Full wwPDB X-ray Structure Validation Report ⓘ

Aug 13, 2026 – 07:20 PM JST

PDB ID	:	8IRE / pdb_00008ire
Title	:	XFEL structure of cyanobacterial photosystem II following two flashes (2F) with a 200-nanosecond delay
Authors	:	Li, H.; Suga, M.; Shen, J.R.
Deposited on	:	2023-03-17
Resolution	:	2.25 Å(reported)

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

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

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

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

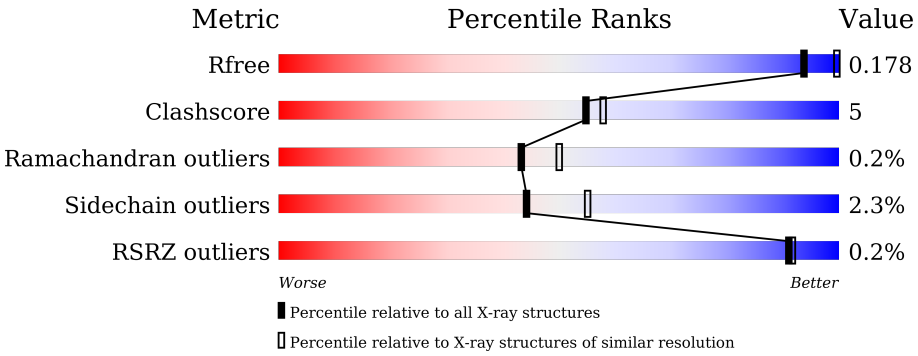
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	344	91% 6% ·
1	a	344	88% 9% ·
2	B	505	93% 7%
2	b	505	91% 8% ·
3	C	455	91% 8% ·
3	c	455	92% 7% ·

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Mol	Chain	Length	Quality of chain
4	D	342	90% 10%
4	d	342	90% 10%
5	E	84	% 81% 15%
5	e	84	% 86% 8% 6%
6	F	44	66% 11% 23%
6	f	44	2% 64% 7% 30%
7	H	65	2% 94% 5%
7	h	65	85% 14%
8	I	38	76% 21%
8	i	38	3% 89% 11%
9	J	39	82% 13%
9	j	39	87% 13%
10	K	37	76% 19% 5%
10	k	37	81% 14% 5%
11	L	37	92% 5%
11	l	37	81% 16%
12	M	36	72% 14% 6% 8%
12	m	36	75% 17% 6%
13	O	244	86% 14%
13	o	244	91% 8%
14	T	32	78% 16% 6%
14	t	32	81% 12% 6%
15	U	104	81% 12% 8%
15	u	104	88% 7%
16	V	137	96%

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Mol	Chain	Length	Quality of chain
16	v	137	92% 8%
17	X	40	88% 8% 5%
17	x	40	92% 5%
18	Y	30	3% 87% 10%
18	y	30	57% 40%
19	Z	62	87% 11%
19	z	62	77% 21%
20	R	34	3% 71% 26%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	GOL	A	701	-	-	X	-
27	GOL	D	701	-	X	-	-
27	GOL	a	801	-	-	X	-
40	HEC	V	202	X	-	-	-
40	HEC	v	202	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 62600 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	221	0
			4330	2830	716	759	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	20	0
			4146	2721	692	720	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	97	0
			4260	2788	713	741	18			
3	c	455	Total	C	N	O	S	0	100	0
			4308	2821	719	750	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	114	0
			3620	2387	596	622	15			
4	d	341	Total	C	N	O	S	0	116	0
			3628	2391	599	623	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	4	0
			807	513	134	160			

- 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).

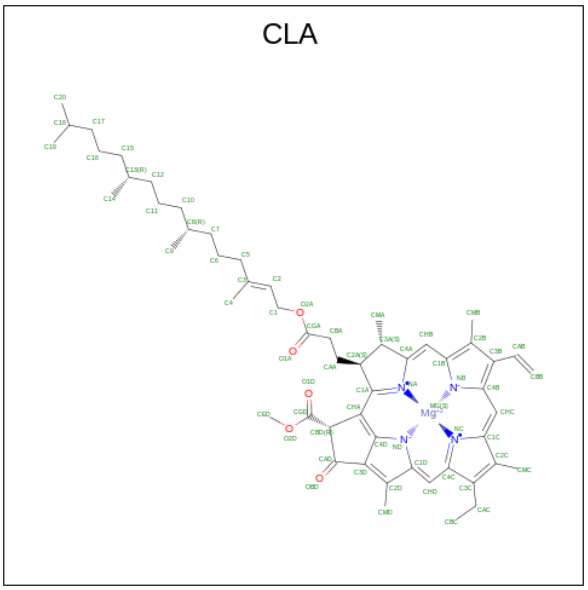
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total 4	Cl 4	0	2

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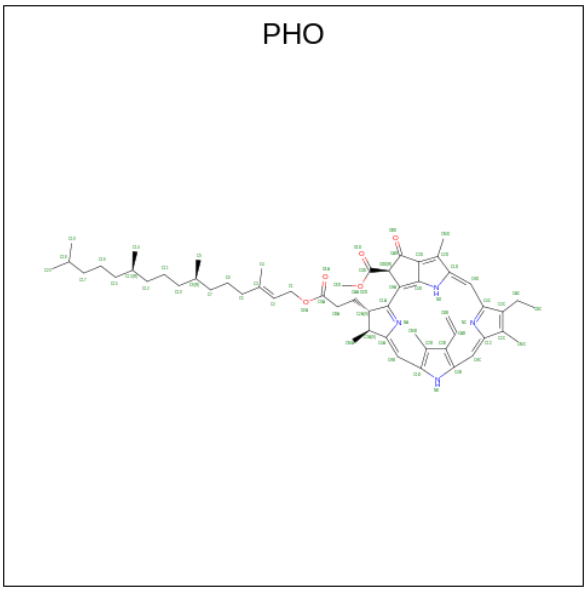
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	D	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	a	1	Total	C	Mg	N	O	0	1
			130	110	2	8	10		
23	a	1	Total	C	Mg	N	O	0	1
			130	110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

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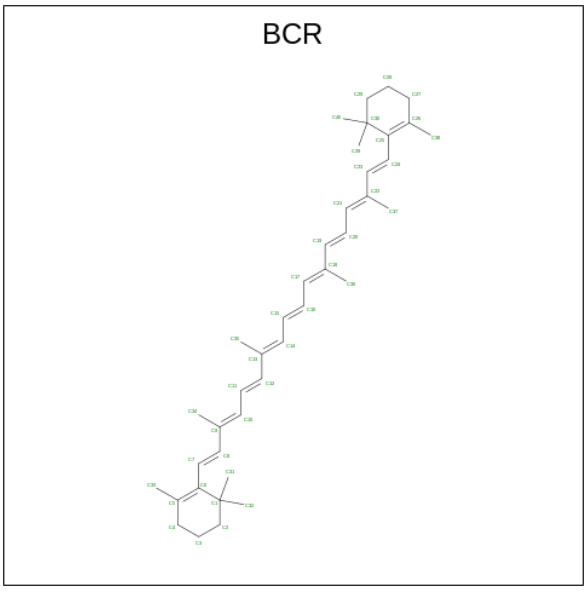
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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



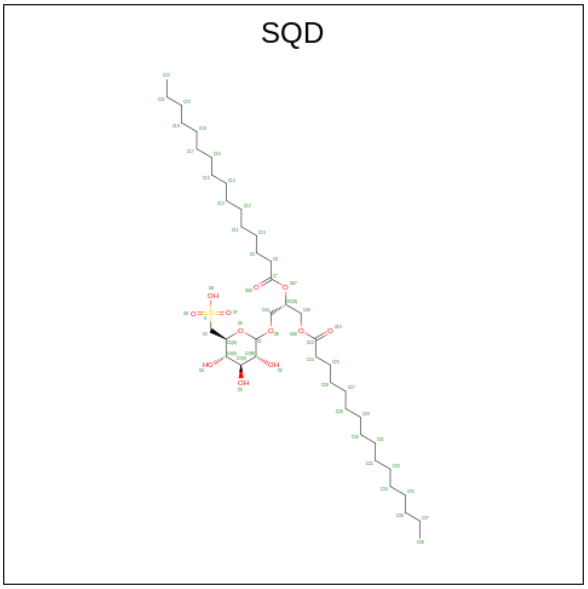
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	A	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		
24	a	1	Total	C	N	O	0	1
			128	110	8	10		

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



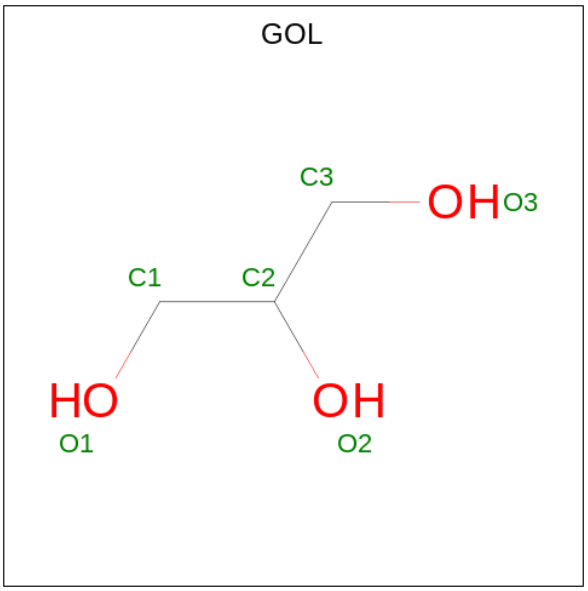
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	H	1	Total C 40 40	0	0
25	K	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total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

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



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

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



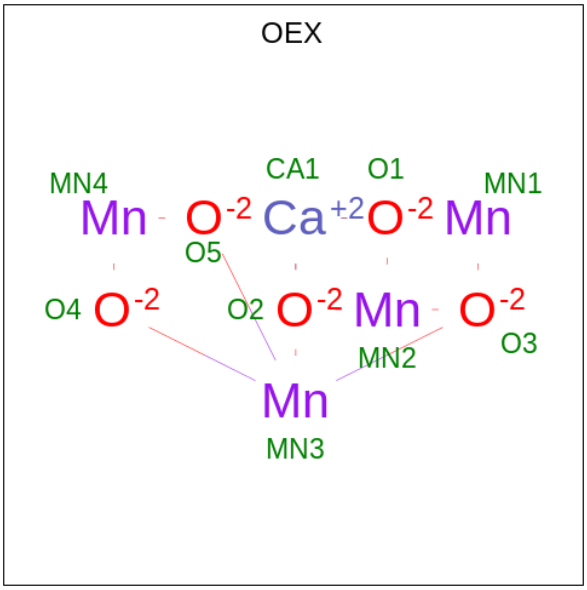
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			6	3	3		
27	A	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	B	1	Total	C	O	0	0
			6	3	3		
27	C	1	Total	C	O	0	1
			12	6	6		
27	D	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27	O	1	Total	C	O	0	0
			6	3	3		
27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

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

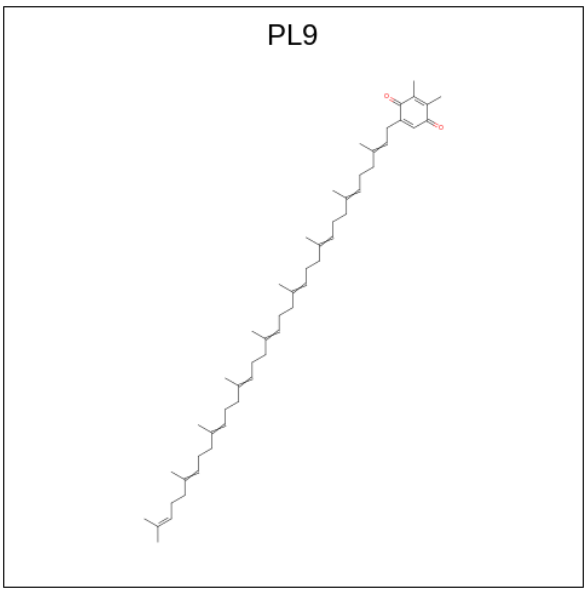
- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$) (labeled as "Ligand of Interest" by depositor).



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:).

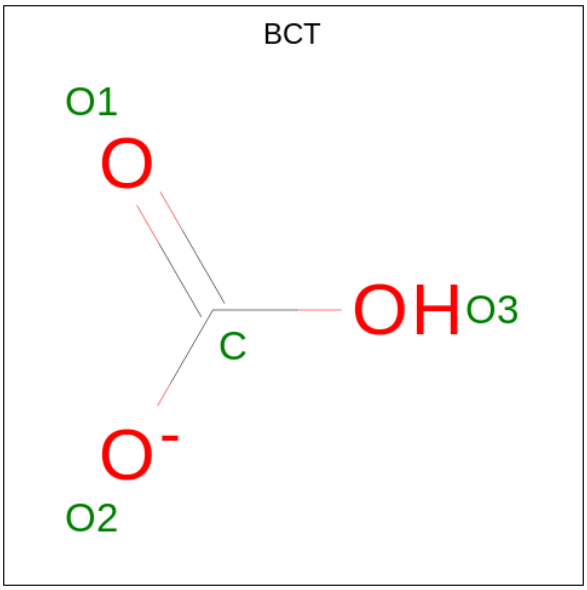
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	A	1	Total C O 28 23 5	0	0
30	B	1	Total C O 33 28 5	0	0
30	D	2	Total C O 57 51 6	0	0
30	I	1	Total C O 40 35 5	0	0
30	J	1	Total C 10 10	0	0
30	K	1	Total C O 68 58 10	0	1
30	M	1	Total C 10 10	0	0

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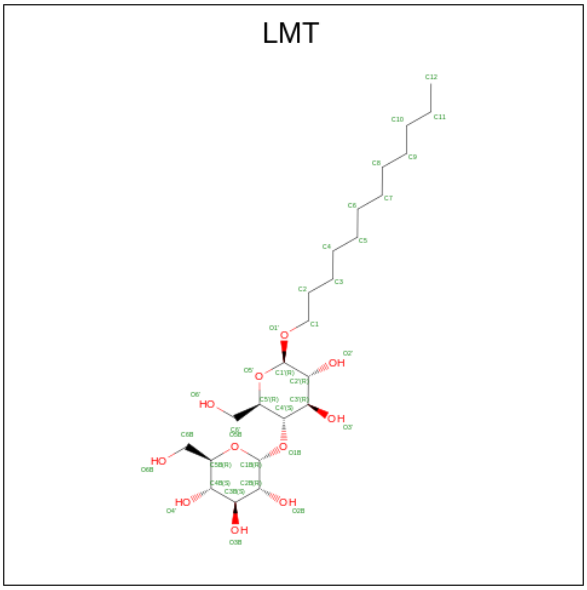
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	1	Total C O 18 16 2	0	0
30	a	1	Total C O 30 25 5	0	0
30	b	1	Total C O 33 28 5	0	0
30	c	1	Total C O 64 54 10	0	1
30	d	2	Total C O 53 47 6	0	0
30	i	1	Total C O 40 35 5	0	0
30	j	1	Total C 10 10	0	0
30	m	1	Total C 10 10	0	0
30	x	1	Total C O 18 16 2	0	0

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 8 2 6	0	1
31	a	1	Total C O 8 2 6	0	1

- Molecule 32 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



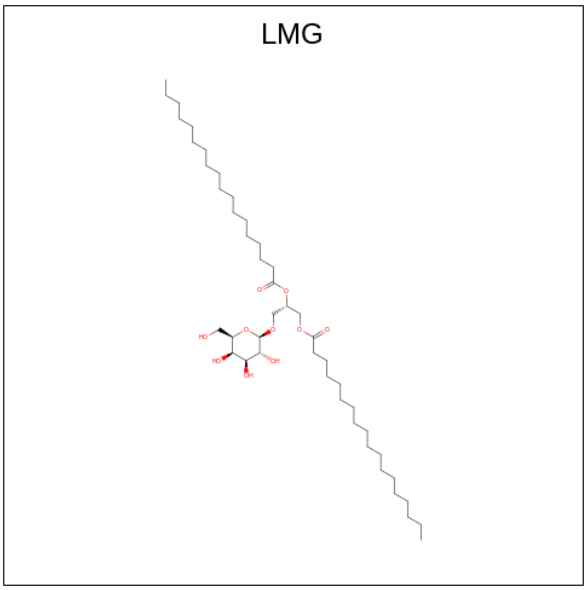
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 35 24 11	0	0
32	D	1	Total C O 35 24 11	0	0
32	E	1	Total C O 35 24 11	0	0
32	I	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	M	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	a	1	Total C O 35 24 11	0	0
32	b	1	Total C O 25 19 6	0	0
32	b	1	Total C O 25 19 6	0	0
32	e	1	Total C O 35 24 11	0	0
32	m	1	Total C O 35 24 11	0	0
32	t	1	Total C O 25 19 6	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	t	1	Total C O 26 19 7	0	0

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



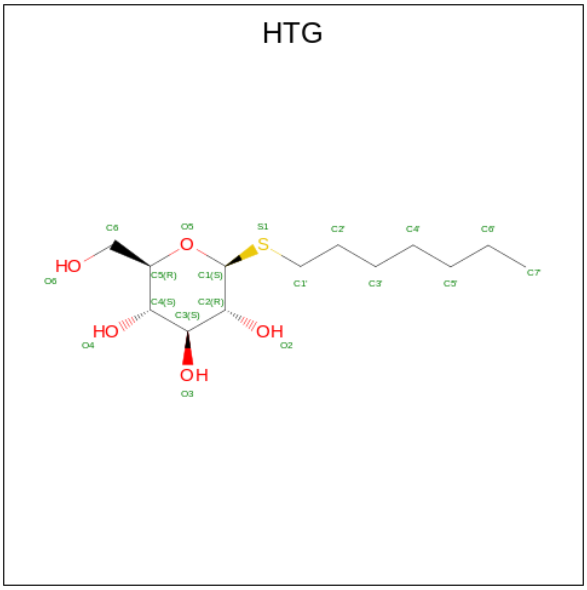
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	C	1	Total C O 51 41 10	0	0
33	D	1	Total C O 51 41 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	m	1	Total C O 51 41 10	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	Z	1	Total C O 37 27 10	0	0
33	z	1	Total C O 39 29 10	0	0

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



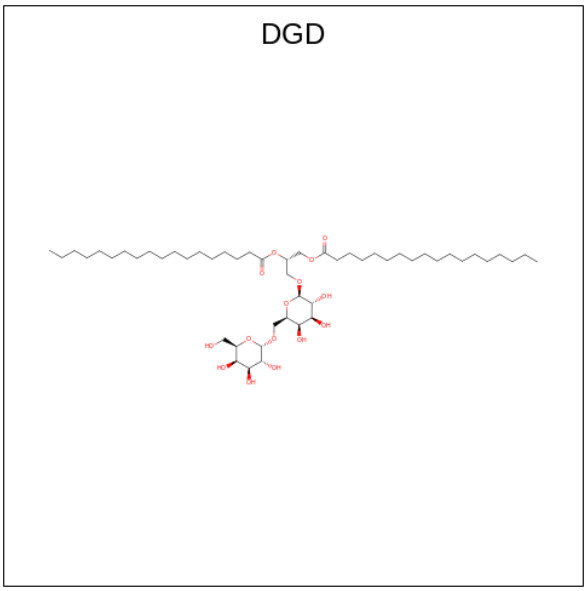
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	B	1	Total C O S 19 13 5 1	0	0
34	C	1	Total C O S 19 13 5 1	0	0
34	D	1	Total C O S 16 10 5 1	0	0
34	V	1	Total C O 11 6 5	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34	b	1	Total C O S 19 13 5 1	0	0
34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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	c	1	Total C O S 19 13 5 1	0	0
34	d	1	Total C O S 16 10 5 1	0	0

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

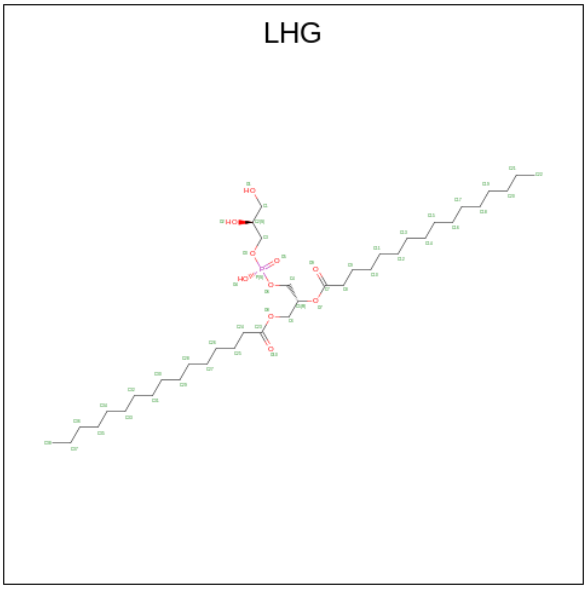


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 124 94 30	0	1
35	C	1	Total C O 62 47 15	0	0
35	H	1	Total C O 62 47 15	0	0
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 124 94 30	0	1
35	c	1	Total C O 62 47 15	0	0
35	h	1	Total C O 62 47 15	0	0

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

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

- Molecule 37 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



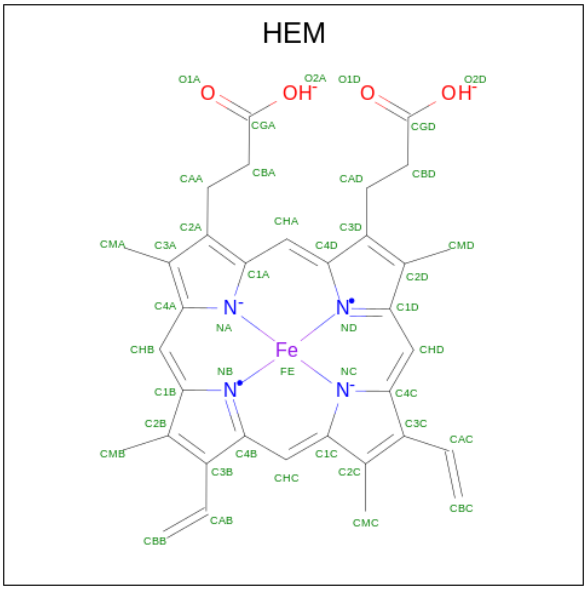
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 98 76 20 2	0	1
37	D	1	Total C O P 98 76 20 2	0	1
37	D	1	Total C O P 98 76 20 2	0	1
37	E	1	Total C O P 84 62 20 2	0	1
37	L	1	Total C O P 98 76 20 2	0	1

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	d	1	Total C O P 98 76 20 2	0	1
37	d	1	Total C O P 98 76 20 2	0	1
37	d	1	Total C O P 98 76 20 2	0	1
37	e	1	Total C O P 84 62 20 2	0	1
37	l	1	Total C O P 98 76 20 2	0	1

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

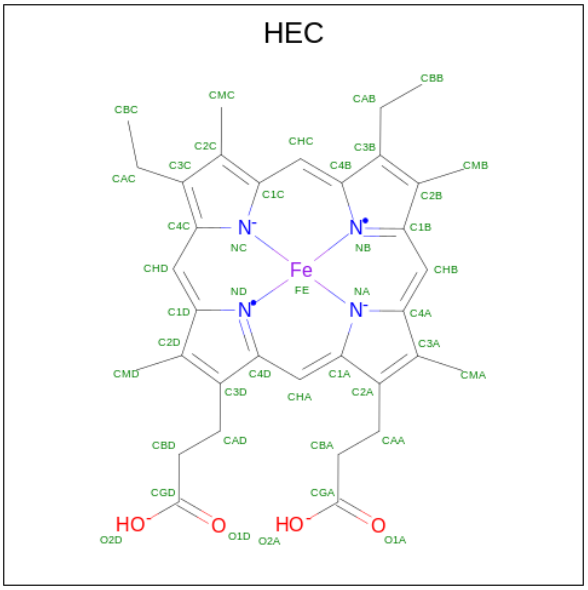


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	E	1	Total C Fe N O 43 34 1 4 4	0	0
38	e	1	Total C Fe N O 43 34 1 4 4	0	0

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

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

- 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	126	Total	O	0	80
			206	206		
41	B	164	Total	O	0	2
			166	166		
41	C	141	Total	O	0	33
			174	174		
41	D	118	Total	O	0	32
			150	150		
41	E	14	Total	O	0	0
			14	14		
41	F	3	Total	O	0	0
			3	3		
41	H	17	Total	O	0	0
			17	17		
41	I	6	Total	O	0	0
			6	6		
41	J	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	K	5	Total O 5 5	0	0
41	L	3	Total O 3 3	0	0
41	M	5	Total O 5 5	0	0
41	O	70	Total O 73 73	0	3
41	T	8	Total O 10 10	0	2
41	U	32	Total O 32 32	0	0
41	V	65	Total O 69 69	0	4
41	X	1	Total O 1 1	0	0
41	a	128	Total O 208 208	0	81
41	b	182	Total O 184 184	0	2
41	c	133	Total O 163 163	0	30
41	d	109	Total O 140 140	0	31
41	e	8	Total O 8 8	0	0
41	f	3	Total O 3 3	0	0
41	h	15	Total O 15 15	0	0
41	i	3	Total O 3 3	0	0
41	j	2	Total O 2 2	0	0
41	k	3	Total O 3 3	0	0
41	l	4	Total O 4 4	0	0
41	m	14	Total O 14 14	0	0
41	o	76	Total O 81 81	0	5

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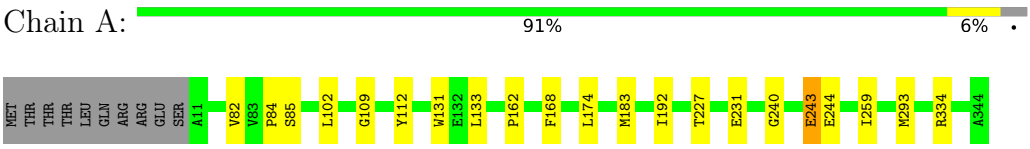
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	t	6	Total O 7 7	0	1
41	u	47	Total O 48 48	0	1
41	v	41	Total O 41 41	0	0
41	x	2	Total O 2 2	0	0
41	y	1	Total O 1 1	0	0
41	G	263	Total O 286 286	0	24

3 Residue-property plots (i)

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

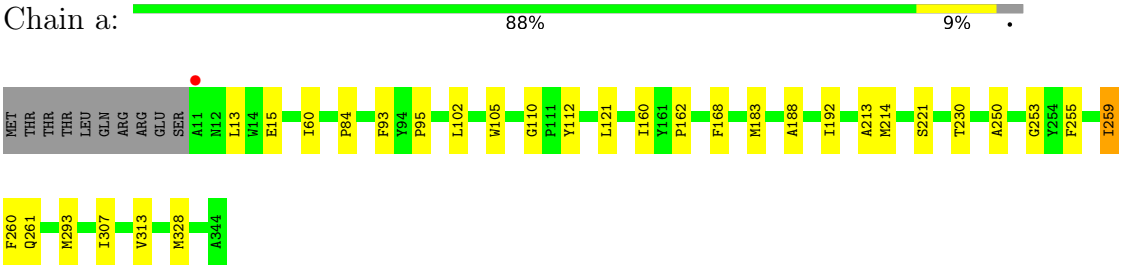
• Molecule 1: Photosystem II protein D1

Chain A:



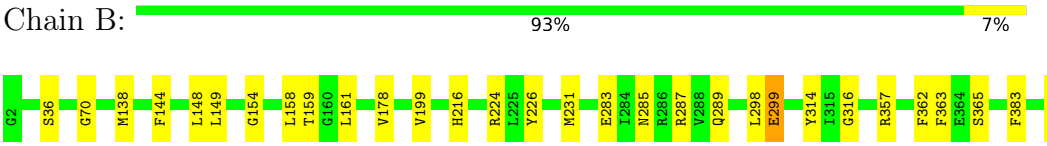
• Molecule 1: Photosystem II protein D1

Chain a:



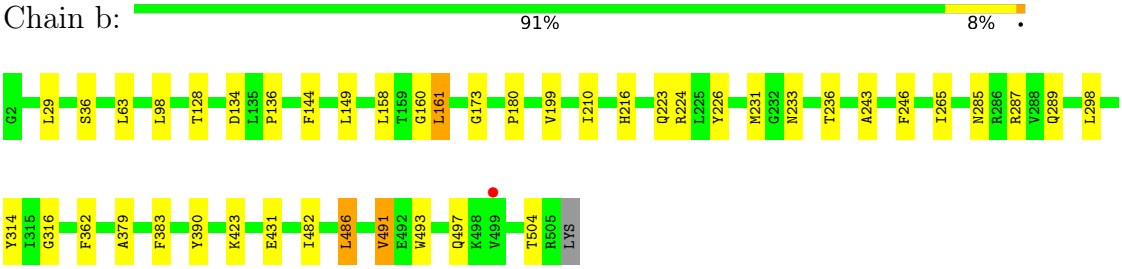
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



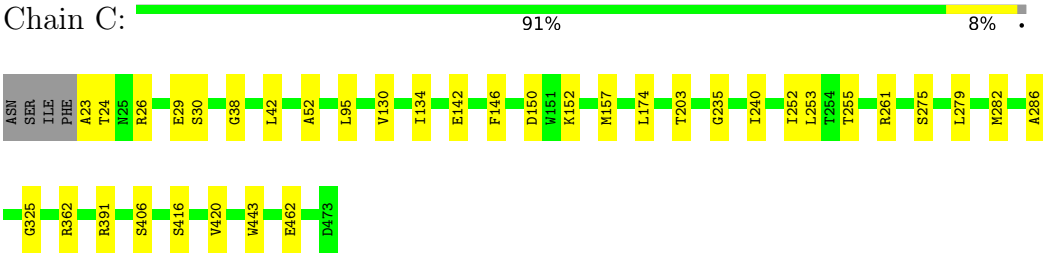
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



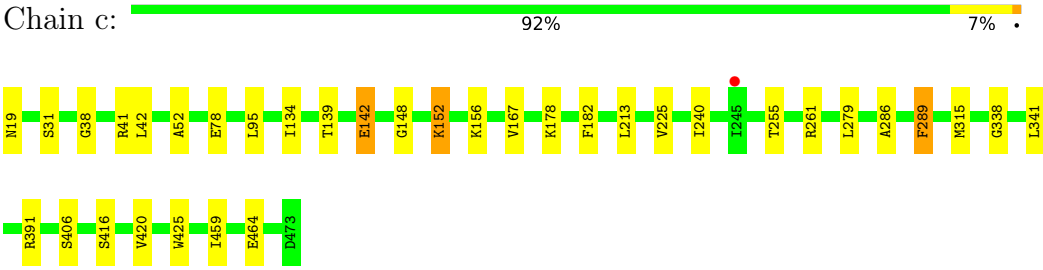
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:



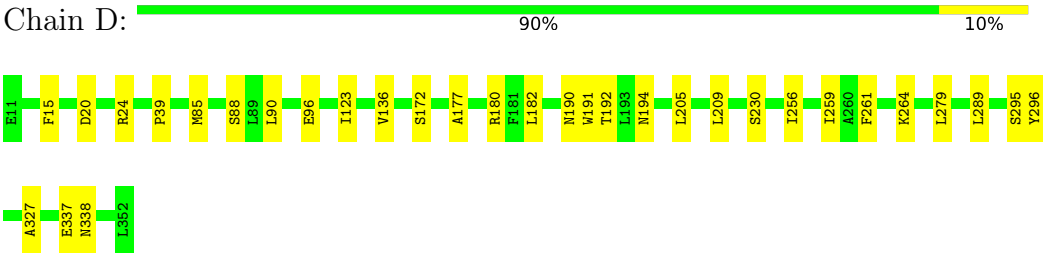
• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:



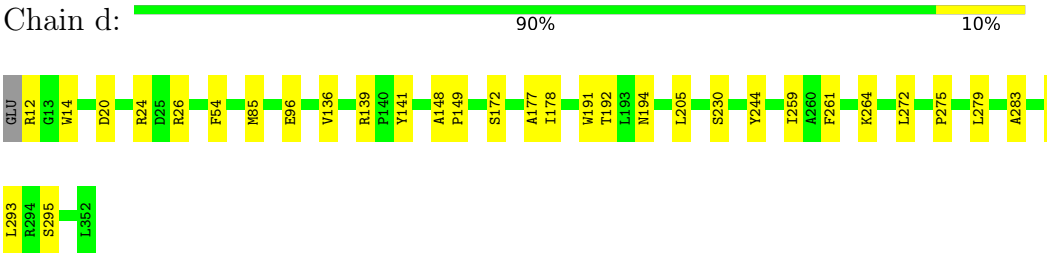
• Molecule 4: Photosystem II D2 protein

Chain D:



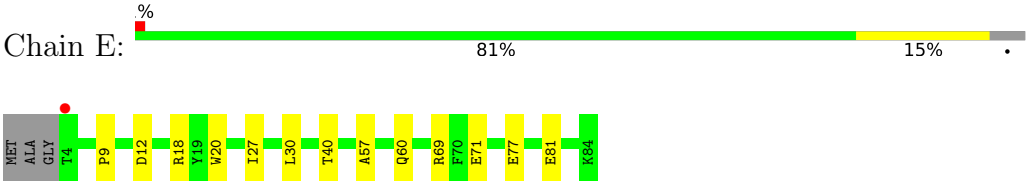
• Molecule 4: Photosystem II D2 protein

Chain d:



• Molecule 5: Cytochrome b559 subunit alpha

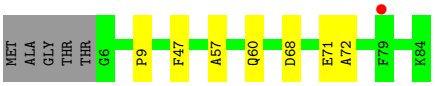
Chain E:



• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

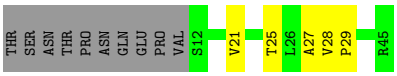




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

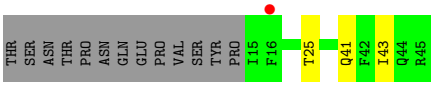




• Molecule 6: Cytochrome b559 subunit beta

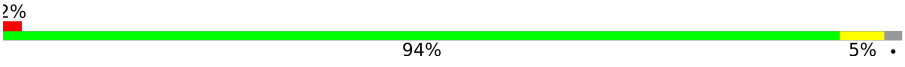
Chain f:

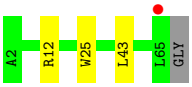




• Molecule 7: Photosystem II reaction center protein H

Chain H:





• Molecule 7: Photosystem II reaction center protein H

Chain h:

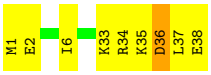




• Molecule 8: Photosystem II reaction center protein I

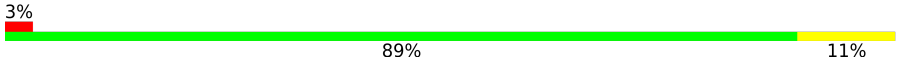
Chain I:

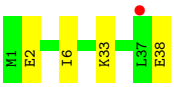




• Molecule 8: Photosystem II reaction center protein I

Chain i:

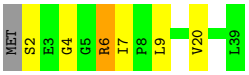




• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:

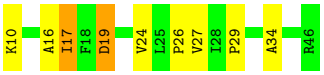




• Molecule 10: Photosystem II reaction center protein K

Chain K:





• Molecule 10: Photosystem II reaction center protein K

Chain k:





• Molecule 11: Photosystem II reaction center protein L

Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:

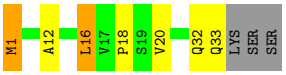




• Molecule 12: Photosystem II reaction center protein M

Chain M:

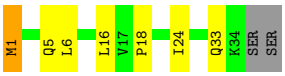




• Molecule 12: Photosystem II reaction center protein M

Chain m:





• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

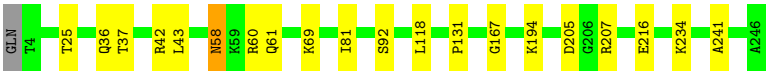




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

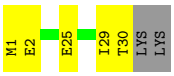




• Molecule 14: Photosystem II reaction center protein T

Chain T:





• Molecule 14: Photosystem II reaction center protein T

Chain t:

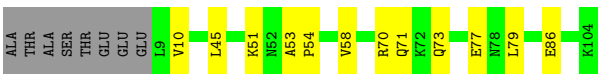




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

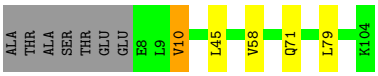




• Molecule 15: Photosystem II 12 kDa extrinsic protein

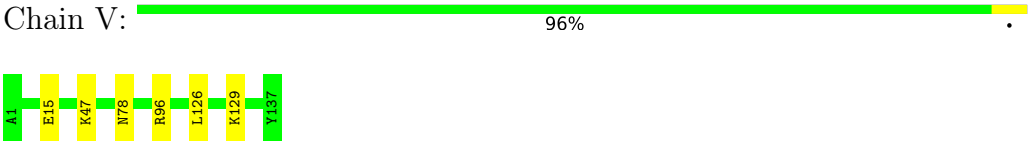
Chain u:





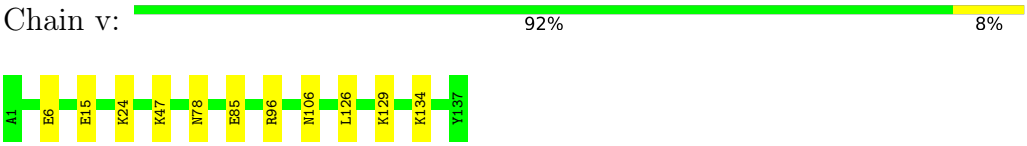
• Molecule 16: Cytochrome c-550

Chain V:



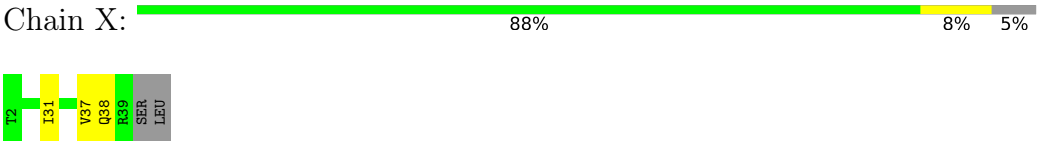
• Molecule 16: Cytochrome c-550

Chain v:



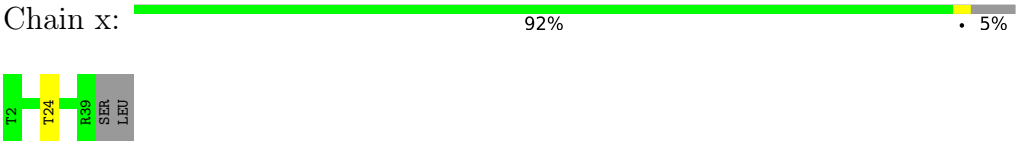
• Molecule 17: Photosystem II reaction center protein X

Chain X:



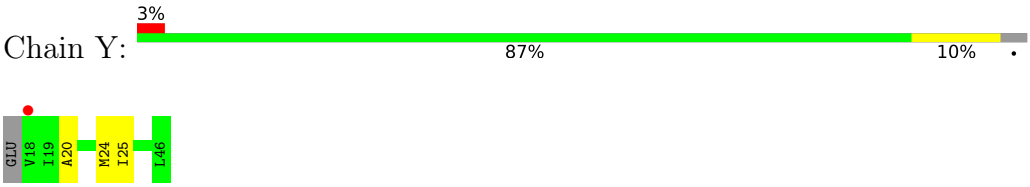
• Molecule 17: Photosystem II reaction center protein X

Chain x:



• Molecule 18: Photosystem II reaction center protein Ycf12

Chain Y:



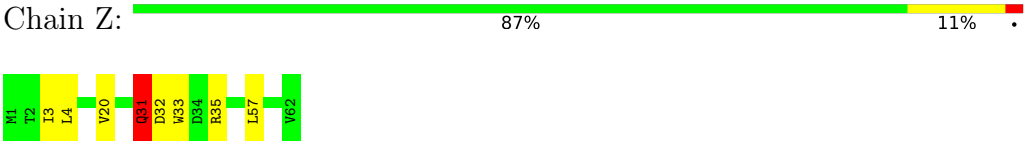
• Molecule 18: Photosystem II reaction center protein Ycf12

Chain y:



• Molecule 19: Photosystem II reaction center protein Z

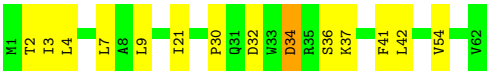
Chain Z:



• Molecule 19: Photosystem II reaction center protein Z

Chain z:

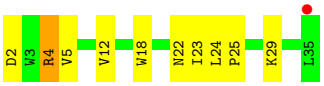




• Molecule 20: Photosystem II protein Y

Chain R:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	125.77Å 231.76Å 288.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.25 19.99 – 2.25	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.25) 99.8 (19.99-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.26Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.139 , 0.177 0.140 , 0.178	Depositor DCC
R_{free} test set	19914 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å^2)	51.0	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 72.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	62600	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 1.65% 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: HEM, DGD, GOL, CA, OEX, LMG, PHO, LHG, MG, LMT, CLA, HTG, BCR, CL, HEC, BCT, UNL, FME, SQD, FE2, PL9

