Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 07:27 PM JST

PDB ID	:	8IR8 / pdb_00008ir8
Title	:	XFEL structure of cyanobacterial photosystem II following one flash (1F) with a 1-microsecond 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:

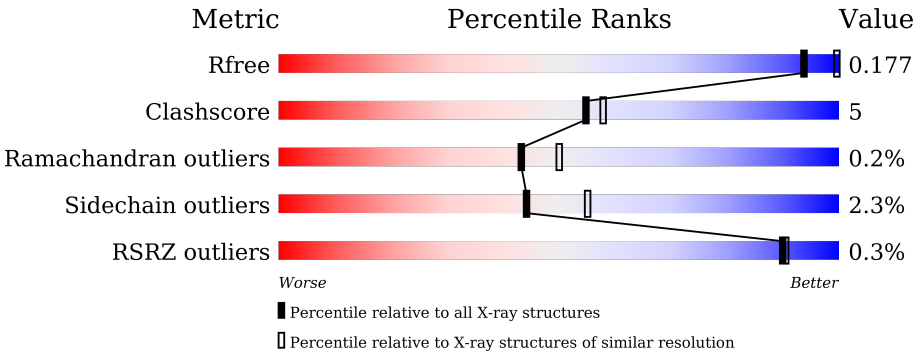
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
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	91% 6% ·
1	a	344	89% 8% ·
2	B	505	93% 6%
2	b	505	93% 6% ·
3	C	455	93% 7% ·
3	c	455	92% 8%

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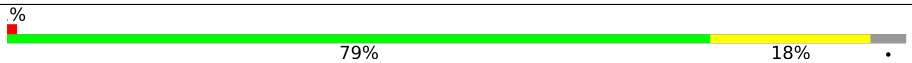
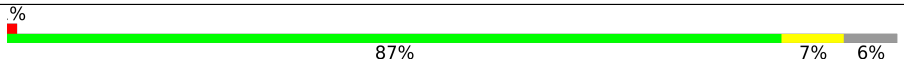
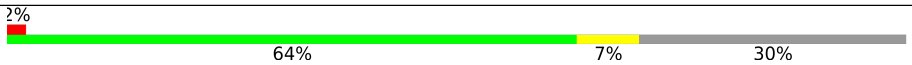
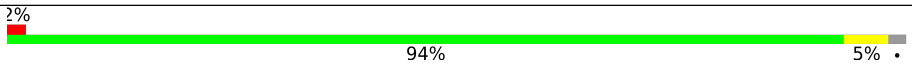
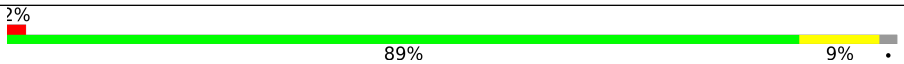
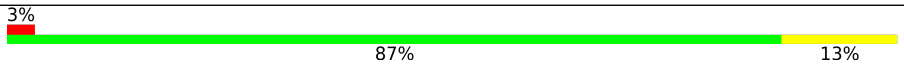
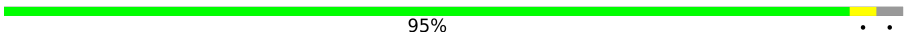
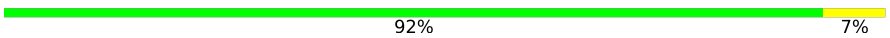
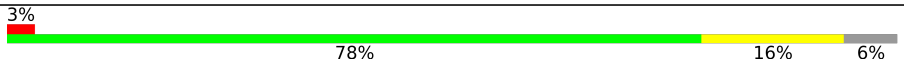
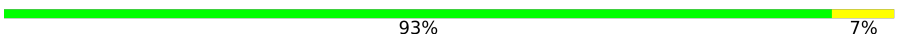
Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	89% 9%
17	X	40	90% 5% 5%
17	x	40	92% 5%
18	Y	30	3% 83% 13%
18	y	30	60% 37%
19	Z	62	90% 8%
19	z	62	81% 16%
20	R	34	3% 71% 29%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	GOL	a	416	-	-	X	-
40	HEC	V	201	X	-	-	-
40	HEC	v	201	X	-	-	-

2 Entry composition (i)

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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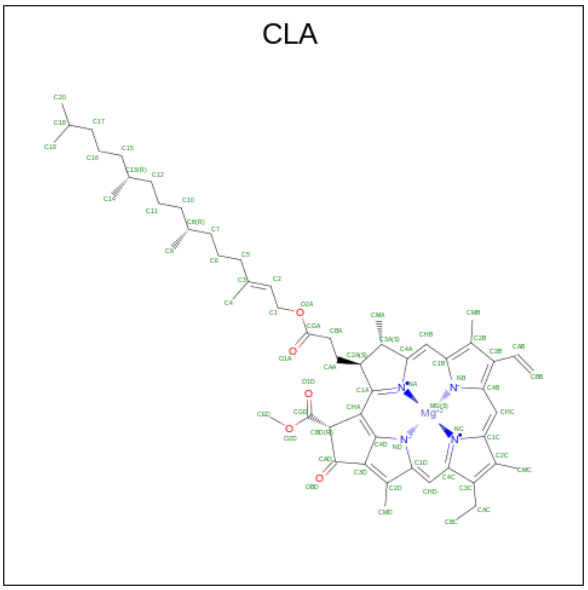
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2

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



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

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

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

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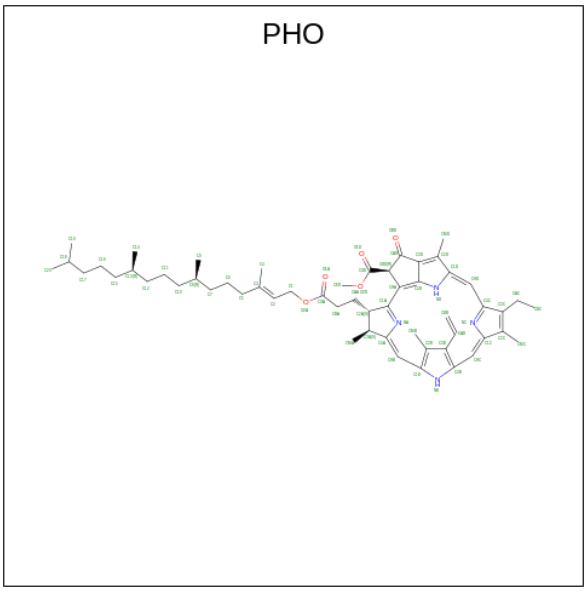
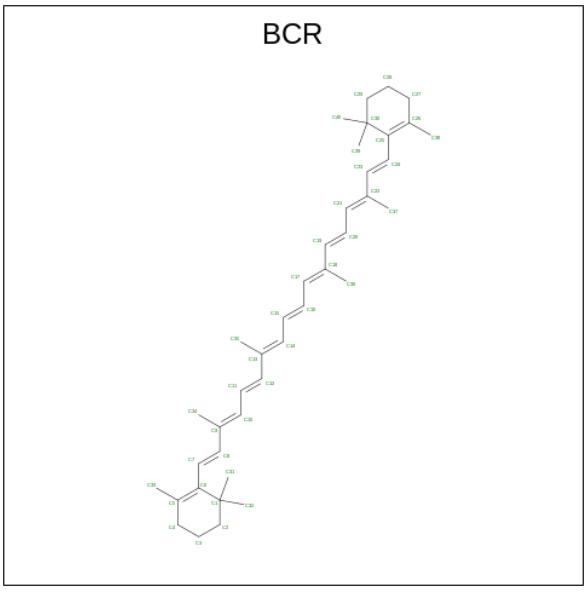
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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



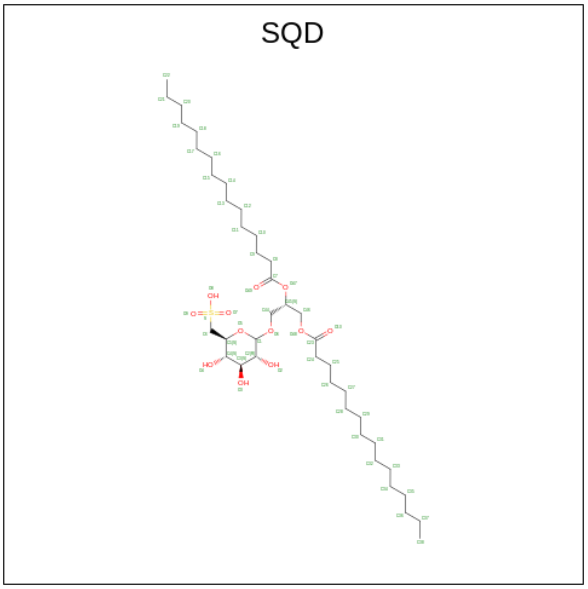
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



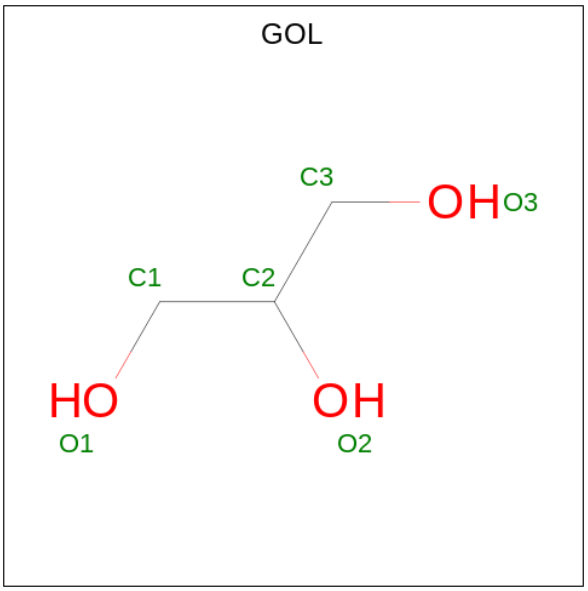
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	X	1	Total C 40 40	0	0
25	Y	1	Total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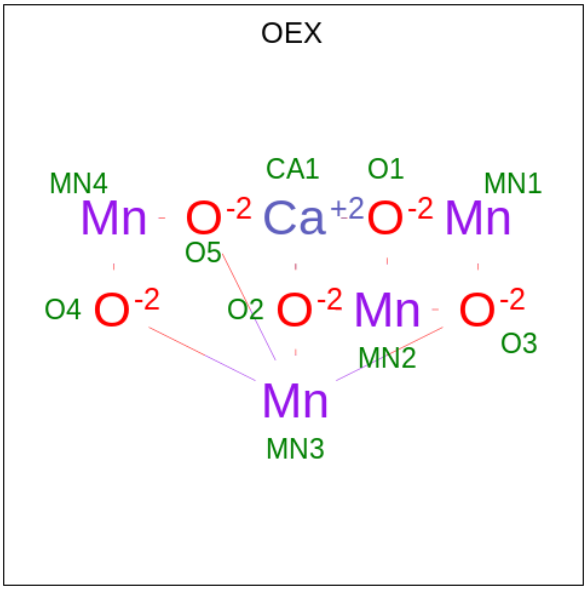
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	c	1	Total C O 12 6 6	0	1
27	c	1	Total C O 6 3 3	0	0
27	d	1	Total C O 6 3 3	0	0
27	l	1	Total C O 12 6 6	0	1
27	o	1	Total C O 6 3 3	0	0
27	o	1	Total C O 6 3 3	0	0
27	v	1	Total C O 12 6 6	0	1

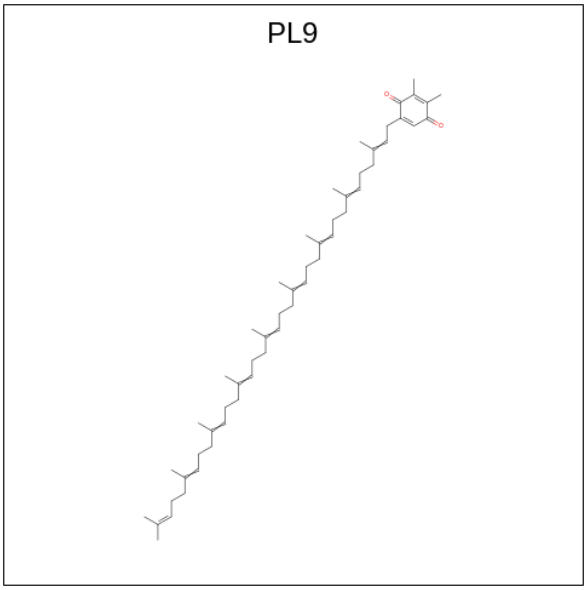
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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	M	1	Total C 10 10	0	0

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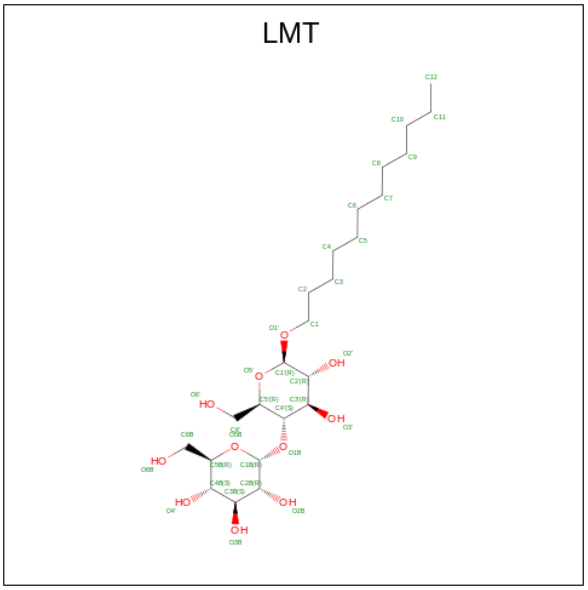
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total C O 18 16 2	0	0
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 64 54 10	0	1
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

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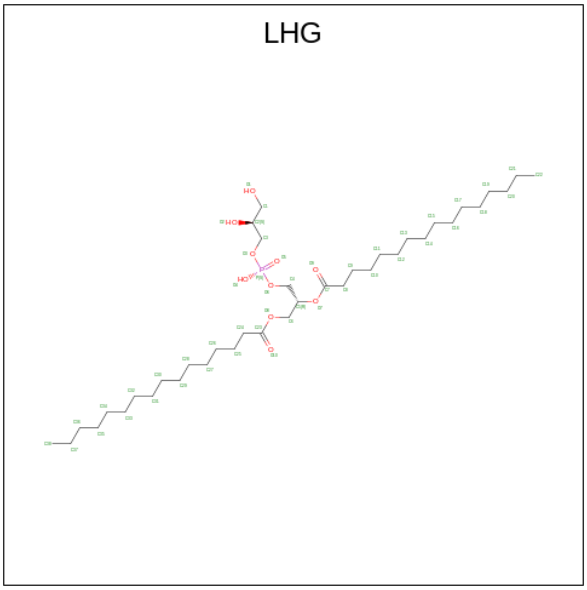
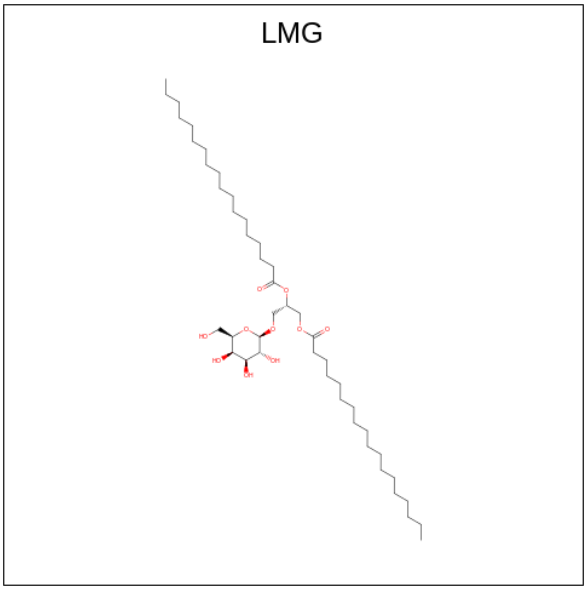
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	B	1	Total C O 25 19 6	0	0
31	F	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	b	1	Total C O 25 19 6	0	0
31	b	1	Total C O 25 19 6	0	0
31	c	1	Total C O 35 24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

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



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

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



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

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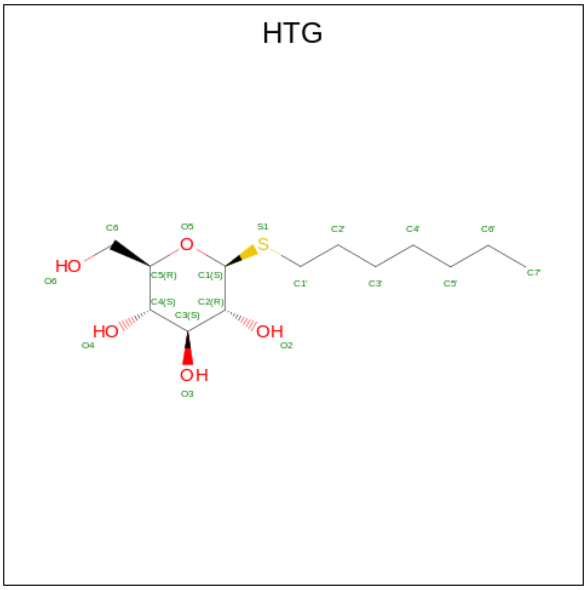
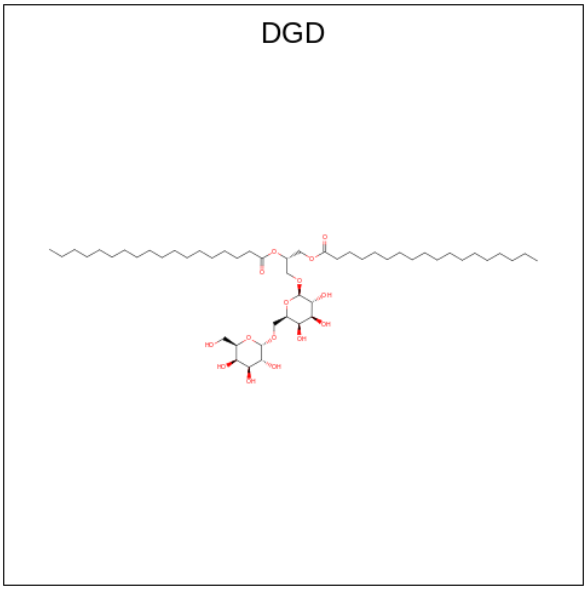
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	D	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	m	1	Total C O 51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

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



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

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

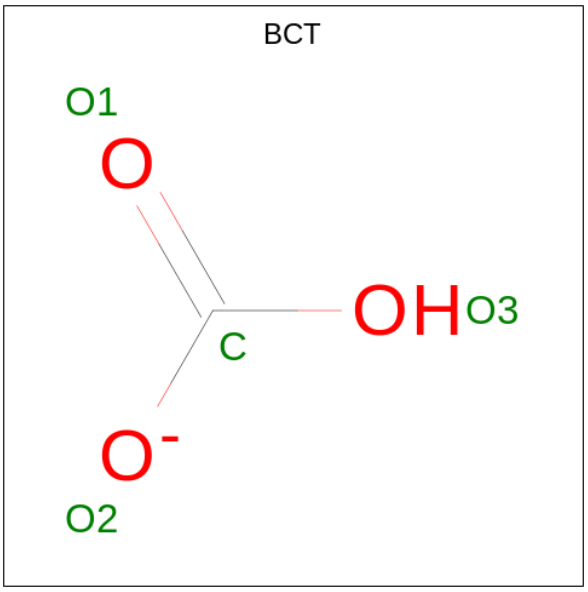


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

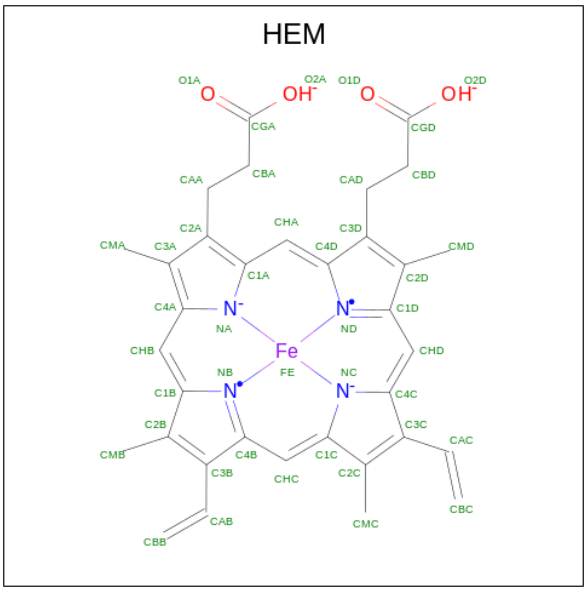
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total Ca 1 1	0	0
36	F	1	Total Ca 1 1	0	0
36	O	1	Total Ca 1 1	0	0
36	c	2	Total Ca 2 2	0	0
36	f	1	Total Ca 1 1	0	0
36	o	1	Total Ca 1 1	0	0

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



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

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



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

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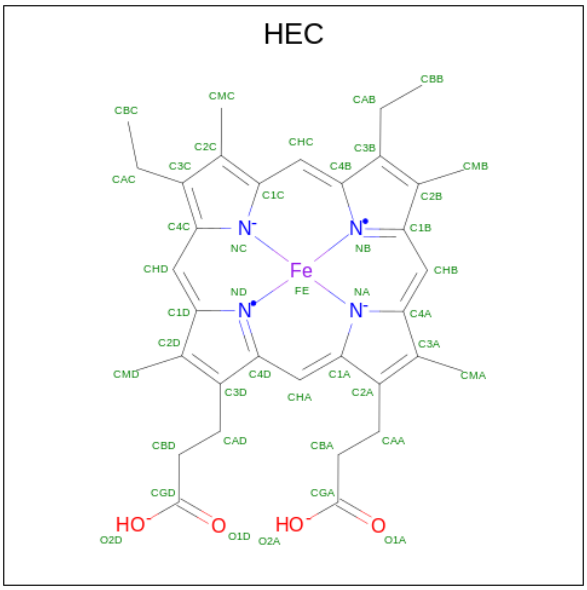
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
38	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	141	Total	O	0	86
			226	226		
41	B	191	Total	O	0	2
			193	193		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	C	168	Total O 205 205	0	38
41	D	117	Total O 151 151	0	34
41	E	17	Total O 17 17	0	0
41	F	5	Total O 5 5	0	0
41	H	21	Total O 21 21	0	0
41	I	6	Total O 6 6	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	103	Total O 108 108	0	5
41	T	10	Total O 13 13	0	3
41	U	46	Total O 48 48	0	2
41	V	79	Total O 80 80	0	1
41	X	7	Total O 7 7	0	0
41	a	126	Total O 206 206	0	81
41	b	200	Total O 203 203	0	3
41	c	160	Total O 193 193	0	34
41	d	119	Total O 151 151	0	32
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0

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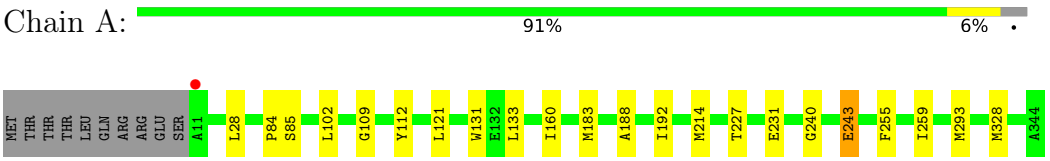
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	h	16	Total O 16 16	0	0
41	i	2	Total O 2 2	0	0
41	j	1	Total O 1 1	0	0
41	k	3	Total O 3 3	0	0
41	l	8	Total O 10 10	0	2
41	m	13	Total O 13 13	0	0
41	o	103	Total O 107 107	0	4
41	t	9	Total O 12 12	0	3
41	u	48	Total O 49 49	0	1
41	v	59	Total O 61 61	0	2
41	x	7	Total 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.

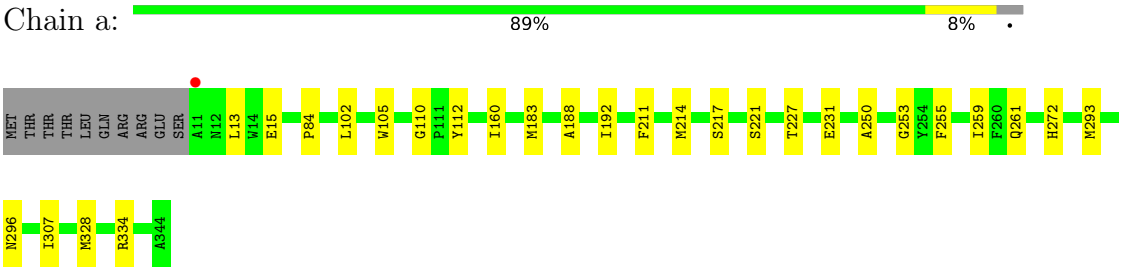
• Molecule 1: Photosystem II protein D1

Chain A:



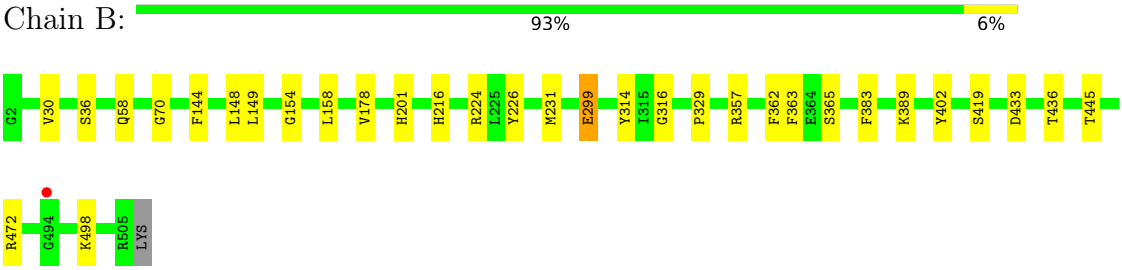
• Molecule 1: Photosystem II protein D1

Chain a:



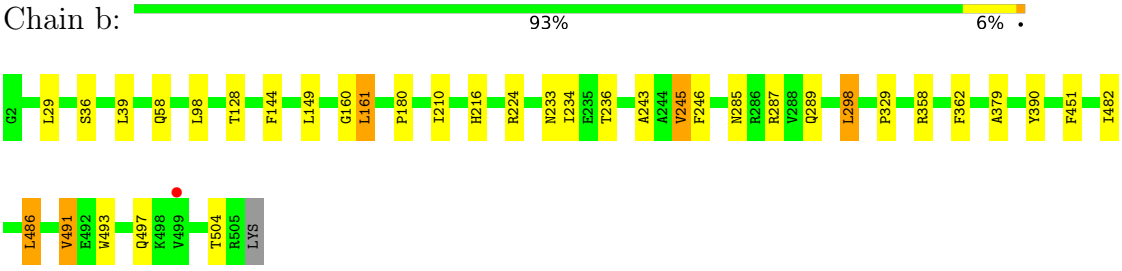
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



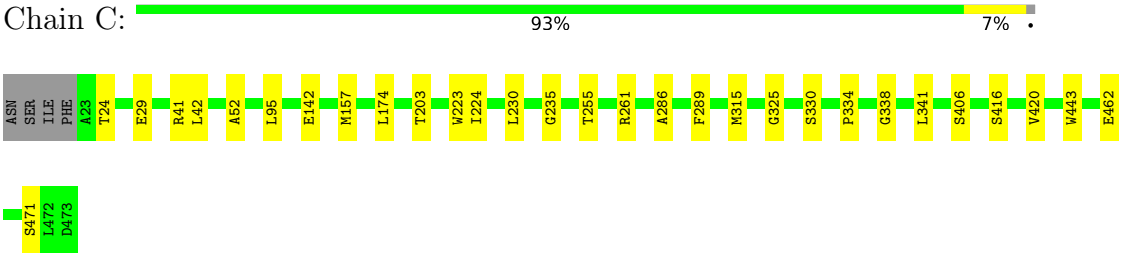
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



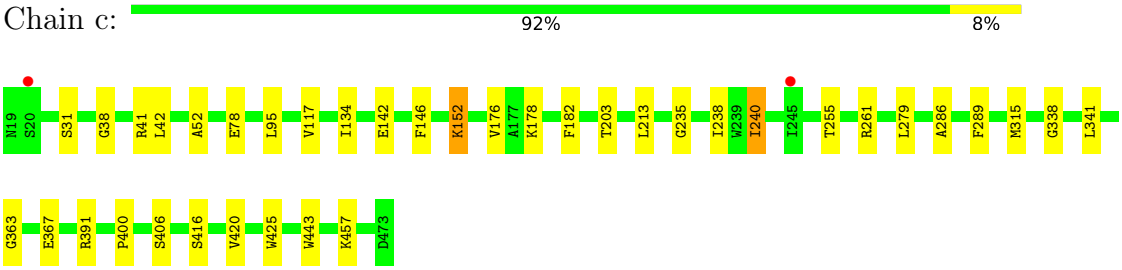
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



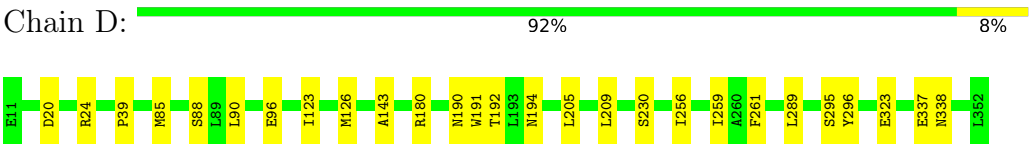
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



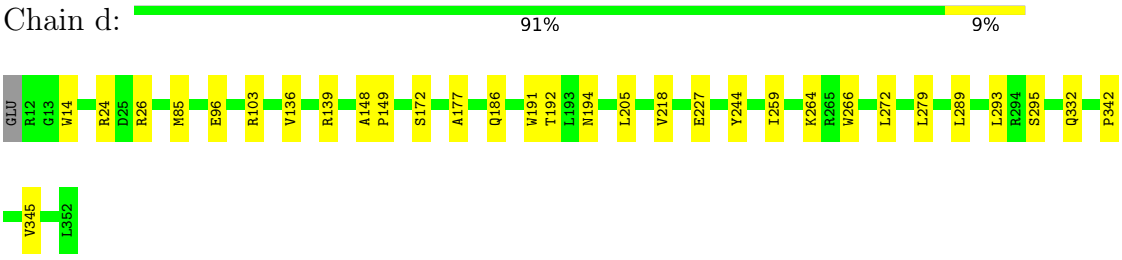
• Molecule 4: Photosystem II D2 protein

Chain D:



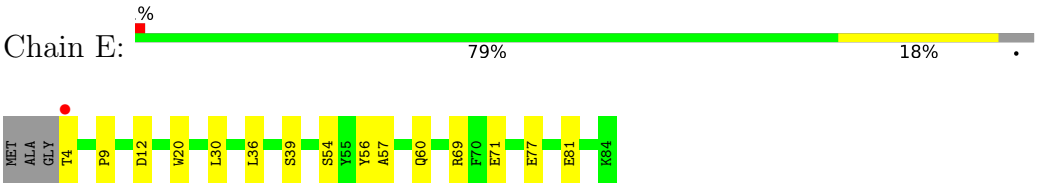
• Molecule 4: Photosystem II D2 protein

Chain d:



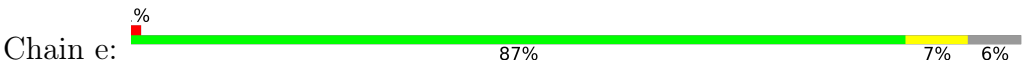
• Molecule 5: Cytochrome b559 subunit alpha

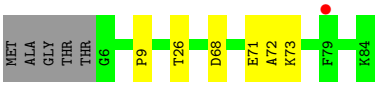
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

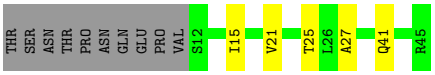
Chain e:





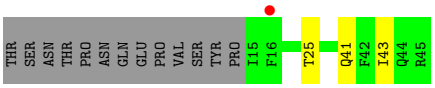
• Molecule 6: Cytochrome b559 subunit beta



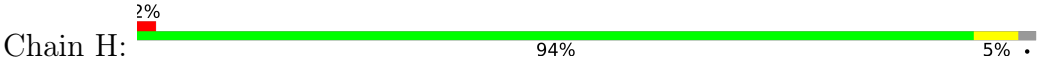


• Molecule 6: Cytochrome b559 subunit beta



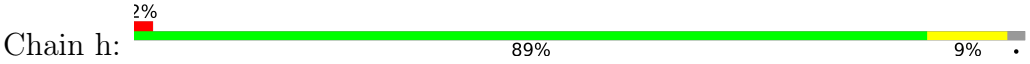


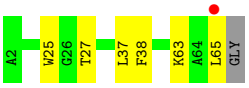
• Molecule 7: Photosystem II reaction center protein H



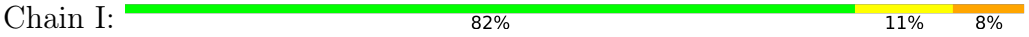


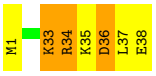
• Molecule 7: Photosystem II reaction center protein H



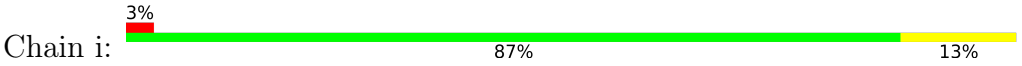


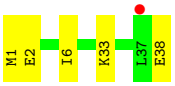
• Molecule 8: Photosystem II reaction center protein I





• Molecule 8: Photosystem II reaction center protein I

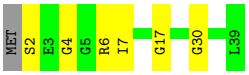




• Molecule 9: Photosystem II reaction center protein J

Chain J:

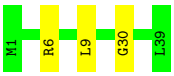




• Molecule 9: Photosystem II reaction center protein J

Chain j:

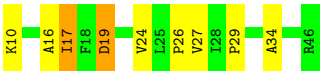




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

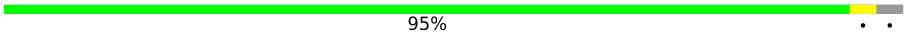
Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:

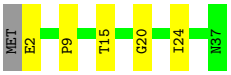




• Molecule 11: Photosystem II reaction center protein L

Chain l:

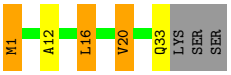




• Molecule 12: Photosystem II reaction center protein M

Chain M:

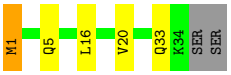




• Molecule 12: Photosystem II reaction center protein M

Chain m:

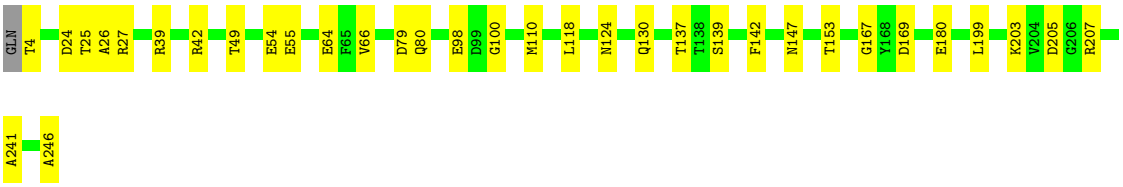




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

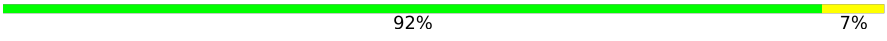
Chain O:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

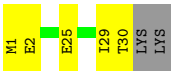




• Molecule 14: Photosystem II reaction center protein T

Chain T:

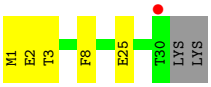




• Molecule 14: Photosystem II reaction center protein T

Chain t:

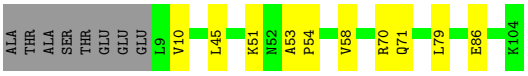




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

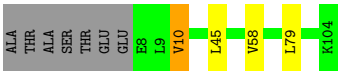




• Molecule 15: Photosystem II 12 kDa extrinsic protein

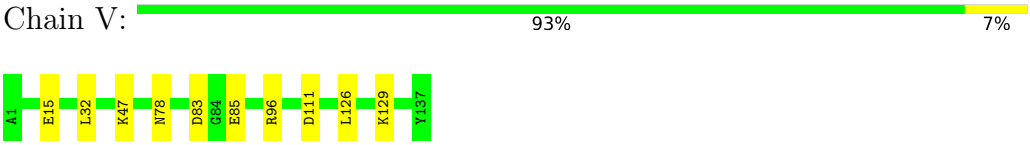
Chain u:





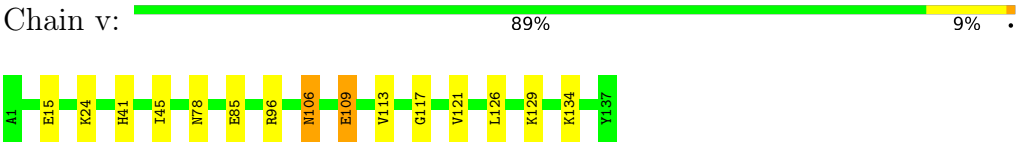
• Molecule 16: Cytochrome c-550

Chain V:



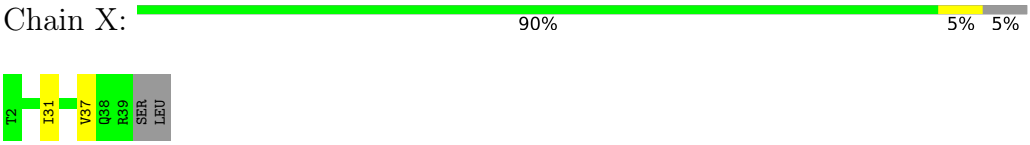
• Molecule 16: Cytochrome c-550

Chain v:



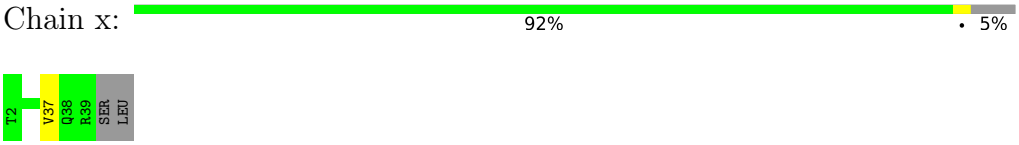
• Molecule 17: Photosystem II reaction center protein X

Chain X:



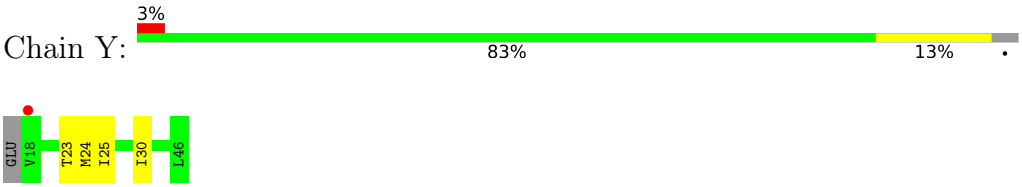
• Molecule 17: Photosystem II reaction center protein X

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



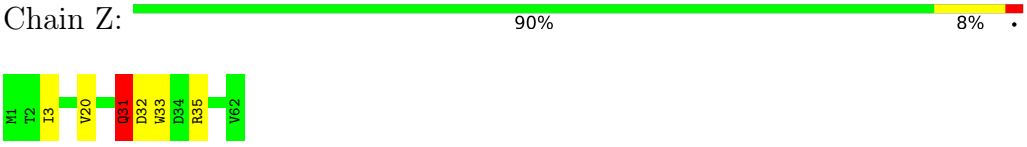
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 19: Photosystem II reaction center protein Z

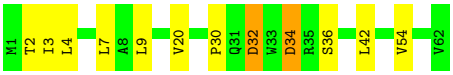
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

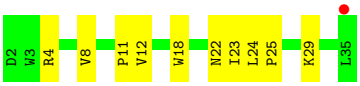




• Molecule 20: Photosystem II protein Y

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.75Å 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]	1.60 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.139 , 0.175 0.140 , 0.177	Depositor DCC
R_{free} test set	19865 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.491	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.8	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)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% 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: PL9, FME, BCR, HEM, CLA, BCT, SQD, LMG, CA, HEC, CL, LMT, UNL, LHG, HTG, DGD, PHO, MG, OEX, GOL, FE2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.27	0/4478	0.45	0/6098
1	a	0.25	0/4457	0.42	0/6069
2	B	0.34	0/4314	0.49	0/5879
2	b	0.32	0/4285	0.48	0/5841
3	C	0.27	0/4416	0.42	0/6013
3	c	0.28	0/4467	0.43	0/6082
4	D	0.32	0/3746	0.46	0/5102
4	d	0.30	0/3780	0.45	0/5147
5	E	0.31	0/681	0.49	0/928
5	e	0.28	0/690	0.46	0/939
6	F	0.31	0/284	0.44	0/387
6	f	0.28	0/269	0.42	0/365
7	H	0.30	0/519	0.50	0/708
7	h	0.29	0/530	0.48	0/722
8	I	0.29	0/311	0.44	0/419
8	i	0.32	0/311	0.45	0/419
9	J	0.29	0/278	0.38	0/376
9	j	0.28	0/283	0.39	0/383
10	K	0.32	0/303	0.50	0/416
10	k	0.32	0/303	0.45	0/416
11	L	0.34	0/318	0.47	0/433
11	l	0.38	0/318	0.47	0/433
12	M	0.38	0/261	0.51	0/357
12	m	0.35	0/279	0.48	0/380
13	O	0.34	0/1991	0.51	0/2698
13	o	0.32	0/1966	0.50	0/2665
14	T	0.32	0/310	0.39	0/419
14	t	0.32	0/301	0.40	0/406
15	U	0.36	0/811	0.52	0/1095
15	u	0.35	0/826	0.52	0/1116
16	V	0.32	0/1142	0.49	0/1545

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
16	v	0.30	0/1139	0.46	0/1542
17	X	0.22	0/292	0.34	0/395
17	x	0.23	0/284	0.37	0/384
18	Y	0.27	0/216	0.43	0/289
18	y	0.24	0/216	0.40	0/289
19	Z	0.22	0/490	0.39	0/669
19	z	0.22	0/490	0.33	0/669
20	R	0.26	0/279	0.37	0/383
All	All	0.30	0/50634	0.46	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	21	0
1	a	4318	0	4124	33	0
2	B	4166	0	3999	23	0
2	b	4134	0	3976	40	0
3	C	4272	0	4138	20	0
3	c	4316	0	4184	30	0
4	D	3625	0	3489	30	0
4	d	3658	0	3522	26	0
5	E	662	0	648	9	0
5	e	670	0	655	5	0
6	F	275	0	282	4	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	6	0
8	I	314	0	328	5	0
8	i	314	0	328	2	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	6	0
10	k	293	0	305	6	0
11	L	311	0	320	2	0
11	l	311	0	320	4	0
12	M	268	0	285	4	0
12	m	286	0	305	7	0
13	O	1958	0	1920	22	0
13	o	1933	0	1900	8	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	3	0
16	V	1120	0	1122	5	0
16	v	1117	0	1131	9	0
17	X	289	0	322	2	0
17	x	281	0	312	1	0
18	Y	215	0	246	2	0
18	y	215	0	246	6	0
19	Z	479	0	516	3	0
19	z	479	0	516	3	0
20	R	273	0	305	5	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	20	0
23	B	1040	0	1152	32	0
23	C	845	0	936	32	0
23	D	195	0	216	5	0
23	a	325	0	360	15	0
23	b	1040	0	1152	25	0
23	c	845	0	936	38	0
23	d	325	0	360	12	0
24	A	256	0	296	7	0
24	a	256	0	296	4	0
25	A	40	0	56	2	0
25	B	120	0	168	6	0
25	C	80	0	112	2	0
25	D	40	0	56	0	0
25	K	40	0	56	1	0
25	T	40	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	X	40	0	56	1	0
25	Y	40	0	56	3	0
25	a	40	0	56	1	0
25	b	120	0	168	10	0
25	c	80	0	112	3	0
25	d	40	0	56	2	0
25	h	40	0	56	5	0
25	k	40	0	56	2	0
25	t	40	0	56	5	0
25	y	40	0	56	3	0
26	A	162	0	233	7	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	162	0	232	10	0
26	b	54	0	78	3	0
26	f	43	0	53	0	0
27	A	12	0	15	3	0
27	B	18	0	24	2	0
27	C	12	0	16	1	0
27	D	6	0	8	2	0
27	O	12	0	16	3	0
27	V	12	0	16	0	0
27	a	12	0	16	5	0
27	b	12	0	16	3	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	18	0
29	D	110	0	160	0	0
29	a	110	0	160	9	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	M	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	X	18	0	0	0	0
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	70	0	92	2	0
31	B	95	0	127	2	0
31	F	35	0	46	0	0
31	M	70	0	91	1	0
31	b	50	0	70	2	0
31	c	35	0	46	1	0
31	e	35	0	46	1	0
31	m	35	0	46	0	0
31	t	26	0	35	0	0
32	A	98	0	148	2	0
32	D	196	0	296	13	0
32	E	84	0	114	7	0
32	L	98	0	148	0	0
32	a	84	0	114	8	0
32	b	98	0	148	0	0
32	d	294	0	444	23	0
33	B	51	0	72	1	0
33	C	153	0	216	3	0
33	D	51	0	72	0	0
33	Z	37	0	44	2	0
33	c	153	0	216	3	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	38	0	52	2	0
34	C	19	0	26	0	0
34	D	16	0	17	0	0
34	V	11	0	10	0	0
34	b	57	0	78	4	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
34	o	19	0	26	2	0
35	C	310	0	410	11	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	9	0
35	h	62	0	82	1	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0
36	O	1	0	0	0	0
36	c	2	0	0	0	0
36	f	1	0	0	0	0
36	o	1	0	0	0	0
37	D	8	0	0	0	0
37	d	8	0	0	0	0
38	E	43	0	30	1	0
38	f	43	0	30	1	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	V	43	0	30	0	0
40	v	43	0	30	0	0
41	A	226	0	0	1	0
41	B	193	0	0	2	0
41	C	205	0	0	2	0
41	D	151	0	0	2	0
41	E	17	0	0	0	0
41	F	5	0	0	0	0
41	H	21	0	0	0	0
41	I	6	0	0	0	0
41	J	7	0	0	1	0
41	K	6	0	0	0	0
41	L	10	0	0	0	0
41	M	5	0	0	0	0
41	O	108	0	0	0	0
41	T	13	0	0	0	0
41	U	48	0	0	0	0
41	V	80	0	0	0	0
41	X	7	0	0	0	0
41	a	206	0	0	3	0
41	b	203	0	0	0	0
41	c	193	0	0	4	0
41	d	151	0	0	1	0
41	e	8	0	0	0	0
41	f	3	0	0	0	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	1	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	107	0	0	0	0
41	t	12	0	0	0	0
41	u	49	0	0	1	0
41	v	61	0	0	0	0
41	x	7	0	0	0	0
41	y	2	0	0	0	0
All	All	62674	0	61528	581	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 (581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:418:GOL:H11	12:M:1:FME:HG2	1.46	0.97
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.53	0.89
23:B:604:CLA:H42	23:B:605:CLA:H2	1.54	0.88
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.53	0.88
23:c:505:CLA:HBB1	23:c:514:CLA:H41	1.57	0.85
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:C:502:CLA:H193	23:C:508:CLA:HBB1	1.67	0.76
23:B:601:CLA:H12	23:B:601:CLA:H71	1.65	0.75
4:d:192[B]:THR:HG23	23:d:403[B]:CLA:HBC2	1.69	0.73
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.22	0.72
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.71	0.72
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.72	0.72
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.72	0.71
23:c:507:CLA:HBB1	23:c:507:CLA:HHC	1.73	0.71
32:D:407[A]:LHG:H112	32:D:407[A]:LHG:H382	1.74	0.70
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.74	0.70
32:d:407[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.73	0.70
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.74	0.69
3:c:213:LEU:HD13	23:c:508:CLA:H202	1.75	0.69
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.73	0.69
27:a:416:GOL:O2	41:a:501:HOH:O	2.09	0.68
27:a:415:GOL:H32	12:m:1:FME:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:407:CLA:H192	23:c:507:CLA:H142	1.74	0.68
23:A:408:CLA:H193	23:C:507:CLA:H101	1.75	0.68
23:c:507:CLA:CMD	23:c:509:CLA:HAB	2.24	0.68
13:O:42:ARG:HH12	27:O:302:GOL:H12	1.59	0.67
23:c:513:CLA:H191	33:z:101:LMG:H241	1.78	0.66
23:C:502:CLA:HHC	23:C:502:CLA:HBB1	1.77	0.66
29:A:414[B]:PL9:H262	32:E:101[B]:LHG:H223	1.78	0.65
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.29	0.64
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.78	0.64
23:a:407:CLA:H152	23:c:508:CLA:H142	1.78	0.64
3:c:279:LEU:HD22	23:c:511:CLA:HED2	1.79	0.64
23:b:601:CLA:H72	23:b:601:CLA:H2	1.78	0.64
29:A:414[A]:PL9:H262	32:E:101[A]:LHG:H223	1.80	0.64
23:C:507:CLA:H142	35:C:517[B]:DGD:HAF2	1.79	0.64
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.81	0.63
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.81	0.63
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.80	0.62
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.82	0.62
23:c:507:CLA:HMD1	23:c:509:CLA:HAB	1.81	0.62
23:d:402[B]:CLA:HHC	23:d:402[B]:CLA:HBB1	1.82	0.62
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H112	1.82	0.62
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.81	0.62
27:A:418:GOL:O2	41:A:501:HOH:O	2.16	0.61
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.82	0.61
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.82	0.61
3:c:134[B]:ILE:HD13	23:c:513:CLA:H43	1.83	0.61
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.31	0.61
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.82	0.61
19:z:32:ASP:O	19:z:36:SER:OG	2.17	0.60
25:C:515:BCR:H352	33:C:521:LMG:H352	1.84	0.60
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.83	0.60
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.84	0.60
10:K:17:ILE:H	10:K:17:ILE:HD13	1.65	0.60
25:T:101:BCR:H311	25:T:101:BCR:HC8	1.84	0.60
23:C:514:CLA:H202	33:C:521:LMG:H402	1.82	0.60
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.32	0.60
16:v:134[A]:LYS:HE2	27:v:202[A]:GOL:H32	1.83	0.60
10:k:17:ILE:HD13	10:k:17:ILE:H	1.67	0.60
2:B:226:TYR:HA	2:B:231:MET:HG3	1.84	0.59
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	1.84	0.59
23:C:507:CLA:H142	35:C:517[A]:DGD:HAF2	1.84	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	1.83	0.59
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.85	0.59
23:c:504:CLA:H61	23:c:514:CLA:H42	1.85	0.59
3:c:134[B]:ILE:HD11	23:c:513:CLA:H71	1.85	0.59
23:b:604:CLA:H42	23:b:605:CLA:H2	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	32:d:408[A]:LHG:H172	1.86	0.58
3:C:286:ALA:HB2	23:C:503:CLA:HMD1	1.84	0.58
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.12	0.58
26:a:409[B]:SQD:H141	32:d:408[B]:LHG:H152	1.85	0.58
23:c:503:CLA:C4D	23:c:505:CLA:H2	2.33	0.58
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.37	0.57
2:b:285:ASN:O	2:b:289:GLN:HG2	2.03	0.57
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.84	0.57
31:A:417:LMT:H71	2:b:39:LEU:HD13	1.86	0.57
31:B:629:LMT:H52	34:o:301:HTG:H4'1	1.86	0.57
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.35	0.56
29:A:414[B]:PL9:H253	23:D:402[B]:CLA:H141	1.87	0.56
13:O:169:ASP:OD1	27:O:303:GOL:H12	2.05	0.56
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.06	0.56
26:a:409[A]:SQD:H141	32:d:408[A]:LHG:H152	1.86	0.56
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.41	0.56
25:t:102:BCR:H382	25:t:102:BCR:H23C	1.88	0.56
4:D:123:ILE:HD11	35:H:101:DGD:HAH2	1.88	0.56
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.18	0.56
33:z:101:LMG:H302	33:z:101:LMG:H141	1.88	0.56
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.39	0.55
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.06	0.55
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.89	0.55
13:O:124:ASN:OD1	13:O:147:ASN:ND2	2.38	0.55
1:a:183[B]:MET:HA	23:a:404[B]:CLA:HMD1	1.89	0.55
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.41	0.55
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.72	0.55
2:B:383[B]:PHE:CZ	13:O:167:GLY:HA2	2.42	0.54
27:a:416:GOL:O3	14:t:2:GLU:OE1	2.26	0.54
26:a:409[B]:SQD:H152	32:d:408[B]:LHG:H172	1.90	0.54
23:a:405[A]:CLA:H191	32:a:417[A]:LHG:H111	1.88	0.54
32:a:417[A]:LHG:HC31	5:e:9:PRO:HA	1.88	0.54
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.90	0.54
15:u:10[A]:VAL:HG12	41:u:240:HOH:O	2.07	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:t:102:BCR:HC8	25:t:102:BCR:H321	1.88	0.54
16:v:134[B]:LYS:HE2	27:v:202[B]:GOL:H32	1.89	0.54
1:a:183[A]:MET:HA	23:a:404[A]:CLA:HMD1	1.90	0.54
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.90	0.54
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.90	0.54
23:B:615:CLA:HHC	23:B:615:CLA:HBB1	1.90	0.54
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.90	0.54
23:c:515:CLA:HBB1	25:c:516:BCR:H24C	1.89	0.54
23:B:606:CLA:H202	26:a:410:SQD:H302	1.91	0.53
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.90	0.53
24:A:416[B]:PHO:H3A	23:D:402[B]:CLA:H142	1.91	0.53
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.08	0.53
32:d:408[B]:LHG:H342	32:d:408[B]:LHG:H151	1.91	0.53
3:C:325:GLY:O	15:U:51:LYS:NZ	2.38	0.53
23:a:404[B]:CLA:H201	32:d:407[B]:LHG:H161	1.91	0.53
4:D:192[A]:THR:HG23	23:D:402[A]:CLA:HBC2	1.90	0.53
27:a:416:GOL:H11	12:m:1:FME:HE3	1.91	0.53
29:A:414[B]:PL9:H472	4:D:39:PRO:HD3	1.92	0.52
23:c:506:CLA:H62	35:c:520:DGD:HB62	1.92	0.52
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.91	0.52
5:E:77:GLU:O	5:E:81:GLU:HG2	2.10	0.52
27:C:523[B]:GOL:O2	16:V:47[B]:LYS:NZ	2.37	0.52
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.92	0.52
25:b:619:BCR:H331	25:b:619:BCR:C8	2.40	0.52
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.43	0.52
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.91	0.52
26:F:102:SQD:H102	17:X:31:ILE:HD11	1.93	0.51
29:a:412[B]:PL9:H28	32:a:417[B]:LHG:H222	1.91	0.51
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.93	0.51
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.45	0.51
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.10	0.51
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.23	0.51
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.45	0.51
32:a:417[B]:LHG:HC31	5:e:9:PRO:HA	1.91	0.51
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.43	0.51
23:c:503:CLA:C3D	23:c:505:CLA:H2	2.39	0.51
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	1.91	0.51
4:D:85:MET:CE	4:D:96:GLU:HG2	2.41	0.51
35:c:518[B]:DGD:HG11	41:c:604[B]:HOH:O	2.11	0.51
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.46	0.51
29:a:412[A]:PL9:H28	32:a:417[A]:LHG:H222	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:520:DGD:HBH2	32:d:408[B]:LHG:H211	1.93	0.51
4:D:261[B]:PHE:CZ	32:D:406[B]:LHG:HC81	2.46	0.51
27:b:628:GOL:HO1	27:b:628:GOL:HO3	1.51	0.51
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.41	0.51
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.93	0.50
2:B:383[A]:PHE:CZ	13:O:167:GLY:HA2	2.46	0.50
31:e:101:LMT:H6'1	6:f:43:ILE:HG12	1.91	0.50
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.93	0.50
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.92	0.50
29:A:414[A]:PL9:H253	23:D:402[A]:CLA:H141	1.92	0.50
24:a:406[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.93	0.50
32:d:407[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.94	0.50
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.45	0.50
32:A:419[B]:LHG:H361	23:B:613:CLA:H51	1.93	0.50
9:J:2:SER:N	41:J:201:HOH:O	2.44	0.50
8:I:35:LYS:O	8:I:37:LEU:N	2.44	0.50
1:A:133:LEU:HD23	4:D:256[B]:ILE:HG12	1.94	0.50
23:b:613:CLA:HBB1	23:b:613:CLA:HMB1	1.92	0.50
4:d:85:MET:CE	4:d:96:GLU:HG2	2.41	0.50
35:c:520:DGD:HBH2	32:d:408[A]:LHG:H211	1.94	0.49
1:A:188[B]:ALA:HB2	1:A:328[B]:MET:HB2	1.94	0.49
29:A:414[A]:PL9:H503	26:F:102:SQD:H341	1.94	0.49
6:F:21:VAL:O	6:F:25:THR:HG23	2.11	0.49
3:c:443[A]:TRP:CE2	23:c:510:CLA:HMD2	2.48	0.49
23:d:404:CLA:H162	7:h:37:LEU:HD21	1.94	0.49
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.12	0.49
4:D:323[A]:GLU:O	27:D:412:GOL:O2	2.31	0.49
1:a:15:GLU:HB2	31:c:502:LMT:H6'2	1.94	0.49
23:d:404:CLA:HHC	23:d:404:CLA:HBB1	1.95	0.49
18:Y:23:THR:HB	18:Y:24:MET:HE2	1.94	0.49
27:l:801[A]:GOL:H32	14:t:25:GLU:HB2	1.93	0.49
29:a:412[A]:PL9:H351	6:f:25:THR:OG1	2.12	0.49
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.12	0.49
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.47	0.49
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.94	0.49
4:D:230[B]:SER:HB2	41:D:547:HOH:O	2.13	0.49
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.93	0.49
23:c:514:CLA:HMB2	23:c:514:CLA:H192	1.95	0.49
23:a:404[A]:CLA:H201	32:d:407[A]:LHG:H161	1.95	0.49
25:T:101:BCR:H19C	25:b:618:BCR:H363	1.95	0.49
12:m:5[B]:GLN:CD	12:m:5[B]:GLN:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:y:20:ALA:O	18:y:24:MET:HG2	2.13	0.49
2:B:30:VAL:HG12	23:B:605:CLA:HHD	1.95	0.48
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.48	0.48
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.95	0.48
3:C:174:LEU:HB3	23:C:503:CLA:H152	1.93	0.48
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.14	0.48
23:b:602:CLA:HHC	23:b:602:CLA:HBB1	1.94	0.48
32:d:408[A]:LHG:H331	32:d:408[A]:LHG:H361	1.55	0.48
2:B:357[A]:ARG:HH12	27:B:623:GOL:H32	1.79	0.48
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:H132	1.96	0.48
2:b:29:LEU:HD23	26:b:620:SQD:H201	1.96	0.48
3:c:286:ALA:HB2	23:c:504:CLA:HMD1	1.94	0.48
13:o:58:ASN:C	13:o:60:ARG:H	2.21	0.48
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	1.96	0.48
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.44	0.48
2:b:233:ASN:O	2:b:236:THR:HG22	2.14	0.48
33:c:521:LMG:H181	10:k:27:VAL:HG11	1.95	0.48
32:d:408[A]:LHG:C38	32:d:408[A]:LHG:H122	2.44	0.48
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.48	0.48
33:d:412:LMG:H221	33:d:412:LMG:H191	1.59	0.48
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.94	0.48
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.96	0.47
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.94	0.47
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.74	0.47
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.96	0.47
1:a:214[B]:MET:HE2	1:a:255[B]:PHE:CE1	2.49	0.47
26:A:410[B]:SQD:H361	10:K:34:ALA:HA	1.96	0.47
10:K:26:PRO:O	10:K:29:PRO:HD2	2.14	0.47
13:O:25:THR:O	13:O:27:ARG:N	2.47	0.47
13:O:42:ARG:O	13:O:241:ALA:HA	2.15	0.47
2:b:245:VAL:HG22	23:b:612:CLA:H202	1.97	0.47
23:c:506:CLA:H151	23:c:510:CLA:H143	1.96	0.47
1:A:240[A]:GLY:HA3	14:T:29[A]:ILE:HG23	1.96	0.47
4:D:323[B]:GLU:O	27:D:412:GOL:O2	2.33	0.47
24:a:414[B]:PHO:HBC3	4:d:279:LEU:HD22	1.95	0.47
9:J:17:GLY:HA3	25:Y:101:BCR:H371	1.97	0.47
1:a:160[A]:ILE:HD11	35:c:518[A]:DGD:HBT1	1.96	0.47
34:B:624:HTG:H61	1:a:102:LEU:HD12	1.96	0.47
1:a:227[B]:THR:HB	1:a:231:GLU:HG3	1.97	0.47
23:a:407:CLA:H172	23:c:508:CLA:H91	1.96	0.47
23:A:404[B]:CLA:HBB1	23:A:404[B]:CLA:HMB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:410[A]:SQD:H152	26:A:410[A]:SQD:H122	1.54	0.47
1:a:214[B]:MET:HB3	29:a:412[B]:PL9:H103	1.97	0.47
23:a:405[B]:CLA:H191	32:a:417[B]:LHG:H111	1.95	0.47
2:b:224:ARG:HH21	31:b:621:LMT:H1'	1.80	0.47
35:C:517[B]:DGD:O1A	41:C:601[B]:HOH:O	2.20	0.47
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.15	0.47
1:A:214[A]:MET:HE2	1:A:255[A]:PHE:CE1	2.49	0.47
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.97	0.47
23:a:405[A]:CLA:H203	33:d:412:LMG:H412	1.97	0.47
3:c:425[A]:TRP:CD1	23:c:506:CLA:HMA3	2.50	0.47
4:d:332[A]:GLN:NE2	41:d:504:HOH:O	2.47	0.47
10:k:20:PRO:HB3	18:y:21:GLN:HG3	1.97	0.47
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.80	0.47
13:O:130:GLN:H	13:O:130:GLN:CD	2.22	0.47
3:c:182:PHE:HA	34:c:523:HTG:H61	1.97	0.47
4:d:342:PRO:O	4:d:345:VAL:HG22	2.15	0.47
32:d:408[A]:LHG:H332	32:d:408[A]:LHG:H302	1.77	0.47
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.97	0.46
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.97	0.46
25:h:101:BCR:C8	25:h:101:BCR:H331	2.45	0.46
26:a:409[B]:SQD:H302	23:c:510:CLA:H71	1.96	0.46
29:a:412[B]:PL9:H171	29:a:412[B]:PL9:H151	1.54	0.46
2:b:234:ILE:HB	27:b:624:GOL:H31	1.98	0.46
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.69	0.46
23:d:402[B]:CLA:HBA1	23:d:402[B]:CLA:C4A	2.44	0.46
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.50	0.46
29:a:412[A]:PL9:H151	29:a:412[A]:PL9:H171	1.57	0.46
4:d:103:ARG:HG3	5:e:73:LYS:HG3	1.96	0.46
1:a:160[B]:ILE:HD11	35:c:518[B]:DGD:HBT1	1.98	0.46
25:d:405:BCR:H15C	25:d:405:BCR:H351	1.79	0.46
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.45	0.46
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.46	0.46
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	1.97	0.46
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.97	0.46
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.98	0.46
23:A:404[B]:CLA:H143	24:A:407[B]:PHO:H61	1.98	0.46
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.51	0.46
23:b:614:CLA:H112	23:b:614:CLA:H72	1.62	0.46
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.96	0.46
23:C:511:CLA:H112	23:C:511:CLA:H152	1.52	0.46
2:b:36:SER:OG	25:b:618:BCR:H362	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.46	0.46
20:R:18:TRP:O	20:R:22:ASN:ND2	2.41	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.15	0.46
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.16	0.46
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.98	0.46
32:D:406[B]:LHG:HC62	11:L:15[B]:THR:HG23	1.98	0.45
1:a:334[B]:ARG:NH2	41:a:509[B]:HOH:O	2.49	0.45
3:c:117:VAL:HG12	33:c:522:LMG:H221	1.98	0.45
23:d:402[A]:CLA:HBA1	23:d:402[A]:CLA:C4A	2.45	0.45
23:b:615:CLA:H61	23:b:615:CLA:H92	1.65	0.45
11:l:20:GLY:O	11:l:24:ILE:HG12	2.15	0.45
16:v:126:LEU:HB3	16:v:129:LYS:HB2	1.97	0.45
25:t:102:BCR:H23C	25:t:102:BCR:C38	2.46	0.45
1:A:28:LEU:HD12	26:A:412:SQD:H121	1.98	0.45
2:B:154:GLY:HA2	2:B:158:LEU:HD12	1.98	0.45
2:b:149[B]:LEU:HD21	23:b:604:CLA:H171	1.99	0.45
32:d:408[B]:LHG:H331	32:d:408[B]:LHG:H361	1.67	0.45
5:e:26:THR:HB	38:f:101:HEM:HAB	1.99	0.45
1:A:231:GLU:HB3	41:B:876:HOH:O	2.17	0.45
35:C:518[A]:DGD:HAT1	35:C:519:DGD:HBE1	1.98	0.45
32:d:408[B]:LHG:H122	32:d:408[B]:LHG:C38	2.47	0.45
18:y:31:ALA:O	18:y:35:ILE:HG13	2.16	0.45
23:B:615:CLA:H71	23:B:616:CLA:H172	1.98	0.45
12:M:20:VAL:HG22	12:m:20:VAL:HG11	1.98	0.45
13:O:142:PHE:HB2	13:O:199:LEU:HB2	1.98	0.45
1:a:105:TRP:CE2	1:a:110[B]:GLY:HA3	2.52	0.45
23:a:405[B]:CLA:H203	33:d:412:LMG:H412	1.99	0.45
25:a:408:BCR:H371	25:a:408:BCR:H24C	1.75	0.45
2:B:363:PHE:HB3	2:B:365:SER:O	2.15	0.45
26:a:409[A]:SQD:H271	32:d:408[A]:LHG:H141	1.98	0.45
4:d:172:SER:HB2	4:d:177:ALA:HB1	1.98	0.45
32:d:408[A]:LHG:H342	32:d:408[A]:LHG:H151	1.99	0.45
26:B:620:SQD:H1	26:B:620:SQD:H462	1.98	0.45
31:B:627:LMT:H62	31:B:627:LMT:H91	1.51	0.45
3:c:443[B]:TRP:CE2	23:c:510:CLA:HMD2	2.52	0.45
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.52	0.45
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.17	0.45
25:d:405:BCR:C8	25:d:405:BCR:H331	2.47	0.45
23:A:404[B]:CLA:HBD	23:A:405[B]:CLA:HAC2	1.99	0.44
23:B:614:CLA:H71	23:B:614:CLA:H112	1.56	0.44
23:B:615:CLA:H112	23:B:615:CLA:H91	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:617:BCR:H11C	25:B:617:BCR:H341	1.87	0.44
13:O:79:ASP:OD1	13:O:80:GLN:N	2.44	0.44
23:b:605:CLA:HAA1	23:b:605:CLA:HBD	1.97	0.44
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.99	0.44
3:C:41:ARG:NH1	23:C:512:CLA:HMD1	2.32	0.44
32:E:101[B]:LHG:H291	32:E:101[B]:LHG:H261	1.73	0.44
26:a:410:SQD:H1	41:a:620:HOH:O	2.17	0.44
2:b:224:ARG:HH21	31:b:621:LMT:H11	1.82	0.44
23:C:505:CLA:H62	23:C:505:CLA:H41	1.73	0.44
23:a:404[A]:CLA:H203	23:a:404[A]:CLA:H162	1.80	0.44
33:Z:101:LMG:H141	33:Z:101:LMG:H111	1.83	0.44
4:D:261[A]:PHE:CZ	32:D:406[A]:LHG:HC81	2.52	0.44
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.44
23:b:615:CLA:H91	23:b:615:CLA:H112	1.77	0.44
23:c:510:CLA:H18	35:c:519[A]:DGD:HAT2	1.99	0.44
4:d:266[A]:TRP:CD1	32:d:407[A]:LHG:HC31	2.52	0.44
13:o:92:SER:HB3	13:o:131:PRO:HA	1.97	0.44
32:A:419[A]:LHG:H361	23:B:613:CLA:H51	1.99	0.44
27:a:416:GOL:H31	12:m:1:FME:HG2	1.99	0.44
23:A:408:CLA:H171	23:C:507:CLA:H121	1.98	0.44
23:A:408:CLA:H41	23:A:408:CLA:H61	1.53	0.44
25:B:619:BCR:H371	25:B:619:BCR:H24C	1.74	0.44
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.48	0.44
32:E:101[A]:LHG:H241	32:E:101[A]:LHG:HC61	1.85	0.44
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.82	0.44
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	1.98	0.44
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.76	0.44
29:A:414[B]:PL9:H151	29:A:414[B]:PL9:H171	1.53	0.44
32:D:407[B]:LHG:H382	32:D:407[B]:LHG:H132	2.00	0.44
5:E:36:LEU:HA	5:E:39:SER:OG	2.17	0.44
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.81	0.44
23:b:607:CLA:H91	23:b:607:CLA:H112	1.71	0.44
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	2.00	0.44
29:A:414[A]:PL9:H322	29:A:414[A]:PL9:H301	1.77	0.44
23:B:614:CLA:H92	23:B:614:CLA:H61	1.77	0.44
5:E:9:PRO:HA	32:E:101[B]:LHG:HC31	1.99	0.44
24:a:414[A]:PHO:HBC3	4:d:279:LEU:HD22	1.98	0.44
23:c:514:CLA:H121	23:c:515:CLA:H142	1.99	0.44
19:Z:31:GLN:CD	19:Z:31:GLN:H	2.26	0.44
25:Y:101:BCR:H15C	25:Y:101:BCR:H351	1.91	0.44
23:d:403[A]:CLA:HAA2	23:d:403[A]:CLA:HBD	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.33	0.44
25:t:102:BCR:HC7	25:t:102:BCR:H331	1.55	0.44
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.53	0.43
3:C:334[A]:PRO:HA	13:O:153:THR:OG1	2.18	0.43
10:K:16:ALA:O	10:K:19:ASP:HB2	2.18	0.43
23:b:601:CLA:HMA2	34:b:623:HTG:H1'1	2.00	0.43
3:c:178:LYS:HA	3:c:182:PHE:HB2	2.00	0.43
35:c:518[A]:DGD:HG11	41:c:604[A]:HOH:O	2.18	0.43
23:C:509:CLA:H142	23:C:509:CLA:H111	1.81	0.43
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.99	0.43
8:I:33:LYS:HB3	8:I:34:ARG:H	1.62	0.43
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CH2	2.54	0.43
3:c:363:GLY:O	3:c:367:GLU:HG2	2.18	0.43
13:o:42:ARG:O	13:o:241:ALA:HA	2.18	0.43
14:t:2:GLU:HG2	14:t:3:THR:N	2.33	0.43
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	2.01	0.43
38:E:102:HEM:HAC	6:F:27:ALA:HB1	2.01	0.43
23:C:507:CLA:H18	23:C:507:CLA:H152	1.44	0.43
23:C:514:CLA:H161	33:C:521:LMG:H421	2.00	0.43
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.53	0.43
23:A:404[A]:CLA:H143	24:A:407[A]:PHO:H61	2.01	0.43
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	2.00	0.43
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.19	0.43
8:I:36:ASP:OD1	8:I:36:ASP:N	2.51	0.43
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.01	0.43
25:c:516:BCR:H15C	25:c:516:BCR:H351	1.84	0.43
32:d:408[A]:LHG:H242	32:d:408[A]:LHG:H272	1.86	0.43
5:e:68:ASP:O	5:e:72:ALA:HB2	2.18	0.43
31:A:420:LMT:O3'	31:A:420:LMT:H6'2	2.19	0.43
2:B:58:GLN:C	2:B:329:PRO:HB3	2.44	0.43
32:D:406[A]:LHG:HC62	11:L:15[A]:THR:HG23	2.00	0.43
25:X:101:BCR:H331	25:X:101:BCR:C8	2.48	0.43
35:C:517[A]:DGD:HG11	41:C:601[A]:HOH:O	2.18	0.43
25:h:101:BCR:H24C	25:h:101:BCR:H371	1.71	0.43
23:B:606:CLA:H72	25:B:619:BCR:H311	2.01	0.43
5:E:56:TYR:HA	5:E:60:GLN:HE21	1.82	0.43
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	2.00	0.43
32:d:408[B]:LHG:H302	32:d:408[B]:LHG:H332	1.81	0.43
10:k:24:VAL:HG21	18:y:25:ILE:HB	2.01	0.43
15:u:45:LEU:HD23	15:u:45:LEU:HA	1.84	0.43
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:405[A]:CLA:HHC	23:A:405[A]:CLA:HBB1	2.01	0.43
24:A:416[A]:PHO:H3A	23:D:402[A]:CLA:H142	1.99	0.43
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.19	0.43
4:D:209[B]:LEU:HD23	4:D:209[B]:LEU:C	2.44	0.43
4:D:230[A]:SER:HB2	41:D:547:HOH:O	2.18	0.43
23:b:609:CLA:NC	25:h:101:BCR:H332	2.34	0.43
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.01	0.43
25:c:517:BCR:H24C	25:c:517:BCR:H371	1.87	0.43
2:B:149:LEU:HG	23:B:606:CLA:HBB2	2.01	0.42
23:C:506:CLA:H93	23:C:506:CLA:H111	1.77	0.42
4:D:180:ARG:HD3	4:D:180:ARG:C	2.44	0.42
5:E:57:ALA:HB3	5:E:60:GLN:HG2	2.01	0.42
32:a:417[B]:LHG:H241	32:a:417[B]:LHG:HC61	1.88	0.42
25:t:102:BCR:H11C	25:t:102:BCR:H341	1.87	0.42
1:A:160[B]:ILE:HD11	35:C:517[B]:DGD:HBT2	2.01	0.42
24:A:407[B]:PHO:HAB	4:D:205[B]:LEU:HD13	2.00	0.42
26:A:410[A]:SQD:H361	10:K:34:ALA:HA	2.01	0.42
3:C:338[B]:GLY:HA3	3:C:341[B]:LEU:O	2.19	0.42
23:C:511:CLA:H2	23:C:511:CLA:HED2	2.00	0.42
35:C:518[B]:DGD:HAT1	35:C:519:DGD:HBE1	2.00	0.42
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.19	0.42
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.86	0.42
2:b:491[A]:VAL:HG13	4:d:136[A]:VAL:HG13	2.02	0.42
23:b:605:CLA:H41	23:b:605:CLA:H62	1.60	0.42
3:c:95:LEU:HD21	23:c:503:CLA:OBD	2.18	0.42
26:A:410[B]:SQD:H171	32:D:407[B]:LHG:H182	2.00	0.42
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.73	0.42
32:a:417[A]:LHG:H241	32:a:417[A]:LHG:HC61	1.89	0.42
3:c:391[B]:ARG:NH2	41:c:612:HOH:O	2.53	0.42
23:c:510:CLA:H18	35:c:519[B]:DGD:HAT2	2.02	0.42
23:c:511:CLA:H142	23:c:511:CLA:H112	1.88	0.42
23:d:404:CLA:H61	23:d:404:CLA:H41	1.67	0.42
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.68	0.42
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.74	0.42
3:C:223:TRP:CG	3:C:224:ILE:H	2.37	0.42
23:C:503:CLA:H151	23:C:504:CLA:HMB2	2.01	0.42
27:l:801[B]:GOL:H32	14:t:25:GLU:HB2	1.99	0.42
29:A:414[A]:PL9:H171	29:A:414[A]:PL9:H151	1.53	0.42
2:B:357[A]:ARG:HH12	27:B:623:GOL:C3	2.33	0.42
1:a:296[B]:ASN:HB2	3:c:400[B]:PRO:O	2.19	0.42
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:338[A]:GLY:HA3	3:C:341[A]:LEU:O	2.20	0.42
25:C:515:BCR:H20C	25:C:515:BCR:H361	1.93	0.42
23:a:407:CLA:H61	23:a:407:CLA:H102	1.88	0.42
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.55	0.42
25:b:618:BCR:H371	25:b:618:BCR:H24C	1.84	0.42
26:b:620:SQD:H462	26:b:620:SQD:H1	2.00	0.42
3:c:176:VAL:HG21	3:c:238:ILE:HG13	2.02	0.42
3:c:457[A]:LYS:HE2	4:d:227:GLU:O	2.20	0.42
32:D:407[A]:LHG:H332	32:D:407[A]:LHG:H302	1.85	0.42
6:F:15:ILE:HD13	20:R:23:ILE:HD11	2.02	0.42
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.97	0.42
16:v:117:GLY:O	16:v:121:VAL:HG23	2.19	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.55	0.42
13:O:39[A]:ARG:HB2	13:O:246:ALA:HB2	2.02	0.42
29:a:412[B]:PL9:H351	6:f:25:THR:OG1	2.18	0.42
2:b:58:GLN:C	2:b:329:PRO:HB3	2.45	0.42
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.87	0.42
25:b:619:BCR:H15C	25:b:619:BCR:H351	1.88	0.42
3:c:203:THR:O	3:c:235:GLY:HA3	2.20	0.42
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.84	0.42
34:o:301:HTG:H6'2	34:o:301:HTG:H3'1	1.90	0.42
20:R:24:LEU:N	20:R:25:PRO:HD2	2.34	0.42
3:C:157:MET:HE2	3:C:157:MET:HA	2.01	0.42
23:A:405[A]:CLA:HBA1	23:A:405[A]:CLA:C4A	2.50	0.42
3:C:330:SER:HB3	13:O:100:GLY:O	2.19	0.42
35:C:518[B]:DGD:HAE2	35:C:518[B]:DGD:HA81	1.86	0.42
32:D:407[A]:LHG:H382	32:D:407[A]:LHG:C11	2.45	0.42
26:a:409[B]:SQD:H271	32:d:408[B]:LHG:H141	2.00	0.42
23:b:603:CLA:H3A	23:b:603:CLA:CGA	2.50	0.42
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.18	0.42
18:y:34:MET:O	18:y:38:LEU:HG	2.19	0.42
3:C:230:LEU:HD23	3:C:230:LEU:HA	1.83	0.41
35:C:519:DGD:HBE2	35:C:519:DGD:HB81	1.78	0.41
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.19	0.41
3:c:31:SER:CB	3:c:41:ARG:HG2	2.49	0.41
16:v:41:HIS:HA	16:v:45[B]:ILE:O	2.20	0.41
23:A:404[A]:CLA:H192	23:A:404[A]:CLA:H161	1.80	0.41
3:C:334[B]:PRO:HA	13:O:153:THR:OG1	2.19	0.41
23:C:509:CLA:H122	23:C:509:CLA:H162	1.85	0.41
35:C:518[B]:DGD:HB61	35:C:518[B]:DGD:HB32	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:MET:HE3	4:D:143[A]:ALA:O	2.20	0.41
32:D:407[A]:LHG:H362	32:D:407[A]:LHG:H331	1.86	0.41
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.46	0.41
26:b:620:SQD:H341	26:b:620:SQD:H311	1.68	0.41
3:c:38:GLY:HA3	23:c:513:CLA:HMD2	2.01	0.41
3:c:52:ALA:HB2	23:c:513:CLA:HMA2	2.01	0.41
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.86	0.41
16:V:32:LEU:HD13	16:V:111:ASP:HB3	2.02	0.41
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.56	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.55	0.41
23:c:508:CLA:HBA1	23:c:508:CLA:H3A	1.83	0.41
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:H121	1.75	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.88	0.41
16:V:83:ASP:CG	16:V:85[B]:GLU:HG3	2.46	0.41
1:a:214[A]:MET:HB3	29:a:412[A]:PL9:H103	2.01	0.41
1:a:261[B]:GLN:HG3	2:b:493[B]:TRP:CZ3	2.55	0.41
26:a:409[A]:SQD:H302	23:c:510:CLA:H71	2.02	0.41
24:a:414[A]:PHO:H42	24:a:414[A]:PHO:H11	1.92	0.41
23:b:605:CLA:H141	23:b:605:CLA:H161	1.90	0.41
3:c:152:LYS:HD2	41:c:746:HOH:O	2.20	0.41
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.72	0.41
23:c:509:CLA:HBD	23:c:509:CLA:HAA2	2.02	0.41
13:O:169:ASP:H	27:O:303:GOL:H12	1.84	0.41
25:T:101:BCR:H331	25:T:101:BCR:HC7	1.66	0.41
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.01	0.41
3:c:42:LEU:HD21	23:c:513:CLA:H2A	2.01	0.41
4:d:148[A]:ALA:HB3	4:d:149[A]:PRO:HD3	2.03	0.41
32:d:408[A]:LHG:H142	32:d:408[A]:LHG:H372	2.03	0.41
23:B:614:CLA:H192	14:t:8:PHE:CE1	2.55	0.41
4:D:126:MET:HE3	4:D:143[B]:ALA:O	2.21	0.41
13:O:54:GLU:HG2	13:O:64:GLU:O	2.20	0.41
4:d:24:ARG:NH1	17:x:37:VAL:HG22	2.36	0.41
1:A:85[A]:SER:HA	1:A:109[A]:GLY:HA3	2.03	0.41
26:A:410[B]:SQD:H152	26:A:410[B]:SQD:H122	1.65	0.41
29:A:414[B]:PL9:H221	29:A:414[B]:PL9:H201	1.85	0.41
27:A:418:GOL:H12	14:T:2:GLU:OE1	2.20	0.41
2:B:201:HIS:CE1	23:B:603:CLA:HMB2	2.55	0.41
23:B:613:CLA:H162	23:B:613:CLA:H121	1.64	0.41
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.20	0.41
1:a:211[B]:PHE:CD1	29:a:412[B]:PL9:H101	2.56	0.41
1:a:307:ILE:HD13	1:a:307:ILE:HG21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.56	0.41
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	2.03	0.41
1:A:214[B]:MET:HE2	1:A:255[B]:PHE:CE1	2.56	0.41
3:C:443[A]:TRP:CZ2	23:C:509:CLA:HMD1	2.55	0.41
4:D:261[B]:PHE:CE1	32:D:406[B]:LHG:HC81	2.55	0.41
32:E:101[A]:LHG:H291	32:E:101[A]:LHG:H261	1.75	0.41
2:b:451:PHE:CD1	2:b:451:PHE:C	2.99	0.41
13:o:153:THR:HA	13:o:190:PHE:HE2	1.86	0.41
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.41
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB1	2.03	0.41
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.83	0.41
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.90	0.41
23:B:613:CLA:H143	23:B:613:CLA:H111	1.84	0.41
34:B:622:HTG:H7'3	34:B:622:HTG:H4'2	1.83	0.41
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.46	0.41
13:O:110:MET:HE2	13:O:110:MET:HB3	1.93	0.41
23:a:407:CLA:H203	23:c:508:CLA:H101	2.03	0.41
25:b:618:BCR:C8	25:b:618:BCR:H331	2.50	0.41
23:c:514:CLA:H142	23:c:514:CLA:H111	1.93	0.41
35:h:102:DGD:HB61	35:h:102:DGD:HB91	1.93	0.41
8:i:2:GLU:O	8:i:6:ILE:HG12	2.21	0.41
10:k:19:ASP:HB3	10:k:20:PRO:HD3	2.03	0.41
19:z:34:ASP:OD1	19:z:34:ASP:N	2.50	0.41
23:A:408:CLA:H18	23:C:506:CLA:H142	2.02	0.41
3:C:42:LEU:HD21	23:C:512:CLA:H2A	2.02	0.41
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.20	0.41
1:a:272[B]:HIS:CD2	4:d:218[B]:VAL:HG21	2.56	0.41
2:b:497:GLN:HB2	2:b:504:THR:HB	2.02	0.41
3:c:146:PHE:HZ	23:c:514:CLA:HBB2	1.86	0.41
7:h:38:PHE:HB2	25:h:101:BCR:H10C	2.03	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:B:601:CLA:C4D	23:B:601:CLA:H72	2.51	0.40
23:B:608:CLA:H3A	23:B:608:CLA:HBA2	1.89	0.40
4:d:186[B]:GLN:HB2	23:d:403[B]:CLA:HBC1	2.03	0.40
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.89	0.40
16:v:45[B]:ILE:HD13	27:v:202[B]:GOL:H11	2.02	0.40
29:A:414[A]:PL9:H121	29:A:414[A]:PL9:HC8	1.78	0.40
23:B:601:CLA:H71	23:B:601:CLA:C1	2.44	0.40
25:B:619:BCR:C8	25:B:619:BCR:H331	2.51	0.40
32:E:101[B]:LHG:H241	32:E:101[B]:LHG:HC61	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:137:THR:C	13:O:139:SER:H	2.29	0.40
23:a:404[B]:CLA:CBD	23:d:402[B]:CLA:HAC2	2.51	0.40
25:y:101:BCR:HC7	25:y:101:BCR:H331	1.95	0.40
23:B:615:CLA:H172	23:B:615:CLA:H13	1.84	0.40
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.04	0.40
4:d:14:TRP:CD1	34:d:411:HTG:H61	2.56	0.40
20:R:8:VAL:O	20:R:11:PRO:HD2	2.22	0.40
1:A:131:TRP:CD2	1:A:131:TRP:C	2.98	0.40
26:A:412:SQD:H222	26:A:412:SQD:H192	1.90	0.40
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:HC2	1.71	0.40
2:B:498:LYS:HE3	4:D:20:ASP:HA	2.02	0.40
23:B:615:CLA:H71	23:B:616:CLA:H192	2.04	0.40
23:C:506:CLA:HBD	23:C:506:CLA:HAA1	2.02	0.40
25:k:101:BCR:C8	25:k:101:BCR:H331	2.52	0.40
16:v:109:GLU:O	16:v:113:VAL:HG23	2.22	0.40
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.86	0.40
24:A:416[B]:PHO:NC	24:A:416[B]:PHO:ND	2.69	0.40
2:B:433:ASP:OD2	2:B:436:THR:OG1	2.37	0.40
2:B:445:THR:HA	41:B:707:HOH:O	2.20	0.40
23:B:601:CLA:H72	23:B:601:CLA:C3D	2.51	0.40
33:B:621:LMG:H141	33:B:621:LMG:H112	1.87	0.40
35:C:518[A]:DGD:HAE2	35:C:518[A]:DGD:HA81	1.86	0.40
2:b:358:ARG:HB2	27:b:628:GOL:H31	2.04	0.40
33:c:501:LMG:H201	33:c:501:LMG:H172	1.88	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	551/344 (160%)	539 (98%)	10 (2%)	2 (0%)	30	31
2	B	524/505 (104%)	515 (98%)	9 (2%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	548/455 (120%)	540 (98%)	7 (1%)	1 (0%)	43	50
3	c	554/455 (122%)	544 (98%)	9 (2%)	1 (0%)	43	50
4	D	454/342 (133%)	439 (97%)	15 (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%)	78 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
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%)	33 (97%)	1 (3%)	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	31
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	99/104 (95%)	96 (97%)	3 (3%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	134 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100 100
17	x	36/40 (90%)	36 (100%)	0	0	100 100
18	Y	27/30 (90%)	24 (89%)	3 (11%)	0	100 100
18	y	27/30 (90%)	27 (100%)	0	0	100 100
19	Z	60/62 (97%)	58 (97%)	1 (2%)	1 (2%)	7 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%)	6035 (98%)	134 (2%)	11 (0%)	43 50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416	SER
8	I	36	ASP
13	O	26	ALA
3	c	416	SER
19	Z	31	GLN
19	z	30	PRO
1	A	259[A]	ILE
1	A	259[B]	ILE
7	h	63	LYS
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%)	410 (98%)	10 (2%)	43 54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	367 (99%)	5 (1%)	61 72
5	E	72/73 (99%)	69 (96%)	3 (4%)	26 31
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%)	54 (98%)	1 (2%)	51 63
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%)	25 (96%)	1 (4%)	29 36
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%)	210 (97%)	6 (3%)	38 48
13	o	213/207 (103%)	206 (97%)	7 (3%)	33 42
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%)	118 (96%)	5 (4%)	27 33
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	21 (96%)	1 (4%)	24 29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	4998 (98%)	112 (2%)	44 56

All (112) 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	299	GLU
2	B	362	PHE
2	B	389	LYS
2	B	419	SER
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
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
3	C	471	SER
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	4	THR
5	E	54	SER
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS
8	I	34	ARG
9	J	6	ARG
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL

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Mol	Chain	Res	Type
12	M	16[A]	LEU
12	M	16[B]	LEU
12	M	20	VAL
13	O	4	THR
13	O	49	THR
13	O	55	GLU
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	118	LEU
14	T	25[A]	GLU
14	T	25[B]	GLU
14	T	30[A]	THR
14	T	30[B]	THR
15	U	10	VAL
15	U	70	ARG
16	V	15	GLU
18	Y	30	ILE
1	a	13	LEU
2	b	128	THR
2	b	161	LEU
2	b	245	VAL
2	b	287	ARG
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	26	ARG
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	71	GLU
7	h	65	LEU

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Mol	Chain	Res	Type
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	37	THR
13	o	58	ASN
13	o	69	LYS
13	o	118	LEU
13	o	194	LYS
15	u	10[A]	VAL
15	u	10[B]	VAL
16	v	15	GLU
16	v	24	LYS
16	v	85	GLU
16	v	106	ASN
16	v	109	GLU
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 (13) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	44	ASN
11	L	8	GLN
13	O	231	HIS
15	U	78	ASN
2	b	14	ASN
2	b	331	ASN
3	c	19	ASN
3	c	201	ASN
11	l	8	GLN
13	o	58	ASN
15	u	78	ASN
16	v	86	GLN
19	Z	31	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.59	2 (28%)
14	FME	T	1	14	8,9,10	0.66	0	7,9,11	1.58	2 (28%)
14	FME	t	1	14	8,9,10	0.75	0	7,9,11	1.70	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.12	1 (14%)
8	FME	I	1	8	8,9,10	0.61	0	7,9,11	1.24	1 (14%)
8	FME	i	1	8	8,9,10	0.63	0	7,9,11	1.42	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	-
14	FME	T	1	14	-	2/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	1/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	1	FME	CA-N-CN	-2.80	118.51	122.82
14	T	1	FME	CG-CB-CA	2.58	120.12	112.95
14	t	1	FME	O-C-CA	-2.54	118.11	124.78
12	m	1	FME	O1-CN-N	-2.53	118.60	125.27
14	t	1	FME	CA-N-CN	-2.52	118.95	122.82
8	i	1	FME	O-C-CA	-2.15	119.14	124.78
8	I	1	FME	O-C-CA	-2.11	119.25	124.78
14	T	1	FME	CA-N-CN	2.10	126.05	122.82
12	M	1	FME	O-C-CA	-2.02	119.48	124.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	3	0
12	M	1	FME	1	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	c	507	3	69,73,73	2.00	19 (27%)	83,113,113	2.81	29 (34%)
32	LHG	b	629[A]	-	48,48,48	0.85	3 (6%)	51,54,54	1.03	4 (7%)
33	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.11	4 (6%)
25	BCR	c	516	-	41,41,41	0.99	1 (2%)	56,56,56	1.59	10 (17%)
23	CLA	b	608	2	69,73,73	2.00	20 (28%)	83,113,113	2.83	32 (38%)
27	GOL	l	801[B]	-	5,5,5	0.92	0	5,5,5	0.98	0
26	SQD	A	412	-	53,54,54	1.01	3 (5%)	62,65,65	1.24	6 (9%)
25	BCR	t	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.61	11 (19%)
31	LMT	b	627	-	25,25,36	0.90	0	30,30,47	1.08	2 (6%)
24	PHO	A	407[B]	-	58,69,69	2.67	12 (20%)	56,99,99	2.78	16 (28%)
32	LHG	D	407[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	4 (7%)
27	GOL	A	411	-	5,5,5	1.24	0	5,5,5	0.71	0
24	PHO	a	406[A]	-	58,69,69	2.72	12 (20%)	56,99,99	2.76	15 (26%)
27	GOL	o	304	-	5,5,5	1.11	1 (20%)	5,5,5	1.04	0
23	CLA	b	616	2	69,73,73	2.03	19 (27%)	83,113,113	2.96	31 (37%)
26	SQD	b	620	-	53,54,54	1.03	3 (5%)	62,65,65	1.68	11 (17%)
27	GOL	b	628	-	5,5,5	0.58	0	5,5,5	1.35	1 (20%)
23	CLA	B	606	2	69,73,73	1.97	20 (28%)	83,113,113	2.96	29 (34%)
25	BCR	d	405	-	41,41,41	1.13	2 (4%)	56,56,56	1.95	17 (30%)
23	CLA	A	406[A]	41	69,73,73	1.99	18 (26%)	83,113,113	2.86	32 (38%)
23	CLA	b	612	2	69,73,73	2.00	20 (28%)	83,113,113	2.77	29 (34%)
34	HTG	b	622	-	19,19,19	1.15	2 (10%)	23,24,24	1.95	8 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	504	3	69,73,73	2.01	20 (28%)	83,113,113	2.79	27 (32%)
24	PHO	a	414[A]	-	58,69,69	2.75	14 (24%)	56,99,99	3.01	17 (30%)
25	BCR	K	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.41	9 (16%)
32	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	0.99	3 (5%)
35	DGD	C	517[A]	-	63,63,67	0.81	2 (3%)	77,77,81	1.21	8 (10%)
28	OEX	a	411[A]	41,3,1	0,14,14	-	-	-		
32	LHG	A	419[A]	-	48,48,48	0.84	2 (4%)	51,54,54	1.31	6 (11%)
25	BCR	k	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.53	12 (21%)
31	LMT	A	417	-	36,36,36	0.92	0	47,47,47	1.06	1 (2%)
31	LMT	c	502	-	36,36,36	1.01	1 (2%)	47,47,47	1.01	1 (2%)
37	BCT	d	401[B]	21	2,3,3	0.66	0	2,3,3	1.24	0
23	CLA	d	402[B]	41	69,73,73	2.04	18 (26%)	83,113,113	2.83	32 (38%)
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.84	10 (16%)
34	HTG	b	623	-	19,19,19	1.08	1 (5%)	23,24,24	1.85	2 (8%)
35	DGD	c	518[B]	-	63,63,67	0.85	2 (3%)	77,77,81	1.04	5 (6%)
23	CLA	C	505	41	69,73,73	1.99	20 (28%)	83,113,113	2.74	27 (32%)
27	GOL	o	303	-	5,5,5	1.03	0	5,5,5	0.94	0
23	CLA	B	601	41	69,73,73	2.10	21 (30%)	83,113,113	2.86	30 (36%)
34	HTG	B	624	-	19,19,19	1.01	2 (10%)	23,24,24	1.22	4 (17%)
37	BCT	D	401[A]	21	2,3,3	0.54	0	2,3,3	1.81	1 (50%)
23	CLA	c	506	41	69,73,73	2.07	21 (30%)	83,113,113	2.81	32 (38%)
23	CLA	d	403[B]	4	69,73,73	2.00	20 (28%)	83,113,113	2.81	31 (37%)
23	CLA	B	605	2	69,73,73	2.03	18 (26%)	83,113,113	2.89	30 (36%)
23	CLA	C	514	3	69,73,73	2.02	20 (28%)	83,113,113	2.83	30 (36%)
33	LMG	m	101	-	51,51,55	0.87	2 (3%)	59,59,63	1.30	8 (13%)
25	BCR	A	409	-	41,41,41	0.99	1 (2%)	56,56,56	1.38	7 (12%)
23	CLA	B	609	2	69,73,73	2.03	18 (26%)	83,113,113	2.80	31 (37%)
23	CLA	B	611	2	69,73,73	2.54	20 (28%)	83,113,113	3.98	30 (36%)
32	LHG	a	417[B]	-	41,41,48	1.03	2 (4%)	44,47,54	0.94	2 (4%)
32	LHG	d	407[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.10	5 (9%)
33	LMG	c	522	-	51,51,55	1.00	2 (3%)	59,59,63	1.38	7 (11%)
25	BCR	B	618	-	41,41,41	0.99	1 (2%)	56,56,56	1.40	9 (16%)
23	CLA	c	503	3	69,73,73	2.02	20 (28%)	83,113,113	2.89	29 (34%)
26	SQD	a	410	-	53,54,54	1.05	3 (5%)	62,65,65	1.23	8 (12%)
29	PL9	D	405[A]	-	55,55,55	0.62	2 (3%)	68,69,69	1.64	18 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.50	8 (13%)
33	LMG	D	411	39	51,51,55	0.81	2 (3%)	59,59,63	1.10	3 (5%)
25	BCR	b	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.40	7 (12%)
27	GOL	B	628	-	5,5,5	0.97	0	5,5,5	1.10	0
38	HEM	f	101	5,6	50,50,50	1.48	6 (12%)	66,82,82	1.72	13 (19%)
32	LHG	L	101[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.09	3 (5%)
23	CLA	B	613	2	69,73,73	1.96	20 (28%)	83,113,113	2.79	30 (36%)
34	HTG	d	411	-	16,16,19	1.00	1 (6%)	20,21,24	1.64	1 (5%)
23	CLA	D	402[A]	4	69,73,73	1.98	19 (27%)	83,113,113	2.88	31 (37%)
35	DGD	c	519[A]	-	63,63,67	0.84	2 (3%)	77,77,81	0.97	5 (6%)
29	PL9	A	414[A]	-	55,55,55	0.68	2 (3%)	68,69,69	2.08	25 (36%)
32	LHG	D	406[A]	-	48,48,48	0.86	2 (4%)	51,54,54	0.99	3 (5%)
23	CLA	C	506	3	69,73,73	2.04	19 (27%)	83,113,113	2.75	29 (34%)
35	DGD	C	518[A]	-	63,63,67	0.89	3 (4%)	77,77,81	1.02	5 (6%)
23	CLA	c	512	3	69,73,73	1.98	19 (27%)	83,113,113	2.89	31 (37%)
27	GOL	D	412	-	5,5,5	1.40	1 (20%)	5,5,5	0.85	0
27	GOL	v	202[B]	-	5,5,5	1.09	0	5,5,5	0.87	0
25	BCR	a	408	-	41,41,41	1.04	1 (2%)	56,56,56	1.33	7 (12%)
26	SQD	F	102	-	42,43,54	1.19	4 (9%)	51,54,65	2.14	14 (27%)
33	LMG	B	621	-	51,51,55	0.92	2 (3%)	59,59,63	1.31	7 (11%)
23	CLA	b	614	2	69,73,73	2.00	19 (27%)	83,113,113	2.90	31 (37%)
23	CLA	a	405[B]	41	69,73,73	2.05	19 (27%)	83,113,113	2.83	29 (34%)
27	GOL	c	527[B]	-	5,5,5	0.97	0	5,5,5	0.95	0
23	CLA	A	404[B]	1	69,73,73	2.05	20 (28%)	83,113,113	2.80	31 (37%)
23	CLA	C	504	3	69,73,73	2.01	19 (27%)	83,113,113	2.92	29 (34%)
25	BCR	C	516	-	41,41,41	1.04	1 (2%)	56,56,56	1.37	7 (12%)
25	BCR	c	517	-	41,41,41	1.04	1 (2%)	56,56,56	1.40	12 (21%)
32	LHG	d	414[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
23	CLA	B	614	2	69,73,73	2.01	18 (26%)	83,113,113	2.94	31 (37%)
27	GOL	C	523[A]	-	5,5,5	1.18	0	5,5,5	0.83	0
23	CLA	A	405[A]	41	69,73,73	1.93	18 (26%)	83,113,113	2.88	33 (39%)
23	CLA	B	603	2	69,73,73	2.04	20 (28%)	83,113,113	2.96	33 (39%)
33	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.11	4 (6%)
29	PL9	a	412[B]	-	55,55,55	0.63	2 (3%)	68,69,69	2.00	22 (32%)
31	LMT	e	101	-	36,36,36	1.04	3 (8%)	47,47,47	0.95	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	HEM	E	102	5,6	50,50,50	1.52	7 (14%)	66,82,82	1.90	16 (24%)
23	CLA	b	607	41	69,73,73	1.99	19 (27%)	83,113,113	2.78	28 (33%)
23	CLA	c	515	3	69,73,73	2.11	21 (30%)	83,113,113	2.88	31 (37%)
27	GOL	V	203[A]	-	5,5,5	1.22	0	5,5,5	0.91	0
23	CLA	b	615	2	69,73,73	2.02	18 (26%)	83,113,113	2.85	31 (37%)
25	BCR	C	515	-	41,41,41	1.04	1 (2%)	56,56,56	1.31	5 (8%)
23	CLA	c	508	3	69,73,73	2.04	20 (28%)	83,113,113	2.80	30 (36%)
23	CLA	a	404[B]	1	69,73,73	1.99	20 (28%)	83,113,113	2.92	33 (39%)
34	HTG	o	301	-	19,19,19	1.16	2 (10%)	23,24,24	1.60	6 (26%)
26	SQD	a	409[B]	-	53,54,54	0.99	3 (5%)	62,65,65	1.64	10 (16%)
24	PHO	a	414[B]	-	58,69,69	2.76	15 (25%)	56,99,99	2.94	17 (30%)
23	CLA	c	505	3	69,73,73	2.06	19 (27%)	83,113,113	2.87	30 (36%)
32	LHG	A	419[B]	-	48,48,48	0.87	2 (4%)	51,54,54	1.19	5 (9%)
23	CLA	B	612	2	69,73,73	1.98	19 (27%)	83,113,113	2.84	29 (34%)
23	CLA	C	510	3	69,73,73	2.07	19 (27%)	83,113,113	2.94	32 (38%)
33	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.34	7 (11%)
31	LMT	M	103	-	36,36,36	1.08	3 (8%)	47,47,47	1.08	2 (4%)
34	HTG	V	202	-	11,11,19	0.36	0	15,15,24	1.12	1 (6%)
27	GOL	d	413	-	5,5,5	1.11	0	5,5,5	0.97	0
23	CLA	B	607	41	69,73,73	1.98	19 (27%)	83,113,113	2.79	29 (34%)
23	CLA	c	510	3	69,73,73	2.13	20 (28%)	83,113,113	2.66	29 (34%)
31	LMT	m	103	-	36,36,36	1.09	3 (8%)	47,47,47	1.11	4 (8%)
23	CLA	C	513	3	69,73,73	2.04	20 (28%)	83,113,113	2.85	33 (39%)
23	CLA	D	403	4	69,73,73	2.11	18 (26%)	83,113,113	2.80	31 (37%)
23	CLA	b	605	2	69,73,73	1.92	18 (26%)	83,113,113	3.02	29 (34%)
27	GOL	A	418	-	5,5,5	1.62	2 (40%)	5,5,5	0.94	1 (20%)
23	CLA	B	608	2	69,73,73	1.96	21 (30%)	83,113,113	2.80	34 (40%)
23	CLA	B	610	41	69,73,73	2.05	19 (27%)	83,113,113	2.91	33 (39%)
29	PL9	d	406[B]	-	55,55,55	0.67	1 (1%)	68,69,69	1.66	21 (30%)
23	CLA	b	611	2	69,73,73	1.99	20 (28%)	83,113,113	2.92	27 (32%)
24	PHO	A	416[B]	-	58,69,69	2.76	15 (25%)	56,99,99	2.95	17 (30%)
23	CLA	A	408	1	69,73,73	1.93	20 (28%)	83,113,113	2.98	34 (40%)
31	LMT	B	627	-	36,36,36	1.16	4 (11%)	47,47,47	1.36	6 (12%)
31	LMT	B	629	-	36,36,36	1.01	3 (8%)	47,47,47	1.19	6 (12%)
35	DGD	c	518[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.12	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
27	GOL	c	528	-	5,5,5	1.22	1 (20%)	5,5,5	0.94	0
25	BCR	T	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.54	10 (17%)
26	SQD	B	620	-	53,54,54	1.04	3 (5%)	62,65,65	1.81	12 (19%)
31	LMT	F	101	-	36,36,36	1.05	1 (2%)	47,47,47	1.05	3 (6%)
25	BCR	y	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.55	10 (17%)
23	CLA	D	402[B]	4	69,73,73	1.97	20 (28%)	83,113,113	2.90	31 (37%)
23	CLA	d	403[A]	4	69,73,73	1.94	20 (28%)	83,113,113	2.78	29 (34%)
32	LHG	D	406[B]	-	48,48,48	0.88	2 (4%)	51,54,54	0.99	3 (5%)
33	LMG	c	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.21	5 (8%)
23	CLA	c	514	3	69,73,73	2.05	19 (27%)	83,113,113	2.88	32 (38%)
34	HTG	B	622	-	19,19,19	0.81	1 (5%)	23,24,24	1.36	1 (4%)
23	CLA	B	604	2	69,73,73	2.04	22 (31%)	83,113,113	2.63	30 (36%)
27	GOL	a	416	-	5,5,5	1.20	1 (20%)	5,5,5	0.93	0
32	LHG	a	417[A]	-	41,41,48	1.04	2 (4%)	44,47,54	0.92	2 (4%)
34	HTG	b	625	-	19,19,19	1.07	2 (10%)	23,24,24	1.57	4 (17%)
23	CLA	B	616	2	69,73,73	2.00	20 (28%)	83,113,113	2.85	24 (28%)
32	LHG	b	629[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.05	4 (7%)
32	LHG	d	407[A]	-	48,48,48	0.86	2 (4%)	51,54,54	1.08	4 (7%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.09	3 (6%)
25	BCR	D	404	-	41,41,41	1.10	1 (2%)	56,56,56	1.83	14 (25%)
32	LHG	E	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	1.11	3 (6%)
33	LMG	Z	101	-	37,37,55	1.01	2 (5%)	45,45,63	1.42	6 (13%)
25	BCR	X	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.40	7 (12%)
23	CLA	a	407	1	69,73,73	1.99	20 (28%)	83,113,113	2.93	30 (36%)
23	CLA	b	603	2	69,73,73	1.97	20 (28%)	83,113,113	2.87	32 (38%)
31	LMT	b	621	-	25,25,36	0.95	1 (4%)	30,30,47	1.20	3 (10%)
32	LHG	D	407[B]	-	48,48,48	0.93	2 (4%)	51,54,54	1.00	3 (5%)
23	CLA	C	511	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	33 (39%)
24	PHO	a	406[B]	-	58,69,69	2.77	13 (22%)	56,99,99	2.76	15 (26%)
23	CLA	c	511	3	69,73,73	2.04	20 (28%)	83,113,113	2.86	31 (37%)
28	OEX	A	413[A]	41,3,1	0,14,14	-	-	-		
23	CLA	b	602	2	69,73,73	2.08	20 (28%)	83,113,113	3.00	34 (40%)
23	CLA	b	601	41	69,73,73	2.11	19 (27%)	83,113,113	2.82	28 (33%)
23	CLA	B	602	2	69,73,73	2.04	20 (28%)	83,113,113	2.88	32 (38%)
25	BCR	h	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	A	405[B]	41	69,73,73	2.00	19 (27%)	83,113,113	2.80	32 (38%)
23	CLA	A	406[B]	41	69,73,73	2.06	19 (27%)	83,113,113	2.83	32 (38%)
27	GOL	v	202[A]	-	5,5,5	1.27	0	5,5,5	0.72	0
25	BCR	b	619	-	41,41,41	1.07	1 (2%)	56,56,56	1.36	8 (14%)
27	GOL	l	801[A]	-	5,5,5	0.96	0	5,5,5	0.97	0
34	HTG	c	523	-	19,19,19	0.97	1 (5%)	23,24,24	1.54	2 (8%)
23	CLA	b	609	2	69,73,73	2.00	19 (27%)	83,113,113	2.82	33 (39%)
34	HTG	C	522	-	19,19,19	0.86	1 (5%)	23,24,24	1.27	1 (4%)
32	LHG	d	408[B]	-	48,48,48	0.95	2 (4%)	51,54,54	1.07	5 (9%)
35	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.10	6 (7%)
28	OEX	a	411[B]	41,3,1	0,14,14	-	-	-		
24	PHO	A	407[A]	-	58,69,69	2.69	14 (24%)	56,99,99	2.78	15 (26%)
25	BCR	b	618	-	41,41,41	1.01	1 (2%)	56,56,56	1.17	5 (8%)
26	SQD	f	102	-	42,43,54	1.18	3 (7%)	51,54,65	1.53	10 (19%)
23	CLA	a	405[A]	41	69,73,73	1.96	19 (27%)	83,113,113	2.86	30 (36%)
27	GOL	V	203[B]	-	5,5,5	1.18	0	5,5,5	0.90	0
27	GOL	c	527[A]	-	5,5,5	0.94	0	5,5,5	0.95	0
23	CLA	A	404[A]	1	69,73,73	1.98	20 (28%)	83,113,113	2.82	32 (38%)
23	CLA	C	507	3	69,73,73	2.03	21 (30%)	83,113,113	2.81	30 (36%)
27	GOL	a	415	-	5,5,5	1.05	0	5,5,5	0.97	0
33	LMG	c	521	-	51,51,55	0.91	2 (3%)	59,59,63	1.15	5 (8%)
23	CLA	b	613	2	69,73,73	1.99	19 (27%)	83,113,113	2.82	29 (34%)
37	BCT	D	401[B]	21	2,3,3	0.61	0	2,3,3	1.21	0
29	PL9	a	412[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.00	22 (32%)
35	DGD	H	101	-	63,63,67	0.88	3 (4%)	77,77,81	1.07	6 (7%)
40	HEC	V	201	16	50,50,50	1.76	7 (14%)	68,82,82	1.51	11 (16%)
35	DGD	C	519	-	63,63,67	0.88	3 (4%)	77,77,81	0.96	3 (3%)
35	DGD	c	520	-	63,63,67	0.88	4 (6%)	77,77,81	1.03	5 (6%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.05	5 (6%)
37	BCT	d	401[A]	21	2,3,3	0.57	0	2,3,3	1.58	1 (50%)
23	CLA	c	509	41	69,73,73	2.04	19 (27%)	83,113,113	2.90	30 (36%)
23	CLA	d	402[A]	41	69,73,73	2.01	17 (24%)	83,113,113	2.80	29 (34%)
27	GOL	O	303	-	5,5,5	0.83	0	5,5,5	1.06	0
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.81	10 (16%)
29	PL9	D	405[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.61	15 (22%)
23	CLA	a	404[A]	1	69,73,73	1.96	19 (27%)	83,113,113	2.88	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	SQD	a	409[A]	-	53,54,54	0.95	3 (5%)	62,65,65	1.77	13 (20%)
35	DGD	c	519[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.98	3 (3%)
27	GOL	O	302	-	5,5,5	0.89	0	5,5,5	0.92	0
29	PL9	A	414[B]	-	55,55,55	0.67	2 (3%)	68,69,69	2.00	25 (36%)
23	CLA	C	512	3	69,73,73	2.03	21 (30%)	83,113,113	2.76	28 (33%)
34	HTG	D	410	-	16,16,19	1.06	2 (12%)	20,21,24	1.47	1 (5%)
23	CLA	C	502	3	69,73,73	1.97	20 (28%)	83,113,113	2.84	32 (38%)
35	DGD	C	518[B]	-	63,63,67	0.87	3 (4%)	77,77,81	1.01	5 (6%)
40	HEC	v	201	16	50,50,50	1.76	8 (16%)	68,82,82	1.38	8 (11%)
23	CLA	C	503	3	69,73,73	2.00	20 (28%)	83,113,113	2.75	29 (34%)
23	CLA	b	604	2	69,73,73	1.98	20 (28%)	83,113,113	2.75	28 (33%)
31	LMT	B	630	-	25,25,36	0.88	1 (4%)	30,30,47	1.16	3 (10%)
23	CLA	B	615	2	69,73,73	2.01	17 (24%)	83,113,113	2.87	31 (37%)
23	CLA	C	509	3	69,73,73	2.05	20 (28%)	83,113,113	2.78	26 (31%)
27	GOL	B	623	-	5,5,5	0.80	0	5,5,5	1.24	1 (20%)
23	CLA	b	606	2	69,73,73	1.97	19 (27%)	83,113,113	2.87	31 (37%)
32	LHG	L	101[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.15	3 (5%)
23	CLA	c	513	3	69,73,73	2.07	20 (28%)	83,113,113	2.80	32 (38%)
31	LMT	M	101	-	36,36,36	1.12	3 (8%)	47,47,47	1.19	4 (8%)
32	LHG	d	414[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.06	5 (9%)
29	PL9	d	406[A]	-	55,55,55	0.65	1 (1%)	68,69,69	1.63	17 (25%)
25	BCR	B	619	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	9 (16%)
27	GOL	C	523[B]	-	5,5,5	1.07	0	5,5,5	0.88	0
24	PHO	A	416[A]	-	58,69,69	2.74	15 (25%)	56,99,99	2.87	17 (30%)
25	BCR	Y	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.62	13 (23%)
23	CLA	d	404	4	69,73,73	2.04	20 (28%)	83,113,113	2.96	32 (38%)
31	LMT	A	420	-	36,36,36	1.06	2 (5%)	47,47,47	1.16	4 (8%)
32	LHG	E	101[B]	-	41,41,48	1.05	2 (4%)	44,47,54	1.09	4 (9%)
25	BCR	B	617	-	41,41,41	1.08	1 (2%)	56,56,56	1.31	6 (10%)
27	GOL	b	624	-	5,5,5	1.23	1 (20%)	5,5,5	0.75	0
31	LMT	t	101	-	26,26,36	0.92	2 (7%)	31,31,47	1.35	2 (6%)
23	CLA	b	610	41	69,73,73	1.99	20 (28%)	83,113,113	2.84	32 (38%)
28	OEX	A	413[B]	41,3,1	0,14,14	-	-	-		
27	GOL	B	626	-	5,5,5	1.11	0	5,5,5	0.98	0
23	CLA	C	508	41	69,73,73	1.98	20 (28%)	83,113,113	2.83	28 (33%)

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	c	507	3	-	7/39/115/115	-
32	LHG	b	629[A]	-	-	20/53/53/53	-
33	LMG	C	520	-	-	9/46/66/70	0/1/1/1
25	BCR	c	516	-	-	1/29/63/63	0/2/2/2
23	CLA	b	608	2	-	4/39/115/115	-
27	GOL	l	801[B]	-	-	2/4/4/4	-
26	SQD	A	412	-	-	14/49/69/69	0/1/1/1
25	BCR	t	102	-	-	4/29/63/63	0/2/2/2
31	LMT	b	627	-	-	11/17/37/61	0/1/1/2
24	PHO	A	407[B]	-	-	5/37/103/103	0/5/6/6
32	LHG	D	407[A]	-	-	14/53/53/53	-
27	GOL	A	411	-	-	2/4/4/4	-
24	PHO	a	406[A]	-	-	5/37/103/103	0/5/6/6
27	GOL	o	304	-	-	4/4/4/4	-
23	CLA	b	616	2	-	8/39/115/115	-
26	SQD	b	620	-	-	17/49/69/69	0/1/1/1
27	GOL	b	628	-	-	0/4/4/4	-
23	CLA	B	606	2	-	10/39/115/115	-
25	BCR	d	405	-	-	6/29/63/63	0/2/2/2
23	CLA	A	406[A]	41	-	7/39/115/115	-
23	CLA	b	612	2	-	3/39/115/115	-
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
23	CLA	c	504	3	-	9/39/115/115	-
24	PHO	a	414[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	K	102	-	-	3/29/63/63	0/2/2/2
32	LHG	d	408[A]	-	-	11/53/53/53	-
35	DGD	C	517[A]	-	-	11/51/91/95	0/2/2/2
32	LHG	A	419[A]	-	-	10/53/53/53	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
31	LMT	A	417	-	-	7/21/61/61	0/2/2/2
31	LMT	c	502	-	-	11/21/61/61	0/2/2/2
23	CLA	d	402[B]	41	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	410[B]	-	-	10/49/69/69	0/1/1/1
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
35	DGD	c	518[B]	-	-	19/51/91/95	0/2/2/2
23	CLA	C	505	41	-	6/39/115/115	-
27	GOL	o	303	-	-	2/4/4/4	-
23	CLA	B	601	41	-	12/39/115/115	-
34	HTG	B	624	-	-	3/10/30/30	0/1/1/1
23	CLA	c	506	41	-	6/39/115/115	-
23	CLA	d	403[B]	4	-	4/39/115/115	-
23	CLA	B	605	2	-	5/39/115/115	-
23	CLA	C	514	3	-	7/39/115/115	-
33	LMG	m	101	-	-	11/46/66/70	0/1/1/1
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	B	609	2	-	1/39/115/115	-
23	CLA	B	611	2	-	2/39/115/115	-
32	LHG	a	417[B]	-	-	16/46/46/53	-
32	LHG	d	407[B]	-	-	19/53/53/53	-
33	LMG	c	522	-	-	9/46/66/70	0/1/1/1
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
23	CLA	c	503	3	-	3/39/115/115	-
26	SQD	a	410	-	-	12/49/69/69	0/1/1/1
29	PL9	D	405[A]	-	-	8/53/73/73	0/1/1/1
33	LMG	C	501	-	-	14/46/66/70	0/1/1/1
33	LMG	D	411	39	-	8/46/66/70	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
27	GOL	B	628	-	-	4/4/4/4	-
38	HEM	f	101	5,6	-	6/14/54/54	-
32	LHG	L	101[B]	-	-	16/53/53/53	-
23	CLA	B	613	2	-	7/39/115/115	-
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	D	402[A]	4	-	0/39/115/115	-
35	DGD	c	519[A]	-	-	17/51/91/95	0/2/2/2
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
32	LHG	D	406[A]	-	-	16/53/53/53	-
23	CLA	C	506	3	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	DGD	C	518[A]	-	-	15/51/91/95	0/2/2/2
23	CLA	c	512	3	-	12/39/115/115	-
27	GOL	D	412	-	-	4/4/4/4	-
27	GOL	v	202[B]	-	-	2/4/4/4	-
25	BCR	a	408	-	-	0/29/63/63	0/2/2/2
26	SQD	F	102	-	-	16/38/58/69	0/1/1/1
33	LMG	B	621	-	-	17/46/66/70	0/1/1/1
23	CLA	b	614	2	-	16/39/115/115	-
23	CLA	a	405[B]	41	-	8/39/115/115	-
27	GOL	c	527[B]	-	-	0/4/4/4	-
23	CLA	A	404[B]	1	-	4/39/115/115	-
23	CLA	C	504	3	-	3/39/115/115	-
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
25	BCR	c	517	-	-	1/29/63/63	0/2/2/2
32	LHG	d	414[A]	-	-	13/53/53/53	-
23	CLA	B	614	2	-	13/39/115/115	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
23	CLA	A	405[A]	41	-	4/39/115/115	-
23	CLA	B	603	2	-	8/39/115/115	-
33	LMG	d	412	39	-	11/46/66/70	0/1/1/1
29	PL9	a	412[B]	-	-	14/53/73/73	0/1/1/1
31	LMT	e	101	-	-	15/21/61/61	0/2/2/2
38	HEM	E	102	5,6	-	5/14/54/54	-
23	CLA	b	607	41	-	3/39/115/115	-
23	CLA	c	515	3	-	9/39/115/115	-
27	GOL	V	203[A]	-	-	2/4/4/4	-
23	CLA	b	615	2	-	7/39/115/115	-
25	BCR	C	515	-	-	1/29/63/63	0/2/2/2
23	CLA	c	508	3	-	9/39/115/115	-
23	CLA	a	404[B]	1	-	3/39/115/115	-
34	HTG	o	301	-	-	4/10/30/30	0/1/1/1
26	SQD	a	409[B]	-	-	10/49/69/69	0/1/1/1
24	PHO	a	414[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	c	505	3	-	3/39/115/115	-
32	LHG	A	419[B]	-	-	10/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	2	-	4/39/115/115	-
23	CLA	C	510	3	-	7/39/115/115	-
33	LMG	C	521	-	-	12/46/66/70	0/1/1/1
31	LMT	M	103	-	-	6/21/61/61	0/2/2/2
34	HTG	V	202	-	-	1/2/19/30	0/1/1/1
27	GOL	d	413	-	-	1/4/4/4	-
23	CLA	B	607	41	-	5/39/115/115	-
23	CLA	c	510	3	-	5/39/115/115	-
31	LMT	m	103	-	-	5/21/61/61	0/2/2/2
23	CLA	C	513	3	-	10/39/115/115	-
23	CLA	D	403	4	-	13/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
27	GOL	A	418	-	-	0/4/4/4	-
23	CLA	B	608	2	-	4/39/115/115	-
23	CLA	B	610	41	-	9/39/115/115	-
29	PL9	d	406[B]	-	-	7/53/73/73	0/1/1/1
23	CLA	b	611	2	-	2/39/115/115	-
24	PHO	A	416[B]	-	-	3/37/103/103	0/5/6/6
23	CLA	A	408	1	-	8/39/115/115	-
31	LMT	B	627	-	-	11/21/61/61	0/2/2/2
31	LMT	B	629	-	-	12/21/61/61	0/2/2/2
35	DGD	c	518[A]	-	-	20/51/91/95	0/2/2/2
27	GOL	c	528	-	-	3/4/4/4	-
25	BCR	T	101	-	-	3/29/63/63	0/2/2/2
26	SQD	B	620	-	-	13/49/69/69	0/1/1/1
31	LMT	F	101	-	-	8/21/61/61	0/2/2/2
25	BCR	y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	D	402[B]	4	-	2/39/115/115	-
23	CLA	d	403[A]	4	-	2/39/115/115	-
32	LHG	D	406[B]	-	-	15/53/53/53	-
33	LMG	c	501	-	-	13/46/66/70	0/1/1/1
23	CLA	c	514	3	-	12/39/115/115	-
34	HTG	B	622	-	-	2/10/30/30	0/1/1/1
23	CLA	B	604	2	-	3/39/115/115	-
27	GOL	a	416	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	a	417[A]	-	-	16/46/46/53	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
23	CLA	B	616	2	-	6/39/115/115	-
32	LHG	b	629[B]	-	-	16/53/53/53	-
32	LHG	d	407[A]	-	-	13/53/53/53	-
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
25	BCR	D	404	-	-	3/29/63/63	0/2/2/2
32	LHG	E	101[A]	-	-	22/46/46/53	-
33	LMG	Z	101	-	-	10/31/51/70	0/1/1/1
25	BCR	X	101	-	-	2/29/63/63	0/2/2/2
23	CLA	a	407	1	-	9/39/115/115	-
23	CLA	b	603	2	-	5/39/115/115	-
31	LMT	b	621	-	-	8/17/37/61	0/1/1/2
32	LHG	D	407[B]	-	-	13/53/53/53	-
23	CLA	C	511	3	-	14/39/115/115	-
24	PHO	a	406[B]	-	-	4/37/103/103	0/5/6/6
23	CLA	c	511	3	-	12/39/115/115	-
23	CLA	b	602	2	-	4/39/115/115	-
23	CLA	b	601	41	-	17/39/115/115	-
23	CLA	B	602	2	-	9/39/115/115	-
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	A	405[B]	41	-	4/39/115/115	-
23	CLA	A	406[B]	41	-	7/39/115/115	-
27	GOL	v	202[A]	-	-	1/4/4/4	-
25	BCR	b	619	-	-	2/29/63/63	0/2/2/2
27	GOL	l	801[A]	-	-	2/4/4/4	-
34	HTG	c	523	-	-	2/10/30/30	0/1/1/1
23	CLA	b	609	2	-	3/39/115/115	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
32	LHG	d	408[B]	-	-	12/53/53/53	-
35	DGD	C	517[B]	-	-	14/51/91/95	0/2/2/2
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	a	405[A]	41	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	V	203[B]	-	-	2/4/4/4	-
27	GOL	c	527[A]	-	-	0/4/4/4	-
23	CLA	A	404[A]	1	-	5/39/115/115	-
23	CLA	C	507	3	-	10/39/115/115	-
27	GOL	a	415	-	-	2/4/4/4	-
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
23	CLA	b	613	2	-	4/39/115/115	-
29	PL9	a	412[A]	-	-	14/53/73/73	0/1/1/1
35	DGD	H	101	-	-	10/51/91/95	0/2/2/2
40	HEC	V	201	16	1/1/3/7	6/14/54/54	-
35	DGD	C	519	-	-	18/51/91/95	0/2/2/2
35	DGD	c	520	-	-	8/51/91/95	0/2/2/2
35	DGD	h	102	-	-	14/51/91/95	0/2/2/2
23	CLA	c	509	41	-	8/39/115/115	-
23	CLA	d	402[A]	41	-	8/39/115/115	-
27	GOL	O	303	-	-	1/4/4/4	-
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
29	PL9	D	405[B]	-	-	8/53/73/73	0/1/1/1
23	CLA	a	404[A]	1	-	3/39/115/115	-
26	SQD	a	409[A]	-	-	10/49/69/69	0/1/1/1
35	DGD	c	519[B]	-	-	16/51/91/95	0/2/2/2
27	GOL	O	302	-	-	2/4/4/4	-
29	PL9	A	414[B]	-	-	16/53/73/73	0/1/1/1
23	CLA	C	512	3	-	4/39/115/115	-
34	HTG	D	410	-	-	3/7/27/30	0/1/1/1
23	CLA	C	502	3	-	5/39/115/115	-
40	HEC	v	201	16	1/1/3/7	6/14/54/54	-
35	DGD	C	518[B]	-	-	14/51/91/95	0/2/2/2
23	CLA	C	503	3	-	10/39/115/115	-
23	CLA	b	604	2	-	10/39/115/115	-
31	LMT	B	630	-	-	10/17/37/61	0/1/1/2
23	CLA	B	615	2	-	7/39/115/115	-
23	CLA	C	509	3	-	5/39/115/115	-
27	GOL	B	623	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	606	2	-	14/39/115/115	-
32	LHG	L	101[A]	-	-	19/53/53/53	-
23	CLA	c	513	3	-	3/39/115/115	-
31	LMT	M	101	-	-	4/21/61/61	0/2/2/2
32	LHG	d	414[B]	-	-	10/53/53/53	-
29	PL9	d	406[A]	-	-	6/53/73/73	0/1/1/1
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	GOL	C	523[B]	-	-	0/4/4/4	-
24	PHO	A	416[A]	-	-	1/37/103/103	0/5/6/6
25	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
23	CLA	d	404	4	-	9/39/115/115	-
31	LMT	A	420	-	-	16/21/61/61	0/2/2/2
32	LHG	E	101[B]	-	-	22/46/46/53	-
25	BCR	B	617	-	-	2/29/63/63	0/2/2/2
27	GOL	b	624	-	-	2/4/4/4	-
31	LMT	t	101	-	-	8/17/38/61	0/1/1/2
23	CLA	b	610	41	-	9/39/115/115	-
27	GOL	B	626	-	-	1/4/4/4	-
23	CLA	C	508	41	-	9/39/115/115	-

