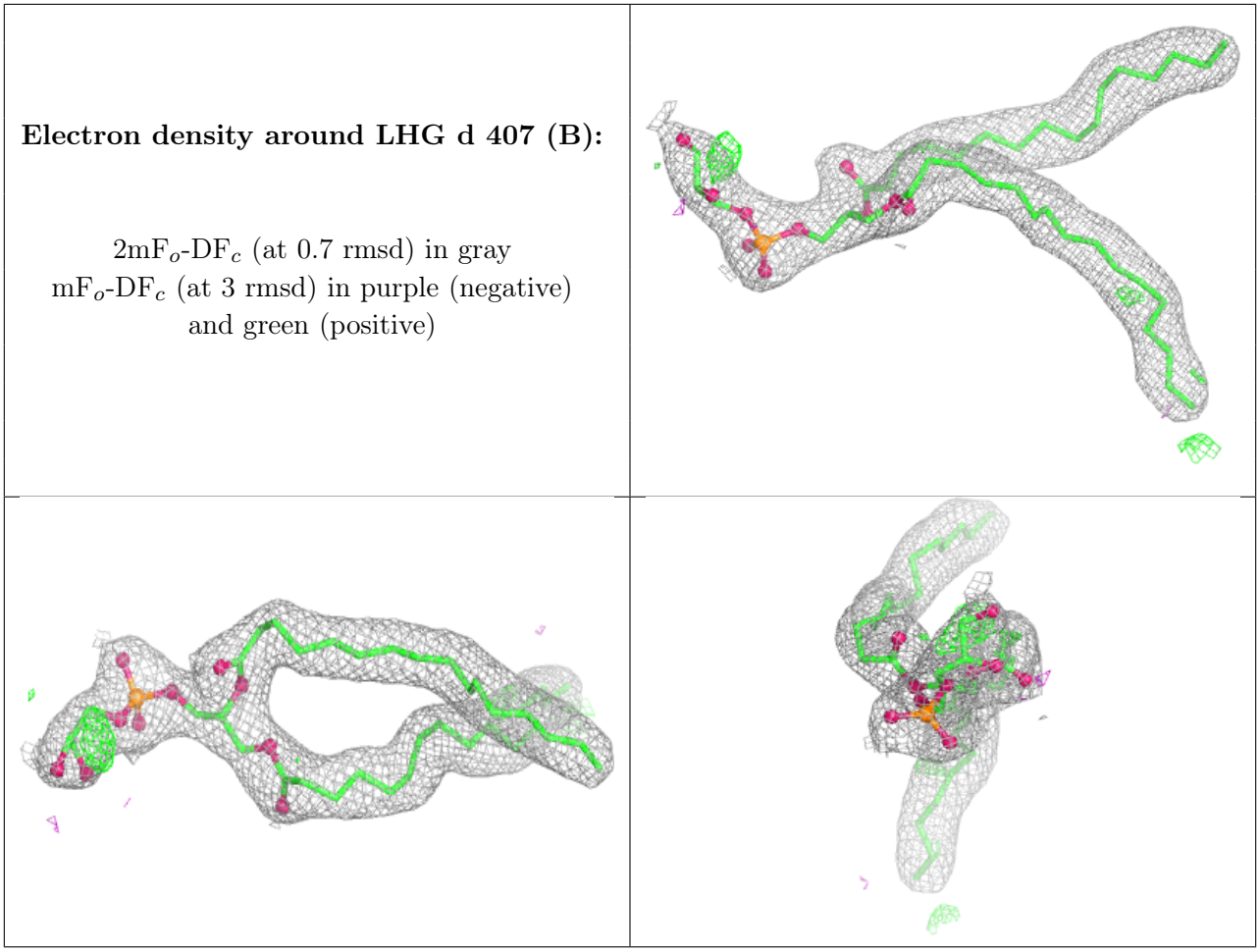






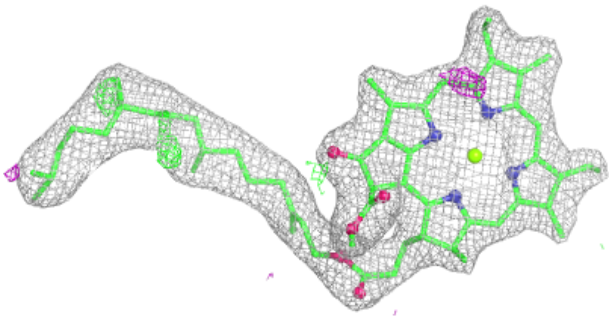
Electron density around LHG d 407 (B):

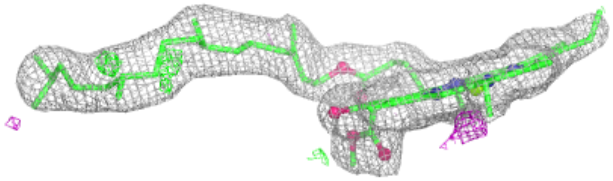
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

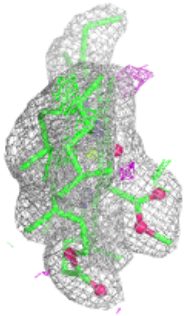


Electron density around CLA B 602:

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

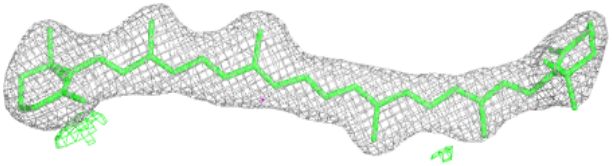


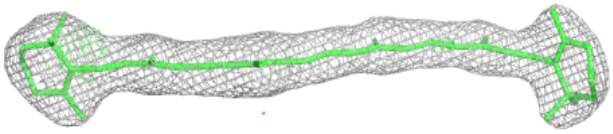


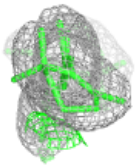


Electron density around BCR c 516:

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

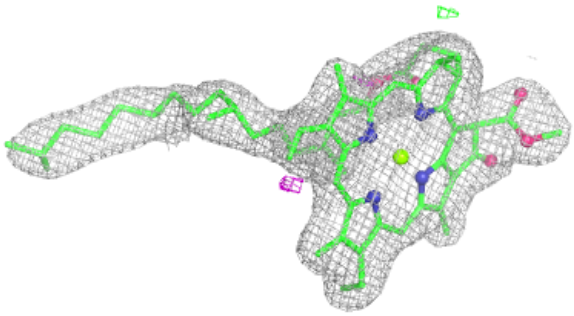


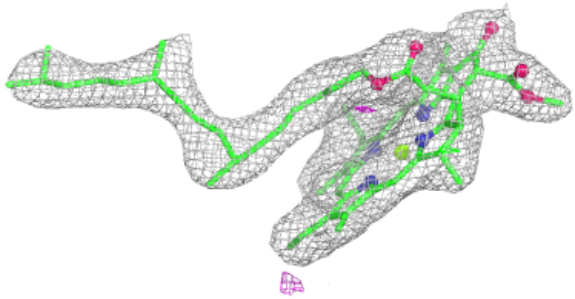


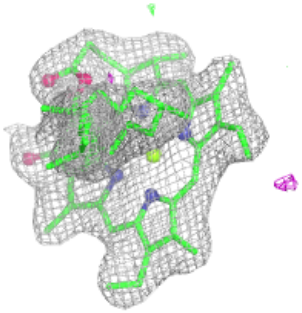


Electron density around CLA C 505:

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

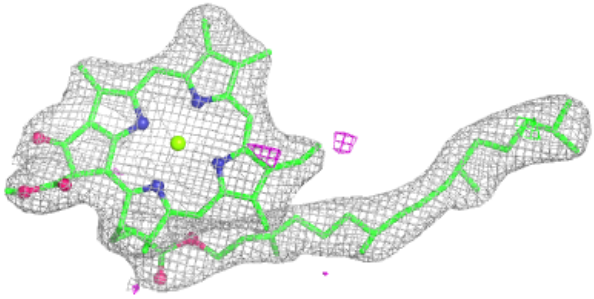


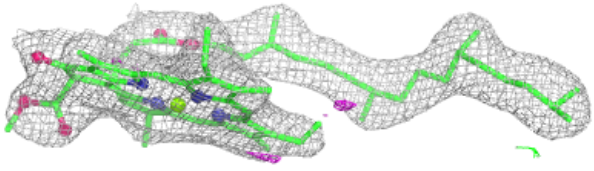


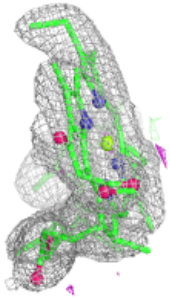


Electron density around CLA c 502:

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

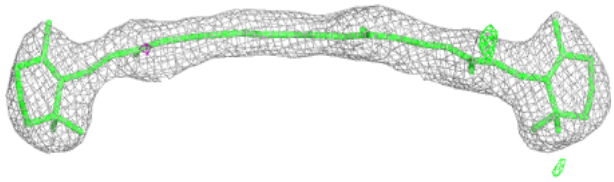


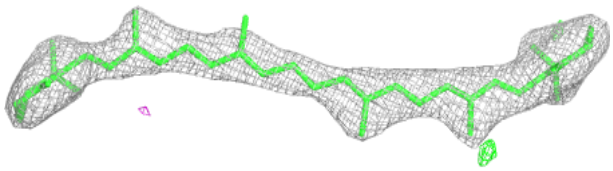


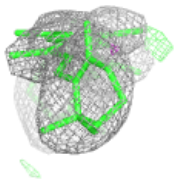


Electron density around BCR k 101:

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

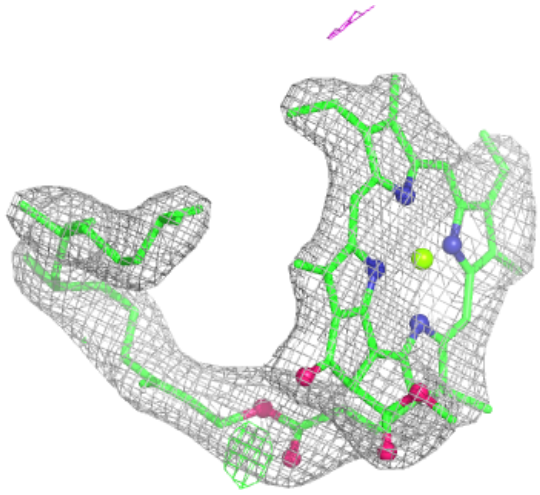


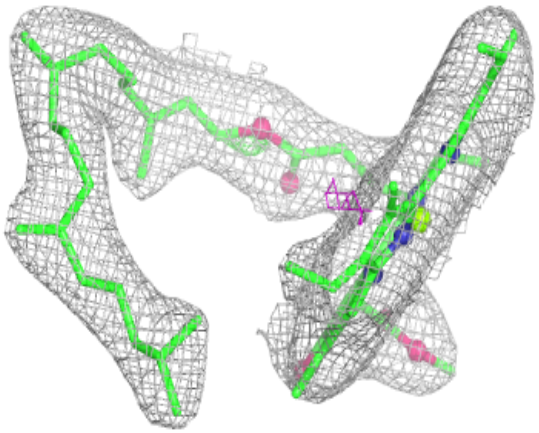


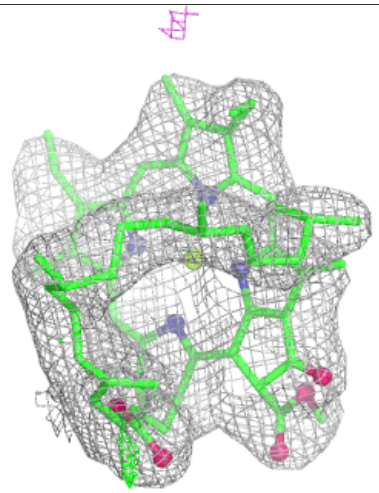


Electron density around CLA c 504:

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

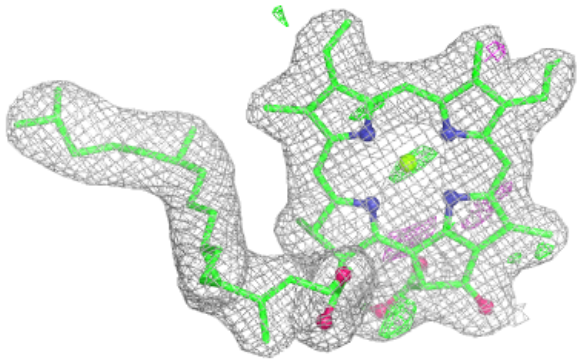


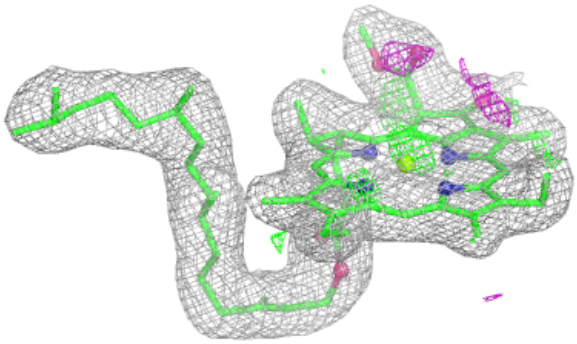


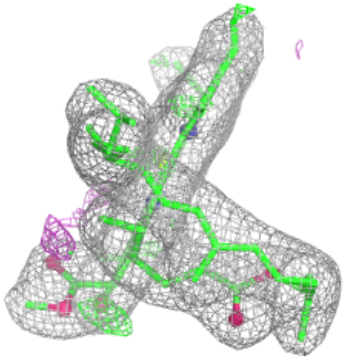


Electron density around CLA A 405 (A):

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

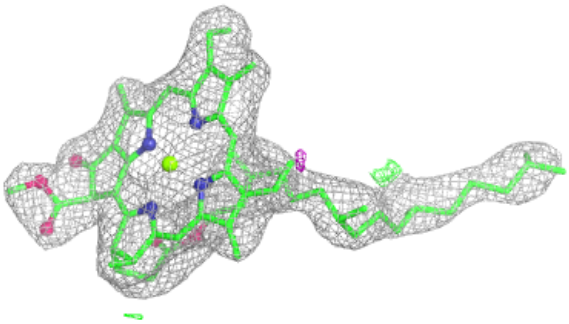


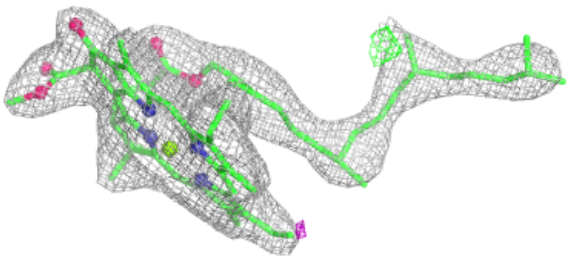


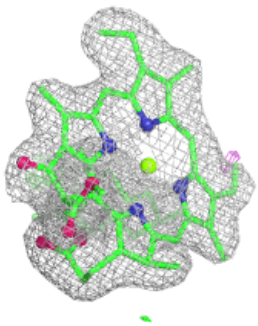


Electron density around CLA c 506:

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

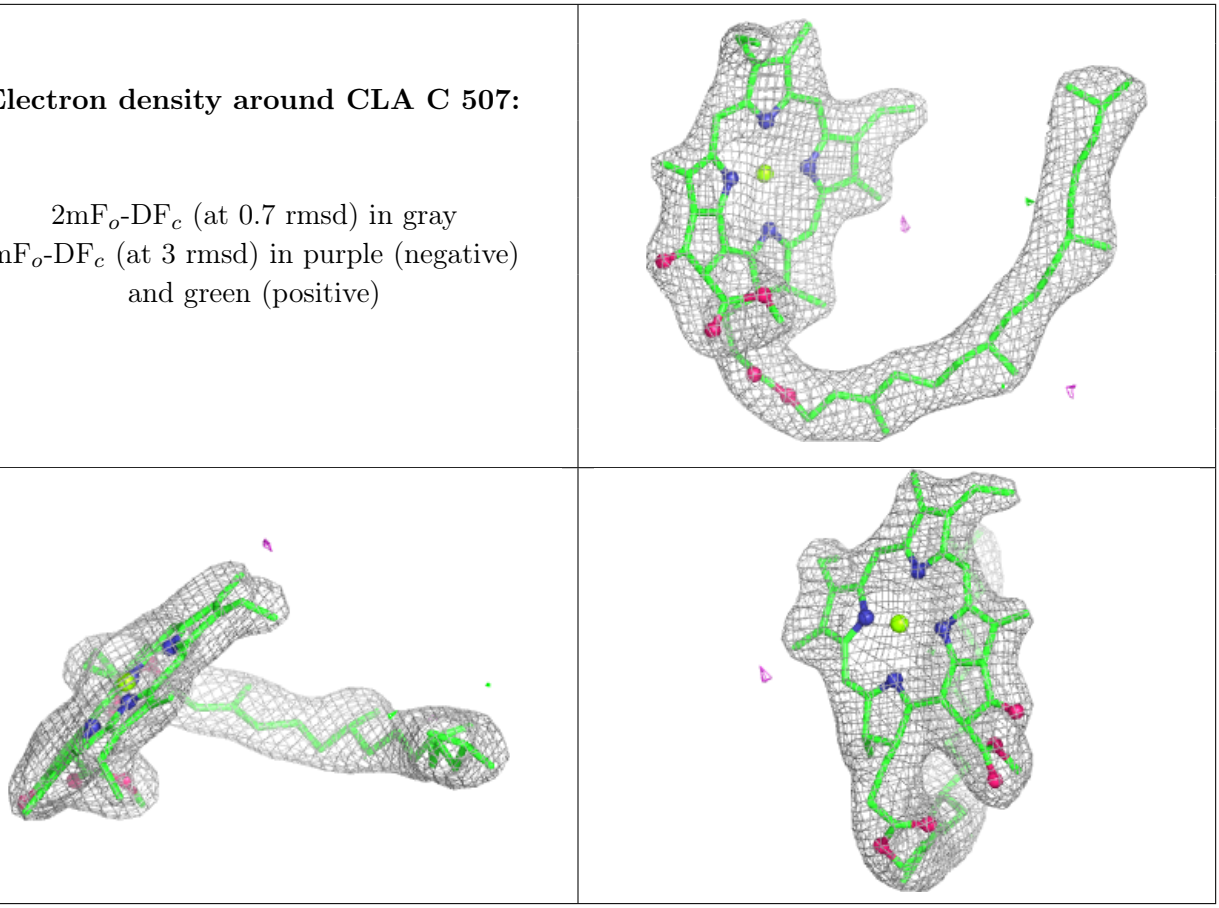






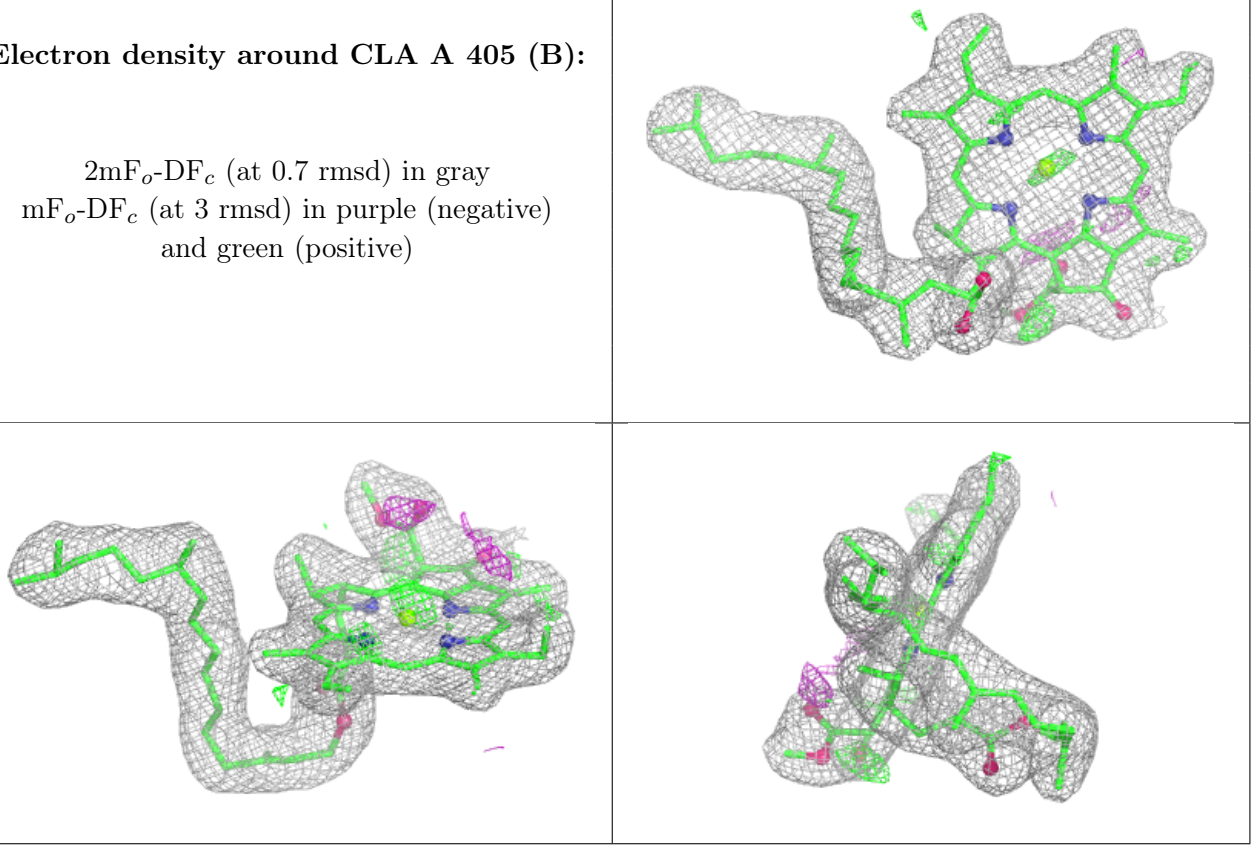
Electron density around CLA C 507:

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



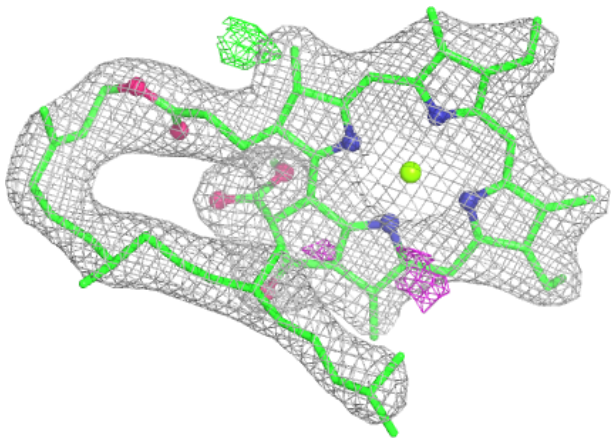
Electron density around CLA A 405 (B):

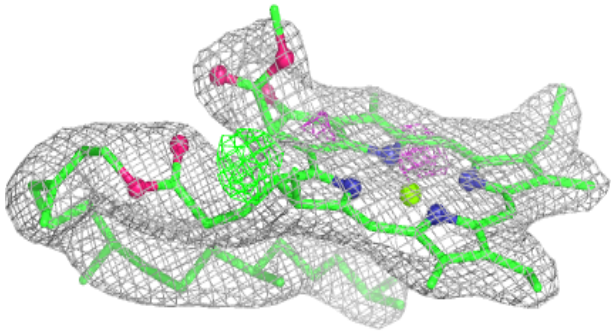
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

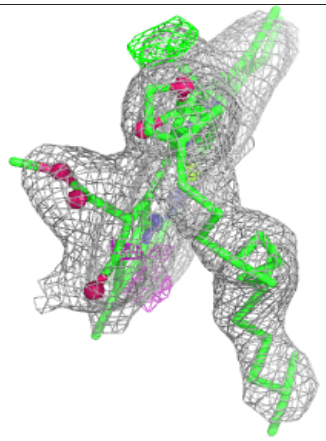


Electron density around CLA C 509:

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

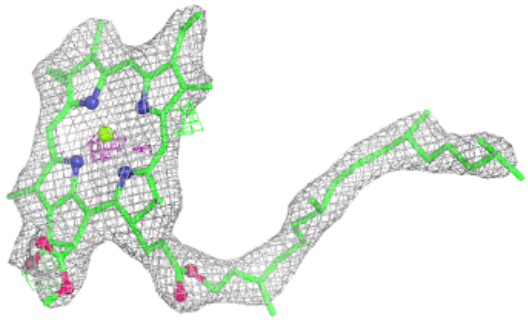


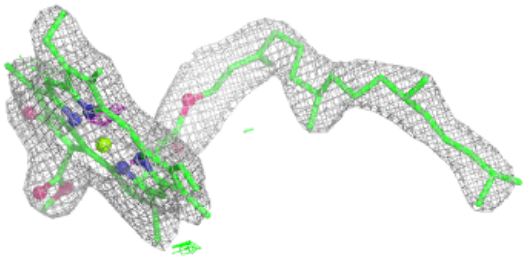


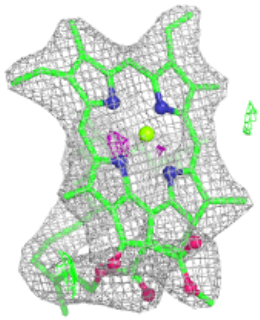


Electron density around CLA c 512:

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

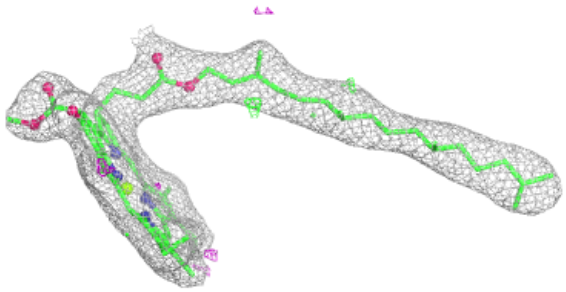


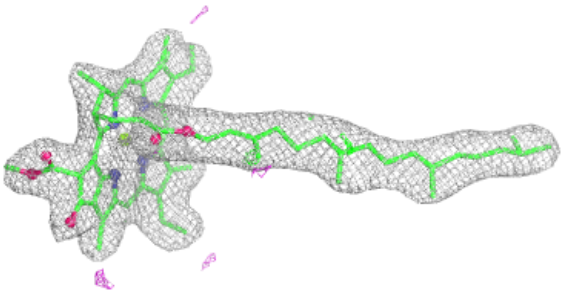


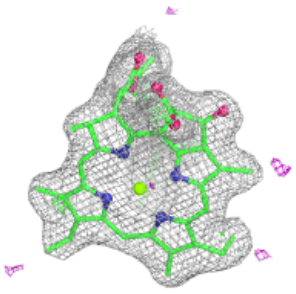


Electron density around CLA B 607:

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

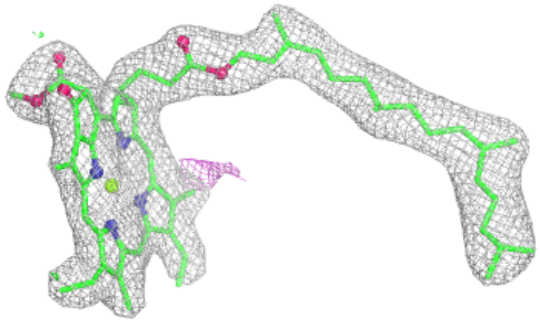


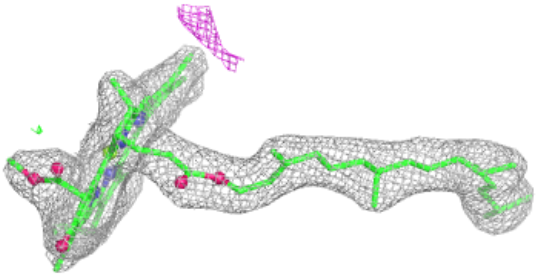


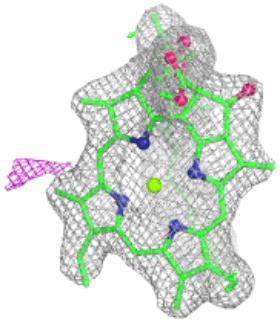


Electron density around CLA B 609:

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

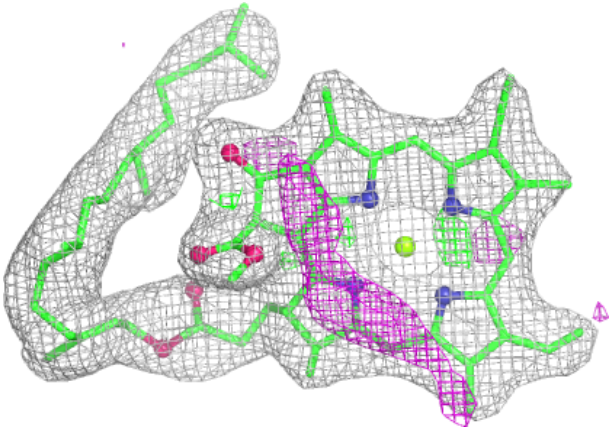


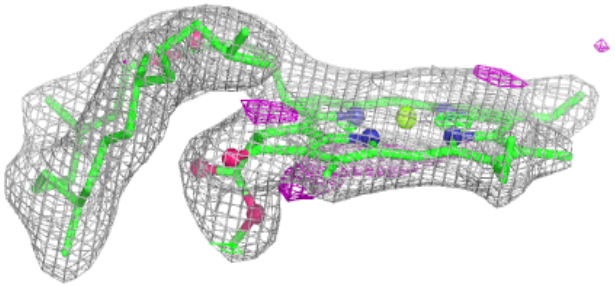


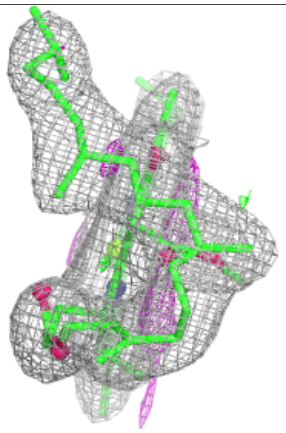


Electron density around CLA B 610:

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

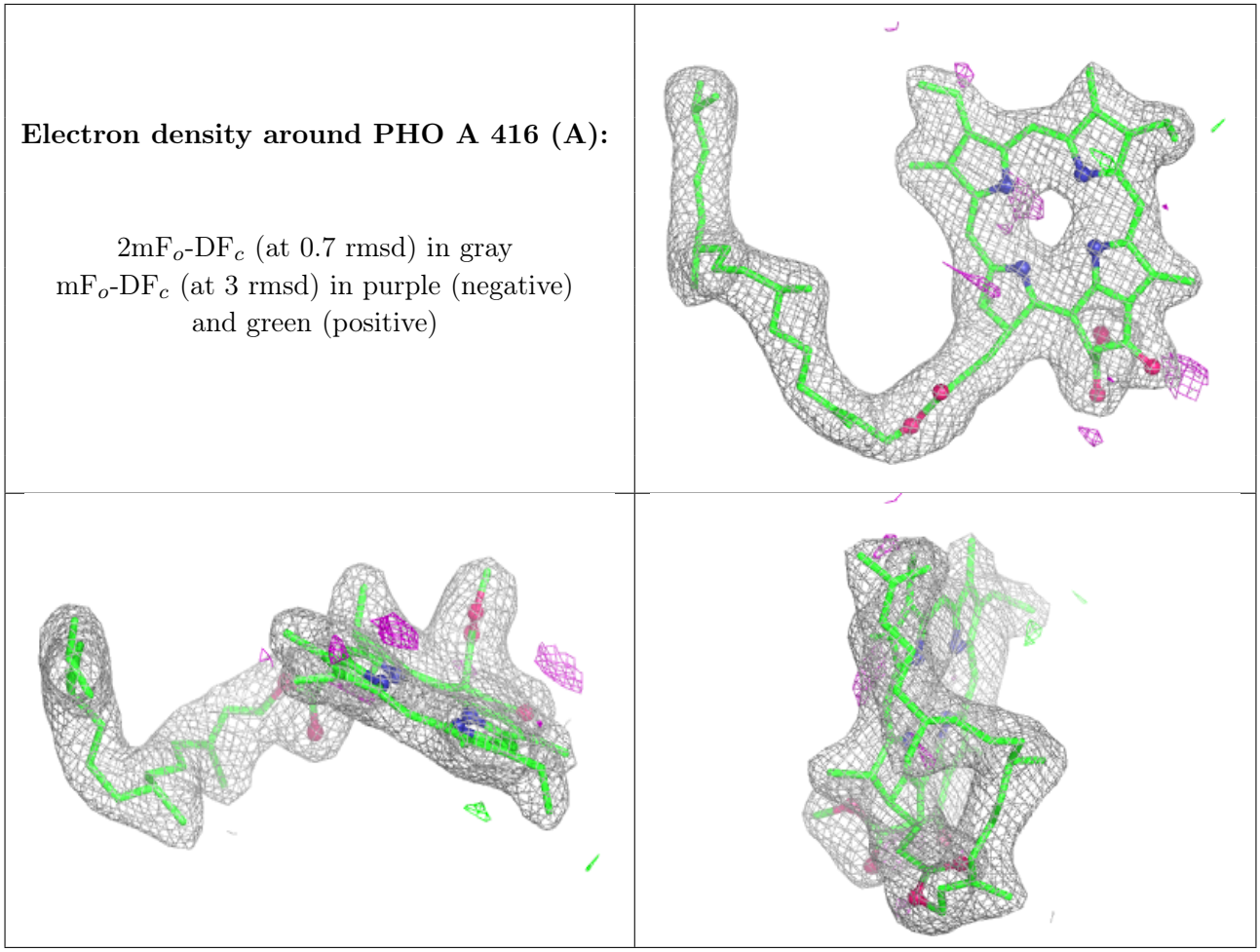






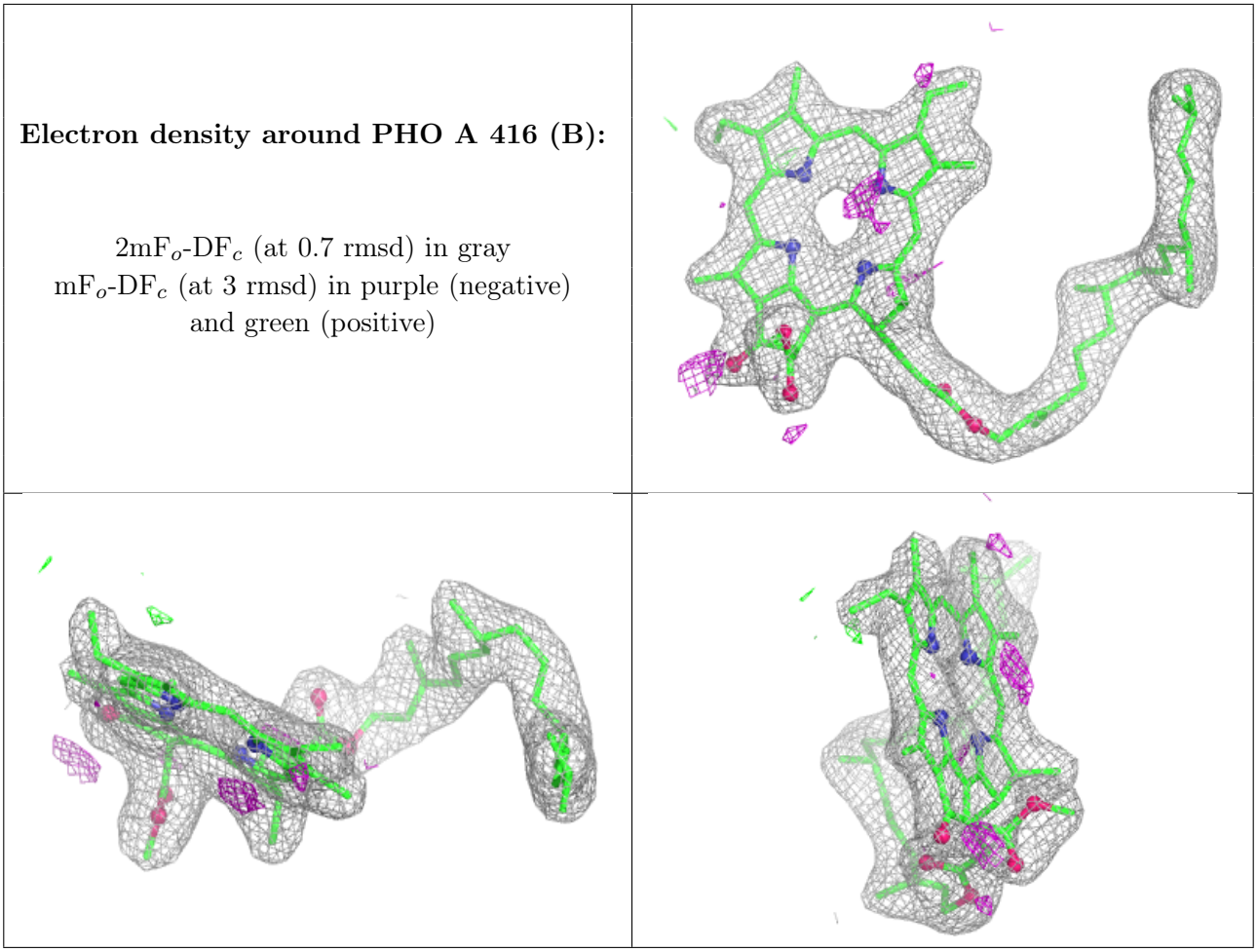
Electron density around PHO A 416 (A):

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



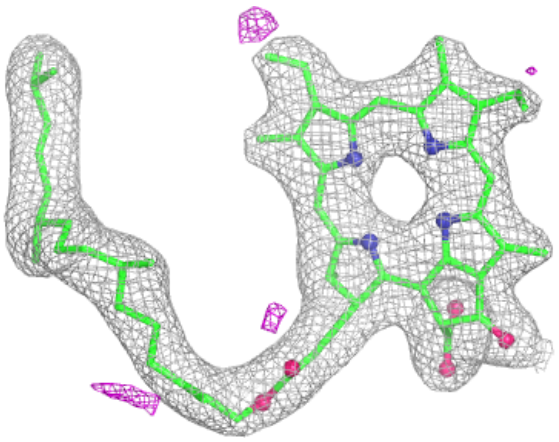
Electron density around PHO A 416 (B):

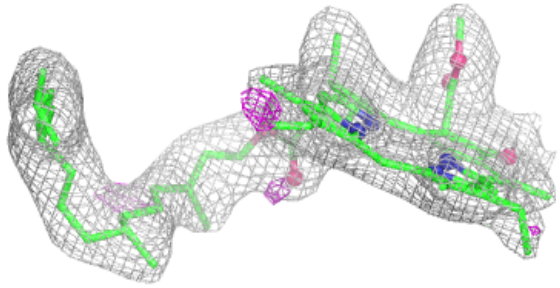
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

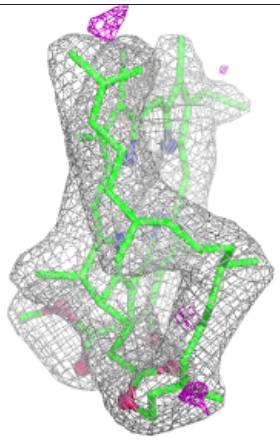


Electron density around PHO a 414 (A):

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

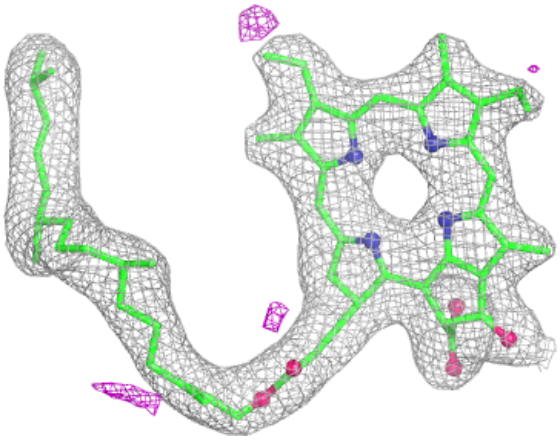


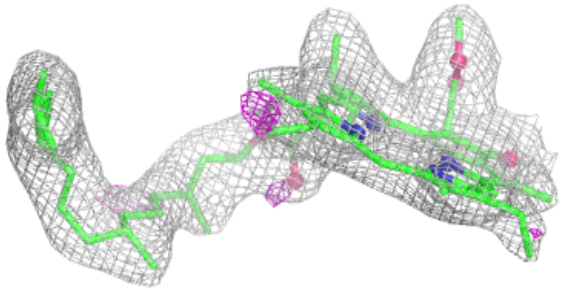


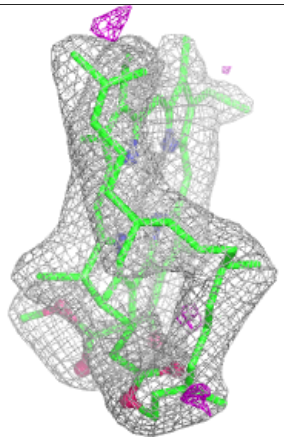


Electron density around PHO a 414 (B):

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

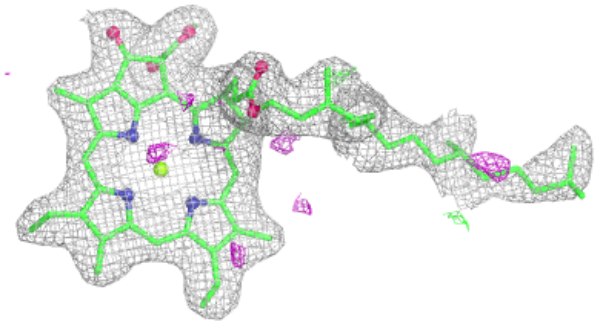


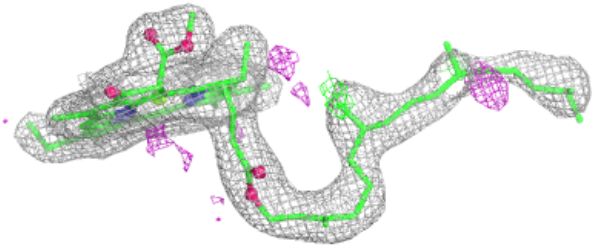


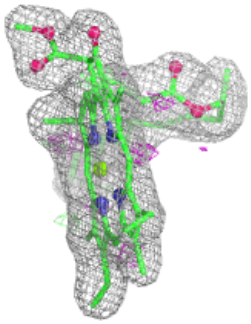


Electron density around CLA A 406 (A):

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

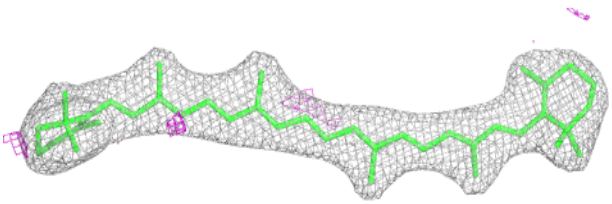


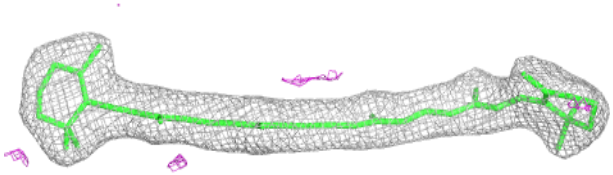


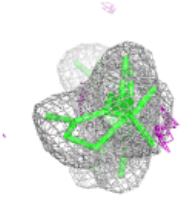


Electron density around BCR B 617:

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

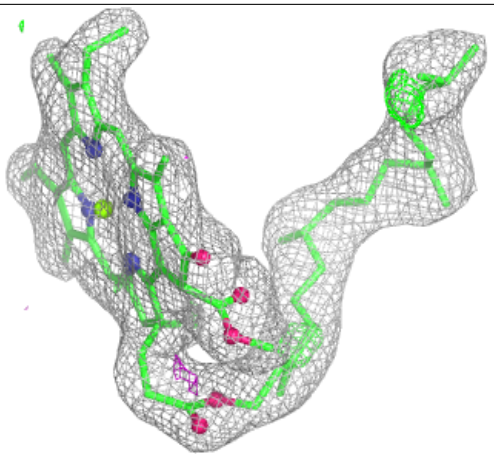


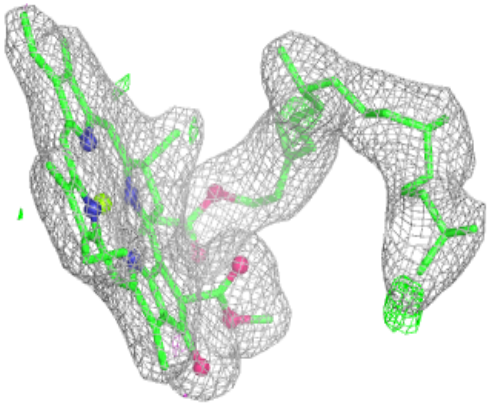


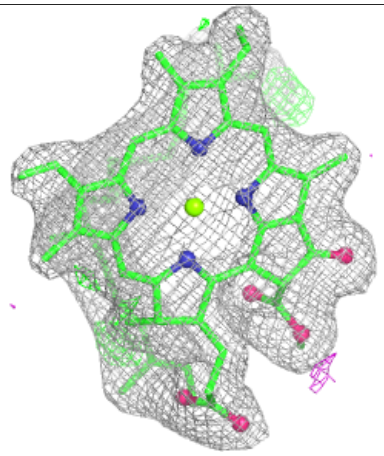


Electron density around CLA B 613:

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

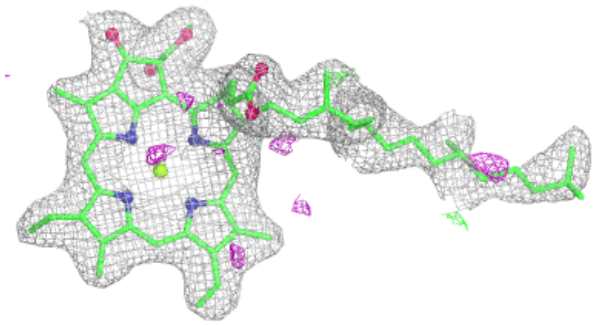


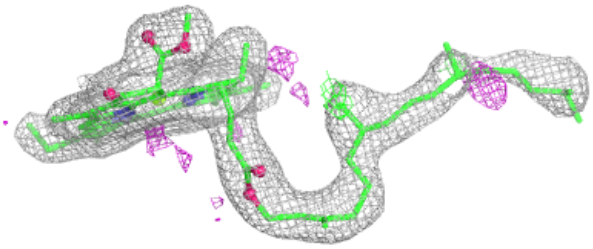


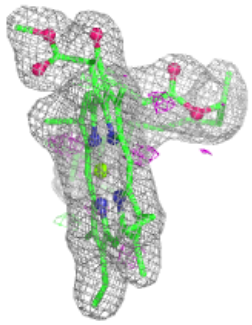


Electron density around CLA A 406 (B):

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

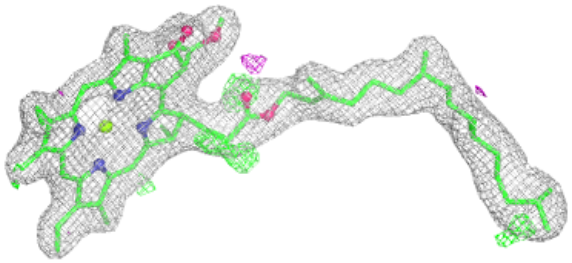


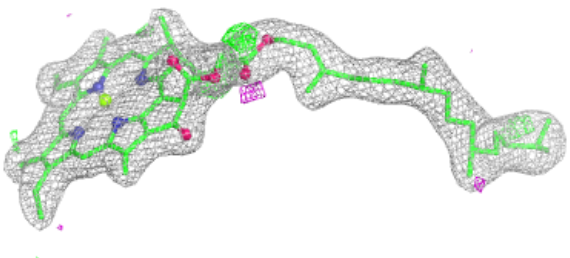




Electron density around CLA A 404 (A):