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	0.43	0/6098
1	a	0.24	0/4470	0.40	0/6087
2	B	0.37	0/4293	0.50	0/5851
2	b	0.34	0/4285	0.49	0/5841
3	C	0.28	0/4404	0.42	0/5997
3	c	0.28	0/4459	0.43	0/6071
4	D	0.34	0/3741	0.46	0/5095
4	d	0.31	0/3749	0.45	0/5106
5	E	0.32	0/681	0.51	0/928
5	e	0.31	0/690	0.49	0/939
6	F	0.42	0/284	0.45	0/387
6	f	0.29	0/269	0.44	0/365
7	H	0.33	0/519	0.51	0/708
7	h	0.29	0/530	0.48	0/722
8	I	0.30	0/311	0.46	0/419
8	i	0.34	0/311	0.51	0/419
9	J	0.30	0/278	0.39	0/376
9	j	0.32	0/283	0.41	0/383
10	K	0.32	0/303	0.47	0/416
10	k	0.33	0/303	0.48	0/416
11	L	0.37	0/318	0.48	0/433
11	l	0.40	0/318	0.45	0/433
12	M	0.43	0/261	0.48	0/357
12	m	0.34	0/279	0.47	0/380
13	O	0.34	0/1991	0.50	0/2698
13	o	0.34	0/1966	0.50	0/2665
14	T	0.34	0/310	0.44	0/419
14	t	0.34	0/301	0.42	0/406
15	U	0.38	0/811	0.53	0/1095
15	u	0.37	0/818	0.54	0/1105
16	V	0.36	0/1142	0.50	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	0.24	0/292	0.37	0/395
17	x	0.24	0/284	0.37	0/384
18	Y	0.25	0/216	0.44	0/289
18	y	0.24	0/216	0.40	0/289
19	Z	0.22	0/490	0.36	0/669
19	z	0.21	0/490	0.35	0/669
20	R	0.25	0/279	0.36	0/383
All	All	0.31	0/50562	0.46	0/68780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4338	0	4142	20	0
1	a	4330	0	4132	31	0
2	B	4146	0	3983	25	0
2	b	4134	0	3976	36	0
3	C	4260	0	4123	25	0
3	c	4308	0	4172	27	0
4	D	3620	0	3484	35	0
4	d	3628	0	3490	24	0
5	E	662	0	648	11	0
5	e	670	0	655	5	0
6	F	275	0	282	3	0
6	f	261	0	269	4	0
7	H	506	0	529	2	0
7	h	517	0	541	7	0
8	I	314	0	328	5	0
8	i	314	0	328	2	0
9	J	272	0	279	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	j	277	0	284	3	0
10	K	293	0	305	5	0
10	k	293	0	305	6	0
11	L	311	0	320	2	0
11	l	311	0	320	5	0
12	M	268	0	285	7	0
12	m	286	0	305	10	0
13	O	1958	0	1920	17	0
13	o	1933	0	1900	10	0
14	T	311	0	318	3	0
14	t	302	0	311	3	0
15	U	800	0	796	8	0
15	u	807	0	805	3	0
16	V	1120	0	1122	3	0
16	v	1117	0	1131	8	0
17	X	289	0	322	3	0
17	x	281	0	312	2	0
18	Y	215	0	246	2	0
18	y	215	0	246	8	0
19	Z	479	0	516	5	0
19	z	479	0	516	4	0
20	R	273	0	305	5	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	a	4	0	0	0	0
23	A	455	0	504	19	0
23	B	1040	0	1152	26	0
23	C	845	0	936	36	0
23	D	195	0	216	8	0
23	a	455	0	504	20	0
23	b	1040	0	1152	26	0
23	c	845	0	936	35	0
23	d	195	0	216	7	0
24	A	256	0	296	6	0
24	a	256	0	296	5	0
25	A	40	0	56	3	0
25	B	120	0	168	5	0
25	C	80	0	112	1	0
25	D	40	0	56	1	0
25	H	40	0	56	2	0
25	K	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	T	40	0	56	7	0
25	Y	40	0	56	1	0
25	a	40	0	56	1	0
25	b	120	0	168	7	0
25	c	80	0	112	4	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	2	0
26	A	162	0	234	3	0
26	B	54	0	78	1	0
26	F	43	0	53	2	0
26	a	162	0	232	7	0
26	b	54	0	78	4	0
26	f	43	0	53	0	0
27	A	12	0	15	7	0
27	B	12	0	16	2	0
27	C	12	0	16	1	0
27	D	6	0	7	3	0
27	O	12	0	16	2	0
27	V	12	0	16	0	0
27	a	18	0	24	6	0
27	b	12	0	16	1	0
27	c	18	0	24	1	0
27	d	18	0	23	1	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	20	0
29	D	110	0	160	1	0
29	a	110	0	160	10	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
30	X	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	30	0	0	0	0
30	b	33	0	0	0	0
30	c	64	0	0	0	0
30	d	53	0	0	0	0
30	i	40	0	0	0	0
30	j	10	0	0	0	0
30	m	10	0	0	0	0
30	x	18	0	0	0	0
31	A	8	0	0	0	0
31	a	8	0	0	0	0
32	A	35	0	46	0	0
32	D	35	0	46	0	0
32	E	35	0	46	0	0
32	I	35	0	46	1	0
32	M	70	0	92	2	0
32	a	70	0	91	2	0
32	b	50	0	70	1	0
32	e	35	0	46	1	0
32	m	35	0	46	1	0
32	t	51	0	70	2	0
33	B	51	0	72	0	0
33	C	153	0	216	2	0
33	D	51	0	72	0	0
33	Z	37	0	44	1	0
33	a	51	0	72	0	0
33	c	102	0	144	1	0
33	d	51	0	72	3	0
33	m	51	0	72	0	0
33	z	39	0	48	2	0
34	B	57	0	78	3	0
34	C	19	0	26	0	0
34	D	16	0	17	1	0
34	V	11	0	10	0	0
34	b	57	0	78	3	0
34	c	19	0	26	1	0
34	d	16	0	17	1	0
35	C	310	0	410	4	0
35	H	62	0	82	1	0
35	c	310	0	410	11	0
35	h	62	0	82	0	0
36	C	1	0	0	0	0
36	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	294	0	444	18	0
37	E	84	0	114	6	0
37	L	98	0	148	0	0
37	d	294	0	444	28	0
37	e	84	0	114	9	0
37	l	98	0	148	0	0
38	E	43	0	30	2	0
38	e	43	0	30	0	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	206	0	0	0	0
41	B	166	0	0	1	0
41	C	174	0	0	1	0
41	D	150	0	0	1	0
41	E	14	0	0	0	0
41	F	3	0	0	0	0
41	G	286	0	0	6	0
41	H	17	0	0	0	0
41	I	6	0	0	0	0
41	J	5	0	0	2	0
41	K	5	0	0	0	0
41	L	3	0	0	0	0
41	M	5	0	0	0	0
41	O	73	0	0	0	0
41	T	10	0	0	1	0
41	U	32	0	0	0	0
41	V	69	0	0	0	0
41	X	1	0	0	0	0
41	a	208	0	0	0	0
41	b	184	0	0	1	0
41	c	163	0	0	2	0
41	d	140	0	0	0	0
41	e	8	0	0	0	0
41	f	3	0	0	0	0
41	h	15	0	0	0	0
41	i	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	j	2	0	0	0	0
41	k	3	0	0	0	0
41	l	4	0	0	0	0
41	m	14	0	0	0	0
41	o	81	0	0	0	0
41	t	7	0	0	1	0
41	u	48	0	0	0	0
41	v	41	0	0	0	0
41	x	2	0	0	0	0
41	y	1	0	0	0	0
All	All	62600	0	61443	590	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 (590) 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)
1:a:250[A]:ALA:HA	2:b:491[A]:VAL:HG11	1.51	0.93
1:a:250[B]:ALA:HA	2:b:491[B]:VAL:HG11	1.51	0.93
23:B:604:CLA:H42	23:B:605:CLA:H2	1.53	0.91
27:A:701:GOL:H11	12:M:1:FME:HG2	1.55	0.87
23:B:601:CLA:H12	23:B:601:CLA:H71	1.62	0.81
23:c:504:CLA:HBB1	23:c:513:CLA:H41	1.64	0.78
4:d:192[A]:THR:HG23	23:d:402[A]:CLA:HBC2	1.66	0.77
4:D:85:MET:HE2	4:D:90:LEU:HD21	1.68	0.76
23:A:406[A]:CLA:H152	29:A:414[A]:PL9:H252	1.67	0.76
23:c:506:CLA:HHC	23:c:506:CLA:HBB1	1.68	0.73
4:d:192[B]:THR:HG23	23:d:402[B]:CLA:HBC2	1.71	0.73
23:a:406[B]:CLA:HBB1	23:a:406[B]:CLA:HHC	1.72	0.72
23:A:406[B]:CLA:H152	29:A:414[B]:PL9:H252	1.71	0.71
23:C:502:CLA:H193	23:C:508:CLA:HBB1	1.72	0.71
2:b:98:LEU:HB2	34:b:622:HTG:H7'1	1.71	0.71
27:a:701:GOL:H32	12:m:1:FME:HG3	1.73	0.70
23:a:409:CLA:H192	23:c:506:CLA:H142	1.72	0.70
27:A:701:GOL:O2	41:T:202:HOH:O	2.10	0.70
23:c:506:CLA:CMD	23:c:508:CLA:HAB	2.22	0.69
1:a:253[B]:GLY:HA3	2:b:491[B]:VAL:HG12	1.74	0.69
1:a:253[A]:GLY:HA3	2:b:491[A]:VAL:HG12	1.75	0.69
3:c:213:LEU:HD13	23:c:507:CLA:H202	1.74	0.69
23:C:514:CLA:H202	33:C:521:LMG:H402	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:609:CLA:HHC	23:B:609:CLA:HBB1	1.73	0.68
37:D:411[A]:LHG:H112	37:D:411[A]:LHG:H382	1.76	0.68
23:a:409:CLA:H152	23:c:507:CLA:H142	1.75	0.67
1:A:102:LEU:HD12	34:b:625:HTG:H61	1.76	0.67
4:D:85:MET:HE1	4:D:96:GLU:HG2	1.76	0.67
23:B:605:CLA:HHC	23:B:605:CLA:HBB1	1.76	0.66
23:C:504:CLA:HBB1	23:C:513:CLA:H41	1.78	0.66
37:D:411[B]:LHG:H382	37:D:411[B]:LHG:H112	1.78	0.65
23:c:503:CLA:H61	23:c:513:CLA:H42	1.77	0.65
27:b:901:GOL:HO1	27:b:901:GOL:HO3	1.42	0.65
25:b:619:BCR:H331	25:b:619:BCR:HC8	1.78	0.64
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:HBB1	1.80	0.64
23:C:506:CLA:HHC	23:C:506:CLA:HBB1	1.78	0.64
25:y:101:BCR:H321	25:y:101:BCR:HC8	1.79	0.64
2:b:482[A]:ILE:HD12	2:b:486[A]:LEU:HD12	1.80	0.64
29:A:414[A]:PL9:H262	37:E:101[A]:LHG:H223	1.80	0.63
23:A:408:CLA:H193	23:C:507:CLA:H101	1.80	0.63
10:K:17:ILE:H	10:K:17:ILE:HD13	1.64	0.63
13:O:42:ARG:HH12	27:O:501:GOL:H12	1.62	0.63
23:B:615:CLA:H2	23:B:616:CLA:HBB2	1.80	0.62
3:c:134[B]:ILE:HD13	23:c:512:CLA:H43	1.81	0.62
10:k:23:ASP:OD2	18:y:21:GLN:NE2	2.31	0.62
26:a:411[A]:SQD:H152	37:d:408[A]:LHG:H172	1.82	0.62
23:b:605:CLA:HHC	23:b:605:CLA:HBB1	1.79	0.62
33:z:101:LMG:H302	33:z:101:LMG:H141	1.79	0.62
3:C:261:ARG:NH1	8:I:38:GLU:OE2	2.32	0.62
2:B:357[B]:ARG:NH2	4:D:337:GLU:O	2.30	0.62
15:U:86[B]:GLU:H	15:U:86[B]:GLU:CD	2.08	0.62
2:B:226:TYR:HA	2:B:231:MET:HG3	1.80	0.62
23:C:509:CLA:HBC3	23:C:511:CLA:H71	1.80	0.62
23:b:604:CLA:H42	23:b:605:CLA:H2	1.80	0.62
20:R:18:TRP:O	20:R:22:ASN:ND2	2.31	0.61
1:a:214[B]:MET:HB3	29:a:416[B]:PL9:H103	1.82	0.61
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.81	0.61
34:B:622:HTG:H4'1	32:a:414:LMT:H52	1.82	0.61
12:M:33:GLN:HB2	12:m:33:GLN:HG3	1.83	0.60
23:C:507:CLA:H142	35:C:517[B]:DGD:HAF2	1.82	0.60
3:c:261:ARG:NH1	8:i:38:GLU:OE2	2.33	0.60
23:C:507:CLA:H142	35:C:517[A]:DGD:HAF2	1.83	0.60
23:C:506:CLA:CMD	23:C:508:CLA:HAB	2.31	0.60
4:D:24:ARG:HD3	17:X:37:VAL:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:801:GOL:H31	12:m:1:FME:HG2	1.84	0.59
1:a:221[B]:SER:HB2	4:d:139[B]:ARG:O	2.02	0.59
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.83	0.59
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.37	0.59
23:B:616:CLA:HED2	23:B:616:CLA:H43	1.85	0.59
26:a:411[A]:SQD:H141	37:d:408[A]:LHG:H152	1.84	0.59
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.35	0.59
23:c:502:CLA:C4D	23:c:504:CLA:H2	2.32	0.58
23:b:601:CLA:H72	23:b:601:CLA:H2	1.85	0.58
10:k:17:ILE:HD13	10:k:17:ILE:H	1.67	0.58
19:Z:32:ASP:OD2	19:Z:35:ARG:HB3	2.04	0.58
23:C:511:CLA:H192	23:C:511:CLA:HBC3	1.86	0.58
23:A:405[B]:CLA:HHC	23:A:405[B]:CLA:HBB1	1.86	0.57
3:C:325:GLY:O	15:U:51:LYS:NZ	2.34	0.57
35:c:519:DGD:HBH2	37:d:408[A]:LHG:H211	1.86	0.57
29:A:414[B]:PL9:H472	4:D:39:PRO:HD3	1.86	0.57
4:D:192[A]:THR:HG23	23:D:405[A]:CLA:HBC2	1.87	0.57
4:D:192[B]:THR:HG23	23:D:405[B]:CLA:HBC2	1.86	0.57
37:d:407[B]:LHG:HC62	11:l:15[B]:THR:HG23	1.86	0.57
23:A:404[B]:CLA:HBB1	23:D:405[B]:CLA:C4B	2.13	0.57
29:A:414[B]:PL9:H262	37:E:101[B]:LHG:H223	1.86	0.57
23:a:407[A]:CLA:H191	37:e:101[A]:LHG:H111	1.85	0.57
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.85	0.57
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.86	0.56
1:a:84[B]:PRO:HA	1:a:112[B]:TYR:CG	2.40	0.56
1:a:192[B]:ILE:HG13	1:a:293[B]:MET:HE1	1.88	0.56
26:F:101:SQD:H102	17:X:31:ILE:HD11	1.86	0.56
27:a:801:GOL:H11	12:m:1:FME:HE3	1.86	0.56
2:b:285:ASN:O	2:b:289:GLN:HG2	2.04	0.56
3:c:78:GLU:OE2	16:v:106:ASN:ND2	2.39	0.56
35:c:517[A]:DGD:HG11	41:c:603[A]:HOH:O	2.06	0.56
35:c:519:DGD:HBH2	37:d:408[B]:LHG:H211	1.88	0.55
13:O:66:VAL:HG21	13:O:110:MET:HE3	1.88	0.55
2:B:357[A]:ARG:HH12	27:B:624:GOL:H32	1.72	0.55
25:Y:101:BCR:H321	25:Y:101:BCR:HC8	1.88	0.55
23:A:404[B]:CLA:H191	37:D:410[B]:LHG:H332	1.87	0.55
34:B:626:HTG:H61	1:a:102:LEU:HD12	1.88	0.55
23:A:406[B]:CLA:HHC	23:A:406[B]:CLA:HBB1	1.88	0.55
23:b:616:CLA:HHC	23:b:616:CLA:HBB1	1.89	0.54
13:o:205:ASP:OD2	13:o:207:ARG:NH2	2.40	0.54
1:a:183[A]:MET:HA	23:a:405[A]:CLA:HMD1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:134[A]:LYS:HE2	27:v:401[A]:GOL:H32	1.88	0.54
3:c:42:LEU:HD21	23:c:512:CLA:H2A	1.89	0.54
25:C:515:BCR:H352	33:C:521:LMG:H352	1.89	0.54
37:D:411[A]:LHG:H382	37:D:411[A]:LHG:H132	1.89	0.54
2:b:216:HIS:HE1	23:b:609:CLA:C1A	2.19	0.54
24:A:353[B]:PHO:H3A	23:D:405[B]:CLA:H142	1.90	0.54
27:a:801:GOL:O3	14:t:2:GLU:OE1	2.25	0.54
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.90	0.54
29:A:414[A]:PL9:H253	23:D:405[A]:CLA:H141	1.89	0.54
23:b:606:CLA:H72	25:b:619:BCR:HC7	1.89	0.53
27:A:701:GOL:H31	12:M:1:FME:HE3	1.90	0.53
1:a:192[A]:ILE:HG13	1:a:293[A]:MET:HE1	1.90	0.53
4:d:85:MET:CE	4:d:96:GLU:HG2	2.38	0.53
4:D:85:MET:CE	4:D:96:GLU:HG2	2.39	0.53
3:c:279:LEU:HD22	23:c:510:CLA:HED2	1.90	0.53
6:f:41:GLN:OE1	9:j:30:GLY:HA3	2.09	0.53
9:J:2:SER:N	41:J:201:HOH:O	2.40	0.53
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.43	0.53
25:b:619:BCR:H331	25:b:619:BCR:C8	2.39	0.53
3:c:338[B]:GLY:HA3	3:c:341[B]:LEU:O	2.09	0.53
29:A:414[A]:PL9:H472	4:D:39:PRO:HD3	1.89	0.53
29:A:414[B]:PL9:H253	23:D:405[B]:CLA:H141	1.90	0.53
13:O:169:ASP:OD1	27:O:601:GOL:H12	2.09	0.53
2:b:482[B]:ILE:HD12	2:b:486[B]:LEU:HD12	1.90	0.53
4:D:323[A]:GLU:O	27:D:701:GOL:O2	2.26	0.52
23:B:615:CLA:H2	23:B:616:CLA:CBB	2.38	0.52
1:a:188[B]:ALA:HB2	1:a:328[B]:MET:HB2	1.91	0.52
2:b:233:ASN:O	2:b:236:THR:HG22	2.10	0.52
37:d:711[B]:LHG:H211	12:m:18:PRO:HG3	1.91	0.52
1:A:183[B]:MET:HA	23:A:404[B]:CLA:HMD1	1.91	0.52
3:c:338[A]:GLY:HA3	3:c:341[A]:LEU:O	2.10	0.52
6:F:21:VAL:O	6:F:25:THR:HG23	2.09	0.52
26:a:411[B]:SQD:H152	37:d:408[B]:LHG:H172	1.92	0.52
1:A:84[A]:PRO:HA	1:A:112[A]:TYR:CG	2.44	0.52
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.45	0.51
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.46	0.51
1:a:15:GLU:HB2	32:a:420:LMT:H6'2	1.92	0.51
26:a:411[B]:SQD:H271	37:d:408[B]:LHG:H141	1.92	0.51
23:B:606:CLA:H202	26:a:413:SQD:H302	1.92	0.51
25:T:101:BCR:H321	25:T:101:BCR:HC8	1.92	0.51
18:y:20:ALA:O	18:y:24:MET:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:a:407[B]:CLA:H191	37:e:101[B]:LHG:H111	1.92	0.51
24:a:408[B]:PHO:HAB	4:d:205[B]:LEU:HD13	1.92	0.51
23:C:502:CLA:C3D	23:C:504:CLA:H2	2.41	0.51
23:a:405[B]:CLA:HBB1	23:d:402[B]:CLA:C4B	2.12	0.51
19:z:32:ASP:O	19:z:36:SER:OG	2.17	0.51
23:a:407[A]:CLA:H203	33:d:412:LMG:H412	1.93	0.50
23:a:409:CLA:H203	23:c:507:CLA:H101	1.94	0.50
13:O:42:ARG:O	13:O:241:ALA:HA	2.12	0.50
26:a:411[B]:SQD:H141	37:d:408[B]:LHG:H152	1.92	0.50
3:C:42:LEU:HD21	23:C:512:CLA:H2A	1.94	0.50
2:b:29:LEU:HD23	26:b:620:SQD:H201	1.93	0.50
33:c:521:LMG:H232	33:c:521:LMG:H391	1.93	0.50
3:c:286:ALA:HB2	23:c:503:CLA:HMD1	1.92	0.50
5:E:57:ALA:H	5:E:60:GLN:HE21	1.58	0.50
35:c:517[B]:DGD:HG11	41:c:603[B]:HOH:O	2.12	0.50
27:d:801[A]:GOL:H32	14:t:25:GLU:HB2	1.94	0.50
1:A:227[B]:THR:HB	1:A:231:GLU:HG3	1.95	0.49
3:C:174:LEU:HB3	23:C:503:CLA:H152	1.94	0.49
5:E:77:GLU:O	5:E:81:GLU:HG2	2.12	0.49
1:A:84[B]:PRO:HA	1:A:112[B]:TYR:CG	2.46	0.49
27:A:701:GOL:H11	12:M:1:FME:CG	2.35	0.49
1:a:221[A]:SER:HB2	4:d:139[A]:ARG:O	2.12	0.49
23:c:502:CLA:C3D	23:c:504:CLA:H2	2.42	0.49
25:B:618:BCR:H363	25:t:103:BCR:H19C	1.95	0.49
13:O:24:ASP:HA	13:O:203:LYS:HE2	1.95	0.49
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.94	0.49
23:a:405[A]:CLA:H201	37:d:407[A]:LHG:H161	1.95	0.49
23:C:502:CLA:C4D	23:C:504:CLA:H2	2.43	0.49
2:b:36:SER:OG	25:b:618:BCR:H362	2.12	0.49
2:b:224:ARG:HH21	32:b:621:LMT:H1'	1.78	0.49
2:B:216:HIS:HE1	23:B:609:CLA:C1A	2.25	0.49
2:b:383[A]:PHE:CZ	13:o:167:GLY:HA2	2.47	0.49
37:d:407[A]:LHG:HC62	11:l:15[A]:THR:HG23	1.95	0.49
16:v:134[B]:LYS:HB3	27:v:401[B]:GOL:H32	1.95	0.49
23:c:510:CLA:HMB1	23:c:510:CLA:HBB1	1.94	0.49
25:d:404:BCR:H331	25:d:404:BCR:C8	2.43	0.49
2:b:158:LEU:HB3	2:b:199:VAL:HG22	1.94	0.49
37:d:408[B]:LHG:H342	37:d:408[B]:LHG:H151	1.95	0.49
5:e:68:ASP:O	5:e:72:ALA:HB2	2.12	0.49
13:o:58:ASN:HB2	13:o:61:GLN:HG2	1.94	0.49
25:t:103:BCR:H321	25:t:103:BCR:HC8	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.95	0.48
12:m:5[B]:GLN:H	12:m:5[B]:GLN:NE2	2.12	0.48
24:A:353[A]:PHO:H3A	23:D:405[A]:CLA:H142	1.94	0.48
5:E:12:ASP:OD1	9:J:4:GLY:HA3	2.14	0.48
37:d:408[A]:LHG:C38	37:d:408[A]:LHG:H122	2.44	0.48
26:B:620:SQD:H1	26:B:620:SQD:H462	1.95	0.48
3:C:203:THR:O	3:C:235:GLY:HA3	2.13	0.48
2:b:98:LEU:HB2	34:b:622:HTG:C7'	2.42	0.48
3:c:95:LEU:HD21	23:c:502:CLA:OBD	2.14	0.48
23:A:408:CLA:H18	23:C:506:CLA:H142	1.96	0.48
4:D:194:ASN:HA	4:D:295[B]:SER:OG	2.14	0.48
9:j:6:ARG:NH1	9:j:6:ARG:HA	2.27	0.48
15:u:45:LEU:HD21	15:u:71:GLN:HB3	1.96	0.48
23:B:612:CLA:HBB1	23:B:612:CLA:HMB1	1.95	0.48
5:e:9:PRO:HA	37:e:101[A]:LHG:HC31	1.94	0.48
37:d:408[B]:LHG:H372	37:d:408[B]:LHG:H142	1.95	0.48
13:o:58:ASN:C	13:o:60:ARG:H	2.21	0.48
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.49	0.48
37:D:410[A]:LHG:HC62	11:L:15[A]:THR:HG23	1.96	0.48
2:B:498:LYS:HE3	4:D:20:ASP:HA	1.95	0.47
1:a:60[B]:ILE:HD12	1:a:84[B]:PRO:HD2	1.95	0.47
25:t:103:BCR:H23C	25:t:103:BCR:H382	1.96	0.47
8:i:2:GLU:O	8:i:6:ILE:HG12	2.14	0.47
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.62	0.47
29:a:416[A]:PL9:H351	6:f:25:THR:OG1	2.14	0.47
23:B:614:CLA:H192	14:t:8:PHE:CE1	2.49	0.47
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.15	0.47
23:C:507:CLA:H18	23:C:507:CLA:H152	1.47	0.47
4:D:180:ARG:HD3	4:D:180:ARG:C	2.40	0.47
5:E:9:PRO:HA	37:E:101[A]:LHG:HC31	1.96	0.47
1:a:84[A]:PRO:HA	1:a:112[A]:TYR:CG	2.49	0.47
1:a:214[A]:MET:HE2	1:a:255[A]:PHE:CE1	2.50	0.47
23:a:405[B]:CLA:H152	24:a:408[B]:PHO:H52	1.96	0.47
37:d:408[A]:LHG:H342	37:d:408[A]:LHG:H151	1.97	0.47
12:m:5[B]:GLN:H	12:m:5[B]:GLN:CD	2.22	0.47
27:A:411:GOL:O3	27:A:411:GOL:O1	2.28	0.47
23:B:601:CLA:HHC	23:B:601:CLA:HBB1	1.97	0.47
3:C:23:ALA:HB1	3:C:26:ARG:HB2	1.97	0.47
3:C:286:ALA:HB2	23:C:503:CLA:HMD2	1.95	0.47
8:I:35:LYS:O	8:I:37:LEU:N	2.48	0.47
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:d:408[B]:LHG:H331	37:d:408[B]:LHG:H361	1.66	0.47
10:k:24:VAL:HG21	18:y:25:ILE:HB	1.97	0.47
23:b:614:CLA:H112	23:b:614:CLA:H72	1.61	0.47
4:d:244[B]:TYR:OH	4:d:264[B]:LYS:HE3	2.14	0.47
4:d:283:ALA:O	4:d:287:VAL:HG23	2.15	0.47
23:d:403:CLA:H162	7:h:37:LEU:HD21	1.97	0.47
37:d:408[A]:LHG:H302	37:d:408[A]:LHG:H332	1.67	0.47
25:h:101:BCR:C8	25:h:101:BCR:H331	2.45	0.47
23:B:613:CLA:H162	23:B:613:CLA:H121	1.63	0.47
29:a:416[A]:PL9:H171	29:a:416[A]:PL9:H151	1.58	0.47
37:d:408[B]:LHG:H122	37:d:408[B]:LHG:C38	2.45	0.47
23:A:405[B]:CLA:H203	23:A:405[B]:CLA:H162	1.70	0.46
3:c:406:SER:HA	3:c:420[B]:VAL:HG23	1.97	0.46
32:t:101:LMT:H6E	32:t:102:LMT:H6D	1.97	0.46
32:t:102:LMT:H112	32:t:102:LMT:H81	1.60	0.46
1:A:192[A]:ILE:HG13	1:A:293[A]:MET:HE1	1.97	0.46
2:B:357[A]:ARG:HH12	27:B:624:GOL:C3	2.27	0.46
23:B:613:CLA:H51	37:D:409[A]:LHG:H361	1.97	0.46
13:O:40:ILE:HD12	13:O:95:PHE:CD1	2.51	0.46
25:a:410:BCR:H24C	25:a:410:BCR:H371	1.73	0.46
3:c:134[B]:ILE:HD11	23:c:512:CLA:H71	1.96	0.46
4:D:230[A]:SER:HB2	41:G:169:HOH:O	2.14	0.46
7:h:38:PHE:HB2	25:h:101:BCR:C10	2.45	0.46
29:A:414[B]:PL9:H471	29:A:414[B]:PL9:H43	1.55	0.46
23:a:406[A]:CLA:HBA1	23:a:406[A]:CLA:C4A	2.45	0.46
3:C:406:SER:HA	3:C:420[A]:VAL:HG23	1.98	0.46
3:C:406:SER:HA	3:C:420[B]:VAL:HG23	1.97	0.46
26:a:411[A]:SQD:H271	37:d:408[A]:LHG:H141	1.97	0.46
3:c:139:THR:OG1	3:c:142:GLU:OE2	2.28	0.46
1:a:183[B]:MET:HA	23:a:405[B]:CLA:HMD1	1.97	0.46
26:b:620:SQD:H311	26:b:620:SQD:H341	1.54	0.46
23:B:602:CLA:H203	23:B:602:CLA:H162	1.72	0.46
4:D:264[B]:LYS:NZ	41:D:526[B]:HOH:O	2.47	0.46
5:E:27:ILE:HD11	38:E:103:HEM:HBC2	1.98	0.46
13:O:25:THR:O	13:O:27:ARG:N	2.48	0.46
33:d:412:LMG:H221	33:d:412:LMG:H191	1.67	0.46
23:B:613:CLA:H141	37:D:409[B]:LHG:H171	1.98	0.46
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.98	0.46
37:E:101[B]:LHG:H241	37:E:101[B]:LHG:HC61	1.81	0.46
37:d:408[A]:LHG:H331	37:d:408[A]:LHG:H361	1.46	0.46
24:A:353[B]:PHO:HBC3	4:D:279:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:24:VAL:HG13	18:Y:25:ILE:HD13	1.97	0.46
19:Z:33:TRP:HZ2	33:Z:101:LMG:HC61	1.81	0.46
29:a:416[B]:PL9:H171	29:a:416[B]:PL9:H151	1.54	0.46
23:c:512:CLA:H191	33:z:101:LMG:H241	1.98	0.46
37:D:411[B]:LHG:H332	37:D:411[B]:LHG:H302	1.83	0.45
5:e:57:ALA:HB3	5:e:60:GLN:HG2	1.97	0.45
1:A:192[B]:ILE:HG13	1:A:293[B]:MET:HE1	1.96	0.45
2:B:149:LEU:HG	23:B:606:CLA:HBB2	1.97	0.45
1:a:188[A]:ALA:HB2	1:a:328[A]:MET:HB2	1.98	0.45
23:a:407[B]:CLA:H203	33:d:412:LMG:H412	1.97	0.45
3:c:178:LYS:HA	3:c:182:PHE:HB2	1.99	0.45
5:e:9:PRO:HA	37:e:101[B]:LHG:HC31	1.97	0.45
9:j:8:PRO:HG2	9:j:11:ILE:HD12	1.98	0.45
1:A:133:LEU:HD23	4:D:256[A]:ILE:HG12	1.99	0.45
29:A:414[A]:PL9:H503	26:F:101:SQD:H341	1.97	0.45
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.51	0.45
25:H:101:BCR:H331	25:H:101:BCR:C8	2.46	0.45
11:l:20:GLY:O	11:l:24:ILE:HG12	2.16	0.45
1:A:227[A]:THR:HB	1:A:231:GLU:HG3	1.98	0.45
23:A:408:CLA:H41	23:A:408:CLA:H61	1.63	0.45
4:D:261[A]:PHE:CZ	37:D:410[A]:LHG:HC81	2.52	0.45
1:a:105:TRP:CE2	1:a:110[A]:GLY:HA3	2.51	0.45
24:a:353[A]:PHO:HBC3	4:d:279:LEU:HD22	1.96	0.45
23:c:509:CLA:H18	35:c:518[A]:DGD:HAT2	1.98	0.45
10:k:21:LEU:HD13	18:y:24:MET:HE3	1.99	0.45
26:A:410[B]:SQD:H122	26:A:410[B]:SQD:H152	1.65	0.45
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.51	0.45
19:Z:31:GLN:CD	19:Z:31:GLN:H	2.24	0.45
2:B:138:MET:HE3	23:B:615:CLA:CHD	2.47	0.45
5:E:20:TRP:CD1	9:J:7:ILE:HD12	2.52	0.45
2:b:497:GLN:HB2	2:b:504:THR:HB	1.98	0.45
37:d:408[A]:LHG:H142	37:d:408[A]:LHG:H372	1.97	0.45
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.52	0.45
12:M:32:GLN:HG2	32:m:103:LMT:H6'2	1.99	0.45
2:b:226:TYR:HA	2:b:231:MET:HG3	1.97	0.45
27:c:742[B]:GOL:O2	16:v:47[B]:LYS:NZ	2.47	0.45
26:b:620:SQD:H462	26:b:620:SQD:H1	1.98	0.45
4:d:54:PHE:HB3	5:e:47:PHE:CD2	2.51	0.45
23:C:510:CLA:HMB1	23:C:510:CLA:HBB1	1.99	0.45
37:E:101[A]:LHG:H241	37:E:101[A]:LHG:HC61	1.83	0.45
23:a:405[B]:CLA:H201	37:d:407[B]:LHG:H161	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:391[B]:ARG:HA	3:C:391[B]:ARG:HD3	1.78	0.44
27:C:523[B]:GOL:O2	16:V:47[B]:LYS:NZ	2.39	0.44
15:U:73:GLN:O	15:U:77:GLU:HG3	2.17	0.44
23:b:606:CLA:H151	23:b:616:CLA:H112	1.98	0.44
3:C:157:MET:HE2	3:C:157:MET:HA	1.98	0.44
23:C:503:CLA:H151	23:C:504:CLA:HMB1	1.99	0.44
4:D:261[B]:PHE:CZ	37:D:410[B]:LHG:HC81	2.51	0.44
4:D:323[B]:GLU:O	27:D:701:GOL:O2	2.34	0.44
4:D:327:ALA:HB2	27:D:701:GOL:H2	1.99	0.44
23:b:615:CLA:H91	23:b:615:CLA:H112	1.73	0.44
19:z:34:ASP:OD1	19:z:34:ASP:N	2.50	0.44
29:A:414[A]:PL9:H151	29:A:414[A]:PL9:H171	1.55	0.44
29:A:414[A]:PL9:H301	29:A:414[A]:PL9:H322	1.76	0.44
3:C:391[A]:ARG:NH1	41:C:612:HOH:O	2.51	0.44
23:a:409:CLA:H61	23:a:409:CLA:H41	1.84	0.44
3:c:391[B]:ARG:NH2	41:G:225:HOH:O	2.50	0.44
23:c:508:CLA:HAA2	23:c:508:CLA:HBD	1.98	0.44
25:d:404:BCR:H15C	25:d:404:BCR:H351	1.79	0.44
23:b:605:CLA:H41	23:b:605:CLA:H62	1.61	0.44
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.98	0.44
1:a:307:ILE:HG22	1:a:313:VAL:HA	1.99	0.44
24:a:353[B]:PHO:HBC3	4:d:279:LEU:HD22	1.99	0.44
2:b:491[B]:VAL:HG13	4:d:136[B]:VAL:HG13	1.99	0.44
25:T:101:BCR:H351	26:b:620:SQD:H211	2.00	0.44
15:U:53:ALA:HB1	15:U:54:PRO:HA	1.99	0.44
1:a:214[A]:MET:HB3	29:a:416[A]:PL9:H103	1.98	0.44
3:c:148:GLY:O	3:c:156:LYS:NZ	2.42	0.44
23:c:506:CLA:HMD1	23:c:508:CLA:HAB	1.96	0.44
23:c:513:CLA:HMB2	23:c:513:CLA:H192	2.00	0.44
4:d:194:ASN:HA	4:d:295[B]:SER:OG	2.18	0.44
23:d:402[B]:CLA:HAA2	23:d:402[B]:CLA:HBD	2.00	0.44
29:A:414[B]:PL9:H151	29:A:414[B]:PL9:H171	1.48	0.44
2:B:363:PHE:HB3	2:B:365:SER:O	2.17	0.44
3:C:146:PHE:HZ	23:C:513:CLA:HBB2	1.82	0.44
3:C:279:LEU:HA	3:C:282:MET:HE3	2.00	0.44
4:D:123:ILE:HD11	35:H:102:DGD:HAH2	2.00	0.44
5:E:18:ARG:H	9:J:2:SER:N	2.15	0.44
37:e:101[B]:LHG:H241	37:e:101[B]:LHG:HC61	1.87	0.44
25:A:409:BCR:H11C	25:A:409:BCR:H341	1.85	0.44
5:E:40:THR:HB	20:R:4:ARG:HG2	2.00	0.44
13:o:92:SER:HB3	13:o:131:PRO:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:134[B]:LYS:HE2	27:v:401[B]:GOL:H32	2.00	0.44
18:y:31:ALA:O	18:y:35:ILE:HG13	2.17	0.44
13:O:205:ASP:OD1	13:O:207:ARG:HG3	2.18	0.44
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.53	0.44
23:c:513:CLA:H142	23:c:513:CLA:H111	1.90	0.44
4:d:20:ASP:O	4:d:24:ARG:HG2	2.18	0.44
2:B:285:ASN:O	2:B:289:GLN:HG2	2.18	0.43
23:B:605:CLA:H192	23:B:605:CLA:H162	1.87	0.43
25:K:102:BCR:H15C	25:K:102:BCR:H351	1.88	0.43
29:a:416[A]:PL9:H28	37:e:101[A]:LHG:H222	1.99	0.43
2:b:314:TYR:CE2	2:b:316:GLY:HA3	2.53	0.43
1:a:259[A]:ILE:HG22	1:a:260[A]:PHE:CD1	2.53	0.43
23:A:404[B]:CLA:H143	24:A:407[B]:PHO:H61	2.01	0.43
2:B:462:PHE:CE2	23:B:613:CLA:HMB2	2.54	0.43
23:C:506:CLA:H93	23:C:506:CLA:H111	1.78	0.43
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.48	0.43
9:J:6:ARG:HG3	41:J:201:HOH:O	2.17	0.43
29:a:416[B]:PL9:H351	6:f:25:THR:OG1	2.18	0.43
23:b:609:CLA:HMD1	7:h:27:THR:HB	1.99	0.43
23:c:510:CLA:H91	23:c:510:CLA:H111	1.81	0.43
23:d:403:CLA:H61	23:d:403:CLA:H41	1.65	0.43
37:d:408[B]:LHG:H131	37:d:408[B]:LHG:H102	1.93	0.43
3:c:406:SER:HA	3:c:420[A]:VAL:HG23	2.00	0.43
29:A:414[A]:PL9:H221	29:A:414[A]:PL9:H201	1.88	0.43
29:A:414[A]:PL9:HC2	29:A:414[A]:PL9:HC8	1.71	0.43
23:C:511:CLA:H152	23:C:511:CLA:H112	1.51	0.43
29:D:408[A]:PL9:H401	29:D:408[A]:PL9:H422	1.75	0.43
13:O:39[B]:ARG:NH1	13:O:244:GLU:OE2	2.42	0.43
27:a:701:GOL:H12	41:t:201:HOH:O	2.17	0.43
13:o:42:ARG:O	13:o:241:ALA:HA	2.18	0.43
20:R:24:LEU:N	20:R:25:PRO:HD2	2.32	0.43
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.91	0.43
23:b:615:CLA:H61	23:b:615:CLA:H92	1.65	0.43
10:k:24:VAL:HG22	18:y:25:ILE:HD13	2.01	0.43
18:y:30:ILE:HD12	18:y:30:ILE:HA	1.91	0.43
23:A:404[B]:CLA:CBD	23:A:405[B]:CLA:HAC2	2.49	0.43
15:U:45:LEU:HD23	15:U:45:LEU:HA	1.89	0.43
23:A:405[B]:CLA:C4A	23:A:405[B]:CLA:HBA1	2.48	0.43
26:A:410[A]:SQD:H122	26:A:410[A]:SQD:H152	1.52	0.43
3:c:38:GLY:HA3	23:c:512:CLA:HMD2	1.99	0.43
3:c:182:PHE:HA	34:c:522:HTG:H61	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:615:CLA:H71	23:B:616:CLA:H172	2.01	0.43
25:H:101:BCR:H24C	25:H:101:BCR:H371	1.75	0.43
25:T:101:BCR:H24C	25:T:101:BCR:H371	1.84	0.43
23:c:509:CLA:H18	35:c:518[B]:DGD:HAT2	2.00	0.43
23:B:613:CLA:H141	37:D:409[A]:LHG:H171	2.00	0.43
8:I:2:GLU:O	8:I:6:ILE:HG12	2.19	0.43
8:I:38:GLU:HG2	8:I:38:GLU:OXT	2.18	0.43
13:O:54:GLU:HG2	13:O:64:GLU:O	2.18	0.43
23:c:509:CLA:HBC3	23:c:511:CLA:H71	2.01	0.43
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.95	0.43
7:h:38:PHE:HB2	25:h:101:BCR:H10C	2.01	0.43
19:Z:4:LEU:HD22	19:Z:57:LEU:HD11	2.01	0.43
20:R:2:ASP:HB3	20:R:5:VAL:HG23	2.01	0.43
1:A:85[B]:SER:HA	1:A:109[B]:GLY:HA3	2.01	0.42
25:B:618:BCR:C8	25:B:618:BCR:H331	2.48	0.42
3:C:52:ALA:HB2	23:C:512:CLA:HMA2	2.01	0.42
23:C:510:CLA:H162	23:C:510:CLA:H192	1.77	0.42
4:D:209[A]:LEU:C	4:D:209[A]:LEU:HD23	2.44	0.42
32:I:101:LMT:O3'	32:I:101:LMT:H6'2	2.19	0.42
10:K:26:PRO:O	10:K:29:PRO:HD2	2.19	0.42
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CH2	2.54	0.42
23:c:514:CLA:HBB1	25:c:515:BCR:H24C	2.01	0.42
25:c:515:BCR:H11C	25:c:515:BCR:H341	1.79	0.42
32:e:102:LMT:H6'1	6:f:43:ILE:HG12	1.99	0.42
24:A:407[A]:PHO:HAB	4:D:205[A]:LEU:HD13	2.00	0.42
23:C:506:CLA:HAA1	23:C:506:CLA:HBD	2.01	0.42
23:C:511:CLA:H52	37:D:411[B]:LHG:H371	2.00	0.42
18:Y:20:ALA:O	18:Y:24:MET:HG2	2.19	0.42
25:c:515:BCR:H15C	25:c:515:BCR:H351	1.81	0.42
2:B:298:LEU:HD12	2:B:298:LEU:HA	1.87	0.42
13:O:137:THR:C	13:O:139:SER:H	2.27	0.42
1:a:230:THR:HG21	11:l:8:GLN:NE2	2.34	0.42
2:b:149[B]:LEU:HD11	23:b:604:CLA:H122	2.02	0.42
3:c:31:SER:CB	3:c:41:ARG:HG2	2.49	0.42
35:c:518[B]:DGD:HAF1	35:c:518[B]:DGD:HA81	2.00	0.42
23:A:405[A]:CLA:H203	23:A:405[A]:CLA:H162	1.76	0.42
23:B:614:CLA:H92	23:B:614:CLA:H61	1.78	0.42
3:C:38:GLY:HA3	23:C:512:CLA:HMD2	2.00	0.42
11:L:24:ILE:HD13	12:M:18:PRO:HB2	2.01	0.42
1:A:131:TRP:CD2	1:A:131:TRP:C	2.96	0.42
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:HC2	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36[B]:SER:OG	25:B:618:BCR:H362	2.19	0.42
32:M:101:LMT:H72	12:m:24:ILE:HD13	2.02	0.42
25:T:101:BCR:H11C	25:T:101:BCR:H341	1.83	0.42
2:b:134:ASP:OD1	2:b:136:PRO:HD2	2.19	0.42
1:A:82[A]:VAL:HB	1:A:174[A]:LEU:HB2	2.01	0.42
2:B:158:LEU:HB3	2:B:199:VAL:HG22	2.02	0.42
23:C:505:CLA:H62	23:C:505:CLA:H41	1.63	0.42
4:D:230[B]:SER:HB2	41:G:169:HOH:O	2.19	0.42
37:D:411[B]:LHG:H382	37:D:411[B]:LHG:H132	2.02	0.42
10:K:16:ALA:O	10:K:19:ASP:HB2	2.19	0.42
1:a:93[A]:PHE:CD2	1:a:95:PRO:HD3	2.54	0.42
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.54	0.42
3:c:167:VAL:HG11	23:c:513:CLA:HBA2	2.02	0.42
3:c:425[A]:TRP:CD1	23:c:505:CLA:HMA3	2.54	0.42
25:t:103:BCR:H11C	25:t:103:BCR:H341	1.89	0.42
23:a:407[B]:CLA:HMB2	23:d:402[B]:CLA:H122	2.00	0.42
23:b:612:CLA:HBB1	23:b:612:CLA:HMB1	2.01	0.42
23:A:404[A]:CLA:HBB1	23:A:404[A]:CLA:HMB3	2.02	0.42
23:A:404[B]:CLA:HBD	23:A:405[B]:CLA:HAC2	2.02	0.42
23:C:503:CLA:HBD	23:C:503:CLA:HAA1	2.02	0.42
38:E:103:HEM:HAC	6:F:27:ALA:HB1	2.02	0.42
13:O:84:GLU:CD	13:O:86:LYS:HG2	2.45	0.42
3:c:459[B]:ILE:HG21	3:c:464[B]:GLU:HG3	2.01	0.42
16:v:126:LEU:HB3	16:v:129:LYS:HB2	2.01	0.42
1:A:85[B]:SER:HB3	1:A:109[B]:GLY:O	2.20	0.42
1:A:183[A]:MET:HA	23:A:404[A]:CLA:HMD1	2.01	0.42
4:D:15:PHE:H	34:D:414:HTG:H61	1.84	0.42
37:D:411[A]:LHG:H302	37:D:411[A]:LHG:H332	1.81	0.42
13:O:130:GLN:H	13:O:130:GLN:CD	2.27	0.42
2:b:173:GLY:HA3	2:b:265:ILE:HD11	2.02	0.42
23:b:611:CLA:H112	23:b:611:CLA:H72	1.80	0.42
37:d:408[B]:LHG:H332	37:d:408[B]:LHG:H302	1.87	0.42
12:m:6:LEU:HD23	12:m:6:LEU:HA	1.86	0.42
27:A:701:GOL:H12	14:T:2:GLU:HG3	2.02	0.42
23:B:613:CLA:H51	37:D:409[B]:LHG:H361	2.02	0.42
2:b:161:LEU:HD12	2:b:161:LEU:HA	1.85	0.42
23:b:607:CLA:H91	23:b:607:CLA:H112	1.58	0.42
15:u:10[A]:VAL:HG12	41:G:214:HOH:O	2.20	0.42
19:Z:57:LEU:HD23	19:Z:57:LEU:HA	1.81	0.42
1:A:243[A]:GLU:CD	1:A:243[A]:GLU:H	2.27	0.41
23:A:404[B]:CLA:HMC3	4:D:182:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:51:LEU:HB3	13:O:65:PHE:HB3	2.02	0.41
29:a:416[B]:PL9:H28	37:e:101[B]:LHG:H222	2.01	0.41
23:b:601:CLA:H92	25:h:101:BCR:H403	2.01	0.41
25:y:101:BCR:H15C	25:y:101:BCR:H351	1.88	0.41
23:C:511:CLA:H52	37:D:411[A]:LHG:H371	2.01	0.41
23:D:405[B]:CLA:HAA2	23:D:405[B]:CLA:HBD	2.01	0.41
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.79	0.41
23:b:609:CLA:HHC	23:b:609:CLA:HBB1	2.02	0.41
23:b:613:CLA:H203	23:b:613:CLA:H161	1.90	0.41
7:h:62:TRP:C	7:h:64:ALA:H	2.28	0.41
13:o:58:ASN:HD22	13:o:61:GLN:HG3	1.84	0.41
1:A:162[B]:PRO:HB3	1:A:168[B]:PHE:HA	2.03	0.41
2:B:497:GLN:HE22	17:X:38:GLN:HB2	1.85	0.41
5:E:9:PRO:HA	37:E:101[B]:LHG:HC31	2.02	0.41
29:a:416[A]:PL9:H503	17:x:24:THR:OG1	2.20	0.41
23:b:614:CLA:H62	23:b:614:CLA:H41	1.72	0.41
37:e:101[A]:LHG:H241	37:e:101[A]:LHG:HC61	1.90	0.41
34:B:623:HTG:H7'3	34:B:623:HTG:H4'2	1.81	0.41
4:D:209[B]:LEU:HD23	4:D:209[B]:LEU:C	2.45	0.41
1:a:213[B]:ALA:HB2	4:d:275[B]:PRO:HG2	2.02	0.41
2:b:216:HIS:CE1	23:b:609:CLA:NA	2.87	0.41
2:b:383[B]:PHE:CZ	13:o:167:GLY:HA2	2.55	0.41
25:b:619:BCR:HC7	25:b:619:BCR:H311	1.66	0.41
18:y:34:MET:O	18:y:38:LEU:HG	2.20	0.41
35:C:519:DGD:HBE2	35:C:519:DGD:HB81	1.79	0.41
23:a:406[A]:CLA:HHC	23:a:406[A]:CLA:CBB	2.48	0.41
23:b:615:CLA:HHC	23:b:615:CLA:HBB1	2.02	0.41
23:b:616:CLA:H13	23:b:616:CLA:H102	1.84	0.41
10:k:19:ASP:HB3	10:k:20:PRO:HD3	2.03	0.41
25:k:101:BCR:H15C	25:k:101:BCR:H351	1.93	0.41
1:A:82[B]:VAL:HB	1:A:174[B]:LEU:HB2	2.02	0.41
29:A:414[A]:PL9:H43	29:A:414[A]:PL9:H471	1.69	0.41
3:C:279:LEU:HD22	23:C:510:CLA:HED2	2.02	0.41
13:O:27:ARG:NH1	13:O:203:LYS:HG2	2.35	0.41
1:a:160[B]:ILE:HD11	35:c:517[B]:DGD:HBT1	2.03	0.41
27:a:801:GOL:C3	12:m:1:FME:HG2	2.49	0.41
2:b:431:GLU:OE2	41:b:819:HOH:O	2.21	0.41
4:d:148[B]:ALA:HB3	4:d:149[B]:PRO:HD3	2.02	0.41
37:d:408[A]:LHG:H131	37:d:408[A]:LHG:H102	1.91	0.41
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.02	0.41
1:A:231:GLU:HB3	41:B:827:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240[B]:GLY:HA3	14:T:29[B]:ILE:HG23	2.02	0.41
23:B:601:CLA:HAA1	23:B:601:CLA:HBD	2.02	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.86	0.41
3:C:362[B]:ARG:NH2	41:G:217:HOH:O	2.46	0.41
25:b:617:BCR:H24C	25:b:617:BCR:H371	1.74	0.41
23:c:505:CLA:H62	35:c:519:DGD:HB62	2.03	0.41
23:c:513:CLA:H121	23:c:514:CLA:H142	2.01	0.41
19:z:37:LYS:HE2	19:z:41:PHE:HE2	1.86	0.41
25:A:409:BCR:H15C	25:A:409:BCR:H351	1.90	0.41
25:A:409:BCR:H371	25:A:409:BCR:H24C	1.71	0.41
3:C:275:SER:HB3	23:C:510:CLA:HED3	2.03	0.41
23:C:509:CLA:HBC2	37:D:411[B]:LHG:H351	2.03	0.41
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.02	0.41
2:B:299:GLU:HG3	2:B:402:TYR:HD1	1.86	0.41
2:B:491[A]:VAL:HG12	4:D:136[A]:VAL:HG13	2.03	0.41
3:C:443[B]:TRP:CE2	23:C:509:CLA:HMD2	2.56	0.41
35:C:518[A]:DGD:HAE2	35:C:518[A]:DGD:HA81	1.91	0.41
4:D:172:SER:HB2	4:D:177:ALA:HB1	2.03	0.41
12:M:12:ALA:O	12:M:16[B]:LEU:HB2	2.21	0.41
13:O:110:MET:HE2	13:O:110:MET:HB3	1.90	0.41
25:T:101:BCR:H19C	25:b:618:BCR:H363	2.03	0.41
1:a:162[A]:PRO:HB3	1:a:168[A]:PHE:HA	2.03	0.41
2:b:216:HIS:CE1	23:b:609:CLA:C1A	3.03	0.41
23:b:610:CLA:H122	23:b:615:CLA:HAA1	2.02	0.41
3:c:363:GLY:O	3:c:367:GLU:HG2	2.21	0.41
35:c:518[A]:DGD:HAT1	35:c:519:DGD:HBF2	2.03	0.41
29:A:414[A]:PL9:HC8	29:A:414[A]:PL9:H121	1.79	0.41
27:A:701:GOL:H12	14:T:2:GLU:OE1	2.20	0.41
23:B:604:CLA:HMD2	23:B:612:CLA:H203	2.02	0.41
3:C:252:ILE:HG22	3:C:253:LEU:HD23	2.03	0.41
23:C:513:CLA:H143	23:C:514:CLA:H142	2.01	0.41
23:b:609:CLA:NC	25:h:101:BCR:H332	2.36	0.41
4:d:141[B]:TYR:OH	37:d:711[B]:LHG:O4	2.32	0.41
25:B:618:BCR:H371	25:B:618:BCR:H24C	1.88	0.40
3:C:150:ASP:OD2	3:C:152:LYS:HB2	2.21	0.40
25:K:102:BCR:H24C	25:K:102:BCR:H371	1.72	0.40
37:e:101[A]:LHG:H142	37:e:101[A]:LHG:H172	1.83	0.40
26:A:410[B]:SQD:H361	10:K:34:ALA:HA	2.03	0.40
29:A:414[B]:PL9:H221	29:A:414[B]:PL9:H201	1.90	0.40
2:B:283:GLU:O	2:B:287:ARG:HG3	2.21	0.40
25:D:407:BCR:H391	9:J:20:VAL:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:M:101:LMT:H6D	11:l:9:PRO:HA	2.03	0.40
15:U:86[B]:GLU:OE1	15:U:86[B]:GLU:N	2.32	0.40
1:a:259[B]:ILE:HG22	1:a:260[B]:PHE:CD1	2.56	0.40
3:c:52:ALA:HB2	23:c:512:CLA:HMA2	2.02	0.40
3:c:225:VAL:HG13	3:c:289:PHE:HA	2.02	0.40
4:d:14:TRP:CD1	34:d:411:HTG:H61	2.56	0.40
4:d:261[B]:PHE:CZ	37:d:407[B]:LHG:HC81	2.56	0.40
37:d:408[A]:LHG:H242	37:d:408[A]:LHG:H272	1.92	0.40
13:o:216:GLU:CD	13:o:234:LYS:HD2	2.46	0.40
25:t:103:BCR:HC7	25:t:103:BCR:H331	1.48	0.40
1:A:334[B]:ARG:HD3	4:D:320[B]:LEU:HD13	2.03	0.40
4:D:261[B]:PHE:CE1	37:D:410[B]:LHG:HC81	2.56	0.40
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.04	0.40
16:V:78:ASN:OD1	16:V:96:ARG:NH1	2.53	0.40
23:a:409:CLA:H3A	23:a:409:CLA:HBA1	1.90	0.40
7:h:43:LEU:O	7:h:47:GLU:HG3	2.21	0.40
16:v:6:GLU:CD	16:v:6:GLU:H	2.29	0.40
29:A:414[B]:PL9:HC8	29:A:414[B]:PL9:H121	1.73	0.40
3:C:130:VAL:O	3:C:134:ILE:HG12	2.21	0.40
25:T:101:BCR:HC8	25:T:101:BCR:H311	2.04	0.40
1:a:261[A]:GLN:HG3	2:b:493[A]:TRP:CZ3	2.55	0.40
24:a:408[B]:PHO:ND	24:a:408[B]:PHO:NC	2.70	0.40
3:c:152:LYS:HD2	41:G:190:HOH:O	2.21	0.40
23:c:510:CLA:H142	23:c:510:CLA:H112	1.79	0.40
35:c:518[A]:DGD:HBF2	35:c:518[A]:DGD:HBE1	1.91	0.40
25:k:101:BCR:H24C	25:k:101:BCR:H371	1.68	0.40
24:A:353[B]:PHO:NC	24:A:353[B]:PHO:ND	2.69	0.40
2:B:144:PHE:CE2	2:B:148[A]:LEU:HD11	2.57	0.40
2:B:154:GLY:O	2:B:159:THR:HG23	2.21	0.40
8:I:36:ASP:OD1	8:I:36:ASP:N	2.55	0.40
29:a:416[B]:PL9:H503	17:x:24:THR:OG1	2.21	0.40
23:c:513:CLA:HBA2	23:c:513:CLA:H3A	1.76	0.40
25:c:516:BCR:H11C	25:c:516:BCR:H341	1.90	0.40
4:d:12:ARG:NE	4:d:12:ARG:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/344 (161%)	544 (98%)	7 (1%)	2 (0%)	30	31
1	a	552/344 (160%)	544 (99%)	6 (1%)	2 (0%)	30	31
2	B	522/505 (103%)	514 (98%)	8 (2%)	0	100	100
2	b	521/505 (103%)	509 (98%)	12 (2%)	0	100	100
3	C	546/455 (120%)	540 (99%)	5 (1%)	1 (0%)	43	50
3	c	553/455 (122%)	540 (98%)	12 (2%)	1 (0%)	43	50
4	D	453/342 (132%)	438 (97%)	15 (3%)	0	100	100
4	d	454/342 (133%)	443 (98%)	11 (2%)	0	100	100
5	E	79/84 (94%)	78 (99%)	1 (1%)	0	100	100
5	e	79/84 (94%)	79 (100%)	0	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	62/65 (95%)	62 (100%)	0	0	100	100
7	h	63/65 (97%)	59 (94%)	3 (5%)	1 (2%)	7	4
8	I	36/38 (95%)	34 (94%)	1 (3%)	1 (3%)	4	2
8	i	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
9	J	36/39 (92%)	35 (97%)	1 (3%)	0	100	100
9	j	37/39 (95%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	36/37 (97%)	36 (100%)	0	0	100	100
12	M	32/36 (89%)	32 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	251/244 (103%)	242 (96%)	8 (3%)	1 (0%)	30	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	249/244 (102%)	244 (98%)	5 (2%)	0	100	100
14	T	33/32 (103%)	33 (100%)	0	0	100	100
14	t	32/32 (100%)	32 (100%)	0	0	100	100
15	U	97/104 (93%)	93 (96%)	4 (4%)	0	100	100
15	u	98/104 (94%)	94 (96%)	4 (4%)	0	100	100
16	V	140/137 (102%)	136 (97%)	4 (3%)	0	100	100
16	v	140/137 (102%)	135 (96%)	5 (4%)	0	100	100
17	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
17	x	36/40 (90%)	36 (100%)	0	0	100	100
18	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
18	y	27/30 (90%)	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	6171/5384 (115%)	6038 (98%)	122 (2%)	11 (0%)	43	50

All (11) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	444/279 (159%)	440 (99%)	4 (1%)	70 79
1	a	443/279 (159%)	441 (100%)	2 (0%)	81 87
2	B	421/403 (104%)	416 (99%)	5 (1%)	63 74
2	b	420/403 (104%)	409 (97%)	11 (3%)	40 50
3	C	430/356 (121%)	421 (98%)	9 (2%)	47 58
3	c	436/356 (122%)	428 (98%)	8 (2%)	51 63
4	D	368/277 (133%)	365 (99%)	3 (1%)	73 80
4	d	369/277 (133%)	361 (98%)	8 (2%)	45 56
5	E	72/73 (99%)	71 (99%)	1 (1%)	59 70
5	e	72/73 (99%)	71 (99%)	1 (1%)	59 70
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	26 (100%)	0	100 100
7	H	54/54 (100%)	52 (96%)	2 (4%)	30 37
7	h	55/54 (102%)	55 (100%)	0	100 100
8	I	34/34 (100%)	32 (94%)	2 (6%)	18 18
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 47
9	J	26/27 (96%)	24 (92%)	2 (8%)	12 10
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%)	208 (96%)	8 (4%)	30 37
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	87/89 (98%)	85 (98%)	2 (2%)	44 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	V	123/117 (105%)	122 (99%)	1 (1%)	73 80
16	v	123/117 (105%)	120 (98%)	3 (2%)	43 54
17	X	32/33 (97%)	32 (100%)	0	100 100
17	x	31/33 (94%)	31 (100%)	0	100 100
18	Y	22/23 (96%)	22 (100%)	0	100 100
18	y	22/23 (96%)	19 (86%)	3 (14%)	3 2
19	Z	52/52 (100%)	49 (94%)	3 (6%)	18 19
19	z	52/52 (100%)	45 (86%)	7 (14%)	4 2
20	R	29/29 (100%)	26 (90%)	3 (10%)	7 5
All	All	5103/4403 (116%)	4987 (98%)	116 (2%)	44 55

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	243[A]	GLU
1	A	243[B]	GLU
1	A	244[A]	GLU
1	A	244[B]	GLU
2	B	161	LEU
2	B	299	GLU
2	B	362	PHE
2	B	389	LYS
2	B	472	ARG
3	C	24	THR
3	C	29	GLU
3	C	30	SER
3	C	142	GLU
3	C	255	THR
3	C	289	PHE
3	C	315[A]	MET
3	C	315[B]	MET
3	C	462	GLU
4	D	259[A]	ILE
4	D	259[B]	ILE
4	D	338	ASN
5	E	71	GLU
7	H	12	ARG
7	H	43	LEU
8	I	33	LYS

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Mol	Chain	Res	Type
8	I	34	ARG
9	J	6	ARG
9	J	9	LEU
10	K	10	LYS
10	K	17	ILE
10	K	19	ASP
10	K	27	VAL
12	M	16[A]	LEU
12	M	16[B]	LEU
12	M	20	VAL
13	O	49	THR
13	O	55	GLU
13	O	69	LYS
13	O	98[A]	GLU
13	O	98[B]	GLU
13	O	115	ARG
13	O	118	LEU
13	O	234	LYS
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
1	a	13	LEU
1	a	121	LEU
2	b	63	LEU
2	b	128	THR
2	b	161	LEU
2	b	223	GLN
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	19	ASN
3	c	142	GLU
3	c	152	LYS
3	c	240	ILE

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Mol	Chain	Res	Type
3	c	255	THR
3	c	289	PHE
3	c	315[A]	MET
3	c	315[B]	MET
4	d	26	ARG
4	d	178	ILE
4	d	230[A]	SER
4	d	230[B]	SER
4	d	259[A]	ILE
4	d	259[B]	ILE
4	d	272[A]	LEU
4	d	272[B]	LEU
5	e	71	GLU
8	i	33	LYS
9	j	9	LEU
10	k	10	LYS
10	k	17	ILE
10	k	24	VAL
11	l	2	GLU
12	m	16[A]	LEU
12	m	16[B]	LEU
13	o	25	THR
13	o	36	GLN
13	o	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
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	23	ILE
20	R	29	LYS

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Mol	Chain	Res	Type
19	z	2	THR
19	z	3	ILE
19	z	4	LEU
19	z	7	LEU
19	z	21	ILE
19	z	34	ASP
19	z	42	LEU

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

Mol	Chain	Res	Type
3	C	322	GLN
5	E	60	GLN
11	L	8	GLN
13	O	231	HIS
15	U	78	ASN
17	X	38	GLN
2	b	14	ASN
2	b	331	ASN
3	c	415	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

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	FME	m	1	12	8,9,10	0.56	0	7,9,11	1.53	2 (28%)
12	FME	M	1	12	8,9,10	0.60	0	7,9,11	1.15	1 (14%)
8	FME	I	1	8	8,9,10	0.59	0	7,9,11	1.19	1 (14%)
8	FME	i	1	8	8,9,10	0.71	0	7,9,11	1.23	0
14	FME	T	1	14	8,9,10	0.60	0	7,9,11	1.49	1 (14%)
14	FME	t	1	14	8,9,10	0.74	0	7,9,11	1.51	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	-	0/7/9/11	-
12	FME	M	1	12	-	1/7/9/11	-
8	FME	I	1	8	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1	14	-	3/7/9/11	-
14	FME	t	1	14	-	1/7/9/11	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	m	1	FME	CA-N-CN	-2.59	118.84	122.82
14	T	1	FME	CG-CB-CA	2.48	119.83	112.95
14	t	1	FME	O-C-CA	-2.46	118.34	124.78
12	m	1	FME	O1-CN-N	-2.34	119.10	125.27
8	I	1	FME	O-C-CA	-2.16	119.11	124.78
12	M	1	FME	O-C-CA	-2.16	119.11	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	m	1	FME	4	0
12	M	1	FME	3	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
23	CLA	d	403	4	69,73,73	2.01	18 (26%)	83,113,113	2.95	32 (38%)
25	BCR	b	619	-	41,41,41	1.04	1 (2%)	56,56,56	1.31	5 (8%)
25	BCR	c	516	-	41,41,41	1.02	1 (2%)	56,56,56	1.32	8 (14%)
37	LHG	l	101[A]	-	48,48,48	0.83	2 (4%)	51,54,54	1.04	4 (7%)
23	CLA	c	503	3	69,73,73	1.92	18 (26%)	83,113,113	2.76	27 (32%)
23	CLA	c	511	3	69,73,73	1.97	17 (24%)	83,113,113	2.83	33 (39%)
23	CLA	C	514	3	69,73,73	2.03	20 (28%)	83,113,113	2.85	31 (37%)
23	CLA	B	608	2	69,73,73	1.88	20 (28%)	83,113,113	2.88	34 (40%)
23	CLA	b	603	2	69,73,73	1.94	19 (27%)	83,113,113	2.91	31 (37%)
25	BCR	k	101	-	41,41,41	1.05	1 (2%)	56,56,56	1.37	7 (12%)
33	LMG	c	521	-	51,51,55	1.01	2 (3%)	59,59,63	1.33	6 (10%)
34	HTG	B	622	-	19,19,19	1.08	2 (10%)	23,24,24	1.56	5 (21%)
23	CLA	b	613	2	69,73,73	1.98	20 (28%)	83,113,113	2.81	31 (37%)
23	CLA	b	608	2	69,73,73	1.99	19 (27%)	83,113,113	2.82	35 (42%)
23	CLA	b	604	2	69,73,73	2.04	19 (27%)	83,113,113	2.77	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	PL9	a	416[B]	-	55,55,55	0.63	2 (3%)	68,69,69	1.95	20 (29%)
27	GOL	A	701	-	5,5,5	1.48	2 (40%)	5,5,5	0.89	0
27	GOL	C	523[A]	-	5,5,5	1.11	0	5,5,5	0.88	0
34	HTG	C	522	-	19,19,19	0.84	1 (5%)	23,24,24	1.23	1 (4%)
32	LMT	b	627	-	25,25,36	0.86	0	30,30,47	1.11	3 (10%)
29	PL9	d	405[A]	-	55,55,55	0.70	1 (1%)	68,69,69	1.63	18 (26%)
33	LMG	a	419	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	3 (5%)
23	CLA	c	512	3	69,73,73	2.06	21 (30%)	83,113,113	2.85	32 (38%)
34	HTG	b	623	-	19,19,19	1.01	1 (5%)	23,24,24	1.97	3 (13%)
25	BCR	C	515	-	41,41,41	1.02	1 (2%)	56,56,56	1.40	5 (8%)
23	CLA	c	514	3	69,73,73	2.08	20 (28%)	83,113,113	2.87	30 (36%)
32	LMT	a	420	-	36,36,36	0.98	2 (5%)	47,47,47	1.04	2 (4%)
35	DGD	c	517[B]	-	63,63,67	0.88	2 (3%)	77,77,81	1.06	6 (7%)
26	SQD	B	620	-	53,54,54	1.08	4 (7%)	62,65,65	1.75	11 (17%)
35	DGD	C	517[B]	-	63,63,67	0.83	2 (3%)	77,77,81	1.05	7 (9%)
23	CLA	B	601	41	69,73,73	2.07	21 (30%)	83,113,113	2.85	27 (32%)
33	LMG	m	101	-	51,51,55	0.86	2 (3%)	59,59,63	1.32	7 (11%)
23	CLA	D	405[B]	4	69,73,73	1.98	20 (28%)	83,113,113	2.87	30 (36%)
27	GOL	b	624	-	5,5,5	1.12	1 (20%)	5,5,5	0.77	0
23	CLA	b	614	2	69,73,73	2.03	20 (28%)	83,113,113	2.99	30 (36%)
35	DGD	c	517[A]	-	63,63,67	0.85	2 (3%)	77,77,81	1.10	7 (9%)
38	HEM	E	103	5,6	50,50,50	1.55	8 (16%)	66,82,82	1.90	16 (24%)
35	DGD	C	517[A]	-	63,63,67	0.83	2 (3%)	77,77,81	1.20	8 (10%)
34	HTG	b	622	-	19,19,19	1.13	2 (10%)	23,24,24	2.01	7 (30%)
25	BCR	b	617	-	41,41,41	1.06	1 (2%)	56,56,56	1.34	3 (5%)
23	CLA	B	610	41	69,73,73	2.07	19 (27%)	83,113,113	2.85	30 (36%)
23	CLA	C	504	3	69,73,73	1.98	19 (27%)	83,113,113	2.83	29 (34%)
23	CLA	c	509	3	69,73,73	2.07	21 (30%)	83,113,113	2.79	29 (34%)
27	GOL	B	624	-	5,5,5	0.94	0	5,5,5	1.12	1 (20%)
26	SQD	A	410[B]	-	53,54,54	0.94	3 (5%)	62,65,65	1.72	11 (17%)
32	LMT	M	101	-	36,36,36	1.12	4 (11%)	47,47,47	1.22	4 (8%)
32	LMT	b	621	-	25,25,36	0.96	1 (4%)	30,30,47	1.21	3 (10%)
23	CLA	b	611	2	69,73,73	1.94	21 (30%)	83,113,113	2.88	27 (32%)
23	CLA	b	610	41	69,73,73	2.02	19 (27%)	83,113,113	2.88	31 (37%)
23	CLA	b	606	2	69,73,73	2.01	20 (28%)	83,113,113	2.93	31 (37%)

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	2.09	20 (28%)	83,113,113	2.83	28 (33%)
35	DGD	C	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	1.02	5 (6%)
23	CLA	C	511	3	69,73,73	2.01	20 (28%)	83,113,113	2.90	34 (40%)
23	CLA	B	603	2	69,73,73	1.98	20 (28%)	83,113,113	2.92	29 (34%)
23	CLA	D	406	4	69,73,73	2.07	18 (26%)	83,113,113	2.75	32 (38%)
23	CLA	a	406[B]	41	69,73,73	2.06	17 (24%)	83,113,113	2.84	32 (38%)
28	OEX	A	413[B]	1,3,41	0,14,14	-	-	-		
31	BCT	A	348[B]	21	2,3,3	0.68	0	2,3,3	1.11	0
23	CLA	C	508	41	69,73,73	1.92	19 (27%)	83,113,113	2.78	32 (38%)
34	HTG	B	626	-	19,19,19	1.10	2 (10%)	23,24,24	1.34	3 (13%)
27	GOL	d	701	-	5,5,5	1.26	1 (20%)	5,5,5	1.00	0
26	SQD	A	410[A]	-	53,54,54	0.93	3 (5%)	62,65,65	1.88	10 (16%)
32	LMT	e	102	-	36,36,36	1.01	2 (5%)	47,47,47	1.02	1 (2%)
29	PL9	A	414[B]	-	55,55,55	0.64	1 (1%)	68,69,69	1.99	23 (33%)
23	CLA	C	505	41	69,73,73	1.94	19 (27%)	83,113,113	2.86	29 (34%)
23	CLA	B	604	2	69,73,73	2.03	21 (30%)	83,113,113	2.70	32 (38%)
27	GOL	O	501	-	5,5,5	0.91	0	5,5,5	0.91	0
27	GOL	o	501	-	5,5,5	0.98	0	5,5,5	0.97	0
23	CLA	A	408	1	69,73,73	2.00	20 (28%)	83,113,113	3.02	33 (39%)
37	LHG	d	711[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.03	4 (7%)
29	PL9	D	408[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.63	17 (25%)
24	PHO	A	353[B]	-	58,69,69	2.78	16 (27%)	56,99,99	2.90	16 (28%)
23	CLA	a	406[A]	41	69,73,73	2.04	17 (24%)	83,113,113	2.86	32 (38%)
25	BCR	a	410	-	41,41,41	1.08	1 (2%)	56,56,56	1.37	9 (16%)
25	BCR	K	102	-	41,41,41	1.03	1 (2%)	56,56,56	1.50	13 (23%)
28	OEX	A	413[A]	1,3,41	0,14,14	-	-	-		
31	BCT	A	348[A]	21	2,3,3	0.64	0	2,3,3	1.30	0
37	LHG	D	411[B]	-	48,48,48	0.92	2 (4%)	51,54,54	0.97	3 (5%)
23	CLA	b	612	2	69,73,73	2.01	19 (27%)	83,113,113	2.74	29 (34%)
23	CLA	B	609	2	69,73,73	1.99	18 (26%)	83,113,113	2.74	31 (37%)
26	SQD	b	620	-	53,54,54	1.06	3 (5%)	62,65,65	1.70	12 (19%)
27	GOL	d	801[B]	-	5,5,5	0.89	0	5,5,5	0.98	0
24	PHO	A	353[A]	-	58,69,69	2.79	15 (25%)	56,99,99	2.85	15 (26%)
29	PL9	a	416[A]	-	55,55,55	0.65	2 (3%)	68,69,69	2.01	22 (32%)
23	CLA	B	614	2	69,73,73	2.02	19 (27%)	83,113,113	3.02	31 (37%)
23	CLA	c	508	41	69,73,73	2.00	20 (28%)	83,113,113	2.87	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
37	LHG	D	411[A]	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
27	GOL	a	412	-	5,5,5	0.88	0	5,5,5	1.00	0
35	DGD	c	518[B]	-	63,63,67	0.86	2 (3%)	77,77,81	0.94	5 (6%)
23	CLA	c	505	41	69,73,73	2.06	21 (30%)	83,113,113	2.84	29 (34%)
27	GOL	d	801[A]	-	5,5,5	0.93	0	5,5,5	0.98	0
27	GOL	D	701	-	5,5,5	1.52	2 (40%)	5,5,5	0.76	0
23	CLA	B	612	2	69,73,73	1.99	21 (30%)	83,113,113	2.69	29 (34%)
23	CLA	a	405[B]	1	69,73,73	2.05	20 (28%)	83,113,113	2.83	33 (39%)
35	DGD	h	102	-	63,63,67	0.87	3 (4%)	77,77,81	1.13	5 (6%)
23	CLA	C	503	3	69,73,73	2.02	19 (27%)	83,113,113	2.73	29 (34%)
23	CLA	B	605	2	69,73,73	2.04	19 (27%)	83,113,113	2.99	31 (37%)
34	HTG	V	203	-	11,11,19	0.29	0	15,15,24	1.28	1 (6%)
23	CLA	D	405[A]	4	69,73,73	2.00	20 (28%)	83,113,113	2.86	32 (38%)
23	CLA	B	607	41	69,73,73	1.96	19 (27%)	83,113,113	2.82	29 (34%)
32	LMT	m	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.19	4 (8%)
25	BCR	B	617	-	41,41,41	1.09	1 (2%)	56,56,56	1.27	8 (14%)
26	SQD	f	102	-	42,43,54	1.21	3 (7%)	51,54,65	1.48	12 (23%)
23	CLA	A	406[B]	41	69,73,73	2.08	19 (27%)	83,113,113	2.86	33 (39%)
32	LMT	M	103	-	36,36,36	1.05	3 (8%)	47,47,47	1.05	2 (4%)
23	CLA	a	405[A]	1	69,73,73	1.99	20 (28%)	83,113,113	2.87	33 (39%)
23	CLA	b	605	2	69,73,73	1.95	19 (27%)	83,113,113	2.97	30 (36%)
26	SQD	A	412	-	53,54,54	1.04	3 (5%)	62,65,65	1.30	7 (11%)
27	GOL	a	801	-	5,5,5	1.32	1 (20%)	5,5,5	1.09	1 (20%)
26	SQD	a	413	-	53,54,54	1.08	4 (7%)	62,65,65	1.18	8 (12%)
40	HEC	v	202	16	50,50,50	1.77	7 (14%)	68,82,82	1.43	12 (17%)
23	CLA	C	506	3	69,73,73	2.04	19 (27%)	83,113,113	2.82	30 (36%)
23	CLA	B	611	2	69,73,73	2.66	19 (27%)	83,113,113	4.21	28 (33%)
32	LMT	t	101	-	25,25,36	0.91	2 (8%)	30,30,47	1.16	3 (10%)
37	LHG	D	409[B]	-	48,48,48	0.88	2 (4%)	51,54,54	1.20	5 (9%)
33	LMG	C	520	-	51,51,55	0.95	2 (3%)	59,59,63	1.10	4 (6%)
34	HTG	D	414	-	16,16,19	0.98	1 (6%)	20,21,24	1.60	1 (5%)
23	CLA	A	406[A]	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	32 (38%)
23	CLA	A	404[B]	1	69,73,73	2.08	19 (27%)	83,113,113	2.80	32 (38%)
25	BCR	D	407	-	41,41,41	1.12	1 (2%)	56,56,56	1.87	17 (30%)
23	CLA	C	512	3	69,73,73	2.04	21 (30%)	83,113,113	2.71	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	c	510	3	69,73,73	2.04	19 (27%)	83,113,113	2.88	32 (38%)
23	CLA	B	616	2	69,73,73	2.03	20 (28%)	83,113,113	2.78	29 (34%)
24	PHO	A	407[B]	-	58,69,69	2.76	11 (18%)	56,99,99	2.70	16 (28%)
24	PHO	a	353[B]	-	58,69,69	2.80	14 (24%)	56,99,99	2.88	15 (26%)
24	PHO	a	408[B]	-	58,69,69	2.73	13 (22%)	56,99,99	2.73	14 (25%)
25	BCR	T	101	-	41,41,41	1.00	1 (2%)	56,56,56	1.53	13 (23%)
26	SQD	a	411[B]	-	53,54,54	0.97	3 (5%)	62,65,65	1.68	12 (19%)
32	LMT	D	404	-	36,36,36	1.18	4 (11%)	47,47,47	1.38	5 (10%)
23	CLA	d	402[B]	4	69,73,73	2.01	20 (28%)	83,113,113	2.84	30 (36%)
34	HTG	b	625	-	19,19,19	1.06	2 (10%)	23,24,24	1.53	3 (13%)
27	GOL	a	701	-	5,5,5	1.07	0	5,5,5	1.02	0
23	CLA	B	602	2	69,73,73	2.05	21 (30%)	83,113,113	2.91	35 (42%)
27	GOL	V	401[B]	-	5,5,5	1.17	0	5,5,5	0.92	0
37	LHG	e	101[B]	-	41,41,48	1.04	2 (4%)	44,47,54	0.91	2 (4%)
33	LMG	C	501	-	51,51,55	0.91	2 (3%)	59,59,63	1.61	8 (13%)
34	HTG	d	411	-	16,16,19	0.92	1 (6%)	20,21,24	1.58	1 (5%)
23	CLA	A	405[B]	41	69,73,73	2.04	19 (27%)	83,113,113	2.85	33 (39%)
27	GOL	A	411	-	5,5,5	1.09	0	5,5,5	0.78	0
29	PL9	A	414[A]	-	55,55,55	0.69	2 (3%)	68,69,69	2.01	24 (35%)
23	CLA	a	407[B]	41	69,73,73	2.02	20 (28%)	83,113,113	2.90	31 (37%)
37	LHG	d	711[A]	-	48,48,48	0.89	2 (4%)	51,54,54	1.11	4 (7%)
25	BCR	Y	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.80	16 (28%)
23	CLA	b	601	41	69,73,73	2.12	20 (28%)	83,113,113	2.81	27 (32%)
24	PHO	A	407[A]	-	58,69,69	2.66	12 (20%)	56,99,99	2.81	14 (25%)
24	PHO	a	353[A]	-	58,69,69	2.77	13 (22%)	56,99,99	2.94	17 (30%)
29	PL9	D	408[A]	-	55,55,55	0.63	1 (1%)	68,69,69	1.61	17 (25%)
24	PHO	a	408[A]	-	58,69,69	2.74	13 (22%)	56,99,99	2.81	14 (25%)
26	SQD	a	411[A]	-	53,54,54	0.96	3 (5%)	62,65,65	1.83	13 (20%)
32	LMT	A	359	-	36,36,36	0.91	0	47,47,47	1.10	1 (2%)
35	DGD	C	518[A]	-	63,63,67	0.90	3 (4%)	77,77,81	1.03	5 (6%)
27	GOL	V	401[A]	-	5,5,5	1.34	0	5,5,5	0.80	0
28	OEX	a	415[B]	1,3,41	0,14,14	-	-	-		
34	HTG	B	623	-	19,19,19	0.76	1 (5%)	23,24,24	1.43	1 (4%)
27	GOL	v	401[B]	-	5,5,5	1.02	0	5,5,5	0.86	0
35	DGD	C	519	-	63,63,67	0.85	3 (4%)	77,77,81	1.01	4 (5%)
37	LHG	L	101[B]	-	48,48,48	0.93	3 (6%)	51,54,54	1.10	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	A	405[A]	41	69,73,73	2.02	18 (26%)	83,113,113	2.85	33 (39%)
23	CLA	c	507	3	69,73,73	2.05	21 (30%)	83,113,113	2.82	30 (36%)
25	BCR	b	618	-	41,41,41	1.04	1 (2%)	56,56,56	1.30	9 (16%)
23	CLA	a	407[A]	41	69,73,73	1.98	19 (27%)	83,113,113	2.83	30 (36%)
25	BCR	H	101	-	41,41,41	1.02	1 (2%)	56,56,56	1.43	8 (14%)
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.10	5 (10%)
26	SQD	F	101	-	42,43,54	1.20	4 (9%)	51,54,65	2.18	14 (27%)
27	GOL	O	601	-	5,5,5	0.79	0	5,5,5	1.12	1 (20%)
34	HTG	c	522	-	19,19,19	0.89	1 (5%)	23,24,24	1.49	2 (8%)
25	BCR	h	101	-	41,41,41	1.04	1 (2%)	56,56,56	1.47	9 (16%)
23	CLA	c	513	3	69,73,73	2.07	20 (28%)	83,113,113	2.84	31 (37%)
28	OEX	a	415[A]	1,3,41	0,14,14	-	-	-		
27	GOL	v	401[A]	-	5,5,5	1.20	0	5,5,5	0.82	0
25	BCR	B	618	-	41,41,41	0.98	1 (2%)	56,56,56	1.48	7 (12%)
35	DGD	c	518[A]	-	63,63,67	0.85	3 (4%)	77,77,81	0.97	3 (3%)
37	LHG	L	101[A]	-	48,48,48	0.88	2 (4%)	51,54,54	1.15	4 (7%)
27	GOL	B	901	-	5,5,5	1.13	0	5,5,5	1.00	0
33	LMG	d	412	39	51,51,55	0.89	2 (3%)	59,59,63	1.14	5 (8%)
27	GOL	C	523[B]	-	5,5,5	1.07	0	5,5,5	0.84	0
37	LHG	d	407[B]	-	48,48,48	0.89	2 (4%)	51,54,54	1.06	4 (7%)
23	CLA	b	616	2	69,73,73	2.01	20 (28%)	83,113,113	2.97	33 (39%)
27	GOL	o	601	-	5,5,5	1.15	1 (20%)	5,5,5	1.09	0
23	CLA	c	502	3	69,73,73	2.00	20 (28%)	83,113,113	2.86	31 (37%)
29	PL9	d	405[B]	-	55,55,55	0.65	1 (1%)	68,69,69	1.65	17 (25%)
33	LMG	D	415	39	51,51,55	0.81	2 (3%)	59,59,63	1.07	3 (5%)
37	LHG	d	408[B]	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
23	CLA	C	502	3	69,73,73	1.97	19 (27%)	83,113,113	2.87	32 (38%)
23	CLA	b	602	2	69,73,73	2.08	18 (26%)	83,113,113	2.96	34 (40%)
37	LHG	E	101[B]	-	41,41,48	1.06	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	a	409	1	69,73,73	1.97	17 (24%)	83,113,113	2.96	30 (36%)
31	BCT	a	404[B]	21	2,3,3	0.61	0	2,3,3	1.19	0
40	HEC	V	202	16	50,50,50	1.75	6 (12%)	68,82,82	1.49	10 (14%)
35	DGD	H	102	-	63,63,67	0.83	3 (4%)	77,77,81	1.07	7 (9%)
23	CLA	B	615	2	69,73,73	2.02	19 (27%)	83,113,113	2.87	29 (34%)
25	BCR	y	101	-	41,41,41	1.06	1 (2%)	56,56,56	1.56	8 (14%)
23	CLA	B	606	2	69,73,73	1.93	19 (27%)	83,113,113	2.98	33 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	C	513	3	69,73,73	2.03	19 (27%)	83,113,113	2.86	34 (40%)
37	LHG	d	407[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.04	4 (7%)
27	GOL	c	742[B]	-	5,5,5	0.98	0	5,5,5	0.90	0
33	LMG	B	621	-	51,51,55	0.90	2 (3%)	59,59,63	1.29	4 (6%)
37	LHG	d	408[A]	-	48,48,48	0.92	2 (4%)	51,54,54	1.01	3 (5%)
23	CLA	c	506	3	69,73,73	2.03	19 (27%)	83,113,113	2.76	28 (33%)
37	LHG	D	410[B]	-	48,48,48	0.91	2 (4%)	51,54,54	0.99	4 (7%)
37	LHG	E	101[A]	-	41,41,48	1.08	2 (4%)	44,47,54	1.10	3 (6%)
23	CLA	b	615	2	69,73,73	2.03	19 (27%)	83,113,113	2.80	31 (37%)
33	LMG	c	520	-	51,51,55	0.90	2 (3%)	59,59,63	1.14	5 (8%)
31	BCT	a	404[A]	21	2,3,3	0.59	0	2,3,3	1.49	0
35	DGD	c	519	-	63,63,67	0.87	4 (6%)	77,77,81	1.06	4 (5%)
33	LMG	C	521	-	51,51,55	1.08	3 (5%)	59,59,63	1.36	7 (11%)
25	BCR	C	516	-	41,41,41	1.05	1 (2%)	56,56,56	1.30	4 (7%)
37	LHG	D	409[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.27	6 (11%)
23	CLA	B	613	2	69,73,73	1.98	19 (27%)	83,113,113	2.78	30 (36%)
25	BCR	t	103	-	41,41,41	1.05	1 (2%)	56,56,56	1.63	11 (19%)
27	GOL	c	742[A]	-	5,5,5	1.00	0	5,5,5	0.98	0
23	CLA	A	404[A]	1	69,73,73	2.00	20 (28%)	83,113,113	2.87	30 (36%)
23	CLA	C	507	3	69,73,73	2.02	21 (30%)	83,113,113	2.84	31 (37%)
33	LMG	Z	101	-	37,37,55	1.02	2 (5%)	45,45,63	1.42	6 (13%)
37	LHG	D	410[A]	-	48,48,48	0.87	2 (4%)	51,54,54	1.01	3 (5%)
32	LMT	E	102	-	36,36,36	1.03	1 (2%)	47,47,47	1.01	2 (4%)
32	LMT	a	414	-	36,36,36	1.02	2 (5%)	47,47,47	1.17	5 (10%)
27	GOL	b	901	-	5,5,5	0.54	0	5,5,5	1.40	1 (20%)
37	LHG	e	101[A]	-	41,41,48	1.06	2 (4%)	44,47,54	0.92	2 (4%)
23	CLA	d	402[A]	4	69,73,73	1.95	20 (28%)	83,113,113	2.76	32 (38%)
25	BCR	d	404	-	41,41,41	1.10	1 (2%)	56,56,56	2.00	17 (30%)
25	BCR	c	515	-	41,41,41	0.99	1 (2%)	56,56,56	1.60	15 (26%)
25	BCR	A	409	-	41,41,41	0.97	1 (2%)	56,56,56	1.42	9 (16%)
23	CLA	C	509	3	69,73,73	2.00	20 (28%)	83,113,113	2.77	29 (34%)
23	CLA	b	607	41	69,73,73	1.96	19 (27%)	83,113,113	2.71	29 (34%)
37	LHG	l	101[B]	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	2 (3%)
25	BCR	B	619	-	41,41,41	1.09	2 (4%)	56,56,56	1.38	8 (14%)
23	CLA	C	510	3	69,73,73	2.08	20 (28%)	83,113,113	2.83	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
23	CLA	b	609	2	69,73,73	2.03	19 (27%)	83,113,113	2.79	30 (36%)
38	HEM	e	87	5,6	50,50,50	1.49	6 (12%)	66,82,82	1.77	13 (19%)
32	LMT	I	101	-	36,36,36	1.04	2 (5%)	47,47,47	1.19	4 (8%)
27	GOL	c	743	-	5,5,5	1.04	0	5,5,5	0.97	0
32	LMT	t	102	-	26,26,36	0.88	2 (7%)	31,31,47	1.33	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	d	403	4	-	8/39/115/115	-
25	BCR	b	619	-	-	4/29/63/63	0/2/2/2
25	BCR	c	516	-	-	0/29/63/63	0/2/2/2
37	LHG	l	101[A]	-	-	14/53/53/53	-
23	CLA	c	503	3	-	7/39/115/115	-
23	CLA	c	511	3	-	11/39/115/115	-
23	CLA	C	514	3	-	6/39/115/115	-
23	CLA	B	608	2	-	3/39/115/115	-
23	CLA	b	603	2	-	8/39/115/115	-
25	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	LMG	c	521	-	-	11/46/66/70	0/1/1/1
34	HTG	B	622	-	-	4/10/30/30	0/1/1/1
23	CLA	b	613	2	-	6/39/115/115	-
23	CLA	b	608	2	-	6/39/115/115	-
23	CLA	b	604	2	-	13/39/115/115	-
29	PL9	a	416[B]	-	-	14/53/73/73	0/1/1/1
27	GOL	A	701	-	-	2/4/4/4	-
27	GOL	C	523[A]	-	-	0/4/4/4	-
34	HTG	C	522	-	-	0/10/30/30	0/1/1/1
32	LMT	b	627	-	-	11/17/37/61	0/1/1/2
29	PL9	d	405[A]	-	-	7/53/73/73	0/1/1/1
33	LMG	a	419	-	-	11/46/66/70	0/1/1/1
23	CLA	c	512	3	-	7/39/115/115	-
34	HTG	b	623	-	-	5/10/30/30	0/1/1/1
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	514	3	-	11/39/115/115	-
32	LMT	a	420	-	-	11/21/61/61	0/2/2/2
35	DGD	c	517[B]	-	-	20/51/91/95	0/2/2/2
26	SQD	B	620	-	-	11/49/69/69	0/1/1/1
35	DGD	C	517[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	B	601	41	-	13/39/115/115	-
33	LMG	m	101	-	-	11/46/66/70	0/1/1/1
23	CLA	D	405[B]	4	-	5/39/115/115	-
27	GOL	b	624	-	-	2/4/4/4	-
23	CLA	b	614	2	-	14/39/115/115	-
35	DGD	c	517[A]	-	-	18/51/91/95	0/2/2/2
38	HEM	E	103	5,6	-	8/14/54/54	-
35	DGD	C	517[A]	-	-	14/51/91/95	0/2/2/2
34	HTG	b	622	-	-	5/10/30/30	0/1/1/1
25	BCR	b	617	-	-	2/29/63/63	0/2/2/2
23	CLA	B	610	41	-	9/39/115/115	-
23	CLA	C	504	3	-	3/39/115/115	-
23	CLA	c	509	3	-	5/39/115/115	-
27	GOL	B	624	-	-	4/4/4/4	-
26	SQD	A	410[B]	-	-	11/49/69/69	0/1/1/1
32	LMT	M	101	-	-	5/21/61/61	0/2/2/2
32	LMT	b	621	-	-	8/17/37/61	0/1/1/2
23	CLA	b	611	2	-	3/39/115/115	-
23	CLA	b	610	41	-	7/39/115/115	-
23	CLA	b	606	2	-	14/39/115/115	-
23	CLA	c	504	3	-	1/39/115/115	-
35	DGD	C	518[B]	-	-	13/51/91/95	0/2/2/2
23	CLA	C	511	3	-	14/39/115/115	-
23	CLA	B	603	2	-	5/39/115/115	-
23	CLA	D	406	4	-	14/39/115/115	-
23	CLA	a	406[B]	41	-	3/39/115/115	-
23	CLA	C	508	41	-	9/39/115/115	-
34	HTG	B	626	-	-	4/10/30/30	0/1/1/1
27	GOL	d	701	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	SQD	A	410[A]	-	-	12/49/69/69	0/1/1/1
32	LMT	e	102	-	-	14/21/61/61	0/2/2/2
29	PL9	A	414[B]	-	-	12/53/73/73	0/1/1/1
23	CLA	C	505	41	-	9/39/115/115	-
23	CLA	B	604	2	-	2/39/115/115	-
27	GOL	O	501	-	-	2/4/4/4	-
27	GOL	o	501	-	-	2/4/4/4	-
23	CLA	A	408	1	-	9/39/115/115	-
37	LHG	d	711[B]	-	-	10/53/53/53	-
29	PL9	D	408[B]	-	-	10/53/73/73	0/1/1/1
24	PHO	A	353[B]	-	-	0/37/103/103	0/5/6/6
23	CLA	a	406[A]	41	-	8/39/115/115	-
25	BCR	a	410	-	-	3/29/63/63	0/2/2/2
25	BCR	K	102	-	-	2/29/63/63	0/2/2/2
37	LHG	D	411[B]	-	-	14/53/53/53	-
23	CLA	b	612	2	-	5/39/115/115	-
23	CLA	B	609	2	-	1/39/115/115	-
26	SQD	b	620	-	-	18/49/69/69	0/1/1/1
27	GOL	d	801[B]	-	-	2/4/4/4	-
24	PHO	A	353[A]	-	-	1/37/103/103	0/5/6/6
29	PL9	a	416[A]	-	-	14/53/73/73	0/1/1/1
23	CLA	B	614	2	-	15/39/115/115	-
23	CLA	c	508	41	-	9/39/115/115	-
37	LHG	D	411[A]	-	-	14/53/53/53	-
27	GOL	a	412	-	-	4/4/4/4	-
35	DGD	c	518[B]	-	-	16/51/91/95	0/2/2/2
23	CLA	c	505	41	-	6/39/115/115	-
27	GOL	d	801[A]	-	-	1/4/4/4	-
27	GOL	D	701	-	-	4/4/4/4	-
23	CLA	B	612	2	-	5/39/115/115	-
23	CLA	a	405[B]	1	-	6/39/115/115	-
35	DGD	h	102	-	-	14/51/91/95	0/2/2/2
23	CLA	C	503	3	-	10/39/115/115	-
23	CLA	B	605	2	-	6/39/115/115	-
34	HTG	V	203	-	-	0/2/19/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	D	405[A]	4	-	2/39/115/115	-
23	CLA	B	607	41	-	3/39/115/115	-
32	LMT	m	103	-	-	6/21/61/61	0/2/2/2
25	BCR	B	617	-	-	1/29/63/63	0/2/2/2
26	SQD	f	102	-	-	12/38/58/69	0/1/1/1
23	CLA	A	406[B]	41	-	4/39/115/115	-
32	LMT	M	103	-	-	7/21/61/61	0/2/2/2
23	CLA	a	405[A]	1	-	4/39/115/115	-
23	CLA	b	605	2	-	7/39/115/115	-
26	SQD	A	412	-	-	13/49/69/69	0/1/1/1
27	GOL	a	801	-	-	0/4/4/4	-
26	SQD	a	413	-	-	14/49/69/69	0/1/1/1
40	HEC	v	202	16	1/1/3/7	6/14/54/54	-
23	CLA	C	506	3	-	7/39/115/115	-
23	CLA	B	611	2	-	2/39/115/115	-
32	LMT	t	101	-	-	9/17/37/61	0/1/1/2
37	LHG	D	409[B]	-	-	14/53/53/53	-
33	LMG	C	520	-	-	11/46/66/70	0/1/1/1
34	HTG	D	414	-	-	3/7/27/30	0/1/1/1
23	CLA	A	406[A]	41	-	5/39/115/115	-
23	CLA	A	404[B]	1	-	8/39/115/115	-
25	BCR	D	407	-	-	4/29/63/63	0/2/2/2
23	CLA	C	512	3	-	4/39/115/115	-
23	CLA	c	510	3	-	14/39/115/115	-
23	CLA	B	616	2	-	7/39/115/115	-
24	PHO	A	407[B]	-	-	3/37/103/103	0/5/6/6
24	PHO	a	353[B]	-	-	2/37/103/103	0/5/6/6
24	PHO	a	408[B]	-	-	5/37/103/103	0/5/6/6
25	BCR	T	101	-	-	1/29/63/63	0/2/2/2
26	SQD	a	411[B]	-	-	8/49/69/69	0/1/1/1
32	LMT	D	404	-	-	12/21/61/61	0/2/2/2
23	CLA	d	402[B]	4	-	5/39/115/115	-
34	HTG	b	625	-	-	3/10/30/30	0/1/1/1
27	GOL	a	701	-	-	2/4/4/4	-
23	CLA	B	602	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	GOL	V	401[B]	-	-	2/4/4/4	-
37	LHG	e	101[B]	-	-	16/46/46/53	-
33	LMG	C	501	-	-	13/46/66/70	0/1/1/1
34	HTG	d	411	-	-	1/7/27/30	0/1/1/1
23	CLA	A	405[B]	41	-	6/39/115/115	-
27	GOL	A	411	-	-	2/4/4/4	-
29	PL9	A	414[A]	-	-	15/53/73/73	0/1/1/1
23	CLA	a	407[B]	41	-	7/39/115/115	-
37	LHG	d	711[A]	-	-	17/53/53/53	-
25	BCR	Y	101	-	-	3/29/63/63	0/2/2/2
23	CLA	b	601	41	-	20/39/115/115	-
24	PHO	A	407[A]	-	-	3/37/103/103	0/5/6/6
24	PHO	a	353[A]	-	-	1/37/103/103	0/5/6/6
29	PL9	D	408[A]	-	-	6/53/73/73	0/1/1/1
24	PHO	a	408[A]	-	-	6/37/103/103	0/5/6/6
26	SQD	a	411[A]	-	-	9/49/69/69	0/1/1/1
32	LMT	A	359	-	-	8/21/61/61	0/2/2/2
35	DGD	C	518[A]	-	-	13/51/91/95	0/2/2/2
27	GOL	V	401[A]	-	-	2/4/4/4	-
34	HTG	B	623	-	-	2/10/30/30	0/1/1/1
27	GOL	v	401[B]	-	-	2/4/4/4	-
35	DGD	C	519	-	-	19/51/91/95	0/2/2/2
37	LHG	L	101[B]	-	-	20/53/53/53	-
23	CLA	A	405[A]	41	-	3/39/115/115	-
23	CLA	c	507	3	-	8/39/115/115	-
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
23	CLA	a	407[A]	41	-	8/39/115/115	-
25	BCR	H	101	-	-	2/29/63/63	0/2/2/2
33	LMG	z	101	-	-	9/34/54/70	0/1/1/1
26	SQD	F	101	-	-	15/38/58/69	0/1/1/1
27	GOL	O	601	-	-	2/4/4/4	-
34	HTG	c	522	-	-	2/10/30/30	0/1/1/1
25	BCR	h	101	-	-	2/29/63/63	0/2/2/2
23	CLA	c	513	3	-	12/39/115/115	-
27	GOL	v	401[A]	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
35	DGD	c	518[A]	-	-	16/51/91/95	0/2/2/2
37	LHG	L	101[A]	-	-	20/53/53/53	-
27	GOL	B	901	-	-	1/4/4/4	-
33	LMG	d	412	39	-	9/46/66/70	0/1/1/1
27	GOL	C	523[B]	-	-	0/4/4/4	-
37	LHG	d	407[B]	-	-	15/53/53/53	-
23	CLA	b	616	2	-	9/39/115/115	-
27	GOL	o	601	-	-	4/4/4/4	-
23	CLA	c	502	3	-	6/39/115/115	-
29	PL9	d	405[B]	-	-	7/53/73/73	0/1/1/1
33	LMG	D	415	39	-	8/46/66/70	0/1/1/1
37	LHG	d	408[B]	-	-	16/53/53/53	-
23	CLA	C	502	3	-	5/39/115/115	-
23	CLA	b	602	2	-	3/39/115/115	-
37	LHG	E	101[B]	-	-	19/46/46/53	-
23	CLA	a	409	1	-	11/39/115/115	-
40	HEC	V	202	16	1/1/3/7	6/14/54/54	-
35	DGD	H	102	-	-	14/51/91/95	0/2/2/2
23	CLA	B	615	2	-	8/39/115/115	-
25	BCR	y	101	-	-	5/29/63/63	0/2/2/2
23	CLA	B	606	2	-	8/39/115/115	-
23	CLA	C	513	3	-	12/39/115/115	-
37	LHG	d	407[A]	-	-	13/53/53/53	-
27	GOL	c	742[B]	-	-	0/4/4/4	-
33	LMG	B	621	-	-	16/46/66/70	0/1/1/1
37	LHG	d	408[A]	-	-	13/53/53/53	-
23	CLA	c	506	3	-	7/39/115/115	-
37	LHG	D	410[B]	-	-	16/53/53/53	-
37	LHG	E	101[A]	-	-	22/46/46/53	-
23	CLA	b	615	2	-	8/39/115/115	-
33	LMG	c	520	-	-	11/46/66/70	0/1/1/1
35	DGD	c	519	-	-	10/51/91/95	0/2/2/2
33	LMG	C	521	-	-	15/46/66/70	0/1/1/1
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	D	409[A]	-	-	14/53/53/53	-
23	CLA	B	613	2	-	8/39/115/115	-
25	BCR	t	103	-	-	0/29/63/63	0/2/2/2
27	GOL	c	742[A]	-	-	0/4/4/4	-
23	CLA	A	404[A]	1	-	3/39/115/115	-
23	CLA	C	507	3	-	13/39/115/115	-
33	LMG	Z	101	-	-	11/31/51/70	0/1/1/1
37	LHG	D	410[A]	-	-	17/53/53/53	-
32	LMT	E	102	-	-	8/21/61/61	0/2/2/2
32	LMT	a	414	-	-	12/21/61/61	0/2/2/2
27	GOL	b	901	-	-	0/4/4/4	-
37	LHG	e	101[A]	-	-	16/46/46/53	-
23	CLA	d	402[A]	4	-	4/39/115/115	-
25	BCR	d	404	-	-	4/29/63/63	0/2/2/2
25	BCR	c	515	-	-	1/29/63/63	0/2/2/2
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
23	CLA	C	509	3	-	6/39/115/115	-
23	CLA	b	607	41	-	4/39/115/115	-
37	LHG	l	101[B]	-	-	17/53/53/53	-
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
23	CLA	C	510	3	-	6/39/115/115	-
23	CLA	b	609	2	-	1/39/115/115	-
38	HEM	e	87	5,6	-	8/14/54/54	-
32	LMT	I	101	-	-	15/21/61/61	0/2/2/2
27	GOL	c	743	-	-	4/4/4/4	-
32	LMT	t	102	-	-	9/17/38/61	0/1/1/2