All (1873) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	406[B]	PHO	C1B-C2B	9.31	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	9.11	1.49	1.39
24	a	406[B]	PHO	C1D-C2D	9.08	1.49	1.39
24	a	406[A]	PHO	C1B-C2B	8.96	1.49	1.39
24	A	407[B]	PHO	C1D-C2D	8.83	1.49	1.39
24	a	414[A]	PHO	C1B-C2B	8.77	1.49	1.39
24	A	416[A]	PHO	C1D-C2D	8.71	1.49	1.39
24	a	414[B]	PHO	C1B-C2B	8.62	1.49	1.39
24	a	414[A]	PHO	C1D-C2D	8.58	1.49	1.39
24	a	414[B]	PHO	C1D-C2D	8.58	1.49	1.39
24	a	406[A]	PHO	C1D-C2D	8.45	1.48	1.39
24	A	416[B]	PHO	C1B-C2B	8.44	1.48	1.39
24	A	407[B]	PHO	C1B-C2B	8.31	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	8.00	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	C3D-C2D	7.99	1.53	1.36
40	V	201	HEC	C3D-C2D	7.45	1.52	1.36
24	A	416[B]	PHO	C3B-C4B	7.22	1.49	1.41
24	a	414[A]	PHO	C3B-C4B	7.11	1.49	1.41
23	B	611	CLA	CMB-C2B	7.02	1.65	1.50
24	a	414[B]	PHO	C3B-C4B	6.99	1.49	1.41
23	B	611	CLA	C1D-ND	6.88	1.46	1.37
24	A	416[B]	PHO	C4D-CHA	6.63	1.50	1.39
24	A	416[A]	PHO	C3B-C4B	6.61	1.49	1.41
23	B	611	CLA	C1B-C2B	6.57	1.58	1.43
24	a	406[A]	PHO	C3B-C4B	6.52	1.49	1.41
24	A	416[B]	PHO	C3B-C2B	6.46	1.49	1.40
24	A	407[A]	PHO	C3B-C4B	6.43	1.48	1.41
24	a	406[B]	PHO	C3B-C4B	6.41	1.48	1.41
24	a	406[A]	PHO	C3B-C2B	6.36	1.49	1.40
24	A	416[A]	PHO	C4D-CHA	6.36	1.49	1.39
24	A	407[A]	PHO	C4D-CHA	6.35	1.49	1.39
24	a	406[A]	PHO	C4D-CHA	6.34	1.49	1.39
24	A	407[B]	PHO	C3B-C2B	6.34	1.49	1.40
24	A	407[B]	PHO	C4D-CHA	6.31	1.49	1.39
24	a	406[B]	PHO	C3B-C2B	6.25	1.49	1.40
24	a	414[B]	PHO	C4D-CHA	6.21	1.49	1.39
24	A	407[A]	PHO	C3B-C2B	6.19	1.49	1.40
24	a	414[B]	PHO	C3B-C2B	6.14	1.48	1.40
24	A	416[A]	PHO	C3B-C2B	6.12	1.48	1.40
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	407[B]	PHO	C3B-C4B	6.02	1.48	1.41
24	a	406[B]	PHO	C4D-CHA	6.01	1.49	1.39
24	a	414[A]	PHO	C3C-C2C	5.98	1.49	1.36
24	a	414[B]	PHO	C3C-C2C	5.93	1.49	1.36
24	a	414[A]	PHO	C3B-C2B	5.90	1.48	1.40
23	B	610	CLA	C3C-C2C	5.90	1.49	1.36
24	A	407[B]	PHO	C3C-C2C	5.81	1.49	1.36
23	B	611	CLA	C3C-C2C	5.73	1.48	1.36
23	c	510	CLA	C3C-C2C	5.73	1.48	1.36
23	d	402[B]	CLA	C3C-C2C	5.73	1.48	1.36
23	D	403	CLA	C1D-ND	5.67	1.44	1.37
23	C	511	CLA	C1D-ND	5.64	1.44	1.37
23	c	510	CLA	C1D-ND	5.64	1.44	1.37
23	c	515	CLA	C1D-ND	5.61	1.44	1.37
23	D	403	CLA	C3C-C2C	5.60	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[A]	PHO	C3C-C2C	5.58	1.48	1.36
23	B	605	CLA	C1D-ND	5.56	1.44	1.37
24	a	406[B]	PHO	C3C-C2C	5.56	1.48	1.36
23	d	404	CLA	C1D-ND	5.56	1.44	1.37
23	B	603	CLA	C1D-ND	5.55	1.44	1.37
23	C	513	CLA	C3C-C2C	5.50	1.48	1.36
24	a	406[A]	PHO	C3C-C2C	5.49	1.48	1.36
23	B	611	CLA	CHC-C1C	5.49	1.49	1.38
23	A	404[B]	CLA	C1D-ND	5.48	1.44	1.37
23	c	514	CLA	C3C-C2C	5.47	1.48	1.36
24	A	416[B]	PHO	C3C-C2C	5.46	1.48	1.36
23	C	510	CLA	C3C-C2C	5.46	1.48	1.36
23	A	404[A]	CLA	C3C-C2C	5.45	1.48	1.36
23	d	402[B]	CLA	C1D-ND	5.44	1.44	1.37
23	C	509	CLA	C3C-C2C	5.43	1.48	1.36
23	b	601	CLA	C1D-ND	5.43	1.44	1.37
23	A	404[B]	CLA	C3C-C2C	5.43	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.42	1.48	1.36
23	a	407	CLA	CHC-C1C	5.42	1.49	1.38
23	c	513	CLA	C1D-ND	5.41	1.44	1.37
24	a	406[A]	PHO	C3D-C2D	5.41	1.49	1.39
23	a	405[B]	CLA	C3C-C2C	5.39	1.48	1.36
23	c	505	CLA	C3C-C2C	5.38	1.48	1.36
23	b	601	CLA	C3C-C2C	5.38	1.48	1.36
23	B	601	CLA	C3C-C2C	5.38	1.48	1.36
23	C	508	CLA	C3C-C2C	5.38	1.48	1.36
23	b	615	CLA	C3C-C2C	5.38	1.48	1.36
24	a	414[B]	PHO	C3D-C2D	5.36	1.49	1.39
23	c	507	CLA	C3C-C2C	5.35	1.48	1.36
24	A	416[B]	PHO	C3D-C2D	5.35	1.49	1.39
23	d	402[A]	CLA	C3C-C2C	5.35	1.48	1.36
23	b	606	CLA	C3C-C2C	5.34	1.48	1.36
23	c	511	CLA	C3C-C2C	5.34	1.48	1.36
23	c	510	CLA	O2D-CGD	5.34	1.46	1.33
23	a	405[A]	CLA	C3C-C2C	5.34	1.48	1.36
23	d	404	CLA	C3C-C2C	5.33	1.48	1.36
23	C	504	CLA	C3C-C2C	5.32	1.48	1.36
23	B	604	CLA	C3C-C2C	5.32	1.48	1.36
23	B	615	CLA	C1D-ND	5.31	1.44	1.37
23	b	610	CLA	C3C-C2C	5.31	1.48	1.36
23	c	512	CLA	C1D-ND	5.30	1.44	1.37
23	B	601	CLA	C1D-ND	5.29	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C3C-C2C	5.29	1.48	1.36
23	c	504	CLA	C3C-C2C	5.29	1.48	1.36
23	c	506	CLA	C1D-ND	5.29	1.44	1.37
24	a	414[A]	PHO	C3D-C2D	5.28	1.48	1.39
23	d	403[B]	CLA	C3C-C2C	5.28	1.48	1.36
23	c	506	CLA	O2D-CGD	5.28	1.46	1.33
24	a	406[B]	PHO	C3D-C2D	5.26	1.48	1.39
24	A	416[A]	PHO	C3D-C2D	5.25	1.48	1.39
23	b	607	CLA	C3C-C2C	5.25	1.47	1.36
23	b	611	CLA	C3C-C2C	5.24	1.47	1.36
23	b	616	CLA	C3C-C2C	5.24	1.47	1.36
23	a	407	CLA	C3C-C2C	5.24	1.47	1.36
23	b	612	CLA	C3C-C2C	5.24	1.47	1.36
23	B	608	CLA	C3C-C2C	5.23	1.47	1.36
23	d	403[A]	CLA	C3C-C2C	5.23	1.47	1.36
23	B	602	CLA	C1D-ND	5.22	1.44	1.37
23	D	402[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	C	505	CLA	C3C-C2C	5.22	1.47	1.36
23	a	404[A]	CLA	C3C-C2C	5.22	1.47	1.36
23	c	514	CLA	C1D-ND	5.21	1.44	1.37
23	b	605	CLA	C3C-C2C	5.21	1.47	1.36
23	c	511	CLA	O2D-CGD	5.21	1.45	1.33
23	B	605	CLA	C3C-C2C	5.21	1.47	1.36
23	b	603	CLA	C3C-C2C	5.20	1.47	1.36
23	c	505	CLA	C1D-ND	5.20	1.44	1.37
23	b	613	CLA	C3C-C2C	5.19	1.47	1.36
23	C	511	CLA	C3C-C2C	5.19	1.47	1.36
23	B	603	CLA	C3C-C2C	5.19	1.47	1.36
23	B	614	CLA	C1D-ND	5.19	1.44	1.37
23	a	404[B]	CLA	C3C-C2C	5.17	1.47	1.36
23	A	408	CLA	C3C-C2C	5.17	1.47	1.36
23	b	616	CLA	C1D-ND	5.17	1.44	1.37
23	d	402[A]	CLA	C1D-ND	5.16	1.44	1.37
23	A	406[B]	CLA	O2D-CGD	5.16	1.45	1.33
23	C	513	CLA	CHC-C1C	5.16	1.49	1.38
23	B	614	CLA	C3C-C2C	5.15	1.47	1.36
23	D	402[B]	CLA	C3C-C2C	5.14	1.47	1.36
23	b	609	CLA	O2D-CGD	5.13	1.45	1.33
23	c	513	CLA	O2D-CGD	5.13	1.45	1.33
23	a	405[B]	CLA	C1D-ND	5.12	1.44	1.37
23	C	503	CLA	C3C-C2C	5.12	1.47	1.36
23	c	513	CLA	C3C-C2C	5.12	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	C1D-ND	5.12	1.44	1.37
40	V	201	HEC	FE-ND	5.11	2.10	1.94
23	c	515	CLA	C3C-C2C	5.11	1.47	1.36
23	b	614	CLA	C3C-C2C	5.10	1.47	1.36
23	C	514	CLA	C3C-C2C	5.10	1.47	1.36
24	a	406[B]	PHO	O2D-CGD	5.10	1.45	1.33
23	B	609	CLA	C3C-C2C	5.10	1.47	1.36
23	C	512	CLA	O2D-CGD	5.09	1.45	1.33
23	c	503	CLA	C3C-C2C	5.09	1.47	1.36
23	c	509	CLA	C3C-C2C	5.09	1.47	1.36
23	C	503	CLA	C1D-ND	5.09	1.44	1.37
25	C	515	BCR	C23-C22	-5.08	1.35	1.45
23	B	609	CLA	O2D-CGD	5.08	1.45	1.33
23	B	601	CLA	O2A-CGA	5.08	1.48	1.33
23	b	609	CLA	C3C-C2C	5.07	1.47	1.36
24	A	416[B]	PHO	O2D-CGD	5.06	1.45	1.33
23	A	406[A]	CLA	C3C-C2C	5.05	1.47	1.36
23	c	512	CLA	C3C-C2C	5.05	1.47	1.36
23	d	402[B]	CLA	O2D-CGD	5.05	1.45	1.33
23	c	508	CLA	O2D-CGD	5.05	1.45	1.33
23	B	605	CLA	O2D-CGD	5.05	1.45	1.33
24	A	407[B]	PHO	O2D-CGD	5.04	1.45	1.33
23	B	613	CLA	O2D-CGD	5.04	1.45	1.33
23	A	405[B]	CLA	C1D-ND	5.04	1.44	1.37
24	a	406[A]	PHO	O2D-CGD	5.03	1.45	1.33
23	b	602	CLA	C3C-C2C	5.02	1.47	1.36
23	C	509	CLA	O2D-CGD	5.02	1.45	1.33
23	B	601	CLA	O2D-CGD	5.02	1.45	1.33
23	b	616	CLA	O2D-CGD	5.02	1.45	1.33
25	k	101	BCR	C23-C22	-5.02	1.35	1.45
23	C	509	CLA	C1D-ND	5.02	1.44	1.37
23	c	504	CLA	O2D-CGD	5.01	1.45	1.33
23	b	615	CLA	C1D-ND	5.01	1.43	1.37
23	c	508	CLA	C1D-ND	5.01	1.43	1.37
24	a	414[B]	PHO	O2D-CGD	5.01	1.45	1.33
25	d	405	BCR	C23-C22	-4.98	1.35	1.45
23	c	515	CLA	O2D-CGD	4.98	1.45	1.33
23	c	508	CLA	C3C-C2C	4.98	1.47	1.36
23	d	402[A]	CLA	O2D-CGD	4.98	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	4.98	1.45	1.33
23	b	603	CLA	CHC-C1C	4.97	1.48	1.38
23	b	601	CLA	O2D-CGD	4.97	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	507	CLA	O2D-CGD	4.97	1.45	1.33
23	b	602	CLA	CHC-C1C	4.96	1.48	1.38
23	C	505	CLA	O2D-CGD	4.96	1.45	1.33
38	f	101	HEM	FE-NB	4.96	2.10	1.94
23	A	405[B]	CLA	C3C-C2C	4.95	1.47	1.36
24	a	414[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	C	502	CLA	C3C-C2C	4.95	1.47	1.36
23	c	514	CLA	CHC-C1C	4.94	1.48	1.38
23	B	602	CLA	C3C-C2C	4.94	1.47	1.36
23	B	606	CLA	CHC-C1C	4.94	1.48	1.38
23	C	508	CLA	CHC-C1C	4.94	1.48	1.38
23	C	510	CLA	O2D-CGD	4.94	1.45	1.33
23	C	506	CLA	C3C-C2C	4.93	1.47	1.36
23	C	507	CLA	C3C-C2C	4.93	1.47	1.36
23	C	504	CLA	C1D-ND	4.93	1.43	1.37
23	B	606	CLA	C3C-C2C	4.93	1.47	1.36
23	B	612	CLA	C3C-C2C	4.93	1.47	1.36
23	A	406[B]	CLA	CHC-C1C	4.93	1.48	1.38
23	B	610	CLA	C1D-ND	4.92	1.43	1.37
23	b	613	CLA	CHC-C1C	4.92	1.48	1.38
23	D	402[B]	CLA	O2D-CGD	4.92	1.45	1.33
24	A	407[B]	PHO	C3D-C2D	4.92	1.48	1.39
23	C	510	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	O2D-CGD	4.90	1.45	1.33
23	B	613	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	b	602	CLA	O2D-CGD	4.90	1.45	1.33
23	c	506	CLA	C3C-C2C	4.90	1.47	1.36
38	E	102	HEM	FE-NB	4.90	2.10	1.94
24	A	407[A]	PHO	C3D-C2D	4.88	1.48	1.39
23	B	611	CLA	C4B-NB	-4.87	1.31	1.37
23	B	615	CLA	C3C-C2C	4.87	1.47	1.36
23	c	503	CLA	CHC-C1C	4.87	1.48	1.38
23	A	405[A]	CLA	C3C-C2C	4.87	1.47	1.36
23	C	514	CLA	C1D-ND	4.86	1.43	1.37
23	d	403[B]	CLA	O2D-CGD	4.85	1.45	1.33
24	a	414[B]	PHO	OBD-CAD	4.85	1.29	1.22
23	A	408	CLA	O2D-CGD	4.85	1.45	1.33
23	c	504	CLA	C1D-ND	4.85	1.43	1.37
23	C	511	CLA	O2D-CGD	4.85	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	C1D-ND	4.85	1.43	1.37
23	c	509	CLA	CHC-C1C	4.84	1.48	1.38
24	a	414[A]	PHO	OBD-CAD	4.84	1.29	1.22
23	B	609	CLA	CHC-C1C	4.84	1.48	1.38
23	B	616	CLA	CHC-C1C	4.84	1.48	1.38
23	B	614	CLA	O2D-CGD	4.84	1.45	1.33
23	a	405[B]	CLA	O2D-CGD	4.84	1.45	1.33
23	b	609	CLA	CHC-C1C	4.83	1.48	1.38
23	B	612	CLA	CHC-C1C	4.83	1.48	1.38
23	c	512	CLA	O2D-CGD	4.83	1.45	1.33
23	C	513	CLA	C1D-ND	4.82	1.43	1.37
23	b	608	CLA	C3C-C2C	4.82	1.47	1.36
23	b	601	CLA	O2A-CGA	4.81	1.47	1.33
23	b	603	CLA	O2D-CGD	4.81	1.44	1.33
23	A	405[B]	CLA	O2D-CGD	4.80	1.44	1.33
23	B	604	CLA	CHD-C1D	4.80	1.47	1.38
23	a	407	CLA	O2D-CGD	4.80	1.44	1.33
23	b	607	CLA	O2D-CGD	4.80	1.44	1.33
25	y	101	BCR	C23-C22	-4.80	1.35	1.45
23	D	402[A]	CLA	O2D-CGD	4.80	1.44	1.33
23	B	613	CLA	CHC-C1C	4.80	1.48	1.38
23	D	403	CLA	O2D-CGD	4.80	1.44	1.33
23	B	606	CLA	O2D-CGD	4.80	1.44	1.33
23	C	513	CLA	O2D-CGD	4.79	1.44	1.33
23	B	608	CLA	C1D-ND	4.79	1.43	1.37
23	B	607	CLA	C3C-C2C	4.78	1.46	1.36
26	F	102	SQD	O47-C7	4.78	1.47	1.34
24	A	416[B]	PHO	OBD-CAD	4.78	1.29	1.22
23	b	610	CLA	O2D-CGD	4.78	1.44	1.33
23	b	614	CLA	CHC-C1C	4.78	1.48	1.38
25	B	617	BCR	C23-C22	-4.78	1.35	1.45
23	d	404	CLA	O2D-CGD	4.77	1.44	1.33
23	C	504	CLA	CHC-C1C	4.77	1.48	1.38
23	c	509	CLA	C1D-ND	4.77	1.43	1.37
23	b	613	CLA	O2D-CGD	4.77	1.44	1.33
23	b	606	CLA	C1D-ND	4.77	1.43	1.37
23	B	604	CLA	O2D-CGD	4.77	1.44	1.33
23	C	502	CLA	C1D-ND	4.77	1.43	1.37
23	b	605	CLA	O2D-CGD	4.77	1.44	1.33
23	a	404[B]	CLA	C1D-ND	4.77	1.43	1.37
23	b	601	CLA	CHC-C1C	4.77	1.48	1.38
25	K	102	BCR	C23-C22	-4.76	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	516	BCR	C23-C22	-4.76	1.35	1.45
25	b	617	BCR	C23-C22	-4.76	1.35	1.45
23	b	615	CLA	O2D-CGD	4.76	1.44	1.33
25	t	102	BCR	C23-C22	-4.76	1.35	1.45
23	C	514	CLA	O2D-CGD	4.76	1.44	1.33
23	b	613	CLA	C1D-ND	4.75	1.43	1.37
23	c	510	CLA	CHC-C1C	4.75	1.48	1.38
23	c	509	CLA	O2D-CGD	4.75	1.44	1.33
23	b	602	CLA	CHD-C1D	4.75	1.47	1.38
23	b	604	CLA	C3C-C2C	4.74	1.46	1.36
23	B	613	CLA	C1D-ND	4.74	1.43	1.37
23	b	616	CLA	CHC-C1C	4.74	1.48	1.38
23	C	502	CLA	CHC-C1C	4.74	1.48	1.38
23	B	601	CLA	CHC-C1C	4.74	1.48	1.38
23	c	505	CLA	CHC-C1C	4.73	1.48	1.38
23	C	512	CLA	C3C-C2C	4.73	1.46	1.36
23	A	404[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	a	405[B]	CLA	CHC-C1C	4.73	1.48	1.38
23	C	506	CLA	O2D-CGD	4.73	1.44	1.33
23	B	610	CLA	CHC-C1C	4.72	1.48	1.38
23	A	406[A]	CLA	CHC-C1C	4.72	1.48	1.38
25	T	101	BCR	C23-C22	-4.71	1.35	1.45
23	C	506	CLA	C1D-ND	4.70	1.43	1.37
25	D	404	BCR	C23-C22	-4.69	1.35	1.45
23	D	403	CLA	CHC-C1C	4.69	1.48	1.38
23	b	604	CLA	C1D-ND	4.69	1.43	1.37
23	B	611	CLA	O2D-CGD	4.68	1.44	1.33
23	c	507	CLA	CHC-C1C	4.68	1.48	1.38
23	b	610	CLA	CHC-C1C	4.68	1.48	1.38
23	c	515	CLA	CHC-C1C	4.67	1.48	1.38
33	C	521	LMG	O7-C10	4.66	1.47	1.34
23	d	403[A]	CLA	O2D-CGD	4.66	1.44	1.33
25	a	408	BCR	C23-C22	-4.66	1.35	1.45
23	b	614	CLA	C1D-ND	4.66	1.43	1.37
23	C	506	CLA	CHC-C1C	4.66	1.48	1.38
23	B	605	CLA	CHC-C1C	4.66	1.48	1.38
23	C	503	CLA	O2D-CGD	4.66	1.44	1.33
33	c	522	LMG	O7-C10	4.66	1.47	1.34
23	B	616	CLA	O2D-CGD	4.65	1.44	1.33
23	C	511	CLA	CHC-C1C	4.65	1.48	1.38
23	C	506	CLA	CHD-C1D	4.65	1.47	1.38
24	a	406[B]	PHO	OBD-CAD	4.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C1B-NB	-4.64	1.32	1.37
25	c	516	BCR	C23-C22	-4.64	1.36	1.45
23	C	508	CLA	C1D-ND	4.64	1.43	1.37
25	c	517	BCR	C23-C22	-4.64	1.36	1.45
25	b	619	BCR	C23-C22	-4.63	1.36	1.45
23	c	507	CLA	O2D-CGD	4.62	1.44	1.33
23	a	404[A]	CLA	C1D-ND	4.62	1.43	1.37
23	B	615	CLA	CHC-C1C	4.62	1.47	1.38
23	b	615	CLA	CHC-C1C	4.61	1.47	1.38
23	b	607	CLA	C1B-NB	-4.61	1.32	1.37
23	a	404[B]	CLA	O2D-CGD	4.61	1.44	1.33
23	b	605	CLA	C1D-ND	4.60	1.43	1.37
25	B	619	BCR	C23-C22	-4.60	1.36	1.45
23	B	609	CLA	CHD-C1D	4.59	1.47	1.38
23	b	604	CLA	CHC-C1C	4.59	1.47	1.38
23	B	606	CLA	C1D-ND	4.58	1.43	1.37
23	d	404	CLA	CHC-C1C	4.58	1.47	1.38
23	c	513	CLA	CHC-C1C	4.58	1.47	1.38
23	B	612	CLA	CHB-C1B	4.58	1.49	1.39
23	a	405[A]	CLA	CHC-C1C	4.58	1.47	1.38
23	A	404[B]	CLA	CHC-C1C	4.58	1.47	1.38
23	b	611	CLA	C1D-ND	4.57	1.43	1.37
23	B	603	CLA	O2D-CGD	4.57	1.44	1.33
23	b	611	CLA	CHC-C1C	4.57	1.47	1.38
23	b	614	CLA	O2D-CGD	4.57	1.44	1.33
23	b	605	CLA	CHC-C1C	4.57	1.47	1.38
23	B	602	CLA	O2D-CGD	4.56	1.44	1.33
23	A	405[A]	CLA	CHC-C1C	4.55	1.47	1.38
23	C	509	CLA	CHC-C1C	4.55	1.47	1.38
33	C	521	LMG	O8-C28	4.54	1.46	1.33
23	a	404[A]	CLA	O2D-CGD	4.54	1.44	1.33
23	B	615	CLA	CHD-C1D	4.54	1.47	1.38
23	d	402[B]	CLA	CHC-C1C	4.54	1.47	1.38
23	B	604	CLA	CHC-C1C	4.52	1.47	1.38
23	b	608	CLA	O2D-CGD	4.52	1.44	1.33
23	C	507	CLA	CHD-C1D	4.51	1.47	1.38
23	c	508	CLA	CHC-C1C	4.51	1.47	1.38
25	A	409	BCR	C23-C22	-4.50	1.36	1.45
23	b	606	CLA	O2D-CGD	4.50	1.44	1.33
23	c	506	CLA	CHC-C1C	4.50	1.47	1.38
23	C	502	CLA	CHD-C1D	4.50	1.47	1.38
23	a	405[A]	CLA	O2D-CGD	4.50	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	604	CLA	O2D-CGD	4.49	1.44	1.33
23	b	607	CLA	CHC-C1C	4.49	1.47	1.38
23	c	514	CLA	O2D-CGD	4.48	1.44	1.33
26	B	620	SQD	O47-C7	4.48	1.46	1.34
23	b	612	CLA	O2D-CGD	4.48	1.44	1.33
32	E	101[A]	LHG	O8-C23	4.48	1.46	1.33
23	D	402[B]	CLA	CHC-C1C	4.47	1.47	1.38
23	b	602	CLA	CHC-C4B	4.47	1.49	1.39
23	B	602	CLA	CHC-C1C	4.47	1.47	1.38
33	C	520	LMG	O8-C28	4.46	1.46	1.33
23	c	515	CLA	CHD-C1D	4.46	1.47	1.38
25	b	618	BCR	C23-C22	-4.45	1.36	1.45
23	C	508	CLA	O2D-CGD	4.45	1.44	1.33
23	C	507	CLA	C1D-ND	4.45	1.43	1.37
23	D	403	CLA	CHD-C1D	4.45	1.47	1.38
23	B	610	CLA	O2D-CGD	4.44	1.44	1.33
23	A	406[B]	CLA	CHD-C1D	4.44	1.47	1.38
23	B	611	CLA	CHC-C4B	4.44	1.49	1.39
23	b	606	CLA	CHC-C1C	4.44	1.47	1.38
23	c	515	CLA	O2A-CGA	4.44	1.46	1.33
33	z	101	LMG	O8-C28	4.43	1.46	1.33
26	f	102	SQD	O47-C7	4.43	1.46	1.34
23	c	514	CLA	O2A-CGA	4.43	1.46	1.33
32	E	101[B]	LHG	O8-C23	4.43	1.46	1.33
25	Y	101	BCR	C23-C22	-4.43	1.36	1.45
23	C	514	CLA	CHC-C1C	4.43	1.47	1.38
23	b	602	CLA	C1D-ND	4.42	1.43	1.37
23	d	402[A]	CLA	CHC-C1C	4.40	1.47	1.38
35	c	520	DGD	O1G-C1A	4.40	1.46	1.33
23	C	505	CLA	CHC-C1C	4.40	1.47	1.38
40	v	201	HEC	FE-ND	4.40	2.08	1.94
23	A	405[B]	CLA	O2A-CGA	4.40	1.46	1.33
23	c	505	CLA	CHD-C1D	4.40	1.46	1.38
32	a	417[A]	LHG	O8-C23	4.39	1.46	1.33
23	B	609	CLA	C1D-ND	4.39	1.43	1.37
26	b	620	SQD	O47-C7	4.39	1.46	1.34
23	A	405[B]	CLA	CHC-C1C	4.39	1.47	1.38
23	C	503	CLA	CHD-C1D	4.38	1.46	1.38
25	h	101	BCR	C23-C22	-4.38	1.36	1.45
23	d	402[A]	CLA	C3D-C2D	4.38	1.51	1.39
38	E	102	HEM	FE-NC	4.37	2.10	1.95
23	c	504	CLA	CHC-C1C	4.37	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	CHD-C1D	4.37	1.46	1.38
23	b	612	CLA	CHC-C1C	4.37	1.47	1.38
32	a	417[B]	LHG	O8-C23	4.37	1.46	1.33
25	X	101	BCR	C23-C22	-4.36	1.36	1.45
23	b	603	CLA	C1D-ND	4.36	1.43	1.37
26	a	410	SQD	O48-C23	4.36	1.46	1.33
23	a	404[A]	CLA	CHC-C1C	4.36	1.47	1.38
23	B	607	CLA	O2D-CGD	4.36	1.43	1.33
24	a	406[A]	PHO	OBD-CAD	4.36	1.28	1.22
23	B	605	CLA	CHC-C4B	4.35	1.49	1.39
23	c	503	CLA	CHD-C1D	4.35	1.46	1.38
23	C	513	CLA	CHD-C1D	4.35	1.46	1.38
23	A	405[A]	CLA	O2D-CGD	4.35	1.43	1.33
23	b	609	CLA	C1D-ND	4.34	1.43	1.37
23	B	614	CLA	CHC-C1C	4.34	1.47	1.38
23	a	407	CLA	O2A-CGA	4.33	1.46	1.33
23	d	403[B]	CLA	CHC-C1C	4.33	1.47	1.38
23	c	510	CLA	CHD-C1D	4.33	1.46	1.38
23	B	616	CLA	C1D-ND	4.33	1.43	1.37
23	B	603	CLA	CHC-C1C	4.32	1.47	1.38
23	C	512	CLA	CHD-C1D	4.32	1.46	1.38
32	d	408[B]	LHG	O8-C23	4.32	1.46	1.33
23	C	505	CLA	CHD-C1D	4.32	1.46	1.38
23	c	512	CLA	CHC-C1C	4.32	1.47	1.38
23	a	404[B]	CLA	CHC-C1C	4.32	1.47	1.38
23	b	610	CLA	CHD-C1D	4.32	1.46	1.38
33	B	621	LMG	O8-C28	4.31	1.45	1.33
24	A	416[A]	PHO	OBD-CAD	4.31	1.28	1.22
23	C	512	CLA	O2A-CGA	4.31	1.45	1.33
23	d	402[B]	CLA	C3D-C2D	4.31	1.50	1.39
23	A	404[A]	CLA	CHC-C1C	4.31	1.47	1.38
23	b	611	CLA	O2A-CGA	4.31	1.45	1.33
32	d	408[A]	LHG	O8-C23	4.31	1.45	1.33
23	C	505	CLA	C1D-ND	4.30	1.43	1.37
23	C	503	CLA	CHC-C1C	4.30	1.47	1.38
23	c	507	CLA	C1D-ND	4.30	1.43	1.37
23	d	404	CLA	O2A-CGA	4.30	1.45	1.33
23	b	612	CLA	C1D-ND	4.29	1.43	1.37
23	B	602	CLA	CHD-C1D	4.29	1.46	1.38
23	c	508	CLA	O2A-CGA	4.29	1.45	1.33
23	b	611	CLA	O2D-CGD	4.29	1.43	1.33
26	a	409[B]	SQD	O48-C23	4.28	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	OBD-CAD	4.28	1.28	1.22
23	A	408	CLA	O2A-CGA	4.28	1.45	1.33
23	D	402[B]	CLA	C1D-ND	4.28	1.43	1.37
23	c	514	CLA	CHD-C1D	4.28	1.46	1.38
23	D	402[A]	CLA	C1D-ND	4.27	1.43	1.37
23	B	601	CLA	CHD-C1D	4.26	1.46	1.38
23	B	608	CLA	CHD-C1D	4.26	1.46	1.38
23	C	509	CLA	O2A-CGA	4.26	1.45	1.33
23	B	608	CLA	O2D-CGD	4.26	1.43	1.33
33	c	522	LMG	O8-C28	4.25	1.45	1.33
23	C	514	CLA	O2A-CGA	4.25	1.45	1.33
23	C	512	CLA	CHC-C1C	4.25	1.47	1.38
23	b	601	CLA	C3D-C2D	4.25	1.50	1.39
23	D	402[A]	CLA	CHC-C1C	4.25	1.47	1.38
23	c	506	CLA	C3D-C2D	4.24	1.50	1.39
23	C	510	CLA	CHC-C1C	4.23	1.47	1.38
23	B	604	CLA	C1D-ND	4.23	1.43	1.37
23	b	608	CLA	CHD-C1D	4.22	1.46	1.38
26	A	412	SQD	O48-C23	4.22	1.45	1.33
23	c	510	CLA	C3D-C2D	4.22	1.50	1.39
23	C	504	CLA	O2D-CGD	4.22	1.43	1.33
23	A	404[A]	CLA	C1D-ND	4.22	1.43	1.37
23	c	513	CLA	CHD-C1D	4.22	1.46	1.38
23	D	402[A]	CLA	O2A-CGA	4.22	1.45	1.33
23	c	509	CLA	O2A-CGA	4.22	1.45	1.33
26	f	102	SQD	O48-C23	4.22	1.45	1.33
23	B	610	CLA	OBD-CAD	4.21	1.29	1.22
23	b	608	CLA	C3D-C2D	4.21	1.50	1.39
23	D	402[B]	CLA	O2A-CGA	4.20	1.45	1.33
23	c	508	CLA	CHD-C1D	4.20	1.46	1.38
33	m	101	LMG	O8-C28	4.20	1.45	1.33
23	D	403	CLA	C3D-C2D	4.20	1.50	1.39
23	c	505	CLA	O2D-CGD	4.19	1.43	1.33
32	E	101[A]	LHG	O7-C7	4.19	1.46	1.34
23	A	406[A]	CLA	CHD-C1D	4.18	1.46	1.38
33	Z	101	LMG	O7-C10	4.18	1.46	1.34
26	B	620	SQD	O48-C23	4.18	1.45	1.33
23	b	608	CLA	CHC-C1C	4.18	1.47	1.38
23	b	615	CLA	O2A-CGA	4.17	1.45	1.33
23	A	404[B]	CLA	CHD-C1D	4.17	1.46	1.38
23	c	504	CLA	CHD-C1D	4.17	1.46	1.38
23	B	612	CLA	O2D-CGD	4.17	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	CHD-C1D	4.17	1.46	1.38
23	C	504	CLA	CHD-C4C	4.17	1.48	1.39
26	b	620	SQD	O48-C23	4.17	1.45	1.33
23	B	607	CLA	C1B-NB	-4.17	1.32	1.37
23	b	614	CLA	CHD-C1D	4.16	1.46	1.38
23	d	404	CLA	CHD-C1D	4.16	1.46	1.38
23	a	404[B]	CLA	CHD-C1D	4.16	1.46	1.38
23	C	509	CLA	C3D-C2D	4.16	1.50	1.39
35	h	102	DGD	O2G-C1B	4.16	1.46	1.34
23	c	509	CLA	CHD-C4C	4.15	1.48	1.39
23	a	405[A]	CLA	C1D-ND	4.15	1.42	1.37
23	b	603	CLA	CHD-C1D	4.15	1.46	1.38
23	A	405[B]	CLA	CHD-C1D	4.15	1.46	1.38
23	B	607	CLA	CHC-C4B	4.14	1.48	1.39
23	B	607	CLA	CHC-C1C	4.14	1.46	1.38
26	a	409[B]	SQD	O47-C7	4.14	1.46	1.34
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
35	C	517[B]	DGD	O2G-C1B	4.14	1.46	1.34
32	a	417[B]	LHG	O7-C7	4.14	1.46	1.34
35	C	519	DGD	O1G-C1A	4.14	1.45	1.33
23	d	402[B]	CLA	O2A-CGA	4.13	1.45	1.33
32	a	417[A]	LHG	O7-C7	4.13	1.46	1.34
23	d	403[A]	CLA	CHC-C1C	4.13	1.46	1.38
35	c	519[B]	DGD	O1G-C1A	4.13	1.45	1.33
23	c	513	CLA	O2A-CGA	4.12	1.45	1.33
23	c	511	CLA	C1B-NB	-4.12	1.32	1.37
25	B	618	BCR	C23-C22	-4.12	1.37	1.45
23	a	405[A]	CLA	O2A-CGA	4.12	1.45	1.33
26	F	102	SQD	O48-C23	4.12	1.45	1.33
23	d	403[A]	CLA	CHB-C1B	4.11	1.48	1.39
23	b	602	CLA	CHD-C4C	4.11	1.48	1.39
32	E	101[B]	LHG	O7-C7	4.11	1.45	1.34
23	c	515	CLA	CHD-C4C	4.11	1.48	1.39
23	d	403[B]	CLA	O2A-CGA	4.11	1.45	1.33
23	C	514	CLA	CHD-C1D	4.11	1.46	1.38
23	b	601	CLA	CHD-C4C	4.11	1.48	1.39
33	z	101	LMG	O7-C10	4.11	1.45	1.34
33	c	521	LMG	O7-C10	4.11	1.45	1.34
23	b	608	CLA	O2A-CGA	4.10	1.45	1.33
23	b	609	CLA	CHB-C1B	4.10	1.48	1.39
23	B	603	CLA	CHB-C1B	4.10	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	CHB-C1B	4.10	1.48	1.39
32	D	407[B]	LHG	O8-C23	4.09	1.45	1.33
23	c	511	CLA	CHD-C1D	4.09	1.46	1.38
23	C	512	CLA	CHB-C1B	4.09	1.48	1.39
23	C	509	CLA	CHD-C1D	4.09	1.46	1.38
23	c	504	CLA	O2A-CGA	4.09	1.45	1.33
35	c	518[A]	DGD	O2G-C1B	4.09	1.45	1.34
23	B	611	CLA	C3B-C2B	4.09	1.55	1.41
23	d	403[B]	CLA	C1D-ND	4.09	1.42	1.37
23	C	505	CLA	CHB-C1B	4.09	1.48	1.39
23	a	404[B]	CLA	CHD-C4C	4.08	1.48	1.39
23	A	406[B]	CLA	CHD-C4C	4.08	1.48	1.39
23	d	402[A]	CLA	O2A-CGA	4.08	1.45	1.33
23	B	607	CLA	CHB-C1B	4.08	1.48	1.39
23	B	614	CLA	CHB-C1B	4.08	1.48	1.39
23	B	611	CLA	CHD-C1D	4.08	1.46	1.38
23	b	616	CLA	O2A-CGA	4.08	1.45	1.33
33	c	521	LMG	O8-C28	4.08	1.45	1.33
23	B	614	CLA	C4B-NB	-4.08	1.32	1.37
23	C	504	CLA	CHC-C4B	4.08	1.48	1.39
23	C	510	CLA	OBD-CAD	4.07	1.29	1.22
23	c	511	CLA	CHC-C1C	4.07	1.46	1.38
26	a	409[A]	SQD	O47-C7	4.07	1.45	1.34
23	c	503	CLA	O2D-CGD	4.07	1.43	1.33
23	C	510	CLA	CHD-C1D	4.07	1.46	1.38
23	B	611	CLA	CHB-C1B	4.07	1.48	1.39
23	B	612	CLA	CHD-C1D	4.06	1.46	1.38
33	c	501	LMG	O7-C10	4.06	1.45	1.34
23	C	512	CLA	C1D-ND	4.06	1.42	1.37
23	c	505	CLA	CHD-C4C	4.06	1.48	1.39
23	a	405[B]	CLA	O2A-CGA	4.06	1.45	1.33
35	C	517[A]	DGD	O2G-C1B	4.06	1.45	1.34
23	D	402[A]	CLA	CHB-C1B	4.06	1.48	1.39
23	b	616	CLA	CHD-C1D	4.06	1.46	1.38
23	c	506	CLA	CHD-C1D	4.06	1.46	1.38
23	C	509	CLA	OBD-CAD	4.05	1.29	1.22
23	B	609	CLA	O2A-CGA	4.05	1.45	1.33
23	c	509	CLA	CHC-C4B	4.05	1.48	1.39
23	a	405[B]	CLA	OBD-CAD	4.05	1.29	1.22
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
26	A	412	SQD	O47-C7	4.05	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CHD-C4C	4.05	1.48	1.39
34	o	301	HTG	C1'-S1	-4.05	1.76	1.81
23	c	509	CLA	CHD-C1D	4.05	1.46	1.38
23	b	610	CLA	C1D-ND	4.05	1.42	1.37
38	f	101	HEM	FE-NC	4.04	2.08	1.95
23	B	615	CLA	CHB-C1B	4.04	1.48	1.39
23	B	606	CLA	CHD-C1D	4.04	1.46	1.38
23	C	514	CLA	C3D-C2D	4.04	1.50	1.39
23	B	602	CLA	CHB-C1B	4.04	1.48	1.39
23	B	609	CLA	C3D-C2D	4.03	1.50	1.39
23	b	608	CLA	OBD-CAD	4.03	1.29	1.22
23	A	404[A]	CLA	CHD-C1D	4.03	1.46	1.38
23	A	406[B]	CLA	O2A-CGA	4.03	1.45	1.33
23	C	507	CLA	O2A-CGA	4.03	1.45	1.33
33	C	501	LMG	O8-C28	4.03	1.45	1.33
33	c	501	LMG	O8-C28	4.03	1.45	1.33
23	A	405[B]	CLA	C3D-C2D	4.03	1.50	1.39
23	A	406[B]	CLA	C1D-ND	4.03	1.42	1.37
23	b	615	CLA	CHD-C1D	4.03	1.46	1.38
33	C	501	LMG	O7-C10	4.02	1.45	1.34
32	L	101[B]	LHG	O8-C23	4.02	1.45	1.33
23	A	406[A]	CLA	C1D-ND	4.02	1.42	1.37
23	B	615	CLA	O2A-CGA	4.02	1.45	1.33
33	C	520	LMG	O7-C10	4.02	1.45	1.34
23	c	503	CLA	CHD-C4C	4.01	1.48	1.39
23	C	512	CLA	C4B-NB	-4.01	1.32	1.37
23	c	511	CLA	O2A-CGA	4.01	1.45	1.33
23	B	602	CLA	CHD-C4C	4.01	1.48	1.39
23	c	507	CLA	CHC-C4B	4.01	1.48	1.39
23	c	507	CLA	CHD-C4C	4.01	1.48	1.39
23	B	616	CLA	O2A-CGA	4.01	1.45	1.33
23	C	504	CLA	CHD-C1D	4.01	1.46	1.38
23	B	604	CLA	CHB-C1B	4.01	1.48	1.39
23	C	506	CLA	CHB-C1B	4.01	1.48	1.39
23	C	502	CLA	O2A-CGA	4.01	1.45	1.33
23	C	503	CLA	O2A-CGA	4.00	1.45	1.33
35	c	518[B]	DGD	O2G-C1B	4.00	1.45	1.34
23	c	503	CLA	C3D-C2D	4.00	1.50	1.39
23	a	405[B]	CLA	C3D-C2D	4.00	1.50	1.39
23	C	508	CLA	O2A-CGA	4.00	1.45	1.33
33	d	412	LMG	O7-C10	4.00	1.45	1.34
23	C	508	CLA	CHD-C1D	4.00	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	OBD-CAD	3.99	1.29	1.22
23	b	608	CLA	C1D-ND	3.99	1.42	1.37
23	b	607	CLA	CHB-C1B	3.99	1.48	1.39
23	C	503	CLA	C3D-C2D	3.99	1.50	1.39
23	a	404[A]	CLA	CHD-C1D	3.99	1.46	1.38
23	B	608	CLA	CHC-C1C	3.99	1.46	1.38
23	C	502	CLA	O2D-CGD	3.99	1.42	1.33
23	B	611	CLA	O2A-CGA	3.99	1.45	1.33
23	b	615	CLA	CHD-C4C	3.99	1.48	1.39
24	A	416[B]	PHO	O2A-CGA	3.99	1.45	1.33
32	D	407[B]	LHG	O7-C7	3.98	1.45	1.34
23	b	604	CLA	CHC-C4B	3.98	1.48	1.39
32	D	407[A]	LHG	O7-C7	3.98	1.45	1.34
23	B	603	CLA	CHC-C4B	3.98	1.48	1.39
23	B	601	CLA	CHC-C4B	3.98	1.48	1.39
32	d	407[B]	LHG	O7-C7	3.98	1.45	1.34
26	a	409[A]	SQD	O48-C23	3.98	1.45	1.33
23	B	605	CLA	CHD-C4C	3.98	1.48	1.39
23	c	504	CLA	C3D-C2D	3.98	1.50	1.39
23	B	611	CLA	OBD-CAD	3.98	1.29	1.22
23	C	506	CLA	CHC-C4B	3.98	1.48	1.39
23	D	403	CLA	CHC-C4B	3.98	1.48	1.39
23	B	616	CLA	CHB-C1B	3.97	1.48	1.39
23	A	408	CLA	CHD-C1D	3.97	1.46	1.38
23	C	510	CLA	CHD-C4C	3.97	1.48	1.39
23	c	503	CLA	O2A-CGA	3.97	1.44	1.33
23	D	403	CLA	CHB-C1B	3.97	1.48	1.39
23	c	507	CLA	CHD-C1D	3.97	1.46	1.38
23	c	513	CLA	OBD-CAD	3.97	1.29	1.22
23	c	513	CLA	CHB-C1B	3.97	1.48	1.39
23	C	511	CLA	CHD-C4C	3.97	1.48	1.39
23	b	610	CLA	CHB-C1B	3.96	1.48	1.39
23	c	514	CLA	CHC-C4B	3.96	1.48	1.39
23	c	514	CLA	CHD-C4C	3.96	1.48	1.39
23	B	610	CLA	C3D-C2D	3.96	1.49	1.39
23	C	511	CLA	O2A-CGA	3.96	1.44	1.33
23	c	510	CLA	OBD-CAD	3.96	1.29	1.22
23	C	504	CLA	O2A-CGA	3.96	1.44	1.33
23	a	404[A]	CLA	CHD-C4C	3.96	1.48	1.39
26	a	410	SQD	O47-C7	3.95	1.45	1.34
23	b	611	CLA	CHB-C1B	3.95	1.48	1.39
23	b	613	CLA	CHB-C1B	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	O2A-CGA	3.95	1.44	1.33
23	c	505	CLA	O2A-CGA	3.95	1.44	1.33
23	C	513	CLA	C3D-C2D	3.95	1.49	1.39
23	c	508	CLA	CHD-C4C	3.95	1.48	1.39
32	d	408[B]	LHG	O7-C7	3.94	1.45	1.34
23	C	507	CLA	CHC-C1C	3.94	1.46	1.38
33	B	621	LMG	O7-C10	3.94	1.45	1.34
23	C	510	CLA	C4B-NB	-3.94	1.32	1.37
23	c	510	CLA	O2A-CGA	3.94	1.44	1.33
23	d	403[B]	CLA	CHD-C1D	3.94	1.46	1.38
23	c	514	CLA	C3D-C2D	3.93	1.49	1.39
23	c	505	CLA	CHC-C4B	3.93	1.48	1.39
23	b	615	CLA	C3D-C2D	3.93	1.49	1.39
23	C	510	CLA	O2A-CGA	3.93	1.44	1.33
23	b	606	CLA	O2A-CGA	3.93	1.44	1.33
23	B	604	CLA	CHD-C4C	3.93	1.48	1.39
26	A	410[B]	SQD	O48-C23	3.93	1.44	1.33
23	b	604	CLA	C3D-C2D	3.93	1.49	1.39
35	C	518[B]	DGD	O1G-C1A	3.93	1.44	1.33
23	A	404[B]	CLA	CHD-C4C	3.92	1.48	1.39
35	c	518[B]	DGD	O1G-C1A	3.92	1.44	1.33
23	D	402[A]	CLA	CHD-C1D	3.92	1.46	1.38
23	b	611	CLA	C3D-C2D	3.92	1.49	1.39
23	b	613	CLA	CHD-C1D	3.92	1.46	1.38
23	C	507	CLA	CHD-C4C	3.92	1.48	1.39
32	d	414[B]	LHG	O8-C23	3.92	1.44	1.33
23	c	512	CLA	CHB-C1B	3.91	1.48	1.39
34	b	623	HTG	C1'-S1	-3.91	1.76	1.81
32	D	407[A]	LHG	O8-C23	3.90	1.44	1.33
35	c	519[B]	DGD	O2G-C1B	3.90	1.45	1.34
23	B	608	CLA	C3D-C2D	3.90	1.49	1.39
23	C	508	CLA	CHC-C4B	3.90	1.48	1.39
23	a	405[A]	CLA	C3D-C2D	3.90	1.49	1.39
23	D	402[A]	CLA	CHD-C4C	3.89	1.48	1.39
23	b	607	CLA	CHD-C1D	3.89	1.45	1.38
23	a	405[B]	CLA	CHD-C1D	3.89	1.45	1.38
23	A	405[A]	CLA	C1D-ND	3.89	1.42	1.37
23	a	404[B]	CLA	OBD-CAD	3.89	1.29	1.22
23	D	402[B]	CLA	CHD-C1D	3.89	1.45	1.38
23	B	606	CLA	O2A-CGA	3.89	1.44	1.33
24	A	407[B]	PHO	O2A-CGA	3.88	1.44	1.33
23	B	613	CLA	C1B-NB	-3.88	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	CHD-C4C	3.88	1.48	1.39
23	c	512	CLA	C3D-C2D	3.88	1.49	1.39
23	c	505	CLA	CHB-C1B	3.88	1.48	1.39
23	c	513	CLA	CHD-C4C	3.88	1.48	1.39
23	b	612	CLA	CHB-C1B	3.88	1.48	1.39
23	b	604	CLA	CHD-C4C	3.87	1.48	1.39
23	C	510	CLA	C3D-C2D	3.87	1.49	1.39
23	B	603	CLA	O2A-CGA	3.87	1.44	1.33
23	b	611	CLA	CHD-C1D	3.87	1.45	1.38
23	d	403[A]	CLA	C1B-NB	-3.87	1.33	1.37
23	C	509	CLA	CHB-C1B	3.87	1.48	1.39
23	B	607	CLA	OBD-CAD	3.87	1.29	1.22
23	c	507	CLA	CHB-C1B	3.86	1.48	1.39
23	B	616	CLA	C3D-C2D	3.86	1.49	1.39
23	c	508	CLA	C3D-C2D	3.86	1.49	1.39
23	A	408	CLA	C1D-ND	3.86	1.42	1.37
23	d	403[B]	CLA	CHB-C1B	3.86	1.48	1.39
23	d	402[B]	CLA	CHD-C1D	3.86	1.45	1.38
23	A	406[B]	CLA	C3D-C2D	3.86	1.49	1.39
23	A	408	CLA	CHC-C1C	3.86	1.46	1.38
24	A	416[A]	PHO	O2A-CGA	3.86	1.44	1.33
23	b	612	CLA	C3D-C2D	3.86	1.49	1.39
23	B	602	CLA	CHC-C4B	3.86	1.48	1.39
23	D	402[B]	CLA	CHD-C4C	3.85	1.48	1.39
23	B	605	CLA	C3D-C2D	3.85	1.49	1.39
23	c	512	CLA	CHC-C4B	3.85	1.48	1.39
35	C	518[A]	DGD	O2G-C1B	3.85	1.45	1.34
33	d	412	LMG	O8-C28	3.85	1.44	1.33
23	C	510	CLA	C1B-NB	-3.85	1.33	1.37
23	B	606	CLA	CHC-C4B	3.85	1.48	1.39
23	B	614	CLA	CHD-C4C	3.85	1.48	1.39
23	C	513	CLA	CHD-C4C	3.85	1.48	1.39
26	A	410[A]	SQD	O48-C23	3.85	1.44	1.33
23	B	609	CLA	CHD-C4C	3.84	1.48	1.39
23	b	611	CLA	CHD-C4C	3.84	1.48	1.39
23	b	603	CLA	CHC-C4B	3.84	1.48	1.39
23	A	405[B]	CLA	CHD-C4C	3.84	1.48	1.39
32	L	101[A]	LHG	O8-C23	3.84	1.44	1.33
23	c	506	CLA	OBD-CAD	3.84	1.29	1.22
23	A	406[A]	CLA	C3D-C2D	3.84	1.49	1.39
23	C	513	CLA	CHC-C4B	3.84	1.48	1.39
35	c	519[A]	DGD	O1G-C1A	3.83	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	505	CLA	C3D-C2D	3.83	1.49	1.39
23	B	606	CLA	CHB-C1B	3.83	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	3.83	1.44	1.33
23	C	502	CLA	CHC-C4B	3.83	1.48	1.39
23	C	503	CLA	CHB-C1B	3.83	1.48	1.39
23	C	512	CLA	C3D-C2D	3.83	1.49	1.39
23	b	616	CLA	C3D-C2D	3.83	1.49	1.39
23	B	615	CLA	OBD-CAD	3.83	1.29	1.22
24	a	414[A]	PHO	O2A-CGA	3.83	1.44	1.33
23	b	610	CLA	CHD-C4C	3.83	1.48	1.39
23	b	613	CLA	CHC-C4B	3.82	1.48	1.39
35	C	518[B]	DGD	O2G-C1B	3.82	1.45	1.34
32	b	629[B]	LHG	O8-C23	3.82	1.44	1.33
23	C	511	CLA	C3D-C2D	3.82	1.49	1.39
23	B	614	CLA	CHC-C4B	3.82	1.48	1.39
23	B	610	CLA	CHB-C1B	3.82	1.48	1.39
23	C	506	CLA	CHD-C4C	3.82	1.48	1.39
24	a	414[B]	PHO	O2A-CGA	3.82	1.44	1.33
32	L	101[A]	LHG	O7-C7	3.82	1.45	1.34
23	B	610	CLA	CHD-C1D	3.82	1.45	1.38
32	L	101[B]	LHG	O7-C7	3.82	1.45	1.34
23	B	613	CLA	C3D-C2D	3.82	1.49	1.39
40	V	201	HEC	FE-NC	3.82	2.08	1.95
23	b	601	CLA	CHC-C4B	3.81	1.48	1.39
23	a	407	CLA	CHD-C4C	3.81	1.47	1.39
23	b	614	CLA	CHB-C1B	3.81	1.48	1.39
23	D	403	CLA	OBD-CAD	3.81	1.29	1.22
23	B	610	CLA	C1B-NB	-3.81	1.33	1.37
23	B	615	CLA	CHD-C4C	3.81	1.47	1.39
23	b	615	CLA	C1B-NB	-3.81	1.33	1.37
23	b	609	CLA	O2A-CGA	3.81	1.44	1.33
23	C	503	CLA	CHC-C4B	3.81	1.47	1.39
23	d	403[A]	CLA	CHD-C1D	3.81	1.45	1.38
32	b	629[B]	LHG	O7-C7	3.81	1.45	1.34
23	B	605	CLA	O2A-CGA	3.80	1.44	1.33
23	a	407	CLA	CHC-C4B	3.80	1.47	1.39
23	b	613	CLA	C3D-C2D	3.80	1.49	1.39
23	d	404	CLA	C3D-C2D	3.80	1.49	1.39
23	b	604	CLA	CHD-C1D	3.80	1.45	1.38
35	C	517[B]	DGD	O1G-C1A	3.80	1.44	1.33
23	d	403[B]	CLA	CHD-C4C	3.80	1.47	1.39
23	c	506	CLA	O2A-CGA	3.80	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	605	CLA	CHD-C4C	3.80	1.47	1.39
23	A	406[A]	CLA	O2A-CGA	3.80	1.44	1.33
23	b	614	CLA	CHD-C4C	3.80	1.47	1.39
23	d	402[B]	CLA	CHD-C4C	3.80	1.47	1.39
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	C	514	CLA	CHD-C4C	3.79	1.47	1.39
23	b	610	CLA	OBD-CAD	3.79	1.29	1.22
23	B	612	CLA	C4B-NB	-3.79	1.33	1.37
23	c	512	CLA	O2A-CGA	3.79	1.44	1.33
23	b	607	CLA	C3D-C2D	3.78	1.49	1.39
23	c	515	CLA	C3D-C2D	3.78	1.49	1.39
23	A	405[A]	CLA	CHB-C1B	3.78	1.47	1.39
23	B	602	CLA	C3D-C2D	3.78	1.49	1.39
23	b	608	CLA	CHB-C1B	3.78	1.47	1.39
23	C	511	CLA	CHB-C1B	3.78	1.47	1.39
23	c	511	CLA	CHD-C4C	3.78	1.47	1.39
23	c	512	CLA	CHD-C4C	3.77	1.47	1.39
23	b	609	CLA	OBD-CAD	3.77	1.29	1.22
23	C	511	CLA	CHD-C1D	3.77	1.45	1.38
23	d	402[A]	CLA	OBD-CAD	3.77	1.29	1.22
23	B	603	CLA	C3D-C2D	3.77	1.49	1.39
23	B	612	CLA	O2A-CGA	3.77	1.44	1.33
23	B	614	CLA	O2A-CGA	3.76	1.44	1.33
23	C	514	CLA	OBD-CAD	3.76	1.29	1.22
23	C	507	CLA	CHB-C1B	3.76	1.47	1.39
23	a	407	CLA	C1D-ND	3.76	1.42	1.37
23	d	404	CLA	CHC-C4B	3.76	1.47	1.39
23	b	614	CLA	C3D-C2D	3.76	1.49	1.39
23	c	508	CLA	OBD-CAD	3.76	1.29	1.22
23	b	614	CLA	CHC-C4B	3.76	1.47	1.39
23	B	601	CLA	CHD-C4C	3.76	1.47	1.39
26	A	410[B]	SQD	O47-C7	3.76	1.44	1.34
23	A	406[B]	CLA	CHC-C4B	3.75	1.47	1.39
23	a	405[A]	CLA	CHB-C1B	3.75	1.47	1.39
23	B	607	CLA	CHD-C4C	3.75	1.47	1.39
23	a	405[B]	CLA	CHD-C4C	3.75	1.47	1.39
23	B	603	CLA	CHD-C4C	3.75	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.75	1.49	1.39
23	A	405[B]	CLA	CHB-C1B	3.75	1.47	1.39
23	c	504	CLA	CHC-C4B	3.75	1.47	1.39
32	d	414[A]	LHG	O8-C23	3.75	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	H	101	DGD	O1G-C1A	3.74	1.44	1.33
23	b	607	CLA	C1D-ND	3.74	1.42	1.37
23	b	612	CLA	OBD-CAD	3.74	1.28	1.22
23	B	611	CLA	C3D-C2D	3.74	1.49	1.39
23	A	406[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	c	511	CLA	OBD-CAD	3.74	1.28	1.22
23	C	504	CLA	CHB-C1B	3.73	1.47	1.39
23	c	508	CLA	CHC-C4B	3.73	1.47	1.39
23	c	503	CLA	CHB-C1B	3.73	1.47	1.39
23	A	404[A]	CLA	CHD-C4C	3.73	1.47	1.39
23	b	606	CLA	CHD-C1D	3.73	1.45	1.38
35	h	102	DGD	O1G-C1A	3.73	1.44	1.33
23	B	607	CLA	CHD-C1D	3.73	1.45	1.38
23	C	502	CLA	CHD-C4C	3.72	1.47	1.39
32	A	419[B]	LHG	O8-C23	3.72	1.44	1.33
23	c	515	CLA	CHB-C1B	3.72	1.47	1.39
23	B	612	CLA	C1D-ND	3.72	1.42	1.37
23	B	609	CLA	CHC-C4B	3.72	1.47	1.39
23	c	513	CLA	CHC-C4B	3.72	1.47	1.39
23	D	402[A]	CLA	C1B-NB	-3.72	1.33	1.37
32	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	C	512	CLA	CHC-C4B	3.72	1.47	1.39
23	c	509	CLA	C3D-C2D	3.71	1.49	1.39
35	C	518[A]	DGD	O1G-C1A	3.71	1.44	1.33
23	C	514	CLA	CHB-C1B	3.71	1.47	1.39
23	b	601	CLA	OBD-CAD	3.71	1.28	1.22
23	B	606	CLA	C3D-C2D	3.71	1.49	1.39
23	d	402[B]	CLA	C1B-NB	-3.71	1.33	1.37
23	C	505	CLA	CHD-C4C	3.70	1.47	1.39
23	B	613	CLA	CHB-C1B	3.70	1.47	1.39
23	c	509	CLA	OBD-CAD	3.70	1.28	1.22
23	b	610	CLA	C1B-NB	-3.70	1.33	1.37
23	a	404[A]	CLA	CHB-C1B	3.69	1.47	1.39
23	b	615	CLA	OBD-CAD	3.69	1.28	1.22
23	C	507	CLA	OBD-CAD	3.69	1.28	1.22
23	B	607	CLA	O2A-CGA	3.69	1.44	1.33
23	B	605	CLA	CHB-C1B	3.69	1.47	1.39
23	A	408	CLA	C3D-C2D	3.69	1.49	1.39
23	a	404[B]	CLA	O2A-CGA	3.69	1.44	1.33
23	c	511	CLA	C3D-C2D	3.69	1.49	1.39
23	b	602	CLA	O2A-CGA	3.68	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	D	406[B]	LHG	O8-C23	3.68	1.44	1.33
23	B	615	CLA	C3D-C2D	3.68	1.49	1.39
23	D	403	CLA	CHD-C4C	3.68	1.47	1.39
23	c	503	CLA	CHC-C4B	3.68	1.47	1.39
23	C	508	CLA	CHB-C1B	3.68	1.47	1.39
23	b	616	CLA	CHC-C4B	3.68	1.47	1.39
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	b	606	CLA	C3D-C2D	3.68	1.49	1.39
23	a	405[A]	CLA	OBD-CAD	3.68	1.28	1.22
23	B	614	CLA	CHD-C1D	3.68	1.45	1.38
23	B	601	CLA	CHB-C1B	3.68	1.47	1.39
23	b	604	CLA	CHB-C1B	3.68	1.47	1.39
23	b	602	CLA	C3D-C2D	3.68	1.49	1.39
23	A	404[A]	CLA	C4B-NB	-3.68	1.33	1.37
23	c	507	CLA	O2A-CGA	3.68	1.44	1.33
32	D	406[B]	LHG	O7-C7	3.67	1.44	1.34
23	B	604	CLA	O2A-CGA	3.67	1.44	1.33
23	b	605	CLA	CHB-C1B	3.67	1.47	1.39
23	c	509	CLA	CHB-C1B	3.67	1.47	1.39
23	C	502	CLA	C3D-C2D	3.67	1.49	1.39
23	D	402[B]	CLA	CHB-C1B	3.67	1.47	1.39
23	b	606	CLA	CHB-C1B	3.67	1.47	1.39
23	A	406[A]	CLA	C1B-NB	-3.67	1.33	1.37
23	d	404	CLA	CHB-C1B	3.67	1.47	1.39
23	A	406[A]	CLA	CHD-C4C	3.67	1.47	1.39
23	b	615	CLA	CHB-C1B	3.66	1.47	1.39
23	b	605	CLA	CHD-C1D	3.66	1.45	1.38
23	b	612	CLA	O2A-CGA	3.66	1.44	1.33
23	B	602	CLA	O2A-CGA	3.66	1.44	1.33
23	a	404[A]	CLA	C3D-C2D	3.66	1.49	1.39
23	d	403[B]	CLA	C3D-C2D	3.66	1.49	1.39
32	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	c	507	CLA	C3D-C2D	3.66	1.49	1.39
23	b	613	CLA	O2A-CGA	3.65	1.44	1.33
23	C	506	CLA	O2A-CGA	3.65	1.44	1.33
23	b	604	CLA	O2A-CGA	3.65	1.44	1.33
23	a	407	CLA	CHD-C1D	3.64	1.45	1.38
24	A	407[A]	PHO	O2A-CGA	3.64	1.44	1.33
32	d	407[B]	LHG	O8-C23	3.64	1.44	1.33
23	a	404[B]	CLA	CHB-C1B	3.64	1.47	1.39
23	C	502	CLA	CHB-C1B	3.64	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	614	CLA	O2A-CGA	3.64	1.44	1.33
23	B	604	CLA	OBD-CAD	3.64	1.28	1.22
23	C	503	CLA	CHD-C4C	3.64	1.47	1.39
23	A	404[A]	CLA	C3D-C2D	3.63	1.49	1.39
23	C	507	CLA	C1B-NB	-3.63	1.33	1.37
23	c	510	CLA	CHB-C1B	3.63	1.47	1.39
23	b	610	CLA	CHC-C4B	3.63	1.47	1.39
23	a	407	CLA	CHB-C1B	3.63	1.47	1.39
23	B	613	CLA	CHD-C1D	3.63	1.45	1.38
23	C	505	CLA	O2A-CGA	3.63	1.43	1.33
33	m	101	LMG	O7-C10	3.63	1.44	1.34
23	B	611	CLA	C1C-C2C	3.63	1.51	1.44
35	C	519	DGD	O2G-C1B	3.62	1.44	1.34
23	C	508	CLA	C3D-C2D	3.62	1.49	1.39
23	b	605	CLA	C3D-C2D	3.62	1.49	1.39
23	B	608	CLA	CHB-C1B	3.62	1.47	1.39
23	C	512	CLA	CHD-C4C	3.62	1.47	1.39
23	D	403	CLA	O2A-CGA	3.62	1.43	1.33
35	c	518[A]	DGD	O1G-C1A	3.62	1.43	1.33
23	B	609	CLA	C1B-NB	-3.62	1.33	1.37
23	d	402[A]	CLA	CHD-C4C	3.62	1.47	1.39
32	b	629[A]	LHG	O7-C7	3.62	1.44	1.34
23	a	405[B]	CLA	CHC-C4B	3.62	1.47	1.39
23	B	616	CLA	CHD-C4C	3.62	1.47	1.39
23	a	404[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	c	504	CLA	OBD-CAD	3.61	1.28	1.22
23	c	508	CLA	CHB-C1B	3.60	1.47	1.39
23	b	610	CLA	C3D-C2D	3.60	1.49	1.39
23	b	608	CLA	C4B-NB	-3.60	1.33	1.37
23	b	615	CLA	CHC-C4B	3.60	1.47	1.39
32	D	406[A]	LHG	O7-C7	3.60	1.44	1.34
23	b	609	CLA	C3D-C2D	3.60	1.48	1.39
23	C	507	CLA	C3D-C2D	3.59	1.48	1.39
23	B	601	CLA	C3D-C2D	3.59	1.48	1.39
23	c	506	CLA	CHD-C4C	3.59	1.47	1.39
23	A	404[B]	CLA	O2A-CGA	3.59	1.43	1.33
23	B	616	CLA	CHD-C1D	3.59	1.45	1.38
23	A	408	CLA	CHD-C4C	3.59	1.47	1.39
23	c	514	CLA	CHB-C1B	3.58	1.47	1.39
23	B	603	CLA	OBD-CAD	3.58	1.28	1.22
23	b	616	CLA	OBD-CAD	3.58	1.28	1.22
23	a	405[A]	CLA	CHD-C4C	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	606	CLA	OBD-CAD	3.58	1.28	1.22
23	b	605	CLA	C1B-NB	-3.58	1.33	1.37
23	B	601	CLA	OBD-CAD	3.58	1.28	1.22
23	c	510	CLA	CHC-C4B	3.58	1.47	1.39
23	b	604	CLA	OBD-CAD	3.57	1.28	1.22
23	b	607	CLA	C1B-C2B	3.57	1.51	1.43
23	b	604	CLA	C1B-NB	-3.57	1.33	1.37
34	b	622	HTG	C1'-S1	-3.57	1.76	1.81
23	d	403[A]	CLA	CHD-C4C	3.57	1.47	1.39
23	B	616	CLA	CHC-C4B	3.57	1.47	1.39
23	B	605	CLA	CHD-C1D	3.57	1.45	1.38
23	B	607	CLA	C1D-ND	3.56	1.42	1.37
23	c	513	CLA	C3D-C2D	3.56	1.48	1.39
35	H	101	DGD	O2G-C1B	3.56	1.44	1.34
23	C	506	CLA	C3D-C2D	3.56	1.48	1.39
23	b	608	CLA	C1B-NB	-3.56	1.33	1.37
23	d	402[B]	CLA	OBD-CAD	3.56	1.28	1.22
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	509	CLA	CHC-C4B	3.56	1.47	1.39
23	A	404[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	B	613	CLA	O2A-CGA	3.55	1.43	1.33
23	C	504	CLA	C3D-C2D	3.55	1.48	1.39
35	C	517[A]	DGD	O1G-C1A	3.55	1.43	1.33
23	a	405[B]	CLA	CHB-C1B	3.55	1.47	1.39
23	b	601	CLA	CHB-C1B	3.55	1.47	1.39
23	d	403[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	b	603	CLA	CHD-C4C	3.55	1.47	1.39
23	b	606	CLA	CHD-C4C	3.55	1.47	1.39
23	d	403[B]	CLA	OBD-CAD	3.55	1.28	1.22
23	B	608	CLA	CHD-C4C	3.54	1.47	1.39
23	b	613	CLA	CHD-C4C	3.54	1.47	1.39
23	a	405[A]	CLA	CHD-C1D	3.54	1.45	1.38
23	b	611	CLA	CHC-C4B	3.54	1.47	1.39
35	c	519[A]	DGD	O2G-C1B	3.53	1.44	1.34
23	B	612	CLA	CHD-C4C	3.53	1.47	1.39
23	b	602	CLA	OBD-CAD	3.53	1.28	1.22
23	A	404[B]	CLA	C4B-NB	-3.53	1.33	1.37
32	d	414[B]	LHG	O7-C7	3.53	1.44	1.34
32	d	407[A]	LHG	O8-C23	3.53	1.43	1.33
23	A	404[B]	CLA	CHB-C1B	3.53	1.47	1.39
32	A	419[B]	LHG	O7-C7	3.53	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHD-C4C	3.53	1.47	1.39
23	b	602	CLA	C1B-NB	-3.53	1.33	1.37
32	D	406[A]	LHG	O8-C23	3.53	1.43	1.33
23	C	510	CLA	CHB-C1B	3.53	1.47	1.39
23	c	514	CLA	OBD-CAD	3.53	1.28	1.22
23	B	603	CLA	CHD-C1D	3.52	1.45	1.38
32	A	419[A]	LHG	O8-C23	3.52	1.43	1.33
23	b	602	CLA	C3B-C4B	3.52	1.51	1.42
23	A	406[B]	CLA	CHB-C1B	3.52	1.47	1.39
23	c	515	CLA	CHC-C4B	3.51	1.47	1.39
23	b	608	CLA	CHD-C4C	3.51	1.47	1.39
23	b	605	CLA	CHC-C4B	3.51	1.47	1.39
23	c	504	CLA	CHB-C1B	3.51	1.47	1.39
23	c	505	CLA	C3D-C2D	3.50	1.48	1.39
32	d	414[A]	LHG	O7-C7	3.50	1.44	1.34
38	E	102	HEM	C1B-NB	-3.50	1.34	1.40
32	A	419[A]	LHG	O7-C7	3.49	1.44	1.34
35	c	520	DGD	O2G-C1B	3.49	1.44	1.34
23	B	610	CLA	CHC-C4B	3.49	1.47	1.39
23	C	513	CLA	OBD-CAD	3.49	1.28	1.22
32	b	629[A]	LHG	O8-C23	3.49	1.43	1.33
23	D	402[B]	CLA	C3D-C2D	3.49	1.48	1.39
23	B	604	CLA	CHC-C4B	3.49	1.47	1.39
23	b	612	CLA	CHC-C4B	3.49	1.47	1.39
23	B	611	CLA	CHD-C4C	3.48	1.47	1.39
23	b	613	CLA	C1B-NB	-3.48	1.33	1.37
23	B	610	CLA	O2A-CGA	3.48	1.43	1.33
23	d	402[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	b	607	CLA	CHC-C4B	3.48	1.47	1.39
23	b	609	CLA	CHC-C4B	3.48	1.47	1.39
23	b	609	CLA	CHD-C4C	3.47	1.47	1.39
23	b	603	CLA	C3D-C2D	3.47	1.48	1.39
23	b	606	CLA	CHC-C4B	3.47	1.47	1.39
23	c	506	CLA	CHB-C1B	3.47	1.47	1.39
33	D	411	LMG	O7-C10	3.47	1.44	1.34
23	d	402[A]	CLA	CHC-C4B	3.47	1.47	1.39
23	A	405[B]	CLA	C1B-NB	-3.47	1.33	1.37
23	B	602	CLA	C1C-C2C	3.46	1.51	1.44
23	D	402[B]	CLA	CHC-C4B	3.46	1.47	1.39
23	c	515	CLA	C1B-NB	-3.46	1.33	1.37
23	B	612	CLA	CHC-C4B	3.46	1.47	1.39
23	b	616	CLA	CHD-C4C	3.45	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C3B-C4B	3.45	1.50	1.42
23	b	607	CLA	CHD-C4C	3.45	1.47	1.39
23	d	403[B]	CLA	CHC-C4B	3.45	1.47	1.39
23	c	508	CLA	C1B-NB	-3.44	1.33	1.37
23	b	614	CLA	OBD-CAD	3.44	1.28	1.22
23	C	507	CLA	C4B-NB	-3.44	1.33	1.37
23	C	513	CLA	CHB-C1B	3.44	1.47	1.39
23	C	502	CLA	C1B-NB	-3.43	1.33	1.37
23	a	404[B]	CLA	C3D-C2D	3.43	1.48	1.39
23	a	407	CLA	C3B-C4B	3.43	1.50	1.42
23	D	402[A]	CLA	C3D-C2D	3.43	1.48	1.39
23	A	406[A]	CLA	CHB-C1B	3.43	1.47	1.39
23	b	612	CLA	C1B-NB	-3.43	1.33	1.37
23	c	512	CLA	CHD-C1D	3.43	1.45	1.38
23	c	506	CLA	CHC-C4B	3.42	1.47	1.39
23	d	403[A]	CLA	CHC-C4B	3.42	1.47	1.39
23	B	608	CLA	O2A-CGA	3.42	1.43	1.33
23	c	512	CLA	OBD-CAD	3.42	1.28	1.22
23	C	510	CLA	CHC-C4B	3.41	1.47	1.39
23	d	403[A]	CLA	OBD-CAD	3.41	1.28	1.22
23	C	508	CLA	CHD-C4C	3.41	1.47	1.39
23	b	603	CLA	OBD-CAD	3.41	1.28	1.22
23	A	405[B]	CLA	CHC-C4B	3.41	1.47	1.39
23	c	511	CLA	C4B-NB	-3.41	1.33	1.37
23	C	511	CLA	OBD-CAD	3.41	1.28	1.22
23	c	509	CLA	C1B-NB	-3.40	1.33	1.37
23	C	506	CLA	C1B-NB	-3.40	1.33	1.37
23	B	606	CLA	CHD-C4C	3.39	1.47	1.39
23	B	611	CLA	C3B-C4B	3.39	1.50	1.42
23	b	602	CLA	C1C-C2C	3.39	1.51	1.44
24	a	406[A]	PHO	O2A-CGA	3.39	1.43	1.33
23	C	505	CLA	C1B-NB	-3.39	1.33	1.37
23	c	507	CLA	OBD-CAD	3.39	1.28	1.22
23	b	616	CLA	CHB-C1B	3.39	1.47	1.39
23	C	504	CLA	OBD-CAD	3.38	1.28	1.22
23	B	604	CLA	C3D-C2D	3.38	1.48	1.39
23	b	603	CLA	CHB-C1B	3.38	1.47	1.39
34	B	624	HTG	C1'-S1	-3.37	1.77	1.81
23	A	408	CLA	OBD-CAD	3.37	1.28	1.22
23	B	613	CLA	OBD-CAD	3.37	1.28	1.22
23	A	404[B]	CLA	C1B-NB	-3.37	1.33	1.37
23	a	404[A]	CLA	CHC-C4B	3.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[B]	CLA	OBD-CAD	3.36	1.28	1.22
23	A	408	CLA	C1B-NB	-3.36	1.33	1.37
23	d	402[A]	CLA	C1B-NB	-3.36	1.33	1.37
23	C	509	CLA	CHD-C4C	3.36	1.46	1.39
23	b	603	CLA	O2A-CGA	3.36	1.43	1.33
23	A	406[B]	CLA	C1B-NB	-3.36	1.33	1.37
23	B	614	CLA	C3D-C2D	3.36	1.48	1.39
23	b	612	CLA	CHD-C4C	3.36	1.46	1.39
23	D	402[B]	CLA	OBD-CAD	3.35	1.28	1.22
23	b	602	CLA	CHB-C1B	3.35	1.46	1.39
23	d	402[B]	CLA	CHB-C1B	3.35	1.46	1.39
23	A	405[B]	CLA	OBD-CAD	3.34	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.34	1.28	1.22
23	d	404	CLA	CHD-C4C	3.34	1.46	1.39
23	D	402[A]	CLA	CHC-C4B	3.33	1.46	1.39
23	C	506	CLA	OBD-CAD	3.33	1.28	1.22
23	A	406[B]	CLA	C3B-C4B	3.33	1.50	1.42
23	c	515	CLA	OBD-CAD	3.32	1.28	1.22
23	c	515	CLA	C4B-NB	-3.32	1.33	1.37
23	C	514	CLA	C1B-NB	-3.32	1.33	1.37
23	a	404[B]	CLA	C4B-NB	-3.32	1.33	1.37
23	d	402[B]	CLA	CHC-C4B	3.32	1.46	1.39
23	b	609	CLA	C1B-NB	-3.30	1.33	1.37
23	C	503	CLA	OBD-CAD	3.30	1.28	1.22
23	a	404[A]	CLA	C1B-NB	-3.30	1.33	1.37
33	D	411	LMG	O8-C28	3.29	1.42	1.33
23	B	609	CLA	OBD-CAD	3.29	1.28	1.22
23	B	614	CLA	OBD-CAD	3.28	1.28	1.22
23	D	403	CLA	C3B-C4B	3.28	1.50	1.42
24	a	406[B]	PHO	O2A-CGA	3.28	1.42	1.33
23	d	404	CLA	OBD-CAD	3.28	1.28	1.22
23	b	614	CLA	C1B-NB	-3.28	1.33	1.37
23	a	404[B]	CLA	CHC-C4B	3.28	1.46	1.39
38	f	101	HEM	C4D-ND	-3.28	1.34	1.40
23	A	408	CLA	CHC-C4B	3.28	1.46	1.39
23	d	403[A]	CLA	C1D-ND	3.27	1.41	1.37
23	B	602	CLA	OBD-CAD	3.27	1.28	1.22
23	c	505	CLA	C3B-C4B	3.27	1.50	1.42
23	C	514	CLA	C4B-NB	-3.27	1.33	1.37
34	c	523	HTG	C1'-S1	-3.27	1.77	1.81
23	B	601	CLA	C3B-C4B	3.27	1.50	1.42
23	c	507	CLA	C1B-NB	-3.27	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	608	CLA	C1B-NB	-3.27	1.33	1.37
23	D	402[A]	CLA	OBD-CAD	3.26	1.28	1.22
23	B	608	CLA	CHC-C4B	3.26	1.46	1.39
23	C	508	CLA	OBD-CAD	3.26	1.28	1.22
23	B	603	CLA	C1B-NB	-3.26	1.33	1.37
40	v	201	HEC	FE-NB	3.25	2.04	1.94
23	b	607	CLA	OBD-CAD	3.25	1.28	1.22
23	b	605	CLA	OBD-CAD	3.25	1.28	1.22
23	b	612	CLA	C4B-NB	-3.24	1.33	1.37
38	f	101	HEM	C1B-NB	-3.24	1.34	1.40
23	a	405[A]	CLA	CHC-C4B	3.24	1.46	1.39
23	D	402[B]	CLA	C4B-NB	-3.24	1.33	1.37
23	B	607	CLA	C3D-C2D	3.23	1.48	1.39
23	C	507	CLA	CHC-C4B	3.23	1.46	1.39
23	d	403[B]	CLA	C1B-NB	-3.22	1.33	1.37
23	C	505	CLA	C4D-CHA	3.22	1.49	1.38
23	C	503	CLA	C4B-NB	-3.22	1.33	1.37
23	b	605	CLA	O2A-CGA	3.22	1.42	1.33
23	b	608	CLA	CHC-C4B	3.22	1.46	1.39
23	D	403	CLA	C1B-NB	-3.22	1.33	1.37
23	C	505	CLA	OBD-CAD	3.21	1.28	1.22
23	b	616	CLA	C1B-NB	-3.20	1.33	1.37
23	C	502	CLA	C3B-C4B	3.20	1.50	1.42
23	B	615	CLA	CHC-C4B	3.20	1.46	1.39
23	C	514	CLA	CHC-C4B	3.20	1.46	1.39
23	A	405[A]	CLA	C3B-C4B	3.20	1.50	1.42
23	C	511	CLA	CHC-C4B	3.20	1.46	1.39
23	B	609	CLA	CHB-C1B	3.20	1.46	1.39
23	A	404[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	c	503	CLA	OBD-CAD	3.18	1.28	1.22
23	b	611	CLA	C1B-NB	-3.18	1.33	1.37
23	B	616	CLA	C1B-NB	-3.18	1.33	1.37
23	c	506	CLA	C1B-NB	-3.17	1.33	1.37
34	b	625	HTG	C1'-S1	-3.17	1.77	1.81
23	D	402[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	a	404[A]	CLA	C4B-NB	-3.17	1.33	1.37
23	B	605	CLA	C3B-C4B	3.17	1.50	1.42
23	a	404[B]	CLA	C1B-NB	-3.17	1.33	1.37
23	C	508	CLA	C4B-NB	-3.16	1.33	1.37
23	b	612	CLA	C1B-C2B	3.16	1.50	1.43
23	C	509	CLA	C4B-NB	-3.16	1.33	1.37
23	A	404[A]	CLA	CHC-C4B	3.15	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	C1B-NB	-3.15	1.33	1.37
23	b	601	CLA	C1B-NB	-3.15	1.33	1.37
23	b	610	CLA	O2A-CGA	3.15	1.42	1.33
23	c	505	CLA	OBD-CAD	3.15	1.27	1.22
23	a	407	CLA	C1B-C2B	3.15	1.50	1.43
23	D	403	CLA	C1C-C2C	3.15	1.50	1.44
24	A	416[B]	PHO	CHA-CBD	-3.15	1.47	1.51
23	B	616	CLA	C4B-NB	-3.15	1.33	1.37
38	E	102	HEM	C4D-ND	-3.14	1.34	1.40
23	C	504	CLA	C3B-C4B	3.14	1.50	1.42
34	D	410	HTG	C1'-S1	-3.14	1.77	1.81
34	d	411	HTG	C1'-S1	-3.14	1.77	1.81
23	B	610	CLA	C3B-C4B	3.13	1.50	1.42
23	c	505	CLA	C1C-C2C	3.13	1.50	1.44
23	a	407	CLA	C3D-C2D	3.13	1.47	1.39
34	b	625	HTG	C1-S1	-3.13	1.75	1.80
23	B	612	CLA	C3D-C2D	3.13	1.47	1.39
23	b	614	CLA	C1B-C2B	3.13	1.50	1.43
23	A	406[A]	CLA	C3B-C4B	3.13	1.50	1.42
23	B	615	CLA	C1B-NB	-3.12	1.33	1.37
23	A	405[A]	CLA	OBD-CAD	3.12	1.27	1.22
23	A	404[B]	CLA	CHC-C4B	3.12	1.46	1.39
23	c	505	CLA	C1B-NB	-3.11	1.34	1.37
23	B	606	CLA	OBD-CAD	3.11	1.27	1.22
23	B	603	CLA	C4B-NB	-3.11	1.34	1.37
23	C	506	CLA	C1B-C2B	3.11	1.50	1.43
23	b	606	CLA	C1B-NB	-3.10	1.34	1.37
23	B	613	CLA	CHD-C4C	3.10	1.46	1.39
24	A	416[A]	PHO	CHA-CBD	-3.10	1.47	1.51
23	b	607	CLA	O2A-CGA	3.10	1.42	1.33
23	b	609	CLA	C3B-C4B	3.10	1.50	1.42
23	b	616	CLA	C3B-C4B	3.09	1.50	1.42
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	513	CLA	C3B-C4B	3.09	1.50	1.42
23	D	402[B]	CLA	C1B-NB	-3.09	1.34	1.37
23	C	505	CLA	CHC-C4B	3.08	1.46	1.39
23	c	507	CLA	C3B-C4B	3.08	1.50	1.42
23	A	408	CLA	CHB-C1B	3.08	1.46	1.39
23	B	602	CLA	C1B-NB	-3.07	1.34	1.37
23	b	614	CLA	C4B-NB	-3.07	1.34	1.37
23	a	404[A]	CLA	O2A-CGA	3.07	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	v	201	HEC	FE-NC	3.07	2.05	1.95
23	C	507	CLA	C4C-C3C	3.07	1.50	1.45
23	c	513	CLA	C1B-C2B	3.07	1.50	1.43
23	c	506	CLA	C1B-C2B	3.06	1.50	1.43
23	C	506	CLA	C3B-C4B	3.05	1.49	1.42
23	C	511	CLA	C4B-NB	-3.05	1.34	1.37
23	d	403[B]	CLA	C4B-NB	-3.05	1.34	1.37
23	b	607	CLA	C1C-C2C	3.05	1.50	1.44
23	B	608	CLA	OBD-CAD	3.05	1.27	1.22
23	a	405[A]	CLA	C3B-C4B	3.05	1.49	1.42
23	b	611	CLA	OBD-CAD	3.05	1.27	1.22
23	C	512	CLA	C1C-C2C	3.03	1.50	1.44
23	a	405[B]	CLA	C1B-NB	-3.03	1.34	1.37
23	B	605	CLA	C1B-C2B	3.03	1.50	1.43
23	B	613	CLA	CHC-C4B	3.03	1.46	1.39
23	B	614	CLA	C1B-NB	-3.03	1.34	1.37
23	B	604	CLA	C1B-C2B	3.03	1.50	1.43
23	b	613	CLA	C4B-NB	-3.03	1.34	1.37
23	c	504	CLA	C4B-NB	-3.02	1.34	1.37
23	b	611	CLA	C1B-C2B	3.02	1.50	1.43
23	c	506	CLA	C4B-NB	-3.02	1.34	1.37
23	B	615	CLA	C1B-C2B	3.01	1.50	1.43
23	b	601	CLA	C3B-C4B	3.01	1.49	1.42
23	c	508	CLA	C4B-NB	-3.01	1.34	1.37
23	c	514	CLA	C3B-C4B	3.01	1.49	1.42
23	c	506	CLA	C4C-C3C	3.00	1.50	1.45
23	d	403[B]	CLA	C1B-C2B	3.00	1.50	1.43
23	c	511	CLA	CHC-C4B	3.00	1.46	1.39
23	c	512	CLA	C1B-NB	-3.00	1.34	1.37
23	c	513	CLA	C4B-NB	-3.00	1.34	1.37
23	B	607	CLA	C4D-CHA	3.00	1.49	1.38
23	a	405[B]	CLA	C4B-NB	-2.99	1.34	1.37
23	d	403[A]	CLA	C4B-NB	-2.99	1.34	1.37
23	c	515	CLA	C3B-C4B	2.98	1.49	1.42
23	B	616	CLA	C1B-C2B	2.97	1.50	1.43
23	c	514	CLA	C1B-NB	-2.97	1.34	1.37
23	c	507	CLA	C1B-C2B	2.97	1.50	1.43
23	B	604	CLA	C1B-NB	-2.96	1.34	1.37
23	B	605	CLA	OBD-CAD	2.96	1.27	1.22
23	a	405[B]	CLA	C3B-C4B	2.96	1.49	1.42
23	A	404[A]	CLA	C4C-C3C	2.96	1.50	1.45
23	c	510	CLA	C3B-C4B	2.96	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	402[A]	CLA	C3B-C4B	2.96	1.49	1.42
23	B	601	CLA	C4B-NB	-2.95	1.34	1.37
23	B	613	CLA	C1B-C2B	2.95	1.50	1.43
23	C	511	CLA	C4C-C3C	2.95	1.50	1.45
23	c	505	CLA	C1B-C2B	2.94	1.50	1.43
23	b	604	CLA	C4D-CHA	2.94	1.48	1.38
23	d	404	CLA	C3B-C4B	2.94	1.49	1.42
23	C	508	CLA	C1B-NB	-2.94	1.34	1.37
23	B	602	CLA	C1B-C2B	2.94	1.50	1.43
23	a	407	CLA	C1B-NB	-2.94	1.34	1.37
23	B	606	CLA	C3B-C4B	2.94	1.49	1.42
23	b	604	CLA	C1B-C2B	2.93	1.50	1.43
23	b	614	CLA	C3B-C4B	2.93	1.49	1.42
23	b	612	CLA	C1C-C2C	2.93	1.50	1.44
23	a	407	CLA	OBD-CAD	2.93	1.27	1.22
23	B	604	CLA	C4D-CHA	2.92	1.48	1.38
23	B	605	CLA	C1B-NB	-2.92	1.34	1.37
23	c	509	CLA	C1C-C2C	2.92	1.50	1.44
23	C	512	CLA	OBD-CAD	2.92	1.27	1.22
23	b	612	CLA	C3B-C4B	2.92	1.49	1.42
23	b	603	CLA	C1B-C2B	2.91	1.50	1.43
23	B	604	CLA	C3B-C4B	2.91	1.49	1.42
23	B	607	CLA	C4B-NB	-2.91	1.34	1.37
23	A	408	CLA	C1B-C2B	2.91	1.50	1.43
23	B	616	CLA	OBD-CAD	2.90	1.27	1.22
34	C	522	HTG	C1'-S1	-2.90	1.77	1.81
23	B	612	CLA	C4D-CHA	2.89	1.48	1.38
23	C	512	CLA	C4D-CHA	2.89	1.48	1.38
23	c	503	CLA	C3B-C4B	2.89	1.49	1.42
23	B	607	CLA	C1C-C2C	2.89	1.50	1.44
23	B	615	CLA	C3B-C4B	2.88	1.49	1.42
23	C	511	CLA	C1B-NB	-2.88	1.34	1.37
23	C	502	CLA	C1C-C2C	2.88	1.50	1.44
23	b	603	CLA	C3B-C4B	2.88	1.49	1.42
23	c	503	CLA	C4B-NB	-2.88	1.34	1.37
27	A	418	GOL	O2-C2	-2.88	1.34	1.43
23	b	610	CLA	C3B-C4B	2.87	1.49	1.42
23	C	505	CLA	C1B-C2B	2.87	1.50	1.43
23	A	406[A]	CLA	C4B-NB	-2.87	1.34	1.37
23	b	613	CLA	OBD-CAD	2.86	1.27	1.22
23	B	607	CLA	C1B-C2B	2.86	1.50	1.43
23	d	404	CLA	C4B-NB	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	510	CLA	C1B-NB	-2.85	1.34	1.37
23	a	407	CLA	C1C-C2C	2.85	1.50	1.44
23	c	509	CLA	C4B-NB	-2.84	1.34	1.37
23	C	511	CLA	C3B-C4B	2.84	1.49	1.42
23	d	402[B]	CLA	C3B-C4B	2.84	1.49	1.42
23	A	405[B]	CLA	C3B-C4B	2.84	1.49	1.42
23	B	601	CLA	C1C-C2C	2.83	1.50	1.44
23	b	616	CLA	C1C-C2C	2.83	1.50	1.44
23	D	402[A]	CLA	C1B-C2B	2.83	1.49	1.43
24	A	407[A]	PHO	CBD-CGD	-2.83	1.48	1.52
23	c	515	CLA	C1C-C2C	2.83	1.50	1.44
23	B	608	CLA	C4B-NB	-2.83	1.34	1.37
23	D	403	CLA	C1B-C2B	2.82	1.49	1.43
23	C	503	CLA	C1B-C2B	2.82	1.49	1.43
23	d	402[B]	CLA	C1B-C2B	2.81	1.49	1.43
23	b	613	CLA	C4D-CHA	2.81	1.48	1.38
23	c	503	CLA	C1B-NB	-2.81	1.34	1.37
23	d	404	CLA	C1B-NB	-2.81	1.34	1.37
23	B	608	CLA	C4D-CHA	2.80	1.48	1.38
23	c	506	CLA	C1C-C2C	2.80	1.50	1.44
23	c	510	CLA	C1B-C2B	2.80	1.49	1.43
23	C	506	CLA	C4D-CHA	2.79	1.48	1.38
23	a	407	CLA	C4B-NB	-2.79	1.34	1.37
23	c	510	CLA	C4C-C3C	2.79	1.49	1.45
23	C	504	CLA	C1B-NB	-2.79	1.34	1.37
23	B	611	CLA	MG-NB	2.79	2.11	2.05
35	H	101	DGD	O5D-C1E	2.78	1.44	1.40
23	b	616	CLA	C1B-C2B	2.77	1.49	1.43
23	d	403[B]	CLA	C4C-C3C	2.77	1.49	1.45
29	A	414[B]	PL9	C6-C5	2.77	1.49	1.35
23	A	404[B]	CLA	C1B-C2B	2.77	1.49	1.43
23	A	406[B]	CLA	C4B-NB	-2.77	1.34	1.37
23	b	601	CLA	C4B-NB	-2.76	1.34	1.37
29	A	414[A]	PL9	C6-C5	2.76	1.49	1.35
23	c	512	CLA	C3B-C4B	2.76	1.49	1.42
23	C	503	CLA	C1C-C2C	2.76	1.49	1.44
23	B	616	CLA	C3B-C4B	2.76	1.49	1.42
26	a	409[B]	SQD	C6-S	-2.76	1.67	1.77
23	C	509	CLA	C3B-C2B	2.76	1.50	1.41
23	C	503	CLA	C3B-C4B	2.76	1.49	1.42
23	c	512	CLA	C1B-C2B	2.75	1.49	1.43
23	c	505	CLA	C4B-NB	-2.75	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	412[A]	PL9	C6-C5	2.75	1.49	1.35
23	B	608	CLA	C1B-C2B	2.75	1.49	1.43
23	C	509	CLA	C4D-CHA	2.75	1.48	1.38
23	A	404[A]	CLA	C1B-C2B	2.75	1.49	1.43
23	C	508	CLA	C1C-C2C	2.75	1.49	1.44
23	C	513	CLA	C4D-CHA	2.75	1.48	1.38
23	a	405[B]	CLA	C1C-C2C	2.75	1.49	1.44
23	C	506	CLA	C1C-C2C	2.75	1.49	1.44
23	b	606	CLA	C3B-C4B	2.75	1.49	1.42
23	C	514	CLA	C1B-C2B	2.75	1.49	1.43
23	b	603	CLA	C1C-C2C	2.75	1.49	1.44
23	b	608	CLA	C3B-C4B	2.74	1.49	1.42
23	C	513	CLA	C1C-C2C	2.74	1.49	1.44
26	a	409[A]	SQD	C6-S	-2.73	1.67	1.77
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	C	504	CLA	C1C-C2C	2.73	1.49	1.44
23	c	515	CLA	C1B-C2B	2.73	1.49	1.43
40	V	201	HEC	FE-NB	2.73	2.03	1.94
23	C	513	CLA	C1B-NB	-2.73	1.34	1.37
23	C	502	CLA	OBD-CAD	2.73	1.27	1.22
23	C	502	CLA	C4D-CHA	2.73	1.48	1.38
23	A	406[A]	CLA	C4D-CHA	2.72	1.48	1.38
23	a	405[A]	CLA	C1C-C2C	2.72	1.49	1.44
23	B	604	CLA	C4B-NB	-2.72	1.34	1.37
23	d	402[A]	CLA	C1B-C2B	2.72	1.49	1.43
23	C	512	CLA	C1B-NB	-2.72	1.34	1.37
23	b	611	CLA	C4C-C3C	2.72	1.49	1.45
33	Z	101	LMG	O8-C28	2.72	1.46	1.33
26	f	102	SQD	C6-S	-2.72	1.67	1.77
23	D	402[A]	CLA	C4D-CHA	2.71	1.48	1.38
23	C	510	CLA	C1B-C2B	2.71	1.49	1.43
23	c	512	CLA	C1C-C2C	2.71	1.49	1.44
23	c	510	CLA	C4D-CHA	2.71	1.48	1.38
23	B	602	CLA	C3D-C4D	-2.71	1.38	1.44
23	c	511	CLA	C4C-C3C	2.71	1.49	1.45
23	c	513	CLA	C1B-NB	-2.71	1.34	1.37
29	a	412[B]	PL9	C6-C5	2.71	1.49	1.35
23	B	606	CLA	C1C-C2C	2.70	1.49	1.44
23	B	614	CLA	C3D-C4D	-2.70	1.38	1.44
23	B	610	CLA	C4D-CHA	2.70	1.48	1.38
23	b	605	CLA	C4B-NB	-2.70	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C4D-CHA	2.70	1.48	1.38
23	c	509	CLA	C4D-CHA	2.70	1.48	1.38
23	C	508	CLA	C4D-CHA	2.69	1.48	1.38
34	b	622	HTG	O5-C1	2.69	1.46	1.42
23	a	405[B]	CLA	C1B-C2B	2.69	1.49	1.43
23	c	513	CLA	C3B-C4B	2.69	1.49	1.42
23	A	405[A]	CLA	C4D-CHA	2.68	1.47	1.38
23	a	405[B]	CLA	C4D-CHA	2.68	1.47	1.38
23	A	408	CLA	C4B-NB	-2.68	1.34	1.37
31	M	101	LMT	O2'-C2'	-2.68	1.36	1.43
23	d	404	CLA	C4D-CHA	2.68	1.47	1.38
23	a	405[A]	CLA	C1B-C2B	2.68	1.49	1.43
23	A	405[B]	CLA	C4D-CHA	2.68	1.47	1.38
23	b	611	CLA	C3B-C4B	2.67	1.49	1.42
23	B	609	CLA	C1B-C2B	2.67	1.49	1.43
23	B	612	CLA	C1C-C2C	2.67	1.49	1.44
23	c	504	CLA	C4D-CHA	2.67	1.47	1.38
23	B	606	CLA	C1B-NB	-2.67	1.34	1.37
23	B	612	CLA	OBD-CAD	2.67	1.27	1.22
23	B	609	CLA	C4D-CHA	2.66	1.47	1.38
26	A	412	SQD	C6-S	-2.66	1.67	1.77
23	B	601	CLA	C1B-NB	-2.66	1.34	1.37
23	d	404	CLA	C1C-C2C	2.66	1.49	1.44
26	a	410	SQD	C6-S	-2.66	1.67	1.77
23	a	404[A]	CLA	C1B-C2B	2.66	1.49	1.43
23	a	404[B]	CLA	C1B-C2B	2.66	1.49	1.43
23	d	403[B]	CLA	C3D-C4D	-2.66	1.38	1.44
23	d	403[A]	CLA	C1B-C2B	2.65	1.49	1.43
23	C	511	CLA	C1B-C2B	2.65	1.49	1.43
23	C	507	CLA	C4D-CHA	2.65	1.47	1.38
23	d	403[B]	CLA	C1C-C2C	2.65	1.49	1.44
23	C	514	CLA	C4D-CHA	2.65	1.47	1.38
23	c	505	CLA	C3D-C4D	-2.64	1.38	1.44
23	A	408	CLA	C4D-CHA	2.64	1.47	1.38
23	b	609	CLA	C4D-CHA	2.64	1.47	1.38
23	C	512	CLA	C4C-C3C	2.64	1.49	1.45
23	A	404[B]	CLA	C4D-CHA	2.64	1.47	1.38
23	C	510	CLA	C1C-C2C	2.64	1.49	1.44
23	C	512	CLA	C3B-C4B	2.64	1.48	1.42
23	B	610	CLA	C1C-C2C	2.63	1.49	1.44
23	b	610	CLA	C4D-CHA	2.63	1.47	1.38
23	b	612	CLA	C4C-C3C	2.63	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[B]	CLA	C1B-C2B	2.63	1.49	1.43
26	A	410[B]	SQD	C6-S	-2.63	1.67	1.77
23	c	512	CLA	C4D-CHA	2.63	1.47	1.38
23	a	405[A]	CLA	C4B-NB	-2.63	1.34	1.37
23	b	606	CLA	C4B-NB	-2.62	1.34	1.37
23	c	514	CLA	C4D-CHA	2.62	1.47	1.38
23	a	405[A]	CLA	C4D-CHA	2.62	1.47	1.38
23	C	511	CLA	C1C-C2C	2.62	1.49	1.44
23	A	405[A]	CLA	C1B-C2B	2.62	1.49	1.43
23	c	503	CLA	C4D-CHA	2.62	1.47	1.38
23	c	504	CLA	C3B-C4B	2.62	1.48	1.42
23	b	616	CLA	C4B-NB	-2.61	1.34	1.37
23	b	602	CLA	C4D-CHA	2.61	1.47	1.38
23	C	505	CLA	C4B-NB	-2.61	1.34	1.37
23	b	607	CLA	C4D-CHA	2.61	1.47	1.38
23	c	510	CLA	C1C-C2C	2.61	1.49	1.44
26	b	620	SQD	C6-S	-2.61	1.67	1.77
23	C	502	CLA	C1B-C2B	2.61	1.49	1.43
23	c	513	CLA	C4D-CHA	2.61	1.47	1.38
23	b	610	CLA	C1B-C2B	2.61	1.49	1.43
23	c	505	CLA	C4D-CHA	2.60	1.47	1.38
23	c	503	CLA	C1C-C2C	2.60	1.49	1.44
23	B	603	CLA	C3B-C4B	2.60	1.48	1.42
23	B	603	CLA	C4D-CHA	2.60	1.47	1.38
23	c	507	CLA	C4D-CHA	2.60	1.47	1.38
23	b	606	CLA	C1C-C2C	2.60	1.49	1.44
23	c	507	CLA	C4C-C3C	2.60	1.49	1.45
23	c	506	CLA	C4D-CHA	2.60	1.47	1.38
31	t	101	LMT	O3'-C3'	-2.60	1.36	1.43
23	C	514	CLA	C1C-C2C	2.60	1.49	1.44
23	b	609	CLA	C4B-NB	-2.59	1.34	1.37
23	b	601	CLA	C1C-C2C	2.59	1.49	1.44
23	D	402[B]	CLA	C1B-C2B	2.59	1.49	1.43
23	c	504	CLA	C3B-C2B	2.59	1.50	1.41
34	B	622	HTG	C1'-S1	-2.59	1.78	1.81
23	c	508	CLA	C1B-C2B	2.59	1.49	1.43
23	B	614	CLA	C4D-CHA	2.58	1.47	1.38
23	b	602	CLA	C4B-NB	-2.58	1.34	1.37
23	A	406[B]	CLA	C1B-C2B	2.58	1.49	1.43
23	B	615	CLA	C4D-CHA	2.58	1.47	1.38
23	B	601	CLA	C1B-C2B	2.58	1.49	1.43
23	a	404[B]	CLA	C4C-C3C	2.57	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C1B-C2B	2.57	1.49	1.43
23	a	404[A]	CLA	C3B-C4B	2.57	1.48	1.42
23	C	506	CLA	C4C-C3C	2.57	1.49	1.45
23	B	613	CLA	C4D-CHA	2.57	1.47	1.38
23	A	404[A]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	606	CLA	C4D-CHA	2.57	1.47	1.38
23	B	605	CLA	C4D-CHA	2.57	1.47	1.38
23	C	511	CLA	C4D-CHA	2.57	1.47	1.38
23	B	602	CLA	C3B-C4B	2.56	1.48	1.42
23	b	608	CLA	C1C-C2C	2.56	1.49	1.44
24	a	406[B]	PHO	C4B-NB	-2.56	1.33	1.38
31	m	103	LMT	O2B-C2B	-2.56	1.37	1.43
23	d	403[A]	CLA	C4C-C3C	2.56	1.49	1.45
23	B	604	CLA	C4C-C3C	2.56	1.49	1.45
23	d	403[B]	CLA	C4D-CHA	2.55	1.47	1.38
23	c	509	CLA	C1B-C2B	2.55	1.49	1.43
40	V	201	HEC	CAC-C3C	2.55	1.57	1.51
23	b	614	CLA	C3D-C4D	-2.55	1.38	1.44
23	b	601	CLA	C4D-CHA	2.55	1.47	1.38
23	b	608	CLA	C1B-C2B	2.55	1.49	1.43
23	b	605	CLA	C3B-C4B	2.55	1.48	1.42
23	C	514	CLA	C3B-C4B	2.55	1.48	1.42
23	D	402[B]	CLA	C4C-C3C	2.55	1.49	1.45
23	C	504	CLA	C4B-NB	-2.55	1.34	1.37
23	B	614	CLA	C1B-C2B	2.55	1.49	1.43
23	c	504	CLA	C1B-C2B	2.55	1.49	1.43
24	a	414[A]	PHO	C3A-C2A	-2.55	1.52	1.54
23	c	511	CLA	C1B-C2B	2.55	1.49	1.43
23	c	513	CLA	C1C-C2C	2.54	1.49	1.44
23	C	506	CLA	C4B-NB	-2.54	1.34	1.37
24	a	414[B]	PHO	C3A-C2A	-2.54	1.52	1.54
23	B	610	CLA	C1B-C2B	2.54	1.49	1.43
23	A	408	CLA	C3D-C4D	-2.54	1.38	1.44
23	b	604	CLA	C3B-C4B	2.54	1.48	1.42
33	C	521	LMG	O1-C1	2.54	1.44	1.40
23	B	613	CLA	C1C-C2C	2.54	1.49	1.44
23	A	406[B]	CLA	C1C-C2C	2.54	1.49	1.44
31	B	627	LMT	C3'-C2'	2.54	1.58	1.52
23	A	405[B]	CLA	C4B-NB	-2.53	1.34	1.37
23	C	512	CLA	C3D-C4D	-2.53	1.38	1.44
23	B	616	CLA	C3D-C4D	-2.53	1.38	1.44
23	C	507	CLA	C3B-C4B	2.53	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1C-C2C	2.53	1.49	1.44
40	v	201	HEC	CAC-C3C	2.53	1.57	1.51
23	b	612	CLA	C3B-C2B	2.52	1.49	1.41
23	b	604	CLA	C1C-C2C	2.52	1.49	1.44
23	C	509	CLA	C1B-C2B	2.52	1.49	1.43
23	B	606	CLA	C4D-CHA	2.52	1.47	1.38
23	b	602	CLA	C3D-C4D	-2.52	1.38	1.44
23	a	404[B]	CLA	C4D-CHA	2.52	1.47	1.38
29	d	406[B]	PL9	C6-C5	2.52	1.48	1.35
23	b	613	CLA	C3B-C4B	2.52	1.48	1.42
23	C	510	CLA	C3B-C4B	2.51	1.48	1.42
38	E	102	HEM	C1C-C2C	-2.51	1.40	1.45
23	c	503	CLA	C4C-C3C	2.51	1.49	1.45
23	C	507	CLA	C1C-C2C	2.51	1.49	1.44
23	B	612	CLA	C1B-C2B	2.51	1.49	1.43
23	C	512	CLA	C1B-C2B	2.51	1.49	1.43
23	C	503	CLA	C4D-CHA	2.51	1.47	1.38
34	B	624	HTG	C1-S1	-2.51	1.76	1.80
23	b	605	CLA	C1B-C2B	2.51	1.49	1.43
23	c	508	CLA	C3B-C4B	2.50	1.48	1.42
23	b	611	CLA	C1C-C2C	2.50	1.49	1.44
23	C	510	CLA	C4D-CHA	2.50	1.47	1.38
23	B	608	CLA	C3D-C4D	-2.50	1.38	1.44
23	B	613	CLA	C3B-C2B	2.50	1.49	1.41
23	B	608	CLA	C3B-C4B	2.50	1.48	1.42
23	B	606	CLA	C3D-C4D	-2.50	1.38	1.44
23	b	615	CLA	C3B-C4B	2.50	1.48	1.42
23	b	606	CLA	C1B-C2B	2.50	1.49	1.43
23	d	402[B]	CLA	C4D-CHA	2.50	1.47	1.38
23	c	505	CLA	C4C-C3C	2.50	1.49	1.45
23	b	610	CLA	C3D-C4D	-2.50	1.38	1.44
26	B	620	SQD	C6-S	-2.50	1.68	1.77
23	A	404[A]	CLA	C1C-C2C	2.49	1.49	1.44
23	a	404[A]	CLA	C4C-C3C	2.49	1.49	1.45
23	A	404[B]	CLA	C4C-C3C	2.49	1.49	1.45
23	b	615	CLA	C4D-CHA	2.49	1.47	1.38
31	A	420	LMT	O3'-C3'	-2.49	1.37	1.43
23	b	615	CLA	C4B-NB	-2.49	1.34	1.37
23	D	403	CLA	C4C-C3C	2.49	1.49	1.45
23	C	503	CLA	C1B-NB	-2.49	1.34	1.37
23	c	509	CLA	C3B-C4B	2.49	1.48	1.42
23	c	515	CLA	C4D-CHA	2.49	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	609	CLA	C1C-NC	-2.48	1.34	1.37
25	B	619	BCR	C30-C25	-2.48	1.50	1.53
23	C	507	CLA	C1B-C2B	2.48	1.49	1.43
23	B	605	CLA	C1C-C2C	2.48	1.49	1.44
23	C	513	CLA	C1B-C2B	2.48	1.49	1.43
23	a	404[A]	CLA	C4D-CHA	2.48	1.47	1.38
23	d	402[A]	CLA	C4D-CHA	2.48	1.47	1.38
31	B	630	LMT	O3'-C3'	-2.47	1.37	1.43
23	A	408	CLA	C3B-C2B	2.47	1.49	1.41
31	e	101	LMT	O3'-C3'	-2.47	1.37	1.43
31	b	621	LMT	C3'-C2'	2.47	1.58	1.52
23	c	507	CLA	C1C-C2C	2.47	1.49	1.44
23	c	506	CLA	C1C-NC	-2.46	1.34	1.37
23	D	402[B]	CLA	C3B-C4B	2.46	1.48	1.42
23	C	511	CLA	C3D-C4D	-2.46	1.38	1.44
23	b	613	CLA	C1B-C2B	2.46	1.49	1.43
23	b	614	CLA	C4D-CHA	2.46	1.47	1.38
23	b	615	CLA	C3D-C4D	-2.46	1.38	1.44
24	A	416[B]	PHO	C3D-C4D	-2.46	1.37	1.41
23	b	610	CLA	C4C-C3C	2.45	1.49	1.45
24	A	416[B]	PHO	C4B-NB	-2.45	1.34	1.38
23	B	603	CLA	C3B-C2B	2.45	1.49	1.41
23	c	507	CLA	C4B-NB	-2.45	1.34	1.37
23	c	511	CLA	C3B-C4B	2.45	1.48	1.42
23	B	602	CLA	C4D-CHA	2.45	1.47	1.38
23	B	615	CLA	C1C-C2C	2.45	1.49	1.44
23	a	405[A]	CLA	C3D-C4D	-2.44	1.38	1.44
38	f	101	HEM	C1C-C2C	-2.44	1.40	1.45
23	b	609	CLA	C1C-C2C	2.44	1.49	1.44
23	B	610	CLA	C4B-NB	-2.44	1.34	1.37
23	A	406[A]	CLA	C1B-C2B	2.44	1.49	1.43
23	B	616	CLA	C1C-C2C	2.44	1.49	1.44
23	C	507	CLA	C3D-C4D	-2.44	1.38	1.44
38	f	101	HEM	C1D-ND	-2.44	1.33	1.38
31	A	420	LMT	O2'-C2'	-2.44	1.37	1.43
23	B	613	CLA	C4C-C3C	2.43	1.49	1.45
23	B	616	CLA	C3B-C2B	2.43	1.49	1.41
23	b	611	CLA	C4B-NB	-2.43	1.34	1.37
23	C	510	CLA	C3B-C2B	2.43	1.49	1.41
23	b	610	CLA	C1C-C2C	2.43	1.49	1.44
23	c	511	CLA	C4D-CHA	2.43	1.47	1.38
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	629	LMT	O2'-C2'	-2.43	1.37	1.43
23	b	603	CLA	C4B-NB	-2.43	1.34	1.37
23	C	509	CLA	C3B-C4B	2.43	1.48	1.42
24	a	406[B]	PHO	C1B-NB	-2.42	1.34	1.38
23	B	602	CLA	C4C-C3C	2.42	1.49	1.45
29	D	405[B]	PL9	C6-C5	2.42	1.47	1.35
23	c	515	CLA	C4C-C3C	2.42	1.49	1.45
23	c	514	CLA	C1B-C2B	2.42	1.49	1.43
31	m	103	LMT	C3'-C2'	2.42	1.58	1.52
23	A	406[B]	CLA	C4D-CHA	2.42	1.47	1.38
23	b	616	CLA	C4D-CHA	2.42	1.47	1.38
34	o	301	HTG	O5-C1	2.41	1.46	1.42
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	B	612	CLA	C3B-C2B	2.41	1.49	1.41
23	A	404[B]	CLA	C3B-C2B	2.41	1.49	1.41
23	c	513	CLA	C3B-C2B	2.41	1.49	1.41
23	C	509	CLA	C1C-C2C	2.41	1.49	1.44
35	C	519	DGD	O2G-C2G	-2.41	1.40	1.46
23	B	601	CLA	C4D-CHA	2.41	1.47	1.38
23	b	608	CLA	C4D-CHA	2.41	1.47	1.38
23	B	616	CLA	C1C-NC	-2.40	1.34	1.37
23	B	606	CLA	C4B-NB	-2.40	1.34	1.37
23	c	509	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	509	CLA	C4C-C3C	2.39	1.49	1.45
23	D	402[A]	CLA	C3D-C4D	-2.39	1.38	1.44
31	c	502	LMT	O3'-C3'	-2.39	1.37	1.43
23	D	403	CLA	C4B-NB	-2.39	1.34	1.37
23	B	605	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	608	CLA	C3D-C4D	-2.39	1.38	1.44
23	D	402[B]	CLA	C3D-C4D	-2.39	1.38	1.44
23	b	612	CLA	C4D-CHA	2.39	1.46	1.38
23	c	506	CLA	C3B-C4B	2.39	1.48	1.42
23	B	606	CLA	C1B-C2B	2.38	1.48	1.43
23	c	503	CLA	C1C-NC	-2.38	1.34	1.37
23	d	403[A]	CLA	C4D-CHA	2.38	1.46	1.38
23	C	514	CLA	C3B-C2B	2.38	1.49	1.41
31	M	103	LMT	O3'-C3'	-2.38	1.37	1.43
24	A	416[B]	PHO	C3A-C2A	-2.37	1.52	1.54
23	B	612	CLA	C3D-C4D	-2.37	1.38	1.44
23	B	614	CLA	C3B-C4B	2.37	1.48	1.42
23	B	607	CLA	C4C-C3C	2.37	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	609	CLA	C1C-C2C	2.37	1.49	1.44
31	B	627	LMT	O3'-C3'	-2.37	1.37	1.43
26	F	102	SQD	C6-S	-2.36	1.68	1.77
23	b	609	CLA	C3D-C4D	-2.36	1.38	1.44
23	C	512	CLA	C3B-C2B	2.36	1.49	1.41
23	B	602	CLA	C3B-C2B	2.36	1.49	1.41
23	a	404[B]	CLA	C1C-C2C	2.36	1.49	1.44
23	b	603	CLA	C4D-CHA	2.36	1.46	1.38
23	A	408	CLA	C3B-C4B	2.36	1.48	1.42
23	C	503	CLA	C3B-C2B	2.36	1.49	1.41
23	d	404	CLA	C1B-C2B	2.36	1.48	1.43
23	c	508	CLA	C4D-CHA	2.35	1.46	1.38
23	c	510	CLA	C3B-C2B	2.35	1.49	1.41
23	b	608	CLA	C4C-C3C	2.35	1.49	1.45
23	c	514	CLA	C4B-NB	-2.35	1.34	1.37
29	d	406[A]	PL9	C6-C5	2.35	1.47	1.35
23	d	403[B]	CLA	C3B-C4B	2.35	1.48	1.42
23	c	515	CLA	C3D-C4D	-2.35	1.38	1.44
23	a	407	CLA	C4D-CHA	2.35	1.46	1.38
23	C	505	CLA	C3B-C2B	2.35	1.49	1.41
23	b	611	CLA	C4D-CHA	2.35	1.46	1.38
23	C	504	CLA	C4D-CHA	2.35	1.46	1.38
24	A	416[A]	PHO	C3D-C4D	-2.35	1.37	1.41
23	C	513	CLA	C3D-C4D	-2.35	1.38	1.44
23	C	514	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[B]	CLA	C4C-C3C	2.34	1.49	1.45
23	A	405[A]	CLA	C3D-C4D	-2.34	1.38	1.44
31	F	101	LMT	O3'-C3'	-2.34	1.37	1.43
23	c	503	CLA	C1B-C2B	2.34	1.48	1.43
29	D	405[A]	PL9	C6-C5	2.34	1.47	1.35
23	C	504	CLA	C1B-C2B	2.34	1.48	1.43
23	C	508	CLA	C1B-C2B	2.33	1.48	1.43
23	b	606	CLA	C3D-C4D	-2.33	1.38	1.44
23	b	613	CLA	C3B-C2B	2.33	1.49	1.41
23	B	604	CLA	C3D-C4D	-2.33	1.38	1.44
23	C	513	CLA	C4B-NB	-2.33	1.34	1.37
23	b	616	CLA	C3D-C4D	-2.33	1.38	1.44
24	a	406[A]	PHO	CBD-CGD	-2.33	1.49	1.52
23	c	512	CLA	C4B-NB	-2.33	1.34	1.37
23	b	611	CLA	C3B-C2B	2.33	1.49	1.41
35	c	520	DGD	O2G-C2G	-2.33	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	C1B-C2B	2.32	1.48	1.43
23	D	402[B]	CLA	C4D-CHA	2.32	1.46	1.38
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	b	603	CLA	C3B-C2B	2.32	1.49	1.41
23	c	508	CLA	C4C-C3C	2.32	1.49	1.45
31	B	629	LMT	O2B-C2B	-2.32	1.37	1.43
23	C	509	CLA	C1B-NB	-2.32	1.34	1.37
31	M	103	LMT	O2'-C2'	-2.32	1.37	1.43
23	C	505	CLA	C3D-C4D	-2.32	1.38	1.44
23	B	605	CLA	C4B-NB	-2.32	1.34	1.37
23	C	502	CLA	C3D-C4D	-2.31	1.39	1.44
23	C	505	CLA	C3B-C4B	2.31	1.48	1.42
23	c	514	CLA	C4C-C3C	2.31	1.49	1.45
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
23	B	609	CLA	C3D-C4D	-2.30	1.39	1.44
23	C	504	CLA	C3D-C4D	-2.30	1.39	1.44
23	B	610	CLA	C3D-C4D	-2.30	1.39	1.44
24	A	407[B]	PHO	C1B-NB	-2.30	1.34	1.38
23	C	502	CLA	C4C-C3C	2.30	1.49	1.45
23	b	605	CLA	C3D-C4D	-2.30	1.39	1.44
23	A	408	CLA	C1C-NC	-2.30	1.34	1.37
27	b	624	GOL	C3-C2	2.30	1.61	1.51
23	B	608	CLA	C4C-C3C	2.30	1.49	1.45
23	c	504	CLA	C1B-NB	-2.29	1.35	1.37
23	d	402[B]	CLA	C4B-NB	-2.29	1.35	1.37
40	v	201	HEC	CMC-C2C	2.28	1.55	1.50
23	c	508	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	611	CLA	C3D-C4D	-2.28	1.39	1.44
26	F	102	SQD	O6-C1	2.28	1.44	1.40
23	C	511	CLA	C3B-C2B	2.28	1.48	1.41
23	B	610	CLA	C4C-C3C	2.28	1.49	1.45
23	c	510	CLA	C4B-NB	-2.28	1.35	1.37
23	b	601	CLA	C3B-C2B	2.28	1.48	1.41
23	b	607	CLA	C4B-NB	-2.28	1.35	1.37
23	c	510	CLA	C3D-C4D	-2.28	1.39	1.44
23	b	607	CLA	C3B-C4B	2.27	1.48	1.42
23	c	506	CLA	C3B-C2B	2.27	1.48	1.41
23	b	602	CLA	C4C-C3C	2.27	1.48	1.45
23	c	511	CLA	C3B-C2B	2.27	1.48	1.41
23	C	504	CLA	C4C-C3C	2.27	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404[B]	CLA	C3B-C4B	2.27	1.48	1.42
23	b	615	CLA	C4C-C3C	2.26	1.48	1.45
23	C	506	CLA	C3D-C4D	-2.26	1.39	1.44
23	b	605	CLA	C4D-CHA	2.26	1.46	1.38
35	h	102	DGD	O5D-C1E	2.26	1.44	1.40
23	D	403	CLA	C4D-CHA	2.26	1.46	1.38
24	A	416[A]	PHO	C4B-NB	-2.26	1.34	1.38
24	a	414[B]	PHO	C4B-NB	-2.26	1.34	1.38
23	B	611	CLA	C4D-CHA	2.26	1.46	1.38
23	B	608	CLA	C3B-C2B	2.26	1.48	1.41
23	B	604	CLA	C1A-CHA	2.26	1.52	1.43
23	b	604	CLA	C4B-NB	-2.25	1.35	1.37
23	c	504	CLA	C1C-C2C	2.25	1.48	1.44
23	a	404[A]	CLA	C1C-C2C	2.25	1.48	1.44
24	a	406[B]	PHO	C1D-ND	-2.25	1.34	1.38
23	b	605	CLA	C1C-C2C	2.25	1.48	1.44
23	B	615	CLA	C4B-NB	-2.25	1.35	1.37
23	D	402[B]	CLA	C1C-C2C	2.25	1.48	1.44
23	A	406[A]	CLA	C3D-C4D	-2.24	1.39	1.44
27	D	412	GOL	C3-C2	2.24	1.60	1.51
23	d	403[A]	CLA	C3B-C4B	2.24	1.48	1.42
23	C	505	CLA	C4C-C3C	2.24	1.48	1.45
23	d	403[B]	CLA	C3B-C2B	2.24	1.48	1.41
23	C	510	CLA	C4C-C3C	2.23	1.48	1.45
23	B	614	CLA	C1C-C2C	2.23	1.48	1.44
23	c	514	CLA	C3D-C4D	-2.23	1.39	1.44
31	M	101	LMT	O2B-C2B	-2.23	1.37	1.43
23	b	612	CLA	C3D-C4D	-2.22	1.39	1.44
23	d	404	CLA	C3D-C4D	-2.22	1.39	1.44
31	M	101	LMT	O3'-C3'	-2.22	1.37	1.43
23	c	503	CLA	C3D-C4D	-2.22	1.39	1.44
23	a	404[B]	CLA	C3B-C4B	2.22	1.48	1.42
23	c	512	CLA	C3B-C2B	2.21	1.48	1.41
23	b	601	CLA	C4C-C3C	2.21	1.48	1.45
23	a	404[B]	CLA	C3B-C2B	2.21	1.48	1.41
23	C	508	CLA	C3D-C4D	-2.21	1.39	1.44
35	C	518[A]	DGD	O5D-C1E	2.21	1.44	1.40
23	D	402[A]	CLA	C4C-C3C	2.21	1.48	1.45
31	t	101	LMT	O2'-C2'	-2.21	1.37	1.43
23	b	613	CLA	C1C-C2C	2.21	1.48	1.44
23	C	507	CLA	C1D-C2D	2.20	1.49	1.45
23	d	402[A]	CLA	C4B-NB	-2.20	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4C-C3C	2.20	1.48	1.45
23	b	616	CLA	C3B-C2B	2.20	1.48	1.41
35	c	520	DGD	O5D-C1E	2.20	1.43	1.40
24	A	416[A]	PHO	C1D-ND	-2.20	1.34	1.38
23	D	402[A]	CLA	C3B-C2B	2.19	1.48	1.41
23	d	402[B]	CLA	C3D-C4D	-2.19	1.39	1.44
29	a	412[A]	PL9	C2-C3	2.19	1.40	1.34
23	A	405[B]	CLA	C3D-C4D	-2.19	1.39	1.44
23	A	405[B]	CLA	C1C-C2C	2.19	1.48	1.44
23	c	514	CLA	C1C-C2C	2.19	1.48	1.44
23	B	613	CLA	C4B-NB	-2.19	1.35	1.37
23	B	608	CLA	C1C-NC	-2.18	1.34	1.37
23	b	609	CLA	C1B-C2B	2.18	1.48	1.43
23	B	606	CLA	C4C-C3C	2.18	1.48	1.45
23	c	504	CLA	C4C-C3C	2.18	1.48	1.45
23	B	601	CLA	C1C-NC	-2.18	1.34	1.37
23	B	601	CLA	C4C-C3C	2.18	1.48	1.45
23	B	602	CLA	C4B-NB	-2.18	1.35	1.37
23	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	604	CLA	MG-NA	2.17	2.11	2.06
27	a	416	GOL	C1-C2	2.17	1.60	1.51
23	c	513	CLA	C4C-C3C	2.17	1.48	1.45
24	A	416[B]	PHO	C1D-ND	-2.17	1.34	1.38
23	D	402[B]	CLA	C3B-C2B	2.17	1.48	1.41
23	A	406[B]	CLA	C3D-C4D	-2.17	1.39	1.44
23	A	404[B]	CLA	C3D-C4D	-2.16	1.39	1.44
23	B	603	CLA	C3D-C4D	-2.16	1.39	1.44
23	c	512	CLA	C3D-C4D	-2.16	1.39	1.44
23	D	402[A]	CLA	C3B-C4B	2.16	1.47	1.42
23	B	603	CLA	C4C-C3C	2.16	1.48	1.45
40	V	201	HEC	CMB-C2B	2.15	1.55	1.50
38	E	102	HEM	C3C-C4C	-2.15	1.42	1.46
23	b	608	CLA	C3B-C2B	2.15	1.48	1.41
23	C	503	CLA	C3D-C4D	-2.15	1.39	1.44
24	a	414[B]	PHO	CHA-CBD	-2.14	1.49	1.51
23	A	406[B]	CLA	C4C-C3C	2.14	1.48	1.45
24	a	406[A]	PHO	C4B-NB	-2.14	1.34	1.38
23	C	508	CLA	C3B-C2B	2.14	1.48	1.41
23	C	507	CLA	C3B-C2B	2.14	1.48	1.41
24	a	414[B]	PHO	C1B-NB	-2.14	1.34	1.38
27	o	304	GOL	C1-C2	2.14	1.60	1.51
23	c	508	CLA	C1C-C2C	2.14	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	405	BCR	C30-C25	-2.14	1.50	1.53
29	a	412[B]	PL9	C2-C3	2.14	1.40	1.34
23	c	509	CLA	C1D-C2D	2.14	1.49	1.45
23	b	613	CLA	C4C-C3C	2.14	1.48	1.45
23	B	604	CLA	C3B-C2B	2.13	1.48	1.41
31	M	103	LMT	O3B-C3B	-2.13	1.38	1.43
24	a	414[A]	PHO	C4B-NB	-2.13	1.34	1.38
23	b	603	CLA	C4C-C3C	2.13	1.48	1.45
23	C	513	CLA	C3B-C2B	2.13	1.48	1.41
23	b	614	CLA	C3B-C2B	2.12	1.48	1.41
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	CMD-C2D	2.12	1.55	1.50
23	b	607	CLA	C3D-C4D	-2.12	1.39	1.44
23	b	614	CLA	C1C-C2C	2.12	1.48	1.44
23	C	505	CLA	C1C-C2C	2.12	1.48	1.44
31	e	101	LMT	O2'-C2'	-2.12	1.38	1.43
23	c	508	CLA	C3B-C2B	2.12	1.48	1.41
23	B	607	CLA	C3D-C4D	-2.12	1.39	1.44
23	b	604	CLA	C1A-CHA	2.12	1.51	1.43
23	d	402[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	b	610	CLA	C3B-C2B	2.12	1.48	1.41
23	B	601	CLA	C3B-C2B	2.11	1.48	1.41
27	c	528	GOL	C3-C2	2.11	1.60	1.51
23	c	511	CLA	C3D-C4D	-2.11	1.39	1.44
31	B	627	LMT	O4'-C4B	-2.11	1.38	1.43
23	b	607	CLA	C4C-C3C	2.11	1.48	1.45
27	A	418	GOL	C3-C2	2.11	1.60	1.51
23	B	613	CLA	C3B-C4B	2.10	1.47	1.42
29	D	405[B]	PL9	C2-C3	2.10	1.40	1.34
23	B	606	CLA	MG-NA	2.10	2.11	2.06
23	C	508	CLA	C4C-C3C	2.10	1.48	1.45
38	E	102	HEM	C3B-C4B	2.10	1.49	1.44
23	C	502	CLA	C3B-C2B	2.10	1.48	1.41
23	c	515	CLA	C1D-C2D	2.09	1.49	1.45
24	A	407[A]	PHO	C1B-NB	-2.09	1.34	1.38
23	B	608	CLA	C1C-C2C	2.09	1.48	1.44
23	b	602	CLA	CHB-C4A	-2.09	1.32	1.37
23	b	604	CLA	C3B-C2B	2.09	1.48	1.41
23	c	506	CLA	C3D-C4D	-2.09	1.39	1.44
23	a	405[B]	CLA	C3D-C4D	-2.09	1.39	1.44
23	d	404	CLA	C4C-C3C	2.09	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	C3D-C4D	-2.09	1.39	1.44
23	b	606	CLA	C3B-C2B	2.08	1.48	1.41
23	a	405[A]	CLA	C4C-C3C	2.08	1.48	1.45
34	D	410	HTG	C1-S1	-2.08	1.77	1.80
23	C	513	CLA	C4C-C3C	2.08	1.48	1.45
24	a	414[B]	PHO	C1D-ND	-2.08	1.34	1.38
23	d	402[B]	CLA	C1C-C2C	2.08	1.48	1.44
23	B	612	CLA	C3B-C4B	2.08	1.47	1.42
23	B	607	CLA	C3B-C2B	2.08	1.48	1.41
23	B	609	CLA	C4C-C3C	2.08	1.48	1.45
23	d	403[A]	CLA	C3B-C2B	2.07	1.48	1.41
23	c	515	CLA	C3B-C2B	2.07	1.48	1.41
29	A	414[B]	PL9	C2-C1	-2.07	1.39	1.44
23	b	603	CLA	C3D-C4D	-2.07	1.39	1.44
24	A	407[A]	PHO	C1D-ND	-2.07	1.34	1.38
31	B	629	LMT	O3'-C3'	-2.06	1.38	1.43
31	B	627	LMT	O5'-C5'	-2.06	1.39	1.44
23	c	504	CLA	C3D-C4D	-2.06	1.39	1.44
31	e	101	LMT	O2B-C2B	-2.06	1.38	1.43
23	C	508	CLA	C3B-C4B	2.06	1.47	1.42
23	b	604	CLA	MG-NA	2.05	2.11	2.06
23	a	407	CLA	C3B-C2B	2.05	1.48	1.41
23	a	404[B]	CLA	C3D-C4D	-2.05	1.39	1.44
23	b	610	CLA	C4B-NB	-2.04	1.35	1.37
29	D	405[A]	PL9	C2-C3	2.04	1.40	1.34
23	A	405[B]	CLA	C3B-C2B	2.04	1.48	1.41
23	B	604	CLA	C1C-C2C	2.04	1.48	1.44
23	d	404	CLA	C3B-C2B	2.04	1.48	1.41
23	b	601	CLA	C1B-C2B	2.04	1.48	1.43
24	a	414[A]	PHO	C1B-NB	-2.03	1.34	1.38
23	B	613	CLA	C1A-CHA	2.03	1.51	1.43
23	b	602	CLA	C1B-C2B	2.03	1.48	1.43
23	A	408	CLA	C4C-C3C	2.03	1.48	1.45
23	C	509	CLA	C1A-CHA	2.03	1.51	1.43
23	C	512	CLA	MG-NA	2.03	2.11	2.06
23	c	513	CLA	MG-NA	2.03	2.11	2.06
40	v	201	HEC	CAB-C3B	2.03	1.56	1.51
32	b	629[A]	LHG	O7-C5	-2.02	1.41	1.46
24	A	407[B]	PHO	C4B-NB	-2.02	1.34	1.38
40	V	201	HEC	CMD-C2D	2.02	1.55	1.50
23	c	511	CLA	C1C-C2C	2.02	1.48	1.44
23	B	611	CLA	C1D-C2D	2.02	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407	CLA	C1D-C2D	2.02	1.49	1.45
23	A	404[A]	CLA	C3D-C4D	-2.02	1.39	1.44
23	A	404[B]	CLA	C1C-C2C	2.01	1.48	1.44
23	a	407	CLA	C4C-C3C	2.01	1.48	1.45
31	m	103	LMT	O3'-C3'	-2.01	1.38	1.43
23	C	514	CLA	C1C-NC	-2.01	1.34	1.37
24	a	414[A]	PHO	CBD-CGD	-2.00	1.49	1.52
35	C	518[B]	DGD	O5D-C1E	2.00	1.43	1.40
23	C	502	CLA	C4B-NB	-2.00	1.35	1.37