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

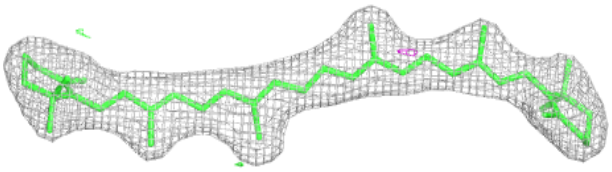


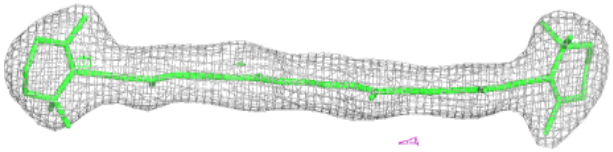


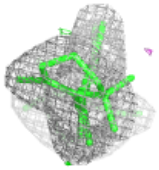


Electron density around BCR C 515:

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

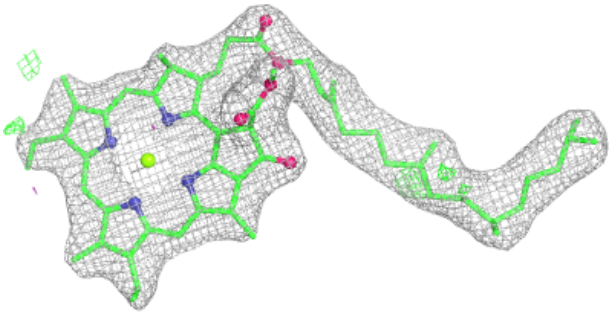


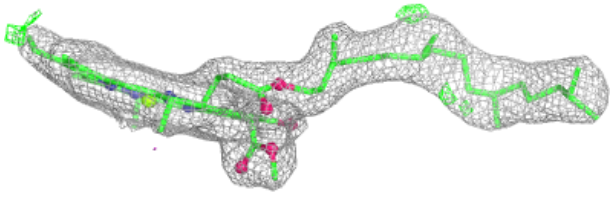


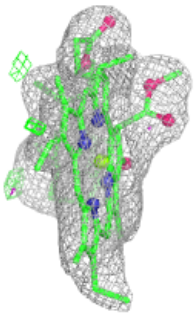


Electron density around CLA b 602:

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

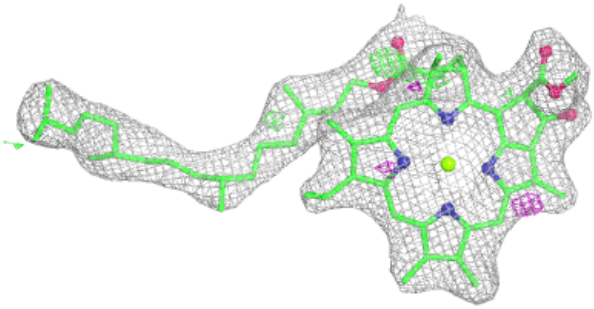


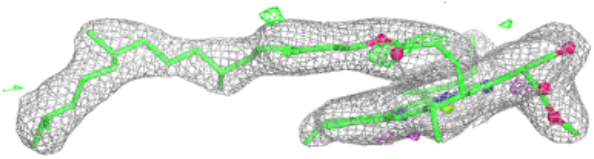


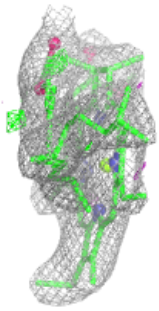


Electron density around CLA b 603:

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

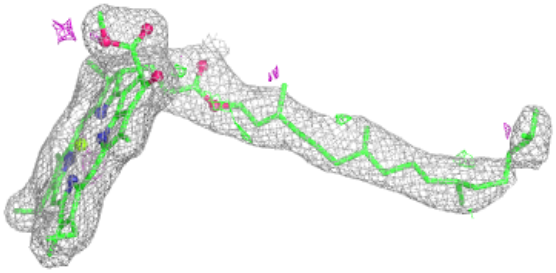


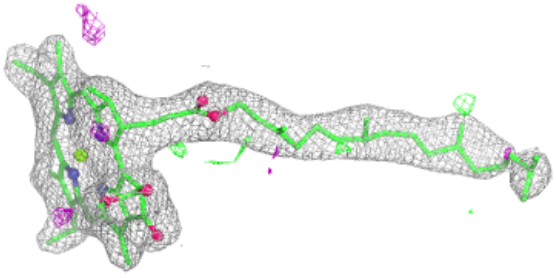


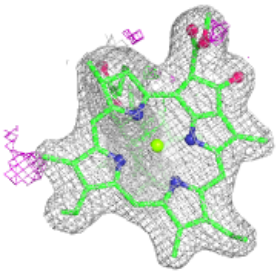


Electron density around CLA b 604:

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

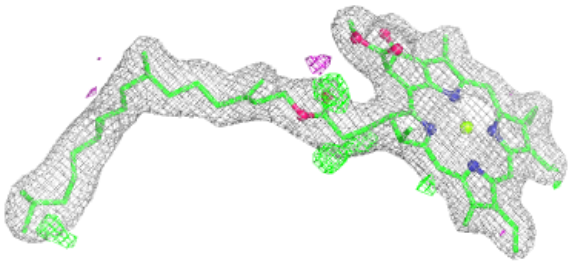


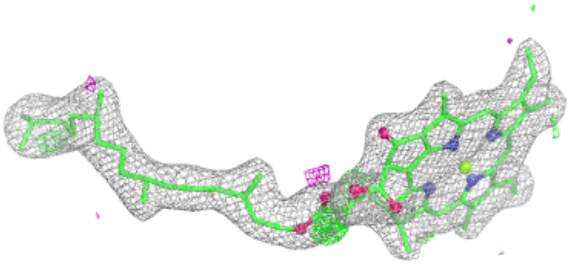


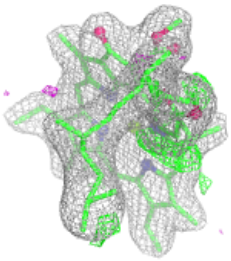


Electron density around CLA A 404 (B):

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

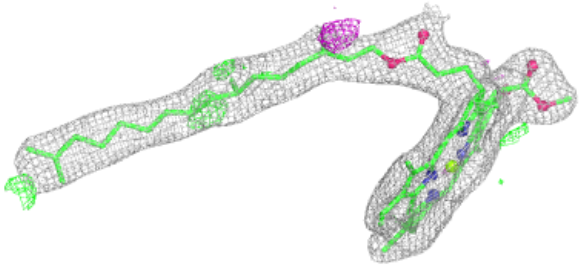


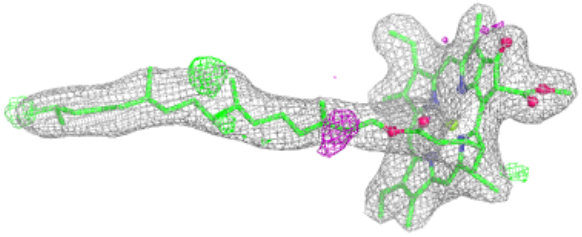


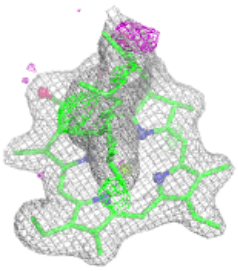


Electron density around CLA b 607:

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

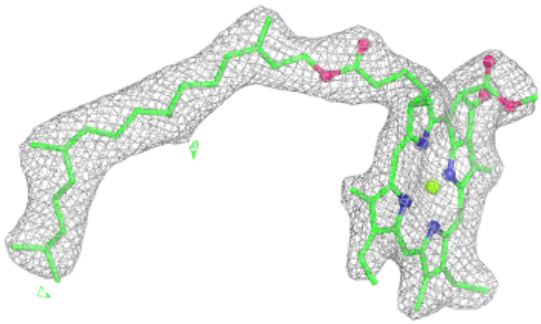


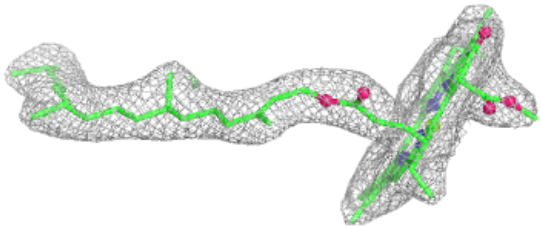


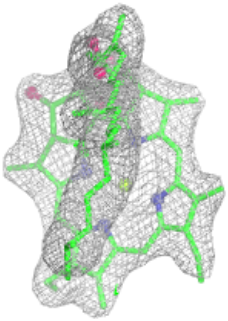


Electron density around CLA b 609:

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

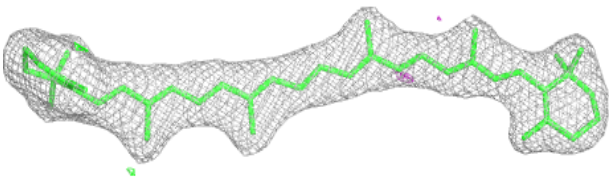


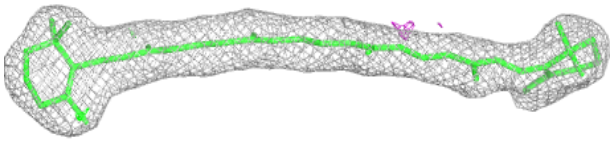


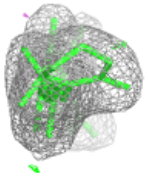


Electron density around BCR b 617:

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

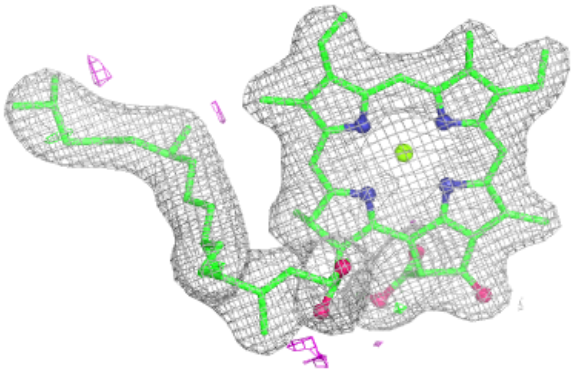


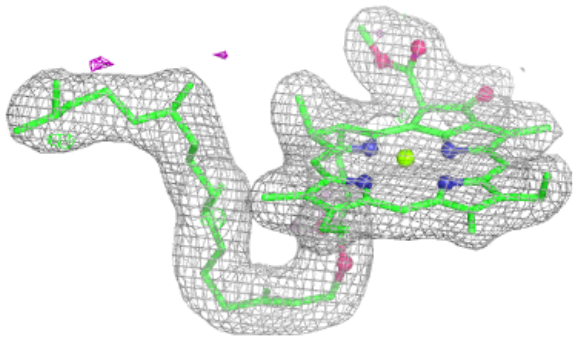


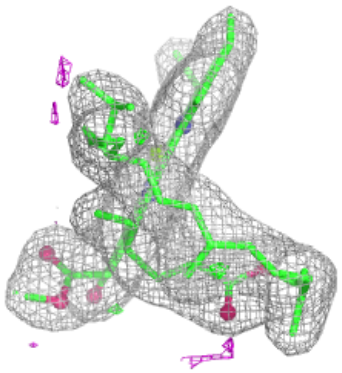


Electron density around CLA d 402 (A):

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

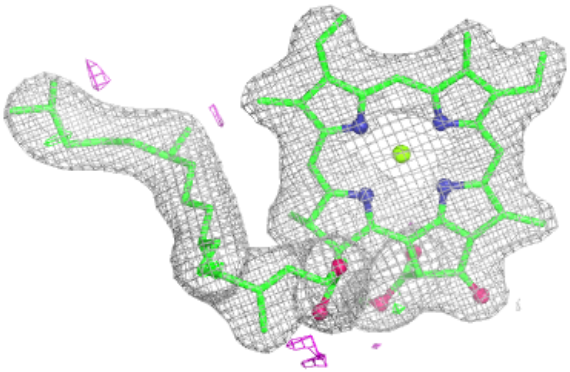


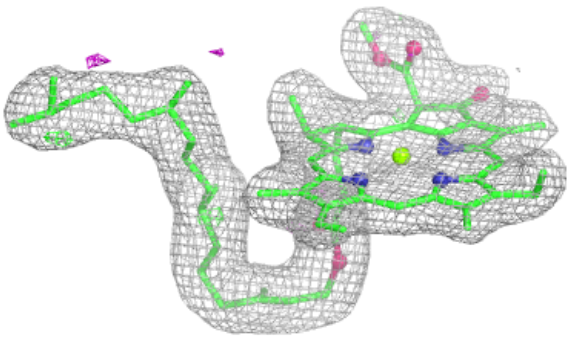


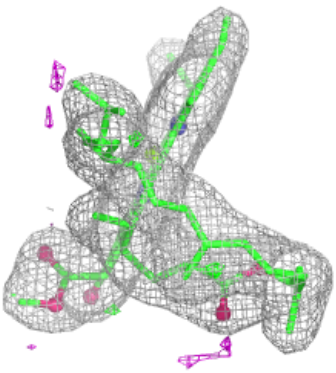


Electron density around CLA d 402 (B):

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

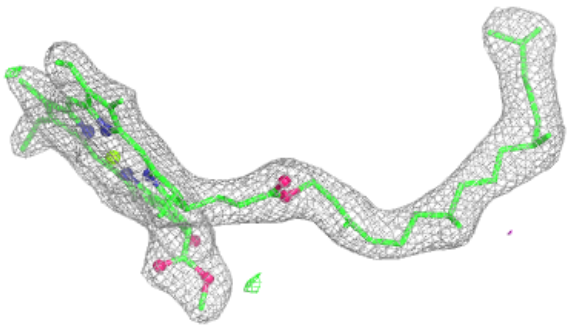


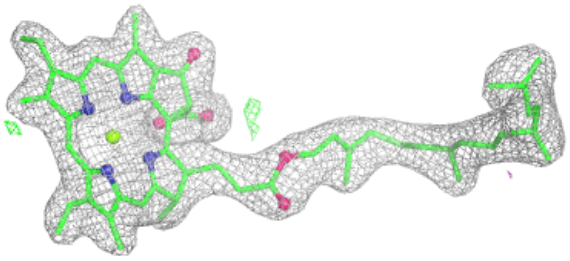


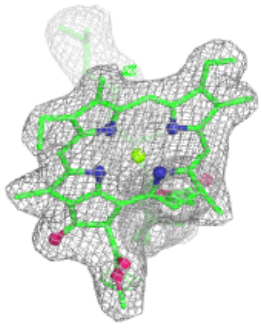


Electron density around CLA d 403 (A):

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

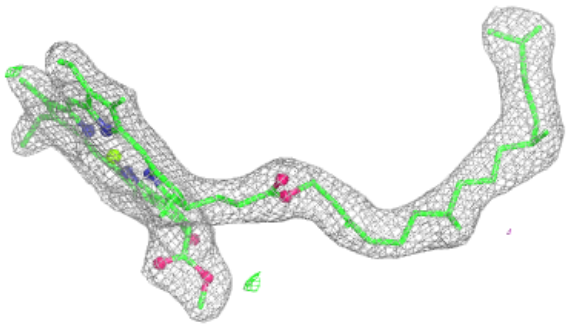


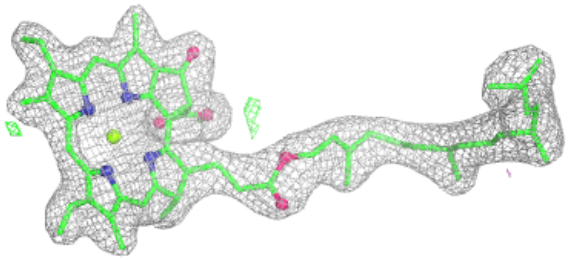


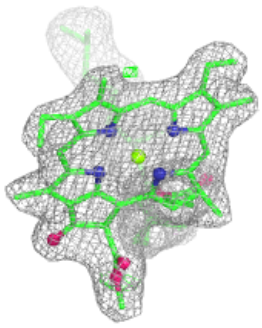


Electron density around CLA d 403 (B):

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

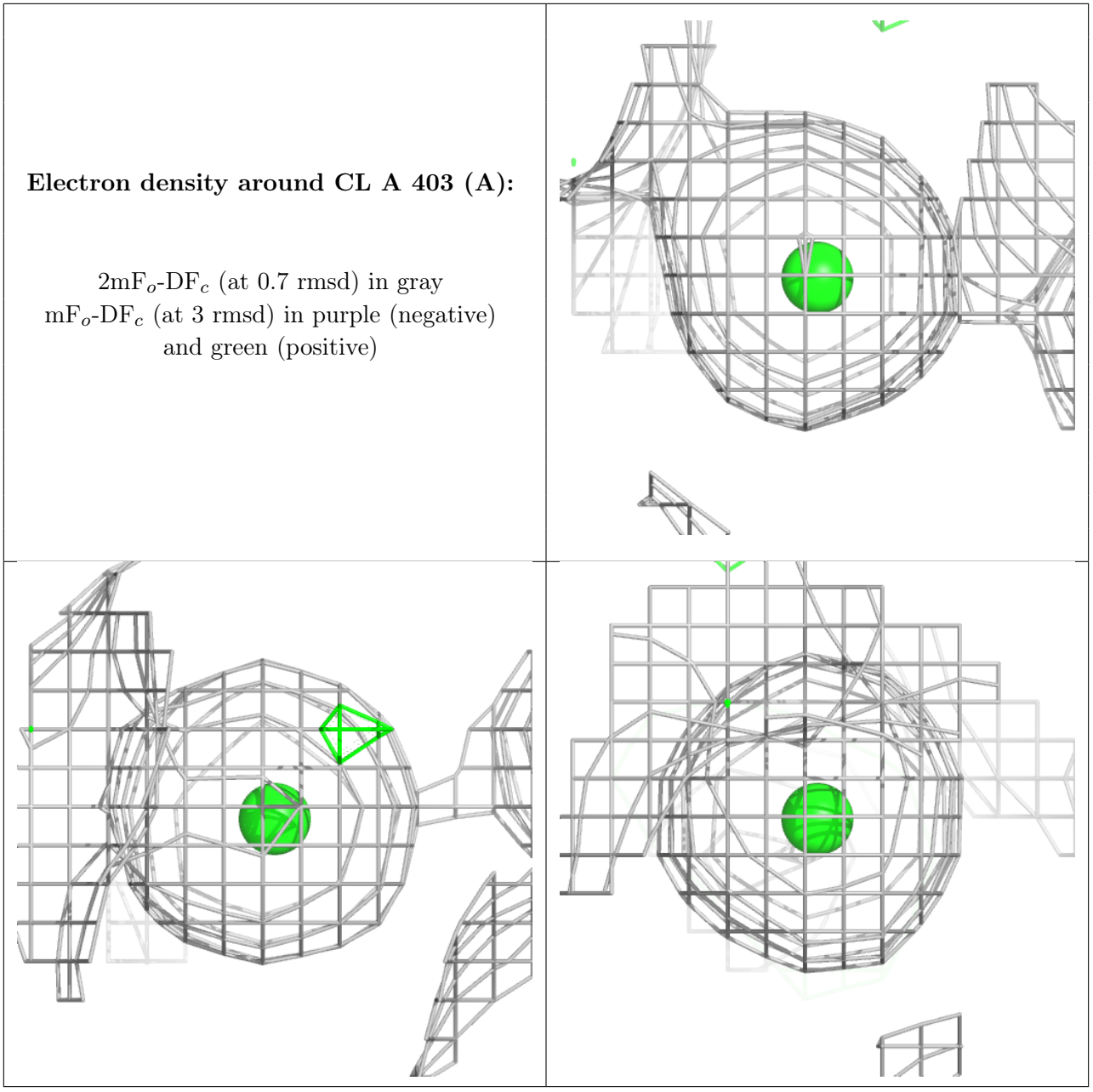






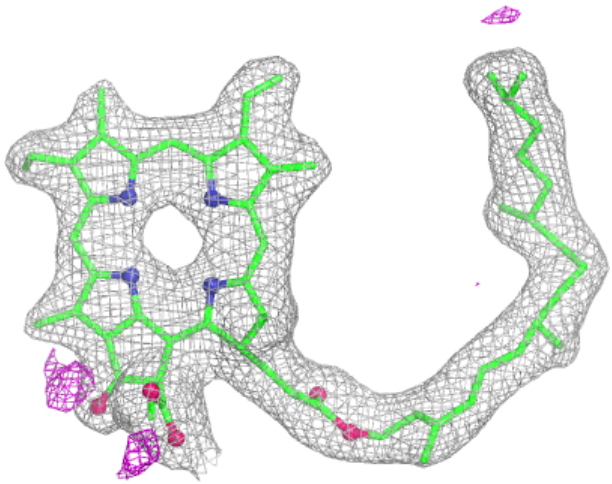
Electron density around CL A 403 (A):

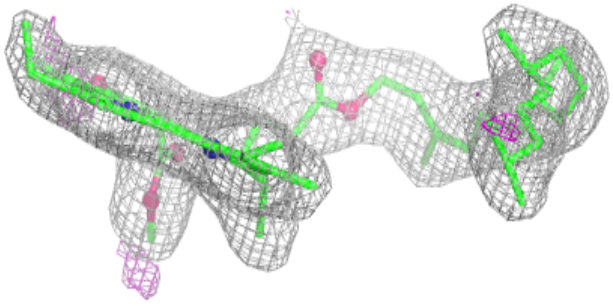
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

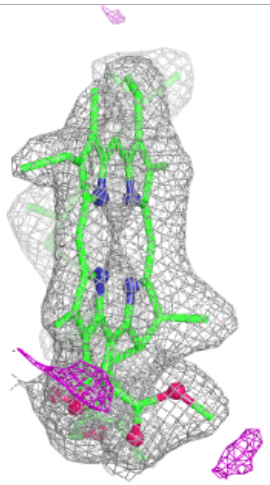


Electron density around PHO A 407 (A):

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

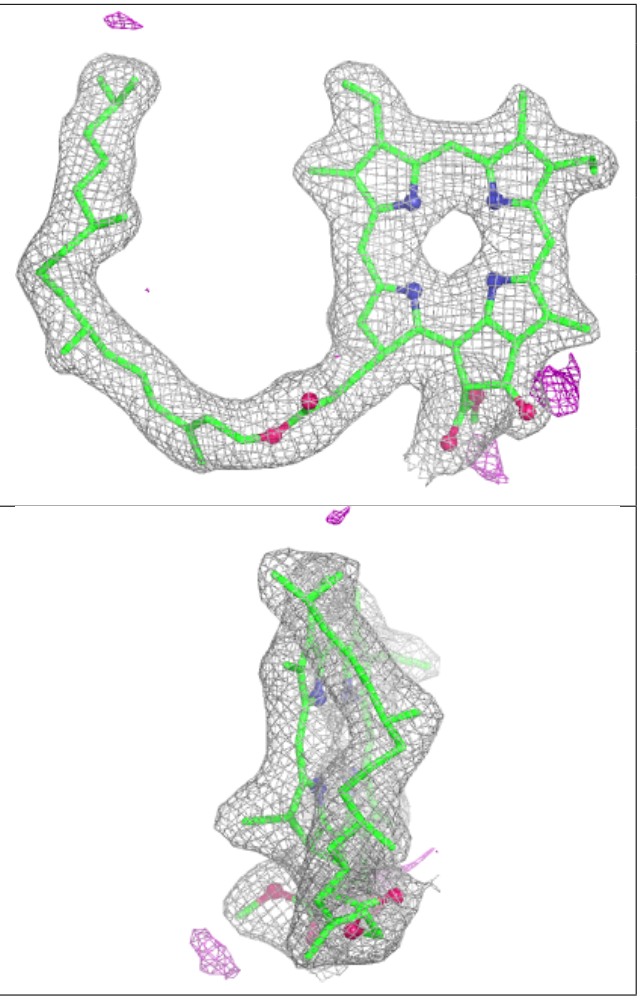






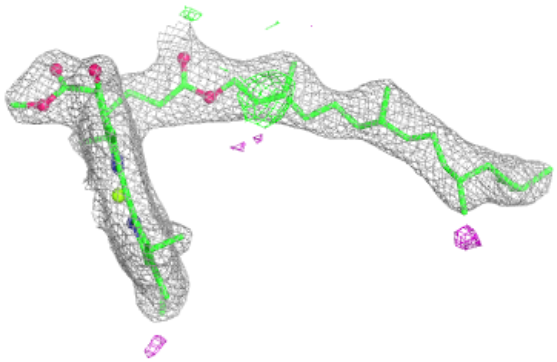
Electron density around PHO A 407 (B):