All (1865) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	407[B]	PHO	C1D-C2D	9.36	1.50	1.39
24	a	408[A]	PHO	C1B-C2B	9.21	1.49	1.39
24	a	353[B]	PHO	C1D-C2D	9.12	1.49	1.39
24	A	407[B]	PHO	C1B-C2B	8.99	1.49	1.39
24	a	408[B]	PHO	C1B-C2B	8.96	1.49	1.39
24	a	353[B]	PHO	C1B-C2B	8.91	1.49	1.39
24	A	407[A]	PHO	C1D-C2D	8.89	1.49	1.39
24	a	353[A]	PHO	C1B-C2B	8.69	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	353[B]	PHO	C1B-C2B	8.68	1.49	1.39
24	A	353[A]	PHO	C1B-C2B	8.65	1.49	1.39
24	a	353[A]	PHO	C1D-C2D	8.62	1.49	1.39
24	A	353[A]	PHO	C1D-C2D	8.53	1.49	1.39
24	a	408[B]	PHO	C1D-C2D	8.52	1.49	1.39
24	A	407[A]	PHO	C1B-C2B	8.45	1.48	1.39
24	a	408[A]	PHO	C1D-C2D	8.40	1.48	1.39
24	A	353[B]	PHO	C1D-C2D	8.35	1.48	1.39
23	B	611	CLA	CMB-C2B	8.20	1.68	1.50
40	v	202	HEC	C3D-C2D	8.12	1.54	1.36
40	V	202	HEC	C3D-C2D	7.48	1.52	1.36
24	a	353[A]	PHO	C3B-C4B	7.31	1.49	1.41
24	A	353[B]	PHO	C3B-C4B	7.22	1.49	1.41
24	A	353[A]	PHO	C3B-C4B	7.11	1.49	1.41
23	B	611	CLA	C1B-C2B	7.09	1.59	1.43
24	a	353[B]	PHO	C3B-C4B	6.76	1.49	1.41
24	a	408[A]	PHO	C3B-C4B	6.66	1.49	1.41
24	a	408[B]	PHO	C3B-C4B	6.65	1.49	1.41
24	a	408[A]	PHO	C4D-CHA	6.54	1.50	1.39
24	a	408[B]	PHO	C4D-CHA	6.44	1.49	1.39
24	A	407[B]	PHO	C3B-C4B	6.43	1.48	1.41
24	a	408[A]	PHO	C3B-C2B	6.39	1.49	1.40
23	B	611	CLA	C1D-ND	6.38	1.45	1.37
24	A	407[B]	PHO	C4D-CHA	6.37	1.49	1.39
24	A	353[B]	PHO	C3B-C2B	6.29	1.49	1.40
24	A	353[A]	PHO	C4D-CHA	6.27	1.49	1.39
24	A	353[B]	PHO	C4D-CHA	6.21	1.49	1.39
24	A	407[A]	PHO	C3B-C4B	6.16	1.48	1.41
24	A	407[A]	PHO	C4D-CHA	6.13	1.49	1.39
24	a	353[B]	PHO	C4D-CHA	6.13	1.49	1.39
24	A	407[A]	PHO	C3B-C2B	6.13	1.48	1.40
24	a	408[B]	PHO	C3B-C2B	6.12	1.48	1.40
23	B	611	CLA	C3C-C2C	6.10	1.49	1.36
24	a	353[B]	PHO	C3B-C2B	6.10	1.48	1.40
24	A	407[B]	PHO	C3B-C2B	6.09	1.48	1.40
24	a	353[A]	PHO	C4D-CHA	6.05	1.49	1.39
24	A	353[A]	PHO	C3B-C2B	5.94	1.48	1.40
24	a	353[A]	PHO	C3B-C2B	5.88	1.48	1.40
24	a	353[A]	PHO	C3C-C2C	5.86	1.49	1.36
23	B	610	CLA	C3C-C2C	5.86	1.49	1.36
24	a	353[B]	PHO	C3C-C2C	5.83	1.49	1.36
24	A	407[B]	PHO	C3C-C2C	5.81	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	353[B]	PHO	C3C-C2C	5.80	1.49	1.36
23	B	611	CLA	CHC-C1C	5.74	1.50	1.38
24	A	353[A]	PHO	C3C-C2C	5.72	1.48	1.36
24	A	407[A]	PHO	C3C-C2C	5.71	1.48	1.36
23	A	404[B]	CLA	C3C-C2C	5.66	1.48	1.36
23	b	601	CLA	C1D-ND	5.66	1.44	1.37
23	B	604	CLA	C3C-C2C	5.63	1.48	1.36
23	C	503	CLA	C1D-ND	5.62	1.44	1.37
24	a	408[B]	PHO	C3D-C2D	5.59	1.49	1.39
23	b	606	CLA	C3C-C2C	5.58	1.48	1.36
23	a	406[A]	CLA	C3C-C2C	5.58	1.48	1.36
23	a	406[B]	CLA	C3C-C2C	5.56	1.48	1.36
23	C	513	CLA	C3C-C2C	5.56	1.48	1.36
23	c	509	CLA	C3C-C2C	5.55	1.48	1.36
23	d	403	CLA	C3C-C2C	5.54	1.48	1.36
23	c	513	CLA	C3C-C2C	5.54	1.48	1.36
23	b	612	CLA	C3C-C2C	5.54	1.48	1.36
23	a	405[B]	CLA	C3C-C2C	5.51	1.48	1.36
23	C	504	CLA	C3C-C2C	5.51	1.48	1.36
23	B	605	CLA	C3C-C2C	5.50	1.48	1.36
23	D	406	CLA	C3C-C2C	5.48	1.48	1.36
23	b	615	CLA	C3C-C2C	5.48	1.48	1.36
23	d	403	CLA	C1D-ND	5.47	1.44	1.37
23	b	614	CLA	C3C-C2C	5.47	1.48	1.36
23	A	408	CLA	C3C-C2C	5.47	1.48	1.36
24	a	353[A]	PHO	C3D-C2D	5.46	1.49	1.39
24	a	408[A]	PHO	C3D-C2D	5.46	1.49	1.39
23	b	605	CLA	C3C-C2C	5.45	1.48	1.36
23	b	601	CLA	C3C-C2C	5.45	1.48	1.36
23	c	504	CLA	C3C-C2C	5.44	1.48	1.36
23	c	507	CLA	C1D-ND	5.44	1.44	1.37
24	a	353[B]	PHO	C3D-C2D	5.43	1.49	1.39
23	A	404[A]	CLA	C3C-C2C	5.43	1.48	1.36
23	a	406[A]	CLA	C1D-ND	5.42	1.44	1.37
24	A	353[B]	PHO	C3D-C2D	5.42	1.49	1.39
23	b	607	CLA	C3C-C2C	5.41	1.48	1.36
23	c	510	CLA	C3C-C2C	5.41	1.48	1.36
23	c	509	CLA	O2D-CGD	5.40	1.46	1.33
23	A	405[B]	CLA	C3C-C2C	5.39	1.48	1.36
23	c	512	CLA	C3C-C2C	5.38	1.48	1.36
23	c	503	CLA	C3C-C2C	5.37	1.48	1.36
23	c	506	CLA	C3C-C2C	5.37	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	C1D-ND	5.37	1.44	1.37
23	B	601	CLA	C3C-C2C	5.36	1.48	1.36
24	a	408[A]	PHO	C3C-C2C	5.36	1.48	1.36
23	C	511	CLA	C1D-ND	5.36	1.44	1.37
23	b	609	CLA	O2D-CGD	5.35	1.46	1.33
23	b	610	CLA	C3C-C2C	5.35	1.48	1.36
23	A	405[B]	CLA	C1D-ND	5.35	1.44	1.37
23	C	511	CLA	C3C-C2C	5.35	1.48	1.36
23	a	406[B]	CLA	C1D-ND	5.34	1.44	1.37
23	b	616	CLA	C3C-C2C	5.34	1.48	1.36
23	a	407[B]	CLA	C3C-C2C	5.34	1.48	1.36
24	A	353[A]	PHO	C3D-C2D	5.33	1.49	1.39
23	C	505	CLA	C3C-C2C	5.33	1.48	1.36
23	B	603	CLA	C3C-C2C	5.32	1.48	1.36
23	A	406[B]	CLA	C3C-C2C	5.32	1.48	1.36
23	a	409	CLA	CHC-C1C	5.32	1.49	1.38
24	a	408[B]	PHO	C3C-C2C	5.31	1.48	1.36
23	a	409	CLA	C3C-C2C	5.31	1.48	1.36
23	a	407[A]	CLA	C3C-C2C	5.31	1.48	1.36
23	D	405[A]	CLA	C3C-C2C	5.30	1.48	1.36
23	b	603	CLA	C3C-C2C	5.30	1.48	1.36
24	a	353[A]	PHO	OBD-CAD	5.30	1.29	1.22
23	c	514	CLA	C3C-C2C	5.29	1.48	1.36
23	d	402[B]	CLA	C3C-C2C	5.29	1.48	1.36
23	c	505	CLA	C1D-ND	5.29	1.44	1.37
24	A	353[A]	PHO	OBD-CAD	5.28	1.29	1.22
24	a	353[B]	PHO	OBD-CAD	5.28	1.29	1.22
23	B	614	CLA	C3C-C2C	5.27	1.47	1.36
23	b	616	CLA	C1D-ND	5.25	1.44	1.37
23	D	406	CLA	C1D-ND	5.25	1.44	1.37
23	b	602	CLA	C3C-C2C	5.25	1.47	1.36
23	c	504	CLA	C1D-ND	5.25	1.44	1.37
24	a	408[A]	PHO	O2D-CGD	5.24	1.46	1.33
23	B	608	CLA	C3C-C2C	5.23	1.47	1.36
23	c	512	CLA	C1D-ND	5.22	1.44	1.37
23	B	614	CLA	C1D-ND	5.22	1.44	1.37
23	B	616	CLA	C3C-C2C	5.21	1.47	1.36
23	c	505	CLA	O2D-CGD	5.21	1.45	1.33
23	C	513	CLA	CHC-C1C	5.21	1.49	1.38
23	C	509	CLA	C1D-ND	5.21	1.44	1.37
23	c	511	CLA	O2D-CGD	5.19	1.45	1.33
23	C	503	CLA	C3C-C2C	5.19	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C1D-ND	5.18	1.44	1.37
23	C	510	CLA	C3C-C2C	5.18	1.47	1.36
23	B	602	CLA	C1D-ND	5.18	1.44	1.37
23	A	406[B]	CLA	CHC-C1C	5.17	1.49	1.38
23	D	405[B]	CLA	C3C-C2C	5.17	1.47	1.36
23	c	506	CLA	CHC-C1C	5.16	1.49	1.38
23	c	510	CLA	O2D-CGD	5.16	1.45	1.33
23	B	604	CLA	O2D-CGD	5.16	1.45	1.33
23	C	508	CLA	C3C-C2C	5.15	1.47	1.36
23	b	602	CLA	O2D-CGD	5.15	1.45	1.33
23	A	405[A]	CLA	O2D-CGD	5.14	1.45	1.33
23	b	604	CLA	C3C-C2C	5.14	1.47	1.36
23	c	502	CLA	C1D-ND	5.14	1.44	1.37
23	c	507	CLA	C3C-C2C	5.13	1.47	1.36
23	A	406[A]	CLA	C3C-C2C	5.13	1.47	1.36
23	c	505	CLA	C3C-C2C	5.13	1.47	1.36
23	a	405[A]	CLA	C1D-ND	5.13	1.44	1.37
23	A	404[A]	CLA	C1D-ND	5.13	1.44	1.37
23	a	405[B]	CLA	C1D-ND	5.12	1.44	1.37
23	A	404[B]	CLA	C1D-ND	5.12	1.44	1.37
23	a	407[B]	CLA	O2D-CGD	5.10	1.45	1.33
23	D	405[B]	CLA	O2D-CGD	5.09	1.45	1.33
23	b	610	CLA	O2D-CGD	5.09	1.45	1.33
23	d	402[A]	CLA	C3C-C2C	5.09	1.47	1.36
23	C	502	CLA	C3C-C2C	5.09	1.47	1.36
23	c	502	CLA	C3C-C2C	5.08	1.47	1.36
23	b	603	CLA	O2D-CGD	5.08	1.45	1.33
23	C	512	CLA	O2D-CGD	5.08	1.45	1.33
23	C	514	CLA	C3C-C2C	5.08	1.47	1.36
23	A	406[B]	CLA	O2D-CGD	5.08	1.45	1.33
23	b	606	CLA	C1D-ND	5.08	1.44	1.37
23	C	502	CLA	C1D-ND	5.07	1.44	1.37
23	B	605	CLA	C1D-ND	5.07	1.44	1.37
23	B	615	CLA	O2D-CGD	5.07	1.45	1.33
23	c	511	CLA	C3C-C2C	5.07	1.47	1.36
23	B	601	CLA	O2A-CGA	5.06	1.48	1.33
23	C	506	CLA	CHC-C1C	5.06	1.48	1.38
24	A	353[B]	PHO	O2D-CGD	5.06	1.45	1.33
23	A	404[B]	CLA	O2D-CGD	5.06	1.45	1.33
40	V	202	HEC	FE-ND	5.05	2.10	1.94
23	b	602	CLA	CHC-C1C	5.04	1.48	1.38
24	a	353[B]	PHO	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	O2D-CGD	5.04	1.45	1.33
24	A	407[B]	PHO	C3D-C2D	5.04	1.48	1.39
23	B	602	CLA	C3C-C2C	5.02	1.47	1.36
23	a	405[A]	CLA	C3C-C2C	5.02	1.47	1.36
23	B	611	CLA	O2D-CGD	5.01	1.45	1.33
23	a	405[B]	CLA	O2D-CGD	5.00	1.45	1.33
23	B	609	CLA	C3C-C2C	5.00	1.47	1.36
23	B	611	CLA	CHC-C4B	5.00	1.50	1.39
23	B	605	CLA	O2D-CGD	5.00	1.45	1.33
23	B	612	CLA	CHC-C1C	5.00	1.48	1.38
23	B	615	CLA	C3C-C2C	4.99	1.47	1.36
23	C	504	CLA	CHC-C1C	4.99	1.48	1.38
24	a	408[B]	PHO	O2D-CGD	4.99	1.45	1.33
23	C	507	CLA	C3C-C2C	4.98	1.47	1.36
23	c	514	CLA	O2D-CGD	4.98	1.45	1.33
23	B	603	CLA	C1D-ND	4.97	1.43	1.37
23	C	507	CLA	O2D-CGD	4.97	1.45	1.33
23	C	510	CLA	CHD-C1D	4.97	1.48	1.38
23	c	507	CLA	O2D-CGD	4.96	1.45	1.33
23	C	506	CLA	C3C-C2C	4.96	1.47	1.36
23	c	504	CLA	CHC-C1C	4.96	1.48	1.38
23	C	510	CLA	O2D-CGD	4.96	1.45	1.33
23	B	610	CLA	O2D-CGD	4.96	1.45	1.33
23	A	405[A]	CLA	C3C-C2C	4.96	1.47	1.36
23	C	509	CLA	C3C-C2C	4.96	1.47	1.36
23	B	601	CLA	C1D-ND	4.96	1.43	1.37
23	C	514	CLA	C1D-ND	4.95	1.43	1.37
23	a	406[A]	CLA	O2D-CGD	4.95	1.45	1.33
24	A	353[A]	PHO	O2D-CGD	4.95	1.45	1.33
23	B	613	CLA	O2D-CGD	4.95	1.45	1.33
25	y	101	BCR	C23-C22	-4.95	1.35	1.45
23	b	613	CLA	O2D-CGD	4.95	1.45	1.33
23	c	513	CLA	C1D-ND	4.95	1.43	1.37
23	A	406[A]	CLA	CHC-C1C	4.95	1.48	1.38
23	b	613	CLA	C3C-C2C	4.94	1.47	1.36
23	c	513	CLA	CHC-C1C	4.94	1.48	1.38
23	B	611	CLA	C4B-NB	-4.93	1.31	1.37
38	e	87	HEM	FE-NB	4.93	2.10	1.94
23	B	615	CLA	C1D-ND	4.92	1.43	1.37
25	k	101	BCR	C23-C22	-4.92	1.35	1.45
23	c	508	CLA	C3C-C2C	4.92	1.47	1.36
24	A	407[B]	PHO	O2D-CGD	4.91	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	O2D-CGD	4.91	1.45	1.33
25	d	404	BCR	C23-C22	-4.91	1.35	1.45
23	B	609	CLA	O2D-CGD	4.91	1.45	1.33
24	A	407[A]	PHO	O2D-CGD	4.91	1.45	1.33
23	C	510	CLA	C1D-ND	4.91	1.43	1.37
25	C	515	BCR	C23-C22	-4.90	1.35	1.45
25	C	516	BCR	C23-C22	-4.90	1.35	1.45
23	D	406	CLA	O2D-CGD	4.90	1.45	1.33
23	b	613	CLA	C1D-ND	4.90	1.43	1.37
23	a	406[B]	CLA	O2D-CGD	4.90	1.45	1.33
23	A	405[B]	CLA	O2D-CGD	4.89	1.45	1.33
23	c	510	CLA	C1D-ND	4.89	1.43	1.37
23	B	612	CLA	C3C-C2C	4.88	1.47	1.36
23	D	405[A]	CLA	O2D-CGD	4.88	1.45	1.33
23	c	511	CLA	C1D-ND	4.88	1.43	1.37
25	K	102	BCR	C23-C22	-4.88	1.35	1.45
23	c	508	CLA	O2D-CGD	4.87	1.45	1.33
23	b	610	CLA	CHC-C1C	4.86	1.48	1.38
23	B	606	CLA	CHC-C1C	4.85	1.48	1.38
23	a	405[B]	CLA	CHC-C1C	4.84	1.48	1.38
24	a	353[A]	PHO	O2D-CGD	4.84	1.45	1.33
23	B	602	CLA	CHC-C1C	4.84	1.48	1.38
23	C	503	CLA	O2D-CGD	4.84	1.45	1.33
23	b	601	CLA	O2A-CGA	4.84	1.47	1.33
23	C	511	CLA	O2D-CGD	4.83	1.45	1.33
23	c	512	CLA	O2D-CGD	4.83	1.45	1.33
23	B	612	CLA	C1B-NB	-4.83	1.31	1.37
23	B	606	CLA	C3C-C2C	4.83	1.47	1.36
23	b	611	CLA	C3C-C2C	4.81	1.47	1.36
23	A	408	CLA	O2D-CGD	4.81	1.44	1.33
23	c	502	CLA	CHC-C1C	4.81	1.48	1.38
23	A	404[B]	CLA	CHC-C1C	4.80	1.48	1.38
23	b	604	CLA	C1D-ND	4.80	1.43	1.37
23	B	601	CLA	O2D-CGD	4.80	1.44	1.33
26	F	101	SQD	O47-C7	4.79	1.47	1.34
24	A	407[A]	PHO	C3D-C2D	4.79	1.48	1.39
23	d	403	CLA	CHC-C1C	4.79	1.48	1.38
23	C	514	CLA	O2D-CGD	4.78	1.44	1.33
23	a	406[B]	CLA	CHC-C1C	4.78	1.48	1.38
25	B	619	BCR	C23-C22	-4.78	1.35	1.45
23	b	605	CLA	C1D-ND	4.78	1.43	1.37
23	b	602	CLA	C1D-ND	4.78	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	504	CLA	CHD-C1D	4.78	1.47	1.38
23	B	604	CLA	CHD-C1D	4.77	1.47	1.38
23	b	614	CLA	CHC-C1C	4.77	1.48	1.38
23	b	612	CLA	C1D-ND	4.77	1.43	1.37
23	A	404[A]	CLA	O2D-CGD	4.77	1.44	1.33
38	E	103	HEM	FE-NB	4.77	2.09	1.94
23	B	615	CLA	CHD-C1D	4.77	1.47	1.38
23	B	610	CLA	CHC-C1C	4.77	1.48	1.38
23	B	606	CLA	O2D-CGD	4.76	1.44	1.33
23	C	506	CLA	C1D-ND	4.76	1.43	1.37
23	b	609	CLA	C3C-C2C	4.76	1.46	1.36
23	a	407[B]	CLA	CHC-C1C	4.76	1.48	1.38
33	c	521	LMG	O7-C10	4.75	1.47	1.34
23	c	509	CLA	C1D-ND	4.75	1.43	1.37
23	d	402[B]	CLA	O2D-CGD	4.75	1.44	1.33
23	B	607	CLA	C3C-C2C	4.74	1.46	1.36
23	B	613	CLA	CHC-C1C	4.74	1.48	1.38
23	B	603	CLA	O2D-CGD	4.74	1.44	1.33
23	c	509	CLA	CHC-C1C	4.74	1.48	1.38
25	D	407	BCR	C23-C22	-4.74	1.35	1.45
23	b	601	CLA	O2D-CGD	4.73	1.44	1.33
23	c	512	CLA	CHC-C1C	4.73	1.48	1.38
25	B	617	BCR	C23-C22	-4.73	1.35	1.45
25	t	103	BCR	C23-C22	-4.73	1.35	1.45
23	A	406[A]	CLA	O2D-CGD	4.73	1.44	1.33
23	b	608	CLA	C3C-C2C	4.72	1.46	1.36
23	b	602	CLA	CHD-C1D	4.72	1.47	1.38
23	c	514	CLA	CHC-C1C	4.71	1.48	1.38
33	C	521	LMG	O7-C10	4.71	1.47	1.34
23	b	609	CLA	C1D-ND	4.70	1.43	1.37
23	b	615	CLA	CHC-C1C	4.70	1.48	1.38
23	C	505	CLA	O2D-CGD	4.70	1.44	1.33
23	b	614	CLA	O2D-CGD	4.70	1.44	1.33
23	A	405[B]	CLA	CHC-C1C	4.70	1.48	1.38
23	c	508	CLA	CHC-C1C	4.69	1.48	1.38
23	B	605	CLA	CHC-C1C	4.69	1.48	1.38
23	b	603	CLA	CHC-C1C	4.68	1.48	1.38
23	c	503	CLA	C1D-ND	4.68	1.43	1.37
26	f	102	SQD	O47-C7	4.68	1.47	1.34
23	C	507	CLA	CHD-C1D	4.67	1.47	1.38
25	T	101	BCR	C23-C22	-4.67	1.35	1.45
23	C	511	CLA	CHC-C1C	4.67	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CHC-C1C	4.66	1.48	1.38
23	b	607	CLA	C1B-NB	-4.66	1.32	1.37
23	b	607	CLA	CHD-C1D	4.66	1.47	1.38
23	B	602	CLA	O2D-CGD	4.65	1.44	1.33
23	B	606	CLA	C1D-ND	4.65	1.43	1.37
23	a	407[A]	CLA	O2D-CGD	4.65	1.44	1.33
23	b	604	CLA	CHC-C1C	4.65	1.48	1.38
23	a	405[A]	CLA	CHC-C1C	4.64	1.47	1.38
23	B	613	CLA	C3C-C2C	4.64	1.46	1.36
23	B	601	CLA	CHC-C1C	4.64	1.47	1.38
23	C	502	CLA	CHC-C1C	4.63	1.47	1.38
23	b	614	CLA	C1D-ND	4.63	1.43	1.37
23	B	609	CLA	CHC-C1C	4.62	1.47	1.38
23	B	614	CLA	CHC-C1C	4.62	1.47	1.38
23	C	504	CLA	O2D-CGD	4.62	1.44	1.33
26	B	620	SQD	O47-C7	4.62	1.47	1.34
24	A	407[B]	PHO	OBD-CAD	4.62	1.28	1.22
23	B	610	CLA	C1D-ND	4.61	1.43	1.37
23	A	405[A]	CLA	CHC-C1C	4.61	1.47	1.38
23	D	406	CLA	CHC-C1C	4.61	1.47	1.38
23	c	503	CLA	O2D-CGD	4.61	1.44	1.33
23	a	407[A]	CLA	CHC-C1C	4.61	1.47	1.38
23	c	508	CLA	C1D-ND	4.61	1.43	1.37
23	b	609	CLA	CHC-C1C	4.61	1.47	1.38
23	a	409	CLA	O2D-CGD	4.61	1.44	1.33
23	C	505	CLA	CHC-C1C	4.60	1.47	1.38
23	C	512	CLA	C3C-C2C	4.60	1.46	1.36
23	D	406	CLA	CHD-C1D	4.60	1.47	1.38
23	C	509	CLA	O2D-CGD	4.60	1.44	1.33
24	a	408[B]	PHO	OBD-CAD	4.60	1.28	1.22
23	a	407[B]	CLA	C1D-ND	4.59	1.43	1.37
26	a	413	SQD	O48-C23	4.59	1.46	1.33
23	d	402[A]	CLA	O2D-CGD	4.59	1.44	1.33
37	E	101[A]	LHG	O8-C23	4.57	1.46	1.33
23	C	506	CLA	O2D-CGD	4.56	1.44	1.33
23	A	406[B]	CLA	C1D-ND	4.56	1.43	1.37
26	A	412	SQD	O48-C23	4.55	1.46	1.33
23	C	507	CLA	C1D-ND	4.55	1.43	1.37
23	A	405[A]	CLA	C1D-ND	4.55	1.43	1.37
25	b	619	BCR	C23-C22	-4.54	1.36	1.45
23	D	405[A]	CLA	CHC-C1C	4.54	1.47	1.38
25	b	618	BCR	C23-C22	-4.53	1.36	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	CHD-C1D	4.53	1.47	1.38
23	b	605	CLA	O2D-CGD	4.53	1.44	1.33
23	B	616	CLA	O2D-CGD	4.53	1.44	1.33
23	c	513	CLA	O2D-CGD	4.53	1.44	1.33
23	C	506	CLA	CHD-C1D	4.53	1.47	1.38
23	B	614	CLA	C4B-NB	-4.52	1.32	1.37
23	C	509	CLA	CHC-C1C	4.52	1.47	1.38
23	B	610	CLA	OBD-CAD	4.52	1.30	1.22
24	A	353[B]	PHO	OBD-CAD	4.51	1.28	1.22
23	C	502	CLA	CHD-C1D	4.51	1.47	1.38
23	b	613	CLA	CHC-C1C	4.51	1.47	1.38
37	e	101[A]	LHG	O8-C23	4.50	1.46	1.33
23	C	508	CLA	CHC-C1C	4.50	1.47	1.38
25	c	516	BCR	C23-C22	-4.49	1.36	1.45
33	z	101	LMG	O8-C28	4.49	1.46	1.33
23	A	408	CLA	O2A-CGA	4.49	1.46	1.33
23	C	512	CLA	CHC-C1C	4.49	1.47	1.38
23	b	601	CLA	CHC-C1C	4.48	1.47	1.38
23	C	514	CLA	CHC-C1C	4.48	1.47	1.38
23	b	616	CLA	CHC-C1C	4.48	1.47	1.38
23	a	407[A]	CLA	C1D-ND	4.48	1.43	1.37
23	A	404[A]	CLA	CHC-C1C	4.48	1.47	1.38
23	B	610	CLA	C3D-C2D	4.48	1.51	1.39
23	d	402[B]	CLA	CHC-C1C	4.48	1.47	1.38
26	b	620	SQD	O47-C7	4.46	1.46	1.34
33	C	521	LMG	O8-C28	4.46	1.46	1.33
25	a	410	BCR	C23-C22	-4.46	1.36	1.45
23	b	612	CLA	O2D-CGD	4.46	1.44	1.33
23	d	403	CLA	O2A-CGA	4.45	1.46	1.33
37	E	101[B]	LHG	O8-C23	4.45	1.46	1.33
25	b	617	BCR	C23-C22	-4.45	1.36	1.45
23	A	408	CLA	C1D-ND	4.45	1.43	1.37
23	b	612	CLA	CHC-C1C	4.44	1.47	1.38
23	B	608	CLA	O2D-CGD	4.44	1.44	1.33
23	a	406[A]	CLA	CHC-C1C	4.44	1.47	1.38
23	b	604	CLA	CHD-C1D	4.44	1.47	1.38
23	b	608	CLA	CHC-C1C	4.43	1.47	1.38
23	B	611	CLA	CHB-C1B	4.43	1.49	1.39
23	b	606	CLA	O2D-CGD	4.42	1.44	1.33
23	B	607	CLA	O2D-CGD	4.42	1.44	1.33
23	b	611	CLA	CHC-C1C	4.42	1.47	1.38
23	d	403	CLA	O2D-CGD	4.41	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	514	CLA	O2A-CGA	4.41	1.46	1.33
23	B	615	CLA	CHC-C1C	4.41	1.47	1.38
23	C	503	CLA	CHC-C1C	4.40	1.47	1.38
23	b	611	CLA	O2D-CGD	4.40	1.43	1.33
25	c	515	BCR	C23-C22	-4.39	1.36	1.45
23	b	614	CLA	CHD-C1D	4.38	1.46	1.38
23	a	405[A]	CLA	O2D-CGD	4.38	1.43	1.33
23	b	607	CLA	CHC-C1C	4.38	1.47	1.38
23	b	616	CLA	O2D-CGD	4.37	1.43	1.33
23	D	405[B]	CLA	CHC-C1C	4.37	1.47	1.38
23	C	513	CLA	O2D-CGD	4.37	1.43	1.33
23	B	614	CLA	O2D-CGD	4.37	1.43	1.33
23	C	507	CLA	CHC-C1C	4.37	1.47	1.38
23	b	604	CLA	CHC-C4B	4.36	1.49	1.39
37	e	101[B]	LHG	O8-C23	4.35	1.46	1.33
23	c	506	CLA	O2D-CGD	4.35	1.43	1.33
23	b	607	CLA	O2D-CGD	4.35	1.43	1.33
23	B	609	CLA	CHD-C1D	4.35	1.46	1.38
23	D	405[B]	CLA	O2A-CGA	4.34	1.46	1.33
23	b	602	CLA	CHC-C4B	4.34	1.49	1.39
23	c	513	CLA	CHD-C1D	4.34	1.46	1.38
25	Y	101	BCR	C23-C22	-4.34	1.36	1.45
23	c	512	CLA	CHD-C1D	4.34	1.46	1.38
23	C	514	CLA	O2A-CGA	4.34	1.46	1.33
23	C	508	CLA	O2D-CGD	4.34	1.43	1.33
23	B	616	CLA	C1D-ND	4.34	1.43	1.37
23	c	506	CLA	CHD-C1D	4.33	1.46	1.38
23	A	406[A]	CLA	C1B-NB	-4.33	1.32	1.37
23	B	604	CLA	CHC-C1C	4.33	1.47	1.38
26	b	620	SQD	O48-C23	4.33	1.46	1.33
23	C	503	CLA	CHD-C1D	4.33	1.46	1.38
23	c	502	CLA	CHD-C1D	4.33	1.46	1.38
23	A	405[B]	CLA	O2A-CGA	4.32	1.46	1.33
23	B	607	CLA	CHC-C1C	4.31	1.47	1.38
23	c	508	CLA	O2A-CGA	4.31	1.45	1.33
23	a	406[A]	CLA	C3D-C2D	4.30	1.50	1.39
23	B	616	CLA	C3D-C2D	4.30	1.50	1.39
23	c	507	CLA	CHD-C1D	4.30	1.46	1.38
23	b	602	CLA	CHD-C4C	4.29	1.49	1.39
23	C	512	CLA	C1D-ND	4.29	1.43	1.37
23	b	611	CLA	C1D-ND	4.29	1.43	1.37
26	f	102	SQD	O48-C23	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	507	CLA	CHD-C4C	4.29	1.49	1.39
23	A	406[B]	CLA	CHD-C1D	4.29	1.46	1.38
23	c	514	CLA	CHD-C1D	4.29	1.46	1.38
23	B	611	CLA	C1C-C2C	4.29	1.52	1.44
23	a	405[B]	CLA	CHD-C1D	4.29	1.46	1.38
23	b	611	CLA	O2A-CGA	4.29	1.45	1.33
37	e	101[A]	LHG	O7-C7	4.28	1.46	1.34
38	E	103	HEM	FE-NC	4.28	2.09	1.95
23	b	606	CLA	CHD-C1D	4.28	1.46	1.38
25	h	101	BCR	C23-C22	-4.28	1.36	1.45
33	C	520	LMG	O8-C28	4.28	1.45	1.33
25	H	101	BCR	C23-C22	-4.28	1.36	1.45
23	B	604	CLA	C1D-ND	4.28	1.43	1.37
26	B	620	SQD	O48-C23	4.27	1.45	1.33
23	b	615	CLA	C1D-ND	4.27	1.43	1.37
23	c	513	CLA	O2A-CGA	4.26	1.45	1.33
23	c	507	CLA	CHC-C1C	4.26	1.47	1.38
23	b	601	CLA	C3D-C2D	4.26	1.50	1.39
23	c	508	CLA	CHD-C1D	4.26	1.46	1.38
23	b	605	CLA	CHC-C1C	4.25	1.47	1.38
23	D	405[A]	CLA	C1D-ND	4.25	1.43	1.37
23	d	402[B]	CLA	O2A-CGA	4.25	1.45	1.33
23	B	607	CLA	C1B-NB	-4.24	1.32	1.37
23	b	610	CLA	CHD-C1D	4.24	1.46	1.38
23	B	611	CLA	C3B-C2B	4.24	1.55	1.41
23	b	613	CLA	C1B-NB	-4.24	1.32	1.37
23	C	512	CLA	CHD-C1D	4.24	1.46	1.38
23	c	505	CLA	CHC-C1C	4.24	1.47	1.38
23	B	607	CLA	CHD-C1D	4.24	1.46	1.38
23	A	405[B]	CLA	CHD-C1D	4.23	1.46	1.38
23	C	514	CLA	CHD-C1D	4.23	1.46	1.38
26	A	412	SQD	O47-C7	4.23	1.46	1.34
23	c	506	CLA	C1D-ND	4.23	1.43	1.37
23	b	606	CLA	CHC-C1C	4.23	1.47	1.38
23	A	404[B]	CLA	CHD-C1D	4.22	1.46	1.38
23	a	409	CLA	O2A-CGA	4.22	1.45	1.33
33	B	621	LMG	O8-C28	4.22	1.45	1.33
23	A	408	CLA	CHD-C1D	4.22	1.46	1.38
23	c	511	CLA	CHC-C1C	4.22	1.47	1.38
37	E	101[B]	LHG	O7-C7	4.22	1.46	1.34
23	C	510	CLA	C4B-NB	-4.22	1.32	1.37
23	C	505	CLA	C1D-ND	4.22	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	CHD-C1D	4.22	1.46	1.38
33	c	521	LMG	O8-C28	4.22	1.45	1.33
23	C	512	CLA	O2A-CGA	4.22	1.45	1.33
37	E	101[A]	LHG	O7-C7	4.22	1.46	1.34
23	C	513	CLA	CHC-C4B	4.21	1.48	1.39
37	e	101[B]	LHG	O7-C7	4.21	1.46	1.34
23	d	402[A]	CLA	CHC-C1C	4.21	1.47	1.38
37	L	101[B]	LHG	O8-C23	4.20	1.45	1.33
23	D	405[B]	CLA	C1D-ND	4.20	1.42	1.37
23	c	512	CLA	CHB-C1B	4.20	1.48	1.39
23	C	511	CLA	CHD-C4C	4.20	1.48	1.39
23	B	609	CLA	C1D-ND	4.20	1.42	1.37
33	Z	101	LMG	O7-C10	4.20	1.46	1.34
23	B	612	CLA	CHB-C1B	4.20	1.48	1.39
23	C	512	CLA	CHD-C4C	4.19	1.48	1.39
37	d	408[A]	LHG	O8-C23	4.19	1.45	1.33
23	D	405[A]	CLA	CHD-C1D	4.19	1.46	1.38
23	d	402[B]	CLA	CHD-C1D	4.19	1.46	1.38
23	B	607	CLA	OBD-CAD	4.19	1.29	1.22
23	B	602	CLA	CHD-C1D	4.19	1.46	1.38
23	b	610	CLA	C1D-ND	4.18	1.42	1.37
23	c	510	CLA	CHC-C1C	4.18	1.47	1.38
23	D	405[A]	CLA	O2A-CGA	4.18	1.45	1.33
23	b	610	CLA	CHB-C1B	4.18	1.48	1.39
25	A	409	BCR	C23-C22	-4.18	1.37	1.45
38	e	87	HEM	FE-NC	4.18	2.09	1.95
23	c	509	CLA	O2A-CGA	4.18	1.45	1.33
23	B	615	CLA	O2A-CGA	4.17	1.45	1.33
23	b	601	CLA	CHD-C4C	4.17	1.48	1.39
26	a	413	SQD	O47-C7	4.16	1.46	1.34
23	C	504	CLA	C1D-ND	4.16	1.42	1.37
23	C	502	CLA	O2D-CGD	4.16	1.43	1.33
23	B	609	CLA	O2A-CGA	4.15	1.45	1.33
23	c	513	CLA	CHD-C4C	4.15	1.48	1.39
23	B	612	CLA	C4B-NB	-4.15	1.32	1.37
23	c	512	CLA	O2A-CGA	4.15	1.45	1.33
23	B	605	CLA	CHC-C4B	4.15	1.48	1.39
23	b	615	CLA	O2A-CGA	4.15	1.45	1.33
23	b	609	CLA	CHD-C1D	4.15	1.46	1.38
23	b	615	CLA	CHD-C1D	4.15	1.46	1.38
23	C	510	CLA	OBD-CAD	4.14	1.29	1.22
33	c	520	LMG	O7-C10	4.14	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	CHD-C1D	4.13	1.46	1.38
35	C	517[A]	DGD	O2G-C1B	4.13	1.46	1.34
24	A	407[A]	PHO	OBD-CAD	4.13	1.28	1.22
23	C	506	CLA	CHD-C4C	4.13	1.48	1.39
35	c	518[B]	DGD	O1G-C1A	4.12	1.45	1.33
40	v	202	HEC	FE-NB	4.12	2.07	1.94
35	c	517[B]	DGD	O2G-C1B	4.12	1.45	1.34
23	a	406[A]	CLA	O2A-CGA	4.12	1.45	1.33
33	m	101	LMG	O8-C28	4.12	1.45	1.33
23	d	402[B]	CLA	CHB-C1B	4.12	1.48	1.39
37	d	408[B]	LHG	O8-C23	4.12	1.45	1.33
23	B	608	CLA	C3D-C2D	4.12	1.50	1.39
23	c	504	CLA	O2A-CGA	4.12	1.45	1.33
23	a	406[B]	CLA	C3D-C2D	4.11	1.50	1.39
23	c	509	CLA	C3D-C2D	4.11	1.50	1.39
23	a	405[A]	CLA	CHD-C1D	4.11	1.46	1.38
23	a	407[B]	CLA	O2A-CGA	4.11	1.45	1.33
23	B	613	CLA	CHB-C1B	4.11	1.48	1.39
23	A	408	CLA	CHC-C1C	4.11	1.46	1.38
37	D	411[B]	LHG	O7-C7	4.11	1.45	1.34
23	a	406[A]	CLA	C1B-NB	-4.11	1.32	1.37
23	C	503	CLA	C3D-C2D	4.11	1.50	1.39
23	A	406[A]	CLA	CHD-C1D	4.10	1.46	1.38
23	A	405[A]	CLA	C3D-C2D	4.10	1.50	1.39
23	b	616	CLA	CHD-C1D	4.10	1.46	1.38
23	c	509	CLA	CHD-C1D	4.10	1.46	1.38
23	b	604	CLA	O2D-CGD	4.10	1.43	1.33
23	a	405[A]	CLA	CHD-C4C	4.10	1.48	1.39
23	d	402[B]	CLA	C1D-ND	4.09	1.42	1.37
23	b	616	CLA	O2A-CGA	4.09	1.45	1.33
23	c	507	CLA	O2A-CGA	4.09	1.45	1.33
35	c	519	DGD	O1G-C1A	4.09	1.45	1.33
23	c	506	CLA	CHC-C4B	4.09	1.48	1.39
23	A	406[A]	CLA	C1D-ND	4.09	1.42	1.37
23	c	504	CLA	O2D-CGD	4.09	1.43	1.33
23	D	406	CLA	C3D-C2D	4.09	1.50	1.39
33	a	419	LMG	O8-C28	4.09	1.45	1.33
23	C	508	CLA	O2A-CGA	4.08	1.45	1.33
23	C	504	CLA	CHD-C1D	4.08	1.46	1.38
23	b	609	CLA	CHB-C1B	4.08	1.48	1.39
23	C	510	CLA	C3D-C2D	4.08	1.50	1.39
33	C	520	LMG	O7-C10	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	411[B]	SQD	O48-C23	4.08	1.45	1.33
23	B	613	CLA	C1D-ND	4.08	1.42	1.37
23	C	505	CLA	CHB-C1B	4.07	1.48	1.39
23	A	405[A]	CLA	O2A-CGA	4.07	1.45	1.33
23	B	603	CLA	CHC-C1C	4.07	1.46	1.38
23	b	612	CLA	CHB-C1B	4.07	1.48	1.39
23	C	509	CLA	CHD-C1D	4.06	1.46	1.38
33	C	501	LMG	O7-C10	4.06	1.45	1.34
35	C	519	DGD	O1G-C1A	4.06	1.45	1.33
23	a	406[B]	CLA	O2A-CGA	4.06	1.45	1.33
23	B	602	CLA	C3D-C2D	4.06	1.50	1.39
23	D	406	CLA	CHB-C1B	4.06	1.48	1.39
23	b	610	CLA	OBD-CAD	4.05	1.29	1.22
23	C	506	CLA	CHC-C4B	4.05	1.48	1.39
23	b	614	CLA	CHC-C4B	4.05	1.48	1.39
40	v	202	HEC	FE-ND	4.05	2.07	1.94
26	a	411[A]	SQD	O47-C7	4.05	1.45	1.34
35	C	517[B]	DGD	O2G-C1B	4.05	1.45	1.34
23	c	504	CLA	CHD-C4C	4.05	1.48	1.39
23	A	404[B]	CLA	CHD-C4C	4.04	1.48	1.39
23	b	608	CLA	CHD-C1D	4.04	1.46	1.38
23	c	504	CLA	CHC-C4B	4.04	1.48	1.39
23	C	512	CLA	CHB-C1B	4.04	1.48	1.39
23	B	601	CLA	CHC-C4B	4.04	1.48	1.39
33	z	101	LMG	O7-C10	4.03	1.45	1.34
23	b	608	CLA	C3D-C2D	4.03	1.50	1.39
23	C	513	CLA	O2A-CGA	4.03	1.45	1.33
23	c	505	CLA	C3D-C2D	4.03	1.50	1.39
23	B	611	CLA	OBD-CAD	4.03	1.29	1.22
23	a	409	CLA	CHC-C4B	4.03	1.48	1.39
23	D	405[A]	CLA	CHB-C1B	4.02	1.48	1.39
23	b	609	CLA	OBD-CAD	4.02	1.29	1.22
35	c	517[B]	DGD	O1G-C1A	4.02	1.45	1.33
23	B	604	CLA	CHD-C4C	4.02	1.48	1.39
23	B	603	CLA	C3D-C2D	4.02	1.50	1.39
24	A	353[A]	PHO	O2A-CGA	4.02	1.45	1.33
23	a	405[A]	CLA	CHB-C1B	4.01	1.48	1.39
23	c	504	CLA	CHB-C1B	4.01	1.48	1.39
23	C	509	CLA	C3D-C2D	4.01	1.50	1.39
23	a	407[B]	CLA	C3D-C2D	4.01	1.50	1.39
23	A	406[B]	CLA	O2A-CGA	4.01	1.45	1.33
23	B	605	CLA	O2A-CGA	4.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	405[B]	CLA	CHB-C1B	4.01	1.48	1.39
35	c	518[A]	DGD	O1G-C1A	4.00	1.45	1.33
23	b	605	CLA	C1B-NB	-4.00	1.32	1.37
37	l	101[B]	LHG	O7-C7	4.00	1.45	1.34
23	A	406[B]	CLA	CHD-C4C	4.00	1.48	1.39
23	d	403	CLA	C3D-C2D	4.00	1.50	1.39
23	c	510	CLA	CHD-C1D	4.00	1.46	1.38
23	b	614	CLA	C3D-C2D	3.99	1.50	1.39
23	b	612	CLA	CHD-C1D	3.99	1.46	1.38
23	d	402[A]	CLA	CHB-C1B	3.99	1.48	1.39
23	c	507	CLA	C3D-C2D	3.99	1.50	1.39
23	c	502	CLA	O2A-CGA	3.98	1.45	1.33
23	a	409	CLA	CHB-C1B	3.98	1.48	1.39
23	b	605	CLA	CHD-C1D	3.98	1.46	1.38
23	c	505	CLA	CHD-C4C	3.98	1.48	1.39
23	c	510	CLA	O2A-CGA	3.98	1.45	1.33
23	b	610	CLA	CHC-C4B	3.98	1.48	1.39
23	c	513	CLA	CHC-C4B	3.97	1.48	1.39
23	A	405[A]	CLA	CHD-C1D	3.97	1.46	1.38
26	a	411[A]	SQD	O48-C23	3.97	1.44	1.33
23	c	503	CLA	O2A-CGA	3.97	1.44	1.33
23	b	608	CLA	OBD-CAD	3.97	1.29	1.22
26	A	410[B]	SQD	O48-C23	3.97	1.44	1.33
23	b	608	CLA	O2A-CGA	3.97	1.44	1.33
23	b	603	CLA	C1D-ND	3.97	1.42	1.37
23	c	502	CLA	CHD-C4C	3.97	1.48	1.39
23	B	602	CLA	CHB-C1B	3.97	1.48	1.39
23	c	514	CLA	CHD-C4C	3.97	1.48	1.39
23	b	611	CLA	CHB-C1B	3.96	1.48	1.39
23	c	503	CLA	CHC-C1C	3.96	1.46	1.38
23	B	614	CLA	CHB-C1B	3.96	1.48	1.39
26	a	411[B]	SQD	O47-C7	3.96	1.45	1.34
23	B	610	CLA	CHD-C1D	3.96	1.46	1.38
23	B	605	CLA	CHD-C1D	3.96	1.46	1.38
23	a	407[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	a	407[A]	CLA	C3D-C2D	3.96	1.49	1.39
23	c	502	CLA	O2D-CGD	3.96	1.42	1.33
35	h	102	DGD	O1G-C1A	3.96	1.44	1.33
23	c	510	CLA	CHB-C1B	3.96	1.48	1.39
23	d	402[A]	CLA	O2A-CGA	3.96	1.44	1.33
23	C	502	CLA	CHD-C4C	3.96	1.48	1.39
23	a	405[B]	CLA	CHD-C4C	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	511	CLA	CHB-C1B	3.95	1.48	1.39
23	b	612	CLA	OBD-CAD	3.95	1.29	1.22
24	A	407[B]	PHO	O2A-CGA	3.95	1.44	1.33
37	l	101[B]	LHG	O8-C23	3.95	1.44	1.33
23	A	406[A]	CLA	OBD-CAD	3.95	1.29	1.22
23	c	508	CLA	CHD-C4C	3.95	1.48	1.39
23	A	406[A]	CLA	C3D-C2D	3.95	1.49	1.39
23	B	604	CLA	OBD-CAD	3.94	1.29	1.22
23	C	507	CLA	O2A-CGA	3.94	1.44	1.33
23	B	613	CLA	C1B-NB	-3.94	1.32	1.37
33	C	501	LMG	O8-C28	3.94	1.44	1.33
23	c	503	CLA	CHD-C1D	3.94	1.46	1.38
23	b	606	CLA	O2A-CGA	3.94	1.44	1.33
23	A	406[B]	CLA	CHC-C4B	3.94	1.48	1.39
33	a	419	LMG	O7-C10	3.94	1.45	1.34
23	A	406[B]	CLA	C3D-C2D	3.94	1.49	1.39
26	F	101	SQD	O48-C23	3.93	1.44	1.33
23	c	509	CLA	CHD-C4C	3.93	1.48	1.39
23	B	613	CLA	CHD-C1D	3.93	1.46	1.38
23	B	602	CLA	CHD-C4C	3.93	1.48	1.39
23	A	404[B]	CLA	C1B-NB	-3.93	1.33	1.37
23	B	608	CLA	C1D-ND	3.93	1.42	1.37
33	c	520	LMG	O8-C28	3.93	1.44	1.33
23	d	402[A]	CLA	CHD-C1D	3.93	1.46	1.38
23	C	513	CLA	C3D-C2D	3.92	1.49	1.39
37	L	101[A]	LHG	O8-C23	3.92	1.44	1.33
23	B	614	CLA	CHD-C4C	3.91	1.48	1.39
23	c	503	CLA	C3D-C2D	3.91	1.49	1.39
23	D	405[B]	CLA	CHD-C1D	3.91	1.46	1.38
23	B	609	CLA	C3D-C2D	3.91	1.49	1.39
23	b	613	CLA	CHC-C4B	3.91	1.48	1.39
23	d	403	CLA	CHD-C1D	3.91	1.46	1.38
23	C	504	CLA	CHC-C4B	3.91	1.48	1.39
37	D	411[A]	LHG	O8-C23	3.91	1.44	1.33
23	b	616	CLA	C3D-C2D	3.90	1.49	1.39
23	c	510	CLA	C3D-C2D	3.90	1.49	1.39
35	C	517[B]	DGD	O1G-C1A	3.90	1.44	1.33
24	a	353[B]	PHO	O2A-CGA	3.90	1.44	1.33
23	B	612	CLA	O2D-CGD	3.90	1.42	1.33
23	c	502	CLA	C3D-C2D	3.90	1.49	1.39
37	d	407[A]	LHG	O7-C7	3.90	1.45	1.34
37	D	410[B]	LHG	O8-C23	3.90	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	CHD-C1D	3.89	1.45	1.38
23	c	506	CLA	CHD-C4C	3.89	1.48	1.39
37	D	411[A]	LHG	O7-C7	3.89	1.45	1.34
23	b	607	CLA	C1D-ND	3.89	1.42	1.37
23	B	603	CLA	C1B-NB	-3.89	1.33	1.37
35	h	102	DGD	O2G-C1B	3.89	1.45	1.34
23	B	603	CLA	O2A-CGA	3.89	1.44	1.33
23	c	506	CLA	CHB-C1B	3.88	1.48	1.39
23	c	511	CLA	O2A-CGA	3.88	1.44	1.33
23	A	405[B]	CLA	CHD-C4C	3.88	1.48	1.39
37	L	101[B]	LHG	O7-C7	3.88	1.45	1.34
23	c	508	CLA	C3D-C2D	3.88	1.49	1.39
37	D	411[B]	LHG	O8-C23	3.88	1.44	1.33
23	B	616	CLA	CHD-C1D	3.88	1.45	1.38
23	c	513	CLA	CHB-C1B	3.88	1.48	1.39
33	d	412	LMG	O8-C28	3.87	1.44	1.33
23	C	512	CLA	C3D-C2D	3.87	1.49	1.39
24	a	408[A]	PHO	OBD-CAD	3.87	1.27	1.22
23	c	505	CLA	CHD-C1D	3.87	1.45	1.38
23	C	509	CLA	O2A-CGA	3.87	1.44	1.33
23	c	511	CLA	C3D-C2D	3.87	1.49	1.39
23	C	503	CLA	O2A-CGA	3.87	1.44	1.33
23	B	616	CLA	O2A-CGA	3.87	1.44	1.33
23	b	607	CLA	C3D-C2D	3.87	1.49	1.39
23	C	507	CLA	CHD-C4C	3.87	1.48	1.39
24	A	353[B]	PHO	O2A-CGA	3.86	1.44	1.33
23	B	615	CLA	CHB-C1B	3.86	1.48	1.39
37	d	407[B]	LHG	O7-C7	3.86	1.45	1.34
37	d	408[B]	LHG	O7-C7	3.86	1.45	1.34
23	b	615	CLA	C3D-C2D	3.86	1.49	1.39
34	B	626	HTG	C1'-S1	-3.86	1.76	1.81
23	a	406[B]	CLA	C1B-NB	-3.86	1.33	1.37
23	B	606	CLA	CHB-C1B	3.86	1.48	1.39
23	c	510	CLA	CHD-C4C	3.85	1.48	1.39
23	c	513	CLA	C3D-C2D	3.85	1.49	1.39
23	a	407[B]	CLA	CHD-C4C	3.85	1.48	1.39
33	B	621	LMG	O7-C10	3.85	1.45	1.34
23	b	615	CLA	CHB-C1B	3.85	1.48	1.39
23	b	614	CLA	CHB-C1B	3.85	1.48	1.39
23	C	502	CLA	O2A-CGA	3.84	1.44	1.33
24	a	353[A]	PHO	O2A-CGA	3.84	1.44	1.33
35	C	518[A]	DGD	O2G-C1B	3.84	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	406[A]	CLA	OBD-CAD	3.84	1.29	1.22
23	C	510	CLA	CHC-C1C	3.84	1.46	1.38
23	B	611	CLA	O2A-CGA	3.84	1.44	1.33
23	b	604	CLA	CHD-C4C	3.84	1.48	1.39
35	C	518[B]	DGD	O2G-C1B	3.84	1.45	1.34
23	C	514	CLA	C3D-C2D	3.83	1.49	1.39
37	D	410[B]	LHG	O7-C7	3.83	1.45	1.34
23	C	504	CLA	CHD-C4C	3.83	1.48	1.39
23	c	514	CLA	C3D-C2D	3.83	1.49	1.39
35	c	518[B]	DGD	O2G-C1B	3.83	1.45	1.34
23	A	405[B]	CLA	C3D-C2D	3.83	1.49	1.39
23	B	604	CLA	CHB-C1B	3.83	1.48	1.39
23	c	510	CLA	C1B-NB	-3.83	1.33	1.37
23	b	615	CLA	OBD-CAD	3.83	1.29	1.22
23	b	610	CLA	CHD-C4C	3.83	1.48	1.39
23	a	405[B]	CLA	O2A-CGA	3.83	1.44	1.33
23	C	506	CLA	CHB-C1B	3.83	1.48	1.39
23	a	407[B]	CLA	CHD-C1D	3.82	1.45	1.38
23	B	607	CLA	CHB-C1B	3.82	1.48	1.39
23	A	408	CLA	CHD-C4C	3.82	1.48	1.39
23	C	511	CLA	O2A-CGA	3.82	1.44	1.33
23	b	613	CLA	O2A-CGA	3.82	1.44	1.33
23	B	601	CLA	CHD-C1D	3.82	1.45	1.38
23	c	505	CLA	O2A-CGA	3.82	1.44	1.33
35	c	517[A]	DGD	O2G-C1B	3.81	1.45	1.34
23	c	511	CLA	CHD-C1D	3.81	1.45	1.38
23	a	406[B]	CLA	CHC-C4B	3.81	1.47	1.39
23	B	616	CLA	CHB-C1B	3.81	1.47	1.39
37	D	409[B]	LHG	O8-C23	3.81	1.44	1.33
23	A	404[A]	CLA	C3D-C2D	3.81	1.49	1.39
23	c	503	CLA	CHD-C4C	3.80	1.47	1.39
37	d	711[B]	LHG	O8-C23	3.80	1.44	1.33
23	b	616	CLA	CHD-C4C	3.80	1.47	1.39
23	a	406[B]	CLA	CHD-C4C	3.80	1.47	1.39
35	C	518[B]	DGD	O1G-C1A	3.80	1.44	1.33
23	a	406[B]	CLA	CHD-C1D	3.80	1.45	1.38
25	B	618	BCR	C23-C22	-3.80	1.37	1.45
23	b	608	CLA	CHD-C4C	3.80	1.47	1.39
23	B	615	CLA	CHD-C4C	3.80	1.47	1.39
23	A	404[A]	CLA	CHB-C1B	3.80	1.47	1.39
23	D	405[B]	CLA	CHD-C4C	3.80	1.47	1.39
23	b	602	CLA	O2A-CGA	3.79	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	CHC-C4B	3.79	1.47	1.39
23	D	406	CLA	OBD-CAD	3.79	1.29	1.22
23	b	614	CLA	O2A-CGA	3.79	1.44	1.33
37	d	711[B]	LHG	O7-C7	3.79	1.45	1.34
35	C	518[A]	DGD	O1G-C1A	3.79	1.44	1.33
23	A	405[A]	CLA	CHD-C4C	3.79	1.47	1.39
23	C	510	CLA	CHD-C4C	3.79	1.47	1.39
23	c	514	CLA	CHB-C1B	3.79	1.47	1.39
23	a	407[A]	CLA	CHD-C4C	3.79	1.47	1.39
23	c	511	CLA	CHD-C4C	3.78	1.47	1.39
23	C	514	CLA	CHD-C4C	3.78	1.47	1.39
23	a	409	CLA	C1D-ND	3.78	1.42	1.37
23	c	513	CLA	OBD-CAD	3.78	1.29	1.22
23	c	508	CLA	CHC-C4B	3.78	1.47	1.39
35	c	517[A]	DGD	O1G-C1A	3.78	1.44	1.33
23	b	605	CLA	CHB-C1B	3.78	1.47	1.39
37	d	407[B]	LHG	O8-C23	3.78	1.44	1.33
23	c	506	CLA	O2A-CGA	3.77	1.44	1.33
23	d	402[B]	CLA	CHD-C4C	3.77	1.47	1.39
23	b	603	CLA	CHD-C1D	3.77	1.45	1.38
23	C	503	CLA	CHB-C1B	3.77	1.47	1.39
33	d	412	LMG	O7-C10	3.77	1.44	1.34
23	A	404[B]	CLA	O2A-CGA	3.77	1.44	1.33
23	a	407[B]	CLA	OBD-CAD	3.77	1.29	1.22
24	A	407[A]	PHO	O2A-CGA	3.77	1.44	1.33
23	b	613	CLA	C3D-C2D	3.77	1.49	1.39
23	b	615	CLA	CHC-C4B	3.77	1.47	1.39
23	c	509	CLA	CHB-C1B	3.77	1.47	1.39
23	A	405[A]	CLA	CHC-C4B	3.76	1.47	1.39
23	C	508	CLA	C3D-C2D	3.76	1.49	1.39
23	b	606	CLA	CHD-C4C	3.76	1.47	1.39
23	D	406	CLA	CHC-C4B	3.76	1.47	1.39
26	A	410[A]	SQD	O48-C23	3.76	1.44	1.33
23	c	512	CLA	CHD-C4C	3.76	1.47	1.39
23	a	405[B]	CLA	C3D-C2D	3.74	1.49	1.39
23	b	602	CLA	C3B-C4B	3.74	1.51	1.42
23	a	405[A]	CLA	OBD-CAD	3.74	1.28	1.22
23	C	502	CLA	CHC-C4B	3.74	1.47	1.39
23	B	605	CLA	C3D-C2D	3.73	1.49	1.39
23	D	406	CLA	CHD-C4C	3.73	1.47	1.39
23	A	406[A]	CLA	O2A-CGA	3.73	1.44	1.33
23	B	613	CLA	OBD-CAD	3.73	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	O2A-CGA	3.73	1.44	1.33
23	b	615	CLA	C1B-NB	-3.73	1.33	1.37
23	B	614	CLA	O2A-CGA	3.73	1.44	1.33
23	C	509	CLA	OBD-CAD	3.73	1.28	1.22
23	b	605	CLA	CHD-C4C	3.73	1.47	1.39
23	B	606	CLA	C3D-C2D	3.73	1.49	1.39
23	B	601	CLA	CHB-C1B	3.72	1.47	1.39
23	b	613	CLA	CHD-C1D	3.72	1.45	1.38
23	C	506	CLA	OBD-CAD	3.72	1.28	1.22
23	B	613	CLA	C3D-C2D	3.72	1.49	1.39
23	C	503	CLA	OBD-CAD	3.72	1.28	1.22
23	b	613	CLA	CHB-C1B	3.71	1.47	1.39
23	d	402[B]	CLA	CHC-C4B	3.71	1.47	1.39
23	d	403	CLA	CHC-C4B	3.71	1.47	1.39
23	b	604	CLA	OBD-CAD	3.71	1.28	1.22
23	c	510	CLA	C4B-NB	-3.71	1.33	1.37
23	A	406[A]	CLA	CHD-C4C	3.70	1.47	1.39
23	b	612	CLA	CHC-C4B	3.70	1.47	1.39
23	b	602	CLA	OBD-CAD	3.70	1.28	1.22
23	B	611	CLA	C3B-C4B	3.70	1.51	1.42
26	A	410[B]	SQD	O47-C7	3.70	1.44	1.34
23	B	614	CLA	CHC-C4B	3.70	1.47	1.39
23	A	404[A]	CLA	CHD-C1D	3.70	1.45	1.38
23	C	508	CLA	CHD-C1D	3.69	1.45	1.38
23	a	405[B]	CLA	OBD-CAD	3.69	1.28	1.22
23	B	601	CLA	OBD-CAD	3.69	1.28	1.22
23	B	605	CLA	CHB-C1B	3.69	1.47	1.39
23	C	511	CLA	C3D-C2D	3.69	1.49	1.39
23	b	608	CLA	CHB-C1B	3.69	1.47	1.39
23	c	508	CLA	CHB-C1B	3.69	1.47	1.39
23	A	406[B]	CLA	C1B-NB	-3.69	1.33	1.37
23	B	609	CLA	CHC-C4B	3.68	1.47	1.39
37	L	101[A]	LHG	O7-C7	3.68	1.44	1.34
26	A	410[A]	SQD	O47-C7	3.68	1.44	1.34
23	b	605	CLA	CHC-C4B	3.68	1.47	1.39
37	d	408[A]	LHG	O7-C7	3.68	1.44	1.34
23	b	610	CLA	C3D-C2D	3.67	1.49	1.39
23	b	602	CLA	C3D-C2D	3.67	1.49	1.39
23	a	406[B]	CLA	OBD-CAD	3.67	1.28	1.22
23	a	405[A]	CLA	C3D-C2D	3.67	1.49	1.39
23	B	607	CLA	O2A-CGA	3.67	1.44	1.33
23	A	404[A]	CLA	CHD-C4C	3.67	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	CHC-C4B	3.66	1.47	1.39
33	m	101	LMG	O7-C10	3.66	1.44	1.34
37	D	410[A]	LHG	O7-C7	3.66	1.44	1.34
34	b	622	HTG	C1'-S1	-3.66	1.76	1.81
23	B	613	CLA	CHD-C4C	3.66	1.47	1.39
23	C	503	CLA	CHC-C4B	3.66	1.47	1.39
23	C	514	CLA	OBD-CAD	3.66	1.28	1.22
23	b	606	CLA	CHB-C1B	3.66	1.47	1.39
23	A	406[B]	CLA	OBD-CAD	3.66	1.28	1.22
23	A	404[B]	CLA	CHB-C1B	3.65	1.47	1.39
23	C	507	CLA	C3D-C2D	3.65	1.49	1.39
23	c	502	CLA	CHB-C1B	3.65	1.47	1.39
35	C	517[A]	DGD	O1G-C1A	3.65	1.44	1.33
23	A	405[A]	CLA	CHB-C1B	3.65	1.47	1.39
23	c	502	CLA	CHC-C4B	3.65	1.47	1.39
23	a	406[A]	CLA	CHD-C1D	3.65	1.45	1.38
23	b	609	CLA	CHD-C4C	3.65	1.47	1.39
23	b	611	CLA	CHD-C4C	3.65	1.47	1.39
37	d	711[A]	LHG	O8-C23	3.64	1.44	1.33
23	D	405[A]	CLA	CHD-C4C	3.64	1.47	1.39
23	B	605	CLA	CHD-C4C	3.64	1.47	1.39
23	C	504	CLA	CHB-C1B	3.64	1.47	1.39
23	b	611	CLA	CHC-C4B	3.64	1.47	1.39
23	C	502	CLA	C1B-NB	-3.64	1.33	1.37
23	c	512	CLA	OBD-CAD	3.64	1.28	1.22
23	A	406[A]	CLA	CHC-C4B	3.64	1.47	1.39
38	e	87	HEM	C4D-ND	-3.64	1.34	1.40
23	b	609	CLA	O2A-CGA	3.64	1.44	1.33
23	C	504	CLA	OBD-CAD	3.64	1.28	1.22
23	B	611	CLA	CHD-C4C	3.64	1.47	1.39
23	B	606	CLA	O2A-CGA	3.64	1.44	1.33
23	B	607	CLA	CHC-C4B	3.63	1.47	1.39
23	B	611	CLA	CHD-C1D	3.63	1.45	1.38
23	C	514	CLA	CHB-C1B	3.63	1.47	1.39
23	A	404[B]	CLA	C3D-C2D	3.63	1.49	1.39
23	c	505	CLA	C1B-NB	-3.63	1.33	1.37
24	A	353[A]	PHO	CHA-CBD	-3.63	1.47	1.51
23	C	510	CLA	O2A-CGA	3.63	1.43	1.33
23	b	608	CLA	C1B-NB	-3.62	1.33	1.37
23	B	601	CLA	C3D-C2D	3.62	1.49	1.39
23	a	405[B]	CLA	C1B-NB	-3.62	1.33	1.37
23	b	606	CLA	OBD-CAD	3.62	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	603	CLA	CHB-C1B	3.62	1.47	1.39
23	d	402[A]	CLA	C1D-ND	3.61	1.42	1.37
23	b	604	CLA	C1B-NB	-3.61	1.33	1.37
23	a	407[A]	CLA	CHD-C1D	3.61	1.45	1.38
23	C	505	CLA	C3D-C2D	3.61	1.49	1.39
23	d	402[A]	CLA	OBD-CAD	3.61	1.28	1.22
23	B	615	CLA	C3D-C2D	3.61	1.49	1.39
37	l	101[A]	LHG	O7-C7	3.60	1.44	1.34
23	A	406[A]	CLA	CHB-C1B	3.60	1.47	1.39
37	D	410[A]	LHG	O8-C23	3.60	1.43	1.33
23	b	614	CLA	OBD-CAD	3.60	1.28	1.22
23	C	508	CLA	CHC-C4B	3.60	1.47	1.39
23	d	402[A]	CLA	CHD-C4C	3.60	1.47	1.39
23	C	506	CLA	O2A-CGA	3.60	1.43	1.33
23	c	509	CLA	OBD-CAD	3.60	1.28	1.22
37	D	409[A]	LHG	O7-C7	3.60	1.44	1.34
23	B	610	CLA	CHB-C1B	3.59	1.47	1.39
23	C	509	CLA	CHB-C1B	3.59	1.47	1.39
23	b	606	CLA	C3D-C2D	3.59	1.48	1.39
34	B	622	HTG	C1'-S1	-3.59	1.76	1.81
23	B	610	CLA	CHD-C4C	3.59	1.47	1.39
23	B	602	CLA	CHC-C4B	3.58	1.47	1.39
23	d	402[B]	CLA	OBD-CAD	3.58	1.28	1.22
23	C	511	CLA	CHB-C1B	3.58	1.47	1.39
23	C	505	CLA	CHD-C4C	3.58	1.47	1.39
23	a	409	CLA	CHD-C1D	3.58	1.45	1.38
23	b	605	CLA	OBD-CAD	3.58	1.28	1.22
37	d	407[A]	LHG	O8-C23	3.58	1.43	1.33
23	b	609	CLA	CHC-C4B	3.58	1.47	1.39
23	C	504	CLA	C3D-C2D	3.58	1.48	1.39
23	b	614	CLA	CHD-C4C	3.57	1.47	1.39
23	A	405[B]	CLA	CHC-C4B	3.57	1.47	1.39
23	b	616	CLA	CHC-C4B	3.57	1.47	1.39
23	C	513	CLA	CHD-C4C	3.57	1.47	1.39
34	b	623	HTG	C1'-S1	-3.57	1.76	1.81
35	c	519	DGD	O2G-C1B	3.57	1.44	1.34
23	b	609	CLA	C3D-C2D	3.57	1.48	1.39
23	B	606	CLA	CHC-C4B	3.56	1.47	1.39
23	b	611	CLA	C3D-C2D	3.56	1.48	1.39
23	b	612	CLA	C3D-C2D	3.56	1.48	1.39
23	c	507	CLA	CHB-C1B	3.56	1.47	1.39