All (3308) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	16.58	121.35	110.23
23	B	611	CLA	C3B-C2B-C1B	-13.51	90.85	107.16
24	A	416[B]	PHO	C2D-C1D-ND	12.19	117.95	109.53
24	a	414[A]	PHO	C2D-C1D-ND	11.91	117.75	109.53
24	a	414[B]	PHO	C2D-C1D-ND	11.59	117.53	109.53
23	B	611	CLA	C1D-ND-C4D	-11.52	98.15	106.33
24	A	407[A]	PHO	C2D-C1D-ND	11.43	117.42	109.53
24	a	406[A]	PHO	C2D-C1D-ND	11.21	117.26	109.53
24	A	407[B]	PHO	C2D-C1D-ND	11.16	117.23	109.53
23	B	611	CLA	CHB-C1B-NB	-10.88	112.74	124.26
24	a	406[B]	PHO	C2D-C1D-ND	10.79	116.97	109.53
24	A	416[A]	PHO	C2D-C1D-ND	10.73	116.93	109.53
23	B	612	CLA	C1D-ND-C4D	-10.49	98.88	106.33
23	a	407	CLA	C1D-ND-C4D	-10.37	98.97	106.33
23	b	605	CLA	C1D-ND-C4D	-10.10	99.16	106.33
23	d	404	CLA	C1D-ND-C4D	-10.04	99.20	106.33
23	C	504	CLA	C1D-ND-C4D	-10.04	99.20	106.33
23	A	408	CLA	C1D-ND-C4D	-9.97	99.25	106.33
23	C	510	CLA	C1D-ND-C4D	-9.83	99.35	106.33
23	B	614	CLA	C1D-ND-C4D	-9.77	99.39	106.33
23	B	615	CLA	C1D-ND-C4D	-9.75	99.41	106.33
23	a	404[B]	CLA	C1D-ND-C4D	-9.71	99.44	106.33
23	a	405[A]	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	c	513	CLA	C1D-ND-C4D	-9.68	99.46	106.33
23	b	603	CLA	C1D-ND-C4D	-9.64	99.49	106.33
23	c	505	CLA	C1D-ND-C4D	-9.62	99.50	106.33
23	B	611	CLA	C2D-C1D-ND	9.59	117.17	110.10
23	B	606	CLA	C1D-ND-C4D	-9.59	99.53	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-9.58	99.53	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	C1D-ND-C4D	-9.56	99.54	106.33
23	A	406[B]	CLA	C1D-ND-C4D	-9.48	99.60	106.33
23	c	503	CLA	C1D-ND-C4D	-9.47	99.61	106.33
23	B	603	CLA	C1D-ND-C4D	-9.45	99.62	106.33
23	C	502	CLA	C1D-ND-C4D	-9.44	99.63	106.33
23	B	607	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	D	402[B]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	b	611	CLA	C1D-ND-C4D	-9.38	99.67	106.33
23	c	515	CLA	C1D-ND-C4D	-9.33	99.71	106.33
23	a	407	CLA	C2D-C1D-ND	9.29	116.95	110.10
23	B	605	CLA	C1D-ND-C4D	-9.28	99.75	106.33
23	C	514	CLA	C1D-ND-C4D	-9.27	99.75	106.33
23	b	615	CLA	C1D-ND-C4D	-9.26	99.76	106.33
23	c	508	CLA	C1D-ND-C4D	-9.24	99.77	106.33
23	B	602	CLA	C1D-ND-C4D	-9.18	99.81	106.33
23	c	507	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	c	511	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	b	614	CLA	C1D-ND-C4D	-9.16	99.82	106.33
23	A	408	CLA	C2D-C1D-ND	9.16	116.85	110.10
23	D	402[A]	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	B	615	CLA	C2D-C1D-ND	9.13	116.83	110.10
23	b	609	CLA	C1D-ND-C4D	-9.13	99.85	106.33
23	B	610	CLA	C1D-ND-C4D	-9.09	99.87	106.33
23	b	610	CLA	C1D-ND-C4D	-9.08	99.88	106.33
23	A	405[A]	CLA	C2D-C1D-ND	9.08	116.79	110.10
23	c	514	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	A	405[A]	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	b	601	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	d	403[A]	CLA	C1D-ND-C4D	-9.03	99.92	106.33
23	d	403[B]	CLA	C1D-ND-C4D	-9.02	99.92	106.33
23	B	612	CLA	C2D-C1D-ND	9.01	116.74	110.10
23	B	606	CLA	C2D-C1D-ND	8.97	116.72	110.10
23	c	504	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	607	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	b	602	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	b	605	CLA	C2D-C1D-ND	8.91	116.67	110.10
23	B	613	CLA	C1D-ND-C4D	-8.88	100.02	106.33
23	b	616	CLA	C1D-ND-C4D	-8.85	100.05	106.33
23	A	405[B]	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	b	606	CLA	C1D-ND-C4D	-8.82	100.07	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[A]	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	b	613	CLA	C2D-C1D-ND	8.81	116.60	110.10
23	b	613	CLA	C1D-ND-C4D	-8.80	100.08	106.33
23	B	613	CLA	C2D-C1D-ND	8.80	116.59	110.10
23	d	404	CLA	C2D-C1D-ND	8.79	116.58	110.10
23	d	402[B]	CLA	C1D-ND-C4D	-8.77	100.11	106.33
23	B	610	CLA	C2D-C1D-ND	8.76	116.56	110.10
23	B	616	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	C	511	CLA	C1D-ND-C4D	-8.76	100.11	106.33
23	C	510	CLA	C2D-C1D-ND	8.74	116.55	110.10
23	D	403	CLA	C1D-ND-C4D	-8.74	100.13	106.33
23	C	508	CLA	C1D-ND-C4D	-8.73	100.13	106.33
23	C	504	CLA	C2D-C1D-ND	8.73	116.54	110.10
23	C	509	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	c	512	CLA	C1D-ND-C4D	-8.72	100.14	106.33
23	B	614	CLA	C2D-C1D-ND	8.71	116.53	110.10
23	b	608	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	B	608	CLA	C1D-ND-C4D	-8.71	100.15	106.33
23	b	611	CLA	C2D-C1D-ND	8.68	116.50	110.10
23	d	402[A]	CLA	C1D-ND-C4D	-8.67	100.18	106.33
23	b	602	CLA	C4A-NA-C1A	-8.66	102.81	106.71
23	b	607	CLA	C2D-C1D-ND	8.65	116.47	110.10
23	C	506	CLA	C1D-ND-C4D	-8.63	100.21	106.33
23	A	406[A]	CLA	C2D-C1D-ND	8.61	116.45	110.10
23	C	507	CLA	C1D-ND-C4D	-8.59	100.23	106.33
23	b	614	CLA	C2D-C1D-ND	8.57	116.42	110.10
23	C	513	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	B	603	CLA	C2D-C1D-ND	8.55	116.40	110.10
23	c	506	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	d	402[A]	CLA	C2D-C1D-ND	8.52	116.39	110.10
23	B	616	CLA	C2D-C1D-ND	8.52	116.38	110.10
23	B	607	CLA	C2D-C1D-ND	8.51	116.38	110.10
23	c	509	CLA	C1D-ND-C4D	-8.50	100.30	106.33
23	a	405[B]	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	D	402[A]	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	513	CLA	C2D-C1D-ND	8.45	116.33	110.10
23	b	602	CLA	C2B-C1B-NB	8.45	115.90	110.23
23	c	503	CLA	C2D-C1D-ND	8.45	116.33	110.10
23	c	514	CLA	C2B-C1B-NB	8.43	115.88	110.23
23	b	612	CLA	C1D-ND-C4D	-8.42	100.35	106.33
23	B	609	CLA	C1D-ND-C4D	-8.39	100.37	106.33
23	B	608	CLA	C2D-C1D-ND	8.36	116.27	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	C2D-C1D-ND	8.36	116.26	110.10
23	b	603	CLA	C2D-C1D-ND	8.36	116.26	110.10
23	D	402[B]	CLA	C2D-C1D-ND	8.35	116.26	110.10
23	C	505	CLA	C2D-C1D-ND	8.35	116.25	110.10
23	C	514	CLA	C2D-C1D-ND	8.34	116.25	110.10
23	d	402[B]	CLA	C2D-C1D-ND	8.33	116.24	110.10
23	b	604	CLA	C1D-ND-C4D	-8.29	100.45	106.33
23	b	604	CLA	C2D-C1D-ND	8.27	116.20	110.10
23	C	505	CLA	C1D-ND-C4D	-8.25	100.47	106.33
23	b	616	CLA	C2D-C1D-ND	8.24	116.18	110.10
23	C	512	CLA	C1D-ND-C4D	-8.23	100.48	106.33
23	c	505	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	c	504	CLA	C2D-C1D-ND	8.20	116.15	110.10
23	C	508	CLA	C2D-C1D-ND	8.16	116.12	110.10
23	b	609	CLA	C2D-C1D-ND	8.16	116.11	110.10
23	C	503	CLA	C1D-ND-C4D	-8.12	100.57	106.33
23	A	405[B]	CLA	C2D-C1D-ND	8.09	116.07	110.10
23	A	404[B]	CLA	C1D-ND-C4D	-8.03	100.63	106.33
23	a	404[A]	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	B	601	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	b	608	CLA	C2D-C1D-ND	8.02	116.02	110.10
23	D	403	CLA	C2D-C1D-ND	8.02	116.01	110.10
23	b	615	CLA	C2D-C1D-ND	8.01	116.00	110.10
23	a	404[B]	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	C	502	CLA	C2D-C1D-ND	7.99	115.99	110.10
23	b	606	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	512	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	A	406[B]	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	B	605	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	C	512	CLA	C2D-C1D-ND	7.96	115.97	110.10
23	c	506	CLA	C2D-C1D-ND	7.95	115.96	110.10
23	d	404	CLA	C2B-C1B-NB	7.93	115.55	110.23
23	d	403[A]	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	b	610	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	B	609	CLA	C4A-NA-C1A	-7.91	103.15	106.71
24	A	407[B]	PHO	O2D-CGD-CBD	7.90	121.00	111.00
23	C	510	CLA	C2B-C1B-NB	7.90	115.53	110.23
23	c	507	CLA	C2D-C1D-ND	7.89	115.92	110.10
23	B	601	CLA	C2B-C1B-NB	7.89	115.52	110.23
23	c	508	CLA	C2D-C1D-ND	7.88	115.91	110.10
23	b	601	CLA	C2D-C1D-ND	7.87	115.90	110.10
23	c	514	CLA	C2D-C1D-ND	7.86	115.90	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C2D-C1D-ND	7.83	115.88	110.10
23	b	614	CLA	C2B-C1B-NB	7.75	115.43	110.23
23	A	408	CLA	C2B-C1B-NB	7.74	115.42	110.23
23	B	611	CLA	CMB-C2B-C1B	7.73	137.14	125.37
23	c	515	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	c	515	CLA	C2D-C1D-ND	7.72	115.79	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-7.69	100.87	106.33
23	c	511	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	B	609	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	c	510	CLA	C1D-ND-C4D	-7.64	100.91	106.33
23	C	504	CLA	C4A-NA-C1A	-7.64	103.27	106.71
23	C	513	CLA	C2D-C1D-ND	7.58	115.69	110.10
23	B	611	CLA	CHD-C4C-C3C	-7.55	113.74	124.84
23	c	509	CLA	O2D-CGD-CBD	7.55	124.68	111.27
23	A	404[A]	CLA	C2D-C1D-ND	7.53	115.66	110.10
23	b	601	CLA	C2B-C1B-NB	7.52	115.28	110.23
23	b	612	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	C	513	CLA	C2B-C1B-NB	7.49	115.25	110.23
23	c	503	CLA	C2B-C1B-NB	7.48	115.25	110.23
23	C	511	CLA	CMD-C2D-C1D	7.47	137.88	124.71
23	B	609	CLA	C2B-C1B-NB	7.46	115.23	110.23
24	a	406[B]	PHO	O2D-CGD-CBD	7.44	120.42	111.00
23	c	509	CLA	C2D-C1D-ND	7.41	115.56	110.10
23	b	616	CLA	C2B-C1B-NB	7.40	115.19	110.23
23	C	503	CLA	C2D-C1D-ND	7.40	115.56	110.10
23	a	404[B]	CLA	C2B-C1B-NB	7.38	115.18	110.23
23	B	606	CLA	C4A-NA-C1A	-7.38	103.39	106.71
24	A	416[A]	PHO	O2D-CGD-CBD	7.38	120.34	111.00
23	C	514	CLA	C2B-C1B-NB	7.34	115.15	110.23
23	B	616	CLA	O2D-CGD-CBD	7.30	124.24	111.27
23	b	606	CLA	C2B-C1B-NB	7.30	115.12	110.23
23	c	506	CLA	C2B-C1B-NB	7.29	115.12	110.23
34	b	623	HTG	C1'-S1-C1	7.28	113.70	100.09
23	c	510	CLA	C2D-C1D-ND	7.28	115.47	110.10
23	C	511	CLA	C2D-C1D-ND	7.27	115.47	110.10
23	C	504	CLA	C2B-C1B-NB	7.27	115.11	110.23
24	A	416[B]	PHO	O2D-CGD-CBD	7.26	120.20	111.00
23	d	403[B]	CLA	C2D-C1D-ND	7.25	115.45	110.10
23	c	509	CLA	CMD-C2D-C1D	7.24	137.48	124.71
23	c	512	CLA	C2B-C1B-NB	7.23	115.08	110.23
23	b	615	CLA	C2B-C1B-NB	7.22	115.07	110.23
23	b	602	CLA	C2D-C1D-ND	7.21	115.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	414[B]	PHO	C2B-C1B-NB	7.21	114.50	109.53
24	a	414[A]	PHO	O2D-CGD-CBD	7.21	120.13	111.00
24	A	416[B]	PHO	C4D-ND-C1D	-7.20	101.50	108.83
23	A	404[A]	CLA	C2B-C1B-NB	7.20	115.06	110.23
23	A	406[B]	CLA	C2B-C1B-NB	7.20	115.06	110.23
23	c	510	CLA	C2B-C1B-NB	7.19	115.06	110.23
24	a	414[B]	PHO	O2D-CGD-CBD	7.18	120.10	111.00
23	B	603	CLA	O2D-CGD-CBD	7.17	124.01	111.27
23	b	608	CLA	C2B-C1B-NB	7.16	115.03	110.23
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	a	405[B]	CLA	C2B-C1B-NB	7.14	115.02	110.23
23	c	504	CLA	C2B-C1B-NB	7.13	115.01	110.23
24	A	416[A]	PHO	C2B-C1B-NB	7.12	114.44	109.53
23	B	606	CLA	CHD-C1D-ND	-7.12	117.91	124.45
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	416[B]	PHO	C2B-C1B-NB	7.09	114.42	109.53
23	C	507	CLA	C2D-C1D-ND	7.08	115.32	110.10
24	a	414[A]	PHO	C4D-ND-C1D	-7.08	101.62	108.83
23	C	512	CLA	C2B-C1B-NB	7.07	114.97	110.23
23	a	407	CLA	C2B-C1B-NB	7.06	114.96	110.23
23	B	604	CLA	C1D-ND-C4D	-7.06	101.32	106.33
23	C	511	CLA	C2B-C1B-NB	7.04	114.95	110.23
23	d	404	CLA	CMD-C2D-C1D	7.03	137.09	124.71
23	D	403	CLA	C2B-C1B-NB	7.01	114.93	110.23
23	B	605	CLA	CHD-C4C-C3C	-7.00	114.55	124.84
23	a	404[A]	CLA	C2B-C1B-NB	6.99	114.92	110.23
23	b	609	CLA	CHD-C4C-C3C	-6.97	114.60	124.84
23	A	404[B]	CLA	C2D-C1D-ND	6.96	115.23	110.10
23	C	508	CLA	CMD-C2D-C1D	6.95	136.97	124.71
23	b	605	CLA	CHD-C4C-C3C	-6.93	114.65	124.84
23	A	404[B]	CLA	C2B-C1B-NB	6.93	114.88	110.23
26	F	102	SQD	O6-C1-C2	6.92	119.10	108.30
24	A	407[A]	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	B	610	CLA	O2D-CGD-CBD	6.90	123.54	111.27
23	c	505	CLA	C2B-C1B-NB	6.90	114.86	110.23
24	a	414[A]	PHO	C1C-C2C-C3C	-6.90	102.87	108.61
23	c	503	CLA	CHD-C1D-ND	-6.89	118.12	124.45
23	b	603	CLA	C2B-C1B-NB	6.89	114.85	110.23
23	c	509	CLA	CHD-C1D-ND	-6.89	118.12	124.45
23	C	503	CLA	C2B-C1B-NB	6.88	114.84	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	CMD-C2D-C1D	6.88	136.84	124.71
23	c	508	CLA	C2B-C1B-NB	6.87	114.84	110.23
23	b	605	CLA	CMD-C2D-C1D	6.87	136.83	124.71
23	a	405[A]	CLA	C2B-C1B-NB	6.86	114.83	110.23
23	c	505	CLA	CMD-C2D-C1D	6.86	136.79	124.71
23	c	505	CLA	C4A-NA-C1A	-6.85	103.62	106.71
23	b	605	CLA	C2B-C1B-NB	6.85	114.83	110.23
24	A	407[A]	PHO	C4D-ND-C1D	-6.85	101.86	108.83
23	C	506	CLA	C2D-C1D-ND	6.85	115.15	110.10
24	a	406[B]	PHO	C1C-C2C-C3C	-6.84	102.92	108.61
23	b	616	CLA	O2D-CGD-CBD	6.84	123.41	111.27
23	B	610	CLA	C2B-C1B-NB	6.83	114.81	110.23
23	C	504	CLA	CMD-C2D-C1D	6.83	136.75	124.71
23	c	503	CLA	CMD-C2D-C1D	6.82	136.74	124.71
23	b	609	CLA	C2B-C1B-NB	6.82	114.80	110.23
23	b	615	CLA	C4A-NA-C1A	-6.81	103.64	106.71
23	C	513	CLA	C4A-NA-C1A	-6.80	103.65	106.71
23	c	515	CLA	CMD-C2D-C1D	6.79	136.67	124.71
23	C	502	CLA	C2B-C1B-NB	6.76	114.77	110.23
23	b	613	CLA	C2B-C1B-NB	6.76	114.77	110.23
24	a	414[B]	PHO	C4D-ND-C1D	-6.76	101.96	108.83
23	B	608	CLA	C2B-C1B-NB	6.75	114.76	110.23
23	c	507	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	A	405[B]	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	d	402[B]	CLA	C2B-C1B-NB	6.74	114.75	110.23
23	C	507	CLA	CMD-C2D-C1D	6.74	136.59	124.71
23	b	611	CLA	C2B-C1B-NB	6.73	114.74	110.23
23	c	511	CLA	C2B-C1B-NB	6.73	114.74	110.23
24	A	407[B]	PHO	C4D-ND-C1D	-6.73	101.99	108.83
23	A	405[A]	CLA	C2B-C1B-NB	6.70	114.72	110.23
23	C	505	CLA	C2C-C1C-NC	6.68	116.23	109.97
23	b	616	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	b	606	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	d	402[A]	CLA	C2B-C1B-NB	6.67	114.71	110.23
23	B	616	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	C	507	CLA	C2C-C1C-NC	6.66	116.21	109.97
23	C	509	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	B	604	CLA	C2C-C1C-NC	6.65	116.20	109.97
23	B	614	CLA	C2B-C1B-NB	6.64	114.68	110.23
23	D	402[B]	CLA	CMD-C2D-C1D	6.64	136.41	124.71
23	b	616	CLA	CMD-C2D-C1D	6.63	136.39	124.71
23	b	601	CLA	O2D-CGD-CBD	6.63	123.04	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	CHD-C4C-C3C	-6.62	115.11	124.84
23	A	404[A]	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	b	606	CLA	CMD-C2D-C1D	6.62	136.38	124.71
23	c	513	CLA	C2B-C1B-NB	6.61	114.66	110.23
23	C	507	CLA	C2B-C1B-NB	6.60	114.66	110.23
23	b	605	CLA	CHD-C1D-ND	-6.60	118.39	124.45
23	b	610	CLA	C2B-C1B-NB	6.58	114.65	110.23
23	b	613	CLA	CHD-C4C-C3C	-6.58	115.16	124.84
24	A	416[A]	PHO	C1C-C2C-C3C	-6.58	103.14	108.61
23	d	404	CLA	CHD-C1D-ND	-6.57	118.41	124.45
23	c	514	CLA	C4A-NA-C1A	-6.56	103.76	106.71
23	b	615	CLA	CMD-C2D-C1D	6.56	136.28	124.71
23	b	616	CLA	C4A-NA-C1A	-6.56	103.76	106.71
23	c	513	CLA	CHD-C4C-C3C	-6.55	115.20	124.84
23	D	402[B]	CLA	C2B-C1B-NB	6.55	114.62	110.23
23	D	402[A]	CLA	C4A-NA-C1A	-6.52	103.77	106.71
23	d	403[A]	CLA	C2C-C1C-NC	6.51	116.07	109.97
23	A	404[B]	CLA	CMD-C2D-C1D	6.50	136.17	124.71
23	B	614	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	D	402[A]	CLA	CMD-C2D-C1D	6.46	136.10	124.71
23	B	603	CLA	C2B-C1B-NB	6.46	114.56	110.23
23	c	515	CLA	CHD-C1D-ND	-6.46	118.52	124.45
23	c	504	CLA	C2C-C1C-NC	6.46	116.02	109.97
24	A	407[B]	PHO	C1C-C2C-C3C	-6.46	103.24	108.61
23	C	506	CLA	C2B-C1B-NB	6.45	114.56	110.23
23	d	402[B]	CLA	CHD-C4C-C3C	-6.44	115.38	124.84
23	a	404[B]	CLA	CMD-C2D-C1D	6.43	136.05	124.71
23	B	601	CLA	CMD-C2D-C1D	6.43	136.04	124.71
23	C	510	CLA	CHD-C1D-ND	-6.43	118.55	124.45
23	C	508	CLA	CHD-C4C-C3C	-6.42	115.40	124.84
24	A	416[A]	PHO	C4D-ND-C1D	-6.42	102.30	108.83
24	a	406[A]	PHO	C2B-C1B-NB	6.41	113.95	109.53
23	B	614	CLA	CMD-C2D-C1D	6.40	136.00	124.71
23	B	616	CLA	C2B-C1B-NB	6.40	114.53	110.23
23	c	512	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	d	403[B]	CLA	C2B-C1B-NB	6.40	114.52	110.23
23	B	605	CLA	CMD-C2D-C1D	6.40	135.98	124.71
23	B	602	CLA	CHD-C4C-C3C	-6.38	115.46	124.84
23	c	507	CLA	O2D-CGD-CBD	6.38	122.60	111.27
23	c	512	CLA	C4A-NA-C1A	-6.37	103.84	106.71
23	B	611	CLA	CMD-C2D-C1D	6.37	135.94	124.71
23	a	404[B]	CLA	C2C-C1C-NC	6.37	115.94	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	CHD-C1D-ND	-6.37	118.60	124.45
23	B	603	CLA	CHD-C4C-C3C	-6.36	115.49	124.84
23	C	504	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
23	C	504	CLA	CHD-C1D-ND	-6.35	118.62	124.45
23	B	604	CLA	C2B-C1B-NB	6.35	114.49	110.23
23	C	509	CLA	C2C-C1C-NC	6.34	115.91	109.97
24	a	406[A]	PHO	C4D-ND-C1D	-6.34	102.38	108.83
23	a	405[A]	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	b	611	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	b	602	CLA	O2D-CGD-CBD	6.33	122.52	111.27
23	d	403[B]	CLA	C2C-C1C-NC	6.33	115.90	109.97
23	c	506	CLA	CHD-C1D-ND	-6.33	118.64	124.45
23	D	402[B]	CLA	CHD-C1D-ND	-6.32	118.64	124.45
23	c	509	CLA	C2B-C1B-NB	6.32	114.47	110.23
24	a	414[B]	PHO	C1C-C2C-C3C	-6.31	103.36	108.61
23	B	601	CLA	CHD-C4C-C3C	-6.31	115.56	124.84
23	a	405[B]	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
23	c	509	CLA	C4A-NA-C1A	-6.31	103.87	106.71
23	a	405[A]	CLA	CHD-C1D-ND	-6.31	118.66	124.45
23	C	509	CLA	CHD-C4C-C3C	-6.30	115.58	124.84
23	b	607	CLA	C2C-C1C-NC	6.30	115.87	109.97
23	b	601	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	b	612	CLA	C2B-C1B-NB	6.29	114.45	110.23
23	A	404[B]	CLA	C4A-NA-C1A	-6.29	103.88	106.71
23	B	613	CLA	C2B-C1B-NB	6.27	114.44	110.23
23	a	407	CLA	CHD-C4C-C3C	-6.26	115.63	124.84
23	D	402[A]	CLA	C2C-C1C-NC	6.26	115.84	109.97
23	a	404[A]	CLA	C2C-C1C-NC	6.26	115.83	109.97
23	c	506	CLA	CMD-C2D-C1D	6.26	135.74	124.71
24	A	407[A]	PHO	C2B-C1B-NB	6.25	113.84	109.53
23	C	505	CLA	C2B-C1B-NB	6.25	114.42	110.23
23	c	512	CLA	CMD-C2D-C1D	6.24	135.71	124.71
23	B	615	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	B	612	CLA	CHD-C4C-C3C	-6.24	115.67	124.84
23	A	406[B]	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	d	403[B]	CLA	CMD-C2D-C1D	6.23	135.68	124.71
23	c	505	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	c	508	CLA	CMD-C2D-C1D	6.22	135.67	124.71
23	c	504	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	d	402[A]	CLA	CHD-C4C-C3C	-6.22	115.70	124.84
23	D	402[B]	CLA	C4A-NA-C1A	-6.21	103.91	106.71
23	b	611	CLA	CHD-C1D-ND	-6.21	118.75	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	CMD-C2D-C1D	6.21	135.66	124.71
23	C	507	CLA	CHD-C1D-ND	-6.21	118.75	124.45
23	A	408	CLA	CMD-C2D-C1D	6.19	135.63	124.71
23	C	502	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	a	404[A]	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	b	611	CLA	CHD-C4C-C3C	-6.18	115.75	124.84
23	B	606	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	C	508	CLA	C2B-C1B-NB	6.18	114.37	110.23
24	a	406[B]	PHO	C4D-ND-C1D	-6.18	102.55	108.83
23	B	603	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	b	612	CLA	CHD-C4C-C3C	-6.17	115.77	124.84
23	D	402[A]	CLA	CHD-C1D-ND	-6.16	118.79	124.45
23	B	605	CLA	C4A-NA-C1A	-6.16	103.94	106.71
24	A	407[A]	PHO	C1C-C2C-C3C	-6.15	103.49	108.61
23	b	607	CLA	CHD-C4C-C3C	-6.15	115.80	124.84
26	B	620	SQD	O6-C1-C2	6.14	117.89	108.30
23	b	601	CLA	CHD-C4C-C3C	-6.14	115.81	124.84
26	F	102	SQD	O47-C7-C8	6.14	124.73	111.50
23	B	612	CLA	CHD-C1D-ND	-6.14	118.82	124.45
23	b	606	CLA	C4A-NA-C1A	-6.13	103.95	106.71
23	b	614	CLA	CHD-C4C-C3C	-6.13	115.83	124.84
23	B	606	CLA	C2B-C1B-NB	6.12	114.33	110.23
23	b	601	CLA	CMD-C2D-C1D	6.11	135.49	124.71
23	b	603	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	B	604	CLA	C2D-C1D-ND	6.11	114.61	110.10
34	c	523	HTG	C1'-S1-C1	6.11	111.51	100.09
23	B	615	CLA	C4A-NA-C1A	-6.10	103.96	106.71
23	b	611	CLA	C4A-NA-C1A	-6.09	103.97	106.71
23	C	514	CLA	CHD-C4C-C3C	-6.09	115.88	124.84
23	C	508	CLA	O2D-CGD-CBD	6.09	122.09	111.27
23	b	603	CLA	CMD-C2D-C1D	6.09	135.44	124.71
23	c	508	CLA	CHD-C1D-ND	-6.08	118.86	124.45
23	B	605	CLA	C2B-C1B-NB	6.08	114.31	110.23
23	A	404[A]	CLA	C2C-C1C-NC	6.08	115.67	109.97
23	B	606	CLA	O2D-CGD-CBD	6.08	122.07	111.27
23	A	405[B]	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	B	602	CLA	C2B-C1B-NB	6.07	114.30	110.23
23	a	404[B]	CLA	CHD-C1D-ND	-6.07	118.88	124.45
23	D	403	CLA	CHD-C4C-C3C	-6.07	115.92	124.84
23	c	509	CLA	CHD-C4C-C3C	-6.06	115.93	124.84
34	d	411	HTG	C1'-S1-C1	6.05	111.41	100.09
23	C	510	CLA	CMD-C2D-C1D	6.05	135.38	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	508	CLA	CHD-C1D-ND	-6.05	118.90	124.45
23	B	615	CLA	CMD-C2D-C1D	6.04	135.36	124.71
23	c	511	CLA	CMD-C2D-C1D	6.04	135.36	124.71
23	b	609	CLA	C4A-NA-C1A	-6.04	103.99	106.71
26	A	410[A]	SQD	O6-C1-C2	6.03	117.72	108.30
23	B	608	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
23	b	610	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	c	513	CLA	CMD-C2D-C1D	6.03	135.34	124.71
23	A	408	CLA	CHD-C4C-C3C	-6.03	115.98	124.84
23	b	604	CLA	O2D-CGD-CBD	6.03	121.98	111.27
23	d	403[A]	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	B	609	CLA	CHD-C1D-ND	-6.02	118.92	124.45
26	A	410[B]	SQD	O6-C1-C2	6.02	117.70	108.30
23	B	602	CLA	O2D-CGD-CBD	6.01	121.94	111.27
40	V	201	HEC	C1D-ND-C4D	6.01	111.28	105.07
23	a	405[B]	CLA	CHD-C1D-ND	-6.00	118.94	124.45
24	A	416[B]	PHO	C1C-C2C-C3C	-6.00	103.62	108.61
23	C	511	CLA	CHD-C1D-ND	-5.99	118.95	124.45
23	B	610	CLA	CMD-C2D-C1D	5.99	135.26	124.71
23	C	512	CLA	CHD-C4C-C3C	-5.98	116.04	124.84
23	A	406[A]	CLA	CHD-C4C-C3C	-5.98	116.05	124.84
23	b	604	CLA	C2C-C1C-NC	5.98	115.58	109.97
23	d	404	CLA	CHD-C4C-C3C	-5.97	116.06	124.84
23	B	601	CLA	O2D-CGD-CBD	5.96	121.86	111.27
23	c	514	CLA	CHD-C1D-ND	-5.96	118.98	124.45
23	C	506	CLA	CMD-C2D-C1D	5.95	135.21	124.71
23	c	507	CLA	CHD-C4C-C3C	-5.95	116.09	124.84
23	b	610	CLA	CMD-C2D-C1D	5.95	135.19	124.71
23	C	506	CLA	CHD-C4C-C3C	-5.94	116.10	124.84
23	c	510	CLA	C2C-C1C-NC	5.94	115.54	109.97
24	a	406[B]	PHO	C2B-C1B-NB	5.93	113.62	109.53
23	A	406[B]	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	C	510	CLA	CHD-C4C-C3C	-5.92	116.13	124.84
23	B	609	CLA	CMD-C2D-C1D	5.92	135.15	124.71
23	C	502	CLA	CMD-C2D-C1D	5.92	135.14	124.71
34	D	410	HTG	C1'-S1-C1	5.91	111.15	100.09
23	C	502	CLA	O2D-CGD-CBD	5.91	121.76	111.27
23	c	514	CLA	CMD-C2D-C1D	5.90	135.12	124.71
23	c	511	CLA	C1-C2-C3	-5.90	115.84	126.04
23	b	608	CLA	CHD-C1D-ND	-5.90	119.03	124.45
23	c	506	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	A	405[A]	CLA	CHD-C4C-C3C	-5.89	116.18	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	CHD-C1D-ND	-5.89	119.04	124.45
23	A	408	CLA	C2C-C1C-NC	5.89	115.49	109.97
29	A	414[A]	PL9	C7-C8-C9	-5.89	116.99	126.79
23	B	605	CLA	CHD-C1D-ND	-5.89	119.05	124.45
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
25	D	404	BCR	C7-C8-C9	-5.88	117.36	126.23
23	b	602	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	b	604	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	B	610	CLA	CHD-C4C-C3C	-5.87	116.22	124.84
23	D	402[A]	CLA	C2B-C1B-NB	5.87	114.17	110.23
23	A	404[B]	CLA	C2C-C1C-NC	5.86	115.47	109.97
23	c	505	CLA	CHD-C1D-ND	-5.86	119.07	124.45
23	C	512	CLA	CMD-C2D-C1D	5.85	135.03	124.71
23	C	514	CLA	CHD-C1D-ND	-5.85	119.08	124.45
23	C	511	CLA	C2C-C1C-NC	5.85	115.45	109.97
23	C	503	CLA	C2C-C1C-NC	5.84	115.45	109.97
23	d	402[B]	CLA	CMD-C2D-C1D	5.84	135.00	124.71
23	c	515	CLA	C4A-NA-C1A	-5.84	104.08	106.71
23	b	610	CLA	O2D-CGD-CBD	5.84	121.64	111.27
23	B	603	CLA	CMD-C2D-C1D	5.83	134.99	124.71
23	A	406[B]	CLA	C4A-NA-C1A	-5.83	104.09	106.71
23	b	601	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	b	602	CLA	CMD-C2D-C1D	5.83	134.98	124.71
23	b	603	CLA	CHD-C1D-ND	-5.83	119.10	124.45
23	b	604	CLA	C2B-C1B-NB	5.82	114.14	110.23
23	B	615	CLA	C2B-C1B-NB	5.82	114.13	110.23
23	b	608	CLA	C2C-C1C-NC	5.82	115.42	109.97
23	b	602	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	615	CLA	C2C-C1C-NC	5.80	115.41	109.97
23	C	503	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	C	502	CLA	CHD-C4C-C3C	-5.79	116.33	124.84
23	b	612	CLA	C2C-C1C-NC	5.79	115.40	109.97
23	B	615	CLA	CHD-C1D-ND	-5.79	119.14	124.45
23	C	506	CLA	C2C-C1C-NC	5.78	115.39	109.97
23	b	613	CLA	C4A-NA-C1A	-5.78	104.11	106.71
23	b	614	CLA	O2D-CGD-CBD	5.77	121.51	111.27
23	b	609	CLA	CMD-C2D-C1D	5.76	134.86	124.71
23	D	402[B]	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	c	511	CLA	C2C-C1C-NC	5.75	115.36	109.97
23	a	404[A]	CLA	CMD-C2D-C1D	5.75	134.84	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[A]	CLA	C4A-NA-C1A	-5.75	104.12	106.71
23	A	405[B]	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	b	613	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	B	609	CLA	CHD-C4C-C3C	-5.74	116.41	124.84
23	b	614	CLA	CMD-C2D-C1D	5.73	134.81	124.71
29	A	414[B]	PL9	C7-C8-C9	-5.73	117.26	126.79
23	A	406[A]	CLA	C4A-NA-C1A	-5.72	104.13	106.71
23	b	606	CLA	CHD-C1D-ND	-5.72	119.20	124.45
23	B	613	CLA	C2C-C1C-NC	5.71	115.32	109.97
23	b	606	CLA	O2D-CGD-CBD	5.70	121.40	111.27
23	b	611	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	b	615	CLA	CHD-C1D-ND	-5.69	119.22	124.45
23	d	402[B]	CLA	C2C-C1C-NC	5.69	115.30	109.97
23	A	404[B]	CLA	CHD-C1D-ND	-5.69	119.23	124.45
23	b	605	CLA	O2D-CGD-CBD	5.69	121.37	111.27
23	B	602	CLA	C2C-C1C-NC	5.68	115.29	109.97
23	B	612	CLA	CMD-C2D-C1D	5.67	134.71	124.71
23	c	515	CLA	CHD-C4C-C3C	-5.67	116.51	124.84
23	B	612	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	c	508	CLA	C2C-C1C-NC	5.66	115.28	109.97
23	A	405[B]	CLA	CMD-C2D-C1D	5.65	134.68	124.71
23	a	407	CLA	CHD-C1D-ND	-5.65	119.26	124.45
40	v	201	HEC	C1D-ND-C4D	5.65	110.91	105.07
23	B	608	CLA	C2C-C1C-NC	5.65	115.26	109.97
23	b	611	CLA	O2D-CGD-CBD	5.64	121.29	111.27
23	d	403[A]	CLA	CMD-C2D-C1D	5.64	134.65	124.71
23	B	614	CLA	C2C-C1C-NC	5.64	115.25	109.97
24	A	407[B]	PHO	C2B-C1B-NB	5.64	113.42	109.53
23	B	607	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	B	607	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
23	b	605	CLA	C4A-NA-C1A	-5.63	104.18	106.71
23	C	502	CLA	CHD-C1D-ND	-5.62	119.29	124.45
23	A	406[B]	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
23	D	402[B]	CLA	CHD-C4C-C3C	-5.61	116.60	124.84
23	d	402[A]	CLA	C2C-C1C-NC	5.61	115.22	109.97
23	C	513	CLA	O2D-CGD-CBD	5.61	121.23	111.27
23	c	511	CLA	CHD-C4C-C3C	-5.60	116.60	124.84
23	B	616	CLA	C4A-NA-C1A	-5.59	104.19	106.71
23	B	614	CLA	CHD-C1D-ND	-5.58	119.32	124.45
23	B	616	CLA	C3C-C4C-NC	5.58	116.83	110.57
26	a	409[A]	SQD	O6-C1-C2	5.58	117.02	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	C2C-C1C-NC	5.58	115.19	109.97
23	D	403	CLA	C4A-NA-C1A	-5.57	104.20	106.71
23	B	613	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	b	603	CLA	C4A-NA-C1A	-5.57	104.20	106.71
26	A	410[A]	SQD	C1-O5-C5	-5.56	102.77	113.69
23	b	607	CLA	CMD-C2D-C1D	5.56	134.51	124.71
23	d	403[A]	CLA	CHD-C1D-ND	-5.56	119.35	124.45
23	c	507	CLA	C2C-C1C-NC	5.56	115.18	109.97
23	a	405[A]	CLA	C4A-NA-C1A	-5.55	104.21	106.71
23	B	611	CLA	O2D-CGD-CBD	5.55	121.13	111.27
23	d	403[A]	CLA	CHD-C4C-C3C	-5.55	116.69	124.84
23	D	403	CLA	CMD-C2D-C1D	5.55	134.49	124.71
24	a	414[B]	PHO	C1-C2-C3	-5.53	116.47	126.04
23	D	402[A]	CLA	CHD-C4C-C3C	-5.53	116.71	124.84
23	A	405[A]	CLA	CHD-C1D-ND	-5.53	119.37	124.45
23	C	503	CLA	C4A-NA-C1A	-5.53	104.22	106.71
23	c	508	CLA	CHD-C4C-C3C	-5.53	116.72	124.84
23	C	510	CLA	C2C-C1C-NC	5.52	115.14	109.97
23	d	403[B]	CLA	CHD-C1D-ND	-5.52	119.38	124.45
23	c	503	CLA	CHD-C4C-C3C	-5.52	116.73	124.84
23	a	405[B]	CLA	CMD-C2D-C1D	5.50	134.41	124.71
23	B	601	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	d	402[B]	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	B	615	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	B	610	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	b	613	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	c	514	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
23	b	608	CLA	CHD-C4C-C3C	-5.47	116.80	124.84
23	C	511	CLA	O2D-CGD-CBD	5.47	120.99	111.27
23	c	507	CLA	C4A-NA-C1A	-5.47	104.25	106.71
23	B	616	CLA	C2C-C1C-NC	5.46	115.09	109.97
23	C	514	CLA	C2C-C1C-NC	5.46	115.09	109.97
38	E	102	HEM	CAD-CBD-CGD	5.46	125.35	113.60
23	C	505	CLA	CHD-C1D-ND	-5.46	119.44	124.45
23	b	607	CLA	C3C-C4C-NC	5.46	116.69	110.57
23	c	514	CLA	O2D-CGD-CBD	5.45	120.96	111.27
23	B	607	CLA	C4A-NA-C1A	-5.45	104.26	106.71
23	c	506	CLA	O2D-CGD-CBD	5.45	120.95	111.27
23	b	615	CLA	CHD-C4C-C3C	-5.44	116.84	124.84
23	c	512	CLA	CHD-C1D-ND	-5.44	119.45	124.45
23	B	608	CLA	CMD-C2D-C1D	5.44	134.30	124.71
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	512	CLA	C2C-C1C-NC	5.44	115.07	109.97
23	b	607	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	a	404[B]	CLA	CHD-C4C-C3C	-5.43	116.85	124.84
23	C	503	CLA	CMD-C2D-C1D	5.43	134.28	124.71
23	C	514	CLA	CMD-C2D-C1D	5.42	134.27	124.71
23	C	511	CLA	CHD-C4C-C3C	-5.42	116.88	124.84
23	B	611	CLA	C3D-C2D-C1D	-5.42	98.44	105.83
23	B	605	CLA	O2D-CGD-CBD	5.42	120.89	111.27
23	c	511	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	c	513	CLA	CHD-C1D-ND	-5.40	119.49	124.45
23	B	604	CLA	CMD-C2D-C1D	5.39	134.21	124.71
23	a	404[A]	CLA	CHD-C4C-C3C	-5.39	116.92	124.84
23	d	404	CLA	O2D-CGD-CBD	5.39	120.84	111.27
23	d	403[B]	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	c	506	CLA	CHD-C4C-C3C	-5.38	116.93	124.84
23	C	505	CLA	CMD-C2D-C1D	5.38	134.19	124.71
23	B	609	CLA	C2C-C1C-NC	5.37	115.00	109.97
23	C	513	CLA	CMD-C2D-C1D	5.37	134.18	124.71
23	B	603	CLA	CHD-C1D-ND	-5.37	119.52	124.45
24	a	414[A]	PHO	C1-C2-C3	-5.37	116.76	126.04
23	B	614	CLA	C3D-C2D-C1D	-5.36	98.51	105.83
23	B	613	CLA	CMD-C2D-C1D	5.36	134.16	124.71
23	b	607	CLA	C2B-C1B-NB	5.36	113.82	110.23
23	A	405[A]	CLA	O2D-CGD-CBD	5.35	120.78	111.27
23	B	614	CLA	O2D-CGD-CBD	5.35	120.77	111.27
23	C	507	CLA	CHD-C4C-C3C	-5.35	116.98	124.84
23	a	405[A]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	a	407	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	616	CLA	CHD-C1D-ND	-5.33	119.56	124.45
26	B	620	SQD	O47-C7-C8	5.33	122.98	111.50
23	b	608	CLA	CMD-C2D-C1D	5.32	134.09	124.71
23	c	504	CLA	O2D-CGD-CBD	5.32	120.72	111.27
26	b	620	SQD	O6-C1-C2	5.31	116.60	108.30
23	C	510	CLA	C3B-C2B-C1B	-5.31	100.75	107.16
23	c	507	CLA	CMD-C2D-C1D	5.31	134.07	124.71
23	c	512	CLA	C2C-C1C-NC	5.31	114.95	109.97
23	A	405[B]	CLA	CHD-C4C-C3C	-5.31	117.04	124.84
23	c	515	CLA	C2C-C1C-NC	5.31	114.94	109.97
23	b	609	CLA	CHD-C1D-ND	-5.31	119.58	124.45
26	a	409[B]	SQD	O6-C1-C2	5.30	116.57	108.30
23	a	404[A]	CLA	CHD-C1D-ND	-5.29	119.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	C4A-NA-C1A	-5.29	104.33	106.71
23	C	503	CLA	CHD-C1D-ND	-5.29	119.60	124.45
23	C	506	CLA	O2D-CGD-CBD	5.28	120.65	111.27
23	c	510	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
23	D	403	CLA	O2D-CGD-CBD	5.26	120.61	111.27
23	B	615	CLA	C3D-C2D-C1D	-5.25	98.66	105.83
23	C	512	CLA	CHD-C1D-ND	-5.25	119.63	124.45
23	b	614	CLA	C2C-C1C-NC	5.25	114.89	109.97
23	C	505	CLA	CHD-C4C-C3C	-5.25	117.13	124.84
26	A	410[A]	SQD	C1-C2-C3	-5.25	99.07	110.00
23	B	608	CLA	CHD-C1D-ND	-5.24	119.64	124.45
23	B	606	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
23	B	602	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	B	603	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	c	507	CLA	CHD-C1D-ND	-5.22	119.66	124.45
23	c	506	CLA	C3B-C2B-C1B	-5.22	100.86	107.16
23	C	508	CLA	C4A-NA-C1A	-5.22	104.36	106.71
25	t	102	BCR	C33-C5-C6	-5.22	118.67	124.53
23	b	605	CLA	C2C-C1C-NC	5.21	114.86	109.97
23	C	512	CLA	C4A-NA-C1A	-5.21	104.36	106.71
26	a	409[A]	SQD	O47-C7-C8	5.21	122.73	111.50
23	B	607	CLA	C2B-C1B-NB	5.21	113.72	110.23
23	a	405[B]	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	C	509	CLA	C3C-C4C-NC	5.20	116.40	110.57
23	B	616	CLA	C3D-C2D-C1D	-5.20	98.74	105.83
23	b	604	CLA	CMD-C2D-C1D	5.19	133.87	124.71
23	A	404[B]	CLA	CHD-C4C-C3C	-5.19	117.21	124.84
23	a	407	CLA	O2D-CGD-CBD	5.19	120.49	111.27
23	A	405[A]	CLA	C3D-C2D-C1D	-5.19	98.75	105.83
23	d	402[A]	CLA	CMD-C2D-C1D	5.19	133.85	124.71
23	B	610	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
23	a	407	CLA	C2C-C1C-NC	5.18	114.83	109.97
23	B	604	CLA	CHD-C4C-C3C	-5.18	117.23	124.84
23	b	605	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
23	B	611	CLA	CHD-C1D-ND	-5.18	119.70	124.45
24	A	407[A]	PHO	C3D-C4D-ND	5.17	114.77	107.72
23	B	613	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	B	602	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	B	604	CLA	C4A-NA-C1A	-5.17	104.38	106.71
23	c	510	CLA	CMD-C2D-C1D	5.17	133.82	124.71
23	C	512	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
23	B	608	CLA	C3D-C2D-C1D	-5.16	98.79	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	613	CLA	C3D-C2D-C1D	-5.16	98.79	105.83
34	B	622	HTG	C1'-S1-C1	5.16	109.74	100.09
23	c	504	CLA	C3B-C2B-C1B	-5.16	100.93	107.16
25	d	405	BCR	C7-C8-C9	-5.15	118.45	126.23
26	F	102	SQD	C1-O5-C5	-5.15	103.58	113.69
23	b	616	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
25	Y	101	BCR	C33-C5-C6	-5.15	118.75	124.53
23	c	503	CLA	O2D-CGD-CBD	5.15	120.41	111.27
23	B	613	CLA	C1-C2-C3	-5.14	117.15	126.04
23	B	607	CLA	CMD-C2D-C1D	5.14	133.78	124.71
23	A	406[B]	CLA	O2D-CGD-CBD	5.14	120.40	111.27
23	b	611	CLA	C3D-C2D-C1D	-5.13	98.84	105.83
24	a	414[B]	PHO	C3D-C4D-ND	5.13	114.71	107.72
23	b	610	CLA	CHD-C1D-ND	-5.12	119.75	124.45
23	D	402[A]	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	d	404	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	b	614	CLA	C3D-C2D-C1D	-5.12	98.84	105.83
23	b	606	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	C	507	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	A	408	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	c	514	CLA	C3B-C2B-C1B	-5.10	101.01	107.16
23	b	612	CLA	C4A-NA-C1A	-5.10	104.41	106.71
23	C	506	CLA	C3C-C4C-NC	5.10	116.29	110.57
24	a	414[A]	PHO	C3D-C4D-ND	5.09	114.66	107.72
23	c	505	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	B	613	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	b	604	CLA	CHD-C1D-ND	-5.08	119.79	124.45
23	c	511	CLA	O2D-CGD-CBD	5.06	120.27	111.27
23	C	505	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
26	b	620	SQD	O47-C7-C8	5.06	122.41	111.50
23	b	610	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	C	508	CLA	C2C-C1C-NC	5.06	114.71	109.97
23	c	509	CLA	C2C-C1C-NC	5.05	114.71	109.97
23	a	404[B]	CLA	C4A-NA-C1A	-5.05	104.43	106.71
23	d	403[B]	CLA	C4A-NA-C1A	-5.05	104.43	106.71
33	C	501	LMG	C7-O1-C1	-5.05	103.87	113.74
23	d	403[B]	CLA	O2D-CGD-CBD	5.05	120.25	111.27
23	C	508	CLA	C3B-C2B-C1B	-5.05	101.06	107.16
23	d	402[B]	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	a	407	CLA	C4A-NA-C1A	-5.05	104.44	106.71
23	D	403	CLA	CHD-C1D-ND	-5.05	119.82	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
23	b	614	CLA	CHD-C1D-ND	-5.03	119.83	124.45
23	c	512	CLA	O2D-CGD-CBD	5.02	120.20	111.27
24	A	416[B]	PHO	C3D-C4D-ND	5.02	114.57	107.72
23	C	506	CLA	CHD-C1D-ND	-5.02	119.84	124.45
23	c	503	CLA	C4A-NA-C1A	-5.02	104.45	106.71
23	B	608	CLA	O2D-CGD-CBD	5.01	120.18	111.27
23	B	603	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	B	611	CLA	CMC-C2C-C1C	5.00	132.65	125.04
23	C	504	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
23	B	607	CLA	O2D-CGD-CBD	5.00	120.15	111.27
23	B	604	CLA	C3C-C4C-NC	5.00	116.17	110.57
23	c	503	CLA	O2D-CGD-O1D	-4.99	114.08	123.84
23	b	612	CLA	CMD-C2D-C1D	4.99	133.50	124.71
23	A	408	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
23	a	405[B]	CLA	O2D-CGD-CBD	4.98	120.12	111.27
23	b	603	CLA	O2D-CGD-CBD	4.97	120.10	111.27
23	b	607	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	C	513	CLA	CHD-C1D-ND	-4.96	119.89	124.45
34	C	522	HTG	C1'-S1-C1	4.95	109.36	100.09
23	c	503	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	a	407	CLA	C3D-C2D-C1D	-4.95	99.07	105.83
23	A	406[B]	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	b	614	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
23	d	404	CLA	C3B-C2B-C1B	-4.95	101.19	107.16
23	B	605	CLA	C3D-C2D-C1D	-4.94	99.08	105.83
23	a	405[A]	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	c	503	CLA	C2C-C1C-NC	4.94	114.60	109.97
23	C	503	CLA	O2D-CGD-CBD	4.93	120.03	111.27
23	B	610	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	C	509	CLA	C4A-NA-C1A	-4.93	104.49	106.71
23	D	402[B]	CLA	O2D-CGD-CBD	4.93	120.02	111.27
23	B	616	CLA	CMD-C2D-C1D	4.92	133.39	124.71
23	b	604	CLA	C3C-C4C-NC	4.92	116.09	110.57
23	a	405[A]	CLA	C3D-C2D-C1D	-4.91	99.12	105.83
24	A	416[A]	PHO	C3D-C4D-ND	4.91	114.42	107.72
23	C	502	CLA	C2C-C1C-NC	4.91	114.57	109.97
23	b	613	CLA	C3C-C4C-NC	4.91	116.08	110.57
23	A	406[B]	CLA	C3D-C4D-ND	4.91	118.18	110.24
23	b	612	CLA	C3C-C4C-NC	4.90	116.07	110.57
23	b	609	CLA	C3C-C4C-NC	4.90	116.07	110.57
23	B	606	CLA	C2C-C1C-NC	4.90	114.56	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407[B]	PHO	C3D-C4D-ND	4.90	114.39	107.72
23	d	402[A]	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
23	C	503	CLA	C3B-C2B-C1B	-4.89	101.26	107.16
23	A	404[A]	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
23	b	602	CLA	C3B-C2B-C1B	-4.88	101.27	107.16
23	C	509	CLA	O2D-CGD-CBD	4.88	119.94	111.27
23	B	601	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
23	C	514	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
23	a	404[B]	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
23	B	604	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	404	CLA	C4A-NA-C1A	-4.87	104.52	106.71
23	b	608	CLA	C1C-C2C-C3C	-4.86	101.84	106.96
23	b	603	CLA	C2C-C1C-NC	4.85	114.52	109.97
23	c	507	CLA	C3C-C4C-NC	4.85	116.02	110.57
24	a	406[B]	PHO	C3D-C4D-ND	4.85	114.34	107.72
23	A	404[B]	CLA	C3B-C2B-C1B	-4.85	101.30	107.16
23	C	504	CLA	O2D-CGD-CBD	4.85	119.89	111.27
23	C	508	CLA	C3D-C2D-C1D	-4.85	99.21	105.83
23	A	405[A]	CLA	C4A-NA-C1A	-4.85	104.53	106.71
23	c	506	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
23	A	404[A]	CLA	CHD-C4C-C3C	-4.84	117.73	124.84
23	c	513	CLA	C2C-C1C-NC	4.84	114.50	109.97
23	b	608	CLA	C4A-NA-C1A	-4.83	104.53	106.71
23	C	512	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
26	f	102	SQD	O47-C7-C8	4.82	121.89	111.50
23	B	604	CLA	C1-C2-C3	-4.82	117.71	126.04
23	B	614	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
23	c	513	CLA	C3B-C2B-C1B	-4.82	101.35	107.16
23	c	515	CLA	C3B-C2B-C1B	-4.81	101.35	107.16
23	b	604	CLA	C1-C2-C3	-4.81	117.72	126.04
23	c	510	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
23	C	505	CLA	O2D-CGD-CBD	4.81	119.81	111.27
23	B	602	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	B	608	CLA	C3C-C4C-NC	4.80	115.96	110.57
23	B	612	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	c	504	CLA	C1C-C2C-C3C	-4.80	101.91	106.96
26	A	410[B]	SQD	C1-O5-C5	-4.79	104.29	113.69
23	B	602	CLA	C3C-C4C-NC	4.79	115.94	110.57
23	c	511	CLA	C4A-NA-C1A	-4.78	104.56	106.71
23	D	402[B]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	b	609	CLA	C3D-C2D-C1D	-4.78	99.31	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	612	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	b	615	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	c	513	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	c	504	CLA	C4A-NA-C1A	-4.77	104.56	106.71
23	D	403	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
23	c	510	CLA	C4A-NA-C1A	-4.76	104.56	106.71
23	C	507	CLA	O2D-CGD-CBD	4.76	119.73	111.27
23	B	612	CLA	C2B-C1B-NB	4.76	113.42	110.23
23	c	505	CLA	C3C-C4C-NC	4.76	115.91	110.57
23	b	607	CLA	O2D-CGD-CBD	4.76	119.73	111.27
23	c	508	CLA	C4A-NA-C1A	-4.76	104.57	106.71
23	C	506	CLA	CMB-C2B-C1B	4.75	132.60	125.37
23	B	611	CLA	C3D-C4D-ND	4.74	117.91	110.24
23	b	606	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	A	408	CLA	C4A-NA-C1A	-4.74	104.57	106.71
23	d	402[B]	CLA	C4A-NA-C1A	-4.74	104.57	106.71
23	d	404	CLA	C2C-C1C-NC	4.74	114.41	109.97
23	A	406[A]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	C	514	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
23	b	609	CLA	C2C-C1C-NC	4.74	114.41	109.97
26	A	410[B]	SQD	C1-C2-C3	-4.73	100.14	110.00
23	d	403[B]	CLA	C3B-C2B-C1B	-4.73	101.45	107.16
23	b	613	CLA	CHD-C1D-ND	-4.73	120.11	124.45
23	c	515	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
38	f	101	HEM	CHC-C4B-NB	4.72	129.54	124.42
23	A	405[B]	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	a	405[B]	CLA	C2C-C1C-NC	4.72	114.39	109.97
26	a	409[B]	SQD	O47-C7-C8	4.71	121.66	111.50
23	b	605	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	A	404[A]	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	B	605	CLA	C2C-C1C-NC	4.71	114.38	109.97
23	C	505	CLA	C4A-NA-C1A	-4.70	104.59	106.71
34	b	622	HTG	C1-O5-C5	4.69	121.24	112.58
23	b	605	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	B	607	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
23	C	513	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	C	509	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
23	B	603	CLA	C3C-C4C-NC	4.68	115.82	110.57
23	a	405[A]	CLA	C3D-C4D-ND	4.68	117.81	110.24
38	E	102	HEM	CHC-C4B-NB	4.67	129.50	124.42
23	c	510	CLA	O2D-CGD-CBD	4.67	119.57	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[B]	CLA	C3B-C2B-C1B	-4.67	101.52	107.16
23	a	405[B]	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	607	CLA	C3B-C4B-NB	4.67	114.85	110.52
23	C	505	CLA	C1C-C2C-C3C	-4.67	102.05	106.96
23	d	403[A]	CLA	C3C-C4C-NC	4.67	115.80	110.57
23	A	405[B]	CLA	C1C-C2C-C3C	-4.66	102.06	106.96
23	b	611	CLA	C3C-C4C-NC	4.66	115.79	110.57
23	c	509	CLA	C3B-C2B-C1B	-4.66	101.54	107.16
23	C	511	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
26	b	620	SQD	C1-O5-C5	-4.64	104.58	113.69
23	C	509	CLA	CMD-C2D-C1D	4.64	132.89	124.71
23	c	509	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	C	508	CLA	C3C-C4C-NC	4.64	115.77	110.57
23	c	514	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	a	407	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
23	b	616	CLA	C3B-C2B-C1B	-4.63	101.58	107.16
23	A	406[A]	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	C	512	CLA	O2D-CGD-CBD	4.62	119.49	111.27
23	c	503	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
23	b	604	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	C	504	CLA	C3B-C2B-C1B	-4.62	101.58	107.16
23	b	606	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
23	B	607	CLA	C1C-C2C-C3C	-4.62	102.10	106.96
23	D	402[B]	CLA	C3B-C2B-C1B	-4.62	101.59	107.16
23	c	508	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
23	B	601	CLA	C4A-NA-C1A	-4.62	104.63	106.71
23	d	403[B]	CLA	C3D-C4D-ND	4.61	117.70	110.24
23	B	601	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	c	512	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
29	a	412[A]	PL9	C7-C8-C9	-4.60	119.13	126.79
23	C	502	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	C	510	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
23	b	602	CLA	C3D-C4D-ND	4.60	117.68	110.24
23	B	601	CLA	C2C-C1C-NC	4.60	114.28	109.97
23	d	402[B]	CLA	C1C-C2C-C3C	-4.59	102.13	106.96
23	B	613	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	B	603	CLA	O2D-CGD-O1D	-4.58	114.88	123.84
23	a	404[A]	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	c	512	CLA	C3B-C2B-C1B	-4.58	101.64	107.16
23	a	405[A]	CLA	O2D-CGD-CBD	4.58	119.40	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[B]	CLA	O2D-CGD-CBD	4.57	119.39	111.27
23	D	403	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	D	403	CLA	C2C-C1C-NC	4.56	114.24	109.97
23	D	402[A]	CLA	O2D-CGD-CBD	4.55	119.36	111.27
23	A	406[A]	CLA	C3D-C4D-ND	4.55	117.61	110.24
23	b	604	CLA	C4A-NA-C1A	-4.55	104.66	106.71
23	A	405[A]	CLA	CMD-C2D-C1D	4.55	132.73	124.71
23	B	610	CLA	C2C-C1C-NC	4.55	114.23	109.97
23	B	605	CLA	C3C-C4C-NC	4.54	115.67	110.57
23	c	504	CLA	CHD-C1D-ND	-4.54	120.28	124.45
23	C	514	CLA	O2D-CGD-CBD	4.54	119.33	111.27
23	B	615	CLA	CMB-C2B-C1B	4.54	132.28	125.37
23	a	407	CLA	C3C-C4C-NC	4.54	115.66	110.57
25	X	101	BCR	C38-C26-C25	-4.54	119.43	124.53
23	A	408	CLA	C3D-C4D-ND	4.53	117.56	110.24
24	A	416[A]	PHO	C1-C2-C3	-4.53	118.22	126.04
23	b	601	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
23	B	608	CLA	C4A-NA-C1A	-4.52	104.67	106.71
23	c	508	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	a	407	CLA	C3D-C4D-ND	4.52	117.55	110.24
23	C	513	CLA	C2C-C1C-NC	4.52	114.20	109.97
23	b	610	CLA	C4A-NA-C1A	-4.52	104.67	106.71
23	b	601	CLA	C2C-C1C-NC	4.51	114.20	109.97
23	C	507	CLA	C1C-C2C-C3C	-4.51	102.21	106.96
23	B	611	CLA	C1D-CHD-C4C	-4.51	116.32	126.06
23	C	502	CLA	C3D-C4D-ND	4.51	117.54	110.24
23	C	510	CLA	C3D-C4D-ND	4.51	117.53	110.24
31	t	101	LMT	C3'-C4'-C5'	-4.50	100.60	110.93
23	c	513	CLA	O2D-CGD-CBD	4.50	119.27	111.27
23	C	513	CLA	C3C-C4C-NC	4.50	115.62	110.57
23	b	603	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
23	C	504	CLA	C2C-C1C-NC	4.50	114.19	109.97
23	b	603	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
23	C	510	CLA	C1-C2-C3	-4.50	118.26	126.04
23	B	614	CLA	C4A-NA-C1A	-4.50	104.69	106.71
23	a	404[B]	CLA	C3D-C4D-ND	4.49	117.50	110.24
23	d	402[A]	CLA	C1C-C2C-C3C	-4.49	102.24	106.96
23	C	513	CLA	C1D-CHD-C4C	-4.49	116.38	126.06
23	b	606	CLA	C3C-C4C-NC	4.49	115.60	110.57
23	b	613	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
23	c	508	CLA	O2D-CGD-CBD	4.49	119.24	111.27
23	a	404[A]	CLA	C3B-C2B-C1B	-4.48	101.75	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	B	607	CLA	C3D-C4D-ND	4.48	117.48	110.24
23	c	504	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
23	A	404[B]	CLA	C3D-C2D-C1D	-4.47	99.72	105.83
23	b	605	CLA	C3C-C4C-NC	4.47	115.59	110.57
23	C	513	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
23	c	503	CLA	C3D-C4D-ND	4.47	117.47	110.24
23	b	601	CLA	C3B-C2B-C1B	-4.47	101.77	107.16
23	a	405[B]	CLA	C3D-C4D-ND	4.47	117.46	110.24
23	C	510	CLA	C4A-NA-C1A	-4.47	104.70	106.71
23	B	609	CLA	C3C-C4C-NC	4.47	115.58	110.57
23	b	615	CLA	C3D-C4D-ND	4.46	117.46	110.24
23	b	610	CLA	C1-C2-C3	-4.46	118.33	126.04
23	C	509	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
23	b	615	CLA	C3B-C2B-C1B	-4.46	101.78	107.16
23	b	603	CLA	C3D-C4D-ND	4.46	117.45	110.24
23	d	404	CLA	C3D-C4D-ND	4.46	117.45	110.24
23	b	607	CLA	C1C-C2C-C3C	-4.45	102.27	106.96
23	C	507	CLA	C3D-C2D-C1D	-4.45	99.75	105.83
23	C	512	CLA	C3C-C4C-NC	4.45	115.56	110.57
23	a	404[B]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
23	C	514	CLA	C3C-C4C-NC	4.45	115.56	110.57
23	B	608	CLA	C3B-C2B-C1B	-4.45	101.79	107.16
23	b	601	CLA	C3D-C4D-ND	4.45	117.44	110.24
23	d	403[A]	CLA	C1C-C2C-C3C	-4.45	102.28	106.96
29	a	412[B]	PL9	C7-C3-C4	4.44	120.49	116.88
23	b	612	CLA	O2D-CGD-CBD	4.44	119.15	111.27
23	d	403[A]	CLA	C3D-C4D-ND	4.44	117.42	110.24
23	b	608	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
23	A	408	CLA	C3C-C4C-NC	4.43	115.54	110.57
23	B	616	CLA	O2D-CGD-O1D	-4.43	115.18	123.84
23	c	508	CLA	C3B-C2B-C1B	-4.42	101.83	107.16
23	c	505	CLA	O2D-CGD-CBD	4.42	119.12	111.27
29	A	414[B]	PL9	C32-C33-C34	-4.42	117.02	127.66
23	c	511	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
23	b	616	CLA	C3C-C4C-NC	4.41	115.52	110.57
23	C	503	CLA	C3D-C2D-C1D	-4.41	99.82	105.83
23	C	504	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	c	515	CLA	O2D-CGD-CBD	4.41	119.10	111.27
23	b	611	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	b	608	CLA	C3D-C4D-ND	4.40	117.36	110.24
33	c	522	LMG	O6-C5-C4	4.40	117.68	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	601	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	d	403[B]	CLA	C1C-C2C-C3C	-4.40	102.33	106.96
23	B	612	CLA	C3B-C2B-C1B	-4.40	101.86	107.16
23	b	610	CLA	C3C-C4C-NC	4.40	115.50	110.57
23	C	505	CLA	C3C-C4C-NC	4.39	115.50	110.57
23	D	402[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	614	CLA	O2D-CGD-O1D	-4.38	115.27	123.84
23	b	608	CLA	O2D-CGD-CBD	4.38	119.05	111.27
23	B	612	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
33	B	621	LMG	O7-C10-C11	4.38	120.94	111.50
23	B	603	CLA	C3B-C2B-C1B	-4.38	101.87	107.16
29	a	412[A]	PL9	C7-C3-C4	4.38	120.44	116.88
23	C	507	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
23	c	514	CLA	C2C-C1C-NC	4.37	114.07	109.97
23	b	610	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	B	602	CLA	C3B-C2B-C1B	-4.37	101.88	107.16
23	c	507	CLA	C3D-C4D-ND	4.37	117.31	110.24
23	c	510	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
23	B	613	CLA	C4A-NA-C1A	-4.37	104.74	106.71
23	b	611	CLA	C3D-C4D-ND	4.37	117.30	110.24
23	b	607	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	c	505	CLA	C1D-CHD-C4C	-4.36	116.65	126.06
23	b	605	CLA	O2D-CGD-O1D	-4.35	115.33	123.84
23	a	404[B]	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
23	b	603	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	B	612	CLA	C3D-C4D-ND	4.35	117.27	110.24
23	B	611	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	A	405[B]	CLA	C4A-NA-C1A	-4.35	104.75	106.71
23	C	505	CLA	C3B-C4B-NB	4.34	114.54	110.52
23	C	511	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	C	503	CLA	C3C-C4C-NC	4.34	115.43	110.57
23	c	512	CLA	C1-C2-C3	-4.33	118.55	126.04
23	B	616	CLA	CHD-C1D-ND	-4.33	120.47	124.45
23	b	612	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
23	c	511	CLA	C3D-C4D-ND	4.33	117.25	110.24
23	B	610	CLA	O2A-CGA-CBA	4.33	125.50	111.91
23	c	507	CLA	C3B-C2B-C1B	-4.33	101.93	107.16
23	c	504	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	b	614	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
23	C	506	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
23	C	514	CLA	C3D-C4D-ND	4.33	117.24	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
32	E	101[A]	LHG	O7-C7-C8	4.32	120.82	111.50
23	A	404[A]	CLA	C1C-C2C-C3C	-4.32	102.41	106.96
23	C	511	CLA	C1-C2-C3	-4.32	118.57	126.04
23	B	613	CLA	C3B-C4B-NB	4.32	114.52	110.52
23	C	507	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	B	601	CLA	C3D-C4D-ND	4.32	117.22	110.24
23	A	404[A]	CLA	C3B-C4B-NB	4.31	114.52	110.52
23	b	610	CLA	O2A-CGA-CBA	4.31	125.45	111.91
23	D	402[A]	CLA	C3C-C4C-NC	4.31	115.41	110.57
23	B	602	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	B	613	CLA	O2D-CGD-CBD	4.30	118.92	111.27
23	A	405[B]	CLA	CBC-CAC-C3C	-4.30	100.57	112.43
23	c	515	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	B	605	CLA	C3D-C4D-ND	4.30	117.19	110.24
23	D	402[B]	CLA	C3C-C4C-NC	4.30	115.39	110.57
23	c	510	CLA	CHD-C1D-ND	-4.30	120.50	124.45
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	b	616	CLA	C2C-C1C-NC	4.30	114.00	109.97
26	A	410[B]	SQD	C44-O6-C1	-4.30	105.35	113.74
23	c	504	CLA	CMD-C2D-C1D	4.30	132.28	124.71
23	B	616	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
26	A	410[B]	SQD	O9-S-C6	4.29	112.04	106.94
23	B	609	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	b	604	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	c	513	CLA	C1D-CHD-C4C	-4.29	116.80	126.06
23	a	404[A]	CLA	C1C-C2C-C3C	-4.29	102.45	106.96
23	c	512	CLA	C3C-C4C-NC	4.28	115.38	110.57
23	A	408	CLA	O2D-CGD-CBD	4.28	118.88	111.27
23	C	510	CLA	C3C-C4C-NC	4.28	115.37	110.57
33	d	412	LMG	O7-C10-C11	4.28	120.72	111.50
23	C	511	CLA	C4A-NA-C1A	-4.28	104.78	106.71
23	D	402[B]	CLA	C3D-C4D-ND	4.27	117.15	110.24
23	c	513	CLA	C4A-NA-C1A	-4.27	104.79	106.71
23	d	403[B]	CLA	C3C-C4C-NC	4.26	115.35	110.57
23	c	505	CLA	C3B-C2B-C1B	-4.26	102.02	107.16
25	y	101	BCR	C33-C5-C6	-4.26	119.75	124.53
23	A	404[B]	CLA	CAA-C2A-C3A	-4.26	101.12	112.78
23	c	509	CLA	C1C-C2C-C3C	-4.26	102.48	106.96
23	a	405[A]	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	B	610	CLA	C3C-C4C-NC	4.25	115.34	110.57
23	C	510	CLA	O2D-CGD-CBD	4.25	118.82	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	509	CLA	CHD-C1D-ND	-4.24	120.55	124.45
23	A	408	CLA	C3B-C4B-NB	4.24	114.45	110.52
23	b	602	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	A	406[B]	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
23	b	608	CLA	C3B-C4B-NB	4.24	114.45	110.52
23	b	609	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	A	405[B]	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	c	505	CLA	C3D-C4D-ND	4.23	117.09	110.24
25	d	405	BCR	C15-C14-C13	-4.23	121.27	127.31
23	A	406[B]	CLA	C3B-C2B-C1B	-4.23	102.05	107.16
38	E	102	HEM	C1B-NB-C4B	4.23	109.44	105.07
26	B	620	SQD	C3-C4-C5	4.23	117.78	110.24
33	C	501	LMG	O7-C10-C11	4.23	120.61	111.50
23	C	506	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	b	612	CLA	C4-C3-C5	4.22	122.37	115.27
23	B	615	CLA	C3C-C4C-NC	4.22	115.30	110.57
23	C	511	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	a	404[A]	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	c	514	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	b	616	CLA	C1D-CHD-C4C	-4.22	116.96	126.06
23	a	405[A]	CLA	C3B-C2B-C1B	-4.21	102.07	107.16
23	c	512	CLA	C1C-C2C-C3C	-4.21	102.53	106.96
23	B	612	CLA	O2D-CGD-O1D	-4.21	115.60	123.84
23	A	404[B]	CLA	C1D-CHD-C4C	-4.21	116.97	126.06
23	a	404[B]	CLA	C3B-C4B-NB	4.21	114.42	110.52
23	d	402[B]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	c	515	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	B	614	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	a	404[A]	CLA	C1D-CHD-C4C	-4.21	116.98	126.06
23	b	606	CLA	C1D-CHD-C4C	-4.20	116.99	126.06
23	B	613	CLA	C3B-C2B-C1B	-4.20	102.09	107.16
23	B	610	CLA	C3D-C4D-ND	4.20	117.03	110.24
33	c	501	LMG	O7-C10-C11	4.20	120.55	111.50
23	B	606	CLA	C3C-C4C-NC	4.20	115.28	110.57
25	C	515	BCR	C7-C8-C9	-4.20	119.90	126.23
23	B	611	CLA	CHD-C4C-NC	4.19	130.81	124.20
23	A	404[B]	CLA	C3B-C4B-NB	4.19	114.41	110.52
29	a	412[B]	PL9	C7-C8-C9	-4.19	119.81	126.79
23	B	607	CLA	C3C-C4C-NC	4.19	115.27	110.57
26	a	409[A]	SQD	C1-C2-C3	-4.19	101.27	110.00
23	c	507	CLA	O2D-CGD-O1D	-4.18	115.66	123.84
23	D	403	CLA	C3B-C2B-C1B	-4.18	102.11	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C3B-C2B-C1B	-4.18	102.12	107.16
23	a	404[A]	CLA	CAA-C2A-C3A	-4.18	101.34	112.78
33	c	522	LMG	O7-C10-C11	4.17	120.50	111.50
23	c	511	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
23	B	603	CLA	C1D-CHD-C4C	-4.17	117.06	126.06
23	B	604	CLA	C3B-C2B-C1B	-4.17	102.13	107.16
23	B	616	CLA	C3B-C4B-NB	4.17	114.38	110.52
23	C	503	CLA	C1C-C2C-C3C	-4.16	102.58	106.96
32	d	408[B]	LHG	O7-C7-C8	4.16	120.47	111.50
23	A	406[A]	CLA	C1C-C2C-C3C	-4.16	102.59	106.96
23	c	508	CLA	C1-C2-C3	-4.16	118.86	126.04
23	c	504	CLA	C3C-C4C-NC	4.16	115.23	110.57
23	C	511	CLA	C1C-C2C-C3C	-4.15	102.59	106.96
23	a	404[B]	CLA	C1D-CHD-C4C	-4.15	117.10	126.06
23	B	602	CLA	CMC-C2C-C1C	4.15	131.36	125.04
23	c	506	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	c	513	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	c	506	CLA	C3C-C4C-NC	4.15	115.22	110.57
23	B	603	CLA	C3D-C4D-ND	4.14	116.94	110.24
33	C	501	LMG	O1-C1-C2	4.14	114.77	108.30
23	D	402[A]	CLA	C1C-C2C-C3C	-4.14	102.60	106.96
23	C	505	CLA	C3B-C2B-C1B	-4.14	102.16	107.16
23	b	611	CLA	C1-C2-C3	-4.14	118.88	126.04
23	c	513	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	d	402[B]	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	B	615	CLA	C3D-C4D-ND	4.14	116.93	110.24
23	b	610	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
23	d	402[B]	CLA	C3B-C2B-C1B	-4.13	102.17	107.16
23	a	407	CLA	C1C-C2C-C3C	-4.13	102.61	106.96
23	b	612	CLA	C1-C2-C3	-4.13	118.90	126.04
25	d	405	BCR	C40-C30-C25	-4.13	103.60	110.30
23	A	405[B]	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
23	b	612	CLA	C3B-C4B-NB	4.13	114.34	110.52
23	b	612	CLA	CHD-C1D-ND	-4.13	120.66	124.45
23	d	403[B]	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
23	C	504	CLA	C1D-CHD-C4C	-4.12	117.16	126.06
23	c	510	CLA	C3C-C4C-NC	4.12	115.19	110.57
23	C	513	CLA	C3D-C4D-ND	4.12	116.90	110.24
23	d	402[A]	CLA	C3D-C4D-ND	4.12	116.90	110.24
38	E	102	HEM	C4C-NC-C1C	4.12	109.38	105.35
29	A	414[A]	PL9	C7-C3-C2	-4.12	117.89	123.30
23	b	614	CLA	C3D-C4D-ND	4.12	116.89	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
23	b	602	CLA	C2C-C1C-NC	4.11	113.82	109.97
23	B	606	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	B	607	CLA	C3B-C2B-C1B	-4.11	102.20	107.16
23	D	403	CLA	C3D-C4D-ND	4.11	116.89	110.24
23	B	601	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
32	E	101[B]	LHG	O7-C7-C8	4.11	120.35	111.50
23	C	504	CLA	C3C-C4C-NC	4.11	115.18	110.57
23	b	612	CLA	CAC-C3C-C4C	4.10	130.13	124.81
23	B	614	CLA	C1D-CHD-C4C	-4.10	117.21	126.06
23	c	509	CLA	C3C-C4C-NC	4.10	115.17	110.57
23	A	405[A]	CLA	C3D-C4D-ND	4.10	116.87	110.24
23	a	404[A]	CLA	C3B-C4B-NB	4.09	114.31	110.52
23	C	502	CLA	O2D-CGD-O1D	-4.09	115.83	123.84
23	c	507	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
25	b	617	BCR	C33-C5-C6	-4.09	119.94	124.53
33	Z	101	LMG	O7-C10-C11	4.09	120.31	111.50
35	C	518[B]	DGD	O2G-C1B-C2B	4.08	120.30	111.50
33	C	521	LMG	O6-C5-C4	4.08	117.10	109.69
23	B	615	CLA	C1D-CHD-C4C	-4.08	117.26	126.06
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	517[A]	DGD	O2G-C1B-C2B	4.08	120.29	111.50
23	A	406[B]	CLA	C1C-C2C-C3C	-4.08	102.67	106.96
23	b	601	CLA	C1D-CHD-C4C	-4.08	117.27	126.06
23	c	504	CLA	C1D-CHD-C4C	-4.07	117.27	126.06
26	a	409[A]	SQD	C1-O5-C5	-4.07	105.69	113.69
23	B	613	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
23	C	509	CLA	C3D-C4D-ND	4.07	116.83	110.24
23	b	609	CLA	O2D-CGD-CBD	4.07	118.50	111.27
23	D	402[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
23	a	405[B]	CLA	C3C-C4C-NC	4.07	115.13	110.57
23	C	503	CLA	C3D-C4D-ND	4.07	116.81	110.24
23	b	603	CLA	C1D-CHD-C4C	-4.06	117.29	126.06
23	A	406[A]	CLA	C3C-C4C-NC	4.06	115.13	110.57
34	b	625	HTG	C1-O5-C5	4.06	120.07	112.58
23	d	402[A]	CLA	C3C-C4C-NC	4.06	115.12	110.57
23	b	612	CLA	C1D-CHD-C4C	-4.05	117.32	126.06
25	c	516	BCR	C11-C10-C9	-4.05	121.53	127.31
38	f	101	HEM	C4C-NC-C1C	4.05	109.31	105.35
23	b	602	CLA	CMC-C2C-C1C	4.04	131.20	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	C	508	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
23	b	609	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
23	C	502	CLA	C1D-CHD-C4C	-4.02	117.38	126.06
23	b	616	CLA	C3D-C4D-ND	4.02	116.74	110.24
23	C	510	CLA	C1C-C2C-C3C	-4.02	102.73	106.96
26	f	102	SQD	C1-O5-C5	4.02	121.57	113.69
23	b	612	CLA	C3D-C4D-ND	4.02	116.73	110.24
23	C	514	CLA	C4A-NA-C1A	-4.01	104.90	106.71
23	b	603	CLA	O2D-CGD-O1D	-4.01	115.99	123.84
23	d	402[A]	CLA	C1D-CHD-C4C	-4.01	117.41	126.06
23	c	509	CLA	O2D-CGD-O1D	-4.01	116.00	123.84
33	C	521	LMG	O7-C10-C11	4.00	120.12	111.50
23	C	511	CLA	C3B-C4B-NB	4.00	114.22	110.52
23	d	404	CLA	C3C-C4C-NC	4.00	115.05	110.57
23	B	604	CLA	C1D-CHD-C4C	-4.00	117.44	126.06
23	d	403[A]	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
23	A	404[B]	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	b	602	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	b	604	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
23	C	514	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	c	515	CLA	C3C-C4C-NC	3.99	115.05	110.57
23	d	402[A]	CLA	C3B-C2B-C1B	-3.99	102.34	107.16
25	b	617	BCR	C7-C8-C9	-3.99	120.21	126.23
23	B	616	CLA	C3D-C4D-ND	3.98	116.67	110.24
23	b	614	CLA	C3C-C4C-NC	3.98	115.03	110.57
23	B	606	CLA	O2D-CGD-O1D	-3.98	116.06	123.84
23	B	602	CLA	C1D-CHD-C4C	-3.97	117.50	126.06
23	c	506	CLA	C1C-C2C-C3C	-3.96	102.79	106.96
23	B	616	CLA	C1D-CHD-C4C	-3.96	117.50	126.06
23	B	614	CLA	C3D-C4D-ND	3.96	116.65	110.24
23	b	612	CLA	C3D-C2D-C1D	-3.96	100.43	105.83
23	b	606	CLA	O2D-CGD-O1D	-3.96	116.11	123.84
23	B	616	CLA	C4C-C3C-C2C	-3.95	101.14	106.90
23	B	615	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	a	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	A	406[A]	CLA	C3B-C2B-C1B	-3.95	102.39	107.16
23	c	506	CLA	C4A-NA-C1A	-3.95	104.93	106.71
23	A	404[A]	CLA	C3C-C4C-NC	3.95	115.00	110.57
35	C	517[B]	DGD	O2G-C1B-C2B	3.94	120.00	111.50
23	B	606	CLA	C3B-C2B-C1B	-3.94	102.40	107.16
23	B	608	CLA	C3D-C4D-ND	3.94	116.61	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	K	102	BCR	C7-C8-C9	-3.94	120.28	126.23
23	B	610	CLA	O2D-CGD-O1D	-3.94	116.14	123.84
23	C	507	CLA	C3C-C4C-NC	3.94	114.98	110.57
29	d	406[A]	PL9	C42-C43-C44	-3.93	118.19	127.66
23	c	509	CLA	CMC-C2C-C1C	3.93	131.03	125.04
23	b	602	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
23	D	402[A]	CLA	C1-C2-C3	-3.93	119.25	126.04
23	a	405[A]	CLA	C1C-C2C-C3C	-3.93	102.83	106.96
23	D	403	CLA	C1D-CHD-C4C	-3.93	117.58	126.06
25	h	101	BCR	C38-C26-C25	-3.93	120.12	124.53
29	a	412[B]	PL9	C32-C33-C34	-3.93	118.21	127.66
23	B	605	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
26	F	102	SQD	O8-S-C6	3.92	111.98	105.74
23	c	509	CLA	C3D-C4D-ND	3.91	116.57	110.24
26	a	409[A]	SQD	C44-O6-C1	-3.91	106.09	113.74
23	A	405[A]	CLA	C3B-C2B-C1B	-3.91	102.44	107.16
23	d	402[B]	CLA	C3C-C4C-NC	3.91	114.95	110.57
29	A	414[A]	PL9	C7-C3-C4	3.91	120.05	116.88
23	b	613	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	b	606	CLA	C3D-C4D-ND	3.90	116.55	110.24
23	a	404[B]	CLA	CAA-C2A-C3A	-3.90	102.09	112.78
24	A	416[B]	PHO	C1-C2-C3	-3.90	119.29	126.04
23	b	614	CLA	C3B-C4B-NB	3.90	114.13	110.52
23	B	609	CLA	C3B-C2B-C1B	-3.90	102.46	107.16
29	a	412[A]	PL9	C32-C33-C34	-3.89	118.28	127.66
23	b	613	CLA	C3D-C4D-ND	3.89	116.53	110.24
23	c	507	CLA	CMB-C2B-C1B	3.89	131.29	125.37
23	c	512	CLA	C3D-C4D-ND	3.89	116.53	110.24
25	k	101	BCR	C29-C30-C25	3.89	116.47	110.48
23	B	614	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	B	602	CLA	C1C-C2C-C3C	-3.88	102.87	106.96
23	D	403	CLA	CMB-C2B-C1B	3.88	131.28	125.37
32	A	419[A]	LHG	O8-C23-O10	-3.88	113.79	123.59
23	B	602	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
35	c	518[A]	DGD	O2G-C1B-C2B	3.88	119.87	111.50
23	A	405[A]	CLA	CMC-C2C-C1C	3.88	130.95	125.04
23	B	604	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	b	611	CLA	O2D-CGD-O1D	-3.88	116.26	123.84
23	b	606	CLA	C4-C3-C5	3.87	121.78	115.27
23	c	511	CLA	C1D-CHD-C4C	-3.87	117.71	126.06
23	C	510	CLA	C3B-C4B-NB	3.87	114.10	110.52
23	d	402[A]	CLA	CAA-C2A-C3A	-3.87	102.19	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	O2A-CGA-CBA	3.87	124.05	111.91
24	A	407[A]	PHO	C1A-C2A-C3A	-3.87	99.16	102.84
23	c	510	CLA	C3D-C4D-ND	3.87	116.49	110.24
23	c	508	CLA	C3C-C4C-NC	3.86	114.90	110.57
23	c	509	CLA	CMB-C2B-C1B	3.86	131.24	125.37
38	E	102	HEM	CHD-C4C-NC	3.85	128.61	124.44
23	A	405[A]	CLA	C3C-C4C-NC	3.85	114.89	110.57
29	a	412[B]	PL9	C7-C3-C2	-3.85	118.24	123.30
23	b	608	CLA	C1-C2-C3	-3.85	119.39	126.04
23	b	615	CLA	C3C-C4C-NC	3.84	114.88	110.57
23	b	611	CLA	C3B-C4B-NB	3.84	114.08	110.52
23	C	502	CLA	C3B-C2B-C1B	-3.84	102.53	107.16
25	d	405	BCR	C29-C30-C25	3.84	116.39	110.48
29	a	412[A]	PL9	C7-C3-C2	-3.84	118.25	123.30
33	c	522	LMG	C3-C4-C5	3.83	117.08	110.24
23	b	608	CLA	C3C-C4C-NC	3.83	114.87	110.57
23	C	506	CLA	C3D-C2D-C1D	-3.83	100.61	105.83
23	b	613	CLA	C1-C2-C3	-3.83	119.42	126.04
23	b	616	CLA	O2D-CGD-O1D	-3.83	116.36	123.84
23	A	404[B]	CLA	C3D-C4D-ND	3.83	116.43	110.24
25	A	409	BCR	C24-C23-C22	-3.82	120.46	126.23
25	d	405	BCR	C38-C26-C25	-3.82	120.23	124.53
26	A	412	SQD	O47-C7-C8	3.82	119.74	111.50
23	b	613	CLA	C1C-C2C-C3C	-3.82	102.94	106.96
32	b	629[B]	LHG	O7-C7-C8	3.81	119.72	111.50
26	F	102	SQD	C44-O6-C1	-3.81	106.29	113.74
23	C	512	CLA	C3D-C4D-ND	3.81	116.40	110.24
23	c	512	CLA	C1D-CHD-C4C	-3.81	117.84	126.06
23	c	503	CLA	C3C-C4C-NC	3.81	114.84	110.57
23	C	502	CLA	C3C-C4C-NC	3.80	114.84	110.57
23	C	514	CLA	C3B-C4B-NB	3.80	114.04	110.52
23	B	613	CLA	C3D-C4D-ND	3.80	116.39	110.24
23	d	402[A]	CLA	CMB-C2B-C1B	3.80	131.16	125.37
32	A	419[A]	LHG	O7-C7-C8	3.80	119.69	111.50
24	A	416[A]	PHO	C1A-C2A-C3A	-3.80	99.22	102.84
23	a	404[B]	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	b	605	CLA	C1D-CHD-C4C	-3.80	117.86	126.06
23	b	609	CLA	C3B-C2B-C1B	-3.80	102.58	107.16
23	D	403	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
23	B	609	CLA	O2D-CGD-CBD	3.79	118.00	111.27
23	C	508	CLA	C3D-C4D-ND	3.79	116.37	110.24
26	F	102	SQD	O7-S-C6	3.79	111.44	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	C3B-C4B-NB	3.79	114.03	110.52
23	D	402[B]	CLA	C1-C2-C3	-3.79	119.50	126.04
23	b	615	CLA	C1D-CHD-C4C	-3.78	117.89	126.06
23	B	615	CLA	C3B-C2B-C1B	-3.78	102.59	107.16
23	c	504	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
23	B	610	CLA	CAA-C2A-C3A	-3.78	102.42	112.78
26	A	410[B]	SQD	O47-C7-C8	3.78	119.65	111.50
23	A	404[B]	CLA	O2D-CGD-CBD	3.78	117.99	111.27
23	B	606	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
26	A	410[A]	SQD	C44-O6-C1	-3.78	106.36	113.74
23	c	508	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	b	608	CLA	CMC-C2C-C1C	3.78	130.79	125.04
23	C	505	CLA	C3D-C4D-ND	3.77	116.34	110.24
23	B	604	CLA	C3D-C2D-C1D	-3.77	100.68	105.83
23	A	405[B]	CLA	CAA-C2A-C3A	-3.77	102.45	112.78
33	C	520	LMG	O7-C10-C11	3.77	119.63	111.50
23	A	405[A]	CLA	CBC-CAC-C3C	-3.77	102.04	112.43
23	C	512	CLA	C1D-CHD-C4C	-3.77	117.93	126.06
33	Z	101	LMG	C1-C2-C3	3.77	117.84	110.00
23	c	511	CLA	CAC-C3C-C4C	3.76	129.69	124.81
23	b	601	CLA	C3C-C4C-NC	3.76	114.79	110.57
23	b	604	CLA	C3D-C4D-ND	3.76	116.32	110.24
23	b	601	CLA	O2D-CGD-O1D	-3.76	116.49	123.84
24	a	414[A]	PHO	C4-C3-C5	3.76	121.59	115.27
23	A	408	CLA	C1C-C2C-C3C	-3.76	103.01	106.96
23	B	604	CLA	C3B-C4B-NB	3.76	114.00	110.52
23	C	509	CLA	C3B-C4B-NB	3.76	114.00	110.52
23	c	511	CLA	C3B-C4B-NB	3.76	114.00	110.52
23	d	402[B]	CLA	CMB-C2B-C1B	3.76	131.09	125.37
23	B	610	CLA	C3B-C2B-C1B	-3.75	102.63	107.16
26	a	409[B]	SQD	C1-C2-C3	-3.75	102.18	110.00
23	C	509	CLA	C1D-CHD-C4C	-3.75	117.96	126.06
33	c	521	LMG	O7-C10-C11	3.75	119.59	111.50
23	C	509	CLA	C1C-C2C-C3C	-3.75	103.01	106.96
23	b	612	CLA	CMC-C2C-C1C	3.75	130.75	125.04
26	A	412	SQD	O8-S-C6	3.75	111.72	105.74
23	B	606	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	c	511	CLA	C1C-C2C-C3C	-3.75	103.02	106.96
23	C	506	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
35	c	519[B]	DGD	O2G-C1B-C2B	3.75	119.58	111.50
23	d	402[B]	CLA	CAA-C2A-C3A	-3.74	102.53	112.78
23	C	509	CLA	C1-C2-C3	-3.74	119.57	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	410[A]	SQD	O47-C7-C8	3.74	119.56	111.50
29	a	412[A]	PL9	C15-C14-C16	3.74	121.56	115.27
26	a	410	SQD	O47-C7-C8	3.74	119.55	111.50
29	A	414[B]	PL9	C7-C3-C2	-3.74	118.39	123.30
23	A	406[A]	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	c	514	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
23	c	515	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	A	406[B]	CLA	C3C-C4C-NC	3.72	114.75	110.57
23	b	607	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
23	A	404[A]	CLA	C3D-C4D-ND	3.72	116.25	110.24
23	b	615	CLA	C1C-C2C-C3C	-3.72	103.05	106.96
24	A	407[B]	PHO	C1A-C2A-C3A	-3.71	99.31	102.84
23	c	505	CLA	CMB-C2B-C1B	3.71	131.02	125.37
23	b	614	CLA	C4A-NA-C1A	-3.71	105.04	106.71
23	B	612	CLA	CMC-C2C-C1C	3.70	130.68	125.04
23	c	506	CLA	C1-O2A-CGA	3.70	126.16	116.44
25	T	101	BCR	C16-C17-C18	-3.70	122.03	127.31
31	B	627	LMT	C1'-O5'-C5'	-3.69	106.44	113.69
35	C	518[A]	DGD	O2G-C1B-C2B	3.69	119.46	111.50
23	C	503	CLA	O2D-CGD-O1D	-3.69	116.62	123.84
23	B	610	CLA	CMB-C2B-C1B	3.69	130.98	125.37
32	L	101[A]	LHG	O7-C7-C8	3.68	119.43	111.50
23	c	508	CLA	C3B-C4B-NB	3.68	113.93	110.52
23	B	608	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
23	A	406[A]	CLA	CMB-C2B-C1B	3.68	130.97	125.37
23	c	511	CLA	C3C-C4C-NC	3.68	114.69	110.57
23	c	510	CLA	C1-C2-C3	-3.67	119.69	126.04
29	A	414[A]	PL9	C37-C38-C39	-3.67	118.82	127.66
23	C	509	CLA	O2D-CGD-O1D	-3.67	116.67	123.84
23	a	404[A]	CLA	O2A-CGA-O1A	-3.67	114.34	123.59
23	b	611	CLA	C1C-C2C-C3C	-3.66	103.10	106.96
23	C	512	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
26	a	409[B]	SQD	C44-O6-C1	-3.66	106.59	113.74
23	D	402[B]	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
33	c	501	LMG	C7-O1-C1	-3.66	106.59	113.74
23	B	608	CLA	C4C-C3C-C2C	-3.66	101.57	106.90
23	b	606	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	a	405[B]	CLA	C1D-CHD-C4C	-3.66	118.17	126.06
23	B	611	CLA	CHB-C4A-NA	3.65	129.56	124.51
23	d	403[B]	CLA	C4-C3-C5	3.65	121.42	115.27
23	B	612	CLA	C4A-NA-C1A	-3.65	105.06	106.71
26	B	620	SQD	O9-S-C6	3.65	111.28	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C4-C3-C5	3.65	121.41	115.27
23	C	514	CLA	C1D-CHD-C4C	-3.64	118.20	126.06
23	B	607	CLA	C3B-C4B-NB	3.64	113.89	110.52
23	D	402[A]	CLA	C3B-C4B-NB	3.64	113.89	110.52
23	b	610	CLA	C1D-CHD-C4C	-3.63	118.22	126.06
23	d	404	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
26	a	409[A]	SQD	O9-S-C6	3.63	111.25	106.94
23	c	510	CLA	C3B-C4B-NB	3.63	113.88	110.52
23	A	408	CLA	C1-C2-C3	-3.63	119.77	126.04
23	b	602	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	a	407	CLA	CMC-C2C-C1C	3.62	130.55	125.04
23	B	609	CLA	C1C-C2C-C3C	-3.62	103.15	106.96
23	C	511	CLA	C3C-C4C-NC	3.62	114.63	110.57
23	A	405[A]	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	a	407	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.61	103.16	106.96
23	A	404[B]	CLA	C3C-C4C-NC	3.61	114.62	110.57
23	B	605	CLA	CMB-C2B-C1B	3.60	130.85	125.37
32	L	101[B]	LHG	O7-C7-C8	3.60	119.25	111.50
35	c	518[B]	DGD	O2G-C1B-C2B	3.60	119.25	111.50
24	A	416[A]	PHO	C4D-CHA-CBD	3.59	110.14	108.52
23	C	502	CLA	CAC-C3C-C4C	3.59	129.47	124.81
23	b	605	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
29	A	414[B]	PL9	C10-C9-C11	3.59	121.30	115.27
23	A	405[A]	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
23	C	511	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
23	b	615	CLA	CMB-C2B-C1B	3.58	130.83	125.37
23	d	403[A]	CLA	C3B-C4B-NB	3.58	113.84	110.52
24	a	414[B]	PHO	C4-C3-C5	3.58	121.29	115.27
23	B	610	CLA	C1D-CHD-C4C	-3.58	118.34	126.06
23	c	514	CLA	C1-C2-C3	-3.58	119.85	126.04
23	d	403[B]	CLA	C1-C2-C3	-3.57	119.86	126.04
23	C	514	CLA	C1-C2-C3	-3.57	119.86	126.04
23	d	403[B]	CLA	C3B-C4B-NB	3.57	113.83	110.52
25	D	404	BCR	C10-C11-C12	-3.57	112.07	123.22
32	d	407[B]	LHG	O7-C7-C8	3.57	119.20	111.50
23	b	616	CLA	CMB-C2B-C1B	3.57	130.81	125.37
29	a	412[B]	PL9	C15-C14-C16	3.57	121.27	115.27
23	B	607	CLA	CBC-CAC-C3C	-3.56	102.61	112.43
33	m	101	LMG	O7-C10-C11	3.56	119.18	111.50
23	C	512	CLA	O2D-CGD-O1D	-3.56	116.88	123.84
23	d	403[A]	CLA	C1-C2-C3	-3.56	119.89	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[B]	CLA	CMB-C2B-C1B	3.56	130.78	125.37
23	a	405[B]	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
23	c	510	CLA	C1D-CHD-C4C	-3.55	118.39	126.06
23	C	509	CLA	C4C-C3C-C2C	-3.55	101.72	106.90
23	a	404[B]	CLA	O2D-CGD-CBD	3.55	117.58	111.27
23	b	615	CLA	C4-C3-C5	3.55	121.24	115.27
23	b	603	CLA	CAA-C2A-C3A	-3.55	103.06	112.78
29	d	406[A]	PL9	C40-C39-C41	3.55	121.23	115.27
23	b	610	CLA	CAA-C2A-C3A	-3.54	103.07	112.78
23	B	608	CLA	CAC-C3C-C4C	3.54	129.41	124.81
29	a	412[A]	PL9	C27-C28-C29	-3.54	119.13	127.66
23	C	507	CLA	C3B-C4B-NB	3.54	113.80	110.52
23	c	506	CLA	C3B-C4B-NB	3.54	113.80	110.52
23	c	504	CLA	CMC-C2C-C1C	3.54	130.43	125.04
23	B	613	CLA	C4-C3-C5	3.54	121.22	115.27
23	B	603	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	A	404[A]	CLA	O2D-CGD-CBD	3.53	117.54	111.27
23	d	403[B]	CLA	C1D-CHD-C4C	-3.53	118.44	126.06
23	B	605	CLA	CHD-C4C-NC	3.53	129.76	124.20
29	A	414[B]	PL9	C22-C23-C24	-3.53	119.17	127.66
23	B	614	CLA	C1-C2-C3	-3.52	119.95	126.04
23	b	605	CLA	CHD-C4C-NC	3.52	129.76	124.20
23	c	513	CLA	C4-C3-C5	3.52	121.20	115.27
23	A	405[B]	CLA	C1D-CHD-C4C	-3.52	118.47	126.06
29	A	414[A]	PL9	C22-C23-C24	-3.52	119.19	127.66
25	Y	101	BCR	C16-C17-C18	-3.51	122.29	127.31
29	a	412[B]	PL9	C27-C28-C29	-3.51	119.20	127.66
38	f	101	HEM	C1B-NB-C4B	3.51	108.70	105.07
34	V	202	HTG	C1-O5-C5	3.51	116.95	112.19
23	b	612	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
23	C	503	CLA	C1D-CHD-C4C	-3.51	118.48	126.06
23	c	507	CLA	C1C-C2C-C3C	-3.51	103.27	106.96
29	A	414[A]	PL9	C15-C14-C16	3.51	121.18	115.27
23	A	406[B]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
32	d	414[B]	LHG	O7-C7-C8	3.51	119.06	111.50
23	A	404[A]	CLA	C1D-CHD-C4C	-3.51	118.49	126.06
23	C	513	CLA	C4-C3-C5	3.51	121.17	115.27
23	c	503	CLA	C1C-C2C-C3C	-3.50	103.27	106.96
23	C	505	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
29	D	405[A]	PL9	C53-C6-C1	3.50	122.15	114.99
23	C	506	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
23	B	615	CLA	O2D-CGD-CBD	3.50	117.48	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	f	101	HEM	CHA-C4D-ND	3.50	128.69	124.37
23	C	511	CLA	CAC-C3C-C4C	3.49	129.34	124.81
23	B	614	CLA	C3B-C4B-NB	3.49	113.75	110.52
38	E	102	HEM	CBD-CAD-C3D	-3.49	102.92	112.63
23	a	405[A]	CLA	C1D-CHD-C4C	-3.49	118.53	126.06
23	b	609	CLA	C4C-C3C-C2C	-3.49	101.81	106.90
23	b	603	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
24	a	406[B]	PHO	O2A-CGA-O1A	-3.48	114.80	123.59
23	B	605	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
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	505	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
38	f	101	HEM	CAD-CBD-CGD	3.47	121.08	113.60
29	D	405[A]	PL9	C42-C43-C44	-3.47	119.29	127.66
29	A	414[B]	PL9	C37-C38-C39	-3.47	119.30	127.66
23	a	404[A]	CLA	O2D-CGD-CBD	3.47	117.43	111.27
24	A	416[B]	PHO	C1A-C2A-C3A	-3.47	99.54	102.84
23	d	402[B]	CLA	CHD-C4C-NC	3.47	129.66	124.20
23	B	612	CLA	C1C-C2C-C3C	-3.46	103.31	106.96
23	c	513	CLA	C3B-C4B-NB	3.46	113.73	110.52
23	A	406[A]	CLA	O2A-CGA-O1A	-3.46	114.85	123.59
23	d	403[A]	CLA	O2A-CGA-CBA	3.46	122.77	111.91
23	b	602	CLA	CAA-C2A-C3A	-3.46	103.30	112.78
26	a	409[B]	SQD	C1-O5-C5	-3.46	106.89	113.69
23	C	511	CLA	C4-C3-C5	3.46	121.09	115.27
23	b	610	CLA	CMB-C2B-C1B	3.46	130.63	125.37
23	A	406[B]	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
29	a	412[B]	PL9	C37-C38-C39	-3.45	119.34	127.66
25	D	404	BCR	C28-C27-C26	-3.45	107.91	114.08
23	C	507	CLA	C1-C2-C3	-3.45	120.07	126.04
23	c	508	CLA	CAC-C3C-C4C	3.45	129.29	124.81
23	c	508	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
40	V	201	HEC	CBD-CAD-C3D	-3.45	103.04	112.63
33	z	101	LMG	O7-C10-C11	3.45	118.93	111.50
23	B	604	CLA	C3D-C4D-ND	3.45	115.82	110.24
23	C	507	CLA	CAC-C3C-C4C	3.45	129.28	124.81
23	B	611	CLA	C4A-NA-C1A	-3.45	105.16	106.71
23	C	503	CLA	C1-C2-C3	-3.44	120.09	126.04
23	d	404	CLA	C1D-CHD-C4C	-3.43	118.65	126.06
32	A	419[B]	LHG	O7-C7-C8	3.43	118.90	111.50
23	B	601	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
23	B	601	CLA	C4C-C3C-C2C	-3.43	101.90	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	502	CLA	C1C-C2C-C3C	-3.43	103.35	106.96
23	c	503	CLA	CMB-C2B-C1B	3.43	130.59	125.37
23	b	616	CLA	O2A-CGA-O1A	-3.43	114.94	123.59
23	b	612	CLA	C4C-C3C-C2C	-3.43	101.90	106.90
23	c	515	CLA	C3B-C4B-NB	3.43	113.69	110.52
23	c	507	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
23	C	513	CLA	C1-C2-C3	-3.42	120.12	126.04
23	c	507	CLA	C1D-CHD-C4C	-3.42	118.68	126.06
23	A	408	CLA	C1D-CHD-C4C	-3.42	118.69	126.06
25	C	516	BCR	C11-C10-C9	-3.42	122.44	127.31
34	B	624	HTG	C1'-S1-C1	3.41	106.48	100.09
29	d	406[B]	PL9	C42-C43-C44	-3.41	119.44	127.66
23	a	404[A]	CLA	O2A-CGA-CBA	3.41	122.61	111.91
23	B	612	CLA	CAC-C3C-C4C	3.41	129.24	124.81
29	a	412[A]	PL9	C35-C34-C36	3.41	121.01	115.27
23	B	604	CLA	CAC-C3C-C4C	3.41	129.23	124.81
33	C	521	LMG	C3-C4-C5	3.41	116.32	110.24
29	d	406[B]	PL9	C7-C8-C9	-3.41	121.12	126.79
25	B	618	BCR	C29-C30-C25	3.41	115.72	110.48
23	c	513	CLA	CHD-C4C-NC	3.41	129.57	124.20
33	B	621	LMG	O8-C28-C29	3.40	122.59	111.91
23	b	607	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	D	402[B]	CLA	CAC-C3C-C4C	3.40	129.22	124.81
23	B	612	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
23	b	608	CLA	CAC-C3C-C4C	3.40	129.22	124.81
23	c	505	CLA	C4C-C3C-C2C	-3.40	101.95	106.90
23	C	507	CLA	C1D-CHD-C4C	-3.39	118.74	126.06
33	Z	101	LMG	O6-C1-C2	3.39	117.53	110.35
23	b	608	CLA	CBC-CAC-C3C	-3.39	103.08	112.43
29	a	412[B]	PL9	C30-C29-C31	3.39	120.97	115.27
23	C	512	CLA	CMC-C2C-C1C	3.39	130.20	125.04
23	b	609	CLA	C1-C2-C3	-3.39	120.18	126.04
29	D	405[A]	PL9	C25-C24-C26	3.39	120.97	115.27
23	C	506	CLA	C4C-C3C-C2C	-3.39	101.96	106.90
23	B	603	CLA	CAA-C2A-C3A	-3.38	103.51	112.78
23	C	507	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
25	C	515	BCR	C33-C5-C6	-3.38	120.73	124.53
23	B	610	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
24	a	406[B]	PHO	C1A-C2A-C3A	-3.38	99.63	102.84
23	B	610	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
35	c	519[A]	DGD	O2G-C1B-C2B	3.37	118.77	111.50
23	b	604	CLA	C3B-C4B-NB	3.37	113.64	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	BCR	C37-C22-C23	3.37	123.38	118.08
23	b	604	CLA	C1D-CHD-C4C	-3.37	118.80	126.06
23	C	508	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
23	b	613	CLA	C4C-C3C-C2C	-3.36	102.00	106.90
23	B	612	CLA	C1-C2-C3	-3.36	120.23	126.04
23	B	609	CLA	CMB-C2B-C1B	3.36	130.48	125.37
23	C	506	CLA	CAC-C3C-C4C	3.36	129.16	124.81
25	D	404	BCR	C38-C26-C25	-3.35	120.77	124.53
29	D	405[B]	PL9	C42-C43-C44	-3.35	119.59	127.66
23	B	606	CLA	C4-C3-C5	3.35	120.91	115.27
23	B	615	CLA	C4-C3-C5	3.35	120.91	115.27
23	B	614	CLA	O2A-CGA-O1A	-3.35	115.14	123.59
23	C	508	CLA	C4C-C3C-C2C	-3.35	102.02	106.90
25	y	101	BCR	C38-C26-C25	-3.34	120.77	124.53
23	B	610	CLA	O2A-CGA-O1A	-3.34	115.15	123.59
23	b	605	CLA	O2A-CGA-O1A	-3.34	115.16	123.59
23	c	514	CLA	C3C-C4C-NC	3.34	114.32	110.57
33	C	520	LMG	O8-C28-C29	3.34	122.39	111.91
23	A	408	CLA	CAA-C2A-C3A	-3.34	103.64	112.78
23	B	604	CLA	C4C-C3C-C2C	-3.34	102.03	106.90
29	A	414[B]	PL9	C15-C14-C16	3.33	120.88	115.27
23	b	610	CLA	C4C-C3C-C2C	-3.33	102.04	106.90
23	b	616	CLA	CHD-C4C-NC	3.33	129.46	124.20
29	D	405[B]	PL9	C10-C9-C11	3.33	120.88	115.27
23	d	403[A]	CLA	C1D-CHD-C4C	-3.33	118.87	126.06
23	b	604	CLA	CMC-C2C-C1C	3.33	130.11	125.04
23	C	513	CLA	C4C-C3C-C2C	-3.33	102.05	106.90
29	a	412[B]	PL9	C25-C24-C26	3.32	120.86	115.27
23	c	514	CLA	O2A-CGA-CBA	3.32	122.34	111.91
23	B	615	CLA	CMC-C2C-C1C	3.32	130.10	125.04
26	F	102	SQD	C1-C2-C3	-3.32	103.08	110.00
29	d	406[B]	PL9	C10-C9-C11	3.32	120.86	115.27
23	A	405[B]	CLA	C3B-C4B-NB	3.32	113.59	110.52
32	D	407[B]	LHG	O7-C7-C8	3.32	118.65	111.50
23	b	602	CLA	C1C-C2C-C3C	-3.32	103.47	106.96
24	A	407[A]	PHO	CMA-C3A-C4A	-3.32	107.11	114.38
23	A	406[A]	CLA	C3B-C4B-NB	3.32	113.59	110.52
25	D	404	BCR	C40-C30-C25	-3.32	104.92	110.30
26	B	620	SQD	C1-O5-C5	-3.31	107.19	113.69
23	b	613	CLA	O2D-CGD-CBD	3.31	117.15	111.27
23	D	403	CLA	C4C-C3C-C2C	-3.31	102.07	106.90
23	b	603	CLA	C3B-C4B-NB	3.31	113.59	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C1-C2-C3	-3.31	120.32	126.04
23	b	614	CLA	CMB-C2B-C1B	3.31	130.41	125.37
29	a	412[B]	PL9	C42-C43-C44	-3.30	119.70	127.66
23	c	506	CLA	CMB-C2B-C1B	3.30	130.40	125.37
32	A	419[B]	LHG	C5-O7-C7	-3.30	109.66	117.79
23	B	614	CLA	CMC-C2C-C1C	3.30	130.06	125.04
38	f	101	HEM	CHD-C1D-ND	3.30	128.00	124.42
23	b	601	CLA	CHD-C4C-NC	3.30	129.40	124.20
32	d	414[A]	LHG	O8-C23-O10	-3.30	115.27	123.59
23	b	610	CLA	C1C-C2C-C3C	-3.29	103.49	106.96
23	c	505	CLA	CAC-C3C-C4C	3.29	129.08	124.81
23	A	404[B]	CLA	O2A-CGA-CBA	3.29	122.24	111.91
25	C	516	BCR	C7-C8-C9	-3.29	121.26	126.23
32	d	408[A]	LHG	O7-C7-C8	3.29	118.59	111.50
23	d	404	CLA	CMB-C2B-C1B	3.29	130.38	125.37
23	b	616	CLA	C4C-C3C-C2C	-3.29	102.10	106.90
23	b	613	CLA	C3B-C4B-NB	3.29	113.56	110.52
23	A	405[B]	CLA	C3C-C4C-NC	3.29	114.26	110.57
23	C	512	CLA	CAC-C3C-C4C	3.29	129.07	124.81
23	b	605	CLA	CMB-C2B-C1B	3.29	130.38	125.37
23	b	604	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
34	b	622	HTG	C1'-S1-C1	3.28	106.23	100.09
23	B	608	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
23	C	506	CLA	C1-C2-C3	-3.28	120.37	126.04
23	c	512	CLA	C3B-C4B-NB	3.28	113.56	110.52
23	c	512	CLA	C4-C3-C5	3.28	120.79	115.27
23	A	405[B]	CLA	CMB-C2B-C1B	3.28	130.36	125.37
23	b	606	CLA	CHD-C4C-NC	3.28	129.37	124.20
23	c	509	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
23	b	611	CLA	C1D-CHD-C4C	-3.27	118.99	126.06
23	b	610	CLA	O2A-CGA-O1A	-3.27	115.34	123.59
23	C	507	CLA	CMC-C2C-C1C	3.27	130.02	125.04
23	a	405[B]	CLA	CMB-C2B-C1B	3.27	130.35	125.37
23	A	408	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
23	B	614	CLA	CHD-C4C-NC	3.27	129.35	124.20
23	d	403[B]	CLA	O2A-CGA-CBA	3.27	122.16	111.91
23	b	616	CLA	CBC-CAC-C3C	-3.26	103.43	112.43
23	c	514	CLA	O2D-CGD-O1D	-3.26	117.46	123.84
23	b	612	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
23	a	404[B]	CLA	O2A-CGA-CBA	3.26	122.13	111.91
23	b	611	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	B	610	CLA	C3B-C4B-NB	3.25	113.53	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	503	CLA	C3B-C4B-NB	3.25	113.53	110.52
23	B	611	CLA	C4C-C3C-C2C	-3.25	102.16	106.90
23	b	608	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
23	c	514	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
23	C	508	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
26	B	620	SQD	O7-S-C6	3.25	110.80	106.94
23	B	611	CLA	C2A-C1A-CHA	-3.25	118.18	123.86
34	b	625	HTG	O5-C5-C4	3.25	115.59	109.69
23	B	613	CLA	O2A-CGA-O1A	-3.25	115.39	123.59
23	b	609	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	a	404[B]	CLA	CHC-C1C-C2C	-3.25	117.71	126.73
32	d	414[A]	LHG	O7-C7-C8	3.25	118.50	111.50
23	D	402[B]	CLA	C1D-CHD-C4C	-3.25	119.05	126.06
23	C	504	CLA	CHD-C4C-NC	3.25	129.32	124.20
23	D	403	CLA	C1C-C2C-C3C	-3.24	103.55	106.96
23	b	615	CLA	C3B-C4B-NB	3.24	113.53	110.52
34	o	301	HTG	C1'-S1-C1	3.24	106.16	100.09
23	B	611	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
34	b	622	HTG	O5-C5-C4	3.24	115.58	109.69
23	B	607	CLA	C4-C3-C5	3.24	120.71	115.27
23	B	604	CLA	CHD-C1D-ND	-3.24	121.48	124.45
25	T	101	BCR	C15-C16-C17	-3.23	116.85	123.47
23	a	405[B]	CLA	CHD-C4C-NC	3.23	129.30	124.20
25	D	404	BCR	C29-C30-C25	3.23	115.46	110.48
23	B	603	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	c	514	CLA	CMB-C2B-C1B	3.23	130.29	125.37
23	C	511	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
23	A	405[A]	CLA	C3B-C4B-NB	3.23	113.51	110.52
23	C	511	CLA	CHC-C1C-C2C	-3.23	117.77	126.73
29	d	406[B]	PL9	C40-C39-C41	3.22	120.69	115.27
23	C	504	CLA	O2D-CGD-O1D	-3.22	117.53	123.84
23	b	615	CLA	C11-C10-C8	-3.22	105.50	115.92
24	A	416[B]	PHO	C4-C3-C5	3.22	120.69	115.27
23	c	513	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
23	c	514	CLA	C4-C3-C5	3.22	120.69	115.27
23	C	507	CLA	CHC-C1C-C2C	-3.22	117.78	126.73
23	B	609	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
24	a	414[A]	PHO	C4A-C3A-C2A	-3.22	99.77	102.84
23	C	513	CLA	CHD-C4C-NC	3.22	129.28	124.20
23	a	407	CLA	C4-C3-C5	3.22	120.68	115.27
32	d	414[A]	LHG	O8-C23-C24	3.22	122.00	111.91
23	B	608	CLA	C1C-C2C-C3C	-3.22	103.58	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C1-C2-C3	-3.21	120.48	126.04
23	C	510	CLA	C1D-CHD-C4C	-3.21	119.14	126.06
23	D	402[B]	CLA	C3B-C4B-NB	3.21	113.49	110.52
26	b	620	SQD	O7-S-C6	3.21	110.75	106.94
31	B	627	LMT	C4B-C3B-C2B	3.20	116.42	110.82
23	c	505	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
23	b	614	CLA	O2A-CGA-O1A	-3.20	115.51	123.59
25	h	101	BCR	C7-C8-C9	-3.20	121.40	126.23
23	b	608	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
23	c	504	CLA	CMB-C2B-C1B	3.20	130.24	125.37
24	a	406[B]	PHO	CMA-C3A-C4A	-3.20	107.38	114.38
23	b	607	CLA	C4C-C3C-C2C	-3.19	102.24	106.90
23	B	605	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
23	a	404[A]	CLA	CHC-C1C-C2C	-3.19	117.86	126.73
26	b	620	SQD	C3-C4-C5	3.19	115.93	110.24
23	a	404[A]	CLA	CAA-C2A-C1A	-3.19	101.52	111.97
23	B	603	CLA	C4-C3-C5	3.19	120.64	115.27
23	a	407	CLA	CAA-C2A-C3A	-3.19	104.05	112.78
23	B	614	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
29	a	412[A]	PL9	C17-C18-C19	-3.19	119.99	127.66
23	C	512	CLA	C1-O2A-CGA	3.18	124.80	116.44
25	B	617	BCR	C33-C5-C6	-3.18	120.95	124.53
23	b	601	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
23	C	503	CLA	CMB-C2B-C1B	3.18	130.22	125.37
23	A	406[A]	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
23	a	407	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	612	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
23	C	505	CLA	C1-O2A-CGA	3.18	124.78	116.44
34	o	301	HTG	O5-C1-C2	3.17	114.31	110.31
23	c	515	CLA	CMC-C2C-C1C	3.17	129.87	125.04
23	c	511	CLA	CHC-C1C-C2C	-3.17	117.92	126.73
23	c	505	CLA	C1C-C2C-C3C	-3.17	103.62	106.96
25	k	101	BCR	C7-C8-C9	-3.17	121.44	126.23
29	a	412[A]	PL9	C25-C24-C26	3.17	120.61	115.27
23	c	510	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
33	m	101	LMG	O8-C28-C29	3.17	121.86	111.91
23	A	404[A]	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	B	602	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
23	D	402[A]	CLA	C1D-CHD-C4C	-3.17	119.22	126.06
23	B	605	CLA	C4C-C3C-C2C	-3.17	102.28	106.90
23	c	512	CLA	CHD-C4C-NC	3.17	129.19	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	E	102	HEM	CHD-C1D-ND	3.17	127.86	124.42
23	c	513	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
23	c	509	CLA	C4-C3-C5	3.16	120.59	115.27
23	c	511	CLA	O2D-CGD-O1D	-3.16	117.65	123.84
29	D	405[B]	PL9	C17-C18-C19	-3.16	120.05	127.66
23	B	609	CLA	C3B-C4B-NB	3.16	113.44	110.52
23	d	402[B]	CLA	C3B-C4B-NB	3.16	113.44	110.52
23	B	604	CLA	CHC-C1C-C2C	-3.15	117.97	126.73
24	A	416[A]	PHO	C4-C3-C5	3.15	120.58	115.27
25	y	101	BCR	C15-C14-C13	-3.15	122.81	127.31
23	d	402[A]	CLA	CHD-C4C-NC	3.15	129.17	124.20
23	A	405[A]	CLA	CMB-C2B-C1B	3.15	130.17	125.37
32	A	419[A]	LHG	C5-O7-C7	-3.15	110.03	117.79
32	A	419[A]	LHG	O8-C23-C24	3.15	121.79	111.91
29	D	405[A]	PL9	C17-C18-C19	-3.15	120.08	127.66
24	a	406[B]	PHO	O1D-CGD-CBD	-3.15	119.50	124.74
23	B	605	CLA	O2A-CGA-O1A	-3.15	115.65	123.59
25	X	101	BCR	C16-C17-C18	-3.14	122.82	127.31
33	c	522	LMG	C9-C8-C7	-3.14	104.35	111.79
23	A	404[B]	CLA	CHC-C1C-C2C	-3.14	118.00	126.73
23	a	405[B]	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
23	c	513	CLA	C4C-C3C-C2C	-3.14	102.32	106.90
23	c	511	CLA	O2A-CGA-CBA	3.14	121.76	111.91
23	c	512	CLA	CMC-C2C-C1C	3.14	129.81	125.04
23	c	503	CLA	C1D-CHD-C4C	-3.13	119.30	126.06
23	b	609	CLA	C1C-C2C-C3C	-3.13	103.66	106.96
23	B	607	CLA	CMC-C2C-C1C	3.13	129.81	125.04
38	E	102	HEM	CHB-C1B-NB	3.13	128.24	124.37
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	614	CLA	CHD-C4C-NC	3.13	129.13	124.20
23	C	504	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
23	B	607	CLA	CAA-C2A-C3A	-3.13	104.22	112.78
23	b	601	CLA	C4-C3-C5	3.12	120.53	115.27
29	d	406[B]	PL9	C37-C38-C39	-3.12	120.14	127.66
26	B	620	SQD	O48-C23-C24	3.12	121.70	111.91
23	c	506	CLA	C1D-CHD-C4C	-3.12	119.33	126.06
23	b	607	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
32	d	414[B]	LHG	O8-C23-C24	3.12	121.70	111.91
23	b	615	CLA	O2D-CGD-CBD	3.12	116.81	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	405[A]	PL9	C51-C49-C50	3.12	121.49	114.60
23	c	512	CLA	O2A-CGA-O1A	-3.11	115.73	123.59
23	C	505	CLA	CHC-C1C-C2C	-3.11	118.08	126.73
23	D	402[B]	CLA	C4C-C3C-C2C	-3.11	102.36	106.90
31	A	417	LMT	O5B-C5B-C4B	3.11	115.34	109.69
23	b	615	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
29	D	405[A]	PL9	C10-C9-C11	3.11	120.50	115.27
23	B	614	CLA	CAC-C3C-C4C	3.10	128.84	124.81
23	c	506	CLA	C4C-C3C-C2C	-3.10	102.37	106.90
33	c	501	LMG	C8-O7-C10	-3.10	110.15	117.79
23	A	405[B]	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
23	c	508	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
23	b	605	CLA	C2A-C1A-CHA	-3.10	118.44	123.86
26	A	412	SQD	O48-C23-C24	3.10	121.64	111.91
31	m	103	LMT	C3'-C4'-C5'	-3.10	103.82	110.93
29	A	414[A]	PL9	C10-C9-C11	3.10	120.48	115.27
23	B	615	CLA	C3B-C4B-NB	3.09	113.39	110.52
25	c	516	BCR	C15-C14-C13	-3.09	122.89	127.31
23	c	512	CLA	O2A-CGA-CBA	3.09	121.62	111.91
23	C	510	CLA	CHB-C1B-NB	-3.09	120.98	124.26
23	C	506	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	A	405[B]	CLA	CAC-C3C-C4C	3.09	128.82	124.81
32	b	629[A]	LHG	O7-C7-C8	3.09	118.16	111.50
23	B	616	CLA	C1C-C2C-C3C	-3.09	103.71	106.96
23	b	605	CLA	C4C-C3C-C2C	-3.09	102.39	106.90
25	d	405	BCR	C10-C11-C12	-3.09	113.58	123.22
23	D	403	CLA	C4-C3-C5	3.09	120.47	115.27
23	c	503	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	C	504	CLA	C4-C3-C5	3.09	120.46	115.27
29	D	405[B]	PL9	C25-C24-C26	3.09	120.46	115.27
26	a	410	SQD	O48-C23-C24	3.09	121.59	111.91
23	c	504	CLA	CHD-C4C-NC	3.08	129.06	124.20
29	a	412[B]	PL9	C17-C18-C19	-3.08	120.24	127.66
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	C	513	CLA	O2A-CGA-CBA	3.08	121.57	111.91
23	a	405[B]	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
38	f	101	HEM	C4D-ND-C1D	3.08	108.25	105.07
23	b	603	CLA	C2A-C1A-CHA	-3.08	118.48	123.86
32	A	419[B]	LHG	O8-C23-O10	-3.07	115.84	123.59
23	a	404[A]	CLA	C1-C2-C3	-3.07	120.73	126.04
35	h	102	DGD	O2G-C1B-C2B	3.07	118.12	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	614	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
23	B	612	CLA	C11-C12-C13	-3.07	106.01	115.92
23	b	608	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
23	B	615	CLA	CHD-C4C-NC	3.06	129.02	124.20
29	a	412[B]	PL9	C35-C34-C36	3.06	120.42	115.27
23	b	607	CLA	CHC-C1C-C2C	-3.06	118.23	126.73
29	d	406[A]	PL9	C10-C9-C11	3.05	120.41	115.27
23	c	505	CLA	C3B-C4B-NB	3.05	113.35	110.52
23	C	502	CLA	CBC-CAC-C3C	-3.05	104.01	112.43
33	C	521	LMG	O8-C28-C29	3.05	121.49	111.91
23	a	404[A]	CLA	C4-C3-C5	3.05	120.41	115.27
23	B	615	CLA	C11-C10-C8	-3.05	106.06	115.92
23	D	402[A]	CLA	O2A-CGA-CBA	3.05	121.48	111.91
23	a	405[A]	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	B	615	CLA	CED-O2D-CGD	3.05	122.84	115.94
23	a	405[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
23	A	406[B]	CLA	CBC-CAC-C3C	-3.05	104.03	112.43
23	B	603	CLA	C3B-C4B-NB	3.05	113.34	110.52
23	d	403[A]	CLA	C2A-C1A-CHA	-3.05	118.53	123.86
25	y	101	BCR	C24-C23-C22	-3.05	121.63	126.23
23	C	509	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
23	A	406[B]	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
23	d	403[A]	CLA	C4C-C3C-C2C	-3.04	102.46	106.90
23	B	614	CLA	O2A-CGA-CBA	3.04	121.45	111.91
23	B	609	CLA	C4C-C3C-C2C	-3.04	102.47	106.90
23	A	405[B]	CLA	CMC-C2C-C1C	3.04	129.67	125.04
31	B	629	LMT	O1'-C1'-C2'	3.04	113.05	108.30
23	c	510	CLA	CHC-C1C-C2C	-3.04	118.29	126.73
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
23	B	601	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
23	b	612	CLA	O2A-CGA-O1A	-3.04	115.93	123.59
23	c	506	CLA	CHC-C1C-C2C	-3.04	118.30	126.73
23	c	510	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
32	a	417[B]	LHG	O7-C7-C8	3.03	118.04	111.50
23	b	615	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	d	403[A]	CLA	O2A-CGA-O1A	-3.03	115.94	123.59
23	A	406[A]	CLA	O2A-CGA-CBA	3.03	121.42	111.91
23	d	402[B]	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
33	D	411	LMG	O7-C10-C11	3.03	118.03	111.50
31	A	420	LMT	O5B-C5B-C4B	3.03	115.19	109.69
23	A	404[A]	CLA	C1-C2-C3	-3.03	120.81	126.04
24	a	406[B]	PHO	O2A-CGA-CBA	3.02	121.40	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	CHB-C1B-NB	-3.02	121.06	124.26
23	d	403[A]	CLA	C4-C3-C5	3.02	120.36	115.27
23	B	606	CLA	CHD-C4C-NC	3.02	128.97	124.20
23	D	402[B]	CLA	O2A-CGA-CBA	3.02	121.39	111.91
29	d	406[A]	PL9	C37-C38-C39	-3.02	120.38	127.66
26	A	410[B]	SQD	O48-C23-C24	3.02	121.39	111.91
25	T	101	BCR	C2-C1-C6	3.02	115.13	110.48
23	C	502	CLA	CMC-C2C-C1C	3.02	129.63	125.04
23	b	616	CLA	C3B-C4B-NB	3.02	113.31	110.52
23	B	602	CLA	C3B-C4B-NB	3.02	113.31	110.52
23	B	602	CLA	CAC-C3C-C4C	3.02	128.72	124.81
23	A	404[A]	CLA	CAA-C2A-C1A	-3.01	102.09	111.97
23	B	613	CLA	O2A-CGA-CBA	3.01	121.37	111.91
23	C	513	CLA	CMB-C2B-C1B	3.01	129.96	125.37
23	d	404	CLA	CBC-CAC-C3C	-3.01	104.12	112.43
29	a	412[A]	PL9	C42-C43-C44	-3.01	120.41	127.66
25	b	619	BCR	C11-C10-C9	-3.01	123.01	127.31
32	d	407[A]	LHG	O7-C7-C8	3.01	117.99	111.50
29	A	414[B]	PL9	C20-C19-C21	3.01	120.33	115.27
23	D	402[A]	CLA	CAC-C3C-C4C	3.01	128.71	124.81
23	c	506	CLA	CAC-C3C-C4C	3.01	128.71	124.81
32	D	406[B]	LHG	O7-C7-C8	3.01	117.98	111.50
25	T	101	BCR	C11-C10-C9	-3.00	123.02	127.31
23	C	502	CLA	C3B-C4B-NB	3.00	113.30	110.52
23	B	601	CLA	CHD-C4C-NC	3.00	128.93	124.20
23	B	607	CLA	C1D-CHD-C4C	-3.00	119.58	126.06
23	C	513	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
23	B	608	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
23	b	614	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
23	c	511	CLA	C1-O2A-CGA	3.00	124.31	116.44
23	c	511	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
29	d	406[B]	PL9	C22-C23-C24	-3.00	120.44	127.66
23	C	514	CLA	CBC-CAC-C3C	-3.00	104.17	112.43
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	b	613	CLA	O2A-CGA-O1A	-3.00	116.03	123.59
23	b	605	CLA	CMC-C2C-C1C	2.99	129.60	125.04
25	a	408	BCR	C38-C26-C25	-2.99	121.17	124.53
33	c	521	LMG	O1-C7-C8	-2.99	103.68	110.90
23	b	603	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	b	613	CLA	CHC-C1C-C2C	-2.99	118.42	126.73
23	b	614	CLA	C1-C2-C3	-2.99	120.87	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	607	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
23	b	604	CLA	CMB-C2B-C1B	2.99	129.92	125.37
23	B	613	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	A	404[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
23	C	504	CLA	C4C-C3C-C2C	-2.99	102.54	106.90
23	D	403	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	b	601	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
32	D	407[A]	LHG	O8-C23-C24	2.98	121.27	111.91
23	d	402[B]	CLA	CBC-CAC-C3C	-2.98	104.21	112.43
33	c	521	LMG	O8-C28-C29	2.98	121.27	111.91
23	B	606	CLA	O2A-CGA-CBA	2.98	121.26	111.91
23	D	403	CLA	O2A-CGA-CBA	2.98	121.25	111.91
23	c	509	CLA	CHD-C4C-NC	2.98	128.89	124.20
23	c	514	CLA	CHD-C4C-NC	2.98	128.89	124.20
23	C	512	CLA	C3B-C4B-NB	2.98	113.28	110.52
23	a	405[B]	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
32	E	101[A]	LHG	O8-C23-C24	2.97	121.23	111.91
23	b	607	CLA	C4-C3-C5	2.97	120.27	115.27
23	d	404	CLA	CHD-C4C-NC	2.97	128.88	124.20
25	t	102	BCR	C11-C10-C9	-2.97	123.07	127.31
26	f	102	SQD	O5-C1-C2	2.97	116.63	110.35
23	C	503	CLA	CHC-C1C-C2C	-2.97	118.49	126.73
23	A	404[B]	CLA	C1-C2-C3	-2.97	120.91	126.04
23	A	408	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
25	Y	101	BCR	C15-C14-C13	-2.96	123.08	127.31
23	C	512	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
23	c	511	CLA	O2A-C1-C2	2.96	116.42	108.64
23	B	613	CLA	C4C-C3C-C2C	-2.96	102.58	106.90
25	c	517	BCR	C32-C1-C6	-2.96	105.50	110.30
25	k	101	BCR	C24-C23-C22	-2.96	121.77	126.23
23	C	510	CLA	C4C-C3C-C2C	-2.96	102.59	106.90
26	b	620	SQD	O8-S-C6	2.96	110.45	105.74
24	A	407[A]	PHO	O1D-CGD-CBD	-2.96	119.81	124.74
23	B	601	CLA	CMB-C2B-C1B	2.95	129.87	125.37
23	c	515	CLA	CAC-C3C-C4C	2.95	128.64	124.81
23	d	402[A]	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
23	b	610	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
29	A	414[B]	PL9	C27-C28-C29	-2.95	120.56	127.66
26	A	410[A]	SQD	O9-S-C6	2.95	110.44	106.94
23	B	604	CLA	C6-C7-C8	-2.94	106.40	115.92
23	C	512	CLA	C4-C3-C5	2.94	120.22	115.27
23	b	605	CLA	C1-C2-C3	-2.94	120.95	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414[A]	PL9	C30-C29-C31	2.94	120.22	115.27
23	C	502	CLA	CHD-C4C-NC	2.94	128.84	124.20
29	D	405[B]	PL9	C53-C6-C1	2.94	121.00	114.99
23	C	512	CLA	C1-C2-C3	-2.94	120.96	126.04
23	b	609	CLA	C3B-C4B-NB	2.94	113.24	110.52
23	B	603	CLA	CAC-C3C-C4C	2.94	128.62	124.81
23	b	606	CLA	C4C-C3C-C2C	-2.94	102.62	106.90
26	F	102	SQD	O5-C1-O6	2.94	116.93	109.97
23	C	508	CLA	CHD-C4C-NC	2.94	128.83	124.20
32	a	417[A]	LHG	O7-C7-C8	2.94	117.83	111.50
23	b	613	CLA	O2A-CGA-CBA	2.93	121.12	111.91
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
32	D	406[A]	LHG	O8-C23-O10	-2.93	116.19	123.59
29	d	406[A]	PL9	C22-C23-C24	-2.93	120.60	127.66
23	A	405[B]	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	B	616	CLA	O2A-CGA-CBA	2.93	121.09	111.91
23	B	609	CLA	CHC-C1C-C2C	-2.93	118.60	126.73
23	b	610	CLA	CAA-CBA-CGA	-2.93	104.70	113.25
29	d	406[A]	PL9	C27-C28-C29	-2.93	120.61	127.66
23	C	506	CLA	C4-C3-C5	2.93	120.19	115.27
23	b	616	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
23	C	504	CLA	CMB-C2B-C1B	2.93	129.82	125.37
23	A	404[A]	CLA	C4C-C3C-C2C	-2.93	102.63	106.90
23	b	609	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
23	d	402[A]	CLA	CBC-CAC-C3C	-2.92	104.38	112.43
23	D	403	CLA	C3B-C4B-NB	2.92	113.22	110.52
23	C	503	CLA	C4-C3-C5	2.92	120.18	115.27
25	B	619	BCR	C24-C23-C22	-2.92	121.82	126.23
23	a	407	CLA	C3B-C4B-NB	2.92	113.22	110.52
23	C	505	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	c	505	CLA	CMC-C2C-C1C	2.92	129.48	125.04
35	C	518[B]	DGD	C2G-O2G-C1B	-2.92	110.61	117.79
29	a	412[B]	PL9	C10-C9-C11	2.92	120.18	115.27
23	d	404	CLA	C4C-C3C-C2C	-2.92	102.65	106.90
29	d	406[A]	PL9	C53-C6-C1	2.92	120.95	114.99
23	a	404[B]	CLA	CAA-C2A-C1A	-2.92	102.42	111.97
29	a	412[A]	PL9	C22-C23-C24	-2.92	120.64	127.66
34	b	622	HTG	O5-C1-C2	2.91	113.98	110.31
25	C	516	BCR	C32-C1-C6	-2.91	105.57	110.30
23	b	602	CLA	C1-C2-C3	-2.91	121.00	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	506	CLA	CHB-C1B-NB	-2.91	121.17	124.26
25	b	619	BCR	C24-C23-C22	-2.91	121.84	126.23
23	b	606	CLA	C3B-C4B-NB	2.91	113.22	110.52
29	a	412[B]	PL9	C53-C6-C1	2.91	120.94	114.99
23	C	503	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
26	A	410[A]	SQD	O48-C23-C24	2.91	121.04	111.91
23	c	515	CLA	O2A-CGA-CBA	2.91	121.04	111.91
32	D	407[A]	LHG	O8-C23-O10	-2.91	116.25	123.59
25	b	617	BCR	C29-C30-C25	2.91	114.96	110.48
23	b	611	CLA	CHC-C1C-C2C	-2.91	118.66	126.73
23	D	402[B]	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	A	405[A]	CLA	C4-C3-C5	2.91	120.16	115.27
38	f	101	HEM	CHD-C4C-NC	2.91	127.58	124.44
26	f	102	SQD	C4-C3-C2	-2.90	105.75	110.82
23	a	404[A]	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	A	408	CLA	CHC-C1C-C2C	-2.90	118.66	126.73
40	V	201	HEC	CBC-CAC-C3C	2.90	120.44	112.43
25	b	618	BCR	C37-C22-C21	-2.90	118.86	122.92
23	a	405[A]	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
25	Y	101	BCR	C28-C27-C26	-2.90	108.90	114.08
24	a	414[B]	PHO	CMB-C2B-C3B	2.90	130.10	124.68
25	C	515	BCR	C15-C14-C13	-2.90	123.17	127.31
23	d	402[A]	CLA	CMA-C3A-C2A	-2.90	102.14	113.83
23	B	608	CLA	CHB-C4A-NA	2.90	128.52	124.51
33	c	522	LMG	O8-C28-C29	2.90	121.00	111.91
25	A	409	BCR	C15-C14-C13	-2.90	123.18	127.31
23	b	602	CLA	C11-C12-C13	-2.90	106.56	115.92
23	a	405[A]	CLA	CMB-C2B-C1B	2.89	129.78	125.37
23	c	514	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
38	f	101	HEM	CBD-CAD-C3D	-2.89	104.59	112.63
23	b	614	CLA	CAC-C3C-C4C	2.89	128.56	124.81
23	B	602	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	C	514	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	B	606	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
23	C	503	CLA	CAC-C3C-C4C	2.89	128.56	124.81
23	B	602	CLA	C2A-C1A-CHA	-2.89	118.81	123.86
23	D	402[A]	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	b	603	CLA	C4-C3-C5	2.89	120.13	115.27
23	b	613	CLA	CHD-C4C-NC	2.89	128.75	124.20
32	E	101[B]	LHG	O8-C23-C24	2.89	120.96	111.91
23	C	514	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	c	503	CLA	CAC-C3C-C4C	2.88	128.55	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	b	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
23	D	402[A]	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	b	605	CLA	C4-C3-C5	2.88	120.12	115.27
23	b	614	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	B	607	CLA	CMB-C2B-C1B	2.88	129.76	125.37
35	c	520	DGD	O2G-C1B-C2B	2.88	117.71	111.50
25	c	516	BCR	C20-C21-C22	-2.88	123.20	127.31
29	A	414[B]	PL9	C17-C18-C19	-2.88	120.73	127.66
23	b	604	CLA	CAC-C3C-C4C	2.88	128.54	124.81
23	b	602	CLA	C1-O2A-CGA	2.88	124.00	116.44
24	a	406[B]	PHO	CBC-CAC-C3C	-2.88	108.67	112.88
23	c	504	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
23	b	611	CLA	CMC-C2C-C1C	2.88	129.42	125.04
26	A	410[B]	SQD	O8-S-C6	2.87	110.32	105.74
23	c	504	CLA	CBC-CAC-C3C	-2.87	104.51	112.43
32	D	407[B]	LHG	O8-C23-C24	2.87	120.93	111.91
23	D	402[B]	CLA	O2A-CGA-O1A	-2.87	116.34	123.59
26	a	409[B]	SQD	O8-S-C6	2.87	110.32	105.74
23	b	616	CLA	CAC-C3C-C4C	2.87	128.54	124.81
23	B	613	CLA	C1D-CHD-C4C	-2.87	119.86	126.06
24	a	406[A]	PHO	O2A-CGA-CBA	2.87	120.92	111.91
23	C	506	CLA	C3B-C4B-NB	2.87	113.18	110.52
23	B	601	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	D	402[A]	CLA	O2A-CGA-O1A	-2.87	116.35	123.59
25	k	101	BCR	C36-C18-C19	2.87	122.60	118.08
29	d	406[B]	PL9	C7-C3-C4	2.87	119.21	116.88
23	c	503	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
33	C	501	LMG	O6-C1-O1	-2.87	103.19	109.97
23	a	404[B]	CLA	C4-C3-C5	2.86	120.09	115.27
23	C	504	CLA	C1-C2-C3	-2.86	121.09	126.04
23	C	514	CLA	CMC-C2C-C1C	2.86	129.40	125.04
34	b	622	HTG	O2-C2-C1	2.86	115.53	110.27
29	D	405[B]	PL9	C27-C28-C29	-2.86	120.77	127.66
29	a	412[A]	PL9	C37-C38-C39	-2.86	120.77	127.66
29	a	412[B]	PL9	C22-C23-C24	-2.86	120.77	127.66
23	c	508	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
23	b	616	CLA	CMC-C2C-C1C	2.86	129.40	125.04
23	b	601	CLA	C1-O2A-CGA	2.86	123.95	116.44
23	b	602	CLA	C2A-C1A-CHA	-2.86	118.86	123.86
23	B	604	CLA	CMB-C2B-C1B	2.86	129.72	125.37
26	B	620	SQD	C4-C3-C2	2.86	115.81	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	O2A-CGA-CBA	2.86	120.88	111.91
23	a	407	CLA	CHD-C4C-NC	2.86	128.71	124.20
23	B	614	CLA	C4C-C3C-C2C	-2.86	102.73	106.90
33	z	101	LMG	O8-C28-C29	2.86	120.88	111.91
23	C	502	CLA	CHC-C1C-C2C	-2.86	118.80	126.73
23	c	511	CLA	CHD-C4C-NC	2.86	128.70	124.20
25	B	617	BCR	C7-C8-C9	-2.85	121.92	126.23
23	A	408	CLA	O2A-CGA-CBA	2.85	120.87	111.91
23	A	405[B]	CLA	CHD-C4C-NC	2.85	128.70	124.20
25	K	102	BCR	C20-C21-C22	-2.85	123.24	127.31
29	A	414[B]	PL9	C7-C3-C4	2.85	119.19	116.88
24	a	406[A]	PHO	C1A-C2A-C3A	-2.85	100.13	102.84
23	A	406[B]	CLA	C2A-C1A-CHA	-2.85	118.87	123.86
31	b	627	LMT	C3'-C4'-C5'	-2.85	104.39	110.93
33	Z	101	LMG	C4-C3-C2	2.85	115.80	110.82
23	b	611	CLA	C2A-C1A-CHA	-2.85	118.88	123.86
32	b	629[A]	LHG	O8-C23-C24	2.85	120.84	111.91
23	B	603	CLA	CHD-C4C-NC	2.85	128.69	124.20
23	c	503	CLA	O2A-CGA-O1A	-2.85	116.41	123.59
23	b	603	CLA	CHD-C4C-NC	2.85	128.69	124.20
24	A	407[B]	PHO	O1D-CGD-CBD	-2.85	120.00	124.74
23	c	507	CLA	C3B-C4B-NB	2.84	113.15	110.52
24	a	406[A]	PHO	O1D-CGD-CBD	-2.84	120.01	124.74
38	E	102	HEM	CHA-C4D-ND	2.84	127.87	124.37
23	A	405[B]	CLA	C4-C3-C5	2.84	120.05	115.27
25	a	408	BCR	C11-C10-C9	-2.84	123.26	127.31
23	c	508	CLA	C4C-C3C-C2C	-2.84	102.76	106.90
23	a	407	CLA	O2A-CGA-CBA	2.84	120.81	111.91
23	A	404[B]	CLA	CAC-C3C-C4C	2.84	128.49	124.81
23	C	510	CLA	O2A-CGA-O1A	-2.83	116.44	123.59
23	c	515	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
23	b	604	CLA	CHC-C1C-C2C	-2.83	118.86	126.73
23	b	611	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
23	D	402[B]	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
23	A	406[B]	CLA	CHD-C4C-NC	2.83	128.66	124.20
40	V	201	HEC	CAD-CBD-CGD	-2.83	107.51	113.60
23	D	403	CLA	O2A-CGA-O1A	-2.83	116.45	123.59
23	c	507	CLA	CHC-C1C-C2C	-2.83	118.87	126.73
26	a	409[B]	SQD	O9-S-C6	2.83	110.30	106.94
25	c	516	BCR	C37-C22-C21	-2.83	118.96	122.92
23	D	402[B]	CLA	CMB-C2B-C1B	2.83	129.68	125.37
29	A	414[B]	PL9	C30-C29-C31	2.83	120.03	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	411	LMG	O8-C28-O10	-2.83	116.46	123.59
23	B	603	CLA	CHC-C1C-C2C	-2.83	118.88	126.73
23	c	513	CLA	CMC-C2C-C1C	2.83	129.34	125.04
24	A	416[B]	PHO	C4D-CHA-CBD	2.83	109.80	108.52
23	a	405[B]	CLA	C4-C3-C5	2.82	120.02	115.27
23	b	606	CLA	C1-C2-C3	-2.82	121.16	126.04
23	b	602	CLA	CHD-C4C-NC	2.82	128.65	124.20
23	a	404[B]	CLA	O2A-CGA-O1A	-2.82	116.47	123.59
23	C	503	CLA	CMC-C2C-C1C	2.82	129.33	125.04
38	f	101	HEM	CHB-C1B-NB	2.82	127.85	124.37
32	b	629[B]	LHG	O8-C23-C24	2.82	120.75	111.91
29	D	405[B]	PL9	C51-C49-C50	2.82	120.83	114.60
23	d	403[B]	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
23	B	616	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	D	403	CLA	CAA-C2A-C3A	-2.82	105.07	112.78
24	A	416[B]	PHO	O2D-CGD-O1D	-2.82	118.33	123.84
23	C	510	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	c	512	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
35	c	518[A]	DGD	O3G-C3G-C2G	-2.82	104.11	110.90
23	C	511	CLA	CMC-C2C-C1C	2.81	129.32	125.04
38	E	102	HEM	CBA-CAA-C2A	-2.81	104.81	112.63
23	b	607	CLA	CBC-CAC-C3C	-2.81	104.68	112.43
23	B	605	CLA	CMC-C2C-C1C	2.81	129.32	125.04
26	a	410	SQD	O7-S-C6	2.81	110.28	106.94
25	B	618	BCR	C37-C22-C21	-2.81	118.99	122.92
23	A	406[B]	CLA	C3B-C4B-NB	2.80	113.12	110.52
23	d	404	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
23	B	606	CLA	CMC-C2C-C1C	2.80	129.30	125.04
23	B	609	CLA	CAC-C3C-C4C	2.80	128.44	124.81
25	b	619	BCR	C38-C26-C25	-2.80	121.39	124.53
31	M	101	LMT	C1'-O5'-C5'	-2.80	108.20	113.69
23	b	612	CLA	O2A-CGA-CBA	2.80	120.68	111.91
23	d	403[A]	CLA	CHC-C1C-C2C	-2.80	118.97	126.73
35	C	517[A]	DGD	O3G-C3G-C2G	-2.79	104.16	110.90
23	b	614	CLA	O2A-CGA-CBA	2.79	120.67	111.91
23	c	511	CLA	C4-C3-C5	2.79	119.97	115.27
24	a	414[B]	PHO	C1A-C2A-C3A	-2.79	100.19	102.84
25	A	409	BCR	C16-C17-C18	-2.79	123.33	127.31
23	B	602	CLA	CHD-C4C-NC	2.79	128.60	124.20
23	A	406[A]	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
23	B	615	CLA	CHC-C1C-C2C	-2.79	118.99	126.73
23	C	506	CLA	O2A-CGA-O1A	-2.79	116.56	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404[B]	CLA	C2A-C1A-CHA	-2.79	118.99	123.86
31	B	627	LMT	C2'-C3'-C4'	2.79	116.04	109.68
32	D	407[A]	LHG	O7-C7-C8	2.79	117.50	111.50
31	c	502	LMT	C3'-C4'-C5'	-2.79	104.54	110.93
23	d	403[B]	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
23	B	612	CLA	O2A-CGA-CBA	2.78	120.64	111.91
23	A	404[B]	CLA	C4C-C3C-C2C	-2.78	102.84	106.90
35	C	517[B]	DGD	C2G-O2G-C1B	-2.78	110.94	117.79
25	B	618	BCR	C37-C22-C23	2.78	122.46	118.08
23	a	405[B]	CLA	C3B-C4B-NB	2.78	113.10	110.52
26	a	409[A]	SQD	O47-C7-O49	-2.78	116.98	123.70
34	o	301	HTG	O2-C2-C3	-2.78	103.92	110.35
25	d	405	BCR	C33-C5-C6	-2.78	121.41	124.53
23	A	404[B]	CLA	CAA-C2A-C1A	-2.78	102.87	111.97
23	B	604	CLA	O2A-CGA-O1A	-2.78	116.58	123.59
23	A	404[A]	CLA	CAA-CBA-CGA	-2.78	105.14	113.25
35	C	517[B]	DGD	O6D-C1D-O3G	-2.78	103.40	109.97
23	B	603	CLA	CMC-C2C-C1C	2.78	129.27	125.04
23	b	609	CLA	CHC-C1C-C2C	-2.77	119.02	126.73
23	b	613	CLA	C4-C3-C5	2.77	119.94	115.27
23	b	612	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
23	A	406[B]	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
23	D	402[B]	CLA	C2A-C1A-CHA	-2.77	119.01	123.86
23	C	506	CLA	O2A-CGA-CBA	2.77	120.60	111.91
23	b	609	CLA	CAC-C3C-C4C	2.77	128.40	124.81
25	B	617	BCR	C11-C10-C9	-2.77	123.36	127.31
23	b	612	CLA	CHB-C1B-NB	-2.77	121.33	124.26
23	B	608	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
23	c	510	CLA	CMB-C2B-C1B	2.76	129.58	125.37
25	B	619	BCR	C21-C20-C19	-2.76	114.60	123.22
23	c	503	CLA	C3B-C4B-NB	2.76	113.08	110.52
23	C	508	CLA	CMB-C2B-C1B	2.76	129.57	125.37
29	a	412[A]	PL9	C53-C6-C1	2.76	120.64	114.99
23	C	514	CLA	CHD-C4C-NC	2.76	128.55	124.20
40	v	201	HEC	CBD-CAD-C3D	-2.76	104.96	112.63
23	a	405[B]	CLA	C1-C2-C3	-2.76	121.27	126.04
23	B	602	CLA	CMA-C3A-C4A	-2.76	104.36	111.77
23	B	615	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
23	b	603	CLA	O2A-CGA-CBA	2.76	120.55	111.91
23	a	404[B]	CLA	C1-C2-C3	-2.76	121.28	126.04
29	A	414[B]	PL9	C53-C6-C1	2.75	120.62	114.99
32	D	406[B]	LHG	O8-C23-O10	-2.75	116.65	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
29	A	414[A]	PL9	C40-C39-C41	2.75	119.90	115.27
23	b	602	CLA	C4C-C3C-C2C	-2.75	102.89	106.90
23	b	603	CLA	CMC-C2C-C1C	2.74	129.22	125.04
25	h	101	BCR	C16-C17-C18	-2.74	123.40	127.31
23	D	402[B]	CLA	CAA-C2A-C3A	-2.74	105.27	112.78
23	b	610	CLA	CHD-C4C-NC	2.74	128.52	124.20
35	H	101	DGD	O1G-C1A-C2A	2.74	120.51	111.91
23	B	611	CLA	C1-C2-C3	-2.74	121.30	126.04
23	B	616	CLA	CAC-C3C-C4C	2.74	128.36	124.81
25	k	101	BCR	C39-C30-C25	-2.74	105.86	110.30
32	A	419[B]	LHG	O8-C23-C24	2.74	120.50	111.91
23	b	607	CLA	CAA-C2A-C3A	-2.74	105.28	112.78
31	b	621	LMT	C1'-O5'-C5'	-2.74	108.32	113.69
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
31	M	103	LMT	C3'-C4'-C5'	-2.73	104.66	110.93
32	d	414[B]	LHG	O8-C23-O10	-2.73	116.69	123.59
23	C	502	CLA	C4C-C3C-C2C	-2.73	102.91	106.90
23	C	508	CLA	C4-C3-C5	2.73	119.87	115.27
23	c	504	CLA	O2A-CGA-CBA	2.73	120.48	111.91
23	C	506	CLA	CHC-C1C-C2C	-2.73	119.14	126.73
23	B	603	CLA	C2A-C1A-CHA	-2.73	119.08	123.86
23	A	406[A]	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	c	511	CLA	CMC-C2C-C1C	2.73	129.20	125.04
24	A	407[B]	PHO	O2A-CGA-CBA	2.73	120.48	111.91
23	B	610	CLA	CAA-CBA-CGA	-2.73	105.27	113.25
23	B	601	CLA	C3B-C4B-NB	2.73	113.05	110.52
23	b	605	CLA	CHC-C1C-C2C	-2.73	119.15	126.73
23	B	613	CLA	CMC-C2C-C1C	2.73	129.20	125.04
25	T	101	BCR	C12-C13-C14	-2.73	114.75	118.94
23	b	602	CLA	C4-C3-C5	2.73	119.86	115.27
35	C	517[A]	DGD	C2G-O2G-C1B	-2.73	111.07	117.79
26	a	410	SQD	C3-C4-C5	2.73	115.11	110.24
23	a	405[B]	CLA	CMC-C2C-C1C	2.73	129.19	125.04
25	h	101	BCR	C24-C23-C22	-2.73	122.12	126.23
32	d	408[A]	LHG	O8-C23-C24	2.73	120.46	111.91
26	f	102	SQD	O7-S-C6	2.73	110.18	106.94
25	d	405	BCR	C28-C27-C26	-2.72	109.21	114.08
23	c	504	CLA	C3B-C4B-NB	2.72	113.04	110.52
23	C	511	CLA	CMB-C2B-C1B	2.72	129.52	125.37
23	C	510	CLA	CHD-C4C-NC	2.72	128.49	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	CHD-C4C-NC	2.72	128.49	124.20
23	b	606	CLA	CMC-C2C-C1C	2.72	129.19	125.04
23	B	603	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
23	d	402[A]	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	D	405[A]	PL9	C42-C41-C39	-2.72	104.03	112.98
23	D	402[A]	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
23	c	515	CLA	CAA-C2A-C3A	-2.72	105.33	112.78
32	A	419[A]	LHG	O7-C7-O9	-2.72	117.13	123.70
23	B	609	CLA	CBC-CAC-C3C	-2.72	104.94	112.43
23	A	408	CLA	CHD-C4C-NC	2.71	128.48	124.20
23	d	403[B]	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
29	d	406[A]	PL9	C36-C34-C33	-2.71	115.63	121.12
29	D	405[B]	PL9	C40-C39-C41	2.71	119.83	115.27
24	a	414[B]	PHO	C4A-C3A-C2A	-2.71	100.26	102.84
23	c	503	CLA	O2A-CGA-CBA	2.71	120.42	111.91
23	d	404	CLA	C2A-C1A-CHA	-2.71	119.12	123.86
23	b	604	CLA	C4C-C3C-C2C	-2.71	102.95	106.90
23	b	606	CLA	CHC-C1C-C2C	-2.71	119.21	126.73
23	a	405[A]	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
23	B	609	CLA	CMC-C2C-C1C	2.71	129.16	125.04
24	a	406[A]	PHO	CMA-C3A-C4A	-2.71	108.45	114.38
23	d	404	CLA	C4-C3-C5	2.71	119.82	115.27
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	609	CLA	O2A-CGA-CBA	2.70	120.39	111.91
23	B	613	CLA	CHC-C1C-C2C	-2.70	119.22	126.73
23	D	402[B]	CLA	CMC-C2C-C1C	2.70	129.16	125.04
25	b	617	BCR	C24-C23-C22	-2.70	122.15	126.23
23	C	510	CLA	C16-C15-C13	-2.70	107.19	115.92
40	V	201	HEC	C4B-NB-C1B	2.70	107.86	105.07
23	A	404[B]	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
35	h	102	DGD	O1G-C1A-C2A	2.70	120.38	111.91
23	B	601	CLA	C1-O2A-CGA	2.70	123.53	116.44
35	C	518[A]	DGD	O1G-C1A-O1A	-2.70	116.78	123.59
23	d	404	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	b	611	CLA	CHD-C4C-NC	2.70	128.45	124.20
23	D	402[A]	CLA	CMC-C2C-C1C	2.70	129.15	125.04
23	B	611	CLA	C3B-C4B-NB	2.69	113.02	110.52
23	c	514	CLA	CAC-C3C-C4C	2.69	128.31	124.81
23	a	404[B]	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
23	C	514	CLA	CHC-C1C-C2C	-2.69	119.25	126.73
23	B	610	CLA	CHD-C4C-NC	2.69	128.44	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	515	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	B	613	CLA	CBC-CAC-C3C	-2.69	105.02	112.43
23	c	514	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	b	610	CLA	CHC-C1C-C2C	-2.69	119.27	126.73
23	a	404[A]	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
23	d	403[B]	CLA	O2A-CGA-O1A	-2.69	116.81	123.59
25	t	102	BCR	C28-C27-C26	-2.69	109.28	114.08
23	b	602	CLA	CHB-C1B-C2B	-2.68	119.66	127.24
25	y	101	BCR	C10-C11-C12	-2.68	114.84	123.22
23	d	403[B]	CLA	CMB-C2B-C1B	2.68	129.46	125.37
24	A	407[B]	PHO	C1-C2-C3	-2.68	121.40	126.04
23	c	503	CLA	CHD-C4C-NC	2.68	128.43	124.20
33	C	501	LMG	C8-O7-C10	-2.68	111.19	117.79
23	A	406[A]	CLA	CMC-C2C-C1C	2.68	129.12	125.04
26	f	102	SQD	O48-C23-C24	2.68	120.32	111.91
23	b	603	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
25	a	408	BCR	C29-C30-C25	2.68	114.61	110.48
23	A	405[A]	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	C	507	CLA	O2A-CGA-O1A	-2.68	116.83	123.59
23	c	507	CLA	CAC-C3C-C4C	2.68	128.29	124.81
23	a	405[A]	CLA	CHC-C1C-C2C	-2.68	119.29	126.73
34	b	623	HTG	O5-C1-C2	2.68	113.68	110.31
23	b	612	CLA	CHC-C1C-C2C	-2.68	119.30	126.73
32	a	417[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	518[A]	DGD	C3G-C2G-C1G	-2.68	105.46	111.79
29	D	405[A]	PL9	C37-C38-C39	-2.67	121.22	127.66
25	c	517	BCR	C11-C10-C9	-2.67	123.49	127.31
23	a	407	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
25	k	101	BCR	C15-C14-C13	-2.67	123.50	127.31
23	A	406[A]	CLA	C1-C2-C3	-2.67	121.42	126.04
26	B	620	SQD	O48-C23-O10	-2.67	116.85	123.59
25	K	102	BCR	C29-C30-C25	2.67	114.59	110.48
25	k	101	BCR	C3-C4-C5	-2.67	109.31	114.08
31	B	629	LMT	O5'-C5'-C6'	2.67	113.08	106.44
25	t	102	BCR	C39-C30-C25	-2.67	105.97	110.30
35	h	102	DGD	O1G-C1A-O1A	-2.67	116.85	123.59
23	C	510	CLA	CMC-C2C-C1C	2.67	129.10	125.04
23	B	610	CLA	CAC-C3C-C4C	2.67	128.27	124.81
23	B	606	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	C	507	CLA	C4-C3-C5	2.67	119.76	115.27
23	b	603	CLA	CBC-CAC-C3C	-2.66	105.09	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	506	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
40	V	201	HEC	CMD-C2D-C1D	2.66	129.10	125.04
31	B	630	LMT	C3'-C4'-C5'	-2.66	104.82	110.93
23	B	610	CLA	CMC-C2C-C1C	2.66	129.09	125.04
23	C	511	CLA	O2A-CGA-O1A	-2.66	116.88	123.59
23	b	614	CLA	CMC-C2C-C1C	2.66	129.09	125.04
23	c	515	CLA	CMB-C2B-C1B	2.66	129.42	125.37
23	B	605	CLA	C2A-C1A-CHA	-2.66	119.21	123.86
23	a	405[B]	CLA	CHC-C1C-C2C	-2.66	119.35	126.73
23	a	405[A]	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
23	b	611	CLA	CAC-C3C-C4C	2.66	128.26	124.81
23	D	403	CLA	CHD-C4C-NC	2.66	128.39	124.20
23	C	512	CLA	CHD-C4C-NC	2.66	128.39	124.20
29	a	412[B]	PL9	C40-C39-C41	2.66	119.74	115.27
26	A	410[A]	SQD	O48-C23-O10	-2.65	116.89	123.59
23	A	406[B]	CLA	O2A-CGA-O1A	-2.65	116.89	123.59
23	b	609	CLA	CMC-C2C-C1C	2.65	129.08	125.04
23	c	510	CLA	CAA-C2A-C3A	-2.65	105.51	112.78
25	T	101	BCR	C33-C5-C6	-2.65	121.55	124.53
23	a	404[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
33	m	101	LMG	C8-O7-C10	-2.65	111.26	117.79
31	A	420	LMT	O5'-C5'-C6'	2.65	113.03	106.44
23	b	609	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
23	A	406[B]	CLA	C4C-C3C-C2C	-2.65	103.03	106.90
23	c	505	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	c	508	CLA	CHD-C4C-NC	2.65	128.38	124.20
23	a	407	CLA	O2A-CGA-O1A	-2.65	116.90	123.59
23	C	513	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
23	b	602	CLA	CMA-C3A-C4A	-2.65	104.65	111.77
29	D	405[A]	PL9	C40-C39-C41	2.65	119.72	115.27
23	C	507	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
35	H	101	DGD	O1G-C1A-O1A	-2.65	116.91	123.59
23	B	612	CLA	CHD-C4C-NC	2.65	128.37	124.20
23	C	503	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	a	407	CLA	CMA-C3A-C2A	-2.65	103.16	113.83
23	B	615	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	c	507	CLA	O2A-CGA-CBA	2.64	120.21	111.91
29	a	412[B]	PL9	C20-C19-C21	2.64	119.72	115.27
23	C	509	CLA	CAC-C3C-C4C	2.64	128.24	124.81
23	b	607	CLA	C4A-NA-C1A	-2.64	105.52	106.71
26	A	412	SQD	C4-C3-C2	-2.64	106.21	110.82
25	k	101	BCR	C2-C1-C6	2.64	114.55	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	606	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
23	C	511	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	A	406[A]	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
23	b	606	CLA	C1-O2A-CGA	2.64	123.36	116.44
25	C	516	BCR	C33-C5-C6	-2.64	121.57	124.53
23	C	514	CLA	O2A-CGA-CBA	2.64	120.18	111.91
23	C	514	CLA	CAA-C2A-C3A	-2.63	105.56	112.78
23	A	406[A]	CLA	C4-C3-C5	2.63	119.70	115.27
23	B	603	CLA	O2A-CGA-CBA	2.63	120.17	111.91
23	d	403[B]	CLA	CBC-CAC-C3C	-2.63	105.17	112.43
23	C	504	CLA	CMC-C2C-C1C	2.63	129.05	125.04
25	K	102	BCR	C24-C23-C22	-2.63	122.26	126.23
24	A	416[A]	PHO	O2D-CGD-O1D	-2.63	118.69	123.84
25	h	101	BCR	C16-C15-C14	-2.63	118.08	123.47
23	b	601	CLA	CMC-C2C-C1C	2.63	129.05	125.04
33	D	411	LMG	O8-C28-C29	2.63	120.16	111.91
23	C	507	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	d	403[B]	CLA	CMC-C2C-C1C	2.63	129.04	125.04
25	b	618	BCR	C29-C30-C25	2.63	114.53	110.48
23	D	403	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
31	M	103	LMT	C1'-O5'-C5'	-2.63	108.53	113.69
25	B	617	BCR	C31-C1-C6	-2.63	106.04	110.30
23	c	509	CLA	O2A-CGA-CBA	2.63	120.16	111.91
23	B	606	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
23	c	515	CLA	C2A-C1A-CHA	-2.63	119.27	123.86
26	F	102	SQD	O48-C23-C24	2.63	120.15	111.91
32	a	417[B]	LHG	O8-C23-C24	2.62	120.14	111.91
23	c	513	CLA	CHC-C1C-C2C	-2.62	119.44	126.73
26	a	410	SQD	C1-O5-C5	2.62	118.84	113.69
23	c	506	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
23	b	610	CLA	CMC-C2C-C1C	2.62	129.03	125.04
23	d	403[B]	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	D	403	CLA	C2A-C1A-CHA	-2.62	119.28	123.86
23	d	403[B]	CLA	CAC-C3C-C4C	2.62	128.21	124.81
23	b	608	CLA	CHD-C4C-NC	2.62	128.33	124.20
23	d	403[A]	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
23	D	403	CLA	CMA-C3A-C2A	-2.62	103.27	113.83
31	M	101	LMT	C3'-C4'-C5'	-2.62	104.93	110.93
23	C	502	CLA	C2A-C1A-CHA	-2.61	119.29	123.86
29	A	414[A]	PL9	C53-C6-C1	2.61	120.33	114.99
23	b	601	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
32	D	406[A]	LHG	O8-C23-C24	2.61	120.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	408[B]	LHG	O8-C23-C24	2.61	120.09	111.91
23	a	404[B]	CLA	CHD-C4C-NC	2.61	128.31	124.20
33	B	621	LMG	C4-C3-C2	-2.61	106.27	110.82
32	D	406[A]	LHG	O7-C7-C8	2.61	117.12	111.50
29	d	406[B]	PL9	C36-C37-C38	-2.61	103.31	111.88
23	C	513	CLA	O2A-CGA-O1A	-2.61	117.01	123.59
35	C	519	DGD	O2G-C1B-C2B	2.61	117.12	111.50
23	d	404	CLA	O2A-CGA-CBA	2.61	120.08	111.91
23	A	408	CLA	CMA-C3A-C2A	-2.61	103.32	113.83
29	A	414[B]	PL9	C2-C3-C4	2.60	122.39	118.80
23	b	608	CLA	CMA-C3A-C4A	-2.60	104.77	111.77
23	C	513	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
40	v	201	HEC	CHA-C4D-ND	2.60	127.25	124.42
29	A	414[B]	PL9	C42-C43-C44	-2.60	121.40	127.66
32	L	101[A]	LHG	O8-C23-C24	2.60	120.06	111.91
23	C	504	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
23	c	515	CLA	CHC-C1C-C2C	-2.60	119.52	126.73
23	C	511	CLA	O2A-CGA-CBA	2.60	120.06	111.91
25	X	101	BCR	C37-C22-C21	-2.60	119.28	122.92
23	D	403	CLA	CMC-C2C-C1C	2.60	128.99	125.04
24	a	414[B]	PHO	O2D-CGD-O1D	-2.59	118.77	123.84
23	B	601	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	d	402[A]	CLA	O2A-CGA-CBA	2.59	120.05	111.91
23	c	508	CLA	CMC-C2C-C1C	2.59	128.99	125.04
23	A	405[A]	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
23	c	510	CLA	C4-C3-C5	2.59	119.63	115.27
23	B	605	CLA	CHC-C1C-C2C	-2.59	119.53	126.73
23	c	511	CLA	C2A-C1A-CHA	-2.59	119.33	123.86
23	A	408	CLA	CBC-CAC-C3C	-2.59	105.30	112.43
23	A	406[B]	CLA	CMC-C2C-C1C	2.59	128.98	125.04
23	A	404[B]	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	a	404[A]	CLA	C2A-C1A-CHA	-2.59	119.34	123.86
25	c	517	BCR	C7-C8-C9	-2.59	122.33	126.23
23	d	402[B]	CLA	C4C-C3C-C2C	-2.59	103.13	106.90
26	a	409[B]	SQD	C45-O47-C7	-2.59	111.42	117.79
32	D	407[B]	LHG	O8-C23-O10	-2.59	117.07	123.59
23	b	615	CLA	CHD-C4C-NC	2.58	128.27	124.20
29	A	414[B]	PL9	C40-C39-C41	2.58	119.62	115.27
23	d	404	CLA	CMA-C3A-C4A	-2.58	104.83	111.77
29	d	406[A]	PL9	C36-C37-C38	-2.58	103.40	111.88
25	t	102	BCR	C1-C6-C7	2.58	123.08	115.78
23	B	614	CLA	C2A-C1A-CHA	-2.58	119.35	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	504	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
23	b	610	CLA	C3B-C4B-NB	2.58	112.91	110.52
23	b	613	CLA	CMA-C3A-C4A	-2.58	104.84	111.77
23	B	613	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	c	510	CLA	O2A-CGA-CBA	2.58	119.99	111.91
33	C	520	LMG	O8-C28-O10	-2.58	117.09	123.59
35	C	519	DGD	O1G-C1A-C2A	2.58	119.99	111.91
23	C	503	CLA	O2A-CGA-O1A	-2.57	117.09	123.59
34	o	301	HTG	C1-O5-C5	2.57	117.33	112.58
25	t	102	BCR	C21-C20-C19	-2.57	115.20	123.22
23	C	509	CLA	C4-C3-C5	2.57	119.59	115.27
23	a	404[A]	CLA	CMA-C3A-C4A	-2.57	104.87	111.77
23	C	503	CLA	CHD-C4C-NC	2.57	128.25	124.20
35	c	520	DGD	O1G-C1A-C2A	2.57	119.96	111.91
23	c	510	CLA	CAC-C3C-C4C	2.57	128.14	124.81
25	k	101	BCR	C20-C21-C22	-2.57	123.65	127.31
26	A	412	SQD	O48-C23-O10	-2.56	117.12	123.59
25	a	408	BCR	C7-C8-C9	-2.56	122.36	126.23
25	A	409	BCR	C33-C5-C6	-2.56	121.65	124.53
23	B	610	CLA	CHC-C1C-C2C	-2.56	119.61	126.73
23	D	402[A]	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
23	D	402[A]	CLA	C2A-C1A-CHA	-2.56	119.38	123.86
23	C	502	CLA	CMB-C2B-C1B	2.56	129.27	125.37
25	B	618	BCR	C38-C26-C25	-2.56	121.65	124.53
35	c	518[A]	DGD	O1G-C1A-O1A	-2.56	117.13	123.59
34	b	622	HTG	C6-C5-C4	-2.56	107.01	113.00
23	d	404	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
25	d	405	BCR	C16-C17-C18	-2.56	123.66	127.31
29	d	406[B]	PL9	C53-C6-C1	2.56	120.22	114.99
23	b	608	CLA	C11-C12-C13	-2.56	107.66	115.92
23	B	612	CLA	C4-C3-C5	2.56	119.57	115.27
23	b	606	CLA	CAA-C2A-C3A	-2.55	105.79	112.78
23	B	607	CLA	CHC-C1C-C2C	-2.55	119.64	126.73
23	d	402[B]	CLA	C4-C3-C5	2.55	119.56	115.27
23	D	402[B]	CLA	C4-C3-C5	2.55	119.56	115.27
23	B	609	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
23	C	507	CLA	C4C-C3C-C2C	-2.55	103.18	106.90
23	B	616	CLA	C1-O2A-CGA	2.55	123.13	116.44
23	A	408	CLA	CHB-C1B-NB	-2.55	121.56	124.26
23	c	513	CLA	CAC-C3C-C4C	2.55	128.12	124.81
23	c	509	CLA	O1D-CGD-CBD	-2.55	119.27	124.48
23	C	505	CLA	OBD-CAD-C3D	-2.55	122.39	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	CHB-C1B-NB	-2.55	121.56	124.26
23	d	404	CLA	C3B-C4B-NB	2.54	112.88	110.52
23	A	405[A]	CLA	CMA-C3A-C2A	-2.54	103.58	113.83
23	B	607	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
23	C	502	CLA	C1-C2-C3	-2.54	121.65	126.04
24	a	414[A]	PHO	O1D-CGD-CBD	-2.54	120.51	124.74
25	b	619	BCR	C16-C17-C18	-2.54	123.69	127.31
23	B	610	CLA	CBC-CAC-C3C	-2.54	105.44	112.43
23	B	606	CLA	C3B-C4B-NB	2.54	112.87	110.52
23	c	508	CLA	O2A-CGA-O1A	-2.54	117.19	123.59
23	A	406[B]	CLA	O2A-CGA-CBA	2.54	119.87	111.91
25	B	618	BCR	C2-C1-C6	2.54	114.38	110.48
26	f	102	SQD	O47-C7-O49	-2.53	117.58	123.70
23	b	603	CLA	CHC-C1C-C2C	-2.53	119.69	126.73
26	f	102	SQD	O8-S-C6	2.53	109.78	105.74
23	c	515	CLA	C1-C2-C3	-2.53	121.66	126.04
29	A	414[A]	PL9	C35-C34-C36	2.53	119.53	115.27
23	C	503	CLA	O2A-CGA-CBA	2.53	119.85	111.91
23	a	404[B]	CLA	C4C-C3C-C2C	-2.53	103.21	106.90
23	b	615	CLA	C6-C7-C8	-2.53	107.74	115.92
23	A	405[A]	CLA	C2A-C1A-CHA	-2.53	119.44	123.86
23	A	406[B]	CLA	C1-C2-C3	-2.53	121.67	126.04
35	c	519[B]	DGD	O1G-C1A-C2A	2.53	119.84	111.91
23	C	514	CLA	C4-C3-C5	2.53	119.52	115.27
23	C	512	CLA	CHC-C1C-C2C	-2.53	119.72	126.73
23	c	512	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
23	b	614	CLA	CBC-CAC-C3C	-2.52	105.47	112.43
23	B	606	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	A	406[A]	CLA	CMA-C3A-C2A	-2.52	103.66	113.83
23	B	601	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	c	504	CLA	C4C-C3C-C2C	-2.52	103.23	106.90
23	B	604	CLA	C11-C12-C13	-2.52	107.78	115.92
23	b	616	CLA	C4-C3-C5	2.52	119.50	115.27
24	A	416[B]	PHO	O2A-CGA-CBA	2.51	119.80	111.91
23	b	602	CLA	CMB-C2B-C1B	2.51	129.20	125.37
29	a	412[A]	PL9	C47-C48-C49	-2.51	119.16	127.75
29	D	405[B]	PL9	C37-C38-C39	-2.51	121.61	127.66
23	d	402[B]	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
23	c	513	CLA	C11-C10-C8	-2.51	107.80	115.92
27	b	628	GOL	C3-C2-C1	-2.51	101.94	111.70
23	B	607	CLA	CHD-C4C-NC	2.51	128.16	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	CHC-C1C-C2C	-2.51	119.75	126.73
23	A	404[B]	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	d	402[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	c	505	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
26	a	410	SQD	O48-C23-O10	-2.51	117.26	123.59
24	A	407[A]	PHO	O2A-CGA-CBA	2.51	119.78	111.91
24	A	407[A]	PHO	CMB-C2B-C3B	2.51	129.37	124.68
23	b	612	CLA	CHD-C4C-NC	2.51	128.16	124.20
35	H	101	DGD	O2G-C1B-C2B	2.51	116.91	111.50
23	a	405[A]	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
23	b	608	CLA	C11-C10-C8	-2.51	107.81	115.92
23	c	507	CLA	C1-C2-C3	-2.51	121.71	126.04
23	b	609	CLA	O2A-CGA-CBA	2.51	119.78	111.91
23	b	609	CLA	O2A-CGA-O1A	-2.51	117.26	123.59
29	D	405[B]	PL9	C7-C8-C9	-2.51	122.62	126.79
23	C	514	CLA	C2A-C1A-CHA	-2.51	119.48	123.86
23	B	615	CLA	C6-C7-C8	-2.51	107.82	115.92
33	C	501	LMG	C6-C5-C4	2.50	118.87	113.00
23	b	610	CLA	CMA-C3A-C4A	-2.50	105.05	111.77
23	b	609	CLA	C7-C6-C5	-2.50	106.57	113.36
23	a	404[B]	CLA	CMA-C3A-C4A	-2.50	105.06	111.77
34	B	624	HTG	O5-C5-C4	2.50	114.23	109.69
24	A	407[B]	PHO	CMA-C3A-C4A	-2.50	108.91	114.38
23	a	405[B]	CLA	O2A-CGA-O1A	-2.50	117.29	123.59
23	a	404[A]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
23	B	616	CLA	CHD-C4C-NC	2.49	128.13	124.20
23	b	601	CLA	C3B-C4B-NB	2.49	112.83	110.52
23	b	610	CLA	C4-C3-C5	2.49	119.47	115.27
23	A	408	CLA	CAC-C3C-C4C	2.49	128.04	124.81
23	A	408	CLA	C4-C3-C5	2.49	119.46	115.27
29	d	406[B]	PL9	C36-C34-C33	-2.49	116.08	121.12
32	A	419[B]	LHG	O7-C7-O9	-2.49	117.68	123.70
23	a	405[A]	CLA	O2A-CGA-CBA	2.49	119.72	111.91
24	A	416[B]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
24	a	406[A]	PHO	CMB-C2B-C3B	2.48	129.33	124.68
23	b	607	CLA	O2A-CGA-O1A	-2.48	117.32	123.59
25	a	408	BCR	C40-C30-C25	-2.48	106.27	110.30
25	A	409	BCR	C8-C7-C6	-2.48	120.23	127.20
25	D	404	BCR	C3-C4-C5	-2.48	109.65	114.08
23	c	512	CLA	C4C-C3C-C2C	-2.48	103.28	106.90
23	b	614	CLA	C2A-C1A-CHA	-2.48	119.52	123.86
35	C	517[A]	DGD	O5D-C6D-C5D	-2.48	104.46	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	406[A]	PL9	C17-C18-C19	-2.48	121.69	127.66
23	c	515	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
23	a	407	CLA	CBC-CAC-C3C	-2.48	105.60	112.43
23	A	408	CLA	CMC-C2C-C1C	2.48	128.81	125.04
24	A	407[A]	PHO	O2A-CGA-O1A	-2.48	117.34	123.59
24	A	407[B]	PHO	O2D-CGD-O1D	-2.48	119.00	123.84
23	d	404	CLA	C1-O2A-CGA	2.47	122.94	116.44
23	d	404	CLA	CAA-C2A-C3A	-2.47	106.00	112.78
23	A	404[A]	CLA	CMA-C3A-C2A	-2.47	103.85	113.83
23	B	614	CLA	CBC-CAC-C3C	-2.47	105.62	112.43
23	B	612	CLA	CHC-C1C-C2C	-2.47	119.86	126.73
25	B	619	BCR	C39-C30-C25	-2.47	106.29	110.30
23	B	608	CLA	CMA-C3A-C4A	-2.47	105.14	111.77
23	C	508	CLA	CHC-C1C-C2C	-2.47	119.87	126.73
23	b	610	CLA	CAC-C3C-C4C	2.47	128.01	124.81
23	a	407	CLA	CHC-C1C-C2C	-2.47	119.88	126.73
23	c	509	CLA	CBC-CAC-C3C	-2.47	105.63	112.43
29	A	414[B]	PL9	C35-C34-C36	2.47	119.42	115.27
38	E	102	HEM	O2A-CGA-CBA	2.47	121.95	114.03
23	b	607	CLA	CMB-C2B-C1B	2.47	129.12	125.37
23	a	404[B]	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
23	B	612	CLA	O2A-CGA-O1A	-2.47	117.37	123.59
23	B	607	CLA	C1-O2A-CGA	2.46	122.91	116.44
23	C	510	CLA	C11-C12-C13	-2.46	107.95	115.92
32	d	407[A]	LHG	O8-C23-O10	-2.46	117.38	123.59
23	d	402[B]	CLA	CMA-C3A-C2A	-2.46	103.90	113.83
26	a	409[B]	SQD	O48-C23-C24	2.46	119.63	111.91
26	a	409[A]	SQD	O7-S-C6	2.46	109.86	106.94
31	F	101	LMT	C1'-O5'-C5'	-2.46	108.86	113.69
23	d	403[B]	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
23	B	606	CLA	C2A-C1A-CHA	-2.46	119.56	123.86
23	b	608	CLA	C4-C3-C5	2.46	119.40	115.27
23	A	406[B]	CLA	CAC-C3C-C4C	2.46	128.00	124.81
23	B	611	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
25	c	516	BCR	C16-C17-C18	-2.45	123.81	127.31
23	d	402[A]	CLA	C4C-C3C-C2C	-2.45	103.32	106.90
32	d	407[B]	LHG	O8-C23-C24	2.45	119.60	111.91
23	B	607	CLA	C2A-C1A-CHA	-2.45	119.57	123.86
33	m	101	LMG	C7-O1-C1	-2.45	108.95	113.74
23	d	404	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	d	402[B]	CLA	O2A-CGA-CBA	2.45	119.60	111.91
23	c	503	CLA	CBC-CAC-C3C	-2.45	105.68	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A	405[A]	CLA	CMA-C3A-C4A	-2.45	105.19	111.77
29	a	412[A]	PL9	C40-C39-C41	2.45	119.39	115.27
29	D	405[A]	PL9	C27-C28-C29	-2.44	121.77	127.66
23	B	608	CLA	CHD-C4C-NC	2.44	128.06	124.20
29	a	412[A]	PL9	C20-C19-C21	2.44	119.38	115.27
23	C	502	CLA	C1-O2A-CGA	2.44	122.86	116.44
25	d	405	BCR	C37-C22-C23	2.44	121.93	118.08
23	c	514	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
23	C	506	CLA	CHB-C1B-NB	-2.44	121.67	124.26
23	C	513	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
23	c	505	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
32	L	101[B]	LHG	O8-C23-C24	2.44	119.57	111.91
38	E	102	HEM	O2D-CGD-CBD	2.44	121.87	114.03
23	c	510	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
23	c	504	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
29	a	412[B]	PL9	C45-C44-C46	2.44	119.38	115.27
23	B	604	CLA	C6-C5-C3	-2.44	107.06	113.45
25	c	516	BCR	C38-C26-C25	-2.44	121.79	124.53
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	613	CLA	CED-O2D-CGD	2.44	121.45	115.94
25	c	516	BCR	C28-C27-C26	-2.44	109.72	114.08
23	B	601	CLA	CMC-C2C-C1C	2.44	128.75	125.04
23	b	602	CLA	C11-C10-C8	-2.44	108.04	115.92
23	c	505	CLA	C4-C3-C5	2.44	119.37	115.27
23	B	608	CLA	CAA-C2A-C3A	-2.44	106.11	112.78
35	C	518[B]	DGD	O1G-C1A-O1A	-2.43	117.45	123.59
25	T	101	BCR	C21-C20-C19	-2.43	115.62	123.22
23	b	611	CLA	O2A-CGA-CBA	2.43	119.55	111.91
25	B	619	BCR	C37-C22-C21	-2.43	119.52	122.92
26	B	620	SQD	C44-O6-C1	-2.43	108.99	113.74
26	a	410	SQD	O8-S-C6	2.43	109.61	105.74
24	a	406[A]	PHO	O2A-CGA-O1A	-2.43	117.46	123.59
35	c	520	DGD	O3G-C3G-C2G	-2.43	105.04	110.90
23	C	507	CLA	CHD-C4C-NC	2.43	128.03	124.20
26	a	409[B]	SQD	O47-C7-O49	-2.43	117.83	123.70
23	c	509	CLA	CHC-C1C-C2C	-2.43	119.99	126.73
23	a	407	CLA	C2A-C1A-CHA	-2.43	119.62	123.86
29	d	406[A]	PL9	C47-C48-C49	-2.42	119.47	127.75
25	b	618	BCR	C15-C14-C13	-2.42	123.85	127.31
31	B	627	LMT	O1'-C1'-C2'	2.42	112.09	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	C16-C15-C13	-2.42	108.09	115.92
23	d	402[B]	CLA	C1-C2-C3	-2.42	121.85	126.04
23	C	509	CLA	CHD-C4C-NC	2.42	128.02	124.20
23	C	510	CLA	C4-C3-C5	2.42	119.34	115.27
23	C	512	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
23	b	601	CLA	C2A-C1A-CHA	-2.42	119.62	123.86
25	B	618	BCR	C15-C14-C13	-2.42	123.86	127.31
23	b	608	CLA	O2A-CGA-CBA	2.42	119.50	111.91
25	X	101	BCR	C10-C11-C12	-2.42	115.67	123.22
25	Y	101	BCR	C24-C23-C22	-2.42	122.58	126.23
23	B	607	CLA	C4C-C3C-C2C	-2.42	103.38	106.90
23	B	609	CLA	CHD-C4C-NC	2.42	128.01	124.20
23	c	506	CLA	O2A-CGA-O1A	-2.42	117.50	123.59
26	a	409[A]	SQD	O8-S-C6	2.41	109.59	105.74
23	B	604	CLA	O2A-CGA-CBA	2.41	119.48	111.91
23	B	602	CLA	C11-C12-C13	-2.41	108.12	115.92
29	A	414[A]	PL9	C35-C34-C33	-2.41	117.49	123.68
29	A	414[B]	PL9	C10-C9-C8	-2.41	117.49	123.68
23	A	405[B]	CLA	C2A-C1A-CHA	-2.41	119.64	123.86
26	b	620	SQD	C1-C2-C3	-2.41	104.97	110.00
29	d	406[B]	PL9	C17-C18-C19	-2.41	121.85	127.66
23	B	611	CLA	C2C-C1C-NC	2.41	112.23	109.97
23	B	602	CLA	CMB-C2B-C1B	2.41	129.04	125.37
25	X	101	BCR	C16-C15-C14	-2.41	118.54	123.47
23	C	508	CLA	CMC-C2C-C1C	2.41	128.71	125.04
25	d	405	BCR	C21-C20-C19	-2.41	115.70	123.22
25	t	102	BCR	C2-C1-C6	2.41	114.19	110.48
26	a	410	SQD	O5-C5-C4	2.41	114.07	109.69
23	C	510	CLA	CAC-C3C-C4C	2.41	127.94	124.81
29	a	412[B]	PL9	C47-C48-C49	-2.41	119.52	127.75
29	A	414[B]	PL9	C12-C13-C14	-2.41	121.86	127.66
25	d	405	BCR	C39-C30-C25	-2.41	106.39	110.30
23	C	502	CLA	O2A-CGA-O1A	-2.41	117.52	123.59
29	A	414[A]	PL9	C42-C43-C44	-2.41	121.87	127.66
23	C	508	CLA	CBC-CAC-C3C	-2.40	105.80	112.43
25	A	409	BCR	C11-C10-C9	-2.40	123.88	127.31
23	D	402[B]	CLA	CHD-C4C-NC	2.40	127.99	124.20
23	c	509	CLA	C4C-C3C-C2C	-2.40	103.39	106.90
35	C	518[B]	DGD	O1G-C1A-C2A	2.40	119.44	111.91
23	c	504	CLA	C1-C2-C3	-2.40	121.89	126.04
33	B	621	LMG	C12-C11-C10	-2.40	104.89	113.62
32	D	406[B]	LHG	O8-C23-C24	2.40	119.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
23	b	601	CLA	CAC-C3C-C4C	2.40	127.92	124.81
29	D	405[B]	PL9	C20-C19-C21	2.40	119.31	115.27
23	a	407	CLA	CAC-C3C-C4C	2.40	127.92	124.81
23	B	602	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	C	508	CLA	C1-C2-C3	-2.40	121.90	126.04
26	f	102	SQD	C44-O6-C1	-2.40	109.06	113.74
23	C	511	CLA	CHB-C1B-NB	-2.40	121.72	124.26
33	C	521	LMG	C9-C8-C7	-2.40	106.12	111.79
25	t	102	BCR	C19-C18-C17	-2.40	115.27	118.94
25	d	405	BCR	C40-C30-C39	2.40	115.88	108.53
23	B	610	CLA	CMA-C3A-C2A	-2.40	104.17	113.83
23	B	601	CLA	CBC-CAC-C3C	-2.39	105.83	112.43
23	B	602	CLA	CMA-C3A-C2A	-2.39	104.17	113.83
24	a	406[B]	PHO	CMB-C2B-C3B	2.39	129.15	124.68
23	C	508	CLA	O2A-CGA-CBA	2.39	119.42	111.91
25	h	101	BCR	C36-C18-C17	-2.39	119.57	122.92
23	B	614	CLA	OBD-CAD-C3D	-2.39	122.76	128.52
31	B	627	LMT	C1B-C2B-C3B	2.39	114.98	110.00
23	c	507	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
23	c	512	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
23	C	513	CLA	CMC-C2C-C1C	2.39	128.68	125.04
23	C	502	CLA	C11-C12-C13	-2.39	108.20	115.92
35	c	518[B]	DGD	O3G-C3G-C2G	-2.39	105.14	110.90
33	B	621	LMG	O1-C7-C8	-2.39	105.14	110.90
23	B	605	CLA	CBC-CAC-C3C	-2.39	105.86	112.43
23	C	512	CLA	CMB-C2B-C1B	2.38	129.00	125.37
23	C	507	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
23	C	504	CLA	CBC-CAC-C3C	-2.38	105.86	112.43
23	B	608	CLA	O2A-CGA-CBA	2.38	119.39	111.91
23	C	511	CLA	C2A-C1A-CHA	-2.38	119.69	123.86
31	A	420	LMT	O1'-C1'-C2'	2.38	112.02	108.30
23	c	507	CLA	CMC-C2C-C1C	2.38	128.66	125.04
32	L	101[A]	LHG	O8-C23-O10	-2.38	117.59	123.59
26	F	102	SQD	O47-C7-O49	-2.38	117.95	123.70
23	b	604	CLA	C4-C3-C5	2.38	119.27	115.27
23	c	512	CLA	C4-C3-C2	-2.38	117.58	123.68
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
29	D	405[A]	PL9	C45-C44-C46	2.38	119.27	115.27
23	B	608	CLA	C11-C12-C13	-2.38	108.24	115.92
23	b	603	CLA	CAC-C3C-C4C	2.38	127.89	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C4-C3-C5	2.37	119.26	115.27
23	B	612	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
23	A	404[B]	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	B	602	CLA	CHC-C1C-C2C	-2.37	120.14	126.73
23	c	515	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
35	h	102	DGD	O4D-C4D-C3D	-2.37	104.87	110.35
23	C	509	CLA	O2A-CGA-CBA	2.37	119.33	111.91
25	C	516	BCR	C38-C26-C25	-2.36	121.87	124.53
29	D	405[B]	PL9	C30-C29-C31	2.36	119.25	115.27
23	d	404	CLA	CAC-C3C-C4C	2.36	127.87	124.81
26	b	620	SQD	O5-C1-C2	-2.36	105.35	110.35
33	B	621	LMG	O8-C28-O10	-2.36	117.64	123.59
29	d	406[B]	PL9	C51-C49-C50	2.36	119.81	114.60
31	B	630	LMT	O1'-C1'-C2'	2.36	111.99	108.30
29	D	405[A]	PL9	C22-C23-C24	-2.36	121.98	127.66
23	B	611	CLA	CAC-C3C-C4C	2.36	127.87	124.81
23	A	408	CLA	C2A-C1A-CHA	-2.36	119.74	123.86
23	B	601	CLA	CHB-C4A-NA	2.36	127.77	124.51
25	b	619	BCR	C7-C8-C9	-2.36	122.67	126.23
25	D	404	BCR	C29-C28-C27	-2.36	106.11	111.38
23	a	405[B]	CLA	O2A-CGA-CBA	2.36	119.30	111.91
25	B	619	BCR	C16-C15-C14	-2.36	118.65	123.47
23	b	603	CLA	CMB-C2B-C1B	2.36	128.96	125.37
23	c	511	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
25	b	619	BCR	C15-C14-C13	-2.35	123.95	127.31
31	B	630	LMT	O5'-C5'-C4'	2.35	114.72	109.75
23	b	615	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
23	b	605	CLA	C3B-C4B-NB	2.35	112.70	110.52
29	A	414[B]	PL9	C47-C48-C49	-2.35	119.71	127.75
35	C	519	DGD	O3G-C3G-C2G	-2.35	105.22	110.90
25	c	517	BCR	C38-C26-C25	-2.35	121.89	124.53
24	A	416[A]	PHO	CMA-C3A-C4A	-2.35	109.23	114.38
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
25	B	619	BCR	C34-C9-C8	2.35	121.78	118.08
35	C	518[A]	DGD	O6E-C5E-C6E	2.35	112.28	106.44
34	c	523	HTG	O5-C1-C2	2.35	113.27	110.31
29	a	412[A]	PL9	C45-C44-C46	2.35	119.22	115.27
25	Y	101	BCR	C37-C22-C23	2.35	121.78	118.08
35	c	518[B]	DGD	C3G-C2G-C1G	-2.35	106.23	111.79
23	d	402[A]	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
23	C	504	CLA	CHB-C1B-C2B	-2.35	120.61	127.24
23	b	607	CLA	CAC-C3C-C4C	2.34	127.85	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	101	BCR	C16-C17-C18	-2.34	123.97	127.31
25	T	101	BCR	C35-C13-C12	2.34	121.76	118.08
40	v	201	HEC	C4B-NB-C1B	2.34	107.49	105.07
23	c	509	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
23	C	513	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
23	C	504	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	c	507	CLA	CHD-C4C-NC	2.34	127.89	124.20
23	b	612	CLA	C11-C12-C13	-2.34	108.37	115.92
26	b	620	SQD	C44-O6-C1	-2.34	109.18	113.74
23	C	510	CLA	CMB-C2B-C1B	2.33	128.92	125.37
35	H	101	DGD	O6E-C5E-C6E	2.33	112.24	106.44
23	b	606	CLA	CMB-C2B-C1B	2.33	128.92	125.37
33	c	522	LMG	O8-C28-O10	-2.33	117.70	123.59
23	c	508	CLA	O2A-CGA-CBA	2.33	119.23	111.91
25	c	516	BCR	C33-C5-C6	-2.33	121.91	124.53
23	c	507	CLA	CHB-C1B-NB	-2.33	121.79	124.26
23	D	402[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	b	607	CLA	C2A-C1A-CHA	-2.33	119.78	123.86
23	B	603	CLA	CMA-C3A-C2A	-2.33	104.43	113.83
23	B	608	CLA	CMC-C2C-C1C	2.33	128.59	125.04
25	Y	101	BCR	C34-C9-C8	2.33	121.75	118.08
29	a	412[A]	PL9	C35-C34-C33	-2.33	117.70	123.68
35	C	518[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
23	C	513	CLA	C2A-C1A-CHA	-2.33	119.79	123.86
35	c	519[A]	DGD	O1G-C1A-C2A	2.33	119.21	111.91
23	c	508	CLA	C4-C3-C5	2.33	119.19	115.27
25	c	517	BCR	C21-C20-C19	-2.33	115.95	123.22
23	C	514	CLA	CHB-C1B-NB	-2.33	121.79	124.26
25	a	408	BCR	C8-C7-C6	-2.33	120.67	127.20
25	t	102	BCR	C29-C28-C27	-2.33	106.18	111.38
32	d	407[A]	LHG	O8-C23-C24	2.33	119.21	111.91
23	B	616	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	c	506	CLA	C2A-C1A-CHA	-2.32	119.80	123.86
23	c	513	CLA	C1-O2A-CGA	2.32	122.54	116.44
35	c	518[A]	DGD	C2G-O2G-C1B	-2.32	112.07	117.79
23	B	603	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
23	c	507	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
23	C	504	CLA	CAC-C3C-C4C	2.32	127.82	124.81
29	D	405[B]	PL9	C45-C44-C46	2.32	119.18	115.27
23	b	615	CLA	O2A-CGA-CBA	2.32	119.19	111.91
33	d	412	LMG	O8-C28-O10	-2.32	117.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	m	103	LMT	C1'-O5'-C5'	-2.32	109.14	113.69
23	C	505	CLA	C4-C3-C5	2.32	119.17	115.27
23	a	405[A]	CLA	C4-C3-C5	2.32	119.17	115.27
23	A	406[B]	CLA	C4-C3-C5	2.32	119.17	115.27
23	C	502	CLA	O2A-CGA-CBA	2.32	119.18	111.91
23	c	505	CLA	O2A-CGA-CBA	2.32	119.18	111.91
33	d	412	LMG	O8-C28-C29	2.32	119.18	111.91
23	A	404[A]	CLA	CMA-C3A-C4A	-2.32	105.54	111.77
23	B	601	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
26	a	409[A]	SQD	O48-C23-C24	2.32	119.17	111.91
25	b	618	BCR	C8-C7-C6	-2.31	120.70	127.20
23	c	505	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
32	d	414[B]	LHG	O7-C7-O9	-2.31	118.11	123.70
26	A	410[B]	SQD	O48-C23-O10	-2.31	117.75	123.59
23	B	602	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
25	D	404	BCR	C30-C25-C24	2.31	122.32	115.78
38	E	102	HEM	C4D-ND-C1D	2.31	107.46	105.07
23	c	506	CLA	CHD-C4C-NC	2.31	127.84	124.20
23	C	513	CLA	C3B-C4B-NB	2.31	112.66	110.52
29	A	414[A]	PL9	C37-C36-C34	-2.31	105.38	112.98
35	c	520	DGD	O3G-C1D-C2D	-2.31	104.70	108.30
23	c	514	CLA	CHB-C4A-NA	2.31	127.70	124.51
35	C	518[B]	DGD	O2G-C1B-O1B	-2.31	118.12	123.70
23	C	506	CLA	CHA-C1A-NA	-2.31	121.11	126.40
23	b	603	CLA	C7-C6-C5	-2.31	107.09	113.36
29	d	406[B]	PL9	C45-C44-C46	2.31	119.15	115.27
23	b	607	CLA	CMC-C2C-C1C	2.31	128.55	125.04
23	B	615	CLA	C2A-C1A-CHA	-2.30	119.83	123.86
24	A	416[B]	PHO	OBD-CAD-C3D	-2.30	124.16	127.98
25	y	101	BCR	C21-C20-C19	-2.30	116.03	123.22
23	d	403[A]	CLA	CMC-C2C-C1C	2.30	128.55	125.04
23	d	402[B]	CLA	CHB-C1B-NB	-2.30	121.82	124.26
29	A	414[B]	PL9	C35-C34-C33	-2.30	117.77	123.68
29	A	414[A]	PL9	C2-C3-C4	2.30	121.97	118.80
23	b	608	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
23	b	608	CLA	C4C-C3C-C2C	-2.30	103.54	106.90
26	B	620	SQD	O5-C1-C2	-2.30	105.48	110.35
40	V	201	HEC	CHA-C4D-ND	2.30	126.92	124.42
23	A	404[A]	CLA	CMC-C2C-C1C	2.30	128.54	125.04
25	c	517	BCR	C37-C22-C23	2.30	121.70	118.08
23	c	514	CLA	C3B-C4B-NB	2.30	112.65	110.52
23	a	407	CLA	CMB-C2B-C1B	2.30	128.87	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	CMC-C2C-C1C	2.29	128.53	125.04
25	K	102	BCR	C38-C26-C25	-2.29	121.95	124.53
34	b	622	HTG	O2-C2-C3	-2.29	105.04	110.35
23	b	613	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
23	b	615	CLA	C2A-C1A-CHA	-2.29	119.85	123.86
29	A	414[A]	PL9	C47-C48-C49	-2.29	119.92	127.75
24	a	414[A]	PHO	O2D-CGD-O1D	-2.29	119.36	123.84
23	B	610	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	c	513	CLA	O2A-C1-C2	-2.29	102.62	108.64
25	c	516	BCR	C34-C9-C10	-2.29	119.72	122.92
32	d	408[A]	LHG	O8-C23-O10	-2.29	117.82	123.59
25	B	619	BCR	C29-C30-C25	2.29	114.00	110.48
23	a	405[A]	CLA	CBC-CAC-C3C	-2.29	106.12	112.43
23	C	504	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
23	C	502	CLA	C4-C3-C5	2.29	119.12	115.27
31	B	629	LMT	O5B-C5B-C4B	2.29	113.85	109.69
33	c	521	LMG	C8-O7-C10	-2.29	112.16	117.79
23	b	615	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
23	c	513	CLA	CMB-C2B-C1B	2.29	128.85	125.37
25	c	517	BCR	C37-C22-C21	-2.29	119.72	122.92
23	B	614	CLA	CAA-C2A-C3A	-2.28	106.52	112.78
23	B	609	CLA	C1-C2-C3	-2.28	122.09	126.04
23	A	406[B]	CLA	CMA-C3A-C2A	-2.28	104.62	113.83
24	a	414[B]	PHO	CBA-CAA-C2A	-2.28	107.15	113.81
35	h	102	DGD	C6D-C5D-C4D	2.28	116.85	112.09
25	b	617	BCR	C21-C20-C19	-2.28	116.10	123.22
23	C	512	CLA	O2A-CGA-CBA	2.28	119.06	111.91
23	c	514	CLA	CMC-C2C-C1C	2.28	128.51	125.04
40	v	201	HEC	C1D-C2D-C3D	-2.28	104.56	106.96
25	Y	101	BCR	C36-C18-C17	-2.28	119.73	122.92
26	A	410[B]	SQD	O9-S-O7	-2.28	106.07	113.95
29	D	405[B]	PL9	C12-C13-C14	-2.28	122.18	127.66
23	b	601	CLA	O2A-CGA-CBA	2.28	119.05	111.91
23	C	513	CLA	CBA-CAA-C2A	-2.28	107.15	113.86
23	C	510	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
23	A	404[B]	CLA	CMA-C3A-C2A	-2.27	104.65	113.83
23	b	615	CLA	C1-C2-C3	-2.27	122.11	126.04
23	a	404[A]	CLA	CMA-C3A-C2A	-2.27	104.66	113.83
23	B	614	CLA	C4-C3-C5	2.27	119.09	115.27
23	B	606	CLA	CHB-C1B-C2B	-2.27	120.82	127.24
29	d	406[A]	PL9	C31-C32-C33	-2.27	104.42	111.88
24	A	407[B]	PHO	C4-C3-C5	2.27	119.09	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	d	407[B]	LHG	O8-C23-O10	-2.27	117.87	123.59
25	y	101	BCR	C34-C9-C8	2.27	121.65	118.08
24	A	407[B]	PHO	CBC-CAC-C3C	-2.27	109.56	112.88
29	A	414[B]	PL9	C51-C49-C50	2.27	119.61	114.60
25	Y	101	BCR	C38-C26-C25	-2.27	121.98	124.53
24	A	416[A]	PHO	O1D-CGD-CBD	-2.27	120.96	124.74
33	m	101	LMG	O1-C7-C8	-2.27	105.43	110.90
23	c	505	CLA	C1-C2-C3	-2.27	122.12	126.04
31	A	420	LMT	O5'-C5'-C4'	2.27	114.53	109.75
23	d	402[B]	CLA	CAC-C3C-C2C	2.26	131.40	127.53
23	a	404[B]	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	b	609	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
23	c	508	CLA	CMB-C2B-C1B	2.26	128.82	125.37
23	C	513	CLA	CAC-C3C-C4C	2.26	127.75	124.81
24	A	407[B]	PHO	CMB-C2B-C3B	2.26	128.91	124.68
25	B	617	BCR	C15-C14-C13	-2.26	124.08	127.31
32	d	407[B]	LHG	C5-O7-C7	-2.26	112.22	117.79
32	d	414[A]	LHG	O7-C7-O9	-2.26	118.24	123.70
25	a	408	BCR	C33-C5-C6	-2.26	121.99	124.53
23	D	402[A]	CLA	C4-C3-C5	2.26	119.07	115.27
32	d	407[A]	LHG	C6-C5-C4	-2.26	106.44	111.79
25	X	101	BCR	C24-C23-C22	-2.26	122.82	126.23
31	e	101	LMT	O1'-C1'-C2'	2.26	111.83	108.30
32	b	629[A]	LHG	O8-C23-O10	-2.26	117.90	123.59
31	M	101	LMT	O5B-C5B-C6B	2.26	112.05	106.44
24	a	414[A]	PHO	C4-C3-C2	-2.26	117.89	123.68
23	A	404[B]	CLA	C4-C3-C5	2.25	119.06	115.27
25	D	404	BCR	C37-C22-C21	-2.25	119.77	122.92
23	B	612	CLA	C3B-C4B-NB	2.25	112.61	110.52
32	d	414[B]	LHG	C5-O7-C7	-2.25	112.25	117.79
23	B	608	CLA	OBD-CAD-C3D	-2.25	123.10	128.52
25	c	517	BCR	C20-C21-C22	-2.25	124.10	127.31
23	c	506	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
29	D	405[A]	PL9	C20-C19-C21	2.25	119.05	115.27
25	K	102	BCR	C37-C22-C21	-2.25	119.77	122.92
27	B	623	GOL	C3-C2-C1	-2.25	102.96	111.70
23	C	503	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
33	m	101	LMG	O3-C3-C2	-2.25	105.15	110.35
23	c	506	CLA	C1-C2-C3	-2.25	122.16	126.04
24	A	416[A]	PHO	CMB-C2B-C3B	2.25	128.88	124.68
35	c	518[B]	DGD	O6D-C1D-O3G	-2.25	104.66	109.97
25	T	101	BCR	C3-C4-C5	-2.25	110.07	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	O1D-CGD-CBD	-2.24	119.89	124.48
23	C	509	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
23	b	613	CLA	CAC-C3C-C4C	2.24	127.72	124.81
38	E	102	HEM	C4A-NA-C1A	2.24	107.54	105.35
23	c	508	CLA	C2A-C1A-CHA	-2.24	119.94	123.86
24	a	414[A]	PHO	CED-O2D-CGD	2.24	121.00	115.94
23	b	604	CLA	C6-C5-C3	-2.24	107.58	113.45
25	b	619	BCR	C39-C30-C25	-2.24	106.67	110.30
31	B	629	LMT	O5'-C5'-C4'	2.24	114.47	109.75
29	a	412[B]	PL9	C51-C49-C50	2.24	119.55	114.60
33	c	501	LMG	O6-C5-C4	2.24	113.76	109.69
25	b	618	BCR	C37-C22-C23	2.24	121.60	118.08
31	t	101	LMT	C1-O1'-C1'	2.24	117.55	113.84
23	b	603	CLA	CMA-C3A-C2A	-2.23	104.82	113.83
25	y	101	BCR	C1-C6-C7	2.23	122.10	115.78
23	B	611	CLA	CMB-C2B-C3B	2.23	132.00	126.59
29	D	405[A]	PL9	C36-C37-C38	-2.23	104.54	111.88
23	c	510	CLA	CHD-C4C-NC	2.23	127.72	124.20
23	B	610	CLA	C1-C2-C3	-2.23	122.18	126.04
24	A	407[B]	PHO	O2A-CGA-O1A	-2.23	117.96	123.59
23	d	403[B]	CLA	CHD-C4C-NC	2.23	127.72	124.20
25	k	101	BCR	C10-C11-C12	-2.23	116.26	123.22
23	d	402[B]	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
33	C	520	LMG	C8-O7-C10	-2.23	112.30	117.79
23	B	615	CLA	CAC-C3C-C4C	2.23	127.70	124.81
23	c	511	CLA	CHB-C1B-NB	-2.23	121.90	124.26
34	b	625	HTG	C1-C2-C3	-2.23	106.19	110.59
23	a	404[A]	CLA	C7-C6-C5	-2.22	107.32	113.36
34	b	625	HTG	C1'-S1-C1	2.22	104.25	100.09
23	B	613	CLA	C2A-C1A-CHA	-2.22	119.97	123.86
29	d	406[B]	PL9	C27-C28-C29	-2.22	122.31	127.66
26	A	410[A]	SQD	O8-S-C6	2.22	109.28	105.74
23	c	509	CLA	C1-C2-C3	-2.22	122.20	126.04
23	b	609	CLA	CAA-C2A-C3A	-2.22	106.70	112.78
23	A	405[A]	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	B	605	CLA	O2A-CGA-CBA	2.22	118.87	111.91
25	B	618	BCR	C7-C8-C9	-2.22	122.88	126.23
23	b	604	CLA	CHD-C4C-NC	2.22	127.70	124.20
23	A	408	CLA	CHB-C4A-NA	2.22	127.58	124.51
35	C	517[A]	DGD	C3G-C2G-C1G	-2.22	106.55	111.79
35	c	519[A]	DGD	O4E-C4E-C3E	-2.22	105.23	110.35
26	B	620	SQD	O8-S-C6	2.21	109.27	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	CMC-C2C-C1C	2.21	128.41	125.04
23	A	405[B]	CLA	CAA-CBA-CGA	2.21	119.72	113.25
25	Y	101	BCR	C10-C11-C12	-2.21	116.31	123.22
23	c	513	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
23	B	611	CLA	O2A-CGA-O1A	-2.21	118.01	123.59
23	c	515	CLA	CHB-C1B-NB	-2.21	121.92	124.26
23	c	509	CLA	C2A-C1A-CHA	-2.21	119.99	123.86
31	F	101	LMT	C3B-C4B-C5B	-2.21	106.30	110.24
31	b	627	LMT	O1'-C1'-C2'	2.21	111.75	108.30
25	d	405	BCR	C38-C26-C27	2.21	117.86	113.62
35	C	517[B]	DGD	O3G-C3G-C2G	-2.21	105.57	110.90
29	d	406[B]	PL9	C7-C3-C2	-2.21	120.40	123.30
23	B	603	CLA	C5-C3-C2	-2.21	116.65	121.12
23	C	510	CLA	C2A-C1A-CHA	-2.20	120.00	123.86
23	B	605	CLA	CAC-C3C-C4C	2.20	127.67	124.81
25	y	101	BCR	C34-C9-C10	-2.20	119.84	122.92
23	a	404[B]	CLA	CMC-C2C-C1C	2.20	128.39	125.04
23	B	611	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
34	o	301	HTG	C6-C5-C4	-2.20	107.85	113.00
34	B	624	HTG	C3-C4-C5	2.20	114.17	110.24
23	b	613	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
23	c	512	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
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
23	b	608	CLA	C2A-C1A-CHA	-2.20	120.01	123.86
25	B	617	BCR	C34-C9-C8	2.20	121.54	118.08
24	a	414[B]	PHO	C4-C3-C2	-2.20	118.03	123.68
25	K	102	BCR	C11-C10-C9	-2.20	124.17	127.31
23	b	609	CLA	C4-C3-C5	2.20	118.97	115.27
23	A	408	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
29	A	414[A]	PL9	C51-C49-C50	2.20	119.46	114.60
35	c	519[B]	DGD	O1G-C1A-O1A	-2.20	118.05	123.59
23	b	615	CLA	CAC-C3C-C4C	2.20	127.66	124.81
24	A	416[A]	PHO	O2A-CGA-CBA	2.20	118.80	111.91
38	E	102	HEM	C4B-C3B-C2B	-2.20	105.37	107.11
23	C	505	CLA	CMC-C2C-C1C	2.20	128.38	125.04
23	b	605	CLA	O2A-CGA-CBA	2.19	118.79	111.91
23	a	404[B]	CLA	CAC-C3C-C4C	2.19	127.66	124.81
23	b	602	CLA	O2A-CGA-CBA	2.19	118.79	111.91
23	b	609	CLA	CHA-C1A-NA	-2.19	121.38	126.40
23	C	507	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
23	c	507	CLA	C4-C3-C5	2.19	118.96	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414[B]	PL9	C45-C44-C46	2.19	118.95	115.27
32	d	407[B]	LHG	C6-C5-C4	-2.19	106.61	111.79
25	y	101	BCR	C16-C17-C18	-2.19	124.19	127.31
23	B	605	CLA	C3B-C4B-NB	2.19	112.54	110.52
25	T	101	BCR	C1-C6-C7	2.19	121.96	115.78
23	D	402[A]	CLA	CED-O2D-CGD	2.19	120.88	115.94
23	d	403[B]	CLA	CHB-C4A-NA	2.19	127.53	124.51
31	b	621	LMT	C1-O1'-C1'	2.18	117.46	113.84
32	b	629[B]	LHG	O8-C23-O10	-2.18	118.08	123.59
26	a	409[A]	SQD	O9-S-O7	-2.18	106.39	113.95
23	c	513	CLA	O2A-CGA-CBA	2.18	118.76	111.91
23	a	404[B]	CLA	CMA-C3A-C2A	-2.18	105.02	113.83
23	b	610	CLA	CHB-C4A-NA	2.18	127.53	124.51
23	b	606	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	c	509	CLA	CAC-C3C-C4C	2.18	127.64	124.81
23	a	405[B]	CLA	C2A-C1A-CHA	-2.18	120.04	123.86
24	a	406[B]	PHO	C1-C2-C3	-2.18	122.27	126.04
23	C	513	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
23	B	605	CLA	OBD-CAD-C3D	-2.18	123.27	128.52
23	c	503	CLA	C2A-C1A-CHA	-2.18	120.05	123.86
33	d	412	LMG	C9-C8-C7	-2.18	106.63	111.79
23	c	515	CLA	CBC-CAC-C3C	-2.18	106.42	112.43
29	d	406[A]	PL9	C51-C49-C50	2.18	119.42	114.60
23	B	603	CLA	C7-C6-C5	-2.18	107.44	113.36
23	A	405[B]	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
23	d	403[A]	CLA	CAC-C3C-C4C	2.18	127.64	124.81
35	c	519[A]	DGD	C2G-O2G-C1B	-2.18	112.43	117.79
23	c	504	CLA	C2A-C1A-CHA	-2.17	120.06	123.86
25	C	516	BCR	C2-C1-C6	2.17	113.83	110.48
25	D	404	BCR	C15-C14-C13	-2.17	124.21	127.31
25	K	102	BCR	C3-C4-C5	-2.17	110.20	114.08
24	A	416[B]	PHO	CMA-C3A-C4A	-2.17	109.62	114.38
24	A	416[B]	PHO	CED-O2D-CGD	2.17	120.85	115.94
23	b	604	CLA	O2A-CGA-CBA	2.17	118.72	111.91
23	B	608	CLA	C2A-C1A-CHA	-2.17	120.07	123.86
23	A	405[B]	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	B	606	CLA	CAA-C2A-C3A	-2.17	106.84	112.78
24	a	406[A]	PHO	CBA-CAA-C2A	-2.17	107.47	113.81
33	c	521	LMG	O8-C28-O10	-2.17	118.12	123.59
23	B	613	CLA	CHD-C4C-NC	2.17	127.62	124.20
32	A	419[A]	LHG	O4-P-O5	2.17	122.95	112.24
23	c	511	CLA	C4-C3-C2	-2.17	118.12	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
23	c	510	CLA	CHB-C1B-NB	-2.17	121.96	124.26
23	b	601	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
23	b	602	CLA	CMA-C3A-C2A	-2.16	105.10	113.83
24	a	414[B]	PHO	O1D-CGD-CBD	-2.16	121.14	124.74
23	A	405[A]	CLA	C4C-C3C-C2C	-2.16	103.75	106.90
33	c	501	LMG	O8-C28-C29	2.16	118.69	111.91
34	b	622	HTG	C3-C4-C5	2.16	114.09	110.24
33	C	521	LMG	O1-C1-C2	2.16	111.67	108.30
23	b	614	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	C	506	CLA	CHD-C4C-NC	2.16	127.61	124.20
35	C	517[B]	DGD	C3G-C2G-C1G	-2.16	106.68	111.79
23	b	605	CLA	O2A-C1-C2	-2.16	102.96	108.64
31	B	627	LMT	O1B-C4'-C5'	-2.16	103.54	109.45
26	A	410[A]	SQD	O9-S-O7	-2.16	106.48	113.95
23	c	508	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
23	C	508	CLA	C6-C7-C8	-2.16	108.95	115.92
23	B	604	CLA	C4-C3-C5	2.16	118.90	115.27
25	K	102	BCR	C36-C18-C19	2.15	121.47	118.08
23	B	613	CLA	CMB-C2B-C1B	2.15	128.65	125.37
23	D	403	CLA	CMA-C3A-C4A	-2.15	105.99	111.77
23	B	613	CLA	C4-C3-C2	-2.15	118.16	123.68
40	v	201	HEC	CBA-CAA-C2A	-2.15	106.65	112.63
23	b	603	CLA	C5-C3-C2	-2.15	116.77	121.12
35	C	518[A]	DGD	C2G-O2G-C1B	-2.15	112.50	117.79
23	c	506	CLA	CMC-C2C-C1C	2.15	128.31	125.04
25	Y	101	BCR	C15-C16-C17	-2.15	119.07	123.47
35	c	518[A]	DGD	O6D-C1D-O3G	-2.15	104.89	109.97
23	C	511	CLA	CBC-CAC-C3C	-2.15	106.51	112.43
25	t	102	BCR	C37-C22-C23	2.15	121.46	118.08
29	d	406[A]	PL9	C35-C34-C36	2.15	118.88	115.27
23	b	608	CLA	CAA-C2A-C3A	-2.15	106.90	112.78
26	b	620	SQD	O48-C23-C24	2.15	118.64	111.91
29	d	406[B]	PL9	C31-C32-C33	-2.14	104.84	111.88
32	E	101[B]	LHG	O7-C7-O9	-2.14	118.53	123.70
25	c	517	BCR	C2-C1-C6	2.14	113.78	110.48
25	C	516	BCR	C34-C9-C10	-2.14	119.92	122.92
38	f	101	HEM	CMD-C2D-C1D	2.14	128.30	125.04
29	A	414[A]	PL9	C25-C24-C26	2.14	118.87	115.27
26	f	102	SQD	O48-C23-O10	-2.14	118.19	123.59
24	A	407[A]	PHO	CBA-CAA-C2A	-2.14	107.57	113.81
33	c	522	LMG	C1-C2-C3	-2.13	105.55	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	608	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
23	B	612	CLA	OBD-CAD-C3D	-2.13	123.38	128.52
33	C	501	LMG	O8-C28-C29	2.13	118.60	111.91
23	c	514	CLA	CHA-C1A-NA	-2.13	121.51	126.40
23	C	514	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
23	b	615	CLA	C11-C12-C13	-2.13	109.03	115.92
25	A	409	BCR	C38-C26-C25	-2.13	122.14	124.53
23	C	508	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
33	m	101	LMG	C3-C4-C5	2.13	114.04	110.24
23	a	404[B]	CLA	CHB-C1B-NB	-2.13	122.00	124.26
33	C	521	LMG	C1-C2-C3	-2.13	105.56	110.00
35	C	517[A]	DGD	O1G-C1A-O1A	-2.13	118.22	123.59
23	b	616	CLA	OBD-CAD-C3D	-2.13	123.40	128.52
26	F	102	SQD	O8-S-O7	-2.13	106.08	111.27
35	c	519[A]	DGD	O1G-C1A-O1A	-2.13	118.23	123.59
35	c	520	DGD	O2G-C1B-O1B	-2.13	118.56	123.70
25	D	404	BCR	C15-C16-C17	-2.13	119.12	123.47
40	V	201	HEC	C4A-NA-C1A	2.13	107.43	105.35
23	c	513	CLA	CMA-C3A-C4A	2.12	117.48	111.77
23	b	601	CLA	CHB-C1B-C2B	-2.12	121.24	127.24
24	a	414[A]	PHO	C1A-C2A-C3A	-2.12	100.82	102.84
26	b	620	SQD	O47-C7-O49	-2.12	118.57	123.70
40	v	201	HEC	C4A-NA-C1A	2.12	107.43	105.35
35	C	517[A]	DGD	O6D-C1D-O3G	-2.12	104.95	109.97
24	a	414[B]	PHO	C11-C12-C13	-2.12	109.06	115.92
24	a	414[B]	PHO	O2A-CGA-CBA	2.12	118.56	111.91
23	A	405[A]	CLA	O2A-CGA-CBA	2.12	118.56	111.91
23	D	402[B]	CLA	CHB-C4A-NA	2.12	127.44	124.51
23	C	514	CLA	CMB-C2B-C1B	2.12	128.60	125.37
29	A	414[A]	PL9	C12-C13-C14	-2.12	122.56	127.66
31	M	101	LMT	C3B-C4B-C5B	-2.12	106.46	110.24
32	d	408[B]	LHG	C5-O7-C7	-2.12	112.58	117.79
26	F	102	SQD	C46-C45-C44	-2.12	106.78	111.79
35	H	101	DGD	C3E-C4E-C5E	-2.11	106.47	110.24
23	b	613	CLA	CBC-CAC-C3C	-2.11	106.61	112.43
31	m	103	LMT	C3B-C4B-C5B	-2.11	106.47	110.24
23	B	609	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
25	d	405	BCR	C29-C28-C27	-2.11	106.66	111.38
23	c	506	CLA	CAA-C2A-C3A	-2.11	107.00	112.78
23	B	615	CLA	O2A-CGA-CBA	2.11	118.53	111.91
25	h	101	BCR	C37-C22-C21	-2.11	119.97	122.92
35	H	101	DGD	C3G-C2G-C1G	-2.11	106.81	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	D	404	BCR	C31-C1-C6	-2.11	106.88	110.30
25	c	517	BCR	C33-C5-C6	-2.11	122.16	124.53
24	A	416[A]	PHO	C6-C5-C3	-2.11	107.94	113.45
23	b	602	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
23	c	505	CLA	OBD-CAD-C3D	-2.10	123.46	128.52
23	B	602	CLA	C11-C10-C8	-2.10	109.12	115.92
32	E	101[B]	LHG	C5-O7-C7	-2.10	112.61	117.79
34	B	624	HTG	C1-O5-C5	2.10	116.46	112.58
25	B	618	BCR	C36-C18-C17	-2.10	119.98	122.92
33	m	101	LMG	O8-C28-O10	-2.10	118.28	123.59
26	F	102	SQD	O48-C23-O10	-2.10	118.29	123.59
29	d	406[A]	PL9	C12-C13-C14	-2.10	122.60	127.66
23	C	502	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
32	b	629[A]	LHG	O7-C7-O9	-2.10	118.63	123.70
38	E	102	HEM	CMD-C2D-C1D	2.10	128.23	125.04
23	B	610	CLA	CHB-C4A-NA	2.10	127.41	124.51
23	D	402[B]	CLA	CED-O2D-CGD	2.10	120.68	115.94
23	b	607	CLA	CHD-C4C-NC	2.10	127.51	124.20
23	b	616	CLA	C11-C12-C13	-2.10	109.15	115.92
34	o	301	HTG	C2'-C1'-S1	-2.09	105.64	112.40
23	b	615	CLA	CHA-C1A-NA	-2.09	121.60	126.40
23	A	405[B]	CLA	O2A-CGA-CBA	2.09	118.48	111.91
32	E	101[A]	LHG	O7-C7-O9	-2.09	118.64	123.70
23	D	402[A]	CLA	CMB-C2B-C1B	2.09	128.56	125.37
23	B	614	CLA	CMA-C3A-C2A	-2.09	105.39	113.83
23	c	508	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
23	b	606	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
23	A	405[B]	CLA	C4C-C3C-C2C	-2.09	103.85	106.90
23	C	511	CLA	C4-C3-C2	-2.09	118.32	123.68
23	A	404[A]	CLA	C7-C6-C5	-2.09	107.69	113.36
25	B	619	BCR	C2-C3-C4	-2.09	106.72	111.38
35	C	517[B]	DGD	O1G-C1A-C2A	2.08	118.45	111.91
23	d	403[A]	CLA	CHD-C4C-NC	2.08	127.49	124.20
23	c	513	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
29	d	406[B]	PL9	C12-C13-C14	-2.08	122.65	127.66
29	d	406[B]	PL9	C20-C19-C21	2.08	118.77	115.27
23	b	616	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
23	c	514	CLA	CBA-CAA-C2A	-2.08	107.72	113.86
23	b	611	CLA	C7-C6-C5	-2.08	107.71	113.36
23	B	611	CLA	C4-C3-C5	2.08	118.77	115.27
23	B	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
23	B	604	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	C	515	BCR	C16-C17-C18	-2.08	124.35	127.31
24	a	406[B]	PHO	CMC-C2C-C1C	2.08	128.65	124.73
33	Z	101	LMG	C9-C8-C7	-2.08	106.88	111.79
25	c	517	BCR	C15-C16-C17	-2.08	119.22	123.47
25	B	618	BCR	C40-C30-C25	-2.08	106.93	110.30
25	d	405	BCR	C36-C18-C17	-2.07	120.02	122.92
23	B	615	CLA	CHA-C1A-NA	-2.07	121.65	126.40
40	V	201	HEC	CBA-CAA-C2A	-2.07	106.87	112.63
25	c	517	BCR	C29-C30-C25	2.07	113.67	110.48
23	b	609	CLA	CGD-CBD-CAD	-2.07	104.03	110.73
23	A	404[A]	CLA	C4-C3-C5	2.07	118.75	115.27
29	D	405[A]	PL9	C12-C13-C14	-2.07	122.68	127.66
23	B	603	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
23	c	512	CLA	C11-C10-C8	-2.07	109.23	115.92
23	C	509	CLA	CAA-C2A-C3A	-2.07	107.12	112.78
29	D	405[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	606	CLA	C4-C3-C2	-2.07	118.38	123.68
23	B	615	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
29	D	405[A]	PL9	C25-C24-C23	-2.06	118.38	123.68
23	c	509	CLA	C3B-C4B-NB	2.06	112.43	110.52
23	B	608	CLA	C1-C2-C3	-2.06	122.47	126.04
32	d	408[B]	LHG	O8-C23-O10	-2.06	118.39	123.59
23	C	511	CLA	CHB-C4A-NA	2.06	127.36	124.51
40	v	201	HEC	CMD-C2D-C1D	2.06	128.18	125.04
25	B	619	BCR	C7-C8-C9	-2.06	123.13	126.23
29	D	405[B]	PL9	C7-C3-C4	2.06	118.55	116.88
23	d	404	CLA	CMA-C3A-C2A	-2.06	105.53	113.83
23	B	609	CLA	C2A-C1A-CHA	-2.06	120.26	123.86
24	A	416[B]	PHO	C4A-C3A-C2A	-2.06	100.88	102.84
23	B	607	CLA	CMA-C3A-C2A	-2.05	105.54	113.83
31	F	101	LMT	C2'-C3'-C4'	2.05	114.37	109.68
25	t	102	BCR	C7-C6-C5	-2.05	116.48	121.46
23	C	508	CLA	CAC-C3C-C4C	2.05	127.47	124.81
23	c	512	CLA	CAC-C3C-C4C	2.05	127.47	124.81
35	C	517[A]	DGD	C3E-C4E-C5E	2.05	113.90	110.24
23	B	609	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
23	B	601	CLA	C4-C3-C5	2.05	118.72	115.27
25	d	405	BCR	C24-C23-C22	-2.05	123.14	126.23
31	b	621	LMT	C2'-C3'-C4'	2.05	114.36	109.68
23	A	406[A]	CLA	CMA-C3A-C4A	-2.05	106.26	111.77
29	d	406[B]	PL9	C30-C29-C31	2.05	118.72	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
23	A	404[A]	CLA	CHB-C4A-NA	2.05	127.34	124.51
23	B	601	CLA	CAA-C2A-C3A	-2.05	107.17	112.78
31	m	103	LMT	O5B-C5B-C6B	2.05	111.53	106.44
25	c	516	BCR	C36-C18-C17	-2.05	120.05	122.92
23	c	513	CLA	CHB-C1B-NB	-2.05	122.09	124.26
40	V	201	HEC	C3D-C4D-ND	-2.05	108.37	110.36
23	c	505	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
25	Y	101	BCR	C21-C20-C19	-2.04	116.84	123.22
25	b	617	BCR	C32-C1-C6	-2.04	106.98	110.30
32	D	407[A]	LHG	O4-P-O5	2.04	122.34	112.24
23	b	604	CLA	CHA-C1A-NA	-2.04	121.72	126.40
23	B	608	CLA	CMB-C2B-C1B	2.04	128.48	125.37
23	A	405[B]	CLA	CMA-C3A-C2A	-2.04	105.59	113.83
38	f	101	HEM	O2A-CGA-CBA	2.04	120.59	114.03
33	Z	101	LMG	C1-O6-C5	2.04	117.70	113.69
24	A	407[A]	PHO	C4-C3-C5	2.04	118.70	115.27
23	d	402[B]	CLA	CHB-C4A-NA	2.04	127.33	124.51
33	B	621	LMG	O6-C5-C4	2.04	113.40	109.69
23	a	405[B]	CLA	CAC-C3C-C4C	2.04	127.45	124.81
23	B	608	CLA	CMA-C3A-C2A	-2.04	105.61	113.83
25	b	617	BCR	C39-C30-C25	-2.04	107.00	110.30
23	c	510	CLA	C2A-C1A-CHA	-2.04	120.30	123.86
23	b	606	CLA	O2A-CGA-CBA	2.04	118.30	111.91
23	A	406[B]	CLA	CHB-C1B-C2B	-2.03	121.49	127.24
23	c	512	CLA	CMA-C3A-C4A	-2.03	106.31	111.77
23	c	506	CLA	O2A-CGA-CBA	2.03	118.29	111.91
23	B	610	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
23	c	506	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
35	c	518[B]	DGD	C2G-O2G-C1B	-2.03	112.79	117.79
29	A	414[B]	PL9	C25-C24-C26	2.03	118.69	115.27
23	a	404[A]	CLA	CMB-C2B-C3B	2.03	131.51	126.59
25	h	101	BCR	C33-C5-C6	-2.03	122.25	124.53
25	X	101	BCR	C29-C30-C25	2.03	113.61	110.48
23	B	609	CLA	CED-O2D-CGD	2.03	120.53	115.94
23	D	403	CLA	CHB-C4A-NA	2.03	127.32	124.51
23	c	514	CLA	CHB-C1B-C2B	-2.03	121.50	127.24
29	A	414[B]	PL9	C37-C36-C34	-2.03	106.30	112.98
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
25	b	619	BCR	C21-C20-C19	-2.03	116.89	123.22
23	A	404[B]	CLA	OBD-CAD-C3D	-2.03	123.64	128.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	406[A]	PHO	CBC-CAC-C3C	-2.03	109.91	112.88
32	L	101[B]	LHG	O8-C23-O10	-2.03	118.47	123.59
23	c	515	CLA	C1-O2A-CGA	2.03	121.76	116.44
23	A	408	CLA	C11-C12-C13	-2.03	109.37	115.92
23	b	614	CLA	C4-C3-C5	2.03	118.68	115.27
29	d	406[A]	PL9	C45-C44-C46	2.03	118.68	115.27
23	B	603	CLA	CMB-C2B-C3B	2.02	131.49	126.59
32	d	408[B]	LHG	O7-C7-O9	-2.02	118.81	123.70
26	F	102	SQD	O5-C1-C2	-2.02	106.07	110.35
23	d	402[B]	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
29	d	406[B]	PL9	C35-C34-C36	2.02	118.67	115.27
29	d	406[B]	PL9	C25-C24-C26	2.02	118.67	115.27
24	a	414[A]	PHO	O2A-CGA-CBA	2.02	118.25	111.91
31	B	629	LMT	O5B-C5B-C6B	2.02	111.46	106.44
23	A	406[A]	CLA	CHB-C4A-NA	2.02	127.30	124.51
29	a	412[B]	PL9	C10-C9-C8	-2.02	118.51	123.68
25	Y	101	BCR	C1-C6-C7	2.02	121.48	115.78
32	b	629[B]	LHG	O7-C7-O9	-2.02	118.83	123.70
24	A	416[A]	PHO	CED-O2D-CGD	2.01	120.49	115.94
23	C	505	CLA	CAC-C3C-C4C	2.01	127.42	124.81
23	d	403[A]	CLA	CBC-CAC-C3C	-2.01	106.88	112.43
23	C	510	CLA	C11-C10-C8	-2.01	109.41	115.92
24	a	406[A]	PHO	O2D-CGD-O1D	-2.01	119.90	123.84
26	A	412	SQD	O6-C1-C2	2.01	111.44	108.30
37	D	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
23	D	402[A]	CLA	CBC-CAC-C3C	-2.01	106.89	112.43
37	d	401[A]	BCT	O2-C-O1	2.01	124.76	119.55
31	B	629	LMT	C3B-C4B-C5B	-2.01	106.65	110.24
25	C	515	BCR	C38-C26-C25	-2.01	122.27	124.53
23	A	408	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
23	C	505	CLA	CHD-C4C-NC	2.01	127.37	124.20
29	D	405[A]	PL9	O2-C1-C6	-2.01	117.11	120.59
33	z	101	LMG	C7-O1-C1	-2.01	109.81	113.74
38	f	101	HEM	CHA-C1A-NA	2.01	127.54	123.85
23	b	605	CLA	CAC-C3C-C4C	2.01	127.42	124.81
27	A	418	GOL	C3-C2-C1	-2.01	103.90	111.70
25	k	101	BCR	C34-C9-C8	2.01	121.24	118.08
23	b	602	CLA	CHC-C1C-C2C	-2.01	121.16	126.73
23	b	606	CLA	C2A-C1A-CHA	-2.00	120.36	123.86
23	B	602	CLA	C4-C3-C5	2.00	118.64	115.27
23	b	616	CLA	CHA-C1A-NA	-2.00	121.81	126.40
33	C	501	LMG	C12-C11-C10	-2.00	106.34	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	514	CLA	CHC-C1C-NC	2.00	127.24	124.20
29	a	412[B]	PL9	C35-C34-C33	-2.00	118.55	123.68
40	V	201	HEC	C2A-C1A-NA	-2.00	108.38	110.32

All (2) chirality outliers are listed below:

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

All (1646) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	408	CLA	C4-C3-C5-C6
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	508	CLA	C2B-C3B-CAB-CBB
23	C	508	CLA	C4B-C3B-CAB-CBB
23	C	509	CLA	CHA-CBD-CGD-O1D
23	C	509	CLA	CHA-CBD-CGD-O2D
23	a	407	CLA	C2-C3-C5-C6
23	a	407	CLA	C4-C3-C5-C6
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CHA-CBD-CGD-O1D
23	b	614	CLA	CHA-CBD-CGD-O2D
23	b	614	CLA	CAD-CBD-CGD-O1D
23	b	614	CLA	CAD-CBD-CGD-O2D
23	c	509	CLA	C4-C3-C5-C6
23	c	510	CLA	CHA-CBD-CGD-O1D
23	c	510	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	C2-C1-O2A-CGA
23	c	511	CLA	C11-C10-C8-C9
23	c	515	CLA	C2B-C3B-CAB-CBB
23	c	515	CLA	C4B-C3B-CAB-CBB
23	d	404	CLA	C2-C3-C5-C6
23	d	404	CLA	C4-C3-C5-C6
25	D	404	BCR	C23-C24-C25-C30
25	T	101	BCR	C11-C12-C13-C35
25	b	617	BCR	C1-C6-C7-C8
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	O49-C7-O47-C45
26	F	102	SQD	C2-C1-O6-C44
26	F	102	SQD	O49-C7-O47-C45
26	F	102	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	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-O2
27	A	411	GOL	O1-C1-C2-C3
27	B	623	GOL	C1-C2-C3-O3
27	B	628	GOL	O1-C1-C2-C3
27	D	412	GOL	C1-C2-C3-O3
27	V	203[A]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	C1-C2-C3-O3
27	V	203[B]	GOL	O2-C2-C3-O3
27	a	415	GOL	O1-C1-C2-C3
27	b	624	GOL	C1-C2-C3-O3
27	b	624	GOL	O2-C2-C3-O3
27	c	528	GOL	C1-C2-C3-O3
27	o	303	GOL	C1-C2-C3-O3
27	o	304	GOL	C1-C2-C3-O3
29	A	414[A]	PL9	C9-C11-C12-C13
29	A	414[A]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C9-C11-C12-C13
29	A	414[B]	PL9	C15-C14-C16-C17
29	A	414[B]	PL9	C14-C16-C17-C18
29	A	414[B]	PL9	C30-C29-C31-C32
29	a	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
29	a	412[B]	PL9	C14-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	A	417	LMT	C2'-C1'-O1'-C1
31	A	417	LMT	O5'-C1'-O1'-C1
31	A	420	LMT	O5'-C1'-O1'-C1
31	A	420	LMT	C2-C1-O1'-C1'
31	B	629	LMT	C2'-C1'-O1'-C1
31	B	630	LMT	O5'-C1'-O1'-C1
31	B	630	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2'-C1'-O1'-C1
31	F	101	LMT	O5'-C1'-O1'-C1
31	M	103	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2'-C1'-O1'-C1
31	b	627	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	O5'-C1'-O1'-C1
31	t	101	LMT	C2-C1-O1'-C1'
32	D	406[A]	LHG	O2-C2-C3-O3
32	D	406[A]	LHG	C3-O3-P-O4
32	D	406[A]	LHG	C3-O3-P-O5
32	D	406[A]	LHG	C3-O3-P-O6
32	D	406[A]	LHG	C4-O6-P-O4
32	D	406[B]	LHG	O2-C2-C3-O3
32	D	406[B]	LHG	C3-O3-P-O4
32	D	406[B]	LHG	C4-O6-P-O4
32	E	101[A]	LHG	C3-O3-P-O4
32	E	101[A]	LHG	C3-O3-P-O5
32	E	101[A]	LHG	O10-C23-O8-C6
32	E	101[A]	LHG	C24-C23-O8-C6
32	E	101[B]	LHG	C3-O3-P-O4
32	E	101[B]	LHG	C3-O3-P-O5
32	E	101[B]	LHG	C3-O3-P-O6
32	E	101[B]	LHG	O10-C23-O8-C6
32	E	101[B]	LHG	C24-C23-O8-C6
32	L	101[A]	LHG	C4-O6-P-O4
32	L	101[A]	LHG	C4-O6-P-O5
32	L	101[B]	LHG	C4-O6-P-O4
32	L	101[B]	LHG	C4-O6-P-O5
32	a	417[A]	LHG	C3-O3-P-O4
32	a	417[A]	LHG	C4-O6-P-O5
32	a	417[A]	LHG	O10-C23-O8-C6
32	a	417[A]	LHG	C24-C23-O8-C6
32	a	417[B]	LHG	C3-O3-P-O4
32	a	417[B]	LHG	C4-O6-P-O5
32	a	417[B]	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
32	a	417[B]	LHG	C24-C23-O8-C6
32	b	629[A]	LHG	C4-O6-P-O3
32	b	629[A]	LHG	C4-O6-P-O4
32	b	629[A]	LHG	C4-O6-P-O5
32	b	629[B]	LHG	C4-O6-P-O3
32	b	629[B]	LHG	C4-O6-P-O4
32	b	629[B]	LHG	C4-O6-P-O5
32	d	407[A]	LHG	C3-O3-P-O5
32	d	407[A]	LHG	C4-O6-P-O4
32	d	407[B]	LHG	C3-O3-P-O4
32	d	407[B]	LHG	C3-O3-P-O5
32	d	407[B]	LHG	C3-O3-P-O6
32	d	407[B]	LHG	C4-O6-P-O4
32	d	407[B]	LHG	C4-O6-P-O5
32	d	414[A]	LHG	C3-O3-P-O5
33	C	521	LMG	C11-C10-O7-C8
33	c	522	LMG	O9-C10-O7-C8
33	c	522	LMG	C11-C10-O7-C8
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
34	b	623	HTG	O5-C1-S1-C1'
34	o	301	HTG	C2'-C1'-S1-C1
38	E	102	HEM	C2C-C3C-CAC-CBC
38	E	102	HEM	C4C-C3C-CAC-CBC
31	A	420	LMT	O5B-C1B-O1B-C4'
34	b	625	HTG	S1-C1'-C2'-C3'
26	A	410[B]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
31	B	629	LMT	C4'-C5'-C6'-O6'
23	B	614	CLA	C3-C5-C6-C7
23	d	404	CLA	C3-C5-C6-C7
31	B	629	LMT	O5B-C5B-C6B-O6B
31	c	502	LMT	O5B-C5B-C6B-O6B
26	A	410[A]	SQD	C8-C7-O47-C45
26	B	620	SQD	C8-C7-O47-C45
23	C	505	CLA	C4-C3-C5-C6
29	a	412[B]	PL9	C25-C24-C26-C27
29	A	414[A]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C28-C29-C31-C32
29	a	412[B]	PL9	C23-C24-C26-C27

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Mol	Chain	Res	Type	Atoms
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	A	408	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	b	616	CLA	C3-C5-C6-C7
31	F	101	LMT	O5'-C5'-C6'-O6'
34	D	410	HTG	O5-C5-C6-O6
31	M	103	LMT	C4B-C5B-C6B-O6B
31	B	627	LMT	C6-C7-C8-C9
33	C	521	LMG	O9-C10-O7-C8
31	B	627	LMT	C4'-C5'-C6'-O6'
31	m	103	LMT	C4B-C5B-C6B-O6B
31	M	103	LMT	O5'-C5'-C6'-O6'
31	b	621	LMT	O5'-C5'-C6'-O6'
23	D	403	CLA	CBD-CGD-O2D-CED
32	E	101[A]	LHG	O2-C2-C3-O3
32	d	407[A]	LHG	O2-C2-C3-O3
32	d	407[B]	LHG	O2-C2-C3-O3
23	D	403	CLA	C3-C5-C6-C7
23	c	514	CLA	C3-C5-C6-C7
33	C	521	LMG	O6-C5-C6-O5
31	B	629	LMT	C4B-C5B-C6B-O6B
33	z	101	LMG	C11-C10-O7-C8
31	m	103	LMT	O5B-C5B-C6B-O6B
34	b	625	HTG	O5-C5-C6-O6
31	B	627	LMT	O5B-C5B-C6B-O6B
31	t	101	LMT	O5'-C5'-C6'-O6'
31	c	502	LMT	C4B-C5B-C6B-O6B
33	c	522	LMG	C4-C5-C6-O5
23	C	510	CLA	CBD-CGD-O2D-CED
23	c	515	CLA	CBD-CGD-O2D-CED
34	D	410	HTG	S1-C1'-C2'-C3'
31	B	627	LMT	O5'-C5'-C6'-O6'
35	C	519	DGD	C6B-C7B-C8B-C9B
31	A	420	LMT	O5B-C5B-C6B-O6B
31	B	629	LMT	O5'-C5'-C6'-O6'
31	M	103	LMT	O5B-C5B-C6B-O6B
33	c	522	LMG	O6-C5-C6-O5
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	614	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	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
31	F	101	LMT	C4'-C5'-C6'-O6'
31	M	103	LMT	C4'-C5'-C6'-O6'
34	D	410	HTG	C4-C5-C6-O6
23	A	408	CLA	C2-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
23	b	603	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	b	614	CLA	C2-C3-C5-C6
23	c	509	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	A	420	LMT	O5'-C5'-C6'-O6'
31	B	630	LMT	O5'-C5'-C6'-O6'
31	b	627	LMT	O5'-C5'-C6'-O6'
29	D	405[A]	PL9	C39-C41-C42-C43
29	d	406[B]	PL9	C39-C41-C42-C43
23	c	512	CLA	CBD-CGD-O2D-CED
31	e	101	LMT	C4'-C5'-C6'-O6'
23	C	514	CLA	CBD-CGD-O2D-CED
33	d	412	LMG	C10-C11-C12-C13
32	D	406[B]	LHG	C1-C2-C3-O3
32	d	407[A]	LHG	C1-C2-C3-O3
33	z	101	LMG	O9-C10-O7-C8
31	A	420	LMT	C4B-C5B-C6B-O6B
31	b	627	LMT	C4'-C5'-C6'-O6'
23	a	404[B]	CLA	C15-C16-C17-C18
33	B	621	LMG	C39-C40-C41-C42
32	D	407[A]	LHG	C33-C34-C35-C36
23	B	606	CLA	C10-C11-C12-C13
31	A	420	LMT	C2'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
31	B	630	LMT	C2'-C1'-O1'-C1
31	t	101	LMT	C2'-C1'-O1'-C1
26	A	410[B]	SQD	O6-C44-C45-O47
23	C	505	CLA	C2-C3-C5-C6
29	a	412[A]	PL9	C23-C24-C26-C27
23	C	503	CLA	C14-C13-C15-C16
23	C	507	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	506	CLA	C11-C12-C13-C14
23	B	602	CLA	C13-C15-C16-C17
23	b	604	CLA	C8-C10-C11-C12
25	b	619	BCR	C7-C8-C9-C34
25	t	102	BCR	C37-C22-C23-C24
25	b	619	BCR	C7-C8-C9-C10
31	b	621	LMT	C4'-C5'-C6'-O6'
26	A	410[B]	SQD	C7-C8-C9-C10
23	b	606	CLA	C10-C11-C12-C13
31	e	101	LMT	O5B-C5B-C6B-O6B
35	h	102	DGD	C6B-C7B-C8B-C9B
23	B	601	CLA	C5-C6-C7-C8
23	b	614	CLA	C8-C10-C11-C12
26	B	620	SQD	C7-C8-C9-C10
33	Z	101	LMG	C10-C11-C12-C13
35	c	519[B]	DGD	C1B-C2B-C3B-C4B
23	A	408	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	b	601	CLA	C10-C11-C12-C13
23	c	514	CLA	C15-C16-C17-C18
32	D	407[B]	LHG	C33-C34-C35-C36
27	B	623	GOL	O2-C2-C3-O3
27	B	628	GOL	O1-C1-C2-O2
27	V	203[A]	GOL	O2-C2-C3-O3
26	F	102	SQD	C23-C24-C25-C26
34	B	624	HTG	O5-C5-C6-O6
31	A	420	LMT	C5'-C4'-O1B-C1B
31	A	420	LMT	O1'-C1-C2-C3
23	C	508	CLA	C5-C6-C7-C8
26	b	620	SQD	C18-C19-C20-C21
23	B	614	CLA	C8-C10-C11-C12
32	E	101[A]	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
35	c	519[A]	DGD	C1B-C2B-C3B-C4B
40	v	201	HEC	C2C-C3C-CAC-CBC
23	D	403	CLA	C10-C11-C12-C13
31	t	101	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C12-C13-C15-C16
23	D	403	CLA	C11-C10-C8-C7
23	b	606	CLA	C12-C13-C15-C16
35	C	519	DGD	C2B-C3B-C4B-C5B
23	B	610	CLA	C2A-CAA-CBA-CGA
23	B	603	CLA	C13-C15-C16-C17
31	B	627	LMT	C5'-C4'-O1B-C1B
35	c	520	DGD	C2B-C3B-C4B-C5B
31	B	630	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
31	B	629	LMT	O5'-C1'-O1'-C1
31	b	621	LMT	O5'-C1'-O1'-C1
31	e	101	LMT	O5'-C1'-O1'-C1
29	A	414[A]	PL9	C44-C46-C47-C48
29	A	414[B]	PL9	C44-C46-C47-C48
29	D	405[B]	PL9	C39-C41-C42-C43
29	d	406[A]	PL9	C39-C41-C42-C43
31	c	502	LMT	O1'-C1-C2-C3
23	C	513	CLA	C10-C11-C12-C13
23	c	515	CLA	C10-C11-C12-C13
23	B	614	CLA	C10-C11-C12-C13
23	C	509	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C13-C15-C16-C17
26	B	620	SQD	C30-C31-C32-C33
31	A	417	LMT	O1'-C1-C2-C3
31	A	420	LMT	C4'-C5'-C6'-O6'
23	C	503	CLA	C13-C15-C16-C17
23	a	404[A]	CLA	C15-C16-C17-C18
23	b	605	CLA	C8-C10-C11-C12
23	b	611	CLA	C8-C10-C11-C12
23	b	611	CLA	C15-C16-C17-C18
32	D	406[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C4-O6-P-O3
32	E	101[A]	LHG	C3-O3-P-O6
32	E	101[A]	LHG	C4-O6-P-O3
32	E	101[B]	LHG	C4-O6-P-O3
32	L	101[A]	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
32	L	101[B]	LHG	C4-O6-P-O3
32	a	417[A]	LHG	C3-O3-P-O6
32	a	417[A]	LHG	C4-O6-P-O3
32	a	417[B]	LHG	C3-O3-P-O6
32	a	417[B]	LHG	C4-O6-P-O3
32	d	407[A]	LHG	C3-O3-P-O6
32	d	407[B]	LHG	C4-O6-P-O3
23	c	511	CLA	C3-C5-C6-C7
23	c	511	CLA	CBA-CGA-O2A-C1
34	b	623	HTG	C1'-C2'-C3'-C4'
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
32	D	406[A]	LHG	C1-C2-C3-O3
32	d	407[B]	LHG	C1-C2-C3-O3
33	B	621	LMG	O9-C10-O7-C8
23	b	606	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C15-C16-C17-C18
32	L	101[A]	LHG	C12-C13-C14-C15
32	d	414[B]	LHG	C16-C17-C18-C19
23	C	502	CLA	CBD-CGD-O2D-CED
33	B	621	LMG	C11-C10-O7-C8
34	o	301	HTG	C1'-C2'-C3'-C4'
26	A	410[B]	SQD	C15-C16-C17-C18
26	F	102	SQD	C30-C31-C32-C33
26	f	102	SQD	C32-C33-C34-C35
31	B	630	LMT	C11-C10-C9-C8
31	b	627	LMT	C7-C8-C9-C10
32	L	101[A]	LHG	C17-C18-C19-C20
32	L	101[B]	LHG	C25-C26-C27-C28
32	d	414[A]	LHG	C16-C17-C18-C19
33	C	501	LMG	C17-C18-C19-C20
33	C	501	LMG	C36-C37-C38-C39
33	D	411	LMG	C12-C13-C14-C15
34	B	622	HTG	C3'-C4'-C5'-C6'
35	c	519[A]	DGD	CAA-CBA-CCA-CDA
35	c	519[B]	DGD	C9A-CAA-CBA-CCA
23	B	615	CLA	C16-C17-C18-C19
23	a	407	CLA	C16-C17-C18-C19
23	b	602	CLA	C16-C17-C18-C20
34	B	624	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
34	b	623	HTG	S1-C1'-C2'-C3'
32	L	101[B]	LHG	C12-C13-C14-C15
32	b	629[B]	LHG	C14-C15-C16-C17
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
35	c	519[A]	DGD	C9A-CAA-CBA-CCA
35	c	519[B]	DGD	CAA-CBA-CCA-CDA
35	c	519[B]	DGD	CBA-CCA-CDA-CEA
31	A	420	LMT	C3-C4-C5-C6
31	B	630	LMT	C3-C4-C5-C6
33	D	411	LMG	C19-C20-C21-C22
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
31	m	103	LMT	O5'-C5'-C6'-O6'
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
32	E	101[B]	LHG	O2-C2-C3-O3
33	C	521	LMG	C18-C19-C20-C21
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
31	e	101	LMT	O5'-C5'-C6'-O6'
26	A	412	SQD	C2-C1-O6-C44
31	b	621	LMT	C2'-C1'-O1'-C1
31	e	101	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
23	a	407	CLA	CBA-CGA-O2A-C1
31	t	101	LMT	C4-C5-C6-C7
32	L	101[B]	LHG	C13-C14-C15-C16
33	B	621	LMG	C34-C35-C36-C37
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
35	h	102	DGD	C7B-C8B-C9B-CAB
23	B	614	CLA	C5-C6-C7-C8
23	b	614	CLA	C16-C17-C18-C20
23	b	615	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
23	c	511	CLA	C16-C17-C18-C20
23	d	404	CLA	C16-C17-C18-C20
29	A	414[A]	PL9	C45-C44-C46-C47
29	d	406[B]	PL9	C15-C14-C16-C17
32	D	406[A]	LHG	C16-C17-C18-C19
32	a	417[A]	LHG	C26-C27-C28-C29
32	a	417[B]	LHG	C26-C27-C28-C29
32	b	629[A]	LHG	C14-C15-C16-C17
33	C	521	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	D	411	LMG	C35-C36-C37-C38
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
29	D	405[B]	PL9	C13-C14-C16-C17
29	d	406[A]	PL9	C13-C14-C16-C17
23	B	603	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9
23	a	405[A]	CLA	C11-C12-C13-C14
23	a	405[B]	CLA	C11-C12-C13-C14
35	c	518[B]	DGD	O6D-C5D-C6D-O5D
32	L	101[B]	LHG	C23-C24-C25-C26
31	e	101	LMT	C4-C5-C6-C7
31	e	101	LMT	C5-C6-C7-C8
32	D	406[B]	LHG	C12-C13-C14-C15
32	D	407[A]	LHG	C32-C33-C34-C35
32	L	101[A]	LHG	C15-C16-C17-C18
32	L	101[B]	LHG	C15-C16-C17-C18
35	c	520	DGD	CBB-CCB-CDB-CEB
23	b	610	CLA	C2A-CAA-CBA-CGA
23	c	509	CLA	C2A-CAA-CBA-CGA
23	c	511	CLA	O1A-CGA-O2A-C1
32	d	414[A]	LHG	C32-C33-C34-C35
33	B	621	LMG	C17-C18-C19-C20
35	c	519[A]	DGD	CBA-CCA-CDA-CEA
35	h	102	DGD	C9A-CAA-CBA-CCA
27	B	628	GOL	C1-C2-C3-O3
27	D	412	GOL	O1-C1-C2-C3
27	O	302	GOL	O1-C1-C2-C3
27	d	413	GOL	O1-C1-C2-C3
27	l	801[B]	GOL	O1-C1-C2-C3
27	v	202[B]	GOL	O1-C1-C2-C3
25	T	101	BCR	C11-C12-C13-C14
23	b	614	CLA	C10-C11-C12-C13
31	B	629	LMT	C2-C3-C4-C5
32	D	407[B]	LHG	C32-C33-C34-C35
32	L	101[A]	LHG	C25-C26-C27-C28
33	C	501	LMG	C12-C13-C14-C15
33	C	501	LMG	C10-C11-C12-C13
26	F	102	SQD	C24-C25-C26-C27
32	A	419[A]	LHG	C34-C35-C36-C37
32	A	419[B]	LHG	C34-C35-C36-C37
32	D	406[B]	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	d	407[A]	LHG	C11-C10-C9-C8
33	c	501	LMG	C34-C35-C36-C37
33	m	101	LMG	C35-C36-C37-C38
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	H	101	DGD	C5B-C6B-C7B-C8B
33	Z	101	LMG	O6-C5-C6-O5
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
40	V	201	HEC	C4C-C3C-CAC-CBC
23	b	604	CLA	C4B-C3B-CAB-CBB
23	c	509	CLA	C4B-C3B-CAB-CBB
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C20
23	a	407	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
26	F	102	SQD	O5-C1-O6-C44
23	B	615	CLA	C5-C6-C7-C8
26	A	410[A]	SQD	C12-C13-C14-C15
31	B	629	LMT	C5-C6-C7-C8
33	d	412	LMG	C29-C30-C31-C32
35	c	520	DGD	CBA-CCA-CDA-CEA
26	B	620	SQD	C11-C10-C9-C8
31	B	627	LMT	C5-C6-C7-C8
31	t	101	LMT	O1'-C1-C2-C3
32	L	101[A]	LHG	C13-C14-C15-C16
32	b	629[B]	LHG	C27-C28-C29-C30
32	d	407[A]	LHG	C34-C35-C36-C37
33	c	521	LMG	C34-C35-C36-C37
33	c	501	LMG	C10-C11-C12-C13
23	c	508	CLA	C15-C16-C17-C18
32	d	407[B]	LHG	C34-C35-C36-C37
32	d	408[A]	LHG	C27-C28-C29-C30
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
26	b	620	SQD	C31-C32-C33-C34
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
25	T	101	BCR	C13-C14-C15-C16
31	B	627	LMT	C2-C1-O1'-C1'
31	F	101	LMT	C2-C1-O1'-C1'
31	b	627	LMT	C2-C1-O1'-C1'
26	A	412	SQD	C17-C18-C19-C20
32	A	419[B]	LHG	C12-C13-C14-C15
32	D	407[B]	LHG	C29-C30-C31-C32
33	c	521	LMG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
23	B	603	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	c	511	CLA	C16-C17-C18-C19
32	A	419[A]	LHG	C12-C13-C14-C15
32	b	629[A]	LHG	C16-C17-C18-C19
33	c	501	LMG	C30-C31-C32-C33
31	c	502	LMT	C1-C2-C3-C4
26	a	410	SQD	C25-C26-C27-C28
32	E	101[A]	LHG	C24-C25-C26-C27
33	C	521	LMG	C13-C14-C15-C16
35	c	518[A]	DGD	O6D-C5D-C6D-O5D
23	D	403	CLA	O1D-CGD-O2D-CED
32	E	101[B]	LHG	C23-C24-C25-C26
33	C	520	LMG	C16-C17-C18-C19
23	c	507	CLA	C4-C3-C5-C6
29	D	405[B]	PL9	C15-C14-C16-C17
29	d	406[A]	PL9	C15-C14-C16-C17
35	c	518[A]	DGD	C2A-C1A-O1G-C1G
23	c	507	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C12-C11-C9-C8
29	A	414[A]	PL9	C43-C44-C46-C47
29	D	405[A]	PL9	C13-C14-C16-C17
29	d	406[B]	PL9	C13-C14-C16-C17
31	M	101	LMT	C3-C4-C5-C6
27	O	302	GOL	O1-C1-C2-O2
27	a	415	GOL	O1-C1-C2-O2
27	c	528	GOL	O2-C2-C3-O3
27	o	304	GOL	O2-C2-C3-O3
27	v	202[B]	GOL	O1-C1-C2-O2
26	a	410	SQD	C31-C32-C33-C34
33	c	521	LMG	C33-C34-C35-C36
35	c	519[A]	DGD	CBB-CCB-CDB-CEB
23	a	407	CLA	O1A-CGA-O2A-C1
31	c	502	LMT	O5'-C5'-C6'-O6'
23	b	614	CLA	C16-C17-C18-C19
23	d	404	CLA	C16-C17-C18-C19
33	C	520	LMG	C17-C18-C19-C20
31	A	420	LMT	C1-C2-C3-C4
23	a	405[A]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
23	c	509	CLA	C2B-C3B-CAB-CBB
26	F	102	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	D	407[A]	LHG	C15-C16-C17-C18
33	C	520	LMG	C34-C35-C36-C37
33	m	101	LMG	C39-C40-C41-C42
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
35	c	518[B]	DGD	C7A-C8A-C9A-CAA
32	E	101[B]	LHG	C24-C25-C26-C27
33	D	411	LMG	C30-C31-C32-C33
34	b	622	HTG	C2'-C3'-C4'-C5'
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
23	B	616	CLA	C2-C1-O2A-CGA
26	B	620	SQD	C34-C35-C36-C37
31	B	630	LMT	C4-C5-C6-C7
31	M	103	LMT	C7-C8-C9-C10
32	D	406[B]	LHG	C10-C11-C12-C13
32	d	414[A]	LHG	C29-C30-C31-C32
32	d	414[B]	LHG	C32-C33-C34-C35
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
23	C	507	CLA	C5-C6-C7-C8
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
31	B	627	LMT	C4B-C5B-C6B-O6B
26	b	620	SQD	C13-C14-C15-C16
31	b	627	LMT	C5-C6-C7-C8
33	C	501	LMG	C19-C20-C21-C22
35	c	518[A]	DGD	C7A-C8A-C9A-CAA
33	c	521	LMG	C10-C11-C12-C13
25	D	404	BCR	C23-C24-C25-C26
25	Y	101	BCR	C1-C6-C7-C8
25	Y	101	BCR	C5-C6-C7-C8
25	t	102	BCR	C23-C24-C25-C26
26	A	412	SQD	C26-C27-C28-C29
26	b	620	SQD	C27-C28-C29-C30
33	C	521	LMG	C19-C20-C21-C22
40	V	201	HEC	C2B-C3B-CAB-CBB
32	d	407[B]	LHG	C24-C23-O8-C6
40	v	201	HEC	C4C-C3C-CAC-CBC
23	B	608	CLA	C13-C15-C16-C17
33	m	101	LMG	C11-C10-O7-C8
35	c	519[A]	DGD	C6A-C7A-C8A-C9A
26	b	620	SQD	C14-C15-C16-C17
33	m	101	LMG	C38-C39-C40-C41
34	b	622	HTG	C3'-C4'-C5'-C6'
35	h	102	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
26	f	102	SQD	C25-C26-C27-C28
35	c	519[B]	DGD	C2B-C3B-C4B-C5B
23	C	506	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C30-C29-C31-C32
29	D	405[A]	PL9	C15-C14-C16-C17
23	B	602	CLA	C11-C12-C13-C15
23	B	603	CLA	C11-C12-C13-C15
23	B	606	CLA	C11-C10-C8-C7
23	C	506	CLA	C2-C3-C5-C6
23	C	511	CLA	C11-C12-C13-C15
23	a	405[A]	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C11-C12-C13-C15
23	b	606	CLA	C11-C10-C8-C7
23	c	506	CLA	C11-C12-C13-C15
23	c	506	CLA	C12-C13-C15-C16
29	A	414[B]	PL9	C12-C11-C9-C8
31	b	627	LMT	C3-C4-C5-C6
32	D	407[B]	LHG	C15-C16-C17-C18
31	B	629	LMT	C6-C7-C8-C9
32	D	407[A]	LHG	C29-C30-C31-C32
35	H	101	DGD	C9B-CAB-CBB-CCB
23	b	601	CLA	C8-C10-C11-C12
32	D	406[A]	LHG	C13-C14-C15-C16
33	D	411	LMG	C36-C37-C38-C39
31	b	621	LMT	C3'-C4'-O1B-C1B
32	L	101[B]	LHG	C17-C18-C19-C20
23	A	406[B]	CLA	C13-C15-C16-C17
23	B	605	CLA	C5-C6-C7-C8
31	A	420	LMT	C3'-C4'-O1B-C1B
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
35	c	518[A]	DGD	O1A-C1A-O1G-C1G
23	C	513	CLA	CBA-CGA-O2A-C1
35	c	518[B]	DGD	C4D-C5D-C6D-O5D
23	b	606	CLA	C16-C17-C18-C20
31	c	502	LMT	C4'-C5'-C6'-O6'
26	A	412	SQD	O5-C1-O6-C44
35	C	518[A]	DGD	O6E-C1E-O5D-C6D
35	C	518[B]	DGD	O6E-C1E-O5D-C6D
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
23	C	511	CLA	C13-C15-C16-C17
31	e	101	LMT	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	a	409[A]	SQD	C9-C10-C11-C12
32	d	408[B]	LHG	C29-C30-C31-C32
35	H	101	DGD	CCB-CDB-CEB-CFB
31	b	621	LMT	C3-C4-C5-C6
33	m	101	LMG	O9-C10-O7-C8
23	C	512	CLA	C3-C5-C6-C7
33	m	101	LMG	C14-C15-C16-C17
35	C	519	DGD	CAB-CBB-CCB-CDB
35	c	519[B]	DGD	C4A-C5A-C6A-C7A
31	B	627	LMT	C1-C2-C3-C4
26	A	410[A]	SQD	O6-C44-C45-O47
35	c	518[B]	DGD	O6E-C5E-C6E-O5E
33	C	501	LMG	C11-C12-C13-C14
33	c	501	LMG	C21-C22-C23-C24
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	519[A]	DGD	C2B-C3B-C4B-C5B
23	C	503	CLA	C15-C16-C17-C18
29	A	414[B]	PL9	C45-C44-C46-C47
23	C	511	CLA	C2-C3-C5-C6
29	d	406[B]	PL9	C28-C29-C31-C32
33	m	101	LMG	C37-C38-C39-C40
23	B	602	CLA	C6-C7-C8-C9
23	B	602	CLA	C11-C12-C13-C14
23	D	403	CLA	C11-C10-C8-C9
23	b	606	CLA	C11-C10-C8-C9
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C14
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
32	b	629[A]	LHG	C13-C14-C15-C16
33	c	501	LMG	C29-C30-C31-C32
23	B	601	CLA	C2A-CAA-CBA-CGA
31	F	101	LMT	C4-C5-C6-C7
26	a	409[B]	SQD	C9-C10-C11-C12
26	b	620	SQD	C26-C27-C28-C29
31	B	627	LMT	C3'-C4'-O1B-C1B
32	d	407[B]	LHG	O10-C23-O8-C6
23	A	405[A]	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C1A-C2A-CAA-CBA
34	b	623	HTG	O5-C5-C6-O6
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
23	c	510	CLA	C16-C17-C18-C20
32	D	406[B]	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
32	D	407[A]	LHG	C17-C18-C19-C20
32	d	408[B]	LHG	C28-C29-C30-C31
23	A	405[B]	CLA	C15-C16-C17-C18
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	615	CLA	C10-C11-C12-C13
35	c	519[B]	DGD	C6A-C7A-C8A-C9A
23	b	605	CLA	C5-C6-C7-C8
32	D	407[B]	LHG	C24-C23-O8-C6
32	d	414[B]	LHG	C25-C26-C27-C28
33	C	501	LMG	C20-C21-C22-C23
35	h	102	DGD	C2B-C3B-C4B-C5B
23	A	404[A]	CLA	C13-C15-C16-C17
23	d	403[A]	CLA	C16-C17-C18-C20
32	b	629[B]	LHG	C16-C17-C18-C19
32	d	408[A]	LHG	C25-C26-C27-C28
32	b	629[B]	LHG	C12-C13-C14-C15
23	B	601	CLA	C13-C15-C16-C17
23	C	511	CLA	C10-C11-C12-C13
23	C	511	CLA	C4-C3-C5-C6
26	b	620	SQD	C11-C10-C9-C8
33	C	521	LMG	C35-C36-C37-C38
35	c	518[B]	DGD	C4B-C5B-C6B-C7B
35	h	102	DGD	C9B-CAB-CBB-CCB
26	A	412	SQD	C27-C28-C29-C30
32	D	407[B]	LHG	C17-C18-C19-C20
35	c	519[A]	DGD	C4A-C5A-C6A-C7A
23	c	515	CLA	O1D-CGD-O2D-CED
23	C	503	CLA	C3-C5-C6-C7
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	a	409[B]	SQD	O6-C44-C45-C46
26	f	102	SQD	O6-C44-C45-C46
33	c	501	LMG	C7-C8-C9-O8
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
32	E	101[A]	LHG	C25-C26-C27-C28
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	C	518[B]	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
35	c	519[A]	DGD	C2G-C3G-O3G-C1D
35	c	519[A]	DGD	C5D-C6D-O5D-C1E
35	c	519[B]	DGD	C5D-C6D-O5D-C1E
23	d	402[B]	CLA	C2C-C3C-CAC-CBC
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
33	c	501	LMG	C35-C36-C37-C38
35	c	518[A]	DGD	C4D-C5D-C6D-O5D
31	A	420	LMT	C5-C6-C7-C8
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
31	e	101	LMT	C4B-C5B-C6B-O6B
27	B	628	GOL	O2-C2-C3-O3
27	D	412	GOL	O1-C1-C2-O2
27	D	412	GOL	O2-C2-C3-O3
27	o	303	GOL	O2-C2-C3-O3
32	d	408[B]	LHG	C27-C28-C29-C30
33	c	521	LMG	C28-C29-C30-C31
33	d	412	LMG	O6-C5-C6-O5
23	A	405[A]	CLA	C15-C16-C17-C18
33	D	411	LMG	O6-C5-C6-O5
35	c	518[A]	DGD	O6E-C5E-C6E-O5E
29	a	412[A]	PL9	C12-C11-C9-C10
29	a	412[B]	PL9	C12-C11-C9-C10
32	d	408[B]	LHG	C9-C10-C11-C12
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
32	D	407[B]	LHG	O10-C23-O8-C6
35	c	518[B]	DGD	C2A-C1A-O1G-C1G
23	A	404[B]	CLA	C13-C15-C16-C17
23	d	402[A]	CLA	C2C-C3C-CAC-CBC
32	d	414[A]	LHG	C33-C34-C35-C36
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	C	510	CLA	C2-C1-O2A-CGA
32	d	408[A]	LHG	C34-C35-C36-C37
34	c	523	HTG	C4'-C5'-C6'-C7'
35	h	102	DGD	CDB-CEB-CFB-CGB
26	a	409[A]	SQD	C12-C13-C14-C15
31	b	621	LMT	C11-C10-C9-C8
32	D	406[A]	LHG	C12-C13-C14-C15
32	d	408[B]	LHG	C34-C35-C36-C37
34	o	301	HTG	C2'-C3'-C4'-C5'
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
23	B	601	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	c	502	LMT	C9-C10-C11-C12
34	B	624	HTG	C4'-C5'-C6'-C7'
35	H	101	DGD	C7A-C8A-C9A-CAA
23	C	511	CLA	CBA-CGA-O2A-C1
23	c	514	CLA	CBA-CGA-O2A-C1
26	b	620	SQD	C24-C23-O48-C46
23	C	513	CLA	O1A-CGA-O2A-C1
23	B	610	CLA	C16-C17-C18-C20
23	B	602	CLA	C15-C16-C17-C18
32	d	414[B]	LHG	C24-C25-C26-C27
33	C	520	LMG	C31-C32-C33-C34
23	B	612	CLA	C10-C11-C12-C13
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
35	c	519[B]	DGD	C2E-C1E-O5D-C6D
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
31	A	420	LMT	C4-C5-C6-C7
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
23	d	403[A]	CLA	C16-C17-C18-C19
32	d	408[A]	LHG	C29-C30-C31-C32
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16
23	C	514	CLA	C11-C10-C8-C7
23	D	403	CLA	C12-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	b	607	CLA	C12-C13-C15-C16
23	c	507	CLA	C11-C12-C13-C15
23	c	511	CLA	C11-C10-C8-C7
23	c	512	CLA	C12-C13-C15-C16
23	c	514	CLA	C12-C13-C15-C16
23	d	403[B]	CLA	C11-C12-C13-C15
35	c	518[B]	DGD	O1A-C1A-O1G-C1G
26	F	102	SQD	C32-C33-C34-C35
33	z	101	LMG	C14-C15-C16-C17
23	B	610	CLA	C14-C13-C15-C16
23	C	505	CLA	C14-C13-C15-C16
23	C	514	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	D	403	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	a	405[B]	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	c	515	CLA	C6-C7-C8-C9
35	C	517[B]	DGD	C1B-C2B-C3B-C4B
32	d	407[B]	LHG	C13-C14-C15-C16
32	d	408[A]	LHG	C28-C29-C30-C31
31	B	630	LMT	O1'-C1-C2-C3
33	B	621	LMG	C15-C16-C17-C18
23	C	510	CLA	O1D-CGD-O2D-CED
25	d	405	BCR	C21-C22-C23-C24
25	t	102	BCR	C21-C22-C23-C24
32	E	101[B]	LHG	C25-C26-C27-C28
33	C	520	LMG	C37-C38-C39-C40
32	b	629[A]	LHG	C27-C28-C29-C30
33	c	522	LMG	C29-C28-O8-C9
23	B	613	CLA	C13-C15-C16-C17
23	C	507	CLA	C15-C16-C17-C18
23	c	514	CLA	C10-C11-C12-C13
32	L	101[B]	LHG	C11-C10-C9-C8
35	C	518[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	402[B]	CLA	C4B-C3B-CAB-CBB
23	a	405[A]	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
23	c	504	CLA	C4B-C3B-CAB-CBB
35	c	519[B]	DGD	O6E-C1E-O5D-C6D
32	E	101[A]	LHG	O6-C4-C5-C6
32	b	629[A]	LHG	O6-C4-C5-C6
32	d	407[B]	LHG	O6-C4-C5-C6
32	D	406[A]	LHG	C10-C11-C12-C13
32	D	407[A]	LHG	C13-C14-C15-C16
32	D	407[B]	LHG	C13-C14-C15-C16
32	d	408[A]	LHG	C9-C10-C11-C12
33	Z	101	LMG	C11-C12-C13-C14
23	d	404	CLA	CBA-CGA-O2A-C1
23	C	514	CLA	O1D-CGD-O2D-CED
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
23	B	603	CLA	C4-C3-C5-C6
23	D	403	CLA	C4-C3-C5-C6
29	d	406[A]	PL9	C45-C44-C46-C47

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Mol	Chain	Res	Type	Atoms
32	A	419[A]	LHG	C26-C27-C28-C29
32	d	407[A]	LHG	C13-C14-C15-C16
40	v	201	HEC	C2B-C3B-CAB-CBB
23	B	610	CLA	C16-C17-C18-C19
31	b	627	LMT	C1-C2-C3-C4
33	z	101	LMG	C10-C11-C12-C13
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
23	c	508	CLA	C3A-C2A-CAA-CBA
31	e	101	LMT	C2-C1-O1'-C1'
31	m	103	LMT	C2-C1-O1'-C1'
32	L	101[B]	LHG	C24-C25-C26-C27
32	d	407[B]	LHG	C11-C10-C9-C8
35	C	519	DGD	CDB-CEB-CFB-CGB
26	F	102	SQD	C34-C35-C36-C37
33	B	621	LMG	C20-C21-C22-C23
32	d	408[B]	LHG	C24-C23-O8-C6
35	c	520	DGD	C2A-C1A-O1G-C1G
32	b	629[B]	LHG	C17-C18-C19-C20
35	c	519[A]	DGD	CDA-CEA-CFA-CGA
23	c	509	CLA	C5-C6-C7-C8
23	c	514	CLA	C13-C15-C16-C17
23	c	512	CLA	O1D-CGD-O2D-CED
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	C44-C45-C46-O48
32	a	417[A]	LHG	C4-C5-C6-O8
32	a	417[B]	LHG	C4-C5-C6-O8
26	a	409[B]	SQD	C12-C13-C14-C15
32	L	101[A]	LHG	C24-C25-C26-C27
32	a	417[A]	LHG	C10-C11-C12-C13
32	A	419[B]	LHG	C23-C24-C25-C26
23	C	511	CLA	O1A-CGA-O2A-C1
32	b	629[A]	LHG	C12-C13-C14-C15
24	a	406[A]	PHO	O2A-C1-C2-C3
31	c	502	LMT	C2-C3-C4-C5
31	e	101	LMT	C3-C4-C5-C6
32	b	629[B]	LHG	C13-C14-C15-C16
35	c	519[A]	DGD	C5A-C6A-C7A-C8A
24	a	406[A]	PHO	C4-C3-C5-C6
29	d	406[B]	PL9	C30-C29-C31-C32
29	A	414[B]	PL9	C43-C44-C46-C47
29	D	405[A]	PL9	C43-C44-C46-C47
32	L	101[A]	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	c	508	CLA	C13-C15-C16-C17
32	a	417[A]	LHG	C7-C8-C9-C10
33	C	501	LMG	C29-C30-C31-C32
35	c	518[B]	DGD	CCB-CDB-CEB-CFB
33	C	520	LMG	C30-C31-C32-C33
32	E	101[A]	LHG	O6-C4-C5-O7
32	E	101[B]	LHG	O6-C4-C5-O7
23	A	406[A]	CLA	C16-C17-C18-C20
23	A	406[B]	CLA	C16-C17-C18-C20
32	b	629[A]	LHG	C31-C32-C33-C34
23	B	602	CLA	C2B-C3B-CAB-CBB
23	D	402[B]	CLA	C2B-C3B-CAB-CBB
23	c	504	CLA	C2B-C3B-CAB-CBB
23	d	404	CLA	O1A-CGA-O2A-C1
35	c	519[B]	DGD	C5A-C6A-C7A-C8A
26	a	409[A]	SQD	C34-C35-C36-C37
26	B	620	SQD	O47-C45-C46-O48
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
23	d	402[B]	CLA	C15-C16-C17-C18
32	d	414[B]	LHG	C33-C34-C35-C36
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
32	E	101[A]	LHG	C17-C18-C19-C20
35	C	519	DGD	CAA-CBA-CCA-CDA
23	b	601	CLA	C13-C15-C16-C17
23	b	610	CLA	C15-C16-C17-C18
29	a	412[A]	PL9	C24-C26-C27-C28
29	a	412[B]	PL9	C24-C26-C27-C28
32	D	407[A]	LHG	C10-C11-C12-C13
32	E	101[B]	LHG	C13-C14-C15-C16
34	b	622	HTG	C1'-C2'-C3'-C4'
23	B	613	CLA	C11-C12-C13-C14
23	B	614	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	511	CLA	C14-C13-C15-C16
23	c	512	CLA	C11-C10-C8-C9
26	F	102	SQD	C24-C23-O48-C46
35	h	102	DGD	CAB-CBB-CCB-CDB
32	d	408[B]	LHG	C2-C3-O3-P
26	b	620	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
33	c	501	LMG	C4-C5-C6-O5
26	a	409[B]	SQD	C34-C35-C36-C37
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
25	B	617	BCR	C5-C6-C7-C8
25	X	101	BCR	C23-C24-C25-C26
25	X	101	BCR	C23-C24-C25-C30
25	b	617	BCR	C5-C6-C7-C8
25	d	405	BCR	C23-C24-C25-C26
25	d	405	BCR	C23-C24-C25-C30
25	h	101	BCR	C23-C24-C25-C26
25	h	101	BCR	C23-C24-C25-C30
25	d	405	BCR	C37-C22-C23-C24
32	d	414[A]	LHG	C25-C26-C27-C28
25	D	404	BCR	C21-C22-C23-C24
32	a	417[B]	LHG	C10-C11-C12-C13
33	m	101	LMG	C32-C33-C34-C35
23	b	606	CLA	C16-C17-C18-C19
32	a	417[B]	LHG	C23-C24-C25-C26
34	b	625	HTG	C4-C5-C6-O6
32	A	419[B]	LHG	C18-C19-C20-C21
23	c	514	CLA	O1A-CGA-O2A-C1
32	E	101[B]	LHG	O6-C4-C5-C6
32	b	629[B]	LHG	O6-C4-C5-C6
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C15
23	C	511	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	c	508	CLA	C11-C10-C8-C7
23	c	511	CLA	C6-C7-C8-C10
24	a	406[A]	PHO	C2-C3-C5-C6
23	B	610	CLA	C13-C15-C16-C17
23	B	608	CLA	C16-C17-C18-C20
32	L	101[A]	LHG	C11-C10-C9-C8
32	d	414[A]	LHG	C24-C25-C26-C27
32	b	629[A]	LHG	C34-C35-C36-C37
32	d	408[B]	LHG	O10-C23-O8-C6
33	c	522	LMG	O10-C28-O8-C9
31	e	101	LMT	C9-C10-C11-C12
33	c	501	LMG	C33-C34-C35-C36
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
32	b	629[A]	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	c	523	HTG	C2'-C1'-S1-C1
26	b	620	SQD	C28-C29-C30-C31
31	c	502	LMT	C3-C4-C5-C6
33	C	501	LMG	C13-C14-C15-C16
35	c	519[B]	DGD	CBB-CCB-CDB-CEB
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	503	CLA	CAD-CBD-CGD-O2D
23	c	512	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
24	a	406[A]	PHO	CAD-CBD-CGD-O2D
38	f	101	HEM	C2B-C3B-CAB-CBB
23	C	502	CLA	O1D-CGD-O2D-CED
32	E	101[A]	LHG	C13-C14-C15-C16
23	b	604	CLA	C10-C11-C12-C13
23	b	612	CLA	C8-C10-C11-C12
26	a	409[A]	SQD	C27-C28-C29-C30
32	D	406[A]	LHG	C34-C35-C36-C37
32	D	407[B]	LHG	C2-C3-O3-P
32	E	101[A]	LHG	C4-C5-C6-O8
32	E	101[B]	LHG	C4-C5-C6-O8
23	b	610	CLA	CBD-CGD-O2D-CED
32	b	629[A]	LHG	O6-C4-C5-O7
23	b	601	CLA	CAA-CBA-CGA-O2A
35	H	101	DGD	O2G-C1B-C2B-C3B
26	a	410	SQD	C16-C17-C18-C19
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
35	h	102	DGD	CBA-CCA-CDA-CEA
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O1D
23	c	505	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O1D
23	C	513	CLA	C3-C5-C6-C7
35	c	520	DGD	O1A-C1A-O1G-C1G
32	a	417[A]	LHG	O7-C5-C6-O8
32	a	417[B]	LHG	O7-C5-C6-O8
33	c	501	LMG	O7-C8-C9-O8
31	M	101	LMT	O1'-C1-C2-C3
33	B	621	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
35	H	101	DGD	CCA-CDA-CEA-CFA
23	C	504	CLA	CBD-CGD-O2D-CED
33	C	520	LMG	C36-C37-C38-C39
27	c	528	GOL	O1-C1-C2-O2
31	t	101	LMT	C7-C8-C9-C10
32	D	407[B]	LHG	C10-C11-C12-C13
33	B	621	LMG	C36-C37-C38-C39
23	c	512	CLA	C4-C3-C5-C6
24	a	406[B]	PHO	C4-C3-C5-C6
29	D	405[A]	PL9	C45-C44-C46-C47
33	C	520	LMG	C29-C30-C31-C32
35	c	519[A]	DGD	C1A-C2A-C3A-C4A
24	a	406[B]	PHO	C2-C3-C5-C6
23	C	507	CLA	C6-C7-C8-C9
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
26	A	412	SQD	C30-C31-C32-C33
32	d	414[B]	LHG	C29-C30-C31-C32
33	C	521	LMG	C12-C13-C14-C15
26	F	102	SQD	O10-C23-O48-C46
23	B	606	CLA	C8-C10-C11-C12
23	C	503	CLA	C16-C17-C18-C19
27	o	304	GOL	O1-C1-C2-C3
23	a	404[A]	CLA	C2C-C3C-CAC-CBC
33	C	501	LMG	C39-C40-C41-C42
25	Y	101	BCR	C21-C22-C23-C24
26	B	620	SQD	C31-C32-C33-C34
23	B	611	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	a	405[B]	CLA	C1A-C2A-CAA-CBA
23	d	402[A]	CLA	C1A-C2A-CAA-CBA
23	d	402[B]	CLA	C1A-C2A-CAA-CBA
32	a	417[B]	LHG	C7-C8-C9-C10
23	b	601	CLA	C2-C1-O2A-CGA
23	c	512	CLA	CBA-CGA-O2A-C1
32	d	408[A]	LHG	C24-C23-O8-C6
32	A	419[A]	LHG	C32-C33-C34-C35
32	E	101[B]	LHG	C17-C18-C19-C20
32	D	406[A]	LHG	C4-O6-P-O3
32	d	414[A]	LHG	C3-O3-P-O6
26	A	410[B]	SQD	C12-C13-C14-C15
33	C	520	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	a	417[A]	LHG	C23-C24-C25-C26
26	a	409[A]	SQD	C35-C36-C37-C38
32	D	407[A]	LHG	C2-C3-O3-P
32	d	408[A]	LHG	C2-C3-O3-P
23	B	603	CLA	C2-C3-C5-C6
31	b	621	LMT	C7-C8-C9-C10
23	c	512	CLA	O1A-CGA-O2A-C1
23	C	513	CLA	C4B-C3B-CAB-CBB
23	a	405[B]	CLA	C4B-C3B-CAB-CBB
32	D	406[A]	LHG	C4-O6-P-O5
32	D	406[B]	LHG	C4-O6-P-O5
32	E	101[A]	LHG	C4-O6-P-O5
32	E	101[B]	LHG	C4-O6-P-O5
32	a	417[A]	LHG	C4-O6-P-O4
32	a	417[B]	LHG	C4-O6-P-O4
32	d	407[A]	LHG	C3-O3-P-O4
23	d	403[B]	CLA	C16-C17-C18-C20
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
32	L	101[A]	LHG	O6-C4-C5-C6
32	L	101[B]	LHG	O6-C4-C5-C6
26	A	410[A]	SQD	C18-C19-C20-C21
35	C	519	DGD	C9A-CAA-CBA-CCA
23	B	611	CLA	C8-C10-C11-C12
33	z	101	LMG	C20-C21-C22-C23
31	B	627	LMT	C9-C10-C11-C12
31	B	629	LMT	C3-C4-C5-C6
23	c	504	CLA	C16-C17-C18-C19
31	b	627	LMT	C6-C7-C8-C9
32	D	406[B]	LHG	C11-C10-C9-C8
32	d	414[A]	LHG	C27-C28-C29-C30
35	c	518[A]	DGD	CCB-CDB-CEB-CFB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	504	CLA	CAD-CBD-CGD-O1D
23	c	508	CLA	CAD-CBD-CGD-O1D
23	C	510	CLA	C3-C5-C6-C7
26	F	102	SQD	C7-C8-C9-C10
33	C	501	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
33	z	101	LMG	C19-C20-C21-C22
32	D	407[A]	LHG	C24-C23-O8-C6
32	E	101[A]	LHG	C1-C2-C3-O3
23	c	515	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C12-C11-C9-C10
23	B	614	CLA	C11-C10-C8-C7
23	B	616	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C6-C7-C8-C10
23	C	514	CLA	C11-C12-C13-C15
23	b	614	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	507	CLA	C12-C13-C15-C16
23	c	512	CLA	C2-C3-C5-C6
23	c	512	CLA	C11-C10-C8-C7
32	b	629[B]	LHG	O6-C4-C5-O7
32	d	407[B]	LHG	O6-C4-C5-O7
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
35	C	519	DGD	C6A-C7A-C8A-C9A
32	d	408[A]	LHG	O10-C23-O8-C6
33	B	621	LMG	O8-C28-C29-C30
35	C	518[A]	DGD	C1A-C2A-C3A-C4A
32	D	407[A]	LHG	O10-C23-O8-C6
32	D	406[B]	LHG	C13-C14-C15-C16
35	c	518[A]	DGD	C8B-C9B-CAB-CBB
23	C	507	CLA	C16-C17-C18-C20
33	C	521	LMG	C4-C5-C6-O5
26	A	410[A]	SQD	C34-C35-C36-C37
31	A	417	LMT	C7-C8-C9-C10
23	c	513	CLA	C8-C10-C11-C12
26	a	410	SQD	O6-C44-C45-C46
33	z	101	LMG	C13-C14-C15-C16
32	E	101[A]	LHG	O7-C5-C6-O8
33	m	101	LMG	C11-C12-C13-C14
26	a	409[A]	SQD	C11-C12-C13-C14
23	B	608	CLA	C16-C17-C18-C19
23	C	503	CLA	C16-C17-C18-C20
23	B	606	CLA	C15-C16-C17-C18
23	b	602	CLA	C10-C11-C12-C13
33	B	621	LMG	C14-C15-C16-C17
35	h	102	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
23	B	601	CLA	O1A-CGA-O2A-C1
23	b	610	CLA	C13-C15-C16-C17
23	b	601	CLA	C4-C3-C5-C6
31	M	101	LMT	C2-C3-C4-C5
23	b	605	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	A	406[A]	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	c	508	CLA	C11-C10-C8-C9
23	c	511	CLA	C6-C7-C8-C9
23	d	403[B]	CLA	C11-C12-C13-C14
35	C	519	DGD	C4A-C5A-C6A-C7A
33	c	521	LMG	C14-C15-C16-C17
34	b	622	HTG	O5-C5-C6-O6
23	B	601	CLA	CAA-CBA-CGA-O2A
24	a	406[A]	PHO	C8-C10-C11-C12
33	c	501	LMG	C31-C32-C33-C34
33	d	412	LMG	C35-C36-C37-C38
23	A	406[A]	CLA	C2B-C3B-CAB-CBB
23	C	513	CLA	C2B-C3B-CAB-CBB
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
31	e	101	LMT	O1'-C1-C2-C3
35	C	519	DGD	CDA-CEA-CFA-CGA
29	a	412[A]	PL9	C12-C11-C9-C8
29	a	412[B]	PL9	C43-C44-C46-C47
32	d	414[A]	LHG	C34-C35-C36-C37
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
23	c	511	CLA	C15-C16-C17-C18
23	b	601	CLA	O1A-CGA-O2A-C1
32	d	408[A]	LHG	C32-C33-C34-C35
23	c	508	CLA	C10-C11-C12-C13
31	A	417	LMT	O5B-C5B-C6B-O6B
23	C	502	CLA	C2A-CAA-CBA-CGA
31	F	101	LMT	C6-C7-C8-C9
32	D	407[B]	LHG	C28-C29-C30-C31
23	B	601	CLA	CBA-CGA-O2A-C1
23	A	408	CLA	C2-C1-O2A-CGA
23	B	613	CLA	C2-C1-O2A-CGA
23	a	404[B]	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	c	515	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
26	A	410[A]	SQD	C16-C17-C18-C19
33	B	621	LMG	C18-C19-C20-C21
23	C	509	CLA	C5-C6-C7-C8
24	a	414[B]	PHO	C2C-C3C-CAC-CBC
23	b	601	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C24-C23-O48-C46
26	A	412	SQD	O10-C23-O48-C46
32	d	407[A]	LHG	O10-C23-O8-C6
32	L	101[A]	LHG	O6-C4-C5-O7
32	L	101[B]	LHG	C11-C12-C13-C14
35	H	101	DGD	CAB-CBB-CCB-CDB
25	B	617	BCR	C1-C6-C7-C8
23	D	403	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C28-C29-C31-C32
29	a	412[B]	PL9	C12-C11-C9-C8
23	d	402[B]	CLA	C4C-C3C-CAC-CBC
35	h	102	DGD	C3B-C4B-C5B-C6B
32	d	407[A]	LHG	C24-C23-O8-C6
23	d	402[A]	CLA	C4C-C3C-CAC-CBC
40	V	201	HEC	C4B-C3B-CAB-CBB
23	b	608	CLA	C16-C17-C18-C20
35	c	519[A]	DGD	O6E-C1E-O5D-C6D
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
35	c	519[A]	DGD	C2E-C1E-O5D-C6D
32	L	101[A]	LHG	C26-C27-C28-C29
32	E	101[B]	LHG	O7-C5-C6-O8
35	H	101	DGD	O1G-C1G-C2G-O2G
23	B	615	CLA	C13-C15-C16-C17
32	d	414[B]	LHG	C3-O3-P-O6
32	D	406[B]	LHG	C28-C29-C30-C31
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
23	C	502	CLA	C16-C17-C18-C20
32	L	101[A]	LHG	C27-C28-C29-C30
33	C	501	LMG	C7-C8-C9-O8
23	C	508	CLA	C11-C12-C13-C15
23	a	405[B]	CLA	C6-C7-C8-C10
23	b	601	CLA	C3-C5-C6-C7
23	b	607	CLA	C3-C5-C6-C7
23	A	406[B]	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	a	407	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	b	607	CLA	C14-C13-C15-C16
23	b	615	CLA	C14-C13-C15-C16
23	c	507	CLA	C14-C13-C15-C16
23	C	508	CLA	C13-C15-C16-C17
26	f	102	SQD	C23-C24-C25-C26
32	d	408[B]	LHG	C11-C10-C9-C8
34	b	623	HTG	C4'-C5'-C6'-C7'
23	a	404[A]	CLA	C4C-C3C-CAC-CBC
32	b	629[B]	LHG	C9-C10-C11-C12
35	c	519[B]	DGD	C9B-CAB-CBB-CCB
23	C	511	CLA	C8-C10-C11-C12
31	A	417	LMT	C9-C10-C11-C12
32	D	407[A]	LHG	C27-C28-C29-C30
25	Y	101	BCR	C37-C22-C23-C24
27	B	623	GOL	O1-C1-C2-C3
27	B	626	GOL	C1-C2-C3-O3
32	d	414[B]	LHG	C13-C14-C15-C16
35	C	519	DGD	C8A-C9A-CAA-CBA
35	c	518[A]	DGD	C4B-C5B-C6B-C7B
32	d	414[A]	LHG	C1-C2-C3-O3
27	l	801[B]	GOL	O1-C1-C2-O2
33	c	521	LMG	C29-C30-C31-C32
23	d	403[B]	CLA	C16-C17-C18-C19
26	a	409[B]	SQD	C11-C12-C13-C14
32	d	414[B]	LHG	C34-C35-C36-C37
33	d	412	LMG	C18-C19-C20-C21
33	C	521	LMG	C10-C11-C12-C13
31	m	103	LMT	C7-C8-C9-C10
32	d	408[A]	LHG	C33-C34-C35-C36
33	c	501	LMG	O8-C28-C29-C30
26	a	409[B]	SQD	C27-C28-C29-C30
23	b	613	CLA	CBD-CGD-O2D-CED
32	b	629[B]	LHG	C34-C35-C36-C37
23	b	604	CLA	C13-C15-C16-C17
23	b	610	CLA	O1D-CGD-O2D-CED
32	b	629[B]	LHG	C28-C29-C30-C31
23	b	612	CLA	C10-C11-C12-C13
32	A	419[B]	LHG	C26-C27-C28-C29
26	A	410[A]	SQD	C11-C10-C9-C8
32	D	407[B]	LHG	C27-C28-C29-C30
32	b	629[A]	LHG	C25-C26-C27-C28
33	d	412	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	H	101	DGD	C8A-C9A-CAA-CBA
23	C	514	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
31	F	101	LMT	C2-C3-C4-C5
32	D	406[A]	LHG	C11-C10-C9-C8
32	a	417[A]	LHG	C24-C25-C26-C27
32	A	419[B]	LHG	C32-C33-C34-C35
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
32	d	408[B]	LHG	C32-C33-C34-C35
33	d	412	LMG	C38-C39-C40-C41
23	b	601	CLA	C2-C3-C5-C6
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	A	408	CLA	C11-C12-C13-C14
23	A	408	CLA	C14-C13-C15-C16
23	C	510	CLA	C6-C7-C8-C9
23	a	405[A]	CLA	C6-C7-C8-C9
23	c	508	CLA	C6-C7-C8-C9
23	d	404	CLA	C11-C12-C13-C14
23	B	613	CLA	C15-C16-C17-C18
23	D	403	CLA	C8-C10-C11-C12
35	c	519[A]	DGD	C7B-C8B-C9B-CAB
23	a	407	CLA	C15-C16-C17-C18
32	d	407[B]	LHG	C4-C5-C6-O8
35	H	101	DGD	O1G-C1G-C2G-C3G
33	B	621	LMG	C37-C38-C39-C40
38	f	101	HEM	CAD-CBD-CGD-O1D
32	L	101[A]	LHG	C23-C24-C25-C26
33	d	412	LMG	C19-C20-C21-C22
23	c	504	CLA	C16-C17-C18-C20
23	B	602	CLA	O2A-C1-C2-C3
24	A	407[B]	PHO	O2A-C1-C2-C3
24	a	406[B]	PHO	O2A-C1-C2-C3
35	C	517[B]	DGD	O6E-C1E-O5D-C6D
26	a	410	SQD	C26-C27-C28-C29
25	C	515	BCR	C7-C8-C9-C34
25	c	517	BCR	C7-C8-C9-C34
25	d	405	BCR	C7-C8-C9-C34
26	B	620	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C3-C5-C6-C7
23	d	402[A]	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C13-C14-C15-C16
31	e	101	LMT	C2-C3-C4-C5
23	C	512	CLA	C8-C10-C11-C12
29	a	412[B]	PL9	C45-C44-C46-C47
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	c	508	CLA	C1A-C2A-CAA-CBA
23	c	513	CLA	C1A-C2A-CAA-CBA
35	c	519[B]	DGD	CDA-CEA-CFA-CGA
23	B	606	CLA	C16-C17-C18-C19
23	B	615	CLA	C12-C13-C15-C16
23	b	609	CLA	C2-C3-C5-C6
23	b	615	CLA	C11-C12-C13-C15
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
31	M	101	LMT	O5'-C5'-C6'-O6'
26	a	409[B]	SQD	C35-C36-C37-C38
35	c	518[B]	DGD	C8B-C9B-CAB-CBB
31	b	627	LMT	O1'-C1-C2-C3
32	A	419[A]	LHG	C18-C19-C20-C21
32	b	629[A]	LHG	C17-C18-C19-C20
35	C	519	DGD	C7A-C8A-C9A-CAA
40	V	201	HEC	CAD-CBD-CGD-O2D
26	a	410	SQD	C24-C25-C26-C27
32	d	408[B]	LHG	C25-C26-C27-C28
33	z	101	LMG	O7-C10-C11-C12
35	h	102	DGD	O2G-C1B-C2B-C3B
32	D	406[A]	LHG	C26-C27-C28-C29
26	A	410[B]	SQD	C16-C17-C18-C19
23	c	505	CLA	C8-C10-C11-C12
26	A	412	SQD	C15-C16-C17-C18
32	d	407[A]	LHG	C16-C17-C18-C19
29	D	405[B]	PL9	C35-C34-C36-C37
29	d	406[A]	PL9	C43-C44-C46-C47
23	A	406[B]	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C2B-C3B-CAB-CBB
33	m	101	LMG	C2-C1-O1-C7
33	Z	101	LMG	C2-C1-O1-C7
31	B	629	LMT	C1-C2-C3-C4
40	V	201	HEC	CAD-CBD-CGD-O1D
32	d	407[B]	LHG	O7-C5-C6-O8
33	C	501	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
26	A	410[B]	SQD	C34-C35-C36-C37
25	K	102	BCR	C19-C20-C21-C22
23	A	406[A]	CLA	C16-C17-C18-C19
23	A	406[B]	CLA	C16-C17-C18-C19
32	a	417[B]	LHG	C24-C25-C26-C27
23	b	616	CLA	C5-C6-C7-C8
29	A	414[A]	PL9	C39-C41-C42-C43
29	A	414[B]	PL9	C39-C41-C42-C43
23	b	616	CLA	C4-C3-C5-C6
29	a	412[A]	PL9	C45-C44-C46-C47
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	C	512	CLA	O1A-CGA-O2A-C1
23	b	613	CLA	O1D-CGD-O2D-CED
23	b	606	CLA	C14-C13-C15-C16
24	a	414[B]	PHO	C6-C7-C8-C9
26	A	410[B]	SQD	C11-C10-C9-C8
40	v	201	HEC	CAD-CBD-CGD-O2D
23	b	604	CLA	C15-C16-C17-C18
32	A	419[A]	LHG	C29-C30-C31-C32
35	c	518[A]	DGD	CAB-CBB-CCB-CDB
35	h	102	DGD	C6A-C7A-C8A-C9A
32	A	419[B]	LHG	C17-C18-C19-C20
25	c	516	BCR	C23-C24-C25-C30
25	t	102	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
40	v	201	HEC	CAD-CBD-CGD-O1D
27	O	303	GOL	O1-C1-C2-C3
27	l	801[A]	GOL	O1-C1-C2-C3
27	v	202[A]	GOL	O1-C1-C2-C3
29	D	405[A]	PL9	C35-C34-C36-C37
29	d	406[B]	PL9	C45-C44-C46-C47
25	K	102	BCR	C7-C8-C9-C10
25	d	405	BCR	C7-C8-C9-C10
32	d	407[B]	LHG	C25-C26-C27-C28
33	Z	101	LMG	C21-C22-C23-C24
29	a	412[A]	PL9	C43-C44-C46-C47
35	C	519	DGD	O1A-C1A-O1G-C1G
35	c	520	DGD	O6D-C5D-C6D-O5D
35	c	519[B]	DGD	C2G-C3G-O3G-C1D
26	b	620	SQD	C30-C31-C32-C33
40	v	201	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	A	404[A]	CLA	C16-C17-C18-C19
32	L	101[B]	LHG	O6-C4-C5-O7
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
32	A	419[A]	LHG	C35-C36-C37-C38
23	C	504	CLA	O1D-CGD-O2D-CED
33	Z	101	LMG	C19-C20-C21-C22
35	c	518[B]	DGD	CAB-CBB-CCB-CDB
23	A	406[B]	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	b	610	CLA	C16-C17-C18-C19
32	b	629[A]	LHG	C10-C11-C12-C13
33	m	101	LMG	O6-C1-O1-C7
23	a	405[A]	CLA	C6-C7-C8-C10
23	b	614	CLA	C11-C10-C8-C7
23	c	504	CLA	C11-C12-C13-C15
24	A	407[B]	PHO	C2-C3-C5-C6
32	L	101[A]	LHG	C16-C17-C18-C19
35	C	517[B]	DGD	C2E-C1E-O5D-C6D
38	f	101	HEM	CAA-CBA-CGA-O2A
26	F	102	SQD	O47-C45-C46-O48
24	A	407[B]	PHO	CBA-CGA-O2A-C1
31	B	630	LMT	C2-C3-C4-C5
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
35	c	518[B]	DGD	CDB-CEB-CFB-CGB
35	c	520	DGD	C2A-C3A-C4A-C5A
38	E	102	HEM	CAD-CBD-CGD-O1D
32	A	419[A]	LHG	O8-C23-C24-C25
23	B	607	CLA	C4-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
29	D	405[B]	PL9	C45-C44-C46-C47
35	c	519[A]	DGD	C9B-CAB-CBB-CCB
35	C	519	DGD	O6D-C5D-C6D-O5D
23	B	610	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	a	405[A]	CLA	C14-C13-C15-C16
23	a	405[B]	CLA	C14-C13-C15-C16
23	b	603	CLA	C11-C10-C8-C9
23	b	605	CLA	C14-C13-C15-C16
23	b	616	CLA	C11-C10-C8-C9
23	c	514	CLA	C6-C7-C8-C9
38	f	101	HEM	CAD-CBD-CGD-O2D
34	B	622	HTG	C4'-C5'-C6'-C7'

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Mol	Chain	Res	Type	Atoms
23	C	513	CLA	CAA-CBA-CGA-O2A
23	B	603	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	c	507	CLA	CAD-CBD-CGD-O2D
23	c	514	CLA	CAD-CBD-CGD-O2D
23	d	404	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	A	416[B]	PHO	CAD-CBD-CGD-O2D
24	a	406[B]	PHO	CAD-CBD-CGD-O2D
24	a	414[A]	PHO	CAD-CBD-CGD-O2D
23	C	507	CLA	C16-C17-C18-C19
23	b	608	CLA	C16-C17-C18-C19
32	D	407[A]	LHG	C28-C29-C30-C31
23	D	403	CLA	C15-C16-C17-C18
23	B	614	CLA	C2A-CAA-CBA-CGA
32	b	629[A]	LHG	C30-C31-C32-C33
23	B	608	CLA	C2-C1-O2A-CGA
33	B	621	LMG	C30-C31-C32-C33
32	L	101[A]	LHG	O7-C7-C8-C9
32	a	417[A]	LHG	O8-C23-C24-C25
32	b	629[B]	LHG	O7-C7-C8-C9
24	A	416[B]	PHO	C2C-C3C-CAC-CBC
29	A	414[A]	PL9	C25-C24-C26-C27
31	e	101	LMT	C2B-C1B-O1B-C4'
23	b	616	CLA	C2-C3-C5-C6
32	L	101[B]	LHG	O7-C7-C8-C9
35	h	102	DGD	CCB-CDB-CEB-CFB
33	B	621	LMG	O1-C7-C8-C9
32	b	629[A]	LHG	O7-C7-C8-C9
33	Z	101	LMG	O7-C10-C11-C12
33	d	412	LMG	C40-C41-C42-C43
23	A	404[A]	CLA	C15-C16-C17-C18
24	A	407[A]	PHO	O2A-C1-C2-C3
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
38	f	101	HEM	C4B-C3B-CAB-CBB
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
32	E	101[B]	LHG	O7-C7-C8-C9
33	c	521	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	b	610	CLA	C16-C17-C18-C20
34	V	202	HTG	O5-C5-C6-O6
26	B	620	SQD	C29-C30-C31-C32
23	A	405[A]	CLA	CHA-CBD-CGD-O1D
23	A	405[A]	CLA	CHA-CBD-CGD-O2D
23	A	405[B]	CLA	CHA-CBD-CGD-O1D
23	A	405[B]	CLA	CHA-CBD-CGD-O2D
23	B	606	CLA	CHA-CBD-CGD-O1D
23	B	606	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O1D
23	C	510	CLA	CHA-CBD-CGD-O2D
23	C	511	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	c	504	CLA	CHA-CBD-CGD-O2D
23	c	506	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	511	CLA	CHA-CBD-CGD-O2D
23	d	402[A]	CLA	CHA-CBD-CGD-O1D
23	d	402[A]	CLA	CHA-CBD-CGD-O2D
35	C	519	DGD	O1G-C1A-C2A-C3A
35	C	519	DGD	C7B-C8B-C9B-CAB
29	d	406[B]	PL9	C43-C44-C46-C47
26	f	102	SQD	C34-C35-C36-C37
32	D	406[B]	LHG	C34-C35-C36-C37
33	B	621	LMG	C29-C30-C31-C32
23	c	512	CLA	CAA-CBA-CGA-O2A
31	A	420	LMT	C7-C8-C9-C10
32	A	419[A]	LHG	C17-C18-C19-C20
32	d	414[A]	LHG	C13-C14-C15-C16
33	c	521	LMG	C32-C33-C34-C35
35	C	518[A]	DGD	CAB-CBB-CCB-CDB
23	c	514	CLA	CAA-CBA-CGA-O2A
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
23	B	606	CLA	C16-C17-C18-C20
24	A	407[A]	PHO	CHA-CBD-CGD-O1D
24	A	416[B]	PHO	CHA-CBD-CGD-O1D
24	a	414[B]	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	a	414[B]	PHO	CHA-CBD-CGD-O2D
27	o	304	GOL	O1-C1-C2-O2
26	a	410	SQD	C18-C19-C20-C21
33	B	621	LMG	C19-C20-C21-C22
23	B	613	CLA	CAA-CBA-CGA-O2A
32	A	419[B]	LHG	O8-C23-C24-C25
32	a	417[B]	LHG	O8-C23-C24-C25
26	A	412	SQD	C7-C8-C9-C10
35	c	519[B]	DGD	C1A-C2A-C3A-C4A
26	F	102	SQD	C33-C34-C35-C36
35	c	520	DGD	C7B-C8B-C9B-CAB
23	B	613	CLA	C11-C12-C13-C15
23	d	402[A]	CLA	C11-C12-C13-C15
29	D	405[B]	PL9	C43-C44-C46-C47
29	A	414[A]	PL9	C4-C3-C7-C8
23	B	615	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C14
23	C	511	CLA	C11-C12-C13-C14
23	b	614	CLA	C11-C12-C13-C14
38	E	102	HEM	CAD-CBD-CGD-O2D
35	C	519	DGD	C2A-C1A-O1G-C1G
23	C	511	CLA	CAA-CBA-CGA-O2A
26	f	102	SQD	C26-C27-C28-C29
26	a	409[B]	SQD	C19-C20-C21-C22
32	d	414[A]	LHG	C18-C19-C20-C21
38	f	101	HEM	CAA-CBA-CGA-O1A
23	B	602	CLA	C2A-CAA-CBA-CGA
23	c	505	CLA	C2A-CAA-CBA-CGA
29	A	414[B]	PL9	C46-C47-C48-C49
29	D	405[B]	PL9	C46-C47-C48-C49
32	b	629[A]	LHG	C24-C25-C26-C27
35	C	518[B]	DGD	C3A-C4A-C5A-C6A
25	K	102	BCR	C7-C8-C9-C34
33	Z	101	LMG	O9-C10-C11-C12
34	o	301	HTG	C3'-C4'-C5'-C6'
27	l	801[A]	GOL	C1-C2-C3-O3
24	A	407[B]	PHO	O1A-CGA-O2A-C1
29	D	405[A]	PL9	C28-C29-C31-C32
33	c	522	LMG	C31-C32-C33-C34
32	b	629[B]	LHG	O9-C7-C8-C9
25	y	101	BCR	C21-C22-C23-C24
23	B	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	b	620	SQD	C10-C11-C12-C13
32	d	407[B]	LHG	C9-C10-C11-C12
23	B	616	CLA	C16-C17-C18-C20
32	A	419[A]	LHG	O10-C23-C24-C25
31	c	502	LMT	C6-C7-C8-C9
23	C	513	CLA	CAA-CBA-CGA-O1A
32	L	101[B]	LHG	O9-C7-C8-C9
32	a	417[A]	LHG	O10-C23-C24-C25
32	b	629[A]	LHG	O9-C7-C8-C9
26	F	102	SQD	C44-C45-C46-O48
35	c	518[A]	DGD	O2G-C1B-C2B-C3B
23	A	404[B]	CLA	C16-C17-C18-C19
32	E	101[B]	LHG	O9-C7-C8-C9
32	a	417[B]	LHG	O10-C23-C24-C25
35	C	519	DGD	O1A-C1A-C2A-C3A
31	B	629	LMT	C7-C8-C9-C10
23	b	609	CLA	C4-C3-C5-C6
32	E	101[A]	LHG	O7-C7-C8-C9
33	D	411	LMG	O7-C10-C11-C12
23	B	604	CLA	C3-C5-C6-C7
33	d	412	LMG	C28-C29-C30-C31
23	D	403	CLA	O1A-CGA-O2A-C1
32	d	407[A]	LHG	C4-O6-P-O5
32	d	414[B]	LHG	C3-O3-P-O5
31	A	417	LMT	C2B-C1B-O1B-C4'
23	B	613	CLA	CAA-CBA-CGA-O1A
33	c	521	LMG	O9-C10-C11-C12
23	b	615	CLA	C10-C11-C12-C13
23	c	514	CLA	CAA-CBA-CGA-O1A
32	A	419[B]	LHG	O10-C23-C24-C25
32	L	101[A]	LHG	O9-C7-C8-C9
24	A	416[A]	PHO	C2C-C3C-CAC-CBC
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
23	C	508	CLA	C2A-CAA-CBA-CGA
23	b	614	CLA	CBD-CGD-O2D-CED
33	d	412	LMG	C11-C12-C13-C14
23	C	509	CLA	C13-C15-C16-C17
35	C	519	DGD	CBA-CCA-CDA-CEA
29	d	406[A]	PL9	C11-C12-C13-C14
23	c	515	CLA	C2-C3-C5-C6
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
23	b	602	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	506	CLA	CAD-CBD-CGD-O1D
26	f	102	SQD	O5-C5-C6-S
23	C	511	CLA	CAA-CBA-CGA-O1A
35	C	518[B]	DGD	O1B-C1B-C2B-C3B
26	a	409[A]	SQD	C10-C11-C12-C13
23	B	614	CLA	C11-C10-C8-C9
23	b	614	CLA	C14-C13-C15-C16
23	c	504	CLA	C11-C12-C13-C14
23	d	402[A]	CLA	C11-C12-C13-C14
27	B	623	GOL	O1-C1-C2-O2
33	C	521	LMG	C38-C39-C40-C41
23	b	613	CLA	CAA-CBA-CGA-O2A
32	D	407[A]	LHG	O8-C23-C24-C25
32	d	408[B]	LHG	O8-C23-C24-C25
33	c	522	LMG	O7-C10-C11-C12
35	c	518[B]	DGD	O2G-C1B-C2B-C3B
23	C	504	CLA	C8-C10-C11-C12
33	c	501	LMG	C13-C14-C15-C16
23	B	612	CLA	O1A-CGA-O2A-C1
33	c	521	LMG	C35-C36-C37-C38
23	a	404[B]	CLA	C2A-CAA-CBA-CGA
26	A	412	SQD	O48-C23-C24-C25
26	a	410	SQD	O48-C23-C24-C25
32	E	101[B]	LHG	O8-C23-C24-C25
29	D	405[B]	PL9	C36-C37-C38-C39
32	A	419[B]	LHG	C1-C2-C3-O3
32	E	101[B]	LHG	C1-C2-C3-O3
26	a	409[A]	SQD	C19-C20-C21-C22
29	D	405[A]	PL9	C40-C39-C41-C42
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
23	B	605	CLA	C11-C12-C13-C15
23	B	607	CLA	C2-C3-C5-C6
23	C	507	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
23	b	603	CLA	C11-C10-C8-C7
23	b	608	CLA	C12-C13-C15-C16
23	c	510	CLA	C12-C13-C15-C16
23	B	612	CLA	CAA-CBA-CGA-O2A
32	E	101[A]	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	O8-C28-C29-C30
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
32	D	406[A]	LHG	C28-C29-C30-C31
23	c	512	CLA	CAA-CBA-CGA-O1A
26	A	412	SQD	O10-C23-C24-C25
32	D	407[A]	LHG	O10-C23-C24-C25
35	c	518[A]	DGD	O1B-C1B-C2B-C3B
26	a	409[B]	SQD	C10-C11-C12-C13
35	C	518[A]	DGD	C3A-C4A-C5A-C6A
23	B	616	CLA	C16-C17-C18-C19
32	D	407[B]	LHG	O8-C23-C24-C25
23	B	601	CLA	C8-C10-C11-C12
31	c	502	LMT	C4-C5-C6-C7
32	E	101[A]	LHG	O9-C7-C8-C9
32	E	101[A]	LHG	O10-C23-C24-C25
32	E	101[B]	LHG	O10-C23-C24-C25
38	E	102	HEM	CAA-CBA-CGA-O2A
23	B	610	CLA	C15-C16-C17-C18
33	D	411	LMG	O9-C10-C11-C12
33	c	522	LMG	O9-C10-C11-C12
35	C	518[A]	DGD	O1B-C1B-C2B-C3B

There are no ring outliers.