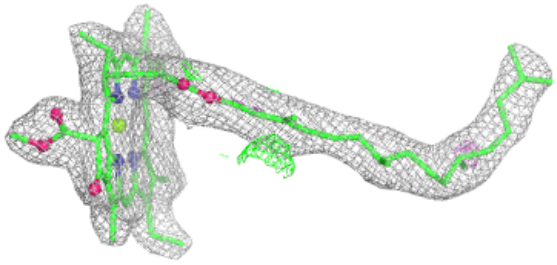
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

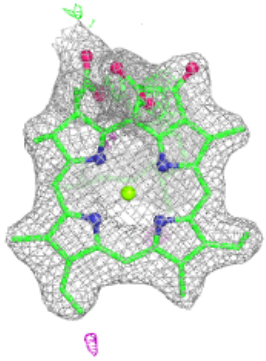


Electron density around CLA b 605:

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

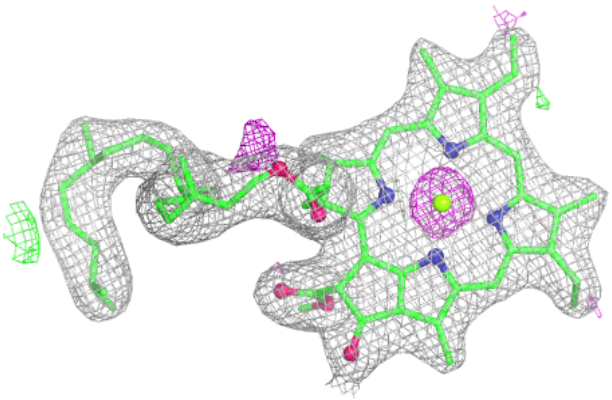


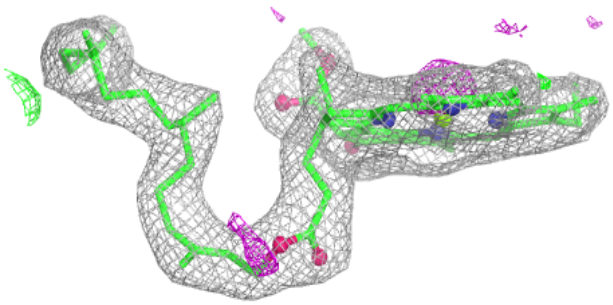


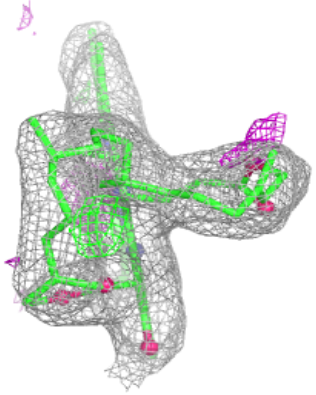


Electron density around CLA B 612:

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

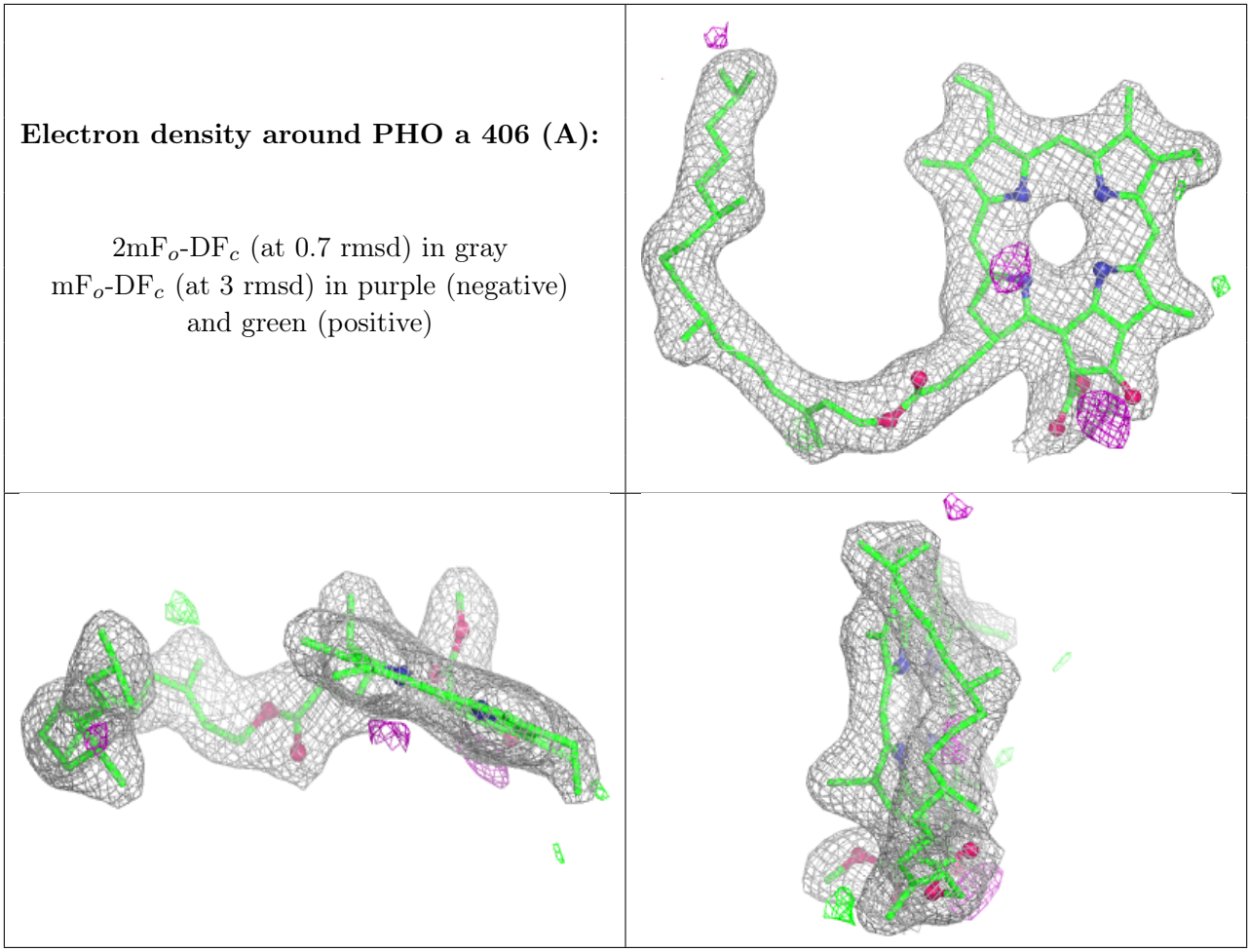






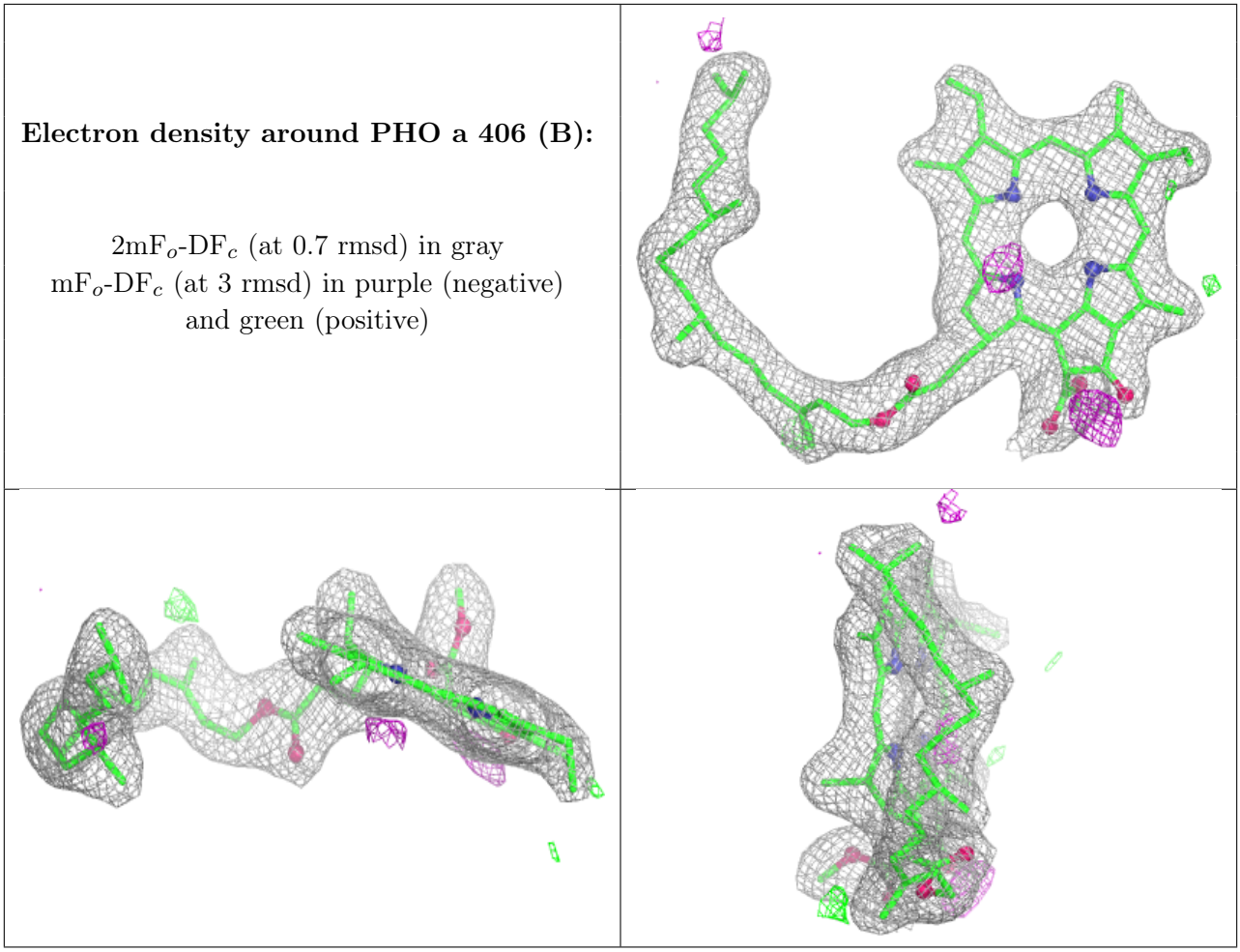
Electron density around PHO a 406 (A):

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



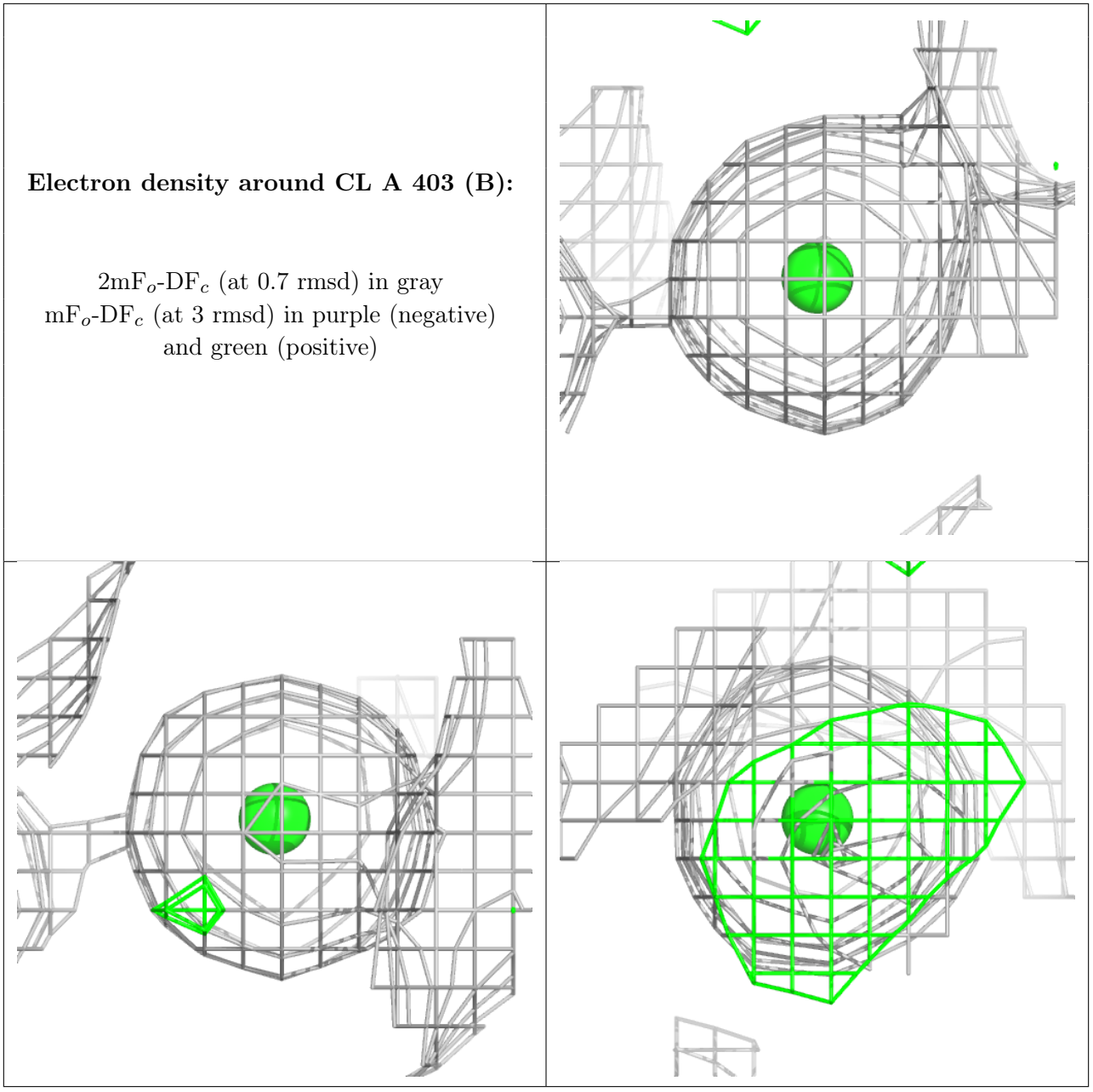
Electron density around PHO a 406 (B):

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



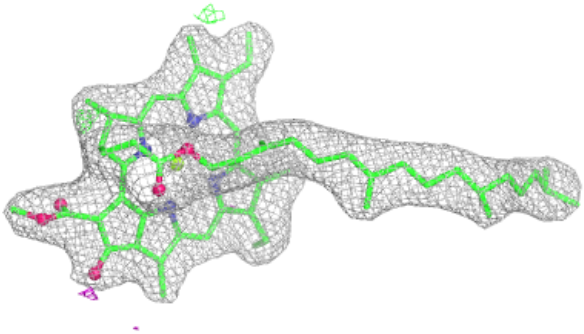
Electron density around CL A 403 (B):

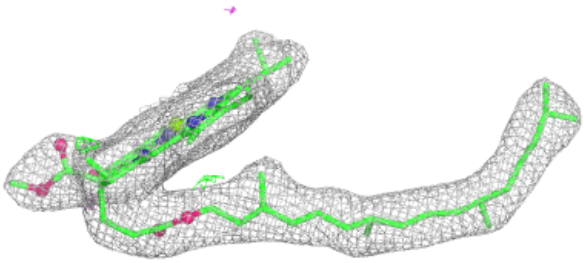
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

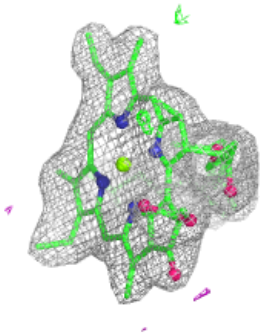


Electron density around CLA b 608:

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

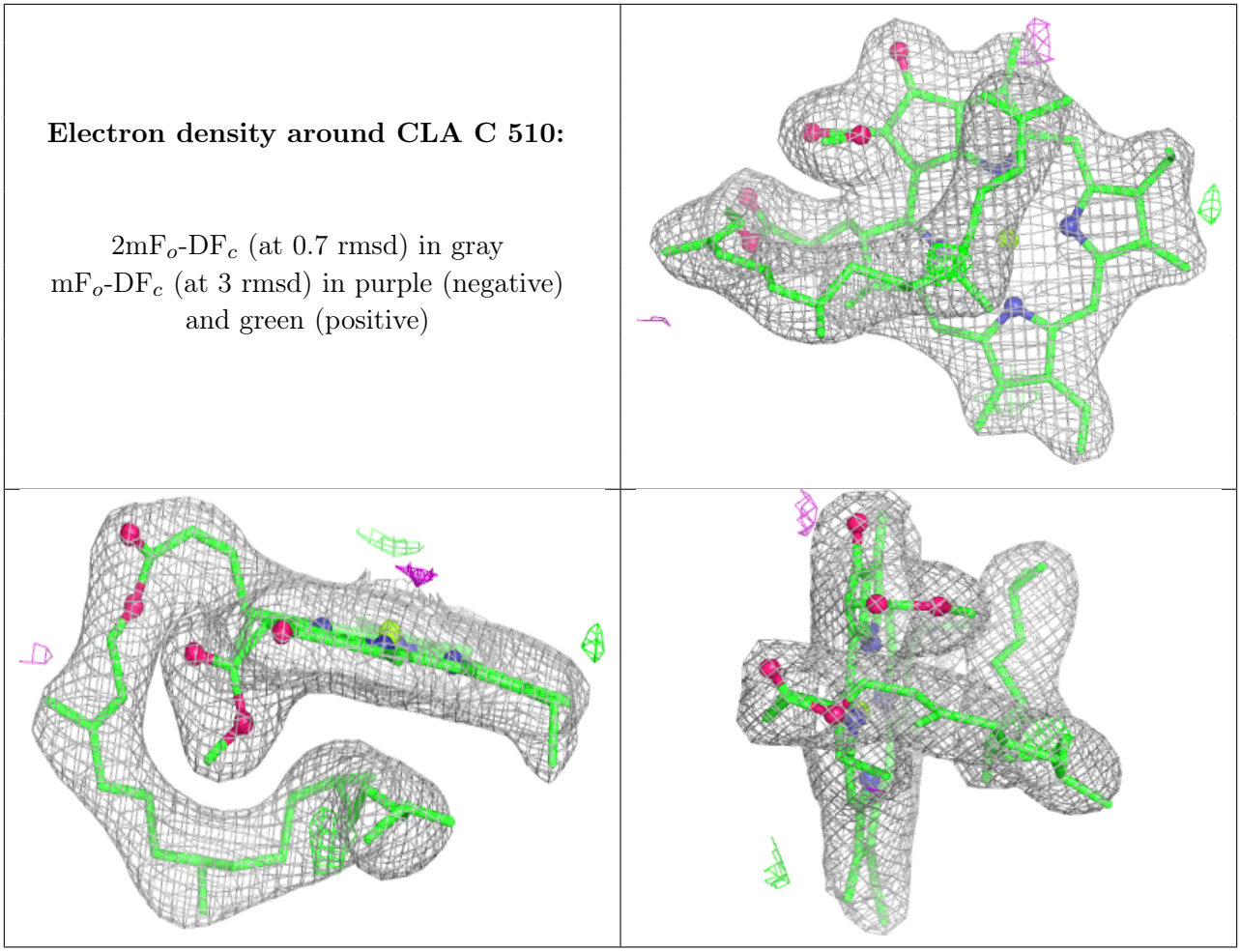






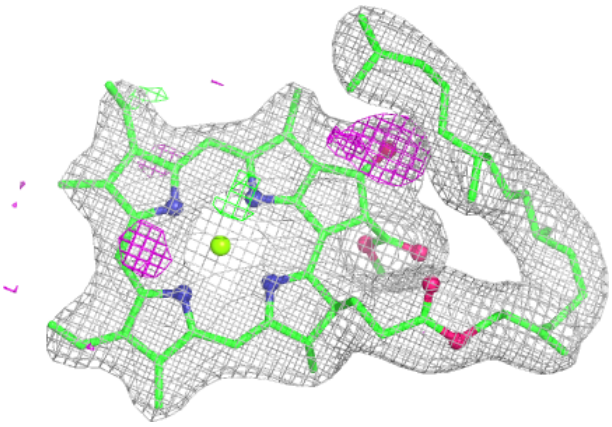
Electron density around CLA C 510:

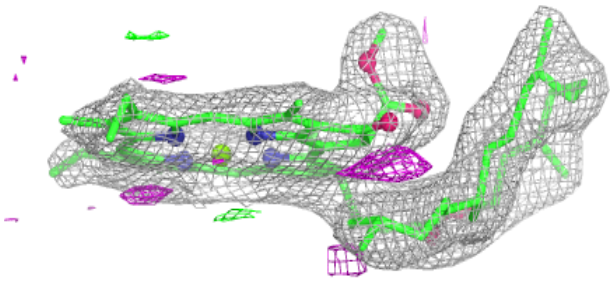
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

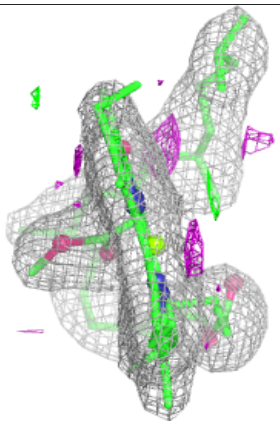


Electron density around CLA b 610:

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

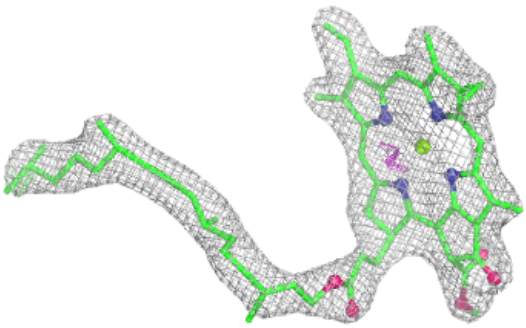


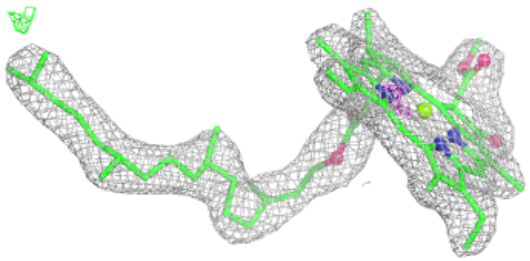


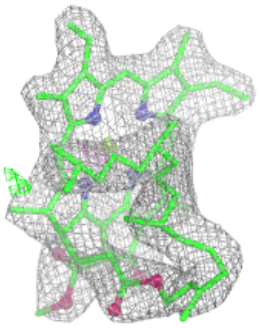


Electron density around CLA C 511:

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

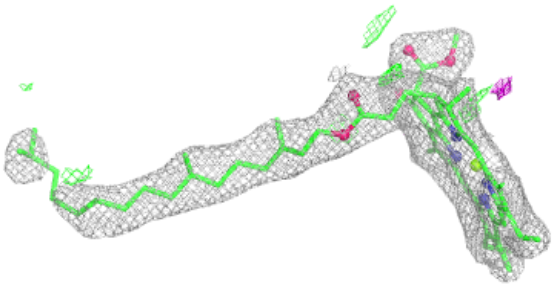


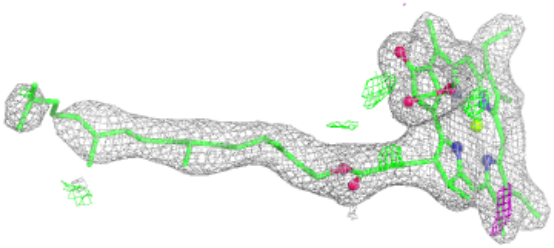


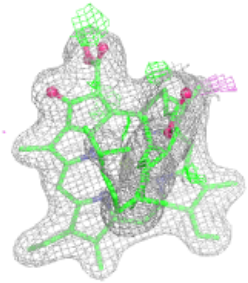


Electron density around CLA B 604:

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

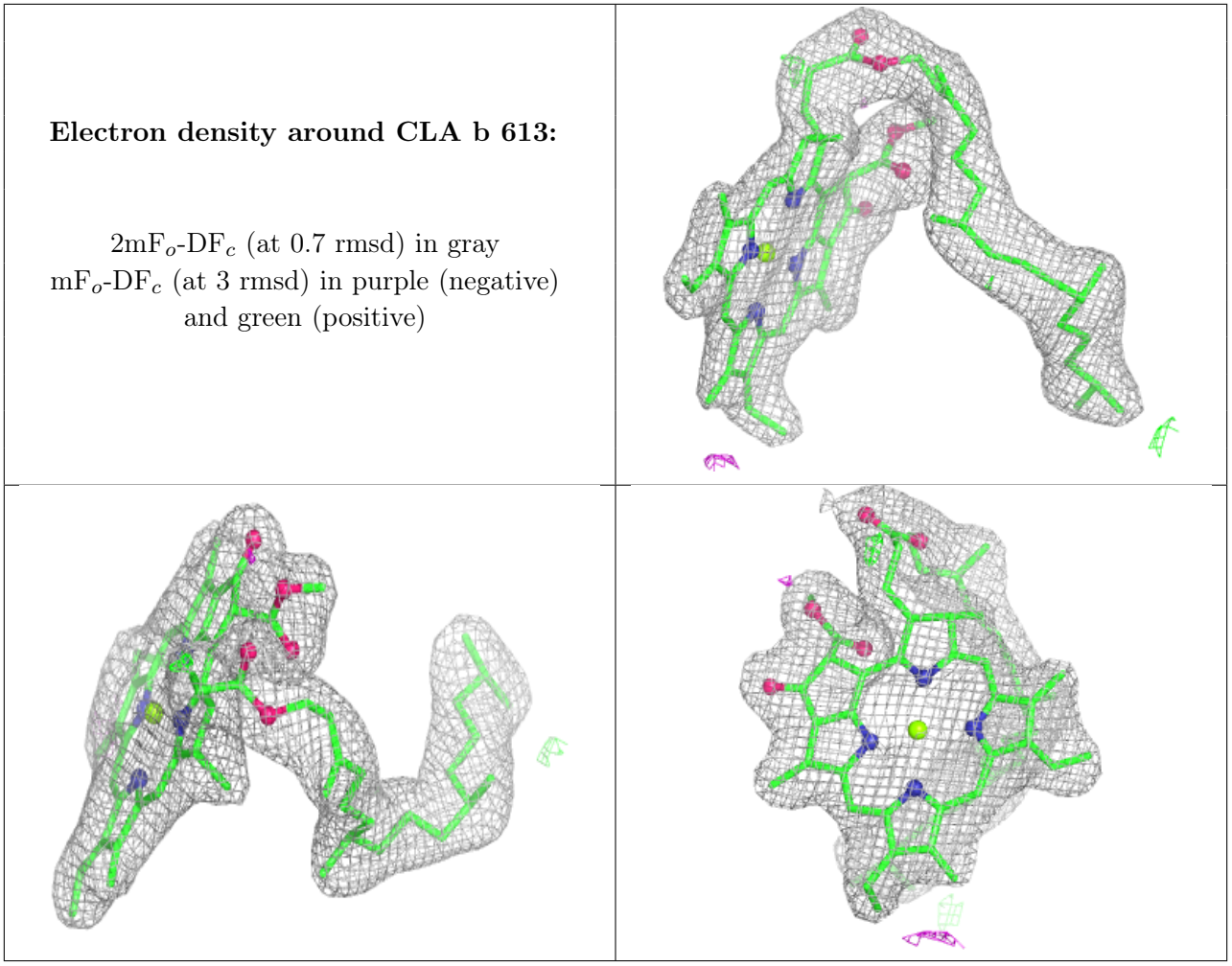






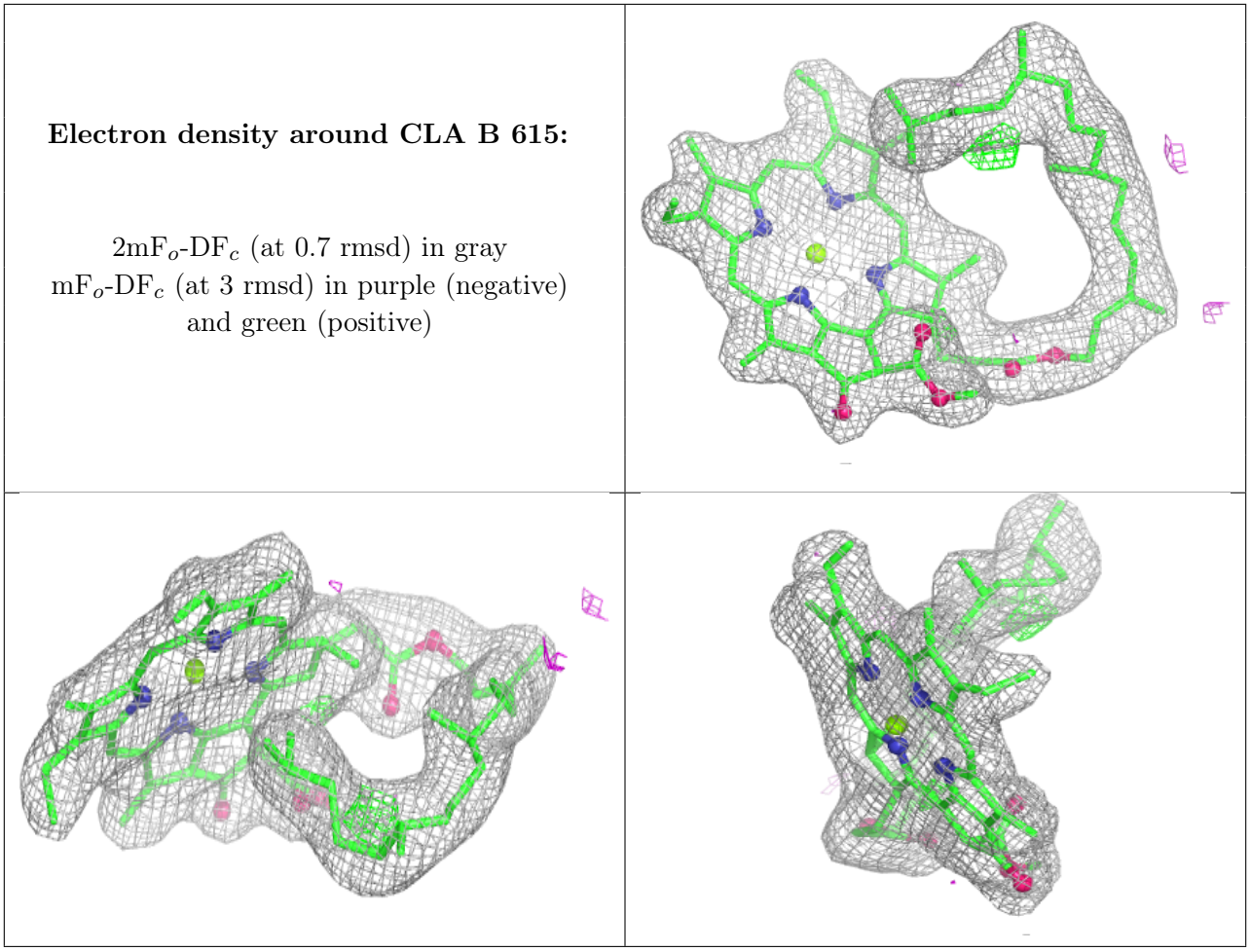
Electron density around CLA b 613:

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



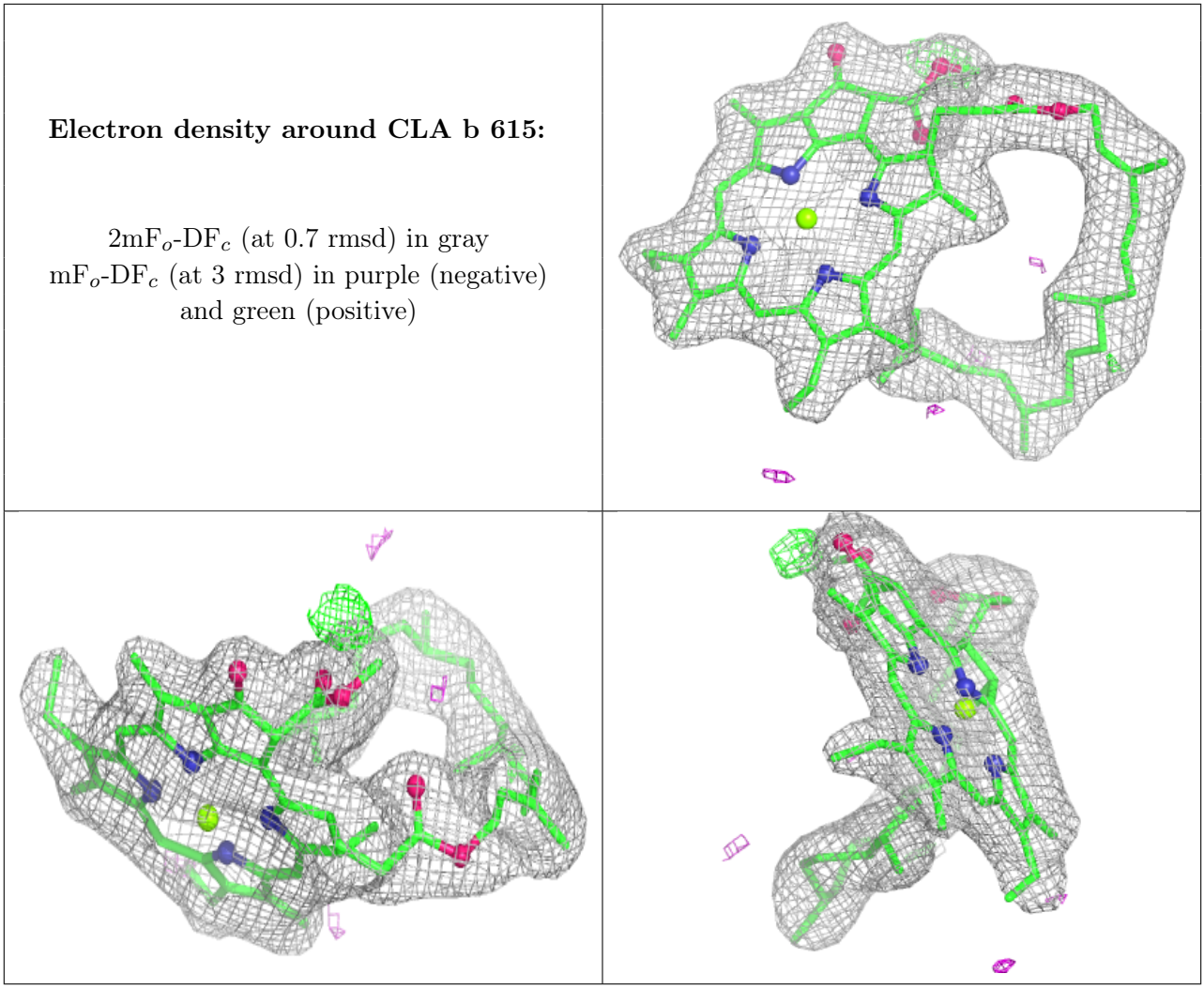
Electron density around CLA B 615:

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



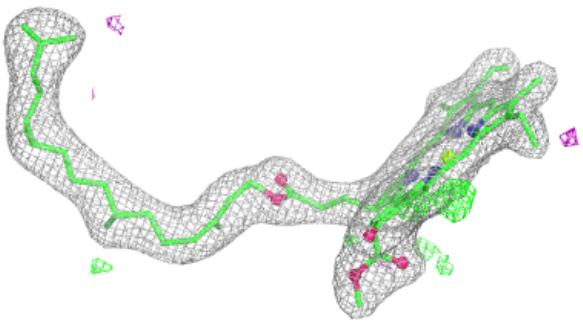
Electron density around CLA b 615:

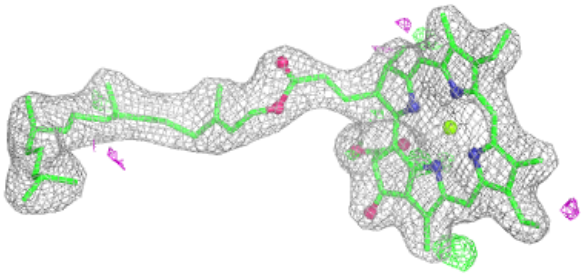
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

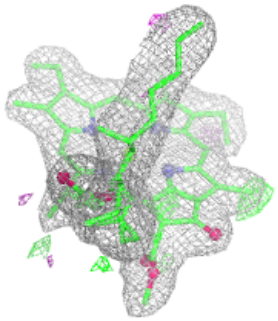


Electron density around CLA D 403 (A):

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

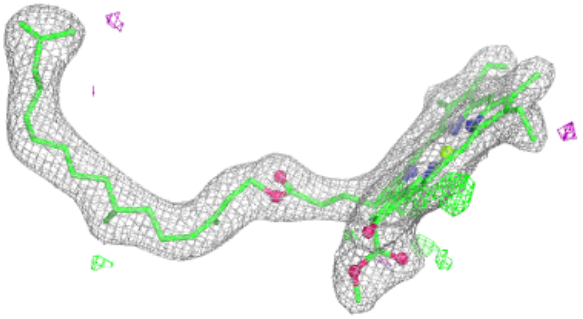


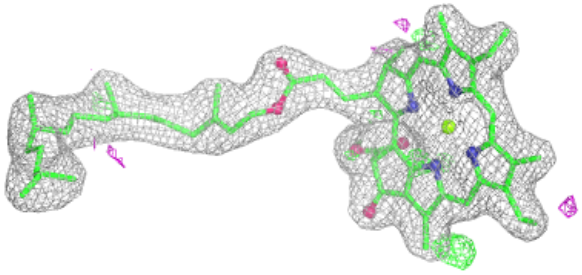


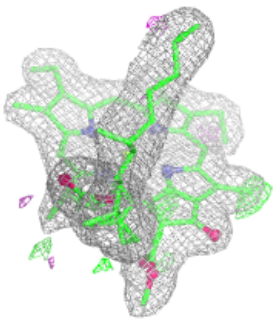


Electron density around CLA D 403 (B):

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

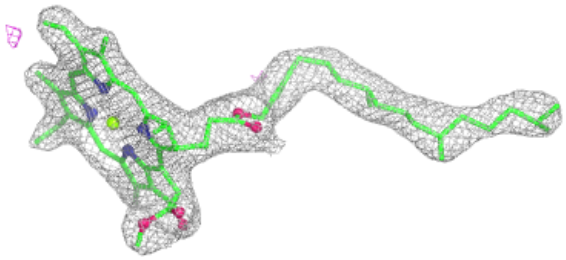


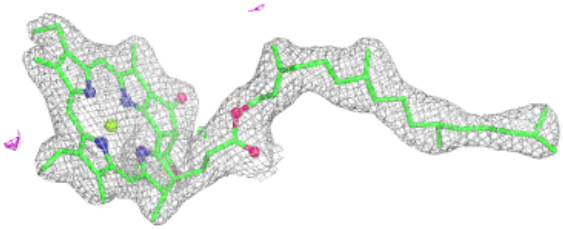


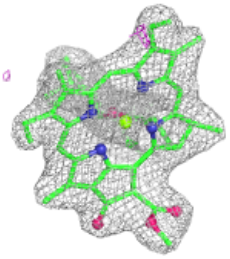


Electron density around CLA c 503:

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

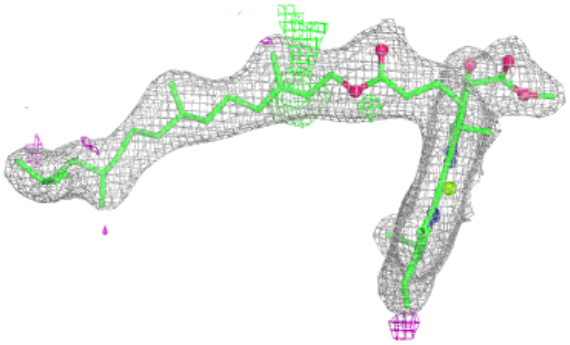


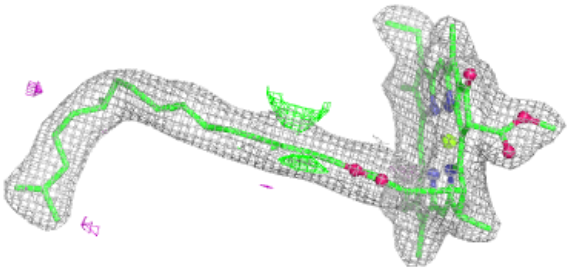


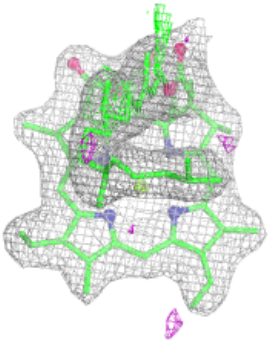


Electron density around CLA B 605:

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

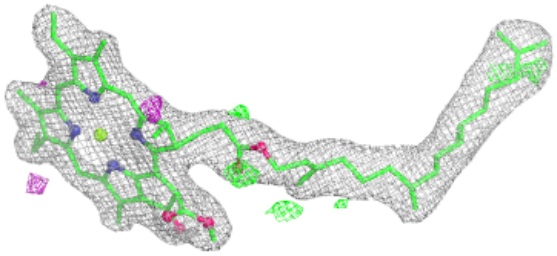


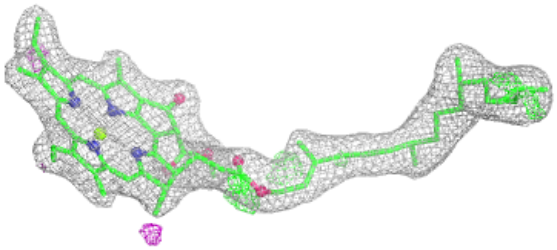


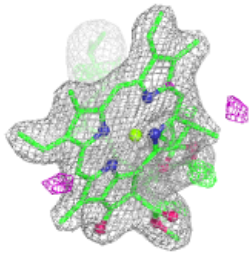


Electron density around CLA a 404 (A):

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

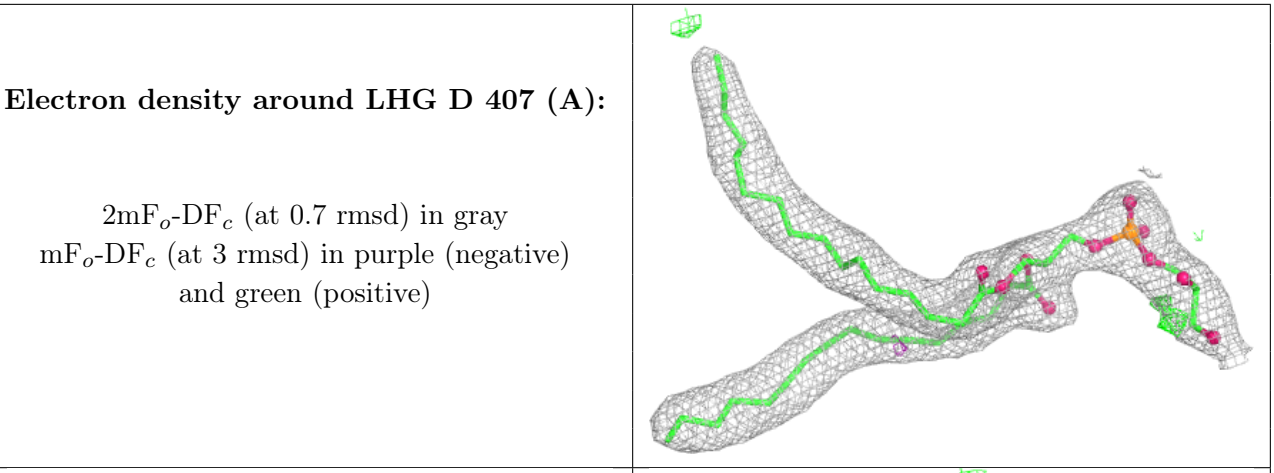


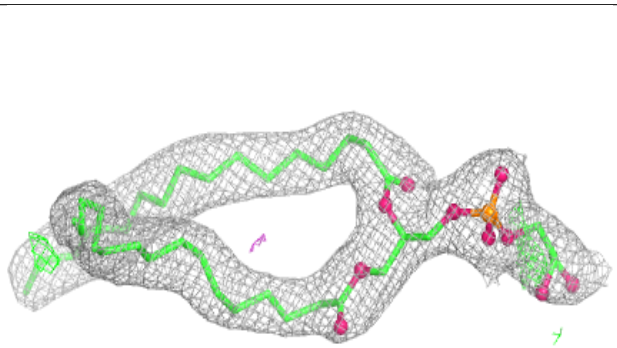


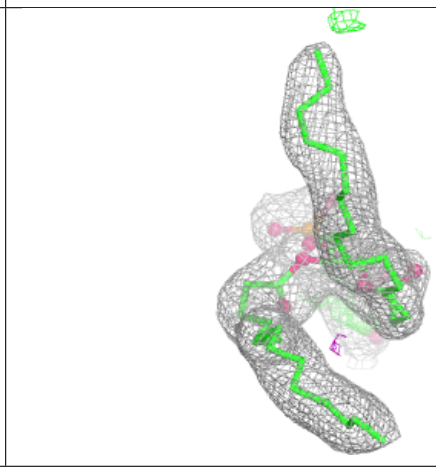


Electron density around LHG D 407 (A):

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

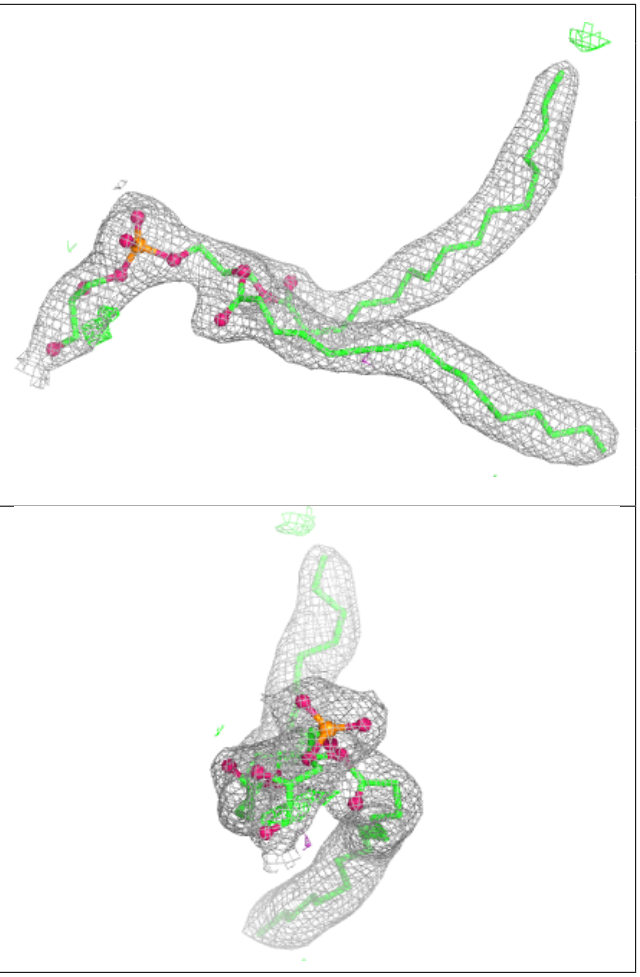






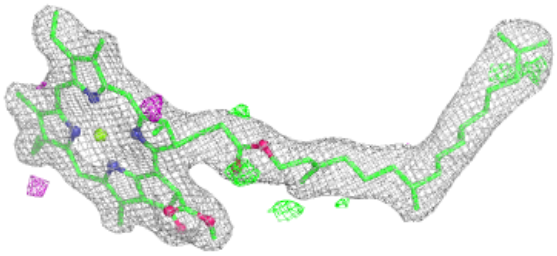
Electron density around LHG D 407 (B):

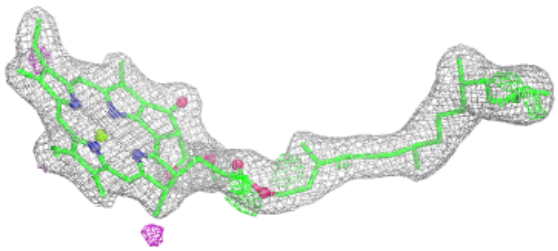
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