23	b	604	CLA	O2A-CGA	3.56	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	D	409[B]	LHG	O7-C7	3.56	1.44	1.34
23	B	607	CLA	CHD-C4C	3.56	1.47	1.39
23	A	404[A]	CLA	C4B-NB	-3.56	1.33	1.37
23	b	607	CLA	CHD-C4C	3.56	1.47	1.39
23	B	603	CLA	CHB-C1B	3.55	1.47	1.39
23	a	405[A]	CLA	CHC-C4B	3.55	1.47	1.39
23	b	601	CLA	C1B-NB	-3.55	1.33	1.37
23	b	614	CLA	C1B-NB	-3.55	1.33	1.37
23	a	407[A]	CLA	CHB-C1B	3.55	1.47	1.39
23	D	405[B]	CLA	C1B-NB	-3.55	1.33	1.37
23	A	408	CLA	C3D-C2D	3.55	1.48	1.39
23	D	405[A]	CLA	C3D-C2D	3.55	1.48	1.39
23	B	615	CLA	OBD-CAD	3.55	1.28	1.22
23	B	606	CLA	CHD-C1D	3.54	1.45	1.38
23	c	505	CLA	OBD-CAD	3.54	1.28	1.22
23	C	505	CLA	CHD-C1D	3.54	1.45	1.38
35	c	518[A]	DGD	O2G-C1B	3.54	1.44	1.34
23	d	402[A]	CLA	C3D-C2D	3.53	1.48	1.39
23	c	508	CLA	OBD-CAD	3.53	1.28	1.22
23	B	609	CLA	CHD-C4C	3.53	1.47	1.39
23	C	502	CLA	C3D-C2D	3.53	1.48	1.39
23	B	614	CLA	CHD-C1D	3.53	1.45	1.38
23	c	511	CLA	CHC-C4B	3.53	1.47	1.39
23	c	512	CLA	C3D-C2D	3.53	1.48	1.39
23	b	615	CLA	CHD-C4C	3.53	1.47	1.39
23	a	406[A]	CLA	CHD-C4C	3.52	1.47	1.39
23	C	509	CLA	CHC-C4B	3.52	1.47	1.39
23	b	601	CLA	OBD-CAD	3.52	1.28	1.22
24	a	408[B]	PHO	O2A-CGA	3.52	1.43	1.33
23	B	608	CLA	CHC-C1C	3.51	1.45	1.38
23	b	603	CLA	C3D-C2D	3.51	1.48	1.39
23	b	608	CLA	C1D-ND	3.51	1.42	1.37
23	B	609	CLA	C1B-NB	-3.51	1.33	1.37
23	b	604	CLA	C3D-C2D	3.51	1.48	1.39
37	d	711[A]	LHG	O7-C7	3.50	1.44	1.34
23	d	403	CLA	CHB-C1B	3.50	1.47	1.39
23	c	504	CLA	C3D-C2D	3.50	1.48	1.39
23	A	406[B]	CLA	CHB-C1B	3.50	1.47	1.39
23	A	405[B]	CLA	C1B-NB	-3.50	1.33	1.37
23	A	406[B]	CLA	C3B-C4B	3.50	1.50	1.42
23	b	607	CLA	CHC-C4B	3.50	1.47	1.39
23	D	405[A]	CLA	CHC-C4B	3.50	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	407[A]	CLA	OBD-CAD	3.50	1.28	1.22
37	D	409[A]	LHG	O8-C23	3.49	1.43	1.33
23	d	402[B]	CLA	C3D-C2D	3.49	1.48	1.39
23	A	405[B]	CLA	OBD-CAD	3.49	1.28	1.22
23	C	502	CLA	CHB-C1B	3.49	1.47	1.39
23	B	610	CLA	O2A-CGA	3.49	1.43	1.33
23	A	405[A]	CLA	C1B-NB	-3.48	1.33	1.37
23	C	510	CLA	CHB-C1B	3.48	1.47	1.39
23	c	514	CLA	CHC-C4B	3.48	1.47	1.39
23	C	503	CLA	CHD-C4C	3.48	1.47	1.39
23	B	602	CLA	O2A-CGA	3.48	1.43	1.33
23	a	406[A]	CLA	CHB-C1B	3.48	1.47	1.39
23	C	508	CLA	C1D-ND	3.48	1.42	1.37
23	B	613	CLA	CHC-C4B	3.48	1.47	1.39
23	D	405[B]	CLA	OBD-CAD	3.47	1.28	1.22
23	B	612	CLA	C3D-C2D	3.47	1.48	1.39
23	c	506	CLA	C3D-C2D	3.47	1.48	1.39
23	B	610	CLA	CHC-C4B	3.47	1.47	1.39
23	C	511	CLA	CHC-C4B	3.47	1.47	1.39
23	A	404[B]	CLA	CHC-C4B	3.47	1.47	1.39
23	b	607	CLA	CHB-C1B	3.47	1.47	1.39
23	b	612	CLA	C4B-NB	-3.47	1.33	1.37
23	c	512	CLA	CHC-C4B	3.46	1.47	1.39
23	C	512	CLA	C4B-NB	-3.46	1.33	1.37
23	b	603	CLA	OBD-CAD	3.46	1.28	1.22
23	C	510	CLA	C1B-NB	-3.46	1.33	1.37
23	b	606	CLA	CHC-C4B	3.46	1.47	1.39
23	c	509	CLA	CHC-C4B	3.46	1.47	1.39
23	b	603	CLA	O2A-CGA	3.46	1.43	1.33
23	b	604	CLA	CHB-C1B	3.46	1.47	1.39
23	A	408	CLA	CHC-C4B	3.45	1.47	1.39
23	B	603	CLA	CHD-C4C	3.45	1.47	1.39
23	c	506	CLA	OBD-CAD	3.45	1.28	1.22
23	B	608	CLA	CHD-C1D	3.45	1.45	1.38
23	C	513	CLA	OBD-CAD	3.44	1.28	1.22
23	b	603	CLA	CHD-C4C	3.44	1.47	1.39
23	B	601	CLA	CHD-C4C	3.44	1.47	1.39
23	b	602	CLA	CHB-C1B	3.44	1.47	1.39
23	c	507	CLA	CHC-C4B	3.43	1.47	1.39
23	C	514	CLA	CHC-C4B	3.43	1.47	1.39
35	H	102	DGD	O2G-C1B	3.43	1.44	1.34
23	b	611	CLA	OBD-CAD	3.43	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	601	CLA	CHB-C1B	3.43	1.47	1.39
23	c	507	CLA	OBD-CAD	3.42	1.28	1.22
23	C	505	CLA	CHC-C4B	3.42	1.47	1.39
23	B	604	CLA	C1B-NB	-3.42	1.33	1.37
33	D	415	LMG	O7-C10	3.42	1.43	1.34
23	b	613	CLA	CHD-C4C	3.41	1.47	1.39
23	d	402[A]	CLA	C1B-NB	-3.41	1.33	1.37
23	C	508	CLA	CHB-C1B	3.41	1.47	1.39
23	A	405[B]	CLA	CHB-C1B	3.40	1.47	1.39
23	B	610	CLA	C4B-NB	-3.40	1.33	1.37
23	C	507	CLA	C4B-NB	-3.40	1.33	1.37
23	b	608	CLA	C4B-NB	-3.40	1.33	1.37
23	C	509	CLA	CHD-C4C	3.40	1.47	1.39
23	B	612	CLA	OBD-CAD	3.40	1.28	1.22
23	d	403	CLA	CHD-C4C	3.40	1.47	1.39
23	D	405[B]	CLA	C3D-C2D	3.40	1.48	1.39
23	c	514	CLA	C4B-NB	-3.39	1.33	1.37
37	l	101[A]	LHG	O8-C23	3.39	1.43	1.33
23	D	406	CLA	O2A-CGA	3.39	1.43	1.33
23	B	609	CLA	OBD-CAD	3.39	1.28	1.22
35	H	102	DGD	O1G-C1A	3.39	1.43	1.33
23	B	603	CLA	CHC-C4B	3.38	1.47	1.39
23	C	505	CLA	OBD-CAD	3.38	1.28	1.22
23	B	606	CLA	CHD-C4C	3.38	1.47	1.39
23	b	601	CLA	CHC-C4B	3.38	1.47	1.39
23	b	612	CLA	CHD-C4C	3.38	1.46	1.39
23	B	604	CLA	O2A-CGA	3.38	1.43	1.33
23	d	402[A]	CLA	CHC-C4B	3.38	1.47	1.39
23	c	507	CLA	C1B-NB	-3.38	1.33	1.37
23	B	612	CLA	O2A-CGA	3.37	1.43	1.33
23	B	611	CLA	C3D-C2D	3.37	1.48	1.39
23	B	603	CLA	CHD-C1D	3.37	1.44	1.38
23	c	505	CLA	CHB-C1B	3.37	1.47	1.39
23	c	504	CLA	C3B-C4B	3.37	1.50	1.42
23	B	609	CLA	CHB-C1B	3.37	1.47	1.39
23	A	406[A]	CLA	C3B-C4B	3.36	1.50	1.42
23	a	407[B]	CLA	CHC-C4B	3.36	1.46	1.39
23	b	605	CLA	O2A-CGA	3.36	1.43	1.33
23	C	507	CLA	CHC-C4B	3.36	1.46	1.39
23	A	405[A]	CLA	OBD-CAD	3.36	1.28	1.22
23	B	608	CLA	CHB-C1B	3.36	1.46	1.39
23	B	607	CLA	C3D-C2D	3.36	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	503	CLA	CHB-C1B	3.35	1.46	1.39
23	B	602	CLA	C1C-C2C	3.35	1.51	1.44
24	a	408[A]	PHO	O2A-CGA	3.35	1.43	1.33
23	B	603	CLA	OBD-CAD	3.35	1.28	1.22
23	A	408	CLA	OBD-CAD	3.35	1.28	1.22
23	a	406[B]	CLA	CHB-C1B	3.35	1.46	1.39
23	B	612	CLA	CHD-C4C	3.35	1.46	1.39
23	C	505	CLA	O2A-CGA	3.34	1.43	1.33
23	C	508	CLA	CHD-C4C	3.34	1.46	1.39
23	b	605	CLA	C3D-C2D	3.34	1.48	1.39
23	B	608	CLA	O2A-CGA	3.34	1.43	1.33
23	C	508	CLA	OBD-CAD	3.33	1.28	1.22
23	A	404[A]	CLA	OBD-CAD	3.33	1.28	1.22
23	C	513	CLA	C3B-C4B	3.33	1.50	1.42
23	c	506	CLA	C1B-NB	-3.32	1.33	1.37
23	B	616	CLA	C4B-NB	-3.32	1.33	1.37
23	C	506	CLA	C3D-C2D	3.32	1.48	1.39
23	a	405[B]	CLA	CHB-C1B	3.32	1.46	1.39
23	C	507	CLA	OBD-CAD	3.32	1.28	1.22
34	b	625	HTG	C1'-S1	-3.31	1.77	1.81
23	b	616	CLA	OBD-CAD	3.31	1.28	1.22
23	B	608	CLA	CHD-C4C	3.30	1.46	1.39
23	B	601	CLA	C3B-C4B	3.30	1.50	1.42
23	A	404[B]	CLA	OBD-CAD	3.30	1.28	1.22
23	C	507	CLA	CHB-C1B	3.30	1.46	1.39
23	C	514	CLA	C1B-NB	-3.30	1.33	1.37
23	b	611	CLA	CHD-C1D	3.29	1.44	1.38
33	D	415	LMG	O8-C28	3.28	1.42	1.33
23	a	407[B]	CLA	C1B-NB	-3.28	1.33	1.37
23	C	512	CLA	CHC-C4B	3.28	1.46	1.39
35	C	519	DGD	O2G-C1B	3.28	1.43	1.34
23	A	404[A]	CLA	O2A-CGA	3.28	1.42	1.33
23	c	514	CLA	OBD-CAD	3.28	1.28	1.22
23	a	409	CLA	CHD-C4C	3.27	1.46	1.39
23	b	611	CLA	C1B-NB	-3.27	1.33	1.37
23	c	510	CLA	OBD-CAD	3.27	1.28	1.22
23	a	407[B]	CLA	CHB-C1B	3.27	1.46	1.39
38	E	103	HEM	C4D-ND	-3.27	1.34	1.40
23	c	505	CLA	CHC-C4B	3.27	1.46	1.39
23	a	407[A]	CLA	CHC-C4B	3.27	1.46	1.39
38	E	103	HEM	C1B-NB	-3.26	1.34	1.40
23	A	405[B]	CLA	C3B-C4B	3.26	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	OBD-CAD	3.26	1.28	1.22
23	C	504	CLA	O2A-CGA	3.25	1.42	1.33
23	B	602	CLA	C1B-NB	-3.25	1.33	1.37
23	B	612	CLA	CHC-C4B	3.24	1.46	1.39
23	C	511	CLA	C4B-NB	-3.24	1.33	1.37
23	D	405[A]	CLA	OBD-CAD	3.24	1.28	1.22
23	A	404[B]	CLA	C3B-C4B	3.24	1.50	1.42
23	a	405[B]	CLA	CHC-C4B	3.24	1.46	1.39
23	b	611	CLA	C4B-NB	-3.24	1.33	1.37
23	a	409	CLA	C3B-C4B	3.23	1.50	1.42
23	b	610	CLA	C1B-NB	-3.23	1.33	1.37
23	B	609	CLA	C3B-C4B	3.23	1.50	1.42
23	a	406[A]	CLA	CHC-C4B	3.23	1.46	1.39
23	b	613	CLA	C4B-NB	-3.23	1.33	1.37
23	c	512	CLA	C1B-C2B	3.23	1.50	1.43
23	B	605	CLA	OBD-CAD	3.23	1.28	1.22
23	B	605	CLA	C3B-C4B	3.22	1.50	1.42
23	b	616	CLA	CHB-C1B	3.22	1.46	1.39
23	B	603	CLA	C4B-NB	-3.21	1.33	1.37
23	B	616	CLA	CHD-C4C	3.21	1.46	1.39
23	C	506	CLA	C1B-NB	-3.21	1.33	1.37
23	B	613	CLA	O2A-CGA	3.21	1.42	1.33
23	D	405[B]	CLA	CHC-C4B	3.21	1.46	1.39
23	b	608	CLA	CHC-C4B	3.21	1.46	1.39
23	c	504	CLA	C1B-NB	-3.20	1.33	1.37
23	c	505	CLA	C1B-C2B	3.20	1.50	1.43
23	B	607	CLA	C1D-ND	3.20	1.41	1.37
23	c	506	CLA	C3B-C4B	3.20	1.50	1.42
23	B	614	CLA	OBD-CAD	3.20	1.28	1.22
23	a	409	CLA	C3D-C2D	3.20	1.47	1.39
23	D	405[A]	CLA	C1B-NB	-3.20	1.33	1.37
23	b	601	CLA	C4B-NB	-3.19	1.33	1.37
23	D	406	CLA	C3B-C4B	3.19	1.50	1.42
23	a	405[A]	CLA	O2A-CGA	3.19	1.42	1.33
23	C	510	CLA	CHC-C4B	3.19	1.46	1.39
23	C	513	CLA	CHB-C1B	3.19	1.46	1.39
23	a	409	CLA	OBD-CAD	3.19	1.28	1.22
23	b	616	CLA	C3B-C4B	3.18	1.50	1.42
23	A	405[A]	CLA	C3B-C4B	3.17	1.50	1.42
23	B	610	CLA	C3B-C4B	3.17	1.50	1.42
23	c	508	CLA	C4B-NB	-3.17	1.33	1.37
23	a	405[B]	CLA	C3B-C4B	3.17	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	513	CLA	C3B-C4B	3.16	1.50	1.42
23	B	614	CLA	C3D-C2D	3.16	1.47	1.39
23	c	510	CLA	C1B-C2B	3.16	1.50	1.43
23	B	608	CLA	C4B-NB	-3.16	1.33	1.37
23	B	608	CLA	C1B-C2B	3.15	1.50	1.43
23	d	403	CLA	OBD-CAD	3.15	1.27	1.22
23	d	402[B]	CLA	C1B-NB	-3.15	1.33	1.37
23	B	613	CLA	C4B-NB	-3.15	1.33	1.37
23	b	610	CLA	O2A-CGA	3.15	1.42	1.33
23	c	503	CLA	CHC-C4B	3.14	1.46	1.39
23	b	606	CLA	C1B-NB	-3.14	1.33	1.37
23	b	612	CLA	C1B-NB	-3.13	1.33	1.37
38	e	87	HEM	C1B-NB	-3.13	1.34	1.40
23	B	604	CLA	C3D-C2D	3.13	1.47	1.39
23	B	604	CLA	CHC-C4B	3.12	1.46	1.39
34	D	414	HTG	C1'-S1	-3.12	1.77	1.81
23	B	601	CLA	C1B-NB	-3.12	1.33	1.37
23	c	504	CLA	OBD-CAD	3.12	1.27	1.22
23	B	616	CLA	C1B-C2B	3.11	1.50	1.43
23	B	604	CLA	C1B-C2B	3.11	1.50	1.43
23	B	610	CLA	C1B-NB	-3.10	1.34	1.37
23	d	402[B]	CLA	C4B-NB	-3.10	1.34	1.37
23	A	404[A]	CLA	C1B-NB	-3.09	1.34	1.37
23	d	402[A]	CLA	C4B-NB	-3.09	1.34	1.37
23	A	408	CLA	C4B-NB	-3.09	1.34	1.37
23	c	507	CLA	C4B-NB	-3.09	1.34	1.37
23	C	505	CLA	C1B-NB	-3.09	1.34	1.37
23	b	616	CLA	C4B-NB	-3.09	1.34	1.37
23	c	511	CLA	OBD-CAD	3.09	1.27	1.22
23	C	511	CLA	OBD-CAD	3.08	1.27	1.22
23	C	506	CLA	C3B-C4B	3.08	1.50	1.42
23	b	606	CLA	C4B-NB	-3.08	1.34	1.37
23	C	507	CLA	C1B-NB	-3.08	1.34	1.37
23	B	615	CLA	CHC-C4B	3.07	1.46	1.39
23	C	504	CLA	C3B-C4B	3.07	1.49	1.42
23	B	615	CLA	C1B-NB	-3.06	1.34	1.37
23	a	405[A]	CLA	C1B-NB	-3.06	1.34	1.37
23	C	514	CLA	C4B-NB	-3.05	1.34	1.37
23	a	405[A]	CLA	C4B-NB	-3.05	1.34	1.37
23	a	407[B]	CLA	C4B-NB	-3.04	1.34	1.37
23	a	407[A]	CLA	C1B-NB	-3.04	1.34	1.37
23	c	503	CLA	OBD-CAD	3.04	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-NC	-3.04	1.33	1.37
23	A	408	CLA	C1B-NB	-3.04	1.34	1.37
23	c	514	CLA	C1B-NB	-3.03	1.34	1.37
23	A	408	CLA	CHB-C1B	3.02	1.46	1.39
40	V	202	HEC	FE-NC	3.01	2.05	1.95
23	B	602	CLA	OBD-CAD	3.01	1.27	1.22
23	A	404[A]	CLA	CHC-C4B	3.01	1.46	1.39
23	C	508	CLA	C4B-NB	-3.01	1.34	1.37
23	b	607	CLA	O2A-CGA	3.01	1.42	1.33
23	b	604	CLA	C1B-C2B	3.01	1.50	1.43
23	D	406	CLA	C1B-NB	-3.01	1.34	1.37
23	C	509	CLA	C1B-C2B	3.00	1.50	1.43
23	B	611	CLA	MG-NB	2.99	2.11	2.05
23	B	601	CLA	C4B-NB	-2.99	1.34	1.37
23	c	502	CLA	OBD-CAD	2.99	1.27	1.22
23	a	407[A]	CLA	C3B-C4B	2.98	1.49	1.42
23	c	502	CLA	C3B-C4B	2.98	1.49	1.42
23	a	406[B]	CLA	C3B-C4B	2.98	1.49	1.42
23	c	511	CLA	C1B-C2B	2.98	1.50	1.43
34	d	411	HTG	C1'-S1	-2.97	1.77	1.81
23	b	609	CLA	C1B-NB	-2.97	1.34	1.37
23	C	512	CLA	C4D-CHA	2.96	1.48	1.38
23	A	406[A]	CLA	C1B-C2B	2.96	1.50	1.43
23	B	615	CLA	C1C-C2C	2.96	1.50	1.44
23	c	509	CLA	C3B-C4B	2.96	1.49	1.42
23	C	508	CLA	C4D-CHA	2.95	1.48	1.38
23	c	514	CLA	C3B-C4B	2.95	1.49	1.42
23	C	513	CLA	C1C-C2C	2.95	1.50	1.44
23	b	604	CLA	C4D-CHA	2.95	1.48	1.38
23	b	608	CLA	C3B-C4B	2.95	1.49	1.42
23	B	606	CLA	C3B-C4B	2.94	1.49	1.42
23	B	605	CLA	C4B-NB	-2.94	1.34	1.37
23	B	606	CLA	OBD-CAD	2.94	1.27	1.22
23	B	612	CLA	C1C-C2C	2.94	1.50	1.44
23	c	511	CLA	C1B-NB	-2.93	1.34	1.37
34	b	625	HTG	C1-S1	-2.93	1.76	1.80
23	C	508	CLA	C1B-NB	-2.93	1.34	1.37
23	B	601	CLA	C1C-C2C	2.93	1.50	1.44
23	b	616	CLA	C1B-NB	-2.93	1.34	1.37
26	a	411[B]	SQD	C6-S	-2.92	1.66	1.77
23	B	614	CLA	C1B-NB	-2.92	1.34	1.37
23	c	510	CLA	C4C-C3C	2.92	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	602	CLA	C1C-C2C	2.92	1.50	1.44
23	b	614	CLA	C1B-C2B	2.91	1.50	1.43
23	C	507	CLA	C4C-C3C	2.91	1.50	1.45
23	b	601	CLA	C3B-C4B	2.91	1.49	1.42
23	b	607	CLA	C4B-NB	-2.91	1.34	1.37
23	a	407[A]	CLA	C1C-C2C	2.91	1.50	1.44
23	d	403	CLA	C4B-NB	-2.91	1.34	1.37
23	C	513	CLA	C1B-NB	-2.90	1.34	1.37
23	a	409	CLA	C1B-C2B	2.90	1.50	1.43
23	a	407[B]	CLA	C3B-C4B	2.90	1.49	1.42
23	d	403	CLA	C3B-C4B	2.90	1.49	1.42
23	b	603	CLA	C1B-C2B	2.89	1.50	1.43
23	b	609	CLA	C3B-C4B	2.89	1.49	1.42
23	A	408	CLA	C1B-C2B	2.89	1.50	1.43
40	v	202	HEC	FE-NC	2.89	2.04	1.95
34	c	522	HTG	C1'-S1	-2.89	1.77	1.81
23	c	514	CLA	C1C-C2C	2.88	1.50	1.44
23	b	606	CLA	C3B-C4B	2.88	1.49	1.42
23	D	406	CLA	C1C-C2C	2.88	1.50	1.44
23	b	604	CLA	C4B-NB	-2.88	1.34	1.37
23	B	616	CLA	C1C-C2C	2.88	1.50	1.44
23	B	608	CLA	C1B-NB	-2.87	1.34	1.37
23	B	605	CLA	C1B-C2B	2.87	1.50	1.43
23	b	604	CLA	C3B-C4B	2.86	1.49	1.42
23	D	405[A]	CLA	C4B-NB	-2.86	1.34	1.37
23	B	602	CLA	C1B-C2B	2.86	1.50	1.43
23	C	504	CLA	C1B-NB	-2.85	1.34	1.37
23	c	508	CLA	C1B-NB	-2.85	1.34	1.37
23	D	406	CLA	C4C-C3C	2.85	1.49	1.45
23	C	502	CLA	C1C-C2C	2.84	1.50	1.44
23	C	514	CLA	C1C-C2C	2.84	1.50	1.44
23	C	512	CLA	C3B-C4B	2.84	1.49	1.42
23	A	404[A]	CLA	C4C-C3C	2.84	1.49	1.45
23	b	615	CLA	C4D-CHA	2.84	1.48	1.38
23	a	406[A]	CLA	C3B-C4B	2.84	1.49	1.42
23	b	614	CLA	C4B-NB	-2.84	1.34	1.37
23	d	402[B]	CLA	C1B-C2B	2.84	1.49	1.43
23	d	402[B]	CLA	C1C-C2C	2.83	1.50	1.44
23	C	512	CLA	OBD-CAD	2.83	1.27	1.22
23	D	406	CLA	C1B-C2B	2.83	1.49	1.43
23	D	405[B]	CLA	C4B-NB	-2.83	1.34	1.37
23	C	505	CLA	C1B-C2B	2.83	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	607	CLA	C1B-C2B	2.83	1.49	1.43
23	b	610	CLA	C3B-C4B	2.83	1.49	1.42
23	B	615	CLA	C1B-C2B	2.83	1.49	1.43
23	D	405[B]	CLA	C1B-C2B	2.82	1.49	1.43
23	a	409	CLA	C1B-NB	-2.82	1.34	1.37
23	C	503	CLA	C1B-C2B	2.81	1.49	1.43
23	c	512	CLA	C1B-NB	-2.81	1.34	1.37
29	A	414[A]	PL9	C6-C5	2.81	1.49	1.35
23	C	512	CLA	C1B-C2B	2.81	1.49	1.43
23	c	511	CLA	C3B-C4B	2.81	1.49	1.42
23	c	505	CLA	C4C-C3C	2.81	1.49	1.45
23	C	502	CLA	C3B-C4B	2.80	1.49	1.42
23	C	506	CLA	C4C-C3C	2.80	1.49	1.45
23	c	514	CLA	C1B-C2B	2.80	1.49	1.43
23	B	612	CLA	C1D-ND	2.80	1.41	1.37
23	B	606	CLA	C1C-C2C	2.80	1.50	1.44
23	C	511	CLA	C1B-C2B	2.80	1.49	1.43
23	c	509	CLA	C4D-CHA	2.80	1.48	1.38
23	B	606	CLA	C1B-NB	-2.79	1.34	1.37
23	D	405[A]	CLA	C1B-C2B	2.79	1.49	1.43
23	d	402[A]	CLA	C4C-C3C	2.79	1.49	1.45
23	c	505	CLA	C4B-NB	-2.79	1.34	1.37
23	B	608	CLA	CHC-C4B	2.79	1.45	1.39
23	B	604	CLA	C4D-CHA	2.78	1.48	1.38
23	c	508	CLA	C4D-CHA	2.78	1.48	1.38
23	B	602	CLA	C4C-C3C	2.78	1.49	1.45
23	C	514	CLA	C1B-C2B	2.78	1.49	1.43
23	c	508	CLA	C1B-C2B	2.78	1.49	1.43
23	B	615	CLA	C3B-C4B	2.78	1.49	1.42
23	B	616	CLA	C1B-NB	-2.78	1.34	1.37
24	A	353[B]	PHO	CHA-CBD	-2.77	1.48	1.51
23	c	509	CLA	C4B-NB	-2.77	1.34	1.37
23	c	504	CLA	C1B-C2B	2.77	1.49	1.43
23	b	614	CLA	C3B-C4B	2.77	1.49	1.42
23	C	502	CLA	C4D-CHA	2.77	1.48	1.38
23	c	506	CLA	C1C-C2C	2.77	1.49	1.44
23	C	505	CLA	C4B-NB	-2.77	1.34	1.37
23	C	507	CLA	C3B-C4B	2.77	1.49	1.42
23	b	612	CLA	C1B-C2B	2.76	1.49	1.43
23	A	404[A]	CLA	C1B-C2B	2.76	1.49	1.43
24	A	407[A]	PHO	CBD-CGD	-2.76	1.48	1.52
29	a	416[B]	PL9	C6-C5	2.76	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406[B]	CLA	C4B-NB	-2.76	1.34	1.37
34	C	522	HTG	C1'-S1	-2.76	1.77	1.81
26	A	410[A]	SQD	C6-S	-2.76	1.67	1.77
23	B	614	CLA	C4D-CHA	2.76	1.48	1.38
23	a	409	CLA	C4B-NB	-2.75	1.34	1.37
40	V	202	HEC	FE-NB	2.75	2.03	1.94
23	B	608	CLA	OBD-CAD	2.75	1.27	1.22
23	C	506	CLA	C1B-C2B	2.75	1.49	1.43
23	C	505	CLA	C4D-CHA	2.75	1.48	1.38
23	C	510	CLA	C1C-C2C	2.75	1.49	1.44
33	Z	101	LMG	O8-C28	2.75	1.46	1.33
23	a	407[A]	CLA	C4B-NB	-2.74	1.34	1.37
23	b	613	CLA	C4D-CHA	2.74	1.48	1.38
29	a	416[A]	PL9	C6-C5	2.74	1.49	1.35
26	a	411[A]	SQD	C6-S	-2.73	1.67	1.77
23	b	603	CLA	C1B-NB	-2.73	1.34	1.37
23	B	605	CLA	C1B-NB	-2.73	1.34	1.37
23	b	609	CLA	C1C-NC	-2.73	1.33	1.37
23	a	406[A]	CLA	C4B-NB	-2.73	1.34	1.37
23	A	405[A]	CLA	C1C-C2C	2.73	1.49	1.44
26	A	410[B]	SQD	C6-S	-2.73	1.67	1.77
23	c	502	CLA	C3D-C4D	-2.72	1.38	1.44
23	c	511	CLA	C4D-CHA	2.72	1.48	1.38
23	b	609	CLA	C4D-CHA	2.72	1.48	1.38
23	B	610	CLA	C1B-C2B	2.72	1.49	1.43
23	c	503	CLA	C1B-C2B	2.72	1.49	1.43
23	A	405[A]	CLA	C4B-NB	-2.72	1.34	1.37
23	B	610	CLA	C4D-CHA	2.71	1.48	1.38
23	b	615	CLA	C3B-C4B	2.71	1.49	1.42
23	c	513	CLA	C4D-CHA	2.71	1.48	1.38
23	C	504	CLA	C1C-C2C	2.71	1.49	1.44
23	c	503	CLA	C4B-NB	-2.71	1.34	1.37
23	c	505	CLA	C1C-C2C	2.71	1.49	1.44
23	C	510	CLA	C1B-C2B	2.70	1.49	1.43
23	A	404[B]	CLA	C4D-CHA	2.70	1.48	1.38
23	c	510	CLA	CHC-C4B	2.70	1.45	1.39
23	B	607	CLA	C1C-C2C	2.70	1.49	1.44
23	A	405[B]	CLA	C1B-C2B	2.70	1.49	1.43
23	c	512	CLA	C4C-C3C	2.70	1.49	1.45
23	A	405[A]	CLA	C1B-C2B	2.69	1.49	1.43
23	C	507	CLA	C1C-C2C	2.69	1.49	1.44
23	c	504	CLA	C1C-C2C	2.69	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405[A]	CLA	C4D-CHA	2.69	1.48	1.38
23	c	513	CLA	C1B-NB	-2.69	1.34	1.37
23	C	506	CLA	C4D-CHA	2.68	1.47	1.38
23	B	607	CLA	C4B-NB	-2.68	1.34	1.37
23	B	612	CLA	C4D-CHA	2.68	1.47	1.38
23	C	510	CLA	C1C-NC	-2.68	1.33	1.37
23	B	602	CLA	C3B-C4B	2.68	1.49	1.42
23	a	407[A]	CLA	C4D-CHA	2.67	1.47	1.38
23	B	610	CLA	C1C-C2C	2.67	1.49	1.44
23	C	512	CLA	C1C-C2C	2.67	1.49	1.44
23	a	407[A]	CLA	C1B-C2B	2.67	1.49	1.43
23	B	605	CLA	C1C-C2C	2.67	1.49	1.44
27	a	801	GOL	C1-C2	2.67	1.62	1.51
32	a	414	LMT	O2'-C2'	-2.67	1.36	1.43
23	A	408	CLA	C4D-CHA	2.66	1.47	1.38
23	a	406[A]	CLA	C1B-C2B	2.66	1.49	1.43
23	B	602	CLA	C3D-C4D	-2.66	1.38	1.44
24	A	353[B]	PHO	C3A-C2A	-2.66	1.52	1.54
23	C	502	CLA	C1B-C2B	2.66	1.49	1.43
23	C	511	CLA	C3B-C4B	2.66	1.49	1.42
23	c	512	CLA	C4D-CHA	2.65	1.47	1.38
23	C	507	CLA	C1B-C2B	2.65	1.49	1.43
23	c	504	CLA	C4B-NB	-2.65	1.34	1.37
23	C	510	CLA	C4D-CHA	2.65	1.47	1.38
29	A	414[B]	PL9	C6-C5	2.65	1.49	1.35
23	C	506	CLA	C4B-NB	-2.65	1.34	1.37
23	c	506	CLA	C4B-NB	-2.65	1.34	1.37
23	a	407[B]	CLA	C4D-CHA	2.64	1.47	1.38
40	V	202	HEC	CAC-C3C	2.64	1.57	1.51
23	B	608	CLA	C3D-C4D	-2.64	1.38	1.44
23	C	505	CLA	C1C-C2C	2.64	1.49	1.44
23	c	506	CLA	C4D-CHA	2.64	1.47	1.38
23	B	614	CLA	C1B-C2B	2.63	1.49	1.43
23	B	602	CLA	C4B-NB	-2.63	1.34	1.37
23	C	508	CLA	C1B-C2B	2.63	1.49	1.43
23	b	613	CLA	C1B-C2B	2.63	1.49	1.43
23	b	612	CLA	C1C-C2C	2.63	1.49	1.44
26	f	102	SQD	C6-S	-2.63	1.67	1.77
23	C	509	CLA	C3B-C4B	2.62	1.48	1.42
23	B	609	CLA	C1B-C2B	2.62	1.49	1.43
23	b	615	CLA	C1B-C2B	2.62	1.49	1.43
23	c	503	CLA	C3B-C4B	2.62	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	C4D-CHA	2.62	1.47	1.38
23	c	506	CLA	C1B-C2B	2.61	1.49	1.43
23	D	405[A]	CLA	C4D-CHA	2.61	1.47	1.38
23	B	612	CLA	C1B-C2B	2.61	1.49	1.43
23	C	507	CLA	C4D-CHA	2.61	1.47	1.38
23	B	603	CLA	C3B-C2B	2.61	1.50	1.41
23	B	608	CLA	C4D-CHA	2.61	1.47	1.38
23	C	512	CLA	C3D-C4D	-2.60	1.38	1.44
23	a	405[B]	CLA	C4C-C3C	2.60	1.49	1.45
23	B	613	CLA	C4C-C3C	2.60	1.49	1.45
23	a	409	CLA	C1C-C2C	2.60	1.49	1.44
23	a	409	CLA	C4D-CHA	2.60	1.47	1.38
23	d	402[A]	CLA	C4D-CHA	2.60	1.47	1.38
23	B	616	CLA	C4D-CHA	2.60	1.47	1.38
23	b	602	CLA	C1B-NB	-2.59	1.34	1.37
23	c	507	CLA	C1B-C2B	2.59	1.49	1.43
23	C	509	CLA	C4C-C3C	2.59	1.49	1.45
23	B	615	CLA	C4D-CHA	2.59	1.47	1.38
23	B	616	CLA	C3B-C4B	2.59	1.48	1.42
23	B	613	CLA	C1B-C2B	2.59	1.49	1.43
32	D	404	LMT	C3'-C2'	2.59	1.58	1.52
23	c	508	CLA	C1C-C2C	2.58	1.49	1.44
23	c	509	CLA	C1C-C2C	2.58	1.49	1.44
23	C	502	CLA	OBD-CAD	2.58	1.26	1.22
23	C	510	CLA	C3B-C4B	2.58	1.48	1.42
23	B	604	CLA	C3B-C4B	2.58	1.48	1.42
32	t	101	LMT	O3'-C3'	-2.58	1.36	1.43
23	B	606	CLA	C3D-C4D	-2.58	1.38	1.44
23	b	609	CLA	C1B-C2B	2.58	1.49	1.43
23	A	406[A]	CLA	C4D-CHA	2.58	1.47	1.38
24	a	408[A]	PHO	CBD-CGD	-2.58	1.49	1.52
26	a	413	SQD	C6-S	-2.58	1.67	1.77
23	C	504	CLA	C4D-CHA	2.57	1.47	1.38
23	b	608	CLA	C4D-CHA	2.57	1.47	1.38
23	b	609	CLA	C4B-NB	-2.57	1.34	1.37
23	B	613	CLA	C4D-CHA	2.57	1.47	1.38
23	C	508	CLA	C1C-C2C	2.57	1.49	1.44
23	b	601	CLA	C4D-CHA	2.57	1.47	1.38
23	C	511	CLA	C1C-C2C	2.57	1.49	1.44
23	A	405[B]	CLA	C4D-CHA	2.57	1.47	1.38
23	b	616	CLA	C1C-C2C	2.57	1.49	1.44
23	C	511	CLA	C1B-NB	-2.56	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C4D-CHA	2.56	1.47	1.38
23	c	510	CLA	C4D-CHA	2.56	1.47	1.38
23	b	607	CLA	C4C-C3C	2.56	1.49	1.45
23	A	404[B]	CLA	C4C-C3C	2.56	1.49	1.45
26	b	620	SQD	C6-S	-2.56	1.67	1.77
23	b	609	CLA	C1C-C2C	2.56	1.49	1.44
38	E	103	HEM	C1C-C2C	-2.56	1.40	1.45
23	b	614	CLA	C4D-CHA	2.56	1.47	1.38
23	d	402[B]	CLA	C4C-C3C	2.55	1.49	1.45
23	a	405[A]	CLA	C4D-CHA	2.55	1.47	1.38
23	B	616	CLA	C3B-C2B	2.55	1.49	1.41
23	d	402[A]	CLA	C1C-C2C	2.55	1.49	1.44
23	B	609	CLA	C1C-C2C	2.55	1.49	1.44
23	A	406[A]	CLA	C4B-NB	-2.55	1.34	1.37
23	c	513	CLA	C4B-NB	-2.54	1.34	1.37
23	b	605	CLA	C1C-C2C	2.54	1.49	1.44
23	b	610	CLA	C3D-C4D	-2.54	1.38	1.44
23	C	512	CLA	C1B-NB	-2.54	1.34	1.37
23	A	404[A]	CLA	C4D-CHA	2.54	1.47	1.38
23	C	514	CLA	C4D-CHA	2.54	1.47	1.38
23	d	403	CLA	C4D-CHA	2.54	1.47	1.38
23	A	408	CLA	C3B-C4B	2.54	1.48	1.42
33	C	521	LMG	O1-C1	2.54	1.44	1.40
23	b	601	CLA	C1C-C2C	2.54	1.49	1.44
23	C	503	CLA	C3B-C2B	2.54	1.49	1.41
23	c	503	CLA	C3B-C2B	2.54	1.49	1.41
23	B	609	CLA	C4D-CHA	2.54	1.47	1.38
23	c	509	CLA	C1B-C2B	2.54	1.49	1.43
23	B	607	CLA	C1B-C2B	2.53	1.49	1.43
23	C	512	CLA	C4C-C3C	2.53	1.49	1.45
23	C	511	CLA	C4D-CHA	2.53	1.47	1.38
35	C	519	DGD	O2G-C2G	-2.53	1.40	1.46
23	d	403	CLA	C1C-C2C	2.53	1.49	1.44
29	D	408[B]	PL9	C6-C5	2.53	1.48	1.35
23	C	504	CLA	C4B-NB	-2.53	1.34	1.37
23	c	502	CLA	C4D-CHA	2.53	1.47	1.38
23	B	608	CLA	C3B-C4B	2.52	1.48	1.42
23	a	406[A]	CLA	C4D-CHA	2.52	1.47	1.38
34	B	626	HTG	C1-S1	-2.52	1.76	1.80
23	C	503	CLA	C3B-C4B	2.52	1.48	1.42
23	B	611	CLA	C4D-CHA	2.52	1.47	1.38
23	a	406[B]	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3D-C4D	-2.52	1.38	1.44
24	a	353[A]	PHO	C3A-C2A	-2.52	1.52	1.54
26	A	412	SQD	C6-S	-2.52	1.68	1.77
23	b	610	CLA	C1C-C2C	2.52	1.49	1.44
23	C	503	CLA	C1B-NB	-2.52	1.34	1.37
23	C	513	CLA	C4B-NB	-2.52	1.34	1.37
23	B	607	CLA	C3D-C4D	-2.52	1.38	1.44
23	b	607	CLA	OBD-CAD	2.51	1.26	1.22
23	b	603	CLA	C1C-C2C	2.51	1.49	1.44
23	c	503	CLA	C1B-NB	-2.51	1.34	1.37
23	B	606	CLA	C1B-C2B	2.51	1.49	1.43
23	b	611	CLA	C3B-C4B	2.51	1.48	1.42
23	d	402[A]	CLA	C1B-C2B	2.51	1.49	1.43
27	A	701	GOL	O2-C2	-2.51	1.35	1.43
23	b	605	CLA	C4D-CHA	2.51	1.47	1.38
23	D	406	CLA	C4D-CHA	2.51	1.47	1.38
23	c	507	CLA	C4D-CHA	2.51	1.47	1.38
23	C	509	CLA	C1B-NB	-2.50	1.34	1.37
23	a	406[B]	CLA	C4B-NB	-2.50	1.34	1.37
23	C	509	CLA	C1C-C2C	2.50	1.49	1.44
23	B	603	CLA	C4D-CHA	2.50	1.47	1.38
23	C	514	CLA	C3B-C4B	2.50	1.48	1.42
23	a	406[B]	CLA	C1B-C2B	2.50	1.49	1.43
23	A	406[B]	CLA	C4D-CHA	2.50	1.47	1.38
23	d	402[B]	CLA	C4D-CHA	2.50	1.47	1.38
23	d	403	CLA	C1B-NB	-2.50	1.34	1.37
23	b	603	CLA	C3B-C4B	2.50	1.48	1.42
23	b	602	CLA	C4B-NB	-2.50	1.34	1.37
29	D	408[A]	PL9	C6-C5	2.50	1.48	1.35
23	A	408	CLA	C3B-C2B	2.49	1.49	1.41
23	D	405[B]	CLA	C4D-CHA	2.49	1.47	1.38
23	A	408	CLA	C3D-C4D	-2.49	1.38	1.44
23	a	407[B]	CLA	C1B-C2B	2.49	1.49	1.43
23	c	504	CLA	C4D-CHA	2.49	1.47	1.38
23	c	513	CLA	C1B-C2B	2.49	1.49	1.43
24	A	353[B]	PHO	C4B-NB	-2.49	1.34	1.38
23	c	507	CLA	C4C-C3C	2.49	1.49	1.45
23	b	606	CLA	C4D-CHA	2.49	1.47	1.38
23	B	608	CLA	C3B-C2B	2.48	1.49	1.41
23	C	509	CLA	C4D-CHA	2.48	1.47	1.38
23	c	514	CLA	C4D-CHA	2.48	1.47	1.38
23	B	606	CLA	C4D-CHA	2.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	612	CLA	C3B-C4B	2.48	1.48	1.42
23	C	502	CLA	C4C-C3C	2.48	1.49	1.45
23	c	502	CLA	C1C-C2C	2.48	1.49	1.44
35	H	102	DGD	O5D-C1E	2.48	1.44	1.40
23	B	605	CLA	C4D-CHA	2.48	1.47	1.38
24	A	353[A]	PHO	C3D-C4D	-2.48	1.37	1.41
23	B	614	CLA	C1C-C2C	2.48	1.49	1.44
23	C	510	CLA	C4C-C3C	2.48	1.49	1.45
23	A	404[B]	CLA	C1C-C2C	2.48	1.49	1.44
23	C	502	CLA	C3D-C4D	-2.47	1.38	1.44
23	c	502	CLA	C1B-NB	-2.47	1.34	1.37
23	a	405[B]	CLA	C4D-CHA	2.47	1.47	1.38
23	b	606	CLA	C1B-C2B	2.47	1.49	1.43
23	a	405[A]	CLA	C1C-C2C	2.47	1.49	1.44
23	c	502	CLA	C1B-C2B	2.47	1.49	1.43
23	a	405[A]	CLA	C1B-C2B	2.47	1.49	1.43
23	B	605	CLA	C3D-C4D	-2.47	1.38	1.44
23	c	512	CLA	C3B-C4B	2.47	1.48	1.42
32	b	621	LMT	C3'-C2'	2.47	1.58	1.52
23	D	405[A]	CLA	C1C-C2C	2.46	1.49	1.44
23	a	405[B]	CLA	C1C-C2C	2.46	1.49	1.44
23	C	509	CLA	C3B-C2B	2.46	1.49	1.41
23	C	513	CLA	C4D-CHA	2.46	1.47	1.38
23	b	611	CLA	C1B-C2B	2.46	1.49	1.43
23	b	609	CLA	C3D-C4D	-2.46	1.38	1.44
26	F	101	SQD	C6-S	-2.46	1.68	1.77
23	c	502	CLA	C4B-NB	-2.46	1.34	1.37
23	b	607	CLA	C4D-CHA	2.46	1.47	1.38
32	t	102	LMT	O3'-C3'	-2.46	1.37	1.43
23	b	605	CLA	C1B-C2B	2.45	1.49	1.43
23	B	613	CLA	C1C-C2C	2.45	1.49	1.44
32	M	101	LMT	O2'-C2'	-2.45	1.37	1.43
23	b	610	CLA	C4D-CHA	2.45	1.47	1.38
23	A	405[B]	CLA	C4B-NB	-2.45	1.34	1.37
23	b	616	CLA	C4D-CHA	2.45	1.47	1.38
23	A	404[B]	CLA	C1B-C2B	2.45	1.49	1.43
23	b	612	CLA	C4D-CHA	2.45	1.47	1.38
23	b	602	CLA	C4D-CHA	2.45	1.47	1.38
23	d	402[A]	CLA	C3D-C4D	-2.45	1.38	1.44
23	c	511	CLA	C1C-C2C	2.45	1.49	1.44
23	B	614	CLA	C3D-C4D	-2.45	1.38	1.44
23	C	506	CLA	C1C-C2C	2.44	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	C4B-NB	-2.44	1.34	1.37
23	c	504	CLA	C3D-C4D	-2.44	1.38	1.44
23	b	611	CLA	C1C-C2C	2.44	1.49	1.44
23	b	604	CLA	C1C-C2C	2.44	1.49	1.44
23	b	603	CLA	C3B-C2B	2.43	1.49	1.41
38	e	87	HEM	C1C-C2C	-2.43	1.40	1.45
23	c	507	CLA	C3B-C4B	2.43	1.48	1.42
23	b	610	CLA	C1B-C2B	2.43	1.49	1.43
29	d	405[B]	PL9	C6-C5	2.43	1.48	1.35
23	A	404[A]	CLA	C3B-C4B	2.43	1.48	1.42
23	D	405[A]	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	509	CLA	C4B-NB	-2.43	1.34	1.37
32	I	101	LMT	O3'-C3'	-2.43	1.37	1.43
23	B	606	CLA	C4B-NB	-2.42	1.34	1.37
23	C	512	CLA	C3B-C2B	2.42	1.49	1.41
23	b	608	CLA	C3D-C4D	-2.42	1.38	1.44
24	a	353[B]	PHO	C3A-C2A	-2.42	1.52	1.54
23	A	404[A]	CLA	C1C-C2C	2.42	1.49	1.44
23	c	514	CLA	C4C-C3C	2.42	1.49	1.45
23	c	512	CLA	C1C-C2C	2.42	1.49	1.44
23	B	604	CLA	C4C-C3C	2.42	1.49	1.45
23	d	402[A]	CLA	C3B-C4B	2.41	1.48	1.42
23	b	603	CLA	C4D-CHA	2.41	1.47	1.38
23	C	508	CLA	C3D-C4D	-2.41	1.38	1.44
23	C	507	CLA	C3D-C4D	-2.40	1.38	1.44
23	b	615	CLA	C3D-C4D	-2.40	1.38	1.44
23	C	514	CLA	C3B-C2B	2.40	1.49	1.41
23	D	405[B]	CLA	C3D-C4D	-2.40	1.38	1.44
32	m	103	LMT	O2B-C2B	-2.40	1.37	1.43
24	a	353[A]	PHO	C4B-NB	-2.40	1.34	1.38
23	C	511	CLA	C3B-C2B	2.40	1.49	1.41
23	C	503	CLA	C1C-C2C	2.40	1.49	1.44
23	b	605	CLA	C3B-C4B	2.40	1.48	1.42
26	B	620	SQD	C6-S	-2.40	1.68	1.77
23	B	612	CLA	C3B-C2B	2.40	1.49	1.41
23	b	603	CLA	C3D-C4D	-2.40	1.38	1.44
23	c	514	CLA	C3D-C4D	-2.40	1.38	1.44
23	b	616	CLA	C3D-C4D	-2.40	1.38	1.44
23	B	601	CLA	C4D-CHA	2.40	1.46	1.38
23	b	606	CLA	C3D-C4D	-2.39	1.38	1.44
23	a	406[B]	CLA	C1C-C2C	2.39	1.49	1.44
23	c	505	CLA	C4D-CHA	2.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	103	LMT	O3'-C3'	-2.39	1.37	1.43
23	c	503	CLA	C4D-CHA	2.39	1.46	1.38
23	a	405[B]	CLA	C3B-C2B	2.39	1.49	1.41
23	d	403	CLA	C1B-C2B	2.39	1.48	1.43
23	c	509	CLA	C1B-NB	-2.39	1.34	1.37
23	B	612	CLA	C3D-C4D	-2.39	1.38	1.44
24	a	408[A]	PHO	C4B-NB	-2.39	1.34	1.38
23	A	404[B]	CLA	C3B-C2B	2.39	1.49	1.41
23	b	603	CLA	C4B-NB	-2.39	1.34	1.37
23	A	406[A]	CLA	C1C-C2C	2.39	1.49	1.44
40	v	202	HEC	CAC-C3C	2.39	1.57	1.51
23	B	615	CLA	C4C-C3C	2.39	1.49	1.45
23	B	608	CLA	C4C-C3C	2.38	1.49	1.45
23	B	601	CLA	C1B-C2B	2.38	1.48	1.43
23	d	402[B]	CLA	C3B-C4B	2.38	1.48	1.42
23	D	405[A]	CLA	C3B-C2B	2.38	1.49	1.41
23	b	612	CLA	C3B-C2B	2.38	1.49	1.41
23	C	514	CLA	C3D-C4D	-2.38	1.38	1.44
23	b	607	CLA	C1C-C2C	2.38	1.49	1.44
24	A	353[A]	PHO	C4B-NB	-2.38	1.34	1.38
23	B	607	CLA	C4C-C3C	2.37	1.49	1.45
23	C	511	CLA	C4C-C3C	2.37	1.49	1.45
23	b	616	CLA	C1B-C2B	2.37	1.48	1.43
23	b	613	CLA	C3B-C4B	2.37	1.48	1.42
23	b	606	CLA	C1C-C2C	2.37	1.49	1.44
23	a	407[A]	CLA	C3D-C4D	-2.36	1.38	1.44
24	a	408[B]	PHO	C4B-NB	-2.36	1.34	1.38
23	d	402[B]	CLA	C3B-C2B	2.36	1.49	1.41
23	b	607	CLA	C3D-C4D	-2.36	1.38	1.44
24	A	353[A]	PHO	C3A-C2A	-2.36	1.52	1.54
23	a	405[A]	CLA	C4C-C3C	2.36	1.49	1.45
32	e	102	LMT	O3'-C3'	-2.36	1.37	1.43
35	h	102	DGD	O5D-C1E	2.35	1.44	1.40
32	I	101	LMT	O2'-C2'	-2.35	1.37	1.43
23	C	503	CLA	C4D-CHA	2.35	1.46	1.38
23	B	609	CLA	C3D-C4D	-2.35	1.38	1.44
23	C	505	CLA	C3B-C2B	2.35	1.49	1.41
23	c	502	CLA	C4C-C3C	2.35	1.49	1.45
23	B	604	CLA	C4B-NB	-2.34	1.34	1.37
23	D	405[B]	CLA	C3B-C4B	2.34	1.48	1.42
23	b	614	CLA	C1C-C2C	2.34	1.49	1.44
23	A	406[B]	CLA	C1B-C2B	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	615	CLA	C1C-C2C	2.34	1.49	1.44
32	D	404	LMT	O4'-C4B	-2.34	1.37	1.43
23	b	605	CLA	C4B-NB	-2.34	1.34	1.37
23	b	610	CLA	C4C-C3C	2.34	1.49	1.45
27	o	601	GOL	C1-C2	2.33	1.61	1.51
35	c	519	DGD	O2G-C2G	-2.33	1.40	1.46
23	c	510	CLA	C3B-C2B	2.33	1.49	1.41
23	c	502	CLA	C1C-NC	-2.33	1.34	1.37
23	c	505	CLA	C1C-NC	-2.33	1.34	1.37
23	d	402[B]	CLA	C3D-C4D	-2.33	1.38	1.44
29	d	405[A]	PL9	C6-C5	2.33	1.47	1.35
23	c	513	CLA	C1C-C2C	2.32	1.49	1.44
32	M	101	LMT	O3'-C3'	-2.32	1.37	1.43
34	B	622	HTG	O5-C1	2.32	1.46	1.42
23	b	601	CLA	C3B-C2B	2.32	1.49	1.41
23	B	607	CLA	C3B-C2B	2.32	1.49	1.41
23	b	613	CLA	C3D-C4D	-2.31	1.38	1.44
23	D	405[B]	CLA	C3B-C2B	2.31	1.49	1.41
23	c	505	CLA	C3B-C4B	2.31	1.48	1.42
23	C	510	CLA	C3B-C2B	2.31	1.49	1.41
23	B	616	CLA	C3D-C4D	-2.31	1.39	1.44
23	b	611	CLA	C3B-C2B	2.30	1.49	1.41
23	c	506	CLA	C4C-C3C	2.30	1.49	1.45
23	C	506	CLA	C3D-C4D	-2.30	1.39	1.44
23	D	405[B]	CLA	C1C-C2C	2.30	1.49	1.44
38	e	87	HEM	C1D-ND	-2.30	1.34	1.38
23	B	604	CLA	C1A-CHA	2.29	1.52	1.43
23	A	406[B]	CLA	C3D-C4D	-2.29	1.39	1.44
34	b	622	HTG	O5-C1	2.29	1.46	1.42
23	C	512	CLA	C1C-NC	-2.29	1.34	1.37
23	C	505	CLA	C3B-C4B	2.29	1.48	1.42
23	B	614	CLA	C3B-C4B	2.29	1.48	1.42
23	c	511	CLA	C3B-C2B	2.28	1.48	1.41
32	D	404	LMT	O3'-C3'	-2.28	1.37	1.43
23	C	505	CLA	C3D-C4D	-2.28	1.39	1.44
23	c	512	CLA	C3B-C2B	2.28	1.48	1.41
23	C	507	CLA	C3B-C2B	2.28	1.48	1.41
23	c	513	CLA	C4C-C3C	2.28	1.49	1.45
23	b	608	CLA	C3B-C2B	2.28	1.48	1.41
23	b	602	CLA	C3D-C4D	-2.28	1.39	1.44
23	B	604	CLA	C3D-C4D	-2.28	1.39	1.44
23	c	510	CLA	C3B-C4B	2.27	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	604	CLA	C1C-C2C	2.27	1.49	1.44
23	b	608	CLA	C1C-C2C	2.27	1.49	1.44
23	c	512	CLA	C4B-NB	-2.27	1.35	1.37
23	A	405[B]	CLA	C1C-C2C	2.27	1.49	1.44
23	A	405[B]	CLA	C3D-C4D	-2.27	1.39	1.44
23	c	508	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	610	CLA	C3D-C4D	-2.27	1.39	1.44
23	a	407[B]	CLA	C1C-C2C	2.27	1.49	1.44
32	m	103	LMT	O3'-C3'	-2.26	1.37	1.43
23	B	603	CLA	C1C-C2C	2.26	1.48	1.44
23	a	407[B]	CLA	C3D-C4D	-2.26	1.39	1.44
23	D	406	CLA	C3D-C4D	-2.26	1.39	1.44
38	E	103	HEM	C3C-C4C	-2.26	1.42	1.46
23	C	513	CLA	C3D-C4D	-2.25	1.39	1.44
23	A	405[A]	CLA	C3D-C4D	-2.25	1.39	1.44
23	B	602	CLA	C3B-C2B	2.25	1.48	1.41
23	B	615	CLA	C3D-C4D	-2.25	1.39	1.44
24	a	408[A]	PHO	C1D-ND	-2.25	1.34	1.38
32	m	103	LMT	C3'-C2'	2.25	1.58	1.52
26	F	101	SQD	O6-C1	2.25	1.44	1.40
27	D	701	GOL	O2-C2	-2.25	1.36	1.43
23	b	611	CLA	C4C-C3C	2.25	1.48	1.45
23	a	405[B]	CLA	C1B-C2B	2.24	1.48	1.43
24	a	353[B]	PHO	C4B-NB	-2.24	1.34	1.38
23	b	613	CLA	OBD-CAD	2.24	1.26	1.22
32	E	102	LMT	O3'-C3'	-2.24	1.37	1.43
23	c	509	CLA	C3B-C2B	2.24	1.48	1.41
23	b	612	CLA	C3D-C4D	-2.24	1.39	1.44
23	b	613	CLA	C1C-C2C	2.24	1.48	1.44
27	d	701	GOL	O2-C2	-2.24	1.36	1.43
23	b	605	CLA	C4C-C3C	2.24	1.48	1.45
24	A	353[B]	PHO	C1D-ND	-2.24	1.34	1.38
23	A	406[B]	CLA	C1C-C2C	2.23	1.48	1.44
23	b	611	CLA	C4D-CHA	2.23	1.46	1.38
23	C	503	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	611	CLA	C3D-C4D	-2.23	1.39	1.44
23	b	601	CLA	C1B-C2B	2.22	1.48	1.43
35	C	518[A]	DGD	O5D-C1E	2.22	1.44	1.40
23	c	504	CLA	MG-NA	2.22	2.11	2.06
23	c	507	CLA	C3B-C2B	2.22	1.48	1.41
23	C	513	CLA	C1B-C2B	2.22	1.48	1.43
23	b	611	CLA	C1D-C2D	2.21	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	C1B-C2B	2.21	1.48	1.43
23	b	608	CLA	C1B-C2B	2.21	1.48	1.43
32	D	404	LMT	O5'-C5'	-2.20	1.39	1.44
23	b	615	CLA	C4B-NB	-2.20	1.35	1.37
23	A	404[A]	CLA	C3B-C2B	2.20	1.48	1.41
24	A	407[B]	PHO	C4B-NB	-2.20	1.34	1.38
23	c	512	CLA	MG-NA	2.20	2.11	2.06
23	b	604	CLA	MG-NA	2.20	2.11	2.06
23	C	513	CLA	C3B-C2B	2.19	1.48	1.41
34	B	623	HTG	C1'-S1	-2.19	1.78	1.81
23	b	602	CLA	C4C-C3C	2.19	1.48	1.45
32	M	103	LMT	O3B-C3B	-2.19	1.37	1.43
23	a	405[A]	CLA	C3B-C4B	2.19	1.47	1.42
23	C	508	CLA	C3B-C2B	2.19	1.48	1.41
38	E	103	HEM	C3B-C4B	2.19	1.49	1.44
23	a	407[B]	CLA	C4C-C3C	2.18	1.48	1.45
24	A	353[A]	PHO	C1D-ND	-2.18	1.34	1.38
23	D	405[A]	CLA	C4C-C3C	2.18	1.48	1.45
23	B	608	CLA	C1C-C2C	2.18	1.48	1.44
23	c	506	CLA	C3D-C4D	-2.17	1.39	1.44
40	v	202	HEC	CMD-C2D	2.17	1.55	1.50
29	D	408[B]	PL9	C2-C3	2.17	1.40	1.34
23	d	403	CLA	C3D-C4D	-2.17	1.39	1.44
23	B	601	CLA	C1C-NC	-2.17	1.34	1.37
23	c	505	CLA	C3B-C2B	2.17	1.48	1.41
23	A	406[B]	CLA	C1D-C2D	2.17	1.49	1.45
23	B	603	CLA	C4C-C3C	2.16	1.48	1.45
23	a	405[A]	CLA	C3B-C2B	2.16	1.48	1.41
23	B	612	CLA	C1C-NC	-2.16	1.34	1.37
26	B	620	SQD	O6-C1	2.16	1.43	1.40
23	B	612	CLA	C3B-C4B	2.15	1.47	1.42
23	D	405[A]	CLA	C3B-C4B	2.15	1.47	1.42
23	B	601	CLA	C3D-C4D	-2.15	1.39	1.44
23	c	514	CLA	C3B-C2B	2.15	1.48	1.41
23	A	408	CLA	C4C-C3C	2.15	1.48	1.45
23	c	503	CLA	C4C-C3C	2.15	1.48	1.45
23	b	607	CLA	C3B-C2B	2.14	1.48	1.41
32	a	420	LMT	O3'-C3'	-2.14	1.37	1.43
23	b	613	CLA	C4C-C3C	2.13	1.48	1.45
23	B	610	CLA	C4C-C3C	2.13	1.48	1.45
23	C	504	CLA	C3D-C4D	-2.13	1.39	1.44
23	c	507	CLA	C1C-NC	-2.13	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	612	CLA	C4C-C3C	2.13	1.48	1.45
23	C	507	CLA	C1D-C2D	2.12	1.49	1.45
23	b	616	CLA	C3B-C2B	2.12	1.48	1.41
23	B	614	CLA	C1C-NC	-2.12	1.34	1.37
29	a	416[A]	PL9	C2-C3	2.12	1.40	1.34
23	a	406[A]	CLA	C1C-C2C	2.12	1.48	1.44
23	B	603	CLA	C1B-C2B	2.12	1.48	1.43
23	A	406[A]	CLA	C1C-NC	-2.12	1.34	1.37
23	B	606	CLA	C3B-C2B	2.11	1.48	1.41
40	v	202	HEC	CMC-C2C	2.11	1.55	1.50
23	C	508	CLA	C4C-C3C	2.11	1.48	1.45
23	b	614	CLA	C3B-C2B	2.11	1.48	1.41
23	b	616	CLA	C1C-NC	-2.11	1.34	1.37
23	A	406[A]	CLA	C3D-C4D	-2.11	1.39	1.44
23	c	509	CLA	C4C-C3C	2.10	1.48	1.45
27	D	701	GOL	C3-C2	2.10	1.60	1.51
23	B	603	CLA	C3B-C4B	2.10	1.47	1.42
23	c	513	CLA	C3D-C4D	-2.10	1.39	1.44
23	C	504	CLA	C4C-C3C	2.10	1.48	1.45
23	a	405[A]	CLA	C3D-C4D	-2.10	1.39	1.44
23	a	407[A]	CLA	C4C-C3C	2.10	1.48	1.45
27	A	701	GOL	C3-C2	2.09	1.60	1.51
23	A	408	CLA	C1C-C2C	2.09	1.48	1.44
32	M	101	LMT	O2B-C2B	-2.09	1.38	1.43
40	V	202	HEC	CMA-C3A	2.09	1.55	1.50
23	a	405[B]	CLA	C4B-NB	-2.09	1.35	1.37
23	d	402[A]	CLA	C3B-C2B	2.09	1.48	1.41
23	c	507	CLA	C1C-C2C	2.09	1.48	1.44
23	B	613	CLA	C3D-C4D	-2.09	1.39	1.44
23	c	508	CLA	C3B-C4B	2.09	1.47	1.42
23	a	405[B]	CLA	C3D-C4D	-2.09	1.39	1.44
23	b	614	CLA	C4C-C3C	2.08	1.48	1.45
23	c	505	CLA	C3D-C4D	-2.08	1.39	1.44
24	a	353[A]	PHO	C1B-NB	-2.08	1.34	1.38
23	c	509	CLA	C1C-NC	-2.08	1.34	1.37
23	B	601	CLA	C4C-C3C	2.08	1.48	1.45
24	A	353[B]	PHO	C3D-C4D	-2.08	1.38	1.41
23	b	605	CLA	C3D-C4D	-2.08	1.39	1.44
23	c	509	CLA	C3D-C4D	-2.07	1.39	1.44
35	c	518[A]	DGD	O2G-C2G	-2.07	1.41	1.46
23	C	502	CLA	C3B-C2B	2.07	1.48	1.41
38	E	103	HEM	C1D-ND	-2.07	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C3B-C2B	2.07	1.48	1.41
23	B	601	CLA	C3B-C2B	2.06	1.48	1.41
23	b	604	CLA	C3B-C2B	2.06	1.48	1.41
35	c	519	DGD	O5D-C1E	2.06	1.43	1.40
24	a	353[B]	PHO	CHA-CBD	-2.06	1.49	1.51
23	a	407[B]	CLA	C3B-C2B	2.05	1.48	1.41
23	c	504	CLA	C4C-C3C	2.05	1.48	1.45
32	a	414	LMT	O3'-C3'	-2.05	1.38	1.43
32	e	102	LMT	O2B-C2B	-2.05	1.38	1.43
23	B	613	CLA	C3B-C2B	2.05	1.48	1.41
23	c	512	CLA	C1D-C2D	2.05	1.49	1.45
23	C	509	CLA	C1A-CHA	2.05	1.51	1.43
23	b	601	CLA	C4C-C3C	2.05	1.48	1.45
23	b	610	CLA	C3B-C2B	2.05	1.48	1.41
32	t	102	LMT	O2'-C2'	-2.05	1.38	1.43
24	A	407[A]	PHO	C1B-NB	-2.05	1.34	1.38
23	C	514	CLA	C1C-NC	-2.04	1.34	1.37
23	b	606	CLA	C3B-C2B	2.04	1.48	1.41
24	A	353[B]	PHO	C1B-NB	-2.04	1.34	1.38
23	B	604	CLA	MG-NA	2.04	2.11	2.06
23	B	602	CLA	O2D-CED	-2.04	1.40	1.45
29	A	414[A]	PL9	C2-C1	-2.04	1.39	1.44
24	a	353[B]	PHO	C1D-ND	-2.04	1.34	1.38
32	M	103	LMT	O2'-C2'	-2.04	1.38	1.43
27	b	624	GOL	C3-C2	2.04	1.60	1.51
24	a	408[B]	PHO	CHA-CBD	-2.03	1.49	1.51
23	c	510	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	603	CLA	C1C-NC	-2.03	1.34	1.37
23	A	404[A]	CLA	C3D-C4D	-2.03	1.39	1.44
23	B	605	CLA	C4C-C3C	2.03	1.48	1.45
23	c	513	CLA	C1D-C2D	2.03	1.49	1.45
32	a	420	LMT	O2'-C2'	-2.03	1.38	1.43
23	b	615	CLA	C4C-C3C	2.03	1.48	1.45
29	a	416[B]	PL9	C2-C3	2.02	1.40	1.34
23	b	601	CLA	C1D-C2D	2.02	1.49	1.45
23	b	606	CLA	C1D-C2D	2.02	1.49	1.45
23	c	508	CLA	C4C-C3C	2.02	1.48	1.45
23	c	508	CLA	C1D-C2D	2.02	1.49	1.45
23	A	405[B]	CLA	C4C-C3C	2.02	1.48	1.45
23	A	404[B]	CLA	C3D-C4D	-2.02	1.39	1.44
25	B	619	BCR	C30-C25	-2.01	1.51	1.53
23	B	615	CLA	MG-NA	2.01	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408[B]	PHO	C3A-C2A	-2.01	1.52	1.54
32	t	101	LMT	O2'-C2'	-2.01	1.38	1.43
37	L	101[B]	LHG	O7-C5	-2.01	1.41	1.46
23	b	614	CLA	CHB-C4A	-2.01	1.32	1.37
23	D	405[B]	CLA	C4C-C3C	2.01	1.48	1.45
26	a	413	SQD	O6-C1	2.01	1.43	1.40
23	c	507	CLA	C1D-C2D	2.00	1.49	1.45
32	M	101	LMT	C1B-C2B	2.00	1.58	1.52
23	B	609	CLA	C3B-C2B	2.00	1.48	1.41