174 monomers are involved in 367 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	507	CLA	4	0
25	c	516	BCR	2	0
27	l	801[B]	GOL	1	0
26	A	412	SQD	2	0
25	t	102	BCR	5	0
24	A	407[B]	PHO	2	0
32	D	407[A]	LHG	5	0
23	b	616	CLA	1	0
26	b	620	SQD	3	0
27	b	628	GOL	2	0
23	B	606	CLA	3	0
25	d	405	BCR	2	0
23	A	406[A]	CLA	1	0
23	b	612	CLA	1	0
34	b	622	HTG	2	0
23	c	504	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	a	414[A]	PHO	2	0
25	K	102	BCR	1	0
32	d	408[A]	LHG	10	0
35	C	517[A]	DGD	2	0
32	A	419[A]	LHG	1	0
25	k	101	BCR	2	0
31	A	417	LMT	1	0
31	c	502	LMT	1	0
23	d	402[B]	CLA	3	0
26	A	410[B]	SQD	3	0
34	b	623	HTG	1	0
35	c	518[B]	DGD	2	0
23	C	505	CLA	1	0
23	B	601	CLA	5	0
34	B	624	HTG	1	0
23	c	506	CLA	3	0
23	d	403[B]	CLA	2	0
23	B	605	CLA	3	0
23	C	514	CLA	2	0
25	A	409	BCR	2	0
23	B	609	CLA	2	0
32	a	417[B]	LHG	4	0
32	d	407[B]	LHG	2	0
33	c	522	LMG	1	0
25	B	618	BCR	2	0
23	c	503	CLA	3	0
26	a	410	SQD	2	0
25	b	617	BCR	1	0
38	f	101	HEM	1	0
23	B	613	CLA	5	0
34	d	411	HTG	1	0
23	D	402[A]	CLA	3	0
35	c	519[A]	DGD	1	0
29	A	414[A]	PL9	10	0
32	D	406[A]	LHG	2	0
23	C	506	CLA	5	0
35	C	518[A]	DGD	2	0
27	D	412	GOL	2	0
27	v	202[B]	GOL	2	0
25	a	408	BCR	1	0
26	F	102	SQD	2	0
33	B	621	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	b	614	CLA	1	0
23	a	405[B]	CLA	2	0
23	A	404[B]	CLA	4	0
23	C	504	CLA	4	0
25	c	517	BCR	1	0
23	B	614	CLA	3	0
23	A	405[A]	CLA	4	0
23	B	603	CLA	1	0
33	d	412	LMG	3	0
29	a	412[B]	PL9	5	0
31	e	101	LMT	1	0
38	E	102	HEM	1	0
23	b	607	CLA	1	0
23	c	515	CLA	2	0
23	b	615	CLA	2	0
25	C	515	BCR	2	0
23	c	508	CLA	5	0
23	a	404[B]	CLA	3	0
34	o	301	HTG	2	0
26	a	409[B]	SQD	4	0
24	a	414[B]	PHO	1	0
23	c	505	CLA	3	0
32	A	419[B]	LHG	1	0
23	B	612	CLA	1	0
33	C	521	LMG	3	0
23	c	510	CLA	7	0
23	C	513	CLA	1	0
23	b	605	CLA	5	0
27	A	418	GOL	3	0
23	B	608	CLA	1	0
24	A	416[B]	PHO	2	0
23	A	408	CLA	4	0
31	B	627	LMT	1	0
31	B	629	LMT	1	0
35	c	518[A]	DGD	2	0
25	T	101	BCR	4	0
26	B	620	SQD	1	0
25	y	101	BCR	3	0
23	D	402[B]	CLA	2	0
23	d	403[A]	CLA	2	0
32	D	406[B]	LHG	3	0
33	c	501	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	c	514	CLA	6	0
34	B	622	HTG	1	0
23	B	604	CLA	1	0
27	a	416	GOL	4	0
32	a	417[A]	LHG	4	0
34	b	625	HTG	1	0
23	B	616	CLA	5	0
32	d	407[A]	LHG	3	0
33	z	101	LMG	2	0
32	E	101[A]	LHG	3	0
33	Z	101	LMG	2	0
25	X	101	BCR	1	0
23	a	407	CLA	5	0
23	b	603	CLA	1	0
31	b	621	LMT	2	0
32	D	407[B]	LHG	3	0
23	C	511	CLA	4	0
24	a	406[B]	PHO	1	0
23	c	511	CLA	2	0
23	b	602	CLA	1	0
23	b	601	CLA	2	0
25	h	101	BCR	5	0
23	A	405[B]	CLA	4	0
23	A	406[B]	CLA	1	0
27	v	202[A]	GOL	1	0
25	b	619	BCR	5	0
27	l	801[A]	GOL	1	0
34	c	523	HTG	1	0
23	b	609	CLA	6	0
32	d	408[B]	LHG	8	0
35	C	517[B]	DGD	3	0
24	A	407[A]	PHO	2	0
25	b	618	BCR	4	0
23	a	405[A]	CLA	2	0
23	A	404[A]	CLA	5	0
23	C	507	CLA	5	0
27	a	415	GOL	1	0
33	c	521	LMG	1	0
23	b	613	CLA	1	0
29	a	412[A]	PL9	4	0
35	H	101	DGD	1	0
35	C	519	DGD	3	0

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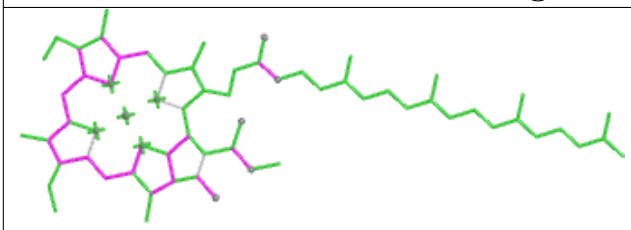
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	c	520	DGD	3	0
35	h	102	DGD	1	0
23	c	509	CLA	3	0
23	d	402[A]	CLA	2	0
27	O	303	GOL	2	0
26	A	410[A]	SQD	2	0
23	a	404[A]	CLA	3	0
26	a	409[A]	SQD	4	0
35	c	519[B]	DGD	1	0
27	O	302	GOL	1	0
29	A	414[B]	PL9	8	0
23	C	512	CLA	3	0
23	C	502	CLA	5	0
35	C	518[B]	DGD	3	0
23	C	503	CLA	3	0
23	b	604	CLA	3	0
23	B	615	CLA	7	0
23	C	509	CLA	4	0
27	B	623	GOL	2	0
23	b	606	CLA	1	0
23	c	513	CLA	6	0
31	M	101	LMT	1	0
25	B	619	BCR	3	0
27	C	523[B]	GOL	1	0
24	A	416[A]	PHO	1	0
25	Y	101	BCR	3	0
23	d	404	CLA	3	0
31	A	420	LMT	1	0
32	E	101[B]	LHG	4	0
25	B	617	BCR	1	0
27	b	624	GOL	1	0
23	C	508	CLA	2	0

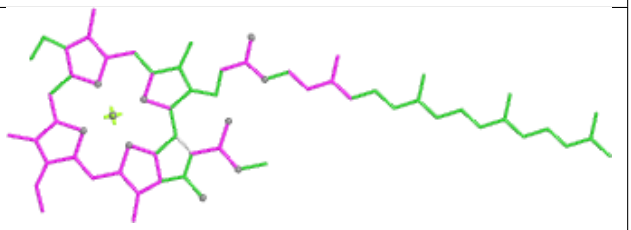
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

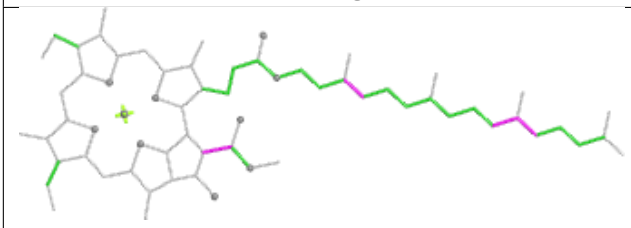
Ligand CLA c 507



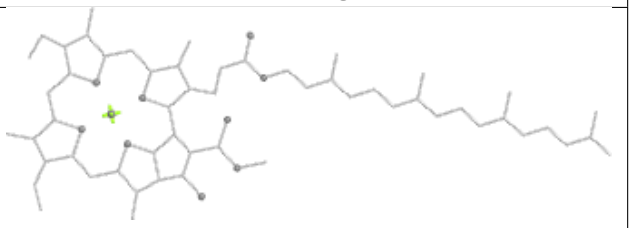
Bond lengths



Bond angles

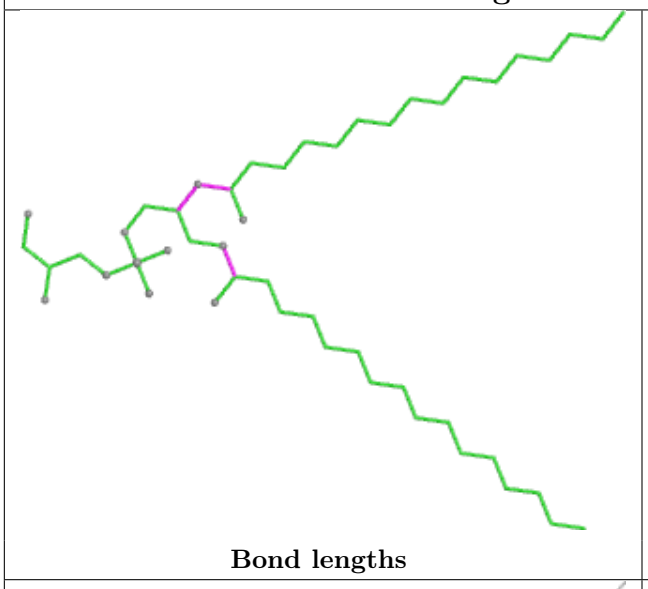


Torsions

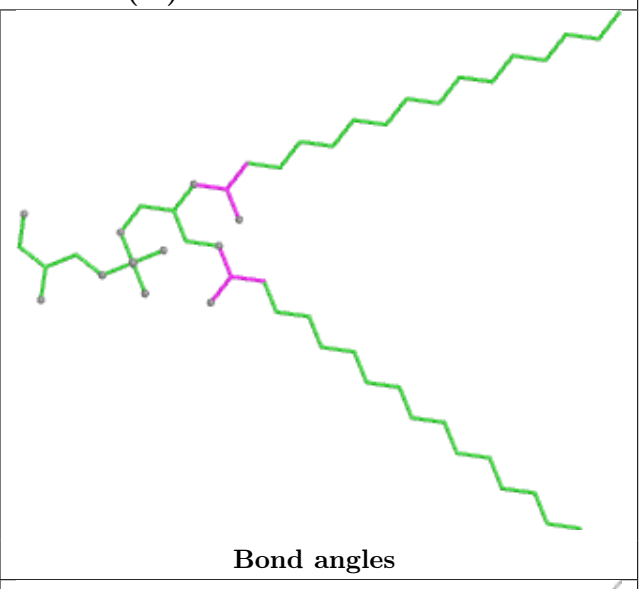


Rings

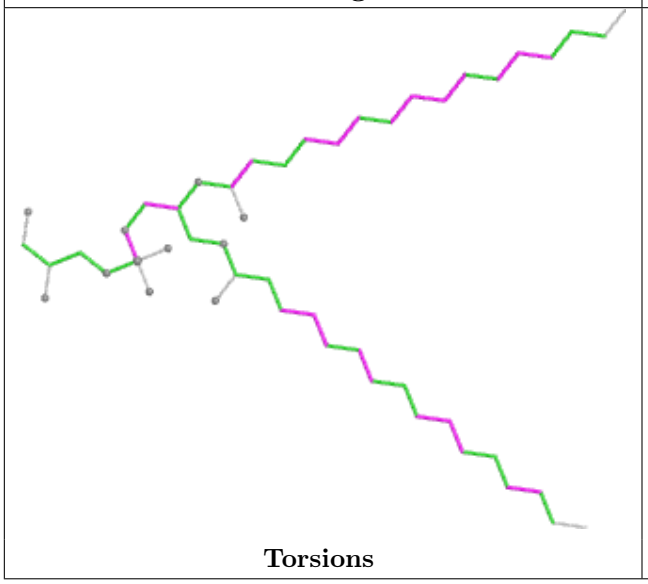
Ligand LHG b 629 (A)



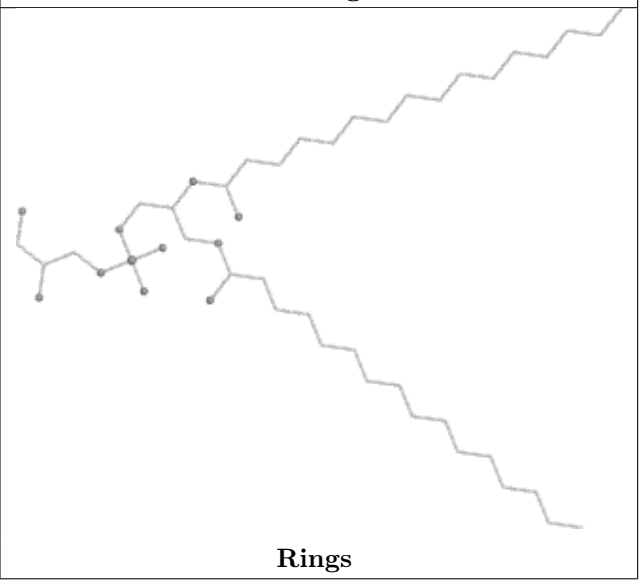
Bond lengths



Bond angles

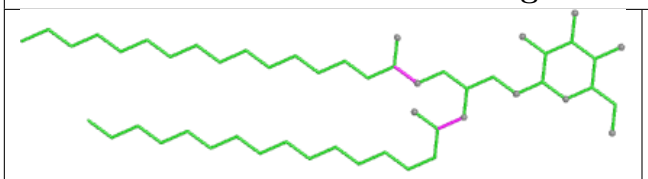


Torsions

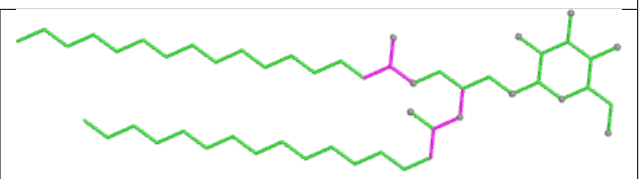


Rings

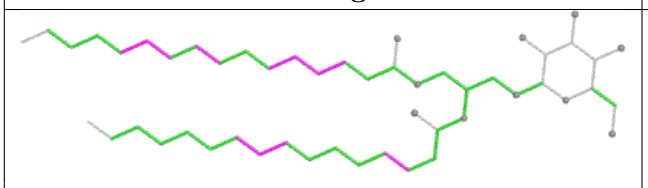
Ligand LMG C 520



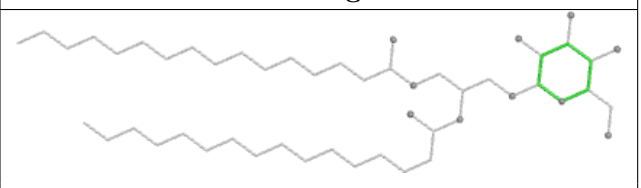
Bond lengths



Bond angles

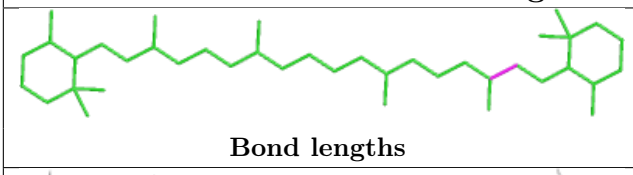


Torsions

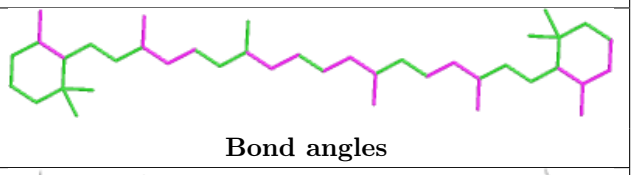


Rings

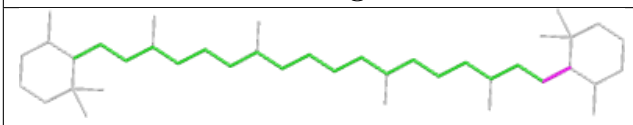
Ligand BCR c 516



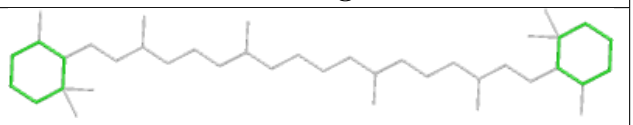
Bond lengths



Bond angles

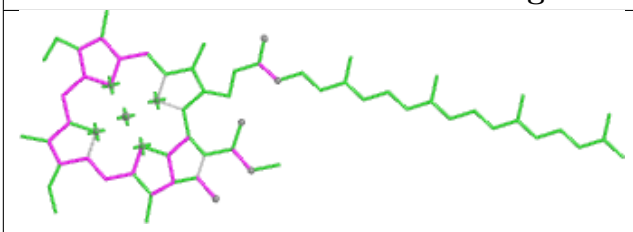


Torsions

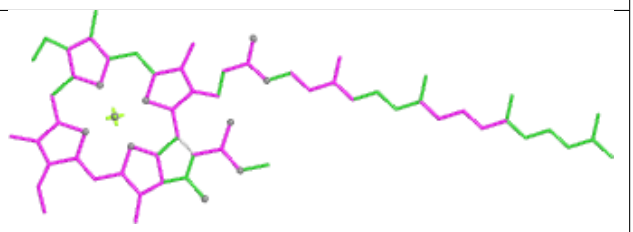


Rings

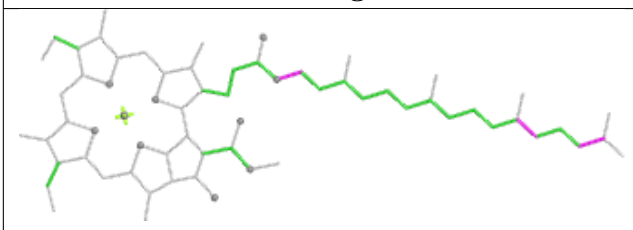
Ligand CLA b 608



Bond lengths



Bond angles



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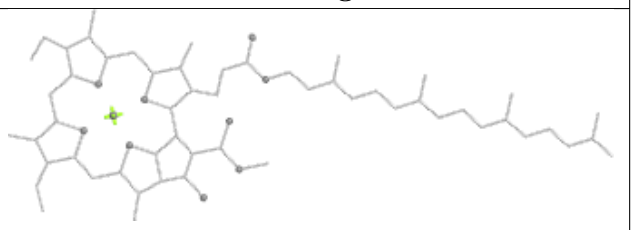
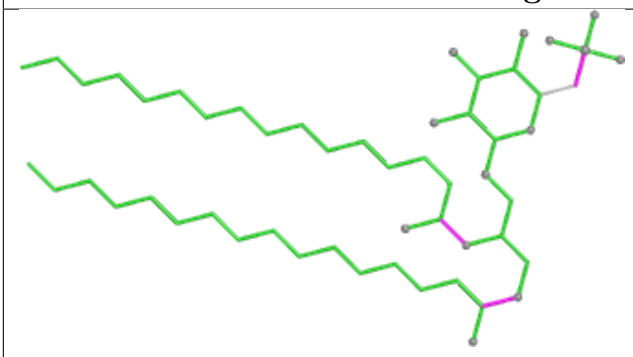


Rings

Ligand SQD A 412



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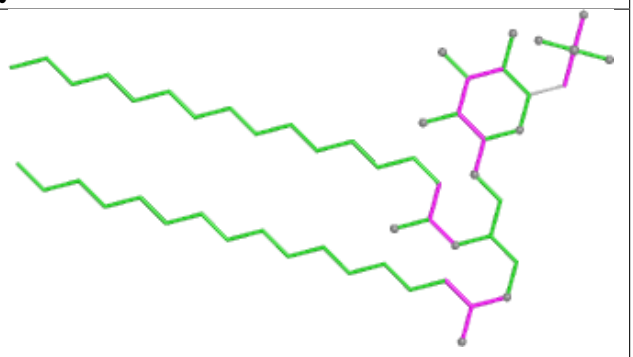
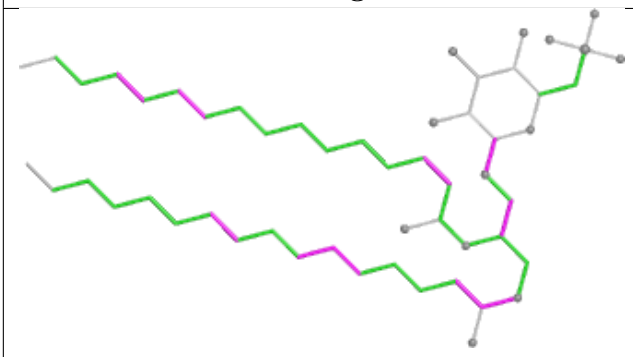
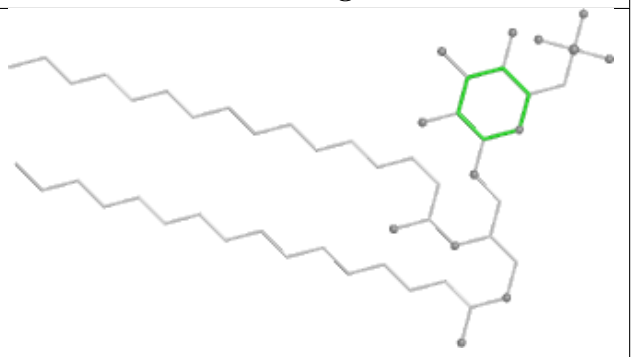


Bond angles

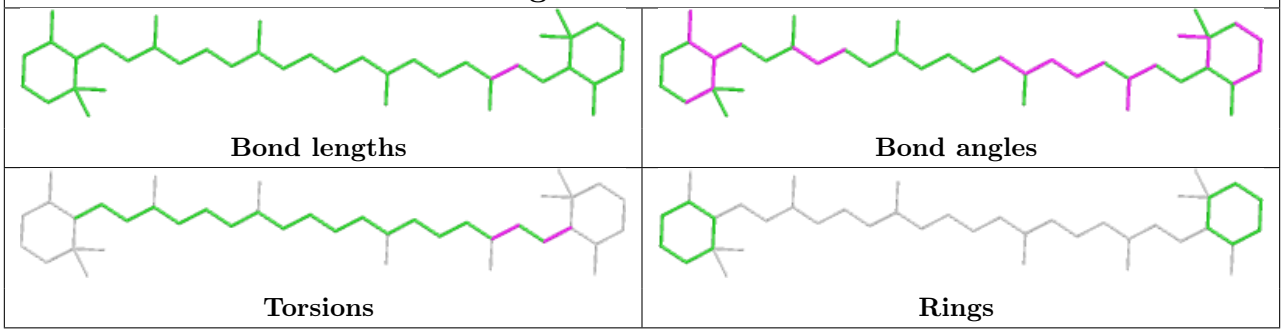


Torsions

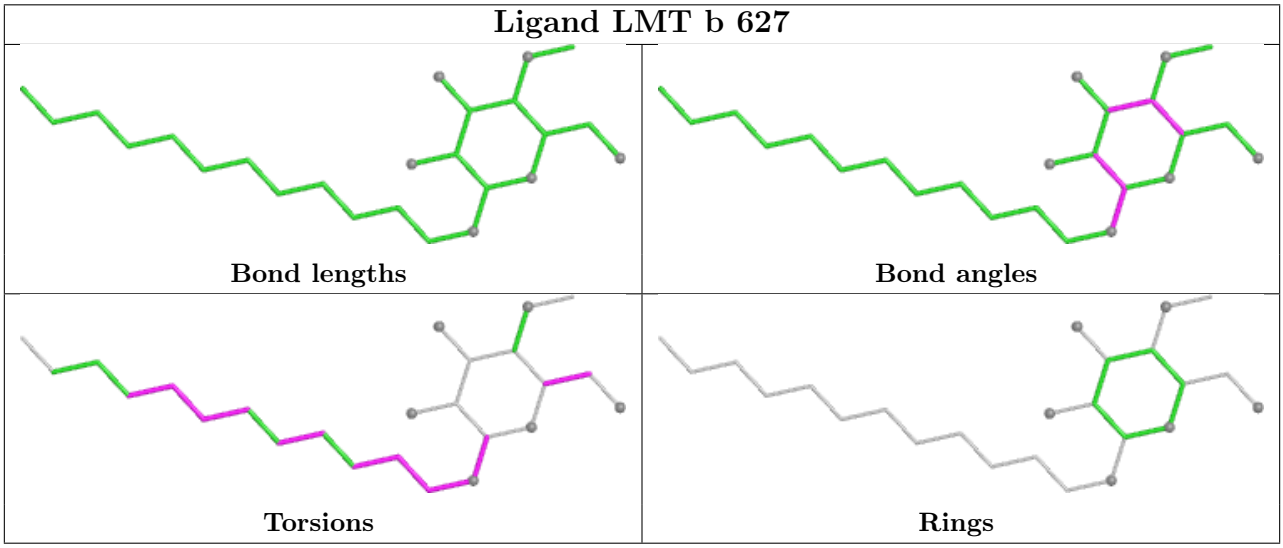


Rings

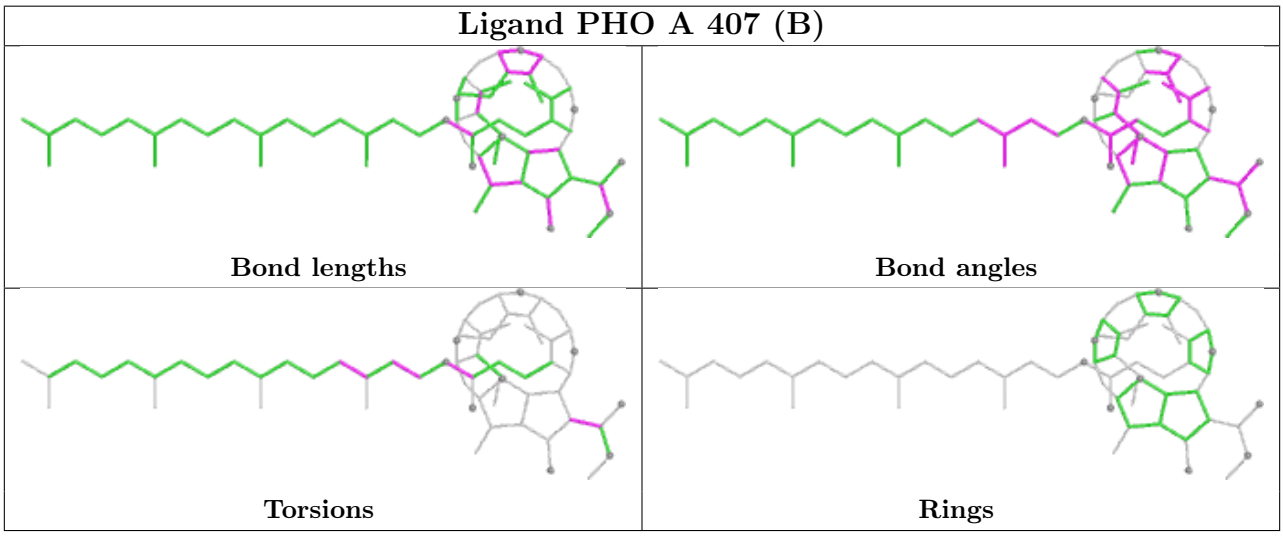
Ligand BCR t 102



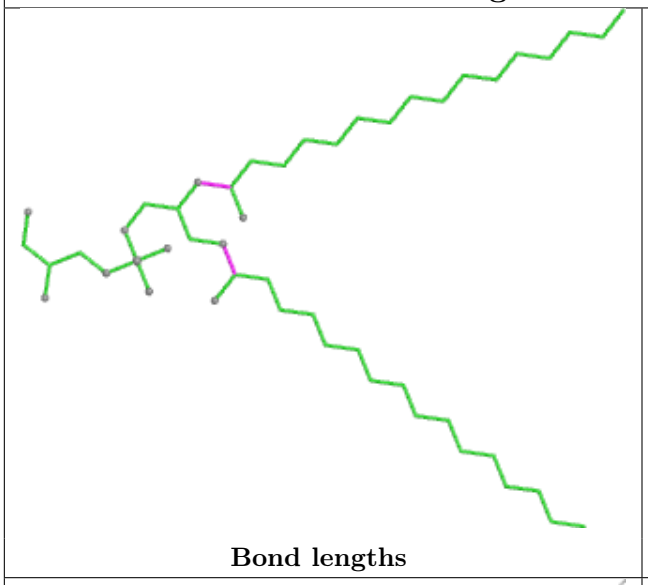
Ligand LMT b 627



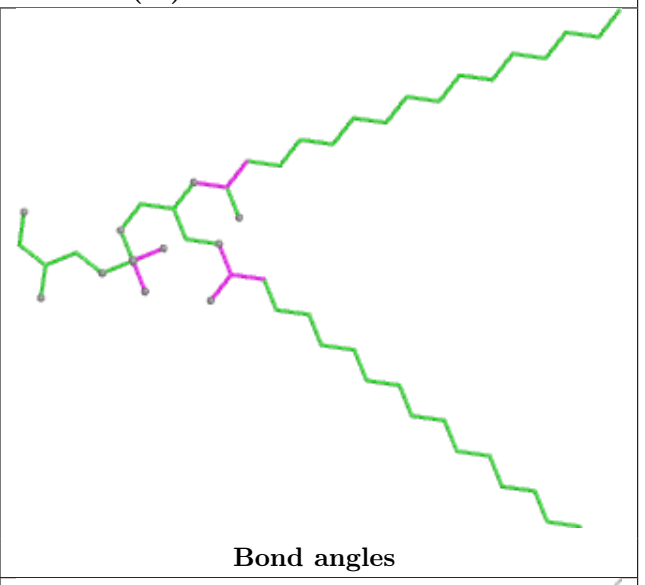
Ligand PHO A 407 (B)



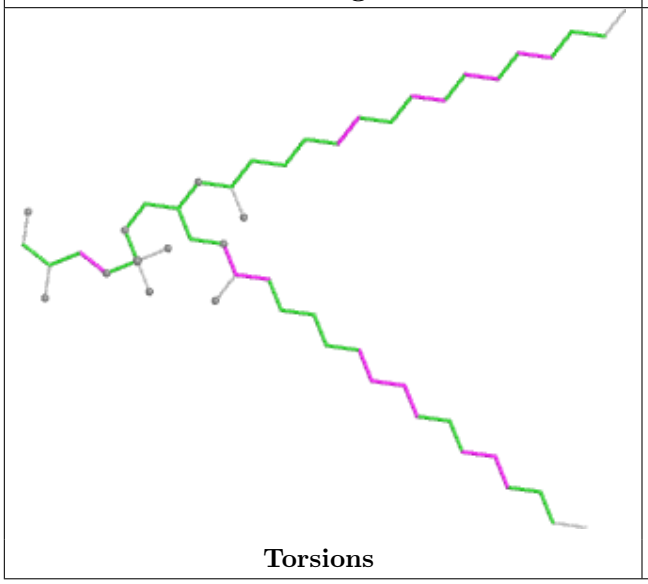
Ligand LHG D 407 (A)



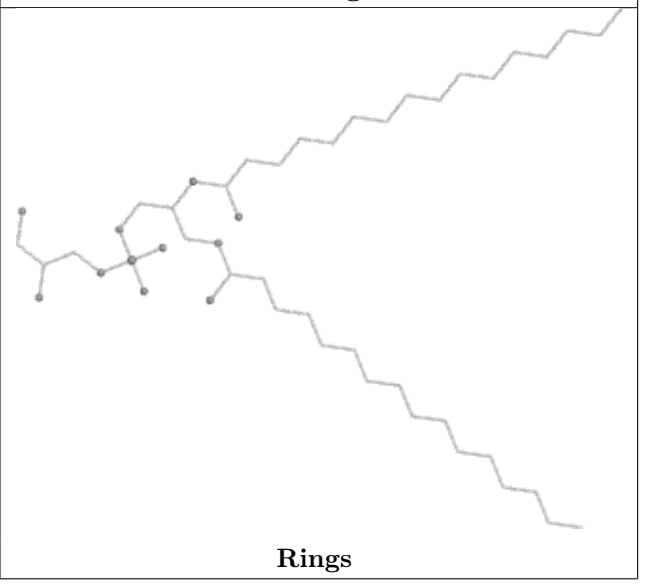
Bond lengths



Bond angles



Torsions



Rings

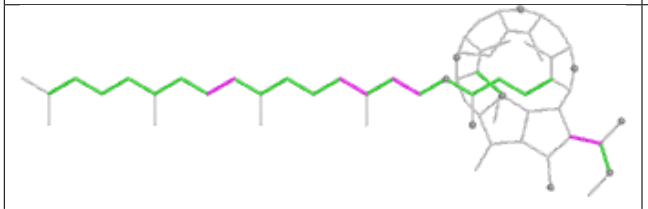
Ligand PHO a 406 (A)



Bond lengths



Bond angles



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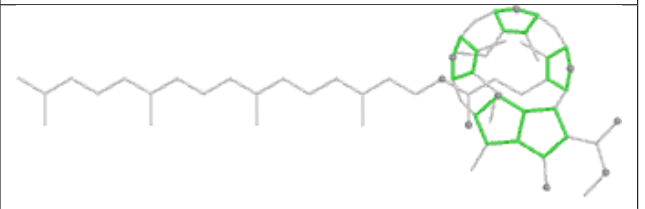
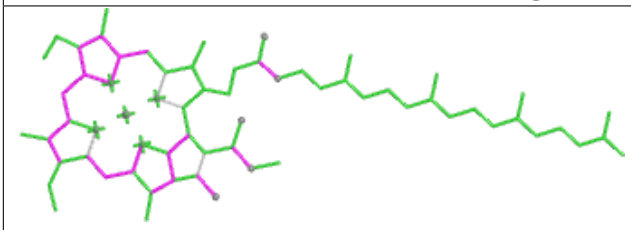
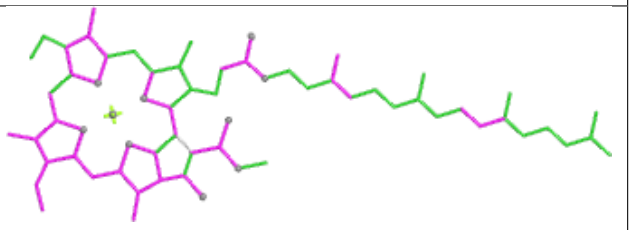


Rings

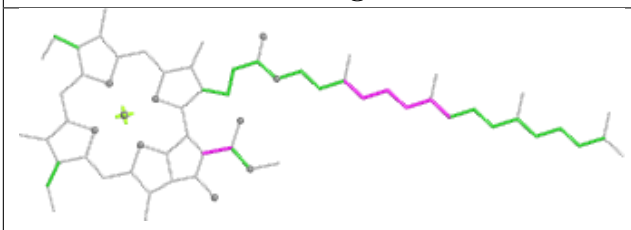
Ligand CLA b 616



Bond lengths



Bond angles



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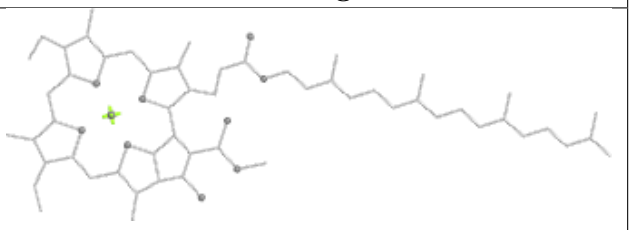
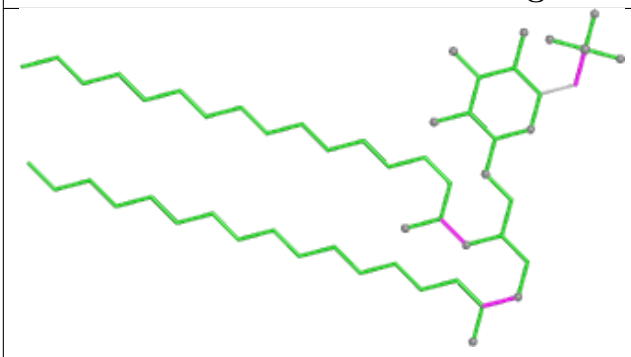


Rings

Ligand SQD b 620



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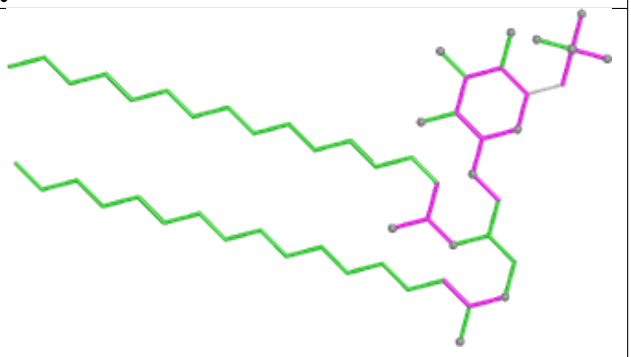
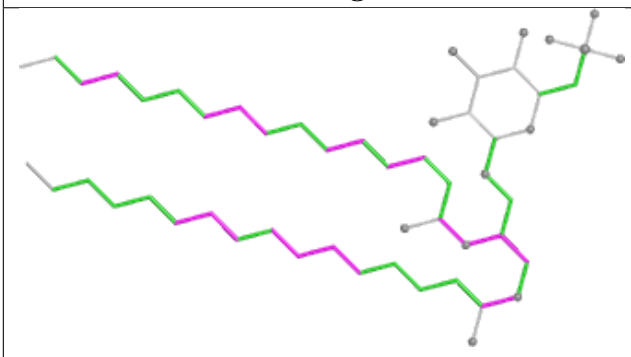


Bond angles



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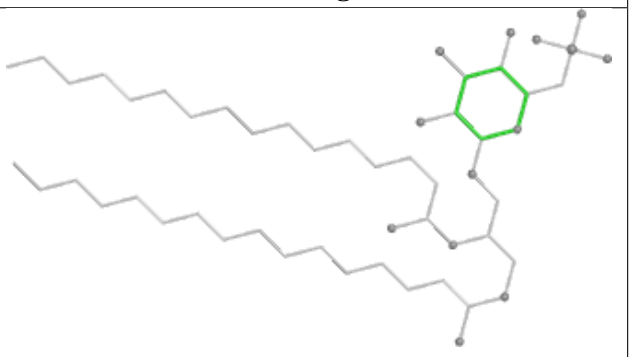
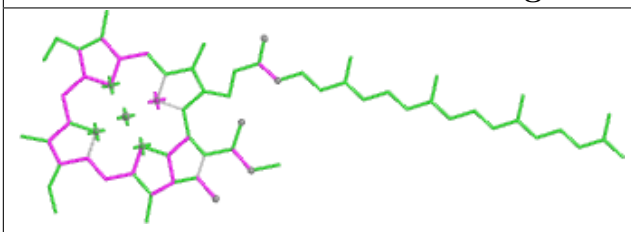


Rings

Ligand CLA B 606



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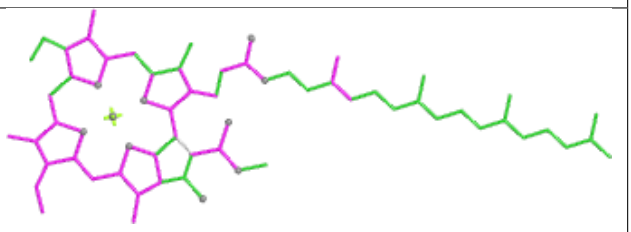
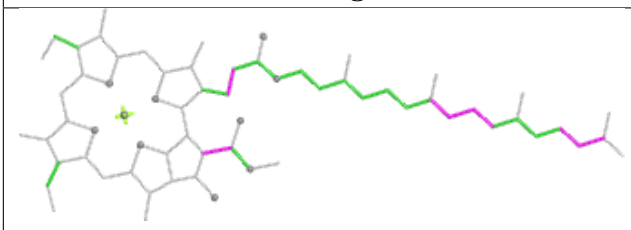


Bond angles



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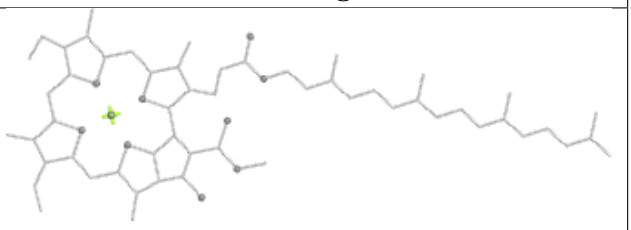
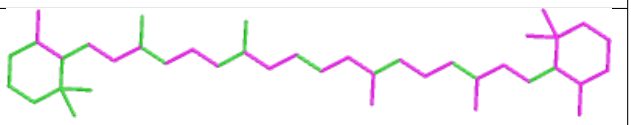


Rings

Ligand BCR d 405



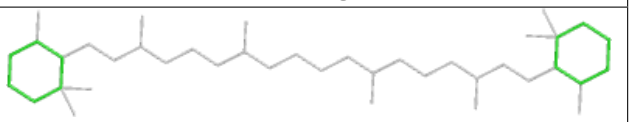
Bond lengths



Bond angles

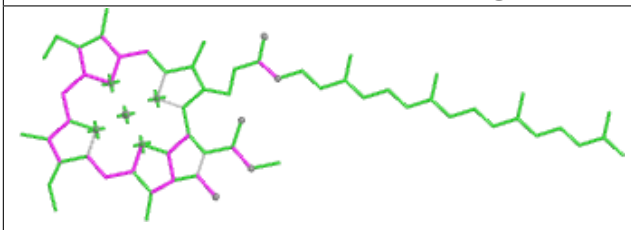


Torsions

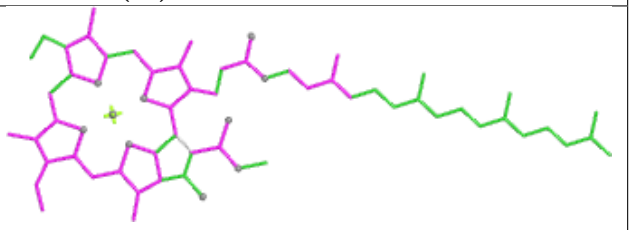


Rings

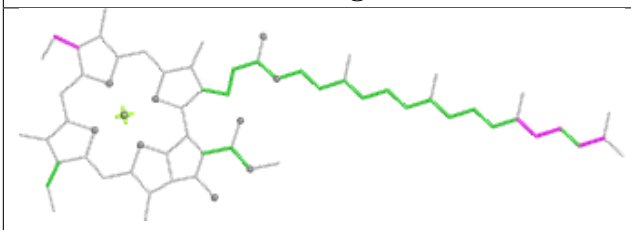
Ligand CLA A 406 (A)



Bond lengths



Bond angles



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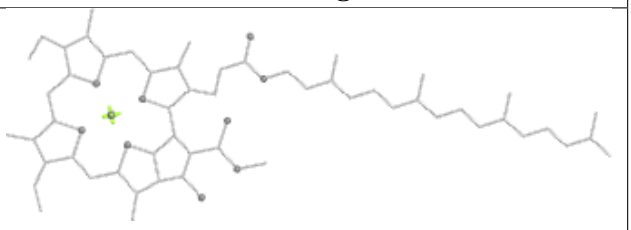
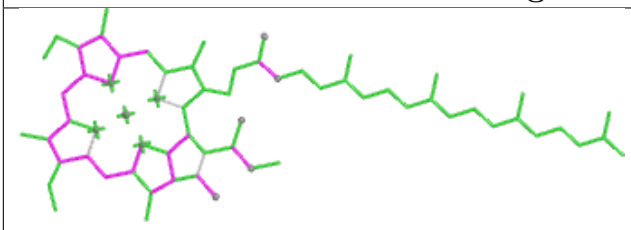


Rings

Ligand CLA b 612



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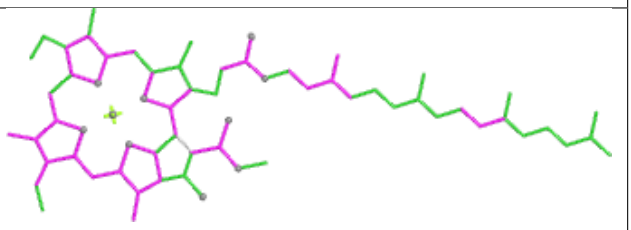
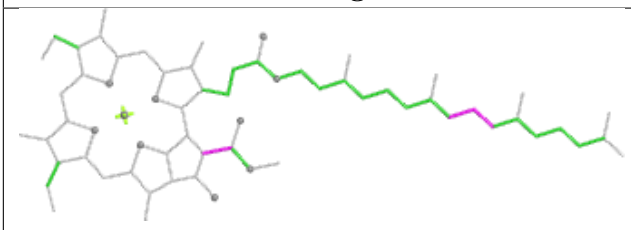


Bond angles



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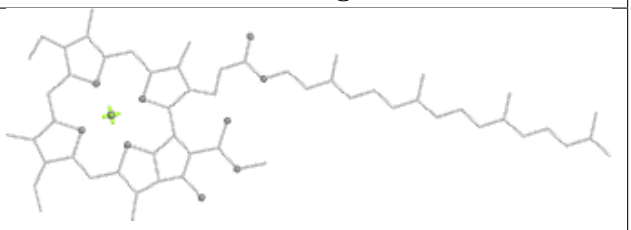
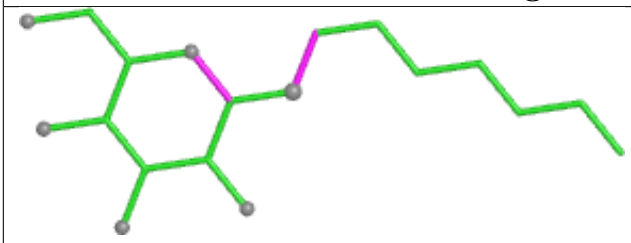


Rings

Ligand HTG b 622



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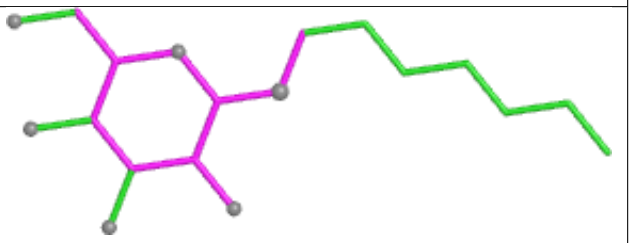
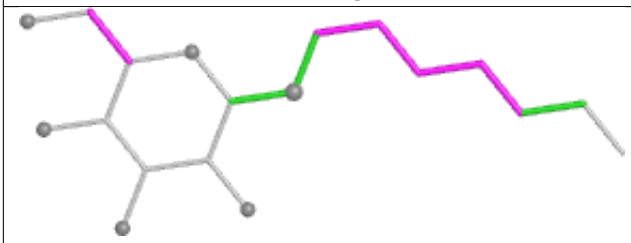


Bond angles



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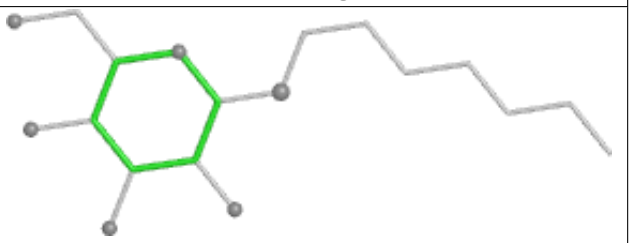
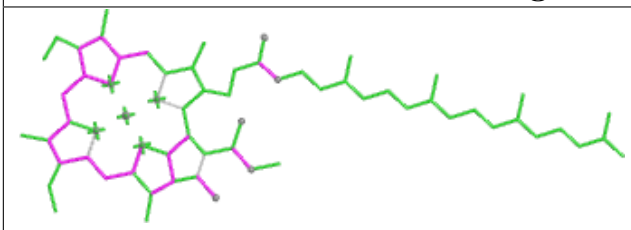


Rings

Ligand CLA c 504



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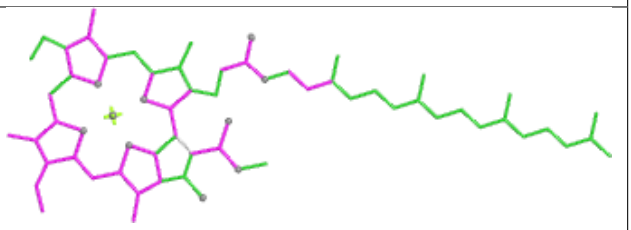
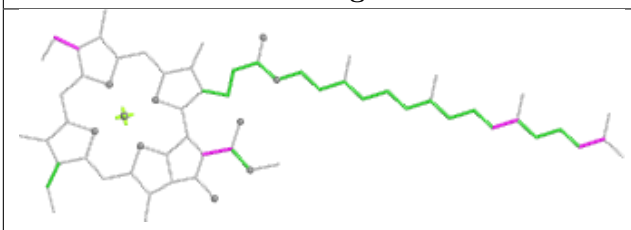


Bond angles



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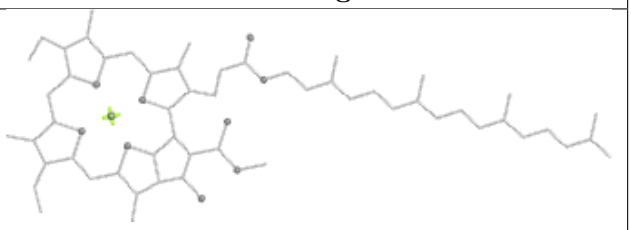
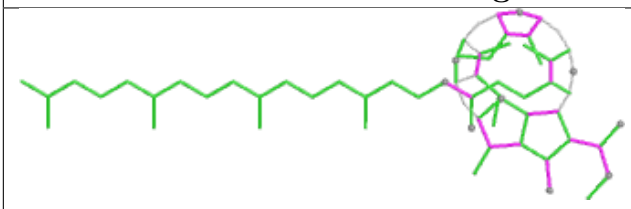


Rings

Ligand PHO a 414 (A)



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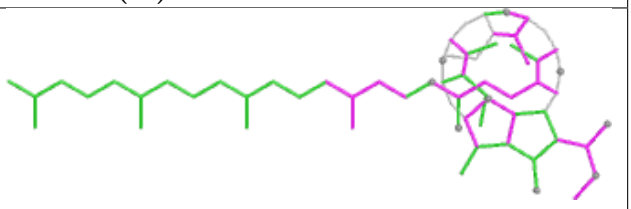
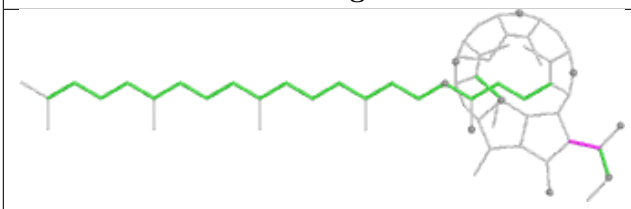


Bond angles



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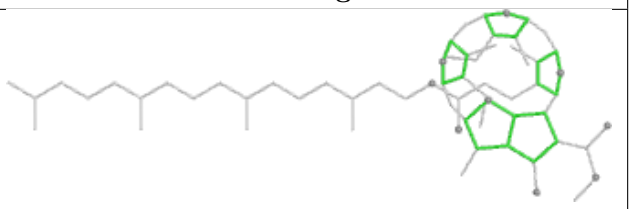
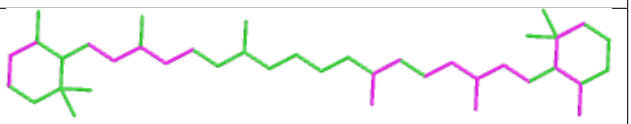


Rings

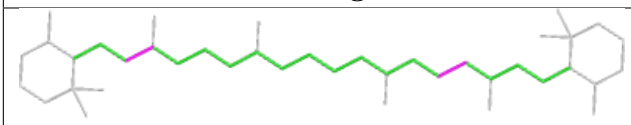
Ligand BCR K 102



Bond lengths



Bond angles



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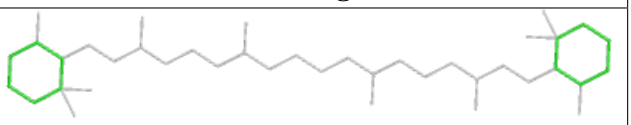
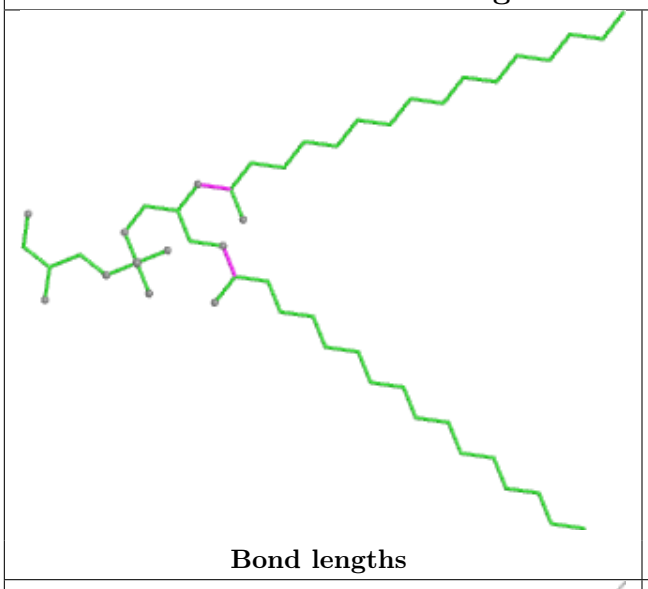


Rings

Ligand LHG d 408 (A)



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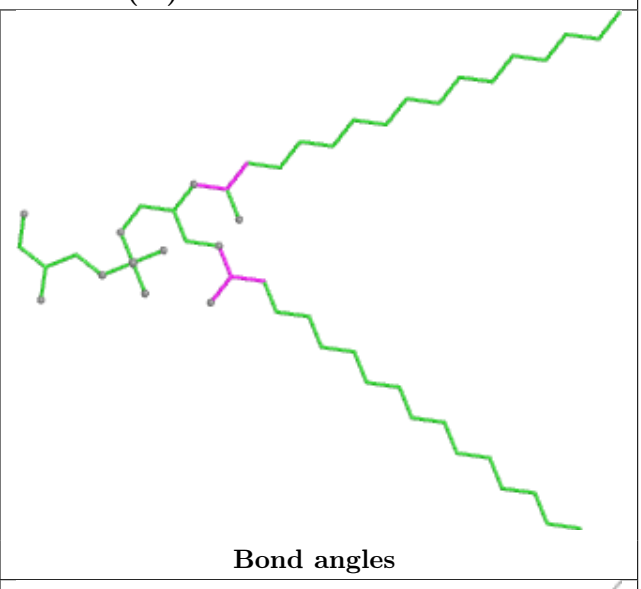
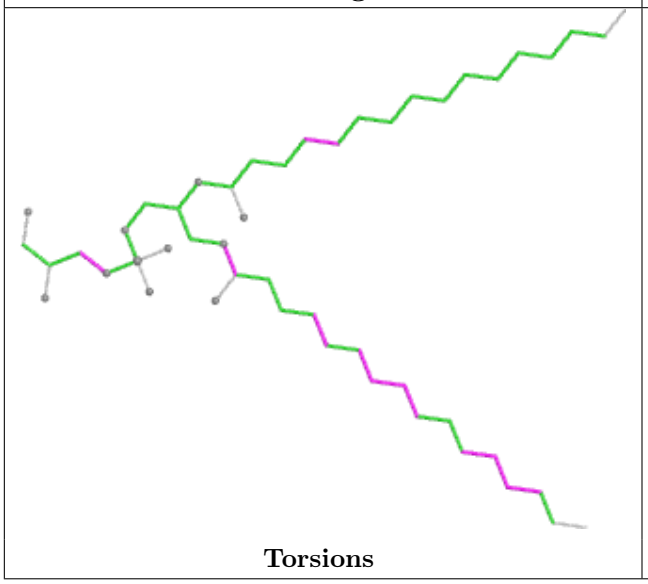


Bond angles



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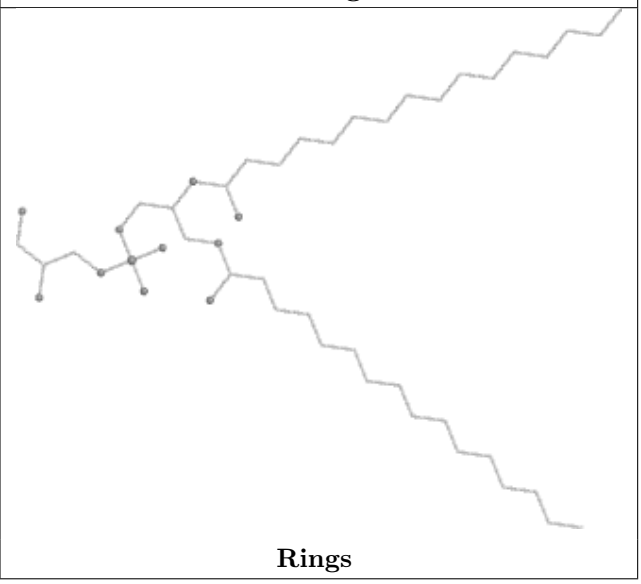
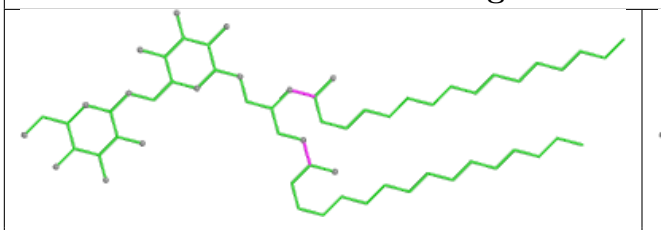


Rings

Ligand DGD C 517 (A)



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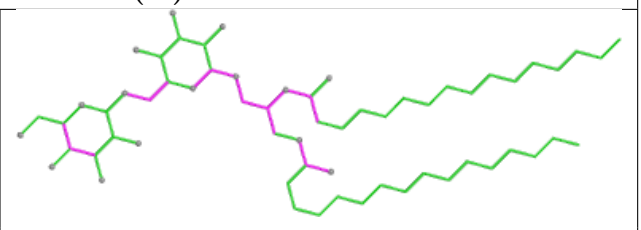
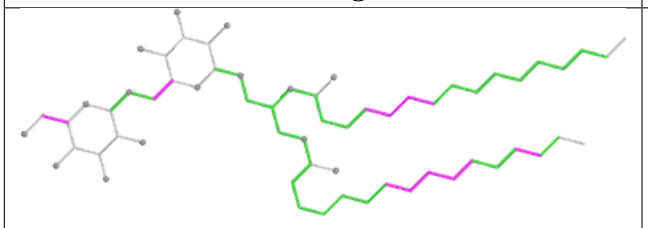


Bond angles



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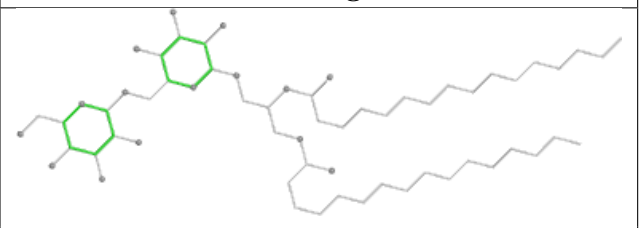
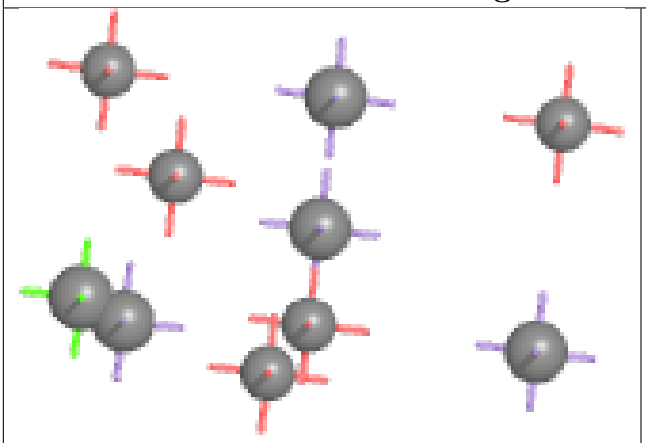


Rings

Ligand OEX a 411 (A)



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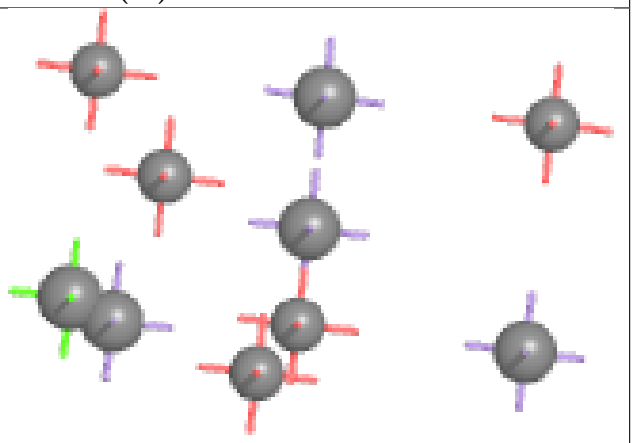
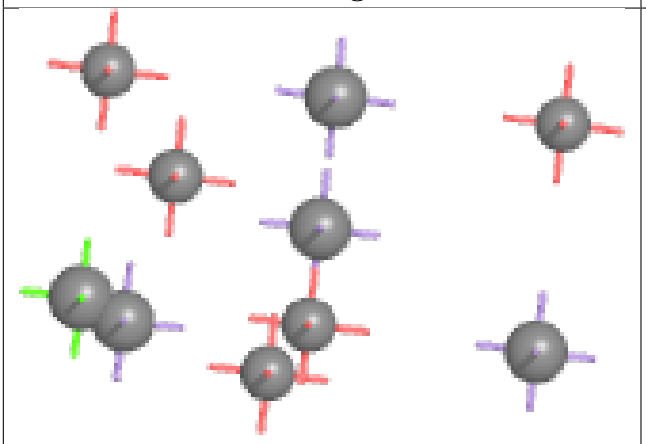


Bond angles



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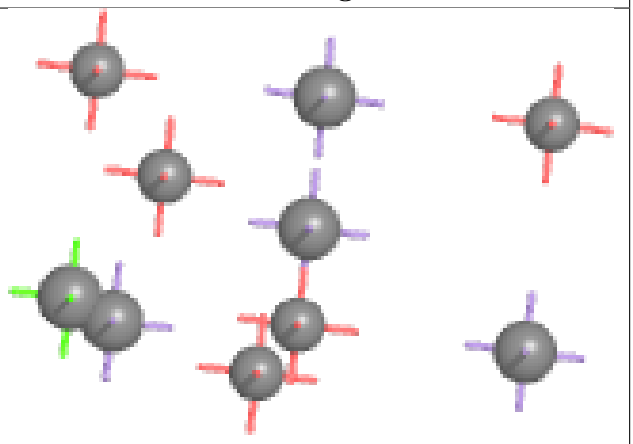
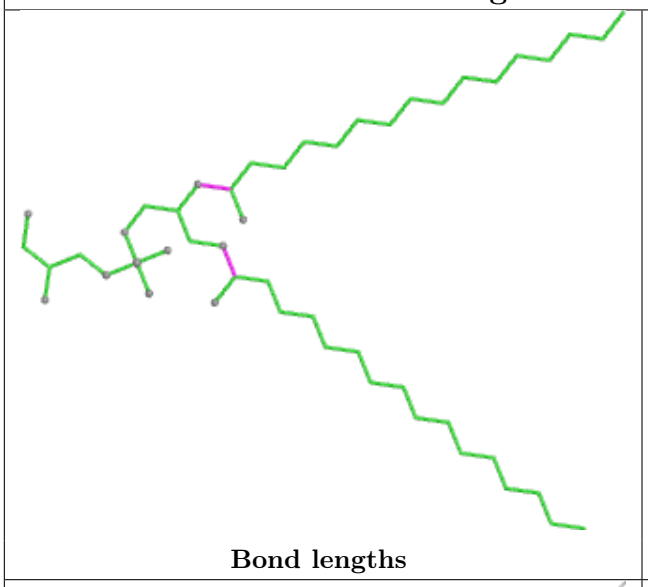


Rings

Ligand LHG A 419 (A)



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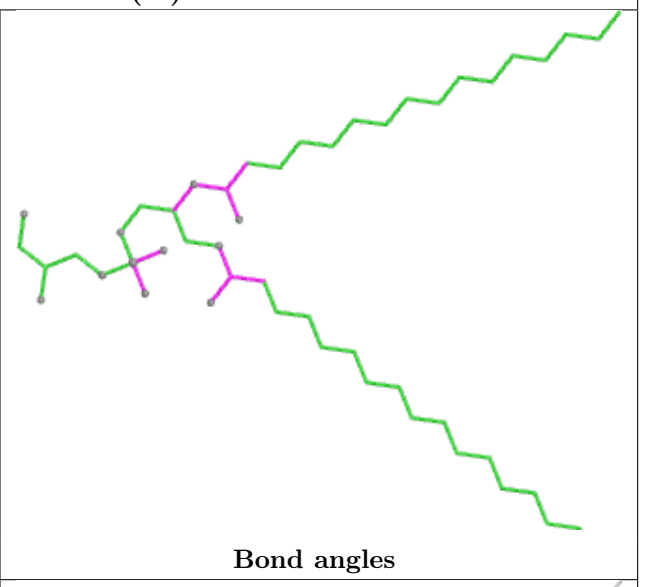
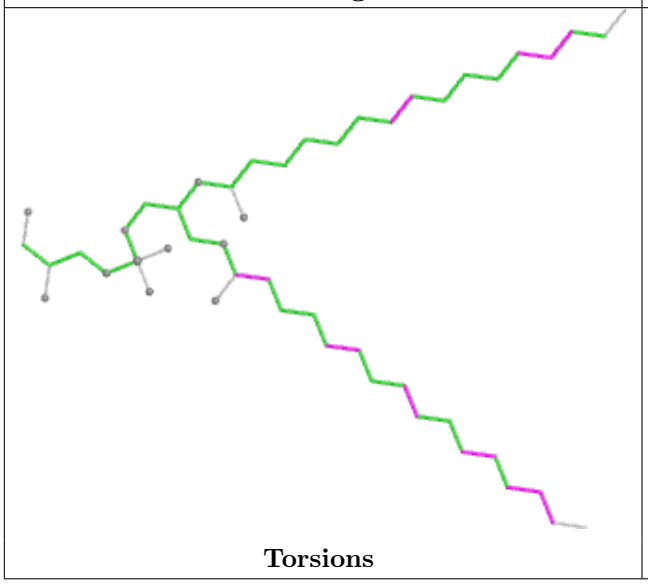


Bond angles



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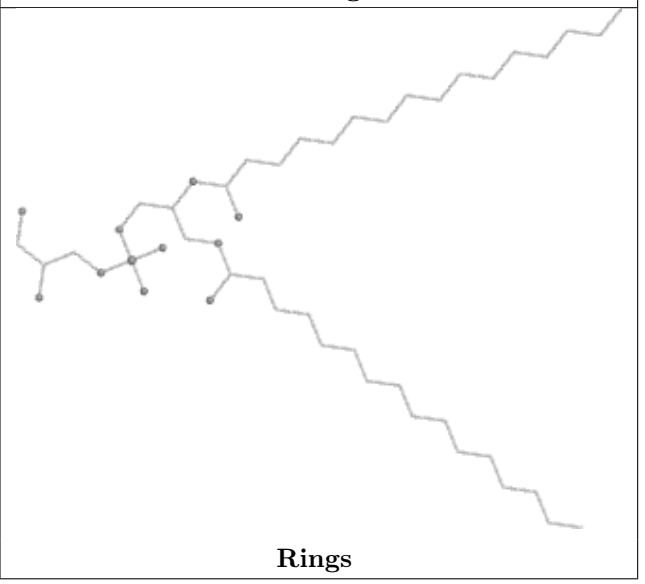


Rings

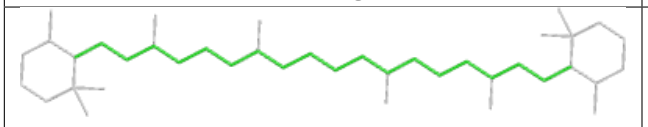
Ligand BCR k 101



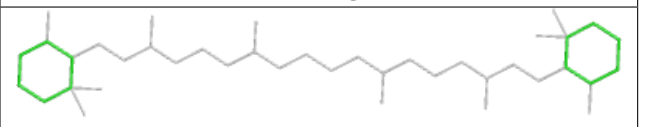
Bond lengths



Bond angles

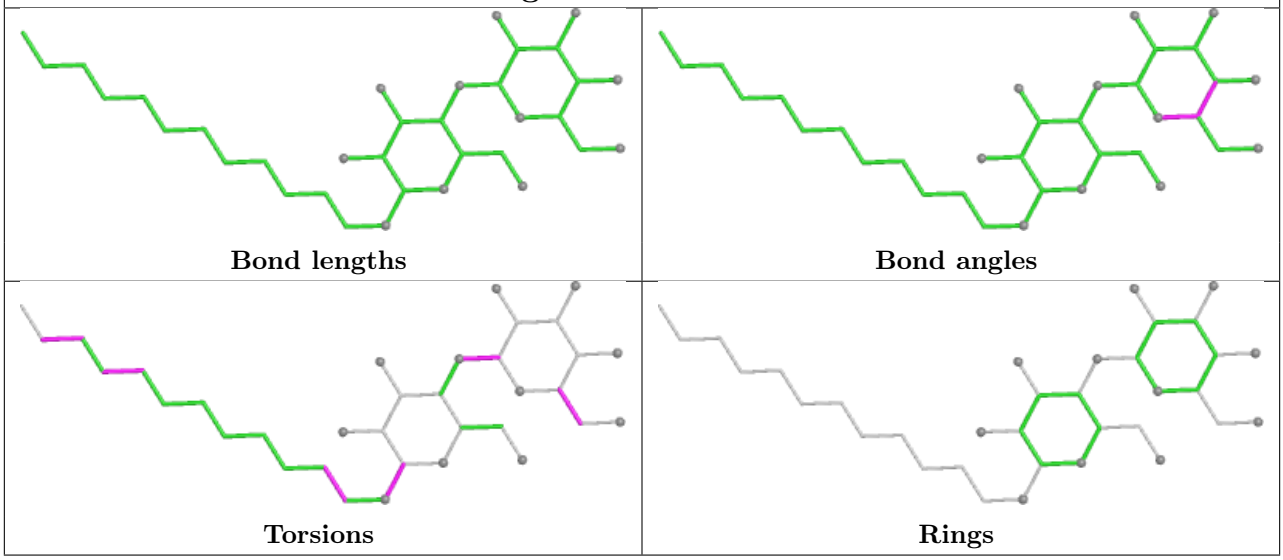


Torsions

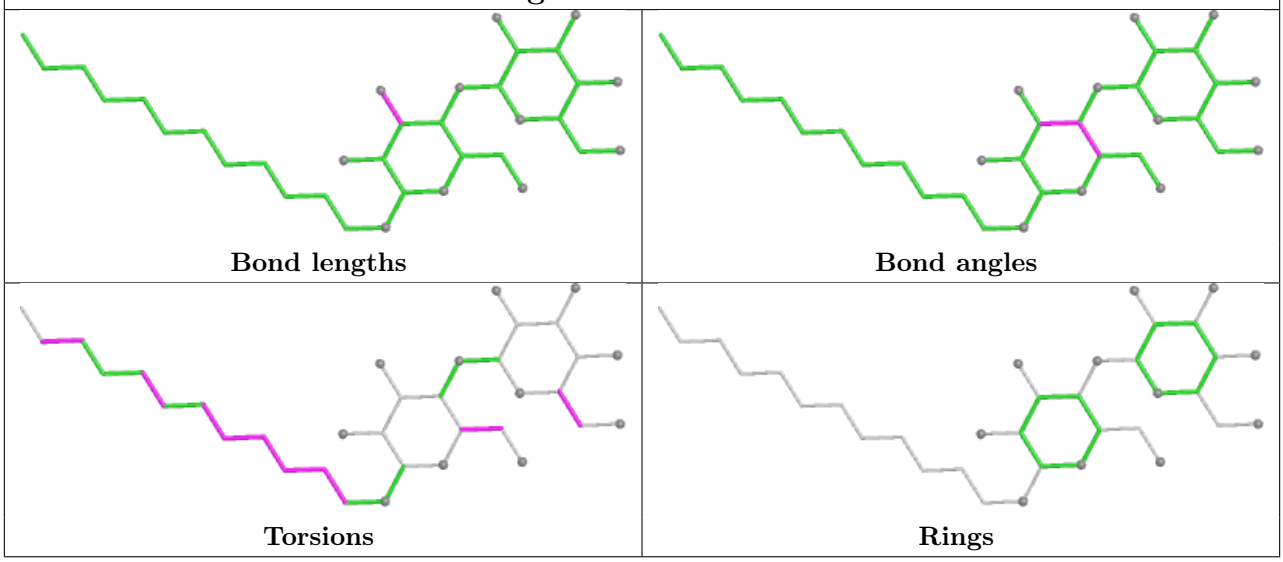


Rings

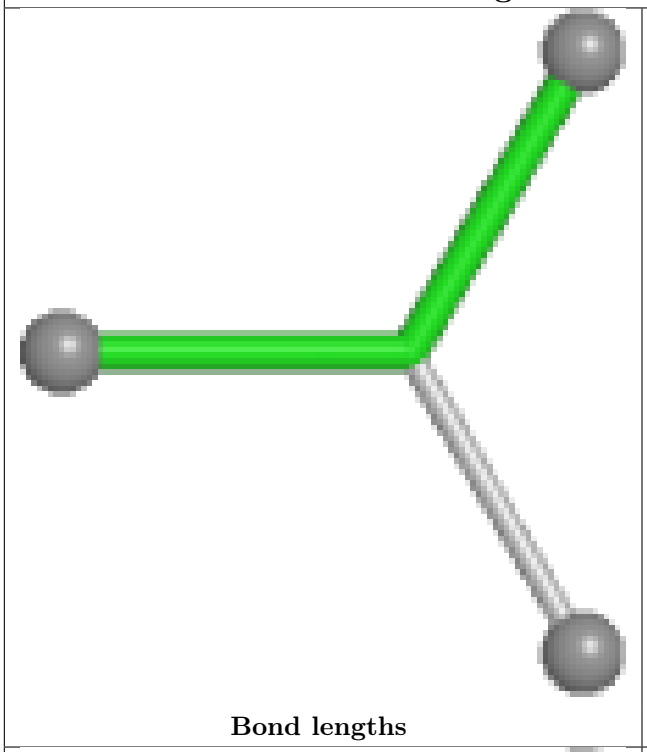
Ligand LMT A 417



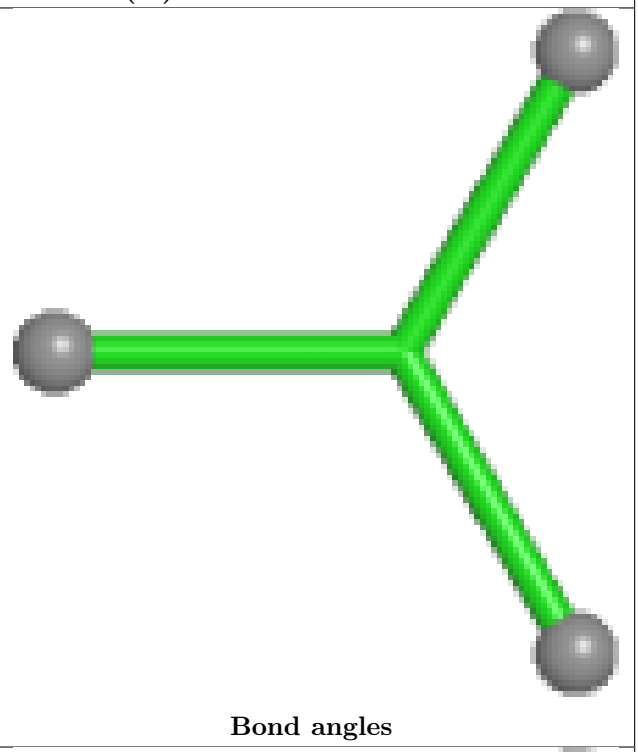
Ligand LMT c 502



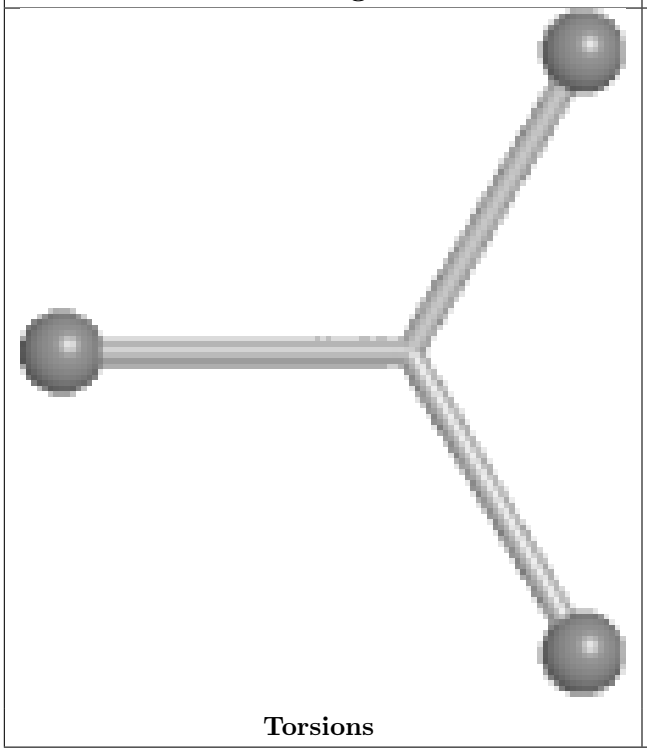
Ligand BCT d 401 (B)



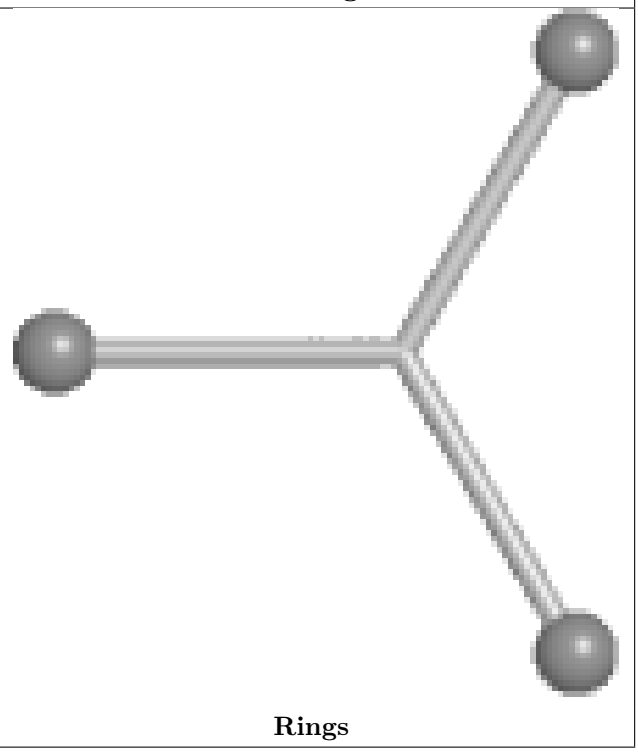
Bond lengths



Bond angles

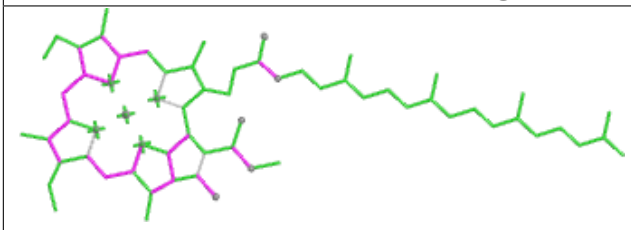


Torsions



Rings

Ligand CLA d 402 (B)



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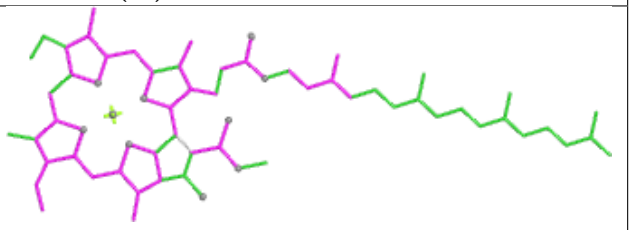
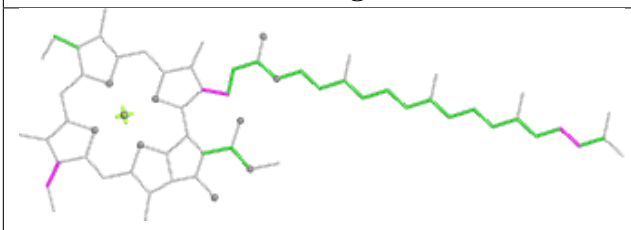
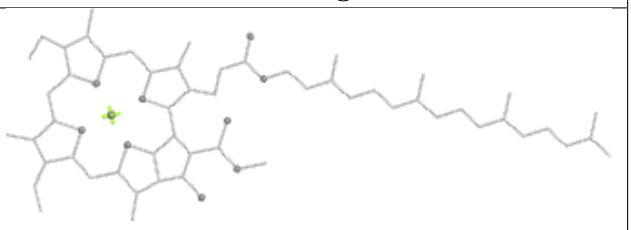


Bond angles

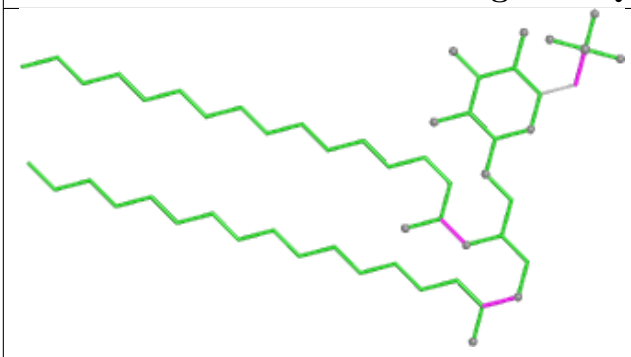


Torsions



Rings

Ligand SQD A 410 (B)



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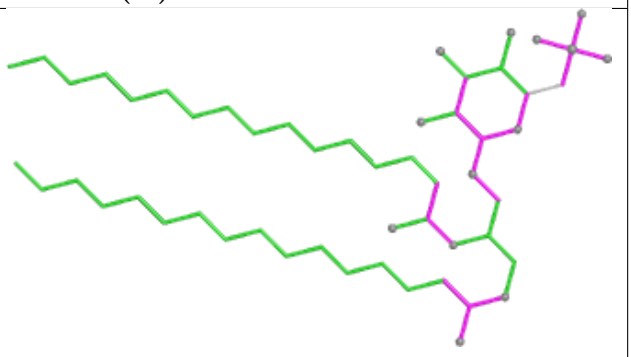
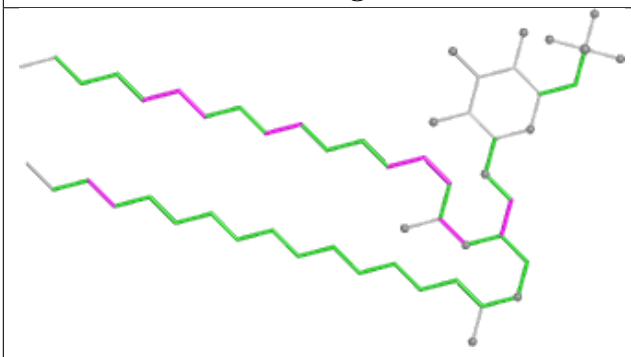


Bond angles



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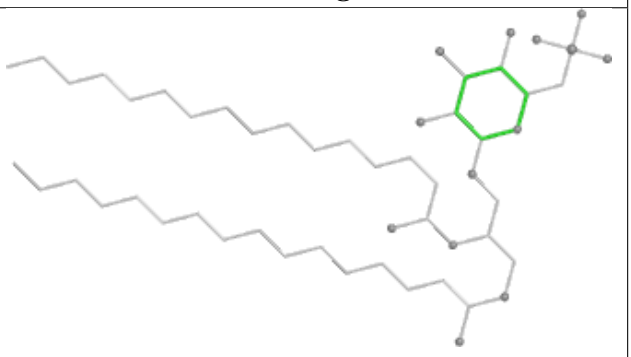
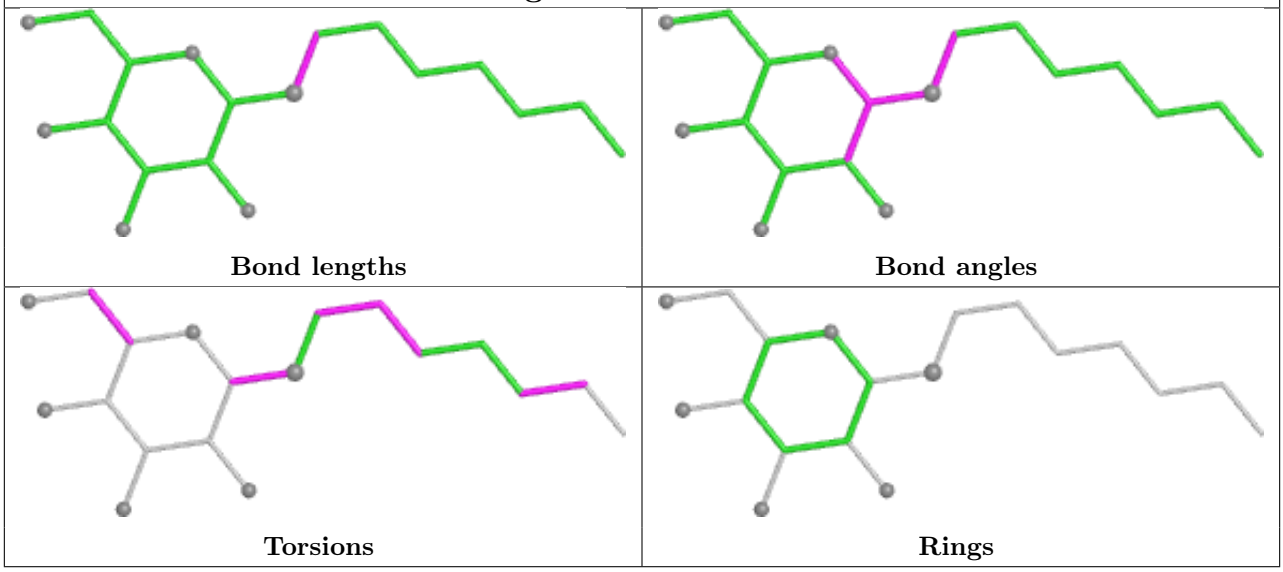
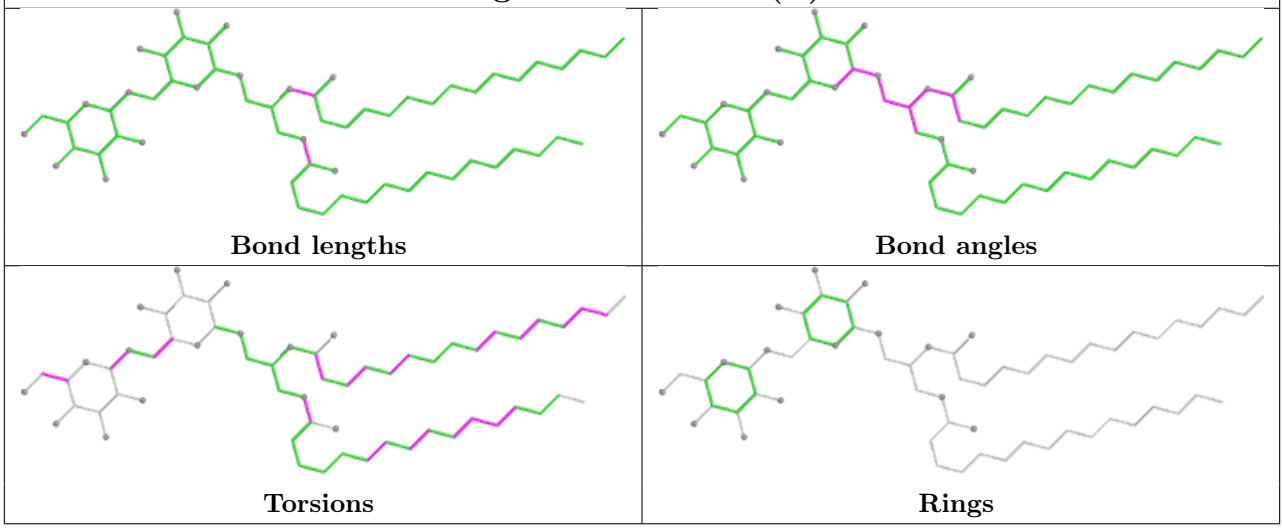


Rings

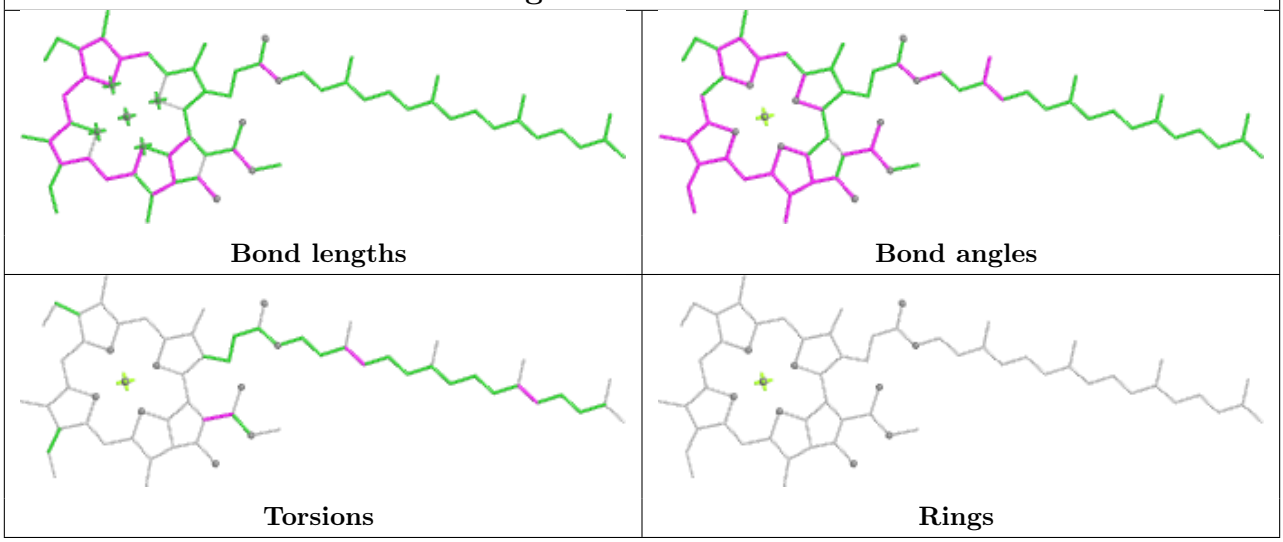
Ligand HTG b 623



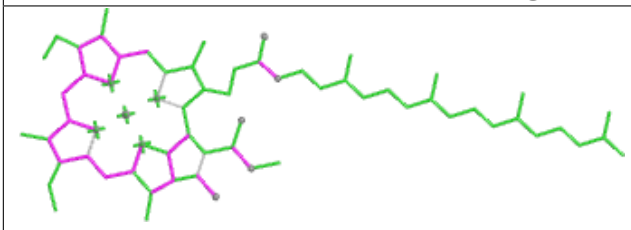
Ligand DGD c 518 (B)



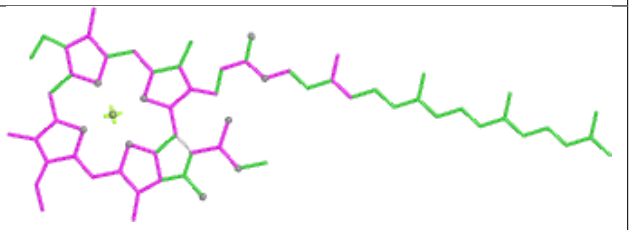
Ligand CLA C 505



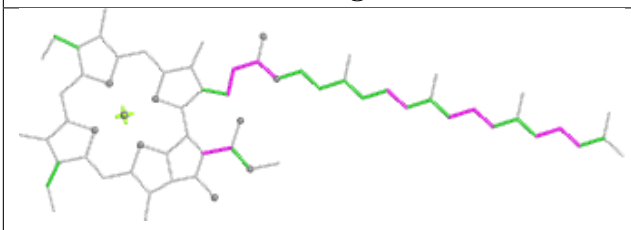
Ligand CLA B 601



Bond lengths



Bond angles



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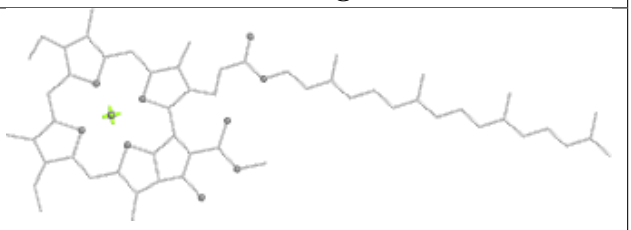
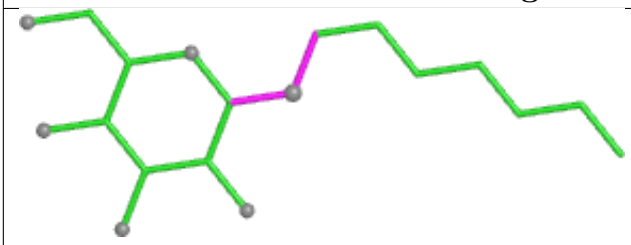


Rings

Ligand HTG B 624



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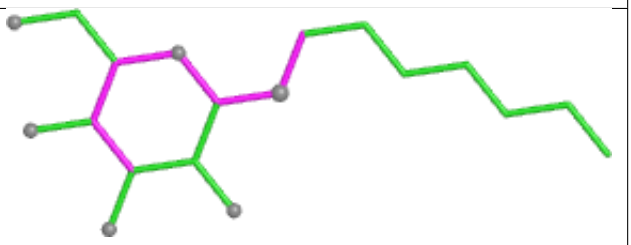
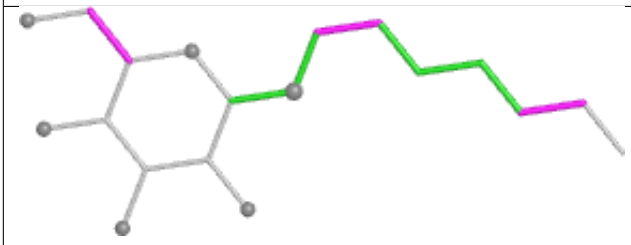


Bond angles



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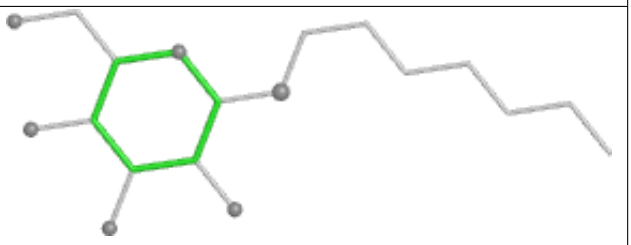
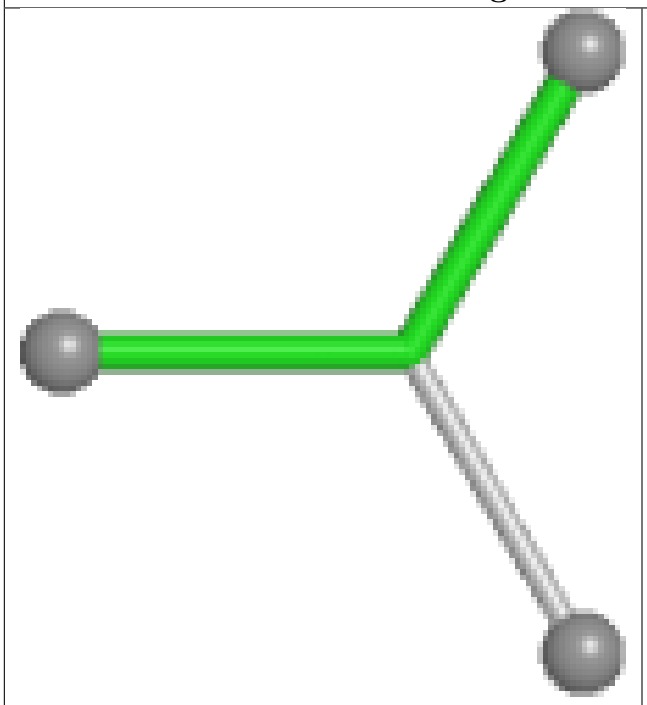


Rings

Ligand BCT D 401 (A)



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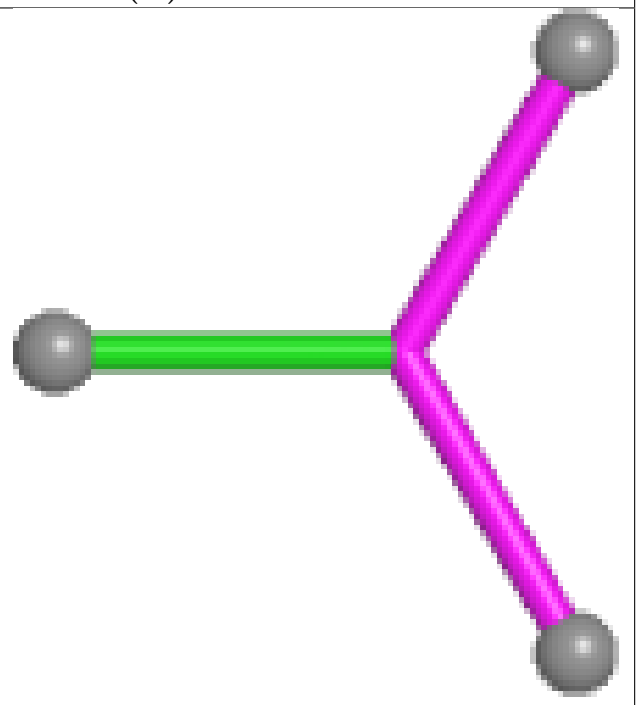
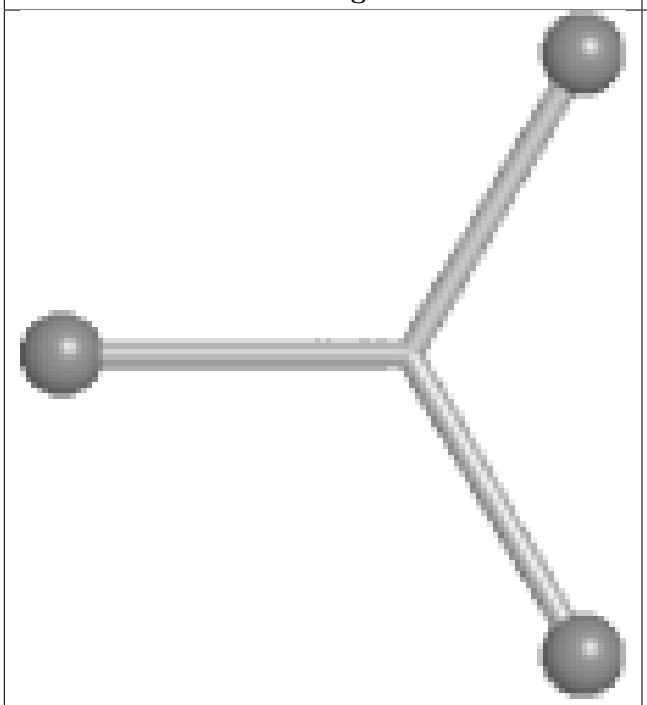


Bond angles



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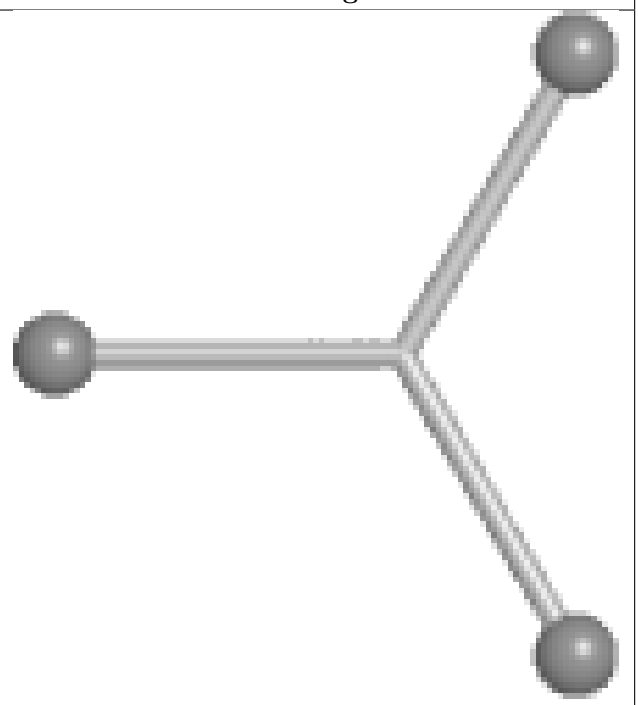
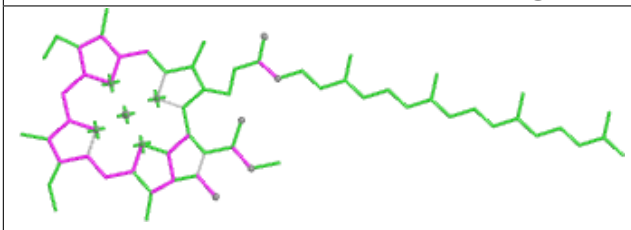


Rings

Ligand CLA c 506



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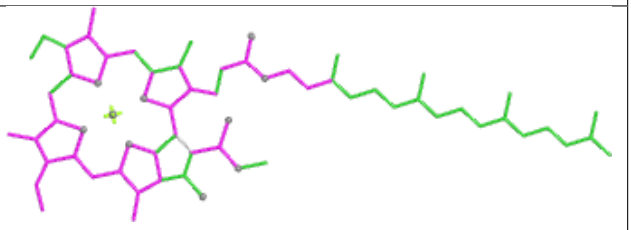
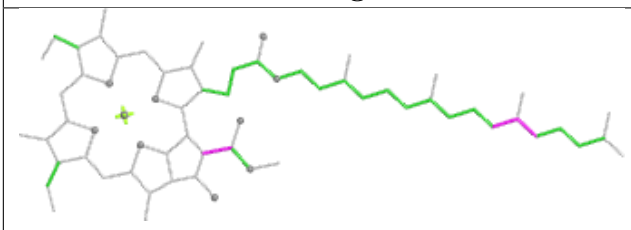


Bond angles



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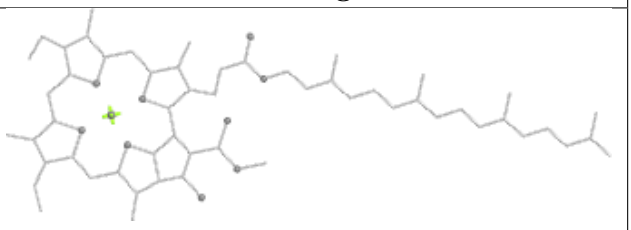
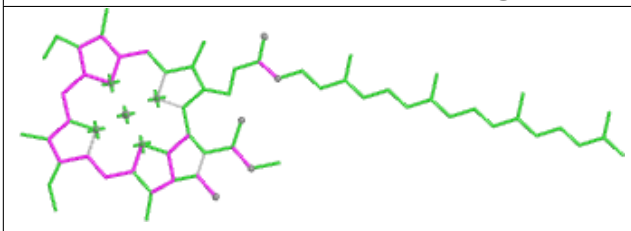


Rings

Ligand CLA d 403 (B)



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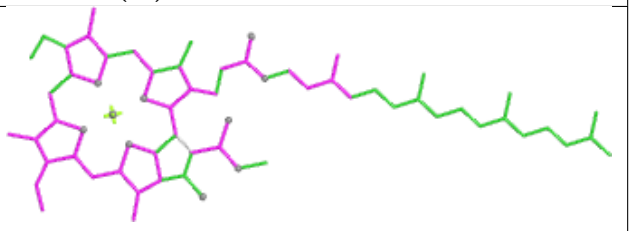
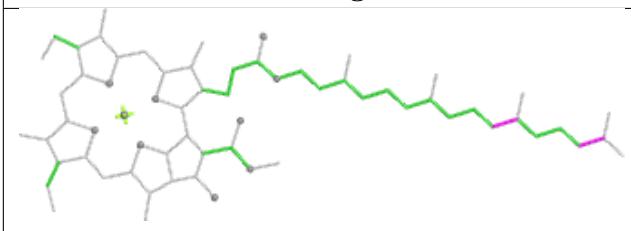
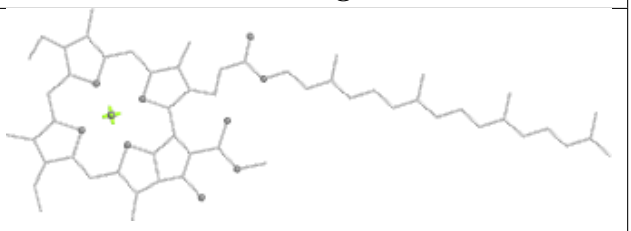


Bond angles

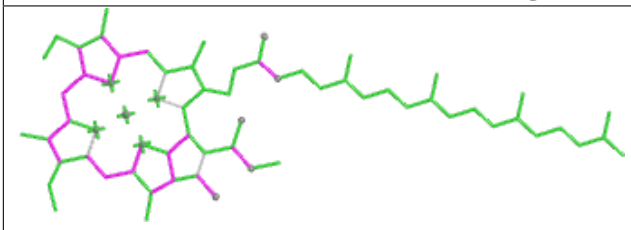


Torsions



Rings

Ligand CLA B 605



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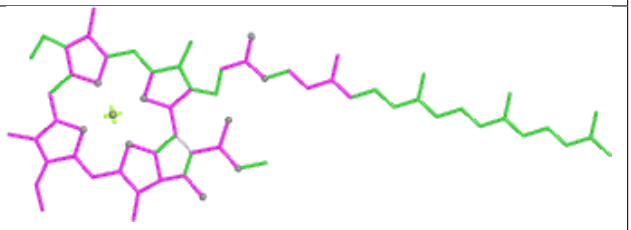
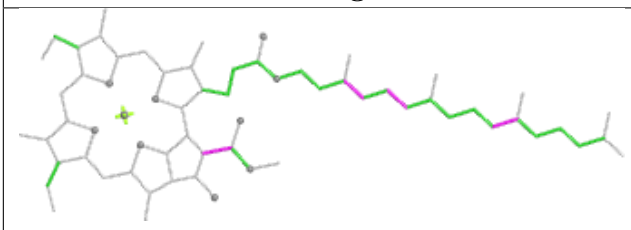


Bond angles



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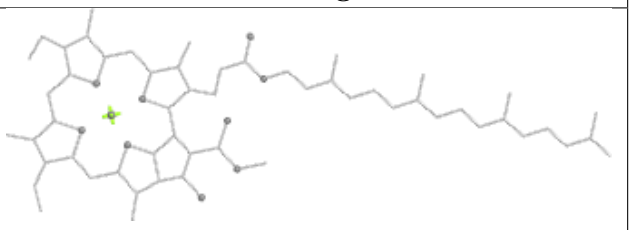
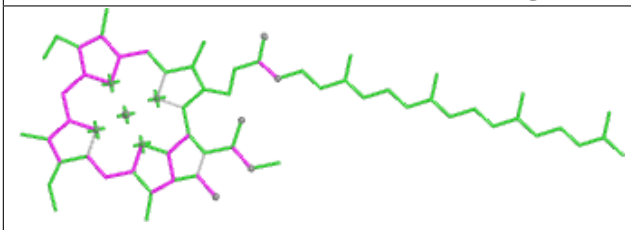


Rings

Ligand CLA C 514



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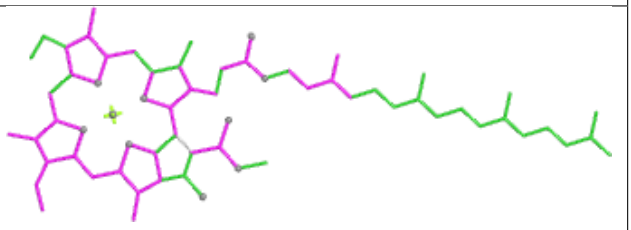
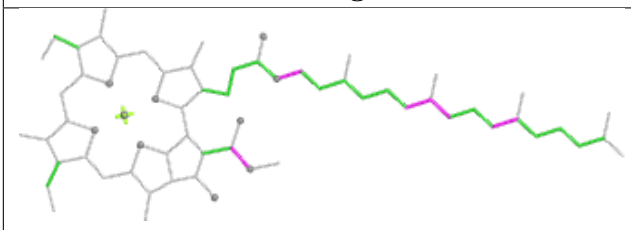


Bond angles



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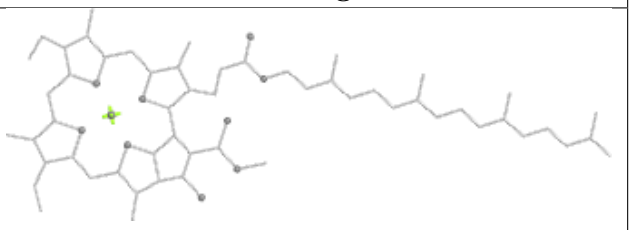
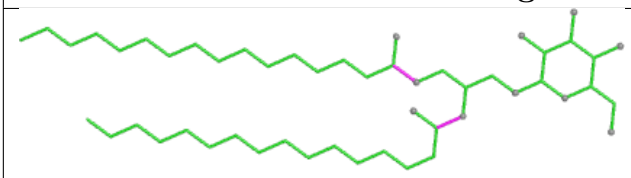


Rings

Ligand LMG m 101



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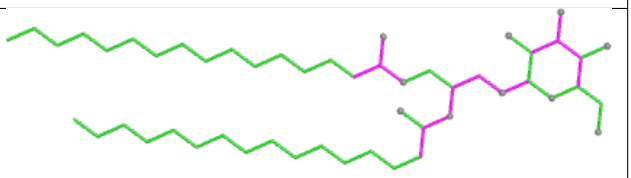
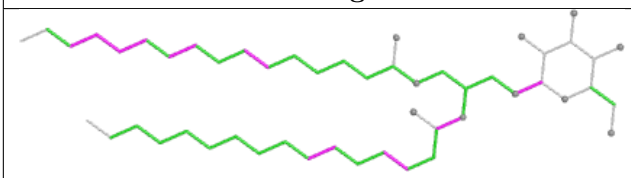


Bond angles



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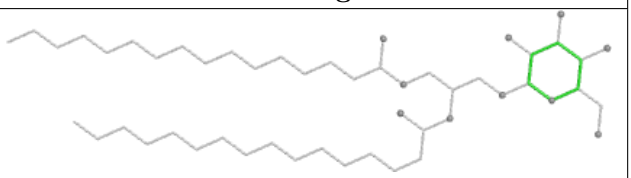
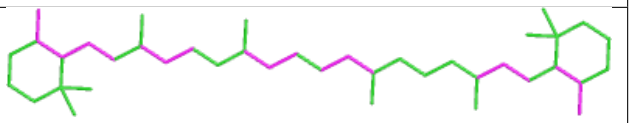


Rings

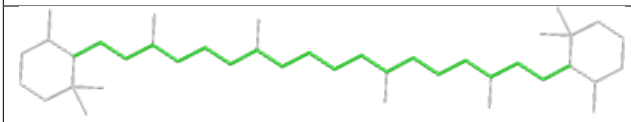
Ligand BCR A 409



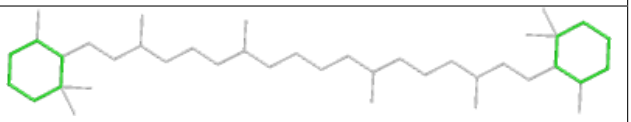
Bond lengths



Bond angles

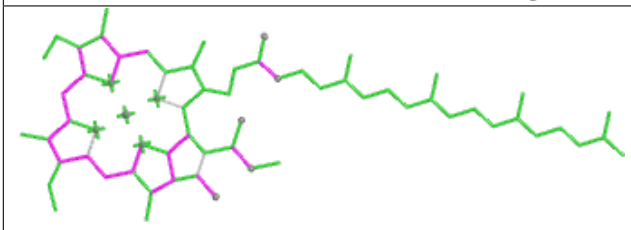


Torsions

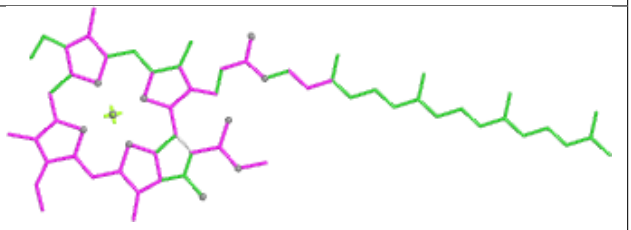


Rings

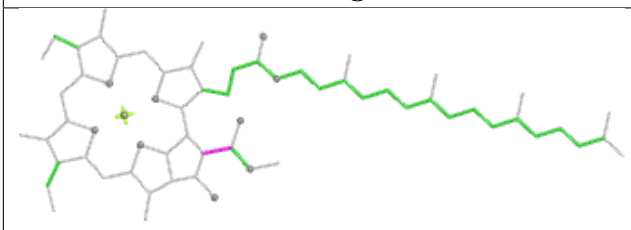
Ligand CLA B 609



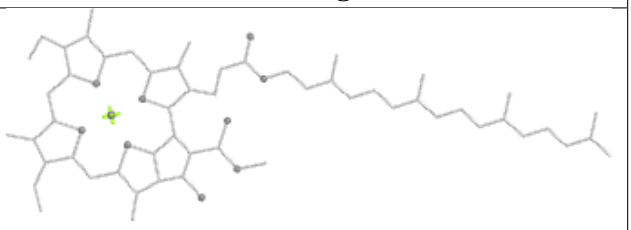
Bond lengths



Bond angles

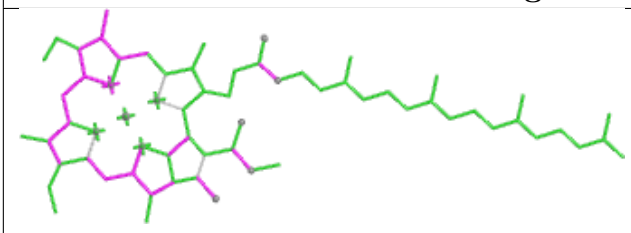


Torsions

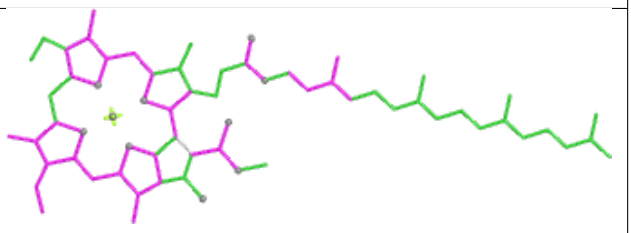


Rings

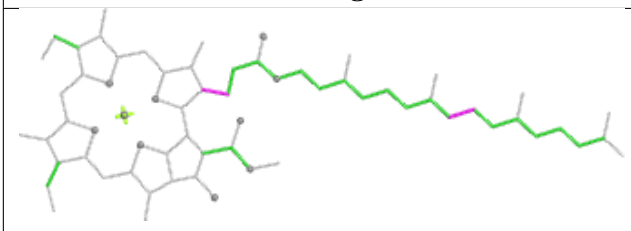
Ligand CLA B 611



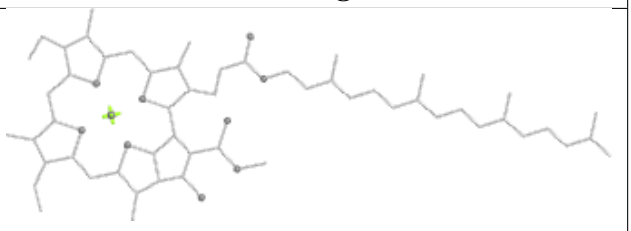
Bond lengths



Bond angles

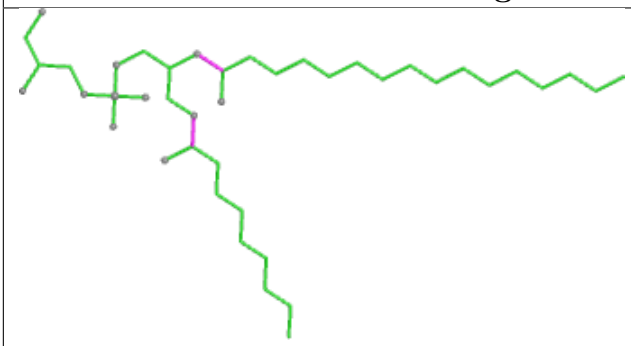


Torsions

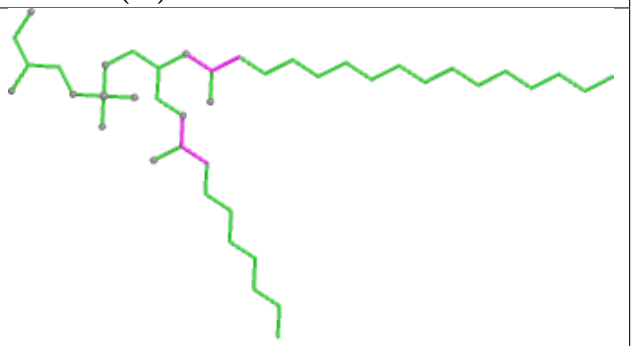


Rings

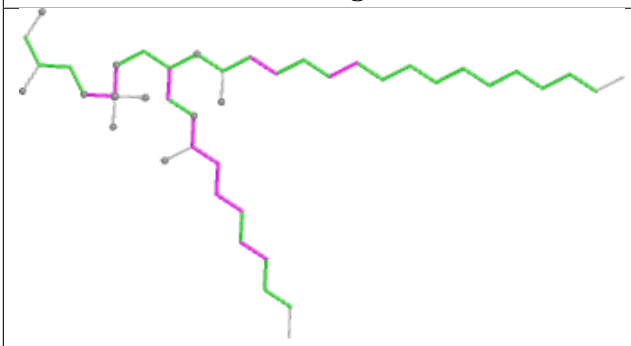
Ligand LHG a 417 (B)



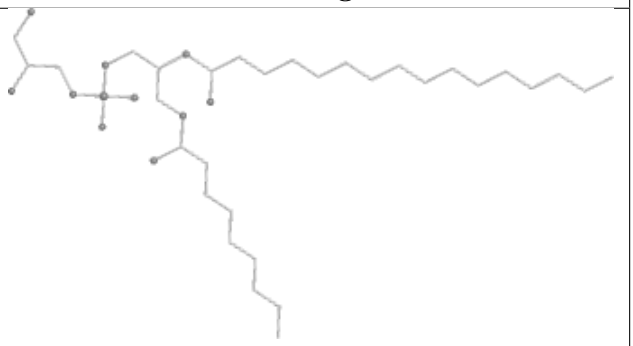
Bond lengths



Bond angles

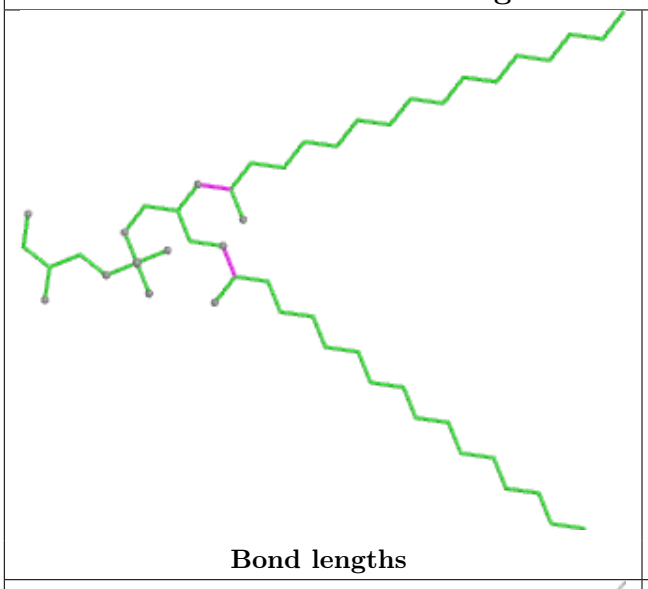


Torsions

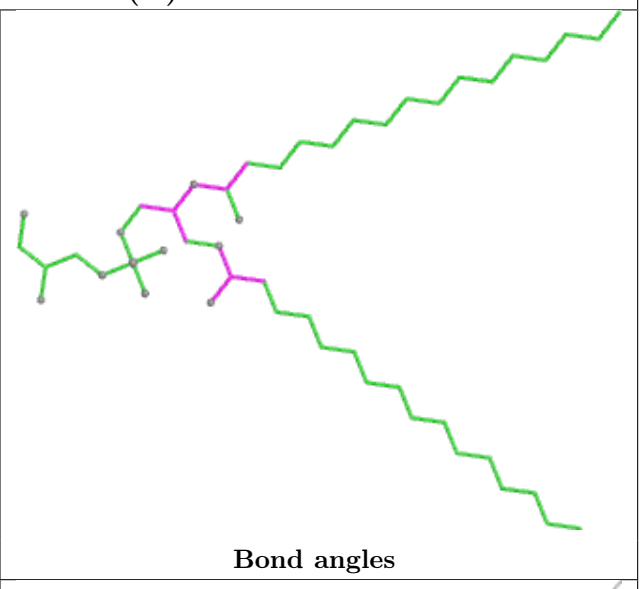


Rings

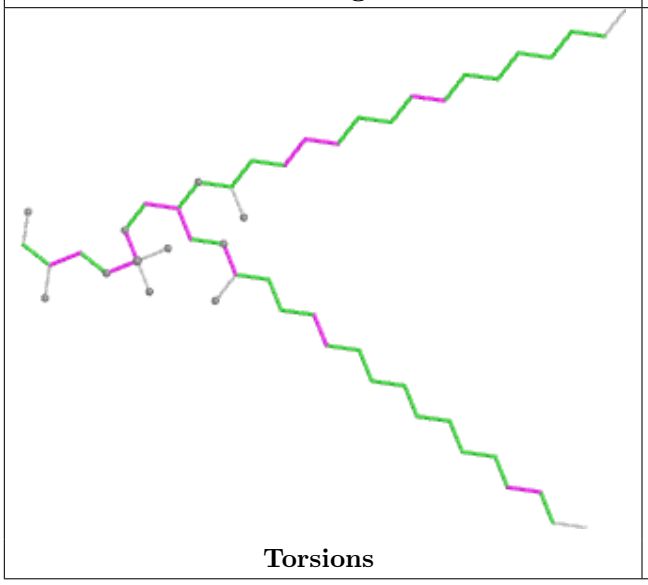
Ligand LHG d 407 (B)



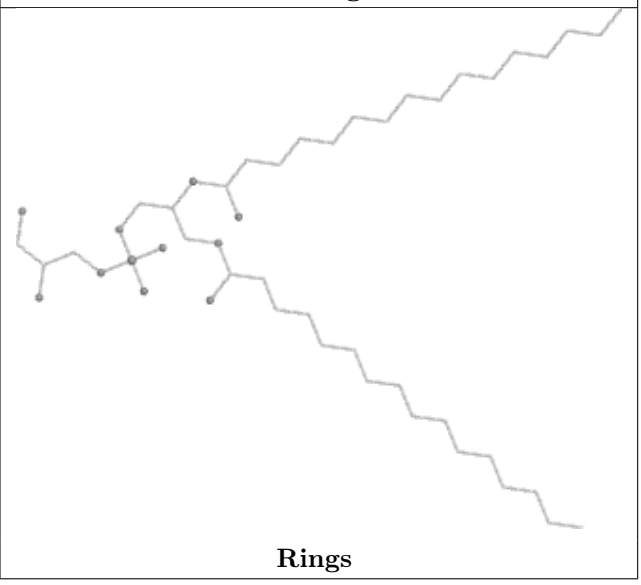
Bond lengths



Bond angles

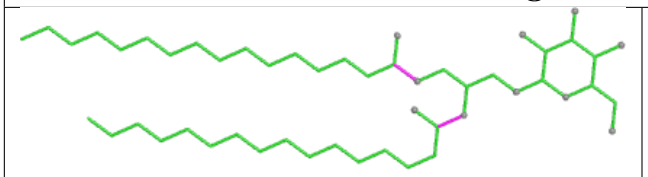


Torsions

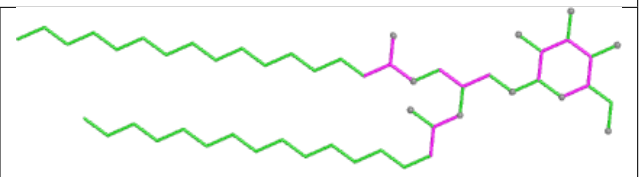


Rings

Ligand LMG c 522



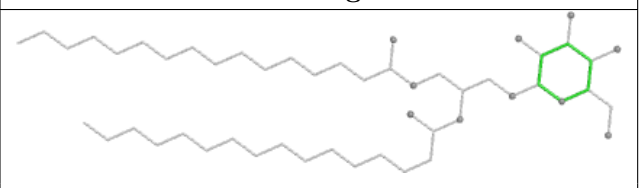
Bond lengths



Bond angles

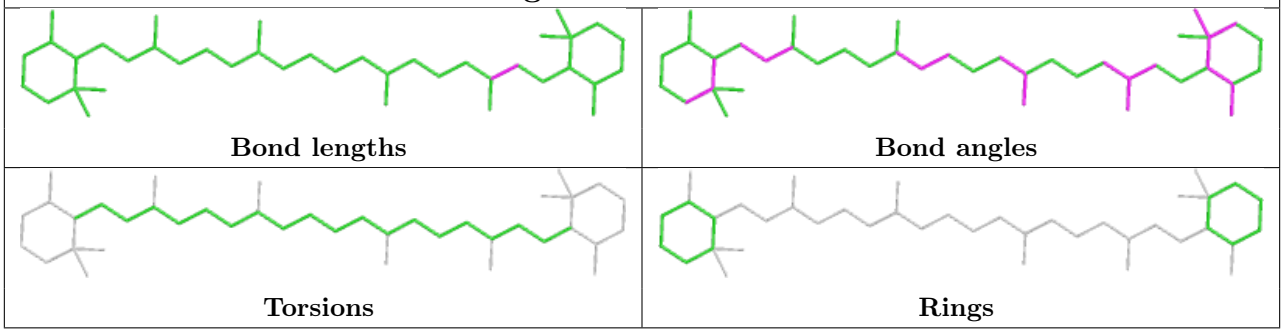


Torsions

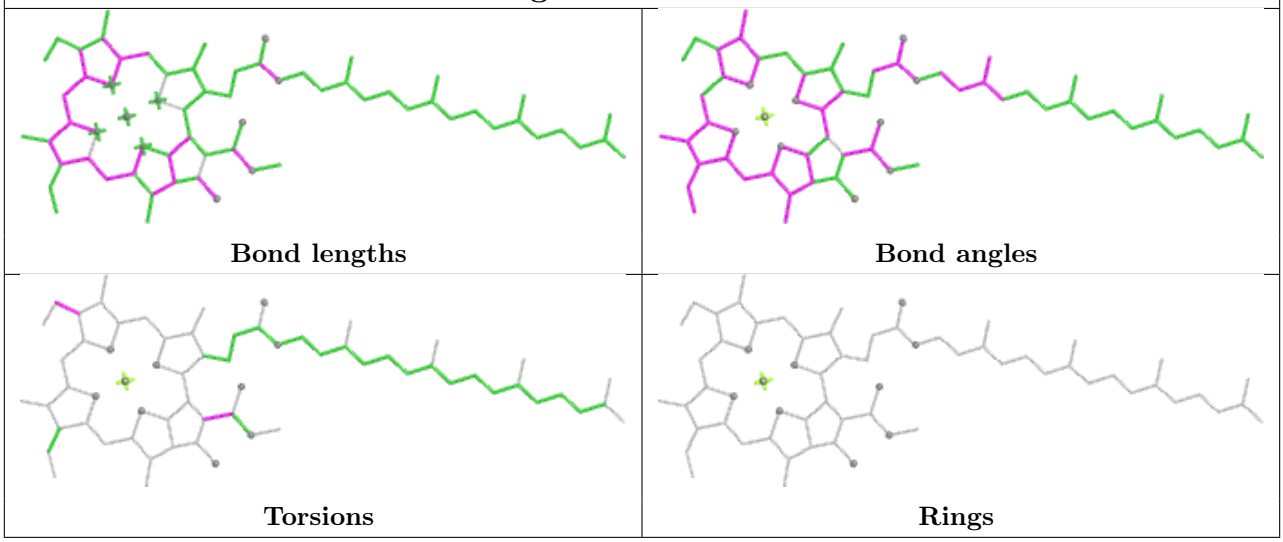


Rings

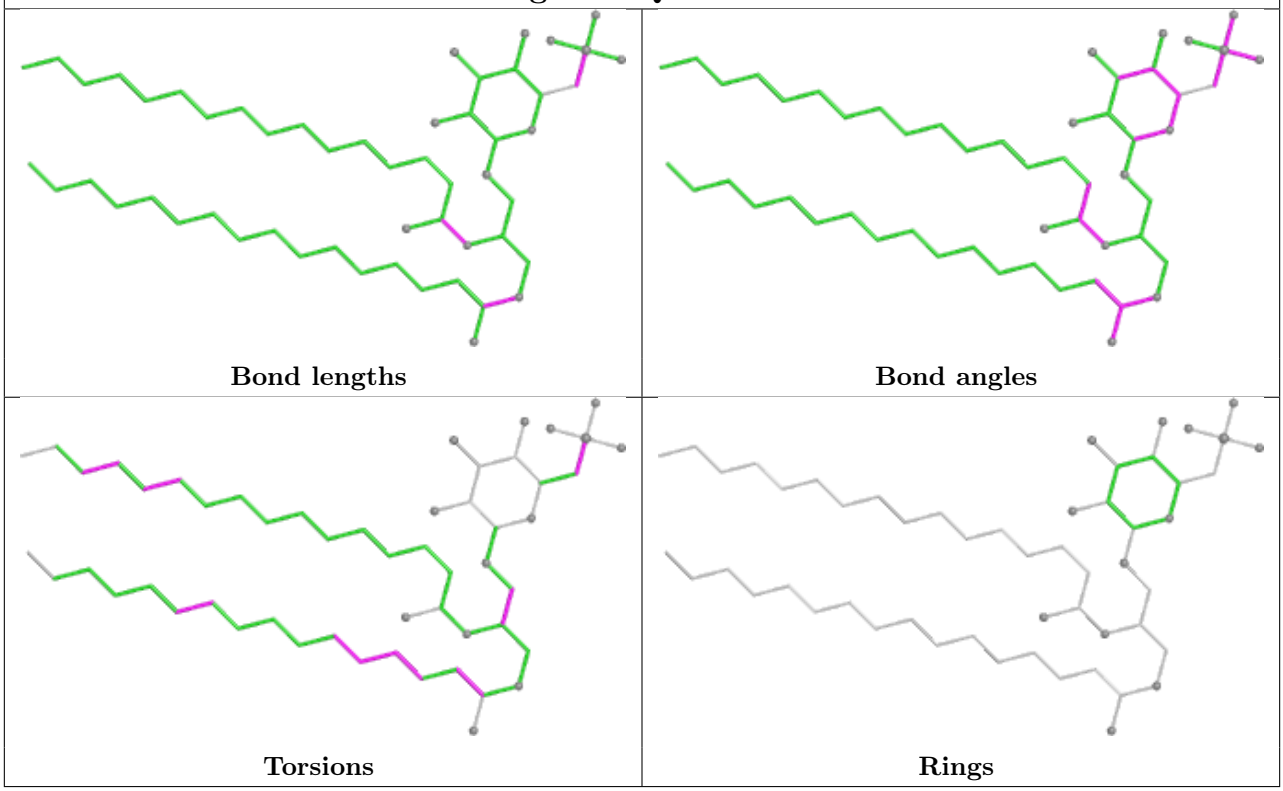
Ligand BCR B 618



Ligand CLA c 503



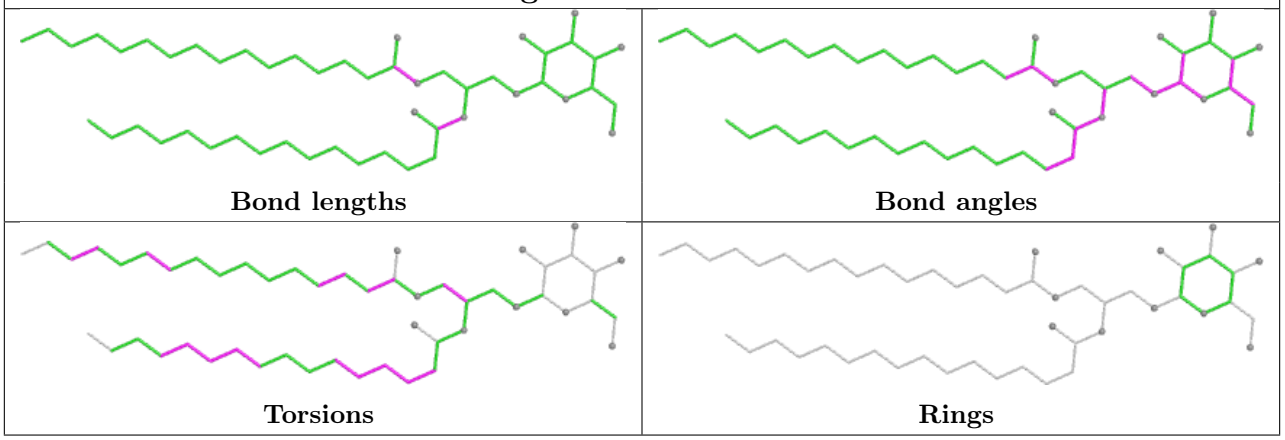
Ligand SQD a 410



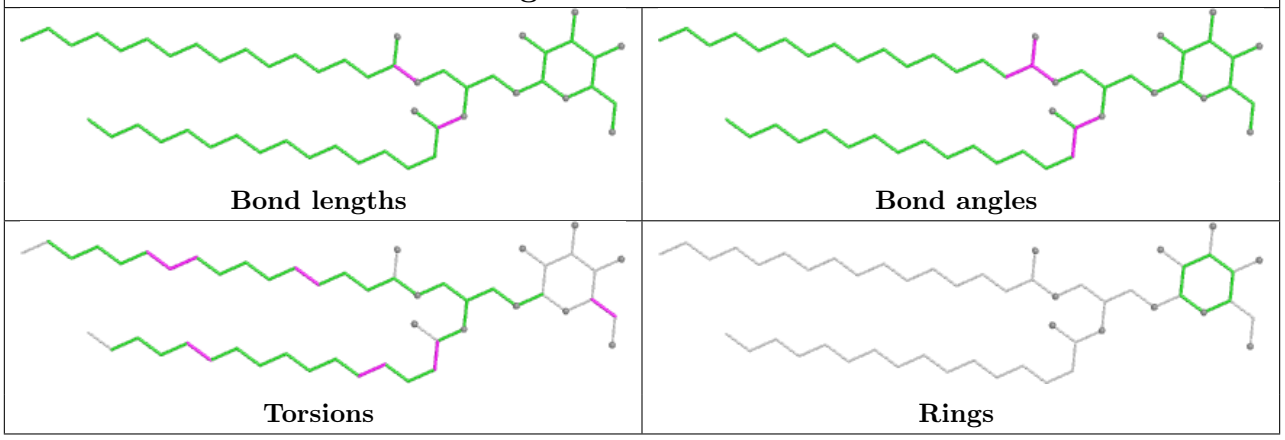
Ligand PL9 D 405 (A)



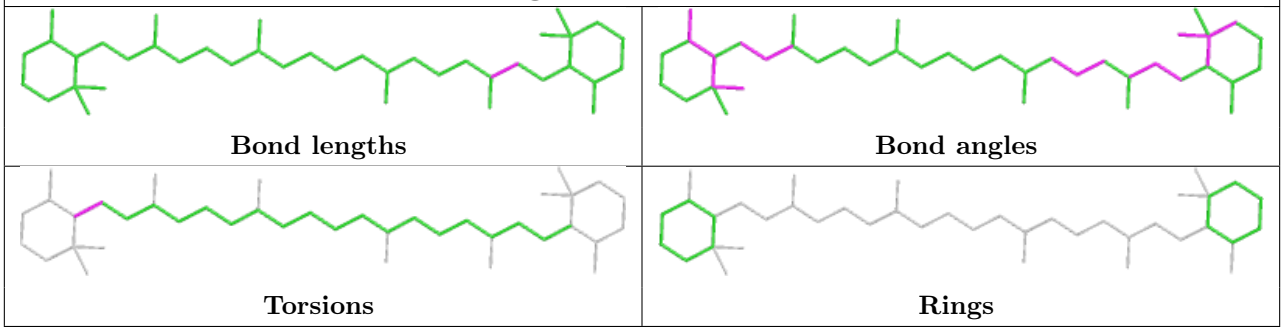
Ligand LMG C 501



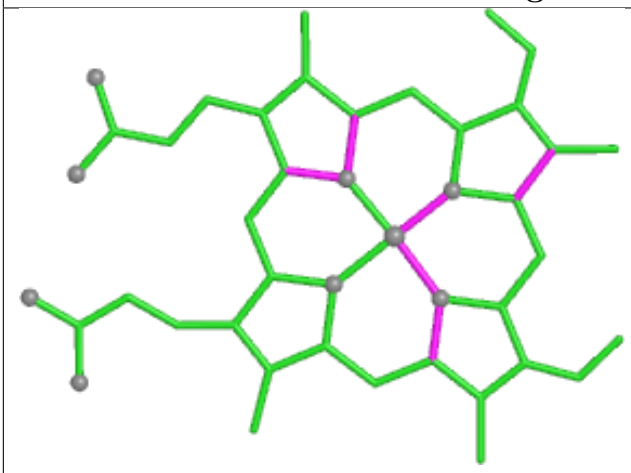
Ligand LMG D 411



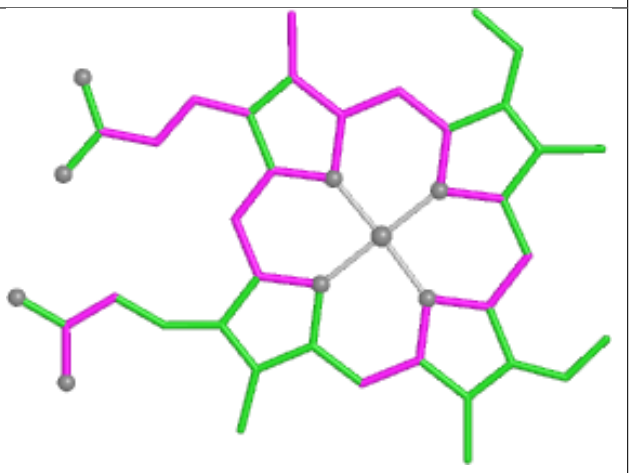
Ligand BCR b 617



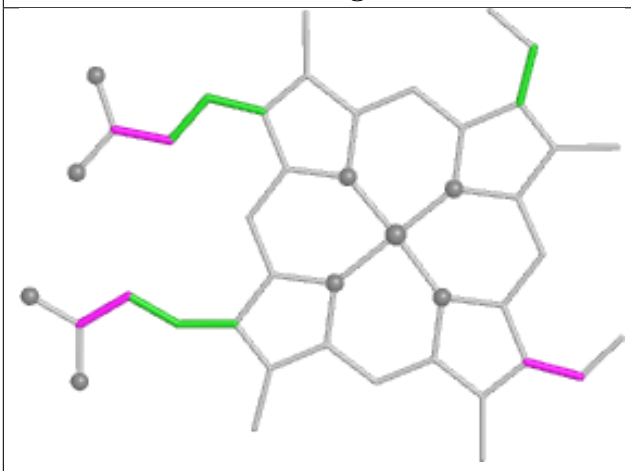
Ligand HEM f 101



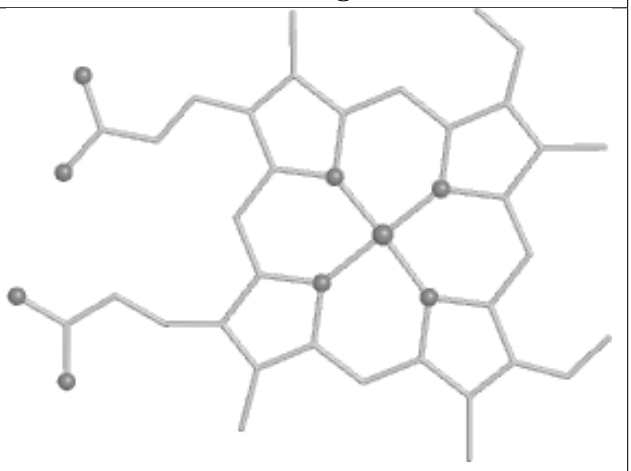
Bond lengths



Bond angles

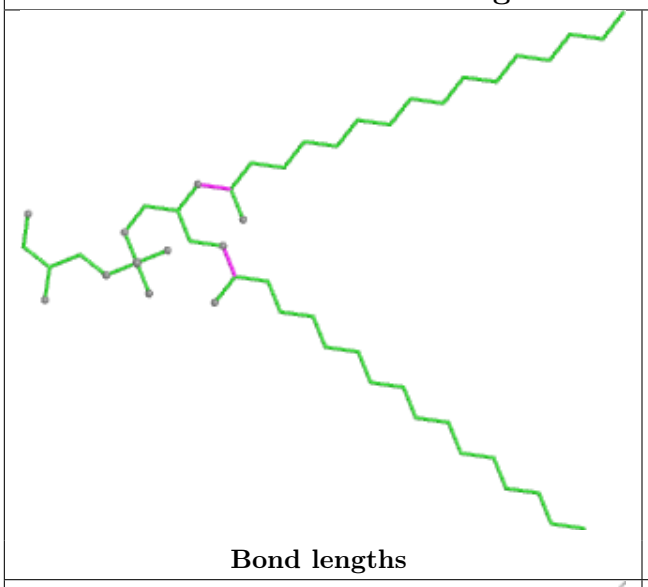


Torsions



Rings

Ligand LHG L 101 (B)



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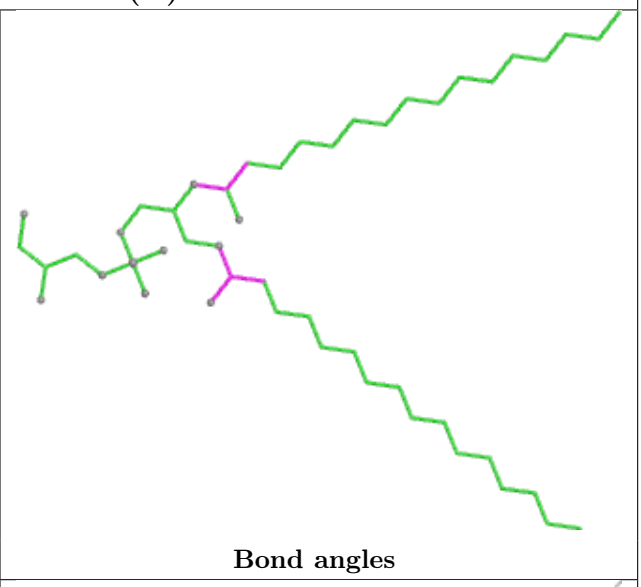
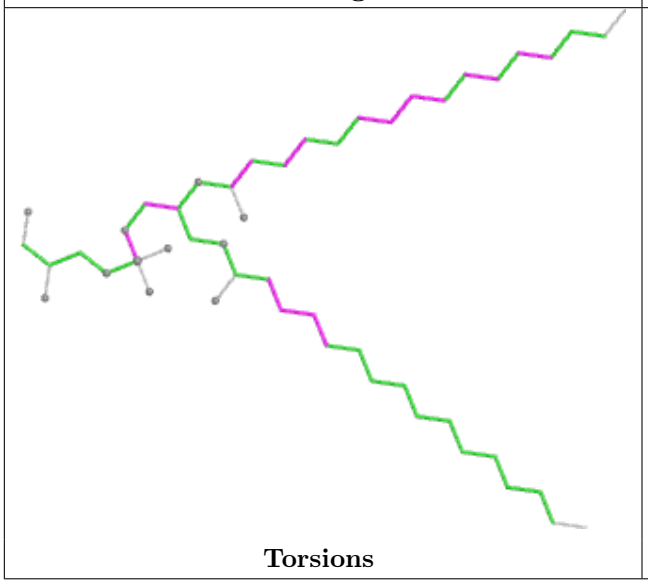


Bond angles



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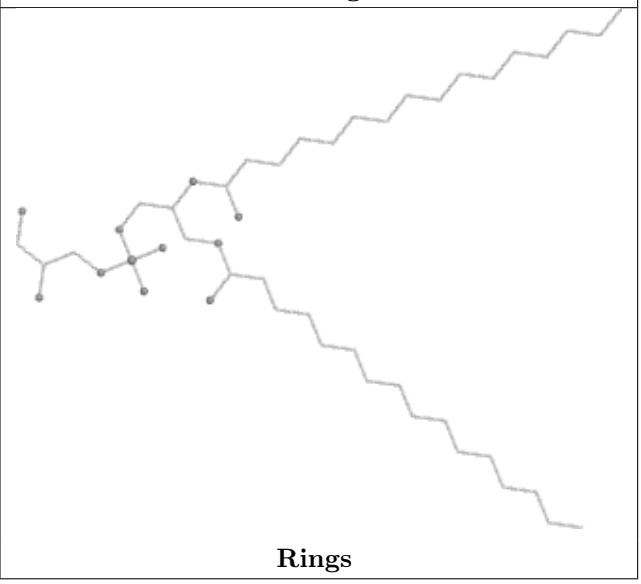
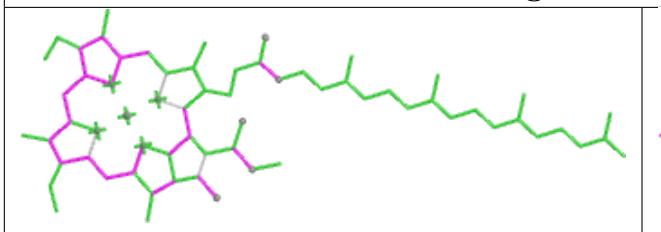
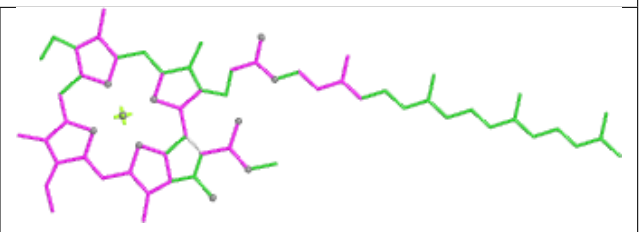


Rings

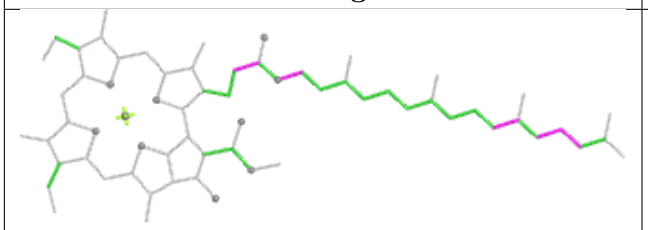
Ligand CLA B 613



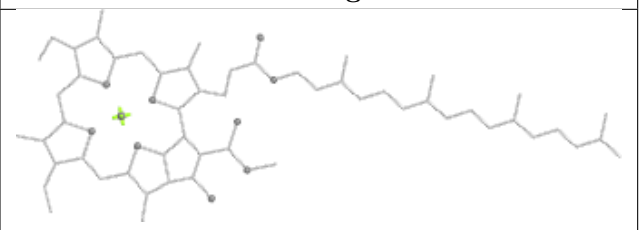
Bond lengths



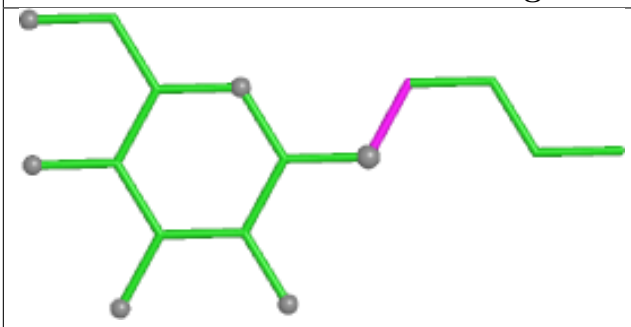
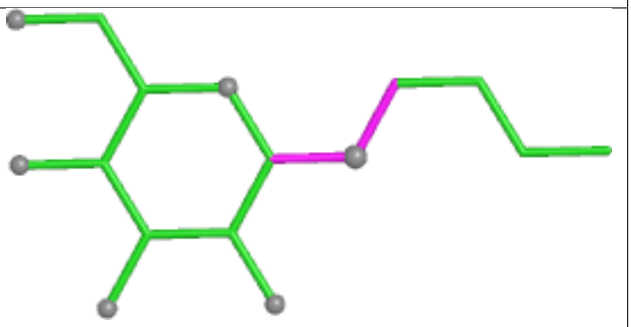
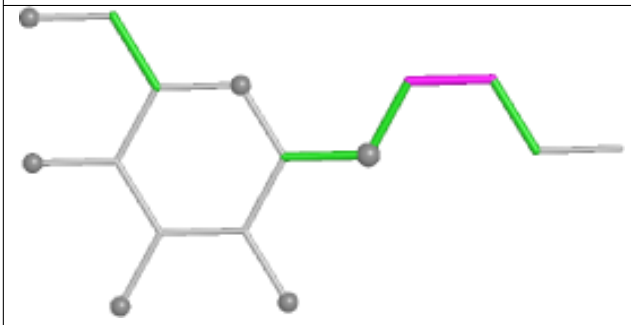
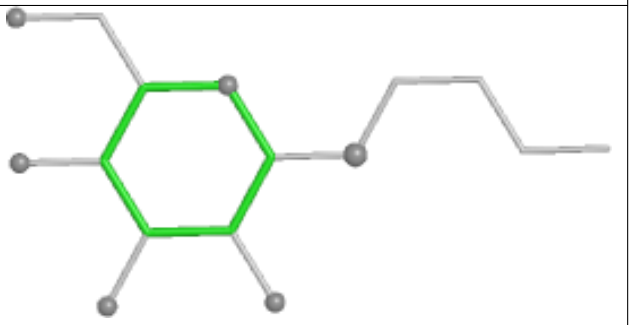
Bond angles

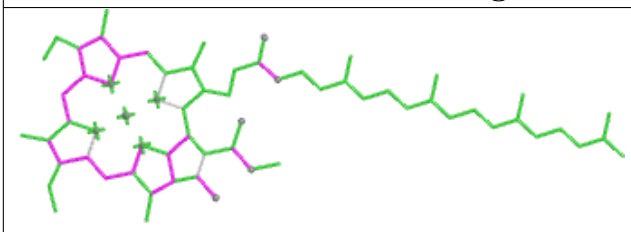
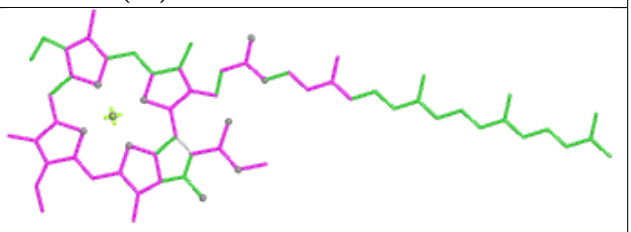
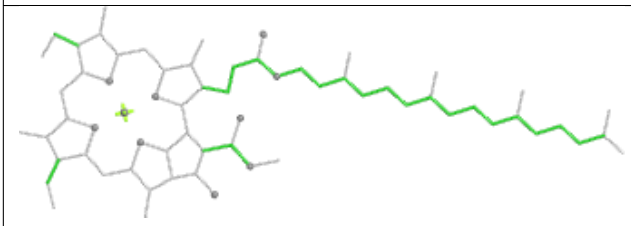
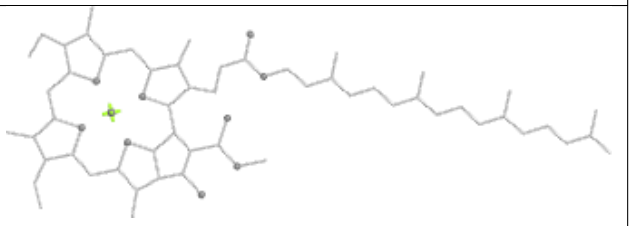


Torsions

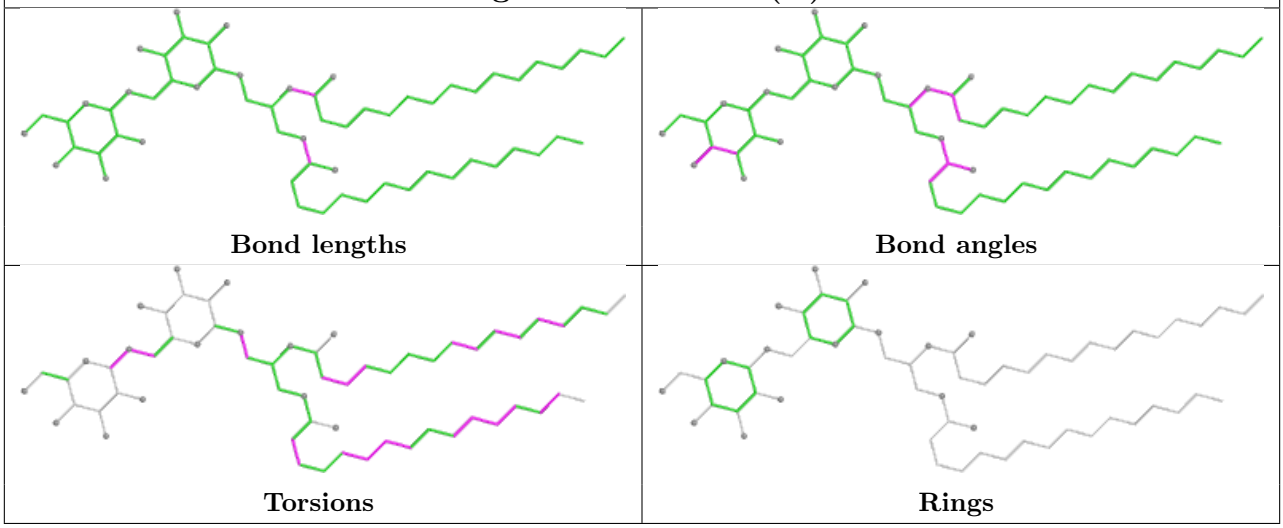


Rings

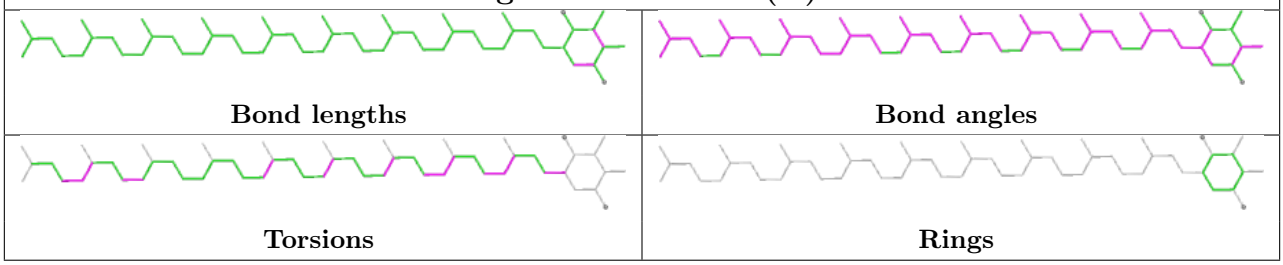
Ligand HTG d 411	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA D 402 (A)	
 Bond lengths	 Bond angles
 Torsions	 Rings

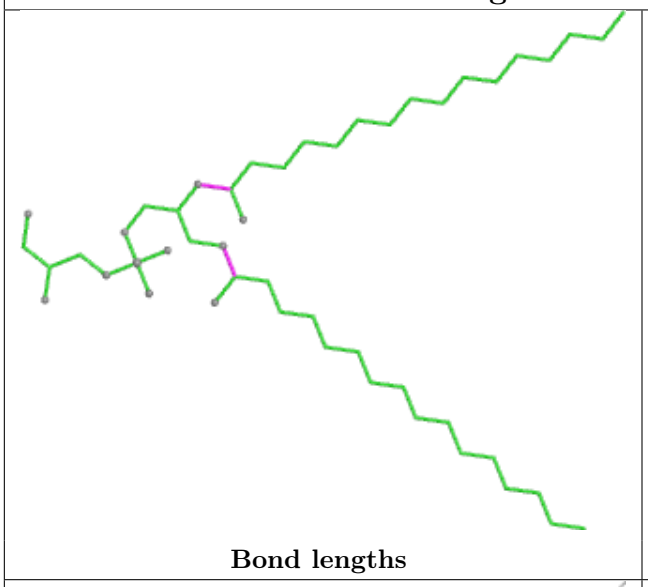
Ligand DGD c 519 (A)



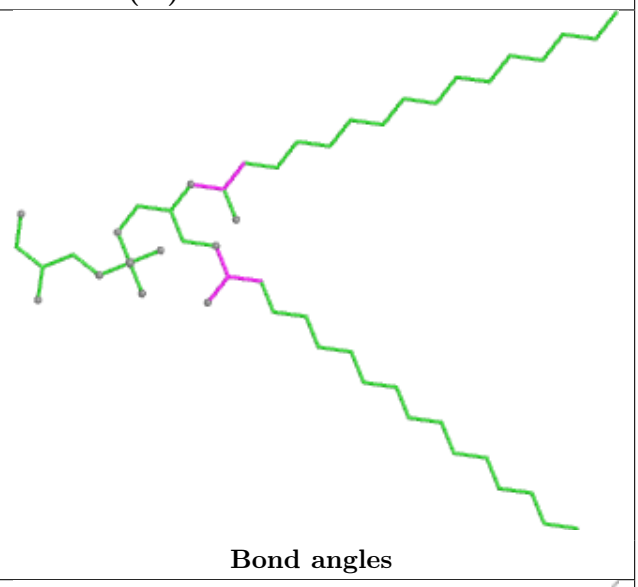
Ligand PL9 A 414 (A)



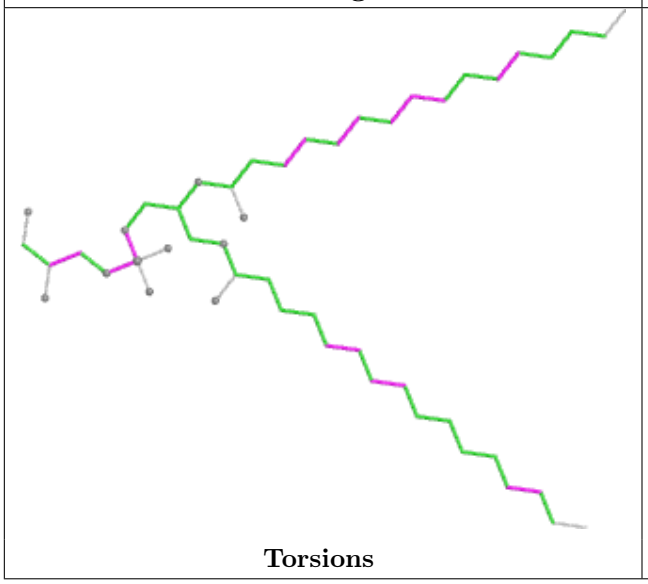
Ligand LHG D 406 (A)



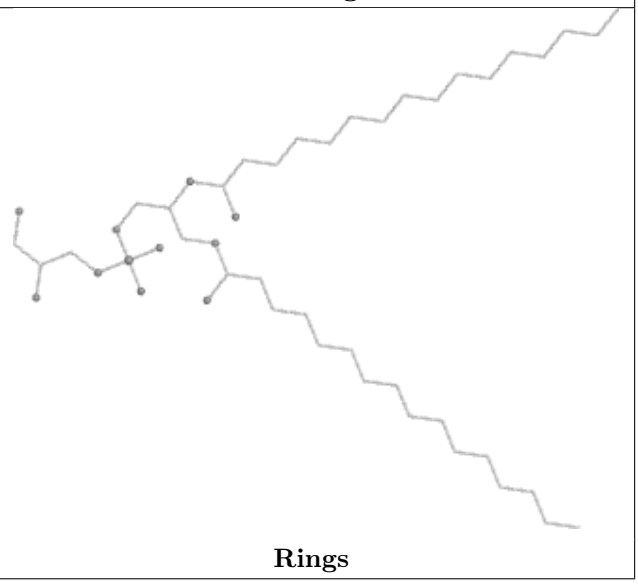
Bond lengths



Bond angles

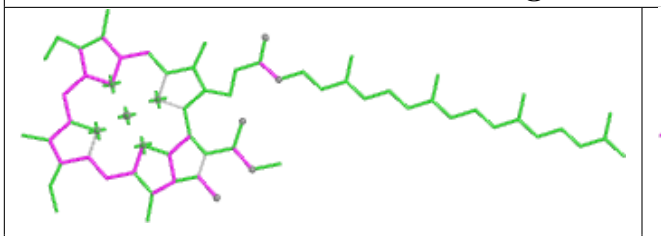


Torsions

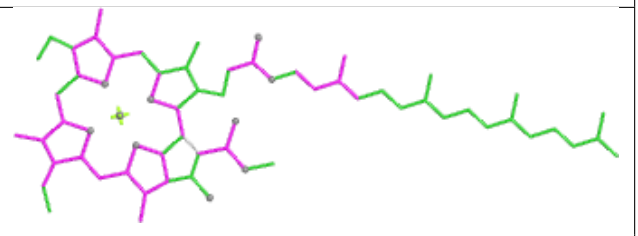


Rings

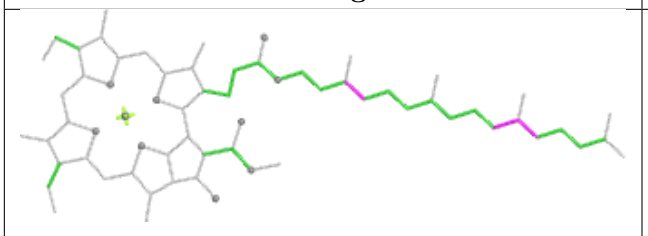
Ligand CLA C 506



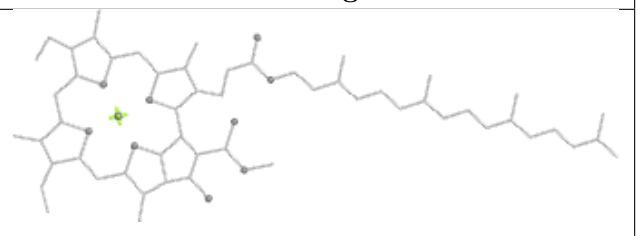
Bond lengths



Bond angles

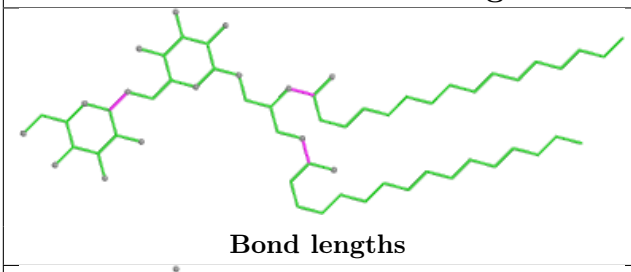


Torsions



Rings

Ligand DGD C 518 (A)



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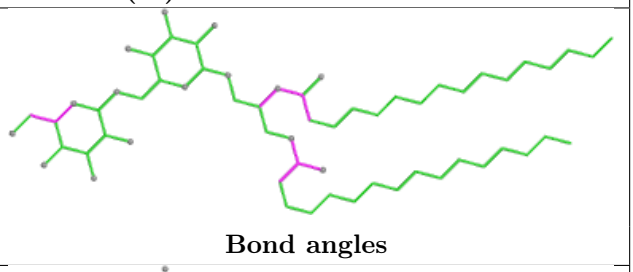
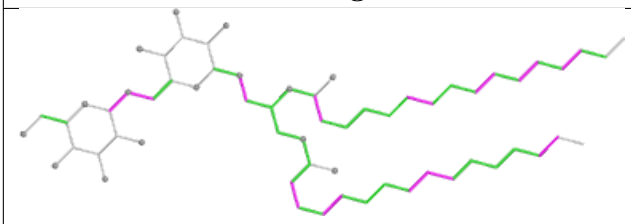


Bond angles



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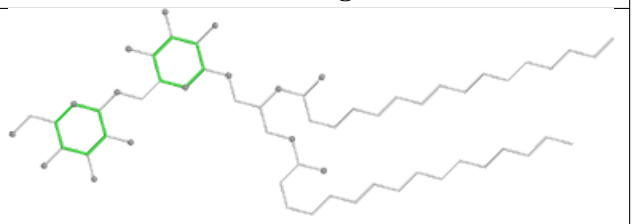
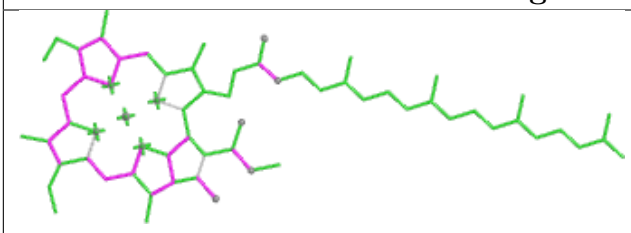
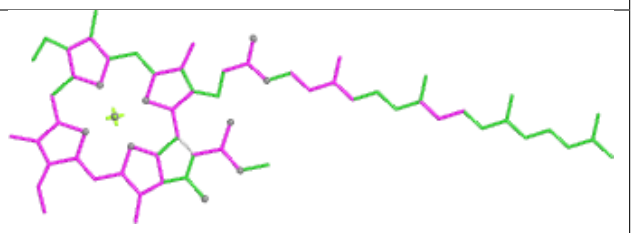


Rings

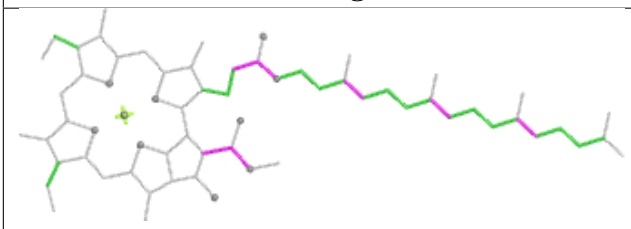
Ligand CLA c 512



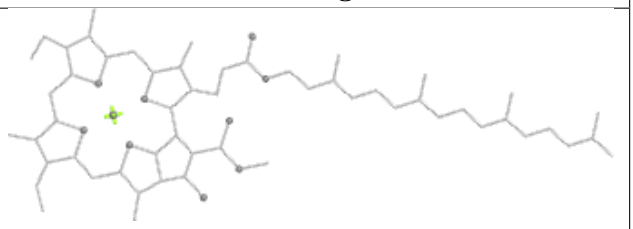
Bond lengths



Bond angles

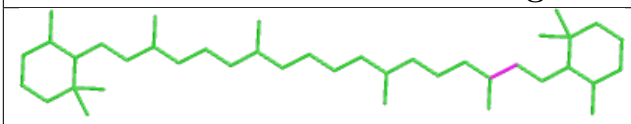


Torsions

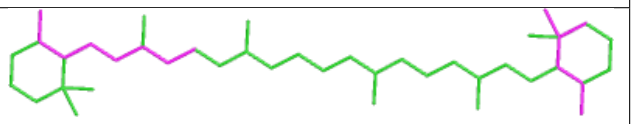


Rings

Ligand BCR a 408



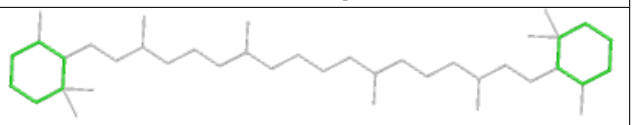
Bond lengths



Bond angles

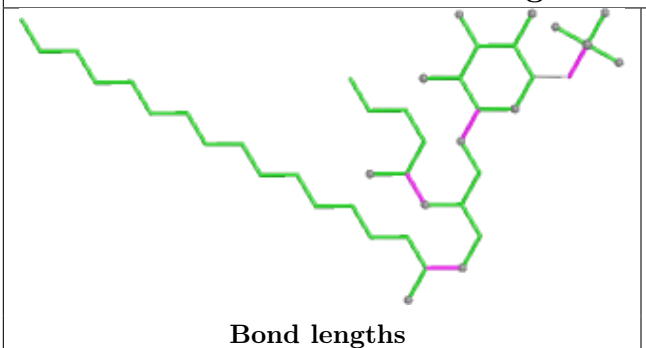


Torsions

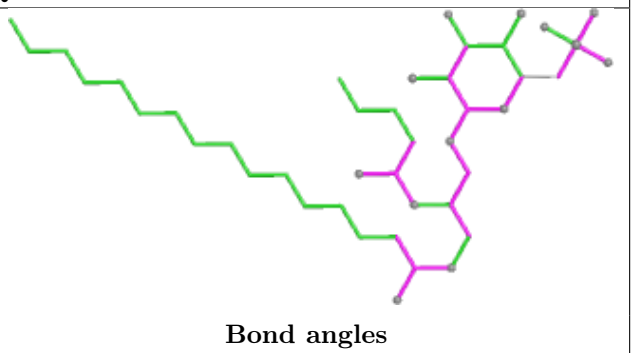


Rings

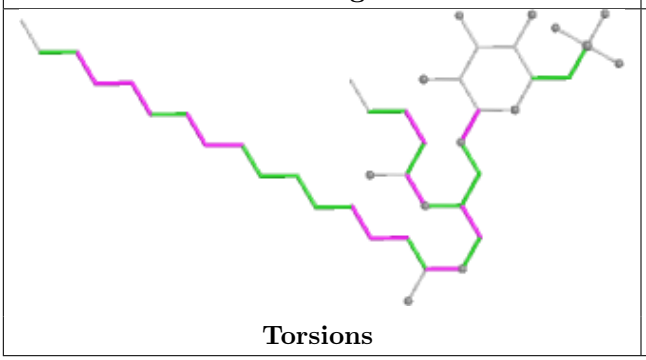
Ligand SQD F 102



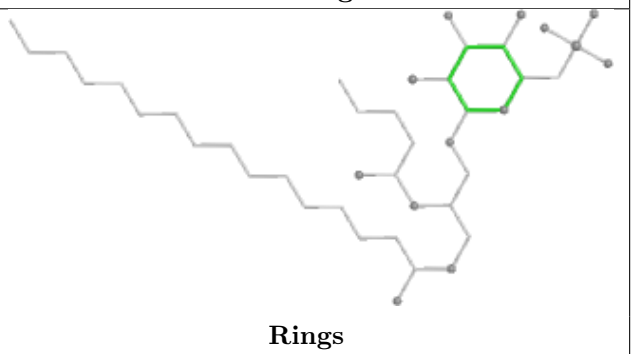
Bond lengths



Bond angles

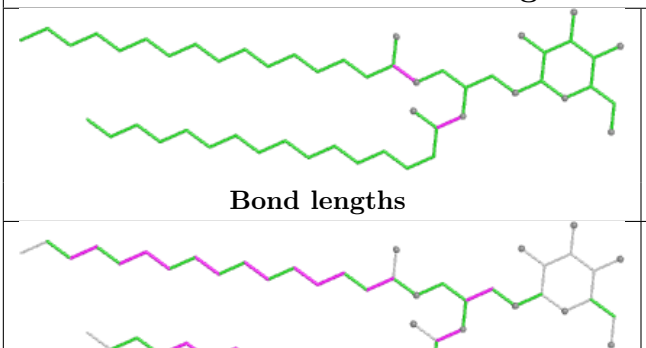


Torsions



Rings

Ligand LMG B 621



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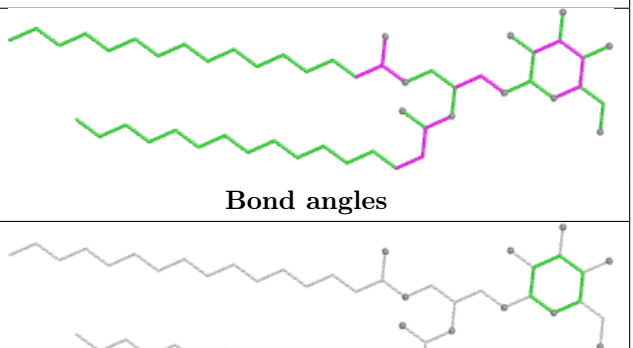
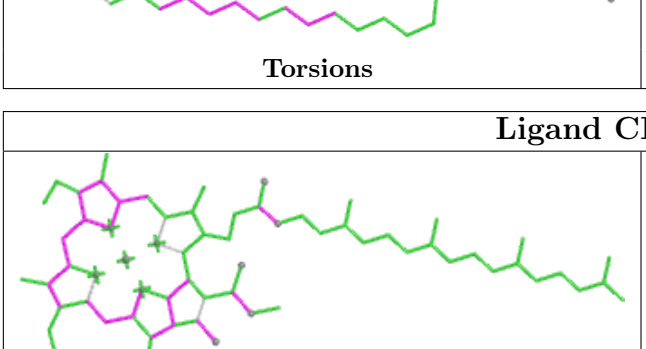


Bond angles



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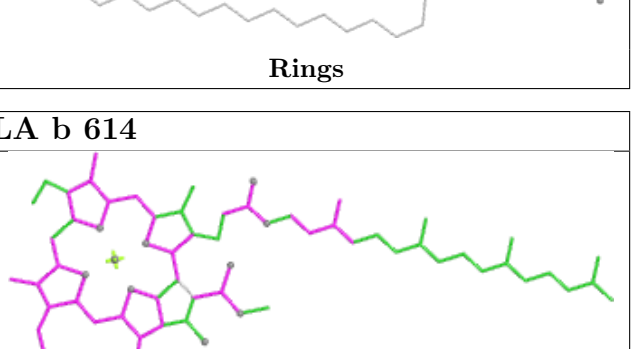
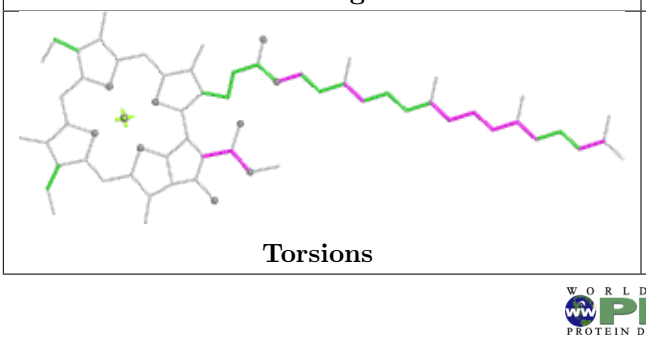


Rings

Ligand CLA b 614

Bond lengths

Bond angles



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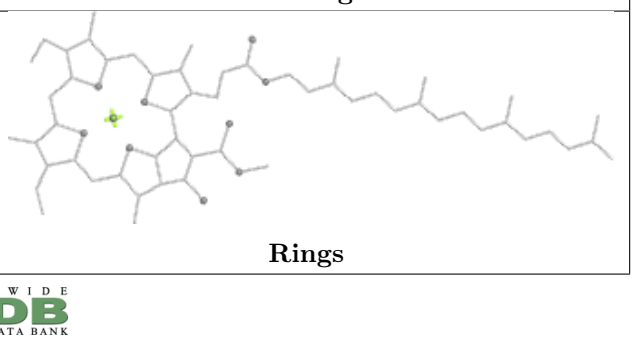
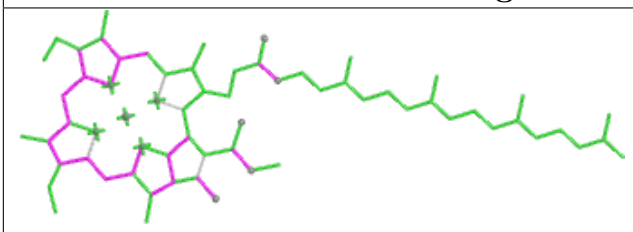


Rings

Ligand CLA a 405 (B)