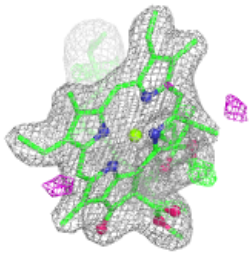


Electron density around CLA a 404 (B):

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

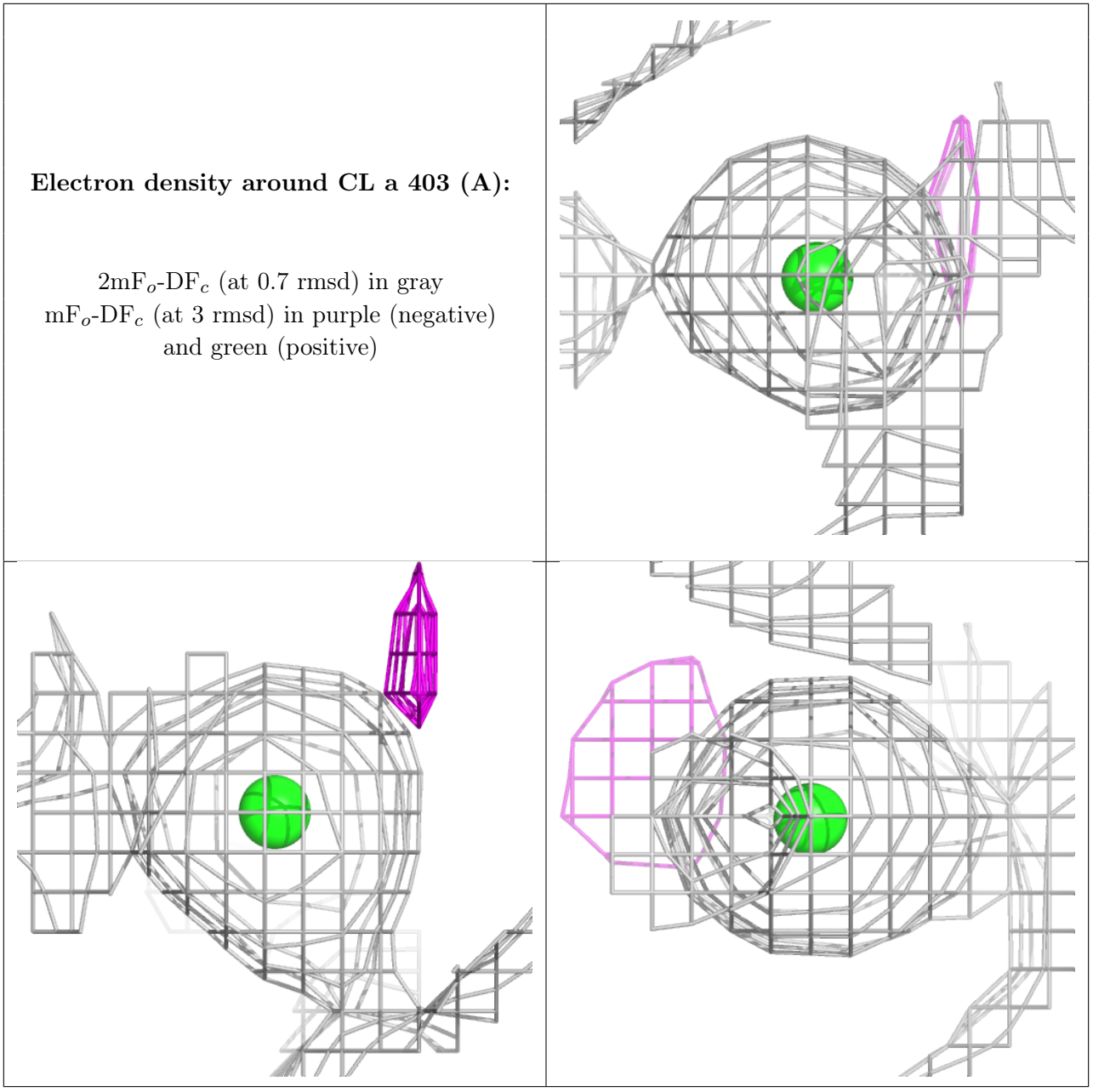






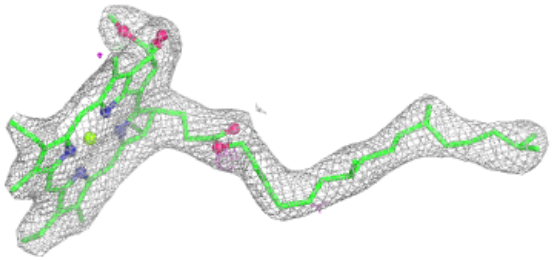
Electron density around CL a 403 (A):

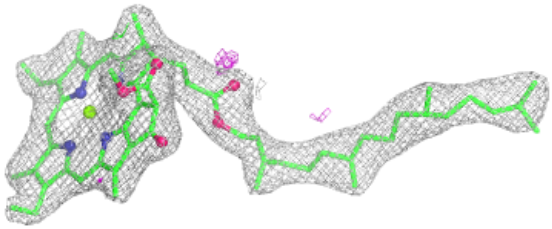
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

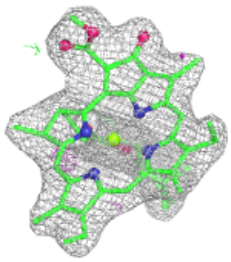


Electron density around CLA C 502:

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

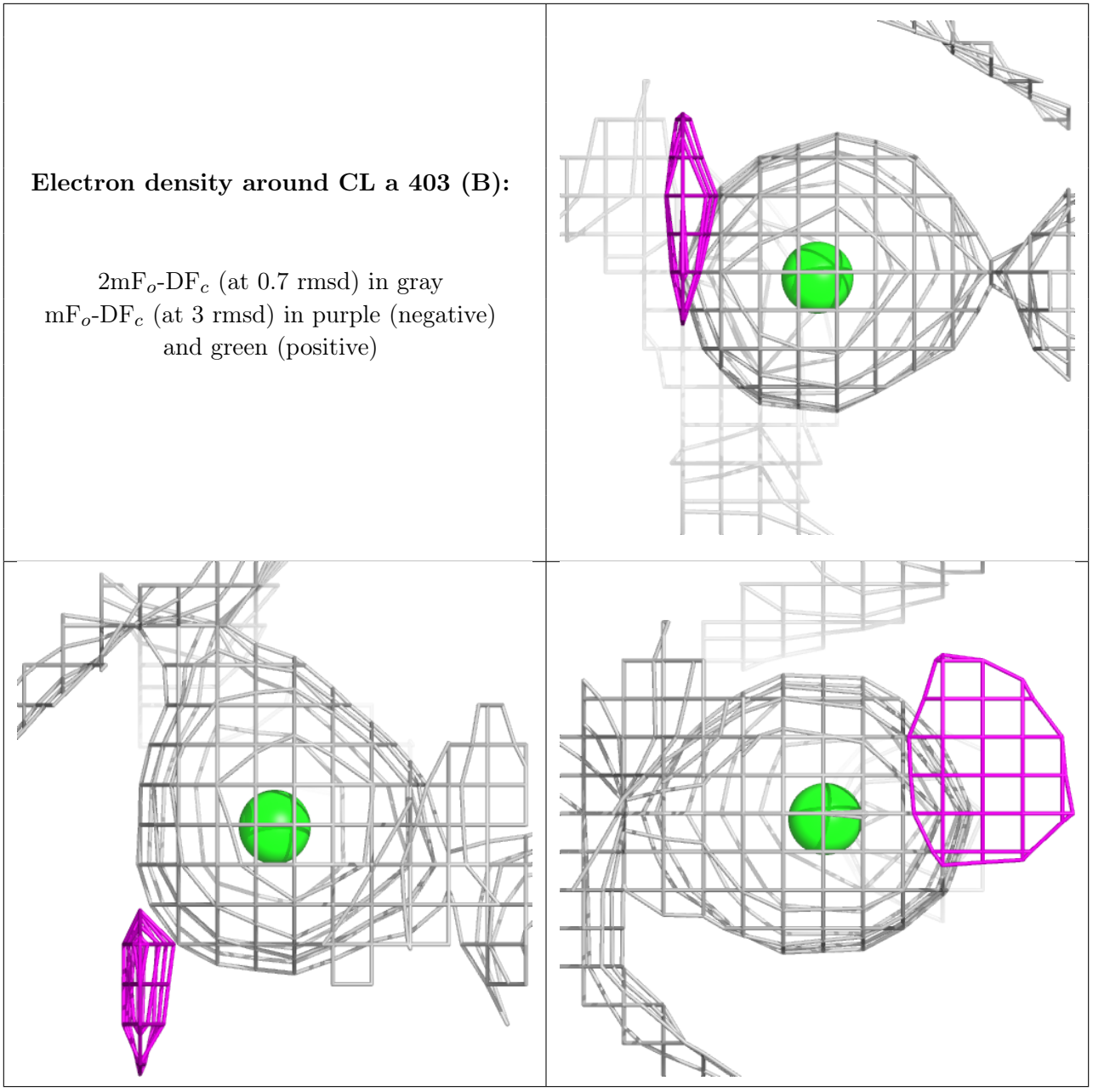






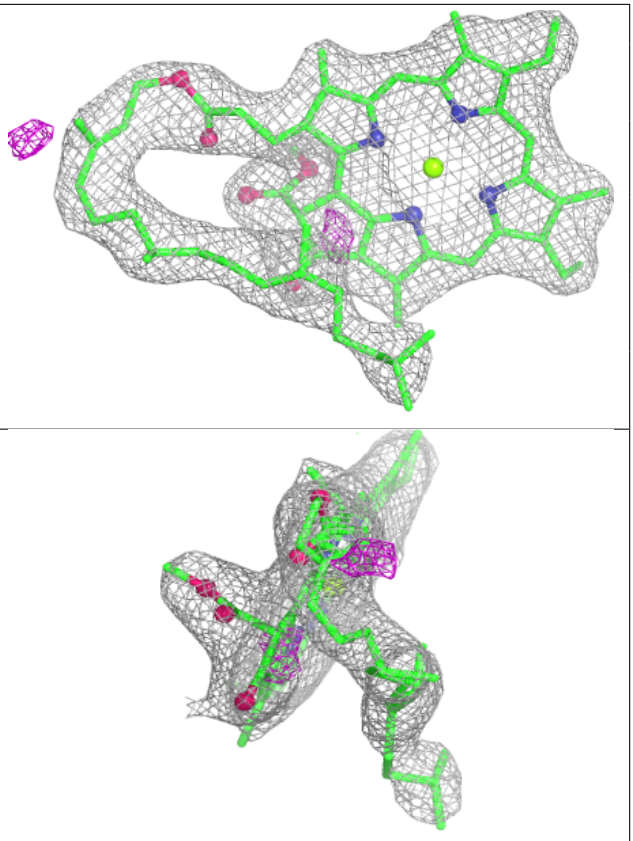
Electron density around CL a 403 (B):

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



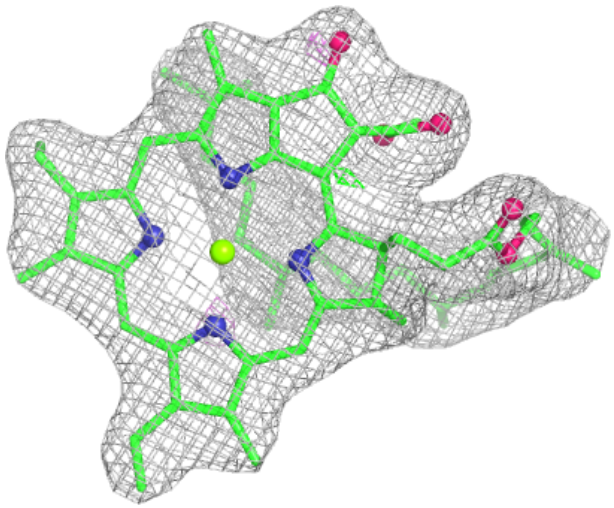
Electron density around CLA c 510:

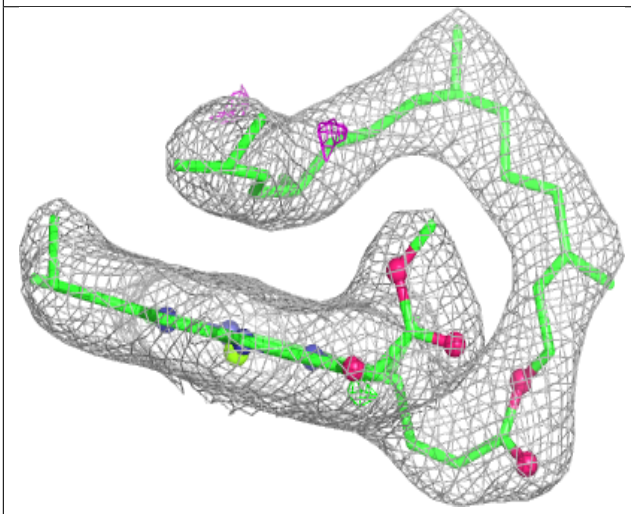
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

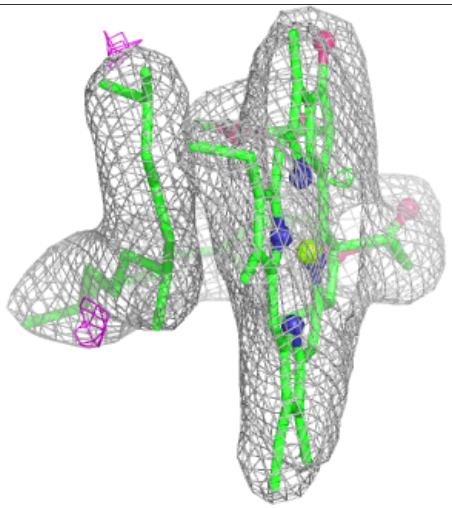


Electron density around CLA c 511:

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

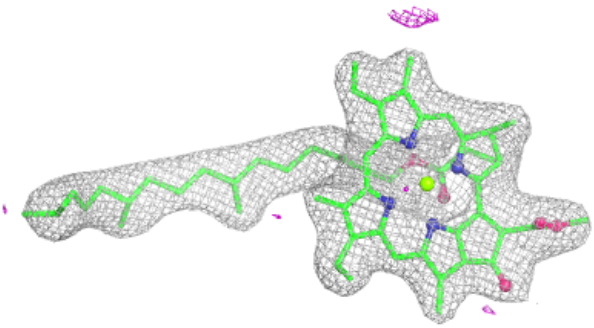


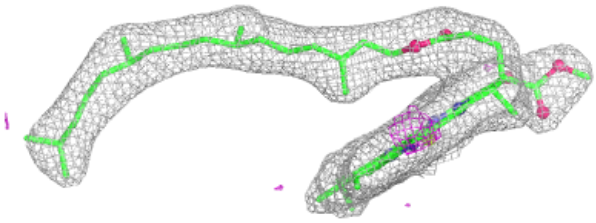


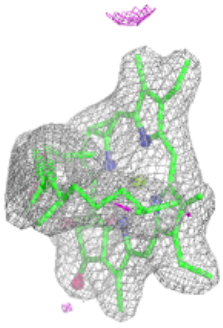


Electron density around CLA B 608:

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

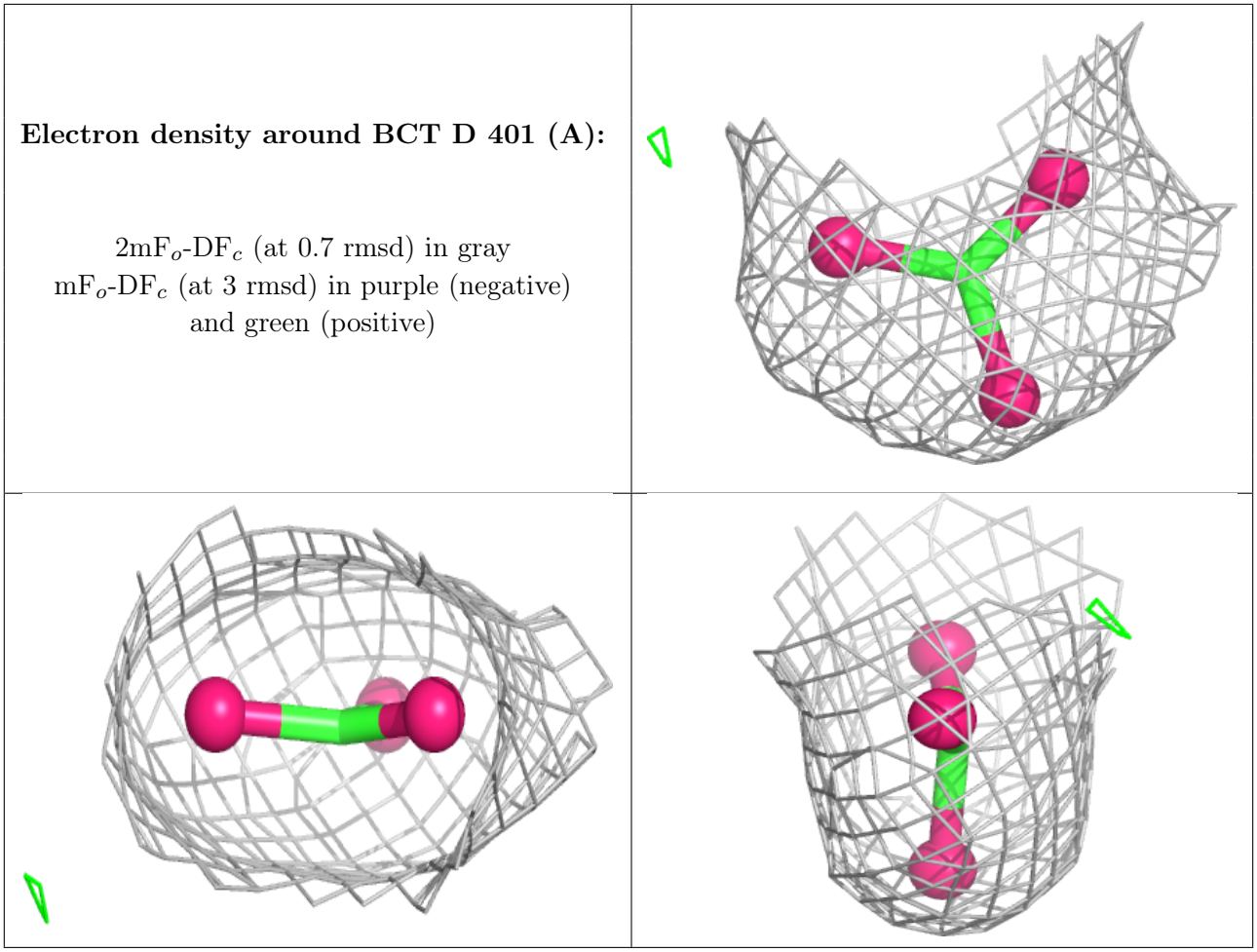






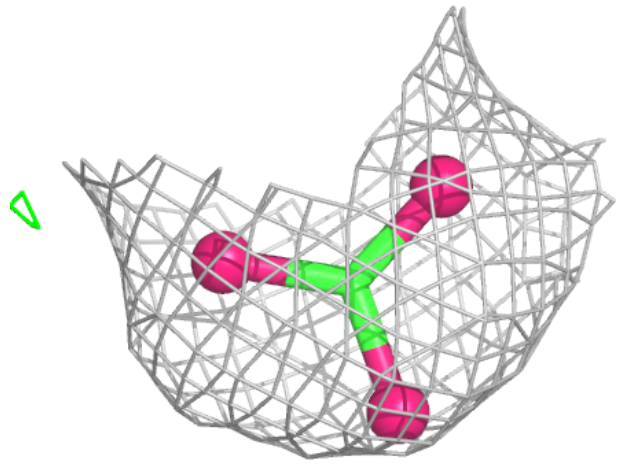
Electron density around BCT D 401 (A):

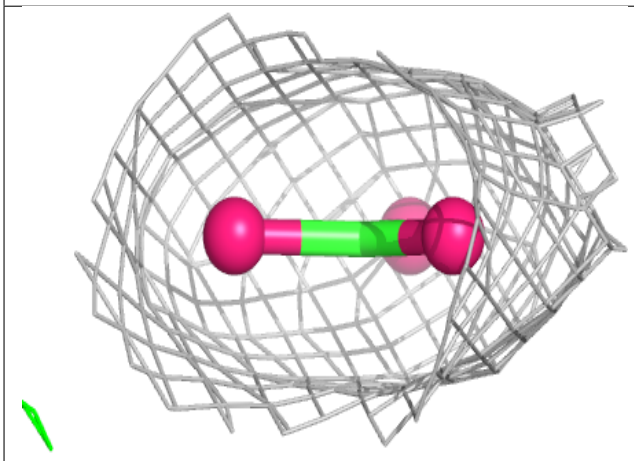
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

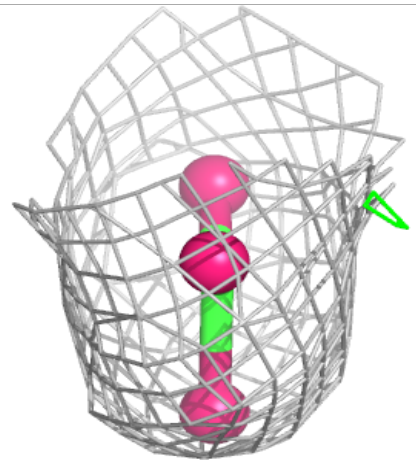


Electron density around BCT D 401 (B):

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

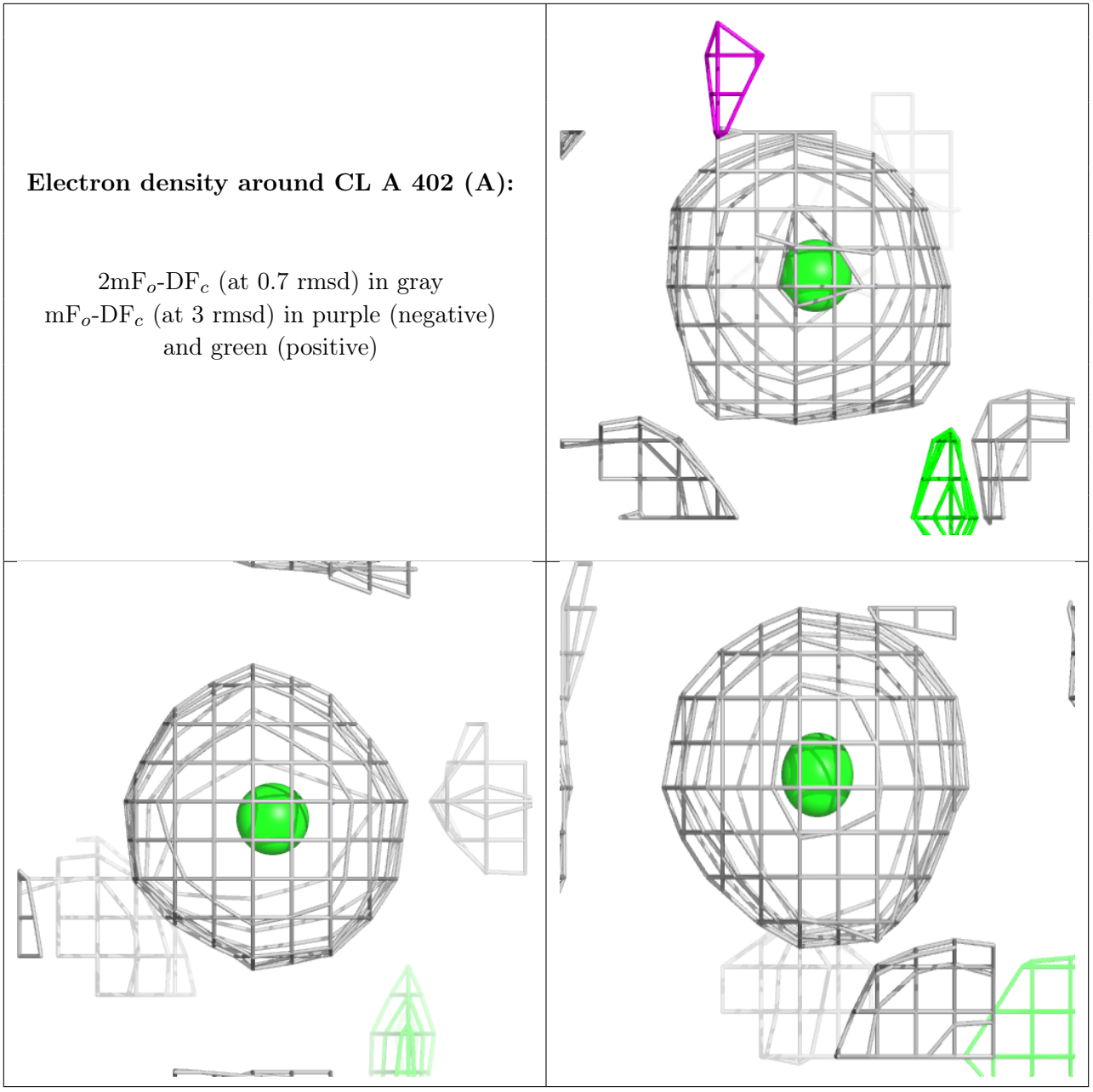






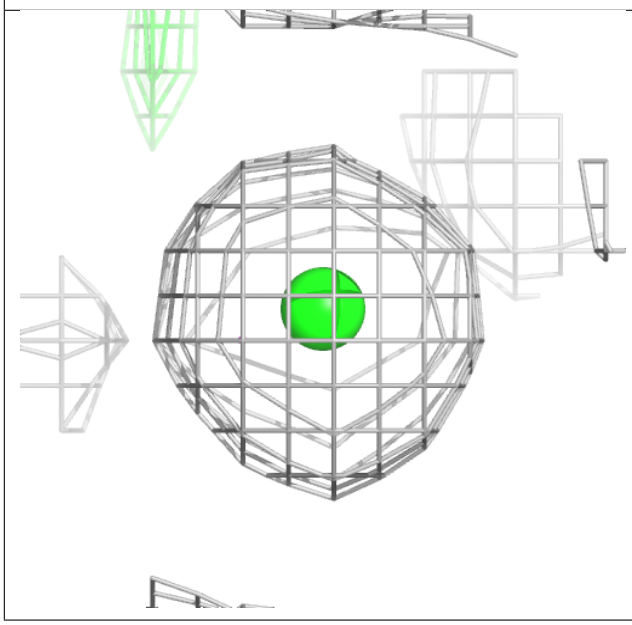
Electron density around CL A 402 (A):