All (3316) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	611	CLA	C2B-C1B-NB	17.87	122.21	110.23
23	B	611	CLA	C3B-C2B-C1B	-14.72	89.39	107.16
24	A	353[B]	PHO	C2D-C1D-ND	11.90	117.74	109.53
24	A	407[A]	PHO	C2D-C1D-ND	11.89	117.73	109.53
23	B	611	CLA	C1D-ND-C4D	-11.73	98.00	106.33
24	a	353[A]	PHO	C2D-C1D-ND	11.37	117.38	109.53
23	B	611	CLA	CHB-C1B-NB	-11.24	112.36	124.26
24	a	408[A]	PHO	C2D-C1D-ND	11.17	117.24	109.53
24	a	353[B]	PHO	C2D-C1D-ND	11.15	117.23	109.53
24	A	353[A]	PHO	C2D-C1D-ND	10.94	117.08	109.53
24	a	408[B]	PHO	C2D-C1D-ND	10.61	116.85	109.53
24	A	407[B]	PHO	C2D-C1D-ND	10.59	116.84	109.53
23	a	409	CLA	C1D-ND-C4D	-10.36	98.98	106.33
23	b	605	CLA	C1D-ND-C4D	-10.18	99.10	106.33
23	a	405[B]	CLA	C1D-ND-C4D	-10.08	99.17	106.33
23	C	504	CLA	C1D-ND-C4D	-10.08	99.18	106.33
23	c	512	CLA	C1D-ND-C4D	-9.99	99.24	106.33
23	d	403	CLA	C1D-ND-C4D	-9.99	99.24	106.33
23	C	505	CLA	C1D-ND-C4D	-9.98	99.24	106.33
23	B	614	CLA	C1D-ND-C4D	-9.96	99.26	106.33
23	B	611	CLA	C2D-C1D-ND	9.88	117.38	110.10
23	b	614	CLA	C2D-C1D-ND	9.86	117.37	110.10
23	A	408	CLA	C1D-ND-C4D	-9.82	99.36	106.33
23	B	615	CLA	C1D-ND-C4D	-9.80	99.37	106.33
23	b	603	CLA	C1D-ND-C4D	-9.75	99.41	106.33
23	a	407[B]	CLA	C1D-ND-C4D	-9.72	99.43	106.33
23	B	601	CLA	C1D-ND-C4D	-9.70	99.45	106.33
23	c	504	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	B	606	CLA	C1D-ND-C4D	-9.68	99.46	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[B]	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	d	402[B]	CLA	C1D-ND-C4D	-9.57	99.54	106.33
23	C	505	CLA	C2D-C1D-ND	9.56	117.15	110.10
23	b	602	CLA	C1D-ND-C4D	-9.53	99.56	106.33
23	D	405[B]	CLA	C1D-ND-C4D	-9.52	99.57	106.33
23	a	406[B]	CLA	C1D-ND-C4D	-9.46	99.61	106.33
23	b	610	CLA	C1D-ND-C4D	-9.42	99.64	106.33
23	C	502	CLA	C1D-ND-C4D	-9.39	99.66	106.33
23	B	605	CLA	C1D-ND-C4D	-9.37	99.68	106.33
23	B	612	CLA	C1D-ND-C4D	-9.35	99.69	106.33
23	B	606	CLA	C2D-C1D-ND	9.35	116.99	110.10
23	c	514	CLA	C1D-ND-C4D	-9.35	99.70	106.33
23	A	404[B]	CLA	C1D-ND-C4D	-9.33	99.70	106.33
23	b	611	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	c	510	CLA	C1D-ND-C4D	-9.31	99.72	106.33
23	C	514	CLA	C1D-ND-C4D	-9.30	99.73	106.33
23	b	614	CLA	C1D-ND-C4D	-9.28	99.75	106.33
23	b	609	CLA	C1D-ND-C4D	-9.25	99.76	106.33
23	c	506	CLA	C1D-ND-C4D	-9.22	99.79	106.33
23	B	603	CLA	C1D-ND-C4D	-9.21	99.79	106.33
23	a	409	CLA	C2D-C1D-ND	9.19	116.88	110.10
23	B	603	CLA	C2D-C1D-ND	9.19	116.88	110.10
23	a	407[A]	CLA	C1D-ND-C4D	-9.17	99.82	106.33
23	D	405[A]	CLA	C1D-ND-C4D	-9.16	99.83	106.33
23	C	511	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	b	615	CLA	C1D-ND-C4D	-9.13	99.85	106.33
23	B	614	CLA	C2D-C1D-ND	9.12	116.83	110.10
23	d	402[A]	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	c	511	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	B	613	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	A	406[A]	CLA	C1D-ND-C4D	-9.08	99.89	106.33
23	C	506	CLA	C1D-ND-C4D	-9.07	99.89	106.33
23	a	406[A]	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	d	403	CLA	C2D-C1D-ND	9.03	116.76	110.10
23	A	408	CLA	C2D-C1D-ND	8.99	116.73	110.10
23	c	502	CLA	C1D-ND-C4D	-8.96	99.97	106.33
23	c	507	CLA	C1D-ND-C4D	-8.95	99.97	106.33
23	C	507	CLA	C1D-ND-C4D	-8.93	99.99	106.33
23	b	601	CLA	C1D-ND-C4D	-8.92	100.00	106.33
23	B	607	CLA	C1D-ND-C4D	-8.91	100.00	106.33
23	A	405[A]	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	b	605	CLA	C2D-C1D-ND	8.89	116.65	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[B]	CLA	C1D-ND-C4D	-8.88	100.03	106.33
23	c	513	CLA	C1D-ND-C4D	-8.87	100.04	106.33
23	C	513	CLA	C1D-ND-C4D	-8.86	100.04	106.33
23	B	610	CLA	C2D-C1D-ND	8.84	116.62	110.10
23	c	505	CLA	C1D-ND-C4D	-8.84	100.06	106.33
23	C	504	CLA	C2D-C1D-ND	8.84	116.61	110.10
23	a	405[A]	CLA	C1D-ND-C4D	-8.83	100.06	106.33
23	B	602	CLA	C1D-ND-C4D	-8.81	100.08	106.33
23	c	509	CLA	C2D-C1D-ND	8.79	116.58	110.10
23	b	606	CLA	C1D-ND-C4D	-8.77	100.11	106.33
23	a	406[A]	CLA	C2D-C1D-ND	8.75	116.56	110.10
23	C	509	CLA	C1D-ND-C4D	-8.75	100.12	106.33
23	b	612	CLA	C1D-ND-C4D	-8.75	100.12	106.33
23	c	503	CLA	C1D-ND-C4D	-8.74	100.13	106.33
23	a	406[B]	CLA	C2D-C1D-ND	8.74	116.54	110.10
23	c	508	CLA	C1D-ND-C4D	-8.69	100.16	106.33
23	a	407[A]	CLA	C2D-C1D-ND	8.65	116.48	110.10
23	B	610	CLA	C1D-ND-C4D	-8.64	100.19	106.33
23	B	613	CLA	C2D-C1D-ND	8.60	116.44	110.10
23	c	512	CLA	C2D-C1D-ND	8.60	116.44	110.10
23	C	510	CLA	C1D-ND-C4D	-8.57	100.25	106.33
23	B	608	CLA	C1D-ND-C4D	-8.56	100.25	106.33
23	B	609	CLA	C1D-ND-C4D	-8.53	100.28	106.33
23	a	407[B]	CLA	C2D-C1D-ND	8.53	116.39	110.10
23	D	405[B]	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	D	405[A]	CLA	C2D-C1D-ND	8.50	116.37	110.10
23	A	404[A]	CLA	C1D-ND-C4D	-8.50	100.30	106.33
23	b	603	CLA	C2D-C1D-ND	8.49	116.36	110.10
23	b	608	CLA	C1D-ND-C4D	-8.48	100.31	106.33
23	B	601	CLA	C2D-C1D-ND	8.48	116.35	110.10
23	c	509	CLA	C1D-ND-C4D	-8.47	100.32	106.33
23	D	406	CLA	C1D-ND-C4D	-8.45	100.33	106.33
23	b	616	CLA	C1D-ND-C4D	-8.42	100.35	106.33
23	c	513	CLA	C2B-C1B-NB	8.41	115.87	110.23
23	b	611	CLA	C2D-C1D-ND	8.36	116.27	110.10
23	B	615	CLA	C2D-C1D-ND	8.36	116.27	110.10
23	b	606	CLA	C2B-C1B-NB	8.36	115.83	110.23
23	C	513	CLA	C2B-C1B-NB	8.32	115.81	110.23
23	B	611	CLA	CHD-C4C-C3C	-8.31	112.62	124.84
23	b	602	CLA	C2B-C1B-NB	8.30	115.79	110.23
23	B	608	CLA	C2D-C1D-ND	8.29	116.21	110.10
23	c	510	CLA	C2D-C1D-ND	8.27	116.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C2D-C1D-ND	8.26	116.19	110.10
23	A	405[A]	CLA	C2D-C1D-ND	8.25	116.18	110.10
23	B	612	CLA	C2D-C1D-ND	8.24	116.18	110.10
23	C	509	CLA	C2D-C1D-ND	8.19	116.14	110.10
23	A	406[A]	CLA	C2D-C1D-ND	8.15	116.11	110.10
23	b	607	CLA	C1D-ND-C4D	-8.15	100.54	106.33
23	b	615	CLA	C2D-C1D-ND	8.15	116.11	110.10
24	a	408[A]	PHO	O2D-CGD-CBD	8.14	121.31	111.00
23	A	404[B]	CLA	C2D-C1D-ND	8.13	116.09	110.10
23	b	610	CLA	C2D-C1D-ND	8.13	116.09	110.10
23	B	616	CLA	C1D-ND-C4D	-8.12	100.56	106.33
23	d	402[B]	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	B	605	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	c	511	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	b	613	CLA	C2D-C1D-ND	8.10	116.08	110.10
23	b	616	CLA	C2B-C1B-NB	8.10	115.66	110.23
23	C	503	CLA	C1D-ND-C4D	-8.09	100.59	106.33
23	C	514	CLA	C2D-C1D-ND	8.09	116.06	110.10
23	c	504	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	a	405[B]	CLA	C2D-C1D-ND	8.06	116.04	110.10
23	c	514	CLA	C2D-C1D-ND	8.03	116.02	110.10
23	C	502	CLA	C2D-C1D-ND	8.02	116.01	110.10
23	A	405[B]	CLA	C2D-C1D-ND	8.01	116.00	110.10
23	a	407[B]	CLA	C2B-C1B-NB	8.01	115.60	110.23
23	c	508	CLA	C2D-C1D-ND	8.00	116.00	110.10
23	B	611	CLA	CMB-C2B-C1B	7.99	137.54	125.37
23	A	408	CLA	C2B-C1B-NB	7.96	115.57	110.23
23	c	507	CLA	C2D-C1D-ND	7.94	115.95	110.10
23	B	602	CLA	C2D-C1D-ND	7.94	115.95	110.10
23	d	403	CLA	C2B-C1B-NB	7.90	115.53	110.23
23	B	607	CLA	C2D-C1D-ND	7.89	115.92	110.10
34	b	623	HTG	C1'-S1-C1	7.87	114.82	100.09
23	B	616	CLA	C2D-C1D-ND	7.87	115.90	110.10
23	C	510	CLA	C2D-C1D-ND	7.87	115.90	110.10
23	c	505	CLA	C2D-C1D-ND	7.86	115.90	110.10
23	b	604	CLA	C1D-ND-C4D	-7.86	100.75	106.33
23	A	406[B]	CLA	C2B-C1B-NB	7.84	115.49	110.23
24	a	353[A]	PHO	O2D-CGD-CBD	7.83	120.91	111.00
23	d	402[A]	CLA	C2D-C1D-ND	7.82	115.87	110.10
23	C	508	CLA	C1D-ND-C4D	-7.81	100.78	106.33
23	b	614	CLA	C2B-C1B-NB	7.81	115.47	110.23
23	C	512	CLA	C1D-ND-C4D	-7.77	100.82	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	513	CLA	C2D-C1D-ND	7.76	115.82	110.10
23	c	504	CLA	C4A-NA-C1A	-7.75	103.22	106.71
23	b	613	CLA	C1D-ND-C4D	-7.74	100.84	106.33
23	c	514	CLA	C2B-C1B-NB	7.73	115.41	110.23
23	b	616	CLA	C4A-NA-C1A	-7.73	103.23	106.71
23	B	609	CLA	C2D-C1D-ND	7.73	115.80	110.10
24	a	408[B]	PHO	O2D-CGD-CBD	7.71	120.77	111.00
23	c	506	CLA	C2D-C1D-ND	7.71	115.78	110.10
23	A	406[B]	CLA	C2D-C1D-ND	7.70	115.78	110.10
23	b	608	CLA	C2B-C1B-NB	7.68	115.38	110.23
23	C	508	CLA	C2D-C1D-ND	7.68	115.76	110.10
23	b	601	CLA	C2D-C1D-ND	7.67	115.76	110.10
23	b	616	CLA	C2D-C1D-ND	7.67	115.75	110.10
23	b	609	CLA	C2D-C1D-ND	7.66	115.75	110.10
23	A	404[A]	CLA	C2D-C1D-ND	7.64	115.73	110.10
23	a	405[B]	CLA	C2B-C1B-NB	7.61	115.34	110.23
23	B	614	CLA	CMD-C2D-C1D	7.61	138.12	124.71
23	b	608	CLA	C2D-C1D-ND	7.60	115.71	110.10
23	A	405[B]	CLA	C2B-C1B-NB	7.60	115.33	110.23
23	b	611	CLA	C2B-C1B-NB	7.60	115.33	110.23
23	B	601	CLA	C2B-C1B-NB	7.59	115.32	110.23
23	C	511	CLA	C2B-C1B-NB	7.59	115.32	110.23
23	b	601	CLA	C2B-C1B-NB	7.58	115.31	110.23
23	C	514	CLA	C2B-C1B-NB	7.55	115.29	110.23
23	c	502	CLA	C2D-C1D-ND	7.52	115.65	110.10
23	A	406[A]	CLA	C2B-C1B-NB	7.52	115.27	110.23
23	b	607	CLA	C2D-C1D-ND	7.51	115.64	110.10
23	C	504	CLA	C4A-NA-C1A	-7.51	103.33	106.71
23	b	602	CLA	C4A-NA-C1A	-7.50	103.33	106.71
23	C	510	CLA	C2B-C1B-NB	7.48	115.24	110.23
23	b	602	CLA	C2D-C1D-ND	7.46	115.61	110.10
24	A	353[A]	PHO	C2B-C1B-NB	7.46	114.68	109.53
24	A	353[A]	PHO	O2D-CGD-CBD	7.46	120.44	111.00
23	c	513	CLA	C2D-C1D-ND	7.45	115.59	110.10
23	C	507	CLA	C2D-C1D-ND	7.44	115.59	110.10
23	c	502	CLA	CMD-C2D-C1D	7.41	137.78	124.71
23	a	406[B]	CLA	C2B-C1B-NB	7.38	115.18	110.23
23	c	505	CLA	C2B-C1B-NB	7.37	115.17	110.23
24	A	407[B]	PHO	O2D-CGD-CBD	7.37	120.33	111.00
24	a	353[B]	PHO	O2D-CGD-CBD	7.36	120.32	111.00
24	A	407[A]	PHO	C4D-ND-C1D	-7.35	101.35	108.83
23	C	511	CLA	C2D-C1D-ND	7.34	115.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	406	CLA	C2D-C1D-ND	7.33	115.50	110.10
23	a	405[A]	CLA	C2D-C1D-ND	7.32	115.50	110.10
23	C	507	CLA	C2B-C1B-NB	7.31	115.13	110.23
24	A	353[B]	PHO	O2D-CGD-CBD	7.30	120.24	111.00
23	b	615	CLA	C4A-NA-C1A	-7.30	103.42	106.71
23	C	511	CLA	CMD-C2D-C1D	7.29	137.56	124.71
23	c	502	CLA	C2B-C1B-NB	7.28	115.11	110.23
23	b	612	CLA	C2D-C1D-ND	7.24	115.44	110.10
23	b	606	CLA	C2D-C1D-ND	7.23	115.43	110.10
23	D	405[A]	CLA	C4A-NA-C1A	-7.21	103.46	106.71
23	a	409	CLA	C2B-C1B-NB	7.19	115.05	110.23
23	C	504	CLA	C2B-C1B-NB	7.19	115.05	110.23
23	C	503	CLA	C2D-C1D-ND	7.18	115.40	110.10
23	b	616	CLA	O2D-CGD-CBD	7.18	124.03	111.27
23	B	605	CLA	C2B-C1B-NB	7.17	115.04	110.23
23	C	512	CLA	C2B-C1B-NB	7.17	115.04	110.23
23	B	604	CLA	C2B-C1B-NB	7.16	115.03	110.23
23	B	604	CLA	C1D-ND-C4D	-7.16	101.25	106.33
23	A	405[A]	CLA	C2B-C1B-NB	7.15	115.03	110.23
23	C	506	CLA	C2D-C1D-ND	7.12	115.35	110.10
23	c	502	CLA	CHD-C1D-ND	-7.10	117.93	124.45
23	c	503	CLA	C2B-C1B-NB	7.09	114.99	110.23
23	c	508	CLA	CMD-C2D-C1D	7.09	137.21	124.71
23	C	512	CLA	C2D-C1D-ND	7.09	115.33	110.10
23	c	506	CLA	C2B-C1B-NB	7.07	114.97	110.23
26	F	101	SQD	O6-C1-C2	7.05	119.30	108.30
23	B	615	CLA	C4A-NA-C1A	-6.98	103.57	106.71
23	c	513	CLA	C4A-NA-C1A	-6.96	103.58	106.71
23	b	613	CLA	C2B-C1B-NB	6.96	114.90	110.23
23	c	509	CLA	C2B-C1B-NB	6.95	114.89	110.23
23	b	604	CLA	C2D-C1D-ND	6.95	115.22	110.10
23	a	407[A]	CLA	C2B-C1B-NB	6.94	114.89	110.23
23	a	406[A]	CLA	C2B-C1B-NB	6.94	114.88	110.23
23	B	611	CLA	CMD-C2D-C1D	6.93	136.93	124.71
23	d	403	CLA	CHD-C1D-ND	-6.93	118.09	124.45
24	a	353[A]	PHO	C2B-C1B-NB	6.92	114.30	109.53
23	c	507	CLA	C2B-C1B-NB	6.92	114.87	110.23
23	c	508	CLA	CHD-C1D-ND	-6.91	118.10	124.45
23	C	502	CLA	C2B-C1B-NB	6.90	114.86	110.23
23	b	606	CLA	C4A-NA-C1A	-6.88	103.61	106.71
23	b	605	CLA	CHD-C4C-C3C	-6.86	114.76	124.84
23	b	615	CLA	C2B-C1B-NB	6.85	114.83	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	602	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	b	604	CLA	C2B-C1B-NB	6.84	114.82	110.23
23	B	616	CLA	CHD-C4C-C3C	-6.83	114.80	124.84
23	b	606	CLA	CMD-C2D-C1D	6.83	136.75	124.71
24	A	353[B]	PHO	C2B-C1B-NB	6.81	114.23	109.53
23	B	606	CLA	C4A-NA-C1A	-6.80	103.65	106.71
23	B	605	CLA	CHD-C4C-C3C	-6.80	114.85	124.84
23	c	504	CLA	CMD-C2D-C1D	6.80	136.69	124.71
23	C	509	CLA	C2B-C1B-NB	6.77	114.77	110.23
23	a	409	CLA	CHD-C4C-C3C	-6.76	114.90	124.84
24	A	353[B]	PHO	C4D-ND-C1D	-6.76	101.95	108.83
24	a	408[B]	PHO	C1C-C2C-C3C	-6.76	102.99	108.61
23	c	507	CLA	CMD-C2D-C1D	6.76	136.62	124.71
23	c	510	CLA	C2B-C1B-NB	6.76	114.76	110.23
23	B	616	CLA	O2D-CGD-CBD	6.75	123.27	111.27
23	a	405[A]	CLA	C2B-C1B-NB	6.74	114.75	110.23
24	a	353[B]	PHO	C2B-C1B-NB	6.74	114.18	109.53
23	B	608	CLA	C2B-C1B-NB	6.73	114.75	110.23
24	a	353[A]	PHO	C4D-ND-C1D	-6.72	101.99	108.83
23	d	403	CLA	CMD-C2D-C1D	6.71	136.54	124.71
23	A	404[A]	CLA	CMD-C2D-C1D	6.70	136.53	124.71
23	B	609	CLA	C4A-NA-C1A	-6.70	103.69	106.71
23	B	606	CLA	CMD-C2D-C1D	6.69	136.50	124.71
23	c	503	CLA	C2C-C1C-NC	6.68	116.23	109.97
23	c	511	CLA	C2B-C1B-NB	6.68	114.71	110.23
23	b	605	CLA	CMD-C2D-C1D	6.67	136.47	124.71
23	b	613	CLA	C4A-NA-C1A	-6.67	103.71	106.71
23	A	406[B]	CLA	C4A-NA-C1A	-6.66	103.71	106.71
23	A	404[A]	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	c	504	CLA	C2B-C1B-NB	6.65	114.69	110.23
23	B	605	CLA	CMD-C2D-C1D	6.65	136.43	124.71
23	B	614	CLA	CHD-C1D-ND	-6.63	118.36	124.45
23	B	609	CLA	C2B-C1B-NB	6.63	114.68	110.23
23	C	506	CLA	C2B-C1B-NB	6.63	114.68	110.23
23	c	508	CLA	O2D-CGD-CBD	6.63	123.05	111.27
24	a	353[B]	PHO	C1C-C2C-C3C	-6.61	103.11	108.61
23	b	601	CLA	O2D-CGD-CBD	6.61	123.02	111.27
23	a	406[A]	CLA	CHD-C4C-C3C	-6.61	115.12	124.84
23	C	513	CLA	CHD-C4C-C3C	-6.61	115.13	124.84
23	c	505	CLA	CHD-C1D-ND	-6.59	118.40	124.45
24	a	353[B]	PHO	C4D-ND-C1D	-6.59	102.12	108.83
23	B	610	CLA	C2B-C1B-NB	6.56	114.63	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	507	CLA	CMD-C2D-C1D	6.56	136.27	124.71
23	c	514	CLA	CMD-C2D-C1D	6.55	136.26	124.71
23	B	606	CLA	C2B-C1B-NB	6.54	114.62	110.23
23	B	603	CLA	CHD-C4C-C3C	-6.54	115.23	124.84
23	a	407[B]	CLA	CHD-C1D-ND	-6.53	118.45	124.45
23	C	503	CLA	C2B-C1B-NB	6.51	114.60	110.23
23	B	601	CLA	CHD-C4C-C3C	-6.51	115.27	124.84
23	B	601	CLA	CMD-C2D-C1D	6.50	136.17	124.71
24	A	407[B]	PHO	C4D-ND-C1D	-6.50	102.22	108.83
23	b	611	CLA	CMD-C2D-C1D	6.50	136.17	124.71
23	B	616	CLA	C2B-C1B-NB	6.50	114.59	110.23
23	b	609	CLA	CHD-C4C-C3C	-6.49	115.30	124.84
23	d	402[A]	CLA	C2C-C1C-NC	6.49	116.05	109.97
24	a	408[A]	PHO	C2B-C1B-NB	6.49	114.01	109.53
23	a	406[B]	CLA	CHD-C4C-C3C	-6.49	115.31	124.84
24	a	408[A]	PHO	C1C-C2C-C3C	-6.48	103.22	108.61
23	B	606	CLA	CHD-C4C-C3C	-6.47	115.33	124.84
23	b	605	CLA	CHD-C1D-ND	-6.46	118.52	124.45
23	A	404[B]	CLA	C2B-C1B-NB	6.46	114.56	110.23
23	b	610	CLA	CHD-C4C-C3C	-6.45	115.36	124.84
23	A	404[A]	CLA	C4A-NA-C1A	-6.44	103.81	106.71
26	A	410[A]	SQD	O6-C1-C2	6.44	118.36	108.30
23	B	606	CLA	CHD-C1D-ND	-6.44	118.54	124.45
24	A	353[A]	PHO	C1C-C2C-C3C	-6.44	103.26	108.61
23	C	509	CLA	C2C-C1C-NC	6.44	116.00	109.97
23	b	616	CLA	CMD-C2D-C1D	6.44	136.06	124.71
24	A	353[A]	PHO	C4D-ND-C1D	-6.43	102.29	108.83
23	B	607	CLA	C4A-NA-C1A	-6.41	103.83	106.71
23	B	614	CLA	C2B-C1B-NB	6.41	114.53	110.23
23	a	407[A]	CLA	CHD-C4C-C3C	-6.40	115.43	124.84
23	D	405[B]	CLA	CMD-C2D-C1D	6.40	135.99	124.71
23	b	603	CLA	CHD-C4C-C3C	-6.39	115.44	124.84
34	D	414	HTG	C1'-S1-C1	6.39	112.05	100.09
26	F	101	SQD	O47-C7-C8	6.38	125.25	111.50
23	C	505	CLA	CHD-C1D-ND	-6.38	118.59	124.45
23	b	607	CLA	C2C-C1C-NC	6.37	115.94	109.97
23	b	605	CLA	C2B-C1B-NB	6.36	114.50	110.23
23	D	405[B]	CLA	C4A-NA-C1A	-6.35	103.85	106.71
23	c	506	CLA	CHD-C4C-C3C	-6.35	115.50	124.84
23	D	406	CLA	C2B-C1B-NB	6.35	114.49	110.23
23	C	508	CLA	CMD-C2D-C1D	6.34	135.88	124.71
23	D	405[B]	CLA	CHD-C1D-ND	-6.33	118.64	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	353[A]	PHO	C1C-C2C-C3C	-6.32	103.36	108.61
23	B	604	CLA	CMD-C2D-C1D	6.31	135.84	124.71
23	b	604	CLA	CMD-C2D-C1D	6.31	135.83	124.71
23	C	514	CLA	CHD-C4C-C3C	-6.31	115.57	124.84
24	A	407[B]	PHO	C2B-C1B-NB	6.30	113.88	109.53
23	b	607	CLA	C2B-C1B-NB	6.30	114.45	110.23
24	a	408[B]	PHO	C2B-C1B-NB	6.29	113.87	109.53
23	B	607	CLA	C2C-C1C-NC	6.29	115.86	109.97
23	B	603	CLA	C2B-C1B-NB	6.29	114.45	110.23
23	C	503	CLA	CMD-C2D-C1D	6.28	135.79	124.71
23	b	614	CLA	CHD-C4C-C3C	-6.27	115.62	124.84
23	b	616	CLA	CHD-C4C-C3C	-6.27	115.63	124.84
23	b	610	CLA	C2B-C1B-NB	6.27	114.43	110.23
23	b	606	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	C	504	CLA	CHD-C1D-ND	-6.26	118.70	124.45
23	C	508	CLA	O2D-CGD-CBD	6.25	122.38	111.27
23	b	613	CLA	C2C-C1C-NC	6.25	115.83	109.97
23	A	405[B]	CLA	CMD-C2D-C1D	6.25	135.72	124.71
23	d	402[B]	CLA	CMD-C2D-C1D	6.25	135.72	124.71
23	b	613	CLA	CHD-C4C-C3C	-6.25	115.66	124.84
23	B	603	CLA	O2D-CGD-CBD	6.24	122.36	111.27
23	C	506	CLA	CMD-C2D-C1D	6.24	135.71	124.71
23	c	507	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	A	408	CLA	CHD-C1D-ND	-6.23	118.73	124.45
24	A	407[A]	PHO	O2D-CGD-CBD	6.23	118.89	111.00
23	B	614	CLA	CHD-C4C-C3C	-6.23	115.69	124.84
23	C	507	CLA	CHD-C1D-ND	-6.23	118.73	124.45
23	B	610	CLA	O2D-CGD-CBD	6.22	122.31	111.27
23	b	612	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
23	C	507	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	A	405[B]	CLA	CHD-C1D-ND	-6.21	118.75	124.45
24	A	407[A]	PHO	C1C-C2C-C3C	-6.21	103.45	108.61
23	c	512	CLA	CHD-C4C-C3C	-6.21	115.71	124.84
23	b	610	CLA	O2D-CGD-CBD	6.21	122.30	111.27
23	a	405[A]	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	B	610	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
23	c	511	CLA	CHD-C4C-C3C	-6.20	115.73	124.84
23	B	611	CLA	O2D-CGD-CBD	6.19	122.27	111.27
23	b	615	CLA	CHD-C4C-C3C	-6.19	115.74	124.84
23	C	513	CLA	C4A-NA-C1A	-6.19	103.92	106.71
23	A	404[B]	CLA	CMD-C2D-C1D	6.18	135.61	124.71
23	a	405[A]	CLA	C4A-NA-C1A	-6.18	103.93	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	408	CLA	CHD-C4C-C3C	-6.18	115.76	124.84
23	c	514	CLA	CHD-C1D-ND	-6.17	118.78	124.45
23	a	407[A]	CLA	C4A-NA-C1A	-6.17	103.93	106.71
23	b	611	CLA	CHD-C4C-C3C	-6.17	115.78	124.84
23	b	603	CLA	C2B-C1B-NB	6.17	114.36	110.23
23	A	406[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
24	a	408[B]	PHO	C4D-ND-C1D	-6.14	102.58	108.83
24	A	407[A]	PHO	C2B-C1B-NB	6.14	113.77	109.53
23	A	406[B]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	C	505	CLA	CMD-C2D-C1D	6.14	135.53	124.71
23	a	407[A]	CLA	CHD-C1D-ND	-6.14	118.81	124.45
23	B	606	CLA	O2D-CGD-CBD	6.12	122.15	111.27
23	A	404[A]	CLA	CHD-C1D-ND	-6.11	118.83	124.45
23	C	502	CLA	CHD-C4C-C3C	-6.11	115.86	124.84
23	b	607	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	D	405[A]	CLA	CMD-C2D-C1D	6.10	135.47	124.71
23	c	504	CLA	CHD-C1D-ND	-6.10	118.85	124.45
23	B	601	CLA	O2D-CGD-CBD	6.10	122.10	111.27
23	B	602	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
23	B	609	CLA	CHD-C4C-C3C	-6.09	115.89	124.84
23	C	508	CLA	C2B-C1B-NB	6.08	114.31	110.23
23	b	602	CLA	CHD-C1D-ND	-6.08	118.87	124.45
23	a	405[A]	CLA	CMD-C2D-C1D	6.07	135.41	124.71
23	b	603	CLA	C4A-NA-C1A	-6.07	103.98	106.71
40	V	202	HEC	C1D-ND-C4D	6.06	111.33	105.07
24	a	408[A]	PHO	C4D-ND-C1D	-6.05	102.68	108.83
23	c	507	CLA	C2C-C1C-NC	6.04	115.63	109.97
23	d	402[B]	CLA	C2B-C1B-NB	6.04	114.28	110.23
23	b	606	CLA	CHD-C4C-C3C	-6.04	115.96	124.84
26	B	620	SQD	O6-C1-C2	6.04	117.73	108.30
23	c	510	CLA	C1-C2-C3	-6.03	115.61	126.04
24	A	407[B]	PHO	C1C-C2C-C3C	-6.03	103.59	108.61
23	b	601	CLA	CMD-C2D-C1D	6.02	135.33	124.71
23	d	402[A]	CLA	C2B-C1B-NB	6.01	114.26	110.23
33	C	501	LMG	C7-O1-C1	-6.01	102.00	113.74
23	d	403	CLA	CHD-C4C-C3C	-6.01	116.01	124.84
23	A	408	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	A	408	CLA	C2C-C1C-NC	6.01	115.60	109.97
23	c	508	CLA	C2B-C1B-NB	6.00	114.26	110.23
23	a	405[B]	CLA	CMD-C2D-C1D	6.00	135.28	124.71
23	B	604	CLA	C2C-C1C-NC	5.99	115.58	109.97
23	C	511	CLA	CHD-C1D-ND	-5.98	118.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	511	CLA	C4A-NA-C1A	-5.98	104.02	106.71
23	a	406[B]	CLA	CHD-C1D-ND	-5.97	118.97	124.45
23	c	504	CLA	CHD-C4C-C3C	-5.96	116.07	124.84
23	a	407[B]	CLA	CMD-C2D-C1D	5.96	135.22	124.71
23	a	407[B]	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	b	602	CLA	CHD-C4C-C3C	-5.96	116.08	124.84
23	b	602	CLA	O2D-CGD-CBD	5.96	121.85	111.27
23	b	608	CLA	O2D-CGD-CBD	5.96	121.85	111.27
23	b	610	CLA	CMD-C2D-C1D	5.95	135.21	124.71
23	B	603	CLA	C2C-C1C-NC	5.95	115.54	109.97
23	C	506	CLA	O2D-CGD-CBD	5.95	121.83	111.27
23	c	512	CLA	C2B-C1B-NB	5.95	114.22	110.23
23	C	508	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	d	402[B]	CLA	CHD-C4C-C3C	-5.94	116.11	124.84
23	B	609	CLA	CMD-C2D-C1D	5.94	135.18	124.71
23	B	608	CLA	CHD-C1D-ND	-5.93	119.00	124.45
23	a	406[A]	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	A	406[B]	CLA	CMD-C2D-C1D	5.93	135.16	124.71
23	B	613	CLA	C2B-C1B-NB	5.92	114.20	110.23
23	B	608	CLA	C2C-C1C-NC	5.92	115.52	109.97
23	b	604	CLA	O2D-CGD-CBD	5.92	121.79	111.27
23	B	616	CLA	C3C-C4C-NC	5.92	117.21	110.57
23	A	406[A]	CLA	C4A-NA-C1A	-5.91	104.05	106.71
23	D	405[A]	CLA	CHD-C1D-ND	-5.91	119.02	124.45
23	c	512	CLA	CMD-C2D-C1D	5.91	135.14	124.71
23	C	511	CLA	CHD-C4C-C3C	-5.91	116.15	124.84
23	D	405[B]	CLA	C2B-C1B-NB	5.91	114.19	110.23
23	C	502	CLA	O2D-CGD-CBD	5.91	121.77	111.27
23	B	614	CLA	O2D-CGD-CBD	5.90	121.76	111.27
40	v	202	HEC	C1D-ND-C4D	5.90	111.17	105.07
23	b	613	CLA	CMD-C2D-C1D	5.90	135.11	124.71
23	B	613	CLA	C2C-C1C-NC	5.90	115.50	109.97
23	C	510	CLA	C2C-C1C-NC	5.89	115.49	109.97
23	b	601	CLA	CHD-C1D-ND	-5.89	119.04	124.45
23	b	608	CLA	C4A-NA-C1A	-5.89	104.06	106.71
23	A	406[A]	CLA	CMD-C2D-C1D	5.89	135.10	124.71
23	b	601	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
23	B	615	CLA	CHD-C4C-C3C	-5.89	116.18	124.84
26	b	620	SQD	O6-C1-C2	5.88	117.48	108.30
23	C	509	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
23	C	506	CLA	C4A-NA-C1A	-5.88	104.06	106.71
23	D	405[A]	CLA	C2C-C1C-NC	5.88	115.48	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	C4A-NA-C1A	-5.87	104.06	106.71
23	d	402[B]	CLA	C2C-C1C-NC	5.87	115.47	109.97
23	B	615	CLA	C2B-C1B-NB	5.87	114.17	110.23
23	C	502	CLA	CMD-C2D-C1D	5.87	135.05	124.71
23	C	506	CLA	CHD-C4C-C3C	-5.86	116.22	124.84
23	C	504	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	c	514	CLA	CHD-C4C-C3C	-5.86	116.23	124.84
23	b	609	CLA	CMD-C2D-C1D	5.86	135.03	124.71
23	B	604	CLA	O2D-CGD-CBD	5.85	121.67	111.27
23	c	509	CLA	CHD-C4C-C3C	-5.85	116.24	124.84
23	b	612	CLA	C2B-C1B-NB	5.85	114.15	110.23
23	c	506	CLA	C4A-NA-C1A	-5.85	104.08	106.71
23	A	406[A]	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	B	605	CLA	CHD-C1D-ND	-5.84	119.08	124.45
23	A	404[A]	CLA	C2C-C1C-NC	5.84	115.44	109.97
25	d	404	BCR	C7-C8-C9	-5.84	117.42	126.23
23	c	505	CLA	CMD-C2D-C1D	5.83	134.99	124.71
23	C	512	CLA	CMD-C2D-C1D	5.82	134.98	124.71
23	b	601	CLA	C4A-NA-C1A	-5.82	104.09	106.71
23	B	601	CLA	CHD-C1D-ND	-5.82	119.11	124.45
23	B	602	CLA	C2C-C1C-NC	5.82	115.42	109.97
23	C	503	CLA	CHD-C4C-C3C	-5.82	116.29	124.84
34	c	522	HTG	C1'-S1-C1	5.81	110.96	100.09
23	B	604	CLA	C2D-C1D-ND	5.81	114.39	110.10
23	C	503	CLA	C2C-C1C-NC	5.81	115.42	109.97
23	B	605	CLA	O2D-CGD-CBD	5.81	121.59	111.27
23	D	405[B]	CLA	CHD-C4C-C3C	-5.80	116.31	124.84
23	A	406[B]	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
23	C	502	CLA	C4A-NA-C1A	-5.80	104.10	106.71
23	D	406	CLA	C4A-NA-C1A	-5.79	104.10	106.71
23	b	605	CLA	C2C-C1C-NC	5.79	115.40	109.97
23	B	602	CLA	CMD-C2D-C1D	5.78	134.90	124.71
23	C	514	CLA	CHD-C1D-ND	-5.78	119.14	124.45
23	b	609	CLA	C2B-C1B-NB	5.77	114.10	110.23
23	A	405[B]	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
23	A	405[A]	CLA	CHD-C4C-C3C	-5.77	116.36	124.84
38	E	103	HEM	CAD-CBD-CGD	5.77	126.02	113.60
34	d	411	HTG	C1'-S1-C1	5.77	110.88	100.09
23	C	514	CLA	CMD-C2D-C1D	5.75	134.85	124.71
25	t	103	BCR	C33-C5-C6	-5.75	118.07	124.53
23	c	508	CLA	CHD-C4C-C3C	-5.75	116.39	124.84
23	B	616	CLA	C4A-NA-C1A	-5.75	104.12	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	C2C-C1C-NC	5.74	115.35	109.97
24	A	353[B]	PHO	C1C-C2C-C3C	-5.74	103.84	108.61
23	B	609	CLA	CHD-C1D-ND	-5.74	119.18	124.45
23	c	510	CLA	C2C-C1C-NC	5.74	115.35	109.97
23	B	602	CLA	C4A-NA-C1A	-5.74	104.13	106.71
23	B	615	CLA	CMD-C2D-C1D	5.73	134.82	124.71
23	b	611	CLA	CHD-C1D-ND	-5.73	119.19	124.45
34	B	623	HTG	C1'-S1-C1	5.73	110.81	100.09
23	c	512	CLA	CHD-C1D-ND	-5.73	119.19	124.45
23	d	402[B]	CLA	CHD-C1D-ND	-5.73	119.19	124.45
23	C	505	CLA	C2B-C1B-NB	5.71	114.06	110.23
23	B	608	CLA	O2D-CGD-CBD	5.71	121.41	111.27
23	D	406	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	C	505	CLA	CHD-C4C-C3C	-5.70	116.46	124.84
26	a	411[A]	SQD	O6-C1-C2	5.69	117.19	108.30
23	C	503	CLA	O2D-CGD-CBD	5.69	121.39	111.27
23	a	409	CLA	O2D-CGD-CBD	5.69	121.38	111.27
23	a	405[B]	CLA	CHD-C1D-ND	-5.69	119.23	124.45
23	C	505	CLA	C2C-C1C-NC	5.68	115.30	109.97
23	B	614	CLA	C3D-C2D-C1D	-5.68	98.08	105.83
23	c	506	CLA	CMD-C2D-C1D	5.66	134.69	124.71
23	a	409	CLA	C4A-NA-C1A	-5.65	104.16	106.71
23	B	613	CLA	CMD-C2D-C1D	5.65	134.67	124.71
23	b	602	CLA	CMD-C2D-C1D	5.65	134.66	124.71
23	B	611	CLA	CMC-C2C-C1C	5.64	133.63	125.04
23	b	603	CLA	CMD-C2D-C1D	5.64	134.66	124.71
23	b	614	CLA	O2D-CGD-CBD	5.64	121.29	111.27
26	A	410[A]	SQD	C1-O5-C5	-5.64	102.61	113.69
23	B	607	CLA	CHD-C1D-ND	-5.64	119.27	124.45
23	C	510	CLA	CHD-C1D-ND	-5.64	119.28	124.45
23	B	612	CLA	CHD-C4C-C3C	-5.63	116.56	124.84
23	B	615	CLA	CHD-C1D-ND	-5.63	119.28	124.45
23	C	512	CLA	C2C-C1C-NC	5.63	115.24	109.97
25	Y	101	BCR	C33-C5-C6	-5.62	118.22	124.53
24	a	353[B]	PHO	C1-C2-C3	-5.62	116.33	126.04
23	B	603	CLA	CHD-C1D-ND	-5.62	119.29	124.45
23	c	513	CLA	CHD-C1D-ND	-5.61	119.30	124.45
25	D	407	BCR	C7-C8-C9	-5.61	117.76	126.23
23	C	510	CLA	CHD-C4C-C3C	-5.61	116.59	124.84
23	b	614	CLA	CHD-C1D-ND	-5.61	119.30	124.45
23	A	404[B]	CLA	CHD-C1D-ND	-5.60	119.30	124.45
23	b	605	CLA	O2D-CGD-CBD	5.60	121.22	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404[B]	CLA	CHD-C4C-C3C	-5.60	116.61	124.84
23	D	405[B]	CLA	C2C-C1C-NC	5.59	115.21	109.97
23	D	406	CLA	CMD-C2D-C1D	5.59	134.57	124.71
23	C	511	CLA	O2D-CGD-CBD	5.59	121.21	111.27
23	c	510	CLA	CMD-C2D-C1D	5.59	134.56	124.71
23	b	607	CLA	CHD-C4C-C3C	-5.58	116.63	124.84
23	b	608	CLA	CHD-C1D-ND	-5.58	119.32	124.45
23	c	509	CLA	C2C-C1C-NC	5.58	115.20	109.97
23	b	603	CLA	CHD-C1D-ND	-5.58	119.33	124.45
23	C	508	CLA	CHD-C1D-ND	-5.57	119.33	124.45
23	B	607	CLA	O2D-CGD-CBD	5.57	121.17	111.27
23	A	405[B]	CLA	C2C-C1C-NC	5.57	115.19	109.97
26	A	410[B]	SQD	O6-C1-C2	5.56	116.98	108.30
23	c	505	CLA	C2C-C1C-NC	5.56	115.18	109.97
23	c	513	CLA	O2D-CGD-CBD	5.56	121.14	111.27
23	C	506	CLA	C2C-C1C-NC	5.55	115.17	109.97
23	c	511	CLA	CHD-C1D-ND	-5.55	119.36	124.45
26	a	411[B]	SQD	O6-C1-C2	5.54	116.96	108.30
23	A	405[A]	CLA	C2C-C1C-NC	5.54	115.17	109.97
23	B	602	CLA	O2D-CGD-CBD	5.54	121.11	111.27
23	C	507	CLA	C4A-NA-C1A	-5.54	104.22	106.71
23	D	405[A]	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	B	608	CLA	CHD-C4C-C3C	-5.52	116.72	124.84
23	c	502	CLA	O2D-CGD-CBD	5.52	121.08	111.27
23	B	613	CLA	C1-C2-C3	-5.52	116.50	126.04
23	B	606	CLA	C3D-C2D-C1D	-5.51	98.31	105.83
23	C	512	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	C	510	CLA	CMD-C2D-C1D	5.51	134.42	124.71
23	a	405[A]	CLA	CHD-C4C-C3C	-5.51	116.74	124.84
23	c	513	CLA	CHD-C4C-C3C	-5.51	116.75	124.84
23	a	406[A]	CLA	C2C-C1C-NC	5.50	115.13	109.97
23	c	503	CLA	CHD-C4C-C3C	-5.50	116.75	124.84
23	c	508	CLA	C2C-C1C-NC	5.50	115.12	109.97
23	d	402[A]	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	C	508	CLA	C2C-C1C-NC	5.49	115.12	109.97
23	B	611	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	a	406[A]	CLA	CHD-C1D-ND	-5.49	119.41	124.45
23	C	513	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	a	407[A]	CLA	CMD-C2D-C1D	5.49	134.38	124.71
23	B	607	CLA	CHD-C4C-C3C	-5.48	116.79	124.84
23	a	405[B]	CLA	CHD-C4C-C3C	-5.47	116.79	124.84
23	b	608	CLA	CHD-C4C-C3C	-5.47	116.80	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	403	CLA	O2D-CGD-CBD	5.47	120.99	111.27
23	C	502	CLA	CHD-C1D-ND	-5.47	119.43	124.45
23	D	405[A]	CLA	C2B-C1B-NB	5.47	113.90	110.23
23	B	603	CLA	CMD-C2D-C1D	5.46	134.34	124.71
23	c	509	CLA	CMD-C2D-C1D	5.46	134.34	124.71
23	b	607	CLA	CHD-C1D-ND	-5.46	119.44	124.45
23	b	614	CLA	C3D-C2D-C1D	-5.46	98.38	105.83
23	B	611	CLA	C3D-C2D-C1D	-5.45	98.39	105.83
23	B	614	CLA	C2C-C1C-NC	5.45	115.08	109.97
23	c	505	CLA	O2D-CGD-CBD	5.44	120.94	111.27
23	d	402[A]	CLA	CMD-C2D-C1D	5.44	134.30	124.71
23	c	510	CLA	CHD-C1D-ND	-5.44	119.46	124.45
23	b	610	CLA	CHD-C1D-ND	-5.43	119.47	124.45
23	b	604	CLA	CHD-C1D-ND	-5.42	119.47	124.45
23	C	508	CLA	C3B-C2B-C1B	-5.41	100.63	107.16
23	A	405[A]	CLA	CHD-C1D-ND	-5.41	119.48	124.45
23	c	510	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
23	B	612	CLA	CHD-C1D-ND	-5.41	119.48	124.45
26	B	620	SQD	O47-C7-C8	5.41	123.15	111.50
23	b	606	CLA	O2D-CGD-CBD	5.41	120.87	111.27
23	C	512	CLA	O2D-CGD-CBD	5.39	120.85	111.27
23	c	507	CLA	C4A-NA-C1A	-5.39	104.28	106.71
23	B	612	CLA	O2D-CGD-CBD	5.39	120.85	111.27
23	b	612	CLA	C2C-C1C-NC	5.39	115.02	109.97
24	a	353[A]	PHO	C1-C2-C3	-5.39	116.72	126.04
23	C	511	CLA	C2C-C1C-NC	5.39	115.02	109.97
23	b	603	CLA	C2C-C1C-NC	5.38	115.01	109.97
23	A	405[A]	CLA	C4A-NA-C1A	-5.38	104.29	106.71
23	C	506	CLA	CHD-C1D-ND	-5.38	119.51	124.45
23	C	504	CLA	CMD-C2D-C1D	5.37	134.18	124.71
23	b	614	CLA	C2C-C1C-NC	5.37	115.00	109.97
23	b	611	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	b	609	CLA	C4A-NA-C1A	-5.36	104.30	106.71
23	b	614	CLA	CMD-C2D-C1D	5.35	134.15	124.71
23	A	404[B]	CLA	C4A-NA-C1A	-5.35	104.30	106.71
26	A	410[A]	SQD	C1-C2-C3	-5.35	98.86	110.00
23	C	507	CLA	CHD-C4C-C3C	-5.34	116.98	124.84
23	b	611	CLA	C2C-C1C-NC	5.34	114.98	109.97
23	c	509	CLA	C3D-C2D-C1D	-5.34	98.54	105.83
23	C	508	CLA	C4A-NA-C1A	-5.34	104.31	106.71
23	a	405[A]	CLA	CHD-C1D-ND	-5.34	119.55	124.45
23	c	506	CLA	C3C-C4C-NC	5.34	116.56	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407[A]	PHO	C3D-C4D-ND	5.34	115.00	107.72
23	a	406[B]	CLA	CMD-C2D-C1D	5.34	134.12	124.71
23	C	514	CLA	C2C-C1C-NC	5.33	114.97	109.97
23	c	513	CLA	CMD-C2D-C1D	5.33	134.11	124.71
23	B	613	CLA	CHD-C1D-ND	-5.32	119.56	124.45
23	b	609	CLA	C2C-C1C-NC	5.32	114.95	109.97
23	b	615	CLA	CMD-C2D-C1D	5.31	134.06	124.71
23	C	503	CLA	CHD-C1D-ND	-5.30	119.58	124.45
23	c	505	CLA	CHD-C4C-C3C	-5.30	117.05	124.84
23	c	509	CLA	O2D-CGD-CBD	5.30	120.69	111.27
23	b	608	CLA	C2C-C1C-NC	5.30	114.93	109.97
23	D	406	CLA	O2D-CGD-CBD	5.29	120.67	111.27
23	B	609	CLA	C2C-C1C-NC	5.29	114.92	109.97
23	A	408	CLA	C3D-C2D-C1D	-5.29	98.62	105.83
23	B	604	CLA	CHD-C4C-C3C	-5.28	117.07	124.84
23	b	604	CLA	C1-C2-C3	-5.28	116.92	126.04
23	C	505	CLA	C3D-C2D-C1D	-5.28	98.63	105.83
23	c	502	CLA	CHD-C4C-C3C	-5.27	117.09	124.84
23	c	502	CLA	O2D-CGD-O1D	-5.27	113.54	123.84
23	A	405[B]	CLA	O2D-CGD-CBD	5.27	120.63	111.27
23	C	503	CLA	C4A-NA-C1A	-5.27	104.34	106.71
23	c	502	CLA	C4A-NA-C1A	-5.27	104.34	106.71
26	F	101	SQD	C1-O5-C5	-5.26	103.36	113.69
23	b	612	CLA	CMD-C2D-C1D	5.26	133.97	124.71
23	D	406	CLA	CHD-C1D-ND	-5.25	119.63	124.45
23	c	514	CLA	C4A-NA-C1A	-5.24	104.35	106.71
23	c	514	CLA	C2C-C1C-NC	5.24	114.88	109.97
23	b	616	CLA	CHD-C1D-ND	-5.24	119.64	124.45
23	B	615	CLA	C2C-C1C-NC	5.23	114.87	109.97
23	c	506	CLA	O2D-CGD-CBD	5.22	120.55	111.27
23	A	408	CLA	C3B-C2B-C1B	-5.22	100.86	107.16
23	b	612	CLA	C4A-NA-C1A	-5.22	104.36	106.71
23	b	613	CLA	C3D-C2D-C1D	-5.22	98.71	105.83
23	B	607	CLA	C2B-C1B-NB	5.22	113.73	110.23
23	a	407[B]	CLA	C4A-NA-C1A	-5.21	104.36	106.71
23	b	609	CLA	CHD-C1D-ND	-5.21	119.67	124.45
23	b	611	CLA	O2D-CGD-CBD	5.20	120.51	111.27
23	D	406	CLA	C2C-C1C-NC	5.19	114.84	109.97
23	b	606	CLA	C2C-C1C-NC	5.19	114.84	109.97
24	a	353[A]	PHO	C3D-C4D-ND	5.19	114.79	107.72
23	B	616	CLA	C2C-C1C-NC	5.19	114.83	109.97
23	d	402[A]	CLA	CHD-C1D-ND	-5.18	119.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C4A-NA-C1A	-5.18	104.38	106.71
24	a	353[B]	PHO	C3D-C4D-ND	5.18	114.78	107.72
23	C	513	CLA	C3B-C2B-C1B	-5.17	100.92	107.16
23	B	613	CLA	CHD-C4C-C3C	-5.17	117.24	124.84
23	b	603	CLA	O2D-CGD-CBD	5.17	120.45	111.27
23	b	615	CLA	CHD-C1D-ND	-5.17	119.70	124.45
23	C	509	CLA	C3C-C4C-NC	5.17	116.37	110.57
23	A	404[B]	CLA	C2C-C1C-NC	5.16	114.81	109.97
23	B	603	CLA	C3D-C2D-C1D	-5.15	98.80	105.83
23	c	503	CLA	C1C-C2C-C3C	-5.15	101.54	106.96
23	d	402[B]	CLA	C4A-NA-C1A	-5.15	104.39	106.71
23	c	509	CLA	CHD-C1D-ND	-5.15	119.72	124.45
23	d	403	CLA	C3D-C2D-C1D	-5.14	98.81	105.83
23	b	614	CLA	C3B-C2B-C1B	-5.13	100.96	107.16
23	A	404[A]	CLA	CHD-C4C-C3C	-5.13	117.30	124.84
23	c	506	CLA	CHD-C1D-ND	-5.13	119.74	124.45
23	c	511	CLA	CMD-C2D-C1D	5.12	133.74	124.71
23	b	611	CLA	C3D-C2D-C1D	-5.11	98.85	105.83
23	B	607	CLA	CMD-C2D-C1D	5.11	133.72	124.71
23	C	502	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	c	512	CLA	C2C-C1C-NC	5.11	114.76	109.97
23	c	509	CLA	C4A-NA-C1A	-5.11	104.41	106.71
23	c	513	CLA	C3B-C2B-C1B	-5.11	101.00	107.16
23	B	612	CLA	C3C-C4C-NC	5.10	116.30	110.57
23	C	511	CLA	C3B-C2B-C1B	-5.10	101.01	107.16
23	c	512	CLA	C4A-NA-C1A	-5.09	104.42	106.71
23	B	612	CLA	CMD-C2D-C1D	5.09	133.68	124.71
26	b	620	SQD	O47-C7-C8	5.09	122.46	111.50
23	B	610	CLA	CMD-C2D-C1D	5.08	133.67	124.71
26	a	411[A]	SQD	O47-C7-C8	5.08	122.45	111.50
23	a	406[A]	CLA	C3D-C2D-C1D	-5.08	98.90	105.83
23	a	409	CLA	CHD-C1D-ND	-5.07	119.79	124.45
23	b	605	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
23	c	512	CLA	O2D-CGD-CBD	5.07	120.28	111.27
23	B	608	CLA	CMD-C2D-C1D	5.07	133.65	124.71
23	b	604	CLA	C4A-NA-C1A	-5.07	104.43	106.71
23	D	405[A]	CLA	C3D-C2D-C1D	-5.06	98.92	105.83
23	a	406[B]	CLA	C2C-C1C-NC	5.06	114.72	109.97
23	b	610	CLA	C2C-C1C-NC	5.05	114.71	109.97
23	c	507	CLA	CHD-C4C-C3C	-5.05	117.41	124.84
26	a	411[B]	SQD	O47-C7-C8	5.05	122.39	111.50
23	C	514	CLA	C3B-C2B-C1B	-5.05	101.06	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	606	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
23	A	406[B]	CLA	C3D-C4D-ND	5.03	118.38	110.24
34	b	622	HTG	C1-O5-C5	5.03	121.85	112.58
23	B	604	CLA	C1-C2-C3	-5.03	117.35	126.04
23	C	510	CLA	C3B-C2B-C1B	-5.03	101.09	107.16
23	B	610	CLA	C2C-C1C-NC	5.02	114.68	109.97
23	c	511	CLA	C2C-C1C-NC	5.02	114.67	109.97
24	A	407[B]	PHO	C3D-C4D-ND	5.01	114.55	107.72
23	C	509	CLA	CMD-C2D-C1D	5.01	133.54	124.71
23	A	405[A]	CLA	O2D-CGD-CBD	5.01	120.17	111.27
23	c	510	CLA	C3B-C2B-C1B	-5.01	101.12	107.16
23	a	405[B]	CLA	C4A-NA-C1A	-5.00	104.46	106.71
23	D	405[A]	CLA	C3C-C4C-NC	5.00	116.18	110.57
23	b	608	CLA	CMD-C2D-C1D	5.00	133.53	124.71
23	B	606	CLA	C2C-C1C-NC	4.99	114.65	109.97
38	e	87	HEM	CHC-C4B-NB	4.99	129.84	124.42
23	c	508	CLA	C4A-NA-C1A	-4.99	104.46	106.71
29	a	416[A]	PL9	C7-C8-C9	-4.98	118.50	126.79
23	c	508	CLA	C3B-C2B-C1B	-4.98	101.15	107.16
23	A	405[B]	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	B	608	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
23	a	407[B]	CLA	C3B-C2B-C1B	-4.97	101.17	107.16
23	a	407[A]	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
24	A	353[B]	PHO	C3D-C4D-ND	4.96	114.49	107.72
23	C	510	CLA	O2D-CGD-CBD	4.96	120.08	111.27
23	B	610	CLA	CHD-C1D-ND	-4.96	119.90	124.45
24	A	353[A]	PHO	C3D-C4D-ND	4.96	114.48	107.72
23	B	605	CLA	C3D-C2D-C1D	-4.96	99.07	105.83
29	A	414[B]	PL9	C7-C8-C9	-4.95	118.54	126.79
23	B	605	CLA	C2C-C1C-NC	4.95	114.61	109.97
23	c	503	CLA	CHD-C1D-ND	-4.95	119.91	124.45
23	B	602	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	b	616	CLA	C3D-C2D-C1D	-4.95	99.08	105.83
23	C	507	CLA	C3B-C2B-C1B	-4.94	101.19	107.16
29	A	414[A]	PL9	C7-C8-C9	-4.94	118.56	126.79
23	B	614	CLA	C3B-C2B-C1B	-4.94	101.19	107.16
23	c	510	CLA	O2D-CGD-CBD	4.94	120.04	111.27
23	d	402[B]	CLA	C3C-C4C-NC	4.94	116.11	110.57
23	a	406[B]	CLA	C3D-C2D-C1D	-4.94	99.10	105.83
23	c	503	CLA	C3B-C2B-C1B	-4.93	101.21	107.16
23	A	406[B]	CLA	O2D-CGD-CBD	4.93	120.02	111.27
23	a	409	CLA	CMD-C2D-C1D	4.93	133.39	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	D	405[B]	CLA	O2D-CGD-CBD	4.92	120.02	111.27
23	C	513	CLA	CHD-C1D-ND	-4.92	119.93	124.45
23	c	505	CLA	C3B-C2B-C1B	-4.92	101.23	107.16
23	C	513	CLA	O2D-CGD-CBD	4.92	120.00	111.27
23	b	615	CLA	C2C-C1C-NC	4.91	114.57	109.97
26	a	411[A]	SQD	C1-O5-C5	-4.91	104.05	113.69
23	d	403	CLA	C3B-C2B-C1B	-4.90	101.24	107.16
23	b	609	CLA	C3C-C4C-NC	4.90	116.06	110.57
33	C	501	LMG	O1-C1-C2	4.90	115.95	108.30
23	B	605	CLA	C3C-C4C-NC	4.89	116.06	110.57
23	d	402[A]	CLA	C4A-NA-C1A	-4.89	104.51	106.71
23	b	612	CLA	O2D-CGD-CBD	4.88	119.94	111.27
33	B	621	LMG	O7-C10-C11	4.88	122.02	111.50
23	b	613	CLA	CHD-C1D-ND	-4.87	119.97	124.45
23	b	604	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
23	D	405[B]	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
23	a	405[B]	CLA	C3D-C4D-ND	4.87	118.12	110.24
23	c	514	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
23	b	601	CLA	C2C-C1C-NC	4.86	114.53	109.97
23	c	514	CLA	C3B-C2B-C1B	-4.86	101.29	107.16
23	c	508	CLA	C3D-C2D-C1D	-4.85	99.22	105.83
23	B	610	CLA	C3D-C2D-C1D	-4.84	99.23	105.83
23	B	610	CLA	C3C-C4C-NC	4.83	115.99	110.57
23	A	406[A]	CLA	C2C-C1C-NC	4.83	114.50	109.97
23	b	602	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
23	a	407[A]	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	C	512	CLA	C3B-C2B-C1B	-4.82	101.34	107.16
23	c	505	CLA	C4A-NA-C1A	-4.82	104.54	106.71
23	B	603	CLA	C3C-C4C-NC	4.81	115.97	110.57
23	a	405[B]	CLA	C2C-C1C-NC	4.81	114.48	109.97
23	A	408	CLA	O2D-CGD-CBD	4.81	119.81	111.27
23	c	507	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
23	B	611	CLA	C3C-C4C-NC	4.80	115.95	110.57
23	B	604	CLA	C3C-C4C-NC	4.79	115.95	110.57
23	C	512	CLA	CHD-C1D-ND	-4.79	120.06	124.45
23	c	502	CLA	C2C-C1C-NC	4.79	114.45	109.97
26	f	102	SQD	O47-C7-C8	4.78	121.81	111.50
23	B	602	CLA	CHD-C1D-ND	-4.78	120.06	124.45
23	A	405[A]	CLA	C3D-C2D-C1D	-4.78	99.31	105.83
23	b	613	CLA	C3C-C4C-NC	4.78	115.93	110.57
23	b	611	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
23	c	504	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	A	405[A]	CLA	CMD-C2D-C1D	4.77	133.12	124.71
23	a	407[B]	CLA	O2D-CGD-CBD	4.77	119.75	111.27
23	b	602	CLA	C3D-C4D-ND	4.77	117.95	110.24
23	c	502	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
23	B	616	CLA	C3B-C4B-NB	4.76	114.93	110.52
23	c	506	CLA	C2C-C1C-NC	4.76	114.43	109.97
23	B	605	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
23	b	616	CLA	C3B-C2B-C1B	-4.76	101.42	107.16
23	a	407[B]	CLA	C2C-C1C-NC	4.75	114.43	109.97
23	C	503	CLA	C3B-C2B-C1B	-4.75	101.43	107.16
23	B	613	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	B	615	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	B	601	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
23	C	512	CLA	C4A-NA-C1A	-4.75	104.57	106.71
23	C	508	CLA	C3C-C4C-NC	4.74	115.89	110.57
23	d	402[B]	CLA	O2D-CGD-CBD	4.74	119.69	111.27
23	a	409	CLA	C3B-C2B-C1B	-4.74	101.44	107.16
23	C	502	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
23	B	612	CLA	C2C-C1C-NC	4.73	114.41	109.97
24	a	408[B]	PHO	C3D-C4D-ND	4.73	114.17	107.72
23	b	607	CLA	C3C-C4C-NC	4.73	115.88	110.57
25	H	101	BCR	C38-C26-C25	-4.73	119.22	124.53
23	A	408	CLA	C3C-C4C-NC	4.72	115.87	110.57
23	B	610	CLA	O2A-CGA-CBA	4.72	126.72	111.91
23	c	503	CLA	O2D-CGD-CBD	4.72	119.65	111.27
23	b	611	CLA	C3C-C4C-NC	4.72	115.86	110.57
23	b	603	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	a	405[A]	CLA	C3B-C2B-C1B	-4.71	101.47	107.16
23	a	409	CLA	C3C-C4C-NC	4.71	115.85	110.57
23	c	512	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
23	b	616	CLA	C2C-C1C-NC	4.70	114.38	109.97
23	B	607	CLA	C1C-C2C-C3C	-4.70	102.01	106.96
23	b	607	CLA	C3D-C2D-C1D	-4.70	99.42	105.83
23	a	409	CLA	C2C-C1C-NC	4.70	114.37	109.97
23	B	609	CLA	C3C-C4C-NC	4.69	115.83	110.57
23	c	504	CLA	C2C-C1C-NC	4.69	114.37	109.97
23	a	407[B]	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	a	409	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	b	603	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
23	C	514	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
23	C	509	CLA	O2D-CGD-CBD	4.67	119.56	111.27
23	a	407[B]	CLA	C3D-C4D-ND	4.66	117.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	610	CLA	C3C-C4C-NC	4.66	115.79	110.57
23	b	605	CLA	C3D-C4D-ND	4.66	117.77	110.24
23	C	504	CLA	C3D-C4D-ND	4.65	117.77	110.24
23	C	504	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	C	508	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
23	B	603	CLA	C4A-NA-C1A	-4.65	104.61	106.71
23	B	608	CLA	C3B-C2B-C1B	-4.65	101.55	107.16
23	C	505	CLA	O2D-CGD-CBD	4.65	119.53	111.27
23	B	604	CLA	C4A-NA-C1A	-4.65	104.62	106.71
23	c	505	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
23	b	615	CLA	C3C-C4C-NC	4.64	115.78	110.57
23	B	615	CLA	CMB-C2B-C1B	4.64	132.44	125.37
24	a	408[A]	PHO	C3D-C4D-ND	4.64	114.04	107.72
23	C	502	CLA	O2D-CGD-O1D	-4.63	114.79	123.84
23	a	406[A]	CLA	O2D-CGD-CBD	4.63	119.49	111.27
23	B	611	CLA	C3D-C4D-ND	4.63	117.73	110.24
23	C	503	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
23	B	608	CLA	C4A-NA-C1A	-4.63	104.63	106.71
23	B	612	CLA	C2B-C1B-NB	4.63	113.33	110.23
23	C	509	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
23	C	513	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
23	c	511	CLA	O2D-CGD-CBD	4.61	119.46	111.27
23	B	611	CLA	C1D-CHD-C4C	-4.60	116.13	126.06
23	d	403	CLA	C4A-NA-C1A	-4.60	104.64	106.71
23	B	608	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	b	610	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	b	605	CLA	C3C-C4C-NC	4.59	115.72	110.57
23	A	404[A]	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
23	b	603	CLA	C3D-C4D-ND	4.59	117.67	110.24
25	d	404	BCR	C15-C14-C13	-4.59	120.76	127.31
23	d	402[B]	CLA	C3B-C2B-C1B	-4.59	101.62	107.16
23	c	503	CLA	CMD-C2D-C1D	4.59	132.80	124.71
23	C	507	CLA	C3D-C2D-C1D	-4.59	99.57	105.83
23	B	611	CLA	CHD-C4C-NC	4.59	131.43	124.20
23	B	608	CLA	C3B-C4B-NB	4.58	114.77	110.52
23	B	601	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	c	509	CLA	C3C-C4C-NC	4.58	115.71	110.57
23	b	615	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
23	b	614	CLA	C4A-NA-C1A	-4.58	104.65	106.71
23	B	602	CLA	C3B-C2B-C1B	-4.58	101.63	107.16
23	b	612	CLA	CHD-C1D-ND	-4.58	120.25	124.45
23	b	601	CLA	C3B-C2B-C1B	-4.58	101.64	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	F	101	SQD	O8-S-C6	4.58	113.03	105.74
23	B	602	CLA	C3C-C4C-NC	4.58	115.70	110.57
23	A	404[A]	CLA	C3B-C2B-C1B	-4.57	101.64	107.16
23	A	404[B]	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
23	A	405[A]	CLA	C1C-C2C-C3C	-4.57	102.15	106.96
23	b	604	CLA	C3B-C2B-C1B	-4.57	101.65	107.16
23	C	514	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	C	513	CLA	C3C-C4C-NC	4.56	115.69	110.57
23	A	408	CLA	C4A-NA-C1A	-4.56	104.66	106.71
23	b	609	CLA	O2D-CGD-CBD	4.56	119.37	111.27
34	C	522	HTG	C1'-S1-C1	4.56	108.61	100.09
23	b	606	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
23	C	509	CLA	CHD-C1D-ND	-4.56	120.27	124.45
23	c	503	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
23	C	505	CLA	C1C-C2C-C3C	-4.55	102.17	106.96
23	d	402[A]	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	b	610	CLA	C3D-C4D-ND	4.54	117.58	110.24
23	C	510	CLA	C3C-C4C-NC	4.54	115.66	110.57
23	A	406[A]	CLA	CMB-C2B-C1B	4.53	132.27	125.37
23	B	614	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	A	406[A]	CLA	C3D-C4D-ND	4.53	117.56	110.24
23	a	406[B]	CLA	C4A-NA-C1A	-4.53	104.67	106.71
23	B	616	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
23	B	609	CLA	C3D-C2D-C1D	-4.53	99.66	105.83
23	C	506	CLA	C3C-C4C-NC	4.52	115.64	110.57
23	C	504	CLA	C3B-C2B-C1B	-4.52	101.70	107.16
25	b	617	BCR	C33-C5-C6	-4.52	119.45	124.53
38	E	103	HEM	CHC-C4B-NB	4.52	129.33	124.42
24	A	353[B]	PHO	C1-C2-C3	-4.52	118.23	126.04
23	B	606	CLA	C3C-C4C-NC	4.51	115.63	110.57
23	b	614	CLA	C3C-C4C-NC	4.51	115.63	110.57
23	B	615	CLA	C3D-C4D-ND	4.51	117.54	110.24
23	C	513	CLA	C1-C2-C3	-4.51	118.24	126.04
23	d	402[B]	CLA	C3D-C4D-ND	4.51	117.54	110.24
23	A	406[A]	CLA	O2D-CGD-CBD	4.51	119.28	111.27
23	b	610	CLA	O2A-CGA-CBA	4.51	126.06	111.91
23	A	405[B]	CLA	C4A-NA-C1A	-4.51	104.68	106.71
23	c	507	CLA	C3B-C2B-C1B	-4.51	101.72	107.16
26	b	620	SQD	C1-O5-C5	-4.51	104.84	113.69
23	a	409	CLA	C3D-C4D-ND	4.50	117.52	110.24
23	B	601	CLA	C4A-NA-C1A	-4.50	104.68	106.71
23	C	514	CLA	C4A-NA-C1A	-4.50	104.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	101	BCR	C33-C5-C6	-4.50	119.48	124.53
23	D	406	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
23	d	402[A]	CLA	C3D-C4D-ND	4.49	117.50	110.24
38	E	103	HEM	C1B-NB-C4B	4.49	109.71	105.07
23	B	615	CLA	C3C-C4C-NC	4.48	115.60	110.57
23	a	409	CLA	CMC-C2C-C1C	4.48	131.87	125.04
23	b	605	CLA	C4A-NA-C1A	-4.48	104.69	106.71
23	B	616	CLA	C3B-C2B-C1B	-4.48	101.76	107.16
23	C	507	CLA	C3D-C4D-ND	4.47	117.47	110.24
23	B	604	CLA	C3B-C2B-C1B	-4.47	101.76	107.16
26	A	410[B]	SQD	C1-C2-C3	-4.47	100.69	110.00
23	C	514	CLA	O2D-CGD-CBD	4.47	119.20	111.27
32	t	102	LMT	C3'-C4'-C5'	-4.46	100.69	110.93
23	C	509	CLA	C3B-C2B-C1B	-4.46	101.77	107.16
23	A	405[B]	CLA	C1C-C2C-C3C	-4.46	102.26	106.96
29	a	416[B]	PL9	C7-C8-C9	-4.46	119.37	126.79
23	b	601	CLA	C3D-C4D-ND	4.46	117.45	110.24
23	b	601	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
23	C	511	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	c	510	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	b	609	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
23	c	507	CLA	O2D-CGD-CBD	4.45	119.17	111.27
23	c	509	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	a	407[A]	CLA	O2D-CGD-CBD	4.44	119.17	111.27
23	b	613	CLA	C3B-C2B-C1B	-4.44	101.80	107.16
23	b	611	CLA	C3D-C4D-ND	4.43	117.40	110.24
23	C	511	CLA	C1-C2-C3	-4.43	118.39	126.04
23	a	406[B]	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	B	601	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	C	503	CLA	C3C-C4C-NC	4.42	115.53	110.57
23	B	603	CLA	C3B-C2B-C1B	-4.41	101.83	107.16
23	b	615	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	C	511	CLA	C3D-C4D-ND	4.41	117.37	110.24
23	b	607	CLA	C3B-C2B-C1B	-4.41	101.84	107.16
23	b	612	CLA	C3C-C4C-NC	4.41	115.51	110.57
23	D	405[B]	CLA	C3C-C4C-NC	4.40	115.51	110.57
33	C	501	LMG	O7-C10-C11	4.40	120.99	111.50
23	c	513	CLA	C2C-C1C-NC	4.40	114.09	109.97
23	c	507	CLA	C3D-C4D-ND	4.40	117.35	110.24
23	B	605	CLA	CMB-C2B-C1B	4.40	132.06	125.37
23	C	505	CLA	C3C-C4C-NC	4.39	115.50	110.57
23	a	405[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[B]	CLA	O2D-CGD-CBD	4.39	119.07	111.27
23	B	613	CLA	C3C-C4C-NC	4.39	115.50	110.57
23	B	607	CLA	C3C-C4C-NC	4.39	115.49	110.57
23	a	406[A]	CLA	C1C-C2C-C3C	-4.39	102.34	106.96
23	b	613	CLA	C1-C2-C3	-4.39	118.46	126.04
23	C	512	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
23	b	606	CLA	C4-C3-C5	4.38	122.64	115.27
23	c	505	CLA	C3B-C4B-NB	4.38	114.58	110.52
23	d	403	CLA	C2C-C1C-NC	4.38	114.08	109.97
23	b	608	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
23	a	406[A]	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	c	510	CLA	C4A-NA-C1A	-4.38	104.74	106.71
23	c	502	CLA	C3B-C2B-C1B	-4.38	101.88	107.16
23	c	506	CLA	C3D-C4D-ND	4.37	117.31	110.24
33	d	412	LMG	O7-C10-C11	4.37	120.92	111.50
23	A	406[A]	CLA	C3D-C2D-C1D	-4.37	99.87	105.83
23	b	603	CLA	C3B-C2B-C1B	-4.37	101.89	107.16
23	B	612	CLA	C3D-C4D-ND	4.37	117.30	110.24
25	B	618	BCR	C29-C30-C25	4.37	117.20	110.48
23	A	405[A]	CLA	C3D-C4D-ND	4.36	117.30	110.24
23	A	406[B]	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	b	616	CLA	C1D-CHD-C4C	-4.36	116.65	126.06
37	E	101[A]	LHG	O7-C7-C8	4.36	120.90	111.50
23	a	405[B]	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
23	c	506	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
23	a	407[A]	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
23	a	407[A]	CLA	C3C-C4C-NC	4.35	115.45	110.57
23	C	509	CLA	C1-C2-C3	-4.35	118.52	126.04
23	c	512	CLA	C3B-C2B-C1B	-4.35	101.92	107.16
23	b	607	CLA	C4A-NA-C1A	-4.34	104.75	106.71
23	c	511	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	d	402[A]	CLA	C1C-C2C-C3C	-4.34	102.39	106.96
23	D	405[B]	CLA	C3B-C2B-C1B	-4.34	101.92	107.16
23	C	506	CLA	C3D-C4D-ND	4.34	117.25	110.24
23	d	403	CLA	C3D-C4D-ND	4.34	117.25	110.24
23	b	616	CLA	O2D-CGD-O1D	-4.34	115.36	123.84
23	B	613	CLA	C3B-C4B-NB	4.33	114.54	110.52
33	a	419	LMG	O7-C10-C11	4.33	120.84	111.50
23	B	605	CLA	C3D-C4D-ND	4.33	117.25	110.24
25	c	515	BCR	C11-C10-C9	-4.33	121.13	127.31
23	C	510	CLA	C4A-NA-C1A	-4.33	104.76	106.71
23	c	508	CLA	C1C-C2C-C3C	-4.33	102.41	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	604	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
23	B	601	CLA	C3D-C4D-ND	4.32	117.23	110.24
23	b	610	CLA	C1-C2-C3	-4.32	118.57	126.04
23	C	506	CLA	C3B-C2B-C1B	-4.31	101.96	107.16
23	b	609	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	b	615	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	c	504	CLA	C3D-C4D-ND	4.31	117.21	110.24
23	B	607	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
23	C	507	CLA	C1C-C2C-C3C	-4.31	102.43	106.96
37	E	101[B]	LHG	O7-C7-C8	4.31	120.79	111.50
26	a	411[A]	SQD	C1-C2-C3	-4.31	101.02	110.00
23	B	607	CLA	C3D-C4D-ND	4.31	117.20	110.24
23	B	616	CLA	O2D-CGD-O1D	-4.30	115.42	123.84
23	c	512	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	a	405[B]	CLA	C1D-CHD-C4C	-4.30	116.78	126.06
23	B	601	CLA	C2C-C1C-NC	4.30	114.00	109.97
29	A	414[A]	PL9	C32-C33-C34	-4.30	117.31	127.66
23	b	609	CLA	C1-C2-C3	-4.29	118.62	126.04
23	b	613	CLA	C1C-C2C-C3C	-4.29	102.44	106.96
23	c	514	CLA	C3D-C4D-ND	4.29	117.18	110.24
23	c	508	CLA	CMC-C2C-C1C	4.29	131.57	125.04
23	a	407[A]	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	b	607	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	c	502	CLA	C3D-C4D-ND	4.29	117.17	110.24
23	a	405[A]	CLA	C3D-C4D-ND	4.28	117.17	110.24
23	c	510	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	C	513	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	C	514	CLA	C3D-C4D-ND	4.28	117.16	110.24
23	A	405[A]	CLA	C3B-C2B-C1B	-4.28	102.00	107.16
23	C	502	CLA	C1D-CHD-C4C	-4.28	116.83	126.06
23	b	604	CLA	C1C-C2C-C3C	-4.28	102.46	106.96
23	c	504	CLA	C3C-C4C-NC	4.28	115.37	110.57
23	D	405[B]	CLA	C3D-C4D-ND	4.28	117.15	110.24
23	c	513	CLA	C3D-C4D-ND	4.27	117.15	110.24
23	A	408	CLA	C3D-C4D-ND	4.27	117.15	110.24
23	B	616	CLA	C4C-C3C-C2C	-4.27	100.67	106.90
23	b	612	CLA	C3B-C2B-C1B	-4.27	102.01	107.16
23	b	614	CLA	O2D-CGD-O1D	-4.27	115.49	123.84
23	B	611	CLA	O2D-CGD-O1D	-4.27	115.49	123.84
26	a	411[A]	SQD	O9-S-C6	4.27	112.01	106.94
23	D	406	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	c	513	CLA	C3D-C2D-C1D	-4.26	100.01	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	608	CLA	C1C-C2C-C3C	-4.26	102.47	106.96
23	a	405[A]	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	c	511	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
23	A	406[B]	CLA	C2C-C1C-NC	4.26	113.96	109.97
23	b	602	CLA	C2C-C1C-NC	4.25	113.96	109.97
23	B	612	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
23	A	405[B]	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
23	A	406[B]	CLA	C3B-C2B-C1B	-4.25	102.03	107.16
25	C	516	BCR	C7-C8-C9	-4.25	119.81	126.23
23	c	504	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
23	a	406[B]	CLA	C1C-C2C-C3C	-4.25	102.49	106.96
23	A	404[B]	CLA	C1D-CHD-C4C	-4.25	116.89	126.06
23	B	612	CLA	O2D-CGD-O1D	-4.25	115.53	123.84
23	c	511	CLA	C1-C2-C3	-4.24	118.71	126.04
23	c	514	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	B	602	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	d	402[B]	CLA	C3D-C2D-C1D	-4.24	100.05	105.83
23	B	609	CLA	C3D-C4D-ND	4.23	117.08	110.24
23	b	603	CLA	C1D-CHD-C4C	-4.23	116.94	126.06
23	C	507	CLA	O2D-CGD-CBD	4.22	118.77	111.27
23	C	502	CLA	C3D-C4D-ND	4.22	117.07	110.24
23	d	402[A]	CLA	C3D-C2D-C1D	-4.22	100.07	105.83
23	B	613	CLA	O2D-CGD-CBD	4.22	118.77	111.27
23	b	607	CLA	C1C-C2C-C3C	-4.22	102.52	106.96
23	c	505	CLA	C3D-C4D-ND	4.22	117.06	110.24
23	c	510	CLA	C3B-C4B-NB	4.21	114.42	110.52
23	C	510	CLA	C3D-C2D-C1D	-4.21	100.08	105.83
23	a	406[A]	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	C	505	CLA	C3D-C4D-ND	4.21	117.05	110.24
26	F	101	SQD	C44-O6-C1	-4.20	105.53	113.74
23	A	404[B]	CLA	C3C-C4C-NC	4.20	115.28	110.57
23	C	504	CLA	C2C-C1C-NC	4.20	113.91	109.97
23	c	514	CLA	C1D-CHD-C4C	-4.20	117.01	126.06
26	A	412	SQD	O47-C7-C8	4.20	120.54	111.50
23	D	406	CLA	O2D-CGD-O1D	-4.20	115.64	123.84
23	b	608	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	A	404[B]	CLA	O2D-CGD-CBD	4.19	118.72	111.27
26	A	410[B]	SQD	C1-O5-C5	-4.19	105.46	113.69
26	A	410[B]	SQD	C44-O6-C1	-4.19	105.55	113.74
23	C	504	CLA	O2D-CGD-CBD	4.19	118.72	111.27
23	a	406[B]	CLA	C3B-C2B-C1B	-4.19	102.11	107.16
23	c	505	CLA	C1-O2A-CGA	4.19	127.42	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	510	CLA	C3B-C4B-NB	4.18	114.40	110.52
23	B	610	CLA	CAA-C2A-C3A	-4.18	101.32	112.78
23	c	503	CLA	C3D-C4D-ND	4.18	117.00	110.24
37	D	409[A]	LHG	O8-C23-O10	-4.18	113.04	123.59
23	A	404[B]	CLA	C3B-C4B-NB	4.18	114.39	110.52
23	c	511	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	A	404[B]	CLA	C3D-C4D-ND	4.18	117.00	110.24
23	C	510	CLA	CAC-C3C-C4C	4.18	130.23	124.81
23	B	603	CLA	C1D-CHD-C4C	-4.18	117.05	126.06
23	b	606	CLA	C3D-C4D-ND	4.18	116.99	110.24
23	D	405[B]	CLA	C1-C2-C3	-4.17	118.82	126.04
23	B	610	CLA	C3B-C2B-C1B	-4.17	102.12	107.16
23	c	511	CLA	C1C-C2C-C3C	-4.17	102.57	106.96
23	b	612	CLA	O2D-CGD-O1D	-4.17	115.69	123.84
23	A	404[A]	CLA	C3B-C4B-NB	4.17	114.38	110.52
23	C	512	CLA	C3C-C4C-NC	4.16	115.24	110.57
38	e	87	HEM	CAD-CBD-CGD	4.16	122.56	113.60
23	B	616	CLA	CHD-C1D-ND	-4.16	120.63	124.45
23	B	616	CLA	CMD-C2D-C1D	4.15	132.03	124.71
23	B	606	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	A	406[A]	CLA	C3B-C2B-C1B	-4.15	102.15	107.16
23	b	606	CLA	O2D-CGD-O1D	-4.15	115.73	123.84
23	b	602	CLA	C3D-C2D-C1D	-4.15	100.17	105.83
23	D	405[A]	CLA	C3B-C2B-C1B	-4.15	102.16	107.16
23	a	405[A]	CLA	C1D-CHD-C4C	-4.14	117.12	126.06
29	A	414[B]	PL9	C32-C33-C34	-4.14	117.68	127.66
23	B	607	CLA	O2D-CGD-O1D	-4.13	115.75	123.84
23	C	509	CLA	C3D-C4D-ND	4.13	116.92	110.24