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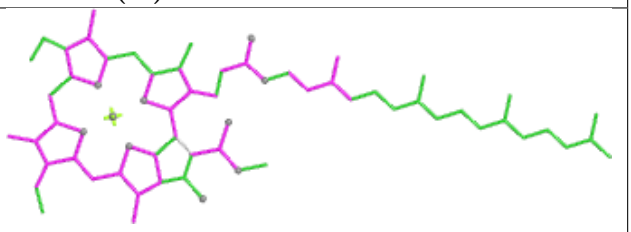
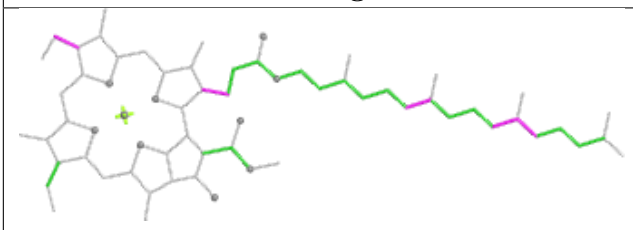


Bond angles



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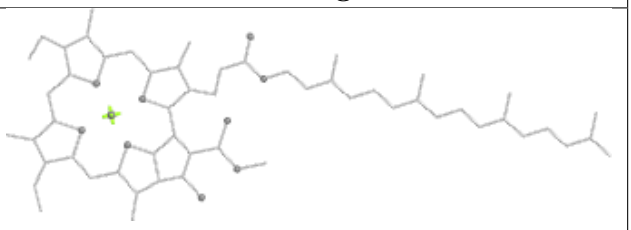
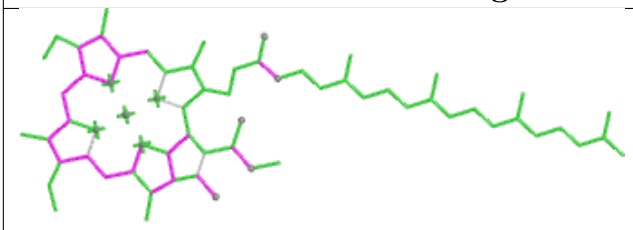


Rings

Ligand CLA A 404 (B)



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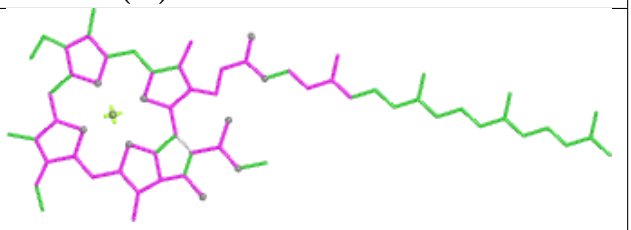
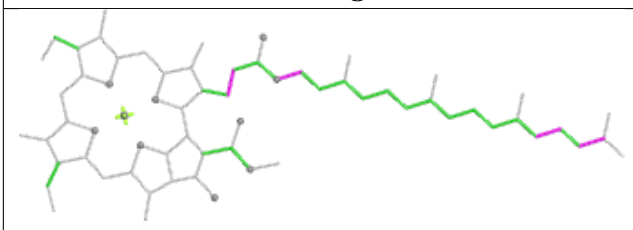


Bond angles



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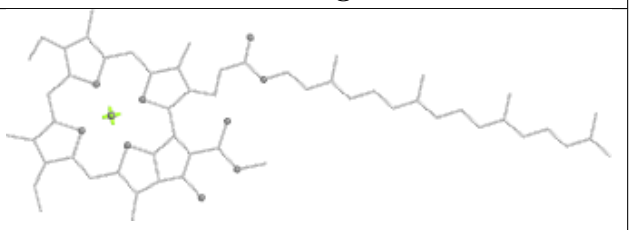
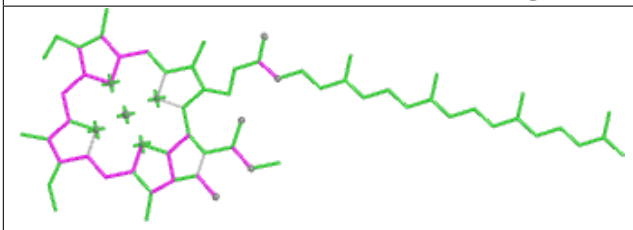


Rings

Ligand CLA C 504



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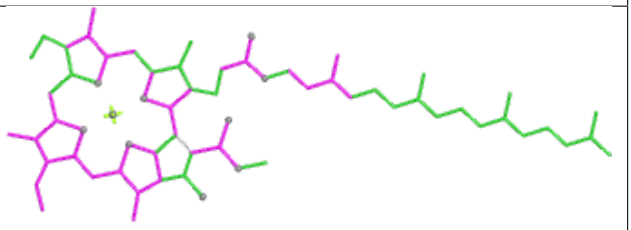

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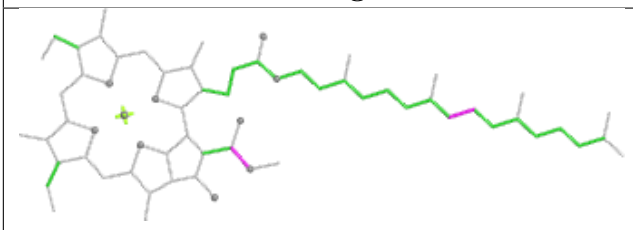

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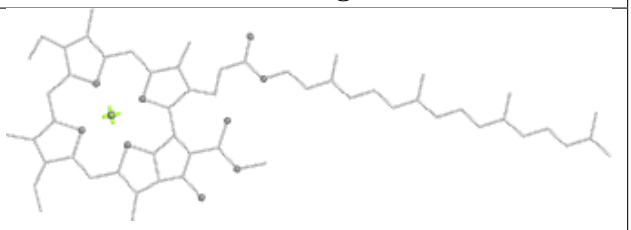
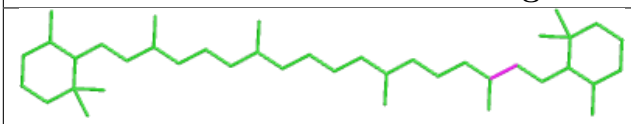
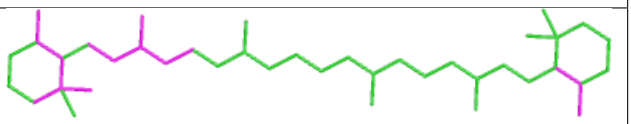
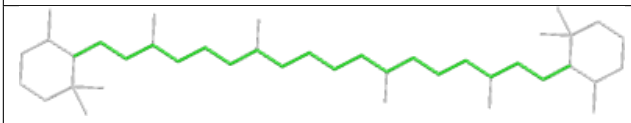
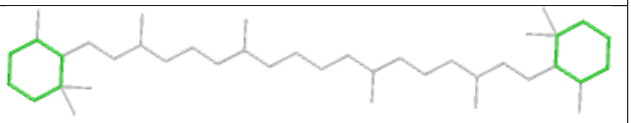


Rings

Ligand BCR C 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

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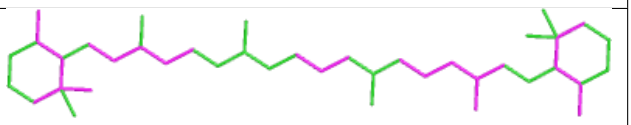
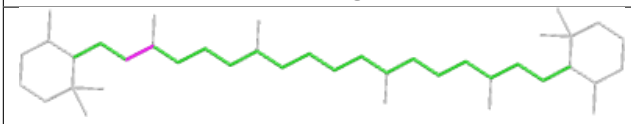
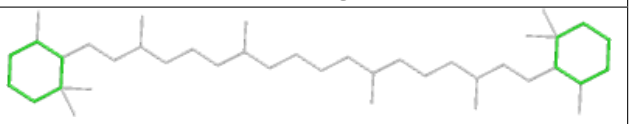
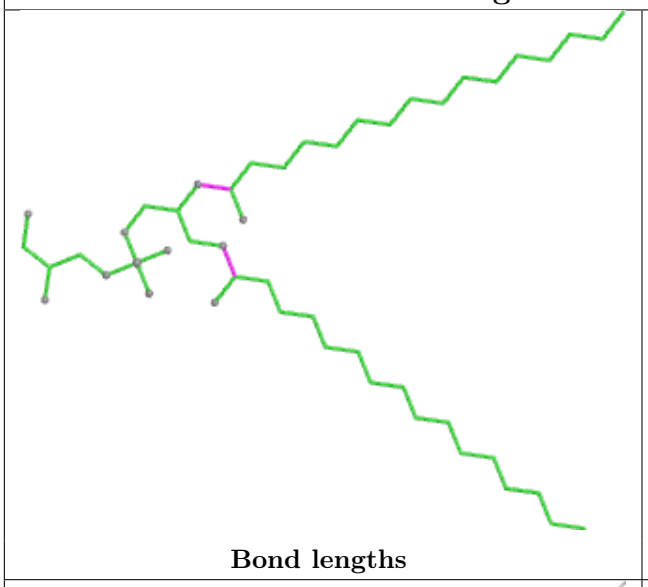
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LHG d 414 (A)



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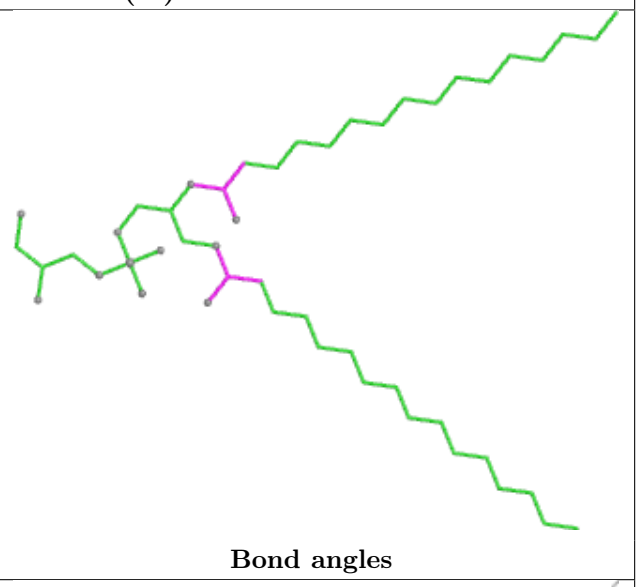
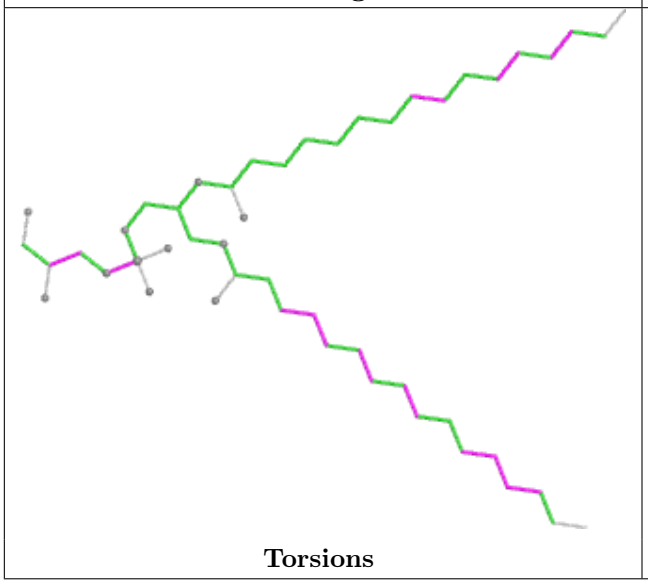
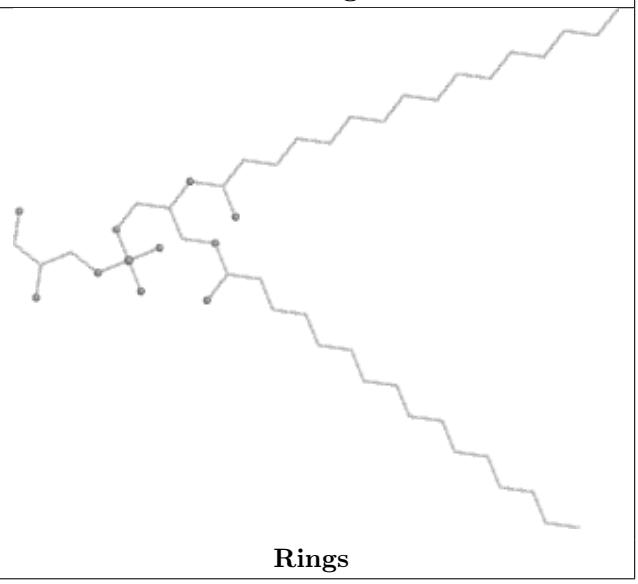


Bond angles

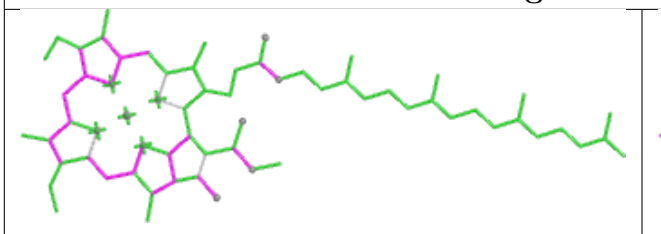


Torsions



Rings

Ligand CLA B 614



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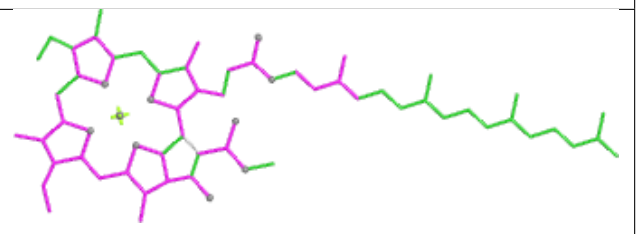
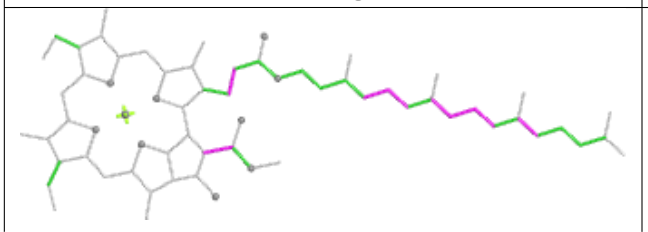


Bond angles



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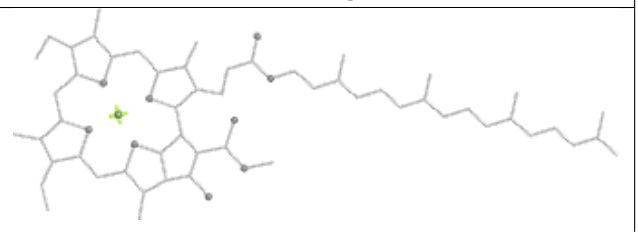
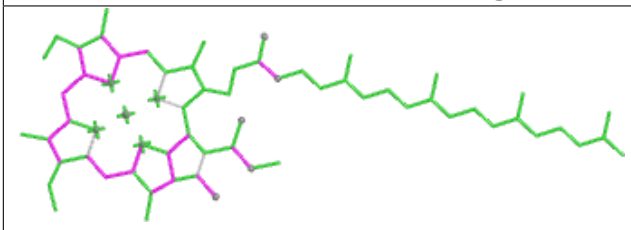


Rings

Ligand CLA A 405 (A)



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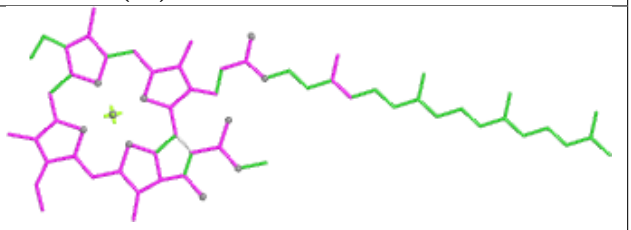
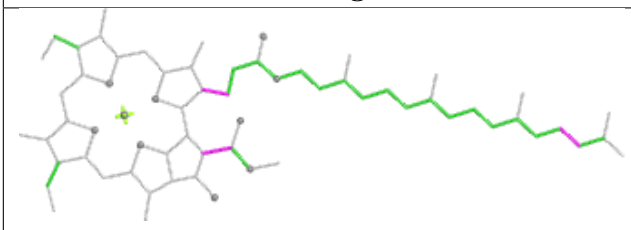


Bond angles



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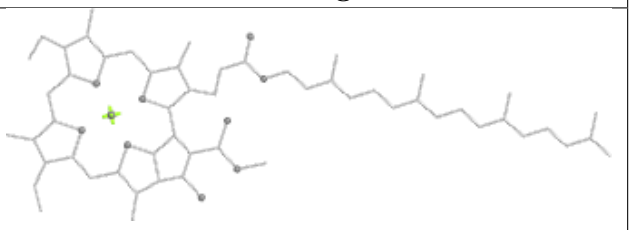
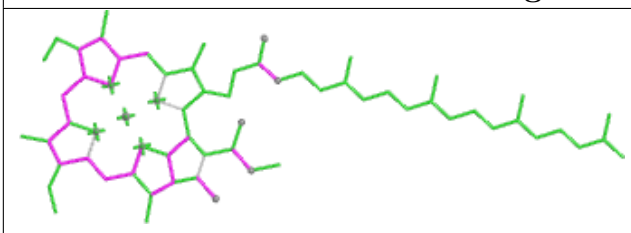


Rings

Ligand CLA B 603



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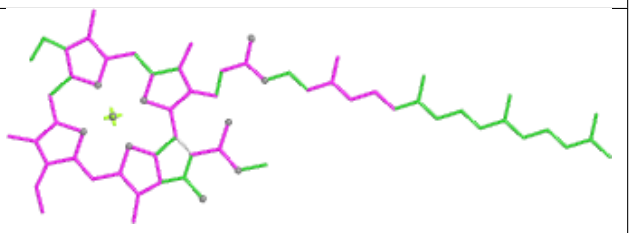
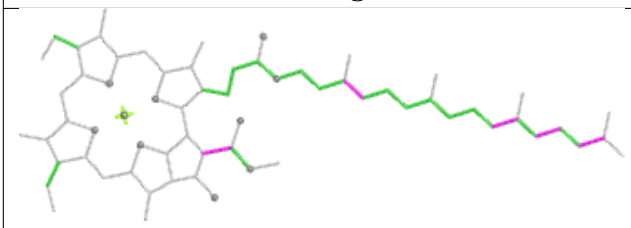


Bond angles



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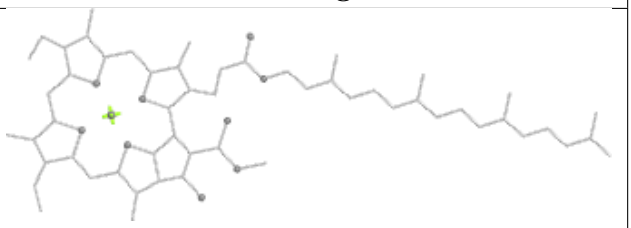
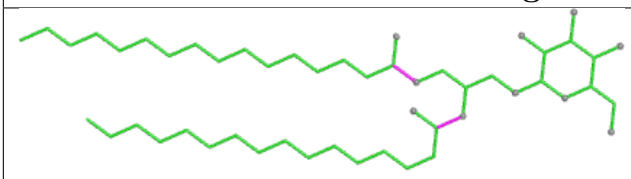


Rings

Ligand LMG d 412



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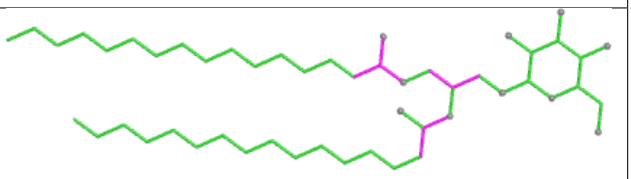
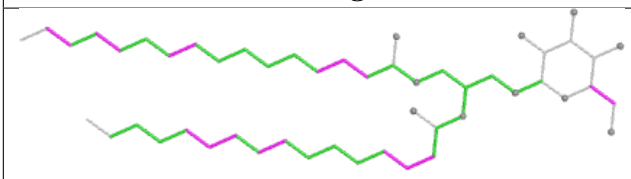


Bond angles



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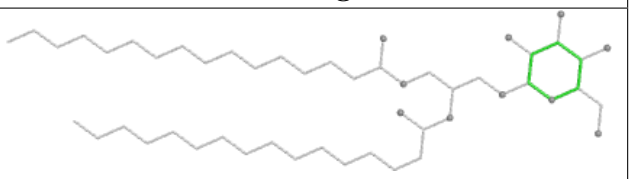
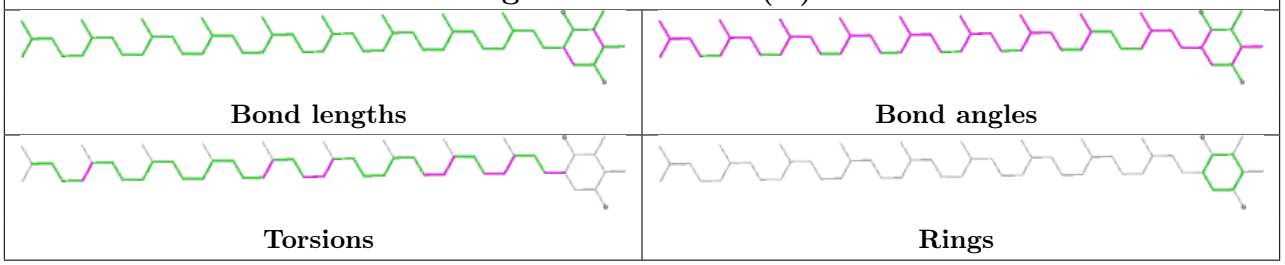
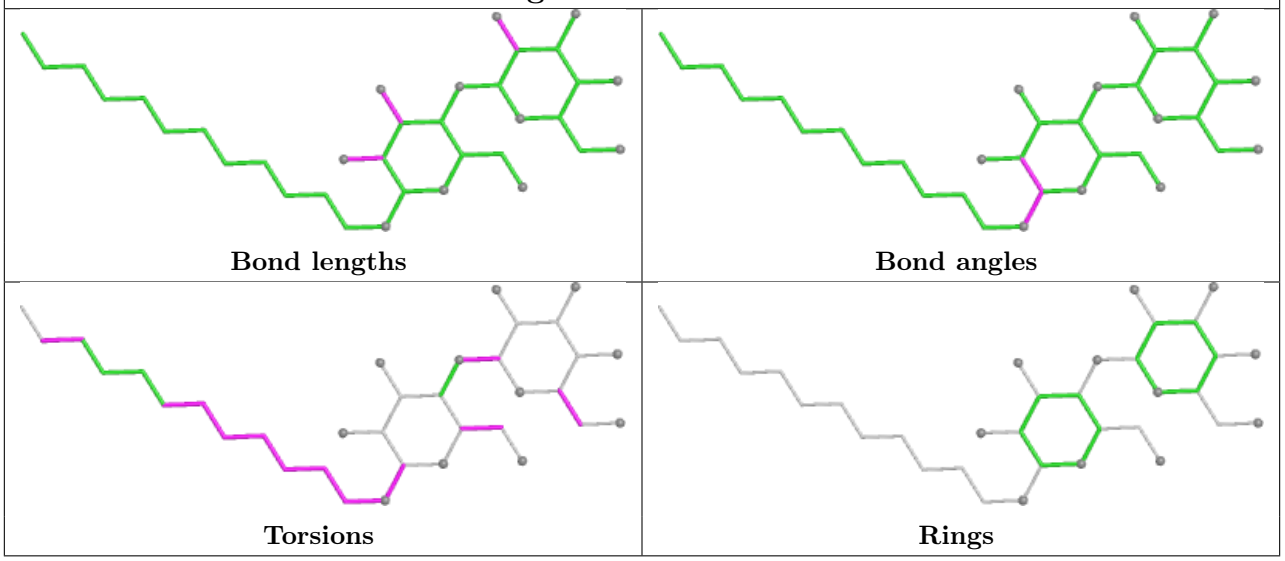


Rings

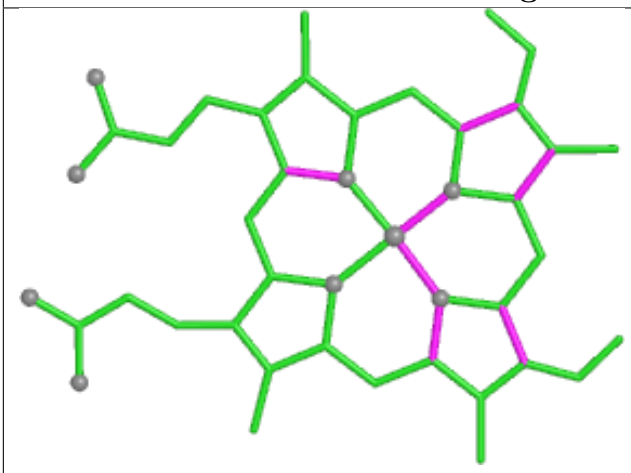
Ligand PL9 a 412 (B)



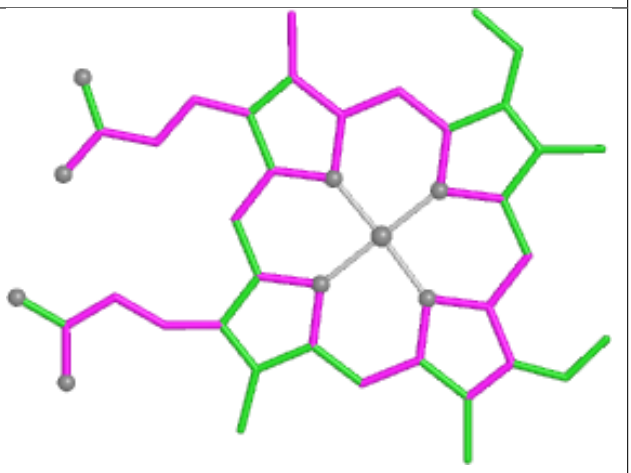
Ligand LMT e 101



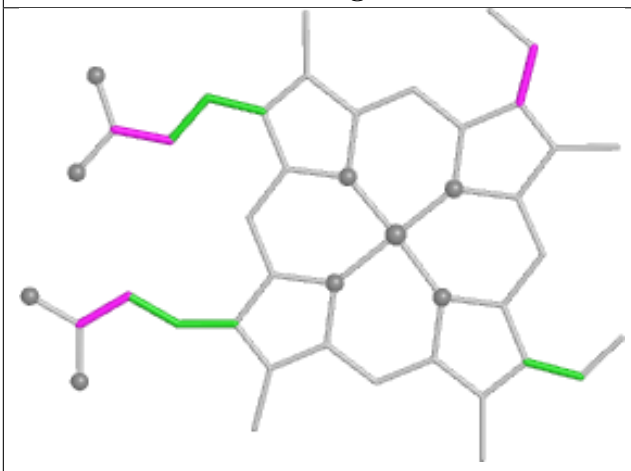
Ligand HEM E 102



Bond lengths



Bond angles



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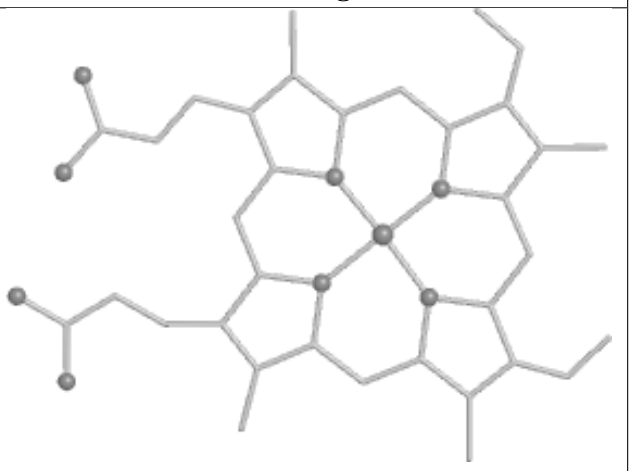
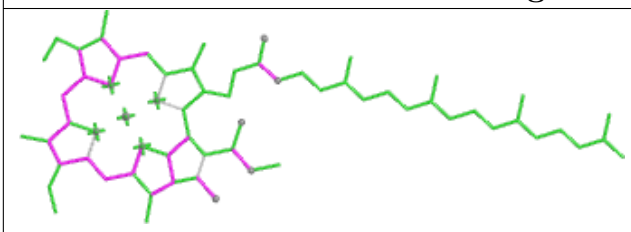
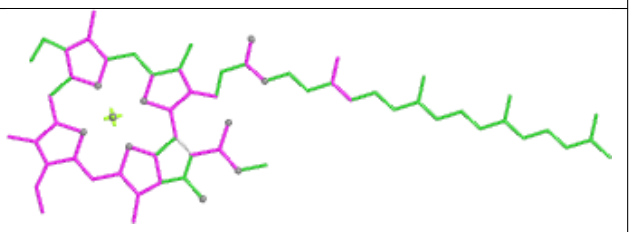


Rings

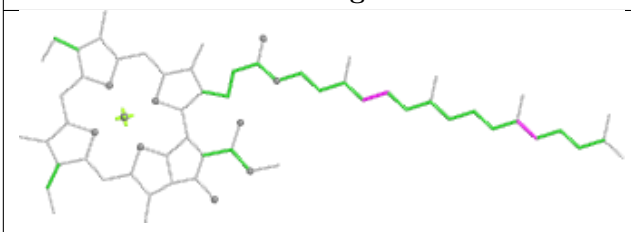
Ligand CLA b 607



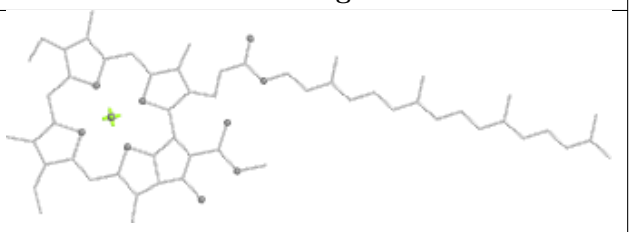
Bond lengths



Bond angles

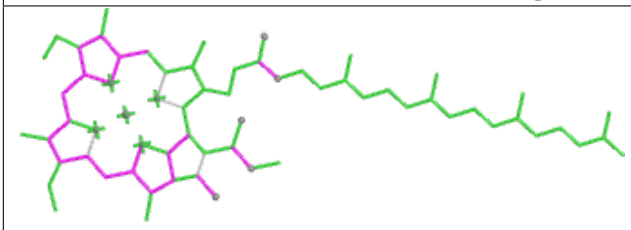


Torsions

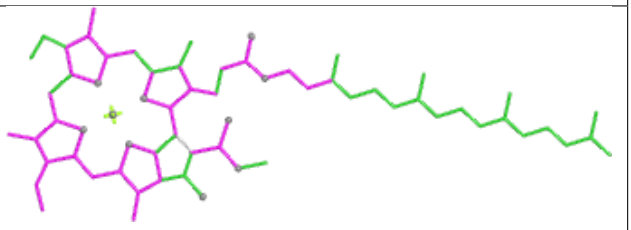


Rings

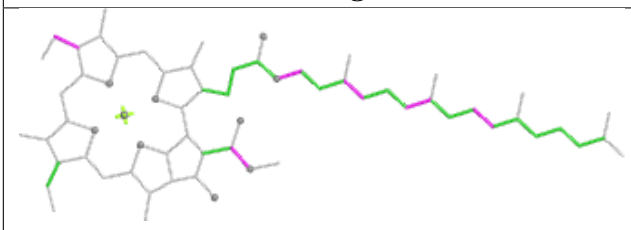
Ligand CLA c 515



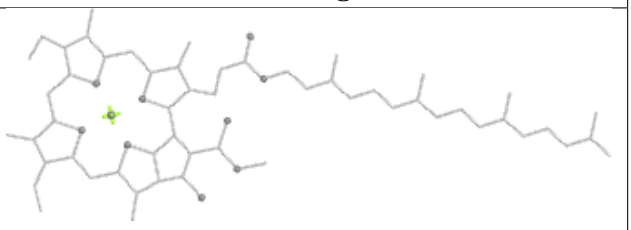
Bond lengths



Bond angles

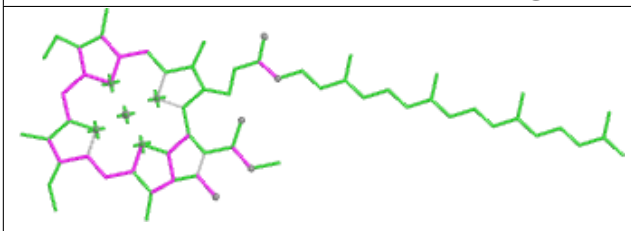


Torsions



Rings

Ligand CLA b 615



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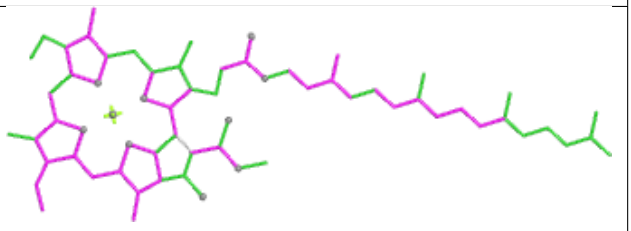
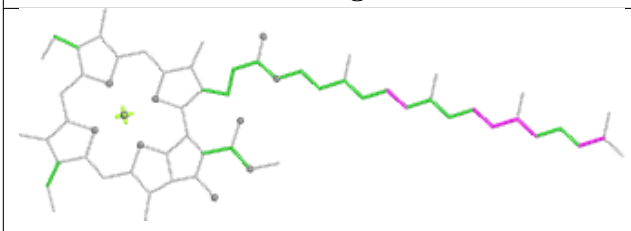


Bond angles



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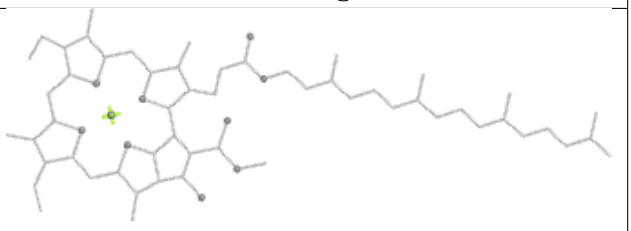
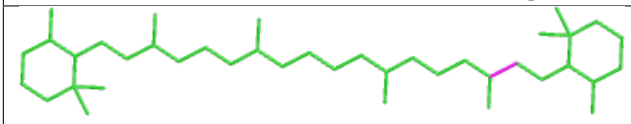


Rings

Ligand BCR C 515



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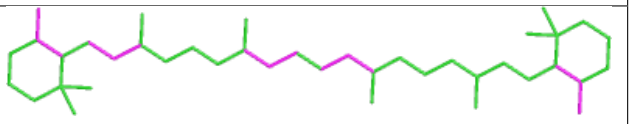
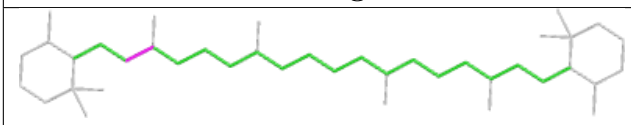


Bond angles



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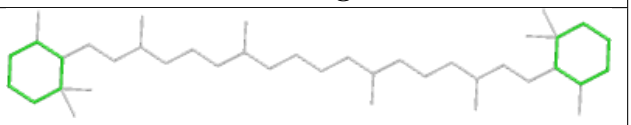
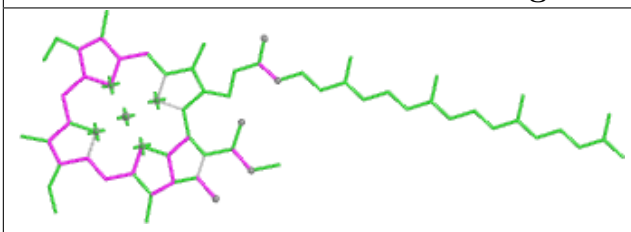


Rings

Ligand CLA c 508



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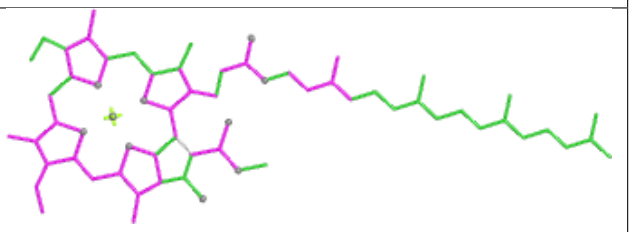
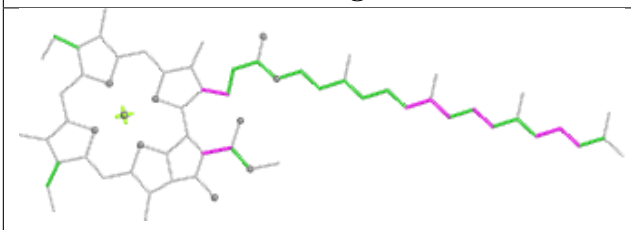


Bond angles



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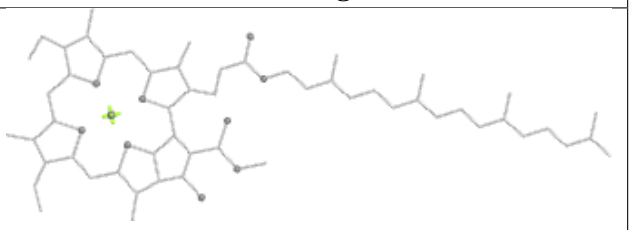
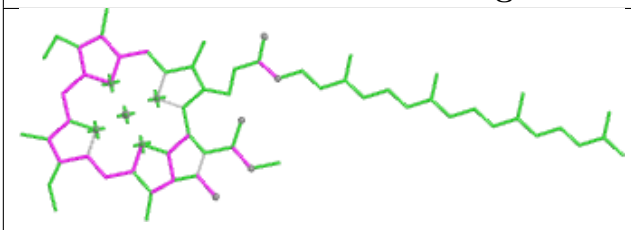


Rings

Ligand CLA a 404 (B)



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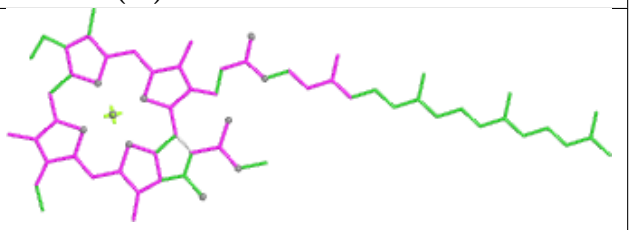
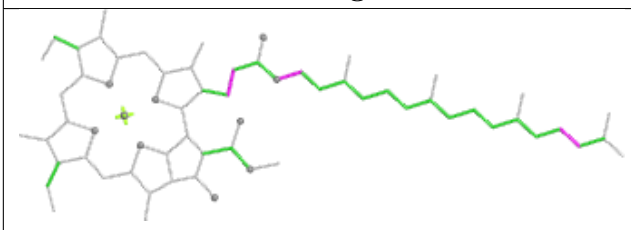


Bond angles



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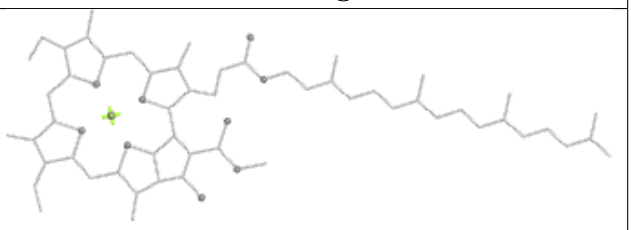
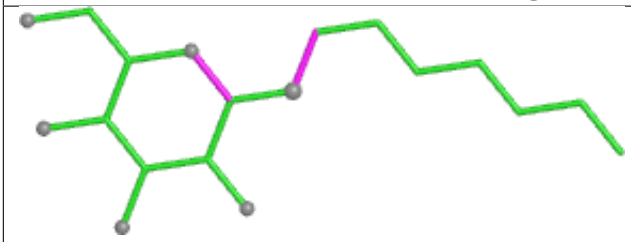


Rings

Ligand HTG o 301



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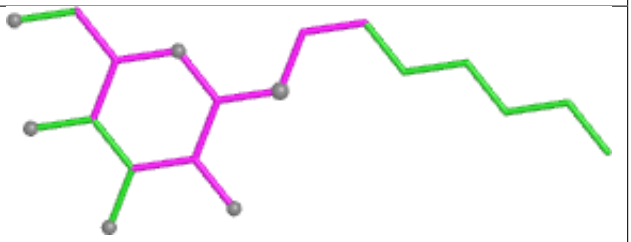
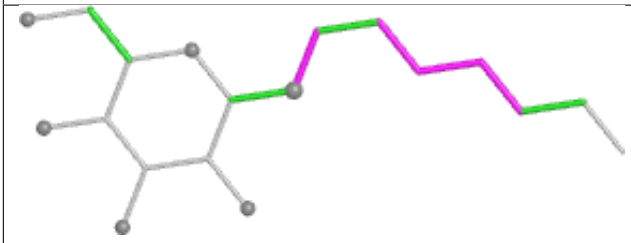


Bond angles



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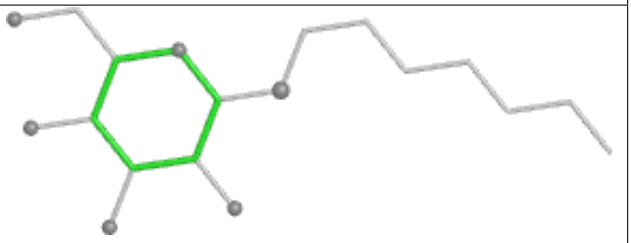
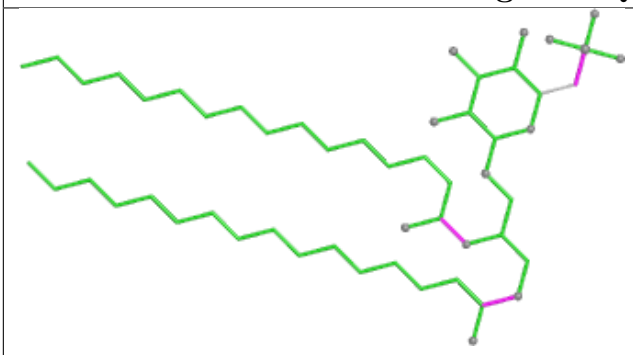


Rings

Ligand SQD a 409 (B)



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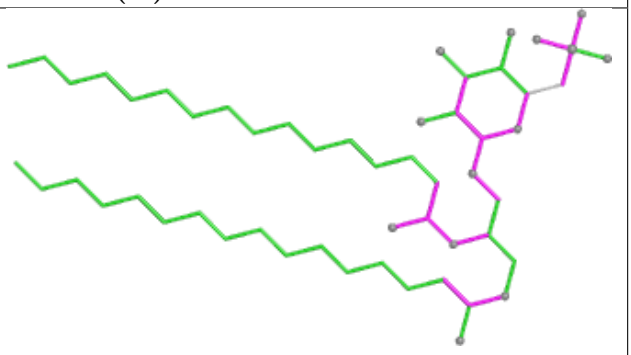
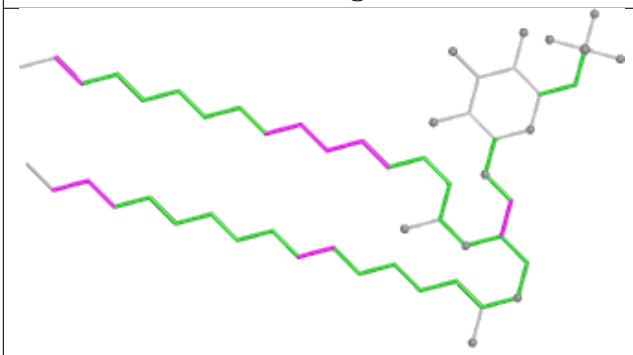


Bond angles



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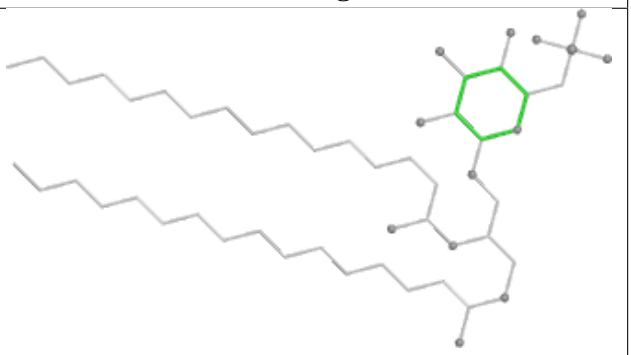
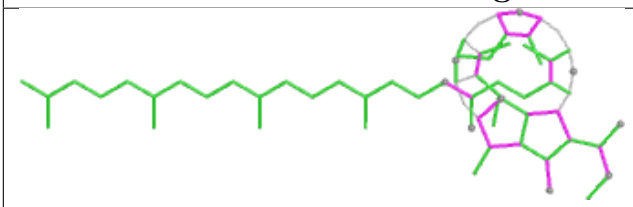


Rings

Ligand PHO a 414 (B)



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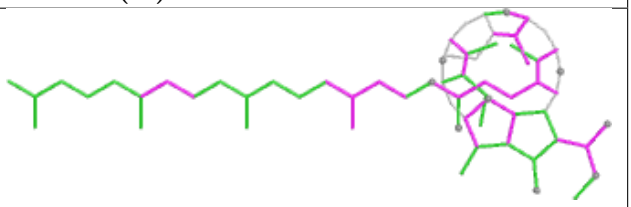
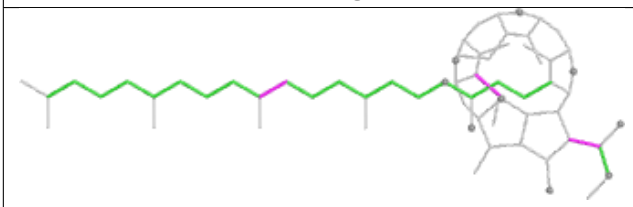


Bond angles



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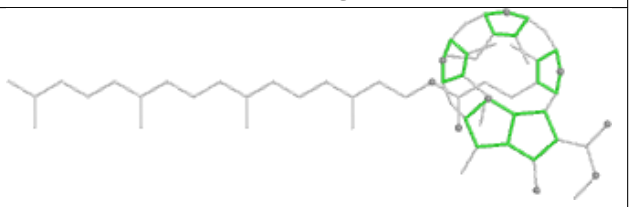
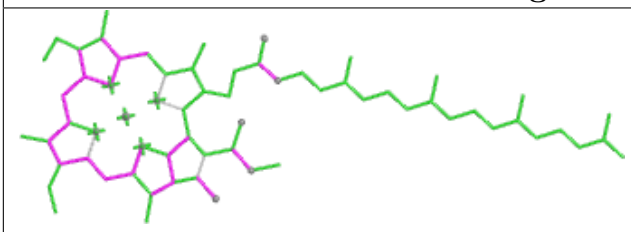


Rings

Ligand CLA c 505



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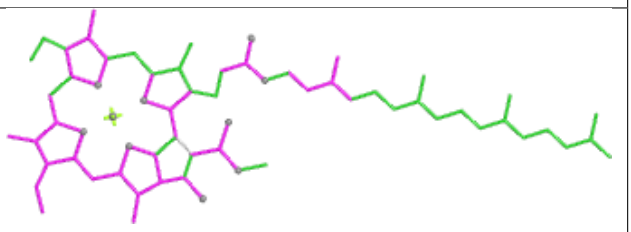
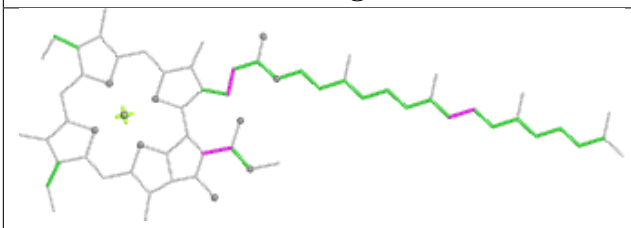


Bond angles



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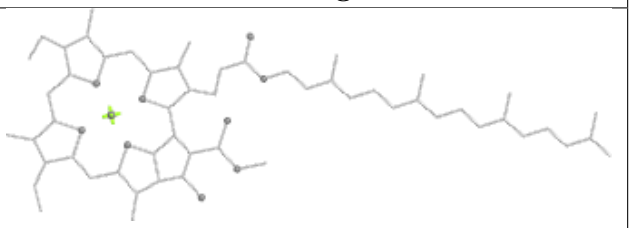
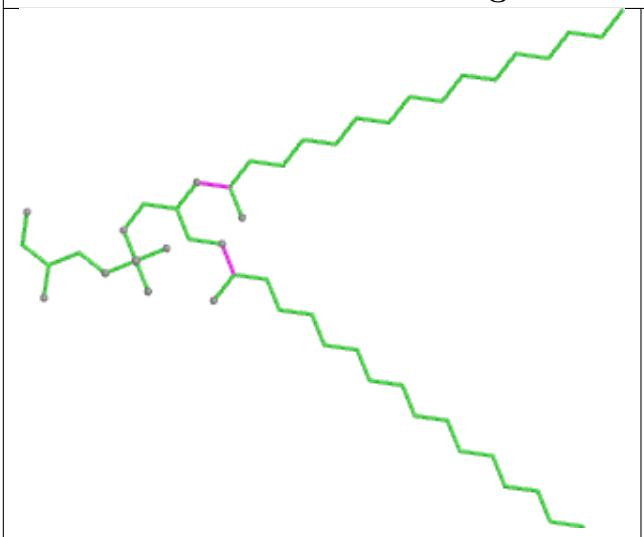


Rings

Ligand LHG A 419 (B)



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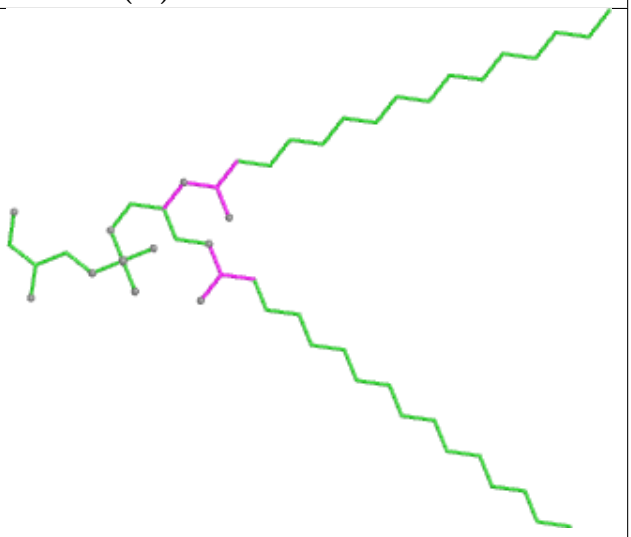
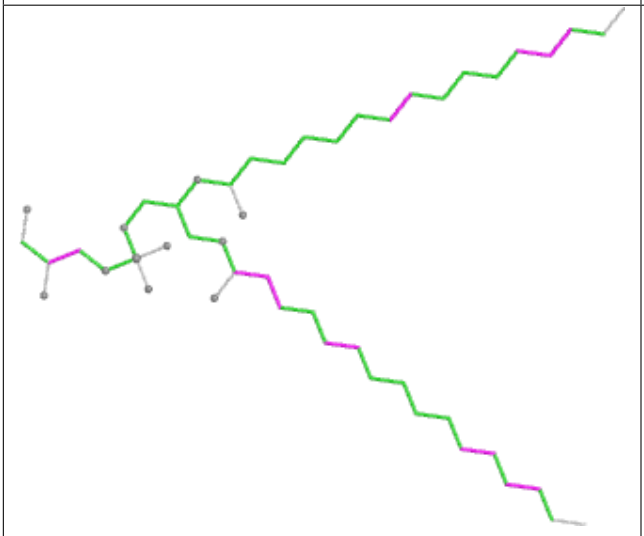


Bond angles



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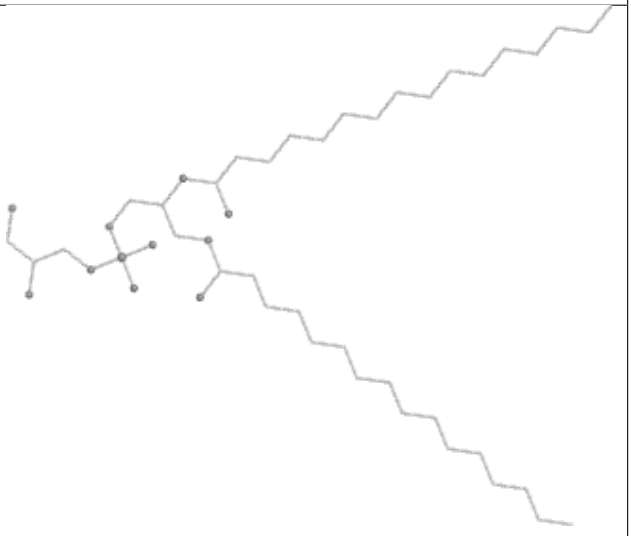
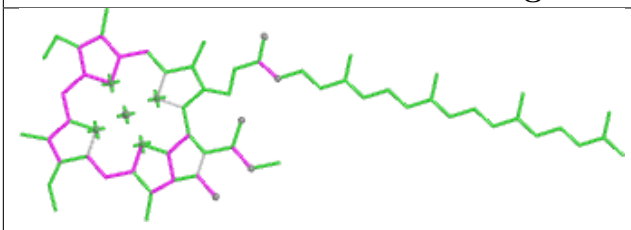


Rings

Ligand CLA B 612



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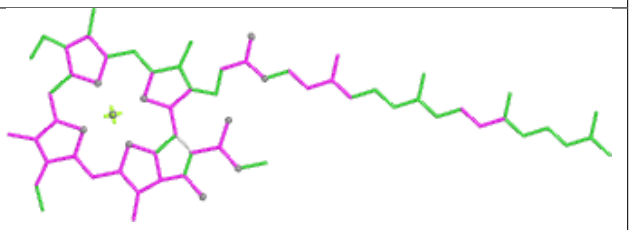
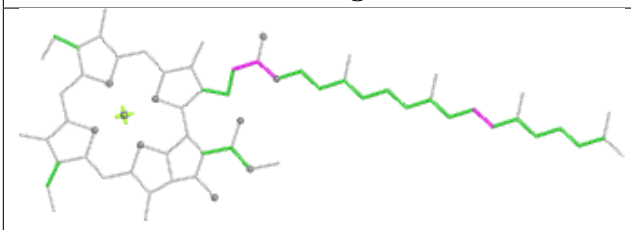


Bond angles



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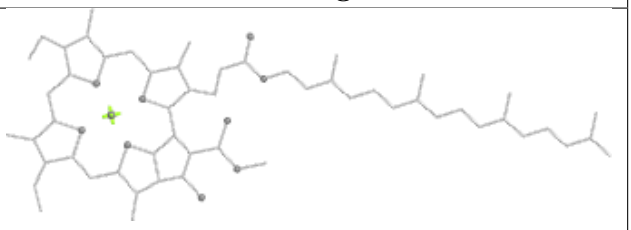
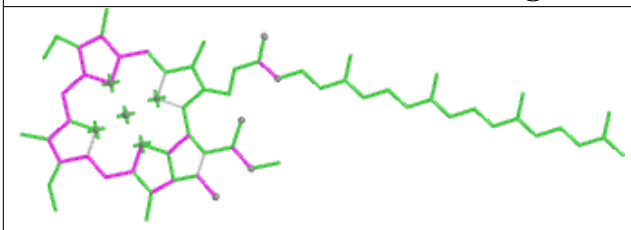


Rings

Ligand CLA C 510



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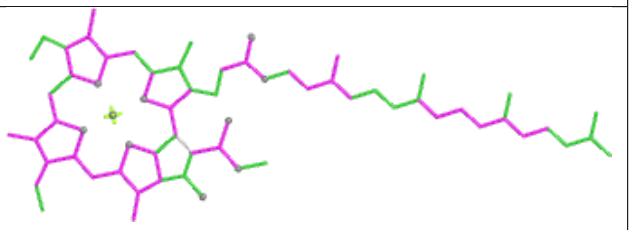
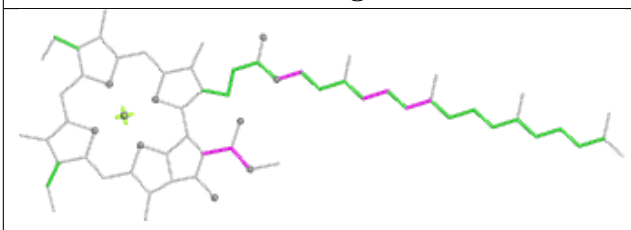


Bond angles



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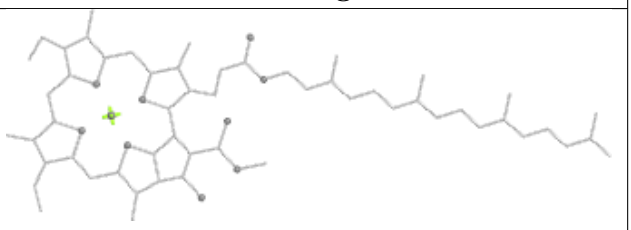
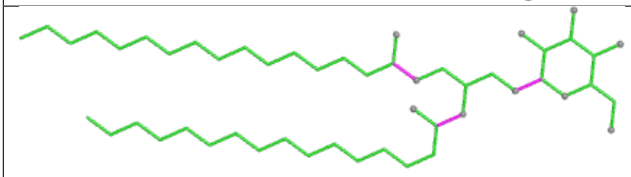
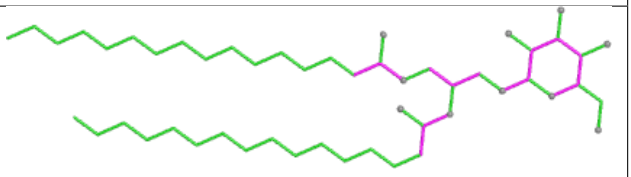


Rings

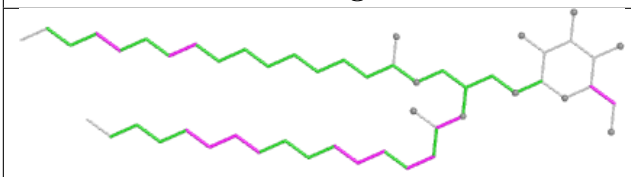
Ligand LMG C 521



Bond lengths



Bond angles



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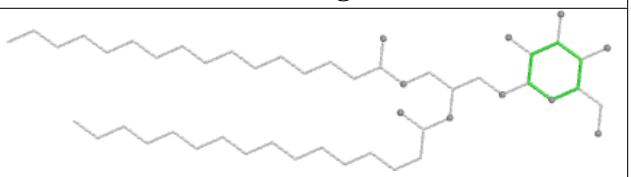
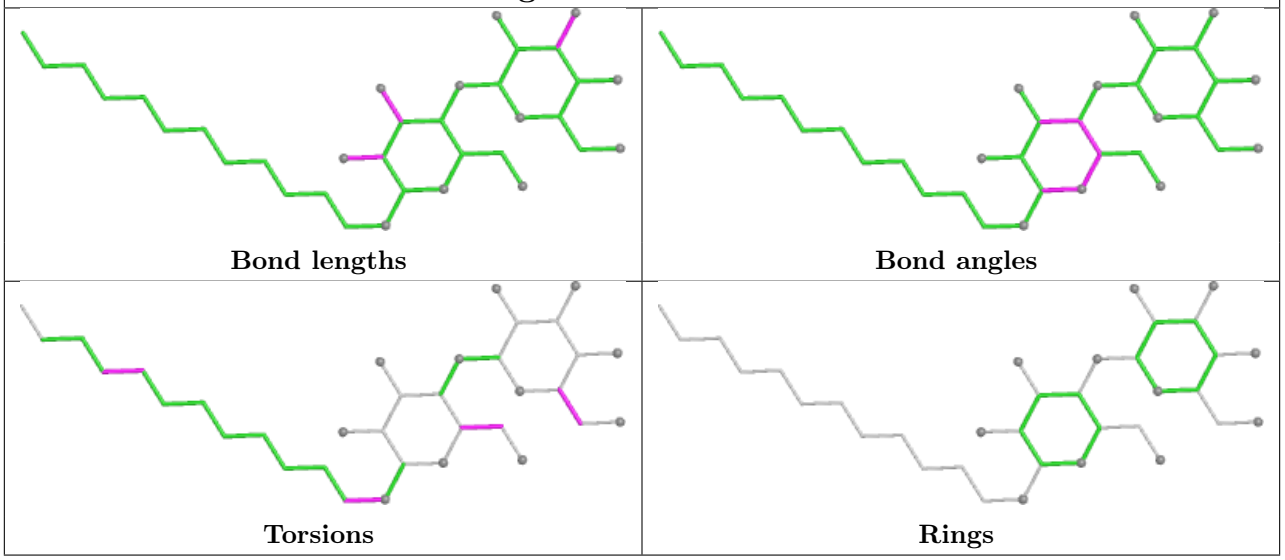
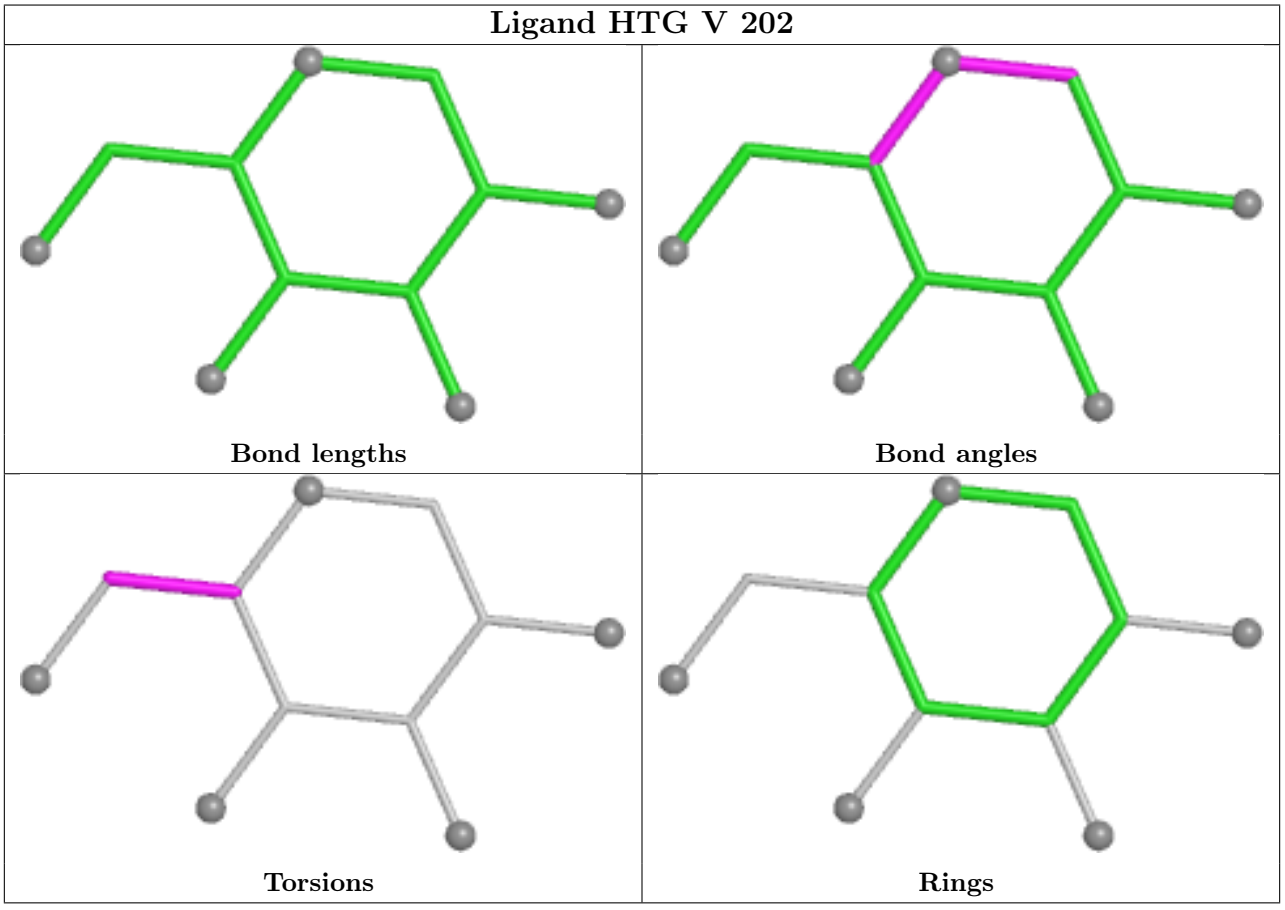


Rings

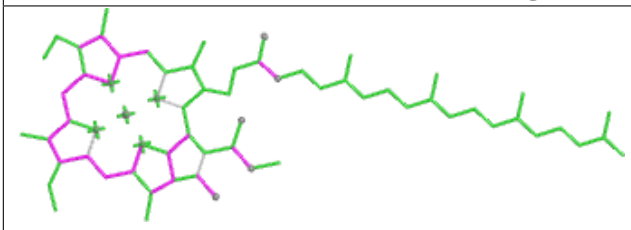
Ligand LMT M 103



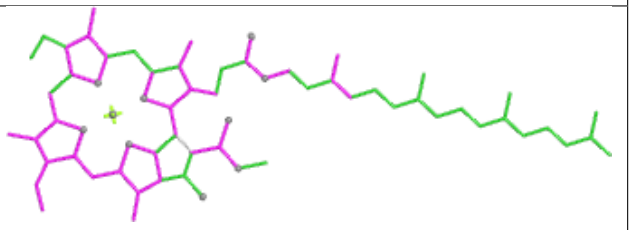
Ligand HTG V 202



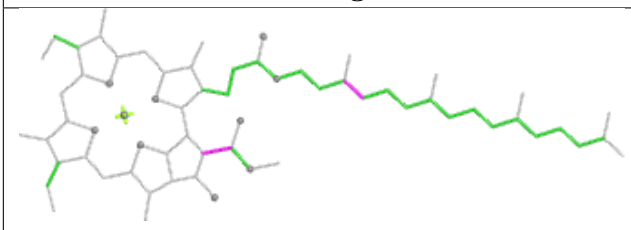
Ligand CLA B 607



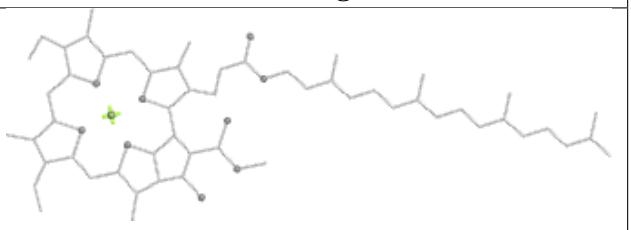
Bond lengths



Bond angles

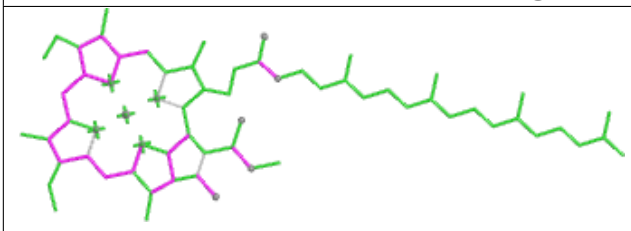


Torsions



Rings

Ligand CLA c 510



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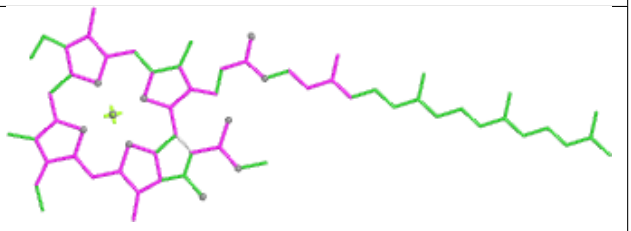
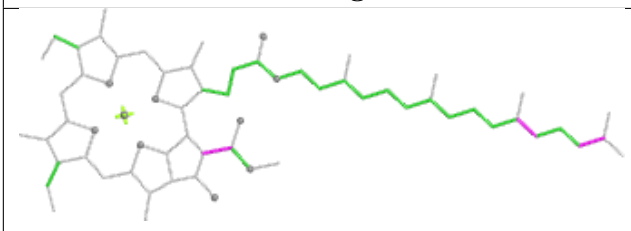


Bond angles



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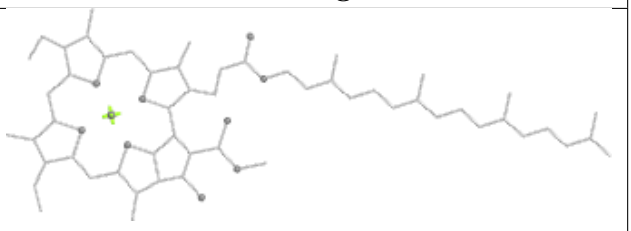
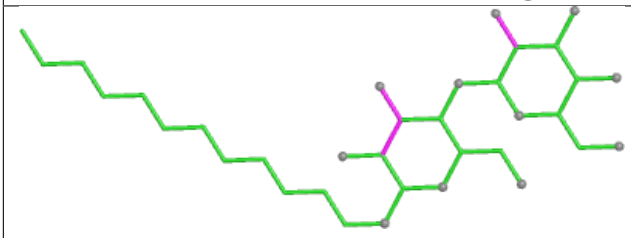


Rings

Ligand LMT m 103



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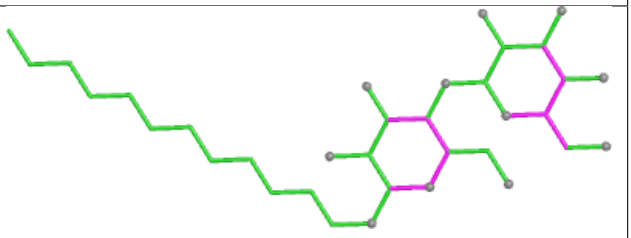
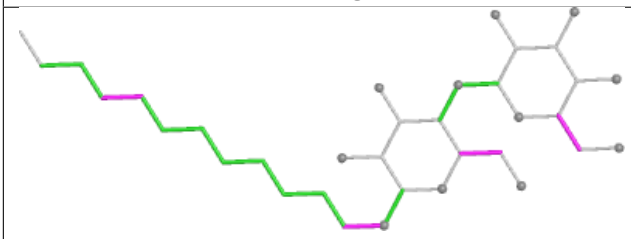


Bond angles



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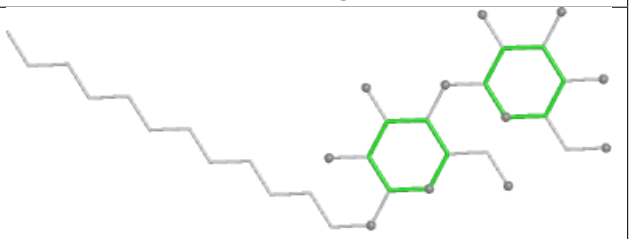
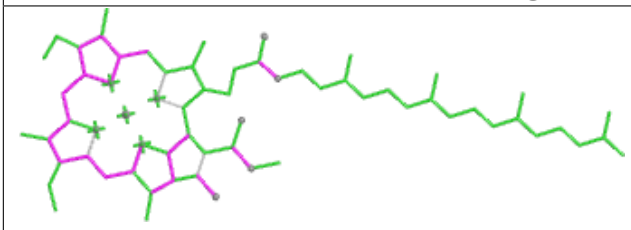


Rings

Ligand CLA C 513



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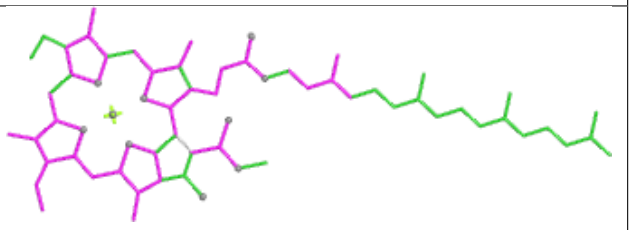
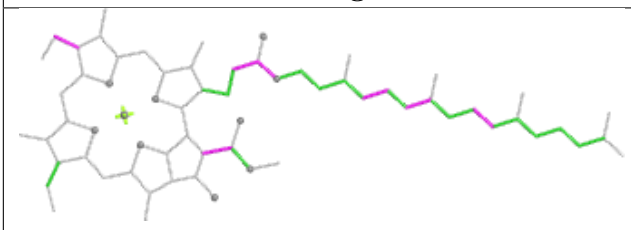


Bond angles



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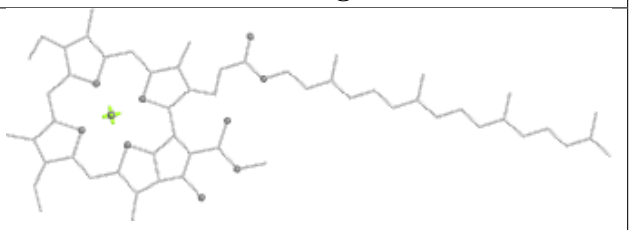
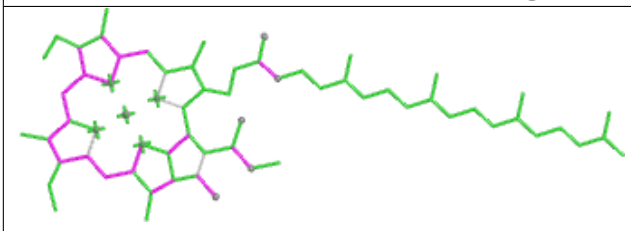


Rings

Ligand CLA D 403



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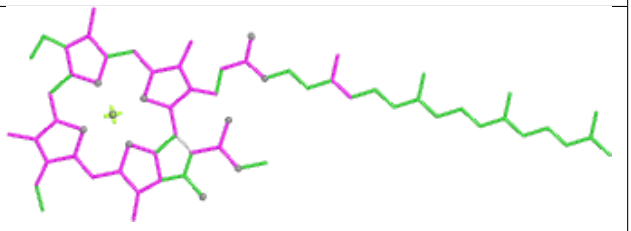
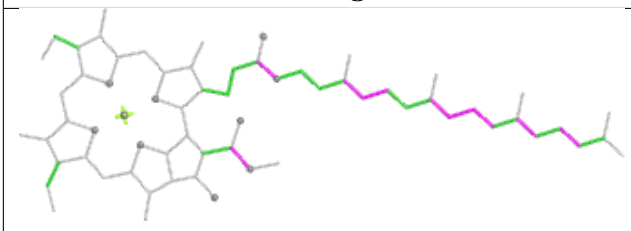


Bond angles



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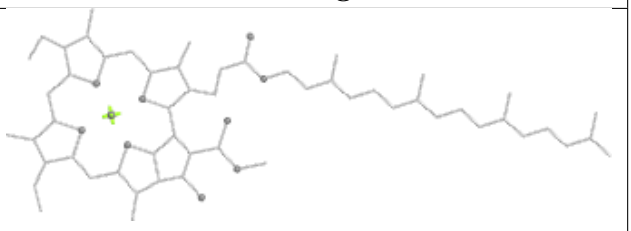
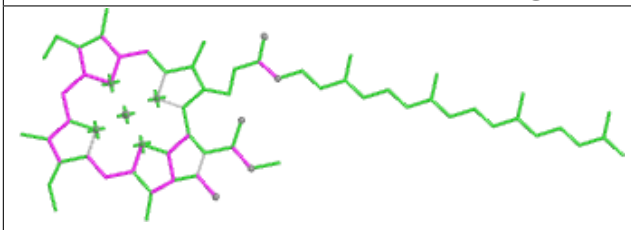


Rings

Ligand CLA b 605



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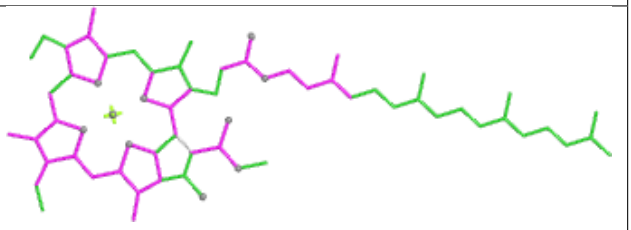

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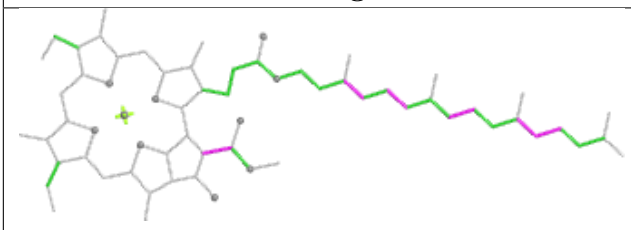

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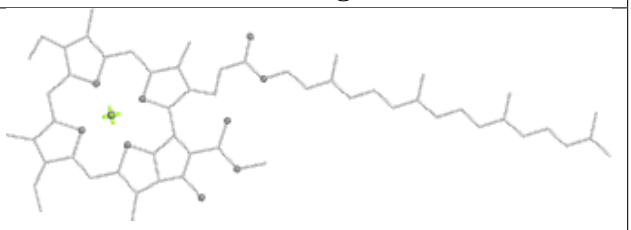
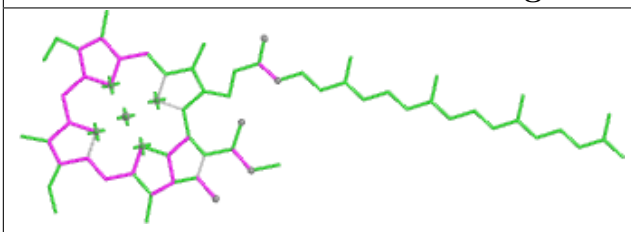


Rings

Ligand CLA B 608



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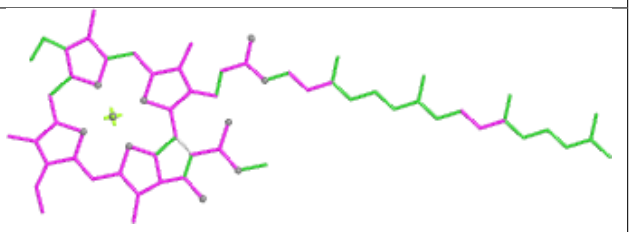
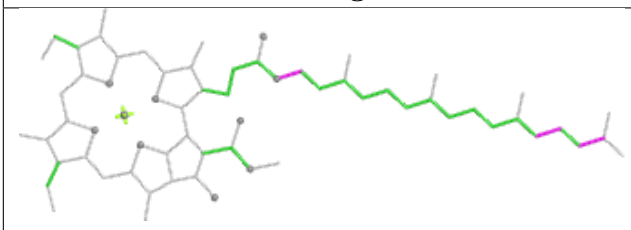


Bond angles



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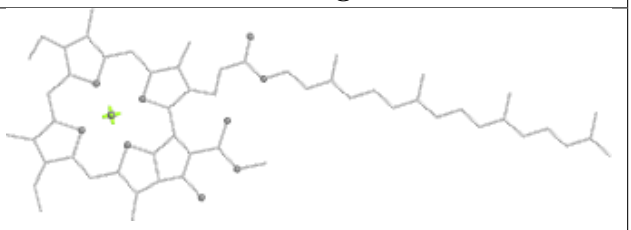
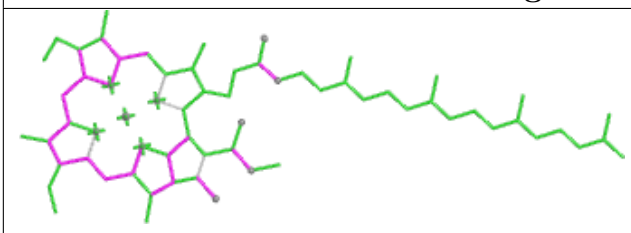


Rings

Ligand CLA B 610



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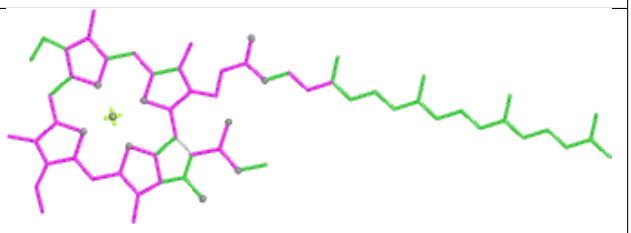
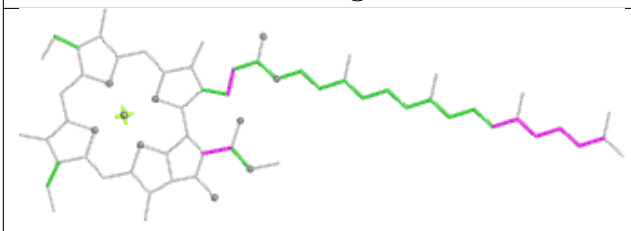


Bond angles



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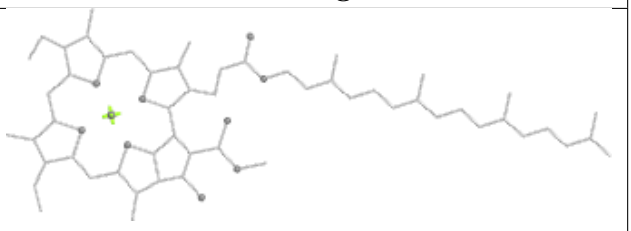
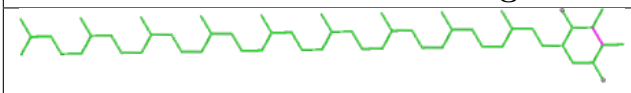


Rings

Ligand PL9 d 406 (B)



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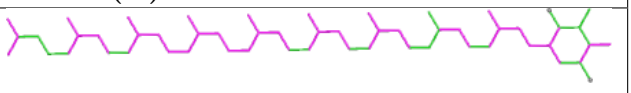
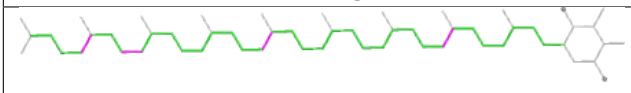


Bond angles



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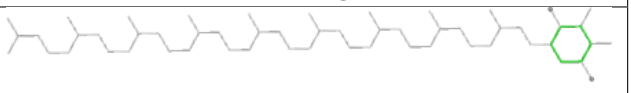
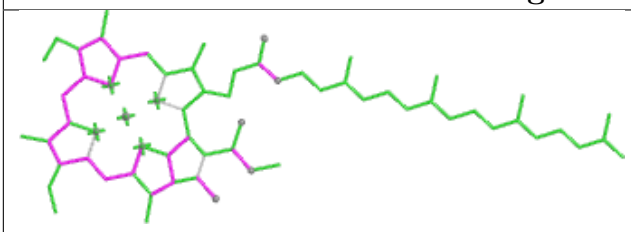


Rings

Ligand CLA b 611



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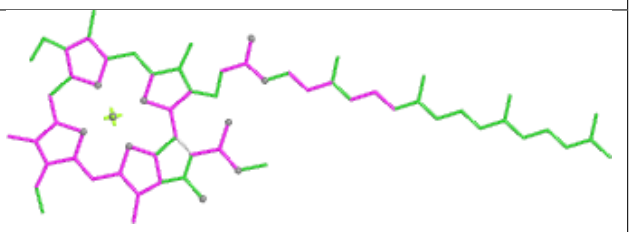
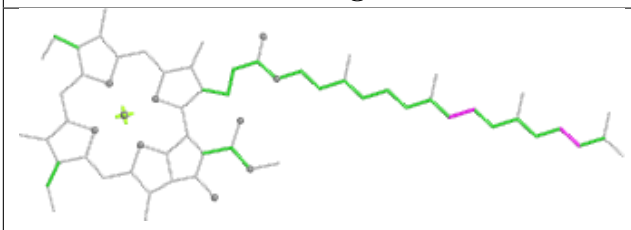


Bond angles



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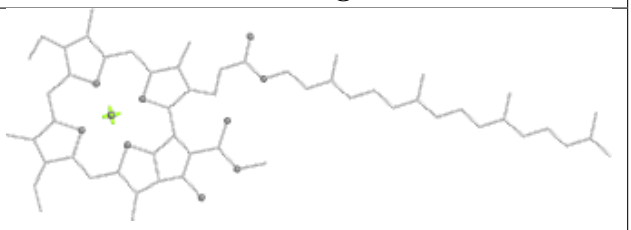
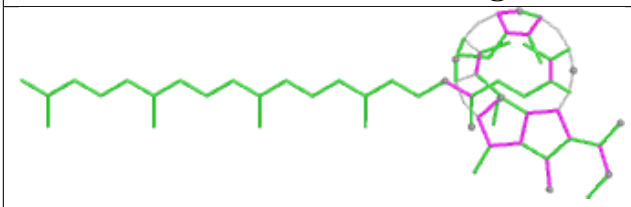


Rings

Ligand PHO A 416 (B)



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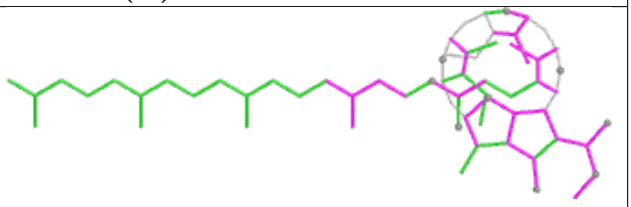
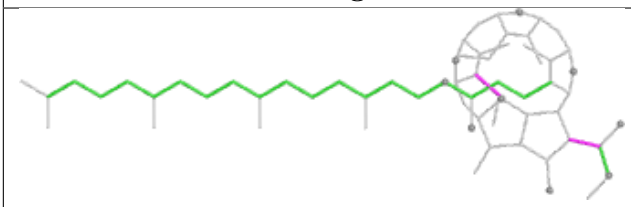


Bond angles



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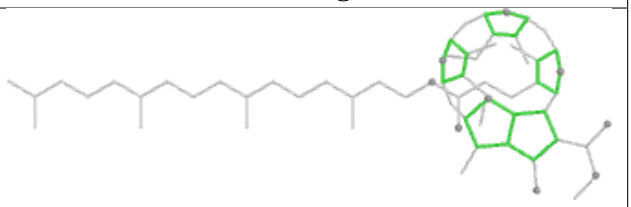
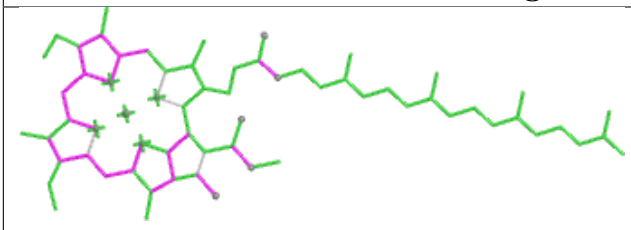


Rings

Ligand CLA A 408



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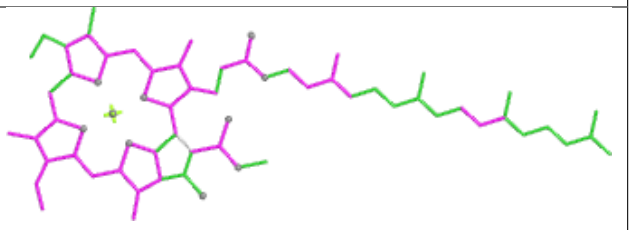
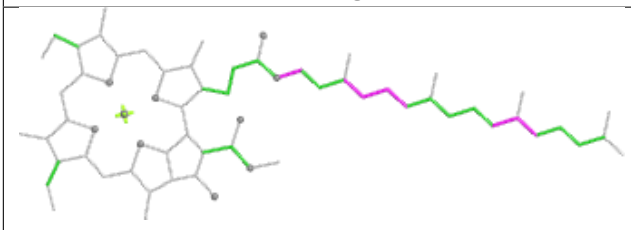


Bond angles



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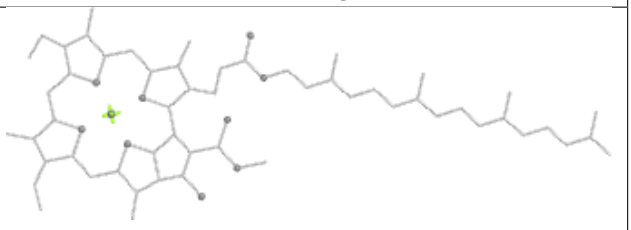
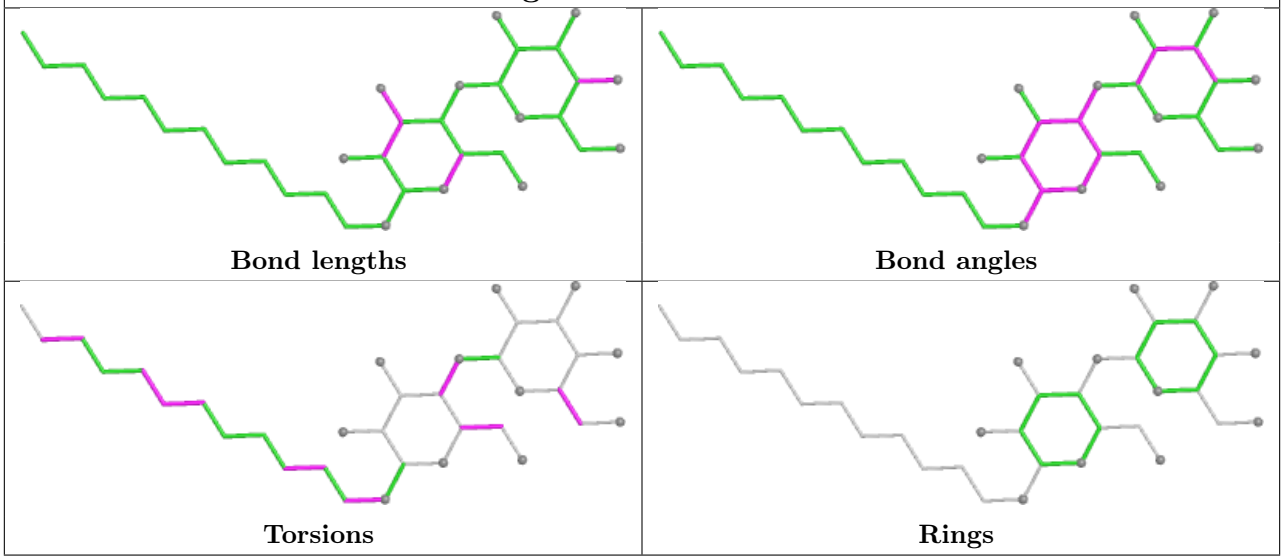
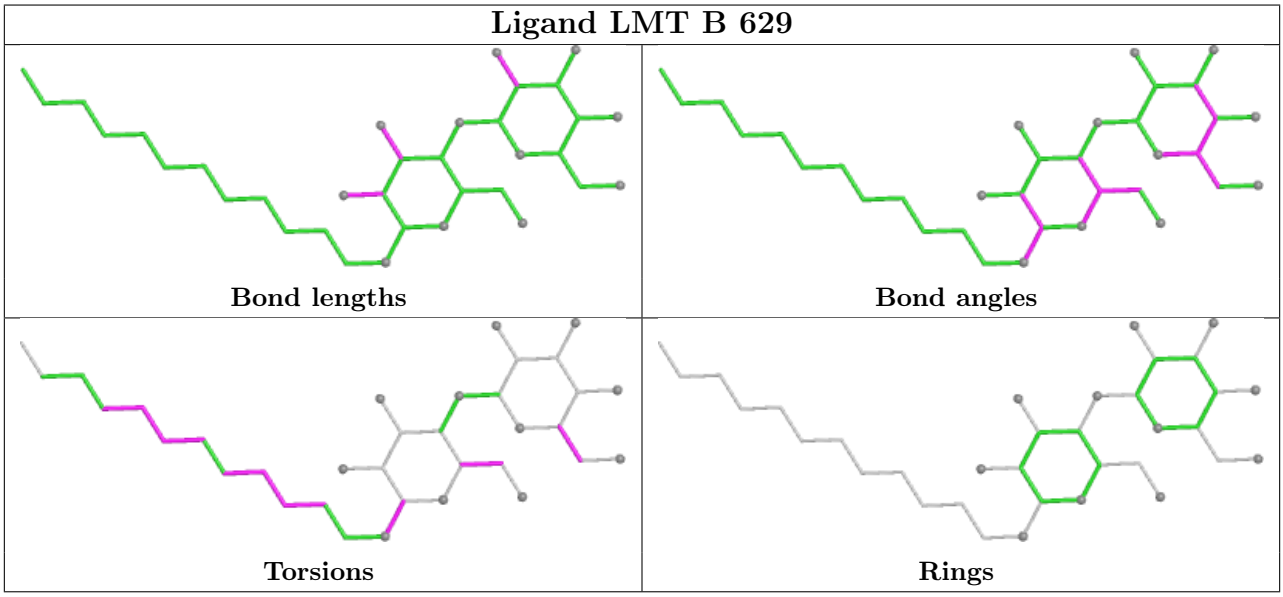


Rings

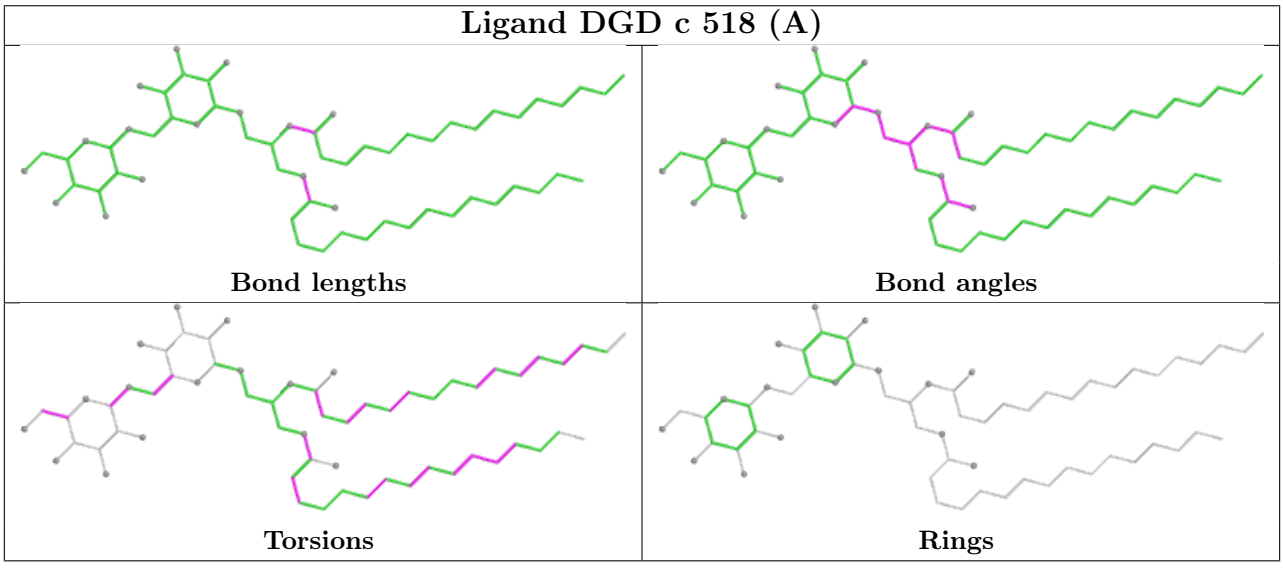
Ligand LMT B 627



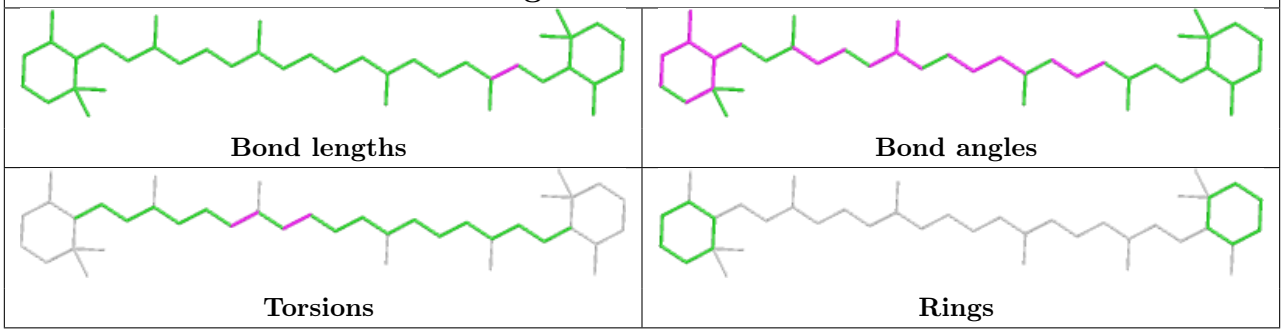
Ligand LMT B 629



Ligand DGD c 518 (A)



Ligand BCR T 101



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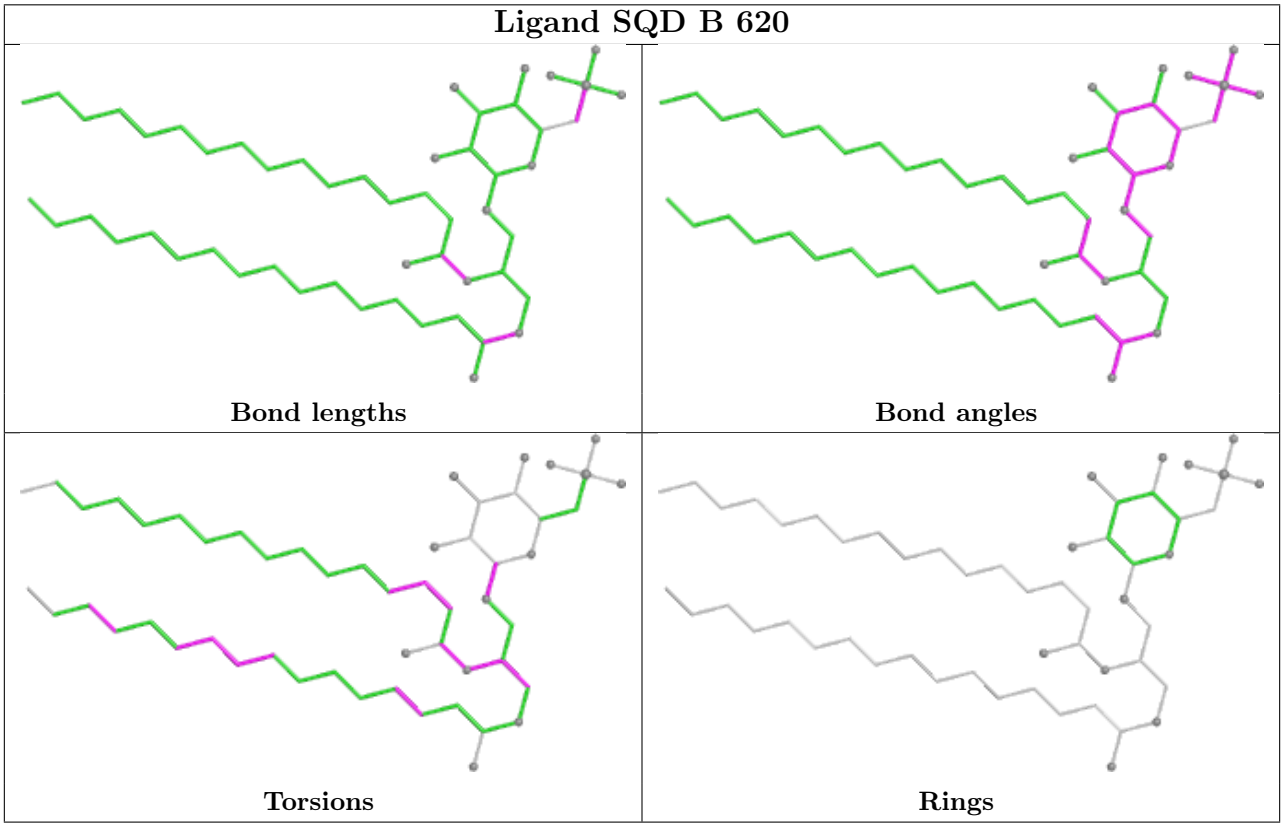

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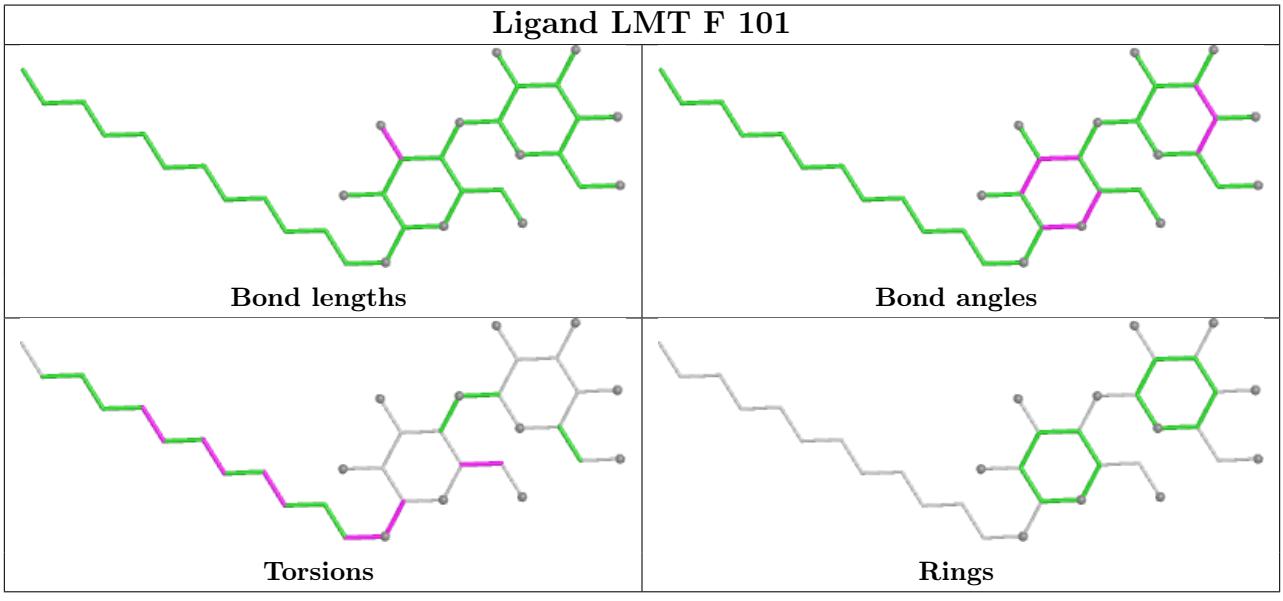

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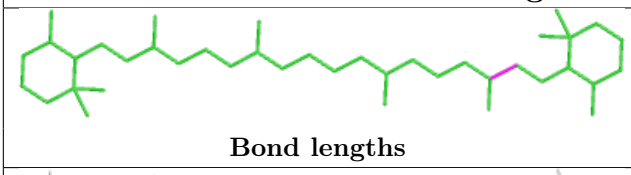
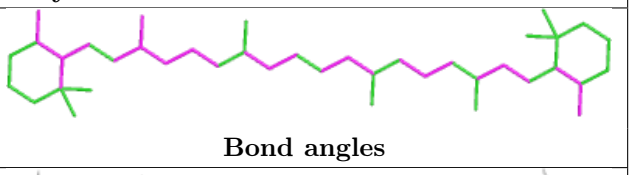
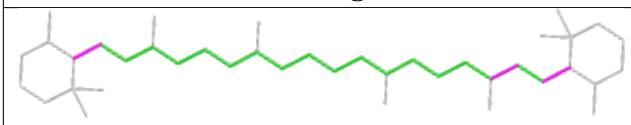


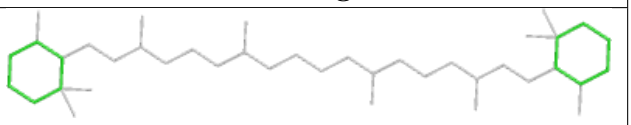
Bond lengths



Bond angles

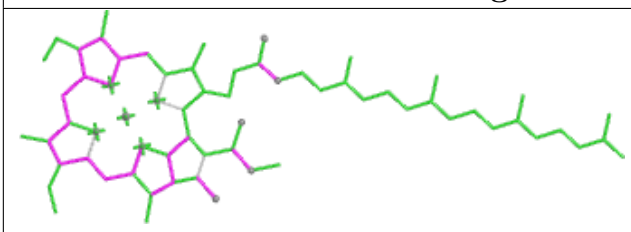


Torsions



Rings

Ligand CLA D 402 (B)



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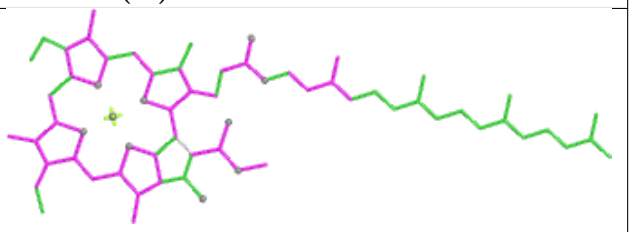
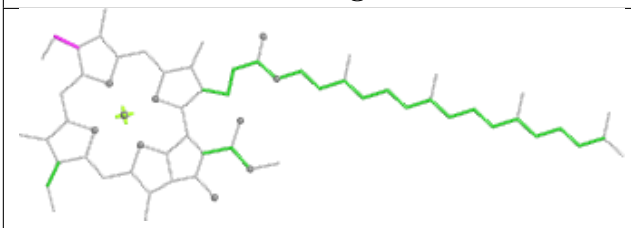
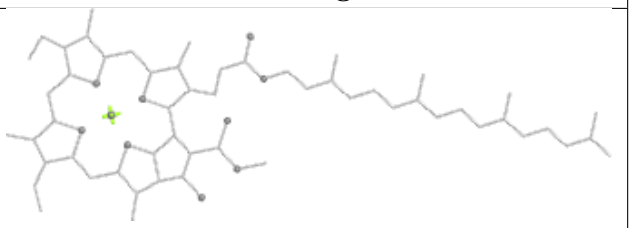


Bond angles

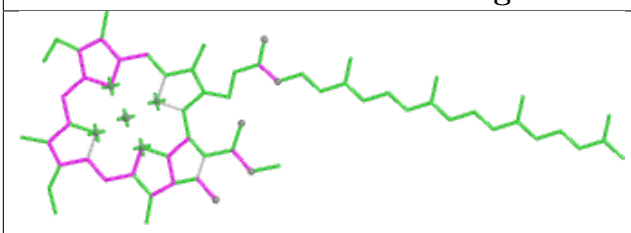


Torsions

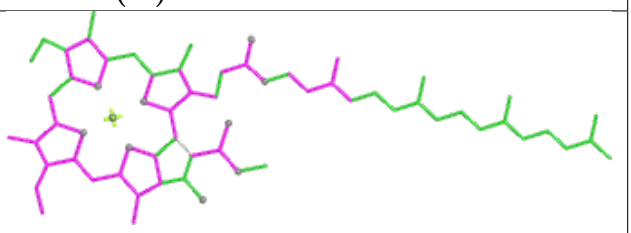


Rings

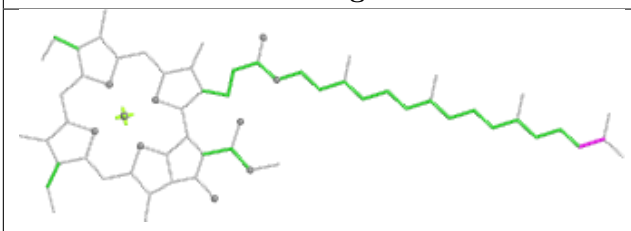
Ligand CLA d 403 (A)



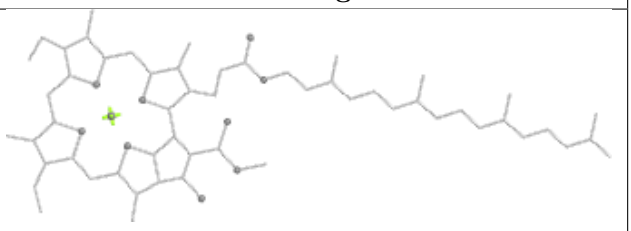
Bond lengths



Bond angles

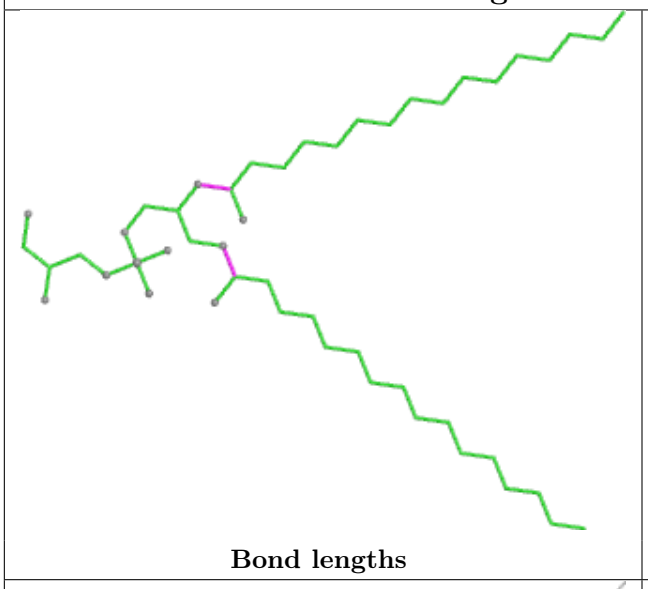


Torsions

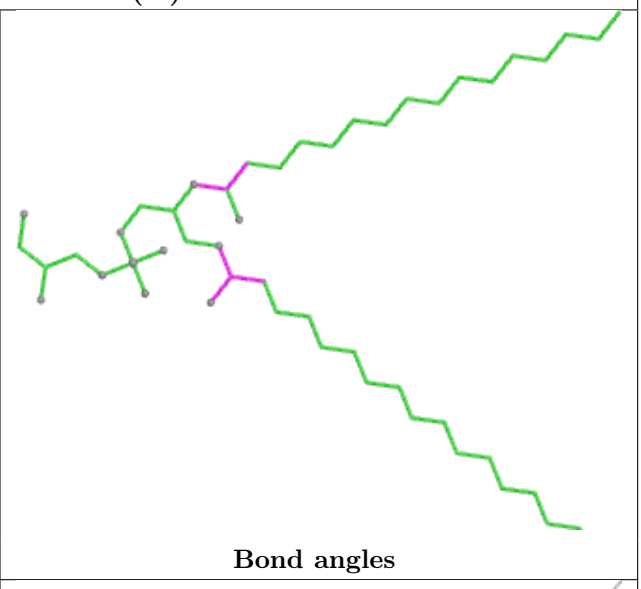


Rings

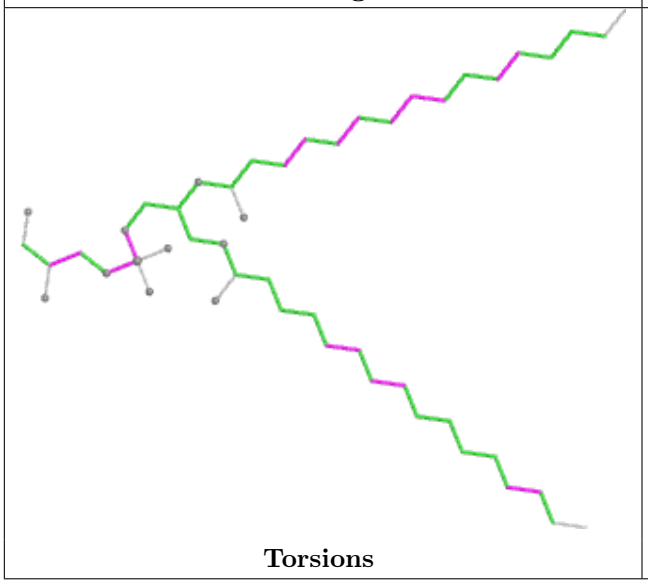
Ligand LHG D 406 (B)



Bond lengths



Bond angles



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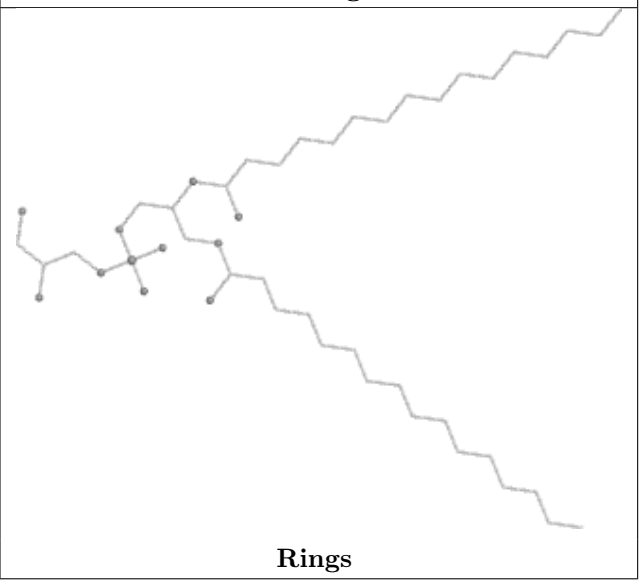
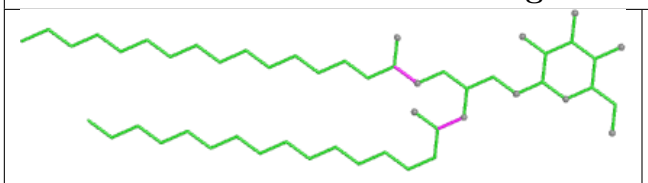


Rings

Ligand LMG c 501



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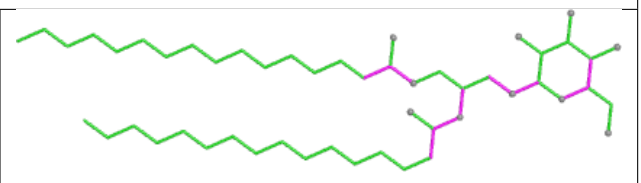
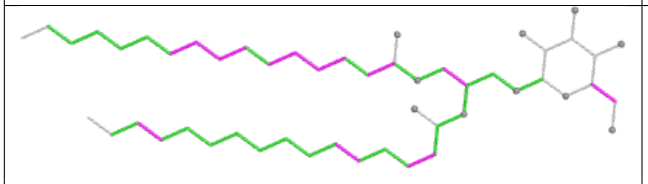


Bond angles



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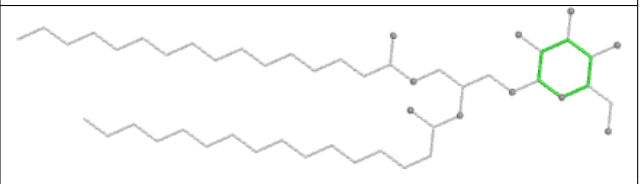
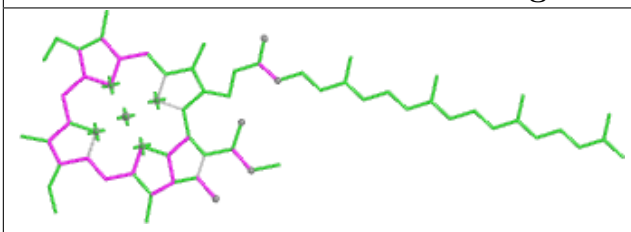


Rings

Ligand CLA c 514



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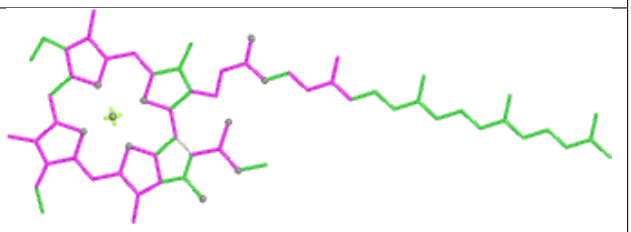
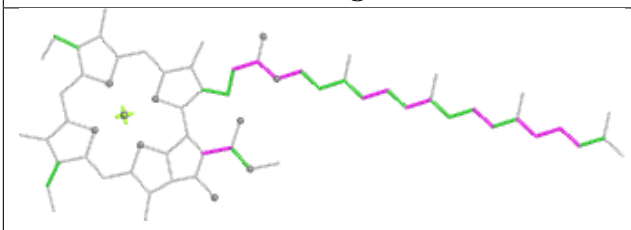
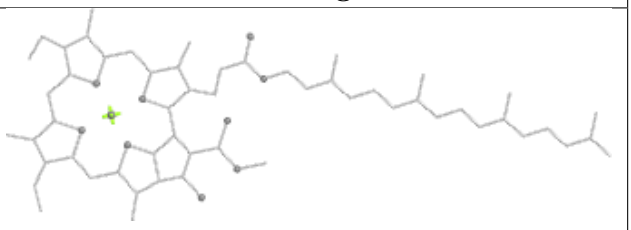


Bond angles

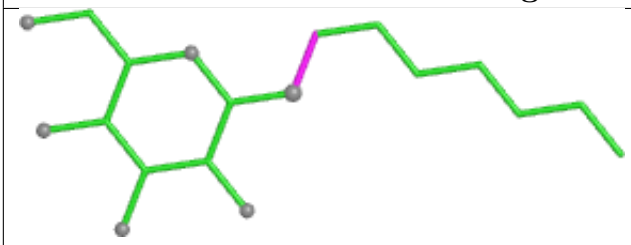


Torsions



Rings

Ligand HTG B 622



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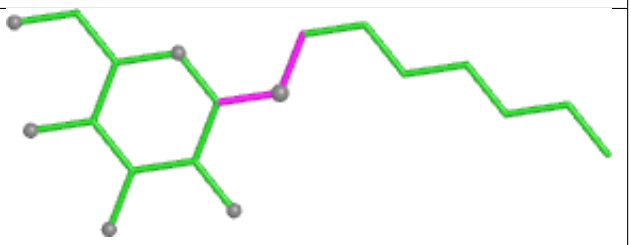
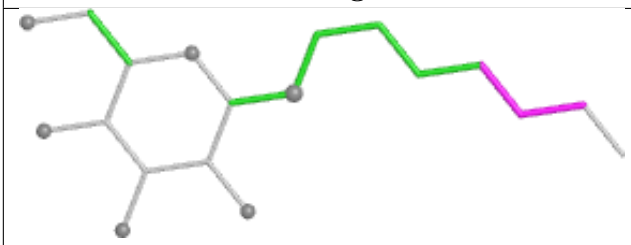


Bond angles



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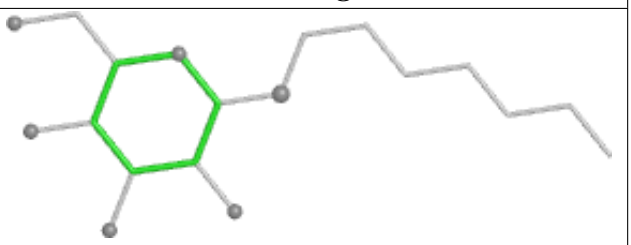
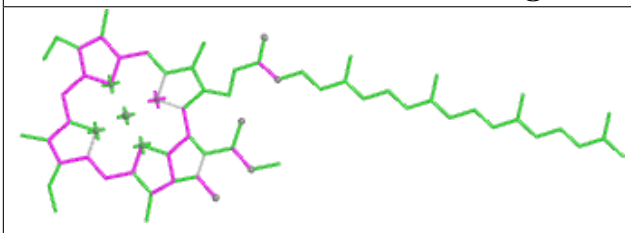


Rings

Ligand CLA B 604



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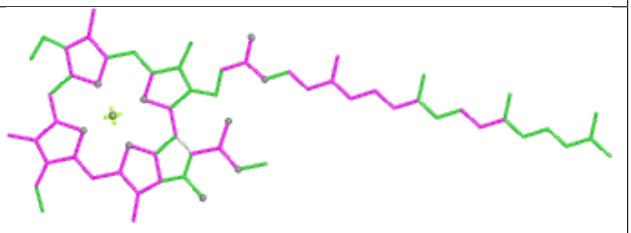
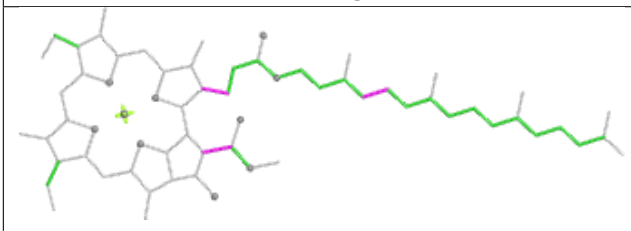


Bond angles



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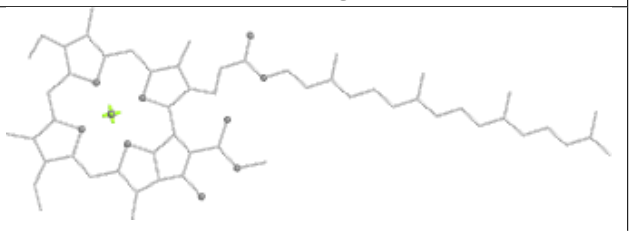
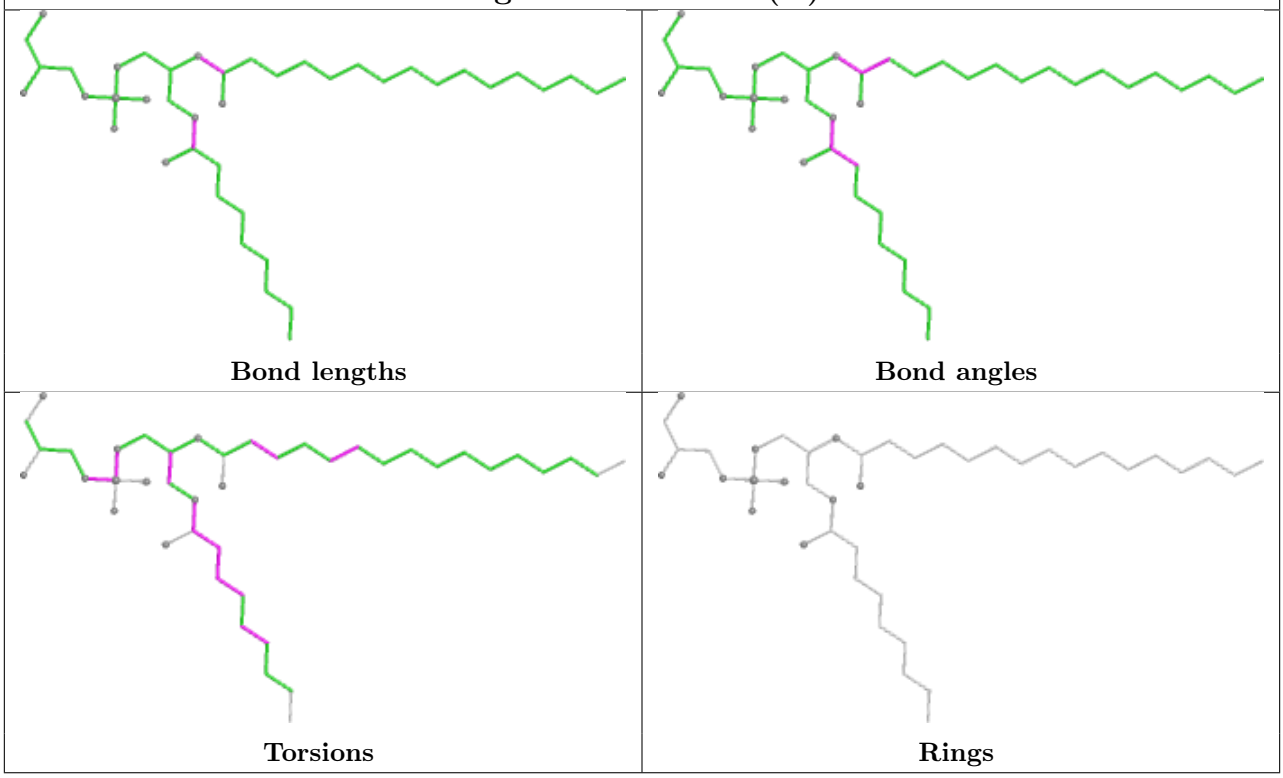
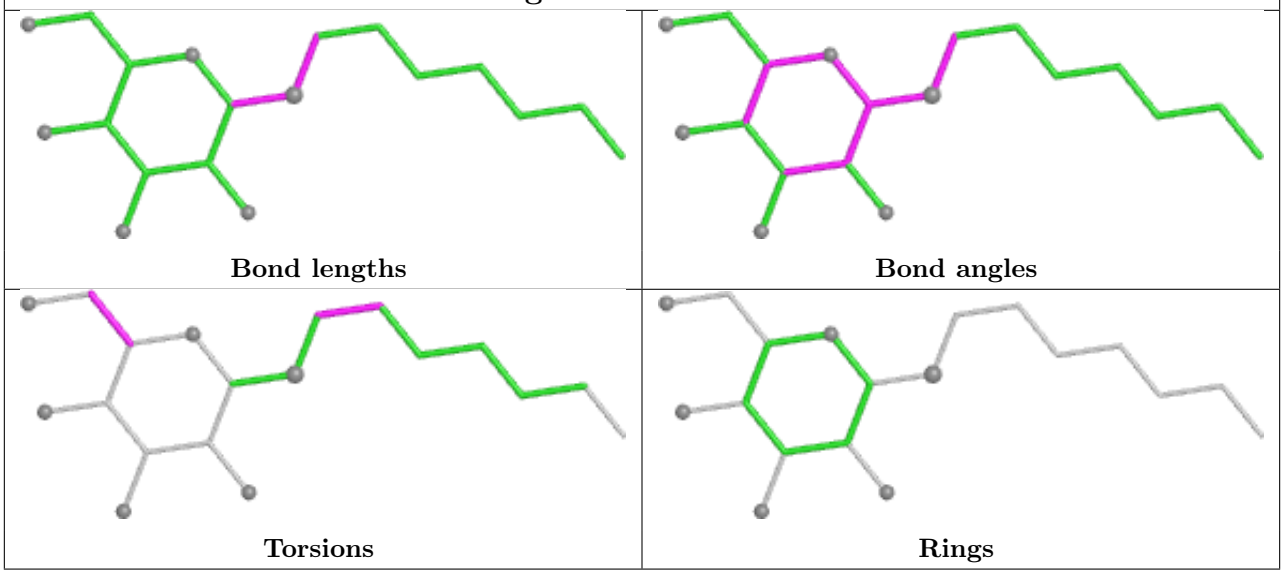


Rings

Ligand LHG a 417 (A)



Ligand HTG b 625



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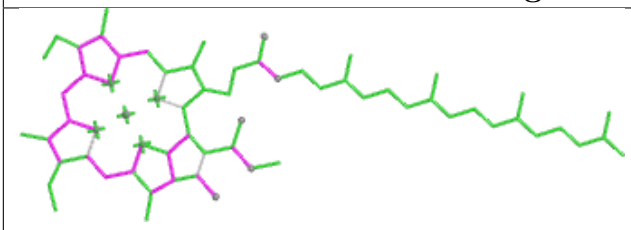

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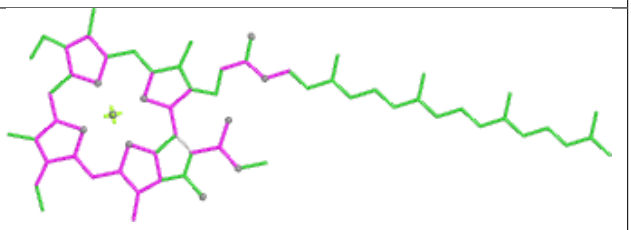
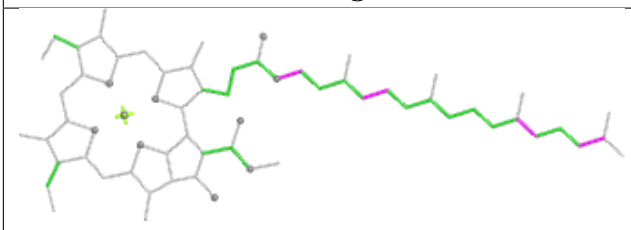


Bond angles



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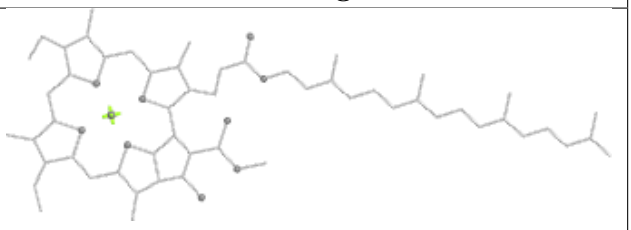
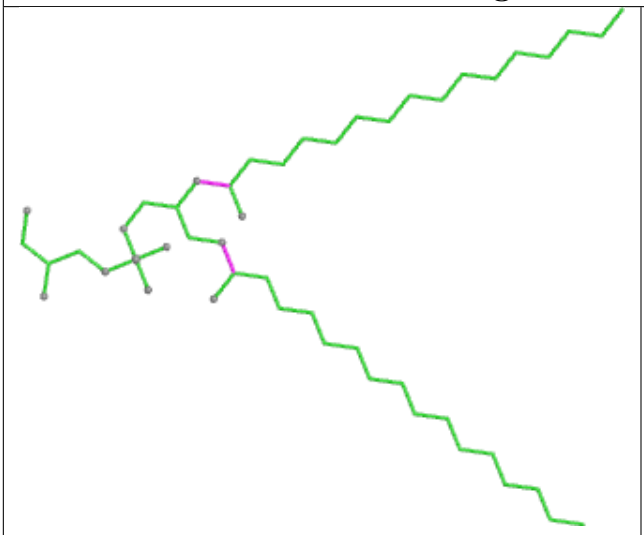


Rings

Ligand LHG b 629 (B)



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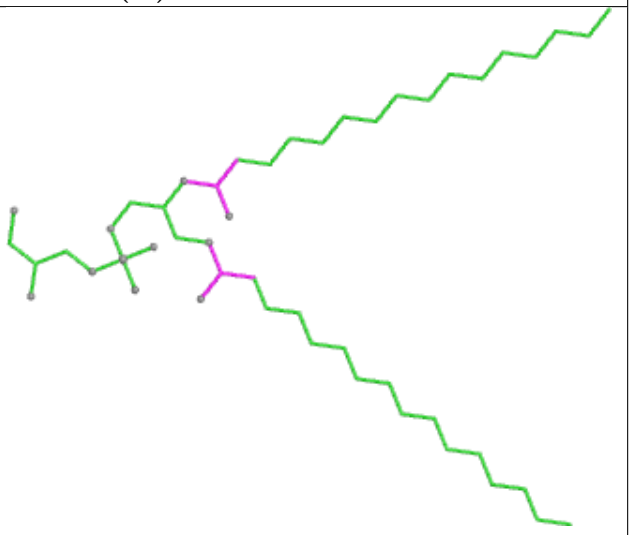
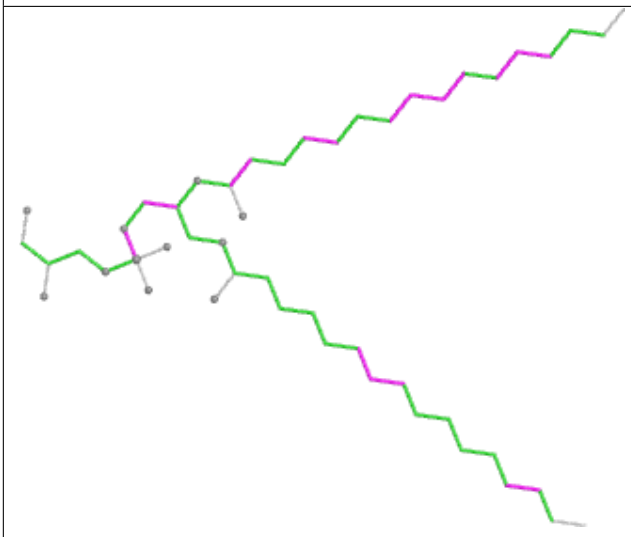


Bond angles



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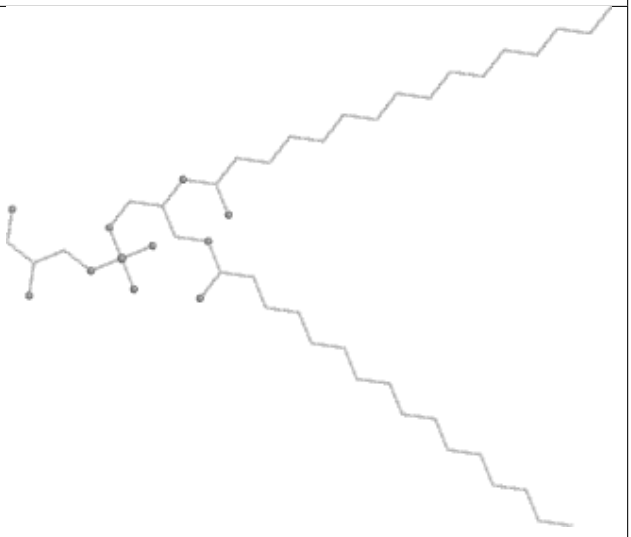
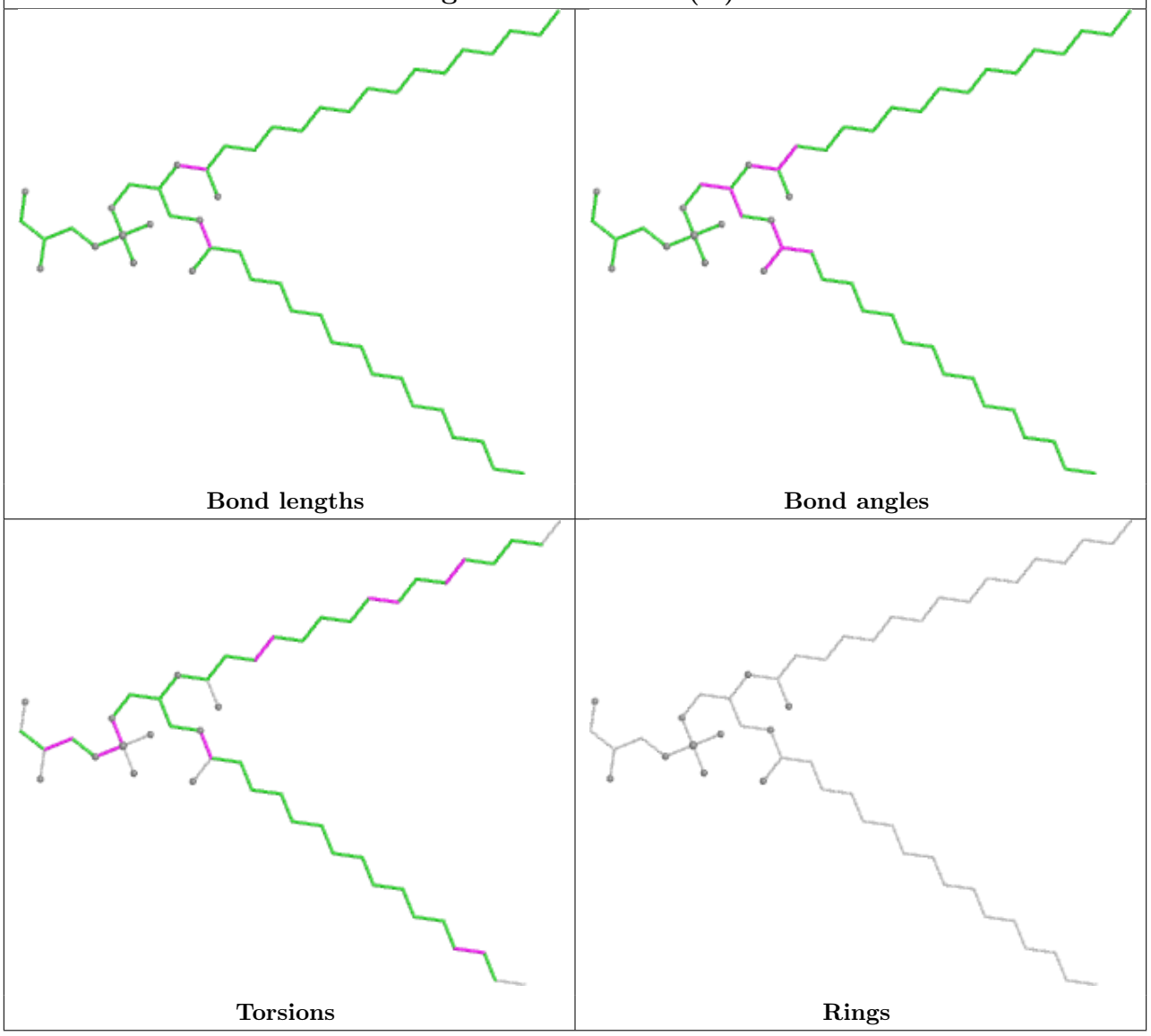
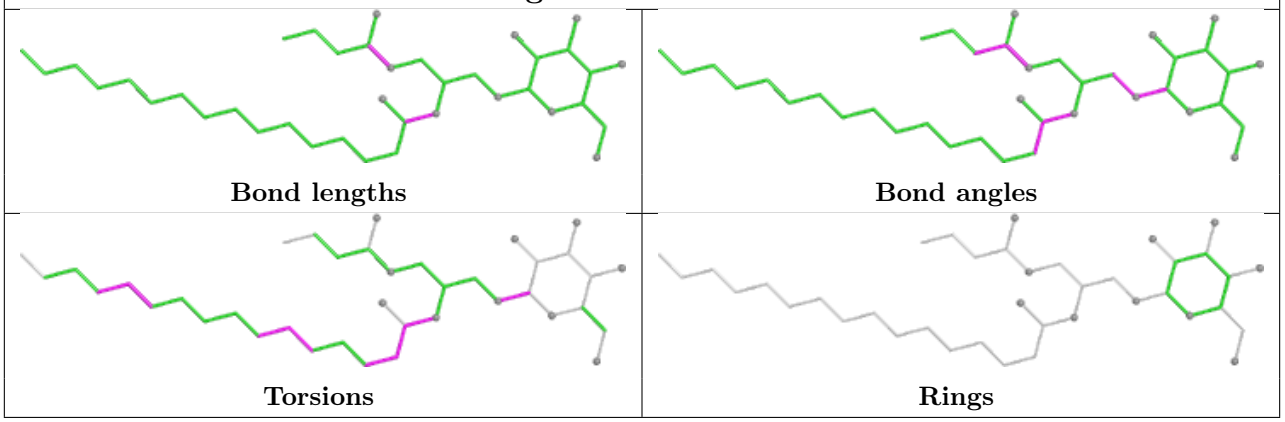


Rings

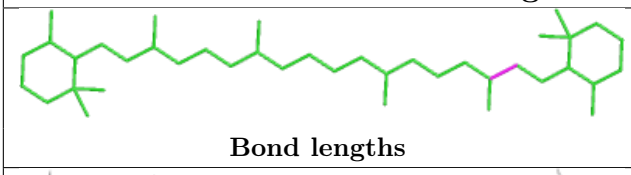
Ligand LHG d 407 (A)

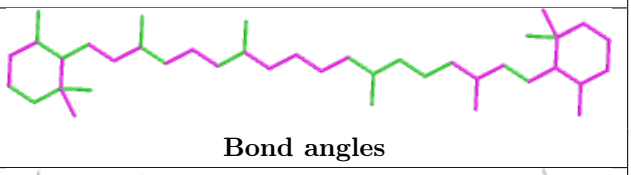


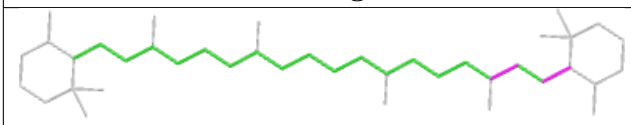
Ligand LMG z 101



Ligand BCR D 404


Bond lengths


Bond angles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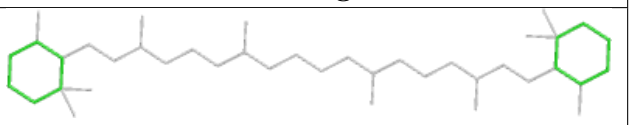
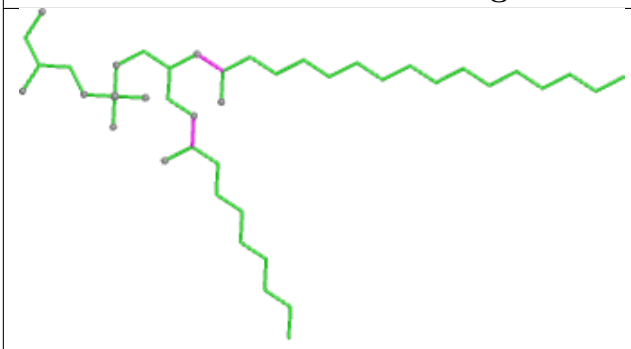

Rings

Ligand LHG E 101 (A)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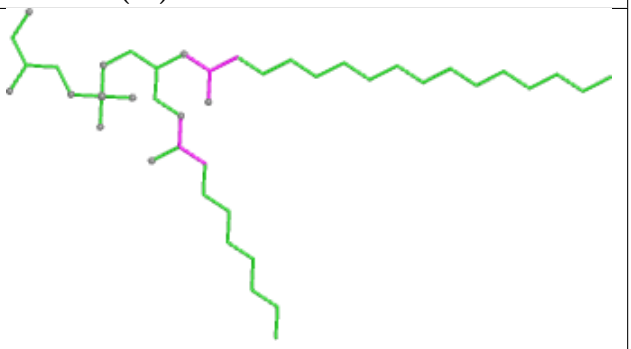
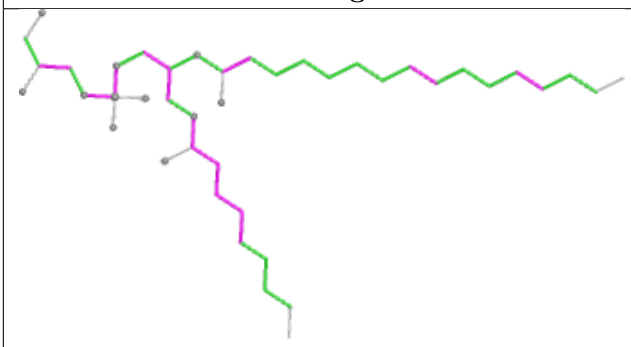

Bond angles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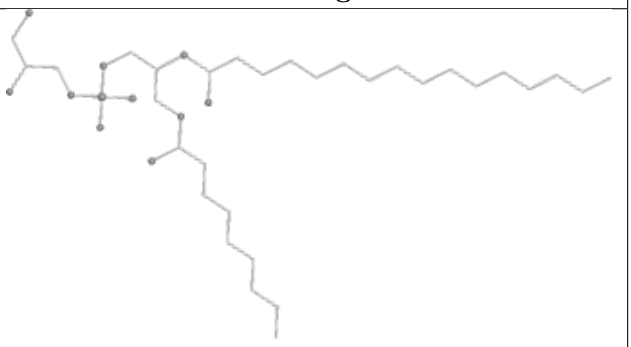
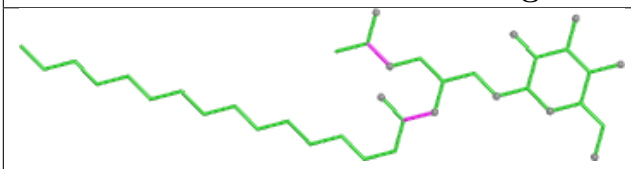

Rings

Ligand LMG Z 101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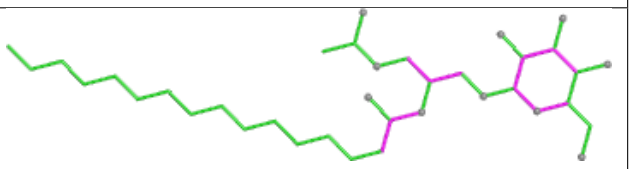
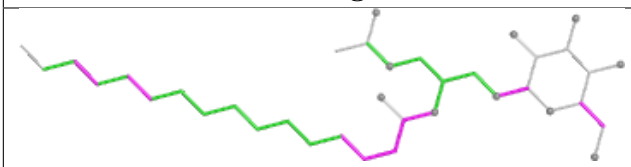

Bond angles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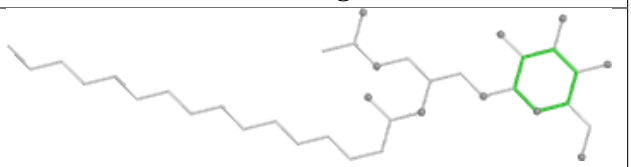
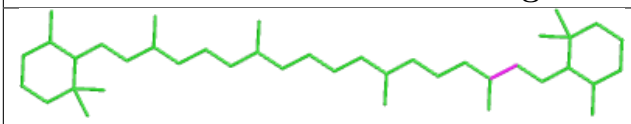
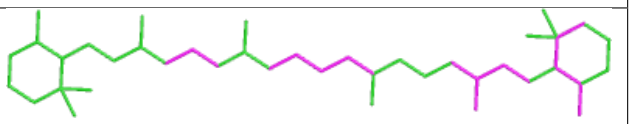

Rings

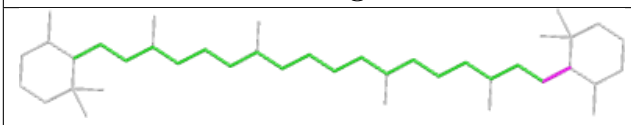
Ligand BCR X 101



Bond lengths



Bond angles



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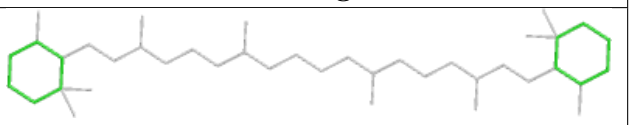
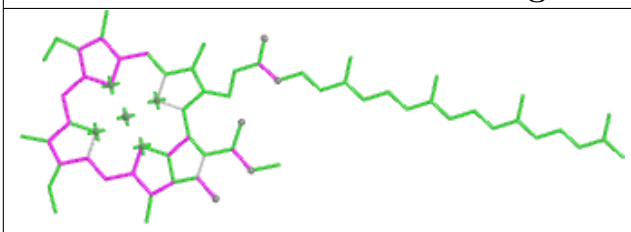
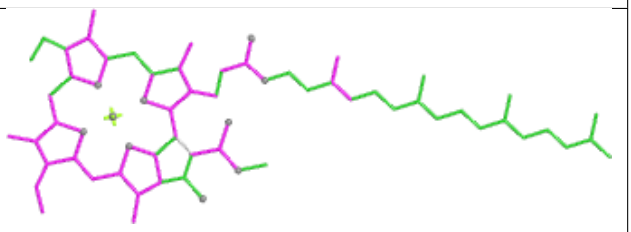


Rings

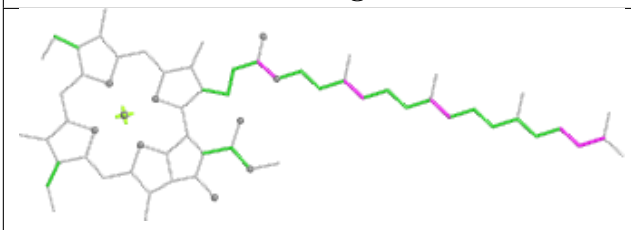
Ligand CLA a 407



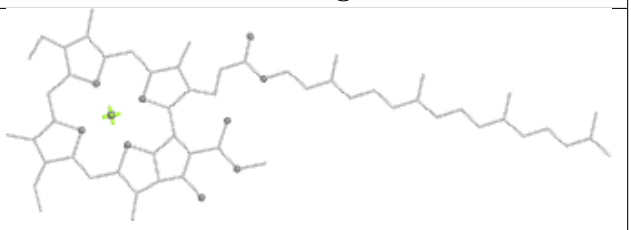
Bond lengths



Bond angles

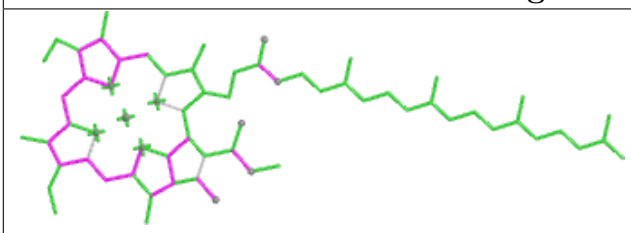


Torsions

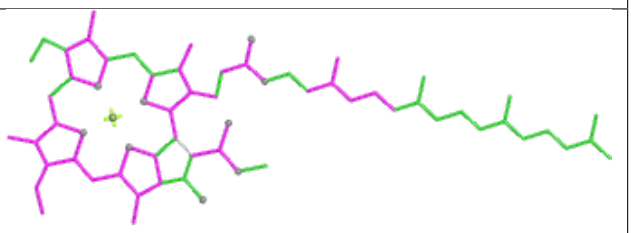


Rings

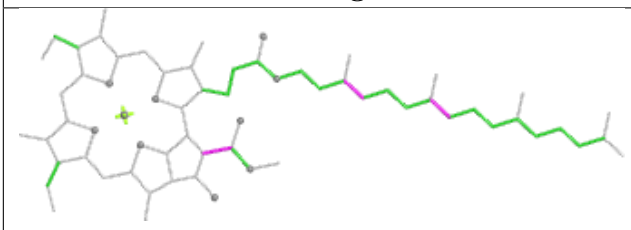
Ligand CLA b 603



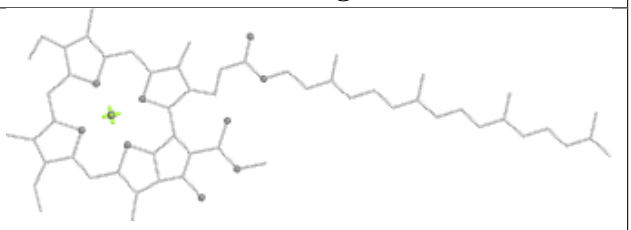
Bond lengths



Bond angles

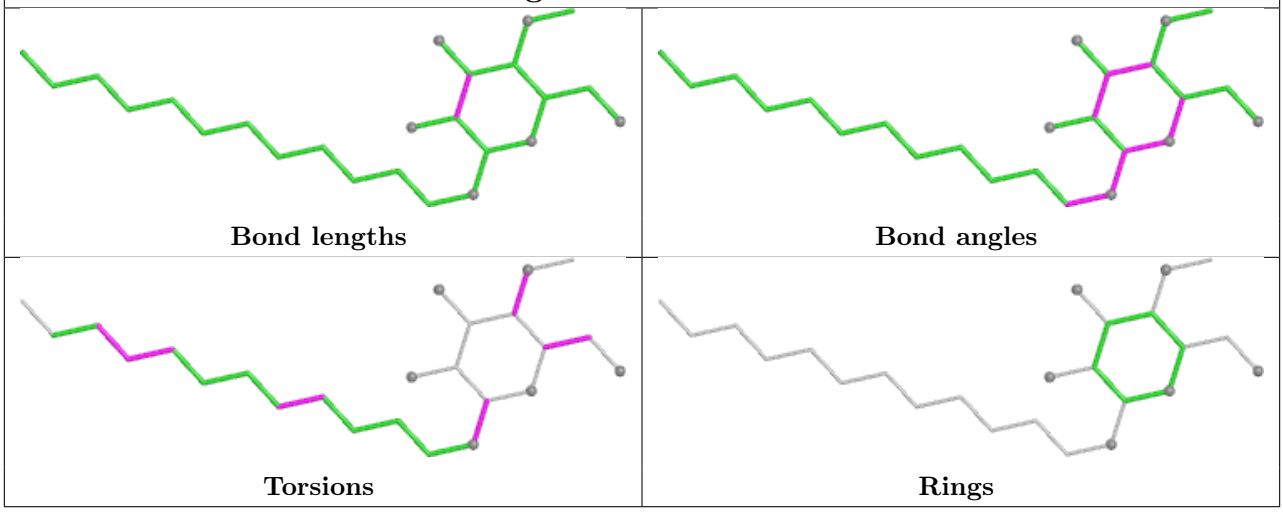


Torsions

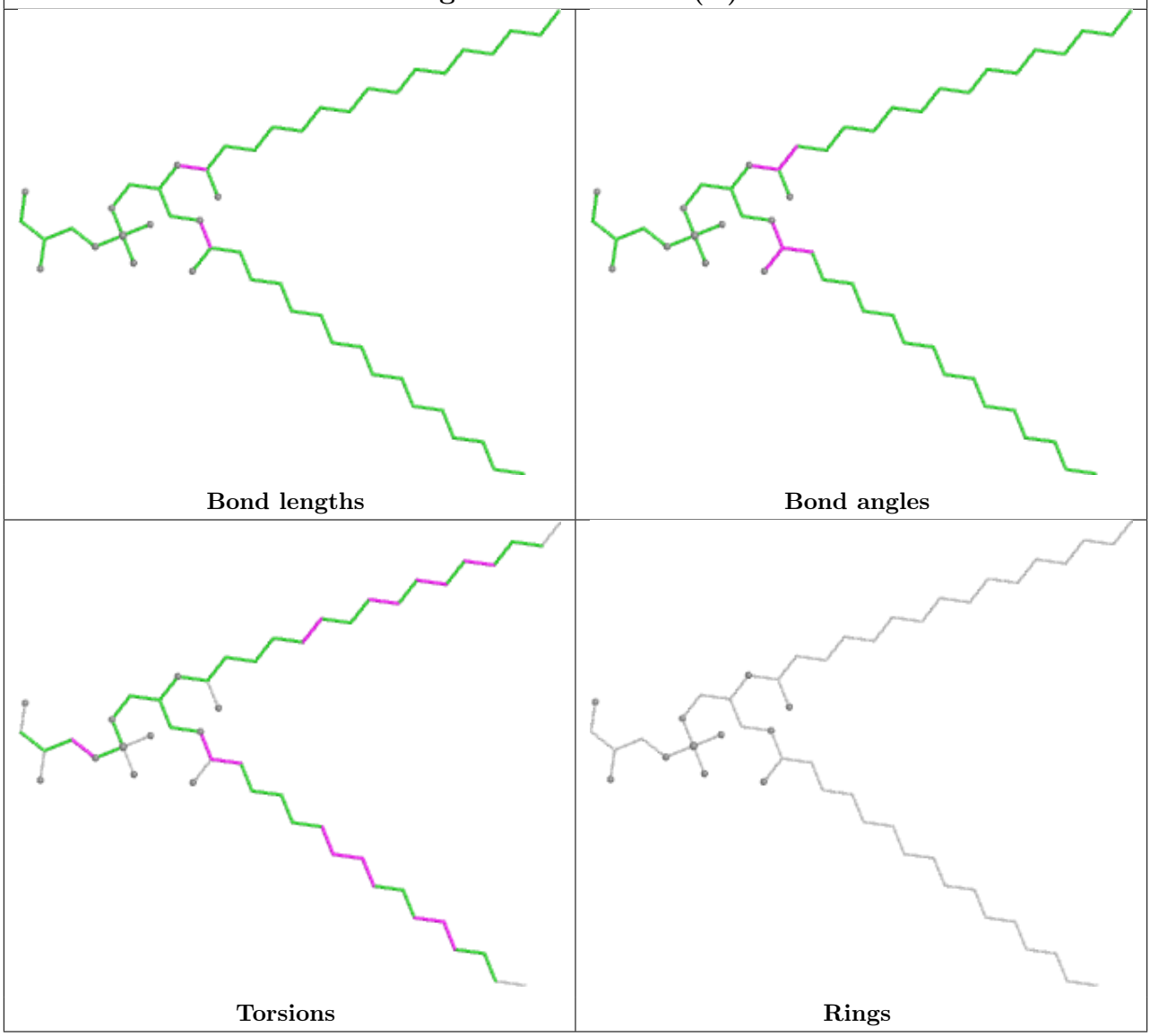


Rings

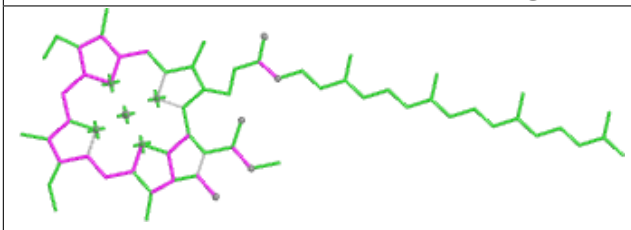
Ligand LMT b 621



Ligand LHG D 407 (B)



Ligand CLA C 511



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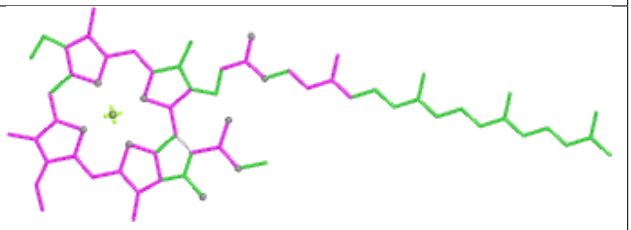
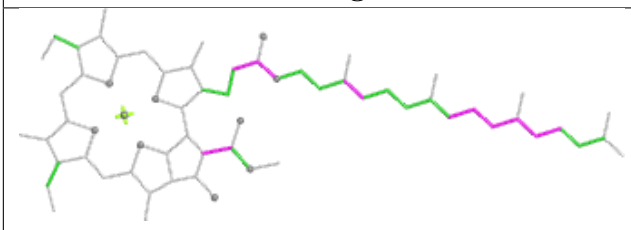


Bond angles



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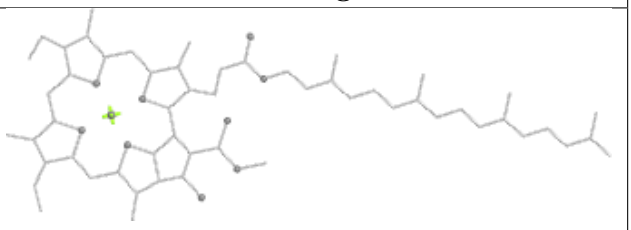
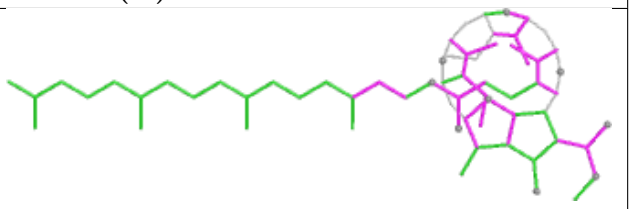


Rings

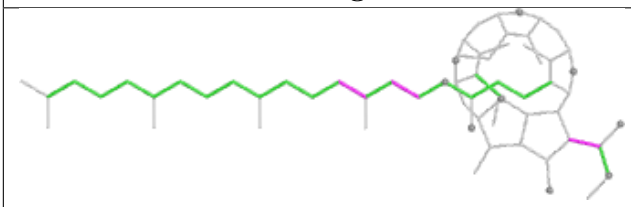
Ligand PHO a 406 (B)



Bond lengths



Bond angles



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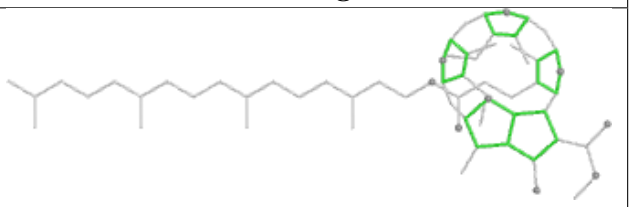
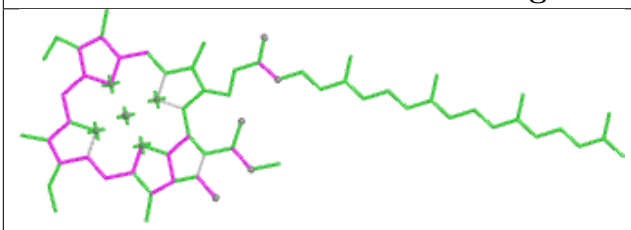


Rings

Ligand CLA c 511



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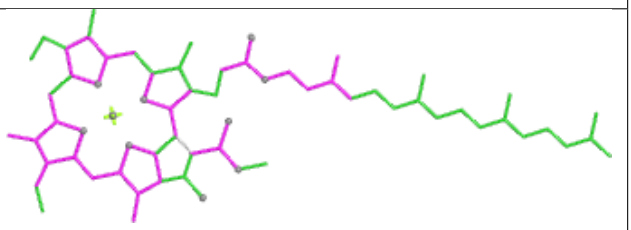
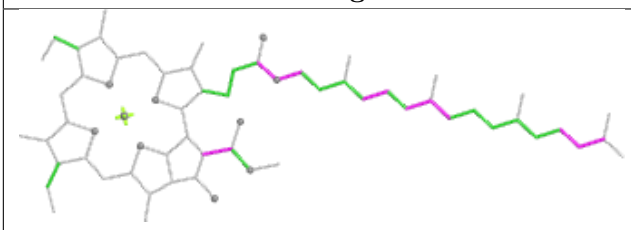


Bond angles



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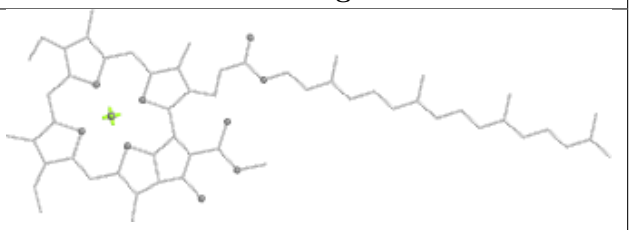
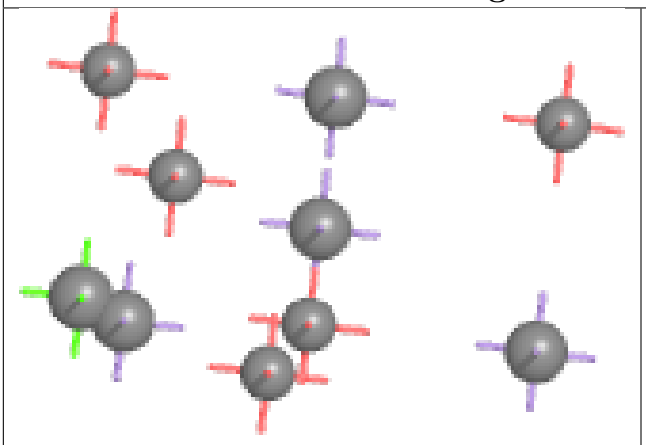


Rings

Ligand OEX A 413 (A)



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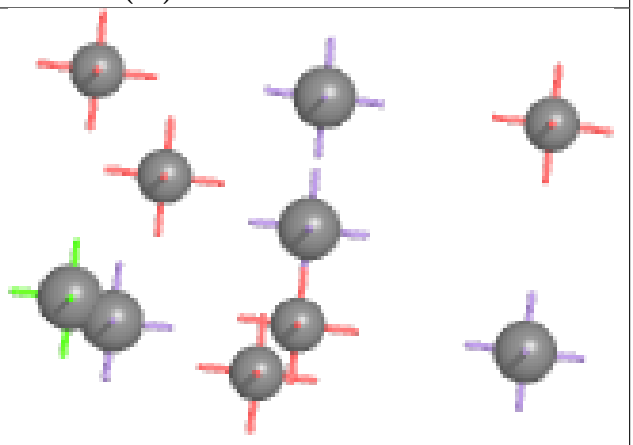
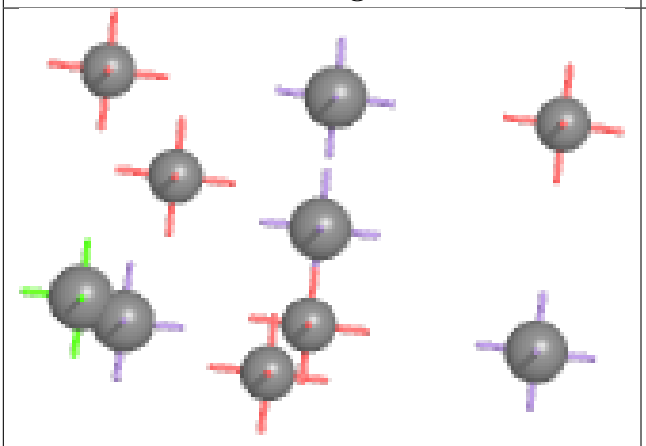
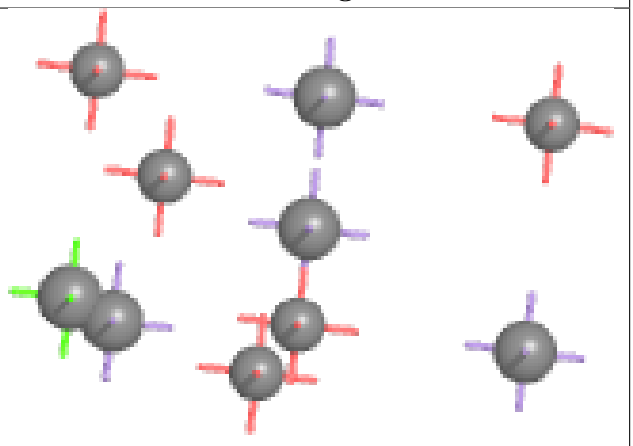


Bond angles

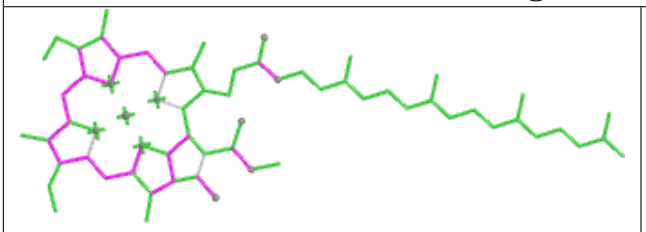


Torsions



Rings

Ligand CLA b 602



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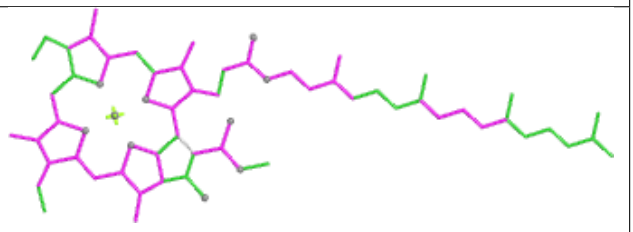
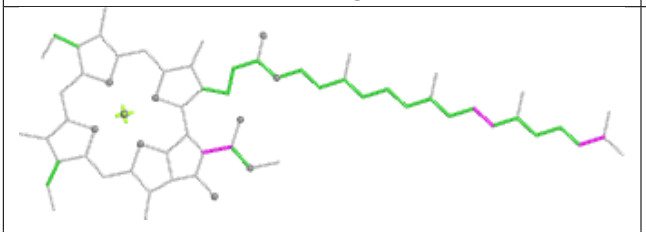


Bond angles



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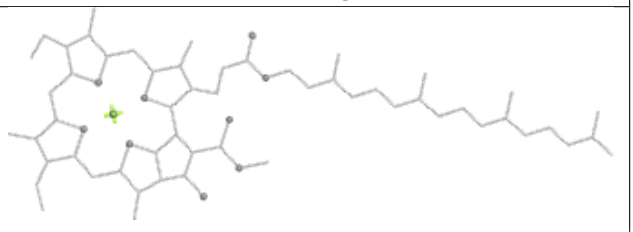
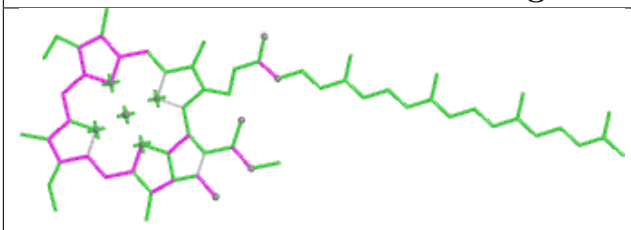


Rings

Ligand CLA b 601



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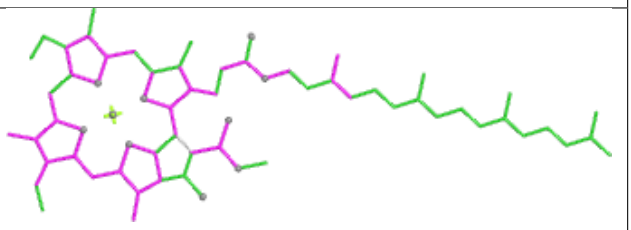
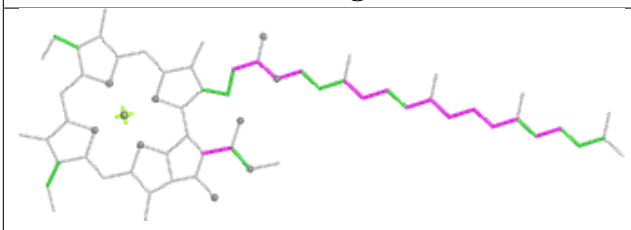


Bond angles



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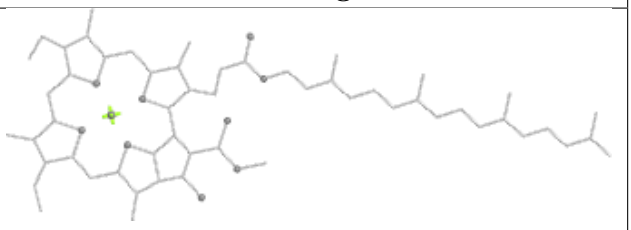
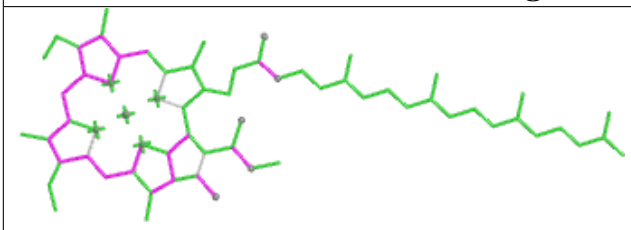


Rings

Ligand CLA B 602



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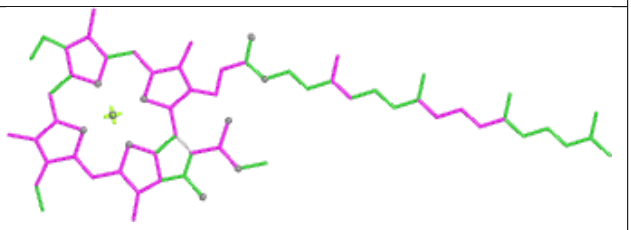
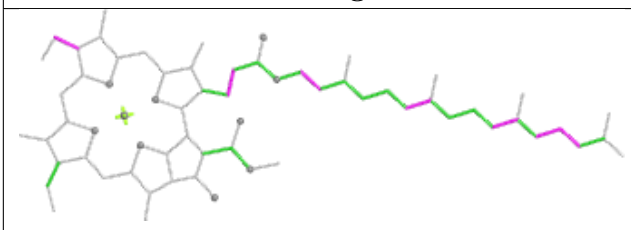


Bond angles



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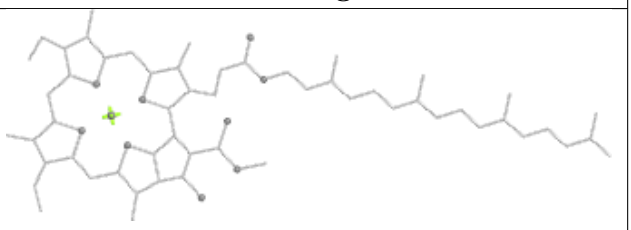
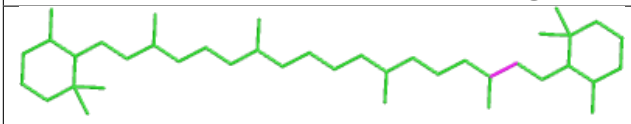


Rings

Ligand BCR h 101



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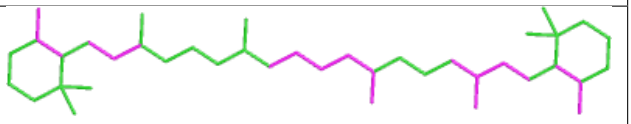
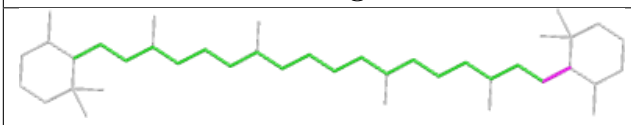


Bond angles



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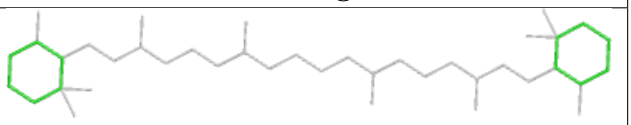
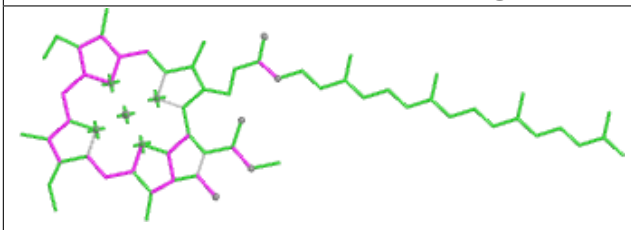


Rings

Ligand CLA A 405 (B)



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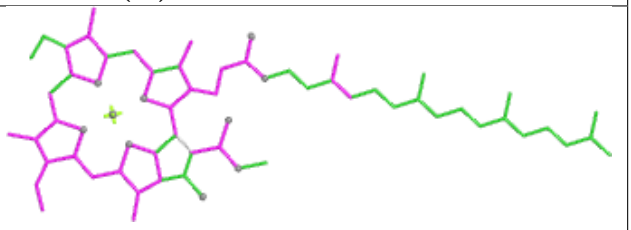

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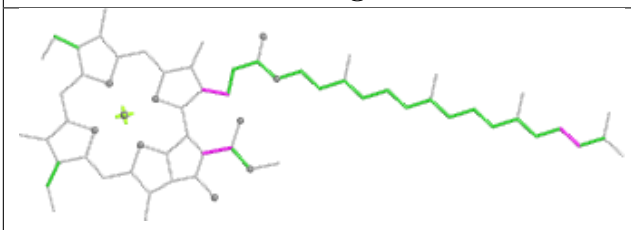

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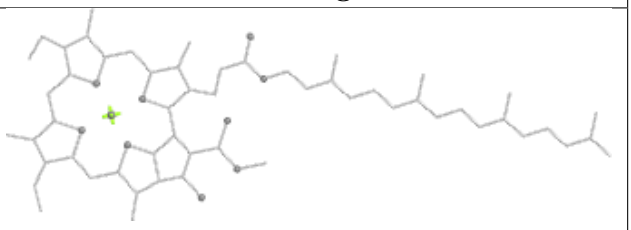
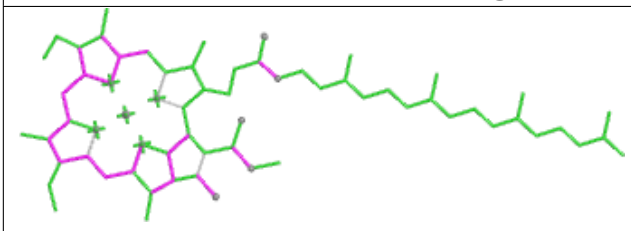


Rings

Ligand CLA A 406 (B)



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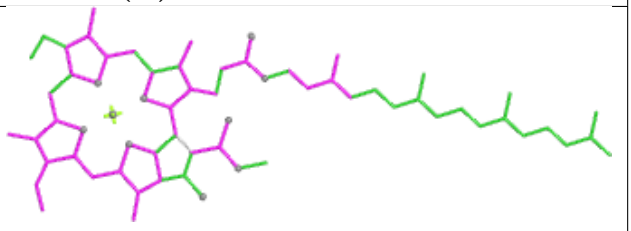
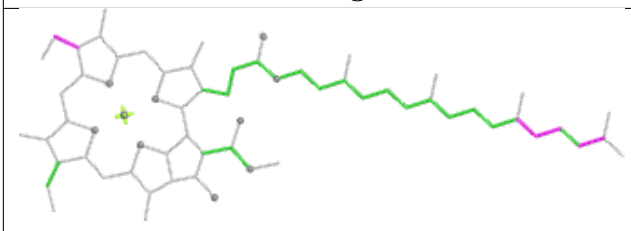


Bond angles



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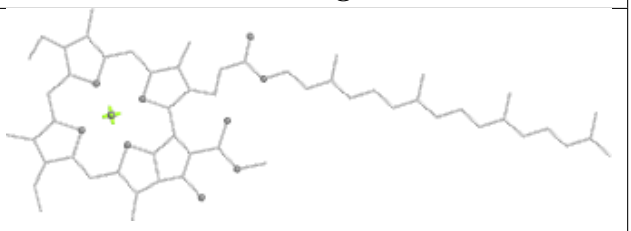
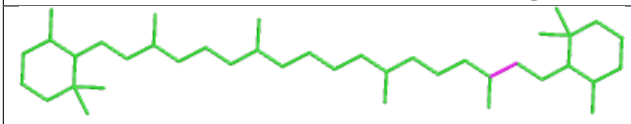


Rings

Ligand BCR b 619



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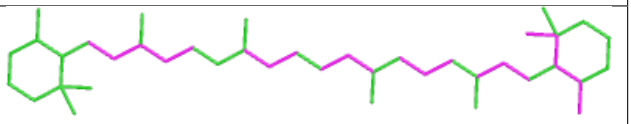
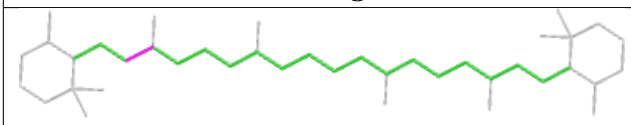


Bond angles



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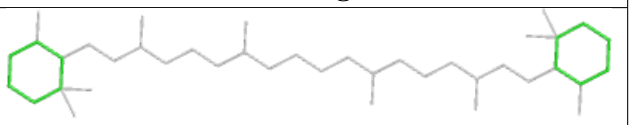
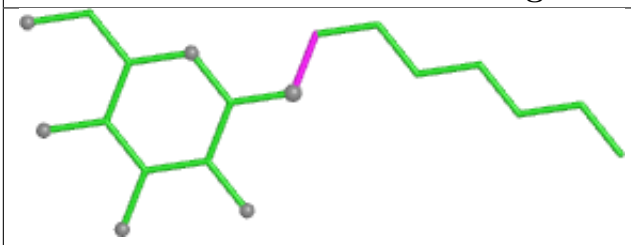


Rings

Ligand HTG c 523



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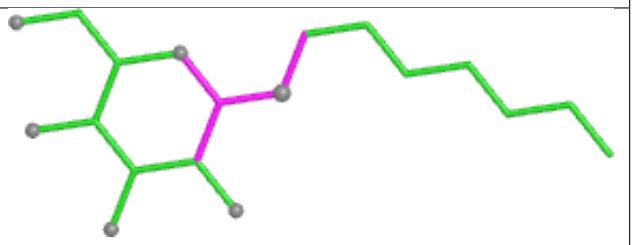
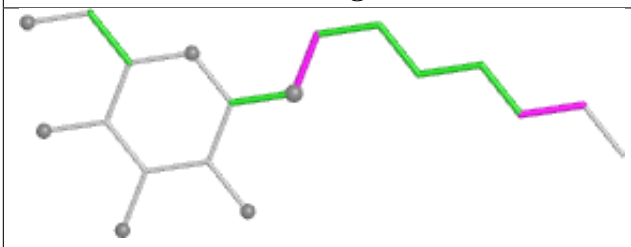


Bond angles



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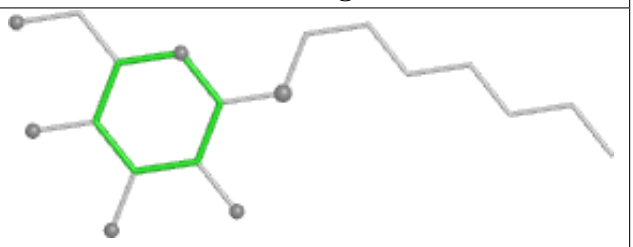
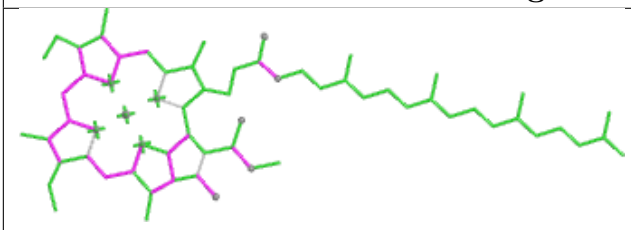
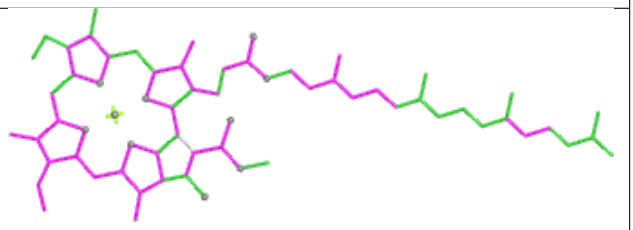


Rings

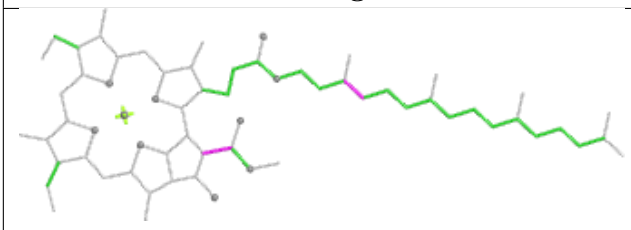
Ligand CLA b 609



Bond lengths



Bond angles



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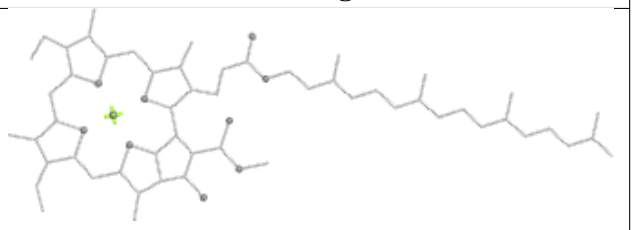
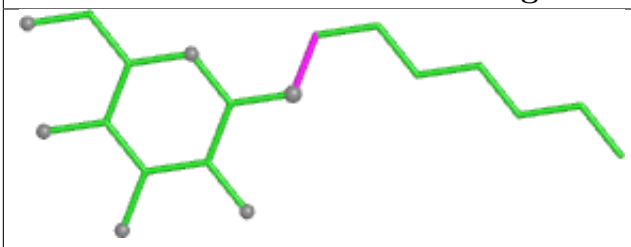
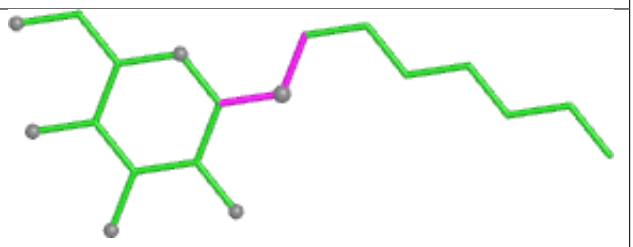


Rings

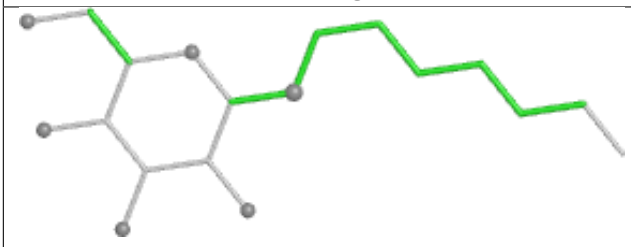
Ligand HTG C 522



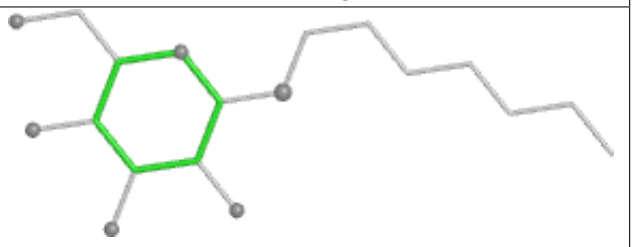
Bond lengths



Bond angles

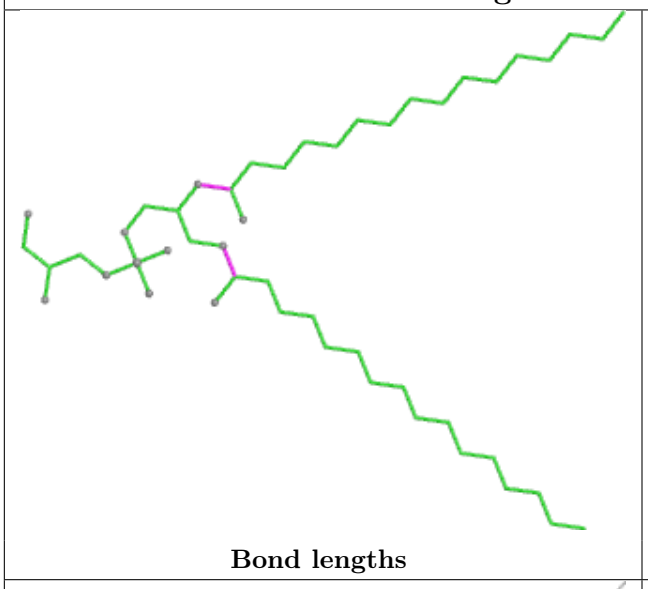


Torsions

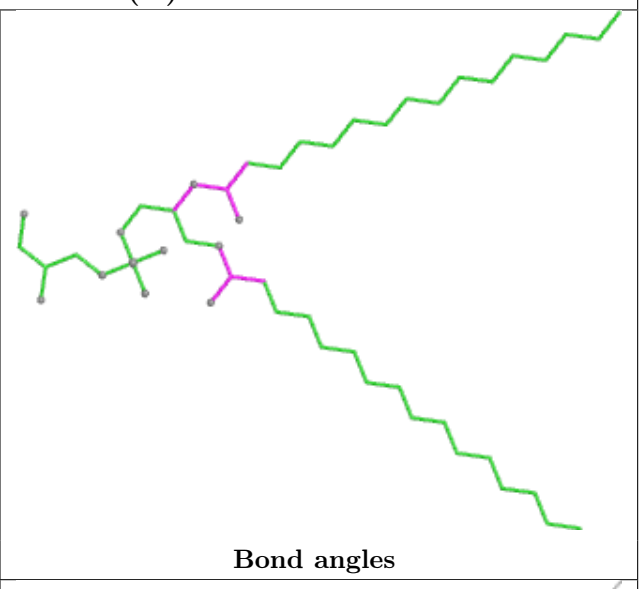


Rings

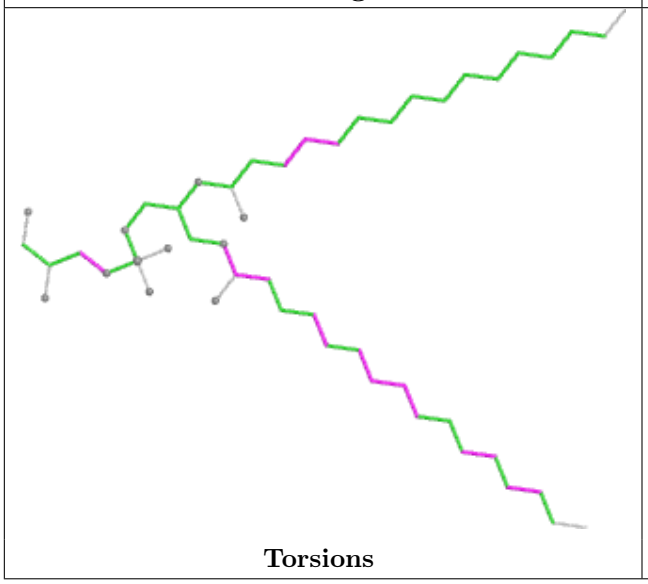
Ligand LHG d 408 (B)