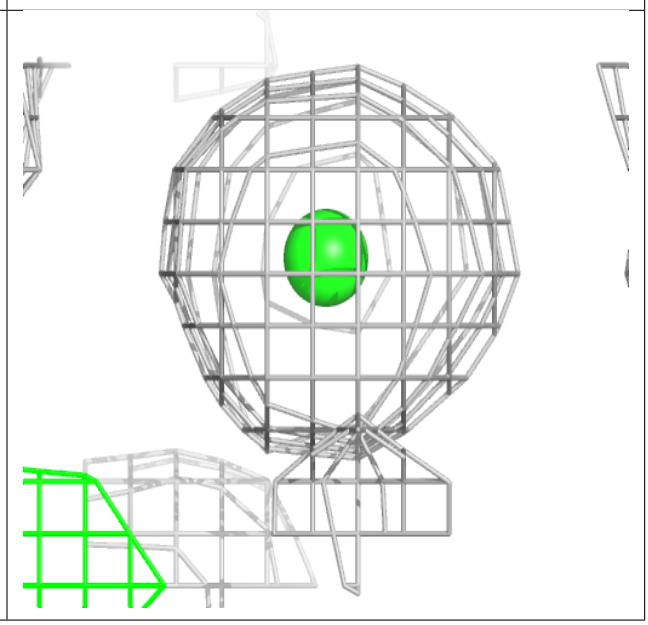
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CL A 402 (B):

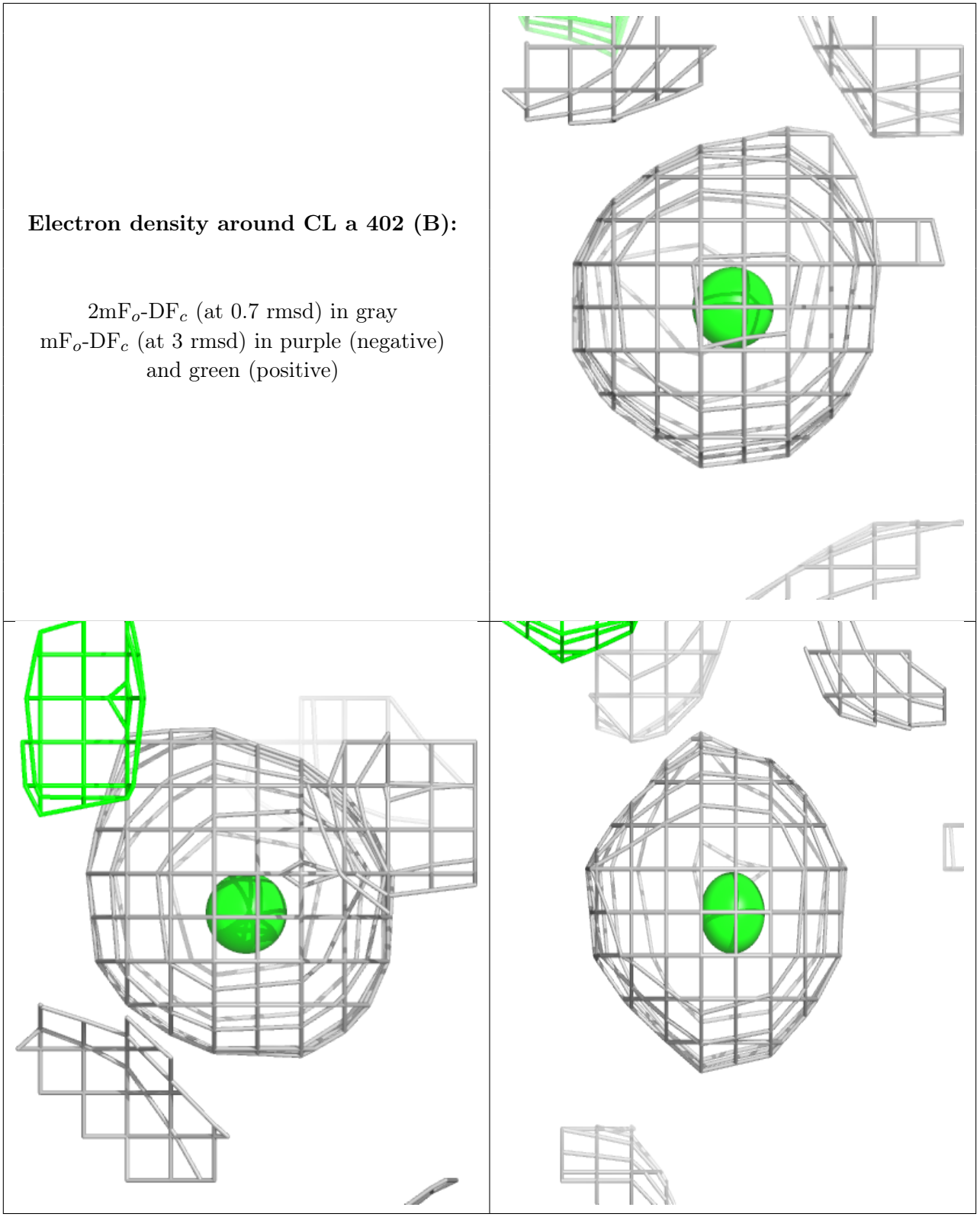
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





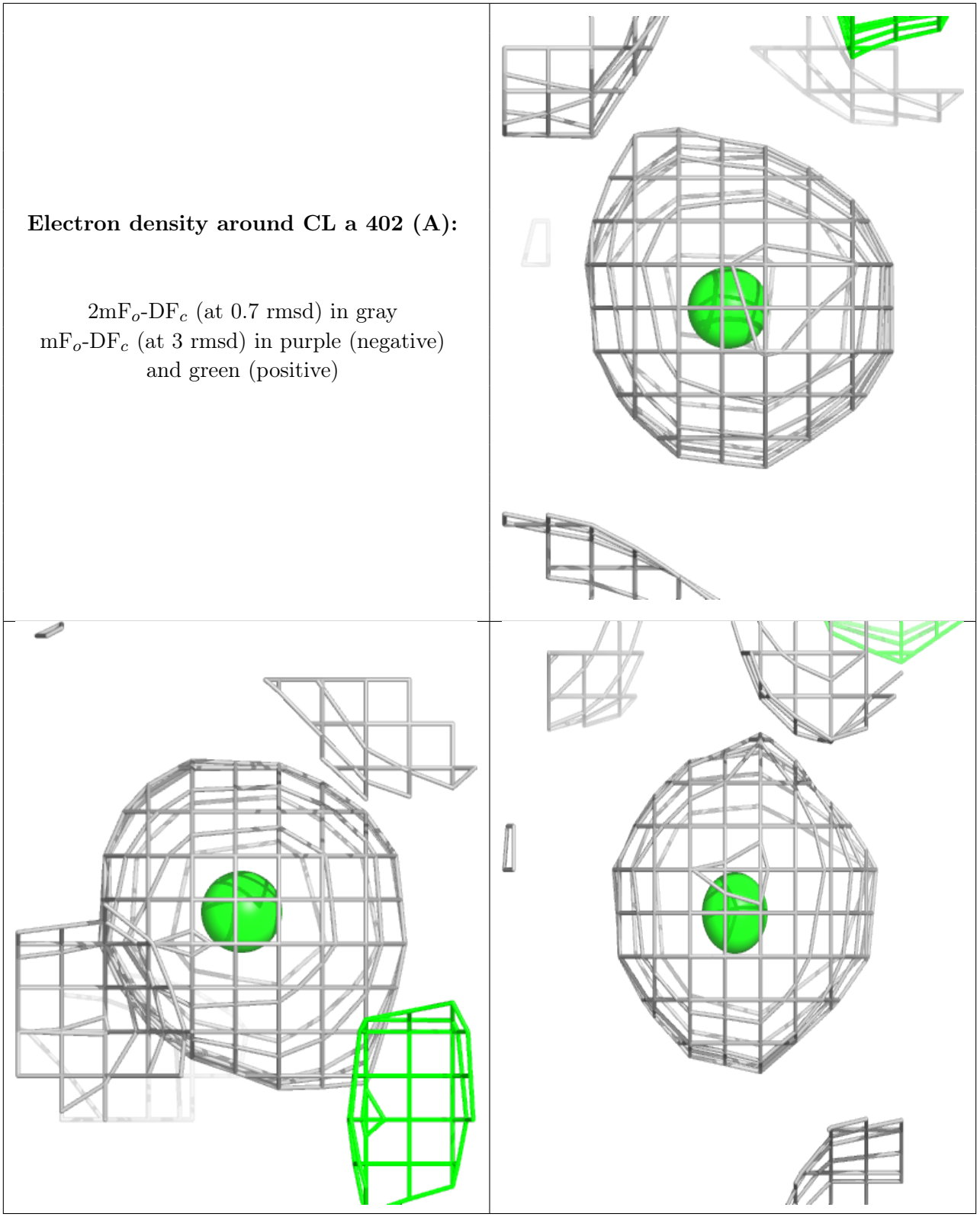
Electron density around CL a 402 (B):

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



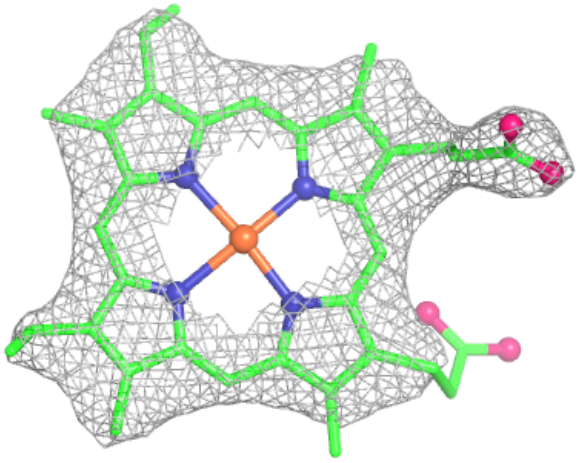
Electron density around CL a 402 (A):

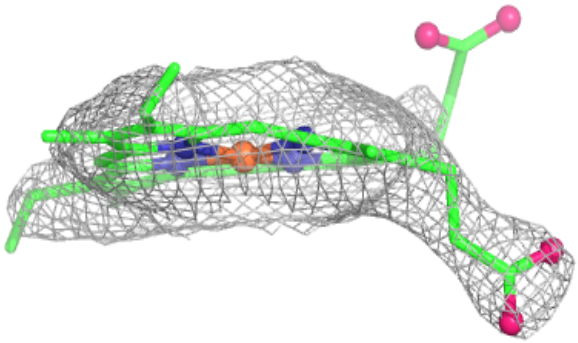
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

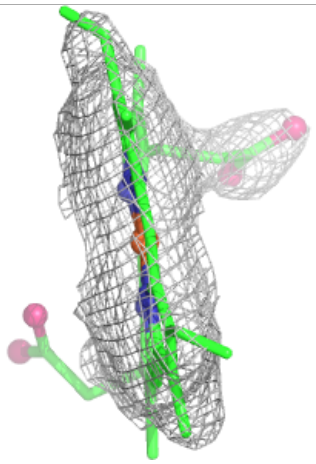


Electron density around HEM f 101:

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

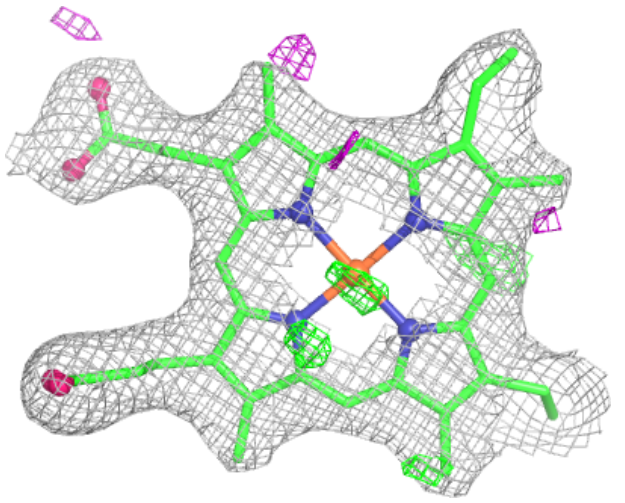


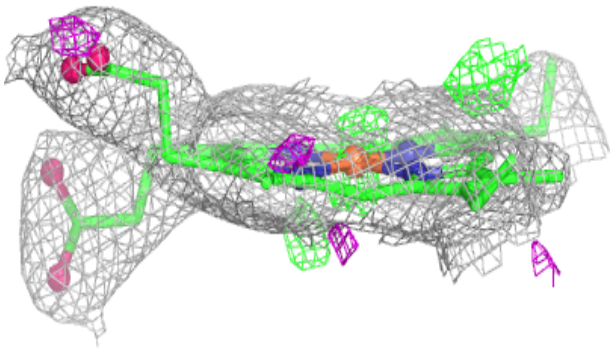


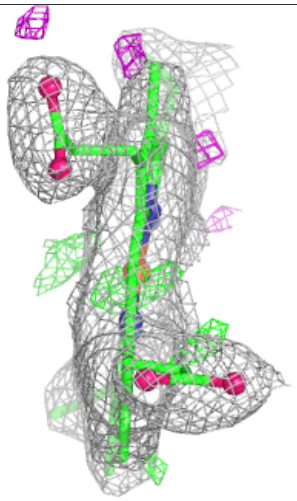


Electron density around HEC V 201:

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

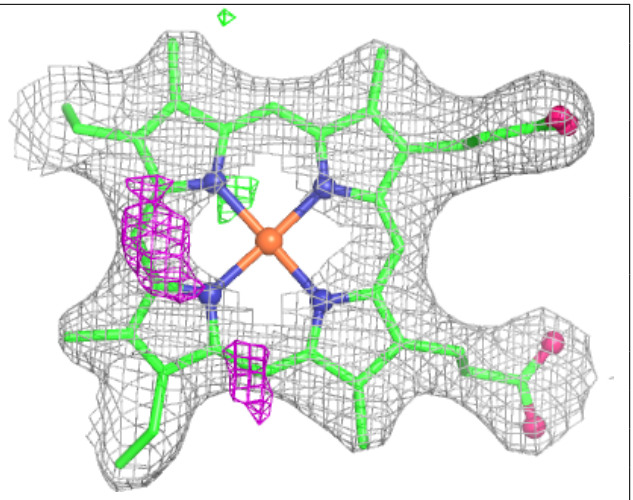


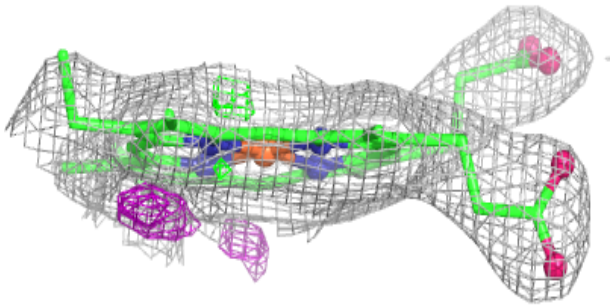


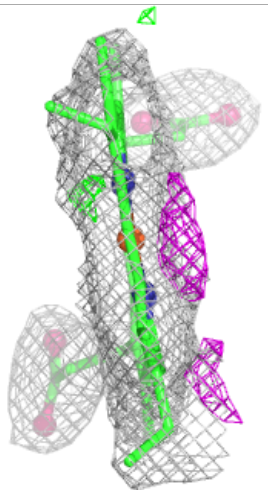


Electron density around HEC v 201:

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

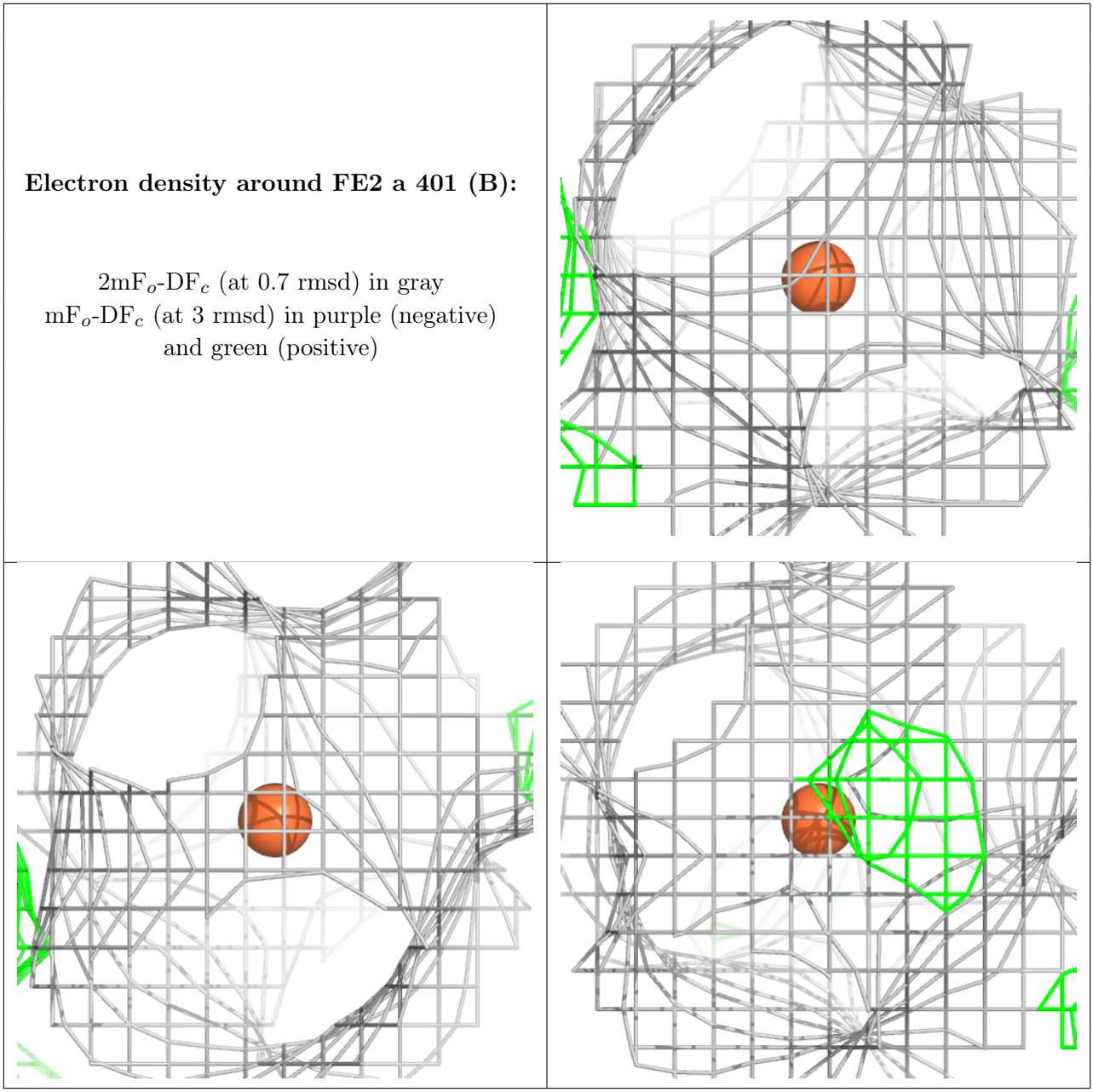






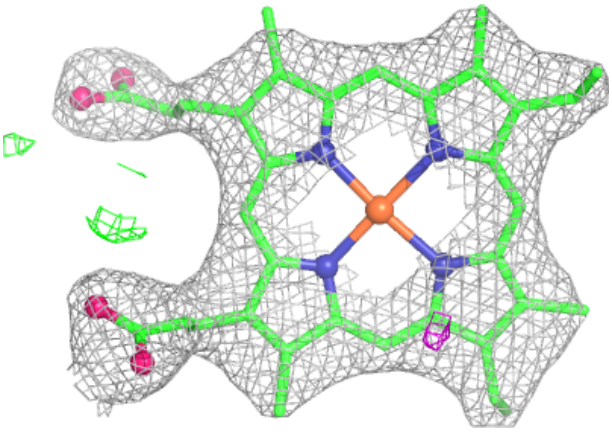
Electron density around FE2 a 401 (B):

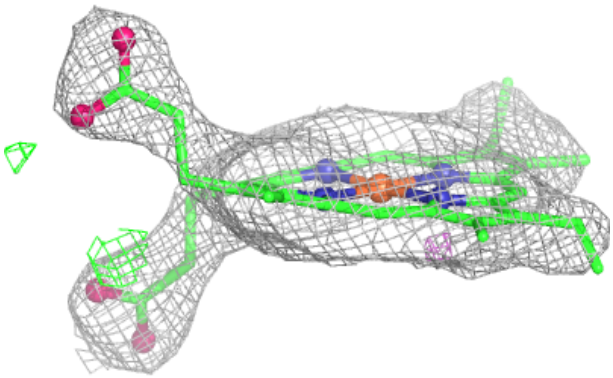
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

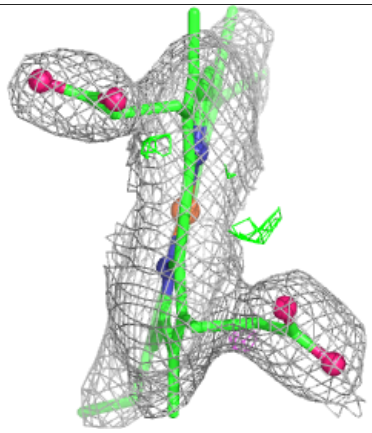


Electron density around HEM F 102:

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

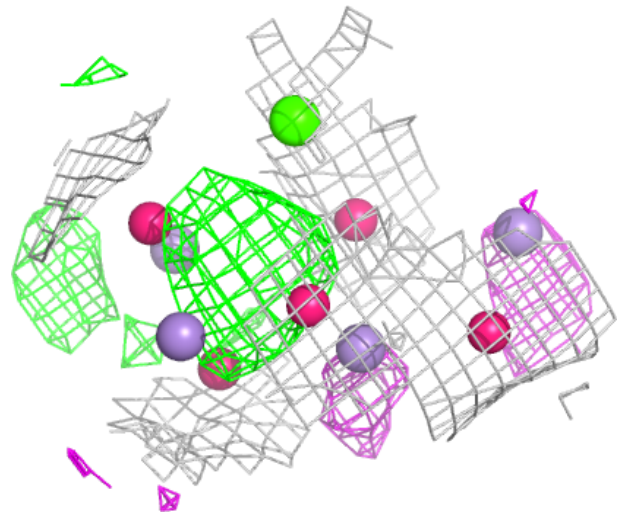


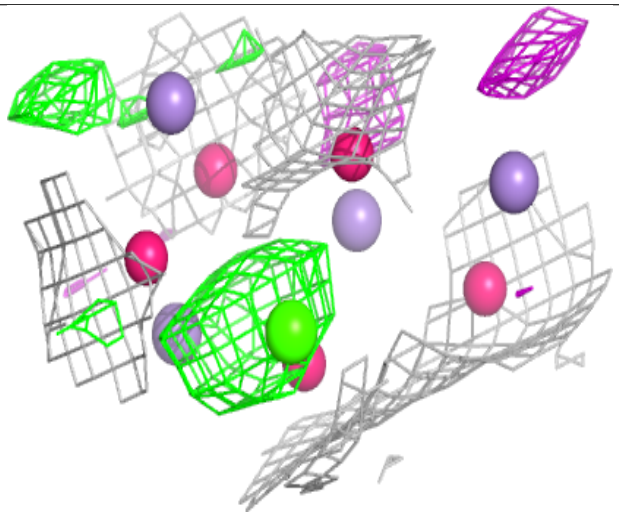


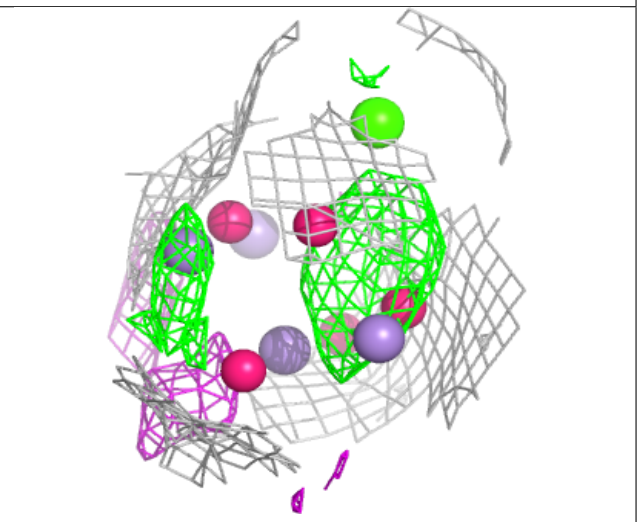


Electron density around OEX A 413 (A):

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

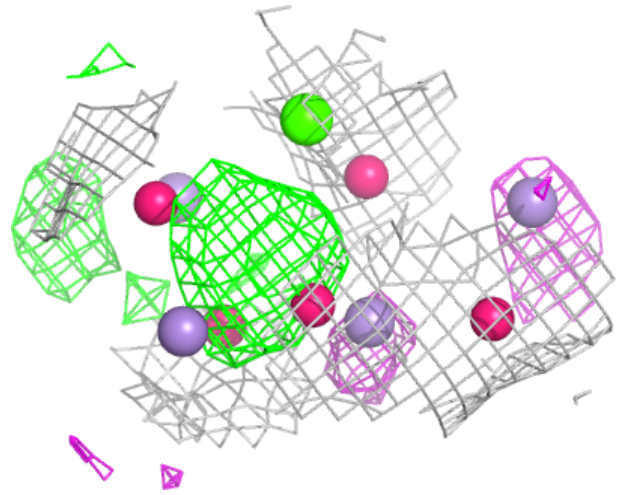


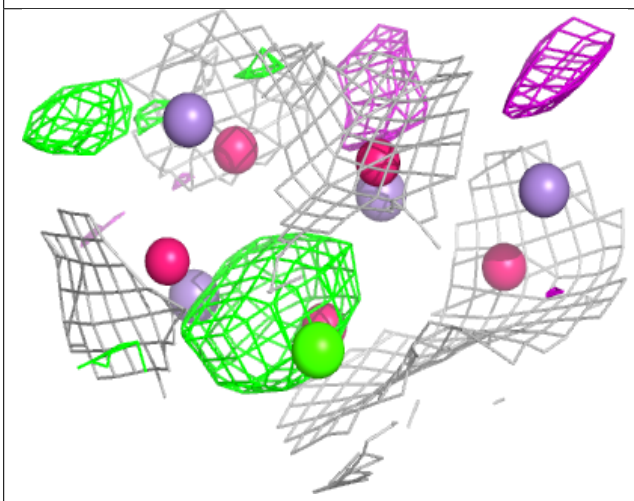


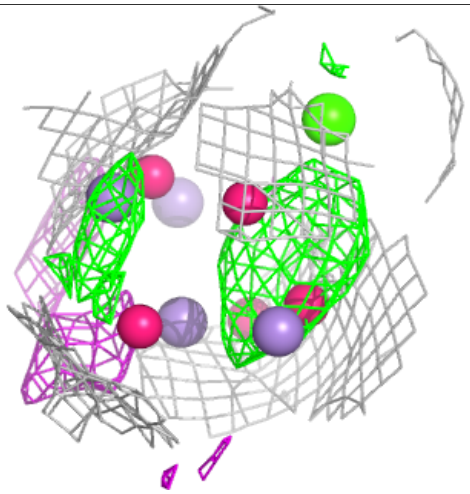


Electron density around OEX A 413 (B):

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

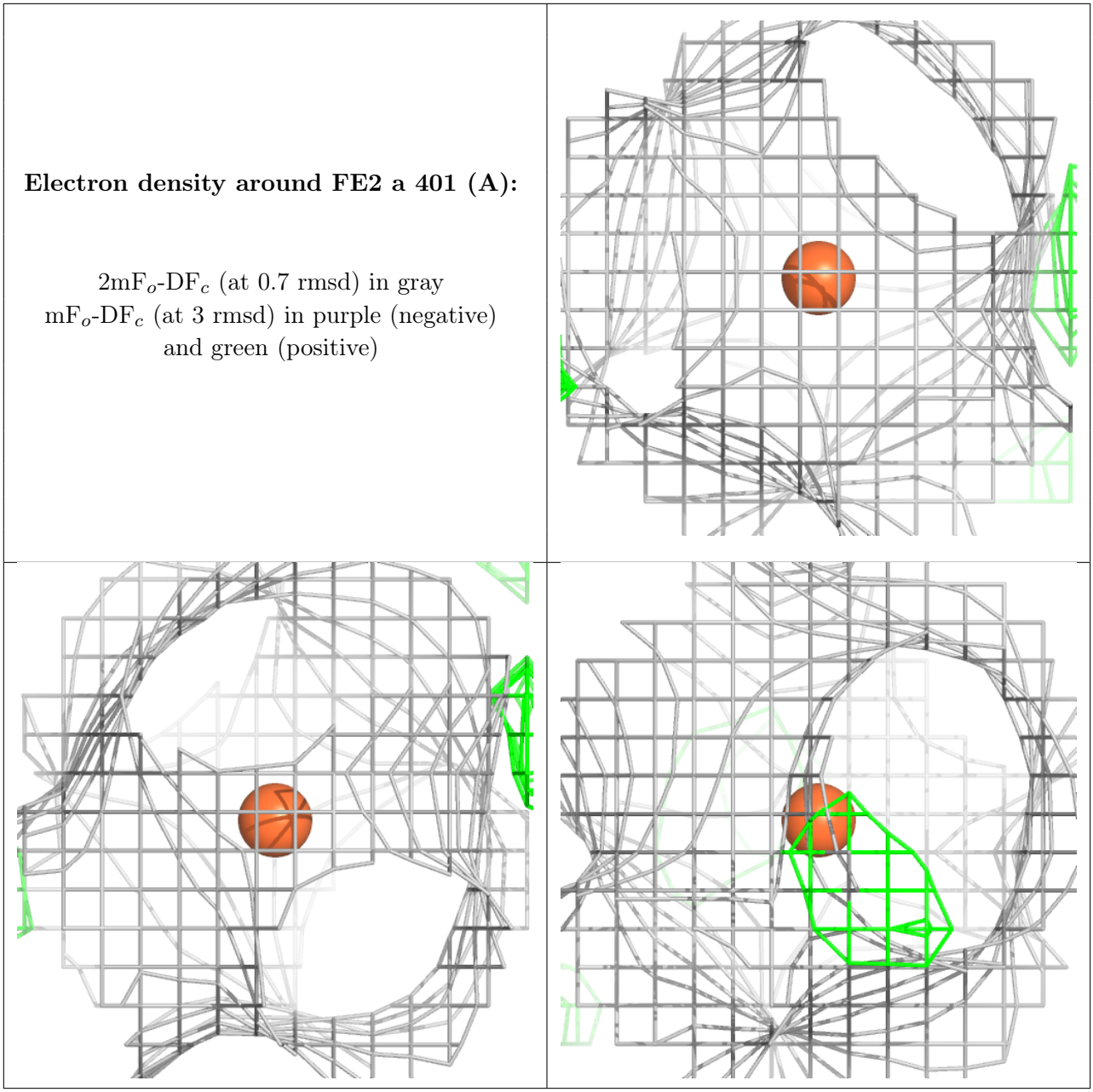






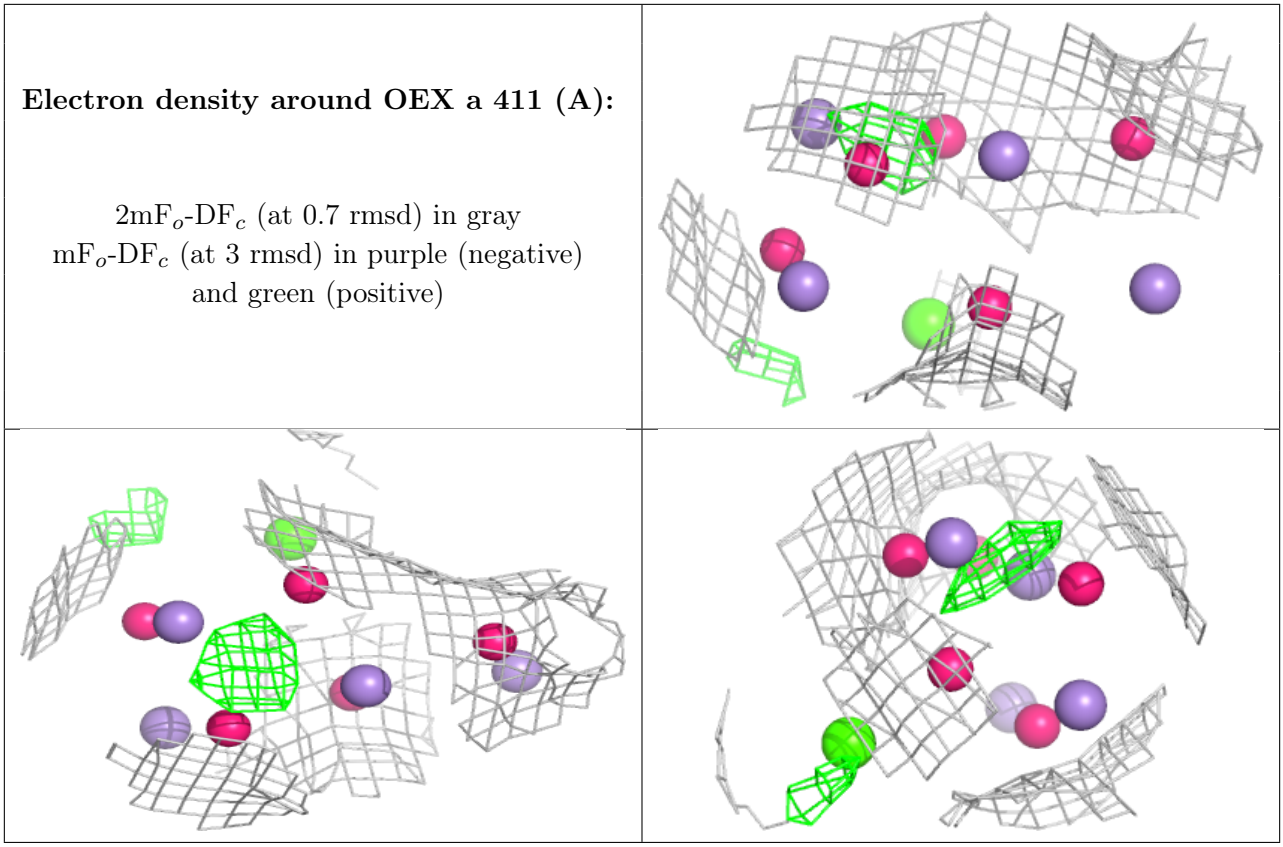
Electron density around FE2 a 401 (A):

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



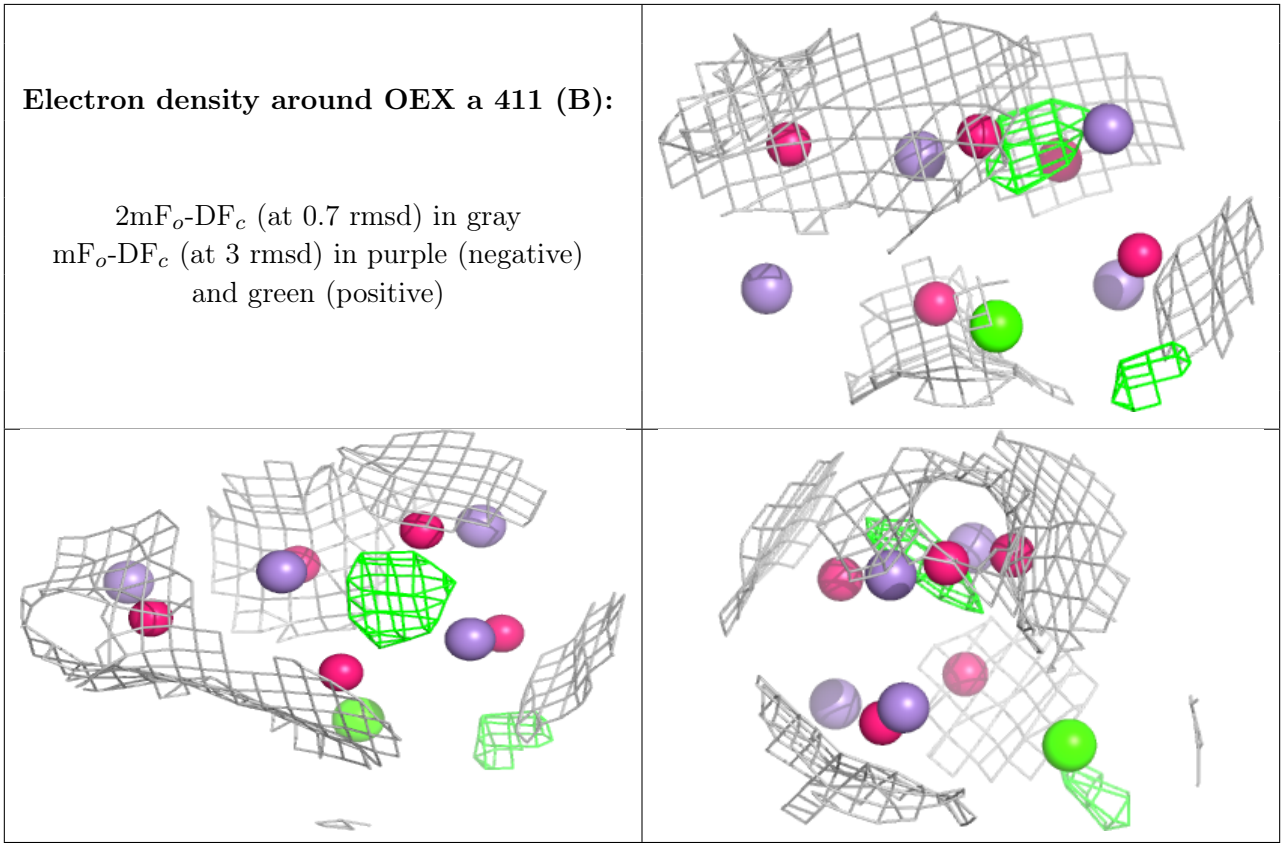
Electron density around OEX a 411 (A):

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



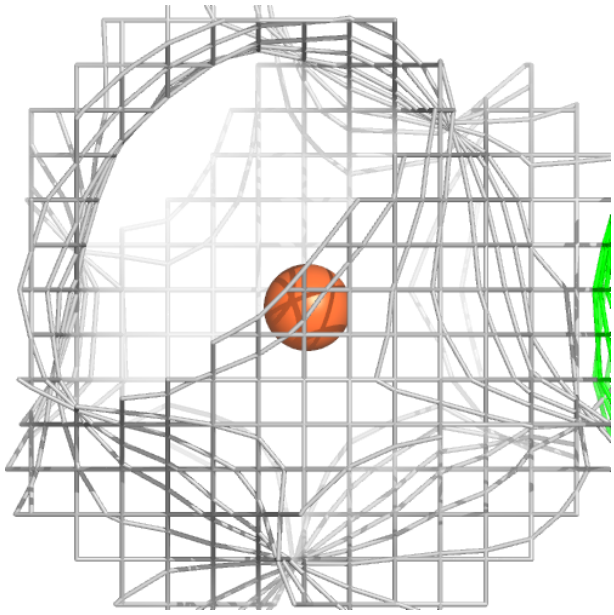
Electron density around OEX a 411 (B):

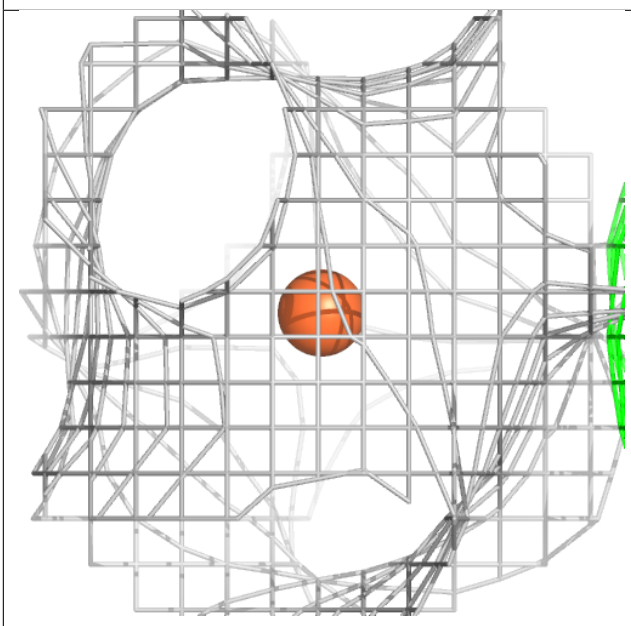
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

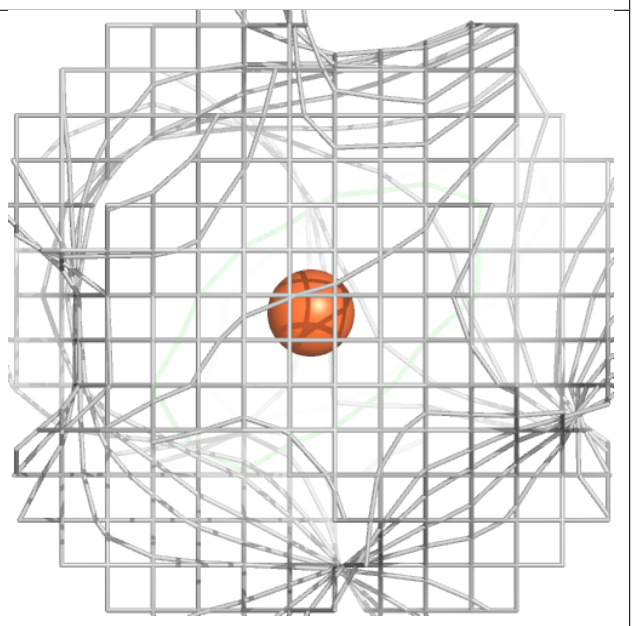


Electron density around FE2 A 401 (A):

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

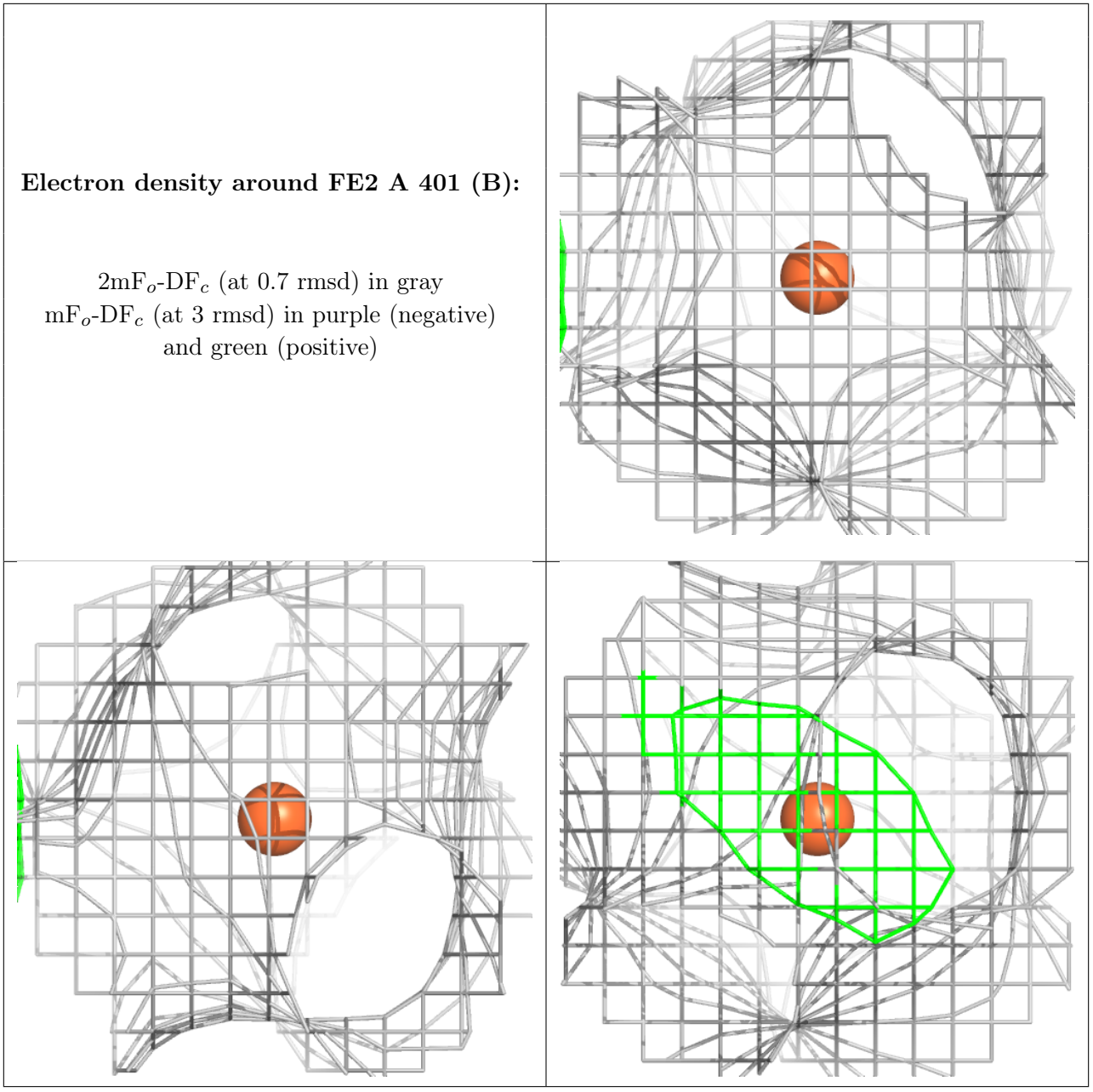






Electron density around FE2 A 401 (B):

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



6.5 Other polymers

There are no such residues in this entry.