29	a	416[A]	PL9	C7-C3-C4	4.13	120.24	116.88
23	B	608	CLA	O2D-CGD-O1D	-4.13	115.77	123.84
23	C	505	CLA	C3B-C2B-C1B	-4.13	102.18	107.16
23	C	509	CLA	C3B-C4B-NB	4.13	114.34	110.52
23	B	608	CLA	C3D-C4D-ND	4.13	116.91	110.24
33	C	521	LMG	O7-C10-C11	4.12	120.39	111.50
23	c	502	CLA	CMB-C2B-C1B	4.12	131.65	125.37
23	a	406[A]	CLA	C3D-C4D-ND	4.12	116.91	110.24
23	B	604	CLA	C3B-C4B-NB	4.12	114.33	110.52
23	C	510	CLA	C3D-C4D-ND	4.12	116.89	110.24
23	B	613	CLA	C3B-C2B-C1B	-4.12	102.19	107.16
23	B	613	CLA	C1C-C2C-C3C	-4.11	102.63	106.96
23	C	511	CLA	C1C-C2C-C3C	-4.11	102.64	106.96
23	b	601	CLA	C1D-CHD-C4C	-4.11	117.20	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	e	87	HEM	C4C-NC-C1C	4.11	109.37	105.35
23	b	612	CLA	C3D-C4D-ND	4.10	116.88	110.24
25	d	404	BCR	C40-C30-C25	-4.09	103.66	110.30
23	a	406[A]	CLA	CMB-C2B-C1B	4.09	131.60	125.37
33	c	521	LMG	O7-C10-C11	4.09	120.32	111.50
23	d	402[A]	CLA	O2D-CGD-CBD	4.09	118.53	111.27
23	C	512	CLA	C1D-CHD-C4C	-4.09	117.24	126.06
23	d	402[A]	CLA	C3B-C2B-C1B	-4.09	102.23	107.16
23	B	614	CLA	C3C-C4C-NC	4.09	115.16	110.57
23	a	406[A]	CLA	CAA-C2A-C3A	-4.09	101.59	112.78
23	C	506	CLA	C3D-C2D-C1D	-4.08	100.27	105.83
24	A	407[A]	PHO	C1A-C2A-C3A	-4.08	98.96	102.84
25	Y	101	BCR	C16-C17-C18	-4.08	121.49	127.31
23	c	507	CLA	C1C-C2C-C3C	-4.07	102.67	106.96
23	D	405[A]	CLA	C3D-C4D-ND	4.07	116.82	110.24
33	Z	101	LMG	O7-C10-C11	4.07	120.27	111.50
24	A	353[A]	PHO	C1-C2-C3	-4.07	119.00	126.04
33	C	521	LMG	O6-C5-C4	4.07	117.08	109.69
23	C	511	CLA	C4A-NA-C1A	-4.07	104.88	106.71
23	c	512	CLA	C1D-CHD-C4C	-4.07	117.29	126.06
23	D	405[A]	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	c	514	CLA	O2D-CGD-CBD	4.06	118.49	111.27
23	a	405[A]	CLA	CAA-C2A-C3A	-4.06	101.65	112.78
23	A	408	CLA	C3B-C4B-NB	4.06	114.28	110.52
25	a	410	BCR	C38-C26-C25	-4.06	119.97	124.53
23	a	406[A]	CLA	C3B-C2B-C1B	-4.06	102.26	107.16
23	c	505	CLA	C1C-C2C-C3C	-4.06	102.69	106.96
23	C	513	CLA	C2C-C1C-NC	4.06	113.78	109.97
23	a	406[A]	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
23	b	606	CLA	C1D-CHD-C4C	-4.06	117.30	126.06
23	C	503	CLA	C3D-C4D-ND	4.06	116.80	110.24
34	V	203	HTG	C1-O5-C5	4.06	117.69	112.19
23	c	508	CLA	CMB-C2B-C1B	4.06	131.55	125.37
34	B	622	HTG	O5-C1-C2	4.05	115.41	110.31
25	h	101	BCR	C38-C26-C25	-4.05	119.98	124.53
23	B	606	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	c	504	CLA	O2D-CGD-CBD	4.05	118.46	111.27
23	A	408	CLA	CAA-C2A-C3A	-4.04	101.70	112.78
33	c	521	LMG	O6-C5-C4	4.04	117.04	109.69
23	A	405[B]	CLA	C3D-C4D-ND	4.04	116.78	110.24
26	a	411[A]	SQD	C44-O6-C1	-4.04	105.84	113.74
23	B	602	CLA	C1C-C2C-C3C	-4.04	102.71	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	e	87	HEM	C1B-NB-C4B	4.04	109.25	105.07
23	B	610	CLA	C3D-C4D-ND	4.04	116.77	110.24
23	b	604	CLA	CAC-C3C-C4C	4.04	130.05	124.81
23	B	606	CLA	C1C-C2C-C3C	-4.04	102.71	106.96
23	B	613	CLA	C3D-C4D-ND	4.04	116.77	110.24
23	B	614	CLA	O2D-CGD-O1D	-4.04	115.95	123.84
23	c	506	CLA	C3D-C2D-C1D	-4.04	100.32	105.83
23	B	601	CLA	C1D-CHD-C4C	-4.03	117.36	126.06
23	A	404[A]	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	C	503	CLA	C1C-C2C-C3C	-4.03	102.72	106.96
23	a	405[A]	CLA	C3C-C4C-NC	4.03	115.09	110.57
29	a	416[A]	PL9	C32-C33-C34	-4.03	117.96	127.66
23	C	504	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	c	508	CLA	C3D-C4D-ND	4.03	116.75	110.24
23	C	502	CLA	C3B-C2B-C1B	-4.02	102.30	107.16
23	B	615	CLA	O2D-CGD-CBD	4.02	118.42	111.27
23	a	409	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
23	b	610	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
23	b	605	CLA	C3B-C2B-C1B	-4.02	102.31	107.16
23	b	614	CLA	C3D-C4D-ND	4.02	116.74	110.24
23	B	612	CLA	C3D-C2D-C1D	-4.01	100.35	105.83
23	B	616	CLA	C3D-C4D-ND	4.01	116.73	110.24
23	D	406	CLA	C3C-C4C-NC	4.01	115.07	110.57
23	c	504	CLA	C3B-C2B-C1B	-4.01	102.32	107.16
23	B	613	CLA	C4A-NA-C1A	-4.01	104.90	106.71
23	A	404[A]	CLA	C1C-C2C-C3C	-4.01	102.74	106.96
23	C	510	CLA	C1-C2-C3	-4.01	119.11	126.04
23	B	608	CLA	CMA-C3A-C4A	-4.00	101.01	111.77
35	C	518[A]	DGD	O2G-C1B-C2B	4.00	120.12	111.50
23	b	616	CLA	O2A-CGA-CBA	4.00	124.46	111.91
23	b	602	CLA	C3C-C4C-NC	4.00	115.06	110.57
23	B	606	CLA	C1D-CHD-C4C	-4.00	117.43	126.06
23	C	503	CLA	O2D-CGD-O1D	-4.00	116.02	123.84
23	B	602	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	B	614	CLA	C1C-C2C-C3C	-3.99	102.77	106.96
25	C	515	BCR	C33-C5-C6	-3.98	120.06	124.53
23	B	604	CLA	CHD-C1D-ND	-3.97	120.80	124.45
23	b	607	CLA	C3B-C4B-NB	3.97	114.20	110.52
23	b	608	CLA	C3D-C2D-C1D	-3.97	100.41	105.83
23	C	512	CLA	O2D-CGD-O1D	-3.97	116.08	123.84
35	C	517[A]	DGD	O2G-C1B-C2B	3.97	120.05	111.50
23	B	603	CLA	C3D-C4D-ND	3.97	116.65	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	512	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	A	406[A]	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	c	508	CLA	C3C-C4C-NC	3.96	115.02	110.57
23	c	509	CLA	C3D-C4D-ND	3.96	116.64	110.24
23	D	405[B]	CLA	C1C-C2C-C3C	-3.96	102.80	106.96
23	b	604	CLA	C3C-C4C-NC	3.96	115.01	110.57
23	b	616	CLA	C3C-C4C-NC	3.96	115.01	110.57
25	d	404	BCR	C29-C30-C25	3.96	116.57	110.48
23	C	513	CLA	C1D-CHD-C4C	-3.96	117.52	126.06
26	A	410[A]	SQD	O9-S-C6	3.96	111.64	106.94
23	b	616	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	C	511	CLA	C1D-CHD-C4C	-3.95	117.53	126.06
23	b	614	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	B	603	CLA	C1C-C2C-C3C	-3.95	102.80	106.96
23	B	614	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	b	610	CLA	C4A-NA-C1A	-3.95	104.93	106.71
23	c	509	CLA	C1C-C2C-C3C	-3.95	102.81	106.96
25	d	404	BCR	C38-C26-C25	-3.95	120.10	124.53
23	c	511	CLA	C3C-C4C-NC	3.95	115.00	110.57
23	A	405[A]	CLA	CMC-C2C-C1C	3.94	131.04	125.04
23	C	514	CLA	C1C-C2C-C3C	-3.94	102.81	106.96
23	a	406[B]	CLA	C1D-CHD-C4C	-3.94	117.56	126.06
23	C	507	CLA	C3C-C4C-NC	3.93	114.98	110.57
32	D	404	LMT	C1'-O5'-C5'	-3.93	105.97	113.69
23	A	404[A]	CLA	C3C-C4C-NC	3.93	114.98	110.57
26	a	411[B]	SQD	C1-O5-C5	-3.93	105.98	113.69
23	c	512	CLA	O2D-CGD-O1D	-3.93	116.16	123.84
23	a	406[B]	CLA	C3C-C4C-NC	3.93	114.97	110.57
23	B	604	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
23	A	408	CLA	C1C-C2C-C3C	-3.92	102.83	106.96
23	B	615	CLA	C1D-CHD-C4C	-3.92	117.60	126.06
25	k	101	BCR	C29-C30-C25	3.92	116.52	110.48
23	b	604	CLA	CMC-C2C-C1C	3.91	131.00	125.04
26	B	620	SQD	O7-S-C6	3.91	111.59	106.94
23	b	612	CLA	C1D-CHD-C4C	-3.91	117.63	126.06
23	C	505	CLA	C3B-C4B-NB	3.91	114.14	110.52
33	m	101	LMG	O7-C10-C11	3.90	119.91	111.50
23	d	402[B]	CLA	C1C-C2C-C3C	-3.90	102.86	106.96
23	C	502	CLA	C3C-C4C-NC	3.90	114.94	110.57
23	b	605	CLA	C1C-C2C-C3C	-3.89	102.86	106.96
23	A	406[A]	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
23	b	603	CLA	C1C-C2C-C3C	-3.89	102.87	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	b	622	HTG	C1'-S1-C1	3.89	107.36	100.09
23	B	607	CLA	C3B-C2B-C1B	-3.88	102.47	107.16
23	b	602	CLA	CAA-C2A-C3A	-3.88	102.15	112.78
23	b	612	CLA	C4-C3-C5	3.88	121.80	115.27
23	d	403	CLA	C3C-C4C-NC	3.88	114.92	110.57
23	a	405[A]	CLA	O2D-CGD-CBD	3.88	118.16	111.27
23	b	612	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
23	C	509	CLA	C1C-C2C-C3C	-3.88	102.88	106.96
23	b	613	CLA	C3B-C4B-NB	3.88	114.11	110.52
23	b	604	CLA	O2D-CGD-O1D	-3.87	116.26	123.84
23	c	507	CLA	C1-C2-C3	-3.87	119.34	126.04
23	b	604	CLA	CMB-C2B-C1B	3.87	131.27	125.37
23	b	603	CLA	O2D-CGD-O1D	-3.87	116.26	123.84
23	c	513	CLA	C1-C2-C3	-3.87	119.34	126.04
33	C	520	LMG	O7-C10-C11	3.87	119.85	111.50
23	b	606	CLA	C1C-C2C-C3C	-3.87	102.89	106.96
26	A	412	SQD	O8-S-C6	3.87	111.91	105.74
23	b	602	CLA	O2D-CGD-O1D	-3.87	116.28	123.84
23	b	605	CLA	C1D-CHD-C4C	-3.87	117.72	126.06
29	a	416[B]	PL9	C32-C33-C34	-3.86	118.36	127.66
33	Z	101	LMG	C1-C2-C3	3.86	118.03	110.00
23	b	605	CLA	O2D-CGD-O1D	-3.86	116.30	123.84
23	B	607	CLA	C4-C3-C5	3.86	121.76	115.27
23	C	506	CLA	CMB-C2B-C1B	3.85	131.24	125.37
23	b	608	CLA	O2D-CGD-O1D	-3.85	116.31	123.84
23	b	612	CLA	C3B-C4B-NB	3.85	114.08	110.52
37	d	408[B]	LHG	O7-C7-C8	3.84	119.77	111.50
33	c	520	LMG	O7-C10-C11	3.84	119.77	111.50
23	C	512	CLA	C3B-C4B-NB	3.83	114.07	110.52
23	b	615	CLA	C1D-CHD-C4C	-3.83	117.79	126.06
23	a	405[B]	CLA	C3C-C4C-NC	3.83	114.87	110.57
23	c	513	CLA	C1D-CHD-C4C	-3.83	117.80	126.06
23	a	405[B]	CLA	C3B-C4B-NB	3.83	114.07	110.52
29	A	414[A]	PL9	C7-C3-C4	3.83	119.99	116.88
23	A	404[A]	CLA	CAA-C2A-C3A	-3.83	102.30	112.78
23	B	610	CLA	C1C-C2C-C3C	-3.83	102.93	106.96
23	A	405[A]	CLA	C3C-C4C-NC	3.83	114.86	110.57
23	c	510	CLA	C1D-CHD-C4C	-3.82	117.82	126.06
23	a	405[B]	CLA	C3B-C2B-C1B	-3.82	102.56	107.16
23	A	408	CLA	C1-C2-C3	-3.81	119.45	126.04
23	B	613	CLA	CAC-C3C-C4C	3.81	129.76	124.81
25	D	407	BCR	C28-C27-C26	-3.81	107.27	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	518[B]	DGD	O2G-C1B-C2B	3.81	119.72	111.50
23	a	409	CLA	C1D-CHD-C4C	-3.81	117.83	126.06
25	b	617	BCR	C7-C8-C9	-3.81	120.47	126.23
23	c	506	CLA	C4C-C3C-C2C	-3.80	101.35	106.90
23	c	507	CLA	C3B-C4B-NB	3.80	114.04	110.52
23	b	606	CLA	C3C-C4C-NC	3.80	114.84	110.57
23	c	503	CLA	C3C-C4C-NC	3.80	114.84	110.57
25	Y	101	BCR	C15-C14-C13	-3.80	121.89	127.31
23	b	601	CLA	O2D-CGD-O1D	-3.80	116.42	123.84
23	b	611	CLA	C3B-C4B-NB	3.79	114.03	110.52
23	c	511	CLA	C1D-CHD-C4C	-3.79	117.87	126.06
23	A	404[A]	CLA	O2A-CGA-CBA	3.79	123.81	111.91
23	B	605	CLA	C4-C3-C5	3.79	121.64	115.27
23	b	604	CLA	C3D-C4D-ND	3.79	116.36	110.24
33	c	521	LMG	C3-C4-C5	3.79	116.99	110.24
23	B	605	CLA	C1D-CHD-C4C	-3.78	117.89	126.06
38	E	103	HEM	C4C-NC-C1C	3.78	109.05	105.35
23	B	606	CLA	O2D-CGD-O1D	-3.78	116.44	123.84
23	a	407[B]	CLA	C1C-C2C-C3C	-3.78	102.98	106.96
23	D	406	CLA	C1D-CHD-C4C	-3.78	117.91	126.06
25	h	101	BCR	C7-C8-C9	-3.77	120.53	126.23
23	A	404[A]	CLA	C1D-CHD-C4C	-3.77	117.92	126.06
38	E	103	HEM	CBD-CAD-C3D	-3.77	102.15	112.63
26	f	102	SQD	C1-O5-C5	3.77	121.09	113.69
23	c	510	CLA	C1C-C2C-C3C	-3.77	103.00	106.96
23	D	405[A]	CLA	C3B-C4B-NB	3.77	114.01	110.52
29	a	416[A]	PL9	C15-C14-C16	3.76	121.60	115.27
25	D	407	BCR	C10-C11-C12	-3.76	111.48	123.22
23	B	602	CLA	CMC-C2C-C1C	3.76	130.77	125.04
23	D	405[A]	CLA	C1-C2-C3	-3.76	119.54	126.04
23	c	514	CLA	C3B-C4B-NB	3.76	114.00	110.52
29	a	416[B]	PL9	C15-C14-C16	3.76	121.59	115.27
23	b	610	CLA	O2A-CGA-O1A	-3.76	114.11	123.59
23	C	514	CLA	C1D-CHD-C4C	-3.75	117.97	126.06
23	A	405[A]	CLA	CBC-CAC-C3C	-3.75	102.10	112.43
34	B	626	HTG	C1'-S1-C1	3.75	107.10	100.09
23	C	511	CLA	C3B-C4B-NB	3.74	113.99	110.52
23	B	604	CLA	C1C-C2C-C3C	-3.74	103.03	106.96
23	C	508	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
23	c	512	CLA	C3B-C4B-NB	3.73	113.98	110.52
23	B	607	CLA	CMC-C2C-C1C	3.73	130.72	125.04
37	d	711[A]	LHG	O8-C23-O10	-3.73	114.17	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	610	CLA	C1D-CHD-C4C	-3.73	118.00	126.06
23	b	607	CLA	O2D-CGD-CBD	3.73	117.90	111.27
23	c	502	CLA	C3C-C4C-NC	3.73	114.76	110.57
23	B	614	CLA	C1D-CHD-C4C	-3.73	118.01	126.06
37	D	409[B]	LHG	O7-C7-C8	3.73	119.54	111.50
23	A	406[B]	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
23	D	406	CLA	C1C-C2C-C3C	-3.72	103.04	106.96
23	B	615	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
23	C	506	CLA	C1-C2-C3	-3.72	119.60	126.04
23	b	614	CLA	C1D-CHD-C4C	-3.72	118.03	126.06
23	c	505	CLA	C3C-C4C-NC	3.72	114.74	110.57
23	A	404[A]	CLA	O2D-CGD-CBD	3.72	117.88	111.27
23	B	609	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
23	C	506	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	b	602	CLA	C1D-CHD-C4C	-3.71	118.05	126.06
23	C	513	CLA	C4-C3-C5	3.71	121.52	115.27
37	L	101[A]	LHG	O7-C7-C8	3.71	119.50	111.50
23	b	608	CLA	C1-C2-C3	-3.71	119.63	126.04
26	B	620	SQD	C3-C4-C5	3.71	116.86	110.24
29	a	416[A]	PL9	C7-C3-C2	-3.71	118.42	123.30
23	b	612	CLA	C1C-C2C-C3C	-3.71	103.06	106.96
23	b	609	CLA	C1D-CHD-C4C	-3.70	118.07	126.06
24	A	407[B]	PHO	C1A-C2A-C3A	-3.70	99.32	102.84
29	A	414[B]	PL9	C37-C38-C39	-3.70	118.76	127.66
23	A	406[B]	CLA	C1D-CHD-C4C	-3.70	118.08	126.06
37	l	101[B]	LHG	O7-C7-C8	3.69	119.46	111.50
24	A	353[B]	PHO	C1A-C2A-C3A	-3.69	99.32	102.84
23	b	603	CLA	CAA-C2A-C3A	-3.69	102.67	112.78
23	b	601	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	C	508	CLA	C3D-C4D-ND	3.69	116.20	110.24
23	B	611	CLA	CHB-C4A-NA	3.69	129.61	124.51
34	b	625	HTG	O5-C5-C4	3.69	116.39	109.69
23	b	612	CLA	C1-C2-C3	-3.69	119.67	126.04
23	B	615	CLA	CAC-C3C-C4C	3.69	129.59	124.81
23	B	616	CLA	C1D-CHD-C4C	-3.68	118.12	126.06
23	B	608	CLA	CAC-C3C-C4C	3.68	129.58	124.81
23	b	610	CLA	CAA-C2A-C3A	-3.68	102.71	112.78
23	b	610	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
26	A	410[A]	SQD	C44-O6-C1	-3.67	106.57	113.74
29	a	416[A]	PL9	C30-C29-C31	3.67	121.44	115.27
29	D	408[A]	PL9	C42-C43-C44	-3.67	118.83	127.66
23	c	514	CLA	C1C-C2C-C3C	-3.67	103.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C1C-C2C-C3C	-3.67	103.10	106.96
23	b	608	CLA	C3B-C4B-NB	3.66	113.92	110.52
23	c	511	CLA	CMC-C2C-C1C	3.66	130.62	125.04
23	C	512	CLA	C3D-C4D-ND	3.66	116.16	110.24
23	D	405[A]	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
23	C	502	CLA	C1C-C2C-C3C	-3.66	103.11	106.96
29	A	414[A]	PL9	C15-C14-C16	3.65	121.41	115.27
34	b	625	HTG	C1-O5-C5	3.65	119.31	112.58
23	C	508	CLA	C1D-CHD-C4C	-3.65	118.19	126.06
23	b	609	CLA	C3B-C2B-C1B	-3.65	102.76	107.16
23	a	407[A]	CLA	C1C-C2C-C3C	-3.64	103.13	106.96
35	c	517[A]	DGD	O2G-C1B-C2B	3.64	119.34	111.50
23	C	512	CLA	CAC-C3C-C4C	3.64	129.53	124.81
23	C	507	CLA	CMC-C2C-C1C	3.63	130.57	125.04
23	C	512	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	a	407[A]	CLA	C1D-CHD-C4C	-3.63	118.23	126.06
23	C	510	CLA	C1C-C2C-C3C	-3.63	103.14	106.96
23	B	610	CLA	CMB-C2B-C1B	3.63	130.89	125.37
23	A	404[B]	CLA	CAA-C2A-C3A	-3.63	102.85	112.78
23	b	609	CLA	CAC-C3C-C4C	3.62	129.51	124.81
23	A	405[B]	CLA	CAA-C2A-C3A	-3.62	102.86	112.78
23	b	613	CLA	O2D-CGD-CBD	3.62	117.70	111.27
23	b	615	CLA	O2D-CGD-CBD	3.62	117.70	111.27
23	B	609	CLA	O2D-CGD-CBD	3.62	117.70	111.27
23	C	508	CLA	CMB-C2B-C1B	3.62	130.88	125.37
23	b	613	CLA	C1D-CHD-C4C	-3.62	118.25	126.06
23	B	602	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
23	A	405[B]	CLA	C1D-CHD-C4C	-3.62	118.26	126.06
23	a	405[A]	CLA	O2A-CGA-O1A	-3.62	114.47	123.59
29	d	405[B]	PL9	C42-C43-C44	-3.61	118.96	127.66
23	b	602	CLA	CMC-C2C-C1C	3.61	130.54	125.04
23	B	604	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
23	C	514	CLA	C3B-C4B-NB	3.61	113.87	110.52
23	C	507	CLA	C1-C2-C3	-3.61	119.80	126.04
23	A	408	CLA	O2D-CGD-O1D	-3.61	116.78	123.84
23	B	610	CLA	O2A-CGA-O1A	-3.61	114.49	123.59
23	B	610	CLA	CAA-CBA-CGA	-3.60	102.73	113.25
23	a	407[B]	CLA	C1D-CHD-C4C	-3.60	118.29	126.06
23	B	614	CLA	C3B-C4B-NB	3.60	113.86	110.52
23	d	403	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
37	d	711[A]	LHG	O8-C23-C24	3.60	123.21	111.91
23	B	615	CLA	CED-O2D-CGD	3.60	124.07	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	503	CLA	C1D-CHD-C4C	-3.60	118.30	126.06
26	a	413	SQD	O47-C7-C8	3.59	119.24	111.50
29	d	405[A]	PL9	C42-C43-C44	-3.59	119.02	127.66
23	B	612	CLA	CAC-C3C-C4C	3.59	129.46	124.81
26	A	410[B]	SQD	O9-S-C6	3.59	111.20	106.94
23	C	504	CLA	C1D-CHD-C4C	-3.58	118.33	126.06
29	A	414[B]	PL9	C7-C3-C2	-3.58	118.59	123.30
29	a	416[B]	PL9	C7-C3-C4	3.58	119.78	116.88
23	B	603	CLA	O2D-CGD-O1D	-3.58	116.85	123.84
29	A	414[A]	PL9	C22-C23-C24	-3.57	119.05	127.66
23	D	406	CLA	C3B-C2B-C1B	-3.57	102.85	107.16
23	B	612	CLA	C4C-C3C-C2C	-3.57	101.69	106.90
29	d	405[A]	PL9	C40-C39-C41	3.57	121.28	115.27
23	A	406[B]	CLA	C3C-C4C-NC	3.57	114.57	110.57
23	c	510	CLA	C3C-C4C-NC	3.57	114.57	110.57
35	c	518[A]	DGD	O2G-C1B-C2B	3.57	119.19	111.50
23	b	609	CLA	C4C-C3C-C2C	-3.57	101.70	106.90
23	C	505	CLA	C4A-NA-C1A	-3.57	105.10	106.71
23	b	608	CLA	C3C-C4C-NC	3.56	114.57	110.57
23	C	508	CLA	C1C-C2C-C3C	-3.56	103.22	106.96
23	A	405[A]	CLA	C1D-CHD-C4C	-3.56	118.38	126.06
35	C	517[B]	DGD	O2G-C1B-C2B	3.56	119.17	111.50
23	C	511	CLA	C3C-C4C-NC	3.56	114.56	110.57
26	A	410[A]	SQD	O47-C7-C8	3.55	119.16	111.50
25	K	102	BCR	C7-C8-C9	-3.55	120.87	126.23
23	C	506	CLA	O2D-CGD-O1D	-3.55	116.89	123.84
23	d	402[B]	CLA	C1D-CHD-C4C	-3.55	118.40	126.06
29	A	414[A]	PL9	C7-C3-C2	-3.55	118.63	123.30
23	b	614	CLA	C1-C2-C3	-3.55	119.91	126.04
38	E	103	HEM	CHD-C4C-NC	3.55	128.27	124.44
23	c	504	CLA	CMB-C2B-C1B	3.54	130.77	125.37
23	A	406[A]	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	c	509	CLA	C1D-CHD-C4C	-3.54	118.43	126.06
23	b	605	CLA	C4-C3-C5	3.54	121.22	115.27
35	c	517[B]	DGD	O2G-C1B-C2B	3.53	119.12	111.50
23	C	514	CLA	CMC-C2C-C1C	3.53	130.42	125.04
26	A	410[B]	SQD	O47-C7-C8	3.53	119.11	111.50
23	b	603	CLA	C3B-C4B-NB	3.53	113.79	110.52
23	B	613	CLA	C4-C3-C5	3.53	121.21	115.27
23	a	409	CLA	C1C-C2C-C3C	-3.53	103.25	106.96
23	c	506	CLA	CMB-C2B-C1B	3.53	130.74	125.37
23	D	406	CLA	CMB-C2B-C1B	3.53	130.74	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	405[A]	CLA	CAA-C2A-C3A	-3.52	103.13	112.78
23	b	608	CLA	C1D-CHD-C4C	-3.52	118.46	126.06
23	d	403	CLA	C1C-C2C-C3C	-3.52	103.25	106.96
23	b	616	CLA	CMB-C2B-C1B	3.52	130.73	125.37
23	B	611	CLA	C2A-C1A-CHA	-3.52	117.70	123.86
23	a	405[B]	CLA	CAA-C2A-C3A	-3.52	103.15	112.78
23	B	608	CLA	C1C-C2C-C3C	-3.52	103.26	106.96
23	b	601	CLA	C1C-C2C-C3C	-3.51	103.26	106.96
23	a	407[B]	CLA	C3C-C4C-NC	3.51	114.51	110.57
23	c	510	CLA	CAC-C3C-C4C	3.51	129.37	124.81
25	T	101	BCR	C11-C10-C9	-3.51	122.30	127.31
23	A	405[B]	CLA	CMB-C2B-C1B	3.51	130.71	125.37
23	B	607	CLA	C3B-C4B-NB	3.51	113.77	110.52
32	A	359	LMT	O5B-C5B-C4B	3.51	116.06	109.69
23	C	506	CLA	CAC-C3C-C4C	3.51	129.36	124.81
29	A	414[B]	PL9	C22-C23-C24	-3.51	119.22	127.66
23	c	507	CLA	C3C-C4C-NC	3.50	114.50	110.57
23	a	406[B]	CLA	CHD-C4C-NC	3.50	129.72	124.20
35	c	518[B]	DGD	O2G-C1B-C2B	3.50	119.04	111.50
37	D	409[A]	LHG	O7-C7-C8	3.50	119.04	111.50
23	B	604	CLA	CAC-C3C-C4C	3.49	129.34	124.81
34	b	622	HTG	O2-C2-C1	3.49	116.68	110.27
23	B	603	CLA	CAA-C2A-C3A	-3.49	103.22	112.78
23	C	503	CLA	C1-C2-C3	-3.49	120.01	126.04
23	B	614	CLA	CMC-C2C-C1C	3.49	130.35	125.04
23	B	609	CLA	CMB-C2B-C1B	3.48	130.68	125.37
23	b	615	CLA	CMB-C2B-C1B	3.48	130.67	125.37
38	E	103	HEM	CHD-C1D-ND	3.48	128.20	124.42
23	d	402[A]	CLA	O2A-CGA-CBA	3.48	122.83	111.91
23	b	611	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
23	A	405[B]	CLA	C3C-C4C-NC	3.47	114.47	110.57
35	h	102	DGD	O2G-C1B-C2B	3.47	118.98	111.50
23	d	402[A]	CLA	C3B-C4B-NB	3.47	113.73	110.52
23	B	601	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
25	D	407	BCR	C29-C30-C25	3.47	115.82	110.48
23	b	610	CLA	C1C-C2C-C3C	-3.47	103.31	106.96
23	B	602	CLA	CAA-C2A-C3A	-3.47	103.29	112.78
23	B	604	CLA	C3D-C4D-ND	3.46	115.84	110.24
24	A	353[A]	PHO	C1A-C2A-C3A	-3.46	99.54	102.84
34	b	622	HTG	O5-C5-C4	3.46	115.98	109.69
29	d	405[A]	PL9	C37-C38-C39	-3.46	119.33	127.66
23	c	512	CLA	C1C-C2C-C3C	-3.46	103.32	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	O2A-CGA-O1A	-3.46	114.86	123.59
33	C	521	LMG	C3-C4-C5	3.46	116.40	110.24
23	B	606	CLA	CMC-C2C-C1C	3.45	130.30	125.04
23	b	608	CLA	CMC-C2C-C1C	3.45	130.30	125.04
23	D	406	CLA	C4-C3-C5	3.45	121.08	115.27
23	c	506	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
23	B	615	CLA	C1C-C2C-C3C	-3.45	103.33	106.96
23	A	404[A]	CLA	O2A-CGA-O1A	-3.45	114.89	123.59
23	c	503	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
33	C	520	LMG	O8-C28-C29	3.45	122.72	111.91
23	b	607	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
23	B	615	CLA	C4-C3-C5	3.45	121.07	115.27
33	a	419	LMG	C8-O7-C10	-3.45	109.31	117.79
23	B	605	CLA	C4C-C3C-C2C	-3.44	101.88	106.90
25	B	617	BCR	C33-C5-C6	-3.44	120.66	124.53
29	a	416[B]	PL9	C27-C28-C29	-3.44	119.38	127.66
33	c	520	LMG	O1-C7-C8	-3.44	102.61	110.90
23	B	601	CLA	C4C-C3C-C2C	-3.44	101.89	106.90
23	c	513	CLA	O2D-CGD-O1D	-3.43	117.12	123.84
23	B	605	CLA	O2D-CGD-O1D	-3.43	117.13	123.84
24	a	408[A]	PHO	C1A-C2A-C3A	-3.43	99.58	102.84
23	A	408	CLA	C1D-CHD-C4C	-3.43	118.67	126.06
37	d	408[A]	LHG	O7-C7-C8	3.42	118.86	111.50
23	C	509	CLA	CAC-C3C-C4C	3.42	129.24	124.81
29	D	408[B]	PL9	C42-C43-C44	-3.42	119.44	127.66
23	C	506	CLA	C1C-C2C-C3C	-3.41	103.37	106.96
23	a	406[A]	CLA	CHD-C4C-NC	3.41	129.58	124.20
25	D	407	BCR	C38-C26-C25	-3.41	120.70	124.53
23	B	609	CLA	CMC-C2C-C1C	3.41	130.23	125.04
23	C	513	CLA	CMC-C2C-C1C	3.41	130.23	125.04
25	A	409	BCR	C24-C23-C22	-3.41	121.09	126.23
24	a	408[A]	PHO	O1D-CGD-CBD	-3.41	119.07	124.74
23	c	507	CLA	CAC-C3C-C4C	3.40	129.23	124.81
23	b	613	CLA	O2A-CGA-O1A	-3.40	115.00	123.59
23	C	510	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
29	A	414[B]	PL9	C27-C28-C29	-3.40	119.48	127.66
37	L	101[B]	LHG	O7-C7-C8	3.40	118.82	111.50
23	c	502	CLA	C1C-C2C-C3C	-3.40	103.39	106.96
23	C	506	CLA	C4-C3-C5	3.39	120.98	115.27
26	a	411[B]	SQD	C44-O6-C1	-3.39	107.11	113.74
23	C	510	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
23	B	611	CLA	C4A-NA-C1A	-3.39	105.18	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	511	CLA	C4-C3-C5	3.39	120.97	115.27
29	a	416[B]	PL9	C7-C3-C2	-3.38	118.85	123.30
29	a	416[B]	PL9	C30-C29-C31	3.38	120.96	115.27
23	A	404[B]	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	D	405[B]	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	b	615	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	a	406[A]	CLA	C3B-C4B-NB	3.38	113.65	110.52
23	d	402[B]	CLA	C1-C2-C3	-3.38	120.20	126.04
29	a	416[A]	PL9	C27-C28-C29	-3.38	119.53	127.66
29	A	414[A]	PL9	C37-C38-C39	-3.37	119.54	127.66
23	B	610	CLA	C4C-C3C-C2C	-3.37	101.98	106.90
29	A	414[B]	PL9	C15-C14-C16	3.37	120.94	115.27
23	b	605	CLA	CHD-C4C-NC	3.37	129.52	124.20
23	C	507	CLA	C1D-CHD-C4C	-3.37	118.78	126.06
23	c	507	CLA	C1D-CHD-C4C	-3.37	118.79	126.06
23	A	406[B]	CLA	C1C-C2C-C3C	-3.37	103.41	106.96
23	b	615	CLA	C4-C3-C5	3.37	120.94	115.27
26	a	411[B]	SQD	C1-C2-C3	-3.36	102.99	110.00
23	C	509	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
29	A	414[A]	PL9	C27-C28-C29	-3.36	119.56	127.66
23	d	402[B]	CLA	O2A-CGA-CBA	3.36	122.46	111.91
23	A	405[B]	CLA	C3B-C4B-NB	3.36	113.63	110.52
23	a	405[A]	CLA	O2A-CGA-CBA	3.36	122.45	111.91
23	c	513	CLA	C1C-C2C-C3C	-3.36	103.43	106.96
40	V	202	HEC	CBD-CAD-C3D	-3.36	103.30	112.63
23	D	405[A]	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
37	d	711[B]	LHG	O7-C7-C8	3.35	118.73	111.50
23	B	602	CLA	C3B-C4B-NB	3.35	113.62	110.52
23	B	610	CLA	C4A-NA-C1A	-3.35	105.20	106.71
23	B	608	CLA	C4C-C3C-C2C	-3.35	102.01	106.90
23	c	508	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
23	A	404[A]	CLA	CAC-C3C-C4C	3.35	129.15	124.81
37	l	101[A]	LHG	O7-C7-C8	3.35	118.72	111.50
37	D	409[B]	LHG	C5-O7-C7	-3.35	109.55	117.79
24	a	353[A]	PHO	C4-C3-C5	3.35	120.90	115.27
29	d	405[B]	PL9	C10-C9-C11	3.35	120.90	115.27
23	b	611	CLA	C1-C2-C3	-3.34	120.26	126.04
25	A	409	BCR	C11-C10-C9	-3.34	122.54	127.31
23	d	402[A]	CLA	C4-C3-C5	3.34	120.89	115.27
23	b	615	CLA	C11-C10-C8	-3.34	105.13	115.92
23	c	505	CLA	C1D-CHD-C4C	-3.33	118.86	126.06
23	C	509	CLA	C4C-C3C-C2C	-3.33	102.04	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	405[A]	CLA	C1-C2-C3	-3.33	120.28	126.04
23	A	404[A]	CLA	CAA-C2A-C1A	-3.33	101.05	111.97
25	d	404	BCR	C16-C17-C18	-3.33	122.56	127.31
25	C	515	BCR	C7-C8-C9	-3.33	121.21	126.23
23	B	614	CLA	C1-C2-C3	-3.33	120.29	126.04
33	m	101	LMG	C7-O1-C1	-3.32	107.25	113.74
23	c	513	CLA	C3C-C4C-NC	3.32	114.30	110.57
37	d	711[B]	LHG	O8-C23-C24	3.32	122.33	111.91
23	a	405[A]	CLA	CAA-C2A-C1A	-3.32	101.10	111.97
23	b	611	CLA	C4C-C3C-C2C	-3.32	102.06	106.90
23	c	510	CLA	CHC-C1C-C2C	-3.32	117.52	126.73
38	e	87	HEM	CBD-CAD-C3D	-3.31	103.42	112.63
23	d	402[B]	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
38	E	103	HEM	CHB-C1B-NB	3.31	128.46	124.37
29	a	416[B]	PL9	C25-C24-C26	3.31	120.84	115.27
26	a	411[B]	SQD	O9-S-C6	3.31	110.87	106.94
23	c	511	CLA	C3B-C4B-NB	3.31	113.58	110.52
23	B	603	CLA	C4C-C3C-C2C	-3.31	102.08	106.90
26	b	620	SQD	O8-S-C6	3.31	111.01	105.74
37	D	409[A]	LHG	O8-C23-C24	3.30	122.28	111.91
23	a	407[B]	CLA	CHD-C4C-NC	3.30	129.41	124.20
23	b	605	CLA	CMC-C2C-C1C	3.30	130.07	125.04
23	c	506	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
29	a	416[A]	PL9	C37-C38-C39	-3.30	119.71	127.66
25	C	516	BCR	C33-C5-C6	-3.30	120.82	124.53
23	a	405[A]	CLA	C3B-C4B-NB	3.30	113.58	110.52
23	d	403	CLA	CMB-C2B-C1B	3.30	130.39	125.37
29	A	414[B]	PL9	C7-C3-C4	3.30	119.56	116.88
23	b	604	CLA	C3B-C4B-NB	3.30	113.58	110.52
29	d	405[B]	PL9	C37-C38-C39	-3.30	119.72	127.66
33	B	621	LMG	O8-C28-C29	3.30	122.25	111.91
23	b	616	CLA	C1C-C2C-C3C	-3.30	103.49	106.96
23	d	402[A]	CLA	C1D-CHD-C4C	-3.29	118.95	126.06
23	B	613	CLA	O2A-CGA-O1A	-3.29	115.28	123.59
23	B	609	CLA	CBC-CAC-C3C	-3.29	103.35	112.43
38	e	87	HEM	CHA-C4D-ND	3.29	128.43	124.37
29	D	408[A]	PL9	C25-C24-C26	3.29	120.81	115.27
23	d	402[B]	CLA	C3B-C4B-NB	3.29	113.56	110.52
23	B	604	CLA	C4C-C3C-C2C	-3.29	102.11	106.90
23	A	406[A]	CLA	C3B-C4B-NB	3.29	113.56	110.52
23	C	505	CLA	O2D-CGD-O1D	-3.29	117.42	123.84
23	b	602	CLA	C1C-C2C-C3C	-3.28	103.50	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	615	CLA	CMC-C2C-C1C	3.28	130.04	125.04
23	A	406[A]	CLA	CAA-C2A-C3A	-3.28	103.78	112.78
23	b	601	CLA	C4-C3-C5	3.28	120.79	115.27
23	c	506	CLA	CAC-C3C-C4C	3.28	129.06	124.81
25	T	101	BCR	C15-C16-C17	-3.28	116.76	123.47
23	C	514	CLA	C1-C2-C3	-3.28	120.37	126.04
23	a	405[A]	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
33	Z	101	LMG	O6-C1-C2	3.27	117.28	110.35
23	b	616	CLA	CHD-C4C-NC	3.27	129.36	124.20
26	A	412	SQD	C4-C3-C2	-3.27	105.11	110.82
23	a	406[B]	CLA	C3B-C4B-NB	3.27	113.55	110.52
23	B	611	CLA	C4C-C3C-C2C	-3.27	102.14	106.90
23	B	614	CLA	CAC-C3C-C4C	3.27	129.05	124.81
23	B	612	CLA	C4A-NA-C1A	-3.27	105.24	106.71
23	C	503	CLA	C1D-CHD-C4C	-3.26	119.02	126.06
23	A	404[B]	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	b	610	CLA	C4C-C3C-C2C	-3.26	102.14	106.90
23	c	513	CLA	C4-C3-C5	3.26	120.76	115.27
25	b	618	BCR	C37-C22-C21	-3.26	118.35	122.92
25	B	619	BCR	C24-C23-C22	-3.26	121.31	126.23
29	a	416[B]	PL9	C37-C38-C39	-3.26	119.81	127.66
23	c	504	CLA	C1C-C2C-C3C	-3.26	103.53	106.96
23	A	408	CLA	C4C-C3C-C2C	-3.26	102.15	106.90
23	D	405[B]	CLA	C1D-CHD-C4C	-3.25	119.04	126.06
23	A	406[B]	CLA	C2A-C1A-CHA	-3.25	118.18	123.86
23	b	612	CLA	CMC-C2C-C1C	3.25	129.99	125.04
23	b	611	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
23	C	508	CLA	C4C-C3C-C2C	-3.25	102.17	106.90
23	C	509	CLA	C1D-CHD-C4C	-3.25	119.06	126.06
23	C	505	CLA	CMC-C2C-C1C	3.25	129.98	125.04
23	c	514	CLA	CMC-C2C-C1C	3.25	129.98	125.04
23	d	402[A]	CLA	C1-C2-C3	-3.24	120.43	126.04
29	d	405[B]	PL9	C7-C3-C4	3.24	119.51	116.88
25	c	515	BCR	C15-C14-C13	-3.24	122.69	127.31
23	b	613	CLA	O2A-CGA-CBA	3.24	122.07	111.91
25	y	101	BCR	C24-C23-C22	-3.24	121.34	126.23
23	C	506	CLA	C4C-C3C-C2C	-3.24	102.18	106.90
23	b	613	CLA	C3D-C4D-ND	3.24	115.47	110.24
29	a	416[B]	PL9	C17-C18-C19	-3.24	119.87	127.66
38	e	87	HEM	CHD-C1D-ND	3.23	127.93	124.42
23	C	513	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
33	c	521	LMG	C9-C8-C7	-3.23	104.15	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	404[B]	CLA	C1-C2-C3	-3.23	120.46	126.04
23	b	615	CLA	C4C-C3C-C2C	-3.23	102.19	106.90
23	A	406[A]	CLA	O2A-CGA-O1A	-3.23	115.45	123.59
23	C	511	CLA	CHD-C4C-NC	3.23	129.29	124.20
26	a	413	SQD	O48-C23-C24	3.23	122.03	111.91
23	d	402[B]	CLA	C4-C3-C5	3.23	120.70	115.27
23	D	406	CLA	O2A-CGA-O1A	-3.22	115.45	123.59
23	b	603	CLA	C4-C3-C5	3.22	120.69	115.27
23	b	606	CLA	C3B-C4B-NB	3.22	113.50	110.52
23	B	602	CLA	C11-C12-C13	-3.22	105.50	115.92
24	a	408[B]	PHO	C1A-C2A-C3A	-3.22	99.77	102.84
23	b	611	CLA	C1D-CHD-C4C	-3.22	119.11	126.06
23	b	607	CLA	C4-C3-C5	3.22	120.69	115.27
23	b	609	CLA	C3B-C4B-NB	3.22	113.50	110.52
29	A	414[B]	PL9	C17-C18-C19	-3.22	119.91	127.66
23	c	512	CLA	CHD-C4C-NC	3.22	129.27	124.20
23	C	507	CLA	CAC-C3C-C4C	3.22	128.98	124.81
23	B	611	CLA	C1-C2-C3	-3.21	120.48	126.04
23	B	609	CLA	C1D-CHD-C4C	-3.21	119.12	126.06
29	D	408[B]	PL9	C17-C18-C19	-3.21	119.92	127.66
26	a	411[A]	SQD	C45-O47-C7	-3.21	109.88	117.79
23	C	504	CLA	C4-C3-C5	3.21	120.68	115.27
33	a	419	LMG	C7-O1-C1	-3.21	107.47	113.74
23	C	505	CLA	C1-O2A-CGA	3.21	124.87	116.44
23	b	616	CLA	O2A-CGA-O1A	-3.21	115.49	123.59
23	C	507	CLA	C3B-C4B-NB	3.21	113.49	110.52
23	c	502	CLA	C1-C2-C3	-3.21	120.50	126.04
29	a	416[A]	PL9	C17-C18-C19	-3.21	119.94	127.66
29	D	408[B]	PL9	C25-C24-C26	3.20	120.66	115.27
40	V	202	HEC	C4B-NB-C1B	3.20	108.38	105.07
23	a	405[B]	CLA	O2D-CGD-CBD	3.20	116.96	111.27
23	c	509	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
24	a	408[A]	PHO	O2A-CGA-O1A	-3.20	115.51	123.59
23	C	502	CLA	CMB-C2B-C1B	3.20	130.24	125.37
23	a	409	CLA	C4-C3-C5	3.20	120.66	115.27
23	a	409	CLA	CHD-C4C-NC	3.20	129.25	124.20
29	a	416[A]	PL9	C25-C24-C26	3.20	120.65	115.27
23	d	402[B]	CLA	C4C-C3C-C2C	-3.20	102.24	106.90
29	D	408[A]	PL9	C17-C18-C19	-3.20	119.96	127.66
23	c	511	CLA	CHD-C4C-NC	3.20	129.24	124.20
23	c	508	CLA	C4-C3-C5	3.20	120.65	115.27
23	c	507	CLA	CHC-C1C-C2C	-3.20	117.85	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	C1D-CHD-C4C	-3.20	119.16	126.06
23	D	406	CLA	C3B-C4B-NB	3.20	113.48	110.52
26	B	620	SQD	O9-S-C6	3.20	110.74	106.94
23	B	605	CLA	C1C-C2C-C3C	-3.19	103.60	106.96
23	c	509	CLA	O2D-CGD-O1D	-3.19	117.59	123.84
24	A	353[A]	PHO	C4-C3-C5	3.19	120.64	115.27
23	B	603	CLA	C3B-C4B-NB	3.19	113.47	110.52
26	b	620	SQD	C3-C4-C5	3.19	115.92	110.24
33	C	521	LMG	O8-C28-C29	3.19	121.91	111.91
23	C	510	CLA	O2A-CGA-CBA	3.19	121.91	111.91
37	d	711[B]	LHG	O8-C23-O10	-3.18	115.56	123.59
23	b	612	CLA	C2A-C1A-CHA	-3.18	118.30	123.86
23	c	508	CLA	C1D-CHD-C4C	-3.18	119.20	126.06
23	a	405[B]	CLA	C4C-C3C-C2C	-3.18	102.27	106.90
23	d	402[A]	CLA	O2A-CGA-O1A	-3.18	115.57	123.59
23	c	503	CLA	CHC-C1C-C2C	-3.18	117.91	126.73
23	c	513	CLA	CMB-C2B-C1B	3.18	130.21	125.37
23	b	603	CLA	C2A-C1A-CHA	-3.17	118.31	123.86
24	a	353[B]	PHO	C4-C3-C5	3.17	120.61	115.27
23	b	612	CLA	O2A-CGA-CBA	3.17	121.87	111.91
23	B	612	CLA	C1-C2-C3	-3.17	120.56	126.04
23	b	606	CLA	CHD-C4C-NC	3.17	129.20	124.20
25	A	409	BCR	C40-C30-C25	-3.17	105.16	110.30
23	b	616	CLA	CBC-CAC-C3C	-3.17	103.69	112.43
23	b	614	CLA	O2A-CGA-O1A	-3.17	115.59	123.59
23	b	608	CLA	CBC-CAC-C3C	-3.17	103.69	112.43
23	B	612	CLA	C1C-C2C-C3C	-3.17	103.63	106.96
23	c	503	CLA	C3B-C4B-NB	3.17	113.45	110.52
23	C	502	CLA	CHD-C4C-NC	3.16	129.19	124.20
25	A	409	BCR	C33-C5-C6	-3.16	120.98	124.53
23	C	504	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
23	B	601	CLA	CHD-C4C-NC	3.16	129.19	124.20
23	A	405[A]	CLA	CMB-C2B-C1B	3.16	130.18	125.37
23	C	513	CLA	CHD-C4C-NC	3.16	129.18	124.20
23	c	510	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
23	A	405[B]	CLA	CHD-C4C-NC	3.16	129.18	124.20
23	c	504	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
37	D	410[B]	LHG	O7-C7-C8	3.15	118.30	111.50
29	A	414[B]	PL9	C20-C19-C21	3.15	120.57	115.27
23	A	405[B]	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
23	a	405[A]	CLA	C4-C3-C5	3.15	120.57	115.27
23	B	610	CLA	C3B-C4B-NB	3.15	113.44	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	609	CLA	CBC-CAC-C3C	-3.15	103.75	112.43
23	d	403	CLA	C1D-CHD-C4C	-3.14	119.28	126.06
23	c	513	CLA	O2A-CGA-CBA	3.14	121.76	111.91
26	B	620	SQD	O48-C23-C24	3.14	121.75	111.91
23	a	409	CLA	O2A-CGA-CBA	3.14	121.75	111.91
23	C	507	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
23	c	503	CLA	CMB-C2B-C1B	3.13	130.14	125.37
37	D	411[B]	LHG	O7-C7-C8	3.13	118.25	111.50
23	b	612	CLA	O2A-CGA-O1A	-3.13	115.69	123.59
23	b	606	CLA	C1-C2-C3	-3.13	120.63	126.04
23	a	406[B]	CLA	CAA-C2A-C3A	-3.13	104.21	112.78
23	A	404[A]	CLA	C1-C2-C3	-3.13	120.63	126.04
23	c	509	CLA	C3B-C4B-NB	3.13	113.42	110.52
23	c	512	CLA	C4-C3-C5	3.13	120.53	115.27
23	a	407[A]	CLA	CMB-C2B-C1B	3.12	130.12	125.37
23	B	614	CLA	O2A-CGA-O1A	-3.12	115.71	123.59
23	C	502	CLA	C3B-C4B-NB	3.12	113.41	110.52
23	A	405[A]	CLA	CAC-C3C-C4C	3.12	128.86	124.81
23	B	615	CLA	C4C-C3C-C2C	-3.12	102.35	106.90
23	C	511	CLA	CHC-C1C-C2C	-3.12	118.07	126.73
23	a	407[A]	CLA	CHD-C4C-NC	3.12	129.12	124.20
23	C	509	CLA	C4A-NA-C1A	-3.12	105.31	106.71
23	c	509	CLA	CAA-C2A-C3A	-3.12	104.25	112.78
23	B	610	CLA	O2D-CGD-O1D	-3.12	117.75	123.84
23	C	510	CLA	O2A-CGA-O1A	-3.11	115.73	123.59
23	A	404[B]	CLA	C3B-C2B-C1B	-3.11	103.40	107.16
23	B	614	CLA	CHD-C4C-NC	3.11	129.11	124.20
23	A	406[B]	CLA	CHD-C4C-NC	3.11	129.11	124.20
32	b	627	LMT	C3'-C4'-C5'	-3.11	103.79	110.93
23	b	601	CLA	CHD-C4C-NC	3.11	129.10	124.20
23	A	404[B]	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
23	D	405[A]	CLA	C1D-CHD-C4C	-3.11	119.36	126.06
23	c	509	CLA	C1-C2-C3	-3.10	120.67	126.04
29	a	416[A]	PL9	C35-C34-C36	3.10	120.49	115.27
23	a	405[B]	CLA	CHC-C1C-C2C	-3.10	118.11	126.73
37	D	411[A]	LHG	O7-C7-C8	3.10	118.19	111.50
23	B	605	CLA	CHD-C4C-NC	3.10	129.09	124.20
24	A	353[B]	PHO	C4-C3-C5	3.10	120.49	115.27
25	C	515	BCR	C15-C14-C13	-3.10	122.88	127.31
23	C	512	CLA	C4-C3-C5	3.10	120.49	115.27
24	a	408[A]	PHO	O2A-CGA-CBA	3.10	121.63	111.91
23	b	614	CLA	C3B-C4B-NB	3.10	113.39	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	407[B]	CLA	CAA-C2A-C3A	-3.10	104.30	112.78
25	t	103	BCR	C21-C20-C19	-3.10	113.56	123.22
23	a	407[A]	CLA	CAA-C2A-C3A	-3.09	104.31	112.78
23	C	510	CLA	CMC-C2C-C1C	3.09	129.75	125.04
23	c	503	CLA	C1-C2-C3	-3.09	120.70	126.04
25	B	618	BCR	C2-C1-C6	3.09	115.24	110.48
23	A	406[B]	CLA	CMB-C2B-C1B	3.09	130.07	125.37
23	C	513	CLA	C4C-C3C-C2C	-3.09	102.40	106.90
23	d	403	CLA	CHD-C4C-NC	3.09	129.07	124.20
23	c	507	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
23	B	615	CLA	C3B-C4B-NB	3.09	113.38	110.52
25	B	619	BCR	C38-C26-C25	-3.08	121.06	124.53
38	e	87	HEM	CHD-C4C-NC	3.08	127.77	124.44
32	I	101	LMT	O5B-C5B-C4B	3.08	115.29	109.69
37	D	410[A]	LHG	O8-C23-O10	-3.08	115.82	123.59
23	A	405[B]	CLA	CHC-C1C-C2C	-3.08	118.18	126.73
23	b	616	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	b	612	CLA	C4C-C3C-C2C	-3.08	102.41	106.90
23	C	512	CLA	C1-C2-C3	-3.08	120.72	126.04
23	C	502	CLA	CAC-C3C-C4C	3.08	128.80	124.81
26	a	411[B]	SQD	C45-O47-C7	-3.08	110.22	117.79
25	d	404	BCR	C10-C11-C12	-3.08	113.62	123.22
23	a	407[A]	CLA	C3B-C4B-NB	3.07	113.37	110.52
23	b	609	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
23	a	407[B]	CLA	C1-C2-C3	-3.07	120.73	126.04
23	a	405[B]	CLA	O2A-CGA-CBA	3.07	121.55	111.91
23	b	610	CLA	CAA-CBA-CGA	-3.07	104.28	113.25
23	b	610	CLA	CMC-C2C-C1C	3.07	129.71	125.04
33	z	101	LMG	O7-C10-C11	3.07	118.11	111.50
23	C	510	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
23	B	604	CLA	CHC-C1C-C2C	-3.07	118.21	126.73
37	D	409[B]	LHG	O8-C23-O10	-3.07	115.85	123.59
23	c	504	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	b	614	CLA	CMB-C2B-C1B	3.07	130.04	125.37
23	b	601	CLA	C3B-C4B-NB	3.07	113.36	110.52
23	C	511	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
23	a	409	CLA	C4C-C3C-C2C	-3.07	102.43	106.90
23	b	609	CLA	CMC-C2C-C1C	3.06	129.70	125.04
23	B	606	CLA	CHD-C4C-NC	3.06	129.03	124.20
23	c	512	CLA	C4C-C3C-C2C	-3.06	102.43	106.90
23	B	607	CLA	C1D-CHD-C4C	-3.06	119.45	126.06
23	b	604	CLA	C1D-CHD-C4C	-3.06	119.45	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	602	CLA	C11-C12-C13	-3.06	106.03	115.92
23	D	405[B]	CLA	O2A-CGA-CBA	3.06	121.51	111.91
29	A	414[B]	PL9	C30-C29-C31	3.06	120.42	115.27
23	c	502	CLA	C4C-C3C-C2C	-3.06	102.44	106.90
23	B	616	CLA	CAC-C3C-C4C	3.06	128.78	124.81
25	a	410	BCR	C40-C30-C25	-3.06	105.34	110.30
37	e	101[A]	LHG	O7-C7-C8	3.05	118.08	111.50
40	V	202	HEC	CAD-CBD-CGD	-3.05	107.03	113.60
23	C	510	CLA	CHB-C1B-NB	-3.05	121.02	124.26
23	B	615	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	a	407[B]	CLA	CBC-CAC-C3C	-3.05	104.03	112.43
23	b	607	CLA	CHC-C1C-C2C	-3.05	118.27	126.73
23	A	404[A]	CLA	CMC-C2C-C1C	3.05	129.68	125.04
37	D	411[A]	LHG	O8-C23-C24	3.05	121.46	111.91
29	A	414[A]	PL9	O1-C4-C3	-3.05	117.37	120.72
23	c	514	CLA	CMB-C2B-C1B	3.04	130.01	125.37
29	a	416[A]	PL9	C10-C9-C11	3.04	120.39	115.27
23	a	405[B]	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
25	D	407	BCR	C16-C17-C18	-3.04	122.97	127.31
23	C	504	CLA	O2A-CGA-O1A	-3.04	115.92	123.59
29	A	414[A]	PL9	C20-C19-C21	3.04	120.38	115.27
37	d	711[A]	LHG	O7-C7-C8	3.03	118.04	111.50
29	a	416[B]	PL9	C42-C43-C44	-3.03	120.36	127.66
23	c	510	CLA	C4C-C3C-C2C	-3.03	102.48	106.90
23	b	616	CLA	C3B-C4B-NB	3.03	113.33	110.52
25	D	407	BCR	C40-C30-C25	-3.03	105.38	110.30
23	b	611	CLA	CHC-C1C-C2C	-3.03	118.32	126.73
25	c	515	BCR	C37-C22-C21	-3.03	118.68	122.92
26	A	412	SQD	O48-C23-C24	3.03	121.41	111.91
23	b	607	CLA	C4C-C3C-C2C	-3.03	102.49	106.90
23	b	603	CLA	O2A-CGA-O1A	-3.03	115.96	123.59
23	c	502	CLA	C1D-CHD-C4C	-3.02	119.53	126.06
23	c	514	CLA	CAC-C3C-C4C	3.02	128.73	124.81
23	c	511	CLA	C4-C3-C5	3.02	120.36	115.27
23	C	502	CLA	CHC-C1C-C2C	-3.02	118.33	126.73
23	A	405[A]	CLA	C3B-C4B-NB	3.02	113.32	110.52
29	D	408[B]	PL9	C20-C19-C21	3.02	120.35	115.27
23	c	513	CLA	CHD-C4C-NC	3.02	128.96	124.20
23	b	603	CLA	O2A-CGA-CBA	3.02	121.38	111.91
24	a	353[A]	PHO	CBA-CAA-C2A	-3.02	105.00	113.81
23	C	503	CLA	C3B-C4B-NB	3.01	113.31	110.52
23	b	605	CLA	O2A-CGA-O1A	-3.01	115.99	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[A]	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
37	D	411[A]	LHG	O8-C23-O10	-3.01	115.99	123.59
23	a	405[B]	CLA	CAC-C3C-C4C	3.01	128.72	124.81
24	a	353[A]	PHO	CMB-C2B-C3B	3.01	130.30	124.68
23	b	605	CLA	C4C-C3C-C2C	-3.01	102.52	106.90
33	D	415	LMG	O8-C28-O10	-3.01	116.00	123.59
23	B	609	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
32	m	103	LMT	C3'-C4'-C5'	-3.00	104.04	110.93
23	B	606	CLA	O2A-CGA-O1A	-3.00	116.01	123.59
23	B	603	CLA	CHC-C1C-C2C	-3.00	118.39	126.73
25	K	102	BCR	C38-C26-C25	-3.00	121.16	124.53
29	D	408[A]	PL9	C53-C6-C1	3.00	121.13	114.99
23	b	614	CLA	CHB-C1B-NB	-3.00	121.08	124.26
23	D	406	CLA	CMC-C2C-C1C	3.00	129.61	125.04
25	y	101	BCR	C38-C26-C25	-3.00	121.16	124.53
23	C	512	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
32	m	103	LMT	C3B-C4B-C5B	-3.00	104.89	110.24
23	A	405[B]	CLA	CBC-CAC-C3C	-3.00	104.16	112.43
23	A	406[B]	CLA	CAA-C2A-C3A	-3.00	104.56	112.78
29	d	405[A]	PL9	C22-C23-C24	-3.00	120.44	127.66
29	d	405[A]	PL9	C36-C34-C33	-3.00	115.05	121.12
23	a	407[A]	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	b	603	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	B	612	CLA	C11-C12-C13	-3.00	106.24	115.92
25	b	618	BCR	C15-C14-C13	-2.99	123.04	127.31
23	C	506	CLA	CMC-C2C-C1C	2.99	129.60	125.04
23	B	603	CLA	C4-C3-C5	2.99	120.31	115.27
29	A	414[A]	PL9	C17-C18-C19	-2.99	120.45	127.66
23	c	505	CLA	CAC-C3C-C4C	2.99	128.69	124.81
23	c	502	CLA	C3B-C4B-NB	2.99	113.29	110.52
23	a	405[A]	CLA	CHC-C1C-C2C	-2.99	118.43	126.73
35	C	518[B]	DGD	C2G-O2G-C1B	-2.99	110.43	117.79
23	c	510	CLA	C4-C3-C5	2.99	120.30	115.27
23	b	609	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	b	613	CLA	CHC-C1C-C2C	-2.99	118.44	126.73
23	c	514	CLA	C4C-C3C-C2C	-2.99	102.55	106.90
33	m	101	LMG	O8-C28-C29	2.98	121.27	111.91
23	d	402[A]	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
23	c	512	CLA	CMB-C2B-C1B	2.98	129.91	125.37
23	B	603	CLA	O2A-CGA-CBA	2.98	121.26	111.91
25	H	101	BCR	C7-C8-C9	-2.98	121.73	126.23
23	a	407[B]	CLA	CMC-C2C-C1C	2.98	129.58	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	C1D-CHD-C4C	-2.98	119.63	126.06
23	C	512	CLA	CHC-C1C-C2C	-2.98	118.46	126.73
23	a	405[A]	CLA	CMA-C3A-C4A	-2.98	103.77	111.77
26	F	101	SQD	C1-C2-C3	-2.98	103.80	110.00
23	A	406[A]	CLA	CMC-C2C-C1C	2.98	129.57	125.04
37	L	101[B]	LHG	O8-C23-C24	2.98	121.25	111.91
35	C	517[A]	DGD	C2G-O2G-C1B	-2.97	110.47	117.79
23	d	402[A]	CLA	C4C-C3C-C2C	-2.97	102.56	106.90
23	B	605	CLA	C1-C2-C3	-2.97	120.90	126.04
25	B	618	BCR	C38-C26-C25	-2.97	121.19	124.53
29	a	416[A]	PL9	C42-C43-C44	-2.97	120.50	127.66
23	a	405[A]	CLA	CMC-C2C-C1C	2.97	129.56	125.04
29	d	405[B]	PL9	C20-C19-C21	2.97	120.27	115.27
23	B	609	CLA	C4C-C3C-C2C	-2.97	102.57	106.90
37	d	407[B]	LHG	O7-C7-C8	2.97	117.90	111.50
23	B	601	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
29	d	405[A]	PL9	C10-C9-C11	2.97	120.27	115.27
23	b	614	CLA	CBC-CAC-C3C	-2.97	104.25	112.43
23	c	512	CLA	CHC-C1C-C2C	-2.97	118.48	126.73
23	a	405[B]	CLA	CAA-C2A-C1A	-2.97	102.26	111.97
23	C	509	CLA	CHC-C1C-C2C	-2.96	118.50	126.73
25	c	516	BCR	C11-C10-C9	-2.96	123.08	127.31
26	A	410[A]	SQD	O8-S-C6	2.96	110.46	105.74
23	B	613	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
32	D	404	LMT	C4B-C3B-C2B	2.96	116.00	110.82
24	a	353[A]	PHO	O2D-CGD-O1D	-2.96	118.05	123.84
23	b	605	CLA	C3B-C4B-NB	2.96	113.26	110.52
23	c	503	CLA	CBC-CAC-C3C	-2.96	104.27	112.43
23	b	602	CLA	CHD-C4C-NC	2.96	128.86	124.20
23	C	504	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
23	b	614	CLA	C4C-C3C-C2C	-2.95	102.59	106.90
23	D	405[A]	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
26	B	620	SQD	C1-O5-C5	-2.95	107.90	113.69
23	b	614	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	B	612	CLA	C1D-CHD-C4C	-2.95	119.70	126.06
23	c	510	CLA	O2A-CGA-CBA	2.95	121.15	111.91
23	b	610	CLA	CHD-C4C-NC	2.95	128.84	124.20
23	B	608	CLA	CHC-C1C-C2C	-2.94	118.55	126.73
33	z	101	LMG	O8-C28-C29	2.94	121.15	111.91
23	C	503	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
23	a	407[B]	CLA	C4-C3-C5	2.94	120.21	115.27
23	C	504	CLA	CMB-C2B-C1B	2.94	129.84	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	618	BCR	C15-C14-C13	-2.94	123.12	127.31
23	b	602	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
23	c	505	CLA	CHC-C1C-C2C	-2.94	118.57	126.73
23	B	607	CLA	C2A-C1A-CHA	-2.94	118.72	123.86
23	B	607	CLA	CBC-CAC-C3C	-2.94	104.33	112.43
23	c	514	CLA	O2A-CGA-CBA	2.94	121.12	111.91
29	D	408[A]	PL9	C10-C9-C11	2.93	120.20	115.27
23	B	608	CLA	C1D-CHD-C4C	-2.93	119.73	126.06
23	a	407[B]	CLA	CMB-C2B-C1B	2.93	129.83	125.37
23	C	502	CLA	CMC-C2C-C1C	2.93	129.50	125.04
23	A	405[A]	CLA	CMA-C3A-C4A	-2.93	103.90	111.77
29	D	408[B]	PL9	C10-C9-C11	2.93	120.19	115.27
29	D	408[B]	PL9	C7-C8-C9	-2.93	121.92	126.79
23	A	404[A]	CLA	C4C-C3C-C2C	-2.92	102.64	106.90
23	b	612	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	a	406[A]	CLA	CMA-C3A-C2A	-2.92	102.03	113.83
23	C	502	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
23	a	406[B]	CLA	CBC-CAC-C3C	-2.92	104.37	112.43
23	b	605	CLA	CHC-C1C-C2C	-2.92	118.61	126.73
23	C	503	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	A	404[B]	CLA	O2A-CGA-CBA	2.92	121.06	111.91
37	E	101[A]	LHG	O8-C23-C24	2.92	121.06	111.91
23	A	408	CLA	CBC-CAC-C3C	-2.91	104.39	112.43
23	D	405[A]	CLA	C4-C3-C5	2.91	120.17	115.27
29	a	416[B]	PL9	C35-C34-C36	2.91	120.17	115.27
23	B	603	CLA	CHD-C4C-NC	2.91	128.79	124.20
23	A	404[A]	CLA	C2A-C1A-CHA	-2.91	118.77	123.86
38	e	87	HEM	CHB-C1B-NB	2.91	127.96	124.37
29	d	405[B]	PL9	C40-C39-C41	2.91	120.17	115.27
23	b	605	CLA	CMB-C2B-C1B	2.90	129.79	125.37
23	D	405[B]	CLA	C4C-C3C-C2C	-2.90	102.66	106.90
23	b	612	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	A	405[A]	CLA	CHD-C4C-NC	2.90	128.78	124.20
23	C	510	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
23	a	407[B]	CLA	C3B-C4B-NB	2.90	113.21	110.52
23	b	602	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	a	409	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
23	d	403	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
23	b	601	CLA	C1-O2A-CGA	2.90	124.05	116.44
37	e	101[B]	LHG	O7-C7-C8	2.90	117.75	111.50
23	D	405[A]	CLA	O2A-CGA-CBA	2.90	121.00	111.91
29	A	414[B]	PL9	C53-C6-C1	2.90	120.91	114.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	514	CLA	C4C-C3C-C2C	-2.90	102.67	106.90
24	a	353[B]	PHO	CMB-C2B-C3B	2.90	130.10	124.68
23	D	406	CLA	CMA-C3A-C2A	-2.89	102.16	113.83
23	B	605	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	C	510	CLA	C16-C15-C13	-2.89	106.58	115.92
23	A	406[B]	CLA	O2A-CGA-O1A	-2.89	116.30	123.59
23	B	613	CLA	C4C-C3C-C2C	-2.89	102.69	106.90
23	d	402[A]	CLA	CHC-C1C-C2C	-2.89	118.71	126.73
23	B	608	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	B	612	CLA	CMC-C2C-C1C	2.89	129.44	125.04
23	B	614	CLA	CBC-CAC-C3C	-2.88	104.48	112.43
23	A	404[B]	CLA	C2A-C1A-CHA	-2.88	118.81	123.86
33	Z	101	LMG	C4-C3-C2	2.88	115.86	110.82
37	d	407[A]	LHG	O7-C7-C8	2.88	117.71	111.50
23	B	614	CLA	CHC-C1C-C2C	-2.88	118.72	126.73
23	A	406[B]	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
32	D	404	LMT	C2'-C3'-C4'	2.88	116.26	109.68
23	D	405[A]	CLA	CAA-C2A-C3A	-2.88	104.89	112.78
23	B	614	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
25	b	619	BCR	C38-C26-C25	-2.88	121.29	124.53
25	k	101	BCR	C7-C8-C9	-2.88	121.88	126.23
23	C	506	CLA	CHC-C1C-C2C	-2.88	118.73	126.73
23	A	406[B]	CLA	O2A-CGA-CBA	2.88	120.94	111.91
23	C	514	CLA	CHD-C4C-NC	2.88	128.74	124.20
24	a	353[A]	PHO	C4A-C3A-C2A	-2.88	100.10	102.84
23	A	408	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
32	a	414	LMT	O1'-C1'-C2'	2.88	112.79	108.30
23	A	406[A]	CLA	CHD-C4C-NC	2.88	128.73	124.20
23	b	614	CLA	CHC-C1C-C2C	-2.88	118.74	126.73
23	b	613	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
26	a	411[A]	SQD	O47-C7-O49	-2.87	116.75	123.70
29	a	416[B]	PL9	C22-C23-C24	-2.87	120.74	127.66
23	b	614	CLA	CHD-C4C-NC	2.87	128.73	124.20
24	A	353[A]	PHO	O2D-CGD-O1D	-2.87	118.22	123.84
25	y	101	BCR	C15-C14-C13	-2.87	123.21	127.31
23	b	601	CLA	C4C-C3C-C2C	-2.87	102.71	106.90
23	c	505	CLA	CHB-C1B-NB	-2.87	121.22	124.26
23	a	406[B]	CLA	C1-C2-C3	-2.87	121.08	126.04
23	d	402[B]	CLA	CMC-C2C-C1C	2.87	129.41	125.04
23	c	505	CLA	C4C-C3C-C2C	-2.87	102.72	106.90
23	C	507	CLA	C4-C3-C5	2.87	120.10	115.27
23	b	606	CLA	CHC-C1C-C2C	-2.87	118.76	126.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	E	101[B]	LHG	O8-C23-C24	2.87	120.91	111.91
23	a	405[A]	CLA	CAC-C3C-C4C	2.87	128.53	124.81
23	C	514	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	C	507	CLA	CHC-C1C-C2C	-2.87	118.77	126.73
23	B	608	CLA	C1-C2-C3	-2.87	121.08	126.04
37	D	409[A]	LHG	C5-O7-C7	-2.87	110.73	117.79
29	A	414[B]	PL9	C35-C34-C36	2.86	120.09	115.27
23	c	509	CLA	CMB-C2B-C1B	2.86	129.73	125.37
23	c	514	CLA	CAA-C2A-C3A	-2.86	104.94	112.78
34	b	622	HTG	O5-C1-C2	2.86	113.91	110.31
26	B	620	SQD	C4-C3-C2	2.86	115.82	110.82
23	B	613	CLA	O2A-CGA-CBA	2.86	120.88	111.91
29	D	408[A]	PL9	C51-C49-C50	2.86	120.92	114.60
23	B	608	CLA	C11-C12-C13	-2.86	106.68	115.92
23	B	609	CLA	C3B-C4B-NB	2.86	113.17	110.52
23	B	614	CLA	O2A-CGA-CBA	2.86	120.87	111.91
25	A	409	BCR	C8-C7-C6	-2.86	119.18	127.20
23	b	603	CLA	CHD-C4C-NC	2.85	128.70	124.20
23	B	604	CLA	CMB-C2B-C1B	2.85	129.72	125.37
23	c	506	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
23	a	406[A]	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
29	a	416[A]	PL9	C53-C6-C1	2.85	120.82	114.99
25	H	101	BCR	C37-C22-C21	-2.85	118.93	122.92
23	b	601	CLA	CHC-C1C-C2C	-2.85	118.81	126.73
23	A	408	CLA	CMC-C2C-C1C	2.85	129.38	125.04
23	d	403	CLA	C3B-C4B-NB	2.85	113.16	110.52
23	c	502	CLA	CHC-C1C-C2C	-2.85	118.82	126.73
23	C	504	CLA	CBC-CAC-C3C	-2.85	104.58	112.43
35	C	517[A]	DGD	O6D-C1D-O3G	-2.85	103.24	109.97
23	C	514	CLA	CBC-CAC-C3C	-2.84	104.59	112.43
23	C	504	CLA	CHD-C4C-NC	2.84	128.68	124.20
23	c	505	CLA	CMC-C2C-C1C	2.84	129.37	125.04
26	A	410[A]	SQD	O48-C23-C24	2.84	120.82	111.91
23	D	406	CLA	CHC-C1C-C2C	-2.84	118.85	126.73
23	a	407[A]	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
26	F	101	SQD	O7-S-C6	2.83	110.31	106.94
23	A	406[A]	CLA	O2A-CGA-CBA	2.83	120.80	111.91
23	a	409	CLA	CMB-C2B-C1B	2.83	129.68	125.37
23	b	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
23	B	602	CLA	C4C-C3C-C2C	-2.83	102.77	106.90
35	c	519	DGD	O1G-C1A-C2A	2.83	120.78	111.91
29	D	408[A]	PL9	C37-C38-C39	-2.83	120.85	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	A	406[B]	CLA	CBC-CAC-C3C	-2.83	104.64	112.43
35	c	517[B]	DGD	O3G-C3G-C2G	-2.83	104.08	110.90
25	b	619	BCR	C7-C8-C9	-2.82	121.97	126.23
25	C	515	BCR	C16-C17-C18	-2.82	123.28	127.31
37	d	407[B]	LHG	O8-C23-O10	-2.82	116.47	123.59
23	d	403	CLA	CMC-C2C-C1C	2.82	129.34	125.04
23	C	508	CLA	CBC-CAC-C3C	-2.82	104.65	112.43
23	d	402[B]	CLA	CAC-C3C-C4C	2.82	128.47	124.81
38	E	103	HEM	CBA-CAA-C2A	-2.82	104.79	112.63
29	A	414[A]	PL9	C35-C34-C36	2.82	120.01	115.27
23	B	613	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
23	C	505	CLA	C2A-C1A-CHA	-2.82	118.93	123.86
23	c	509	CLA	CHC-C1C-C2C	-2.82	118.90	126.73
37	L	101[A]	LHG	O8-C23-C24	2.82	120.75	111.91
23	c	511	CLA	CHC-C1C-C2C	-2.82	118.91	126.73
23	d	403	CLA	CBC-CAC-C3C	-2.82	104.67	112.43
32	M	101	LMT	C3'-C4'-C5'	-2.82	104.47	110.93
23	B	612	CLA	O2A-CGA-CBA	2.82	120.74	111.91
23	c	505	CLA	CMB-C2B-C1B	2.81	129.65	125.37
25	h	101	BCR	C37-C22-C21	-2.81	118.98	122.92
37	d	408[B]	LHG	O8-C23-C24	2.81	120.73	111.91
23	A	404[A]	CLA	CHC-C1C-C2C	-2.81	118.92	126.73
25	T	101	BCR	C12-C13-C14	-2.81	114.63	118.94
35	C	519	DGD	O1G-C1A-C2A	2.81	120.73	111.91
23	A	406[A]	CLA	C4C-C3C-C2C	-2.81	102.80	106.90
35	h	102	DGD	O1G-C1A-C2A	2.81	120.73	111.91
23	B	603	CLA	CMC-C2C-C1C	2.81	129.32	125.04
23	b	608	CLA	CHD-C4C-NC	2.81	128.63	124.20
23	B	614	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
23	C	503	CLA	CMC-C2C-C1C	2.81	129.31	125.04
23	A	406[A]	CLA	C4-C3-C5	2.81	119.99	115.27
29	A	414[A]	PL9	C30-C29-C31	2.81	119.99	115.27
23	a	405[B]	CLA	C2A-C1A-CHA	-2.81	118.95	123.86
23	B	601	CLA	O2A-CGA-CBA	2.81	120.71	111.91
23	B	606	CLA	C3B-C4B-NB	2.80	113.12	110.52
29	a	416[A]	PL9	C22-C23-C24	-2.80	120.92	127.66
35	c	519	DGD	O2G-C1B-C2B	2.80	117.54	111.50
23	b	609	CLA	CHD-C4C-NC	2.80	128.61	124.20
23	C	511	CLA	CHB-C4A-NA	2.80	128.38	124.51
23	a	407[B]	CLA	CHC-C1C-C2C	-2.80	118.96	126.73
24	a	408[B]	PHO	O1D-CGD-CBD	-2.79	120.08	124.74
23	a	409	CLA	C2A-C1A-CHA	-2.79	118.97	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	505	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
32	a	420	LMT	C3'-C4'-C5'	-2.79	104.52	110.93
23	A	405[A]	CLA	CHC-C1C-C2C	-2.79	118.97	126.73
23	B	602	CLA	C2A-C1A-CHA	-2.79	118.98	123.86
33	C	501	LMG	C6-C5-C4	2.79	119.54	113.00
38	e	87	HEM	C4D-ND-C1D	2.79	107.95	105.07
23	c	513	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
23	B	615	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
23	a	407[A]	CLA	CHC-C1C-C2C	-2.79	118.98	126.73
23	c	504	CLA	C3B-C4B-NB	2.79	113.10	110.52
23	C	503	CLA	C4-C3-C5	2.79	119.96	115.27
23	B	612	CLA	O2A-CGA-O1A	-2.79	116.56	123.59
34	B	622	HTG	C1-O5-C5	2.79	117.72	112.58
23	c	508	CLA	CHD-C4C-NC	2.78	128.59	124.20
25	B	618	BCR	C36-C18-C17	-2.78	119.03	122.92
23	d	403	CLA	C4-C3-C5	2.78	119.95	115.27
23	b	609	CLA	C16-C15-C13	-2.78	106.93	115.92
23	A	404[B]	CLA	CAC-C3C-C4C	2.78	128.42	124.81
25	H	101	BCR	C16-C17-C18	-2.78	123.34	127.31
25	K	102	BCR	C15-C14-C13	-2.78	123.34	127.31
35	H	102	DGD	O6E-C5E-C6E	2.78	113.35	106.44
25	B	618	BCR	C37-C22-C23	2.78	122.46	118.08
23	B	607	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
23	C	507	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
23	c	513	CLA	CMC-C2C-C1C	2.78	129.27	125.04
23	C	509	CLA	O2A-CGA-O1A	-2.78	116.59	123.59
23	c	511	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
23	C	505	CLA	CBC-CAC-C3C	-2.77	104.78	112.43
29	A	414[B]	PL9	C10-C9-C11	2.77	119.94	115.27
23	b	608	CLA	CHC-C1C-C2C	-2.77	119.03	126.73
32	e	102	LMT	O1'-C1'-C2'	2.77	112.63	108.30
23	a	409	CLA	CAC-C3C-C4C	2.77	128.41	124.81
23	A	405[A]	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	D	406	CLA	C4C-C3C-C2C	-2.77	102.86	106.90
24	a	408[A]	PHO	CMB-C2B-C3B	2.77	129.86	124.68
33	D	415	LMG	O8-C28-C29	2.77	120.60	111.91
23	B	608	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	b	619	BCR	C24-C23-C22	-2.77	122.05	126.23
23	b	603	CLA	CMA-C3A-C2A	-2.77	102.67	113.83
23	c	503	CLA	CMC-C2C-C1C	2.77	129.25	125.04
26	b	620	SQD	O9-S-C6	2.77	110.23	106.94
26	a	411[B]	SQD	O8-S-C6	2.77	110.15	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[A]	CLA	O2A-CGA-CBA	2.76	120.58	111.91
23	B	616	CLA	O2A-CGA-CBA	2.76	120.57	111.91
37	D	409[B]	LHG	O8-C23-C24	2.76	120.57	111.91
23	a	407[A]	CLA	O2A-CGA-O1A	-2.76	116.62	123.59
25	B	618	BCR	C37-C22-C21	-2.76	119.06	122.92
25	H	101	BCR	C24-C23-C22	-2.76	122.07	126.23
35	h	102	DGD	O1G-C1A-O1A	-2.76	116.63	123.59
24	A	407[B]	PHO	CMA-C3A-C4A	-2.76	108.34	114.38
23	b	602	CLA	CMB-C2B-C1B	2.76	129.57	125.37
37	D	410[A]	LHG	O7-C7-C8	2.75	117.44	111.50
23	C	513	CLA	O2A-CGA-CBA	2.75	120.54	111.91
23	c	504	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	c	510	CLA	CHD-C4C-NC	2.75	128.54	124.20
23	b	611	CLA	CAC-C3C-C4C	2.75	128.38	124.81
35	C	519	DGD	O3G-C3G-C2G	-2.75	104.27	110.90
23	D	406	CLA	CAA-C2A-C3A	-2.75	105.25	112.78
32	b	621	LMT	C1'-O5'-C5'	-2.75	108.30	113.69
25	K	102	BCR	C20-C21-C22	-2.75	123.39	127.31
23	b	609	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
23	B	616	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
25	h	101	BCR	C36-C18-C17	-2.75	119.08	122.92
37	D	411[B]	LHG	O8-C23-C24	2.75	120.53	111.91
23	c	510	CLA	C1-O2A-CGA	2.75	123.65	116.44
29	d	405[A]	PL9	C36-C37-C38	-2.74	102.86	111.88
23	b	616	CLA	CHC-C1C-C2C	-2.74	119.12	126.73
23	D	406	CLA	C2A-C1A-CHA	-2.74	119.08	123.86
23	c	509	CLA	O2A-CGA-CBA	2.74	120.49	111.91
23	b	610	CLA	C4-C3-C5	2.73	119.87	115.27
23	A	405[B]	CLA	C4-C3-C5	2.73	119.87	115.27
35	C	519	DGD	O2G-C1B-C2B	2.73	117.39	111.50
24	a	408[B]	PHO	O2A-CGA-CBA	2.73	120.48	111.91
23	c	506	CLA	CMC-C2C-C1C	2.73	129.20	125.04
23	c	508	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
23	C	509	CLA	O2A-CGA-CBA	2.73	120.48	111.91
23	B	612	CLA	C3B-C4B-NB	2.73	113.04	110.52
26	f	102	SQD	O48-C23-C24	2.72	120.45	111.91
23	C	507	CLA	C2A-C1A-CHA	-2.72	119.10	123.86
26	A	410[B]	SQD	O48-C23-C24	2.72	120.45	111.91
25	b	618	BCR	C33-C5-C6	-2.72	121.47	124.53