Bond lengths



Bond angles



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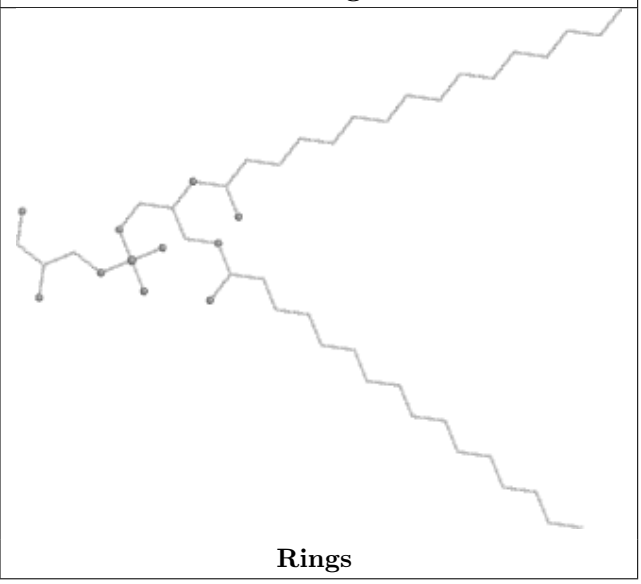
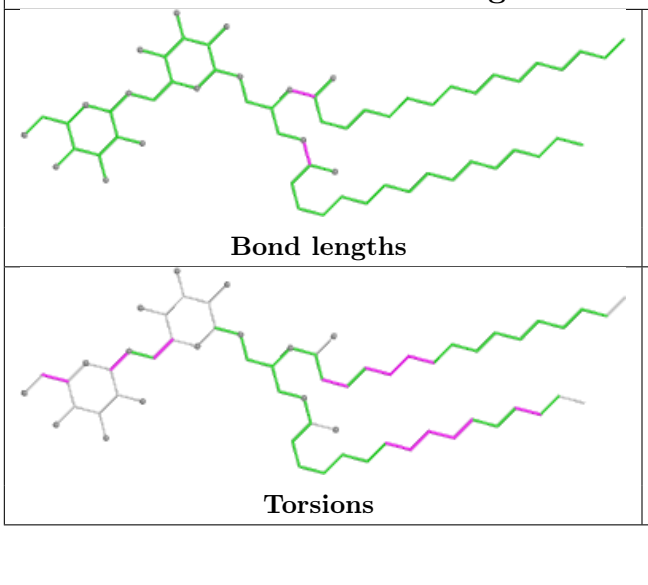


Rings

Ligand DGD C 517 (B)



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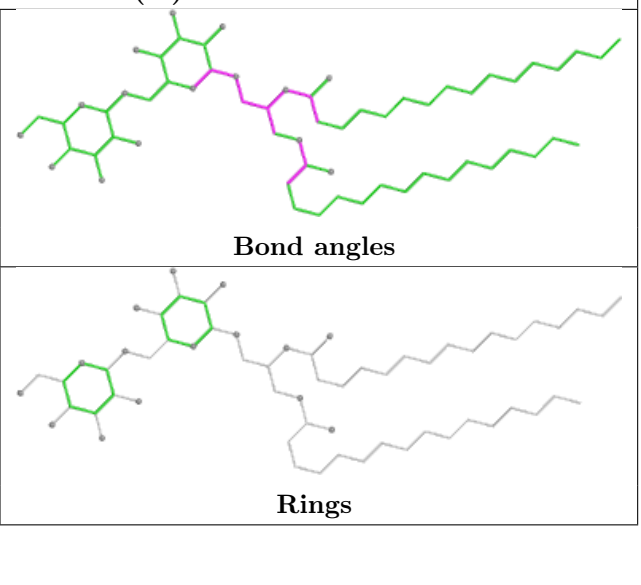
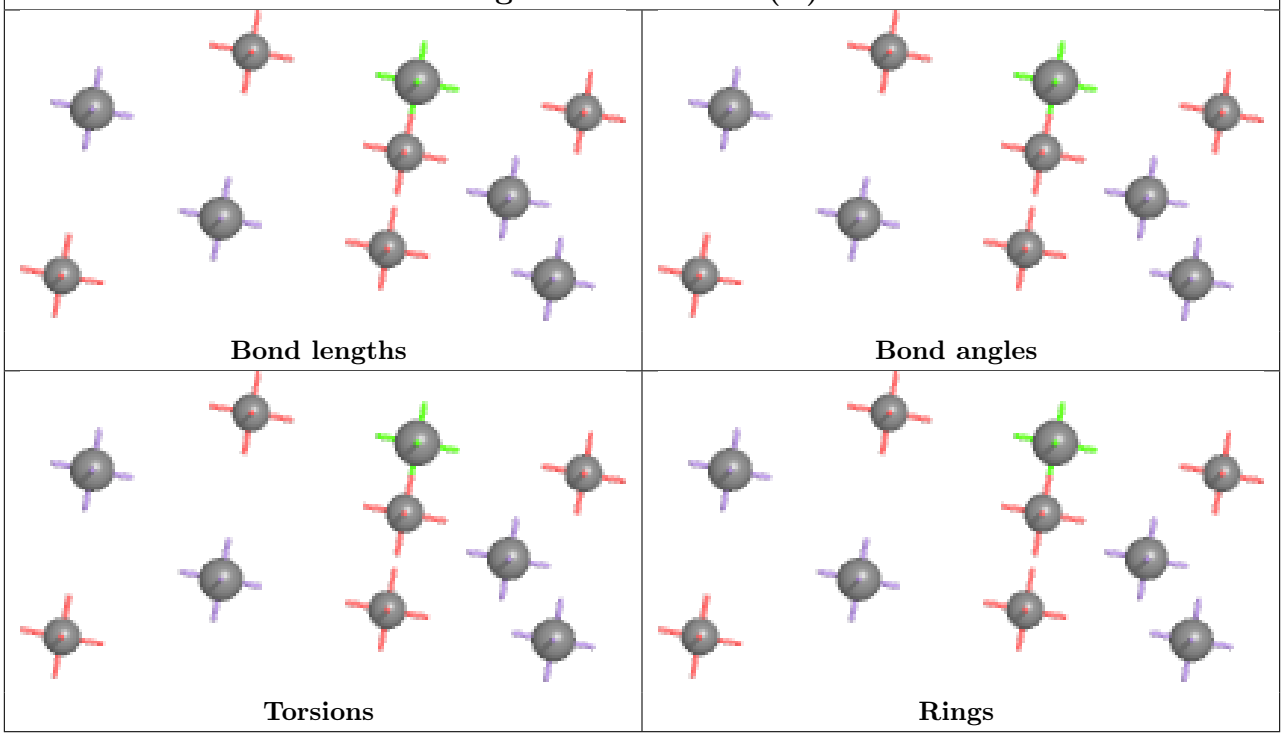


Bond angles

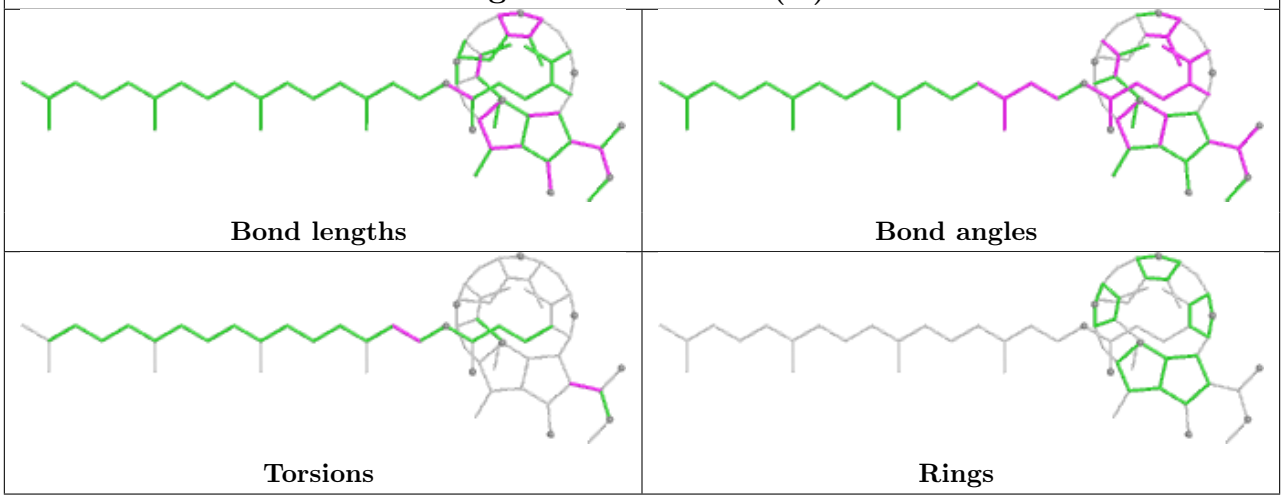
Torsions

Rings

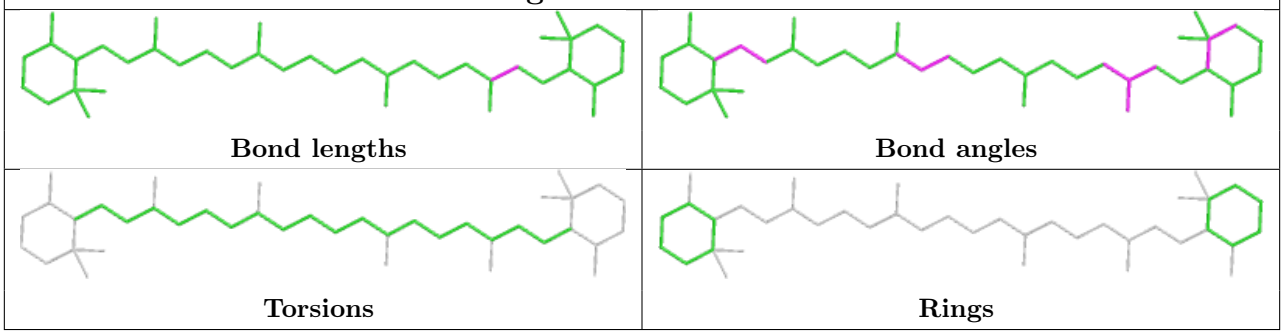
Ligand OEX a 411 (B)



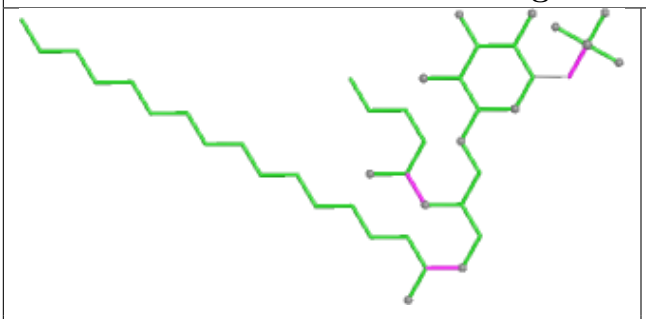
Ligand PHO A 407 (A)



Ligand BCR b 618



Ligand SQD f 102



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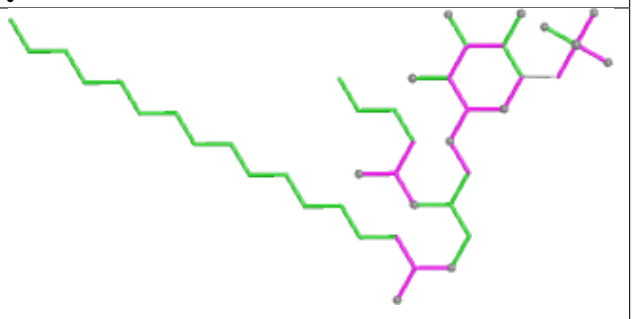
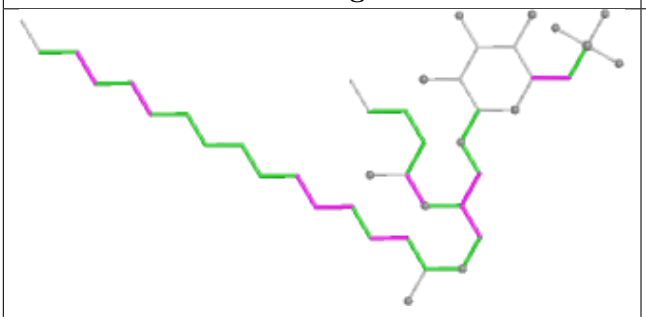


Bond angles



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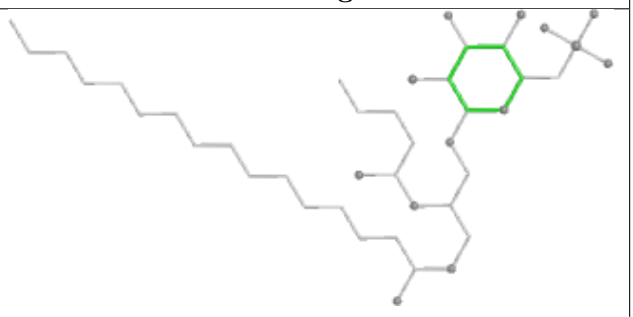
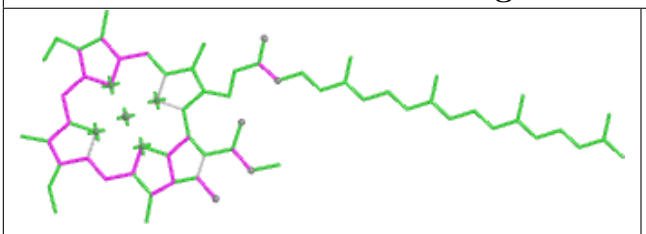


Rings

Ligand CLA a 405 (A)



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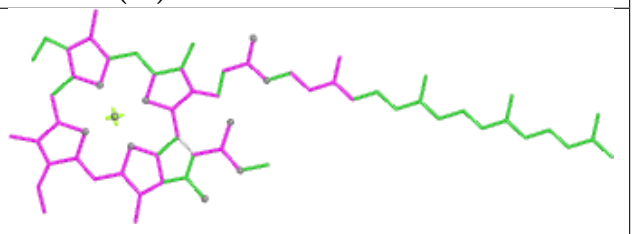
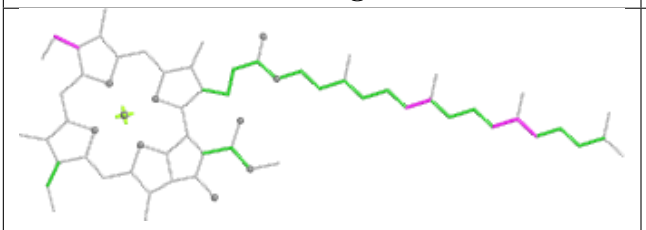


Bond angles



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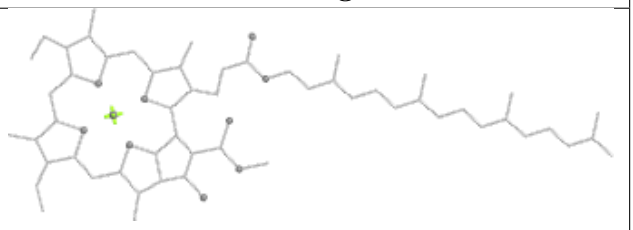
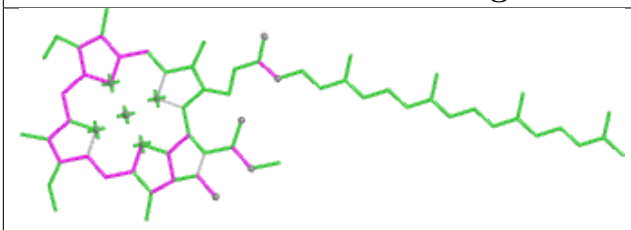


Rings

Ligand CLA A 404 (A)



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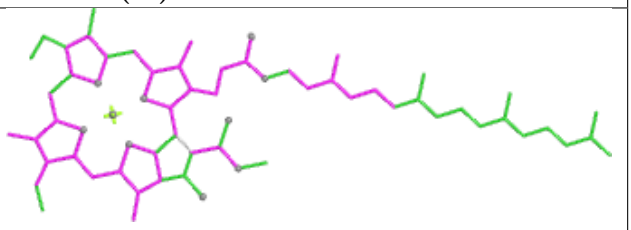
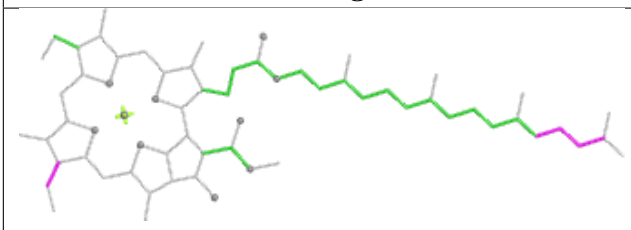


Bond angles



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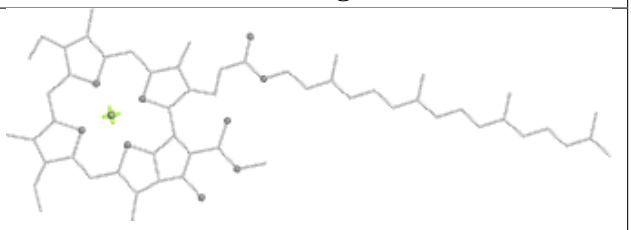
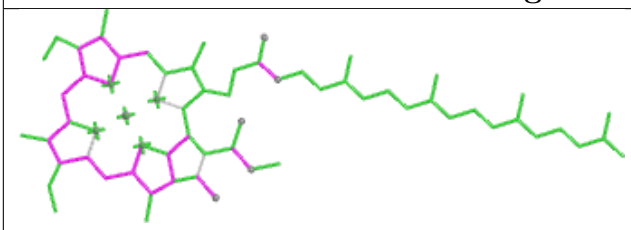


Rings

Ligand CLA C 507



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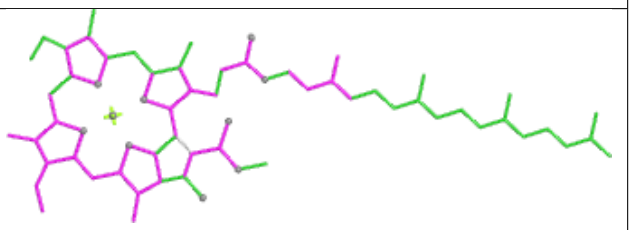
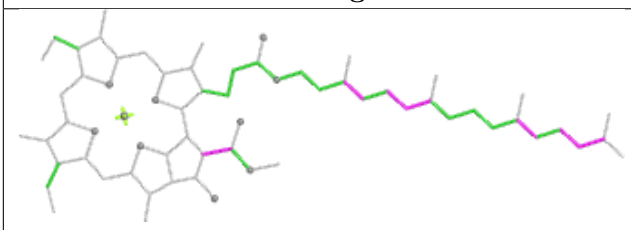


Bond angles



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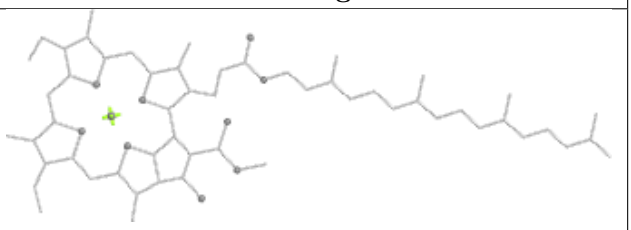
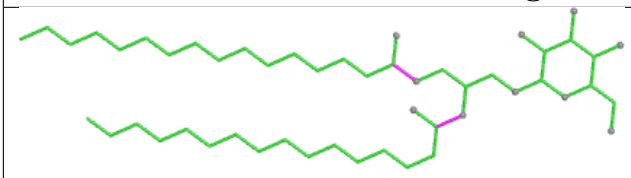


Rings

Ligand LMG c 521



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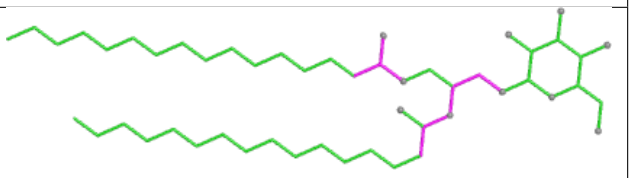
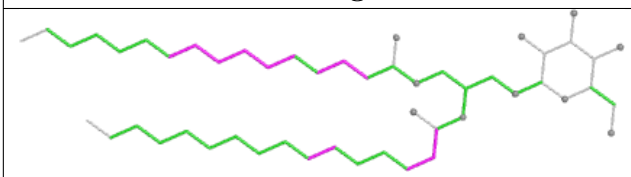


Bond angles



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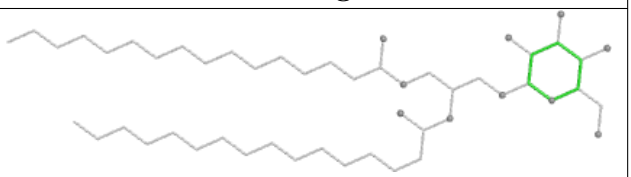
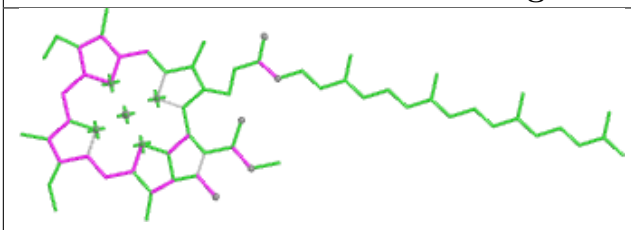


Rings

Ligand CLA b 613



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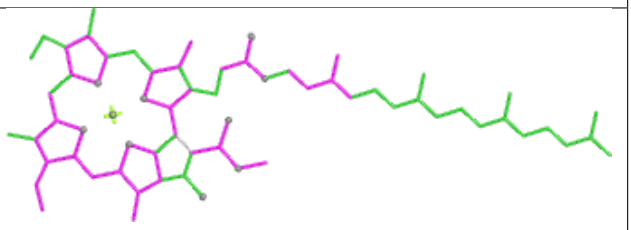
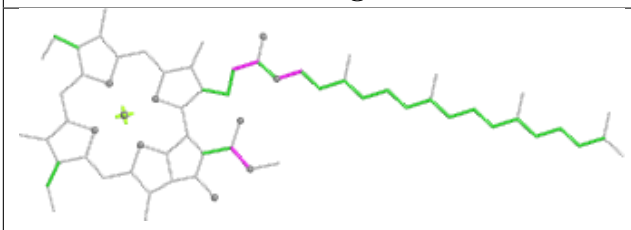


Bond angles



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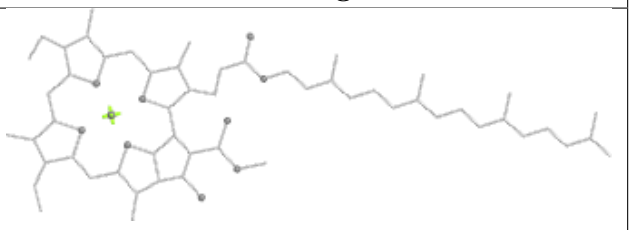
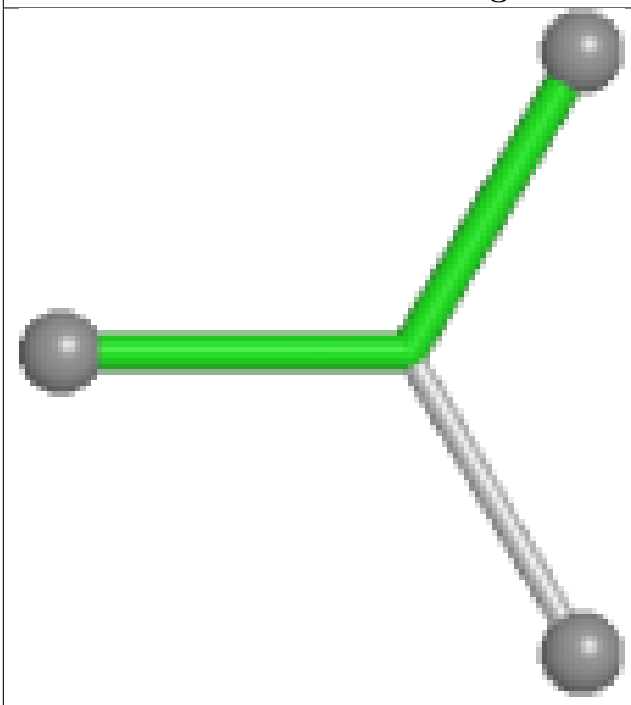


Rings

Ligand BCT D 401 (B)



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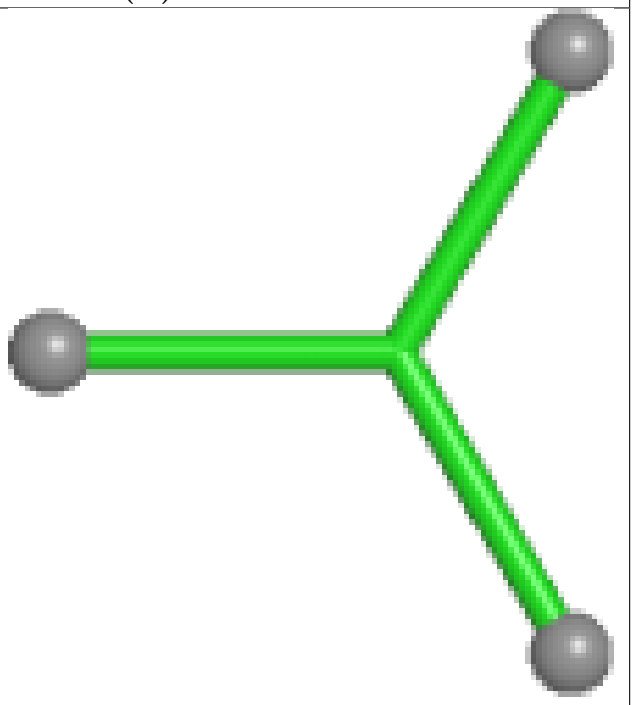
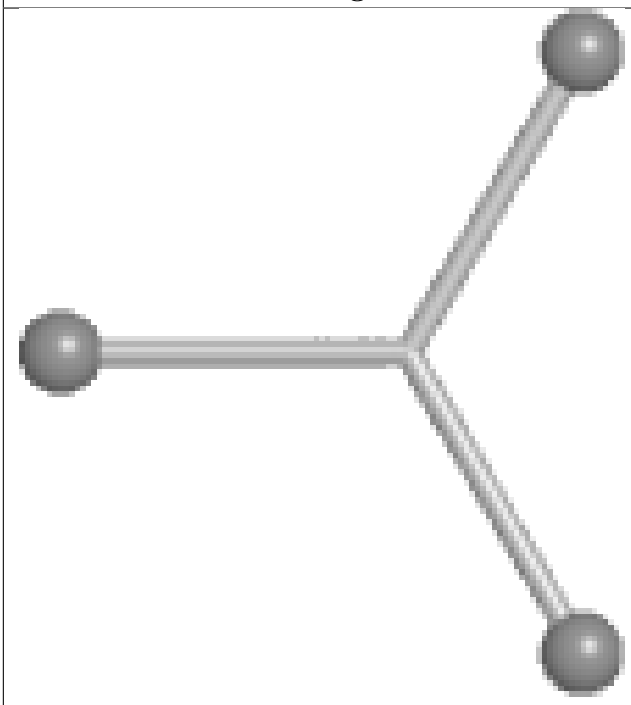


Bond angles



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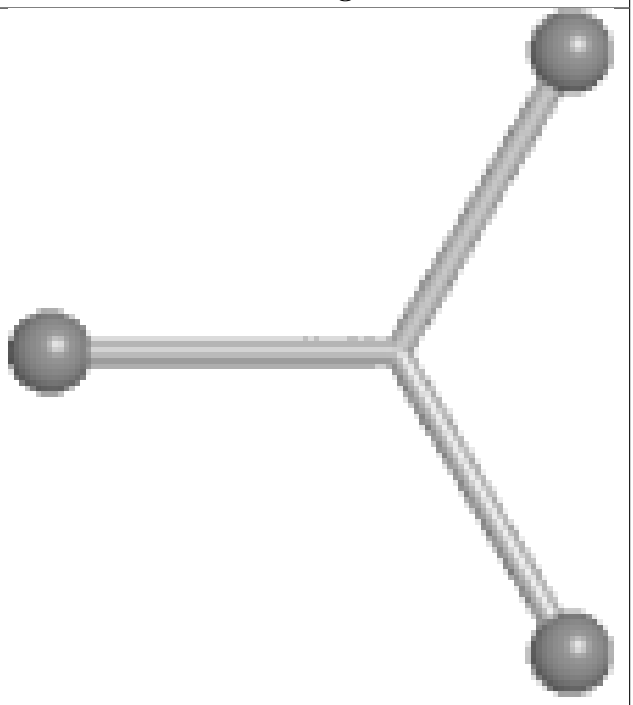
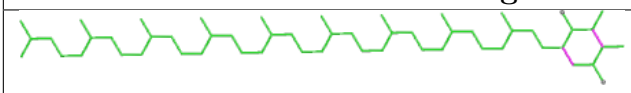


Rings

Ligand PL9 a 412 (A)



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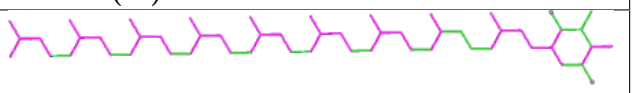
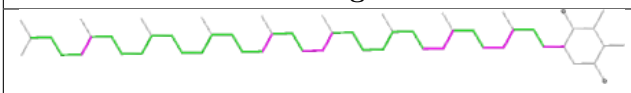


Bond angles



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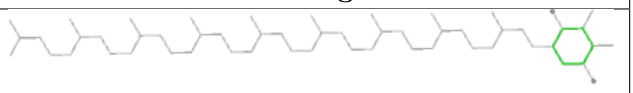
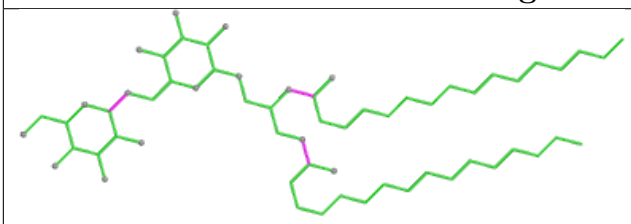


Rings

Ligand DGD H 101



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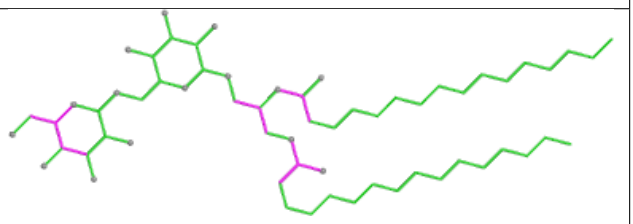
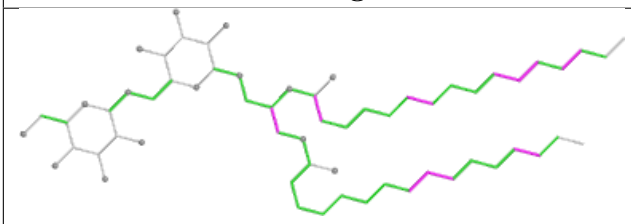


Bond angles



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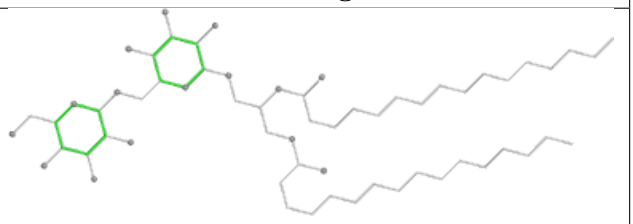
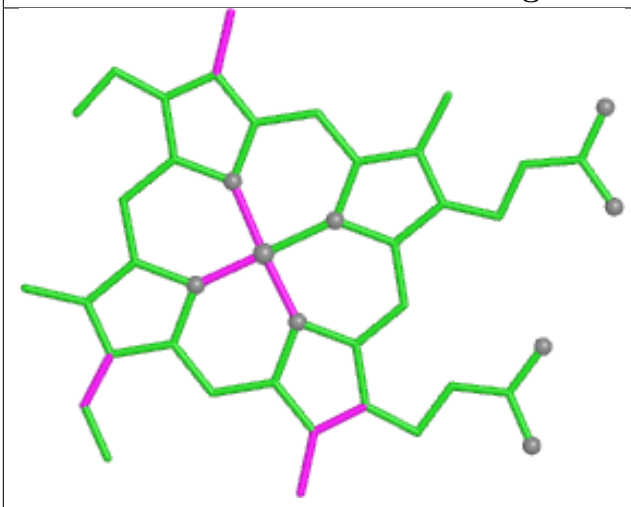


Rings

Ligand HEC V 201



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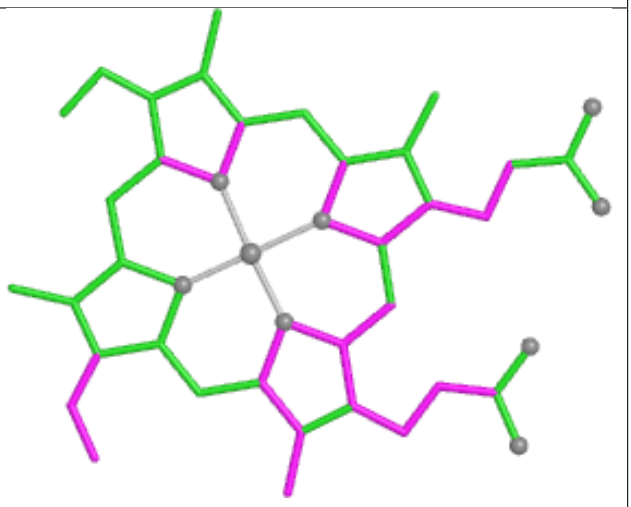
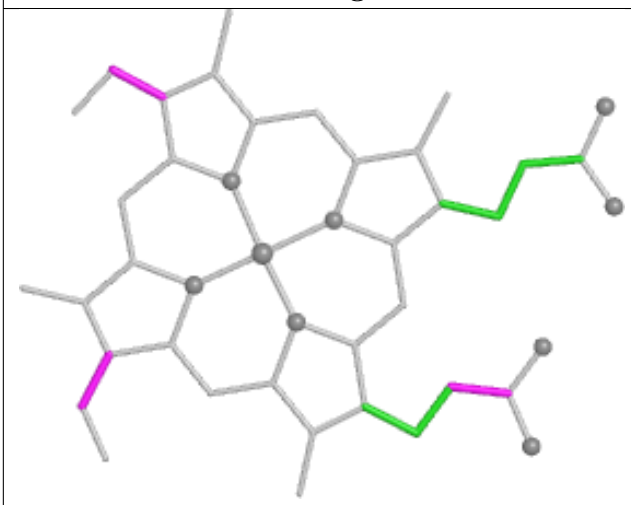


Bond angles



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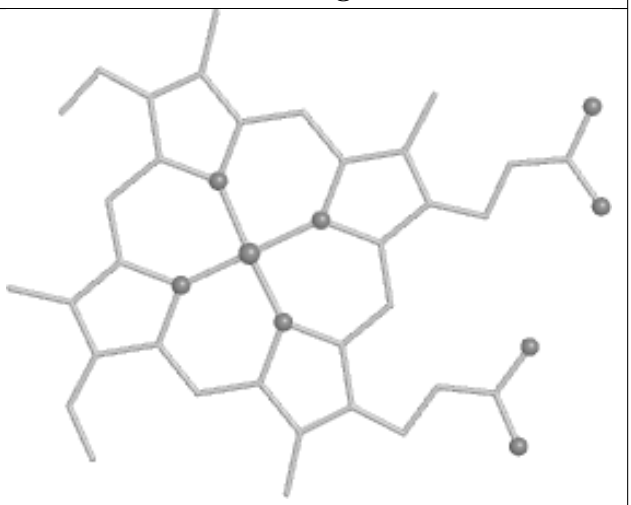
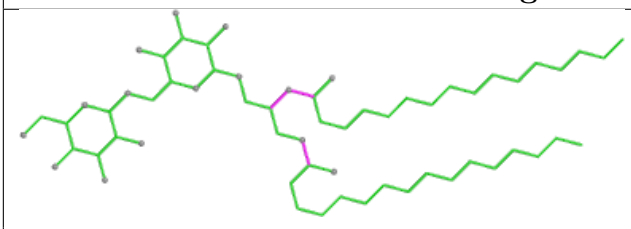


Rings

Ligand DGD C 519



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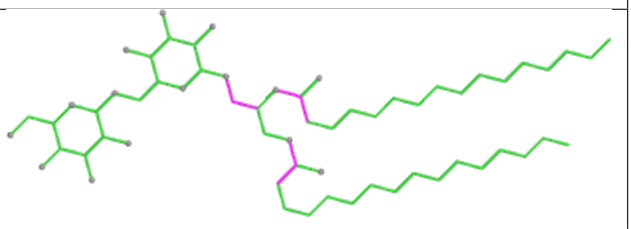
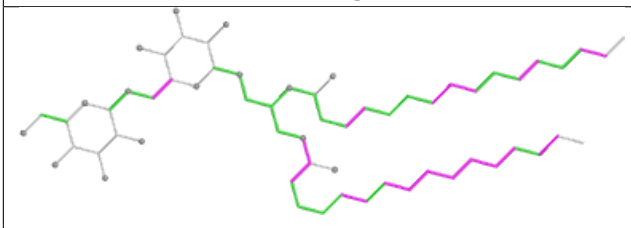


Bond angles



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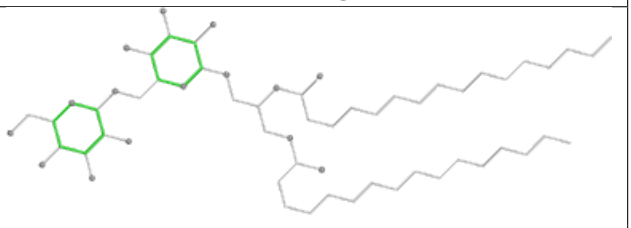

Rings

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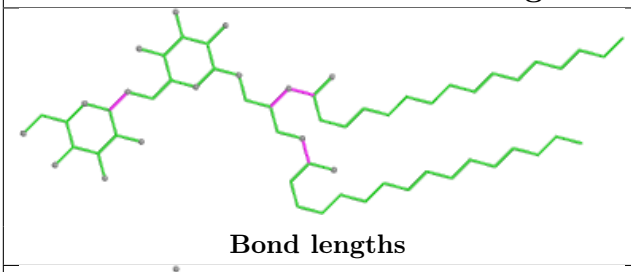
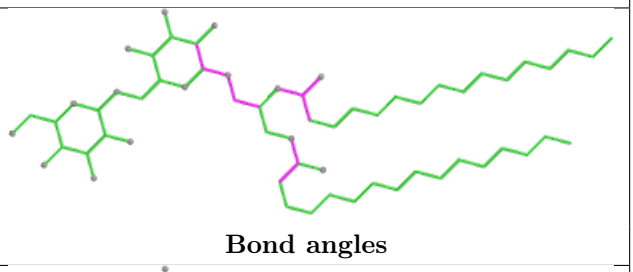
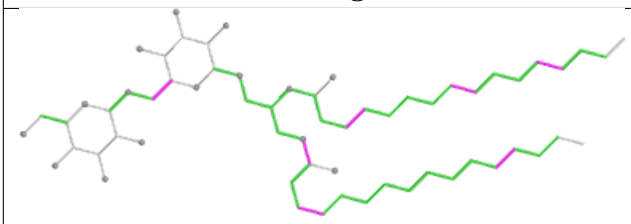


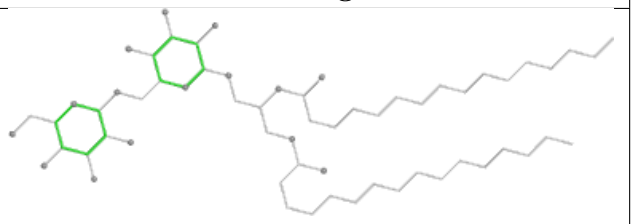
Bond lengths



Bond angles

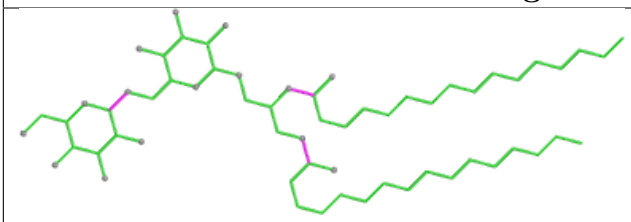


Torsions

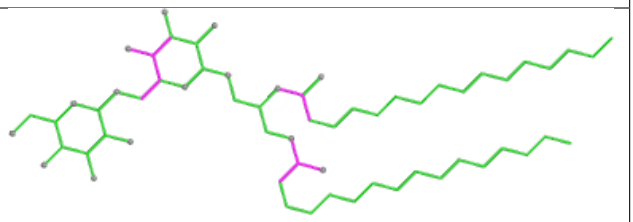


Rings

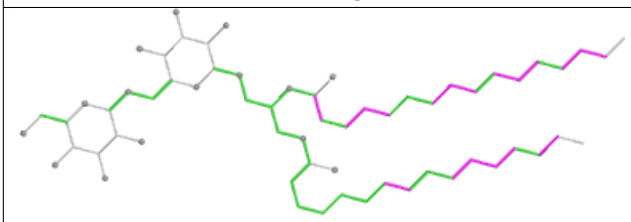
Ligand DGD h 102



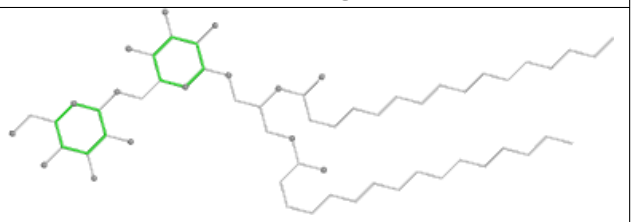
Bond lengths



Bond angles

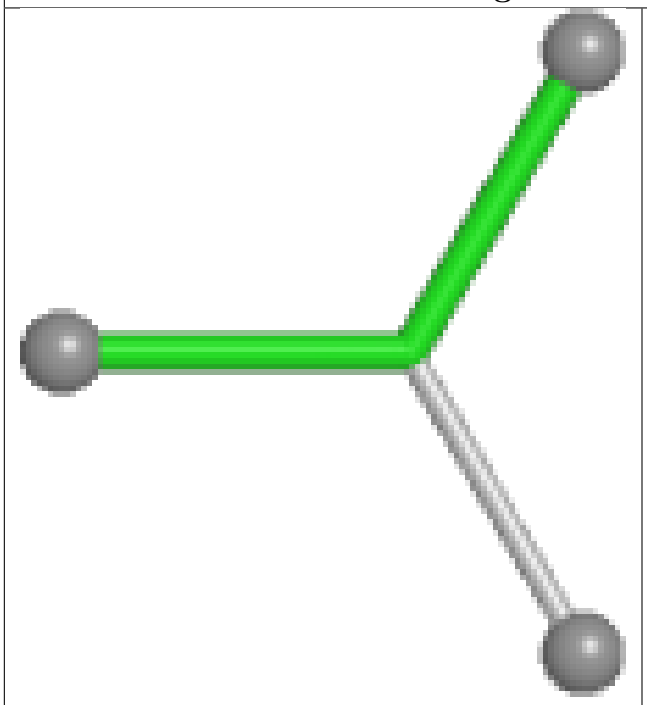


Torsions

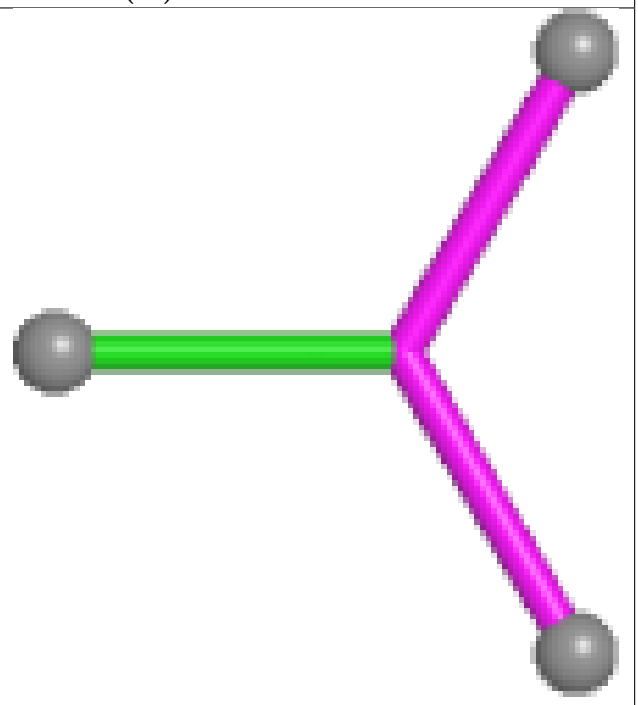


Rings

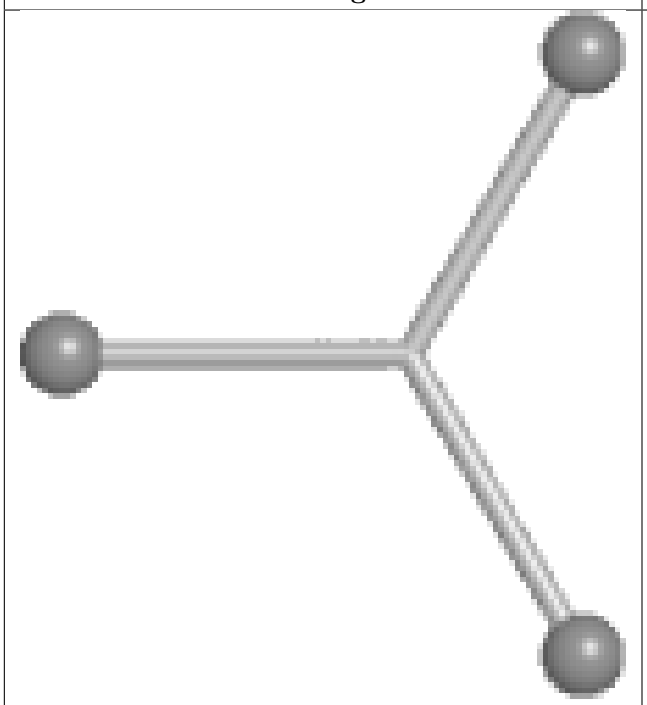
Ligand BCT d 401 (A)



Bond lengths



Bond angles



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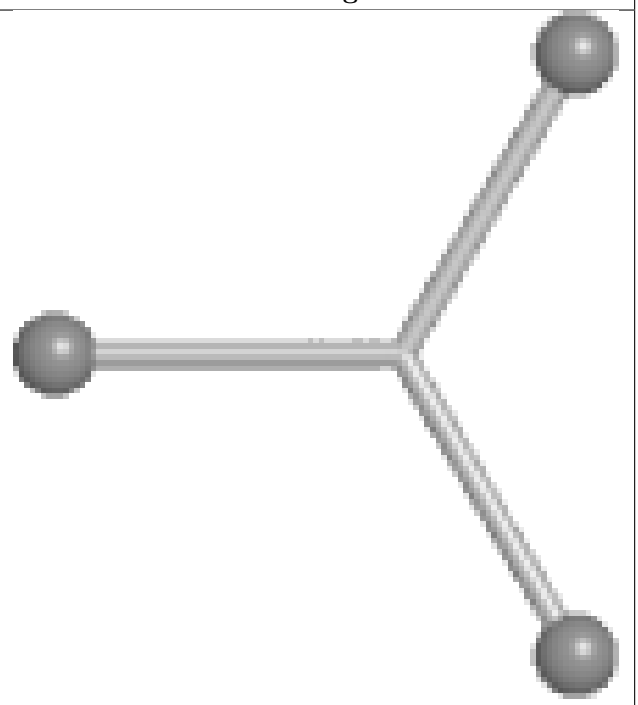
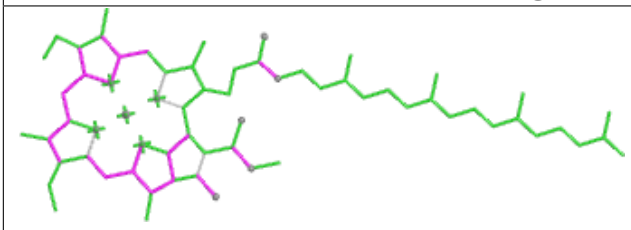
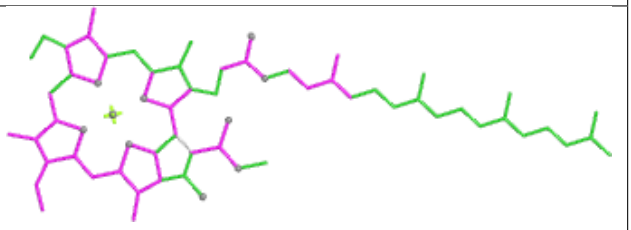


Rings

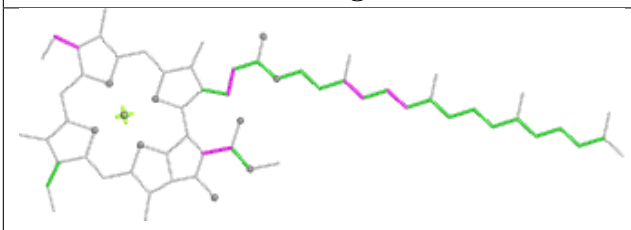
Ligand CLA c 509



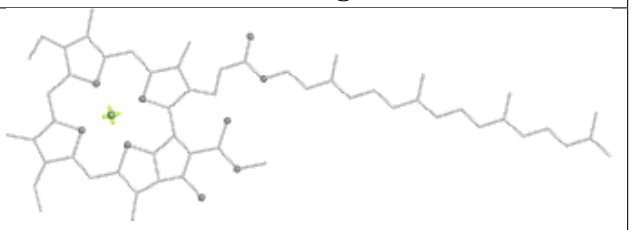
Bond lengths



Bond angles

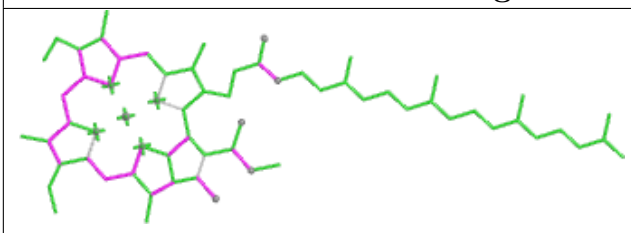


Torsions

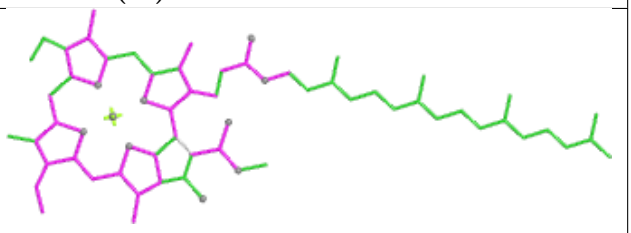


Rings

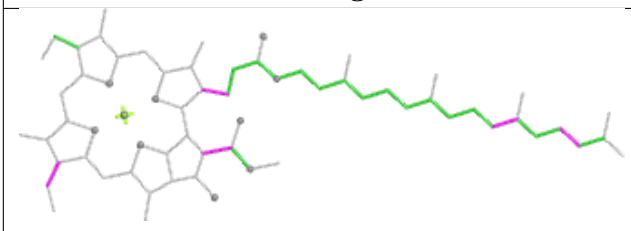
Ligand CLA d 402 (A)



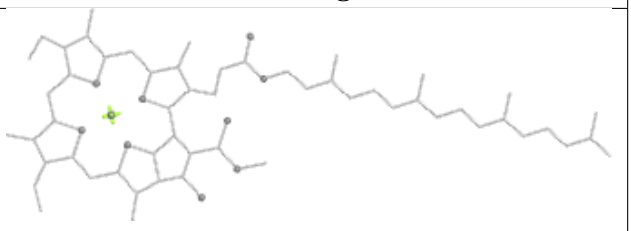
Bond lengths



Bond angles

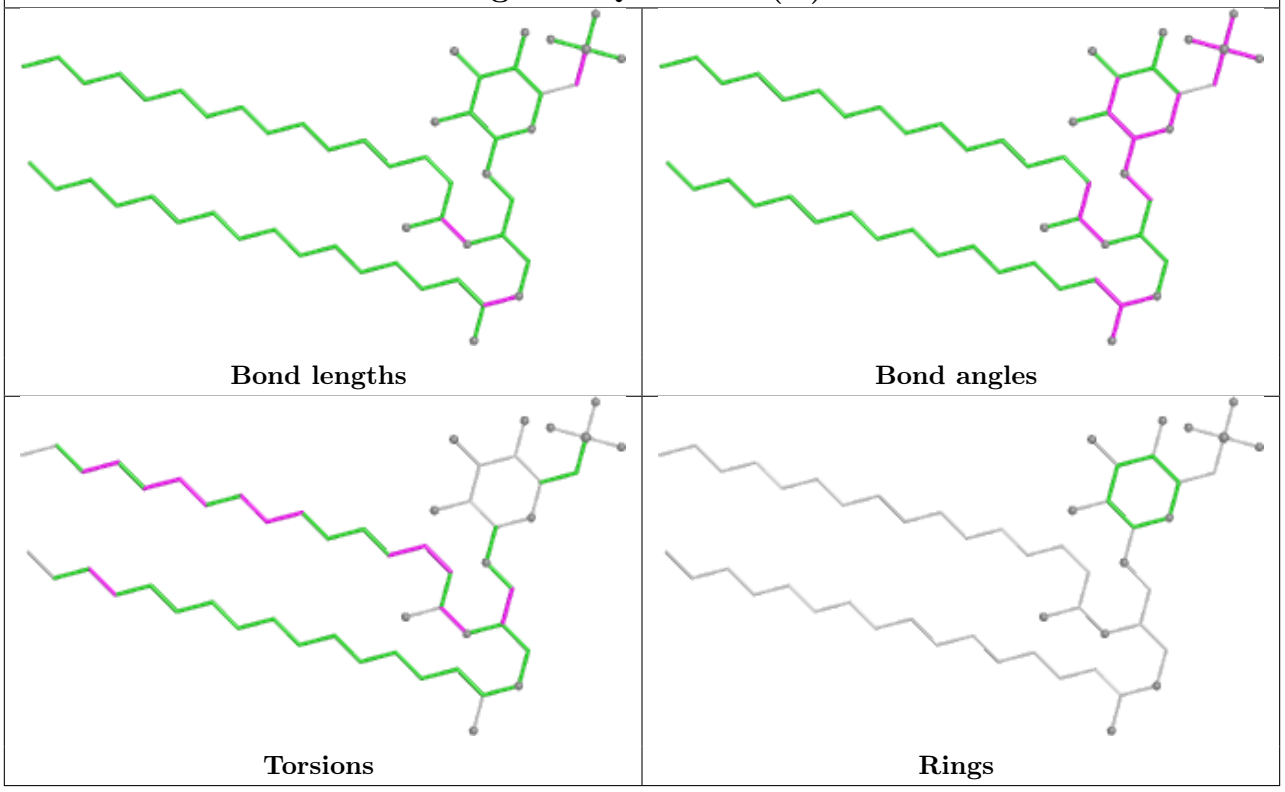


Torsions

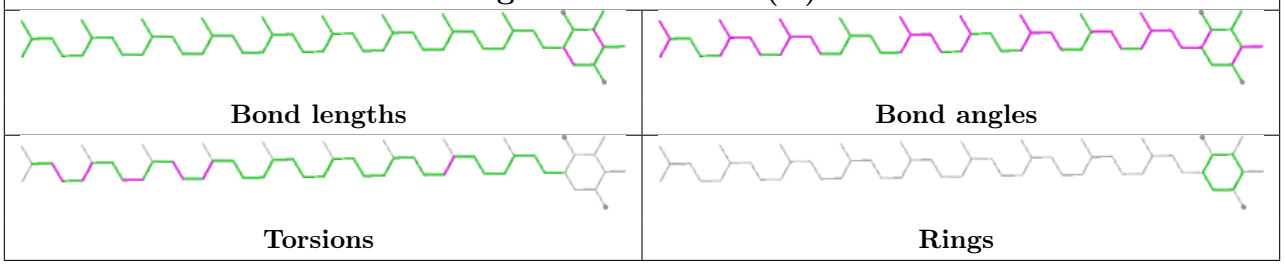


Rings

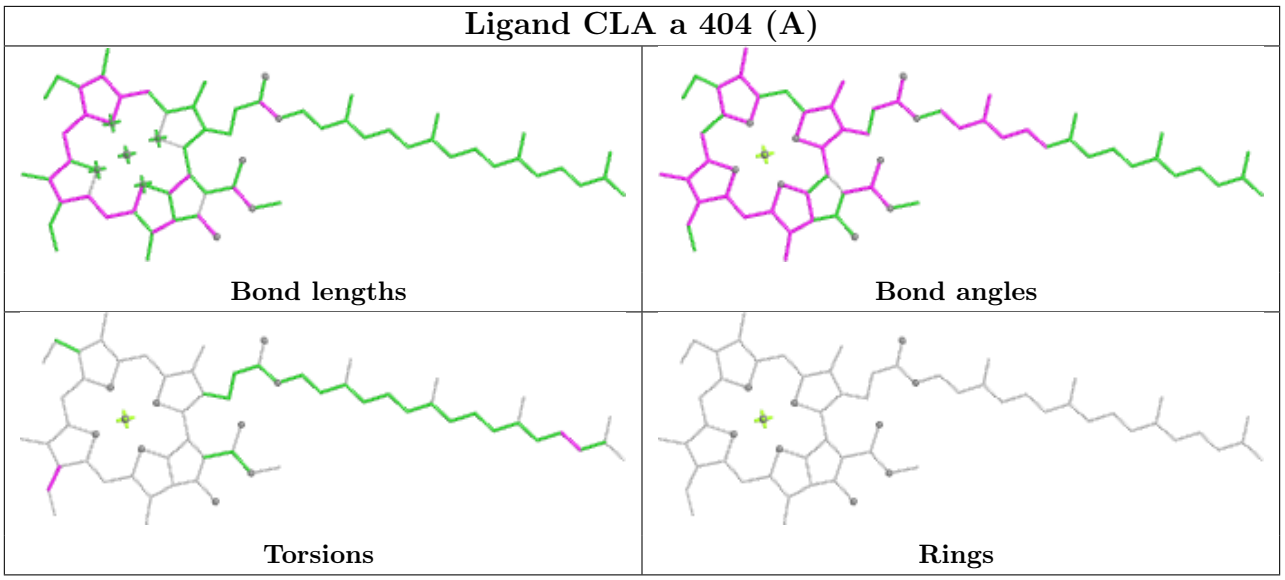
Ligand SQD A 410 (A)



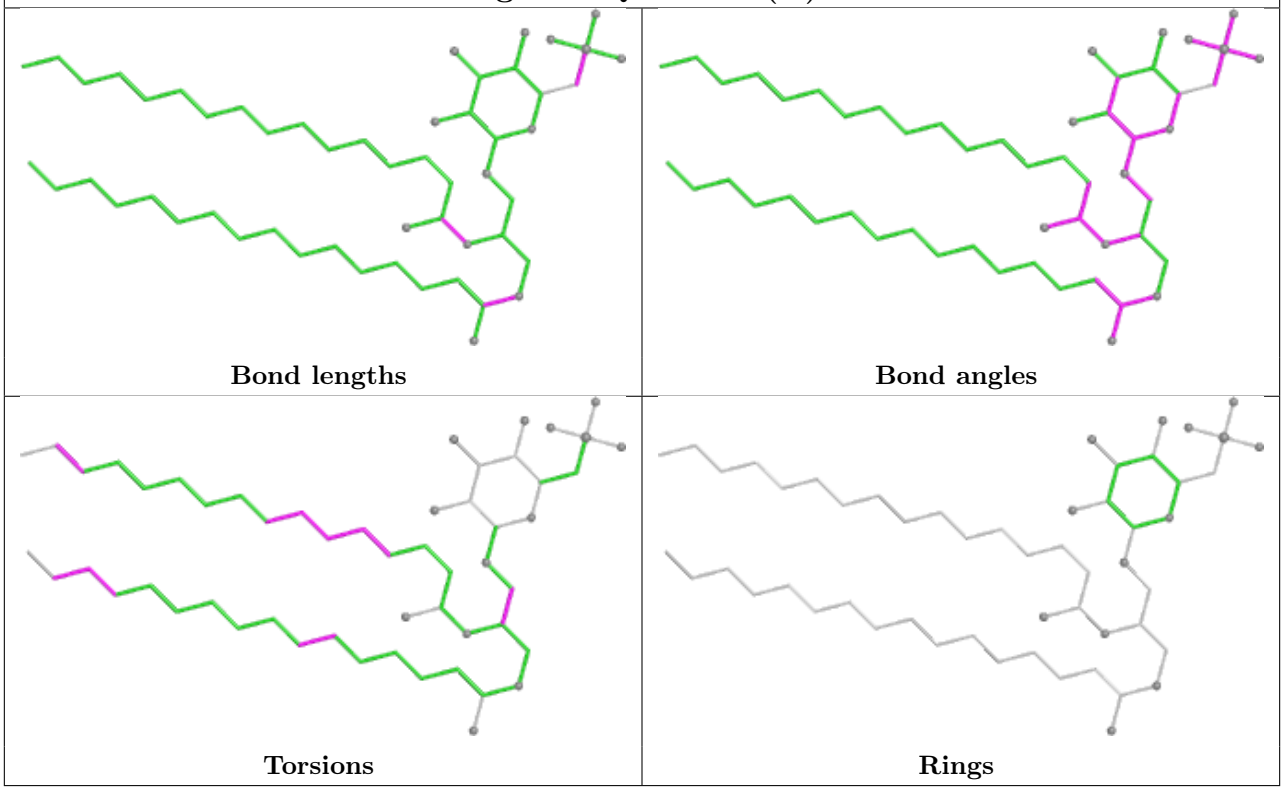
Ligand PL9 D 405 (B)



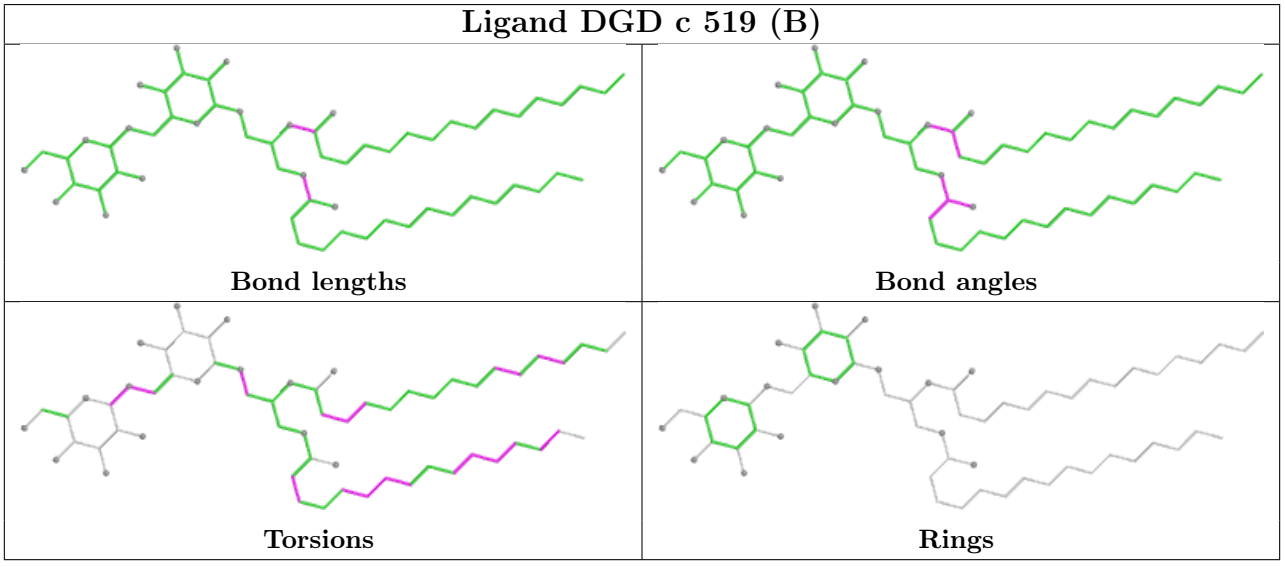
Ligand CLA a 404 (A)



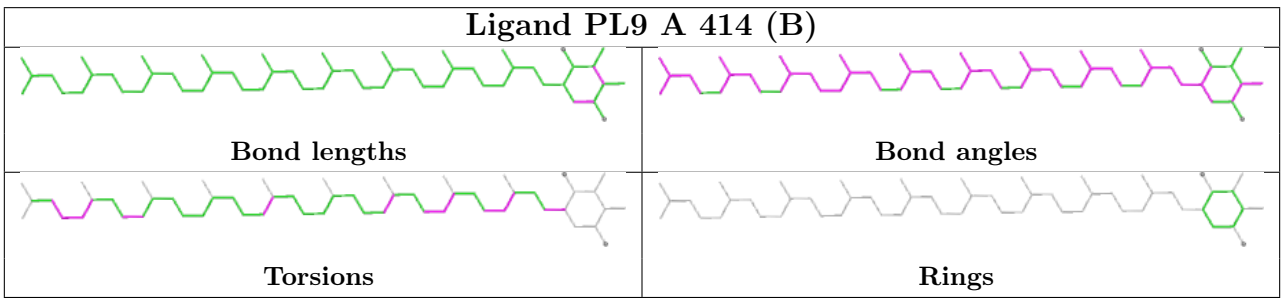
Ligand SQD a 409 (A)



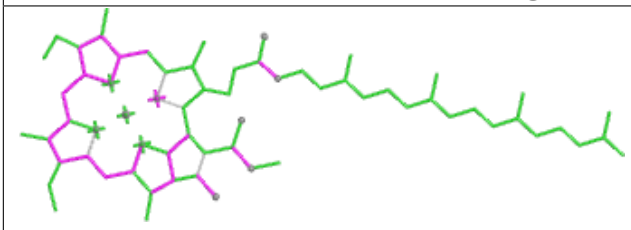
Ligand DGD c 519 (B)



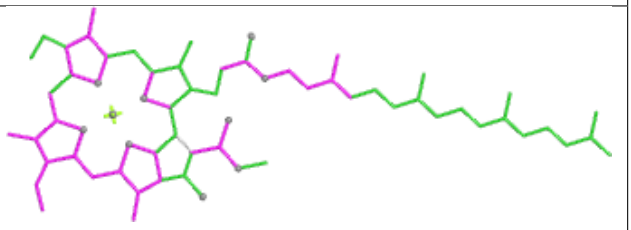
Ligand PL9 A 414 (B)



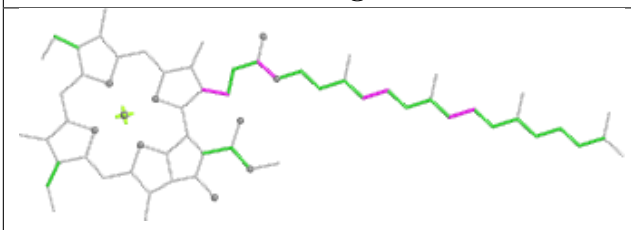
Ligand CLA C 512



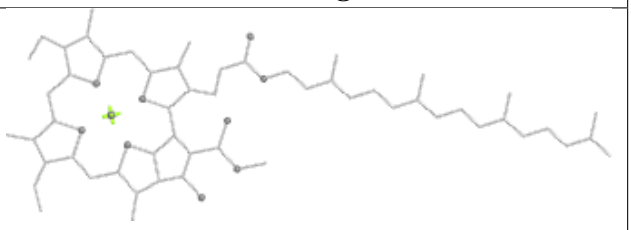
Bond lengths



Bond angles

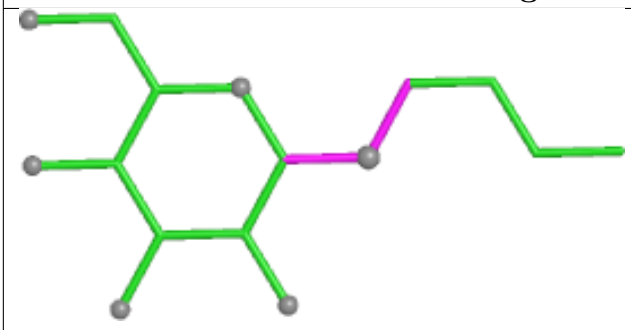


Torsions



Rings

Ligand HTG D 410



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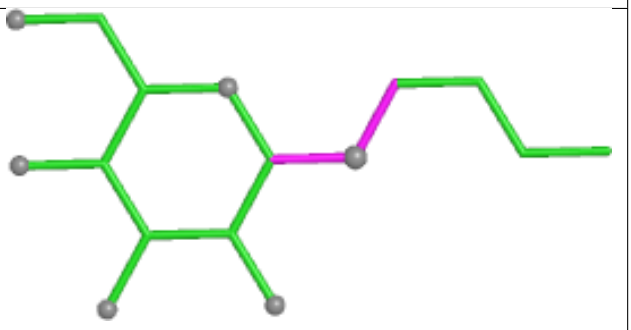
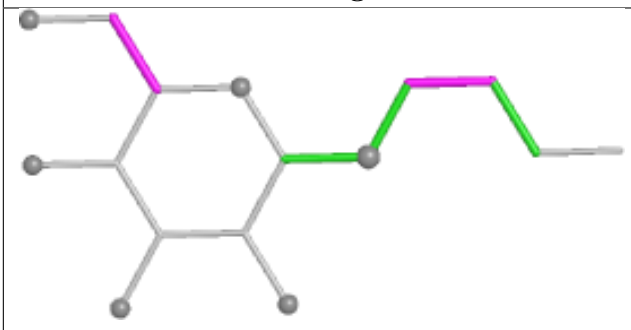


Bond angles



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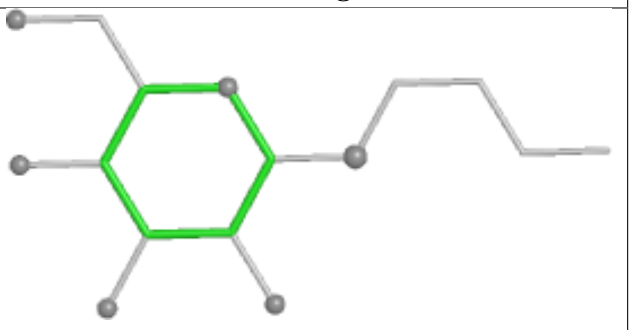
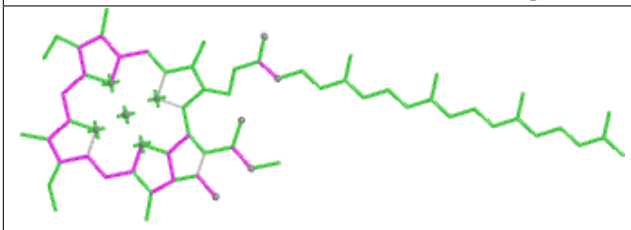


Rings

Ligand CLA C 502



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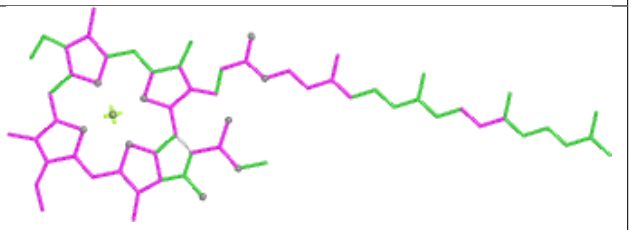
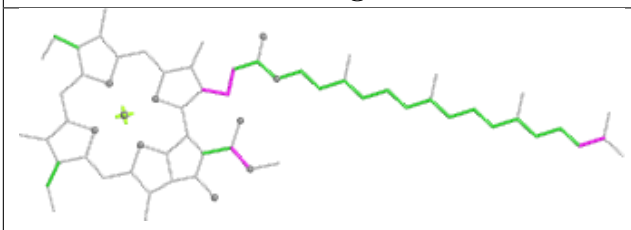


Bond angles



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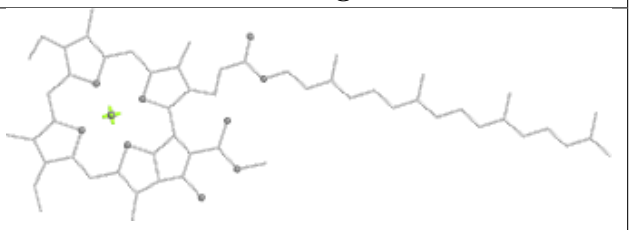
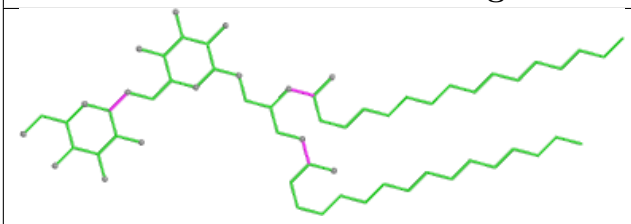


Rings

Ligand DGD C 518 (B)



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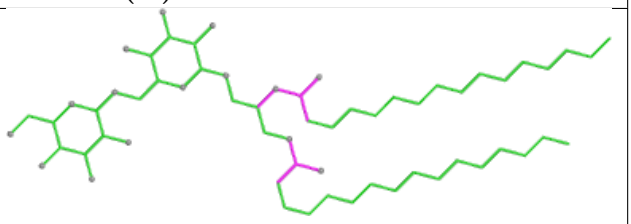
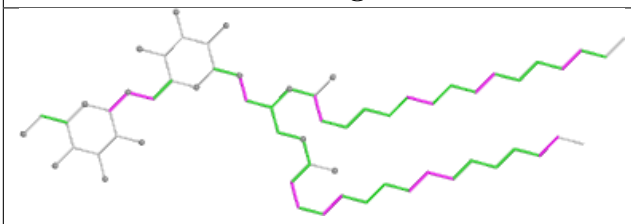


Bond angles



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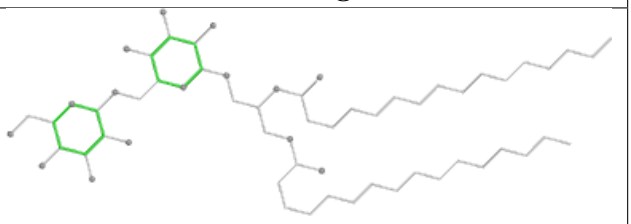
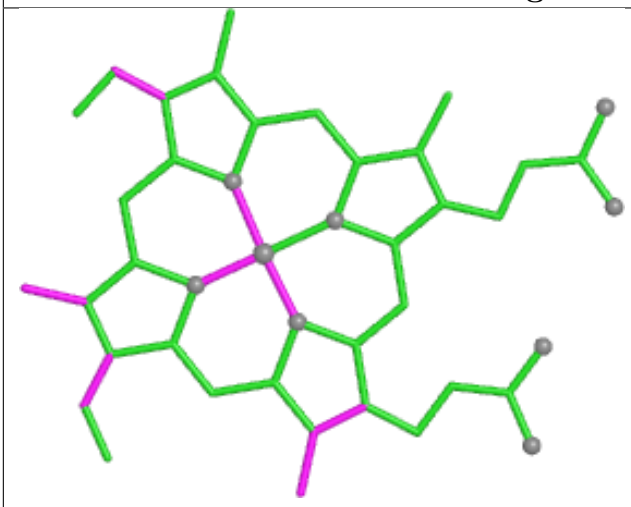


Rings

Ligand HEC v 201



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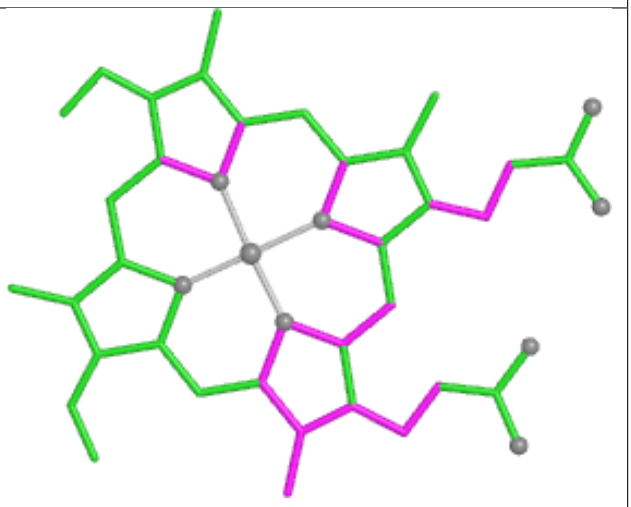
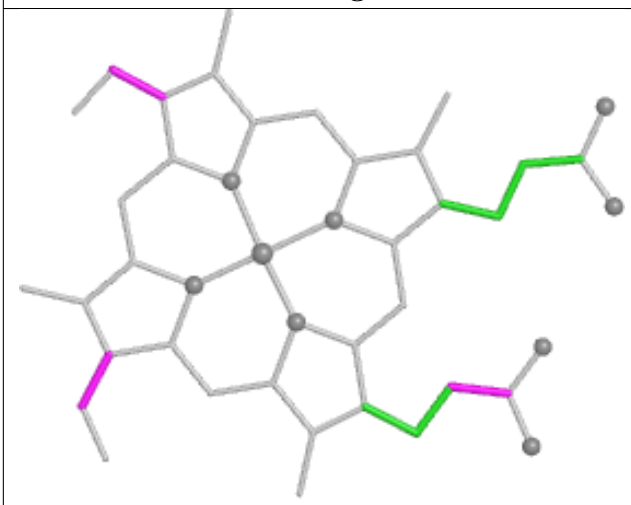


Bond angles



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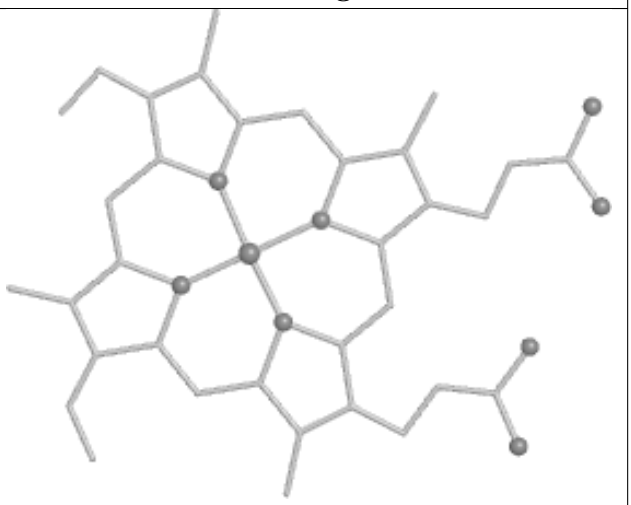
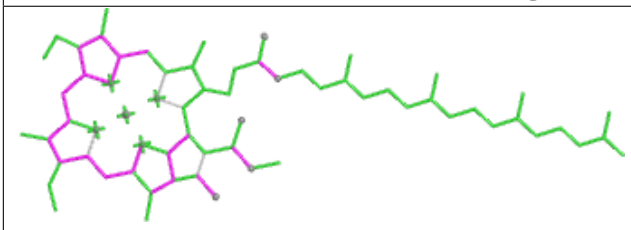


Rings

Ligand CLA C 503



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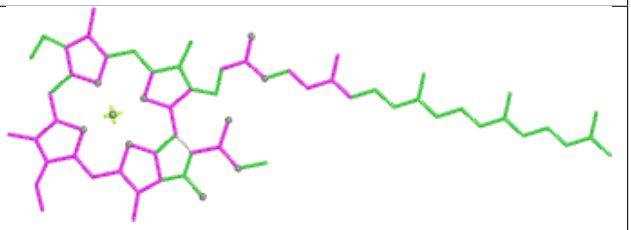
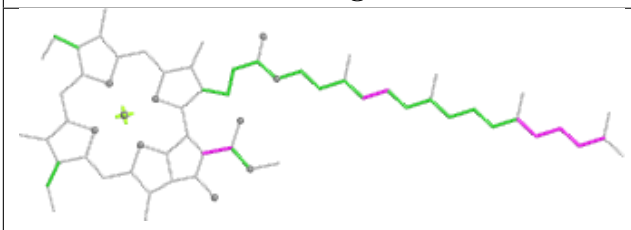


Bond angles



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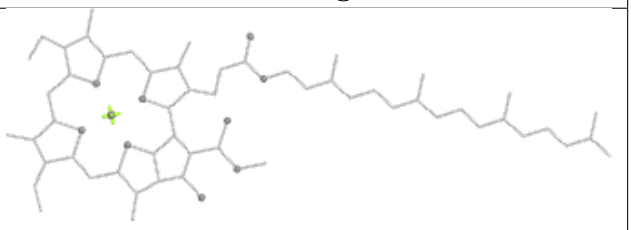
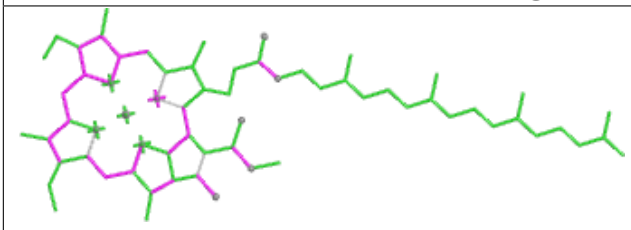
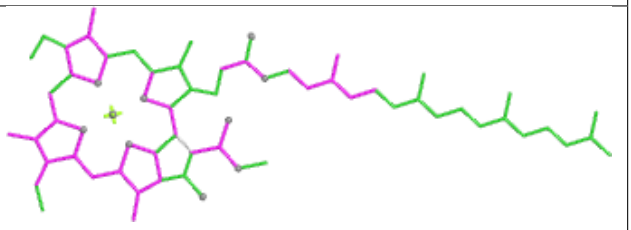


Rings

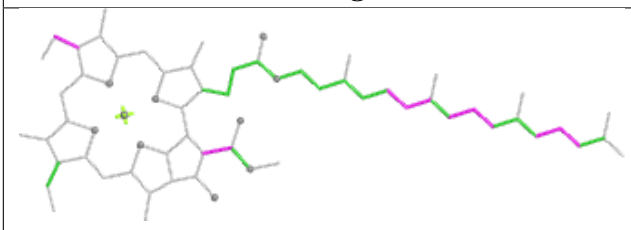
Ligand CLA b 604



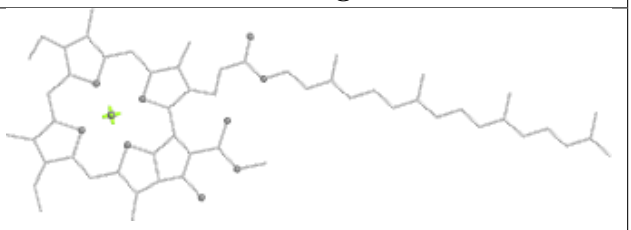
Bond lengths



Bond angles



Torsions

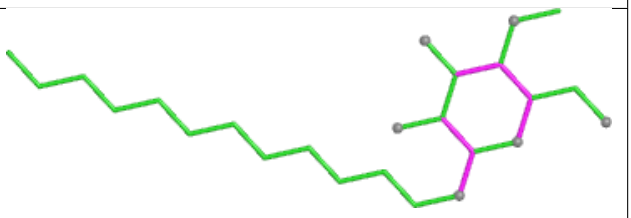


Rings

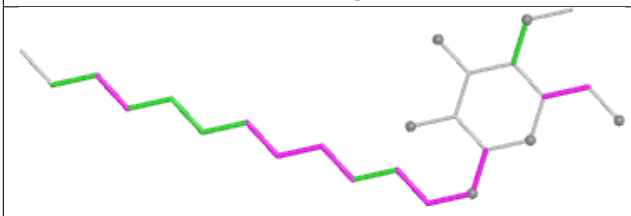
Ligand LMT B 630



Bond lengths



Bond angles



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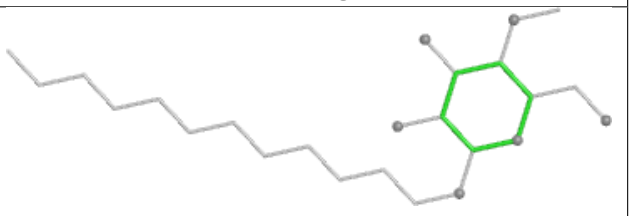
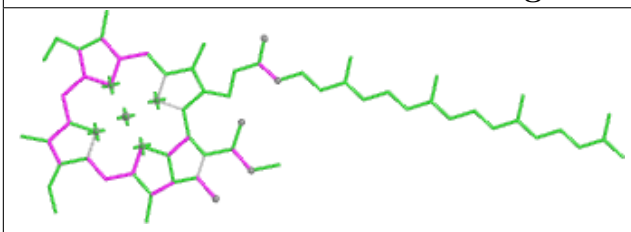
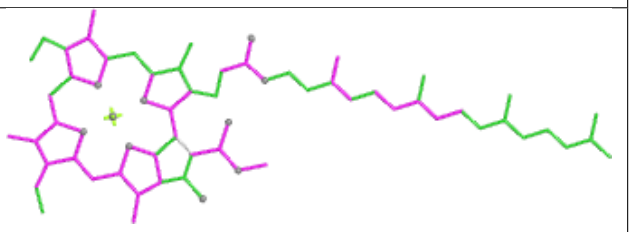


Rings

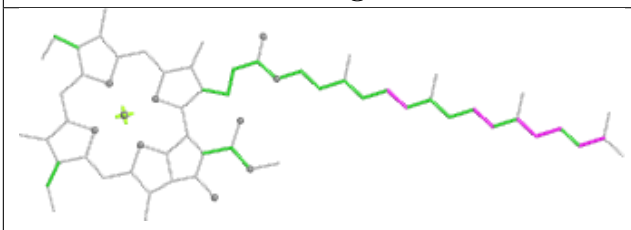
Ligand CLA B 615



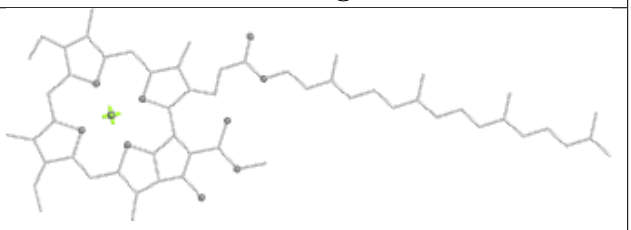
Bond lengths



Bond angles

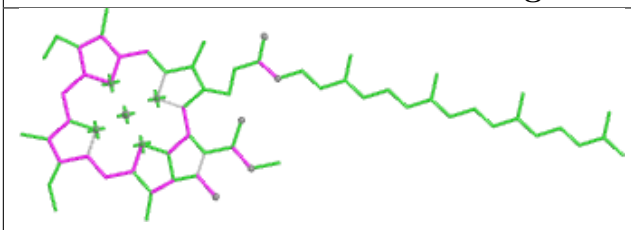


Torsions

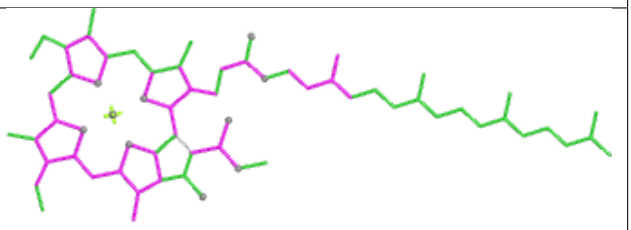


Rings

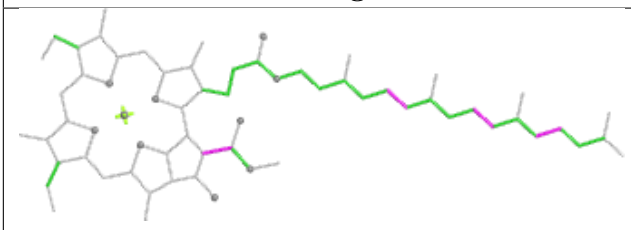
Ligand CLA C 509



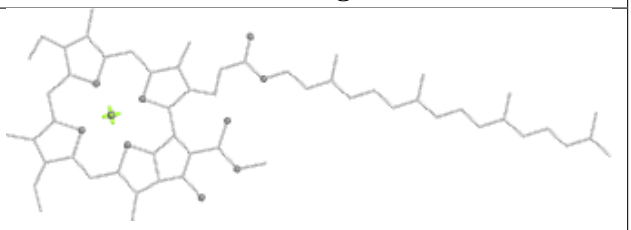
Bond lengths



Bond angles

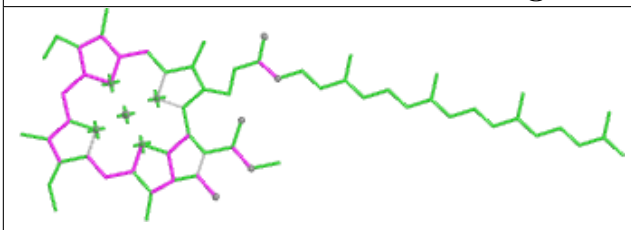


Torsions

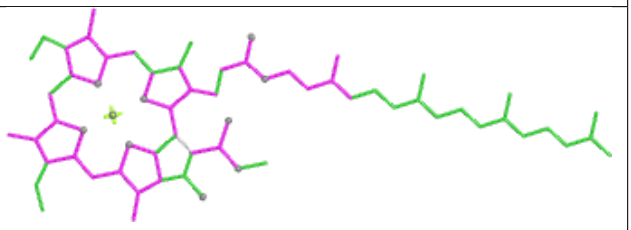


Rings

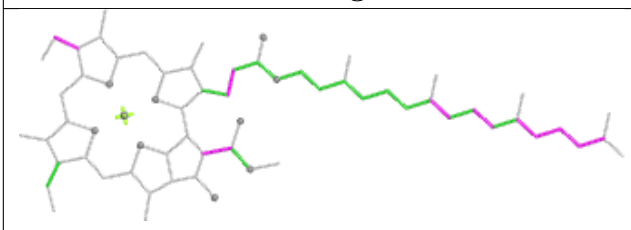
Ligand CLA b 606



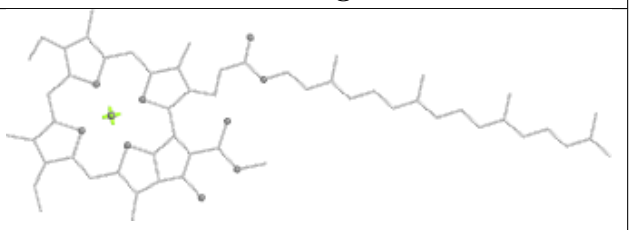
Bond lengths



Bond angles

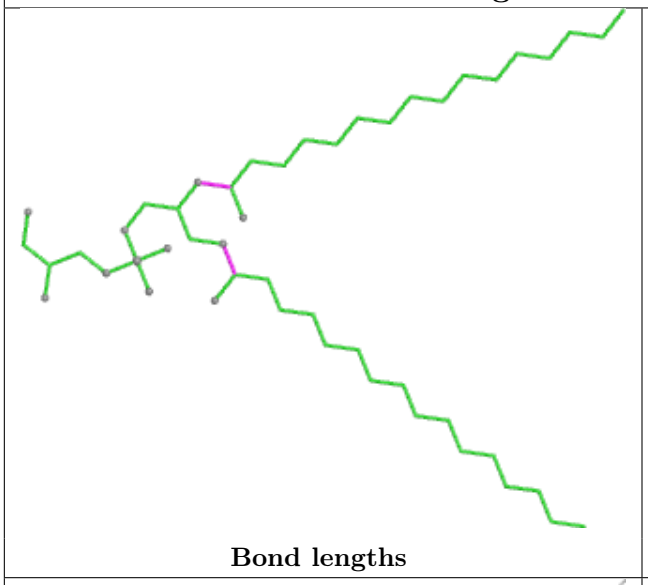


Torsions

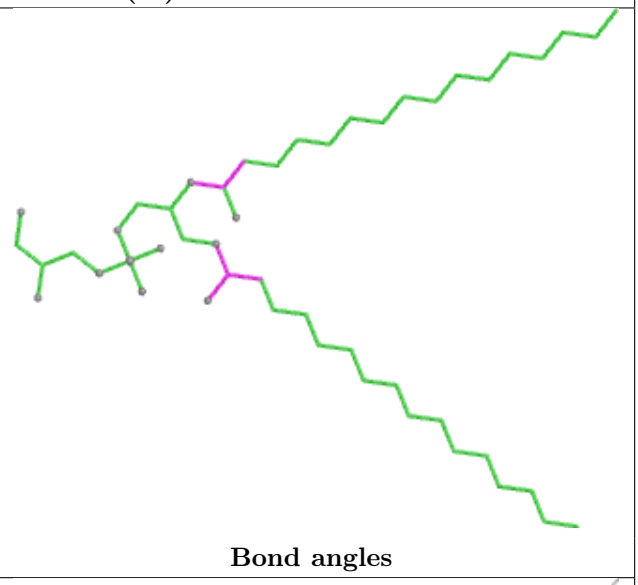


Rings

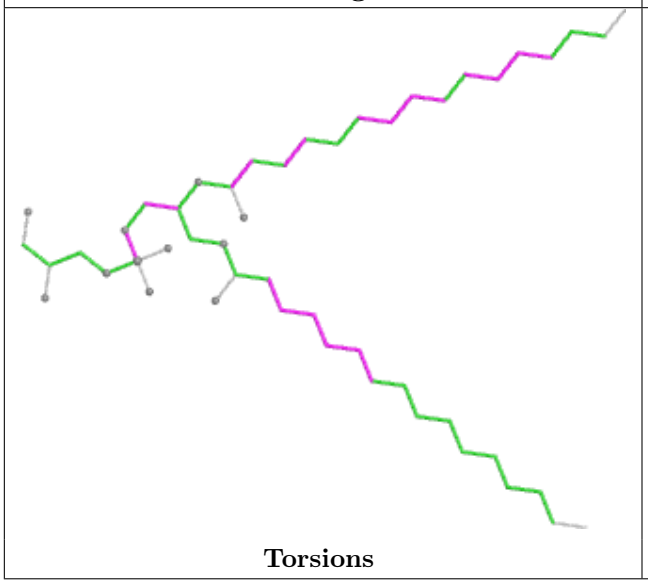
Ligand LHG L 101 (A)



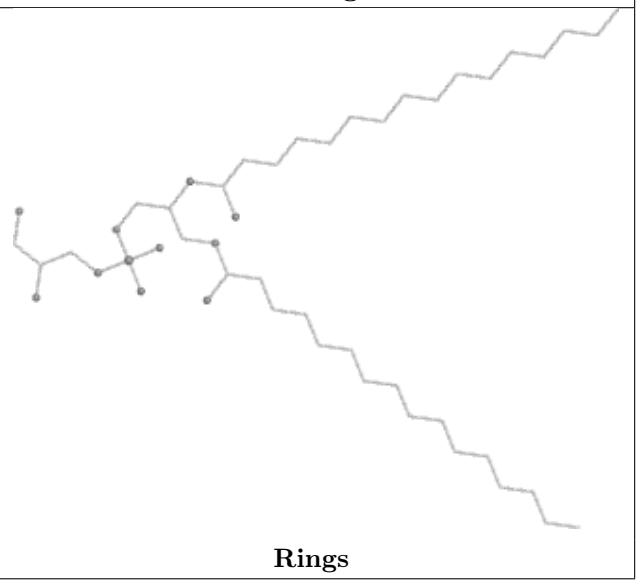
Bond lengths



Bond angles

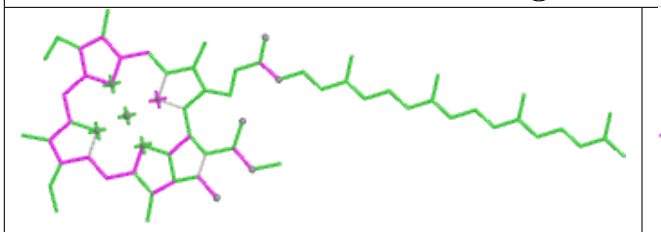


Torsions

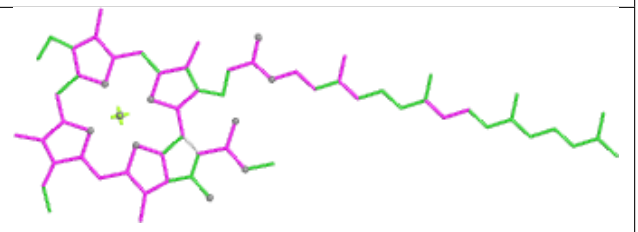


Rings

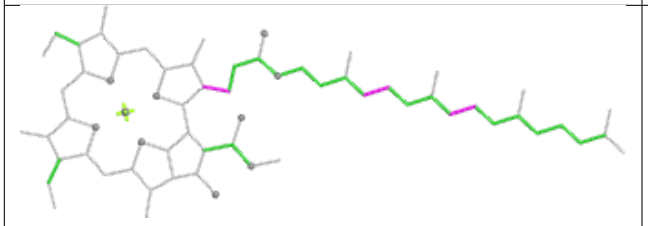
Ligand CLA c 513



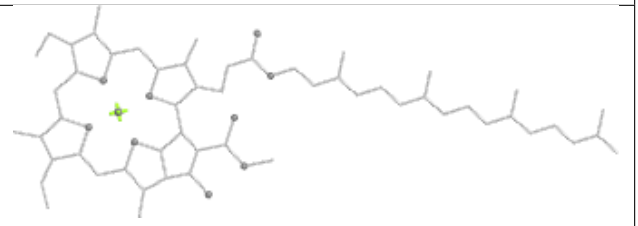
Bond lengths



Bond angles

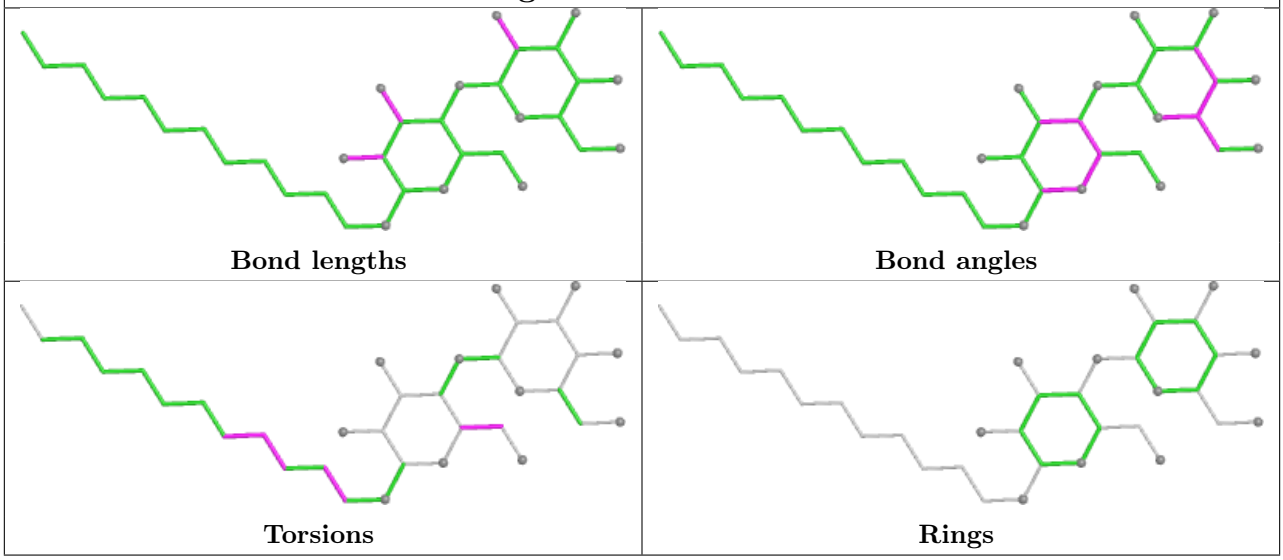


Torsions

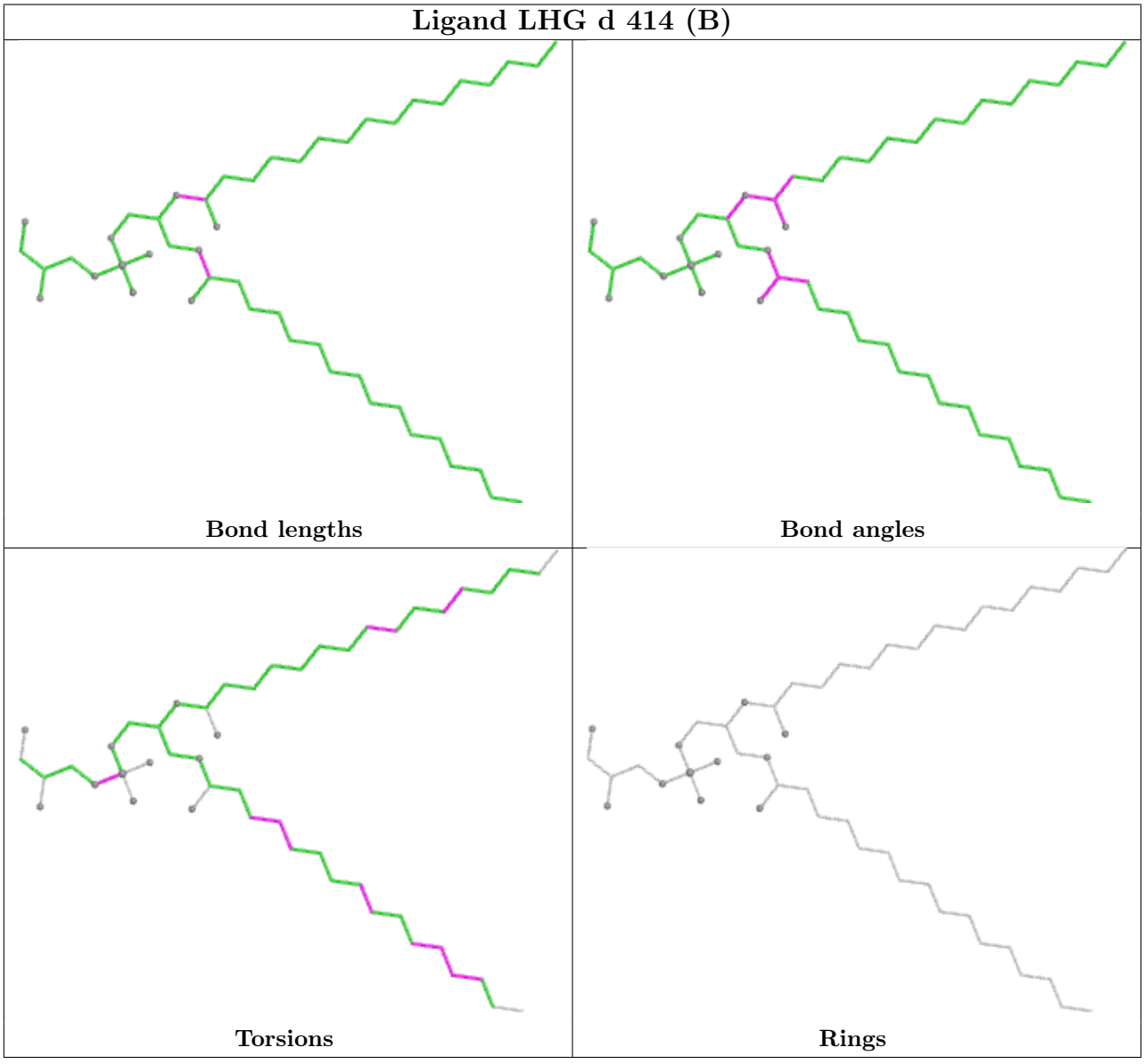


Rings

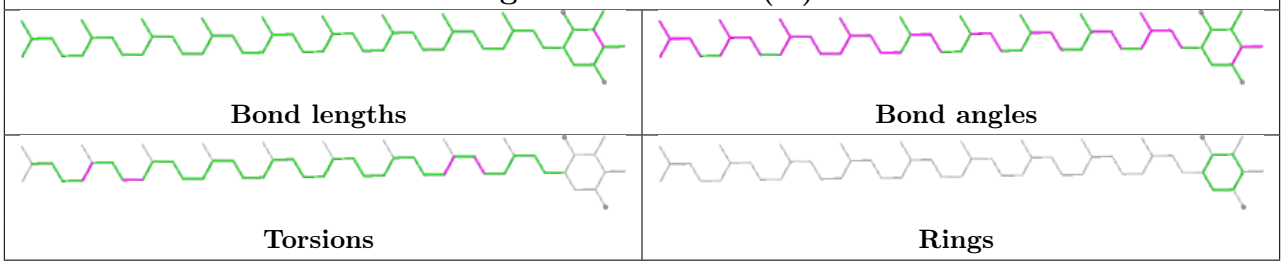
Ligand LMT M 101



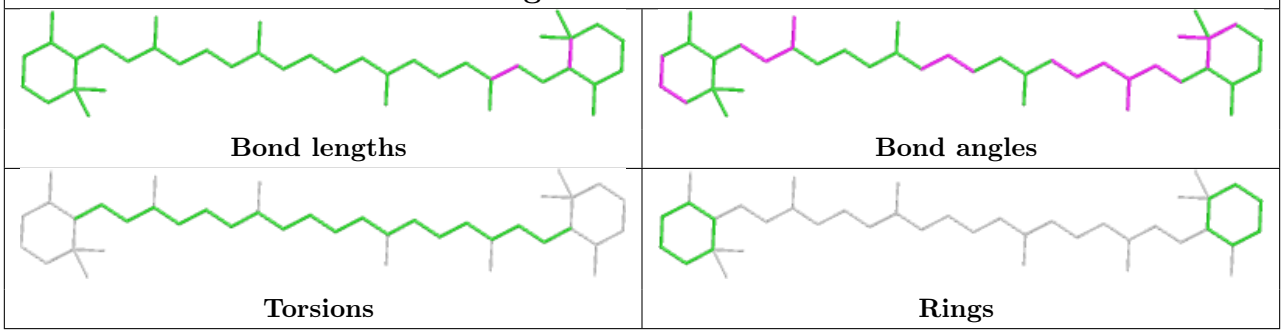
Ligand LHG d 414 (B)



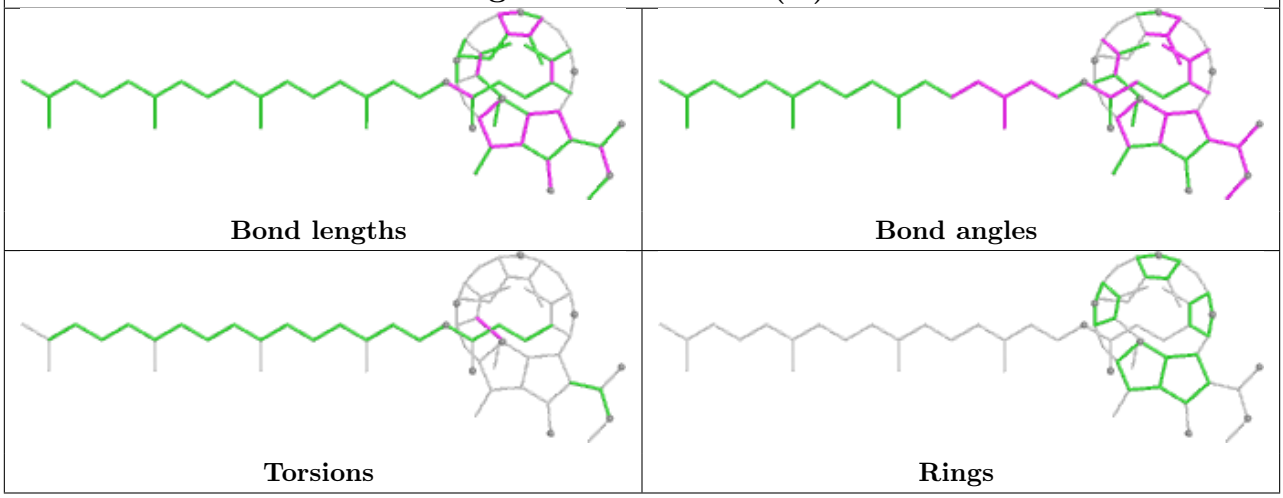
Ligand PL9 d 406 (A)



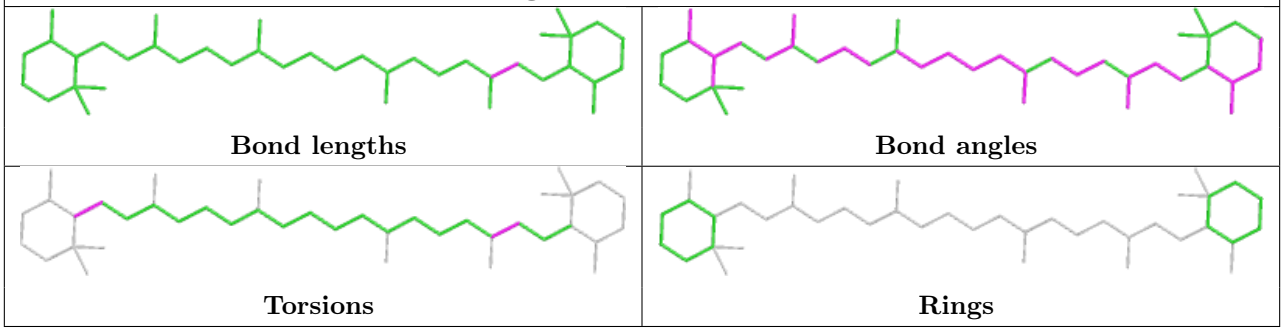
Ligand BCR B 619



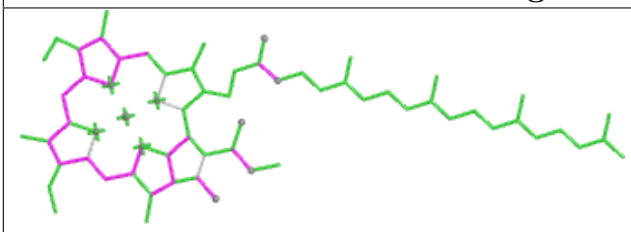
Ligand PHO A 416 (A)



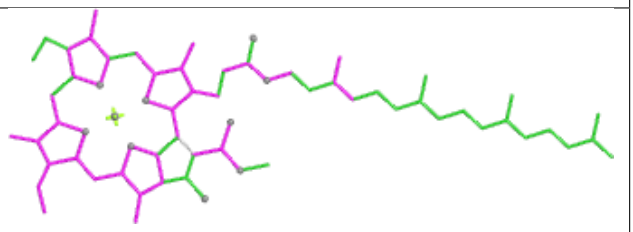
Ligand BCR Y 101



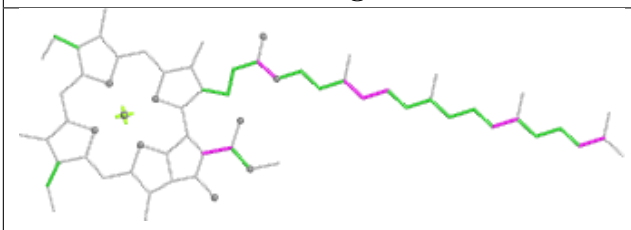
Ligand CLA d 404



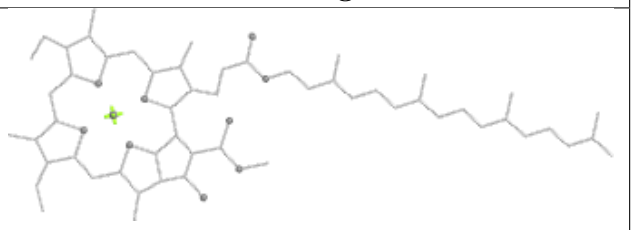
Bond lengths



Bond angles

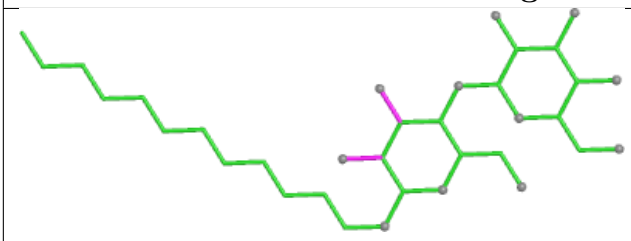


Torsions

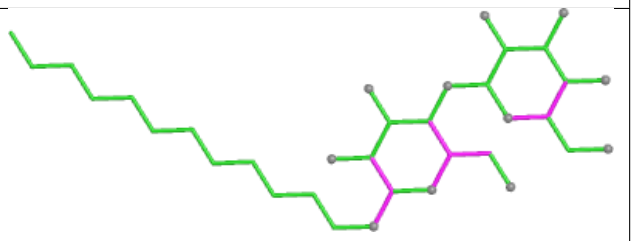


Rings

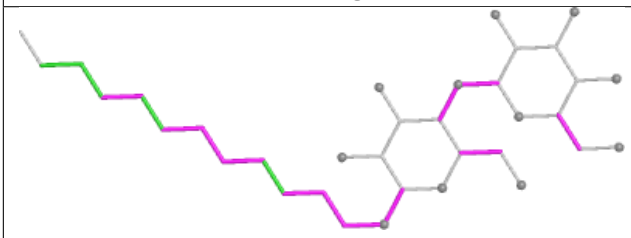
Ligand LMT A 420



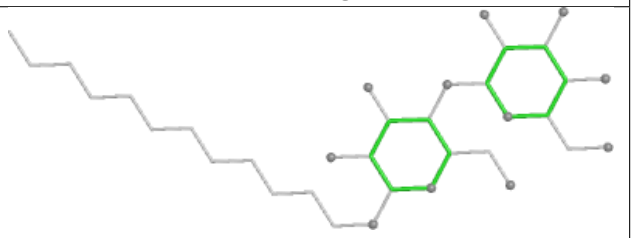
Bond lengths



Bond angles

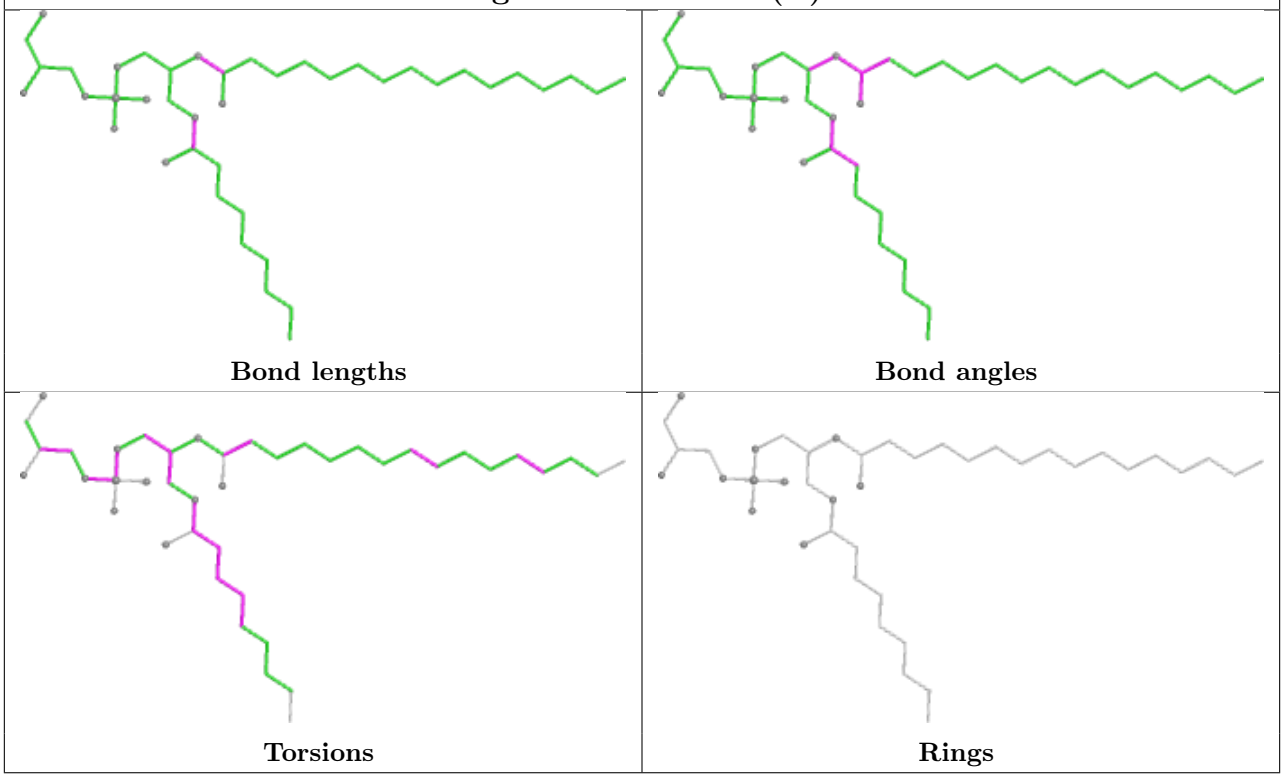


Torsions

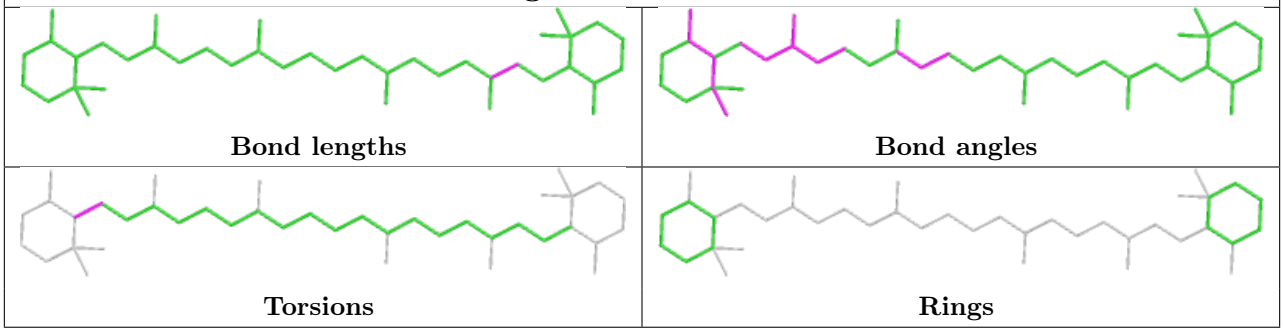


Rings

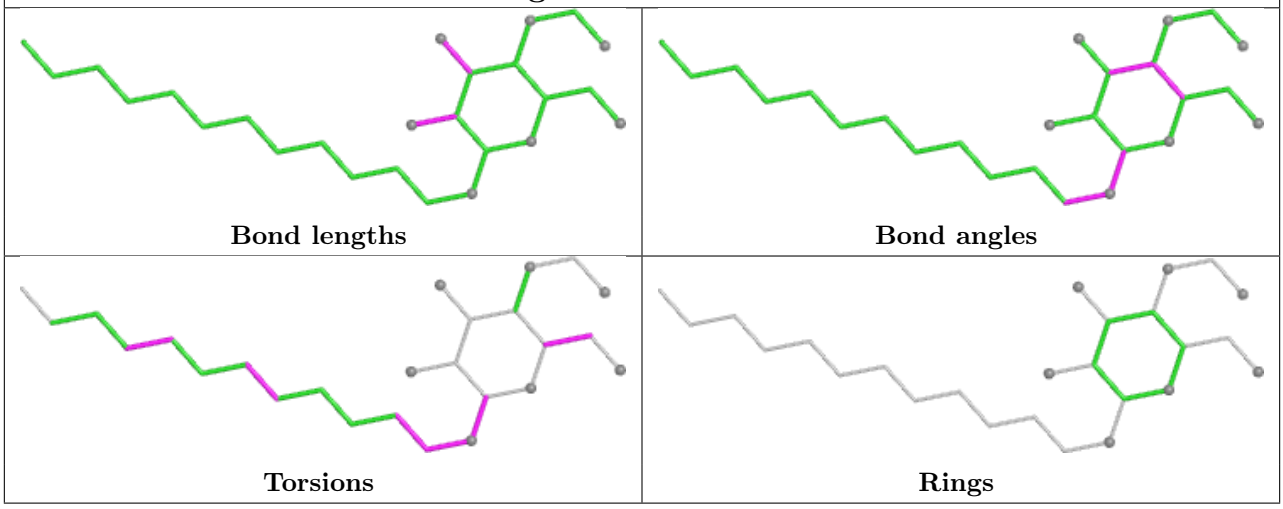
Ligand LHG E 101 (B)



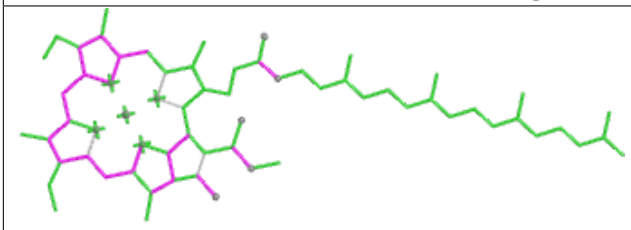
Ligand BCR B 617



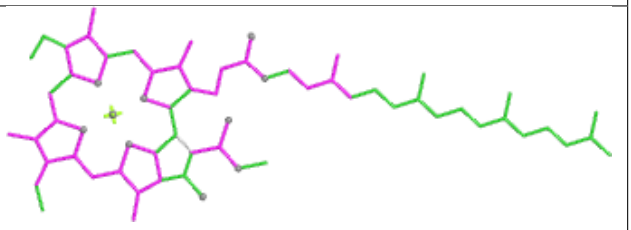
Ligand LMT t 101



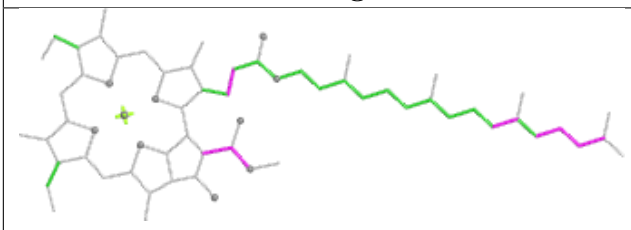
Ligand CLA b 610



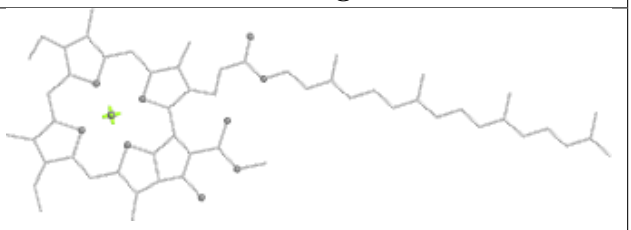
Bond lengths



Bond angles

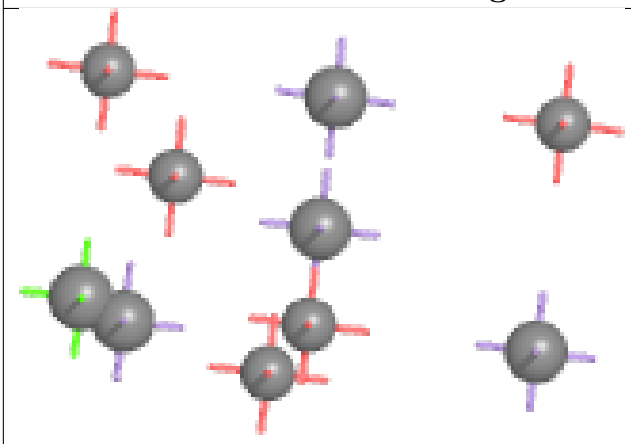


Torsions

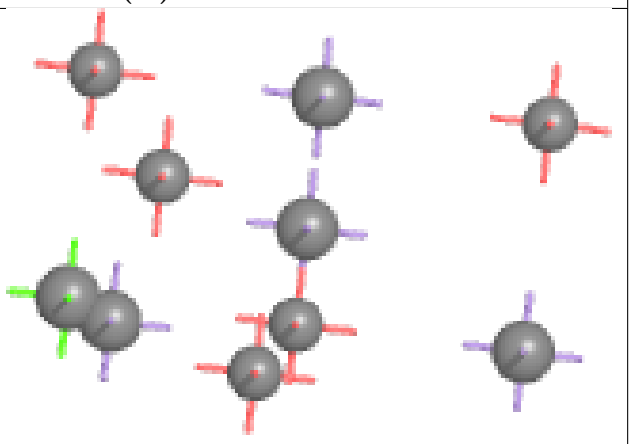


Rings

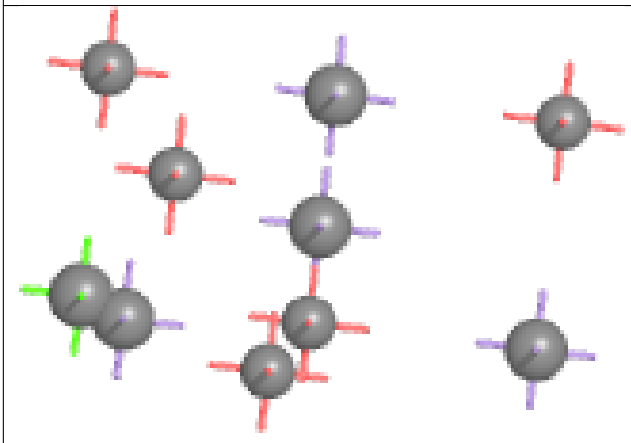
Ligand OEX A 413 (B)



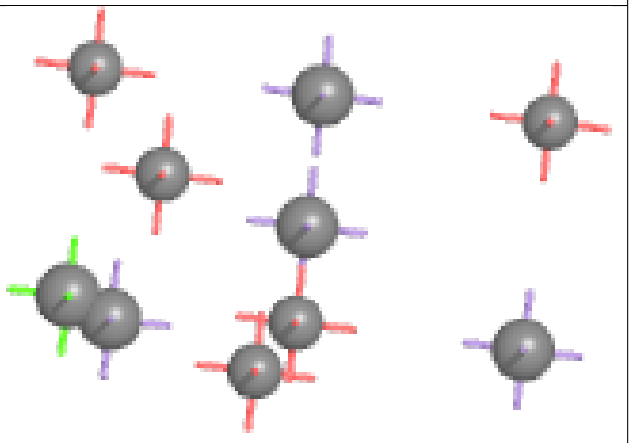
Bond lengths



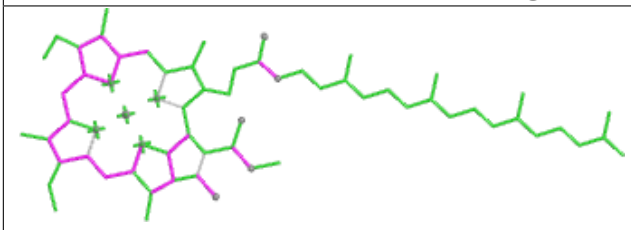
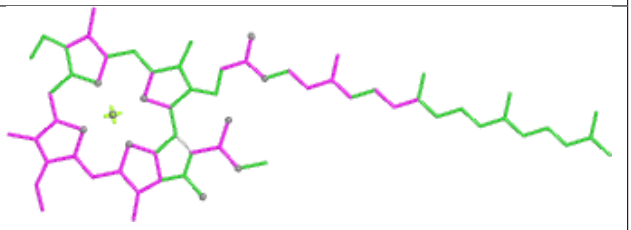
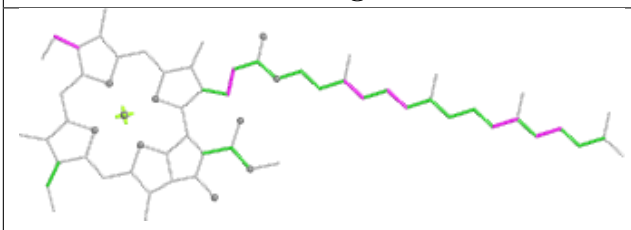
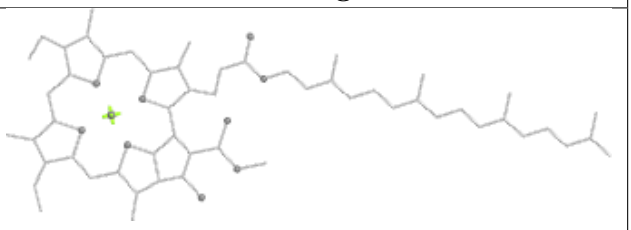
Bond angles



Torsions



Rings

Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.71	1 (0%) 90 90	21, 26, 58, 119	222 (66%)
1	a	334/344 (97%)	-0.67	1 (0%) 90 90	21, 28, 66, 122	220 (65%)
2	B	504/505 (99%)	-0.65	1 (0%) 91 92	23, 53, 81, 113	22 (4%)
2	b	504/505 (99%)	-0.58	1 (0%) 91 92	24, 56, 92, 146	19 (3%)
3	C	451/455 (99%)	-0.66	0 100 100	22, 59, 79, 145	99 (21%)
3	c	455/455 (100%)	-0.62	2 (0%) 88 89	25, 65, 84, 123	101 (22%)
4	D	342/342 (100%)	-0.73	0 100 100	21, 46, 64, 135	115 (33%)
4	d	341/342 (99%)	-0.73	0 100 100	22, 50, 72, 131	119 (34%)
5	E	81/84 (96%)	-0.43	1 (1%) 76 77	52, 69, 97, 160	0
5	e	79/84 (94%)	-0.45	1 (1%) 75 76	33, 74, 112, 139	2 (2%)
6	F	34/44 (77%)	-0.67	0 100 100	54, 63, 84, 110	0
6	f	31/44 (70%)	-0.44	1 (3%) 50 50	55, 65, 93, 144	1 (3%)
7	H	64/65 (98%)	-0.41	1 (1%) 70 71	49, 61, 81, 106	0
7	h	64/65 (98%)	-0.54	1 (1%) 70 71	39, 67, 90, 105	1 (1%)
8	I	37/38 (97%)	-0.40	0 100 100	55, 62, 118, 153	0
8	i	37/38 (97%)	-0.39	1 (2%) 56 57	55, 63, 114, 137	0
9	J	38/39 (97%)	-0.48	0 100 100	53, 68, 115, 163	0
9	j	39/39 (100%)	-0.37	0 100 100	60, 77, 117, 150	0
10	K	37/37 (100%)	-0.78	0 100 100	60, 67, 86, 109	0
10	k	37/37 (100%)	-0.63	0 100 100	66, 73, 97, 108	0
11	L	36/37 (97%)	-0.74	0 100 100	23, 46, 98, 137	2 (5%)
11	l	36/37 (97%)	-0.67	0 100 100	24, 48, 97, 118	2 (5%)
12	M	32/36 (88%)	-0.69	0 100 100	27, 49, 72, 137	1 (3%)
12	m	33/36 (91%)	-0.62	0 100 100	24, 49, 70, 142	2 (6%)

Continued on next page...

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.62	0 100 100	21, 63, 115, 173	10 (4%)
13	o	243/244 (99%)	-0.56	0 100 100	23, 66, 120, 164	8 (3%)
14	T	29/32 (90%)	-0.68	0 100 100	27, 47, 56, 64	6 (20%)
14	t	29/32 (90%)	-0.71	1 (3%) 48 48	28, 47, 64, 72	5 (17%)
15	U	96/104 (92%)	-0.66	0 100 100	25, 59, 89, 94	4 (4%)
15	u	97/104 (93%)	-0.71	0 100 100	29, 62, 82, 133	5 (5%)
16	V	137/137 (100%)	-0.76	0 100 100	24, 57, 81, 106	6 (4%)
16	v	137/137 (100%)	-0.68	0 100 100	27, 70, 102, 130	6 (4%)
17	X	38/40 (95%)	-0.39	0 100 100	34, 70, 92, 111	1 (2%)
17	x	38/40 (95%)	-0.27	0 100 100	64, 76, 115, 152	0
18	Y	29/30 (96%)	-0.04	1 (3%) 48 48	70, 83, 122, 128	0
18	y	29/30 (96%)	-0.34	0 100 100	75, 92, 108, 116	0
19	Z	62/62 (100%)	-0.45	0 100 100	66, 80, 133, 155	0
19	z	62/62 (100%)	-0.02	0 100 100	80, 94, 139, 191	0
20	R	34/34 (100%)	0.36	1 (2%) 53 54	82, 99, 125, 134	0
All	All	5283/5384 (98%)	-0.61	15 (0%) 90 90	21, 57, 97, 191	979 (18%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.0
5	e	79[A]	PHE	3.8
6	f	16[A]	PHE	3.4
14	t	30[A]	THR	2.7
3	c	245[A]	ILE	2.5
2	b	499	VAL	2.5
20	R	35	LEU	2.4
18	Y	18	VAL	2.4
1	a	11	ALA	2.4
2	B	494	GLY	2.4
8	i	37	LEU	2.2
1	A	11	ALA	2.1
3	c	20	SER	2.0
7	h	65	LEU	2.0
5	E	4	THR	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	FME	I	1	10/11	0.95	0.07	59,67,78,85	0
14	FME	T	1	10/11	0.95	0.07	46,53,69,73	0
14	FME	t	1	10/11	0.96	0.07	45,48,65,80	0
8	FME	i	1	10/11	0.97	0.06	54,68,77,86	0
12	FME	m	1	10/11	0.97	0.07	48,62,89,110	0
12	FME	M	1	10/11	0.97	0.07	43,64,87,109	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	415	6/6	0.63	0.16	69,88,99,108	0
31	LMT	B	629	35/35	0.64	0.15	57,108,139,145	0
30	UNL	a	413	30/-	0.68	0.14	91,117,135,149	0
30	UNL	j	101	10/-	0.69	0.19	72,89,103,104	0
30	UNL	J	101	10/-	0.69	0.25	76,81,94,98	0
31	LMT	F	101	35/35	0.69	0.15	89,132,181,189	0
30	UNL	A	415	28/-	0.70	0.14	93,115,130,146	0
30	UNL	m	102	10/-	0.71	0.20	70,77,94,97	0
31	LMT	A	417	35/35	0.72	0.13	64,111,132,139	0
31	LMT	A	420	35/35	0.72	0.12	91,134,160,167	0
31	LMT	c	502	35/35	0.73	0.14	99,135,153,158	0
31	LMT	e	101	35/35	0.73	0.14	105,143,191,202	0
30	UNL	I	101	40/-	0.75	0.15	66,107,159,166	0
30	UNL	K	101[A]	34/-	0.75	0.14	85,106,123,126	34
30	UNL	K	101[B]	34/-	0.75	0.14	85,106,123,127	34
31	LMT	b	621	25/35	0.78	0.12	72,110,159,162	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	UNL	M	102	10/-	0.78	0.17	72,78,86,87	0
26	SQD	f	102	43/54	0.78	0.13	96,127,168,182	0
34	HTG	B	622	19/19	0.78	0.15	67,88,107,120	0
30	UNL	d	410	36/-	0.79	0.11	70,91,130,143	0
30	UNL	i	101	40/-	0.79	0.13	72,107,159,163	0
27	GOL	B	626	6/6	0.79	0.13	67,79,94,115	0
30	UNL	D	409	40/-	0.79	0.12	62,93,134,146	0
30	UNL	c	526[A]	32/-	0.79	0.15	97,112,129,132	32
30	UNL	c	526[B]	32/-	0.79	0.15	97,112,129,132	32
34	HTG	D	410	16/19	0.79	0.12	80,104,130,149	0
27	GOL	o	303	6/6	0.80	0.15	82,98,113,117	0
34	HTG	C	522	19/19	0.80	0.12	107,121,154,156	0
33	LMG	C	521	51/55	0.80	0.11	59,121,154,164	0
27	GOL	O	303	6/6	0.81	0.12	80,92,96,101	0
27	GOL	b	624	6/6	0.81	0.15	85,92,97,98	0
32	LHG	a	417[A]	42/49	0.81	0.11	87,142,151,156	42
32	LHG	a	417[B]	42/49	0.81	0.11	87,142,151,156	42
34	HTG	V	202	11/19	0.81	0.10	76,110,122,123	0
36	CA	F	103	1/1	0.81	0.23	123,123,123,123	0
30	UNL	b	626	33/-	0.82	0.12	64,96,170,174	0
31	LMT	B	627	35/35	0.82	0.11	66,104,133,139	0
27	GOL	d	413	6/6	0.82	0.24	51,71,80,86	0
30	UNL	B	625	33/-	0.82	0.14	61,108,138,141	0
27	GOL	o	304	6/6	0.82	0.14	84,87,96,106	0
31	LMT	M	103	35/35	0.83	0.11	69,130,181,184	0
34	HTG	c	523	19/19	0.83	0.10	104,126,144,148	0
27	GOL	O	302	6/6	0.83	0.09	73,85,93,100	0
29	PL9	A	414[A]	55/55	0.84	0.15	70,94,112,116	55
34	HTG	d	411	16/19	0.84	0.12	91,113,133,153	0
29	PL9	A	414[B]	55/55	0.84	0.15	70,94,112,116	55
27	GOL	A	411	6/6	0.85	0.12	62,77,80,84	0
26	SQD	a	410	54/54	0.85	0.10	61,96,133,146	0
36	CA	f	103	1/1	0.85	0.12	121,121,121,121	0
33	LMG	Z	101	37/55	0.86	0.13	65,125,151,166	0
26	SQD	A	412	54/54	0.86	0.10	65,87,121,141	0
31	LMT	b	627	25/35	0.86	0.12	56,99,149,162	0
29	PL9	a	412[A]	55/55	0.86	0.15	82,105,120,125	55
29	PL9	a	412[B]	55/55	0.86	0.15	82,105,120,125	55
34	HTG	b	623	19/19	0.86	0.10	86,133,158,165	0
31	LMT	t	101	26/35	0.86	0.12	66,105,152,163	0
31	LMT	B	630	25/35	0.86	0.12	55,83,149,173	0
27	GOL	l	801[A]	6/6	0.86	0.17	69,97,102,105	6

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
27	GOL	l	801[B]	6/6	0.86	0.17	69,97,103,105	6
27	GOL	D	412	6/6	0.87	0.16	50,64,75,85	0
34	HTG	b	622	19/19	0.87	0.12	60,85,107,122	0
33	LMG	c	522	51/55	0.87	0.10	76,135,166,173	0
31	LMT	m	103	35/35	0.87	0.10	62,86,103,106	0
27	GOL	c	528	6/6	0.87	0.16	103,113,122,124	0
27	GOL	B	628	6/6	0.87	0.12	71,75,94,95	0
31	LMT	M	101	35/35	0.87	0.10	57,90,104,109	0
33	LMG	z	101	39/55	0.88	0.11	76,122,156,170	0
34	HTG	o	301	19/19	0.88	0.11	56,84,108,111	0
32	LHG	E	101[B]	42/49	0.89	0.12	70,102,120,127	42
27	GOL	V	203[A]	6/6	0.89	0.12	58,66,71,73	6
27	GOL	V	203[B]	6/6	0.89	0.12	58,66,71,74	6
27	GOL	A	418	6/6	0.89	0.27	51,77,78,88	0
26	SQD	B	620	54/54	0.89	0.09	57,89,120,138	0
32	LHG	E	101[A]	42/49	0.89	0.12	70,102,119,127	42
34	HTG	B	624	19/19	0.90	0.07	67,78,94,96	0
27	GOL	v	202[B]	6/6	0.90	0.11	67,78,84,84	6
23	CLA	b	601	65/65	0.90	0.09	61,84,128,149	0
27	GOL	C	523[A]	6/6	0.90	0.10	57,59,60,66	6
27	GOL	C	523[B]	6/6	0.90	0.10	57,59,60,66	6
33	LMG	C	501	51/55	0.90	0.09	66,89,113,123	0
26	SQD	b	620	54/54	0.90	0.09	61,90,111,124	0
27	GOL	a	416	6/6	0.90	0.25	57,74,81,82	0
26	SQD	F	102	43/54	0.90	0.10	66,102,129,143	0
30	UNL	D	408	17/-	0.90	0.10	59,76,100,119	0
27	GOL	v	202[A]	6/6	0.90	0.11	66,78,83,84	6
33	LMG	c	501	51/55	0.91	0.08	62,89,109,115	0
23	CLA	B	601	65/65	0.91	0.09	54,74,116,147	0
23	CLA	c	515	65/65	0.92	0.09	66,88,128,143	0
33	LMG	C	520	51/55	0.92	0.09	52,83,121,135	0
30	UNL	d	409	17/-	0.92	0.09	63,80,111,112	0
27	GOL	c	527[A]	6/6	0.92	0.08	62,66,67,70	6
33	LMG	c	521	51/55	0.92	0.09	59,92,124,153	0
27	GOL	c	527[B]	6/6	0.92	0.08	62,66,69,71	6
33	LMG	m	101	51/55	0.92	0.08	50,72,93,115	0
33	LMG	B	621	51/55	0.93	0.07	50,70,94,110	0
27	GOL	B	623	6/6	0.93	0.08	70,82,87,88	0
25	BCR	D	404	40/40	0.93	0.09	47,61,105,111	0
25	BCR	T	101	40/40	0.93	0.07	46,56,70,73	0
33	LMG	D	411	51/55	0.93	0.08	50,67,119,138	0
32	LHG	A	419[A]	49/49	0.93	0.09	50,62,83,89	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LHG	A	419[B]	49/49	0.93	0.09	50,63,84,89	49
34	HTG	b	625	19/19	0.93	0.07	62,76,95,98	0
26	SQD	A	410[A]	54/54	0.93	0.08	58,78,116,119	54
33	LMG	d	412	51/55	0.93	0.08	56,72,115,135	0
26	SQD	A	410[B]	54/54	0.93	0.08	59,78,117,119	54
35	DGD	C	518[A]	62/66	0.93	0.08	50,63,118,122	62
35	DGD	C	518[B]	62/66	0.93	0.08	49,63,118,122	62
23	CLA	b	616	65/65	0.93	0.08	45,62,127,136	0
23	CLA	C	514	65/65	0.93	0.08	60,80,114,122	0
36	CA	o	302	1/1	0.93	0.06	103,103,103,103	0
27	GOL	b	628	6/6	0.94	0.07	77,82,88,92	0
23	CLA	d	404	65/65	0.94	0.08	53,63,122,147	0
32	LHG	D	407[A]	49/49	0.94	0.09	51,60,106,112	49
32	LHG	D	407[B]	49/49	0.94	0.09	51,60,106,113	49
23	CLA	C	505	65/65	0.94	0.07	42,56,103,124	0
25	BCR	K	102	40/40	0.94	0.09	54,64,75,75	0
23	CLA	c	514	65/65	0.94	0.09	61,79,125,135	0
26	SQD	a	409[A]	54/54	0.94	0.09	62,81,121,124	54
30	UNL	X	102	18/-	0.94	0.10	59,73,102,109	0
35	DGD	c	519[A]	62/66	0.94	0.07	54,68,124,138	62
35	DGD	c	519[B]	62/66	0.94	0.07	54,68,124,138	62
26	SQD	a	409[B]	54/54	0.94	0.09	62,81,121,124	54
25	BCR	d	405	40/40	0.94	0.07	52,66,98,102	0
23	CLA	C	507	65/65	0.94	0.07	57,69,125,136	0
32	LHG	d	414[A]	49/49	0.95	0.08	49,66,83,89	49
32	LHG	d	414[B]	49/49	0.95	0.08	49,66,83,89	49
25	BCR	A	409	40/40	0.95	0.07	39,53,63,66	0
25	BCR	B	619	40/40	0.95	0.07	47,62,87,94	0
25	BCR	C	515	40/40	0.95	0.07	63,74,89,91	0
30	UNL	x	101	18/-	0.95	0.10	64,77,119,131	0
23	CLA	B	614	65/65	0.95	0.07	41,51,103,120	0
23	CLA	a	405[A]	65/65	0.95	0.07	44,52,123,132	65
29	PL9	D	405[A]	55/55	0.95	0.06	39,48,57,67	55
29	PL9	D	405[B]	55/55	0.95	0.06	38,48,57,67	55
23	CLA	a	405[B]	65/65	0.95	0.07	43,53,123,132	65
25	BCR	X	101	40/40	0.95	0.07	50,65,78,82	0
25	BCR	Y	101	40/40	0.95	0.07	55,68,80,83	0
25	BCR	c	516	40/40	0.95	0.07	74,83,92,99	0
23	CLA	a	407	65/65	0.95	0.09	46,55,138,152	0
25	BCR	h	101	40/40	0.95	0.07	53,69,85,87	0
25	BCR	t	102	40/40	0.95	0.06	39,59,75,79	0
25	BCR	y	101	40/40	0.95	0.07	56,71,86,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	B	616	65/65	0.95	0.08	48,57,130,136	0
23	CLA	b	614	65/65	0.95	0.07	41,51,102,113	0
23	CLA	A	408	65/65	0.95	0.08	43,52,128,143	0
23	CLA	c	506	65/65	0.95	0.07	50,62,107,131	0
23	CLA	c	508	65/65	0.95	0.07	54,71,122,133	0
23	CLA	c	509	65/65	0.95	0.08	54,66,81,89	0
23	CLA	c	510	65/65	0.95	0.07	44,62,129,146	0
23	CLA	B	606	65/65	0.95	0.07	43,55,121,129	0
23	CLA	C	509	65/65	0.95	0.07	46,56,116,136	0
35	DGD	C	519	62/66	0.95	0.07	45,59,98,111	0
35	DGD	H	101	62/66	0.95	0.08	48,61,73,78	0
35	DGD	c	518[A]	62/66	0.95	0.07	50,64,105,112	62
35	DGD	c	518[B]	62/66	0.95	0.07	50,64,105,112	62
23	CLA	C	513	65/65	0.95	0.08	58,74,111,124	0
32	LHG	b	629[A]	49/49	0.95	0.08	51,58,71,93	49
35	DGD	c	520	62/66	0.95	0.07	51,63,104,131	0
35	DGD	h	102	62/66	0.95	0.07	53,64,73,78	0
32	LHG	b	629[B]	49/49	0.95	0.08	51,58,71,93	49
32	LHG	d	408[A]	49/49	0.95	0.08	53,65,115,128	49
32	LHG	d	408[B]	49/49	0.95	0.08	53,65,115,128	49
23	CLA	A	406[A]	65/65	0.96	0.06	40,48,115,121	65
23	CLA	C	508	65/65	0.96	0.07	48,60,80,90	0
29	PL9	d	406[A]	55/55	0.96	0.07	40,50,59,69	55
29	PL9	d	406[B]	55/55	0.96	0.07	40,50,59,69	55
25	BCR	a	408	40/40	0.96	0.06	45,53,64,69	0
25	BCR	b	617	40/40	0.96	0.05	47,54,64,70	0
25	BCR	b	618	40/40	0.96	0.06	45,57,74,78	0
25	BCR	b	619	40/40	0.96	0.06	51,63,84,87	0
23	CLA	c	503	65/65	0.96	0.07	52,66,77,88	0
23	CLA	c	505	65/65	0.96	0.06	51,67,78,87	0
23	CLA	B	609	65/65	0.96	0.06	49,58,69,80	0
25	BCR	k	101	40/40	0.96	0.08	59,72,86,88	0
32	LHG	D	406[A]	49/49	0.96	0.07	47,54,65,78	49
32	LHG	D	406[B]	49/49	0.96	0.07	47,54,65,78	49
23	CLA	B	610	65/65	0.96	0.07	41,55,66,81	0
23	CLA	B	611	65/65	0.96	0.06	35,47,64,71	0
23	CLA	D	403	65/65	0.96	0.07	47,58,119,130	0
23	CLA	A	406[B]	65/65	0.96	0.06	40,48,115,121	65
23	CLA	B	602	65/65	0.96	0.07	43,55,76,96	0
35	DGD	C	517[A]	62/66	0.96	0.06	47,58,100,107	62
35	DGD	C	517[B]	62/66	0.96	0.06	46,58,100,107	62
23	CLA	C	502	65/65	0.96	0.06	48,60,73,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	PHO	a	414[A]	64/64	0.96	0.06	46,54,60,66	64
24	PHO	a	414[B]	64/64	0.96	0.06	46,54,60,66	64
32	LHG	d	407[A]	49/49	0.96	0.07	48,56,68,80	49
32	LHG	d	407[B]	49/49	0.96	0.07	48,56,68,80	49
23	CLA	B	603	65/65	0.96	0.07	41,53,72,79	0
25	BCR	B	618	40/40	0.96	0.05	43,55,70,79	0
23	CLA	b	603	65/65	0.96	0.06	45,55,76,89	0
23	CLA	b	606	65/65	0.96	0.07	44,56,108,125	0
25	BCR	C	516	40/40	0.96	0.06	54,64,75,81	0
23	CLA	b	607	65/65	0.96	0.06	38,48,79,91	0
36	CA	c	524	1/1	0.96	0.08	74,74,74,74	0
23	CLA	b	611	65/65	0.96	0.06	42,49,72,81	0
23	CLA	b	612	65/65	0.96	0.07	42,52,64,70	0
37	BCT	d	401[A]	4/4	0.96	0.06	55,57,64,73	4
37	BCT	d	401[B]	4/4	0.96	0.06	56,57,65,74	4
23	CLA	C	512	65/65	0.97	0.07	50,65,79,86	0
23	CLA	c	507	65/65	0.97	0.06	49,61,89,102	0
23	CLA	A	404[B]	65/65	0.97	0.06	38,43,60,67	65
23	CLA	B	612	65/65	0.97	0.06	37,49,62,70	0
23	CLA	D	402[A]	65/65	0.97	0.06	35,43,68,76	65
23	CLA	c	511	65/65	0.97	0.07	49,61,87,93	0
23	CLA	c	512	65/65	0.97	0.05	49,63,78,94	0
23	CLA	c	513	65/65	0.97	0.07	56,67,82,90	0
23	CLA	D	402[B]	65/65	0.97	0.06	35,43,68,77	65
23	CLA	B	613	65/65	0.97	0.05	38,47,96,106	0
23	CLA	d	402[A]	65/65	0.97	0.05	40,45,61,73	65
23	CLA	d	402[B]	65/65	0.97	0.05	40,45,61,73	65
23	CLA	d	403[A]	65/65	0.97	0.06	40,47,73,87	65
23	CLA	d	403[B]	65/65	0.97	0.06	40,47,73,87	65
23	CLA	a	404[A]	65/65	0.97	0.06	41,47,64,78	65
24	PHO	A	407[A]	64/64	0.97	0.04	39,45,50,53	64
24	PHO	A	407[B]	64/64	0.97	0.04	39,45,50,53	64
24	PHO	A	416[A]	64/64	0.97	0.06	42,51,57,62	64
24	PHO	A	416[B]	64/64	0.97	0.06	42,51,57,62	64
24	PHO	a	406[A]	64/64	0.97	0.05	42,48,53,57	64
24	PHO	a	406[B]	64/64	0.97	0.05	42,48,53,57	64
23	CLA	a	404[B]	65/65	0.97	0.06	41,47,65,79	65
23	CLA	B	604	65/65	0.97	0.06	37,47,107,124	0
23	CLA	B	615	65/65	0.97	0.06	41,52,77,89	0
25	BCR	B	617	40/40	0.97	0.05	43,52,63,67	0
23	CLA	B	605	65/65	0.97	0.06	39,49,67,80	0
23	CLA	A	405[A]	65/65	0.97	0.05	35,44,55,66	65

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	b	602	65/65	0.97	0.06	48,60,78,87	0
23	CLA	C	503	65/65	0.97	0.06	48,56,74,84	0
23	CLA	b	604	65/65	0.97	0.06	42,51,101,112	0
23	CLA	b	605	65/65	0.97	0.06	42,50,71,74	0
23	CLA	C	504	65/65	0.97	0.06	52,60,72,87	0
23	CLA	B	607	65/65	0.97	0.06	38,47,75,85	0
23	CLA	b	608	65/65	0.97	0.05	45,56,76,83	0
23	CLA	b	609	65/65	0.97	0.06	51,60,78,93	0
23	CLA	b	610	65/65	0.97	0.06	48,56,70,77	0
23	CLA	C	506	65/65	0.97	0.06	49,57,91,103	0
23	CLA	B	608	65/65	0.97	0.05	42,52,66,76	0
23	CLA	b	613	65/65	0.97	0.05	42,50,89,101	0
25	BCR	c	517	40/40	0.97	0.06	54,67,78,83	0
23	CLA	A	405[B]	65/65	0.97	0.05	35,44,55,66	65
32	LHG	L	101[A]	49/49	0.97	0.06	49,57,70,88	49
36	CA	O	301	1/1	0.97	0.03	103,103,103,103	0
32	LHG	L	101[B]	49/49	0.97	0.06	49,57,70,88	49
23	CLA	A	404[A]	65/65	0.97	0.06	38,43,60,67	65
23	CLA	C	510	65/65	0.97	0.07	50,59,82,87	0
37	BCT	D	401[A]	4/4	0.97	0.06	54,55,59,64	4
37	BCT	D	401[B]	4/4	0.97	0.06	54,55,59,65	4
23	CLA	c	504	65/65	0.97	0.06	45,59,86,106	0
23	CLA	C	511	65/65	0.97	0.06	49,60,80,86	0
22	CL	a	403[A]	1/1	0.98	0.07	52,52,52,52	1
22	CL	a	403[B]	1/1	0.98	0.07	52,52,52,52	1
36	CA	C	524	1/1	0.98	0.05	71,71,71,71	0
22	CL	A	402[A]	1/1	0.98	0.05	43,43,43,43	1
22	CL	A	402[B]	1/1	0.98	0.05	42,42,42,42	1
23	CLA	b	615	65/65	0.98	0.05	44,57,81,89	0
38	HEM	f	101	43/43	0.98	0.07	62,80,114,125	0
40	HEC	v	201	43/43	0.98	0.06	50,62,70,75	0
22	CL	a	402[A]	1/1	0.99	0.04	49,49,49,49	1
22	CL	a	402[B]	1/1	0.99	0.04	50,50,50,50	1
22	CL	A	403[A]	1/1	0.99	0.03	47,47,47,47	1
22	CL	A	403[B]	1/1	0.99	0.03	47,47,47,47	1
28	OEX	A	413[A]	10/10	0.99	0.03	42,44,49,50	10
38	HEM	E	102	43/43	0.99	0.06	57,67,78,91	0
36	CA	c	525	1/1	0.99	0.03	78,78,78,78	0
39	MG	J	102	1/1	0.99	0.03	59,59,59,59	0
39	MG	j	102	1/1	0.99	0.05	62,62,62,62	0
40	HEC	V	201	43/43	0.99	0.05	41,51,57,61	0
28	OEX	A	413[B]	10/10	0.99	0.03	41,44,50,50	10

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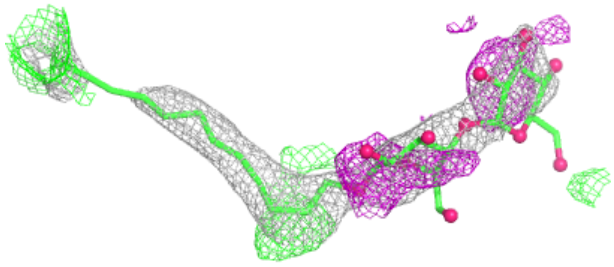
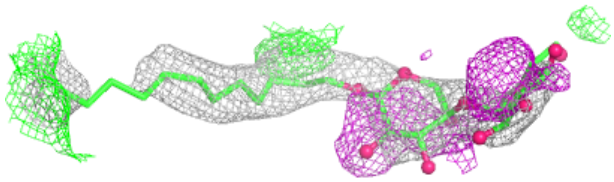
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
21	FE2	a	401[A]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	a	401[B]	1/1	1.00	0.01	53,53,53,53	1
21	FE2	A	401[A]	1/1	1.00	0.01	51,51,51,51	1
21	FE2	A	401[B]	1/1	1.00	0.01	51,51,51,51	1
28	OEX	a	411[A]	10/10	1.00	0.02	46,49,50,56	10
28	OEX	a	411[B]	10/10	1.00	0.02	46,49,50,56	10

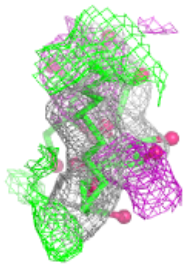
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 629:

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

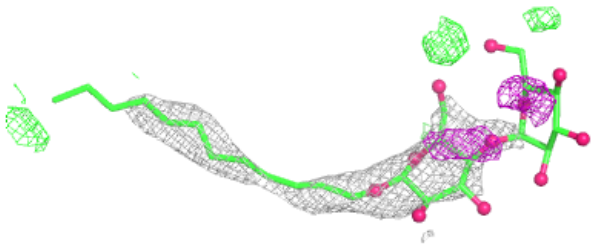


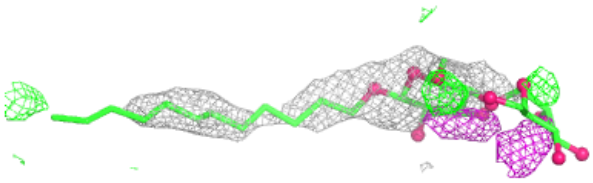


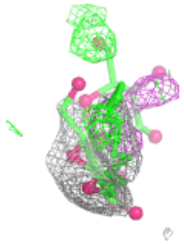


Electron density around LMT F 101:

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

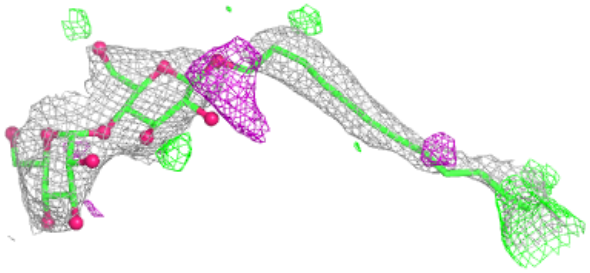


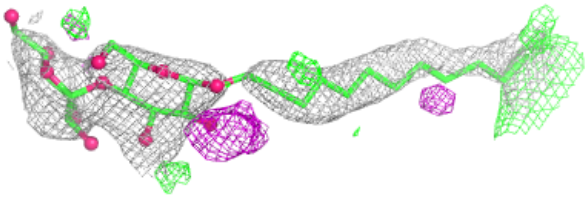


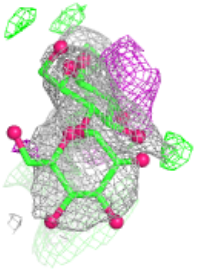


Electron density around LMT A 417:

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

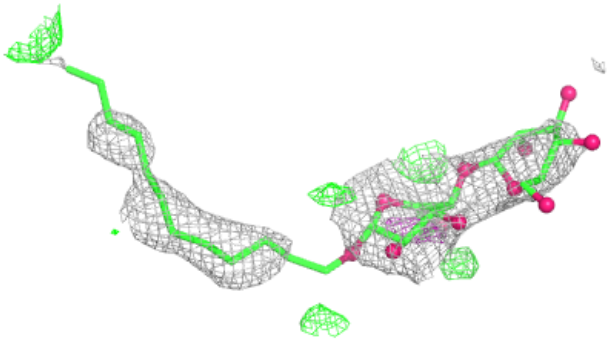


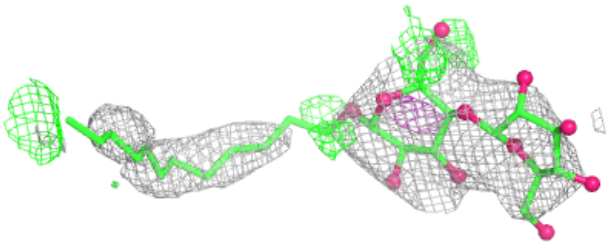


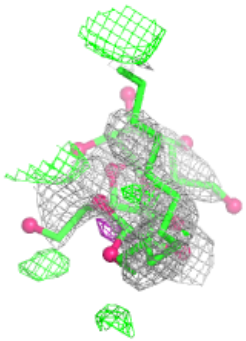


Electron density around LMT A 420:

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

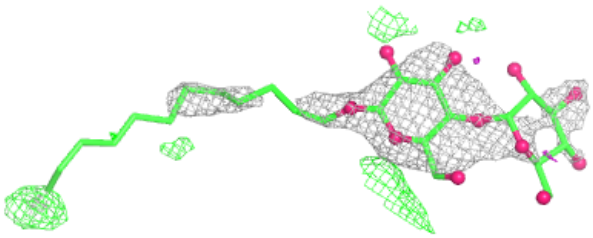


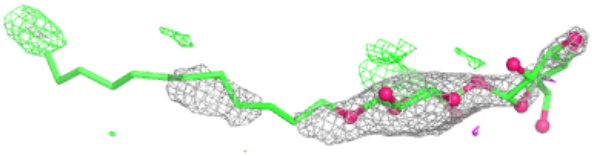


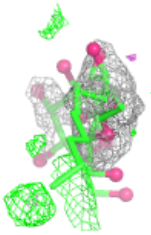


Electron density around LMT c 502:

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

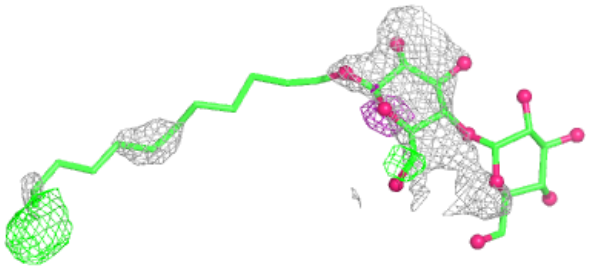


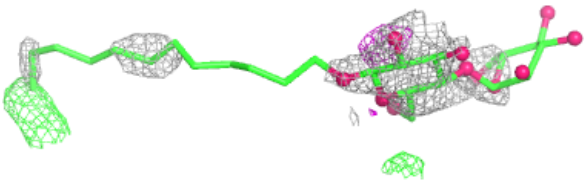


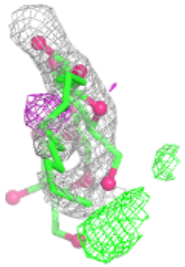


Electron density around LMT e 101:

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

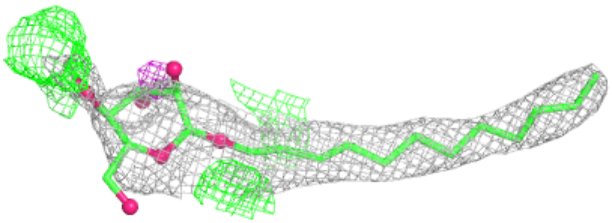


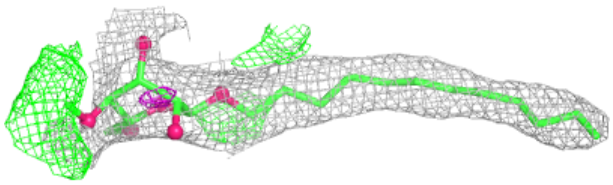


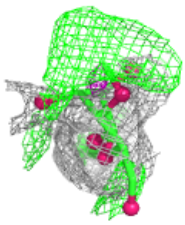


Electron density around LMT b 621:

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

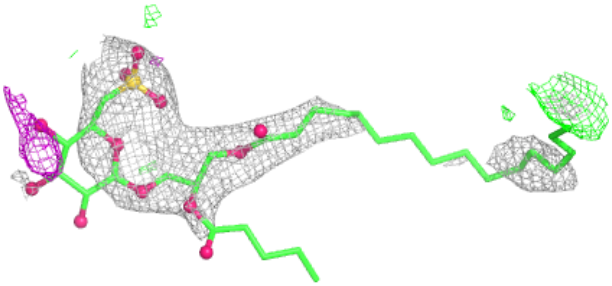


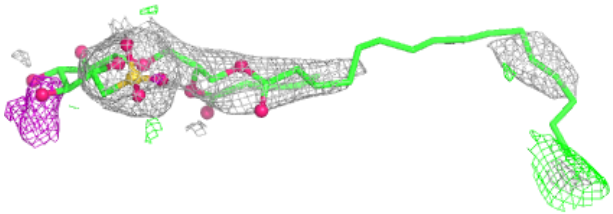


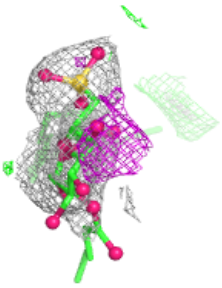


Electron density around SQD f 102:

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

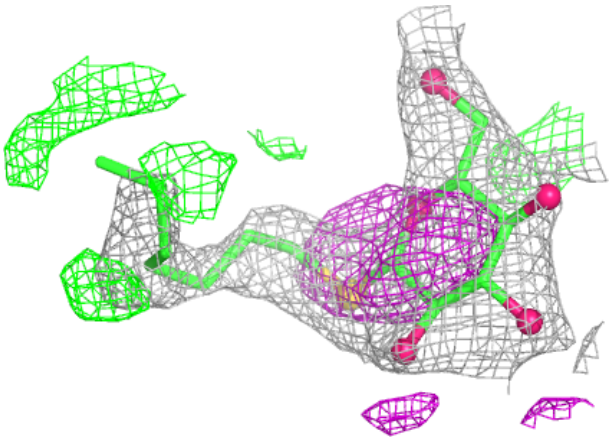


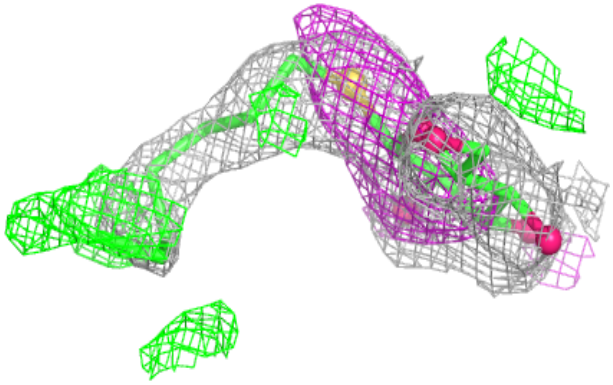


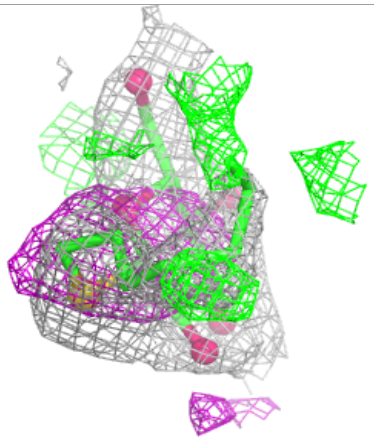


Electron density around HTG B 622:

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

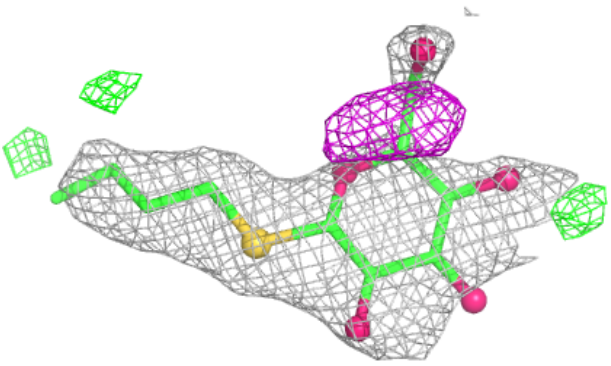


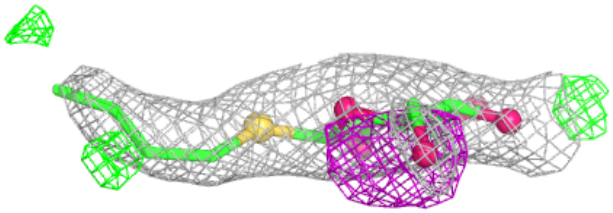


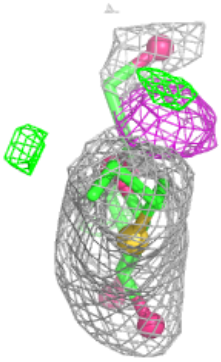


Electron density around HTG D 410:

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

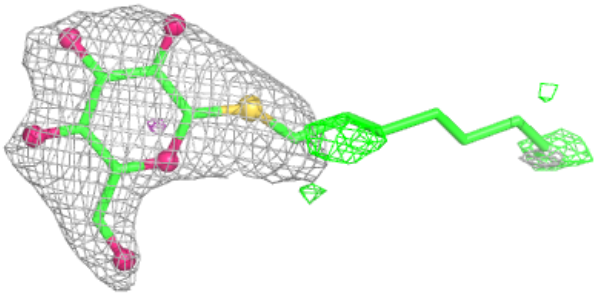


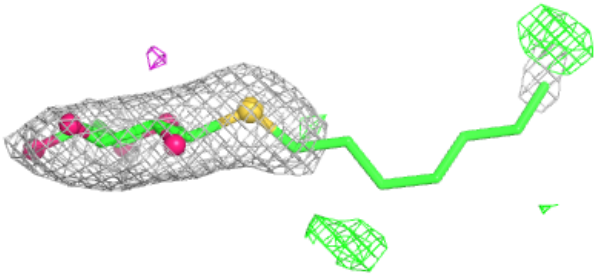


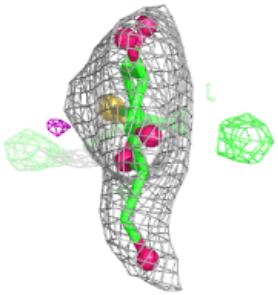


Electron density around HTG C 522:

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

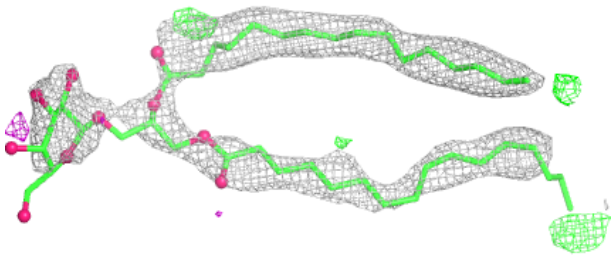


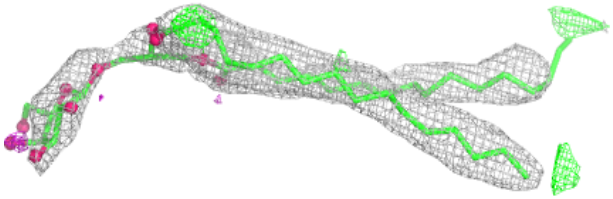


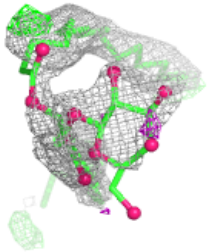


Electron density around LMG C 521:

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

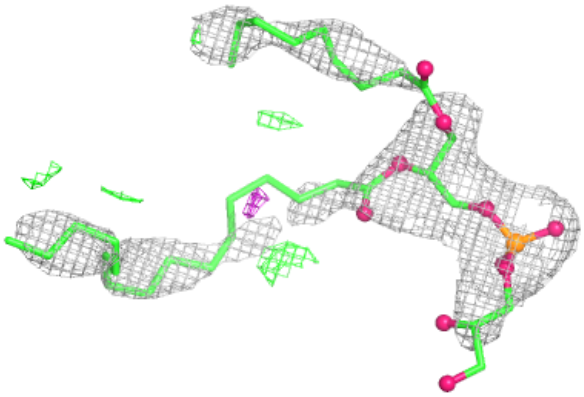


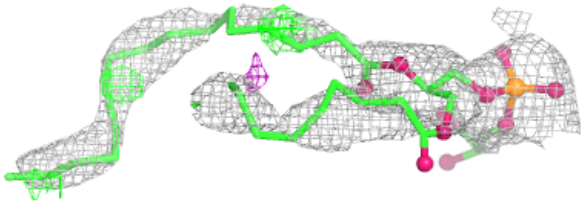


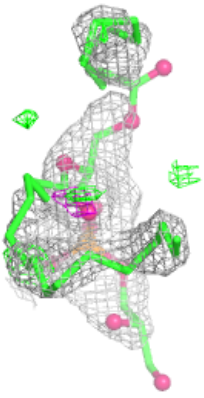


Electron density around LHG a 417 (A):

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

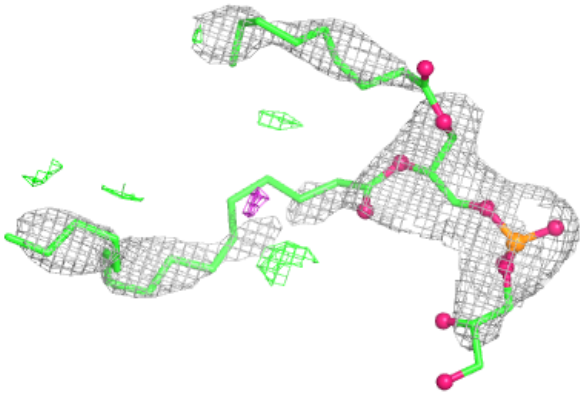


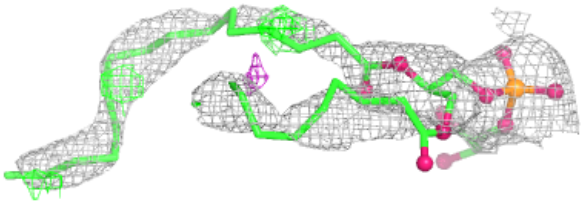


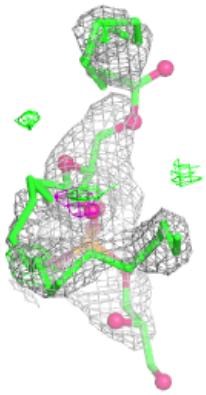


Electron density around LHG a 417 (B):

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

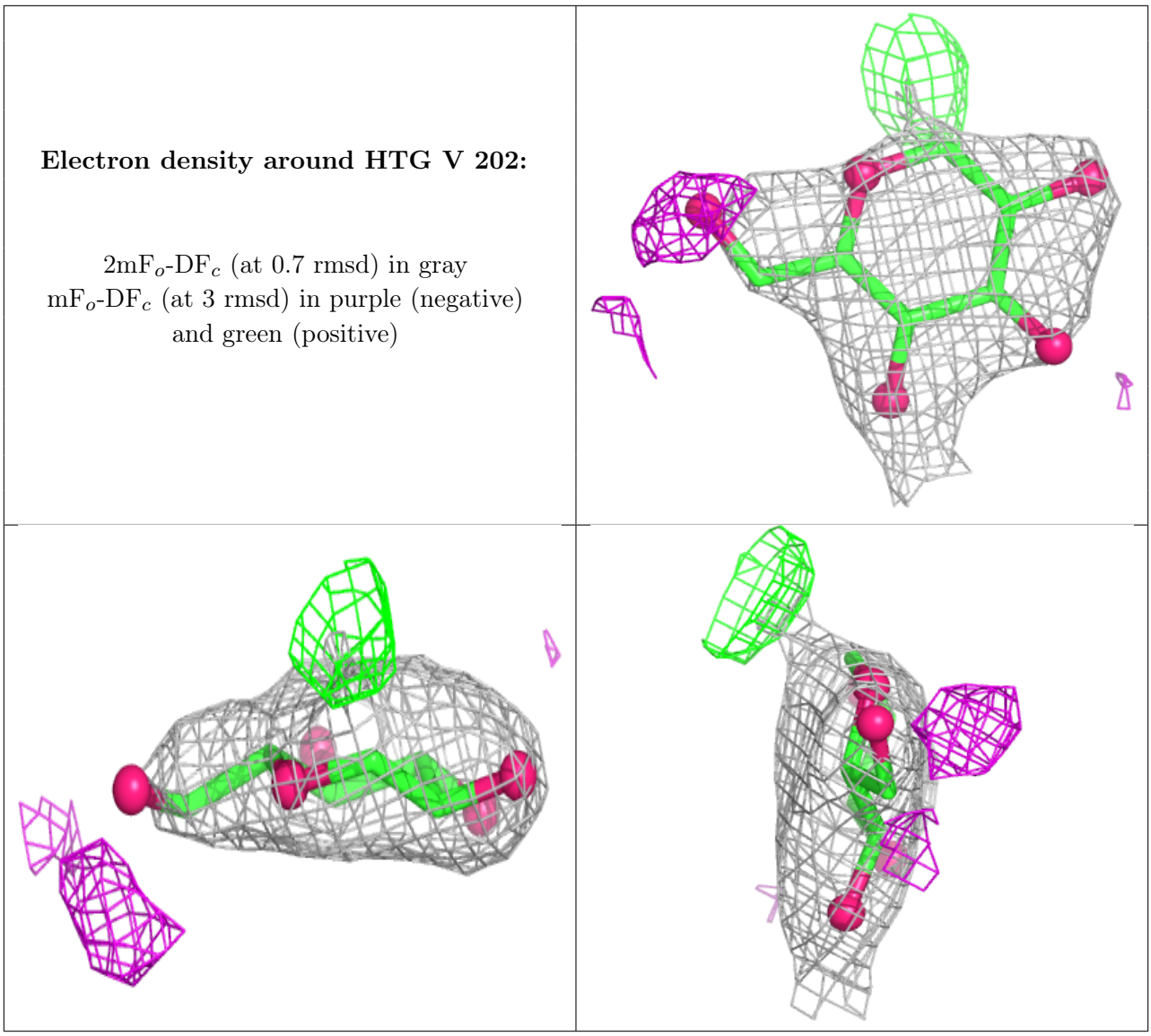






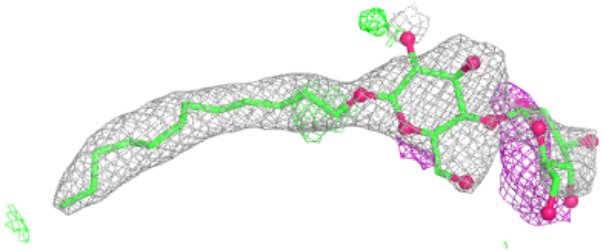
Electron density around HTG V 202:

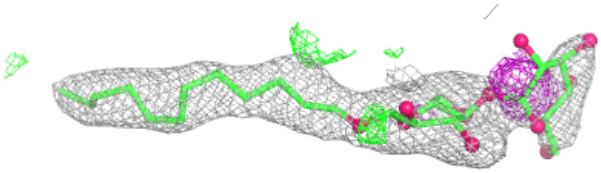
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

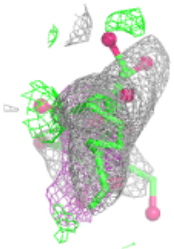


Electron density around LMT B 627:

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

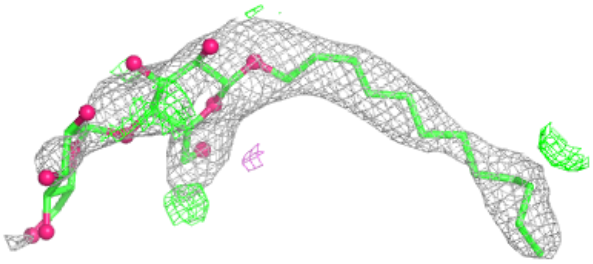


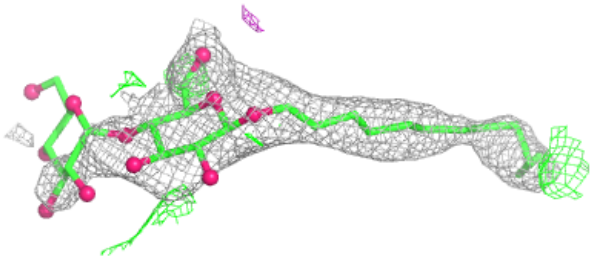


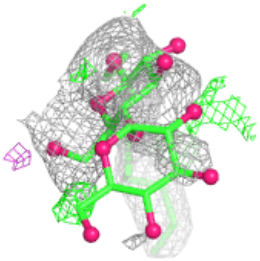


Electron density around LMT M 103:

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

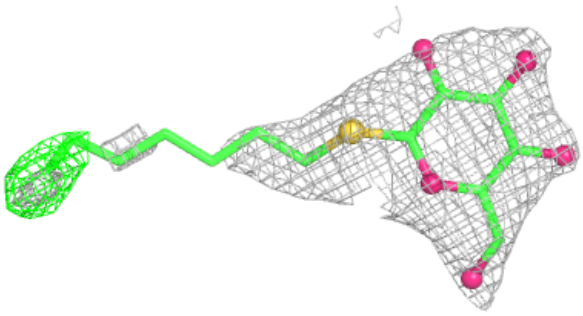


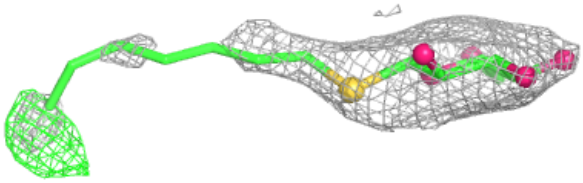


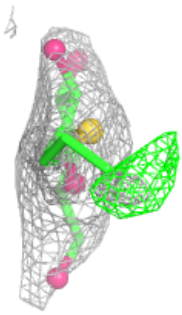


Electron density around HTG c 523:

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

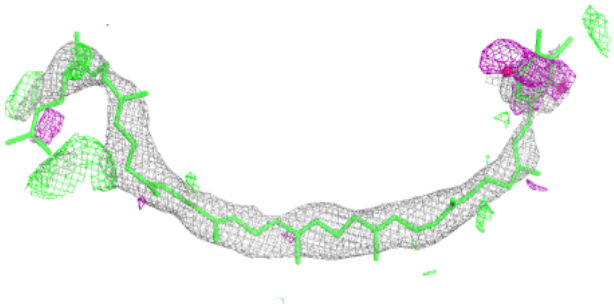


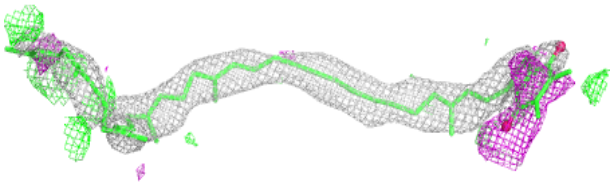


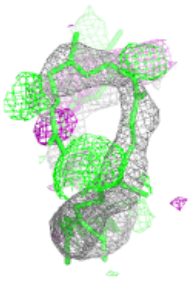


Electron density around PL9 A 414 (A):

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

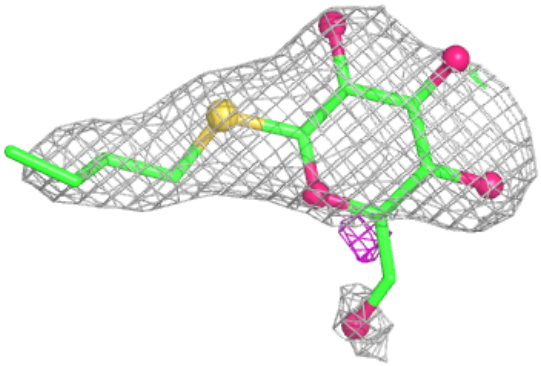


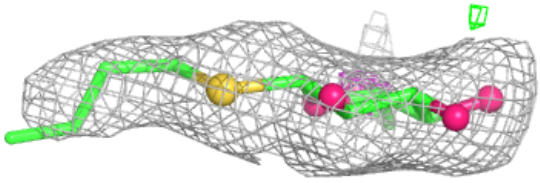


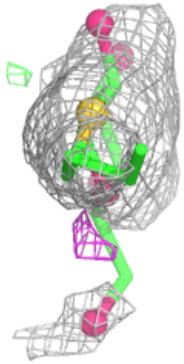


Electron density around HTG d 411:

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

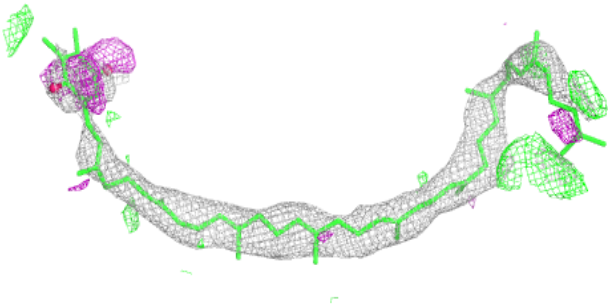


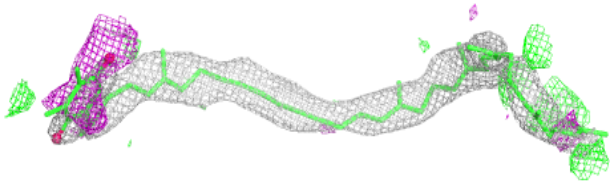


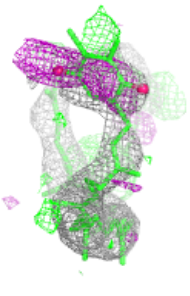


Electron density around PL9 A 414 (B):

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

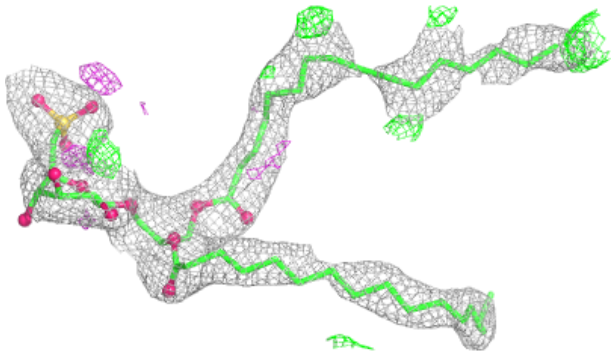


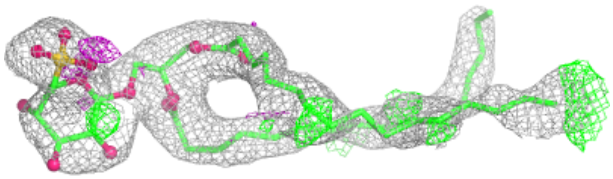


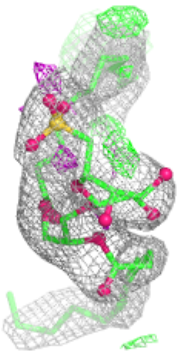


Electron density around SQD a 410:

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

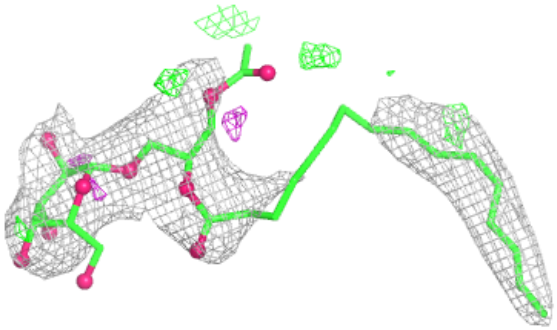


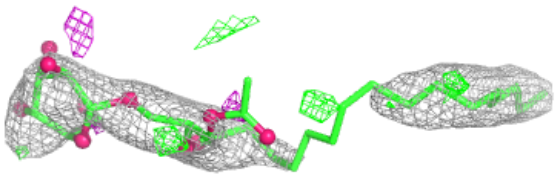


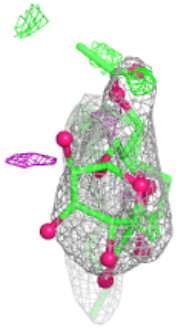


Electron density around LMG Z 101:

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

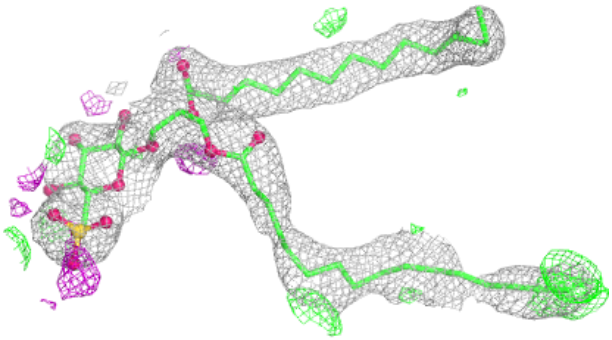


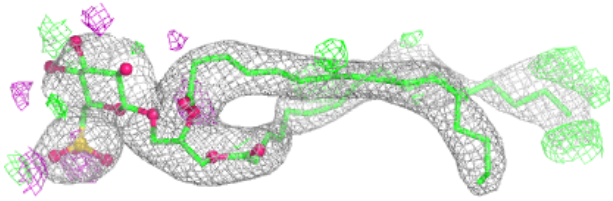




Electron density around SQD A 412:

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

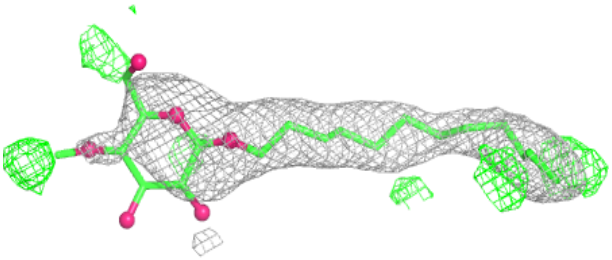


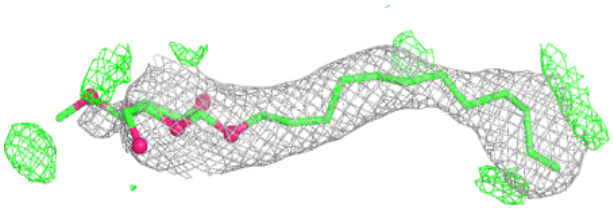


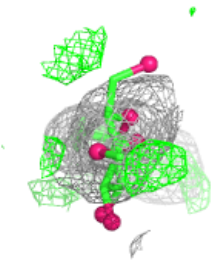


Electron density around LMT b 627:

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

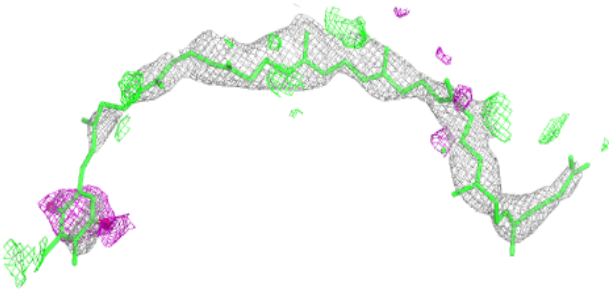


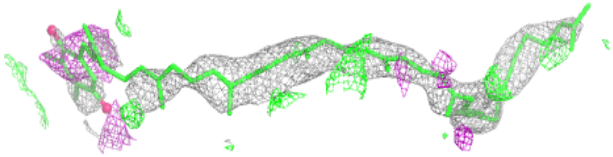


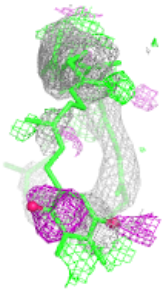


Electron density around PL9 a 412 (A):

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

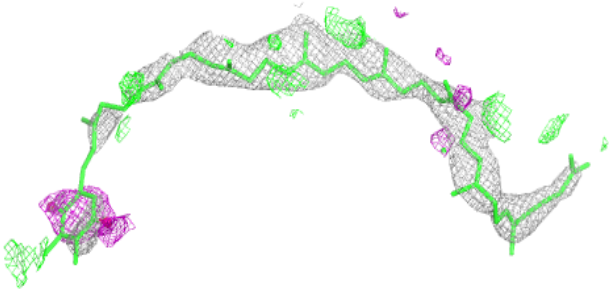


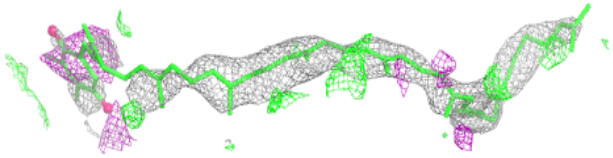


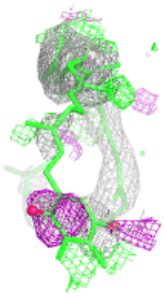


Electron density around PL9 a 412 (B):

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

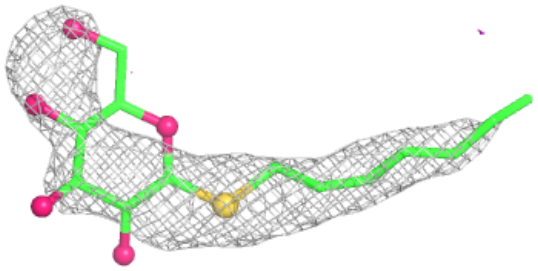


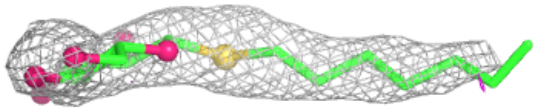


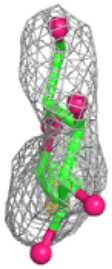


Electron density around HTG b 623:

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

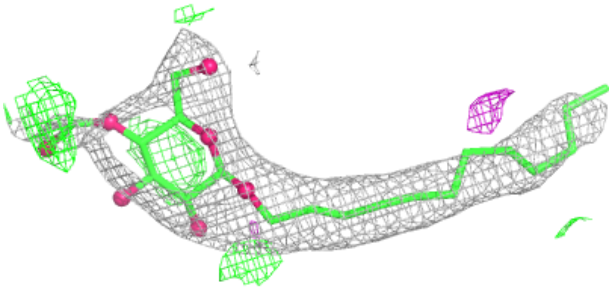


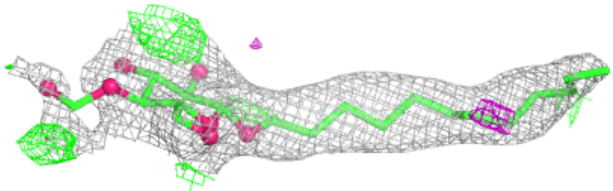


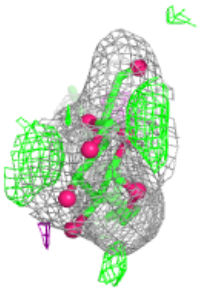


Electron density around LMT t 101:

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

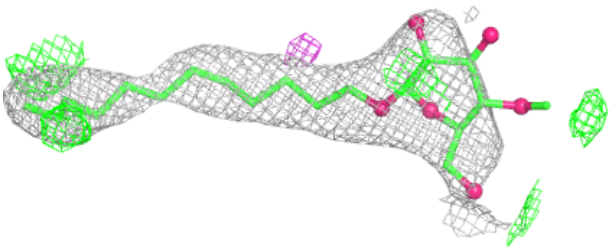


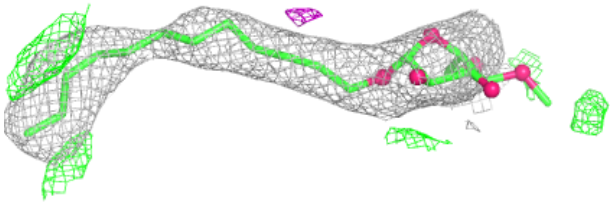


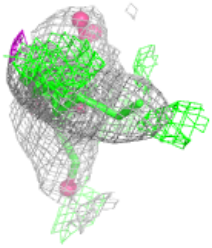


Electron density around LMT B 630:

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

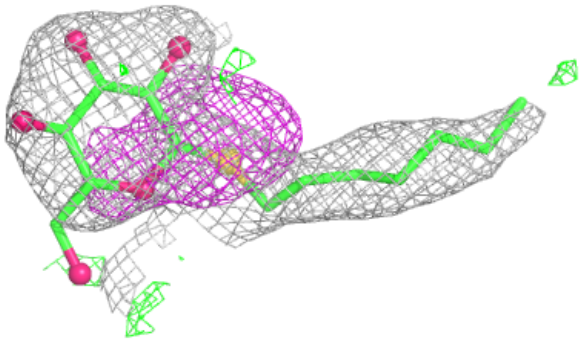


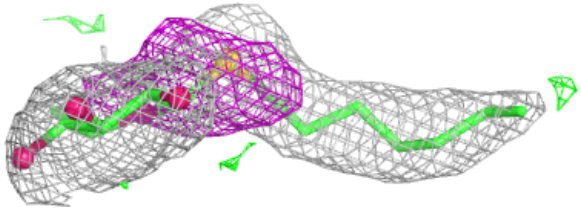


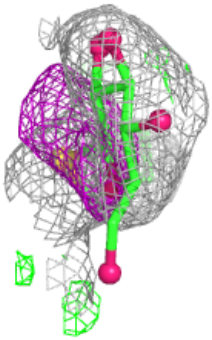


Electron density around HTG b 622:

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

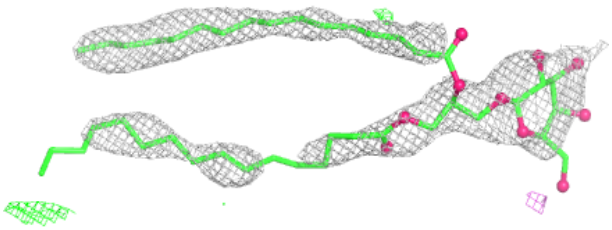


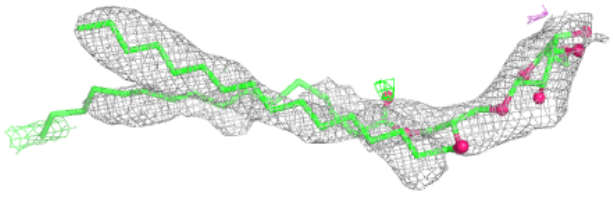


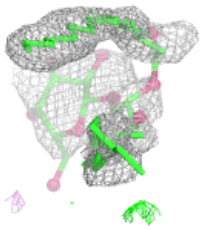


Electron density around LMG c 522:

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

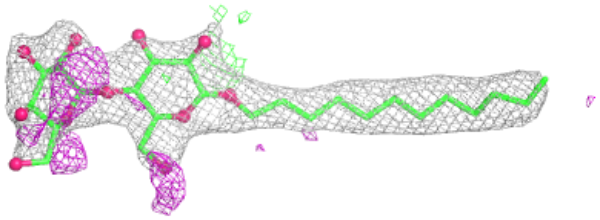


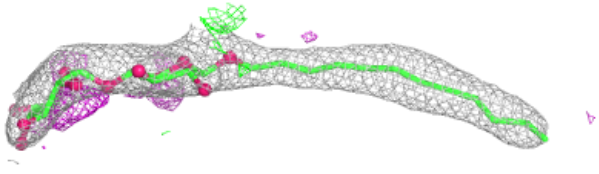


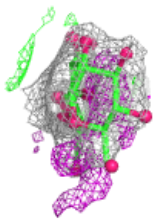


Electron density around LMT m 103:

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

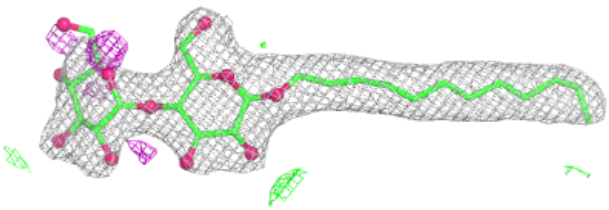


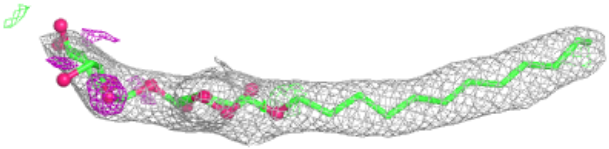


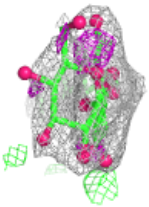


Electron density around LMT M 101:

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

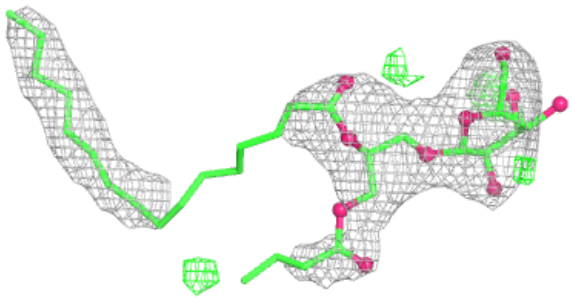


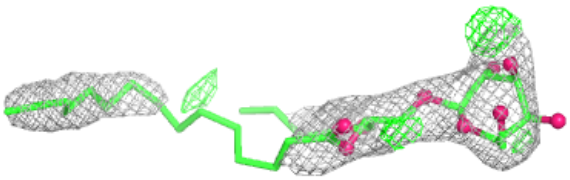


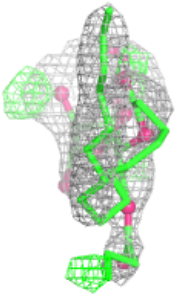


Electron density around LMG z 101:

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

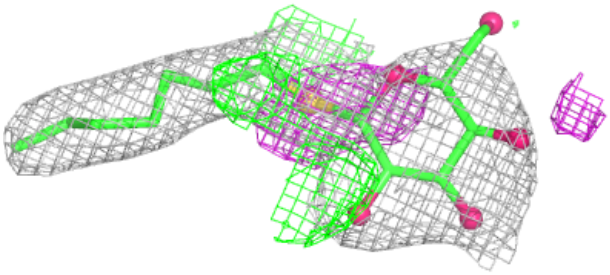


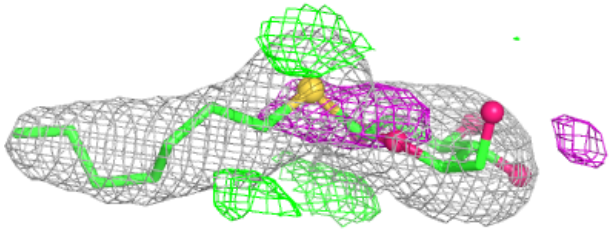


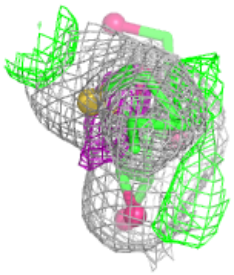


Electron density around HTG o 301:

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

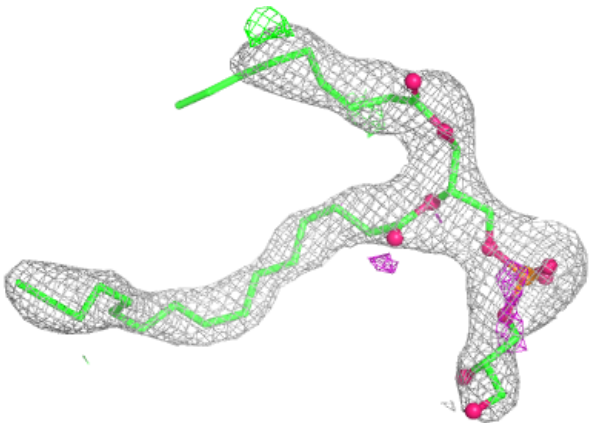


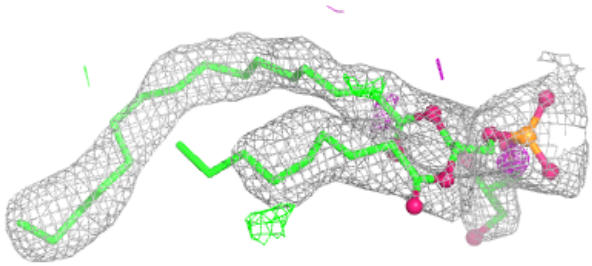


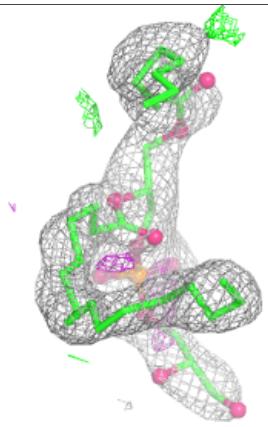


Electron density around LHG E 101 (B):

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

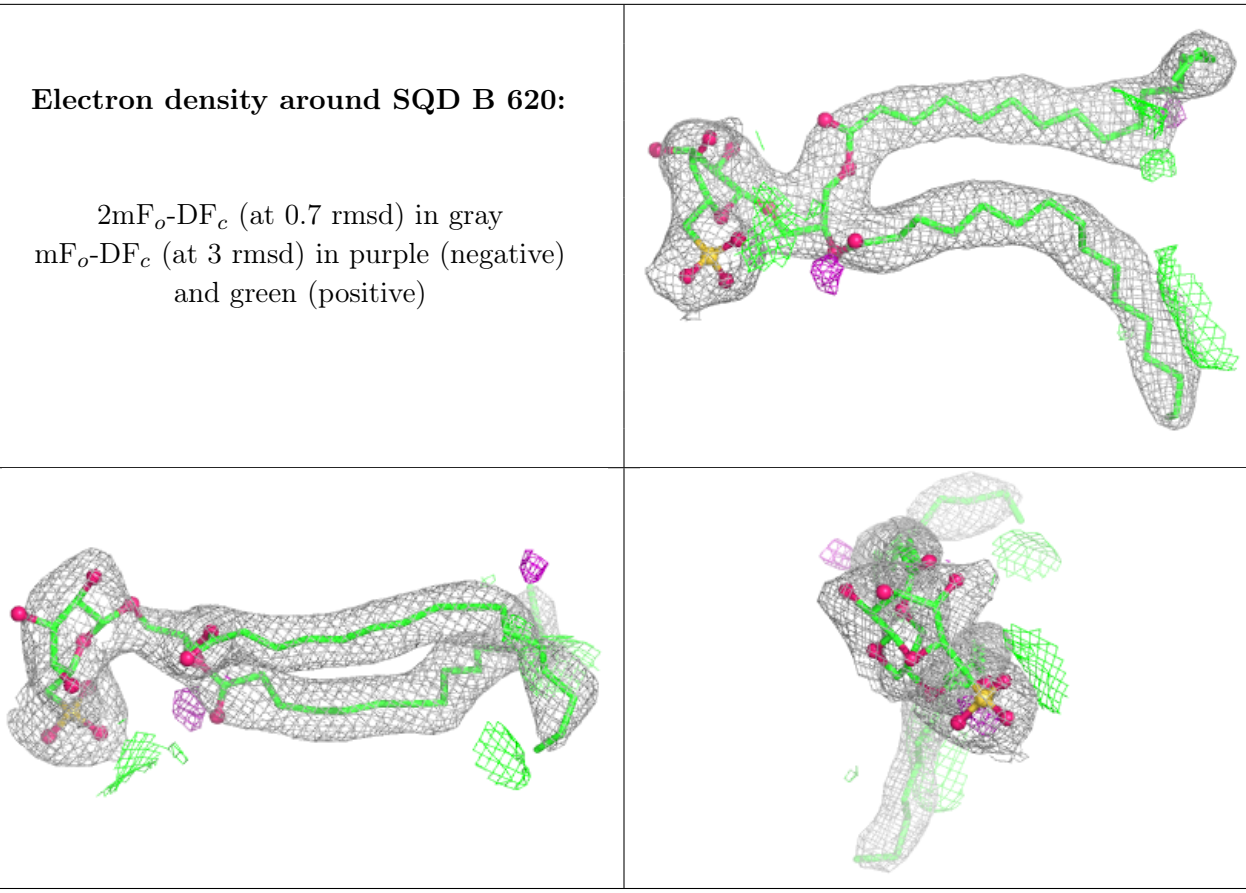






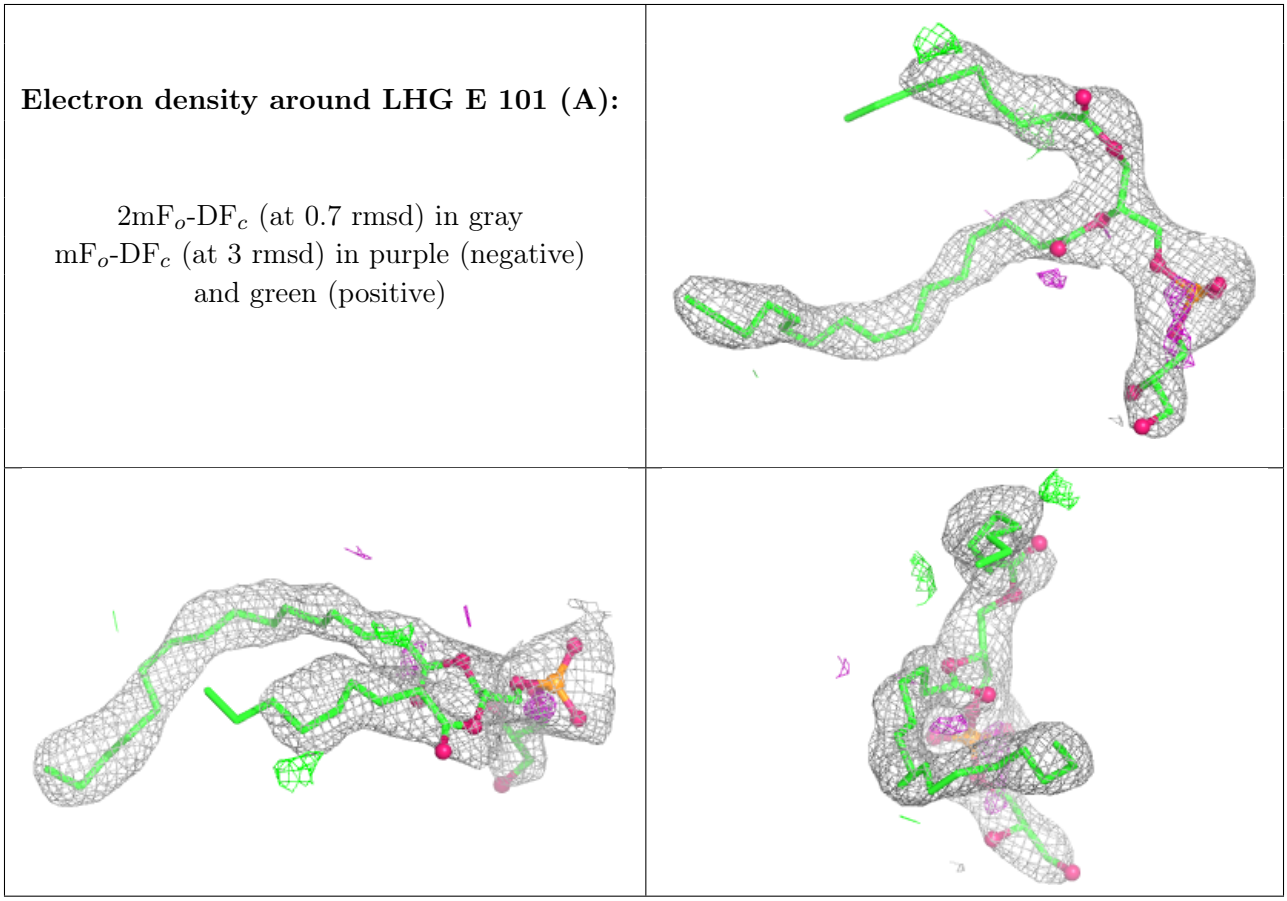
Electron density around SQD B 620:

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



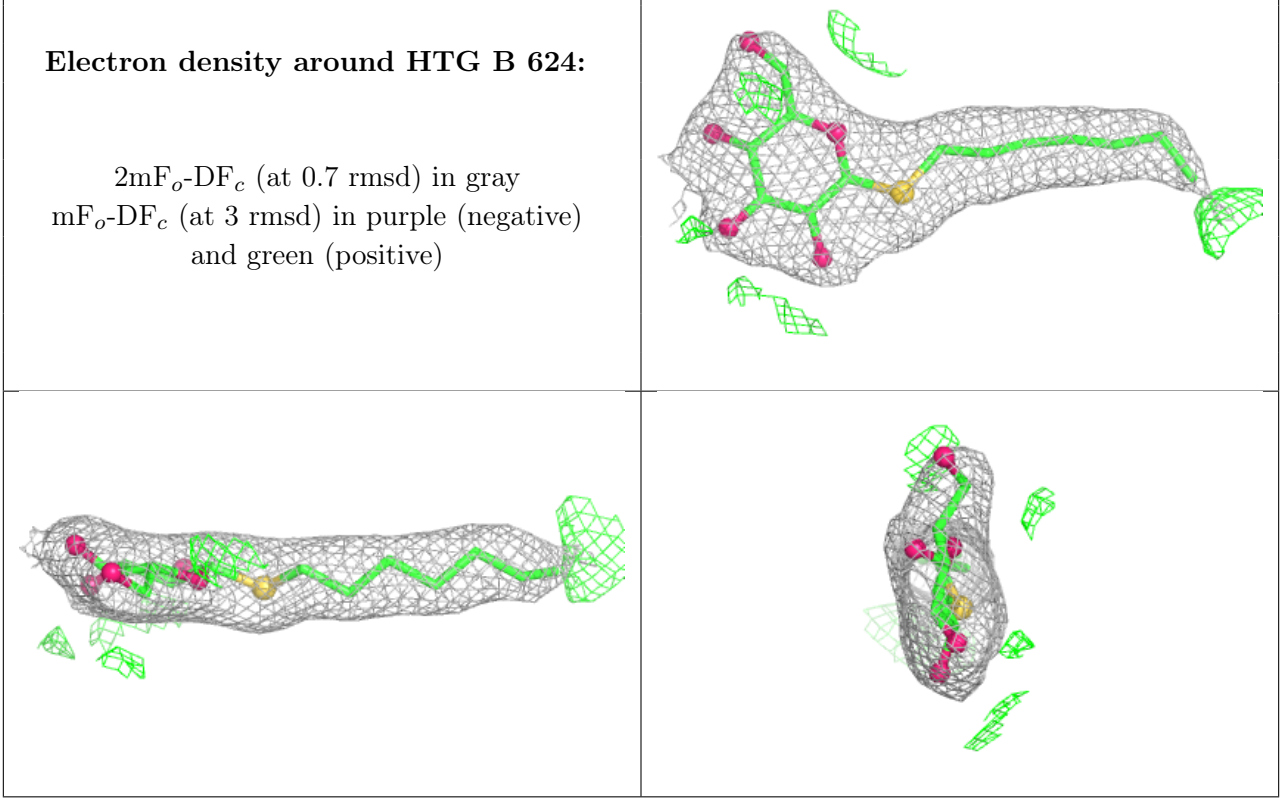
Electron density around LHG E 101 (A):

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



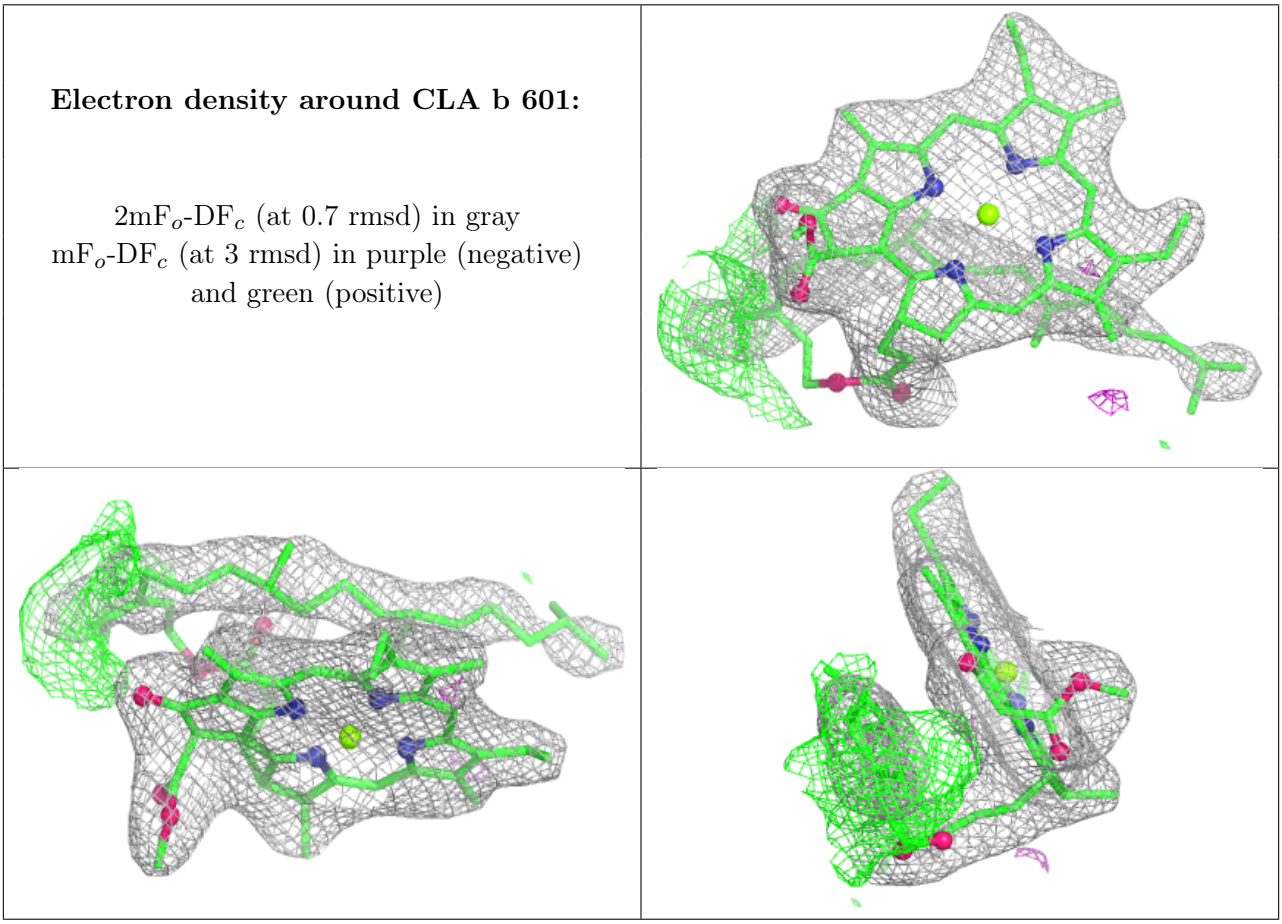
Electron density around HTG B 624:

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



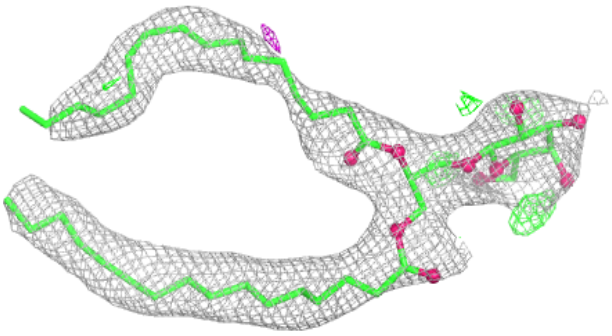
Electron density around CLA b 601:

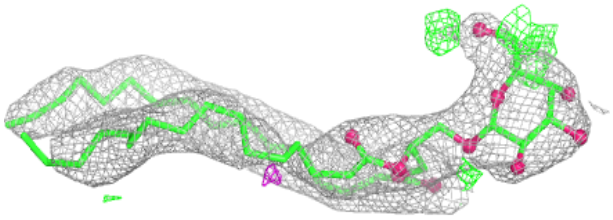
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMG C 501:

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

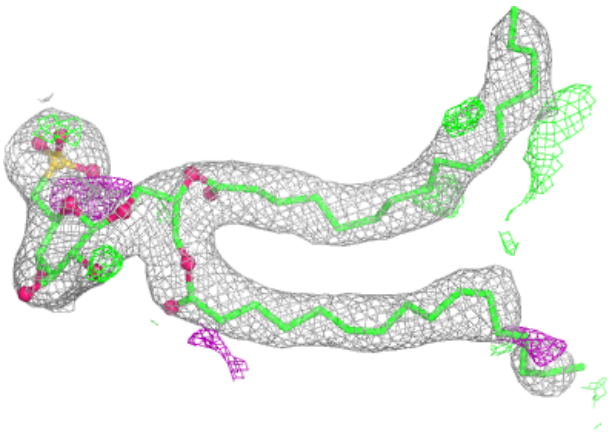


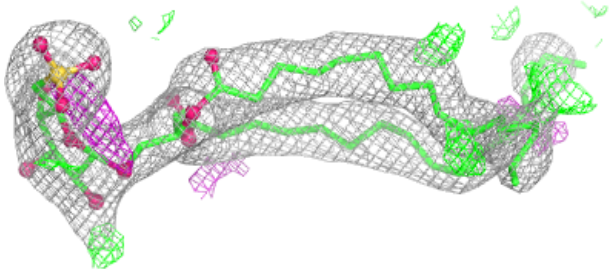


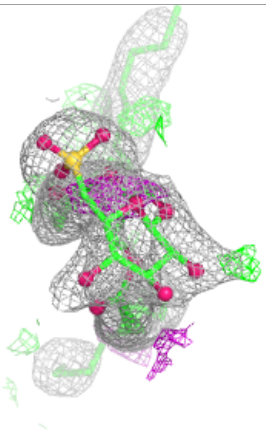


Electron density around SQD b 620:

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

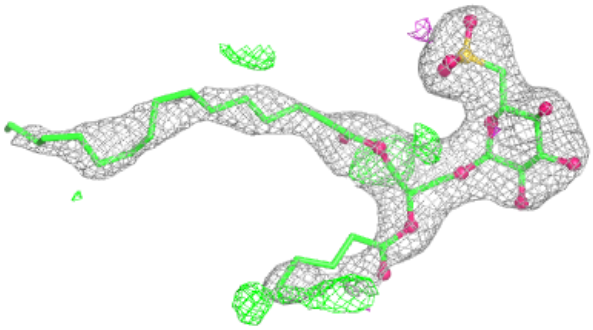


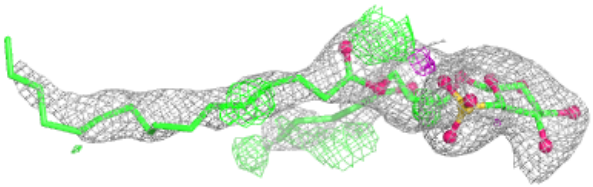


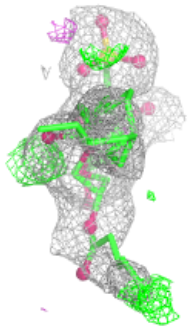


Electron density around SQD F 102:

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

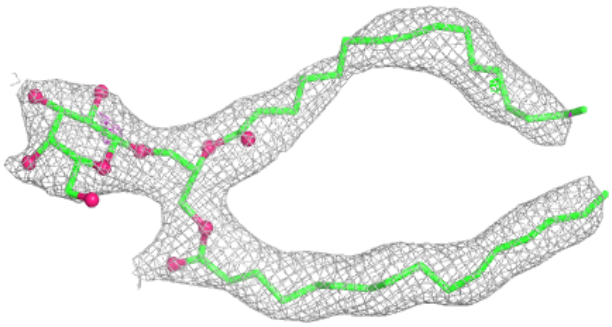


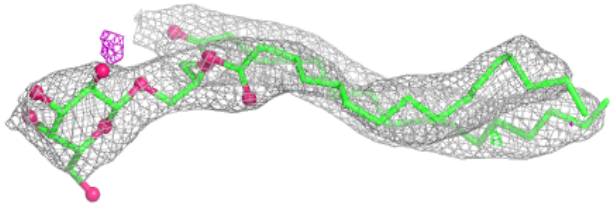


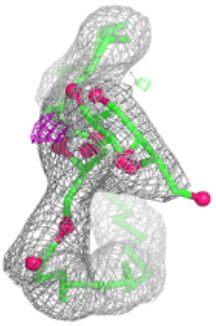


Electron density around LMG c 501:

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

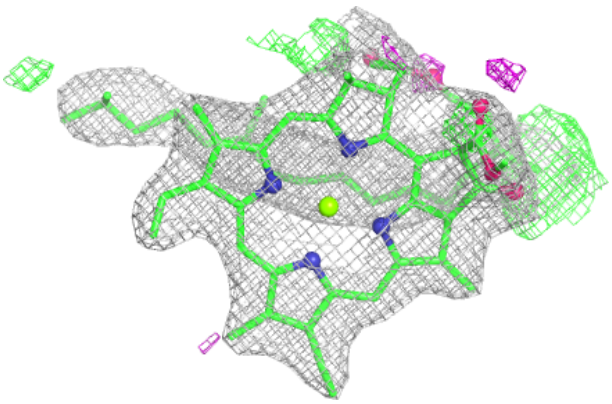


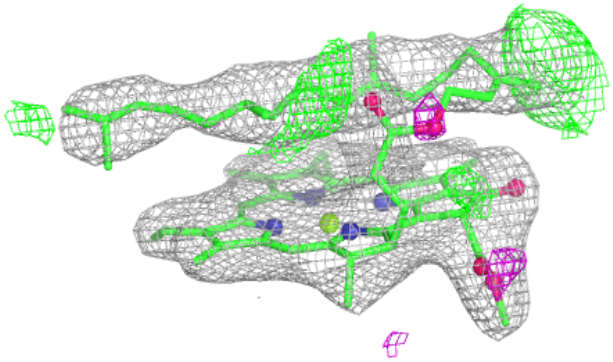




Electron density around CLA B 601:

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

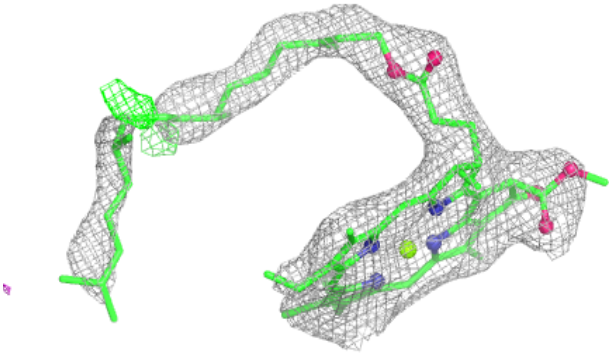


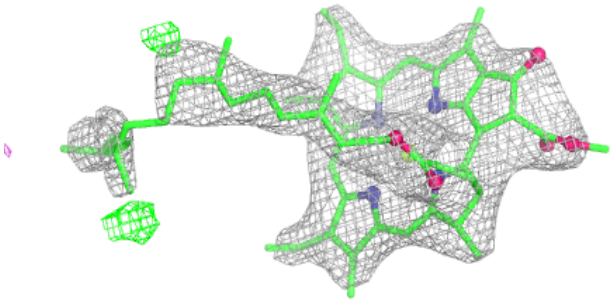


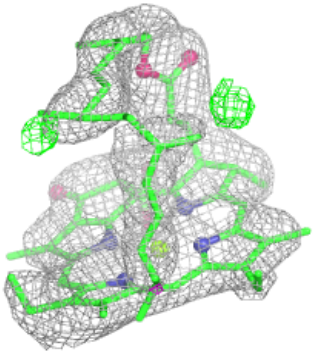


Electron density around CLA c 515:

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

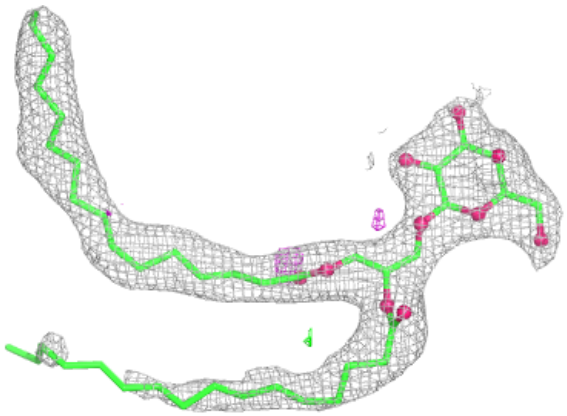


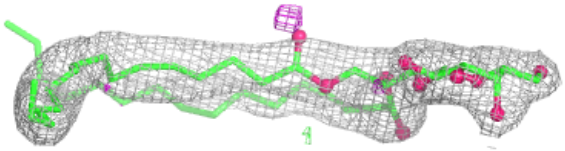


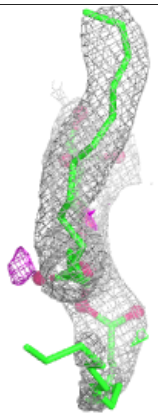


Electron density around LMG C 520:

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

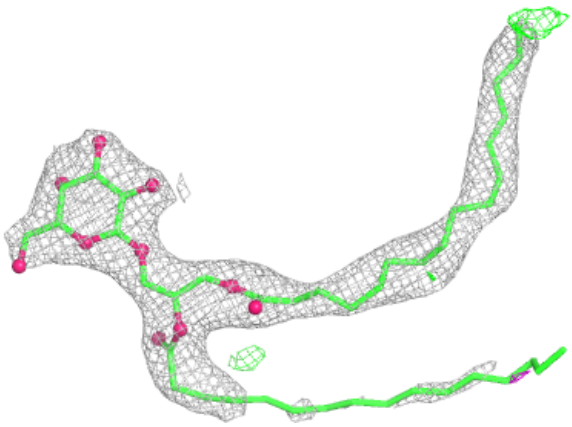


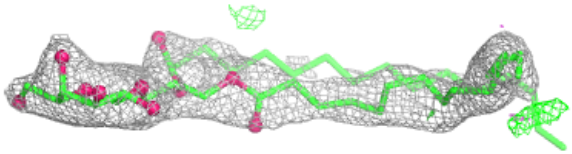


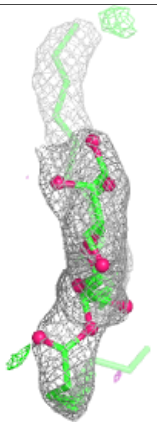


Electron density around LMG c 521:

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

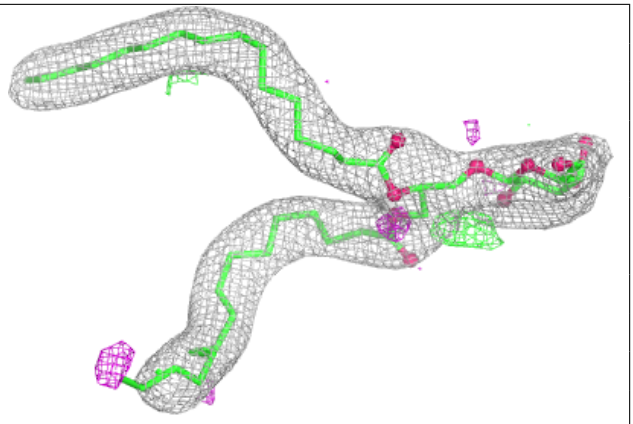


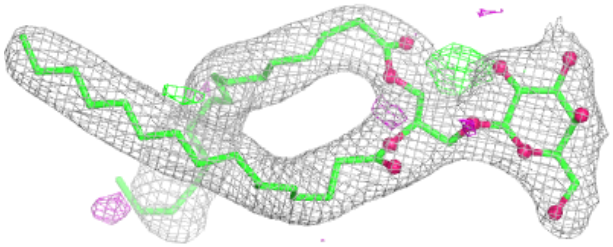


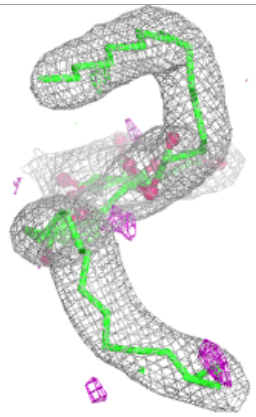


Electron density around LMG m 101:

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

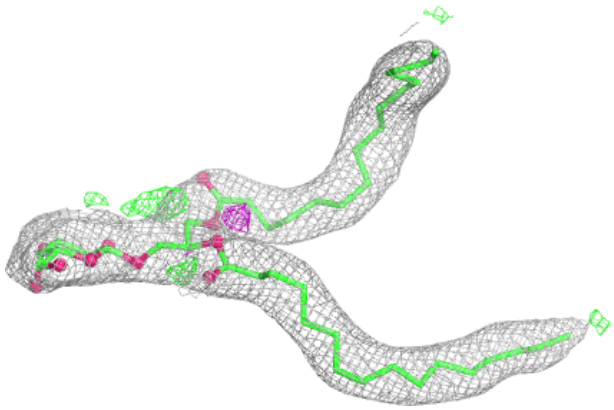


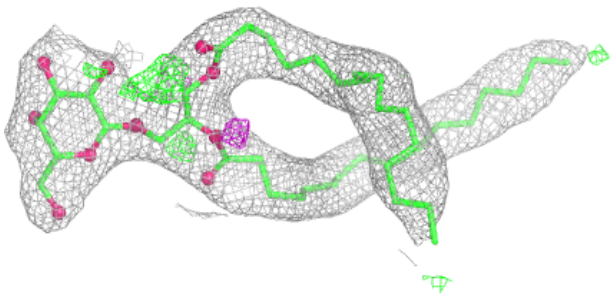




Electron density around LMG B 621:

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

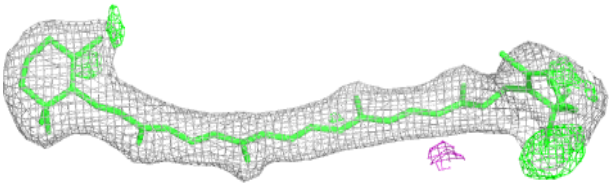


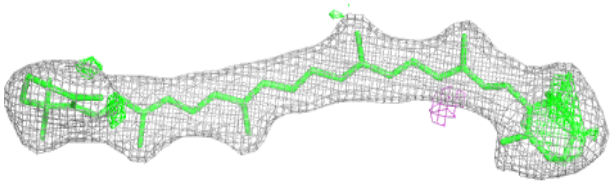


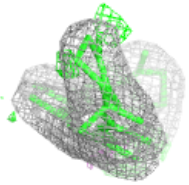


Electron density around BCR D 404:

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

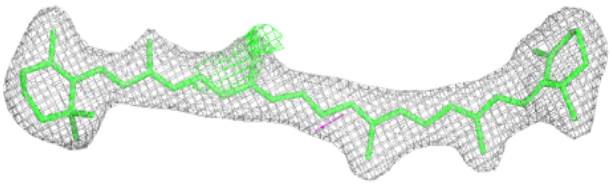


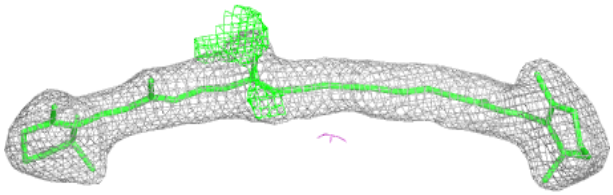


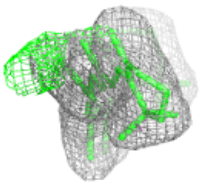


Electron density around BCR T 101:

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

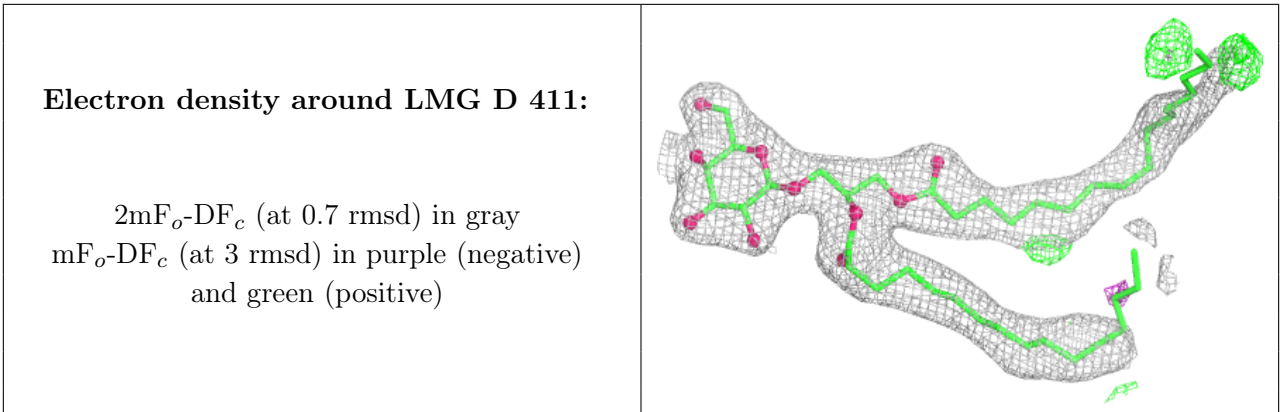


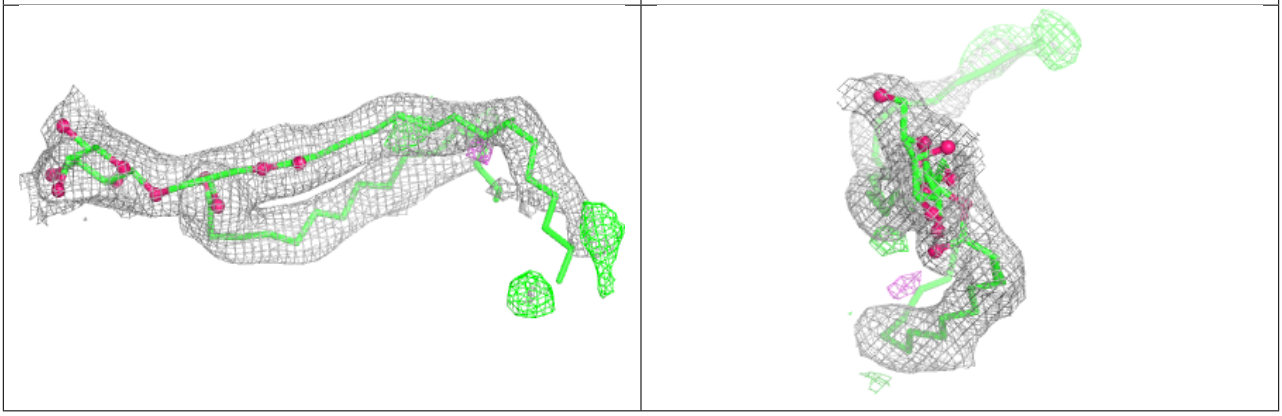




Electron density around LMG D 411:

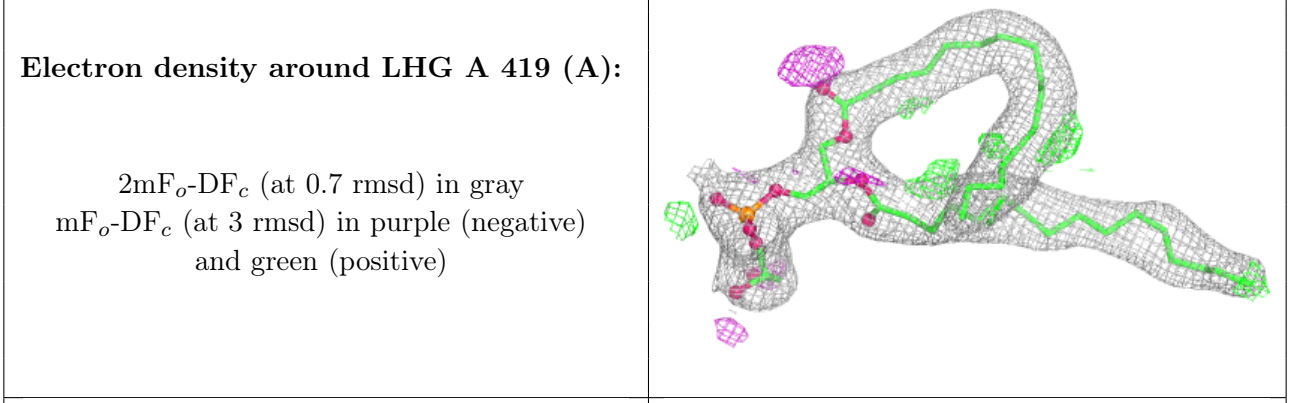
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

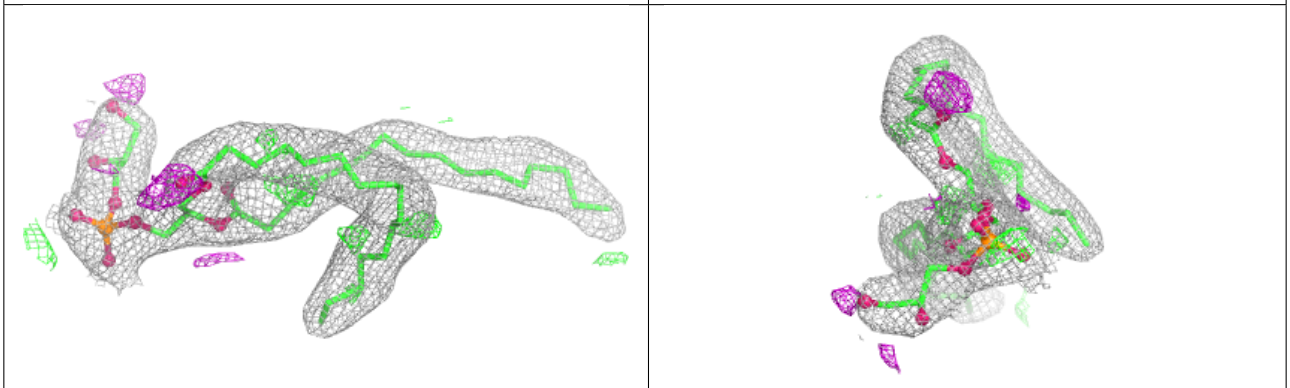




Electron density around LHG A 419 (A):

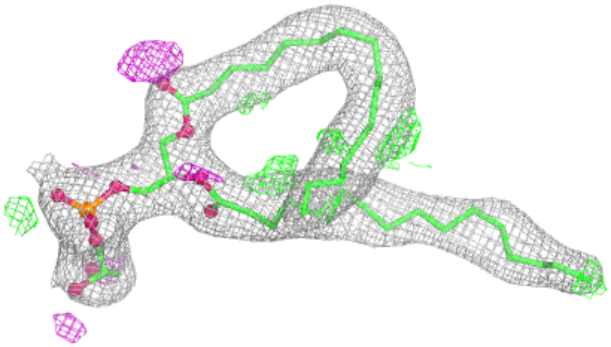
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

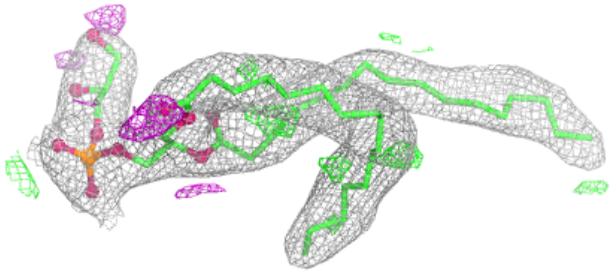


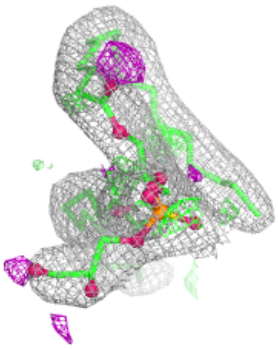


Electron density around LHG A 419 (B):

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

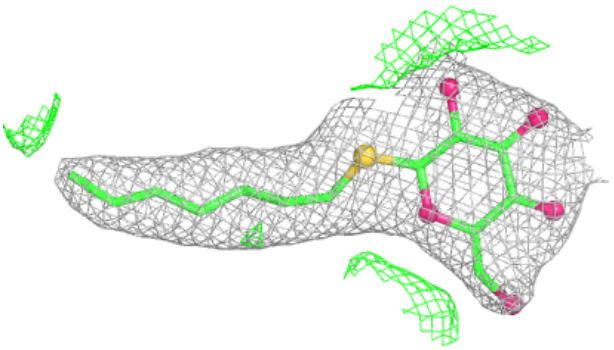


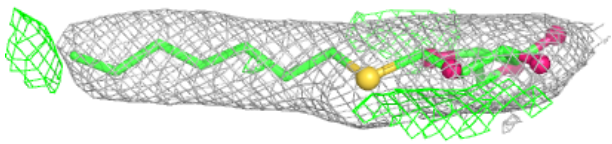


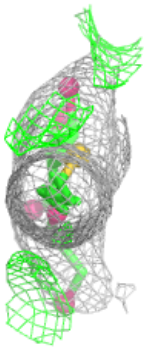


Electron density around HTG b 625:

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

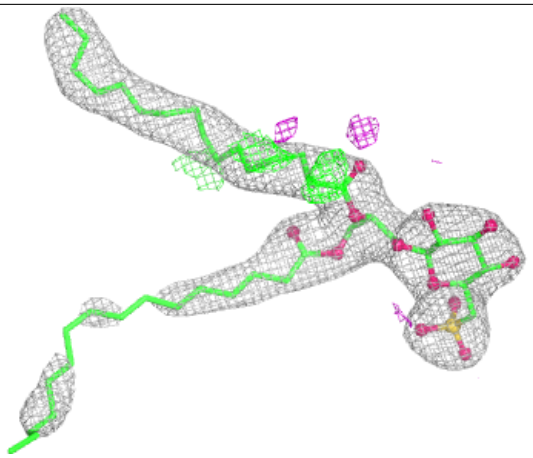


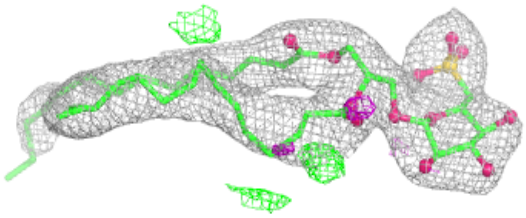


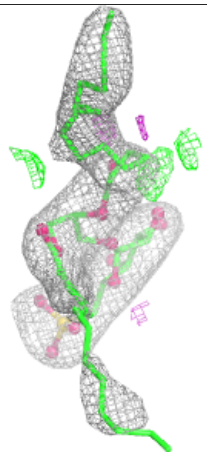


Electron density around SQD A 410 (A):

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

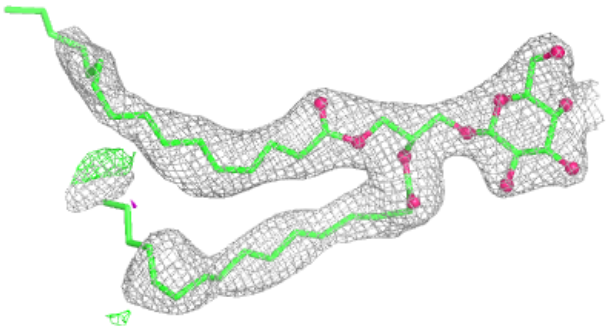


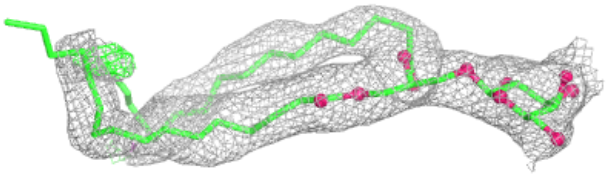


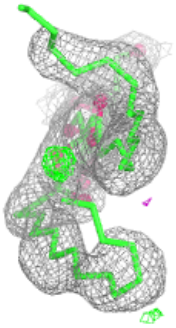


Electron density around LMG d 412:

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

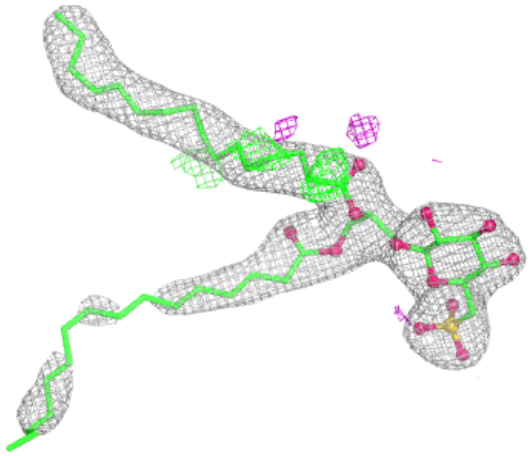


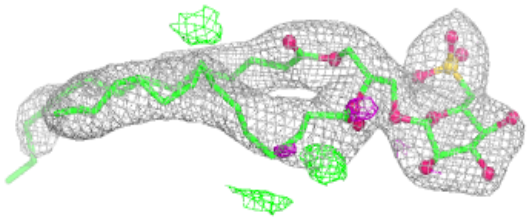


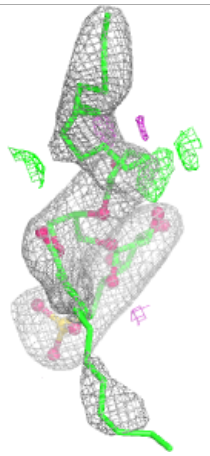


Electron density around SQD A 410 (B):

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

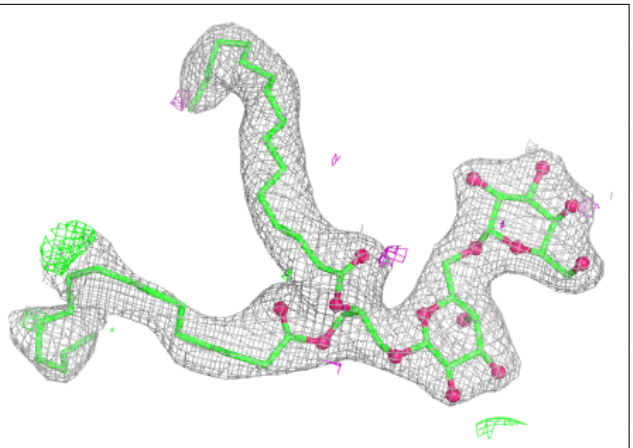


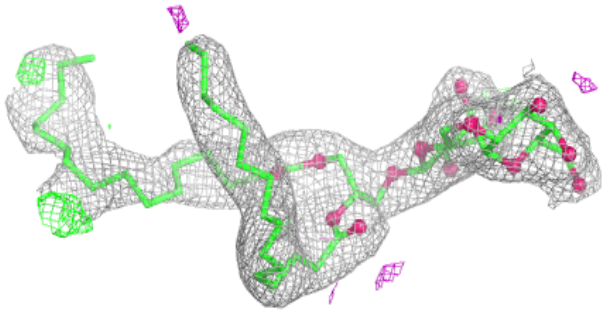


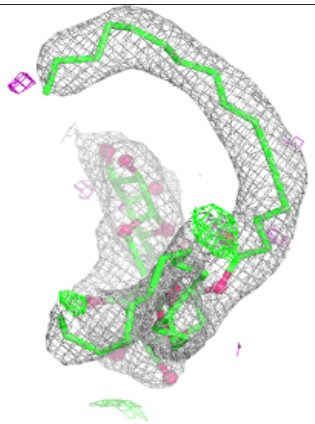


Electron density around DGD C 518 (A):

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



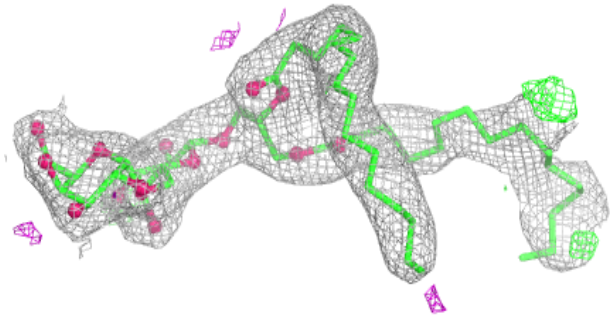


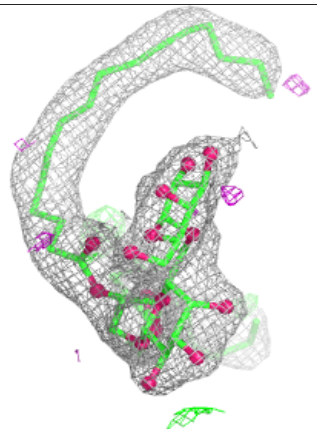


Electron density around DGD C 518 (B):

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

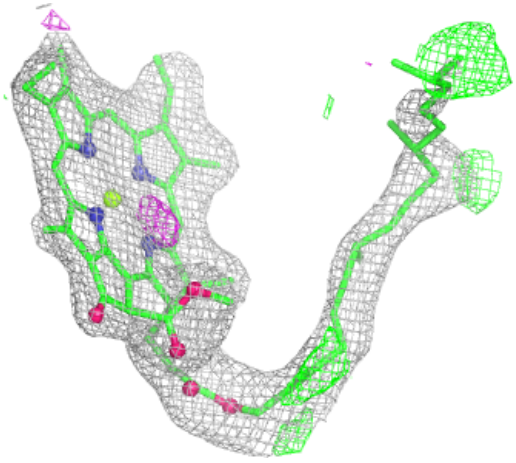


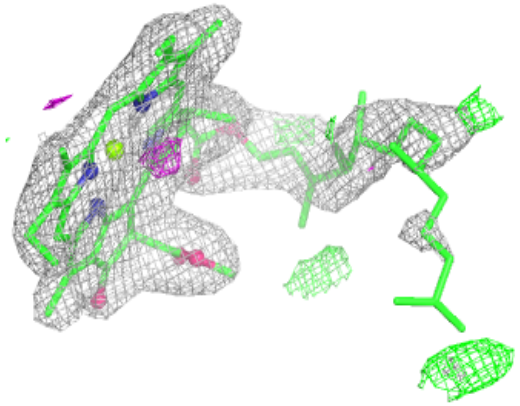


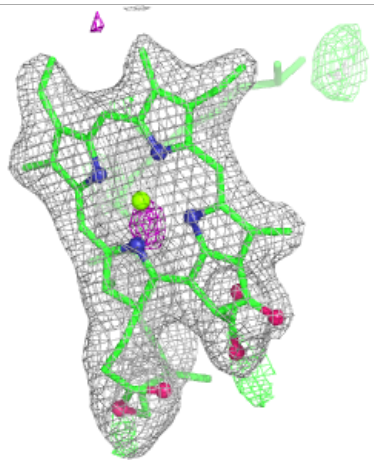


Electron density around CLA b 616:

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

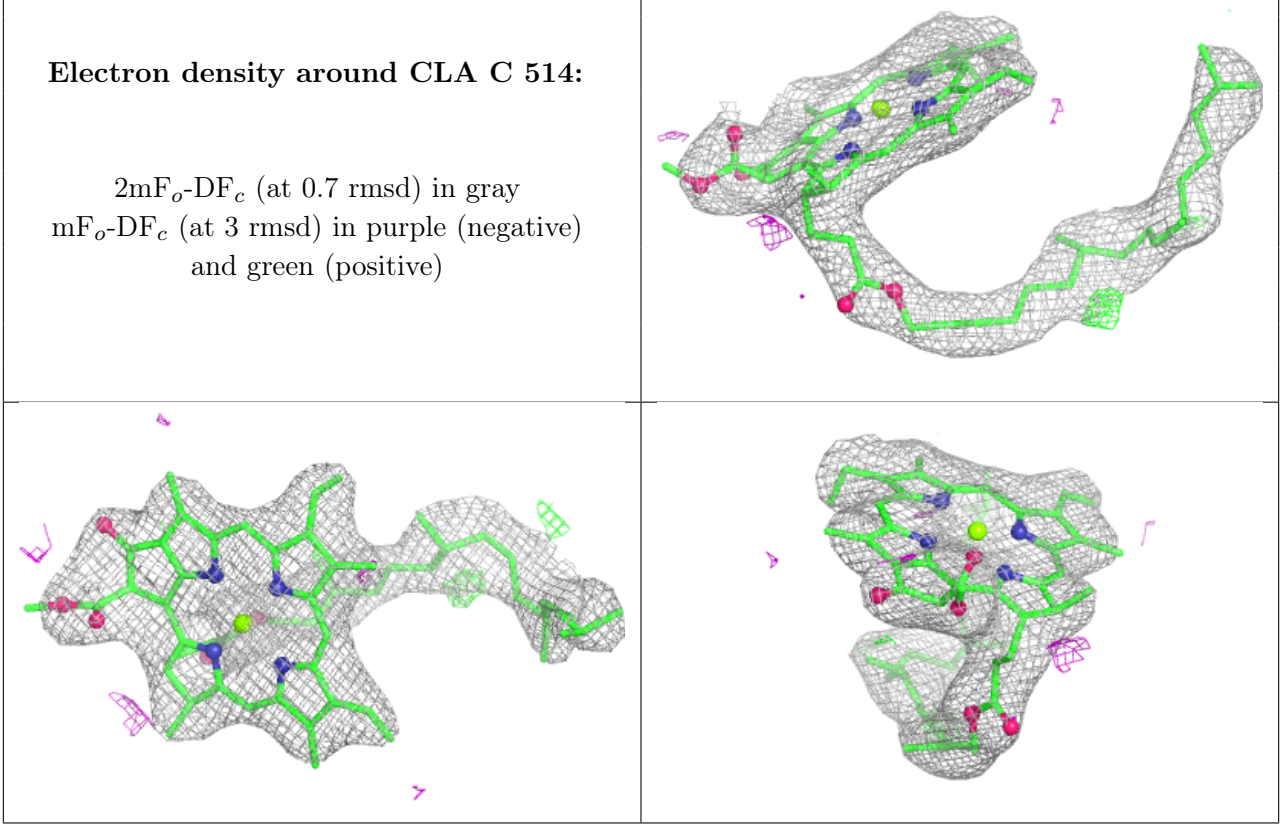






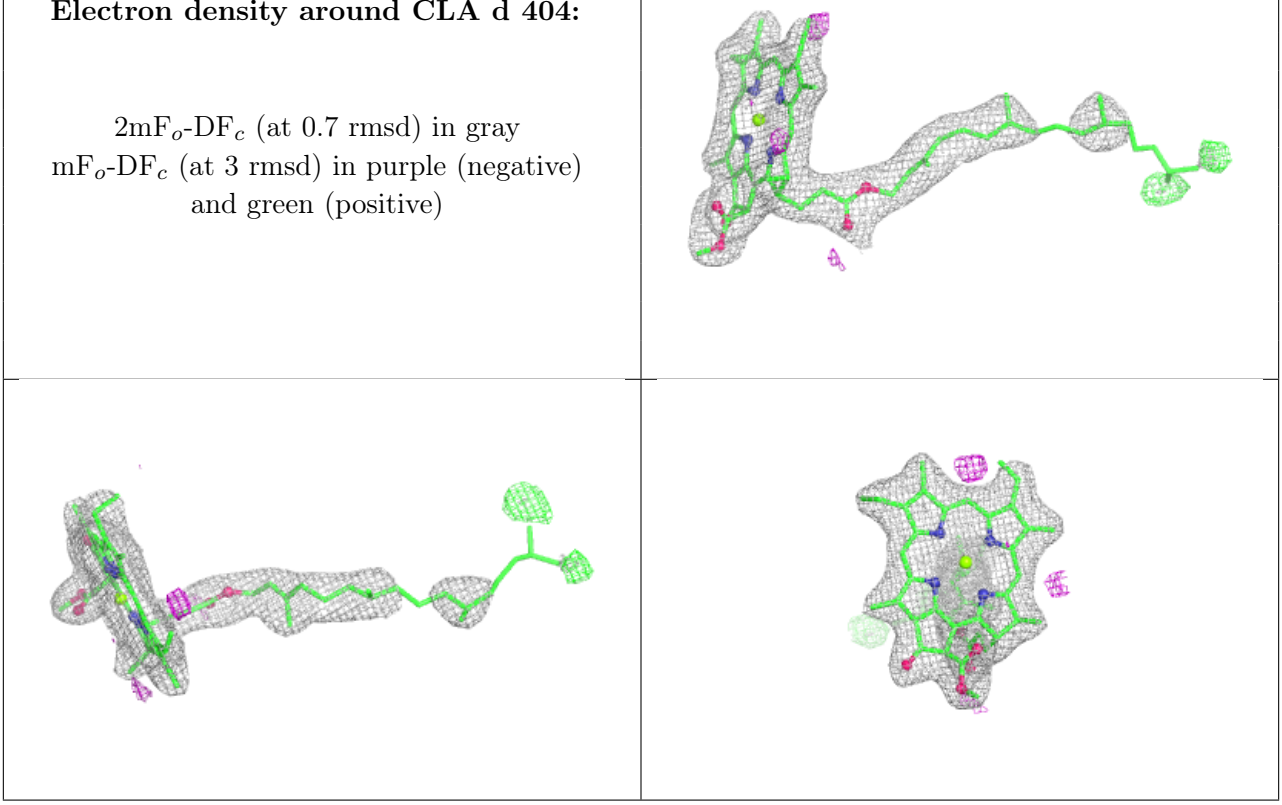
Electron density around CLA C 514:

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



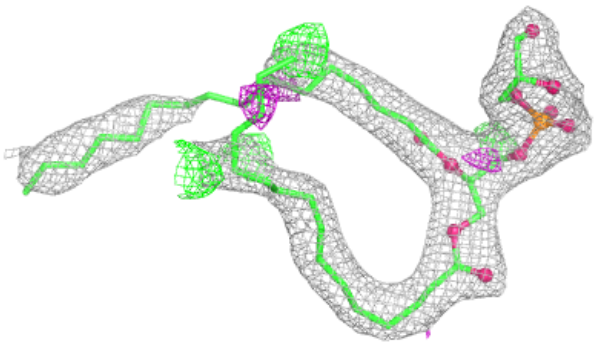
Electron density around CLA d 404:

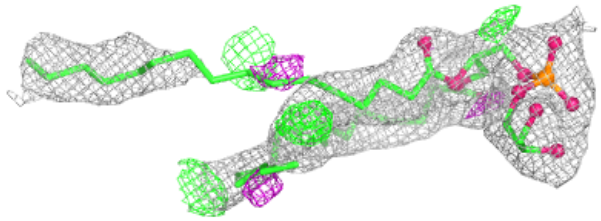
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

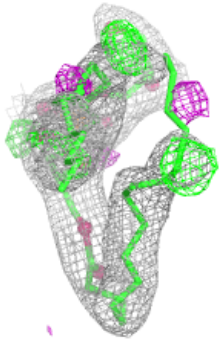


Electron density around LHG D 407 (A):

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

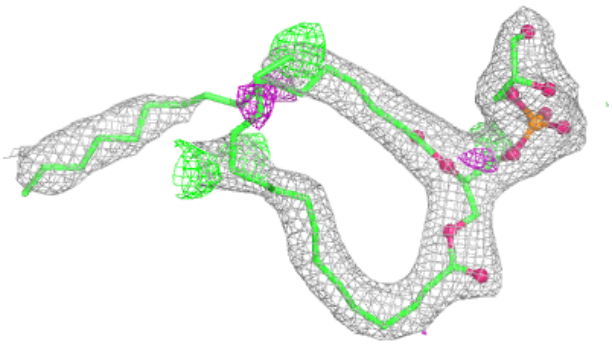


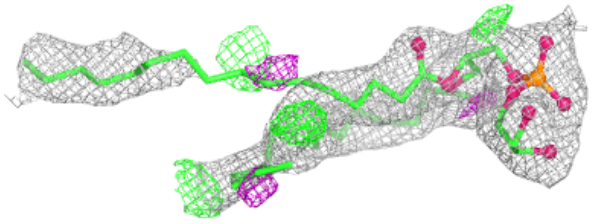


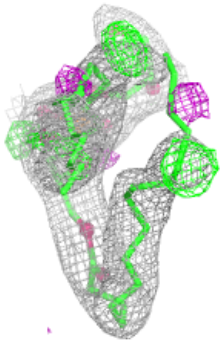


Electron density around LHG D 407 (B):

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

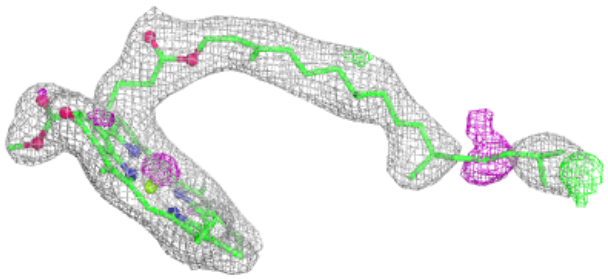


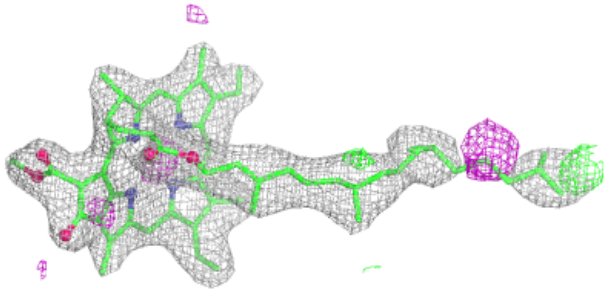


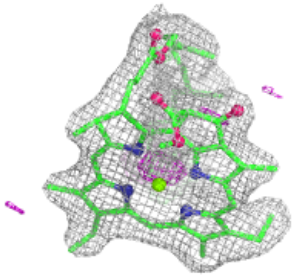


Electron density around CLA C 505:

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

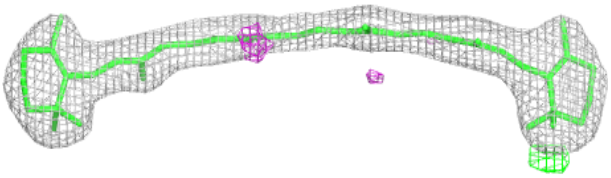


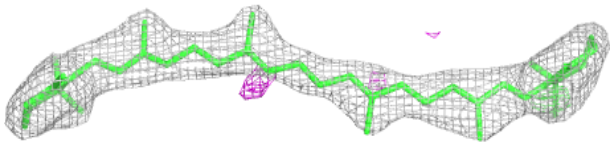


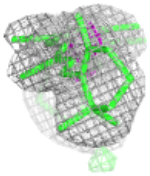


Electron density around BCR K 102:

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

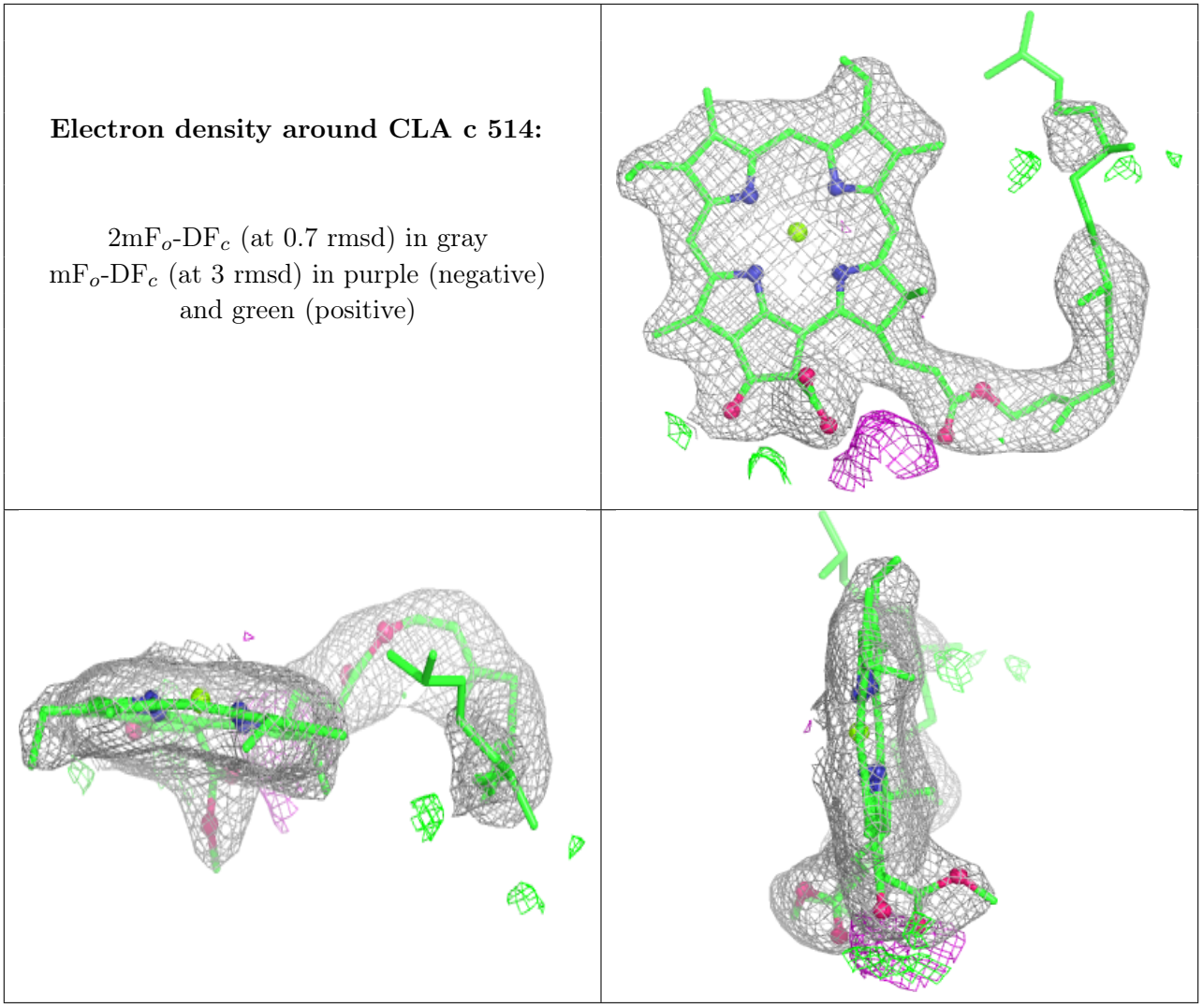






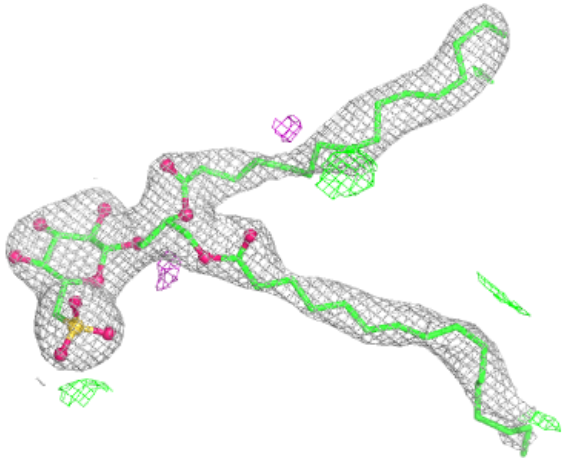
Electron density around CLA c 514:

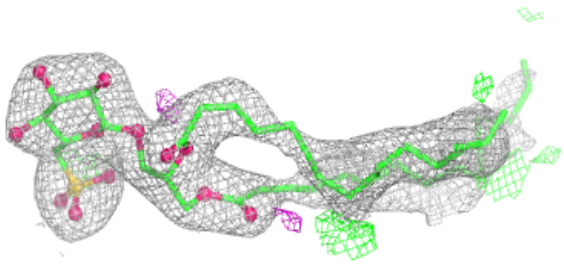
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

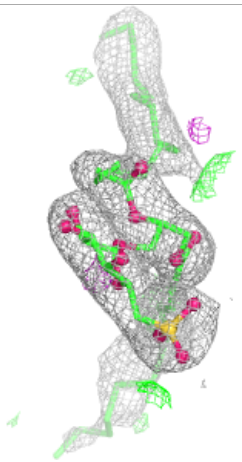


Electron density around SQD a 409 (A):

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

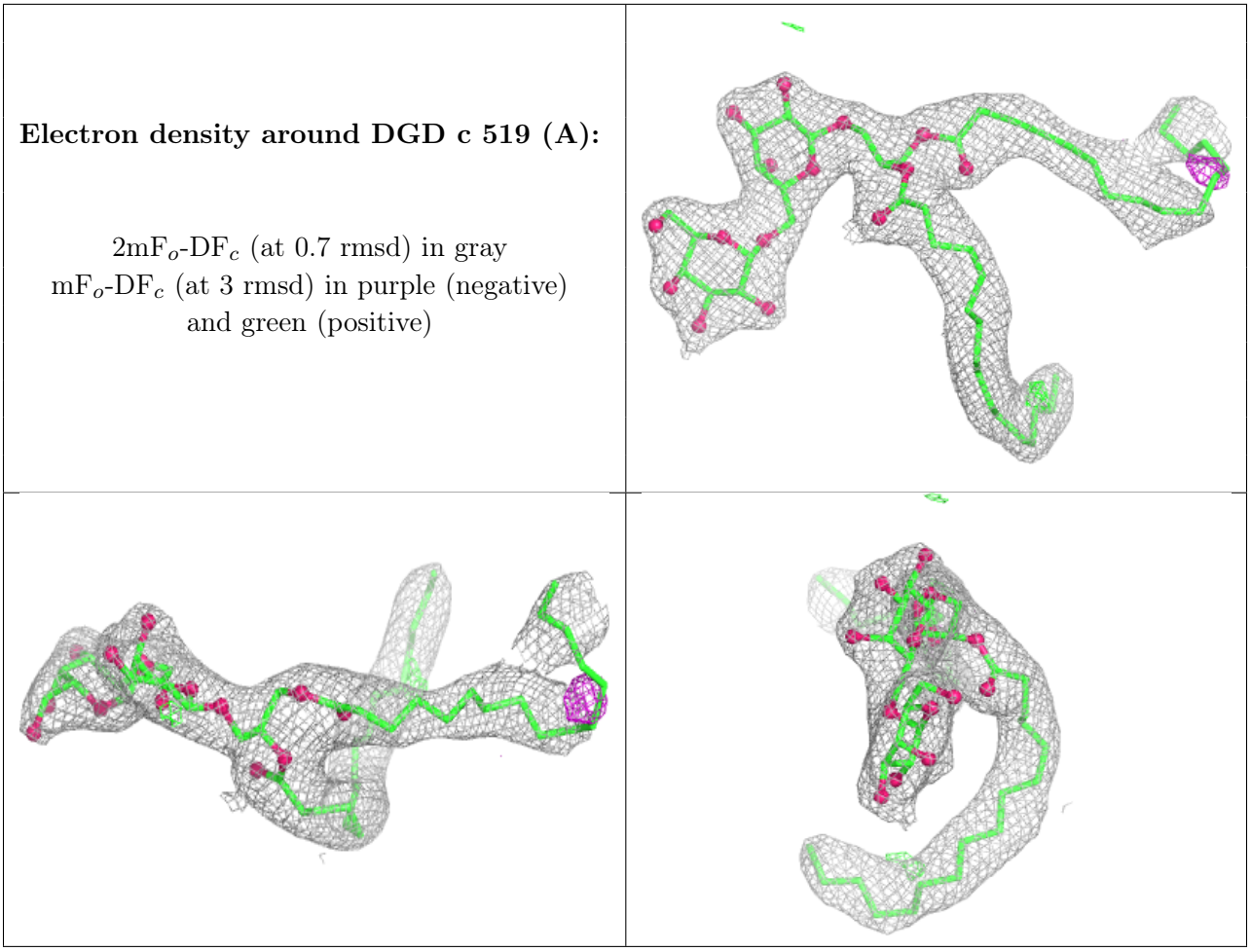






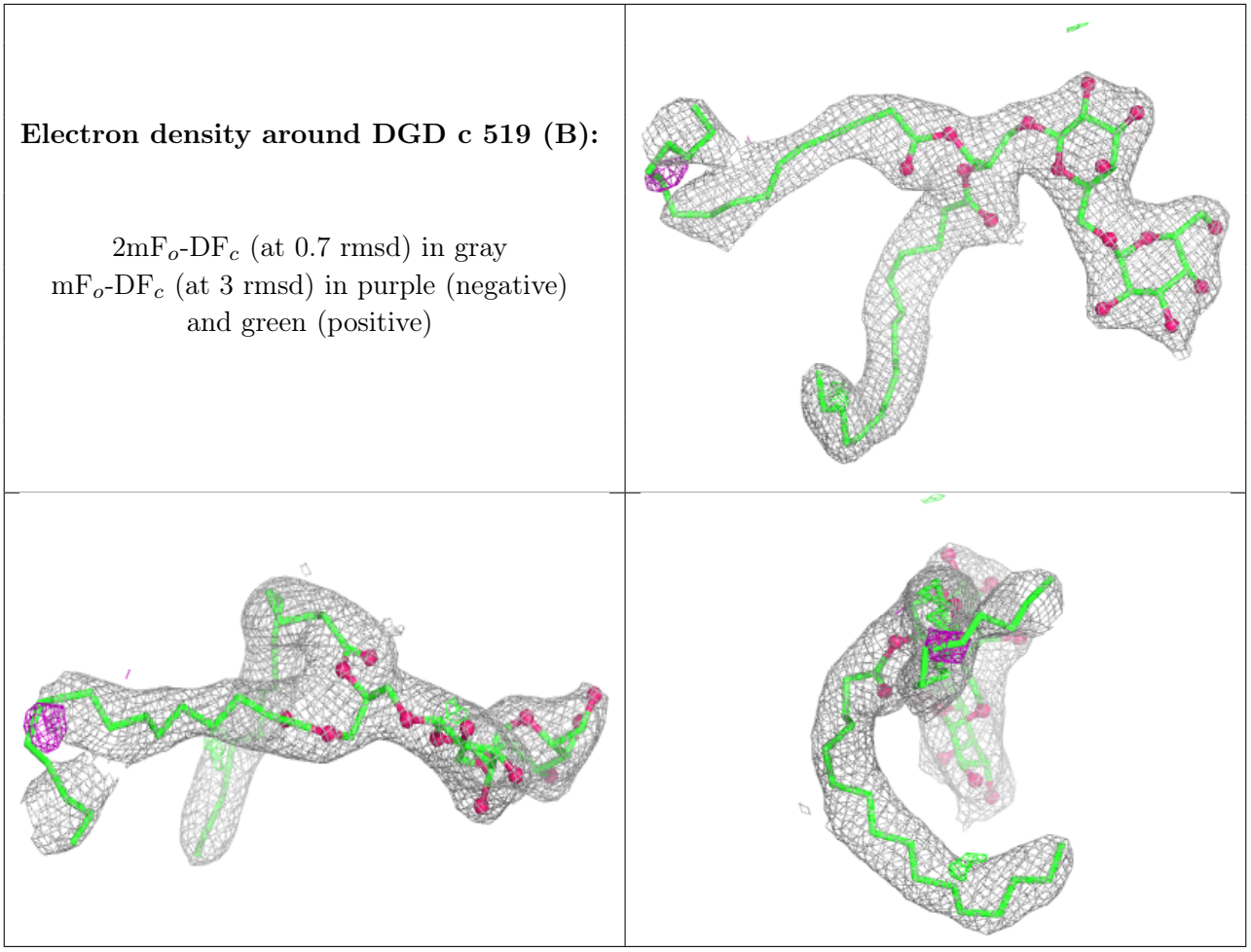
Electron density around DGD c 519 (A):

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



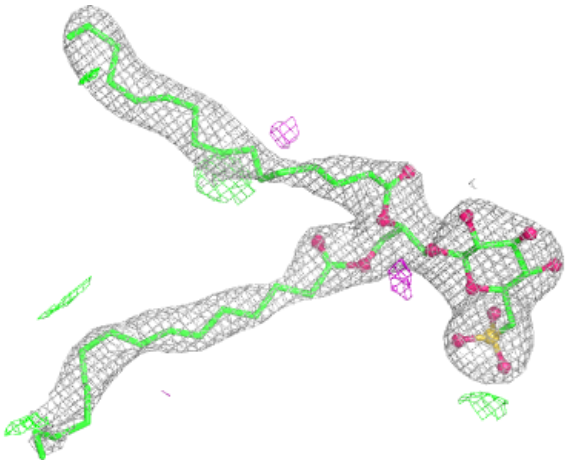
Electron density around DGD c 519 (B):

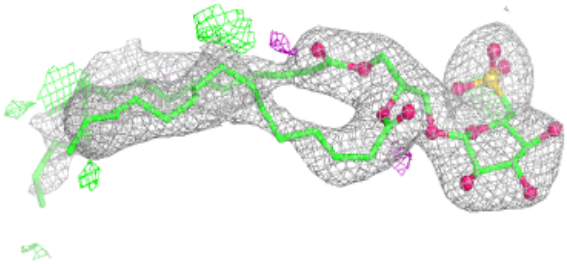
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

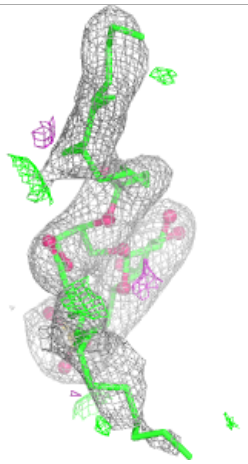


Electron density around SQD a 409 (B):

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

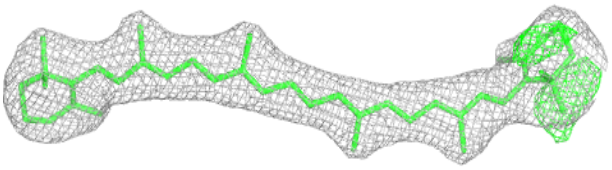


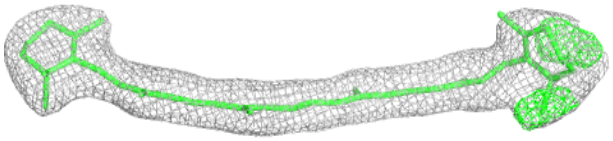


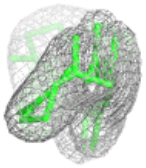


Electron density around BCR d 405:

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

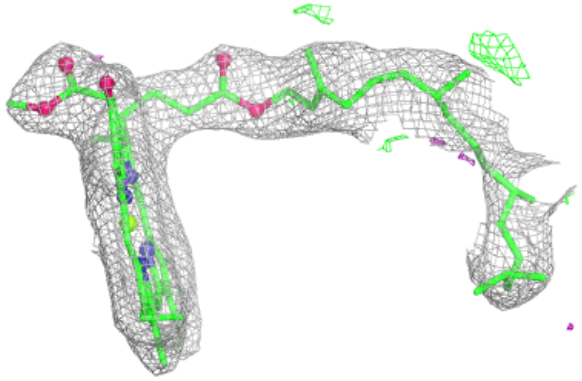


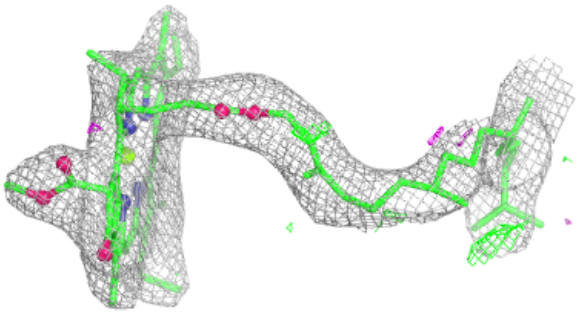


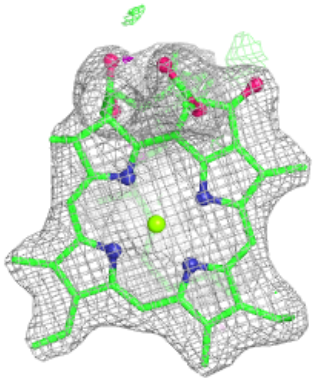


Electron density around CLA C 507:

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

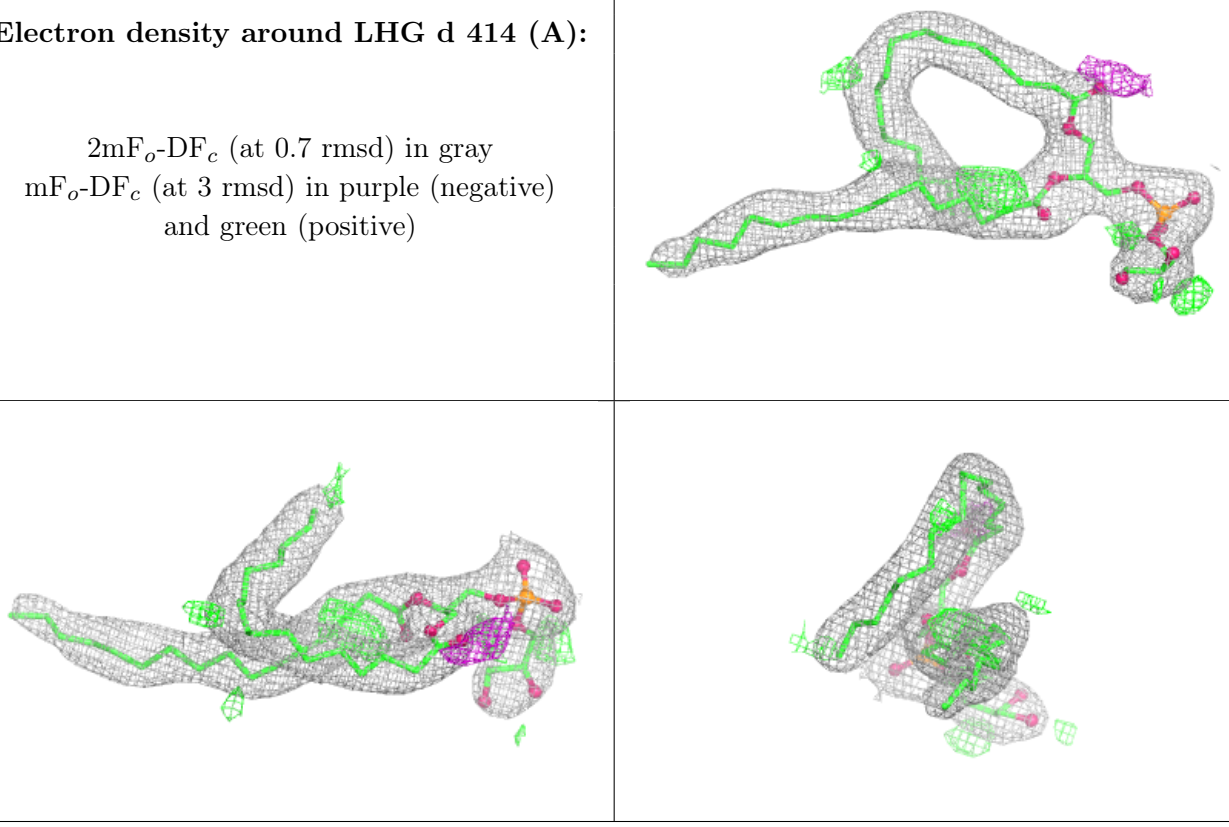






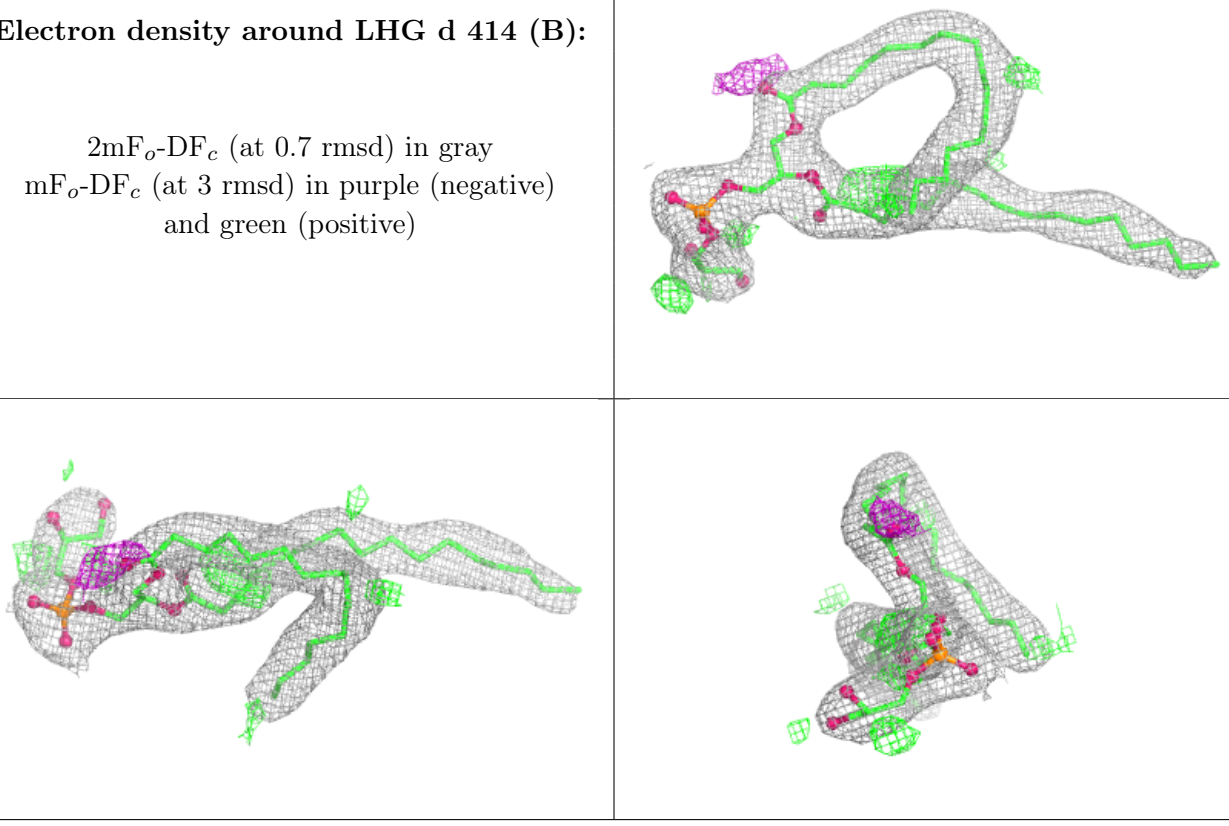
Electron density around LHG d 414 (A):

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



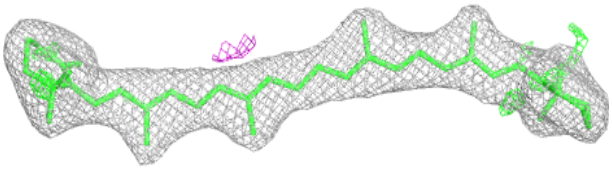
Electron density around LHG d 414 (B):

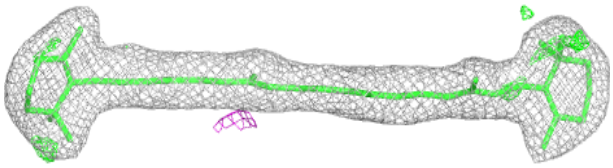
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

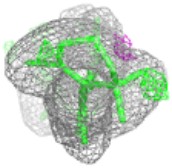


Electron density around BCR A 409:

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

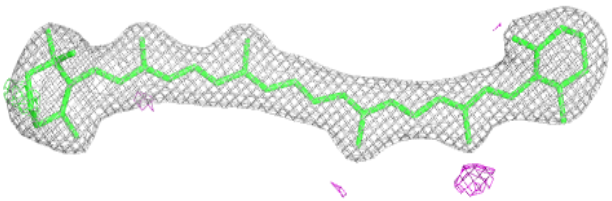


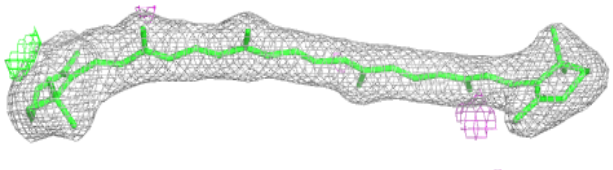


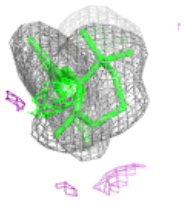


Electron density around BCR B 619:

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

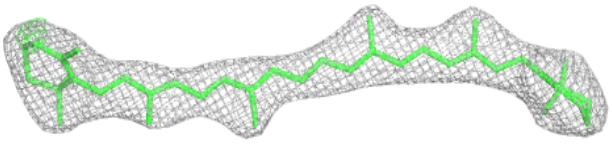


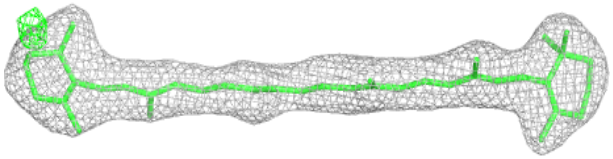


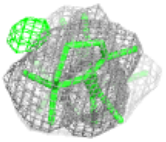


Electron density around BCR C 515:

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

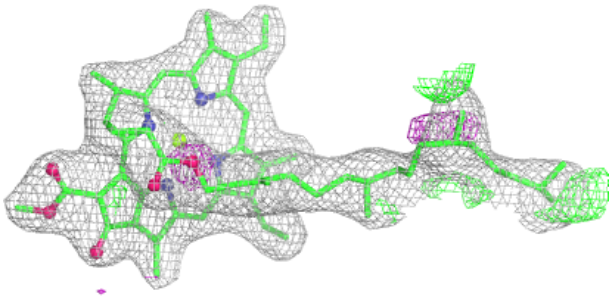


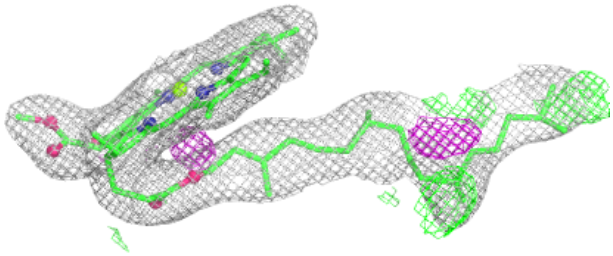


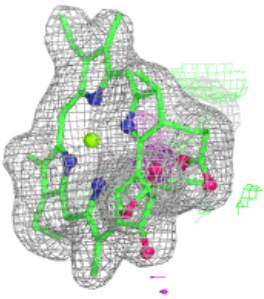


Electron density around CLA B 614:

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

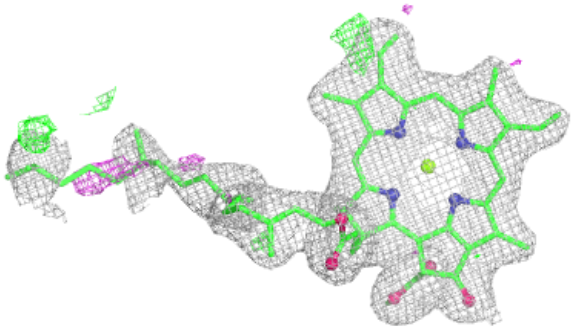


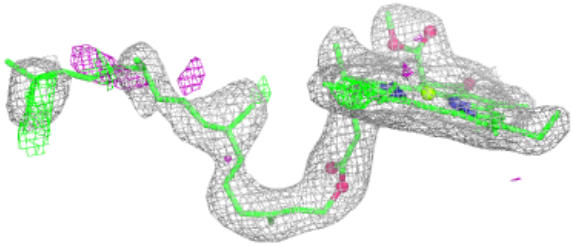




Electron density around CLA a 405 (A):

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

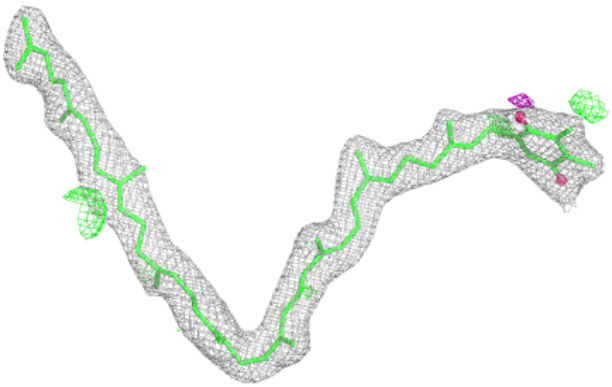


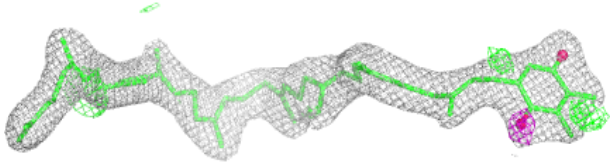


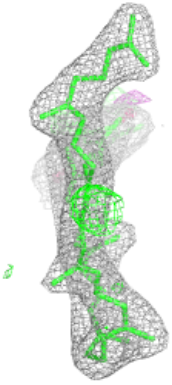


Electron density around PL9 D 405 (A):

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

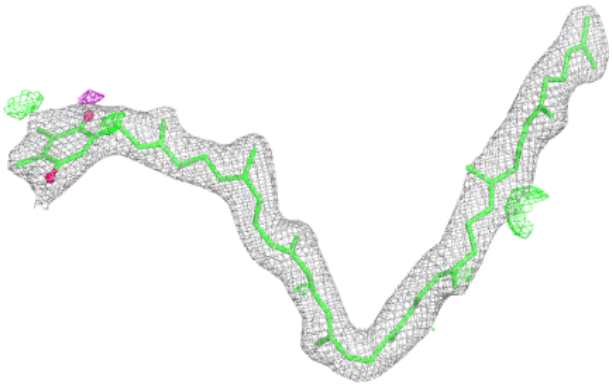


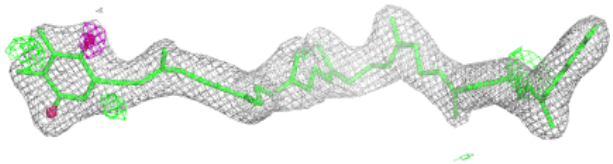




Electron density around PL9 D 405 (B):

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

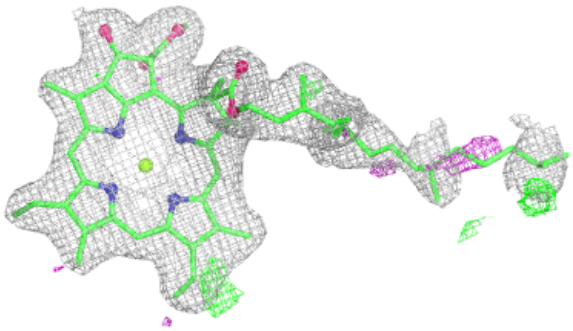


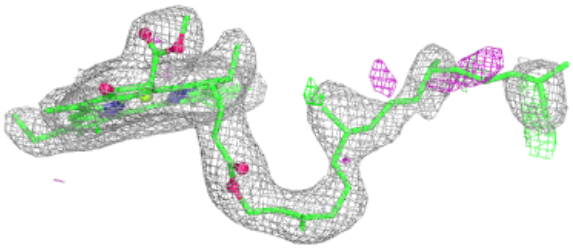


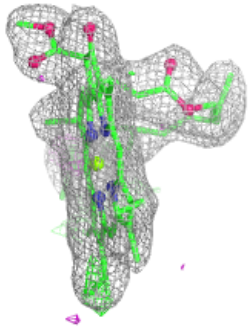


Electron density around CLA a 405 (B):

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

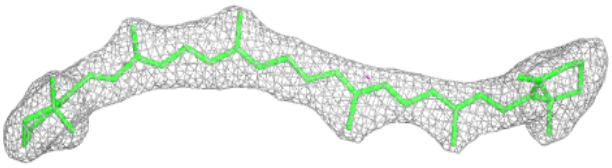


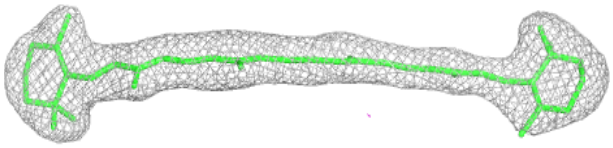


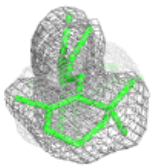


Electron density around BCR X 101:

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

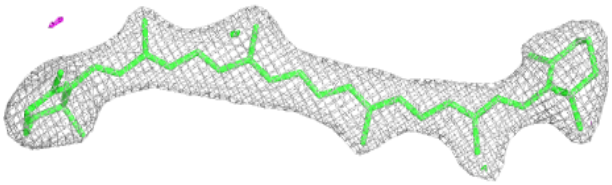


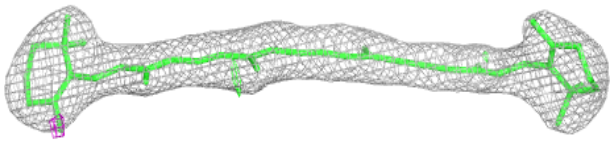


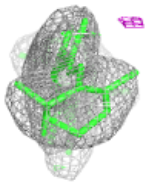


Electron density around BCR Y 101:

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

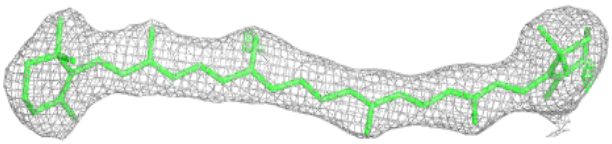


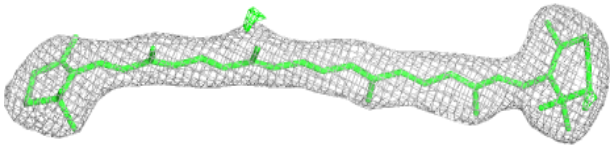


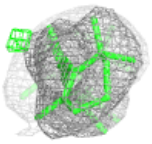


Electron density around BCR c 516:

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

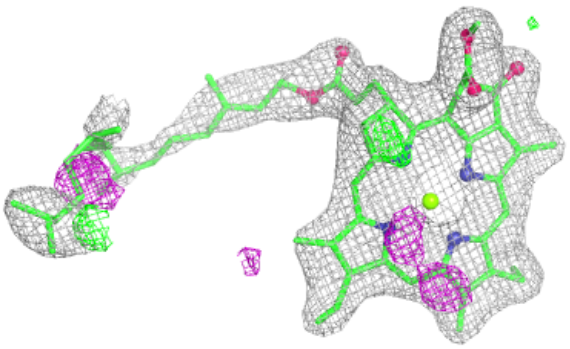


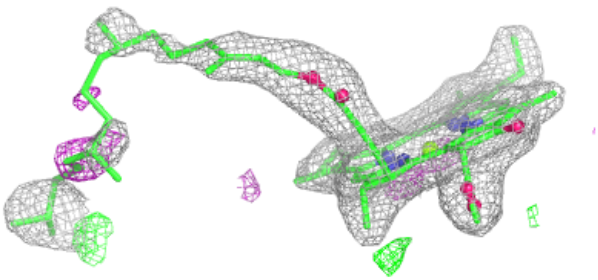




Electron density around CLA a 407:

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

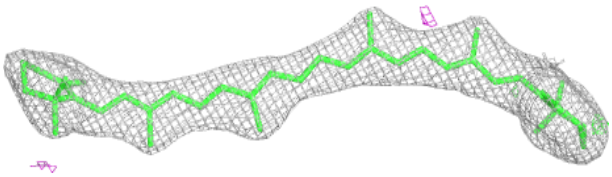


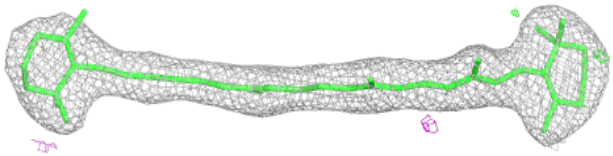


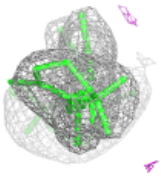


Electron density around BCR h 101:

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

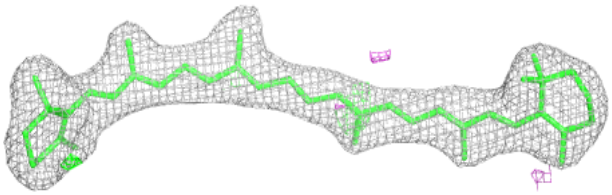


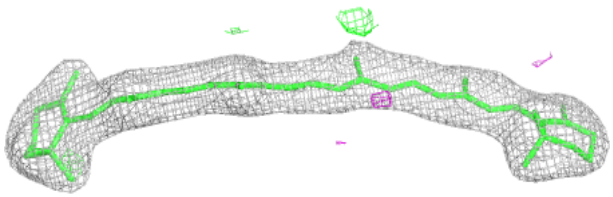


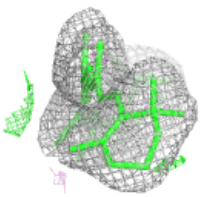


Electron density around BCR t 102:

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

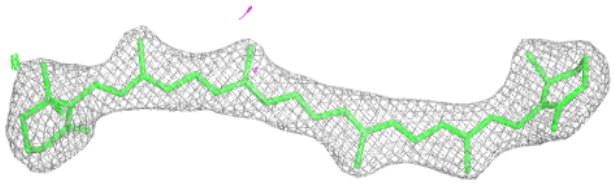


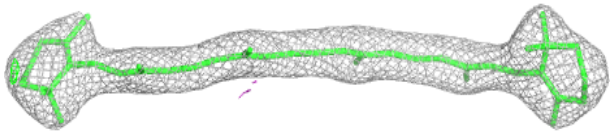


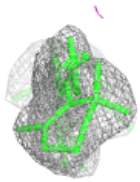


Electron density around BCR y 101:

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

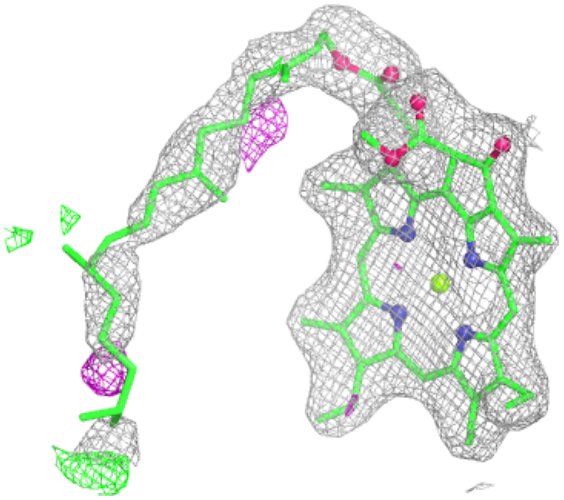


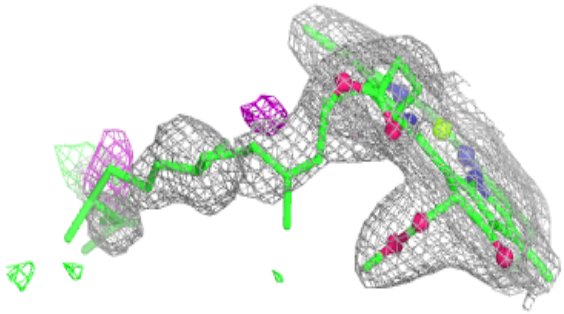


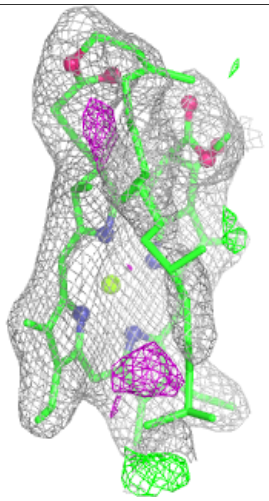


Electron density around CLA B 616:

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

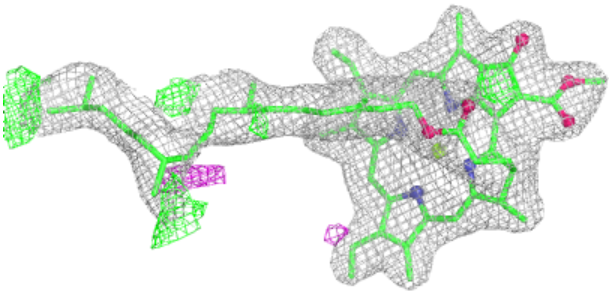


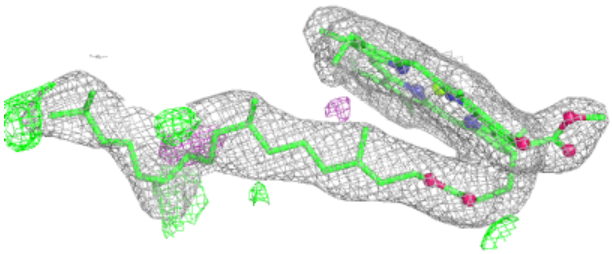


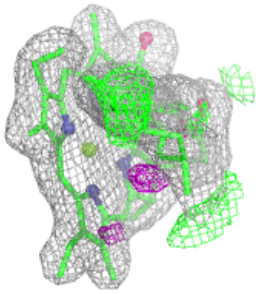


Electron density around CLA b 614:

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

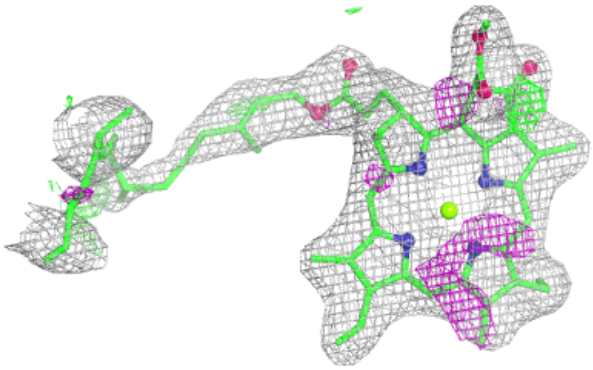


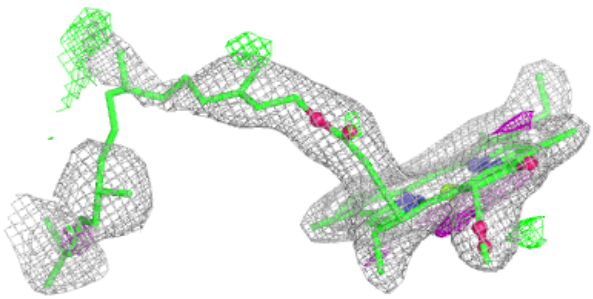




Electron density around CLA A 408:

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

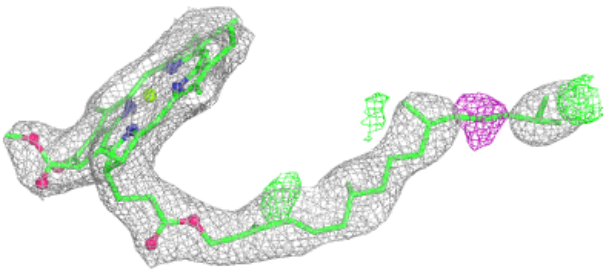


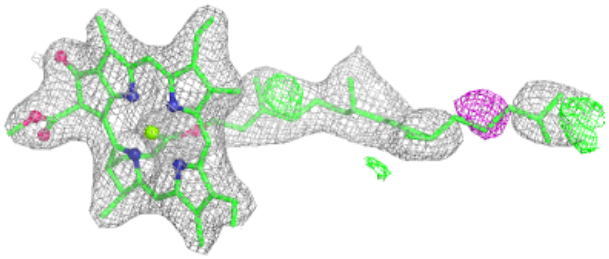


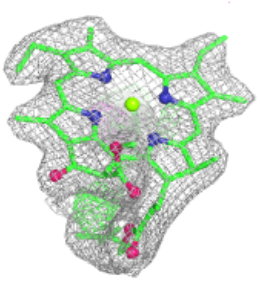


Electron density around CLA c 506:

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

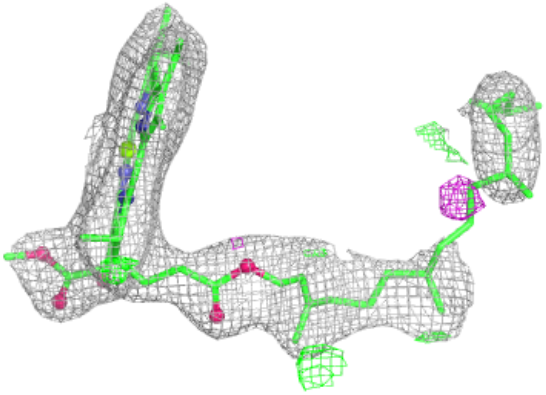


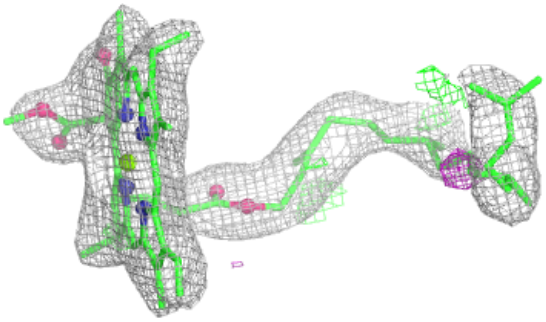


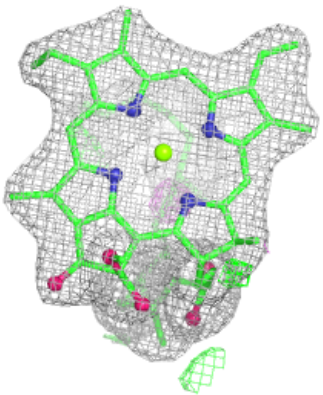


Electron density around CLA c 508:

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

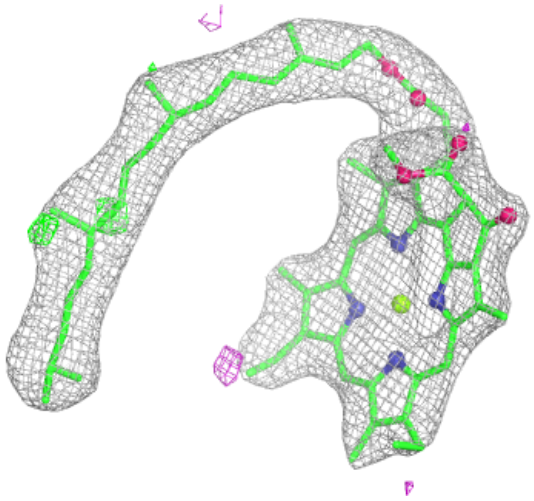


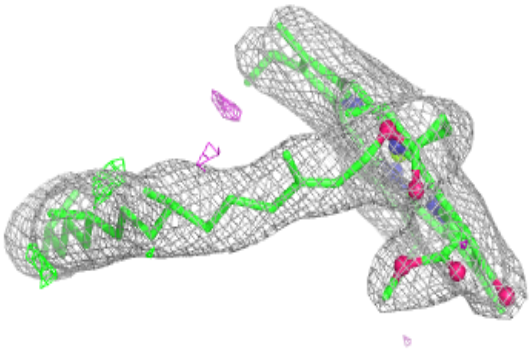


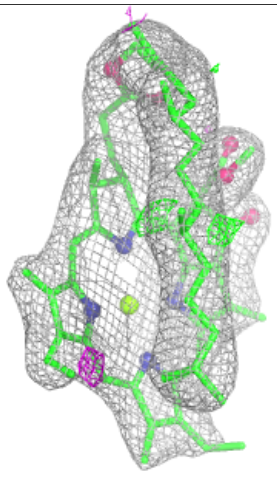


Electron density around CLA c 509:

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

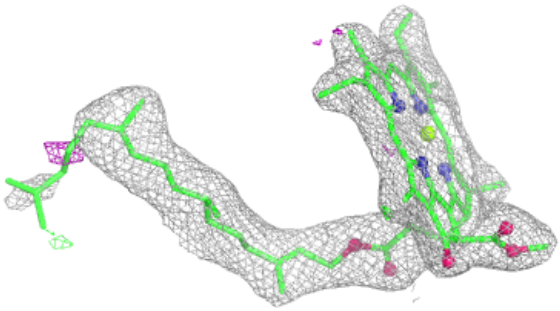


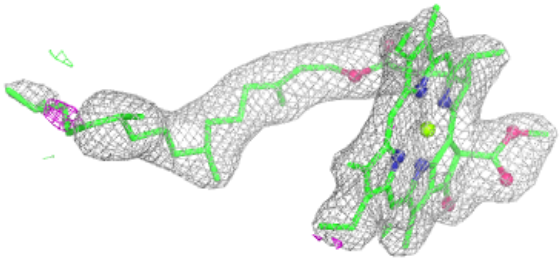


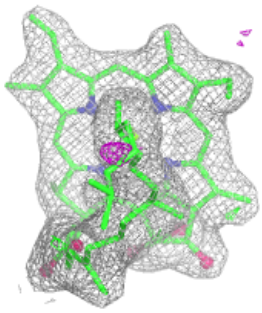


Electron density around CLA c 510:

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

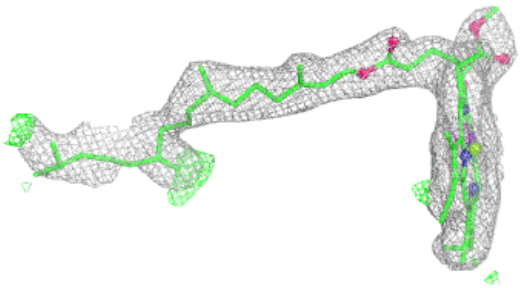


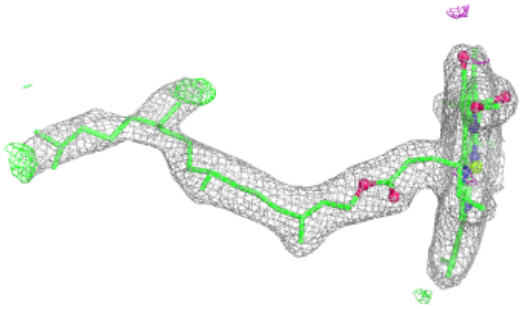


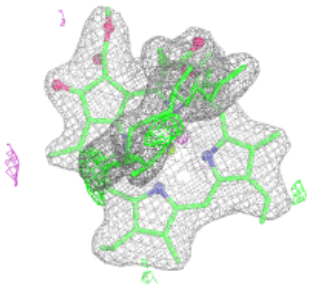


Electron density around CLA B 606:

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

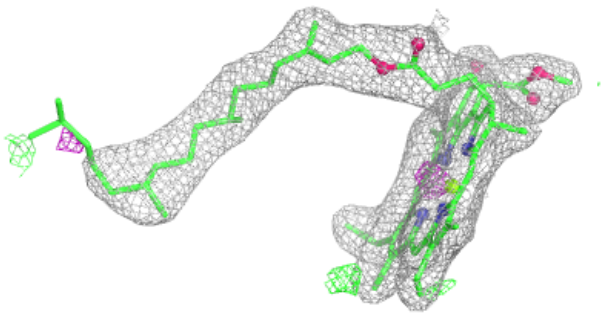


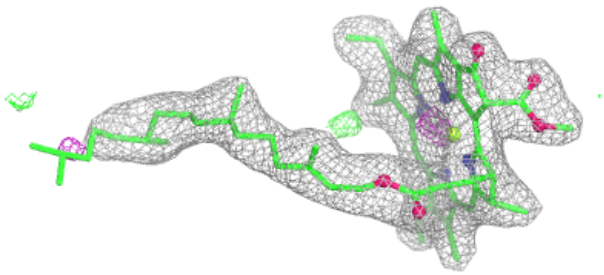


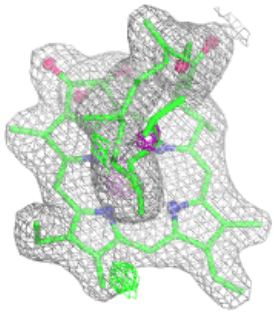


Electron density around CLA C 509:

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

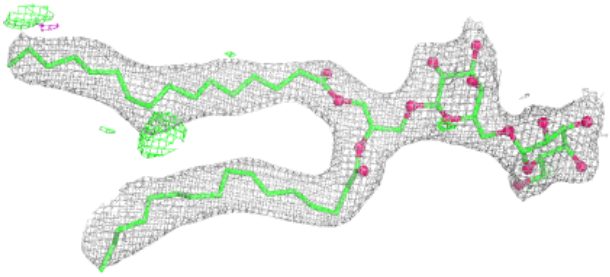


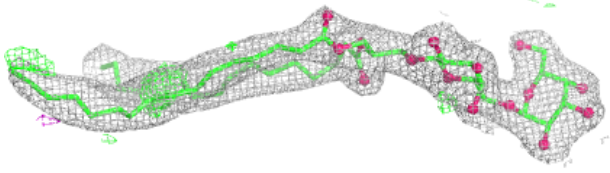


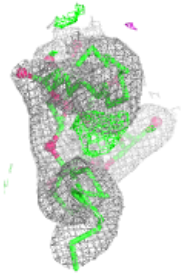


Electron density around DGD C 519:

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

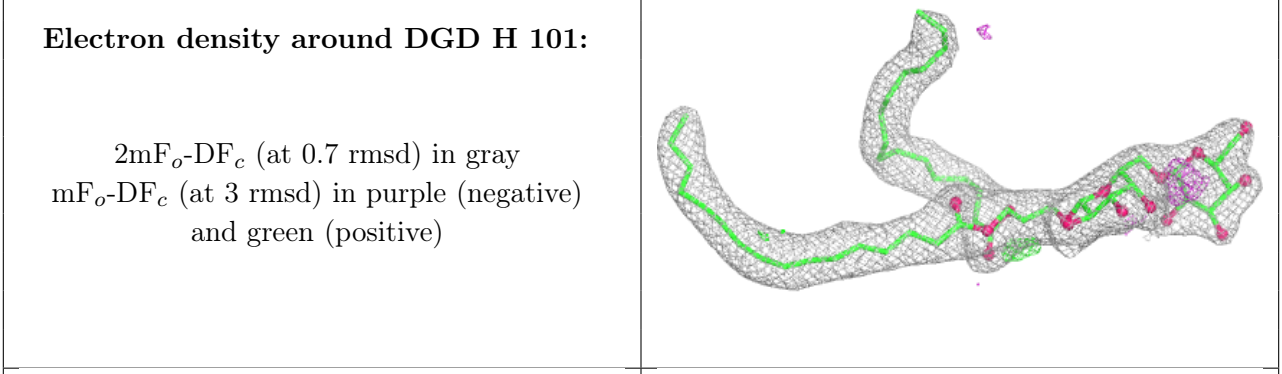






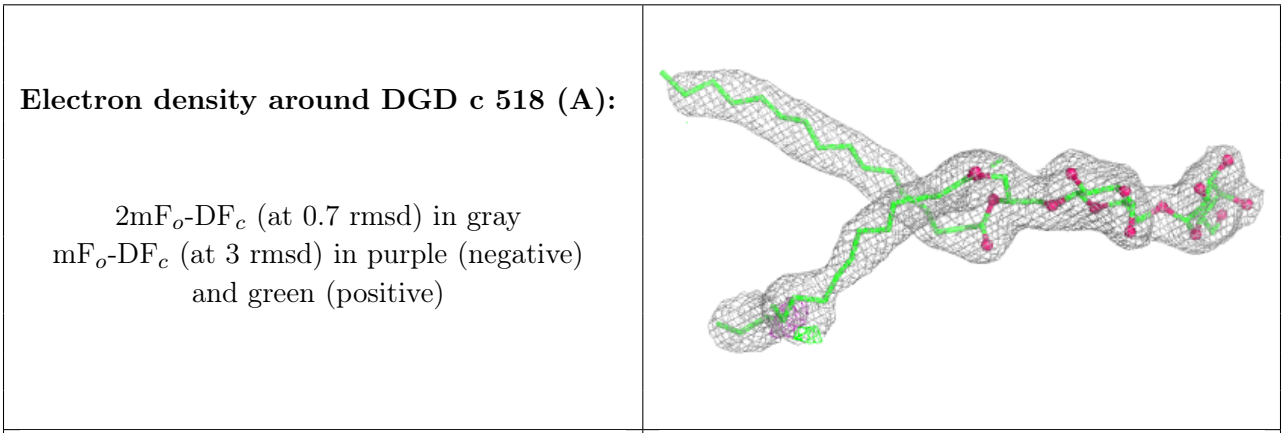
Electron density around DGD H 101:

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



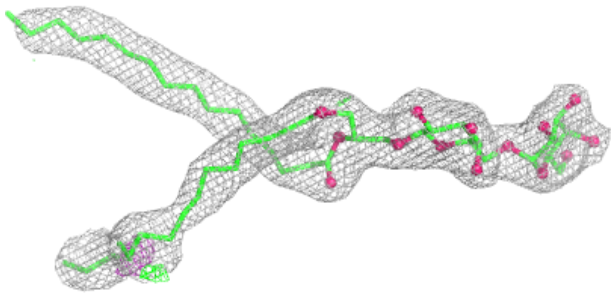
Electron density around DGD c 518 (A):

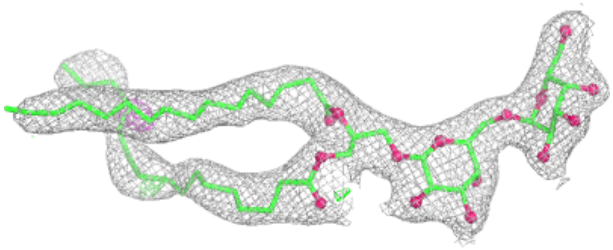
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD c 518 (B):

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

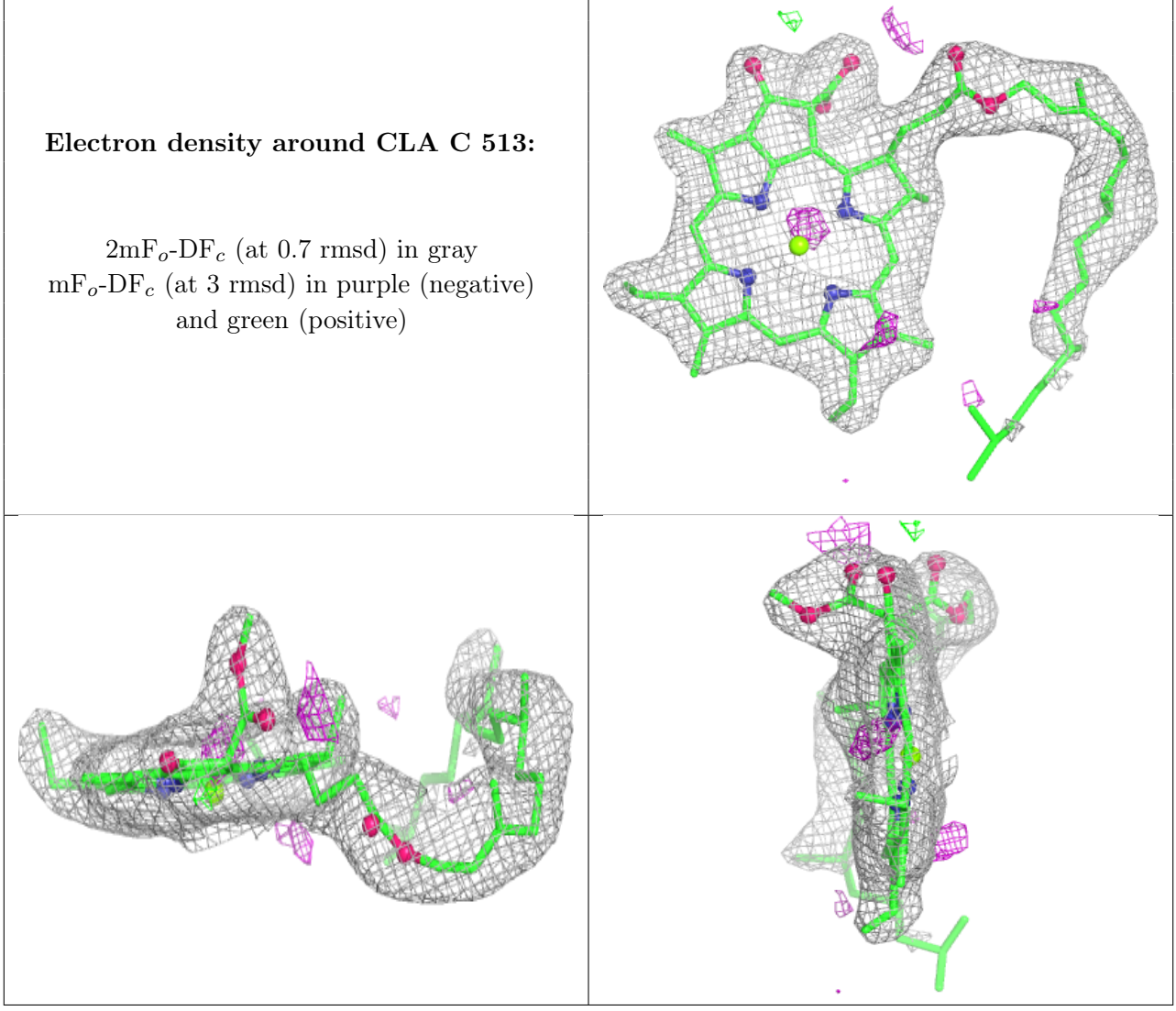






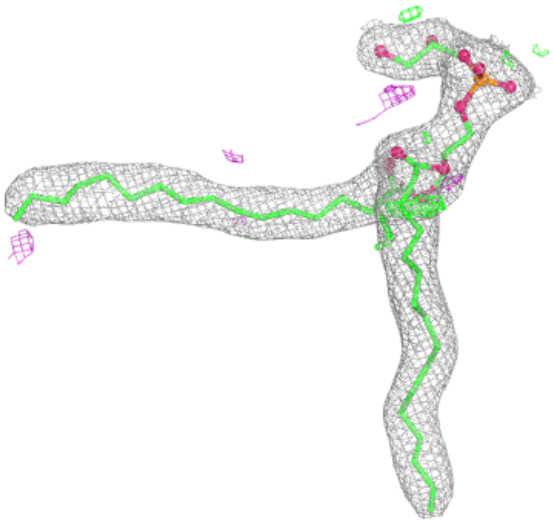
Electron density around CLA C 513:

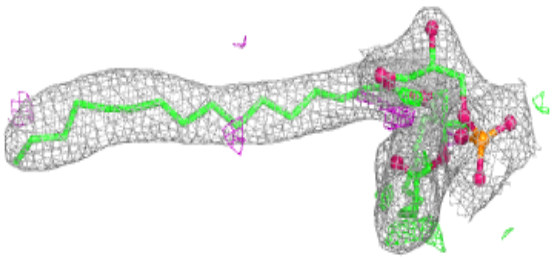
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

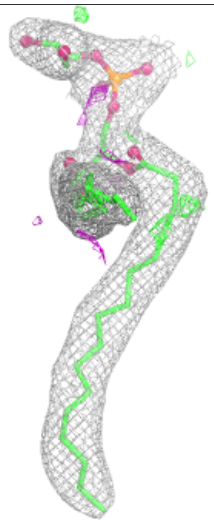


Electron density around LHG b 629 (A):

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

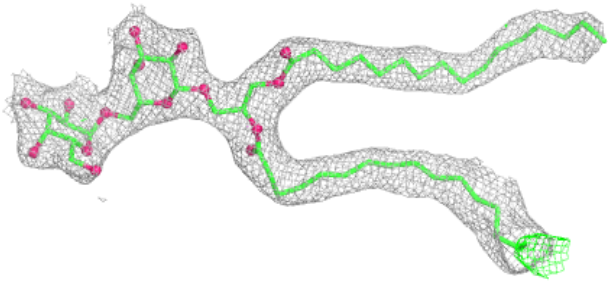


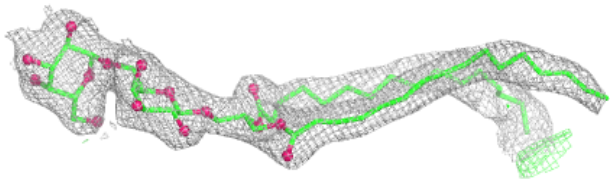


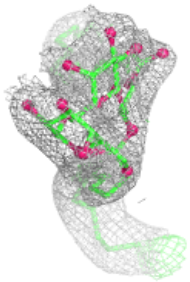


Electron density around DGD c 520:

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

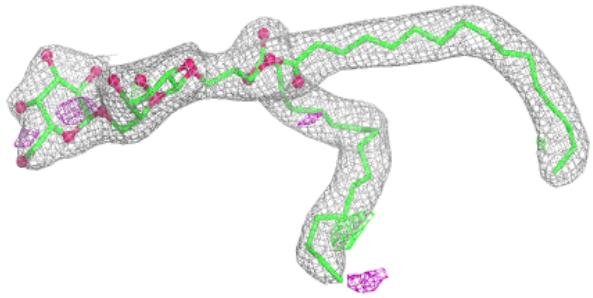


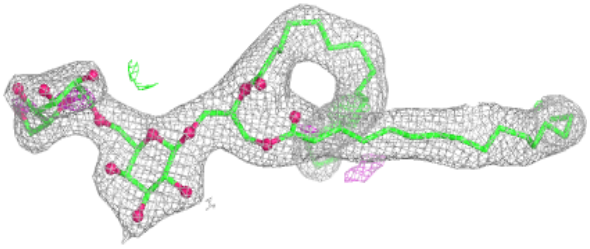




Electron density around DGD h 102:

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

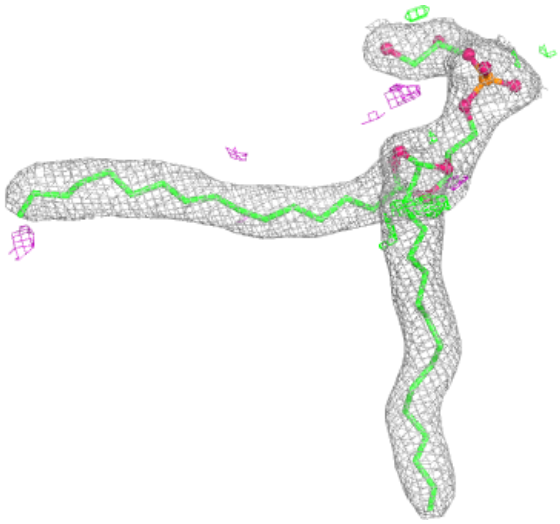


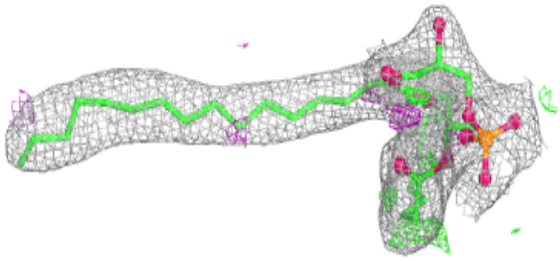


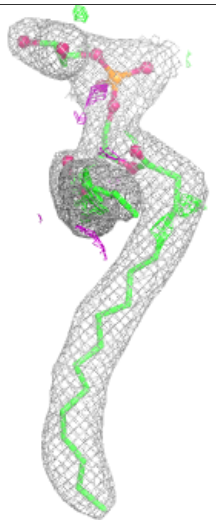


Electron density around LHG b 629 (B):

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

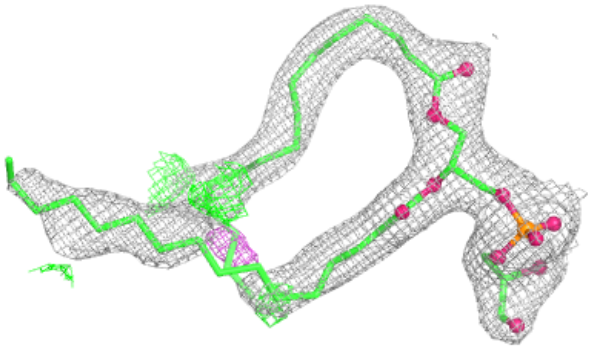


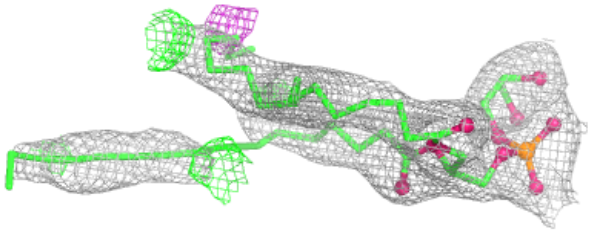


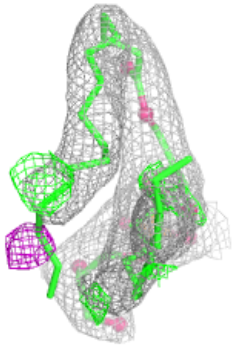


Electron density around LHG d 408 (A):

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

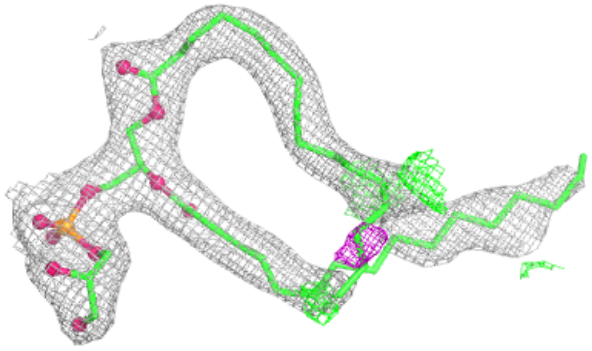


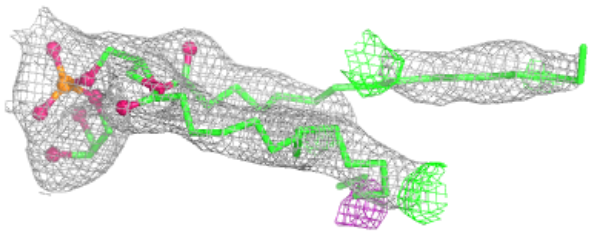


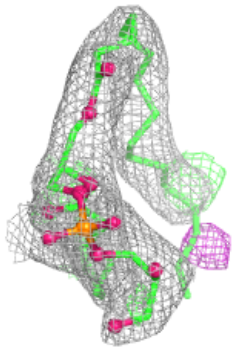


Electron density around LHG d 408 (B):

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

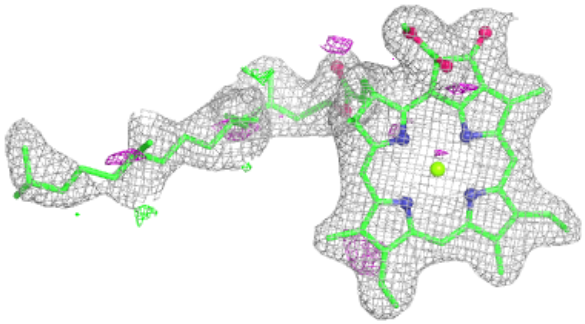


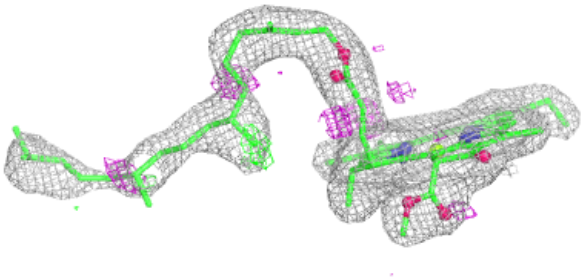




Electron density around CLA A 406 (A):

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

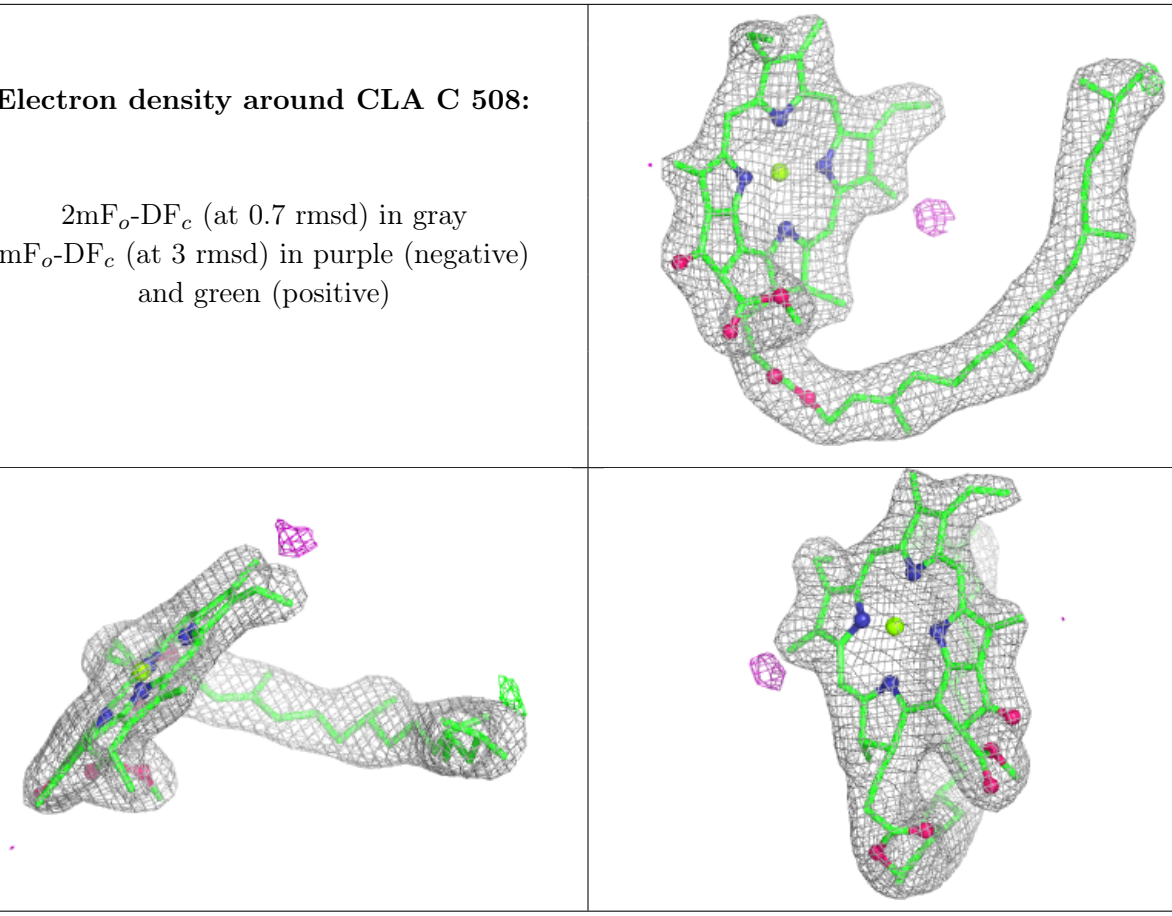






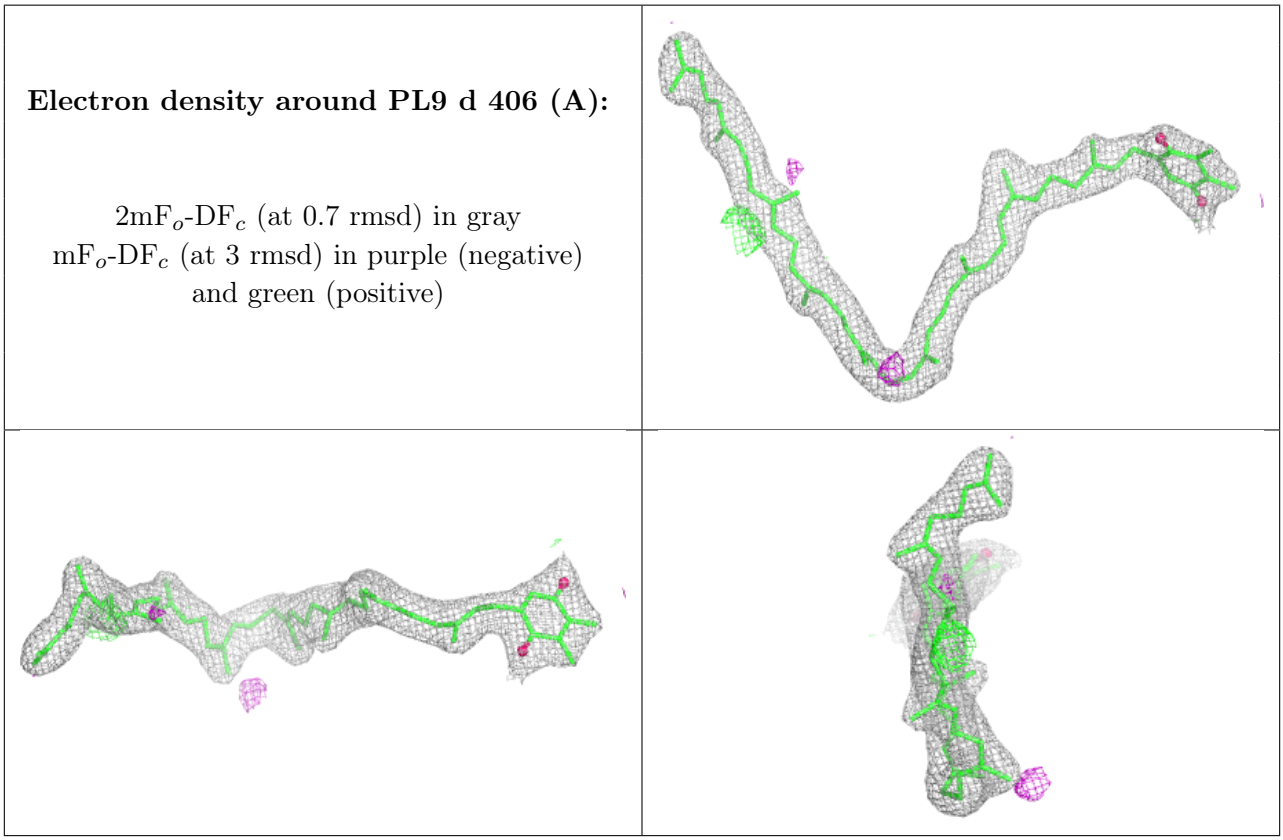
Electron density around CLA C 508:

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



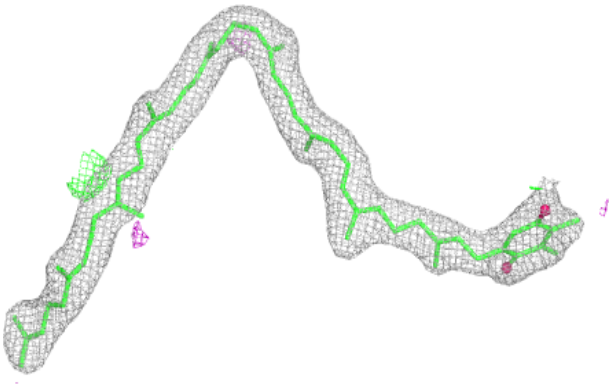
Electron density around PL9 d 406 (A):

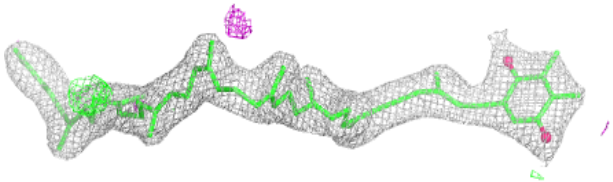
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

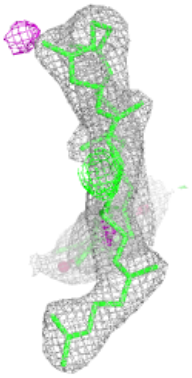


Electron density around PL9 d 406 (B):

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

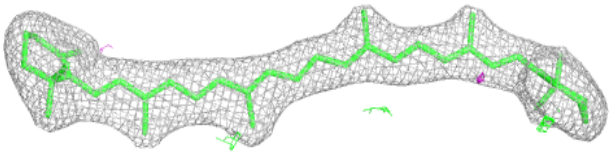


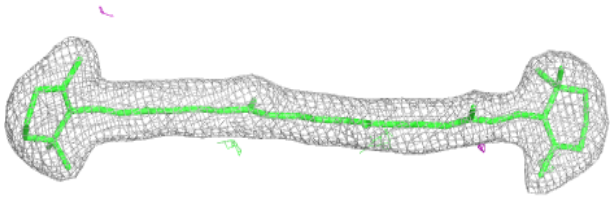


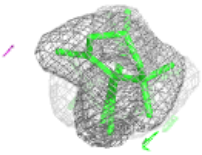


Electron density around BCR a 408:

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

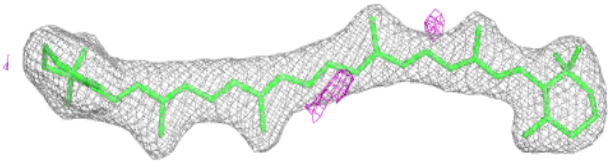


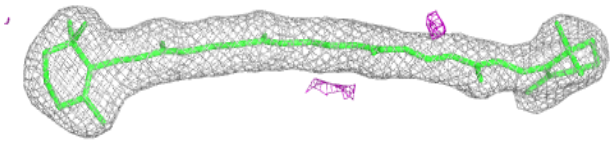


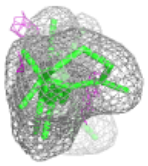


Electron density around BCR b 617:

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

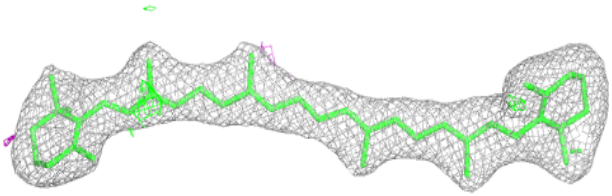


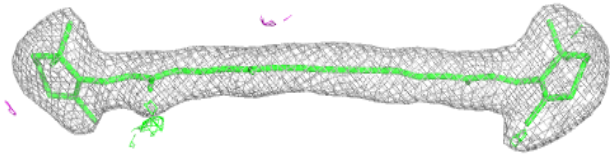


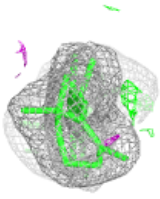


Electron density around BCR b 618:

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

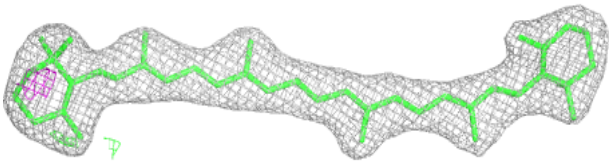


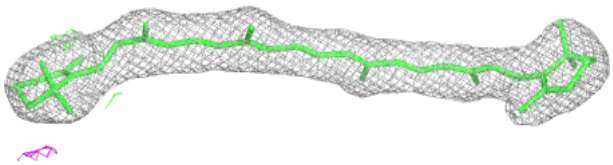


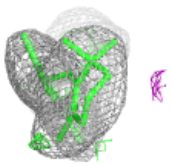


Electron density around BCR b 619:

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

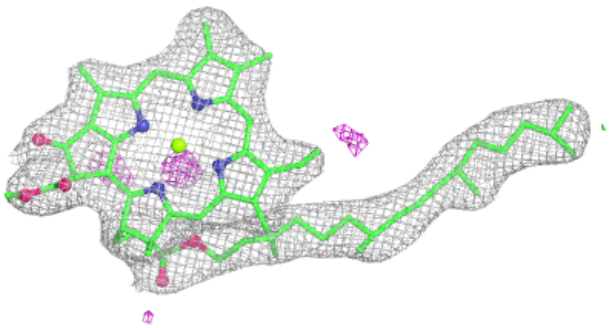


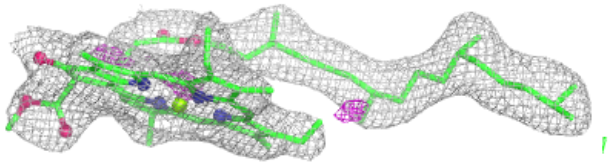


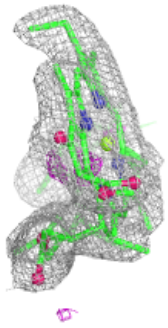


Electron density around CLA c 503:

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

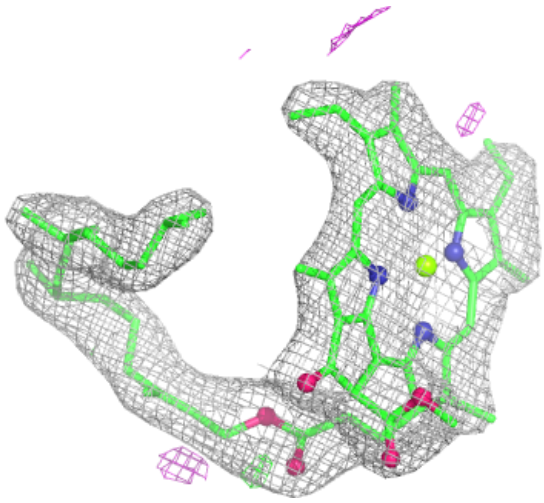


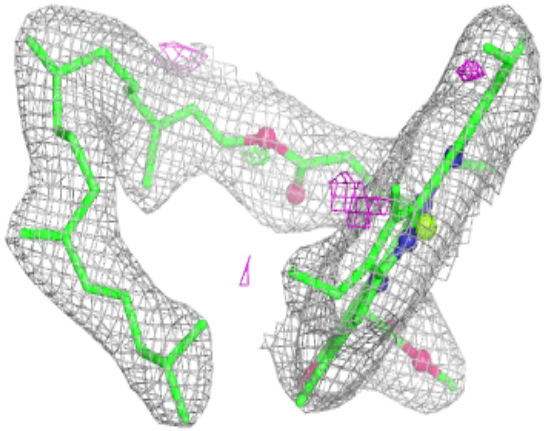


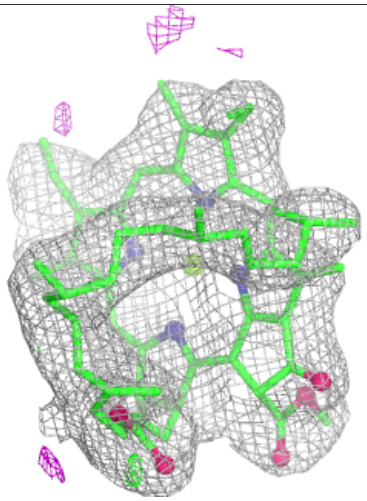


Electron density around CLA c 505:

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

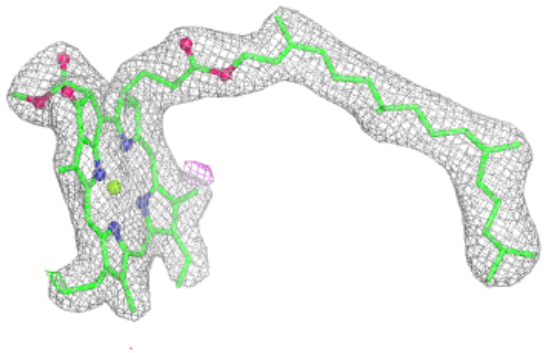


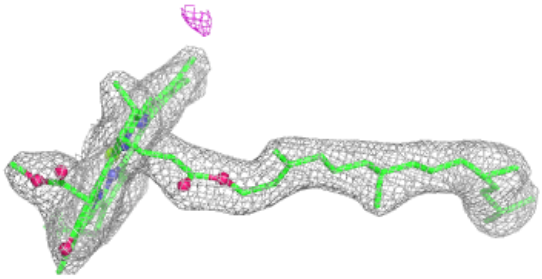


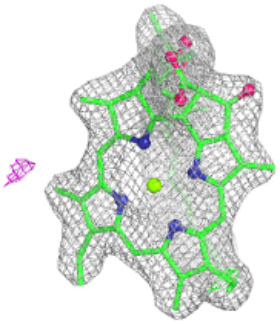


Electron density around CLA B 609:

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

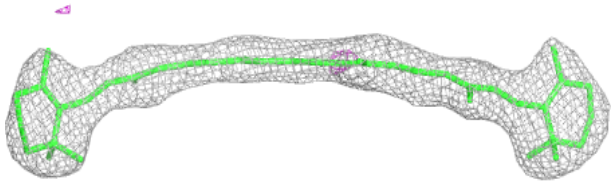


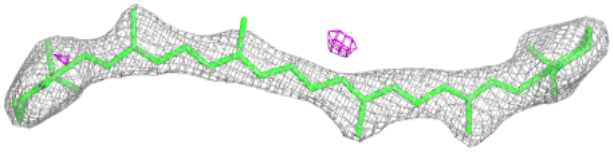


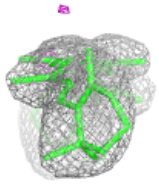


Electron density around BCR k 101:

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

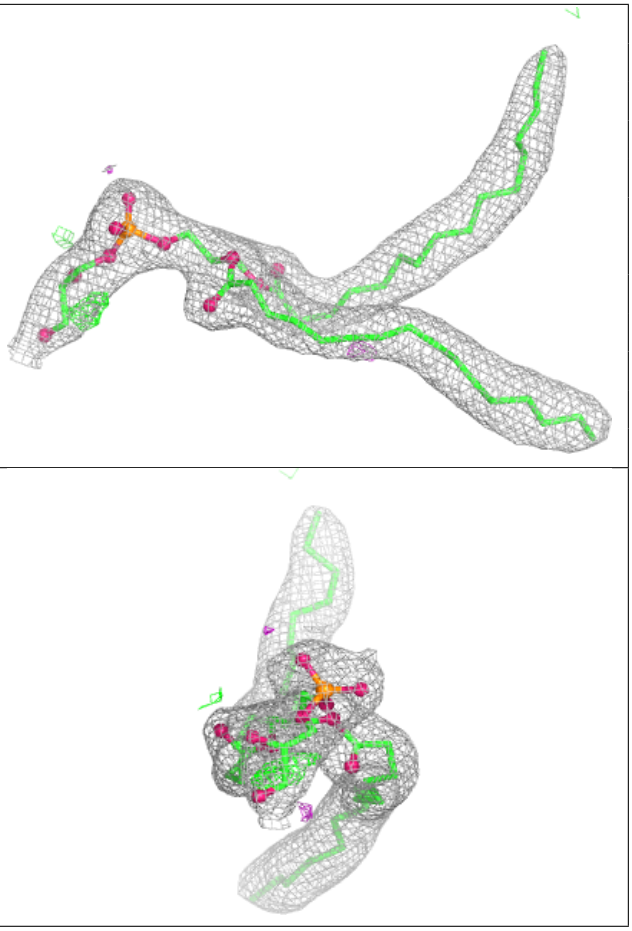






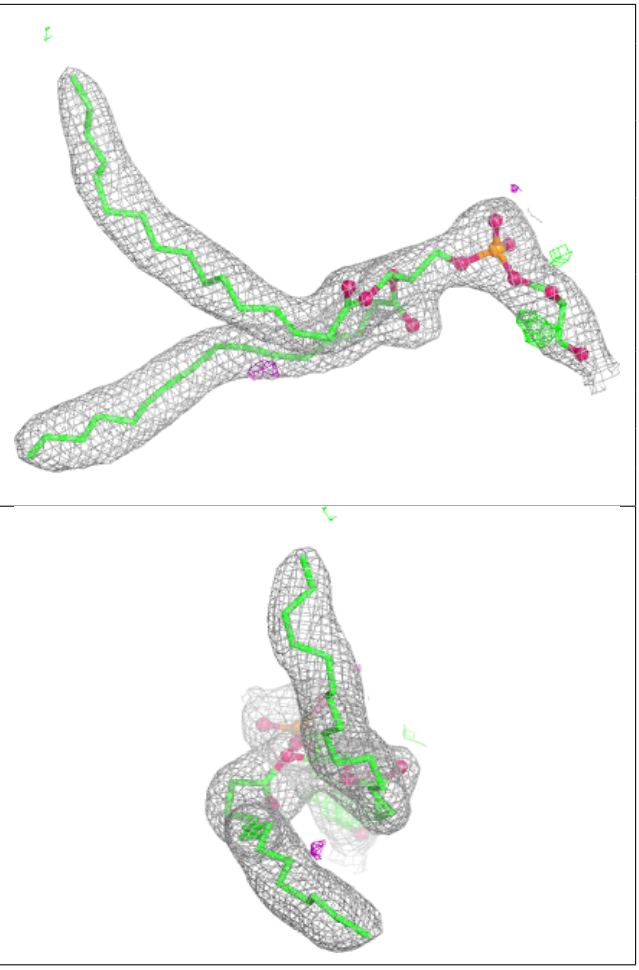
Electron density around LHG D 406 (A):

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



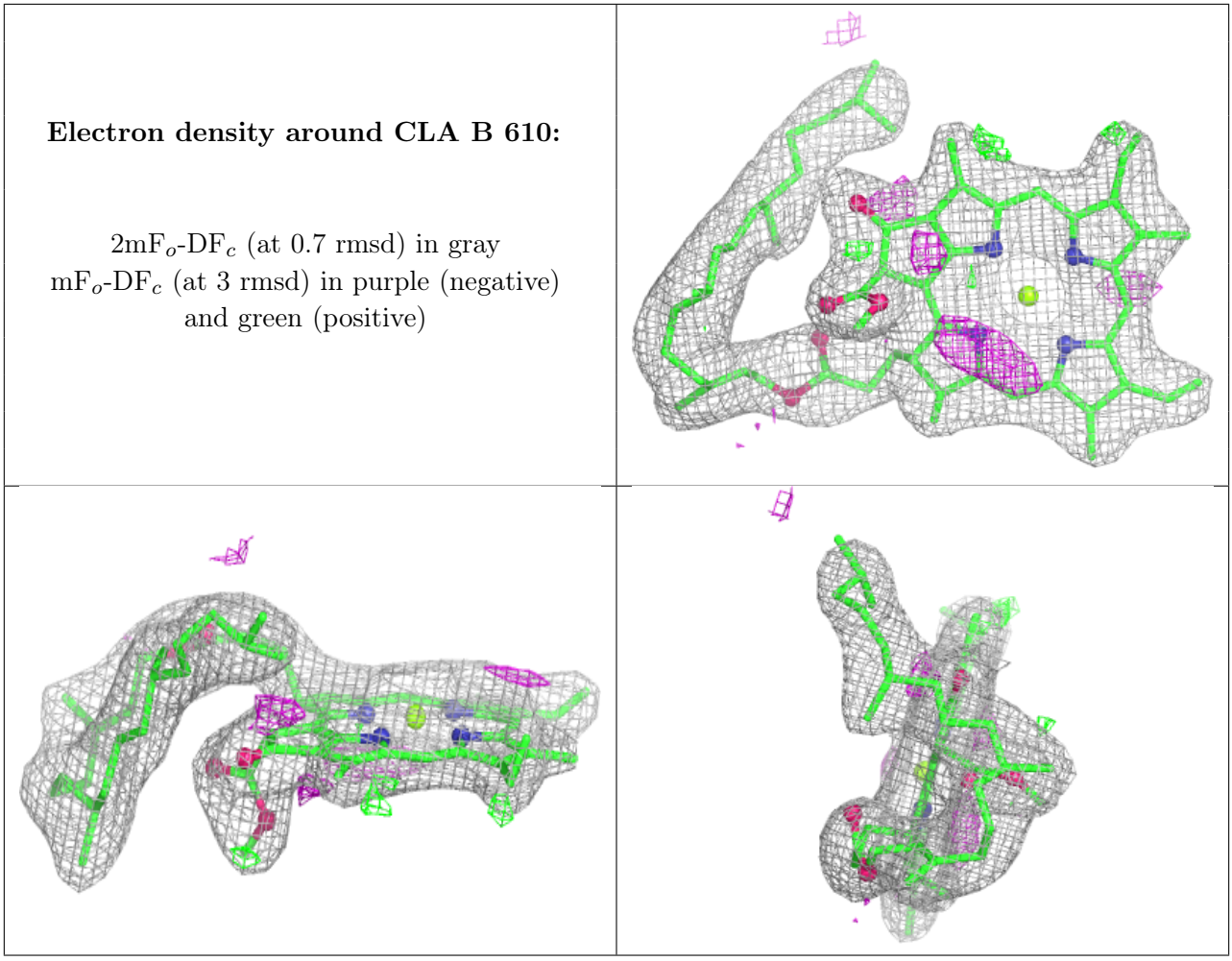
Electron density around LHG D 406 (B):

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



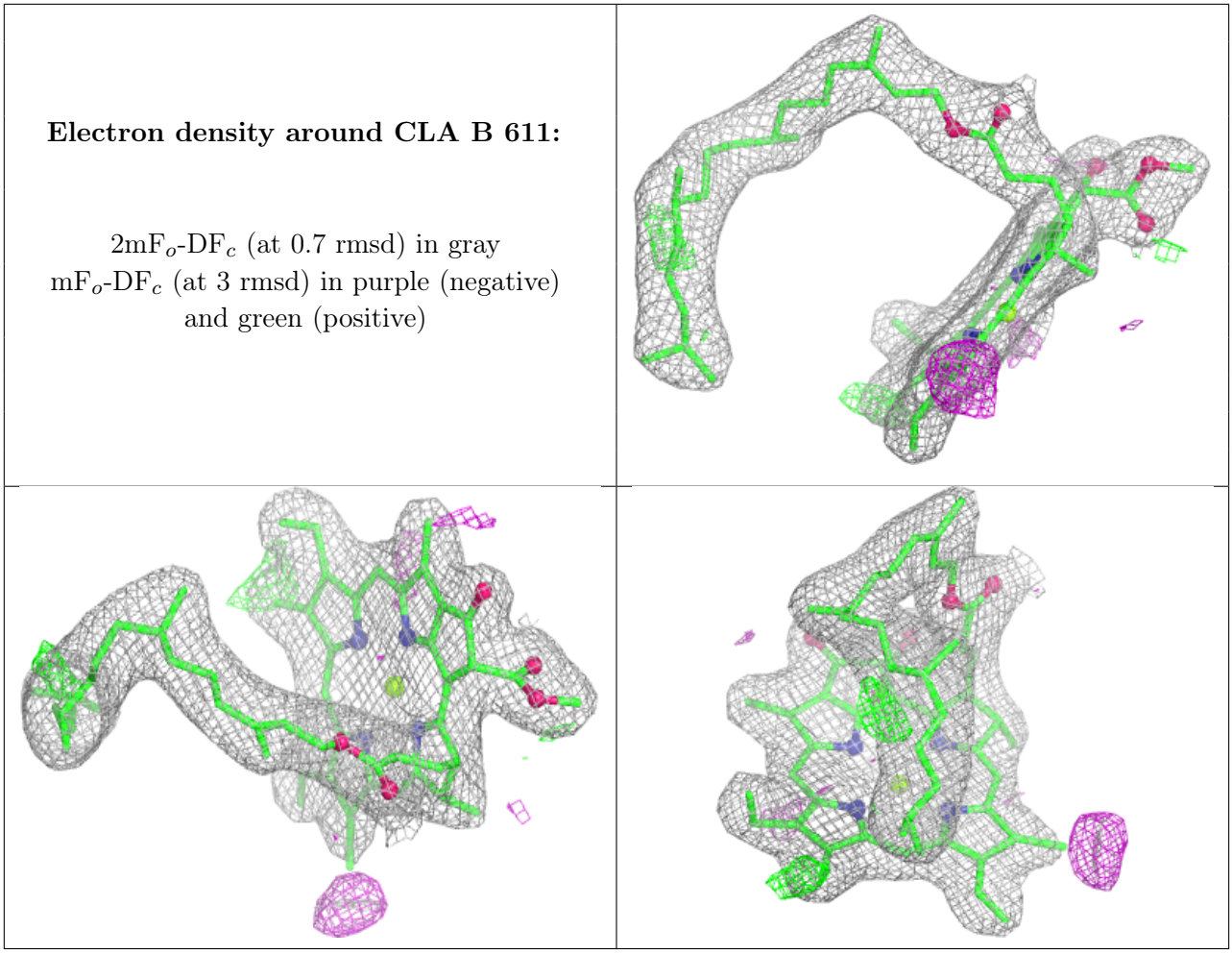
Electron density around CLA B 610:

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



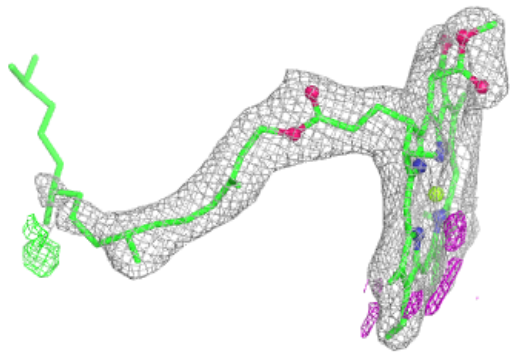
Electron density around CLA B 611:

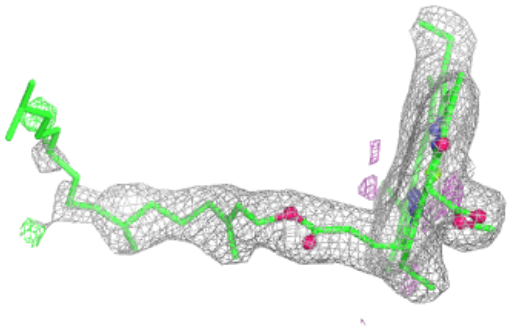
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

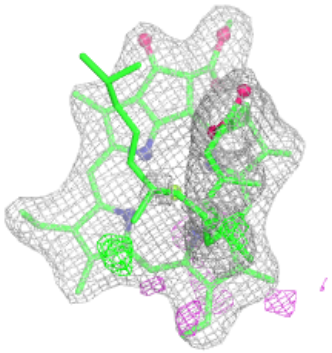


Electron density around CLA D 403:

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

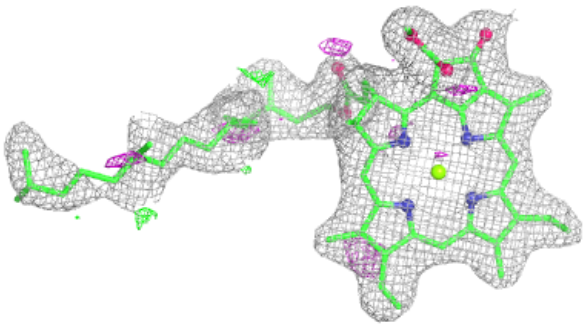


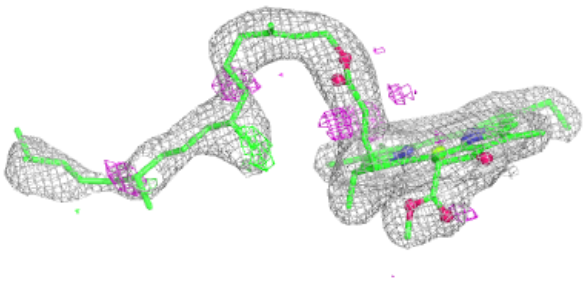


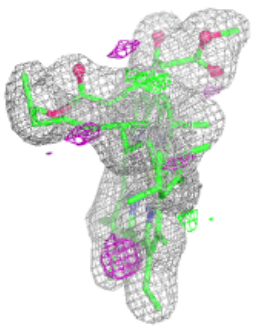


Electron density around CLA A 406 (B):

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

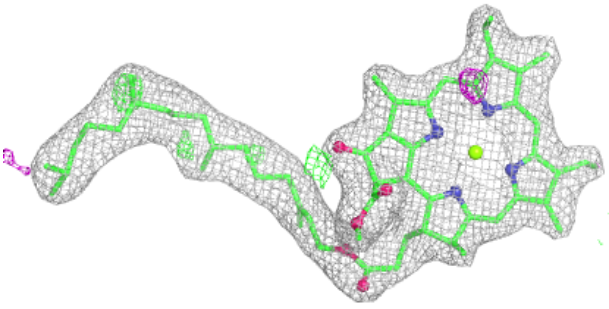


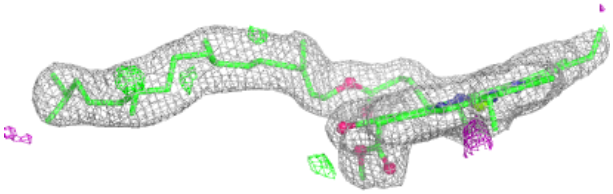


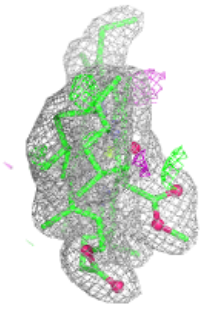


Electron density around CLA B 602:

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

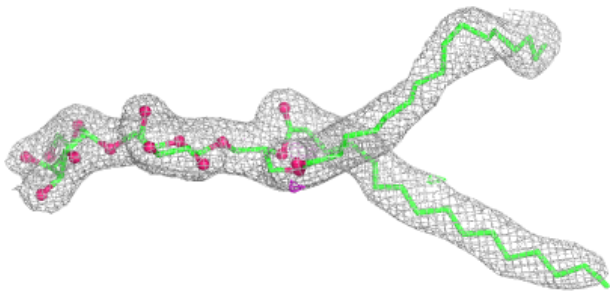


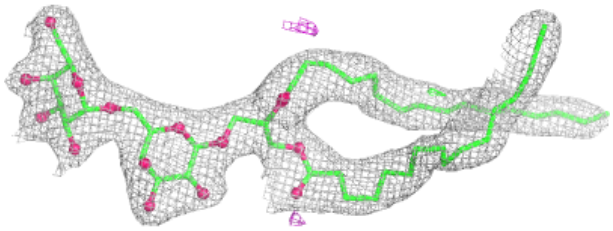


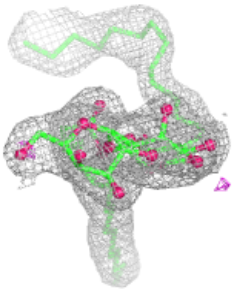


Electron density around DGD C 517 (A):