29	d	405[A]	PL9	C27-C28-C29	-2.72	121.11	127.66
23	A	408	CLA	C4-C3-C5	2.72	119.85	115.27
33	c	521	LMG	O8-C28-C29	2.72	120.44	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	a	406[B]	CLA	CHC-C1C-C2C	-2.72	119.18	126.73
23	c	510	CLA	CHB-C1B-NB	-2.72	121.38	124.26
25	H	101	BCR	C10-C11-C12	-2.72	114.74	123.22
29	D	408[B]	PL9	C27-C28-C29	-2.72	121.12	127.66
23	B	602	CLA	CAC-C3C-C4C	2.71	128.33	124.81
23	b	606	CLA	CMB-C2B-C1B	2.71	129.50	125.37
23	C	502	CLA	C4-C3-C5	2.71	119.84	115.27
23	D	406	CLA	CHD-C4C-NC	2.71	128.48	124.20
32	M	101	LMT	C1'-O5'-C5'	-2.71	108.37	113.69
23	b	602	CLA	C1-O2A-CGA	2.71	123.56	116.44
23	b	615	CLA	CHD-C4C-NC	2.71	128.47	124.20
23	c	512	CLA	CAC-C3C-C4C	2.71	128.32	124.81
23	C	504	CLA	CMC-C2C-C1C	2.71	129.16	125.04
23	A	406[B]	CLA	CMA-C3A-C2A	-2.71	102.91	113.83
23	b	604	CLA	O2A-CGA-CBA	2.71	120.40	111.91
25	T	101	BCR	C16-C17-C18	-2.71	123.45	127.31
23	d	402[B]	CLA	O2A-CGA-O1A	-2.70	116.77	123.59
40	v	202	HEC	CHA-C1A-NA	2.70	127.36	124.44
37	d	407[B]	LHG	O8-C23-C24	2.70	120.37	111.91
26	B	620	SQD	O48-C23-O10	-2.70	116.79	123.59
23	D	406	CLA	O2A-CGA-CBA	2.70	120.37	111.91
25	D	407	BCR	C24-C23-C22	-2.69	122.16	126.23
23	c	507	CLA	C4C-C3C-C2C	-2.69	102.97	106.90
23	a	405[A]	CLA	C2A-C1A-CHA	-2.69	119.15	123.86
34	B	626	HTG	O5-C5-C4	2.69	114.58	109.69
26	F	101	SQD	O48-C23-C24	2.69	120.36	111.91
29	a	416[B]	PL9	C10-C9-C11	2.69	119.80	115.27
37	L	101[A]	LHG	O8-C23-O10	-2.69	116.80	123.59
23	c	514	CLA	CHD-C4C-NC	2.69	128.44	124.20
23	D	405[A]	CLA	CAC-C3C-C4C	2.69	128.30	124.81
23	C	503	CLA	C4C-C3C-C2C	-2.69	102.98	106.90
25	Y	101	BCR	C28-C27-C26	-2.69	109.28	114.08
23	B	604	CLA	CED-O2D-CGD	2.69	122.01	115.94
35	H	102	DGD	O1G-C1A-O1A	-2.69	116.81	123.59
23	B	605	CLA	CED-O2D-CGD	2.68	122.01	115.94
23	C	514	CLA	C2A-C1A-CHA	-2.68	119.17	123.86
23	c	513	CLA	CAC-C3C-C4C	2.68	128.29	124.81
26	a	411[B]	SQD	O47-C7-O49	-2.68	117.22	123.70
25	D	407	BCR	C15-C14-C13	-2.68	123.48	127.31
23	b	602	CLA	C1-C2-C3	-2.68	121.40	126.04
37	l	101[A]	LHG	O8-C23-C24	2.68	120.32	111.91
23	c	508	CLA	O2A-CGA-CBA	2.68	120.31	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	k	101	BCR	C2-C1-C6	2.68	114.60	110.48
23	D	405[B]	CLA	CHC-C1C-C2C	-2.67	119.30	126.73
23	b	607	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
23	A	404[A]	CLA	CMA-C3A-C2A	-2.67	103.05	113.83
23	D	405[B]	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	a	407[B]	CLA	C4C-C3C-C2C	-2.67	103.00	106.90
25	C	515	BCR	C38-C26-C25	-2.67	121.53	124.53
23	c	503	CLA	CHD-C4C-NC	2.67	128.41	124.20
23	C	509	CLA	CMC-C2C-C1C	2.67	129.10	125.04
26	f	102	SQD	O8-S-C6	2.67	109.99	105.74
23	b	613	CLA	CHD-C4C-NC	2.67	128.41	124.20
23	B	611	CLA	CMB-C2B-C3B	2.67	133.05	126.59
23	b	607	CLA	CBC-CAC-C3C	-2.67	105.08	112.43
23	A	406[B]	CLA	C3B-C4B-NB	2.67	112.99	110.52
25	a	410	BCR	C33-C5-C6	-2.67	121.53	124.53
23	B	602	CLA	CHD-C4C-NC	2.67	128.40	124.20
23	a	406[A]	CLA	C4C-C3C-C2C	-2.67	103.01	106.90
23	a	409	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
24	a	408[B]	PHO	CBC-CAC-C3C	-2.66	108.98	112.88
23	C	506	CLA	C3B-C4B-NB	2.66	112.99	110.52
23	B	604	CLA	O1D-CGD-CBD	-2.66	119.03	124.48
25	t	103	BCR	C1-C6-C7	2.66	123.31	115.78
23	B	612	CLA	C4-C3-C5	2.66	119.75	115.27
23	B	606	CLA	O2A-CGA-CBA	2.66	120.26	111.91
24	a	408[B]	PHO	CMA-C3A-C4A	-2.66	108.55	114.38
29	A	414[B]	PL9	C45-C44-C46	2.66	119.75	115.27
23	B	610	CLA	CHC-C1C-C2C	-2.66	119.34	126.73
37	e	101[A]	LHG	O8-C23-C24	2.66	120.25	111.91
23	b	608	CLA	CMA-C3A-C4A	-2.66	104.63	111.77
23	b	603	CLA	CMB-C2B-C1B	2.66	129.42	125.37
29	a	416[B]	PL9	C20-C19-C21	2.66	119.74	115.27
23	A	408	CLA	O2A-CGA-CBA	2.66	120.25	111.91
24	A	407[A]	PHO	C1-C2-C3	-2.66	121.45	126.04
23	a	409	CLA	CMA-C3A-C2A	-2.66	103.12	113.83
29	a	416[B]	PL9	C53-C6-C1	2.66	120.42	114.99
23	B	609	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
23	B	608	CLA	O2A-CGA-O1A	-2.65	116.89	123.59
35	h	102	DGD	O4D-C4D-C3D	-2.65	104.21	110.35
23	D	405[A]	CLA	CHC-C1C-C2C	-2.65	119.36	126.73
34	b	623	HTG	O5-C1-C2	2.65	113.65	110.31
23	c	510	CLA	O2A-C1-C2	2.65	115.60	108.64
23	a	406[A]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[A]	CLA	CAC-C3C-C4C	2.65	128.25	124.81
35	C	518[A]	DGD	O1G-C1A-O1A	-2.65	116.90	123.59
33	C	501	LMG	O6-C1-O1	-2.65	103.70	109.97
23	d	402[A]	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	D	405[B]	CLA	CMC-C2C-C1C	2.65	129.07	125.04
23	A	405[A]	CLA	C4-C3-C5	2.65	119.73	115.27
23	A	408	CLA	CMB-C2B-C1B	2.65	129.40	125.37
23	D	405[B]	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
23	b	608	CLA	O2A-CGA-CBA	2.65	120.22	111.91
24	A	407[B]	PHO	C1-C2-C3	-2.65	121.46	126.04
23	A	408	CLA	CHD-C4C-NC	2.65	128.37	124.20
29	a	416[A]	PL9	C40-C39-C41	2.65	119.72	115.27
37	e	101[B]	LHG	O8-C23-C24	2.65	120.21	111.91
23	d	403	CLA	C2A-C1A-CHA	-2.65	119.23	123.86
23	B	603	CLA	O2A-CGA-O1A	-2.64	116.92	123.59
23	D	405[A]	CLA	C2A-C1A-CHA	-2.64	119.24	123.86
37	D	410[A]	LHG	O8-C23-C24	2.64	120.20	111.91
25	c	516	BCR	C21-C20-C19	-2.64	114.97	123.22
26	F	101	SQD	O47-C7-O49	-2.64	117.32	123.70
25	T	101	BCR	C35-C13-C12	2.64	122.24	118.08
23	C	502	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
33	B	621	LMG	C12-C11-C10	-2.64	104.02	113.62
23	B	602	CLA	CMB-C2B-C1B	2.64	129.39	125.37
23	b	611	CLA	CHD-C4C-NC	2.64	128.36	124.20
23	d	402[B]	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
23	B	607	CLA	O2A-CGA-O1A	-2.64	116.94	123.59
23	c	512	CLA	O2A-CGA-CBA	2.63	120.17	111.91
23	C	508	CLA	CHC-C1C-C2C	-2.63	119.42	126.73
23	C	505	CLA	C4-C3-C5	2.63	119.70	115.27
29	A	414[A]	PL9	C40-C39-C41	2.63	119.70	115.27
37	D	411[B]	LHG	O8-C23-O10	-2.63	116.95	123.59
33	c	520	LMG	O8-C28-C29	2.63	120.16	111.91
29	d	405[B]	PL9	C7-C8-C9	-2.63	122.42	126.79
23	a	406[B]	CLA	C4C-C3C-C2C	-2.63	103.07	106.90
23	b	602	CLA	CHB-C1B-C2B	-2.63	119.82	127.24
23	c	502	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	c	504	CLA	CAC-C3C-C4C	2.63	128.22	124.81
40	V	202	HEC	CBC-CAC-C3C	2.63	119.67	112.43
34	B	622	HTG	C1'-S1-C1	2.63	105.00	100.09
23	A	404[B]	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	D	408[B]	PL9	C40-C39-C41	2.63	119.69	115.27
29	D	408[B]	PL9	C51-C49-C50	2.62	120.40	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	d	402[B]	CLA	C2A-C1A-CHA	-2.62	119.27	123.86
23	a	405[B]	CLA	CHD-C4C-NC	2.62	128.34	124.20
35	h	102	DGD	O3G-C1D-C2D	2.62	112.39	108.30
26	F	101	SQD	O9-S-C6	-2.62	103.83	106.94
23	d	403	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
25	K	102	BCR	C3-C4-C5	-2.62	109.41	114.08
23	C	511	CLA	CMB-C2B-C1B	2.61	129.35	125.37
32	D	404	LMT	O1'-C1'-C2'	2.61	112.38	108.30
29	a	416[A]	PL9	C47-C48-C49	-2.61	118.83	127.75
23	a	407[A]	CLA	O2A-CGA-CBA	2.61	120.10	111.91
23	B	608	CLA	C2A-C1A-CHA	-2.61	119.30	123.86
24	A	353[B]	PHO	O2D-CGD-O1D	-2.61	118.74	123.84
37	d	408[A]	LHG	O8-C23-C24	2.61	120.09	111.91
23	b	612	CLA	CHC-C1C-C2C	-2.61	119.48	126.73
23	B	608	CLA	CMA-C3A-C2A	-2.61	103.31	113.83
37	l	101[B]	LHG	O8-C23-C24	2.61	120.08	111.91
23	b	606	CLA	C4C-C3C-C2C	-2.61	103.10	106.90
23	C	503	CLA	C2A-C1A-CHA	-2.60	119.31	123.86
23	C	511	CLA	O2A-CGA-O1A	-2.60	117.02	123.59
23	c	505	CLA	CBC-CAC-C3C	-2.60	105.25	112.43
23	B	603	CLA	CAC-C3C-C4C	2.60	128.19	124.81
23	A	405[A]	CLA	CMA-C3A-C2A	-2.60	103.33	113.83
23	C	505	CLA	CHC-C1C-C2C	-2.60	119.50	126.73
29	a	416[A]	PL9	C10-C9-C8	-2.60	117.01	123.68
23	B	602	CLA	C1-C2-C3	-2.60	121.55	126.04
23	C	506	CLA	CBC-CAC-C3C	-2.60	105.27	112.43
23	c	513	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	a	407[A]	CLA	CMC-C2C-C1C	2.60	128.99	125.04
23	b	615	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
24	A	407[A]	PHO	O2A-CGA-CBA	2.59	120.05	111.91
23	b	611	CLA	C2A-C1A-CHA	-2.59	119.32	123.86
27	b	901	GOL	C3-C2-C1	-2.59	101.62	111.70
24	a	408[B]	PHO	O2A-CGA-O1A	-2.59	117.05	123.59
23	B	601	CLA	C1-O2A-CGA	2.59	123.25	116.44
33	c	520	LMG	C8-O7-C10	-2.59	111.41	117.79
25	a	410	BCR	C29-C30-C25	2.59	114.47	110.48
32	M	103	LMT	C1'-O5'-C5'	-2.59	108.61	113.69
33	m	101	LMG	C8-O7-C10	-2.59	111.42	117.79
23	B	606	CLA	C4C-C3C-C2C	-2.59	103.12	106.90
23	a	406[A]	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
23	B	610	CLA	CHD-C4C-NC	2.59	128.28	124.20
23	B	601	CLA	CMB-C2B-C1B	2.59	129.31	125.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	614	CLA	O2A-CGA-CBA	2.59	120.03	111.91
23	b	608	CLA	CAC-C3C-C4C	2.59	128.17	124.81
25	k	101	BCR	C39-C30-C25	-2.59	106.11	110.30
32	t	101	LMT	C3'-C4'-C5'	-2.58	105.00	110.93
25	K	102	BCR	C29-C30-C25	2.58	114.46	110.48
23	B	607	CLA	CMB-C2B-C1B	2.58	129.30	125.37
25	K	102	BCR	C24-C23-C22	-2.58	122.33	126.23
25	K	102	BCR	C11-C10-C9	-2.58	123.63	127.31
23	C	511	CLA	C4C-C3C-C2C	-2.58	103.14	106.90
26	F	101	SQD	O5-C1-O6	2.58	116.08	109.97
40	v	202	HEC	C4B-NB-C1B	2.58	107.74	105.07
23	C	502	CLA	O2A-CGA-O1A	-2.58	117.08	123.59
23	B	609	CLA	CHD-C4C-NC	2.58	128.27	124.20
24	a	353[B]	PHO	O2D-CGD-O1D	-2.58	118.80	123.84
23	A	406[A]	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
23	a	407[B]	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
23	B	609	CLA	O2A-CGA-CBA	2.58	120.00	111.91
23	b	615	CLA	CHC-C1C-C2C	-2.58	119.57	126.73
23	A	405[A]	CLA	C2A-C1A-CHA	-2.58	119.35	123.86
23	c	504	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
23	b	614	CLA	CAC-C3C-C4C	2.58	128.15	124.81
23	A	404[B]	CLA	CAA-C2A-C1A	-2.58	103.53	111.97
23	a	406[B]	CLA	CMB-C2B-C1B	2.58	129.29	125.37
23	D	405[B]	CLA	C2A-C1A-CHA	-2.57	119.36	123.86
25	t	103	BCR	C19-C18-C17	-2.57	114.99	118.94
29	A	414[B]	PL9	C40-C39-C41	2.57	119.60	115.27
23	c	512	CLA	CMC-C2C-C1C	2.57	128.96	125.04
23	D	405[A]	CLA	O2A-CGA-O1A	-2.57	117.10	123.59
26	f	102	SQD	O7-S-C6	2.57	110.00	106.94
25	B	619	BCR	C2-C1-C6	2.57	114.44	110.48
23	c	504	CLA	C1-C2-C3	-2.57	121.60	126.04
23	c	506	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
23	b	602	CLA	CAC-C3C-C4C	2.57	128.15	124.81
23	a	405[B]	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
24	A	407[A]	PHO	O1D-CGD-CBD	-2.57	120.46	124.74
23	B	602	CLA	CED-O2D-CGD	2.57	121.75	115.94
25	d	404	BCR	C33-C5-C6	-2.57	121.64	124.53
23	b	603	CLA	CHC-C1C-C2C	-2.57	119.59	126.73
26	A	410[A]	SQD	O48-C23-O10	-2.57	117.11	123.59
23	A	406[B]	CLA	CHC-C1C-C2C	-2.57	119.60	126.73
23	a	409	CLA	C3B-C4B-NB	2.57	112.90	110.52
23	B	606	CLA	CBC-CAC-C3C	-2.57	105.35	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	604	CLA	O2A-CGA-O1A	-2.57	117.11	123.59
24	A	407[A]	PHO	O2A-CGA-O1A	-2.57	117.12	123.59
24	A	407[B]	PHO	O1D-CGD-CBD	-2.57	120.47	124.74
33	C	501	LMG	C8-O7-C10	-2.57	111.47	117.79
23	C	502	CLA	C2A-C1A-CHA	-2.56	119.37	123.86
29	D	408[B]	PL9	C53-C6-C1	2.56	120.23	114.99
23	B	609	CLA	CAC-C3C-C4C	2.56	128.14	124.81
23	C	507	CLA	C4C-C3C-C2C	-2.56	103.16	106.90
38	E	103	HEM	C4A-NA-C1A	2.56	107.86	105.35
24	A	407[B]	PHO	O2A-CGA-CBA	2.56	119.95	111.91
23	C	508	CLA	C4-C3-C5	2.56	119.58	115.27
23	B	607	CLA	CHC-C1C-C2C	-2.56	119.62	126.73
29	A	414[A]	PL9	C10-C9-C8	-2.56	117.11	123.68
23	C	505	CLA	C4C-C3C-C2C	-2.56	103.17	106.90
23	b	606	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
23	B	602	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
38	E	103	HEM	CHA-C4D-ND	2.56	127.53	124.37
23	c	511	CLA	CAC-C3C-C4C	2.56	128.13	124.81
23	c	504	CLA	O2A-CGA-CBA	2.56	119.93	111.91
23	c	508	CLA	C3B-C4B-NB	2.55	112.89	110.52
23	c	514	CLA	C2A-C1A-CHA	-2.55	119.39	123.86
25	t	103	BCR	C28-C27-C26	-2.55	109.52	114.08
23	B	613	CLA	C4-C3-C2	-2.55	117.13	123.68
23	c	504	CLA	C2A-C1A-CHA	-2.55	119.40	123.86
23	c	503	CLA	O2A-CGA-CBA	2.55	119.91	111.91
23	B	615	CLA	C11-C10-C8	-2.55	107.68	115.92
23	B	616	CLA	C1-O2A-CGA	2.55	123.13	116.44
23	D	405[B]	CLA	CBC-CAC-C3C	-2.55	105.41	112.43
23	C	506	CLA	O2A-CGA-O1A	-2.55	117.17	123.59
23	B	615	CLA	CHD-C4C-NC	2.55	128.22	124.20
25	A	409	BCR	C15-C14-C13	-2.55	123.68	127.31
37	D	410[B]	LHG	O8-C23-C24	2.55	119.89	111.91
23	c	505	CLA	CHD-C4C-NC	2.55	128.21	124.20
23	A	405[A]	CLA	O2A-CGA-O1A	-2.54	117.17	123.59
23	d	402[A]	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
29	A	414[A]	PL9	C47-C48-C49	-2.54	119.05	127.75
25	B	617	BCR	C7-C8-C9	-2.54	122.39	126.23
23	B	607	CLA	C4C-C3C-C2C	-2.54	103.19	106.90
23	C	514	CLA	C4-C3-C5	2.54	119.55	115.27
29	a	416[B]	PL9	C40-C39-C41	2.54	119.55	115.27
29	d	405[B]	PL9	C53-C6-C1	2.54	120.19	114.99
25	t	103	BCR	C35-C13-C12	2.54	122.08	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	512	CLA	CMC-C2C-C1C	2.54	128.91	125.04
23	C	511	CLA	O2A-CGA-CBA	2.54	119.88	111.91
23	a	406[B]	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
23	b	609	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
23	c	514	CLA	O2A-CGA-O1A	-2.54	117.18	123.59
25	Y	101	BCR	C37-C22-C23	2.54	122.08	118.08
23	b	613	CLA	CED-O2D-CGD	2.54	121.68	115.94
23	b	615	CLA	C6-C7-C8	-2.54	107.72	115.92
23	B	605	CLA	CAC-C3C-C4C	2.54	128.10	124.81
25	c	515	BCR	C16-C17-C18	-2.54	123.69	127.31
23	c	506	CLA	O2A-CGA-CBA	2.54	119.87	111.91
32	I	101	LMT	O5'-C5'-C6'	2.54	112.74	106.44
23	C	509	CLA	C4-C3-C5	2.54	119.54	115.27
23	C	502	CLA	O2A-CGA-CBA	2.54	119.86	111.91
23	A	408	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	b	608	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
23	a	407[B]	CLA	O2A-CGA-CBA	2.53	119.86	111.91
29	D	408[B]	PL9	C45-C44-C46	2.53	119.53	115.27
23	b	611	CLA	O2A-CGA-O1A	-2.53	117.20	123.59
23	C	512	CLA	CMB-C2B-C1B	2.53	129.22	125.37
23	b	604	CLA	CHC-C1C-C2C	-2.53	119.70	126.73
25	Y	101	BCR	C34-C9-C8	2.53	122.06	118.08
23	b	615	CLA	C3B-C4B-NB	2.53	112.86	110.52
23	B	606	CLA	CHC-C1C-C2C	-2.53	119.70	126.73
23	D	406	CLA	CAC-C3C-C4C	2.53	128.09	124.81
23	B	606	CLA	C4-C3-C5	2.53	119.52	115.27
23	B	604	CLA	C11-C12-C13	-2.53	107.75	115.92
24	A	353[B]	PHO	CMB-C2B-C3B	2.53	129.41	124.68
23	C	511	CLA	CBC-CAC-C3C	-2.53	105.47	112.43
23	C	503	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	C	504	CLA	CHC-C1C-C2C	-2.52	119.72	126.73
23	A	408	CLA	CMA-C3A-C2A	-2.52	103.65	113.83
23	B	608	CLA	C11-C10-C8	-2.52	107.76	115.92
23	B	608	CLA	O2A-CGA-CBA	2.52	119.82	111.91
23	D	405[B]	CLA	CHD-C4C-NC	2.52	128.18	124.20
23	c	512	CLA	C2A-C1A-CHA	-2.52	119.45	123.86
23	C	513	CLA	CBA-CAA-C2A	-2.52	106.42	113.86
34	c	522	HTG	O5-C1-C2	2.52	113.48	110.31
23	B	616	CLA	CHC-C1C-C2C	-2.52	119.73	126.73
23	C	512	CLA	O2A-CGA-CBA	2.52	119.81	111.91
29	A	414[B]	PL9	C42-C43-C44	-2.52	121.60	127.66
23	b	605	CLA	C2A-C1A-CHA	-2.52	119.46	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	605	CLA	CBC-CAC-C3C	-2.52	105.49	112.43
23	C	512	CLA	C1-O2A-CGA	2.52	123.05	116.44
23	b	609	CLA	CMA-C3A-C4A	-2.52	105.01	111.77
23	C	504	CLA	C1-C2-C3	-2.51	121.69	126.04
23	C	514	CLA	O2A-CGA-CBA	2.51	119.80	111.91
25	B	619	BCR	C21-C20-C19	-2.51	115.38	123.22
23	a	406[A]	CLA	CAA-CBA-CGA	2.51	120.59	113.25
23	d	403	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
23	c	504	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	d	402[A]	CLA	CMC-C2C-C1C	2.51	128.86	125.04
23	c	514	CLA	CHB-C1B-NB	-2.51	121.60	124.26
25	b	618	BCR	C8-C7-C6	-2.51	120.16	127.20
25	D	407	BCR	C37-C22-C23	2.51	122.03	118.08
23	B	605	CLA	CHC-C1C-C2C	-2.51	119.76	126.73
23	C	514	CLA	CAA-C2A-C3A	-2.51	105.91	112.78
23	A	406[A]	CLA	C2A-C1A-CHA	-2.51	119.47	123.86
23	c	502	CLA	CHD-C4C-NC	2.51	128.16	124.20
23	b	602	CLA	C11-C10-C8	-2.51	107.81	115.92
23	c	514	CLA	CHC-C1C-C2C	-2.51	119.77	126.73
34	b	622	HTG	O2-C2-C3	-2.51	104.55	110.35
23	a	405[A]	CLA	CHD-C4C-NC	2.51	128.15	124.20
23	c	513	CLA	O2A-CGA-O1A	-2.51	117.27	123.59
23	B	601	CLA	C3B-C4B-NB	2.50	112.84	110.52
29	a	416[B]	PL9	C45-C44-C46	2.50	119.48	115.27
37	D	409[B]	LHG	O7-C7-O9	-2.50	117.65	123.70
32	I	101	LMT	O1'-C1'-C2'	2.50	112.21	108.30
29	D	408[A]	PL9	C42-C41-C39	-2.50	104.75	112.98
23	d	403	CLA	O2A-CGA-CBA	2.50	119.76	111.91
25	Y	101	BCR	C15-C16-C17	-2.50	118.35	123.47
25	Y	101	BCR	C10-C11-C12	-2.50	115.42	123.22
23	a	406[B]	CLA	CMC-C2C-C1C	2.50	128.84	125.04
35	c	518[A]	DGD	O1G-C1A-C2A	2.50	119.74	111.91
23	B	615	CLA	C2A-C1A-CHA	-2.50	119.50	123.86
23	D	405[B]	CLA	C4-C3-C5	2.49	119.47	115.27
23	a	405[A]	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
23	B	606	CLA	C2A-C1A-CHA	-2.49	119.50	123.86
23	b	605	CLA	CED-O2D-CGD	2.49	121.58	115.94
23	b	610	CLA	CMB-C2B-C1B	2.49	129.16	125.37
23	c	504	CLA	C4-C3-C5	2.49	119.46	115.27
23	C	506	CLA	CHD-C4C-NC	2.49	128.13	124.20
25	h	101	BCR	C16-C17-C18	-2.49	123.75	127.31
23	C	504	CLA	CAC-C3C-C4C	2.49	128.04	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	t	103	BCR	C11-C10-C9	-2.49	123.76	127.31
24	A	353[B]	PHO	O2A-CGA-CBA	2.49	119.72	111.91
29	d	405[B]	PL9	C35-C34-C36	2.49	119.46	115.27
35	H	102	DGD	O1G-C1A-C2A	2.49	119.72	111.91
23	A	406[B]	CLA	C4-C3-C5	2.49	119.46	115.27
23	c	509	CLA	C4-C3-C5	2.49	119.46	115.27
23	b	610	CLA	O1D-CGD-CBD	-2.49	119.40	124.48
23	a	406[B]	CLA	C2A-C1A-CHA	-2.49	119.51	123.86
23	b	608	CLA	C11-C12-C13	-2.49	107.89	115.92
26	a	411[A]	SQD	O8-S-C6	2.49	109.70	105.74
37	d	407[B]	LHG	C6-C5-C4	-2.48	105.91	111.79
23	B	604	CLA	CHB-C1B-NB	-2.48	121.63	124.26
23	a	406[A]	CLA	CBC-CAC-C3C	-2.48	105.59	112.43
23	C	503	CLA	O2A-CGA-CBA	2.48	119.70	111.91
23	C	507	CLA	O2A-CGA-O1A	-2.48	117.33	123.59
25	B	619	BCR	C7-C8-C9	-2.48	122.48	126.23
32	a	414	LMT	O5'-C5'-C6'	2.48	112.60	106.44
35	c	518[B]	DGD	O1G-C1A-C2A	2.48	119.69	111.91
35	c	517[B]	DGD	C3G-C2G-C1G	-2.48	105.93	111.79
23	B	602	CLA	CHC-C1C-C2C	-2.48	119.85	126.73
25	c	515	BCR	C20-C21-C22	-2.48	123.78	127.31
23	B	604	CLA	C6-C7-C8	-2.48	107.92	115.92
23	b	607	CLA	C2A-C1A-CHA	-2.48	119.53	123.86
25	h	101	BCR	C16-C15-C14	-2.48	118.40	123.47
29	D	408[A]	PL9	C20-C19-C21	2.47	119.43	115.27
26	f	102	SQD	O47-C7-O49	-2.47	117.72	123.70
34	B	626	HTG	C3-C4-C5	2.47	114.65	110.24
23	A	404[B]	CLA	CHD-C4C-NC	2.47	128.10	124.20
35	c	517[A]	DGD	C2G-O2G-C1B	-2.47	111.70	117.79
23	c	507	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	B	610	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	B	612	CLA	C2A-C1A-CHA	-2.47	119.54	123.86
23	c	511	CLA	O2A-CGA-CBA	2.47	119.65	111.91
23	c	507	CLA	CHD-C4C-NC	2.47	128.09	124.20
23	C	503	CLA	CMB-C2B-C1B	2.47	129.13	125.37
32	t	101	LMT	O5'-C5'-C4'	2.47	114.95	109.75
35	c	519	DGD	O3G-C1D-C2D	-2.46	104.46	108.30
32	a	414	LMT	O5B-C5B-C4B	2.46	114.17	109.69
23	C	505	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
23	a	407[B]	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
24	A	407[A]	PHO	CMB-C2B-C3B	2.46	129.29	124.68
23	A	404[B]	CLA	C4-C3-C5	2.46	119.41	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	D	415	LMG	O7-C10-C11	2.46	116.81	111.50
25	c	515	BCR	C31-C1-C6	-2.46	106.31	110.30
23	c	508	CLA	CHC-C1C-C2C	-2.46	119.89	126.73
23	C	508	CLA	O2A-CGA-CBA	2.46	119.63	111.91
26	A	410[B]	SQD	O8-S-C6	2.46	109.66	105.74
38	E	103	HEM	O2A-CGA-CBA	2.46	121.93	114.03
33	C	520	LMG	O8-C28-O10	-2.46	117.39	123.59
26	a	411[B]	SQD	O48-C23-C24	2.46	119.62	111.91
25	c	515	BCR	C36-C18-C17	-2.46	119.48	122.92
29	d	405[B]	PL9	C12-C13-C14	-2.46	121.75	127.66
23	c	510	CLA	CMB-C2B-C1B	2.46	129.11	125.37
24	a	353[B]	PHO	CBA-CAA-C2A	-2.46	106.64	113.81
23	b	609	CLA	CMB-C2B-C1B	2.45	129.11	125.37
32	I	101	LMT	O5'-C5'-C4'	2.45	114.92	109.75
23	c	502	CLA	CBC-CAC-C3C	-2.45	105.67	112.43
23	B	612	CLA	CHC-C1C-C2C	-2.45	119.92	126.73
23	C	513	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	d	404	BCR	C36-C18-C17	-2.45	119.49	122.92
33	z	101	LMG	C7-O1-C1	-2.45	108.95	113.74
23	c	506	CLA	C3B-C4B-NB	2.45	112.79	110.52
23	A	404[A]	CLA	CAA-CBA-CGA	-2.45	106.09	113.25
25	b	618	BCR	C29-C30-C25	2.45	114.25	110.48
23	b	606	CLA	C1-O2A-CGA	2.45	122.87	116.44
23	b	609	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	d	405[B]	PL9	C17-C18-C19	-2.45	121.77	127.66
29	D	408[A]	PL9	C40-C39-C41	2.45	119.39	115.27
23	C	513	CLA	CMB-C2B-C1B	2.45	129.09	125.37
23	C	514	CLA	CHC-C1C-C2C	-2.44	119.94	126.73
23	b	614	CLA	C2A-C1A-CHA	-2.44	119.59	123.86
25	K	102	BCR	C10-C11-C12	-2.44	115.59	123.22
23	d	403	CLA	C1-O2A-CGA	2.44	122.85	116.44
23	b	610	CLA	CHC-C1C-C2C	-2.44	119.95	126.73
25	Y	101	BCR	C38-C26-C25	-2.44	121.79	124.53
25	C	516	BCR	C11-C10-C9	-2.44	123.83	127.31
23	c	509	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	T	101	BCR	C21-C20-C19	-2.44	115.61	123.22
23	C	509	CLA	CMB-C2B-C1B	2.44	129.08	125.37
23	A	408	CLA	CAC-C3C-C4C	2.44	127.97	124.81
25	d	404	BCR	C21-C20-C19	-2.44	115.61	123.22
26	f	102	SQD	O5-C1-C2	2.44	115.50	110.35
23	B	615	CLA	C6-C7-C8	-2.43	108.05	115.92
23	c	507	CLA	O2A-CGA-O1A	-2.43	117.45	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	y	101	BCR	C21-C20-C19	-2.43	115.62	123.22
23	b	604	CLA	C4C-C3C-C2C	-2.43	103.35	106.90
23	C	508	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
23	c	503	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
23	c	504	CLA	CHC-C1C-C2C	-2.43	119.98	126.73
29	D	408[B]	PL9	C37-C38-C39	-2.43	121.81	127.66
23	c	510	CLA	C2A-C1A-CHA	-2.43	119.61	123.86
23	c	511	CLA	O2A-CGA-O1A	-2.43	117.46	123.59
23	C	505	CLA	CHD-C4C-NC	2.43	128.03	124.20
23	B	609	CLA	O2A-CGA-O1A	-2.43	117.47	123.59
23	C	507	CLA	CHD-C4C-NC	2.43	128.03	124.20
23	c	510	CLA	C4-C3-C2	-2.43	117.45	123.68
25	b	618	BCR	C37-C22-C23	2.42	121.90	118.08
23	A	405[A]	CLA	CAA-CBA-CGA	2.42	120.34	113.25
25	k	101	BCR	C24-C23-C22	-2.42	122.57	126.23
35	C	518[B]	DGD	O1G-C1A-O1A	-2.42	117.47	123.59
23	B	613	CLA	CMC-C2C-C1C	2.42	128.73	125.04
35	H	102	DGD	O2G-C1B-C2B	2.42	116.72	111.50
25	c	516	BCR	C32-C1-C6	-2.42	106.37	110.30
23	D	406	CLA	CBC-CAC-C3C	-2.42	105.75	112.43
23	C	506	CLA	O2A-CGA-CBA	2.42	119.50	111.91
25	a	410	BCR	C7-C8-C9	-2.42	122.58	126.23
23	C	512	CLA	CHD-C4C-NC	2.42	128.02	124.20
23	b	615	CLA	O2A-CGA-O1A	-2.42	117.49	123.59
26	a	413	SQD	C1-O5-C5	2.42	118.44	113.69
23	A	406[A]	CLA	C1-C2-C3	-2.42	121.86	126.04
38	e	87	HEM	CMD-C2D-C1D	2.42	128.72	125.04
25	c	516	BCR	C16-C17-C18	-2.42	123.86	127.31
23	b	606	CLA	CMC-C2C-C1C	2.42	128.72	125.04
23	A	405[B]	CLA	CMC-C2C-C1C	2.42	128.72	125.04
29	D	408[A]	PL9	C7-C8-C9	-2.41	122.77	126.79
23	c	505	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
33	B	621	LMG	O8-C28-O10	-2.41	117.50	123.59
23	C	511	CLA	C4-C3-C2	-2.41	117.48	123.68
23	C	514	CLA	CMB-C2B-C1B	2.41	129.05	125.37
23	B	601	CLA	CHC-C1C-C2C	-2.41	120.02	126.73
25	t	103	BCR	C7-C6-C5	-2.41	115.62	121.46
37	D	409[A]	LHG	O7-C7-O9	-2.41	117.87	123.70
23	c	508	CLA	CAC-C3C-C4C	2.41	127.94	124.81
23	C	514	CLA	CHB-C1B-NB	-2.41	121.71	124.26
23	c	507	CLA	CMB-C2B-C1B	2.41	129.04	125.37
24	A	407[A]	PHO	CMA-C3A-C4A	-2.41	109.11	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	C	505	CLA	CHB-C1B-NB	-2.41	121.71	124.26
23	B	614	CLA	OBD-CAD-C3D	-2.41	122.73	128.52
23	b	608	CLA	C2A-C1A-CHA	-2.41	119.65	123.86
23	C	508	CLA	CHD-C4C-NC	2.41	128.00	124.20
35	c	517[B]	DGD	O6D-C1D-O3G	-2.40	104.29	109.97
23	B	616	CLA	CHD-C4C-NC	2.40	127.99	124.20
37	l	101[A]	LHG	O8-C23-O10	-2.40	117.53	123.59
25	H	101	BCR	C16-C15-C14	-2.40	118.56	123.47
24	a	408[B]	PHO	O2D-CGD-O1D	-2.40	119.15	123.84
29	d	405[B]	PL9	C27-C28-C29	-2.40	121.88	127.66
37	d	408[A]	LHG	O8-C23-O10	-2.40	117.54	123.59
29	d	405[A]	PL9	C17-C18-C19	-2.40	121.89	127.66
23	c	512	CLA	CBC-CAC-C3C	-2.40	105.82	112.43
26	a	413	SQD	O7-S-C6	2.40	109.79	106.94
23	b	606	CLA	CBC-CAC-C3C	-2.40	105.83	112.43
23	c	512	CLA	CMA-C3A-C4A	2.40	118.21	111.77
33	d	412	LMG	O7-C10-O9	-2.39	117.92	123.70
23	c	502	CLA	O2A-CGA-CBA	2.39	119.42	111.91
25	t	103	BCR	C37-C22-C23	2.39	121.85	118.08
29	d	405[A]	PL9	C7-C8-C9	-2.39	122.81	126.79
25	d	404	BCR	C28-C27-C26	-2.39	109.81	114.08
23	c	506	CLA	C4-C3-C5	2.39	119.29	115.27
26	b	620	SQD	C44-O6-C1	-2.39	109.07	113.74
23	c	512	CLA	O2A-CGA-O1A	-2.39	117.57	123.59
24	a	353[B]	PHO	C1A-C2A-C3A	-2.39	100.57	102.84
23	B	603	CLA	CMA-C3A-C2A	-2.39	104.20	113.83
26	f	102	SQD	C4-C3-C2	-2.39	106.66	110.82
23	a	409	CLA	CBC-CAC-C3C	-2.39	105.86	112.43
38	E	103	HEM	C4D-ND-C1D	2.38	107.53	105.07
25	y	101	BCR	C1-C6-C7	2.38	122.52	115.78
23	D	405[A]	CLA	CMC-C2C-C1C	2.38	128.67	125.04
23	b	607	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
23	d	402[A]	CLA	CMB-C2B-C1B	2.38	129.00	125.37
23	a	405[A]	CLA	CMA-C3A-C2A	-2.38	104.22	113.83
23	c	505	CLA	O2A-CGA-CBA	2.38	119.38	111.91
29	a	416[A]	PL9	C20-C19-C21	2.38	119.28	115.27
37	D	410[B]	LHG	O8-C23-O10	-2.38	117.58	123.59
23	b	603	CLA	CMC-C2C-C1C	2.38	128.66	125.04
23	B	613	CLA	C2A-C1A-CHA	-2.38	119.70	123.86
25	Y	101	BCR	C1-C6-C7	2.38	122.51	115.78
32	M	103	LMT	C3'-C4'-C5'	-2.38	105.47	110.93
23	b	607	CLA	C1-O2A-CGA	2.38	122.68	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407[B]	PHO	O2D-CGD-O1D	-2.38	119.19	123.84
29	D	408[A]	PL9	C36-C37-C38	-2.38	104.07	111.88
23	D	405[B]	CLA	CMB-C2B-C1B	2.38	128.99	125.37
32	b	621	LMT	C2'-C3'-C4'	2.38	115.11	109.68
32	E	102	LMT	C1'-O5'-C5'	-2.38	109.03	113.69
40	v	202	HEC	CHA-C4D-ND	2.38	127.00	124.42
23	C	502	CLA	C1-O2A-CGA	2.37	122.67	116.44
25	c	516	BCR	C7-C8-C9	-2.37	122.65	126.23
35	C	517[B]	DGD	O1G-C1A-O1A	-2.37	117.60	123.59
23	C	502	CLA	C11-C12-C13	-2.37	108.25	115.92
23	b	604	CLA	C4-C3-C5	2.37	119.26	115.27
23	C	513	CLA	C2A-C1A-CHA	-2.37	119.71	123.86
23	A	406[A]	CLA	CAC-C3C-C4C	2.37	127.89	124.81
23	c	513	CLA	C3B-C4B-NB	2.37	112.72	110.52
33	d	412	LMG	O8-C28-O10	-2.37	117.61	123.59
23	c	508	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
23	c	514	CLA	C1-C2-C3	-2.37	121.95	126.04
23	b	613	CLA	CMC-C2C-C1C	2.37	128.65	125.04
33	z	101	LMG	C8-O7-C10	-2.37	111.96	117.79
25	d	404	BCR	C40-C30-C39	2.37	115.79	108.53
23	b	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
23	B	615	CLA	C1-O2A-CGA	2.37	122.65	116.44
24	A	353[A]	PHO	C4D-CHA-CBD	2.37	109.59	108.52
23	b	615	CLA	O2A-CGA-CBA	2.37	119.33	111.91
23	c	506	CLA	CHD-C4C-NC	2.36	127.93	124.20
23	b	607	CLA	C1-C2-C3	-2.36	121.95	126.04
32	m	103	LMT	C1'-O5'-C5'	-2.36	109.05	113.69
24	a	353[A]	PHO	C1A-C2A-C3A	-2.36	100.59	102.84
23	b	606	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
23	B	609	CLA	C16-C15-C13	-2.36	108.29	115.92
25	h	101	BCR	C20-C21-C22	-2.36	123.94	127.31
35	c	517[A]	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
23	c	502	CLA	C1-O2A-CGA	2.36	122.63	116.44
23	C	513	CLA	CMA-C3A-C4A	-2.36	105.44	111.77
29	d	405[A]	PL9	C12-C13-C14	-2.36	121.99	127.66
23	A	404[B]	CLA	CMA-C3A-C2A	-2.36	104.33	113.83
23	c	505	CLA	C2A-C1A-CHA	-2.35	119.74	123.86
24	a	353[B]	PHO	C4A-C3A-C2A	-2.35	100.60	102.84
23	B	616	CLA	C2A-C1A-CHA	-2.35	119.75	123.86
23	a	407[A]	CLA	C1-C2-C3	-2.35	121.98	126.04
29	A	414[B]	PL9	C10-C9-C8	-2.35	117.65	123.68
23	c	507	CLA	CAA-C2A-C3A	-2.35	106.34	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	A	414[A]	PL9	C45-C44-C46	2.35	119.22	115.27
23	d	403	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	a	416[B]	PL9	C47-C48-C49	-2.35	119.73	127.75
23	C	511	CLA	CAC-C3C-C4C	2.35	127.86	124.81
23	B	611	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
23	b	608	CLA	C4-C3-C5	2.35	119.22	115.27
33	C	521	LMG	C9-C8-C7	-2.34	106.25	111.79
23	c	511	CLA	C4C-C3C-C2C	-2.34	103.48	106.90
23	A	406[A]	CLA	CMA-C3A-C2A	-2.34	104.38	113.83
23	C	510	CLA	C4-C3-C5	2.34	119.21	115.27
25	b	617	BCR	C29-C30-C25	2.34	114.09	110.48
26	b	620	SQD	O48-C23-C24	2.34	119.26	111.91
24	A	407[B]	PHO	CMB-C2B-C3B	2.34	129.06	124.68
23	c	507	CLA	CMC-C2C-C1C	2.34	128.60	125.04
23	A	405[B]	CLA	OBD-CAD-C3D	-2.34	122.89	128.52
25	B	617	BCR	C11-C10-C9	-2.34	123.97	127.31
23	C	507	CLA	CMB-C2B-C1B	2.34	128.93	125.37
23	A	405[B]	CLA	CHB-C1B-NB	-2.34	121.78	124.26
29	A	414[A]	PL9	C42-C43-C44	-2.34	122.03	127.66
25	c	515	BCR	C28-C27-C26	-2.34	109.90	114.08
40	V	202	HEC	CHA-C4D-ND	2.33	126.95	124.42
37	d	407[A]	LHG	C6-C5-C4	-2.33	106.27	111.79
29	d	405[A]	PL9	C20-C19-C21	2.33	119.20	115.27
23	b	604	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
23	B	611	CLA	OBD-CAD-C3D	-2.33	122.90	128.52
23	B	608	CLA	CMB-C2B-C1B	2.33	128.92	125.37
25	c	516	BCR	C29-C30-C25	2.33	114.07	110.48
23	d	403	CLA	CHB-C4A-NA	2.33	127.74	124.51
23	B	604	CLA	C6-C5-C3	-2.33	107.34	113.45
33	d	412	LMG	O8-C28-C29	2.33	119.23	111.91
40	v	202	HEC	CMC-C2C-C1C	-2.33	121.82	125.37
23	c	508	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
33	C	521	LMG	O1-C1-C2	2.33	111.94	108.30
25	K	102	BCR	C33-C5-C6	-2.33	121.91	124.53
23	D	405[A]	CLA	CMB-C2B-C1B	2.33	128.92	125.37
33	c	521	LMG	O8-C28-O10	-2.33	117.71	123.59
24	A	407[B]	PHO	O2A-CGA-O1A	-2.33	117.72	123.59
23	B	604	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
23	b	612	CLA	OBD-CAD-C3D	-2.33	122.92	128.52
23	b	615	CLA	C1-C2-C3	-2.32	122.02	126.04
26	a	413	SQD	C3-C4-C5	2.32	114.38	110.24
23	a	407[B]	CLA	C2A-C1A-CHA	-2.32	119.80	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	405[B]	PL9	C51-C49-C50	2.32	119.73	114.60
23	C	508	CLA	CBB-CAB-C3B	-2.32	116.06	127.62
23	c	512	CLA	C1-C2-C3	-2.32	122.03	126.04
33	C	501	LMG	C9-C8-C7	-2.32	106.30	111.79
24	a	408[B]	PHO	CMB-C2B-C3B	2.32	129.02	124.68
23	B	605	CLA	C3B-C4B-NB	2.32	112.67	110.52
23	b	601	CLA	O2A-CGA-CBA	2.32	119.19	111.91
25	a	410	BCR	C24-C23-C22	-2.32	122.73	126.23
25	D	407	BCR	C11-C10-C9	-2.32	124.00	127.31
23	B	602	CLA	CHB-C4A-NA	2.32	127.72	124.51
35	C	518[B]	DGD	O1G-C1A-C2A	2.32	119.18	111.91
24	a	353[B]	PHO	O1D-CGD-CBD	-2.32	120.88	124.74
23	b	616	CLA	C2A-C1A-CHA	-2.32	119.81	123.86
25	T	101	BCR	C15-C14-C13	2.32	130.62	127.31
23	C	507	CLA	O2A-CGA-CBA	2.31	119.17	111.91
23	B	605	CLA	C2A-C1A-CHA	-2.31	119.81	123.86
40	V	202	HEC	CMD-C2D-C1D	2.31	128.56	125.04
23	A	406[B]	CLA	CHC-C4B-NB	-2.31	121.81	124.26
23	a	406[A]	CLA	CMC-C2C-C1C	2.31	128.56	125.04
23	a	406[B]	CLA	C4-C3-C5	2.31	119.16	115.27
26	a	413	SQD	O5-C5-C4	2.31	113.89	109.69
23	B	611	CLA	CAC-C3C-C2C	2.31	131.48	127.53
23	B	604	CLA	CMC-C2C-C1C	2.31	128.56	125.04
25	A	409	BCR	C37-C22-C21	-2.31	119.69	122.92
25	b	618	BCR	C3-C4-C5	-2.31	109.95	114.08
23	b	608	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	b	611	CLA	O2A-CGA-CBA	2.31	119.15	111.91
23	C	507	CLA	CGD-CBD-CAD	-2.31	103.26	110.73
35	C	518[A]	DGD	C2G-O2G-C1B	-2.31	112.11	117.79
25	T	101	BCR	C33-C5-C6	-2.30	121.94	124.53
23	B	602	CLA	C11-C10-C8	-2.30	108.47	115.92
23	a	405[B]	CLA	C1-C2-C3	-2.30	122.06	126.04
35	C	517[A]	DGD	O6E-C5E-C4E	2.30	113.88	109.69
25	y	101	BCR	C10-C11-C12	-2.30	116.03	123.22
26	f	102	SQD	C44-O6-C1	-2.30	109.24	113.74
23	A	406[B]	CLA	C1-C2-C3	-2.30	122.06	126.04
25	Y	101	BCR	C40-C30-C25	-2.30	106.57	110.30
23	C	504	CLA	C2A-C1A-CHA	-2.30	119.84	123.86
23	b	602	CLA	CMA-C3A-C4A	-2.30	105.60	111.77
23	b	615	CLA	CMC-C2C-C1C	2.30	128.54	125.04
26	a	411[A]	SQD	O48-C23-C24	2.30	119.11	111.91
23	c	511	CLA	C11-C10-C8	-2.30	108.50	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	A	410[B]	SQD	O7-S-C6	2.29	109.67	106.94
23	c	514	CLA	C4-C3-C5	2.29	119.13	115.27
23	C	513	CLA	C4-C3-C2	-2.29	117.80	123.68
29	D	408[B]	PL9	C22-C23-C24	-2.29	122.15	127.66
23	A	404[B]	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
23	C	511	CLA	C2A-C1A-CHA	-2.29	119.86	123.86
32	D	404	LMT	C1B-C2B-C3B	2.29	114.76	110.00
23	c	509	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
25	d	404	BCR	C37-C22-C23	2.29	121.68	118.08
35	C	517[A]	DGD	C3G-C2G-C1G	-2.29	106.38	111.79
23	b	613	CLA	OBD-CAD-C3D	-2.29	123.02	128.52
33	m	101	LMG	O8-C28-O10	-2.28	117.83	123.59
32	a	420	LMT	O5B-C5B-C4B	2.28	113.84	109.69
23	B	614	CLA	C4-C3-C5	2.28	119.11	115.27
23	c	508	CLA	C4C-C3C-C2C	-2.28	103.58	106.90
29	d	405[A]	PL9	C51-C49-C50	2.28	119.63	114.60
23	d	402[B]	CLA	CAA-C2A-C3A	-2.28	106.55	112.78
25	T	101	BCR	C2-C1-C6	2.27	113.98	110.48
23	d	402[B]	CLA	CHD-C4C-NC	2.27	127.79	124.20
35	c	519	DGD	O3G-C3G-C2G	-2.27	105.41	110.90
23	b	608	CLA	C4C-C3C-C2C	-2.27	103.58	106.90
23	C	504	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
23	b	608	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
29	A	414[B]	PL9	C25-C24-C26	2.27	119.09	115.27
33	C	520	LMG	C8-O7-C10	-2.27	112.20	117.79
24	a	353[A]	PHO	O2A-CGA-CBA	2.27	119.03	111.91
29	A	414[A]	PL9	C35-C34-C33	-2.27	117.86	123.68
40	v	202	HEC	C1D-C2D-C3D	-2.27	104.57	106.96
23	a	405[A]	CLA	C7-C6-C5	-2.27	107.20	113.36
25	K	102	BCR	C36-C18-C19	2.27	121.65	118.08
25	A	409	BCR	C31-C1-C6	-2.27	106.62	110.30
25	k	101	BCR	C15-C14-C13	-2.27	124.08	127.31
23	a	407[B]	CLA	CAC-C3C-C4C	2.27	127.75	124.81
23	b	615	CLA	C2A-C1A-CHA	-2.26	119.90	123.86
23	B	605	CLA	O2A-CGA-CBA	2.26	119.01	111.91
23	C	511	CLA	CMC-C2C-C1C	2.26	128.49	125.04
23	b	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
23	b	607	CLA	CAC-C3C-C4C	2.26	127.75	124.81
23	c	511	CLA	C4-C3-C2	-2.26	117.88	123.68
23	c	508	CLA	C2A-C1A-CHA	-2.26	119.91	123.86
35	C	518[A]	DGD	O2G-C1B-O1B	-2.26	118.24	123.70
23	b	603	CLA	C7-C6-C5	-2.26	107.22	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	T	101	BCR	C3-C4-C5	-2.26	110.04	114.08
25	c	515	BCR	C38-C26-C25	-2.26	121.99	124.53
23	c	503	CLA	C4C-C3C-C2C	-2.26	103.61	106.90
23	b	606	CLA	C4-C3-C2	-2.26	117.89	123.68
23	C	505	CLA	OBD-CAD-C3D	-2.26	123.09	128.52
23	A	404[B]	CLA	CHB-C1B-C2B	-2.26	120.86	127.24
26	A	412	SQD	C1-C2-C3	-2.26	105.30	110.00
25	D	407	BCR	C32-C1-C6	-2.26	106.64	110.30
23	b	613	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
26	F	101	SQD	O48-C23-O10	-2.25	117.91	123.59
23	b	605	CLA	CAC-C3C-C4C	2.25	127.73	124.81
25	B	617	BCR	C16-C17-C18	-2.25	124.09	127.31
24	A	407[A]	PHO	C4-C3-C5	2.25	119.06	115.27
23	D	405[A]	CLA	CED-O2D-CGD	2.25	121.03	115.94
24	a	408[A]	PHO	CMA-C3A-C4A	-2.25	109.45	114.38
23	a	406[A]	CLA	C2A-C1A-CHA	-2.25	119.92	123.86
23	c	514	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
23	b	603	CLA	C5-C3-C2	-2.25	116.56	121.12
23	C	510	CLA	CHD-C4C-NC	2.25	127.75	124.20
26	a	413	SQD	O8-S-C6	2.25	109.32	105.74
32	b	627	LMT	O1'-C1'-C2'	2.25	111.81	108.30
26	a	411[B]	SQD	C3-C4-C5	2.25	114.25	110.24
37	d	408[B]	LHG	O8-C23-O10	-2.25	117.92	123.59
23	C	502	CLA	OBD-CAD-C3D	-2.25	123.11	128.52
23	C	510	CLA	C11-C12-C13	-2.25	108.66	115.92
23	B	611	CLA	CAA-C2A-C3A	-2.25	106.63	112.78
23	c	511	CLA	C2A-C1A-CHA	-2.24	119.93	123.86
35	c	517[A]	DGD	O3G-C3G-C2G	-2.24	105.48	110.90
25	Y	101	BCR	C24-C23-C22	-2.24	122.84	126.23
23	B	601	CLA	CAC-C3C-C4C	2.24	127.72	124.81
29	d	405[A]	PL9	C47-C48-C49	-2.24	120.08	127.75
23	B	603	CLA	CBC-CAC-C3C	-2.24	106.25	112.43
26	B	620	SQD	C44-O6-C1	-2.24	109.36	113.74
23	A	408	CLA	CHB-C1B-NB	-2.24	121.88	124.26
23	a	406[B]	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	A	405[B]	CLA	C4C-C3C-C2C	-2.24	103.63	106.90
23	C	504	CLA	CHB-C1B-C2B	-2.24	120.91	127.24
24	A	353[B]	PHO	O1D-CGD-CBD	-2.24	121.01	124.74
23	B	614	CLA	CAA-C2A-C3A	-2.24	106.65	112.78
35	c	518[B]	DGD	C2G-O2G-C1B	-2.24	112.28	117.79
23	C	513	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
37	D	410[B]	LHG	C5-O7-C7	-2.24	112.29	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	a	416[B]	PL9	C51-C49-C50	2.24	119.54	114.60
25	C	516	BCR	C32-C1-C6	-2.24	106.67	110.30
23	C	513	CLA	CBC-CAC-C3C	-2.23	106.27	112.43
29	A	414[B]	PL9	C35-C34-C33	-2.23	117.95	123.68
29	a	416[A]	PL9	C35-C34-C33	-2.23	117.95	123.68
23	a	405[B]	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
23	a	405[B]	CLA	C7-C6-C5	-2.23	107.30	113.36
23	B	607	CLA	CHD-C4C-NC	2.23	127.72	124.20
25	b	619	BCR	C7-C6-C5	2.23	126.86	121.46
23	b	606	CLA	CHB-C1B-C2B	-2.23	120.94	127.24
40	V	202	HEC	C3B-C4B-NB	-2.23	107.69	110.17
23	b	606	CLA	C2A-C1A-CHA	-2.23	119.96	123.86
29	A	414[A]	PL9	C25-C24-C26	2.23	119.02	115.27
23	B	611	CLA	C7-C6-C5	-2.23	107.31	113.36
23	b	601	CLA	CBC-CAC-C3C	-2.23	106.30	112.43
23	c	511	CLA	CED-O2D-CGD	2.23	120.97	115.94
25	b	619	BCR	C15-C14-C13	-2.23	124.13	127.31
23	B	606	CLA	CHB-C1B-C2B	-2.23	120.95	127.24
29	A	414[A]	PL9	C12-C13-C14	-2.23	122.30	127.66
23	B	607	CLA	C1-C2-C3	-2.22	122.19	126.04
23	b	610	CLA	C3B-C4B-NB	2.22	112.58	110.52
24	A	353[A]	PHO	CED-O2D-CGD	2.22	120.97	115.94
29	A	414[A]	PL9	C53-C6-C1	2.22	119.54	114.99
26	A	410[A]	SQD	O9-S-O7	-2.22	106.25	113.95
23	a	405[B]	CLA	CMB-C2B-C1B	2.22	128.76	125.37
23	A	404[A]	CLA	CHD-C4C-NC	2.22	127.71	124.20
23	B	610	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
24	a	353[A]	PHO	O1D-CGD-CBD	-2.22	121.04	124.74
23	A	405[A]	CLA	C4C-C3C-C2C	-2.22	103.66	106.90
23	C	513	CLA	CHB-C1B-C2B	-2.22	120.97	127.24
40	v	202	HEC	CMB-C2B-C1B	-2.22	121.66	125.04
37	d	407[A]	LHG	O8-C23-O10	-2.22	117.99	123.59
38	E	103	HEM	O2D-CGD-CBD	2.22	121.16	114.03
23	B	601	CLA	C2A-C1A-CHA	-2.22	119.98	123.86
23	B	608	CLA	C4-C3-C5	2.22	119.00	115.27
23	A	408	CLA	OBD-CAD-C3D	-2.22	123.19	128.52
23	C	503	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
33	C	501	LMG	C12-C11-C10	-2.21	105.57	113.62
23	D	405[A]	CLA	CMA-C3A-C4A	-2.21	105.82	111.77
26	a	413	SQD	O48-C23-O10	-2.21	118.01	123.59
23	b	605	CLA	C1-O2A-CGA	2.21	122.25	116.44
26	A	410[B]	SQD	O9-S-O7	-2.21	106.29	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	b	616	CLA	CAC-C3C-C4C	2.21	127.68	124.81
25	h	101	BCR	C10-C11-C12	-2.21	116.32	123.22
24	A	353[B]	PHO	CED-O2D-CGD	2.21	120.94	115.94
23	C	503	CLA	CBC-CAC-C3C	-2.21	106.34	112.43
23	B	606	CLA	C11-C10-C8	-2.21	108.78	115.92
25	c	515	BCR	C36-C18-C19	2.21	121.56	118.08
25	Y	101	BCR	C21-C20-C19	-2.21	116.33	123.22
37	E	101[A]	LHG	O7-C7-O9	-2.21	118.37	123.70
29	A	414[B]	PL9	C2-C3-C4	2.21	121.84	118.80
23	A	406[B]	CLA	CHB-C1B-C2B	-2.20	121.02	127.24
32	b	621	LMT	C1-O1'-C1'	2.20	117.49	113.84
23	C	514	CLA	CAC-C3C-C4C	2.20	127.67	124.81
35	C	517[A]	DGD	O3G-C3G-C2G	-2.20	105.59	110.90
23	c	509	CLA	CAC-C3C-C4C	2.20	127.66	124.81
23	c	507	CLA	C4-C3-C5	2.20	118.97	115.27
26	a	411[A]	SQD	O9-S-O7	-2.20	106.34	113.95
23	b	609	CLA	C7-C6-C5	-2.20	107.39	113.36
26	b	620	SQD	O47-C7-O49	-2.20	118.39	123.70
32	t	102	LMT	C1-O1'-C1'	2.20	117.48	113.84
25	A	409	BCR	C16-C17-C18	-2.20	124.18	127.31
37	L	101[B]	LHG	O8-C23-O10	-2.20	118.05	123.59
23	C	509	CLA	C2A-C1A-CHA	-2.19	120.02	123.86
23	c	511	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
35	c	518[A]	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
23	d	402[B]	CLA	CMB-C2B-C1B	2.19	128.71	125.37
32	m	103	LMT	O5B-C5B-C6B	2.19	111.89	106.44
29	d	405[B]	PL9	C22-C23-C24	-2.19	122.39	127.66
23	b	602	CLA	O2A-CGA-CBA	2.19	118.78	111.91
23	C	507	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
29	D	408[B]	PL9	C12-C13-C14	-2.19	122.39	127.66
23	b	610	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	b	611	CLA	CMB-C2B-C1B	2.19	128.70	125.37
24	a	353[A]	PHO	C4-C3-C2	-2.19	118.07	123.68
23	b	612	CLA	CHB-C1B-NB	-2.19	121.94	124.26
25	B	617	BCR	C15-C14-C13	-2.18	124.20	127.31
23	a	405[B]	CLA	C4-C3-C5	2.18	118.94	115.27
25	a	410	BCR	C38-C26-C27	2.18	117.80	113.62
25	d	404	BCR	C38-C26-C27	2.18	117.80	113.62
23	a	405[B]	CLA	CMC-C2C-C1C	2.18	128.36	125.04
23	b	603	CLA	CBC-CAC-C3C	-2.18	106.43	112.43
23	c	506	CLA	C1-O2A-CGA	2.18	122.16	116.44
38	E	103	HEM	C4B-C3B-C2B	-2.18	105.39	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	517[B]	DGD	O6D-C1D-O3G	-2.18	104.82	109.97
23	c	502	CLA	C4-C3-C5	2.18	118.93	115.27
25	D	407	BCR	C21-C20-C19	-2.18	116.42	123.22
23	b	602	CLA	CHC-C1C-C2C	-2.18	120.68	126.73
40	V	202	HEC	CBB-CAB-C3B	-2.18	106.43	112.43
23	C	508	CLA	C1-C2-C3	-2.18	122.28	126.04
25	b	618	BCR	C38-C26-C25	-2.18	122.08	124.53
26	f	102	SQD	O6-C1-C2	2.18	111.70	108.30
23	C	508	CLA	CAC-C3C-C4C	2.17	127.63	124.81
23	A	405[B]	CLA	O2A-CGA-O1A	-2.17	118.10	123.59
25	T	101	BCR	C1-C6-C7	2.17	121.93	115.78
23	b	613	CLA	C4-C3-C5	2.17	118.93	115.27
35	C	517[B]	DGD	C3G-C2G-C1G	-2.17	106.65	111.79
26	A	412	SQD	O6-C44-C45	-2.17	105.66	110.90
23	a	407[A]	CLA	C4-C3-C5	2.17	118.92	115.27
25	B	617	BCR	C37-C22-C23	2.17	121.50	118.08
26	f	102	SQD	O5-C5-C4	2.17	113.64	109.69
40	v	202	HEC	CBA-CAA-C2A	-2.17	106.60	112.63
23	b	616	CLA	OBD-CAD-C3D	-2.17	123.30	128.52
23	b	614	CLA	CED-O2D-CGD	2.17	120.84	115.94
37	D	409[A]	LHG	O4-P-O5	2.17	122.96	112.24
23	C	513	CLA	CAC-C3C-C4C	2.17	127.62	124.81
40	v	202	HEC	CAD-CBD-CGD	-2.17	108.94	113.60
32	a	414	LMT	O5'-C5'-C4'	2.17	114.32	109.75
29	a	416[A]	PL9	C45-C44-C46	2.16	118.91	115.27
23	A	406[B]	CLA	CMC-C2C-C1C	2.16	128.33	125.04
23	B	604	CLA	CHA-C1A-NA	-2.16	121.44	126.40
23	B	613	CLA	CHB-C4A-NA	2.16	127.50	124.51
25	k	101	BCR	C10-C11-C12	-2.16	116.48	123.22
23	A	405[A]	CLA	O2A-CGA-CBA	2.16	118.68	111.91
24	a	408[A]	PHO	O2D-CGD-O1D	-2.16	119.62	123.84
23	B	602	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
23	c	512	CLA	C1-O2A-CGA	2.15	122.10	116.44
23	A	404[B]	CLA	CMC-C2C-C1C	2.15	128.32	125.04
25	a	410	BCR	C8-C7-C6	-2.15	121.16	127.20
23	c	511	CLA	CHB-C1B-NB	-2.15	121.98	124.26
29	D	408[A]	PL9	C12-C13-C14	-2.15	122.48	127.66
37	d	711[A]	LHG	O7-C7-O9	-2.15	118.51	123.70
23	d	403	CLA	OBD-CAD-C3D	-2.15	123.35	128.52
23	c	510	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
23	C	506	CLA	CHA-C1A-NA	-2.15	121.48	126.40
23	d	403	CLA	CMA-C3A-C4A	-2.15	106.01	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	c	510	CLA	CMC-C2C-C1C	2.15	128.31	125.04
32	a	414	LMT	O5B-C5B-C6B	2.15	111.77	106.44
23	C	513	CLA	CHC-C1C-C2C	-2.14	120.77	126.73
27	a	801	GOL	C3-C2-C1	-2.14	103.37	111.70
23	C	511	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
23	B	601	CLA	CHB-C4A-NA	2.14	127.47	124.51
29	d	405[A]	PL9	C45-C44-C46	2.14	118.87	115.27
23	D	405[A]	CLA	OBD-CAD-C3D	-2.14	123.37	128.52
23	C	504	CLA	O2A-CGA-CBA	2.14	118.62	111.91
35	H	102	DGD	O3G-C3G-C2G	-2.14	105.74	110.90
23	b	601	CLA	C2A-C1A-CHA	-2.14	120.12	123.86
23	C	505	CLA	CAC-C3C-C4C	2.14	127.58	124.81
23	C	513	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
23	A	405[B]	CLA	O2A-CGA-CBA	2.14	118.61	111.91
23	C	508	CLA	CHC-C4B-NB	2.14	126.52	124.26
23	b	615	CLA	C11-C12-C13	-2.14	109.02	115.92
23	b	616	CLA	C4-C3-C5	2.14	118.86	115.27
23	B	602	CLA	CMA-C3A-C2A	-2.13	105.22	113.83
23	b	615	CLA	CHA-C1A-NA	-2.13	121.51	126.40
25	T	101	BCR	C7-C8-C9	-2.13	123.01	126.23
25	c	515	BCR	C33-C5-C6	-2.13	122.13	124.53
25	B	619	BCR	C31-C1-C6	-2.13	106.84	110.30
23	B	616	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
23	b	608	CLA	CMB-C2B-C3B	2.13	131.75	126.59
26	b	620	SQD	O7-S-C6	2.13	109.47	106.94
35	c	517[A]	DGD	O6D-C1D-O3G	-2.13	104.93	109.97
26	A	412	SQD	O48-C23-O10	-2.13	118.22	123.59
23	A	406[A]	CLA	CHB-C4A-NA	2.13	127.46	124.51
26	b	620	SQD	C1-C2-C3	-2.13	105.56	110.00
35	C	517[A]	DGD	O5D-C6D-C5D	-2.13	105.11	109.05
37	d	407[A]	LHG	O8-C23-C24	2.13	118.59	111.91
32	E	102	LMT	C2'-C3'-C4'	2.13	114.54	109.68
38	E	103	HEM	CHA-C1A-NA	2.13	127.76	123.85
29	D	408[B]	PL9	C15-C14-C16	2.13	118.85	115.27
23	C	508	CLA	CMC-C2C-C1C	2.13	128.28	125.04
23	c	511	CLA	CMB-C2B-C1B	2.13	128.61	125.37
23	B	608	CLA	CHD-C4C-NC	2.13	127.56	124.20
23	c	513	CLA	CHB-C4A-NA	2.13	127.45	124.51
37	E	101[B]	LHG	O7-C7-O9	-2.13	118.57	123.70
23	a	407[A]	CLA	CBC-CAC-C3C	-2.12	106.57	112.43
25	c	515	BCR	C29-C30-C25	2.12	113.75	110.48
25	D	407	BCR	C15-C16-C17	-2.12	119.12	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	613	CLA	CBC-CAC-C3C	-2.12	106.58	112.43
23	a	406[B]	CLA	O2A-CGA-CBA	2.12	118.57	111.91
25	B	617	BCR	C31-C1-C6	-2.12	106.85	110.30
26	f	102	SQD	O48-C23-O10	-2.12	118.23	123.59
23	d	402[A]	CLA	CHD-C4C-NC	2.12	127.55	124.20
23	B	606	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
25	t	103	BCR	C29-C28-C27	-2.12	106.64	111.38
23	a	405[B]	CLA	CMA-C3A-C2A	-2.12	105.27	113.83
23	A	405[A]	CLA	CHB-C4A-NA	2.12	127.44	124.51
23	A	405[B]	CLA	C2A-C1A-CHA	-2.12	120.15	123.86
23	c	507	CLA	CBC-CAC-C3C	-2.12	106.59	112.43
23	B	604	CLA	O2A-CGA-CBA	2.12	118.55	111.91
23	b	613	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
33	m	101	LMG	O6-C1-C2	2.12	114.83	110.35
26	B	620	SQD	O5-C1-C2	-2.12	105.87	110.35
40	v	202	HEC	CMD-C2D-C1D	2.12	128.26	125.04
29	A	414[B]	PL9	C47-C48-C49	-2.11	120.52	127.75
23	a	405[B]	CLA	CHC-C1C-NC	2.11	127.41	124.20
23	B	606	CLA	C7-C6-C5	-2.11	107.62	113.36
33	d	412	LMG	C7-O1-C1	-2.11	109.61	113.74
34	B	622	HTG	O2-C2-C3	-2.11	105.46	110.35
35	C	517[B]	DGD	O1G-C1A-C2A	2.11	118.54	111.91
35	c	517[A]	DGD	O1G-C1A-O1A	-2.11	118.26	123.59
23	a	406[A]	CLA	CHB-C4A-NA	2.11	127.43	124.51
23	a	407[B]	CLA	CHB-C4A-NA	2.11	127.43	124.51
25	t	103	BCR	C20-C21-C22	-2.11	124.30	127.31
23	d	402[A]	CLA	CMA-C3A-C2A	-2.11	105.31	113.83
23	A	405[B]	CLA	CED-O2D-CGD	2.11	120.71	115.94
35	C	517[B]	DGD	O6E-C5E-C4E	2.11	113.53	109.69
35	C	518[A]	DGD	O1G-C1A-C2A	2.11	118.53	111.91
26	a	411[A]	SQD	C3-C4-C5	2.11	114.00	110.24
23	B	601	CLA	CMC-C2C-C1C	2.11	128.25	125.04
23	b	605	CLA	C1-C2-C3	-2.11	122.40	126.04
34	b	623	HTG	C1-C2-C3	2.11	114.75	110.59
23	b	613	CLA	CHA-C1A-NA	-2.11	121.57	126.40
23	A	404[B]	CLA	CAA-CBA-CGA	-2.11	107.10	113.25
26	F	101	SQD	C46-C45-C44	-2.11	106.81	111.79
29	d	405[A]	PL9	C31-C32-C33	-2.10	104.97	111.88
34	B	622	HTG	C2'-C1'-S1	-2.10	105.60	112.40
23	a	406[A]	CLA	CAC-C3C-C2C	2.10	131.13	127.53
23	C	512	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
29	a	416[A]	PL9	C51-C49-C50	2.10	119.25	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	B	609	CLA	C16-C17-C18	-2.10	106.07	115.98
23	A	404[A]	CLA	C7-C6-C5	-2.10	107.65	113.36
23	B	612	CLA	C7-C6-C5	-2.10	107.65	113.36
35	C	518[B]	DGD	O2G-C1B-O1B	-2.10	118.63	123.70
40	v	202	HEC	C2A-C1A-NA	-2.10	108.28	110.32
26	b	620	SQD	O5-C1-C2	-2.10	105.91	110.35
23	C	502	CLA	CHB-C1B-NB	-2.10	122.03	124.26
35	H	102	DGD	O2G-C1B-O1B	-2.10	118.63	123.70
29	D	408[B]	PL9	C7-C3-C4	2.10	118.58	116.88
23	b	601	CLA	CHB-C1B-C2B	-2.10	121.31	127.24
23	B	607	CLA	C6-C7-C8	-2.10	109.14	115.92
27	O	601	GOL	C3-C2-C1	-2.09	103.56	111.70
33	Z	101	LMG	C9-O8-C28	2.09	122.36	117.10
29	A	414[A]	PL9	C51-C49-C50	2.09	119.22	114.60
25	B	619	BCR	C34-C9-C8	2.09	121.37	118.08
23	c	503	CLA	C2A-C1A-CHA	-2.09	120.20	123.86
23	b	608	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
29	d	405[B]	PL9	C36-C37-C38	-2.09	105.02	111.88
23	c	506	CLA	C1-C2-C3	-2.09	122.43	126.04
23	b	605	CLA	O2A-CGA-CBA	2.09	118.46	111.91
23	b	607	CLA	CHD-C4C-NC	2.09	127.49	124.20
24	A	353[A]	PHO	OBD-CAD-C3D	-2.09	124.52	127.98
25	h	101	BCR	C36-C18-C19	2.09	121.36	118.08
23	a	407[A]	CLA	CAC-C3C-C4C	2.08	127.52	124.81
23	C	508	CLA	CHA-C1A-NA	-2.08	121.62	126.40
23	a	406[A]	CLA	CHB-C1B-NB	-2.08	122.05	124.26
25	c	515	BCR	C34-C9-C10	-2.08	120.00	122.92
23	B	613	CLA	CMA-C3A-C4A	-2.08	106.18	111.77
32	t	102	LMT	O5'-C1'-O1'	-2.08	105.05	109.97
29	A	414[B]	PL9	C12-C13-C14	-2.08	122.65	127.66
23	C	510	CLA	C2A-C1A-CHA	-2.08	120.22	123.86
25	b	618	BCR	C21-C20-C19	-2.08	116.73	123.22
29	A	414[A]	PL9	C10-C9-C11	2.08	118.77	115.27
35	C	517[B]	DGD	C2G-O2G-C1B	-2.08	112.68	117.79
25	c	516	BCR	C15-C14-C13	-2.08	124.34	127.31
32	b	627	LMT	C1'-O5'-C5'	-2.08	109.61	113.69
25	d	404	BCR	C39-C30-C25	-2.08	106.93	110.30
32	t	101	LMT	O1'-C1'-C2'	2.08	111.55	108.30
23	D	405[A]	CLA	CBC-CAC-C3C	-2.07	106.71	112.43
23	C	511	CLA	CMA-C3A-C4A	-2.07	106.20	111.77
25	Y	101	BCR	C36-C18-C17	-2.07	120.02	122.92
24	A	407[B]	PHO	CBC-CAC-C3C	-2.07	109.84	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	d	405[A]	PL9	C40-C39-C38	-2.07	118.37	123.68
35	c	518[B]	DGD	O6E-C5E-C6E	2.07	111.58	106.44
23	d	402[A]	CLA	CBB-CAB-C3B	-2.07	117.32	127.62
23	c	513	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
25	c	515	BCR	C37-C22-C23	2.07	121.34	118.08
35	c	517[B]	DGD	C2G-O2G-C1B	-2.07	112.70	117.79
25	D	407	BCR	C30-C25-C24	2.07	121.63	115.78
23	c	502	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
23	a	409	CLA	CHC-C1C-C2C	-2.07	120.99	126.73
23	b	607	CLA	C11-C10-C8	-2.07	109.24	115.92
40	V	202	HEC	CHA-C1A-NA	2.07	126.67	124.44
23	C	508	CLA	C7-C6-C5	-2.07	107.75	113.36
25	D	407	BCR	C38-C26-C27	2.07	117.59	113.62
34	b	625	HTG	C1-C2-C3	-2.07	106.51	110.59
23	a	406[B]	CLA	CAA-CBA-CGA	2.06	119.28	113.25
23	c	507	CLA	CAA-CBA-CGA	2.06	119.28	113.25
23	c	513	CLA	CHA-C1A-NA	-2.06	121.67	126.40
23	b	611	CLA	CMC-C2C-C1C	2.06	128.18	125.04
23	b	616	CLA	CMC-C2C-C1C	2.06	128.18	125.04
23	B	606	CLA	OBD-CAD-C3D	-2.06	123.56	128.52
23	A	405[B]	CLA	CAA-CBA-CGA	2.06	119.28	113.25
23	C	506	CLA	C4-C3-C2	-2.06	118.39	123.68
23	d	402[A]	CLA	CBC-CAC-C3C	-2.06	106.75	112.43
25	d	404	BCR	C16-C15-C14	-2.06	119.26	123.47
23	A	406[B]	CLA	CAC-C3C-C4C	2.06	127.48	124.81
25	B	617	BCR	C21-C20-C19	-2.06	116.79	123.22
35	c	518[B]	DGD	O1G-C1A-O1A	-2.06	118.40	123.59
29	D	408[A]	PL9	C27-C28-C29	-2.06	122.71	127.66
23	b	616	CLA	CHB-C1B-C2B	-2.06	121.43	127.24
23	B	616	CLA	C4-C3-C2	-2.06	118.40	123.68
23	c	502	CLA	OBD-CAD-C3D	-2.06	123.57	128.52
23	c	513	CLA	CBA-CAA-C2A	-2.06	107.80	113.86
23	c	502	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
23	D	405[B]	CLA	CAC-C3C-C4C	2.05	127.48	124.81
25	H	101	BCR	C20-C21-C22	-2.05	124.38	127.31
23	B	616	CLA	CHB-C1B-NB	-2.05	122.08	124.26
23	c	512	CLA	C11-C10-C8	-2.05	109.28	115.92
23	A	405[B]	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
29	d	405[A]	PL9	O2-C1-C6	-2.05	117.04	120.59
38	e	87	HEM	O2A-CGA-CBA	2.05	120.62	114.03
26	A	410[B]	SQD	O48-C23-O10	-2.05	118.41	123.59
23	C	509	CLA	C6-C7-C8	-2.05	109.29	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	C	519	DGD	O2G-C1B-O1B	-2.05	118.75	123.70
23	b	602	CLA	CMA-C3A-C2A	-2.05	105.55	113.83
24	A	353[A]	PHO	O1D-CGD-CBD	-2.05	121.33	124.74
25	c	516	BCR	C37-C22-C23	2.05	121.31	118.08
23	b	608	CLA	C11-C10-C8	-2.05	109.30	115.92
24	A	353[B]	PHO	C4D-CHA-CBD	2.05	109.44	108.52
29	D	408[A]	PL9	C45-C44-C46	2.05	118.72	115.27
25	Y	101	BCR	C29-C30-C25	2.05	113.64	110.48
23	C	509	CLA	CHD-C4C-NC	2.05	127.43	124.20
23	c	502	CLA	C2A-C1A-CHA	-2.05	120.28	123.86
23	c	509	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	B	605	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	D	406	CLA	CMA-C3A-C4A	-2.05	106.27	111.77
37	L	101[A]	LHG	O4-P-O5	2.05	122.36	112.24
23	B	602	CLA	C16-C15-C13	-2.05	109.31	115.92
23	b	613	CLA	CBC-CAC-C3C	-2.05	106.79	112.43
23	a	405[A]	CLA	CMB-C2B-C3B	2.05	131.54	126.59
23	A	406[A]	CLA	CBC-CAC-C3C	-2.04	106.79	112.43
25	d	404	BCR	C24-C23-C22	-2.04	123.15	126.23
23	b	602	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	b	601	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
23	A	408	CLA	C11-C12-C13	-2.04	109.31	115.92
23	b	610	CLA	C4-C3-C2	-2.04	118.44	123.68
23	a	406[B]	CLA	CMA-C3A-C2A	-2.04	105.59	113.83
23	B	606	CLA	C1-C2-C3	-2.04	122.51	126.04
24	a	353[A]	PHO	O2A-CGA-O1A	-2.04	118.44	123.59
24	a	408[A]	PHO	C1-C2-C3	-2.04	122.51	126.04
37	l	101[A]	LHG	O7-C7-O9	-2.04	118.77	123.70
23	b	616	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	D	408[B]	PL9	C47-C48-C49	-2.04	120.78	127.75
33	c	520	LMG	O8-C28-O10	-2.04	118.45	123.59
33	C	521	LMG	O8-C28-O10	-2.04	118.45	123.59
23	b	616	CLA	CHC-C4B-NB	-2.04	122.10	124.26
23	D	405[B]	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
23	B	616	CLA	CMC-C2C-C1C	2.04	128.14	125.04
33	m	101	LMG	O7-C10-O9	-2.04	118.78	123.70
25	K	102	BCR	C2-C1-C6	2.04	113.61	110.48
27	B	624	GOL	C3-C2-C1	-2.03	103.80	111.70
23	C	513	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
23	B	614	CLA	CMA-C3A-C2A	-2.03	105.63	113.83
26	F	101	SQD	O8-S-O7	-2.03	106.31	111.27
33	z	101	LMG	O8-C28-O10	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	D	408[A]	PL9	C47-C48-C49	-2.03	120.81	127.75
29	D	408[A]	PL9	C21-C22-C23	-2.03	105.21	111.88
23	B	608	CLA	OBD-CAD-C3D	-2.03	123.63	128.52
23	a	406[B]	CLA	C1-O2A-CGA	2.03	121.77	116.44
23	B	609	CLA	CHA-C1A-NA	-2.03	121.75	126.40
35	c	517[B]	DGD	O1G-C1A-C2A	2.03	118.27	111.91
29	d	405[B]	PL9	C30-C29-C31	2.03	118.68	115.27
29	d	405[B]	PL9	C31-C32-C33	-2.03	105.22	111.88
25	a	410	BCR	C2-C1-C6	2.03	113.60	110.48
25	B	619	BCR	C3-C4-C5	-2.03	110.46	114.08
23	B	609	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
32	M	101	LMT	C1-O1'-C1'	2.02	117.20	113.84
24	a	353[B]	PHO	C4-C3-C2	-2.02	118.49	123.68
23	a	407[A]	CLA	CHA-C1A-NA	-2.02	121.77	126.40
23	B	616	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
26	a	411[A]	SQD	O4-C4-C3	-2.02	105.68	110.35
26	a	411[B]	SQD	O48-C23-O10	-2.02	118.50	123.59
23	B	602	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
40	v	202	HEC	CBD-CAD-C3D	-2.02	107.03	112.63
23	c	509	CLA	CMC-C2C-C1C	2.02	128.11	125.04
23	B	606	CLA	CMB-C2B-C1B	2.02	128.44	125.37
25	T	101	BCR	C7-C6-C5	-2.01	116.58	121.46
23	B	610	CLA	CMA-C3A-C2A	-2.01	105.70	113.83
38	e	87	HEM	C4A-NA-C1A	2.01	107.32	105.35
25	Y	101	BCR	C11-C10-C9	-2.01	124.44	127.31
23	C	508	CLA	C6-C7-C8	-2.01	109.41	115.92
35	c	517[A]	DGD	O1G-C1A-C2A	2.01	118.23	111.91
23	b	604	CLA	C4-C3-C2	-2.01	118.51	123.68
23	c	506	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
23	b	607	CLA	CMC-C2C-C1C	2.01	128.10	125.04
25	y	101	BCR	C35-C13-C14	-2.01	120.10	122.92
25	K	102	BCR	C37-C22-C21	-2.01	120.11	122.92
23	B	610	CLA	CAC-C3C-C2C	2.01	130.97	127.53
35	H	102	DGD	C2G-O2G-C1B	-2.01	112.84	117.79
32	M	101	LMT	O5B-C5B-C6B	2.01	111.43	106.44
23	C	514	CLA	CGD-CBD-CAD	-2.01	104.22	110.73
24	A	353[B]	PHO	C4A-C3A-C2A	-2.01	100.93	102.84
34	b	622	HTG	C6-C5-C4	-2.01	108.30	113.00
23	B	612	CLA	CMA-C3A-C4A	-2.01	106.37	111.77
23	D	406	CLA	CHB-C4A-NA	2.01	127.29	124.51
23	B	603	CLA	C2A-C3A-C4A	-2.01	98.63	101.87
33	Z	101	LMG	C1-O6-C5	2.01	117.63	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	d	711[B]	LHG	O7-C7-O9	-2.01	118.85	123.70
23	C	511	CLA	CAA-C2A-C3A	-2.01	107.28	112.78
24	A	407[B]	PHO	C4-C3-C5	2.01	118.65	115.27
25	c	515	BCR	C35-C13-C14	-2.01	120.11	122.92
23	d	402[B]	CLA	CHB-C4A-NA	2.01	127.28	124.51
24	A	353[A]	PHO	CMB-C2B-C3B	2.00	128.43	124.68
35	C	517[A]	DGD	C4E-C3E-C2E	-2.00	107.33	110.82
23	B	609	CLA	C7-C6-C5	-2.00	107.92	113.36
25	D	407	BCR	C39-C30-C25	-2.00	107.05	110.30
23	B	610	CLA	CMC-C2C-C1C	2.00	128.09	125.04
23	b	616	CLA	C11-C12-C13	-2.00	109.45	115.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
40	V	202	HEC	NA
40	v	202	HEC	NA