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

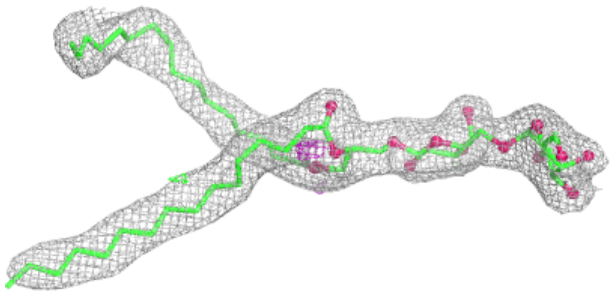


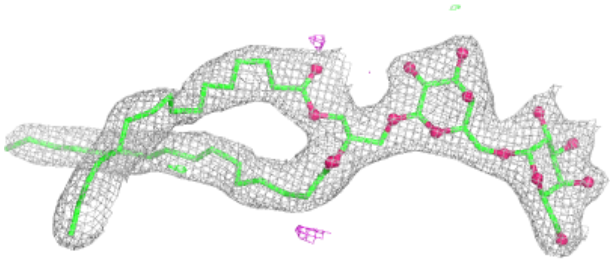


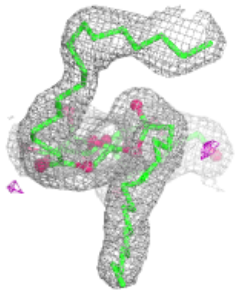


Electron density around DGD C 517 (B):

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

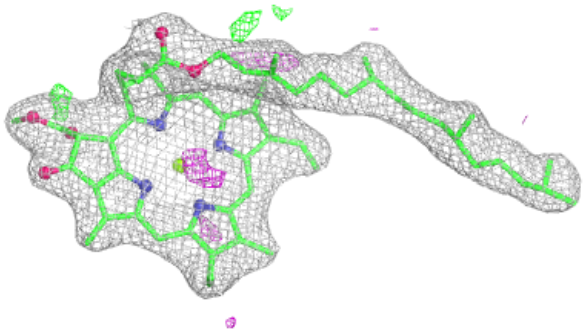


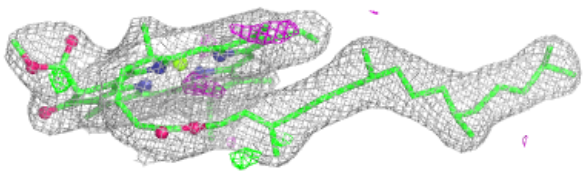


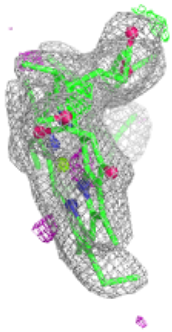


Electron density around CLA C 502:

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

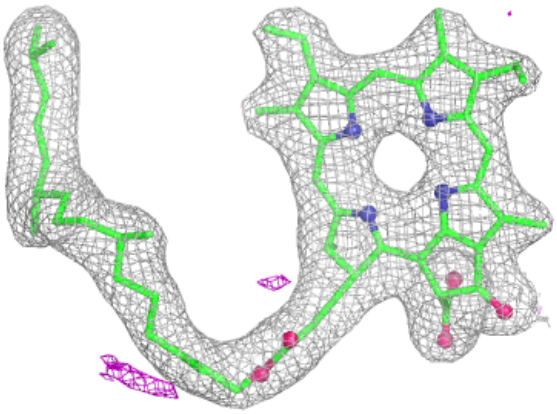


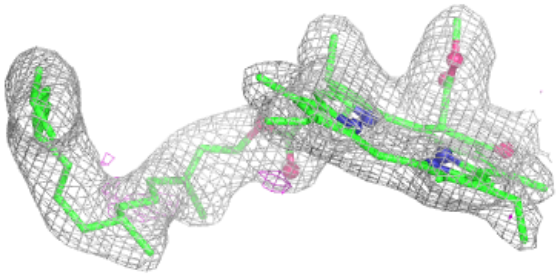


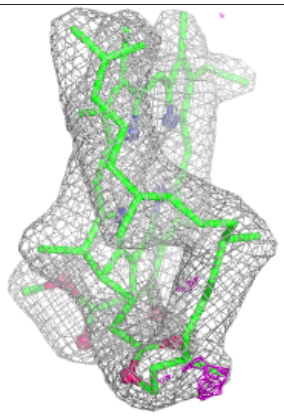


Electron density around PHO a 414 (A):

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

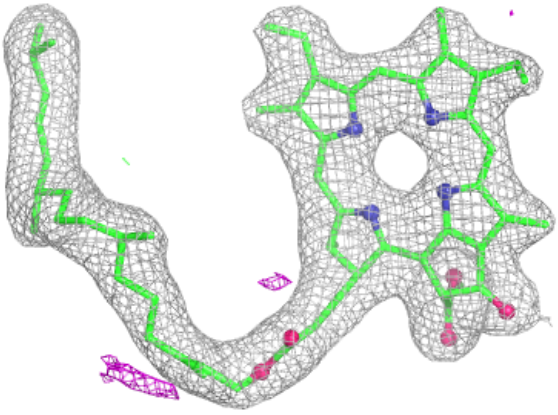


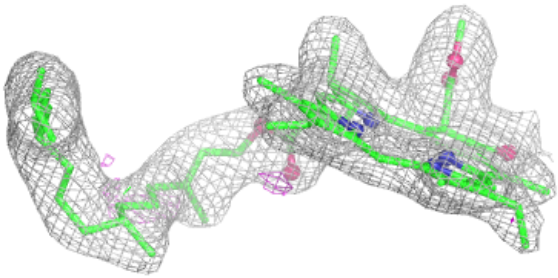


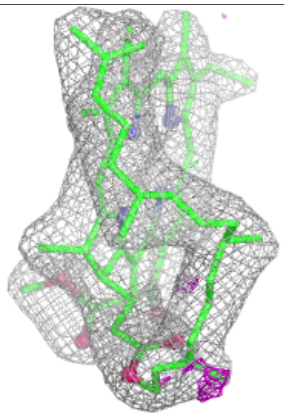


Electron density around PHO a 414 (B):

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

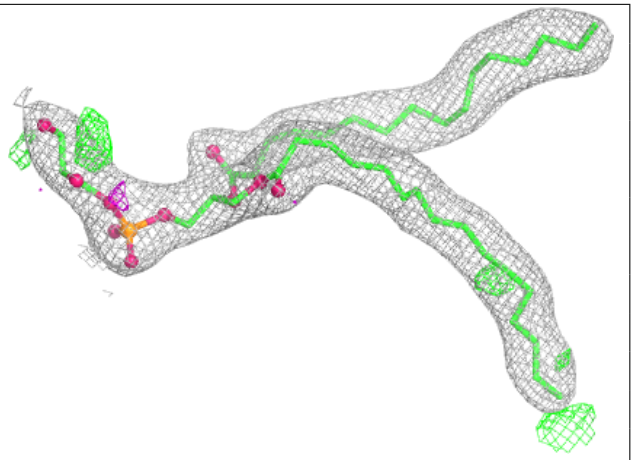


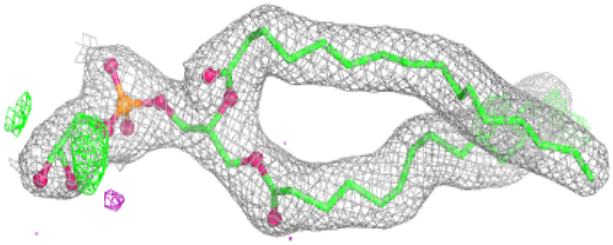




Electron density around LHG d 407 (A):

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

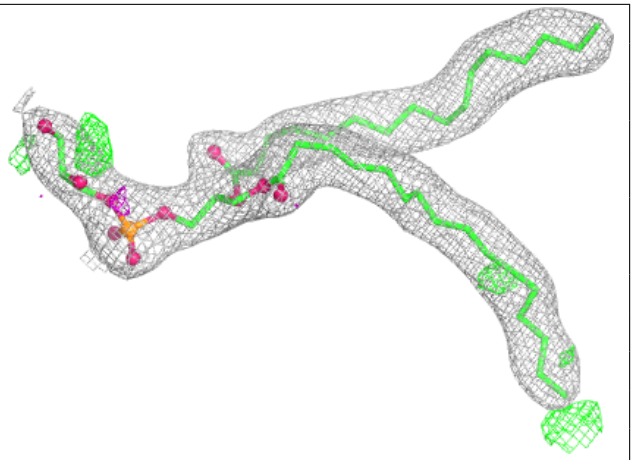


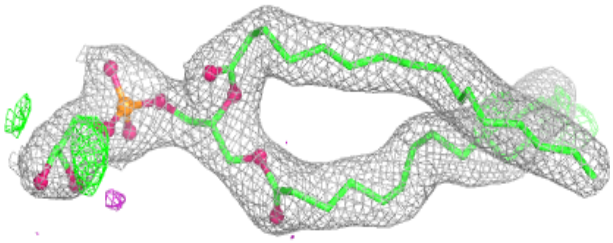


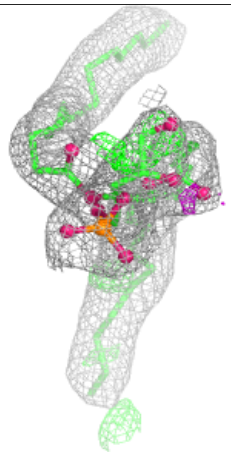


Electron density around LHG d 407 (B):

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

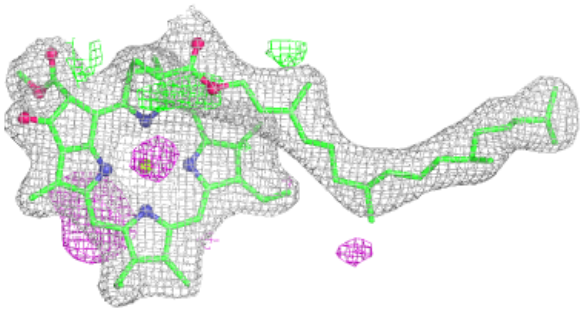


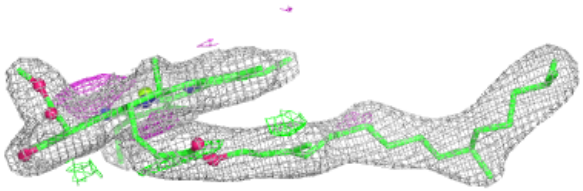


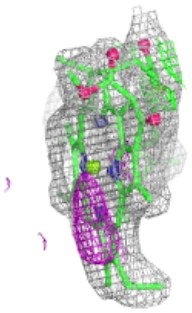


Electron density around CLA B 603:

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

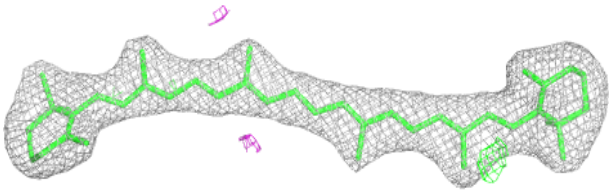


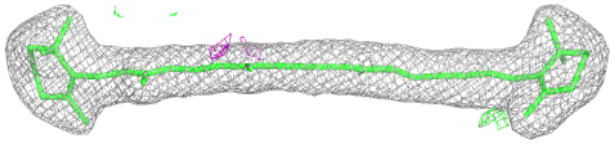


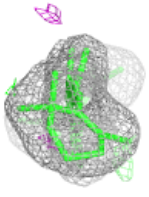


Electron density around BCR B 618:

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

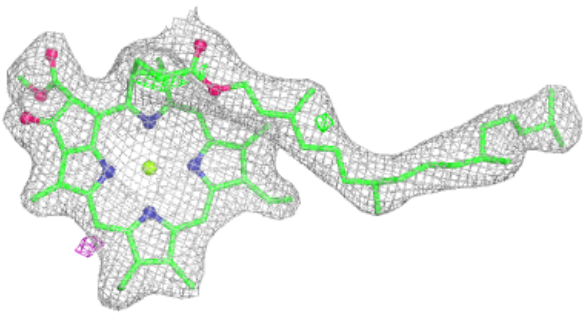


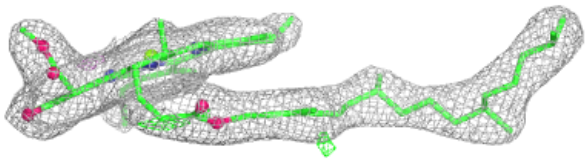


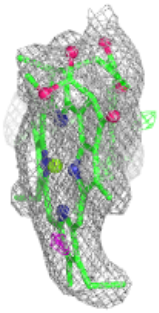


Electron density around CLA b 603:

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

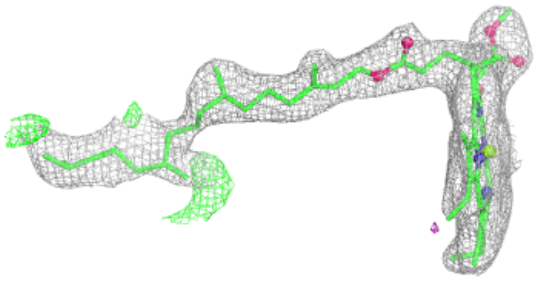


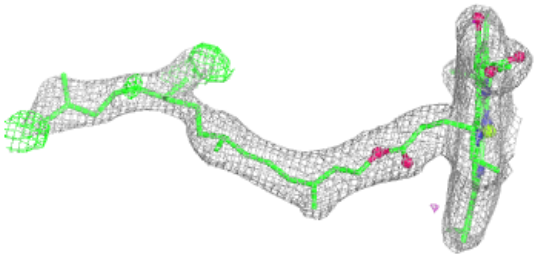


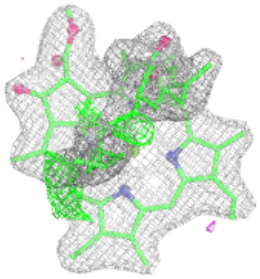


Electron density around CLA b 606:

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

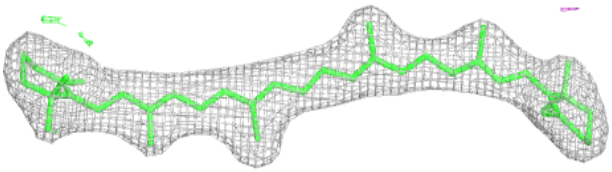


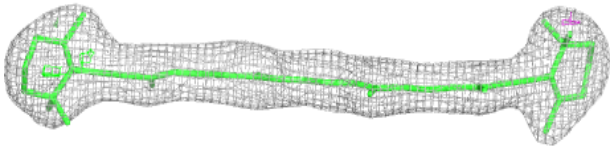


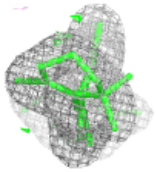


Electron density around BCR C 516:

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

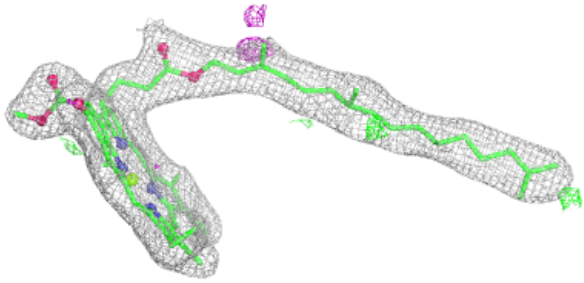


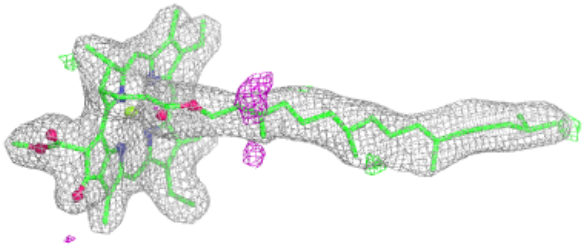


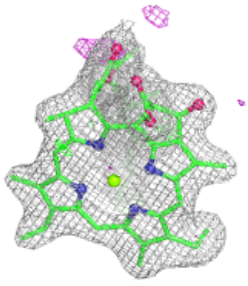


Electron density around CLA b 607:

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

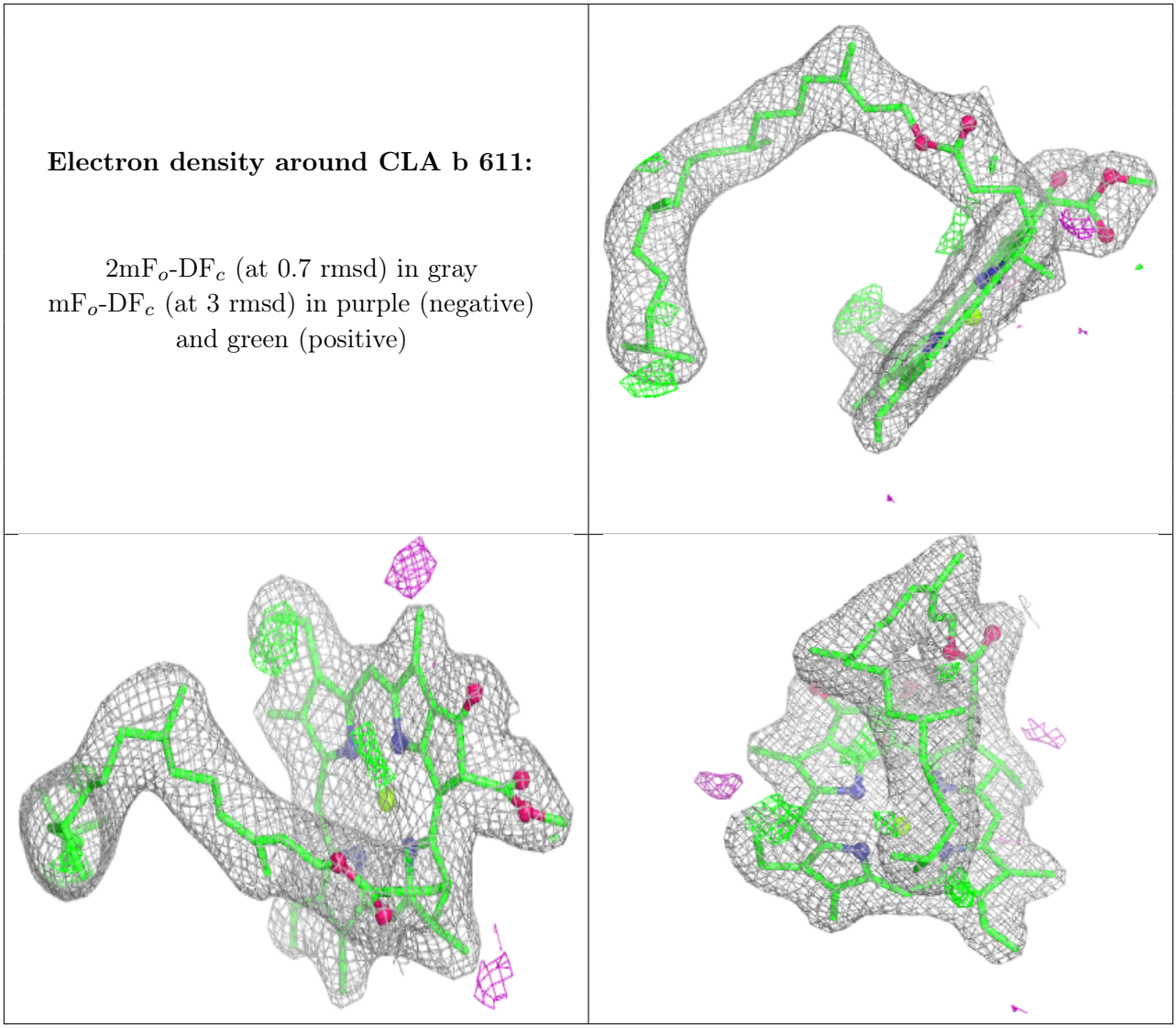






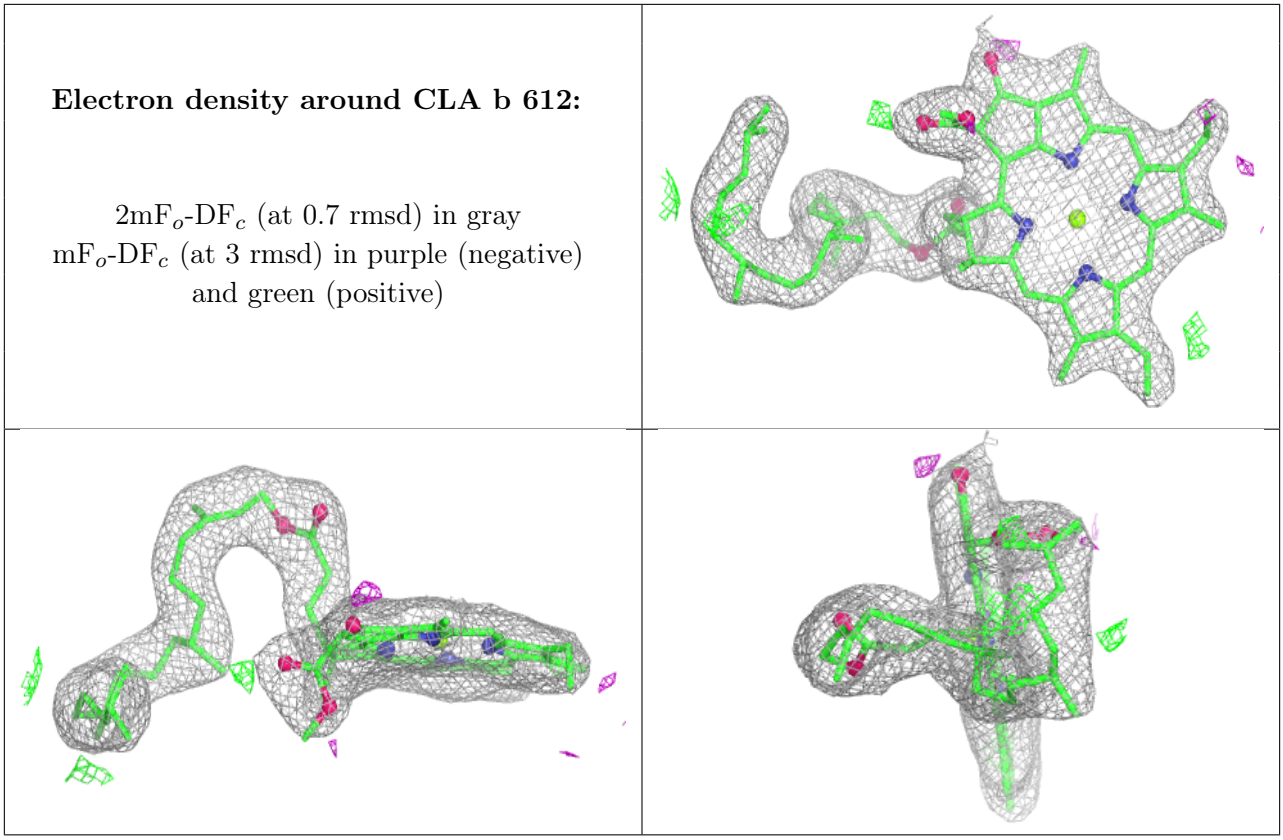
Electron density around CLA b 611:

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



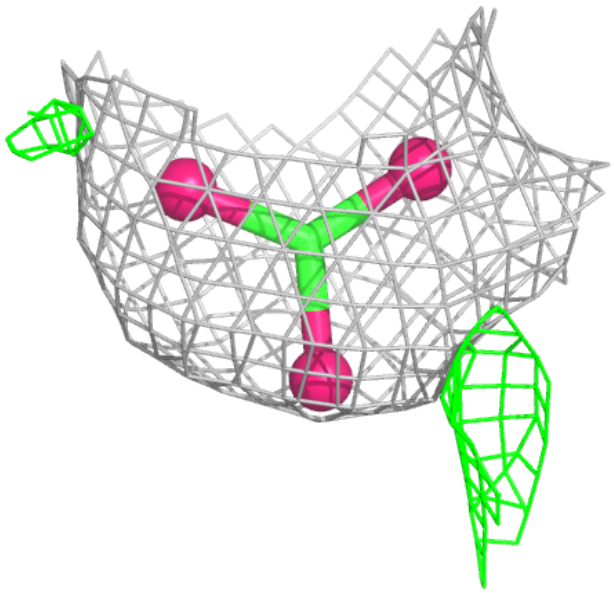
Electron density around CLA b 612:

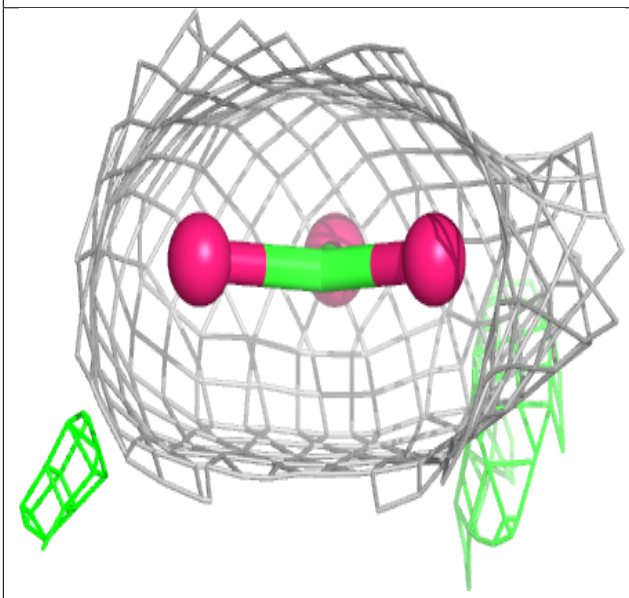
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

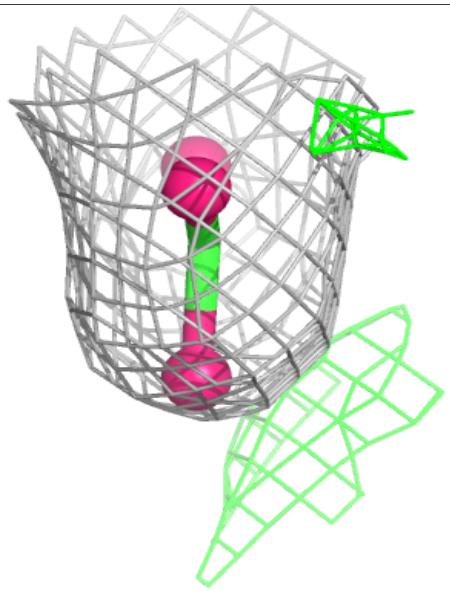


Electron density around BCT d 401 (A):

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

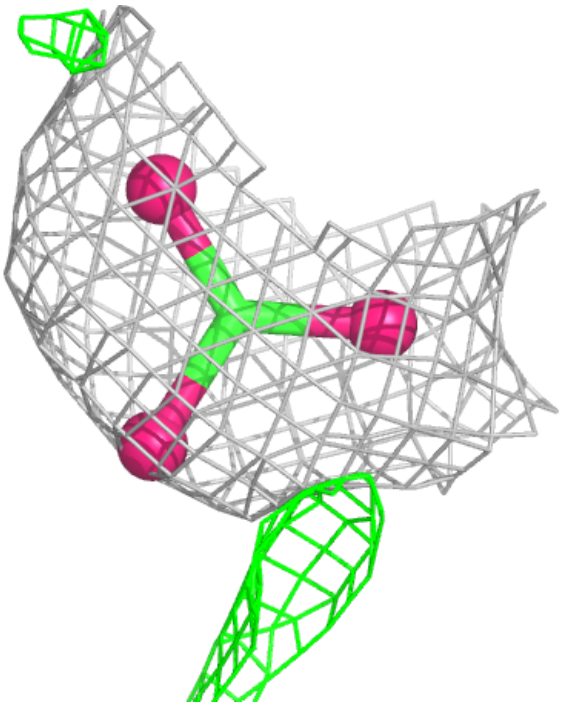


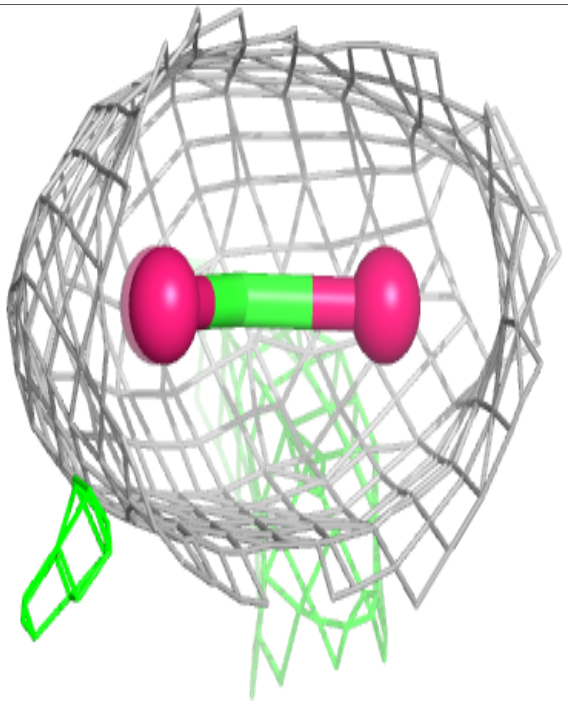


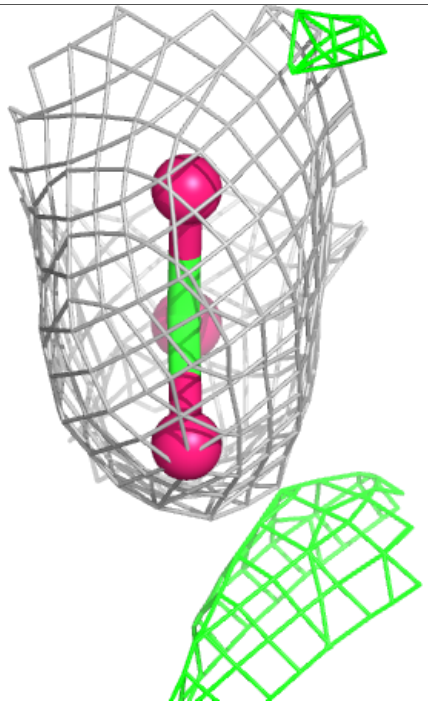


Electron density around BCT d 401 (B):

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

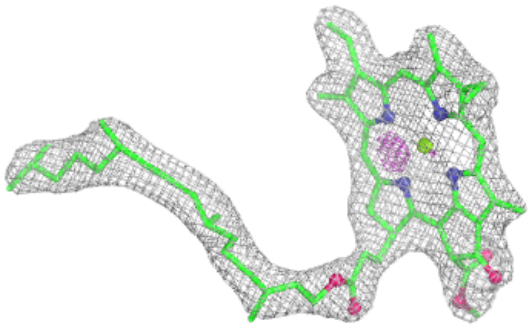


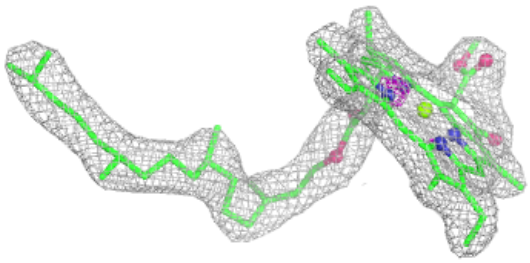


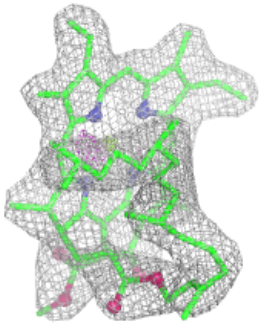


Electron density around CLA C 512:

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

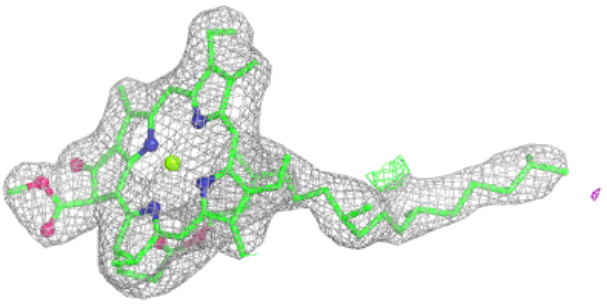


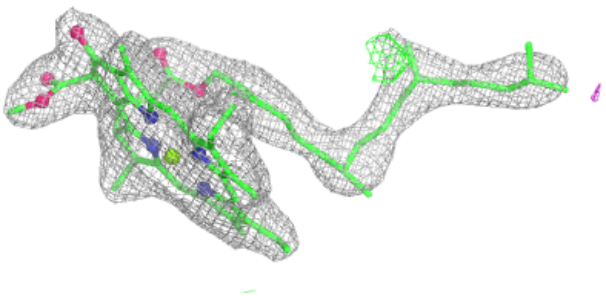


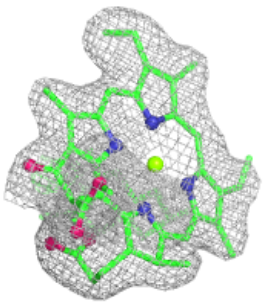


Electron density around CLA c 507:

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

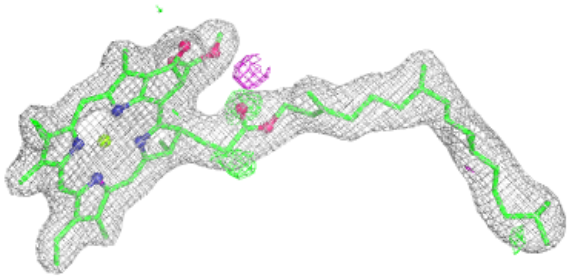


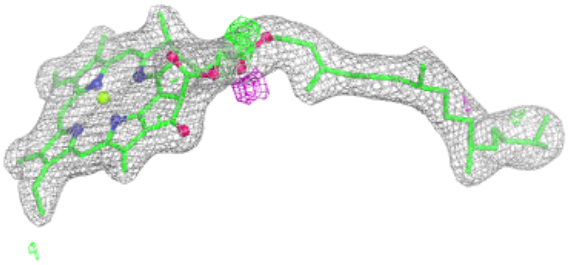


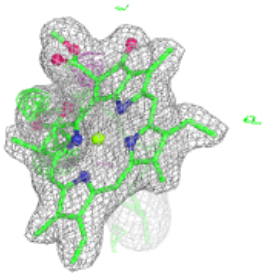


Electron density around CLA A 404 (B):

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

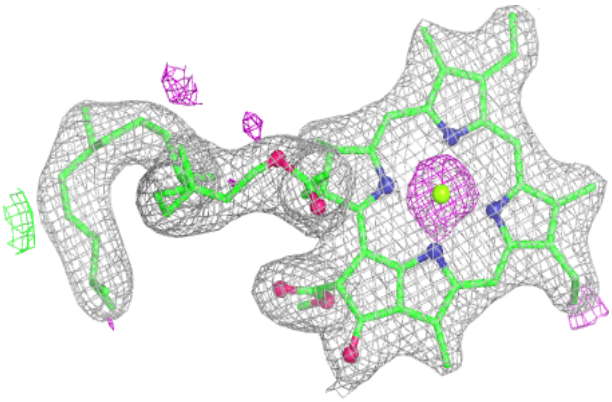


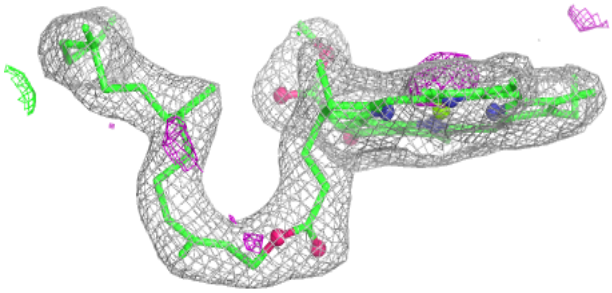




Electron density around CLA B 612:

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

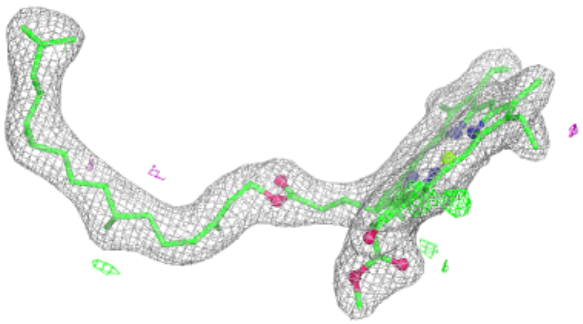


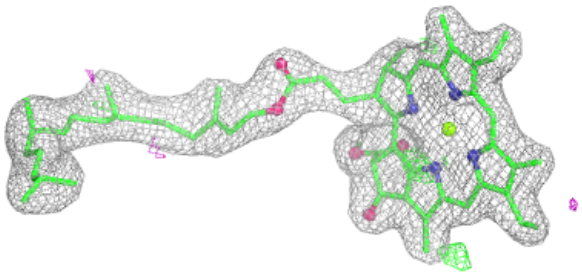


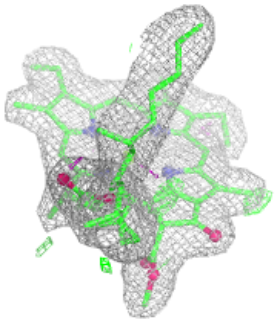


Electron density around CLA D 402 (A):

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

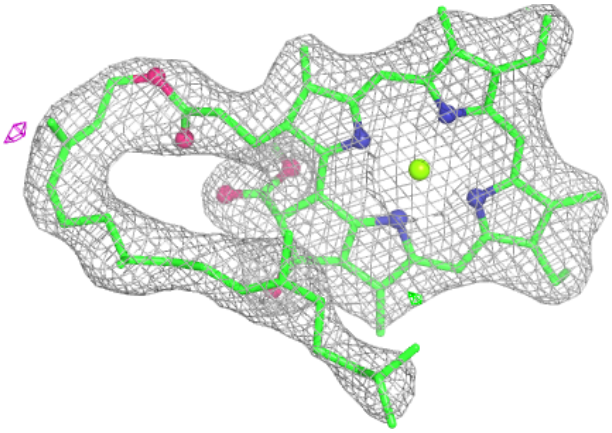


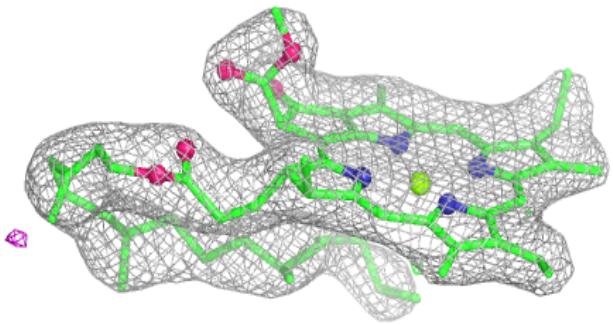


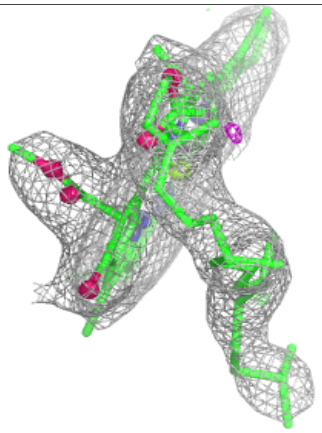


Electron density around CLA c 511:

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

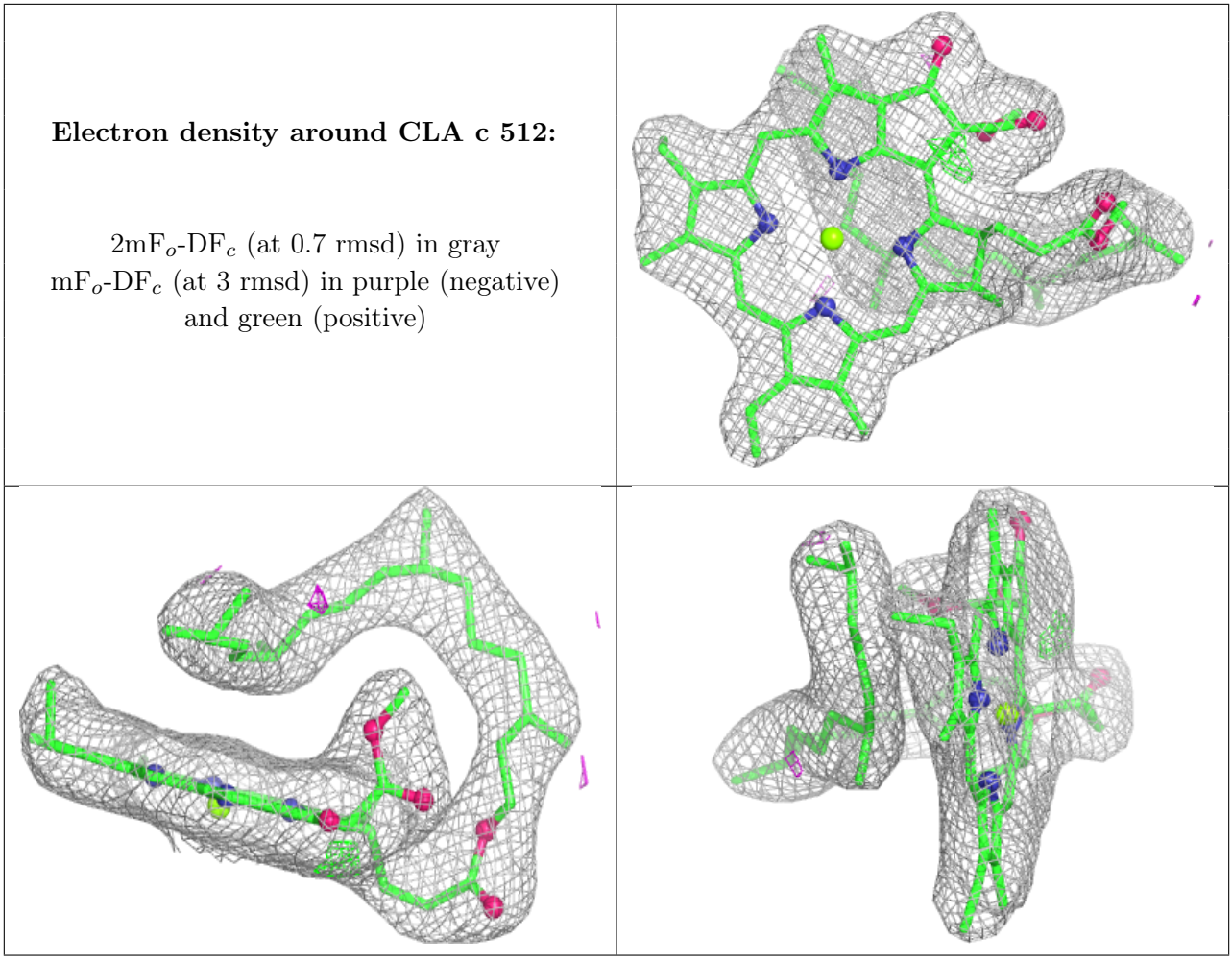






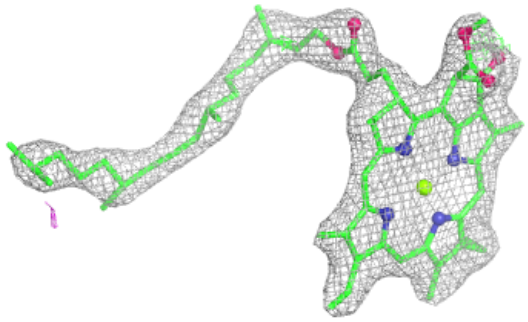
Electron density around CLA c 512:

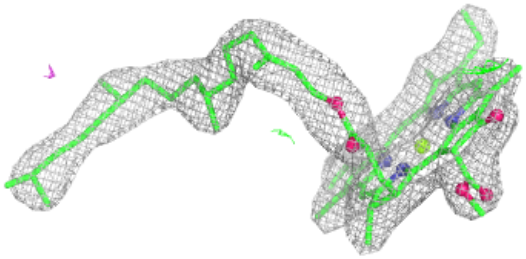
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

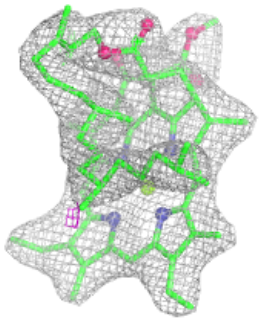


Electron density around CLA c 513:

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

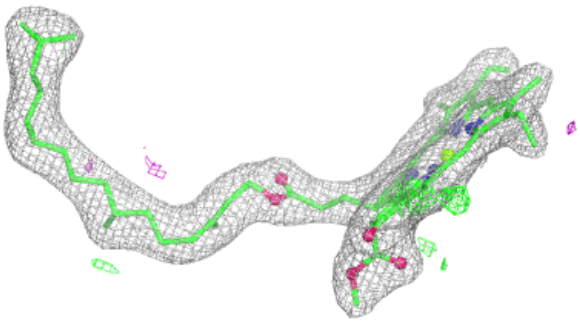


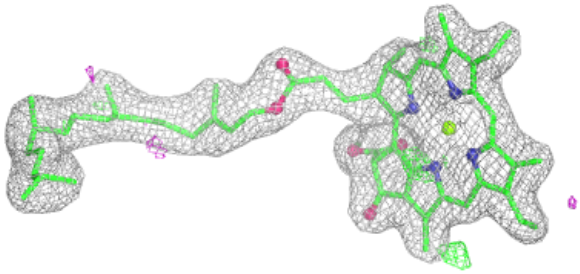


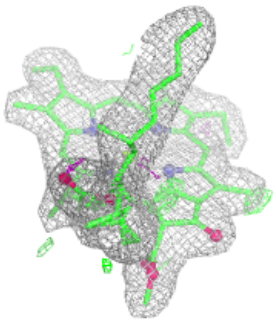


Electron density around CLA D 402 (B):

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

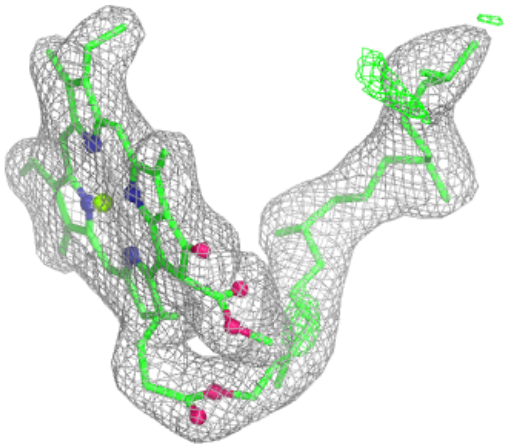


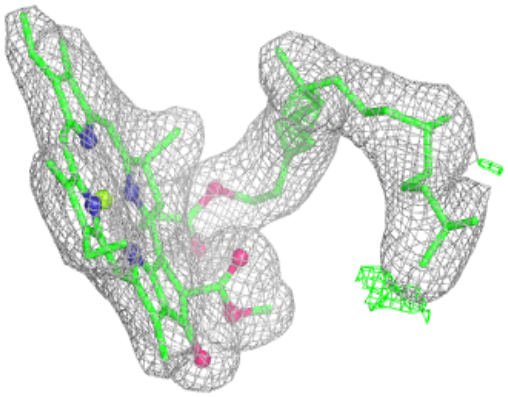


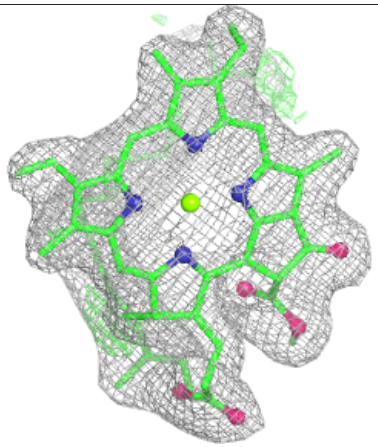


Electron density around CLA B 613:

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

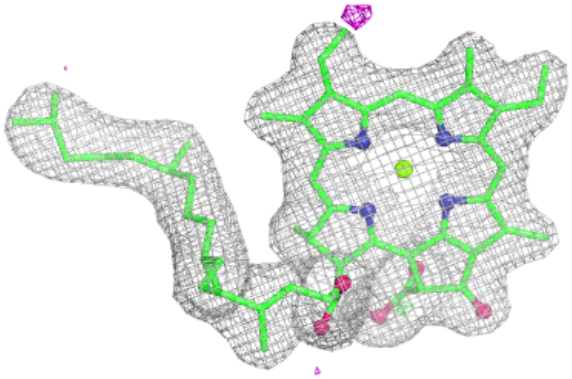


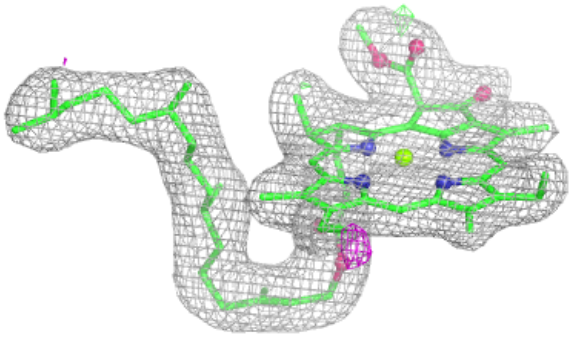


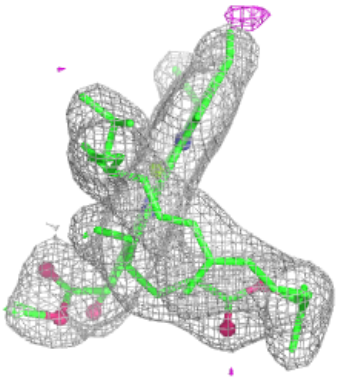


Electron density around CLA d 402 (A):

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

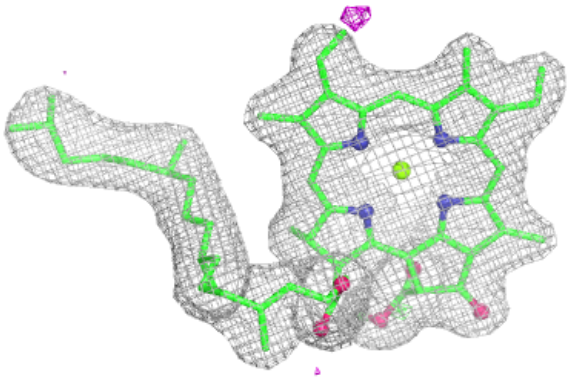


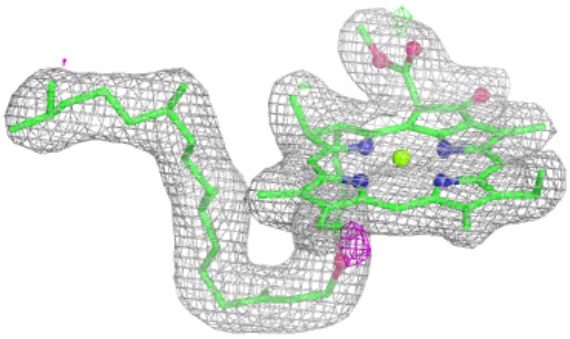


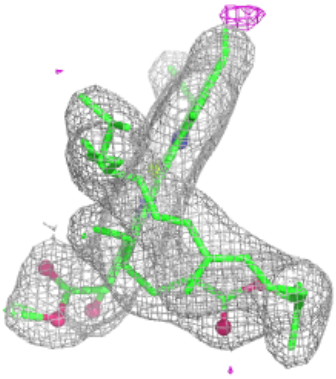


Electron density around CLA d 402 (B):

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

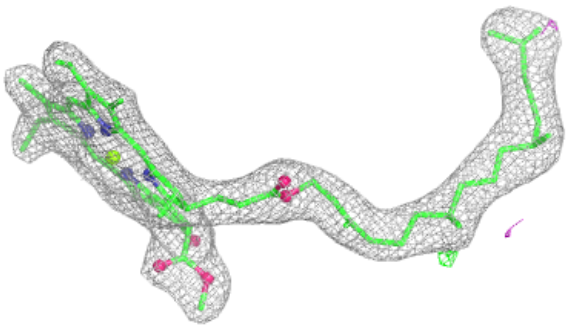


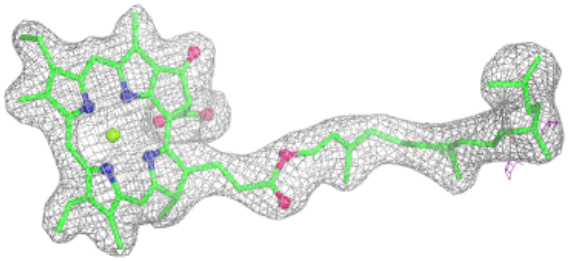


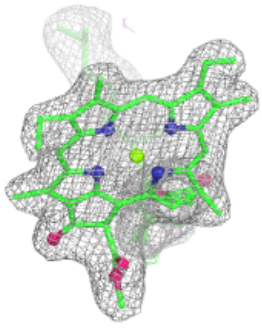


Electron density around CLA d 403 (A):

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

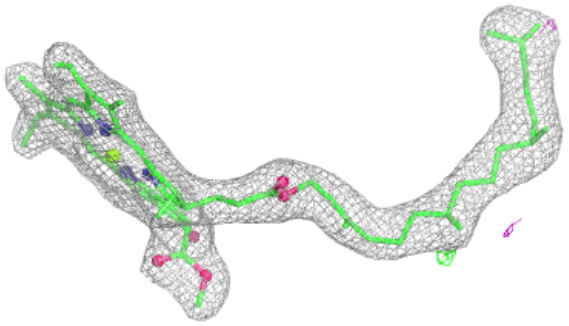


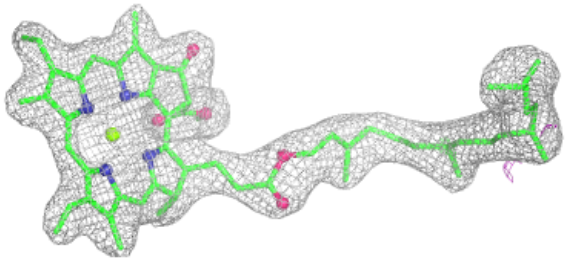


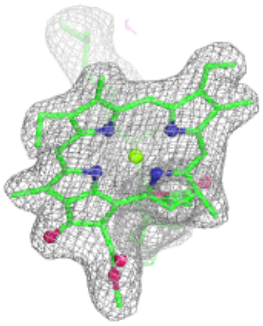


Electron density around CLA d 403 (B):

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

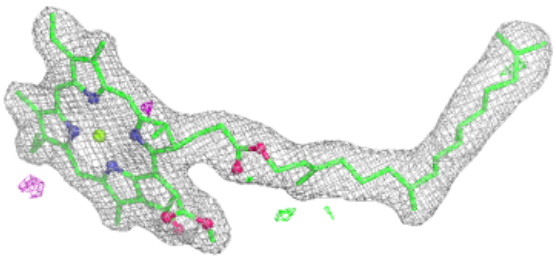


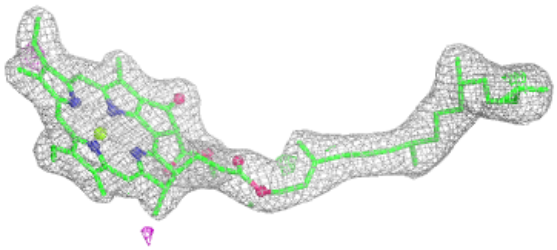


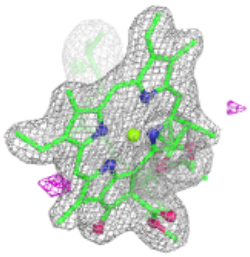


Electron density around CLA a 404 (A):

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

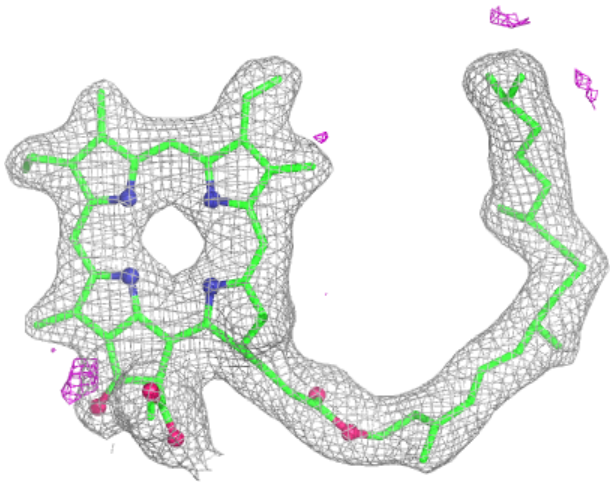


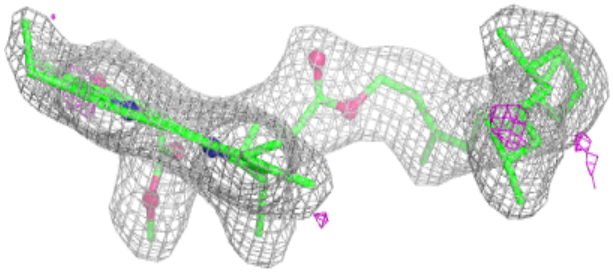


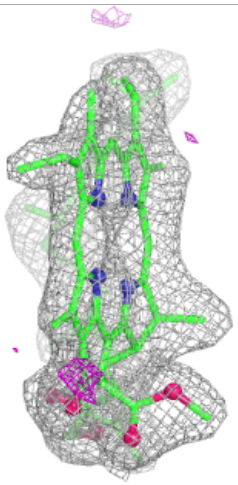


Electron density around PHO A 407 (A):

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

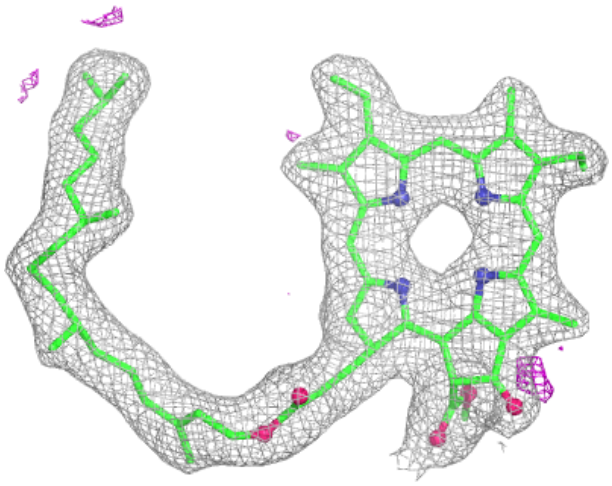


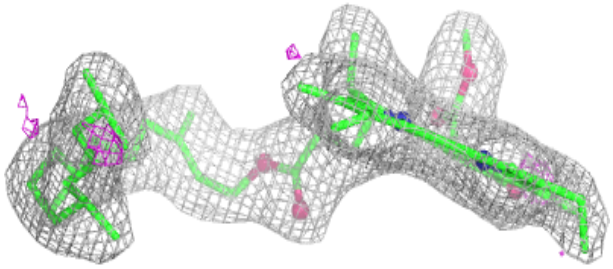


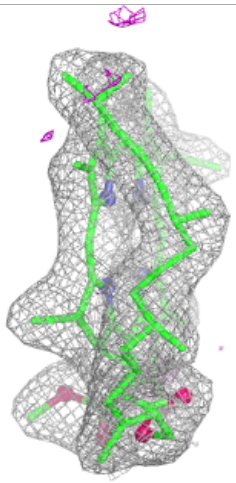


Electron density around PHO A 407 (B):

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

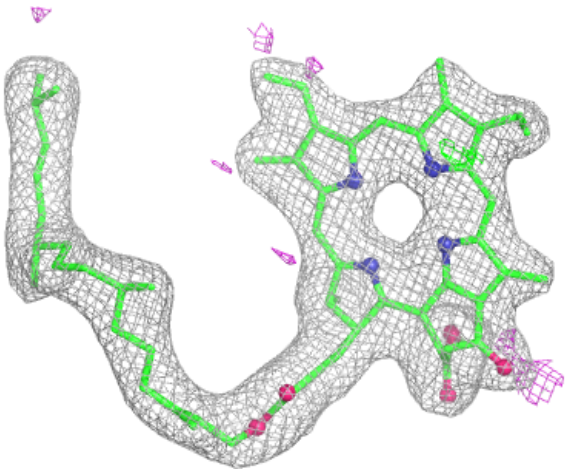


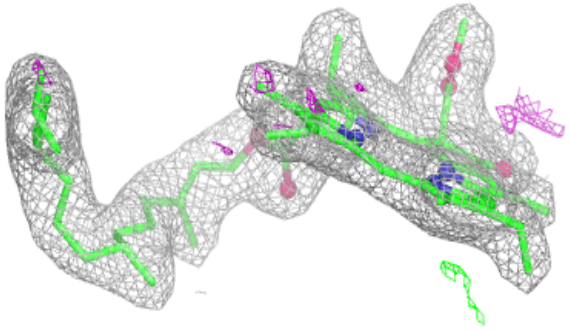


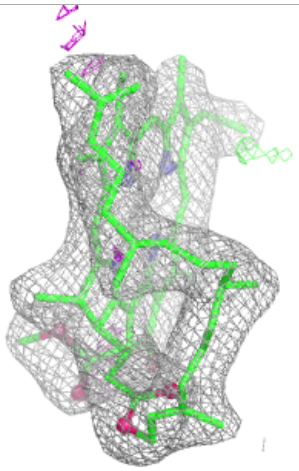


Electron density around PHO A 416 (A):

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

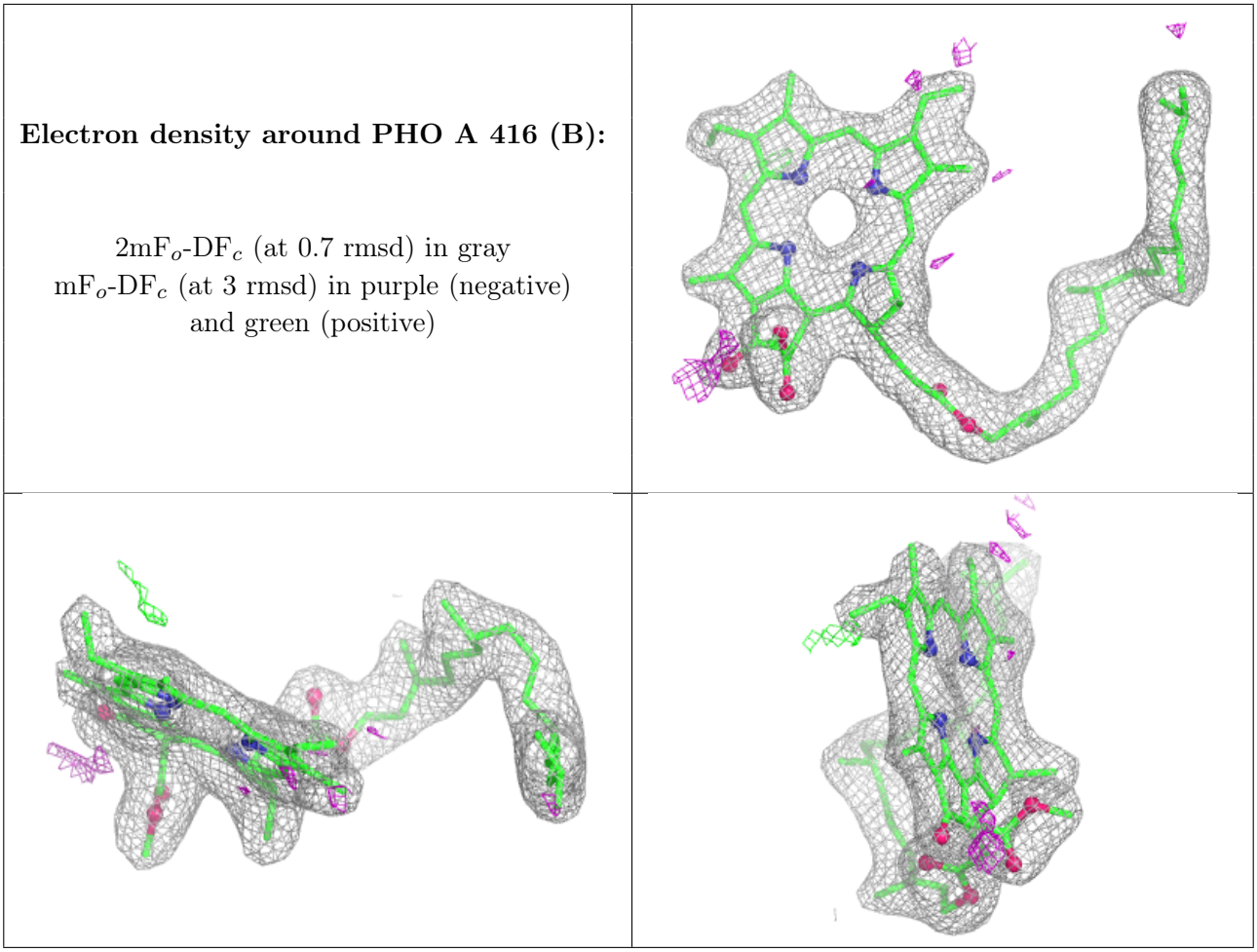






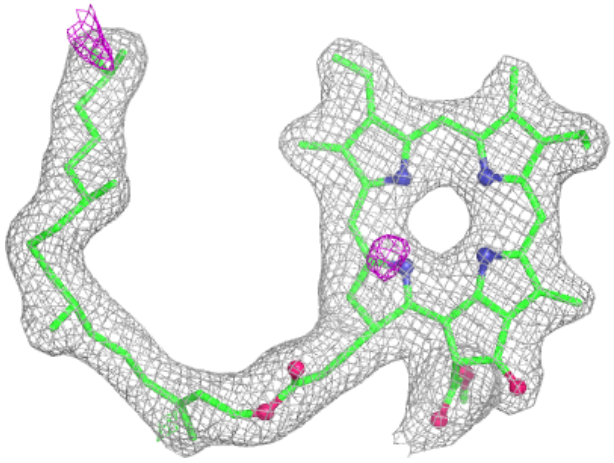
Electron density around PHO A 416 (B):

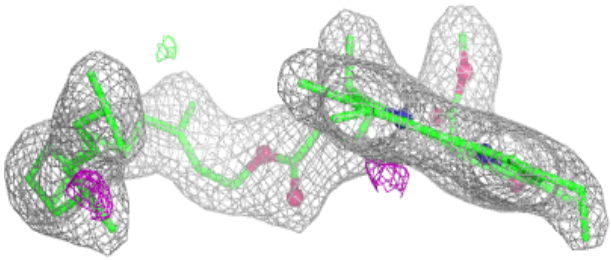
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

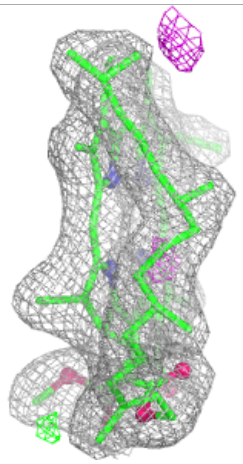


Electron density around PHO a 406 (A):

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

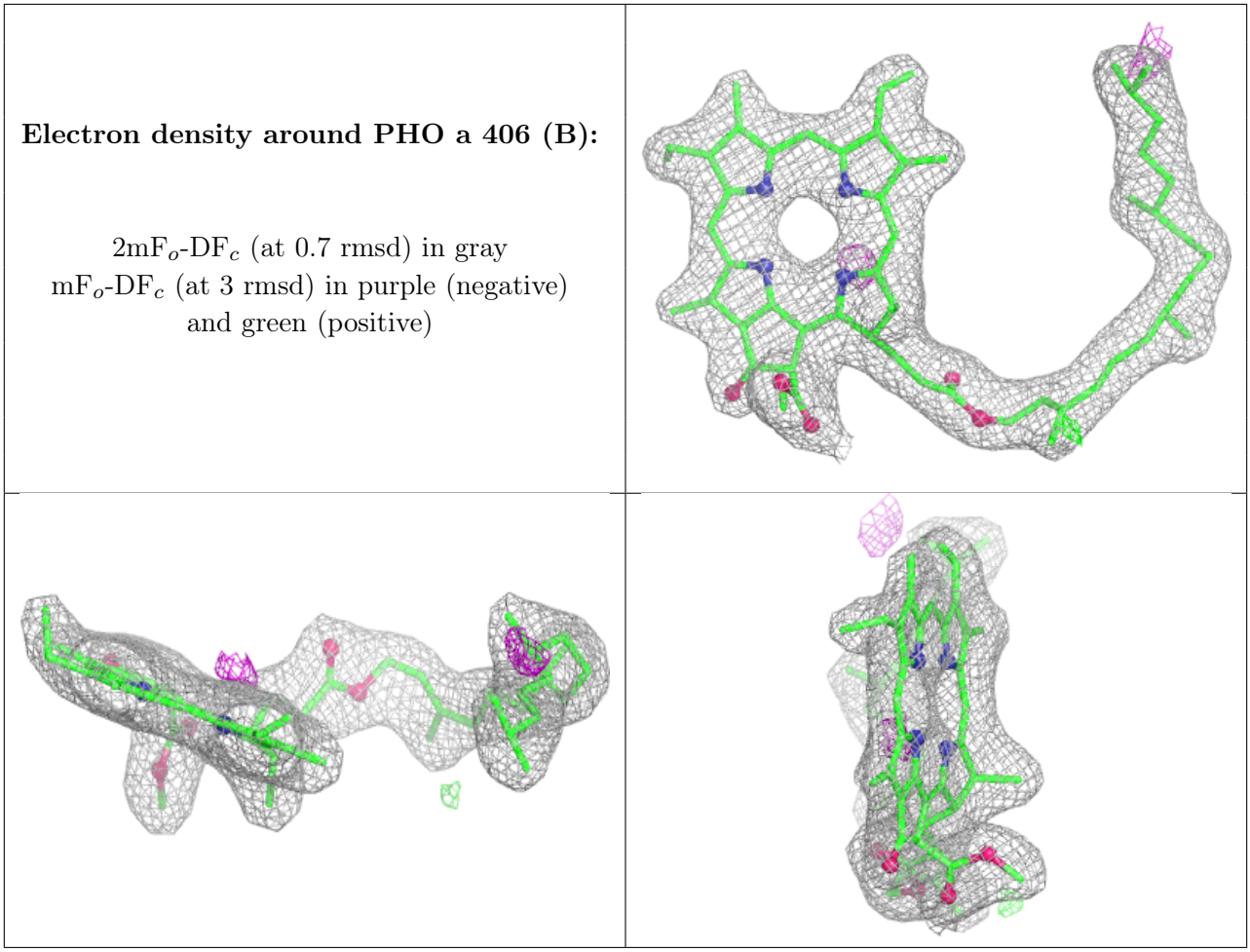






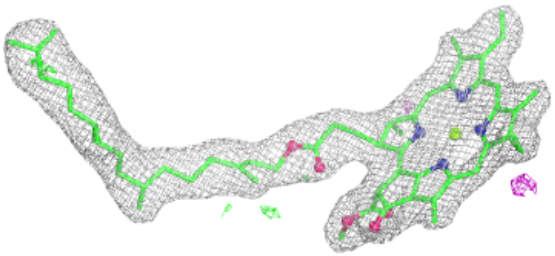
Electron density around PHO a 406 (B):

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

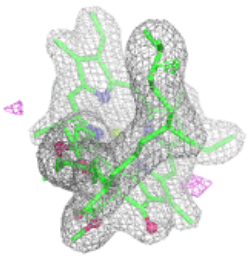


Electron density around CLA a 404 (B):

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

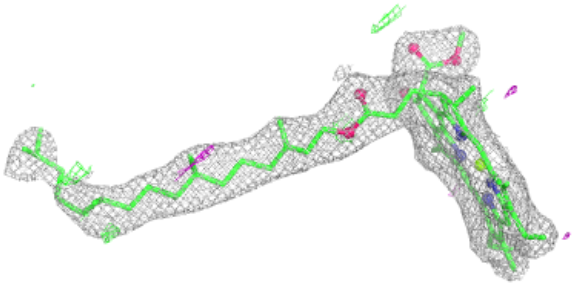


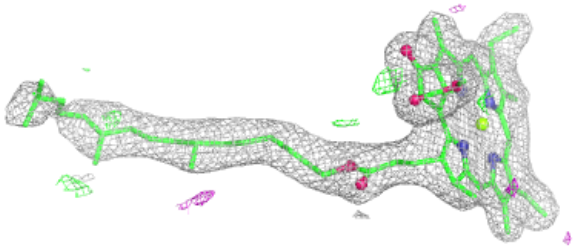


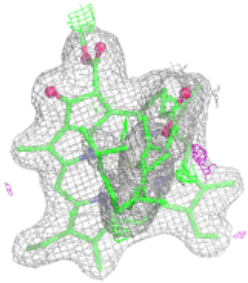


Electron density around CLA B 604:

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

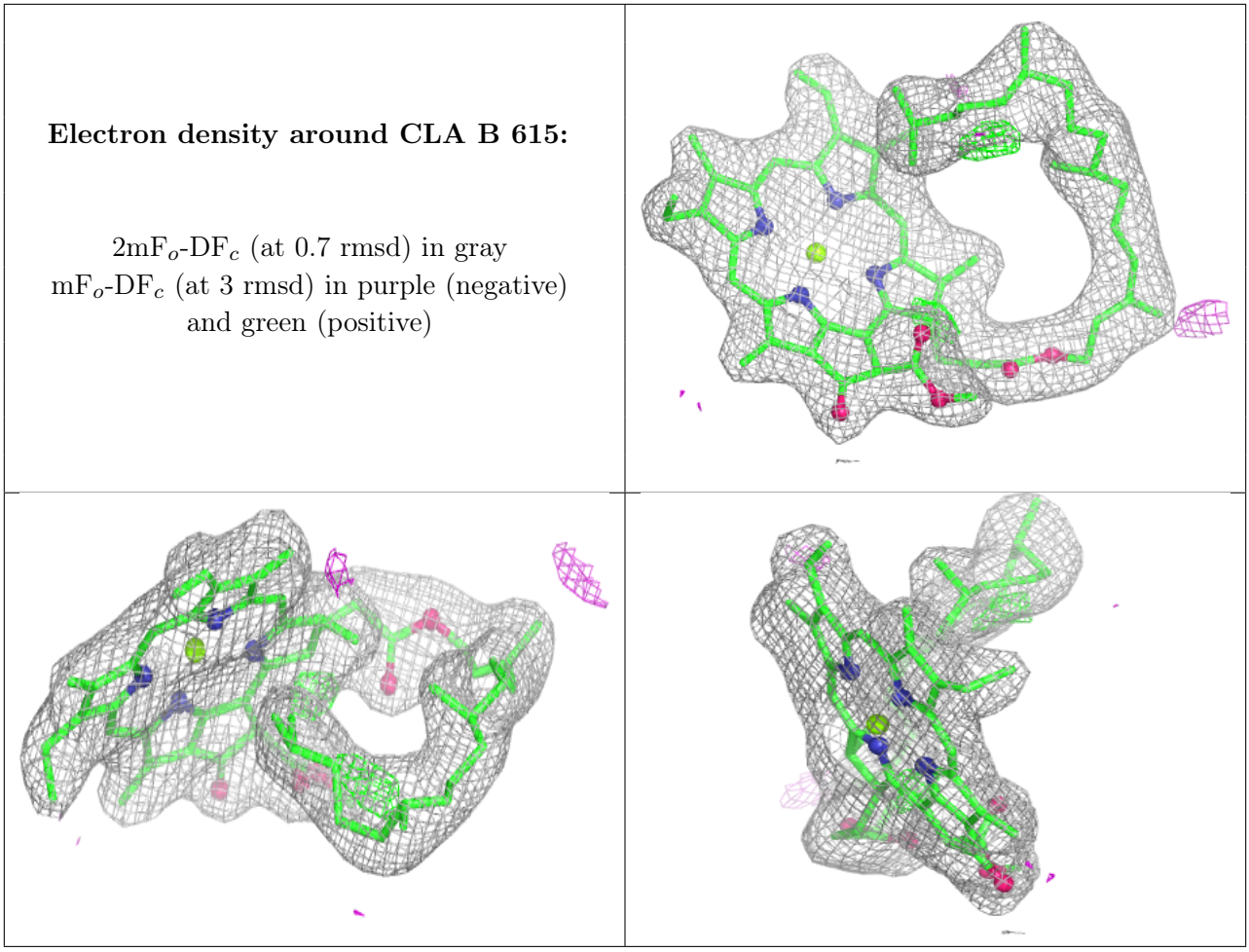






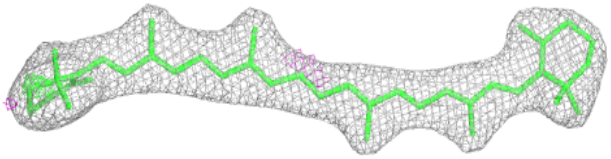
Electron density around CLA B 615:

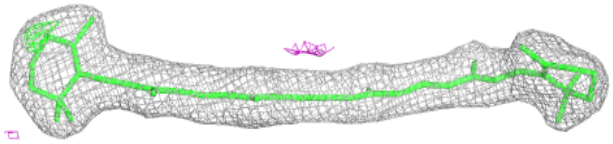
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

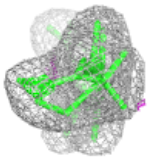


Electron density around BCR B 617:

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

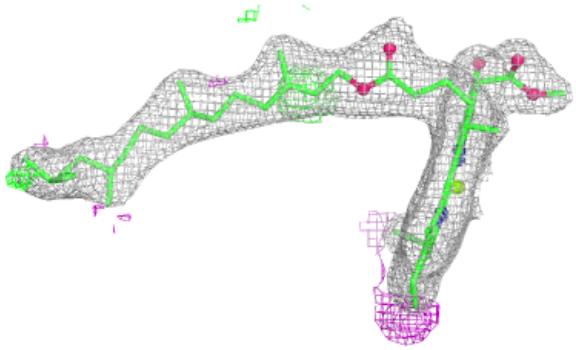


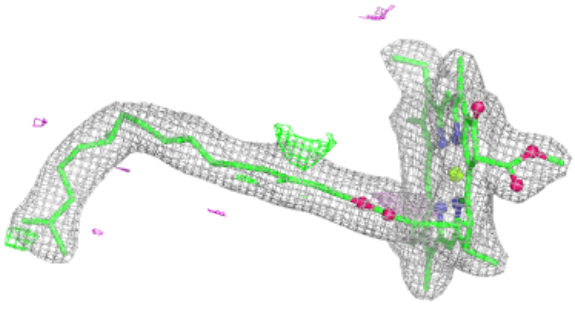


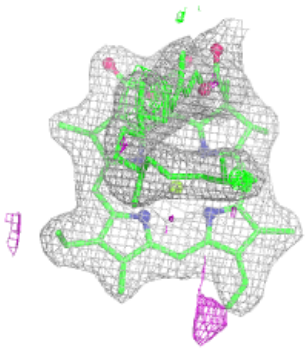


Electron density around CLA B 605:

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

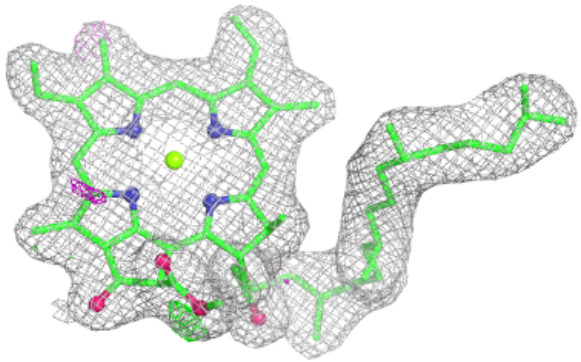


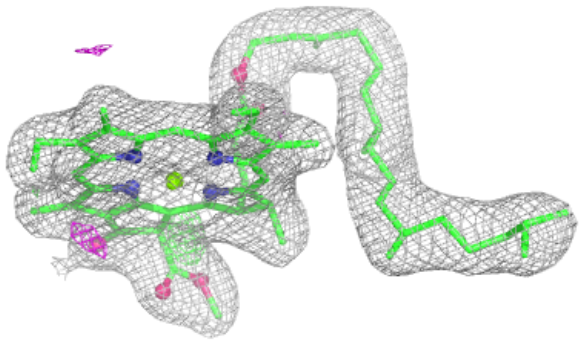


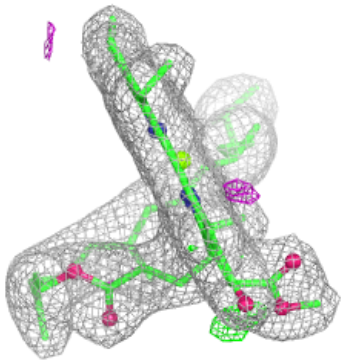


Electron density around CLA A 405 (A):

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

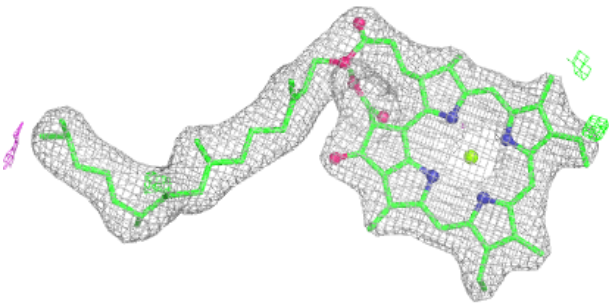


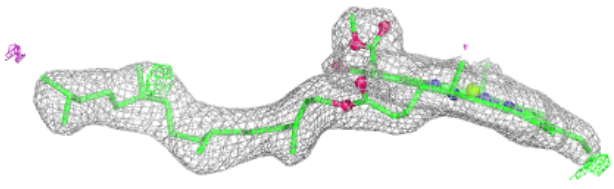




Electron density around CLA b 602:

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

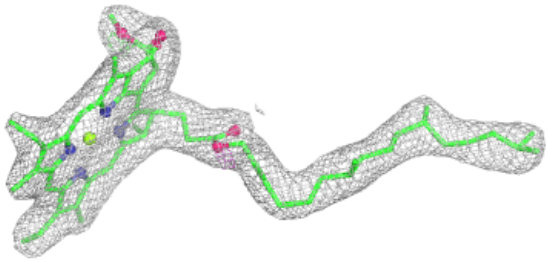


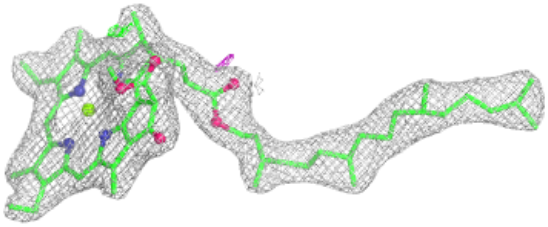


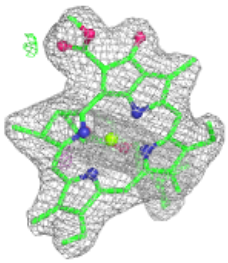


Electron density around CLA C 503:

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

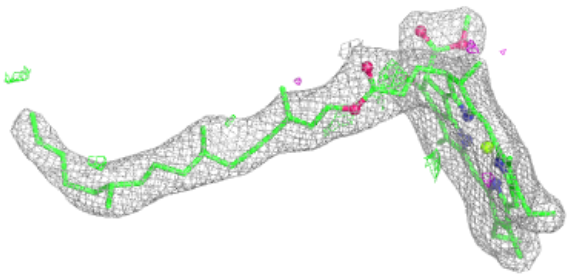


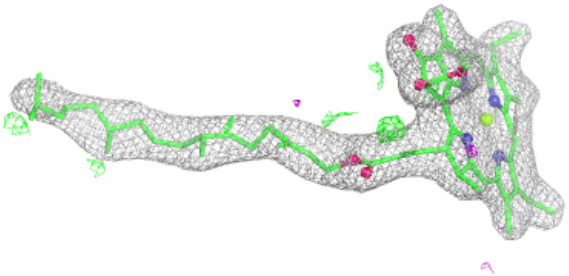


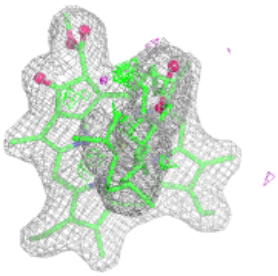


Electron density around CLA b 604:

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

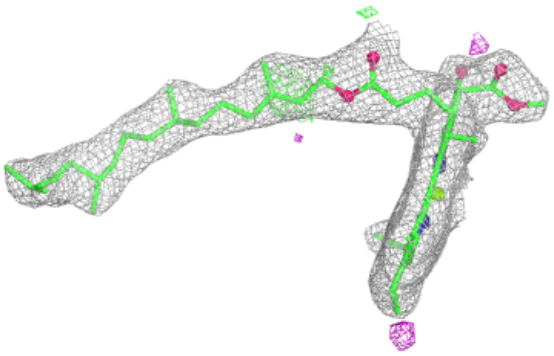


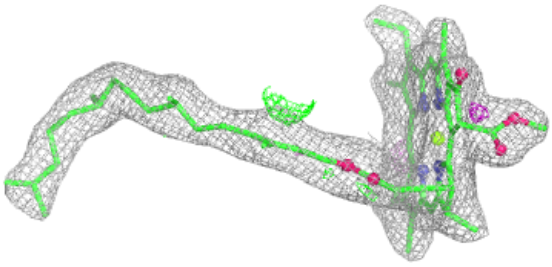


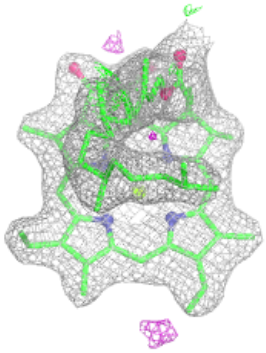


Electron density around CLA b 605:

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

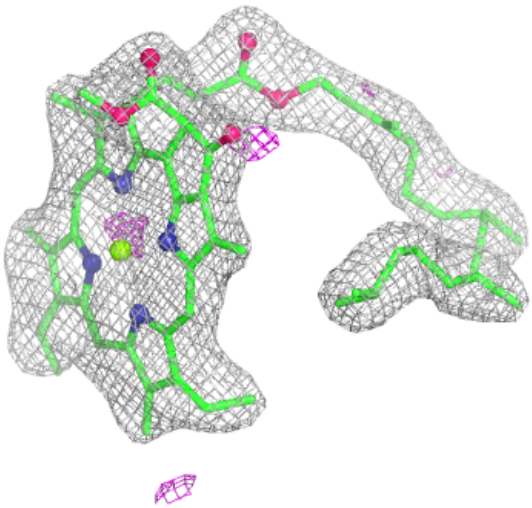


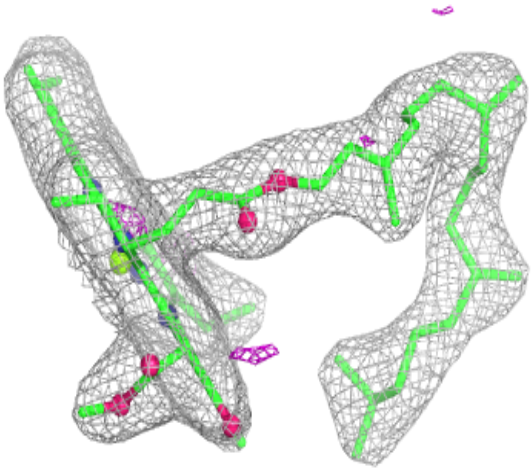


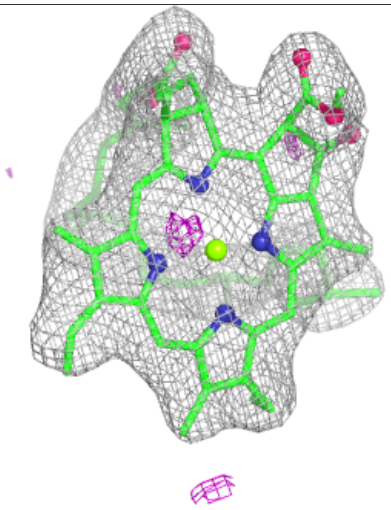


Electron density around CLA C 504:

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

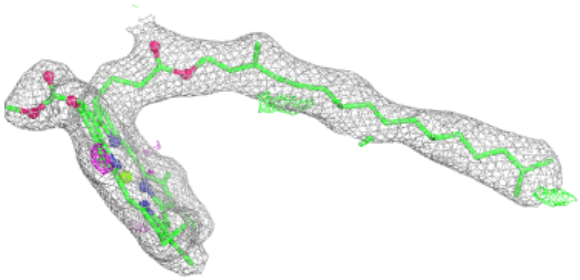


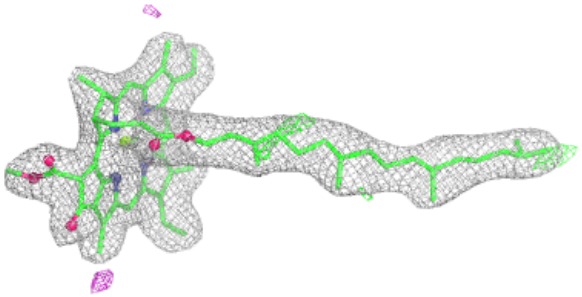


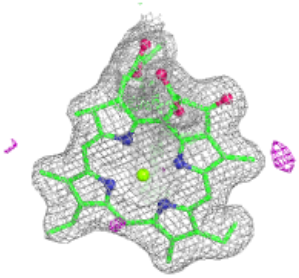


Electron density around CLA B 607:

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

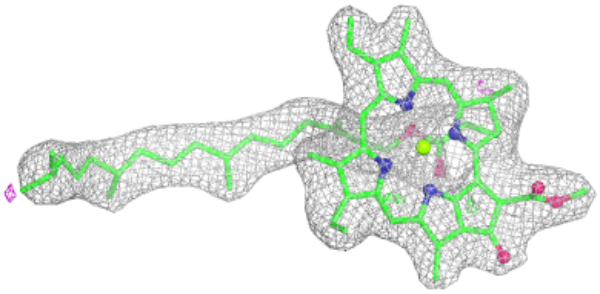


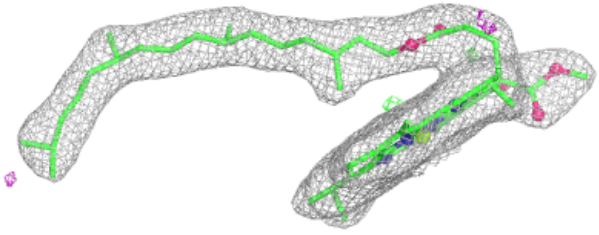


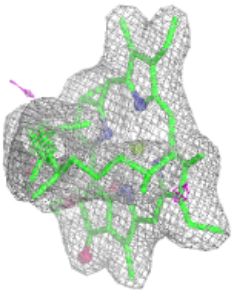


Electron density around CLA b 608:

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

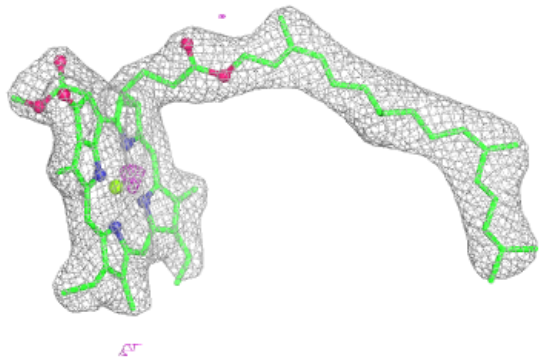


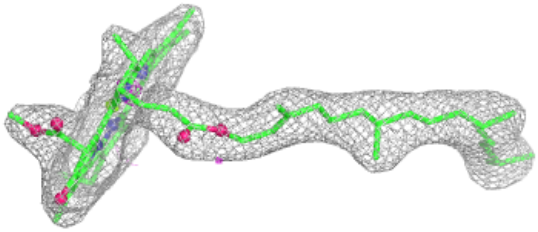


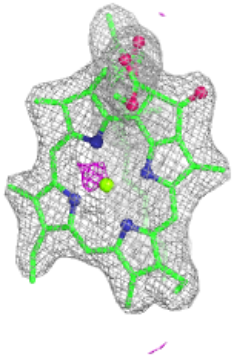


Electron density around CLA b 609:

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

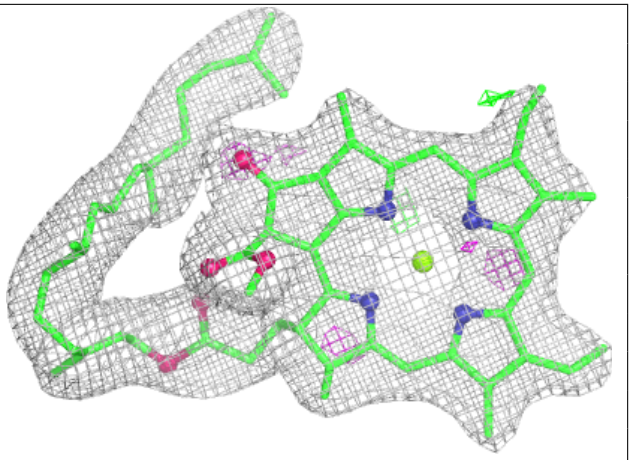


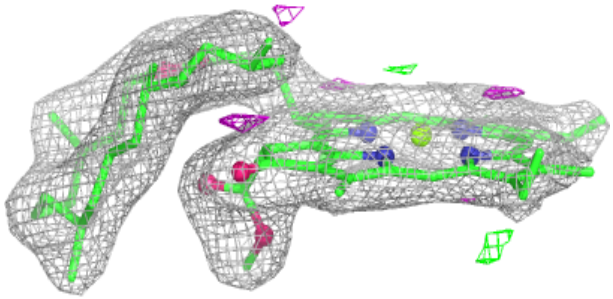




Electron density around CLA b 610:

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

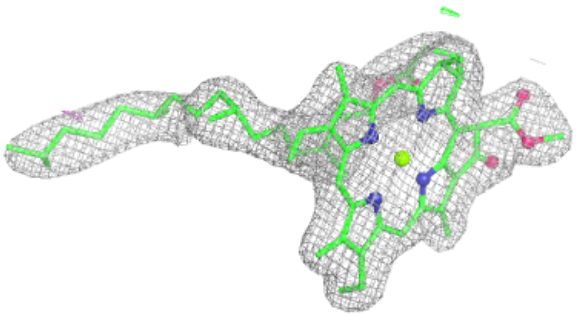


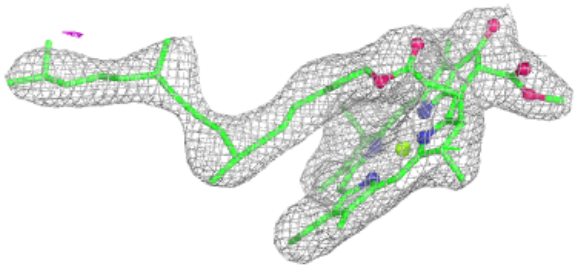


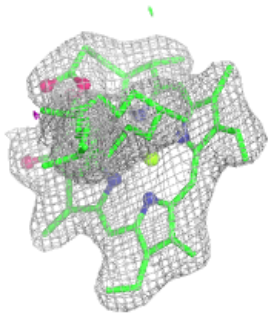


Electron density around CLA C 506:

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

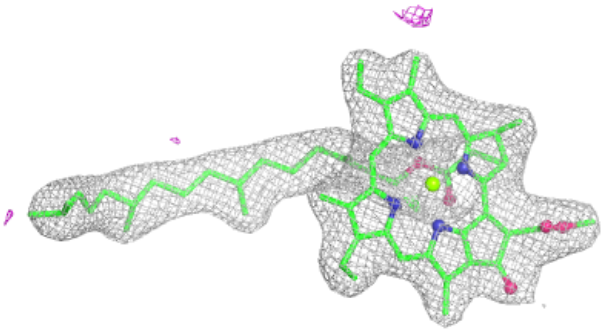


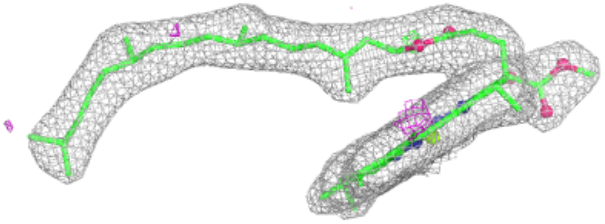


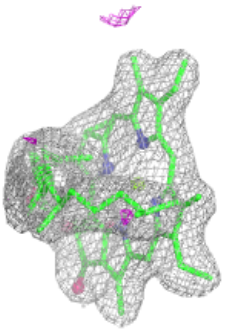


Electron density around CLA B 608:

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

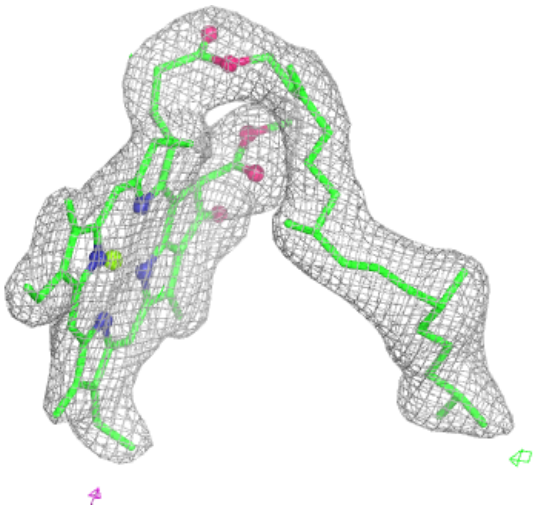


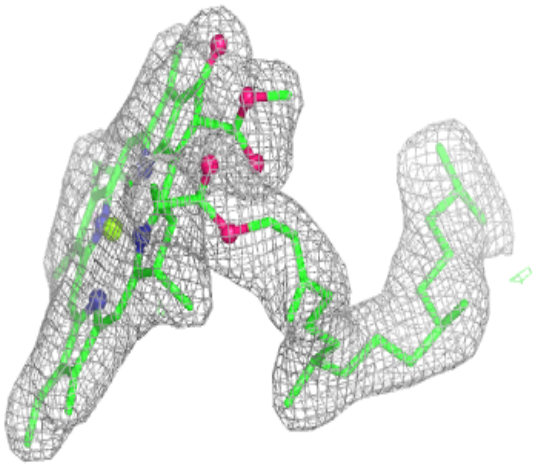


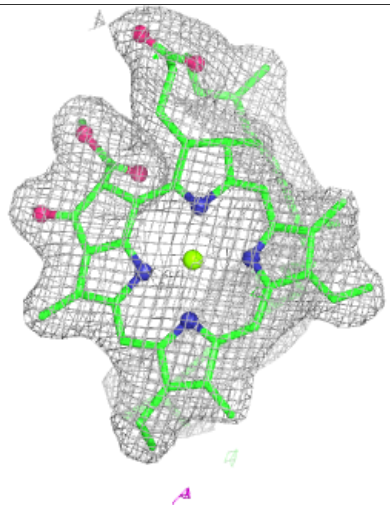


Electron density around CLA b 613:

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

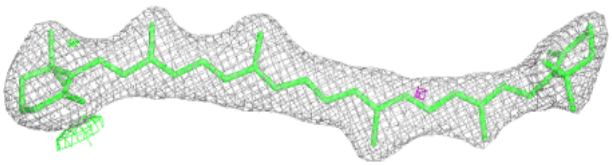


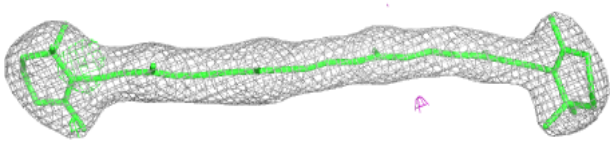


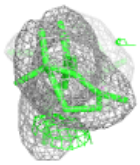


Electron density around BCR c 517:

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

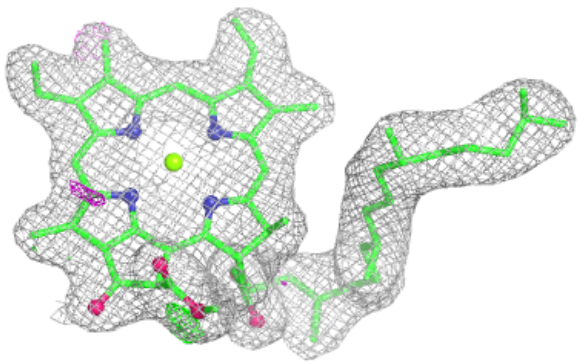


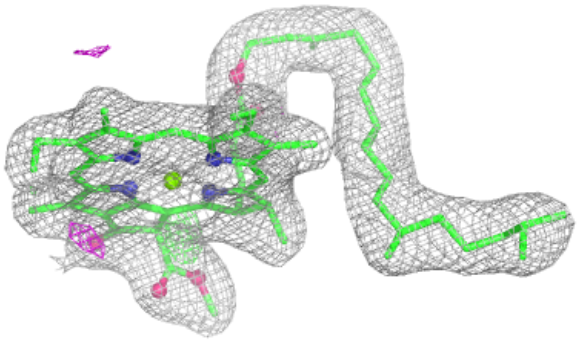


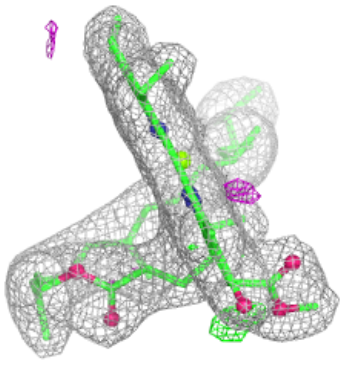


Electron density around CLA A 405 (B):

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



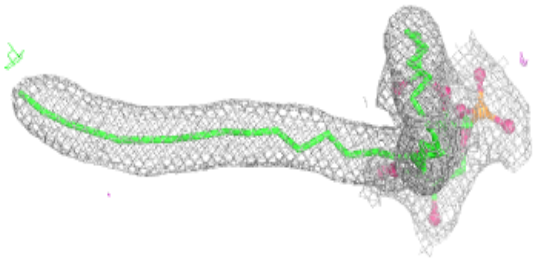


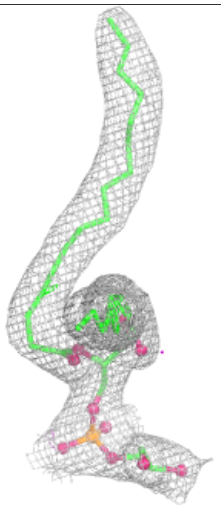


Electron density around LHG L 101 (A):

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

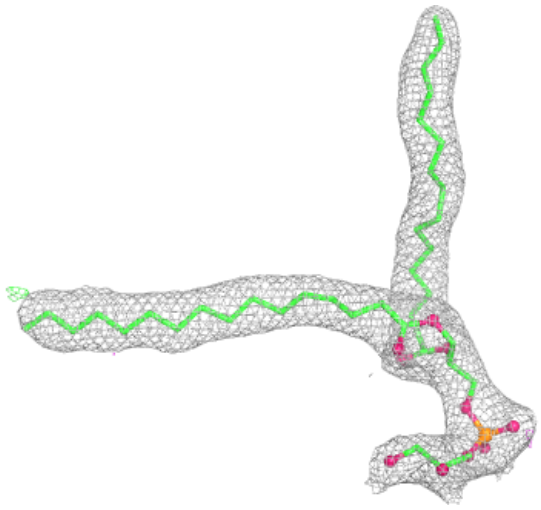


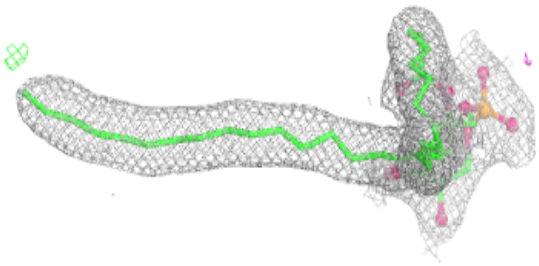


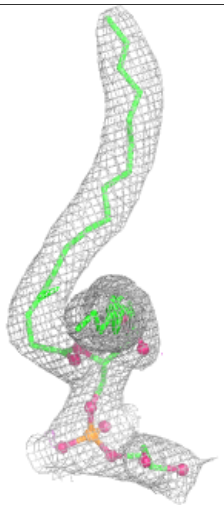


Electron density around LHG L 101 (B):

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

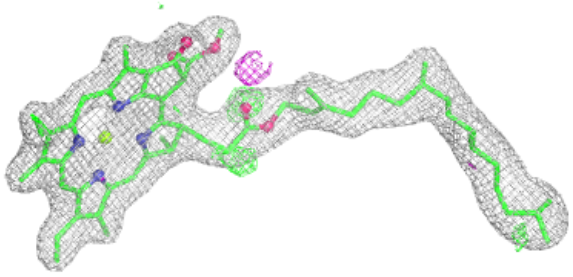


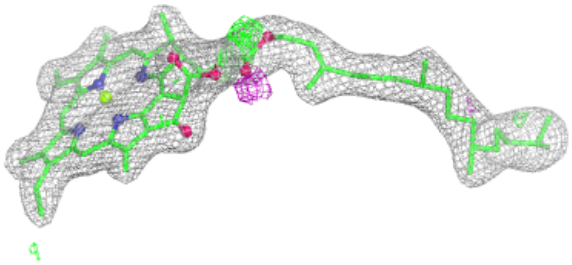


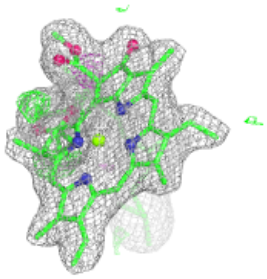


Electron density around CLA A 404 (A):

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

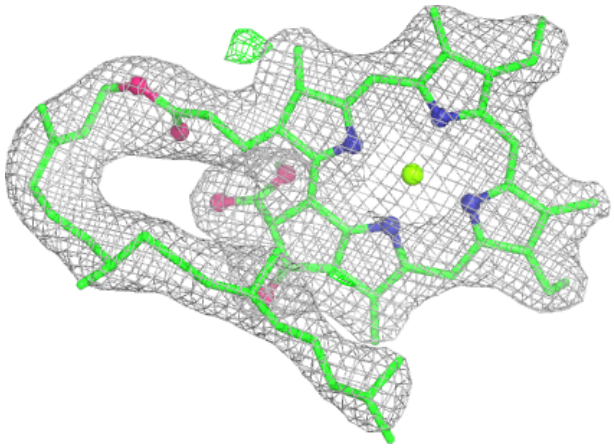


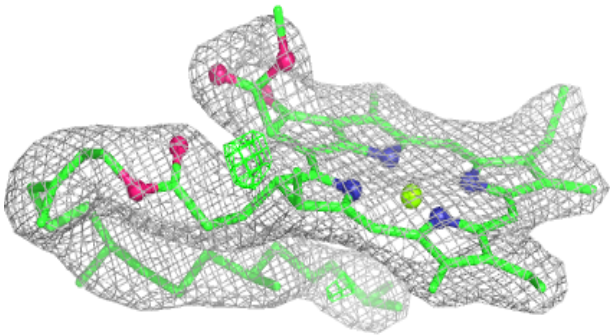




Electron density around CLA C 510:

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

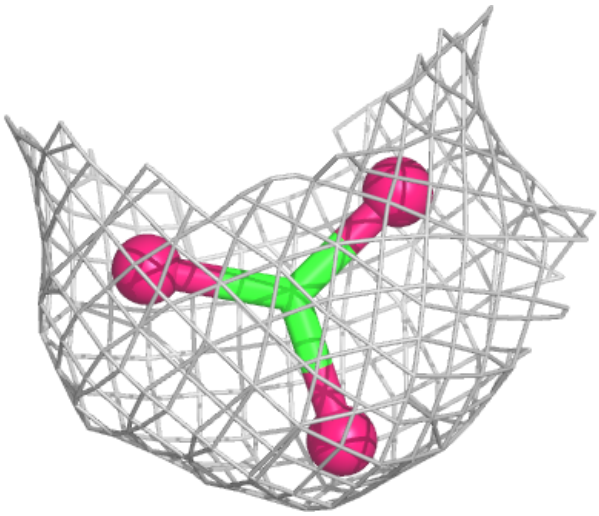


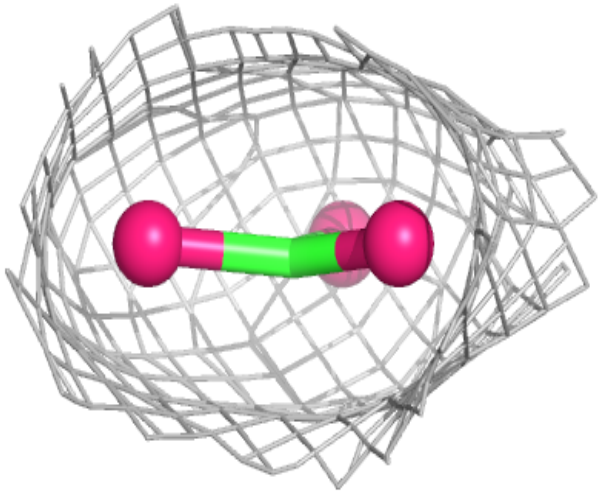


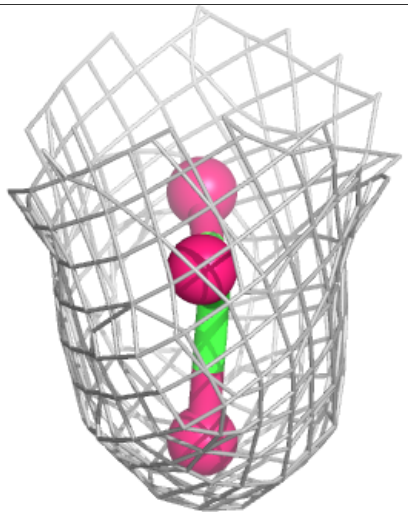


Electron density around BCT D 401 (A):

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

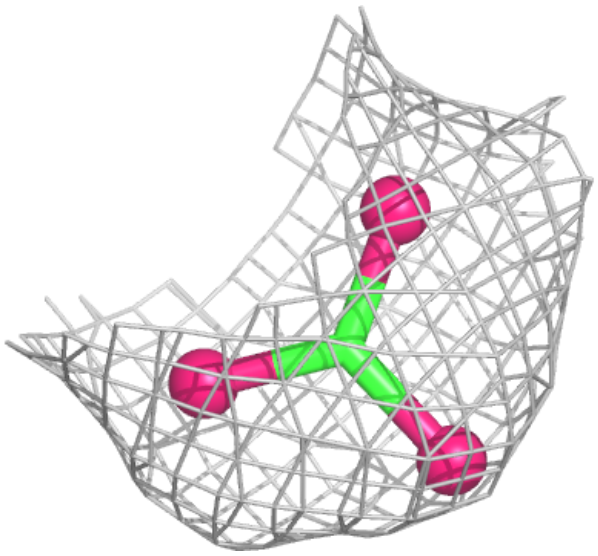


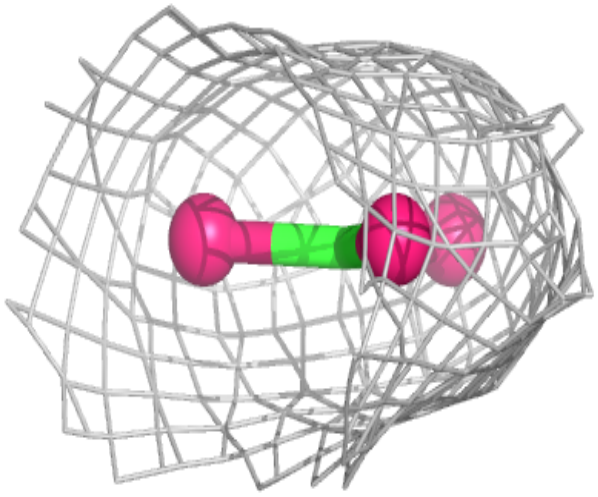


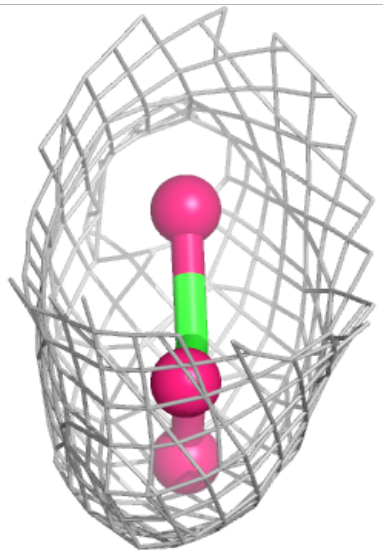


Electron density around BCT D 401 (B):

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

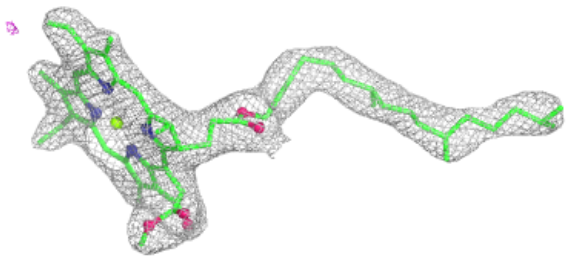


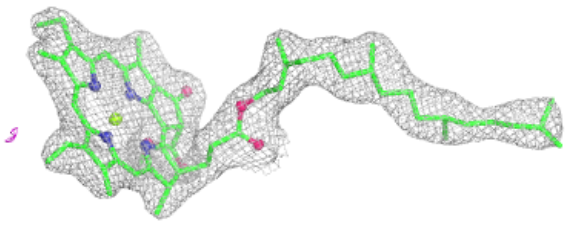


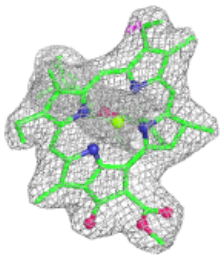


Electron density around CLA c 504:

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

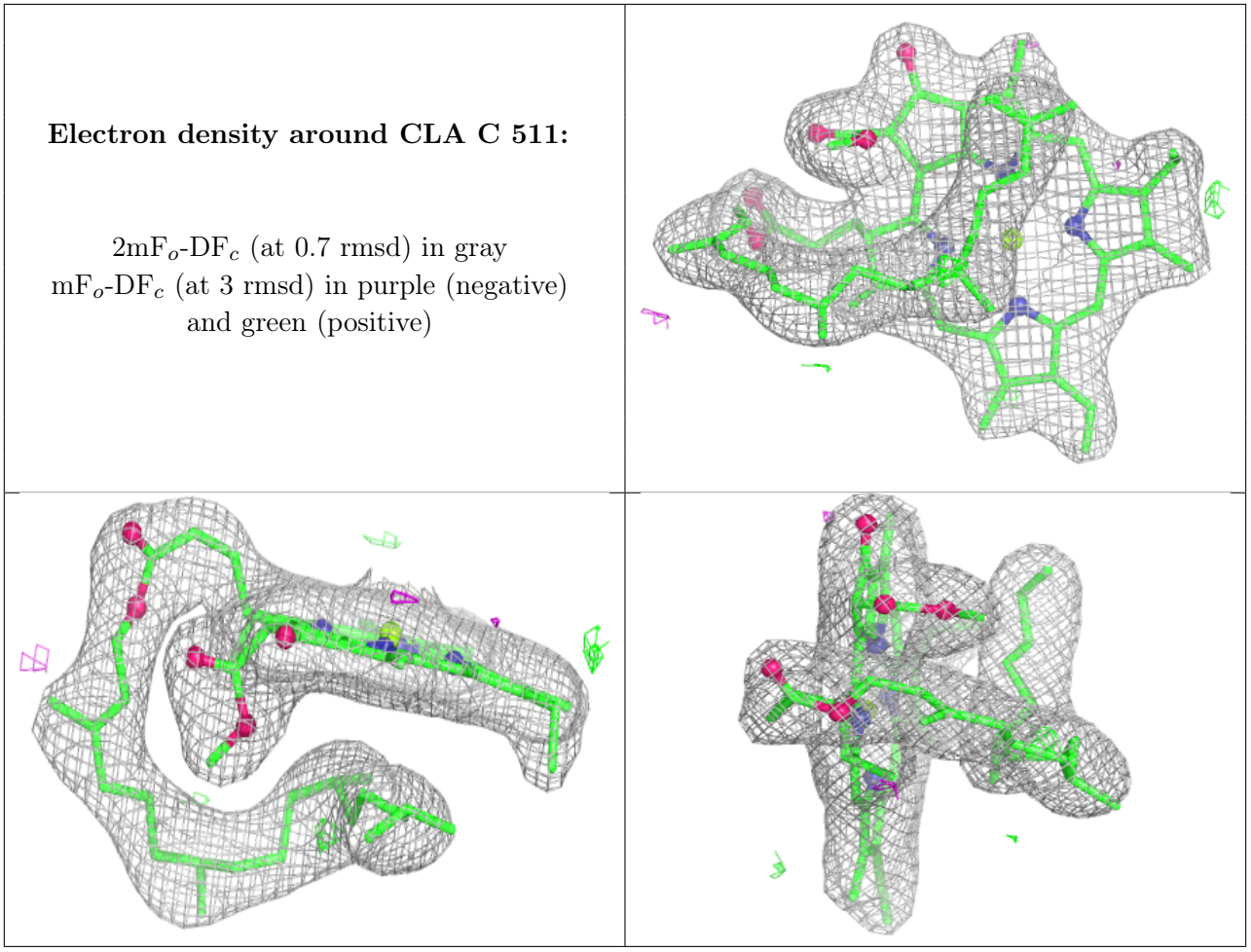






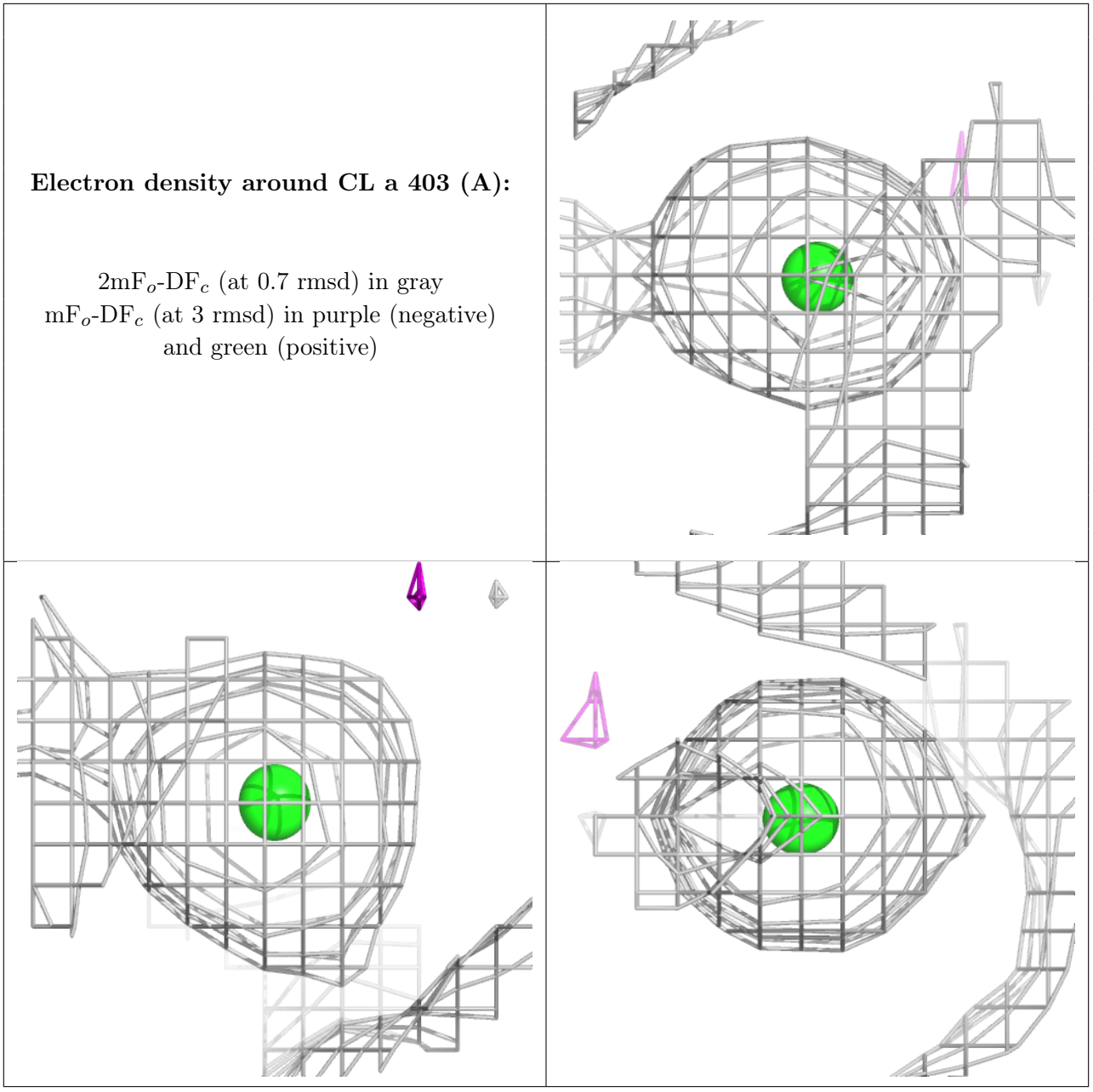
Electron density around CLA C 511:

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



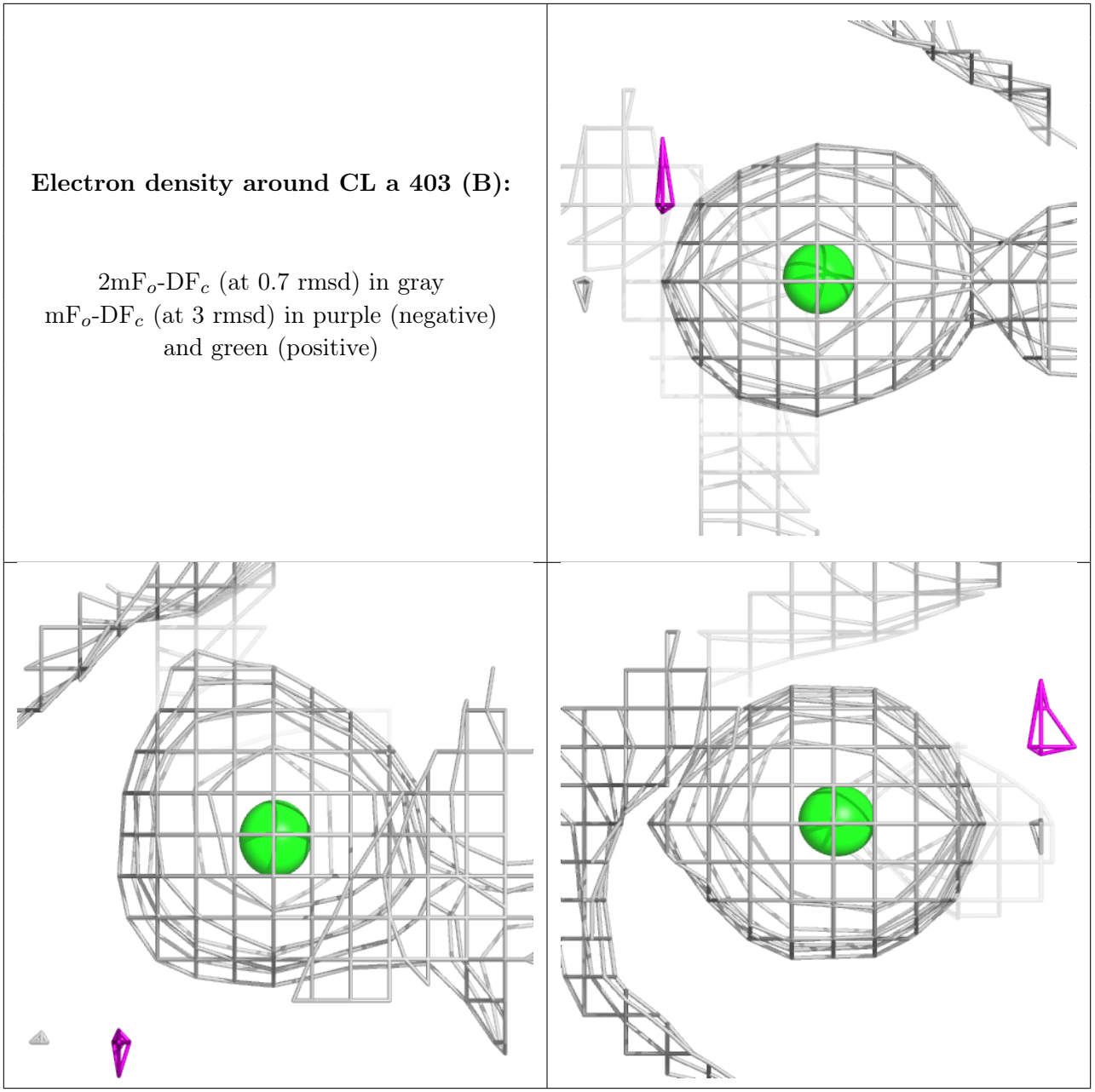
Electron density around CL a 403 (A):

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



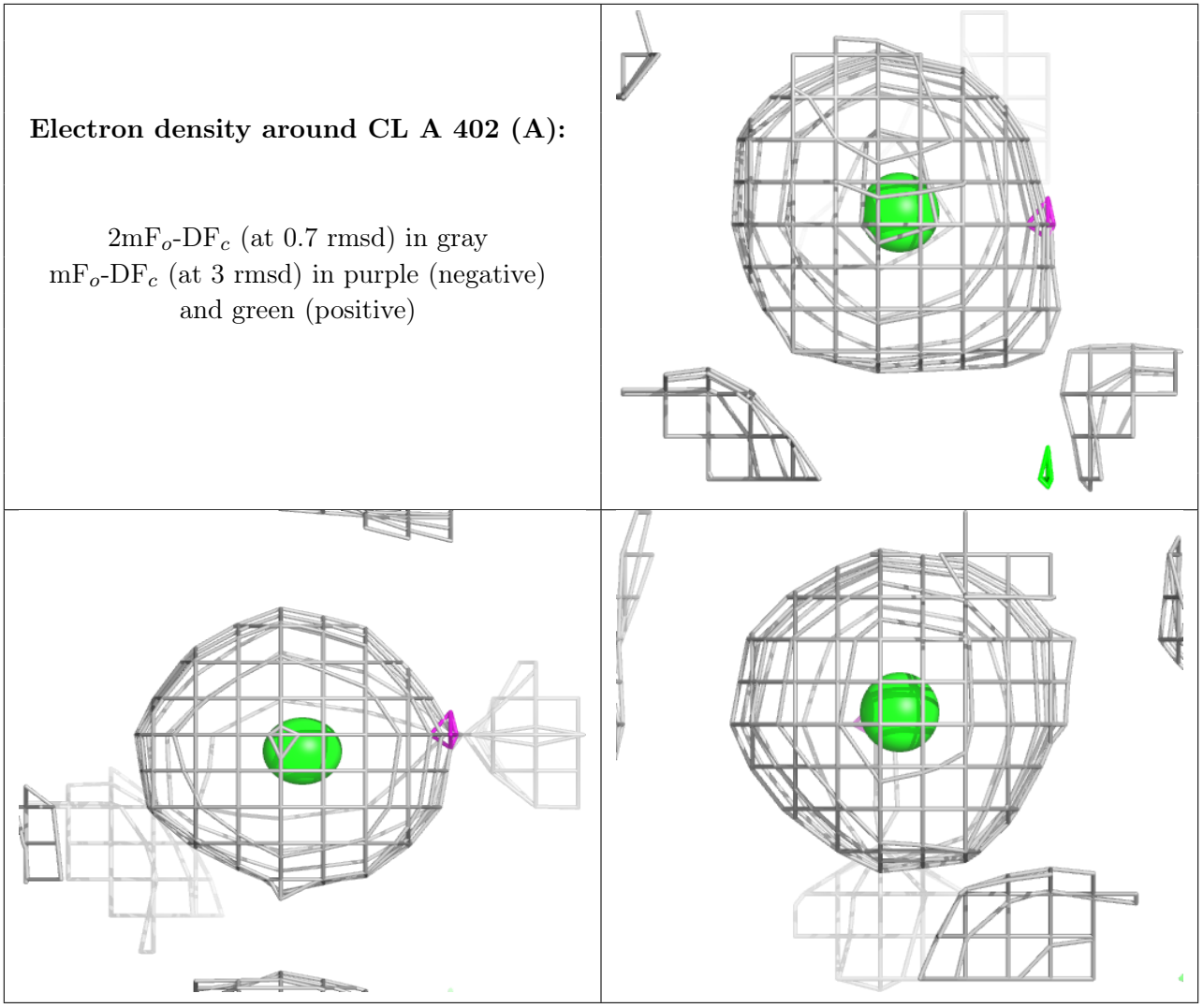
Electron density around CL a 403 (B):

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



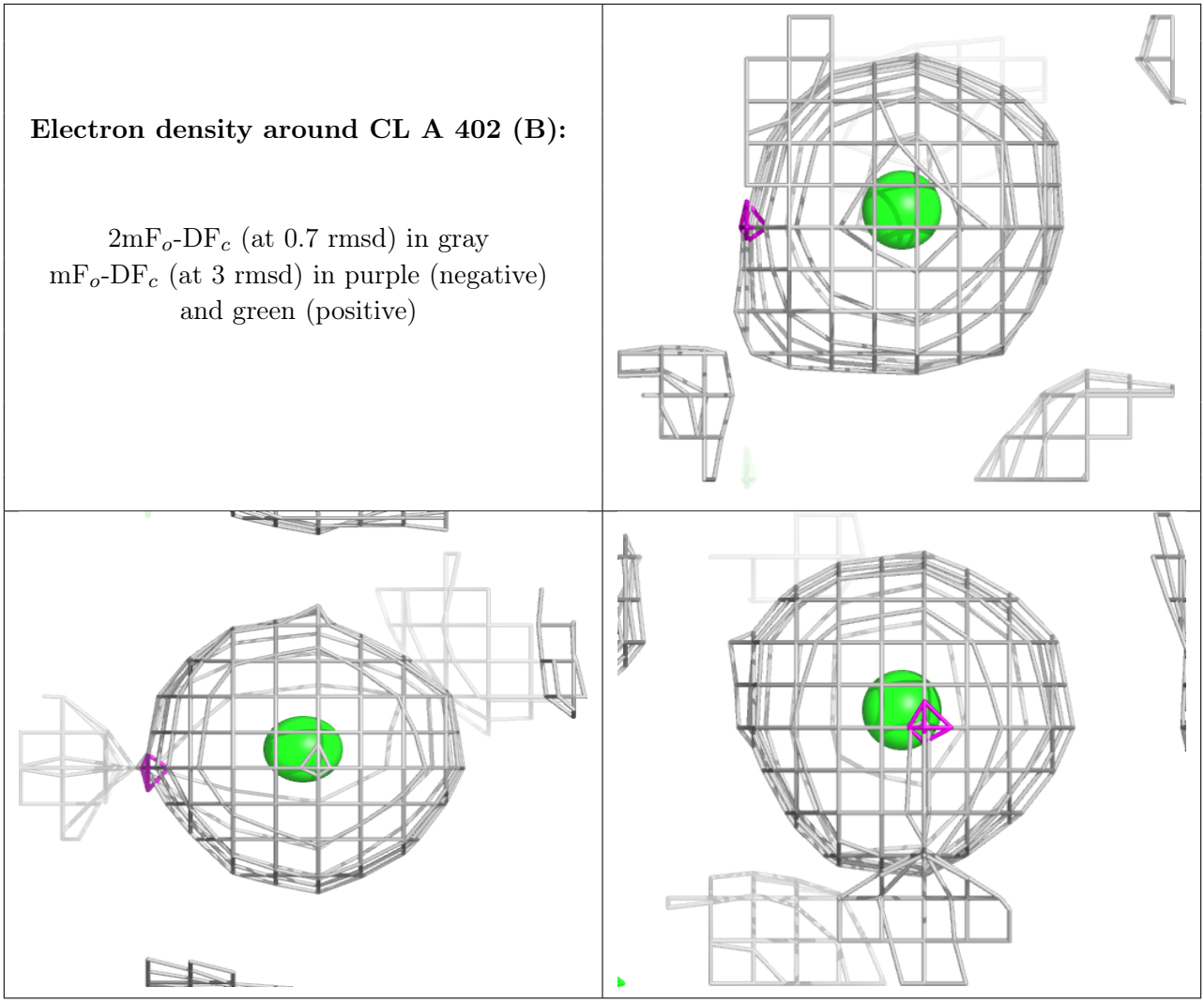
Electron density around CL A 402 (A):

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



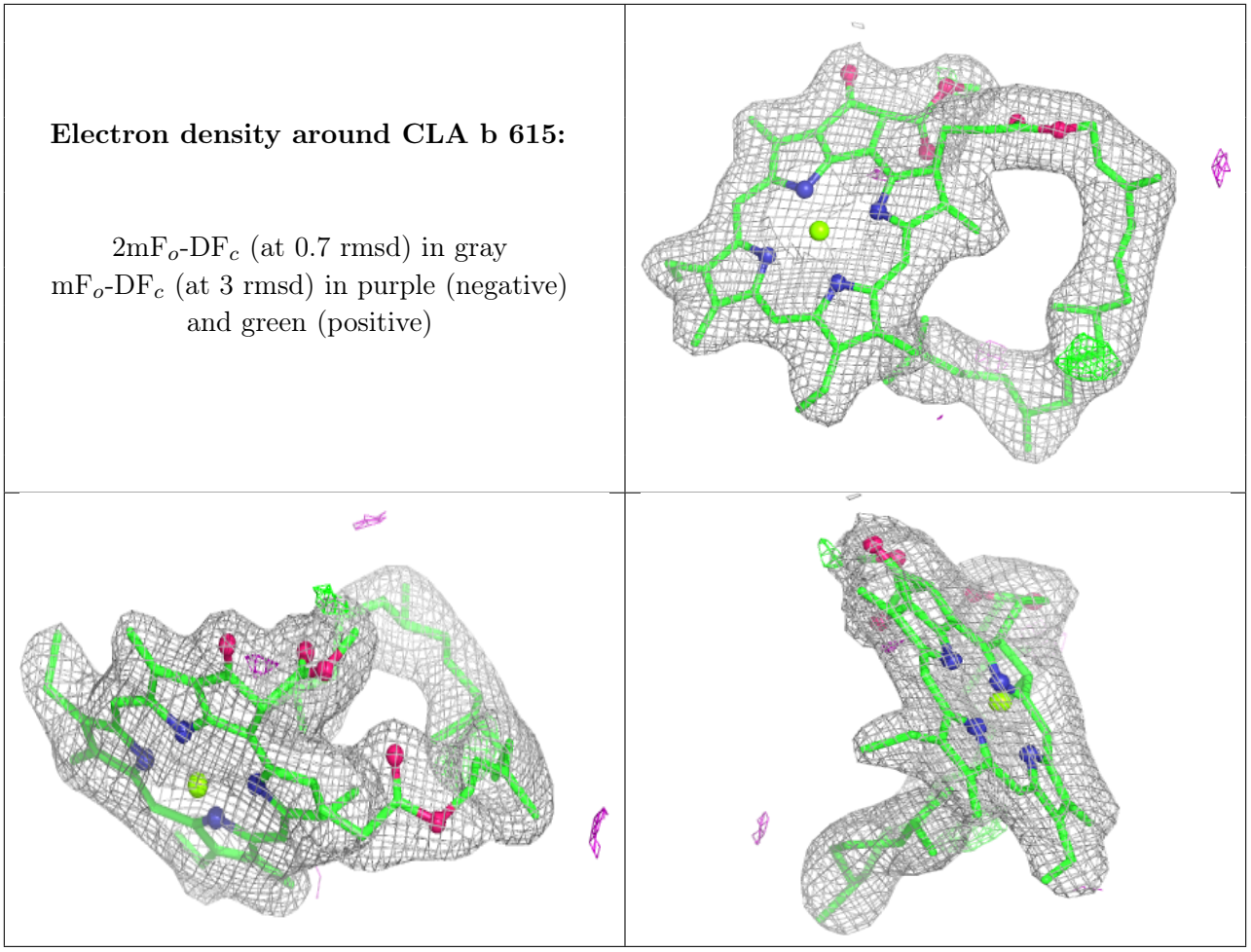
Electron density around CL A 402 (B):

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



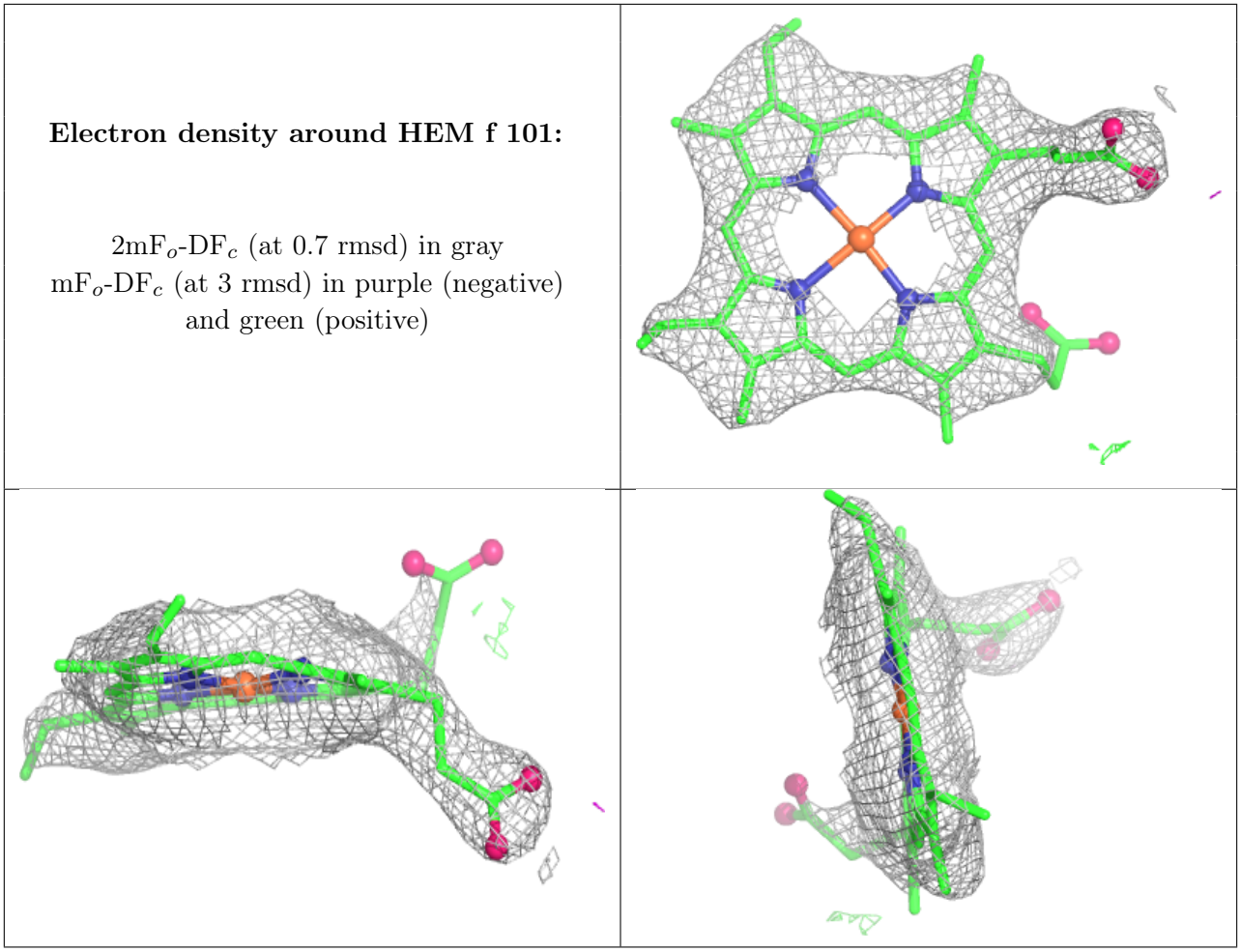
Electron density around CLA b 615:

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



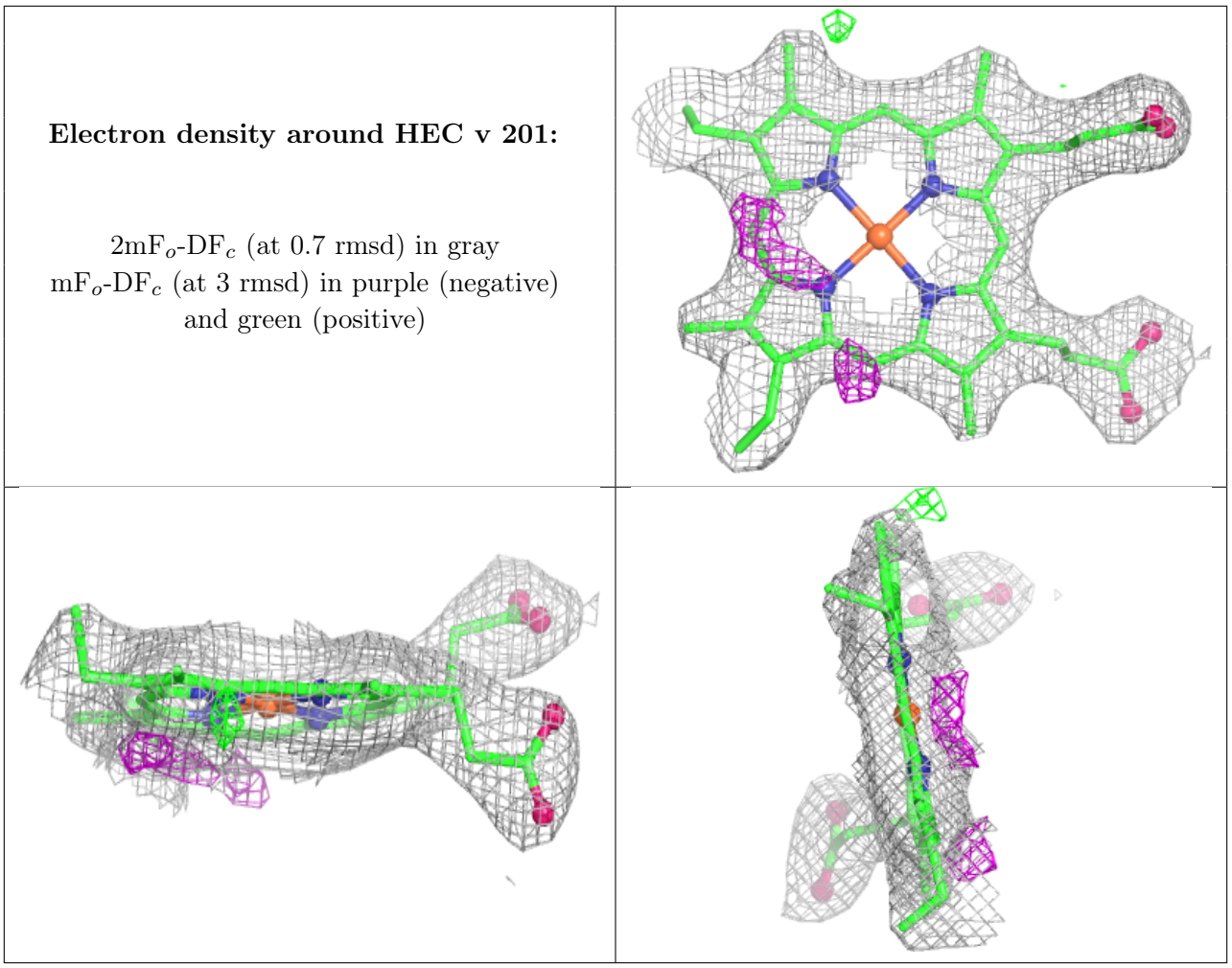
Electron density around HEM f 101:

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



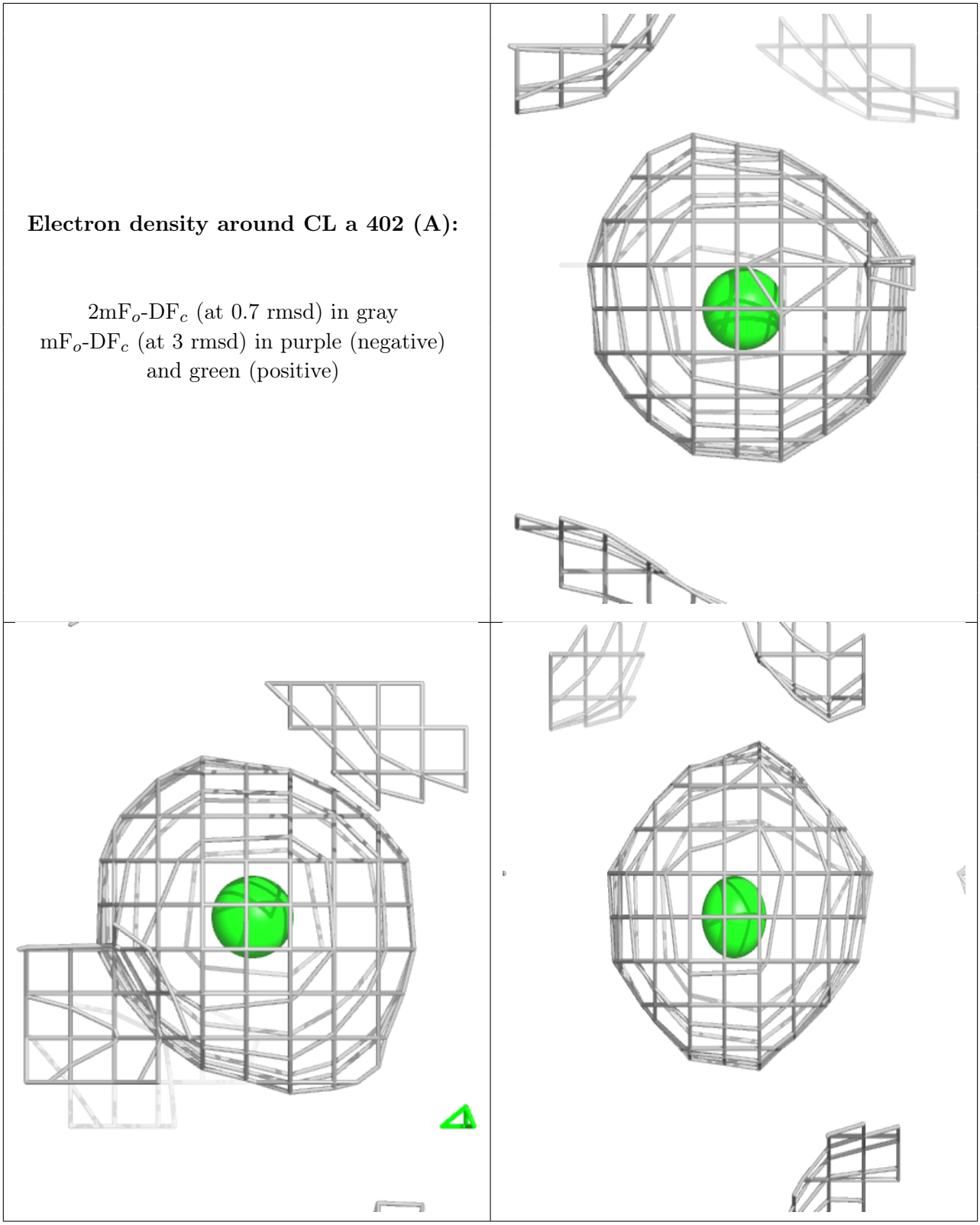
Electron density around HEC v 201:

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



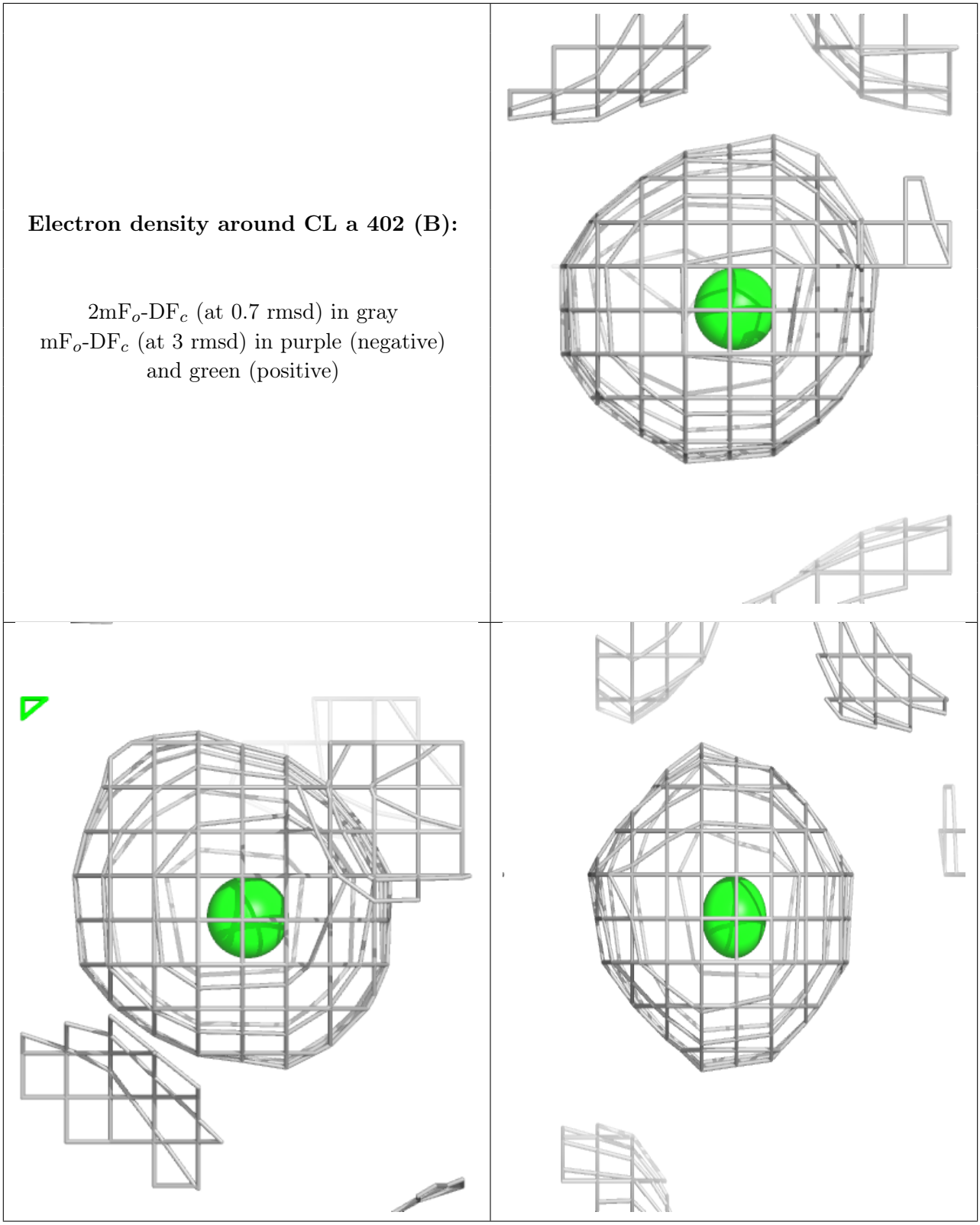
Electron density around CL a 402 (A):

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



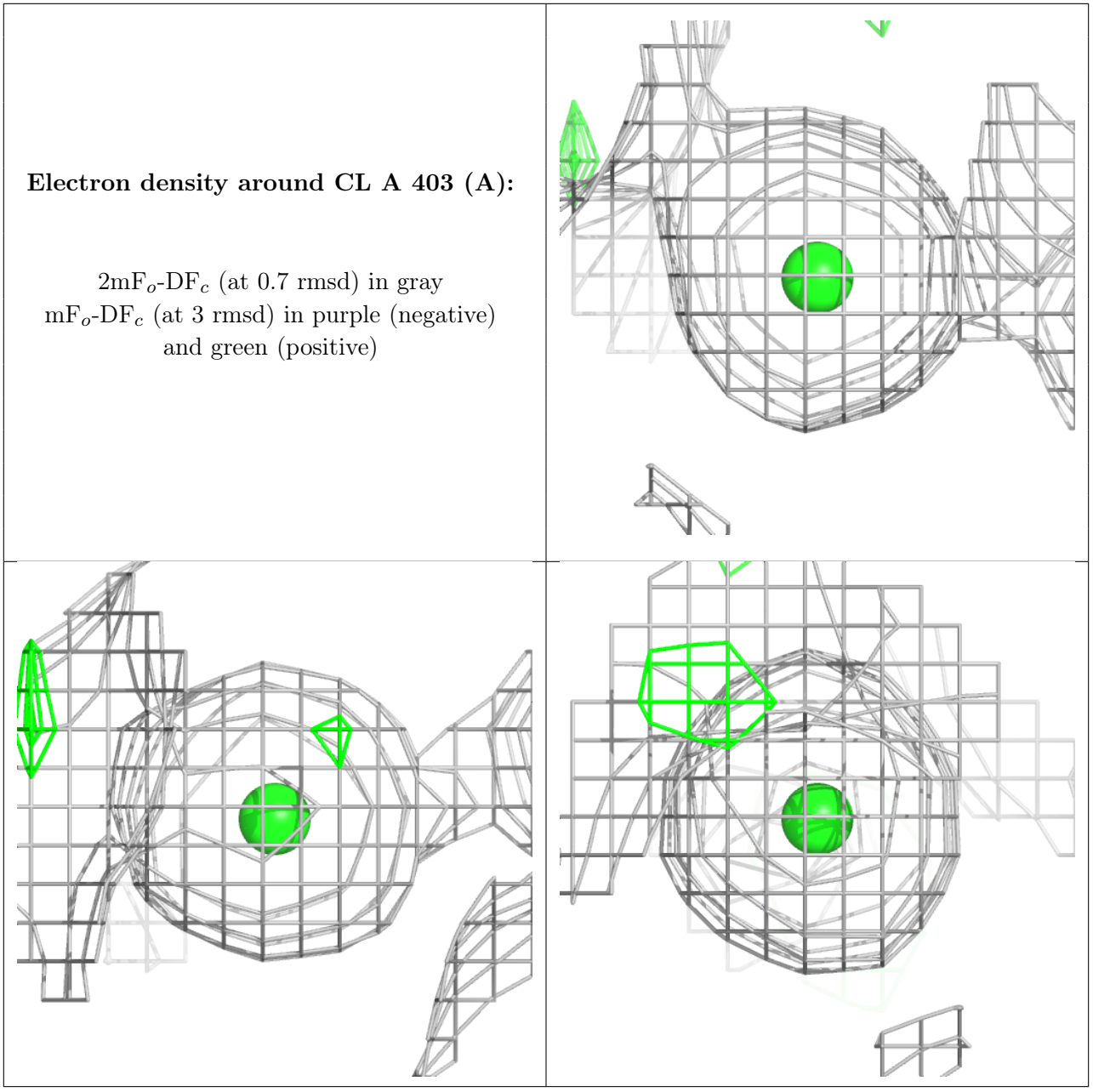
Electron density around CL a 402 (B):

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



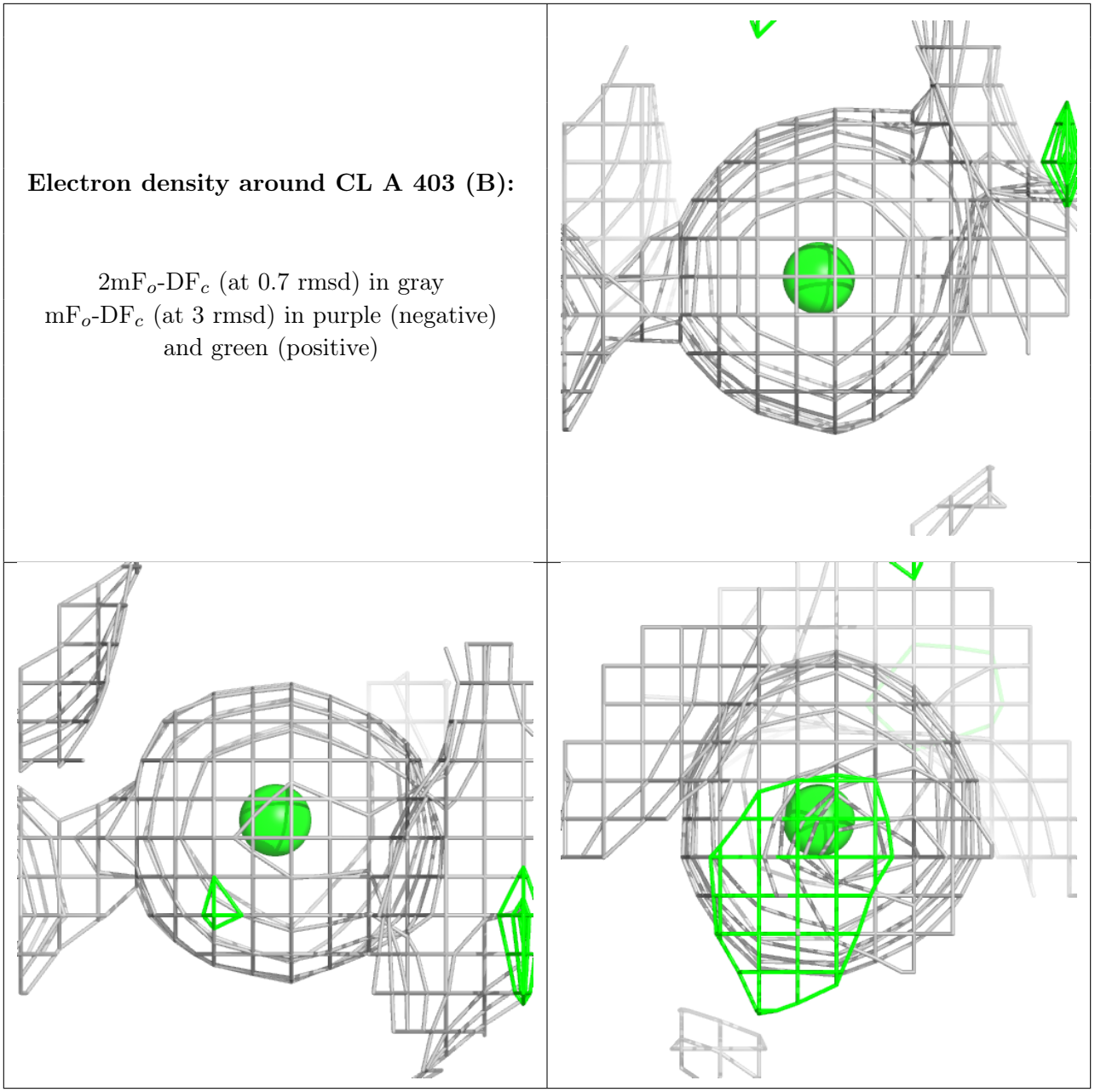
Electron density around CL A 403 (A):

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



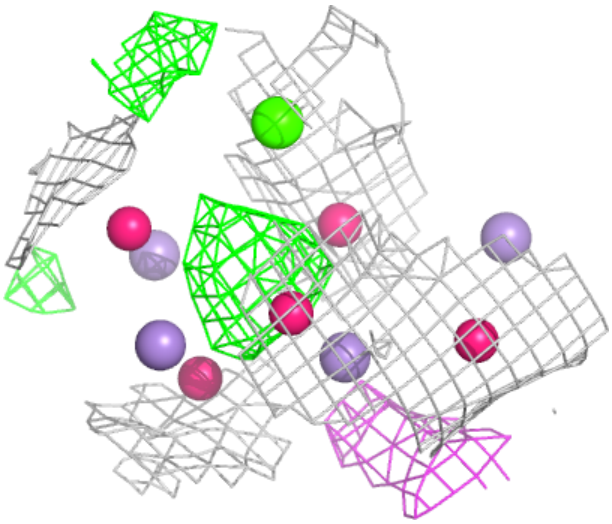
Electron density around CL A 403 (B):

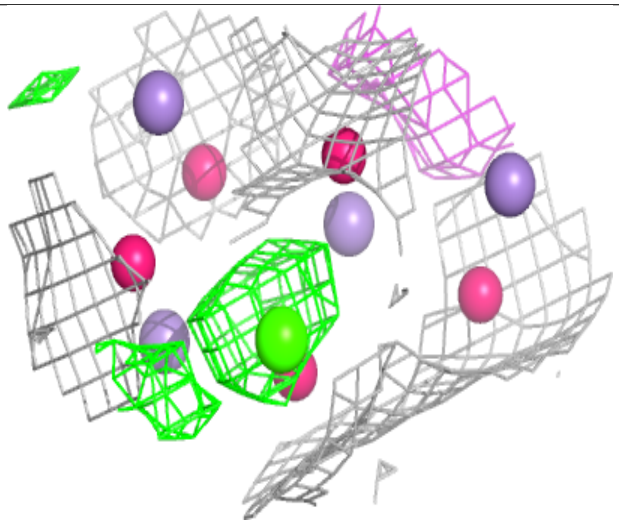
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

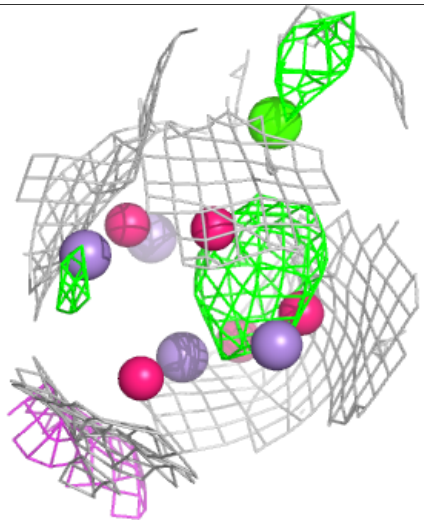


Electron density around OEX A 413 (A):

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

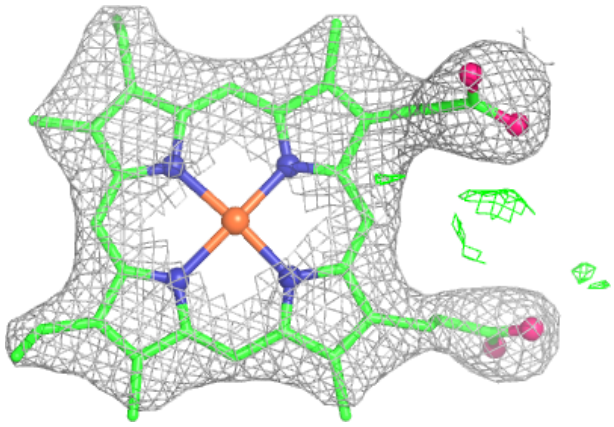


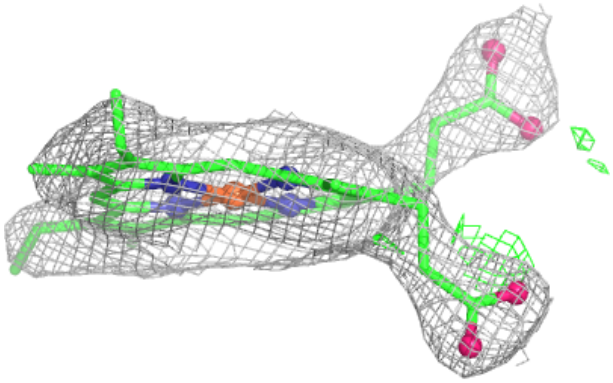


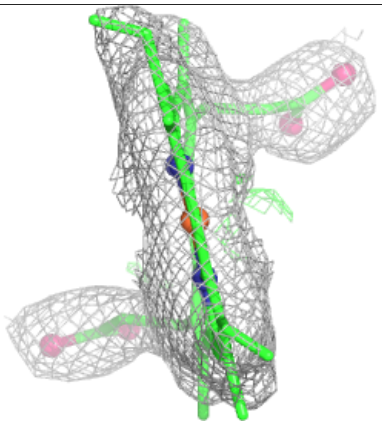


Electron density around HEM E 102:

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

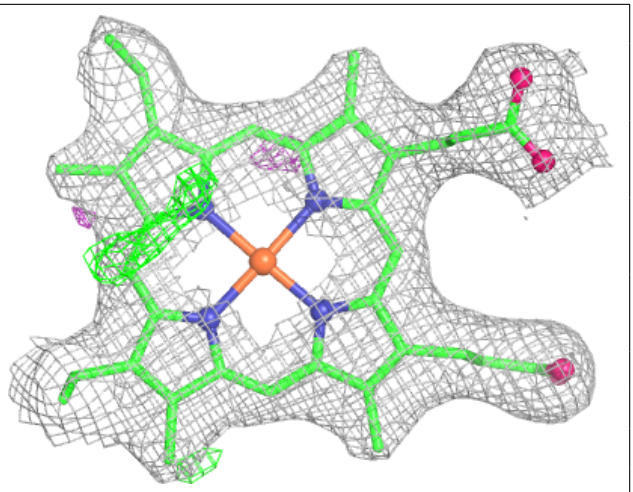


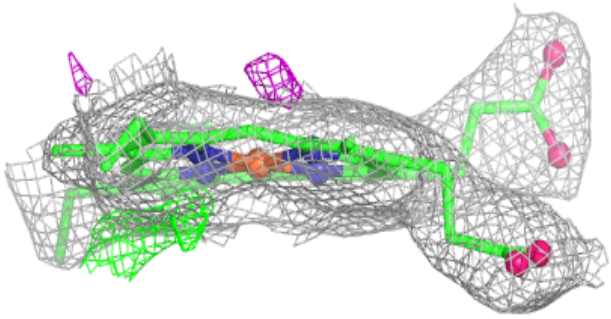




Electron density around HEC V 201:

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

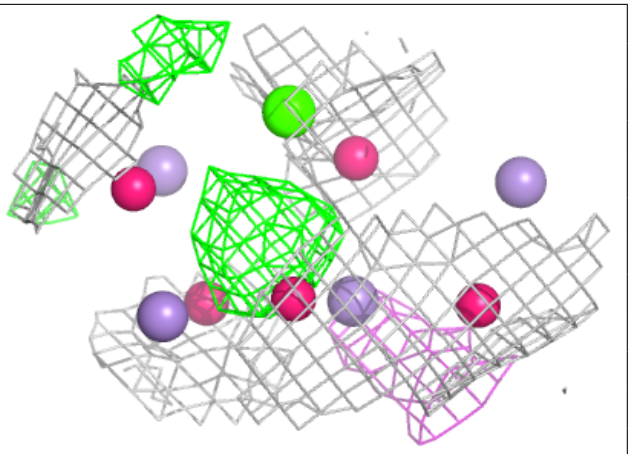


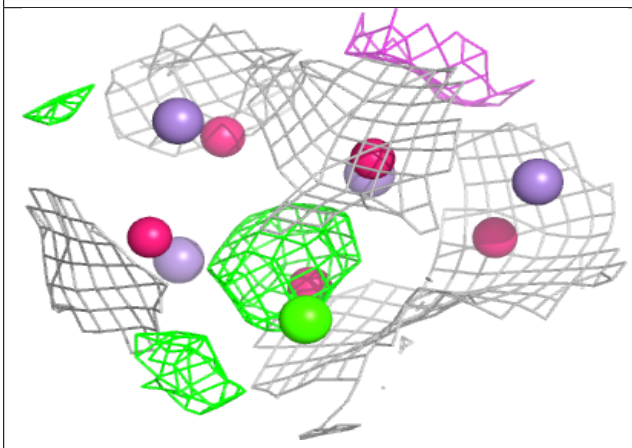


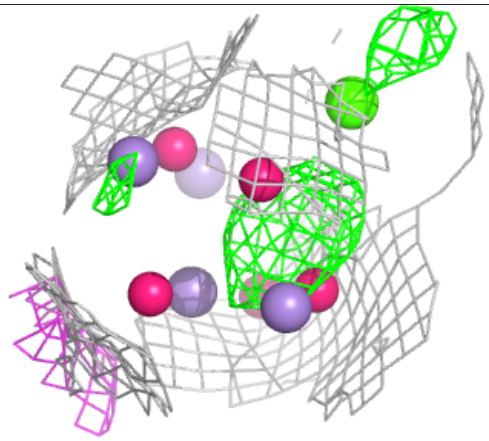


Electron density around OEX A 413 (B):

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

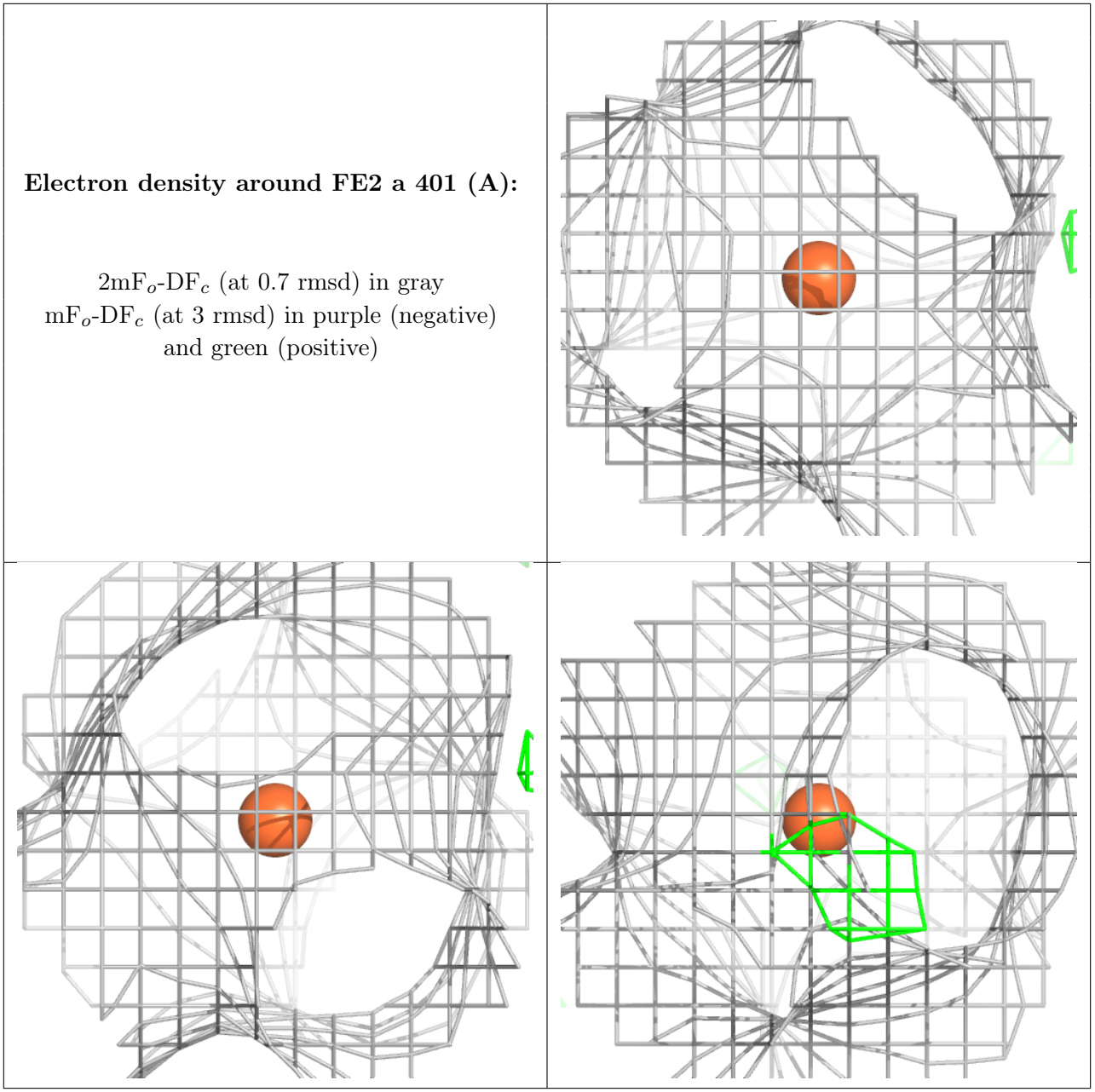






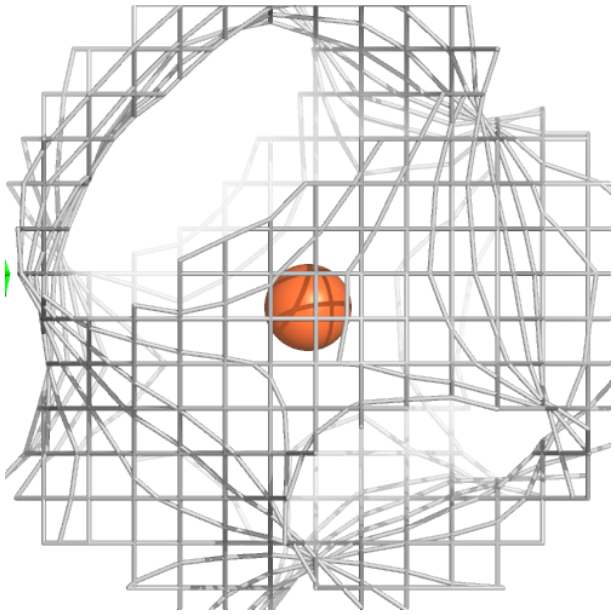
Electron density around FE2 a 401 (A):

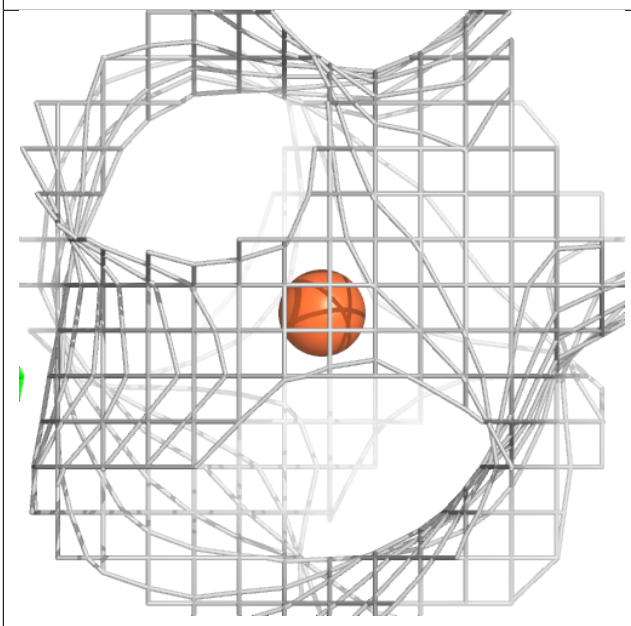
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

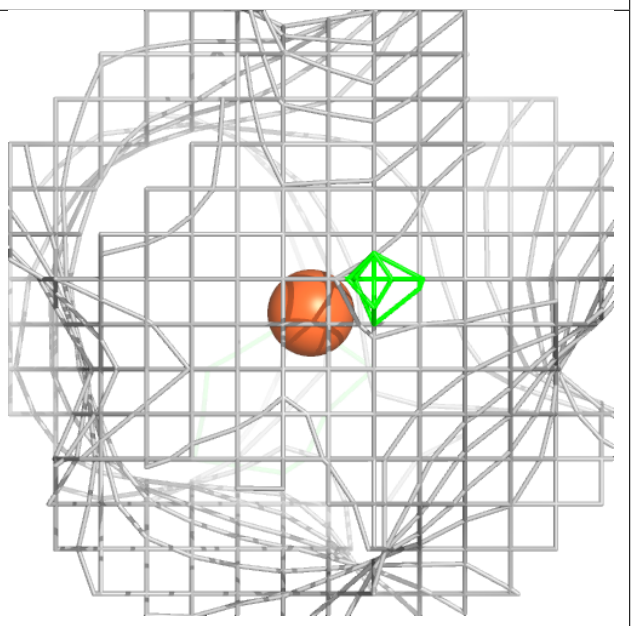


Electron density around FE2 a 401 (B):

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

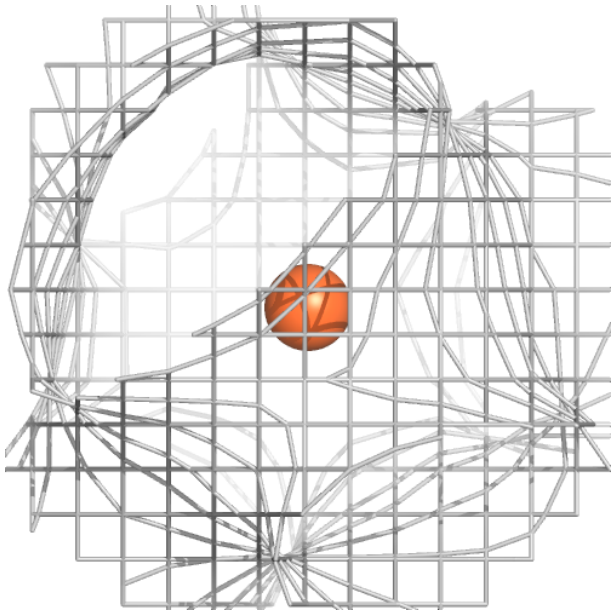


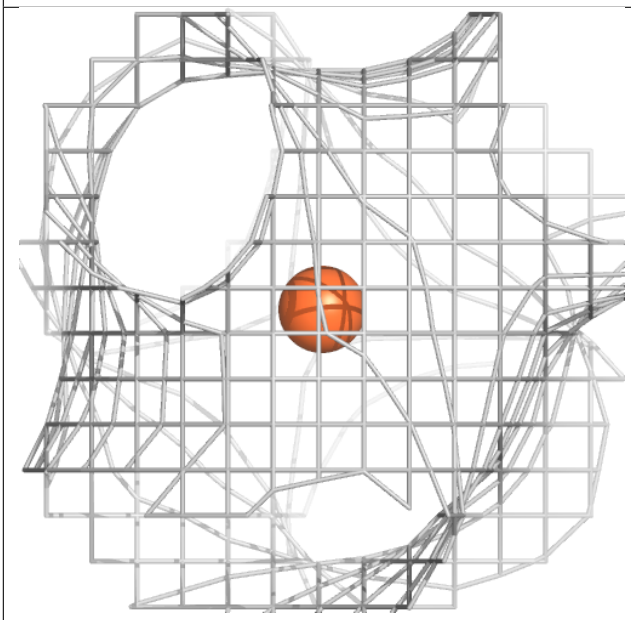


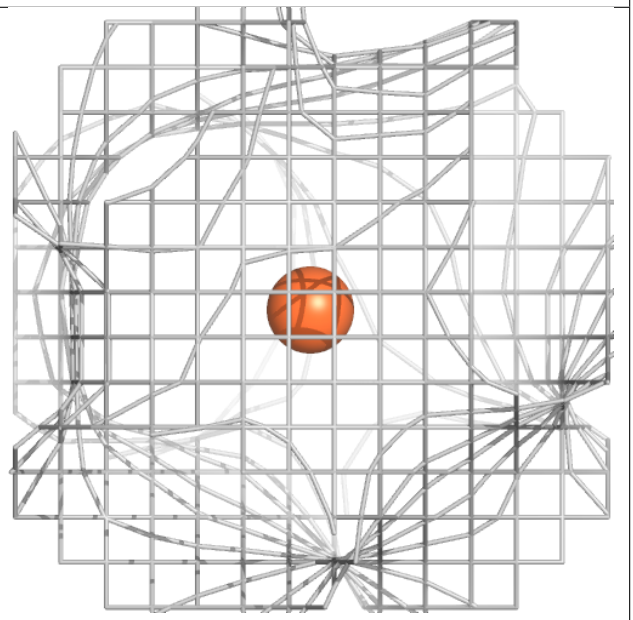


Electron density around FE2 A 401 (A):

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

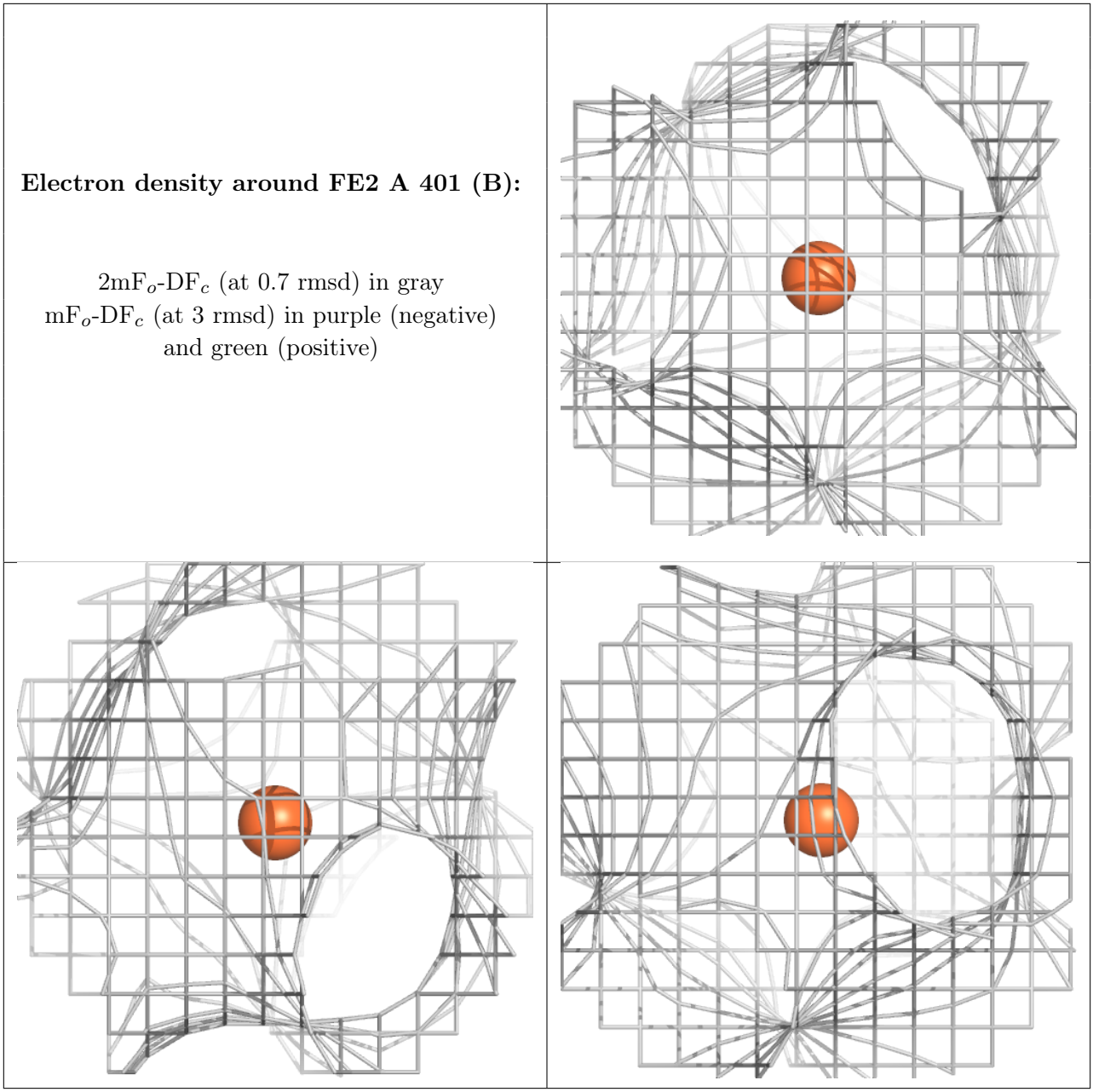






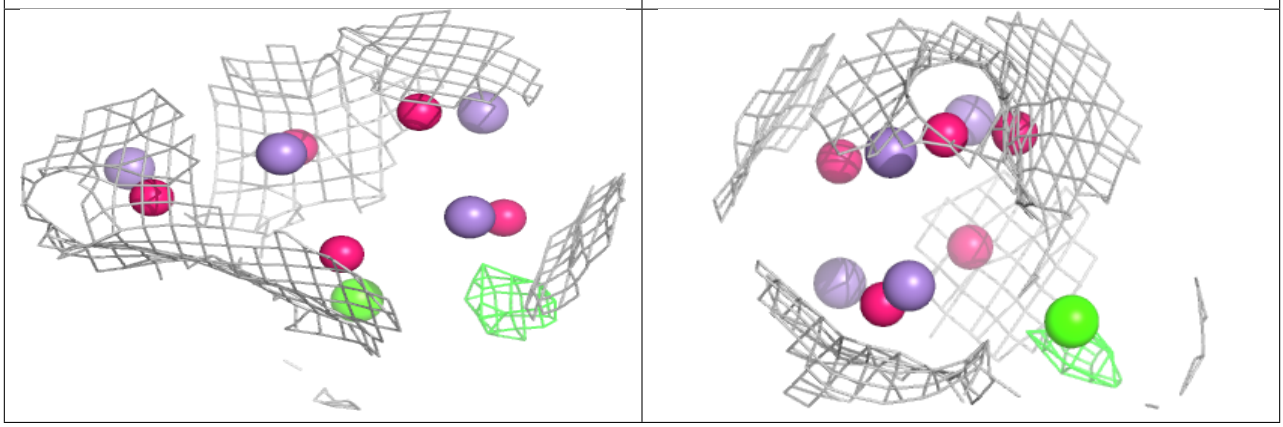
Electron density around FE2 A 401 (B):

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



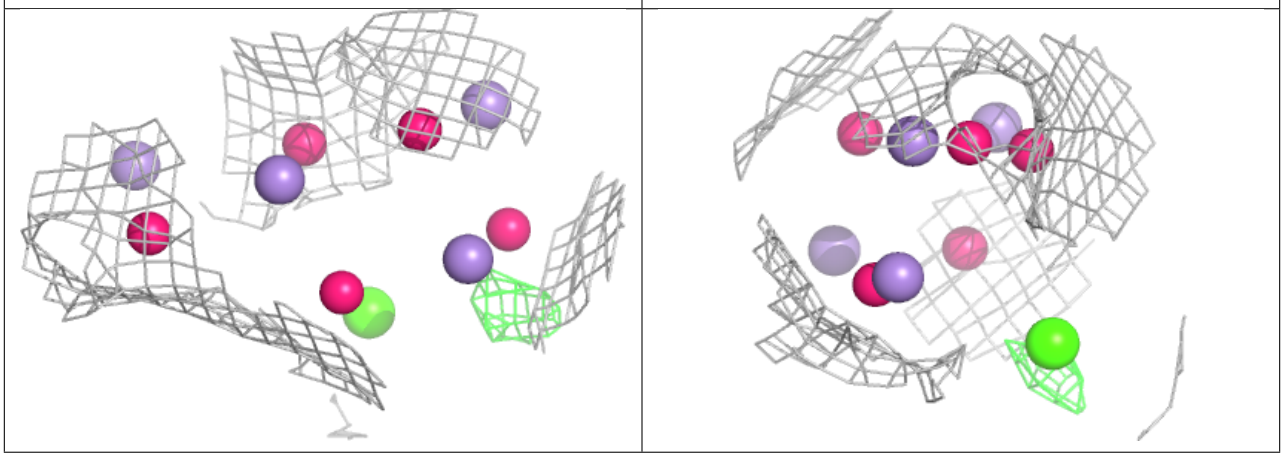
Electron density around OEX a 411 (A):

$2mF_o$-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)



6.5 Other polymers (i)

There are no such residues in this entry.