All (1699) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	404[B]	CLA	C2B-C3B-CAB-CBB
23	A	404[B]	CLA	C4B-C3B-CAB-CBB
23	A	408	CLA	C2-C3-C5-C6
23	A	408	CLA	C4-C3-C5-C6
23	B	601	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O1D
23	B	614	CLA	CHA-CBD-CGD-O2D
23	B	614	CLA	CAD-CBD-CGD-O1D
23	B	614	CLA	CAD-CBD-CGD-O2D
23	C	505	CLA	C2-C3-C5-C6
23	C	505	CLA	C4-C3-C5-C6
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	405[B]	CLA	C2B-C3B-CAB-CBB
23	a	405[B]	CLA	C4B-C3B-CAB-CBB
23	a	409	CLA	C2-C3-C5-C6
23	a	409	CLA	C4-C3-C5-C6
23	b	601	CLA	C11-C10-C8-C9
23	b	605	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C12-C13-C15-C16
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	505	CLA	C11-C12-C13-C14
23	c	508	CLA	C2B-C3B-CAB-CBB
23	c	508	CLA	C4B-C3B-CAB-CBB
23	c	508	CLA	C4-C3-C5-C6
23	c	509	CLA	CHA-CBD-CGD-O1D
23	c	509	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2B-C3B-CAB-CBB
23	c	514	CLA	C4B-C3B-CAB-CBB
23	d	403	CLA	C2-C3-C5-C6
23	d	403	CLA	C4-C3-C5-C6
25	D	407	BCR	C21-C22-C23-C24
25	D	407	BCR	C37-C22-C23-C24
25	D	407	BCR	C23-C24-C25-C30
25	Y	101	BCR	C5-C6-C7-C8
25	d	404	BCR	C21-C22-C23-C24
25	d	404	BCR	C37-C22-C23-C24
25	d	404	BCR	C23-C24-C25-C30
25	y	101	BCR	C5-C6-C7-C8
26	A	410[B]	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	101	SQD	C2-C1-O6-C44
26	F	101	SQD	O49-C7-O47-C45
26	F	101	SQD	C8-C7-O47-C45
26	a	413	SQD	O6-C44-C45-O47
26	a	413	SQD	C5-C6-S-O7
26	a	413	SQD	C5-C6-S-O8
26	a	413	SQD	C5-C6-S-O9
26	b	620	SQD	C8-C7-O47-C45
26	f	102	SQD	O6-C44-C45-O47
26	f	102	SQD	O49-C7-O47-C45
26	f	102	SQD	C8-C7-O47-C45
27	A	411	GOL	O1-C1-C2-C3
27	A	701	GOL	O1-C1-C2-C3
27	B	624	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
27	D	701	GOL	O1-C1-C2-C3
27	D	701	GOL	C1-C2-C3-O3
27	O	501	GOL	O1-C1-C2-C3
27	O	601	GOL	O1-C1-C2-C3
27	V	401[A]	GOL	C1-C2-C3-O3
27	V	401[B]	GOL	C1-C2-C3-O3
27	V	401[B]	GOL	O2-C2-C3-O3
27	a	412	GOL	O1-C1-C2-C3
27	a	412	GOL	C1-C2-C3-O3
27	b	624	GOL	C1-C2-C3-O3
27	c	743	GOL	C1-C2-C3-O3
27	o	501	GOL	C1-C2-C3-O3
27	o	601	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	C14-C16-C17-C18
29	A	414[B]	PL9	C18-C19-C21-C22
29	A	414[B]	PL9	C20-C19-C21-C22
29	a	416[A]	PL9	C9-C11-C12-C13
29	a	416[A]	PL9	C14-C16-C17-C18
29	a	416[A]	PL9	C23-C24-C26-C27
29	a	416[A]	PL9	C25-C24-C26-C27
29	a	416[B]	PL9	C9-C11-C12-C13
29	a	416[B]	PL9	C14-C16-C17-C18
32	A	359	LMT	C2'-C1'-O1'-C1
32	A	359	LMT	O5'-C1'-O1'-C1
32	D	404	LMT	C2-C1-O1'-C1'
32	E	102	LMT	C2'-C1'-O1'-C1
32	E	102	LMT	O5'-C1'-O1'-C1
32	I	101	LMT	C2'-C1'-O1'-C1
32	I	101	LMT	O5'-C1'-O1'-C1
32	I	101	LMT	C2-C1-O1'-C1'
32	M	103	LMT	C2-C1-O1'-C1'
32	a	414	LMT	C2'-C1'-O1'-C1
32	b	621	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	C2'-C1'-O1'-C1
32	b	627	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	O5'-C1'-O1'-C1
32	t	101	LMT	C2-C1-O1'-C1'
32	t	102	LMT	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
32	t	102	LMT	C2-C1-O1'-C1'
33	C	521	LMG	C11-C10-O7-C8
33	c	521	LMG	O9-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	622	HTG	C2'-C1'-S1-C1
37	D	410[A]	LHG	O2-C2-C3-O3
37	D	410[A]	LHG	C3-O3-P-O4
37	D	410[A]	LHG	C3-O3-P-O5
37	D	410[A]	LHG	C3-O3-P-O6
37	D	410[A]	LHG	C4-O6-P-O4
37	D	410[B]	LHG	C3-O3-P-O4
37	D	410[B]	LHG	C4-O6-P-O4
37	D	410[B]	LHG	C4-O6-P-O5
37	E	101[A]	LHG	C3-O3-P-O4
37	E	101[A]	LHG	C3-O3-P-O5
37	E	101[A]	LHG	O10-C23-O8-C6
37	E	101[A]	LHG	C24-C23-O8-C6
37	E	101[B]	LHG	C3-O3-P-O4
37	E	101[B]	LHG	C3-O3-P-O5
37	E	101[B]	LHG	C4-O6-P-O3
37	E	101[B]	LHG	C4-O6-P-O5
37	E	101[B]	LHG	O10-C23-O8-C6
37	E	101[B]	LHG	C24-C23-O8-C6
37	L	101[A]	LHG	C4-O6-P-O4
37	L	101[A]	LHG	C4-O6-P-O5
37	L	101[B]	LHG	C4-O6-P-O4
37	L	101[B]	LHG	C4-O6-P-O5
37	d	407[A]	LHG	C3-O3-P-O4
37	d	407[A]	LHG	C3-O3-P-O5
37	d	407[A]	LHG	C4-O6-P-O4
37	d	407[B]	LHG	C3-O3-P-O4
37	d	407[B]	LHG	C4-O6-P-O4
37	d	408[B]	LHG	C4-O6-P-O4
37	d	711[A]	LHG	C3-O3-P-O5
37	d	711[B]	LHG	C3-O3-P-O5
37	e	101[A]	LHG	C3-O3-P-O4
37	e	101[A]	LHG	C4-O6-P-O5
37	e	101[A]	LHG	O10-C23-O8-C6
37	e	101[A]	LHG	C24-C23-O8-C6
37	e	101[B]	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
37	e	101[B]	LHG	C4-O6-P-O5
37	e	101[B]	LHG	O10-C23-O8-C6
37	e	101[B]	LHG	C24-C23-O8-C6
37	l	101[A]	LHG	C4-O6-P-O4
37	l	101[A]	LHG	C4-O6-P-O5
37	l	101[B]	LHG	C4-O6-P-O4
37	l	101[B]	LHG	C4-O6-P-O5
38	E	103	HEM	C2C-C3C-CAC-CBC
38	E	103	HEM	C4C-C3C-CAC-CBC
32	a	414	LMT	C4'-C5'-C6'-O6'
32	I	101	LMT	O5B-C1B-O1B-C4'
26	A	410[A]	SQD	O49-C7-O47-C45
26	b	620	SQD	O49-C7-O47-C45
23	B	614	CLA	C3-C5-C6-C7
23	D	406	CLA	C3-C5-C6-C7
23	c	513	CLA	C3-C5-C6-C7
23	d	403	CLA	C3-C5-C6-C7
32	a	420	LMT	O5B-C5B-C6B-O6B
32	M	103	LMT	C4B-C5B-C6B-O6B
26	B	620	SQD	C8-C7-O47-C45
33	c	521	LMG	C11-C10-O7-C8
23	D	406	CLA	CBD-CGD-O2D-CED
32	E	102	LMT	O5'-C5'-C6'-O6'
23	D	406	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C20-C19-C21-C22
29	a	416[B]	PL9	C25-C24-C26-C27
23	D	406	CLA	C2-C3-C5-C6
23	b	605	CLA	C2-C3-C5-C6
23	c	508	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C18-C19-C21-C22
23	C	502	CLA	CBD-CGD-O2D-CED
23	B	606	CLA	C2A-CAA-CBA-CGA
23	b	606	CLA	C2A-CAA-CBA-CGA
23	b	616	CLA	C3-C5-C6-C7
34	D	414	HTG	O5-C5-C6-O6
33	C	521	LMG	O9-C10-O7-C8
33	z	101	LMG	O9-C10-O7-C8
32	m	103	LMT	C4B-C5B-C6B-O6B
32	M	103	LMT	O5'-C5'-C6'-O6'
32	b	621	LMT	O5'-C5'-C6'-O6'
23	c	513	CLA	CBD-CGD-O2D-CED
23	c	514	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
37	d	407[A]	LHG	O2-C2-C3-O3
37	d	407[B]	LHG	O2-C2-C3-O3
23	A	408	CLA	C3-C5-C6-C7
32	a	414	LMT	O5B-C5B-C6B-O6B
33	C	521	LMG	O6-C5-C6-O5
26	A	410[A]	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
23	C	514	CLA	CBD-CGD-O2D-CED
32	a	420	LMT	C4B-C5B-C6B-O6B
32	D	404	LMT	C6-C7-C8-C9
34	b	625	HTG	O5-C5-C6-O6
33	c	521	LMG	C4-C5-C6-O5
34	D	414	HTG	S1-C1'-C2'-C3'
34	b	625	HTG	S1-C1'-C2'-C3'
32	I	101	LMT	O5B-C5B-C6B-O6B
32	I	101	LMT	O5'-C5'-C6'-O6'
32	m	103	LMT	O5B-C5B-C6B-O6B
32	t	102	LMT	O5'-C5'-C6'-O6'
32	D	404	LMT	C4'-C5'-C6'-O6'
32	M	103	LMT	C4'-C5'-C6'-O6'
34	D	414	HTG	C4-C5-C6-O6
32	M	103	LMT	O5B-C5B-C6B-O6B
23	B	605	CLA	C4-C3-C5-C6
23	C	508	CLA	C4-C3-C5-C6
23	b	603	CLA	C4-C3-C5-C6
23	b	614	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C15-C14-C16-C17
29	a	416[A]	PL9	C15-C14-C16-C17
29	a	416[A]	PL9	C30-C29-C31-C32
29	a	416[B]	PL9	C15-C14-C16-C17
29	a	416[B]	PL9	C30-C29-C31-C32
32	E	102	LMT	C4'-C5'-C6'-O6'
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	614	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	416[A]	PL9	C13-C14-C16-C17
29	a	416[A]	PL9	C28-C29-C31-C32
29	a	416[B]	PL9	C13-C14-C16-C17
29	a	416[B]	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
40	v	202	HEC	C2C-C3C-CAC-CBC
32	D	404	LMT	O5B-C5B-C6B-O6B
32	a	414	LMT	O5'-C5'-C6'-O6'
32	t	101	LMT	O5'-C5'-C6'-O6'
32	b	621	LMT	C4'-C5'-C6'-O6'
32	e	102	LMT	C4'-C5'-C6'-O6'
26	B	620	SQD	O5-C1-O6-C44
32	b	621	LMT	O5'-C1'-O1'-C1
32	e	102	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	408[A]	PL9	C39-C41-C42-C43
29	D	408[B]	PL9	C39-C41-C42-C43
23	c	510	CLA	C3-C5-C6-C7
37	d	407[A]	LHG	C1-C2-C3-O3
32	a	414	LMT	C4B-C5B-C6B-O6B
23	C	504	CLA	CBD-CGD-O2D-CED
32	b	627	LMT	C4'-C5'-C6'-O6'
32	I	101	LMT	C4B-C5B-C6B-O6B
26	b	620	SQD	C18-C19-C20-C21
32	t	101	LMT	C2'-C1'-O1'-C1
32	t	102	LMT	C2'-C1'-O1'-C1
29	A	414[A]	PL9	C30-C29-C31-C32
32	D	404	LMT	C4B-C5B-C6B-O6B
29	a	416[B]	PL9	C23-C24-C26-C27
23	C	503	CLA	C14-C13-C15-C16
23	C	507	CLA	C14-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C9
23	b	610	CLA	C11-C12-C13-C14
23	b	616	CLA	C6-C7-C8-C9
23	c	510	CLA	C11-C10-C8-C9
34	b	622	HTG	S1-C1'-C2'-C3'
33	B	621	LMG	C39-C40-C41-C42
26	B	620	SQD	C7-C8-C9-C10
26	F	101	SQD	C23-C24-C25-C26
37	E	101[A]	LHG	C23-C24-C25-C26
23	B	601	CLA	C5-C6-C7-C8
23	B	601	CLA	C10-C11-C12-C13
23	B	602	CLA	C13-C15-C16-C17
23	c	513	CLA	C15-C16-C17-C18
32	b	627	LMT	O5'-C5'-C6'-O6'
23	a	405[B]	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	b	611	CLA	C15-C16-C17-C18
26	b	620	SQD	C31-C32-C33-C34
35	c	518[B]	DGD	C1B-C2B-C3B-C4B
32	D	404	LMT	O5'-C5'-C6'-O6'
33	c	521	LMG	O6-C5-C6-O5
23	A	408	CLA	C5-C6-C7-C8
23	b	601	CLA	C10-C11-C12-C13
23	b	606	CLA	C10-C11-C12-C13
23	b	606	CLA	C13-C15-C16-C17
23	b	614	CLA	C8-C10-C11-C12
27	A	411	GOL	O1-C1-C2-O2
35	c	518[A]	DGD	C1B-C2B-C3B-C4B
34	B	626	HTG	O5-C5-C6-O6
23	B	614	CLA	C8-C10-C11-C12
23	C	508	CLA	C5-C6-C7-C8
32	I	101	LMT	O1'-C1-C2-C3
32	a	420	LMT	O1'-C1-C2-C3
40	V	202	HEC	C4C-C3C-CAC-CBC
37	D	411[A]	LHG	C33-C34-C35-C36
23	b	604	CLA	C8-C10-C11-C12
23	b	605	CLA	C8-C10-C11-C12
33	Z	101	LMG	C10-C11-C12-C13
32	I	101	LMT	C4'-C5'-C6'-O6'
23	A	408	CLA	C12-C13-C15-C16
23	B	606	CLA	C11-C10-C8-C7
25	T	101	BCR	C13-C14-C15-C16
23	D	406	CLA	C10-C11-C12-C13
23	c	514	CLA	C10-C11-C12-C13
23	C	513	CLA	CBD-CGD-O2D-CED
26	F	101	SQD	O5-C1-O6-C44
32	a	414	LMT	O5'-C1'-O1'-C1
23	a	405[A]	CLA	C15-C16-C17-C18
29	d	405[A]	PL9	C39-C41-C42-C43
29	d	405[B]	PL9	C39-C41-C42-C43
26	A	410[B]	SQD	C7-C8-C9-C10
32	t	101	LMT	C4'-C5'-C6'-O6'
34	b	625	HTG	C4-C5-C6-O6
23	B	606	CLA	C10-C11-C12-C13
23	b	604	CLA	C15-C16-C17-C18
32	I	101	LMT	C5'-C4'-O1B-C1B
23	C	503	CLA	C13-C15-C16-C17
23	C	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	D	411[B]	LHG	C33-C34-C35-C36
32	e	102	LMT	O5'-C5'-C6'-O6'
35	h	102	DGD	C6B-C7B-C8B-C9B
23	B	614	CLA	C10-C11-C12-C13
23	b	604	CLA	C5-C6-C7-C8
23	b	606	CLA	C15-C16-C17-C18
37	D	410[B]	LHG	C3-O3-P-O6
37	D	410[B]	LHG	C4-O6-P-O3
37	E	101[A]	LHG	C3-O3-P-O6
37	E	101[A]	LHG	C4-O6-P-O3
37	E	101[B]	LHG	C3-O3-P-O6
37	L	101[A]	LHG	C4-O6-P-O3
37	L	101[B]	LHG	C4-O6-P-O3
37	d	407[A]	LHG	C3-O3-P-O6
37	d	407[B]	LHG	C3-O3-P-O6
37	e	101[A]	LHG	C3-O3-P-O6
37	e	101[A]	LHG	C4-O6-P-O3
37	e	101[B]	LHG	C3-O3-P-O6
37	e	101[B]	LHG	C4-O6-P-O3
37	l	101[A]	LHG	C4-O6-P-O3
37	l	101[B]	LHG	C4-O6-P-O3
26	A	410[A]	SQD	C7-C8-C9-C10
37	E	101[B]	LHG	C23-C24-C25-C26
32	t	102	LMT	C4'-C5'-C6'-O6'
23	c	510	CLA	CBA-CGA-O2A-C1
34	B	622	HTG	C1'-C2'-C3'-C4'
34	b	623	HTG	C1'-C2'-C3'-C4'
40	V	202	HEC	C2C-C3C-CAC-CBC
37	D	410[A]	LHG	C1-C2-C3-O3
37	d	407[B]	LHG	C1-C2-C3-O3
23	C	511	CLA	C4-C3-C5-C6
29	A	414[B]	PL9	C30-C29-C31-C32
26	A	410[A]	SQD	C12-C13-C14-C15
23	b	611	CLA	C8-C10-C11-C12
23	c	509	CLA	C16-C17-C18-C19
23	B	616	CLA	C3-C5-C6-C7
23	a	409	CLA	CBA-CGA-O2A-C1
23	b	614	CLA	C10-C11-C12-C13
32	b	621	LMT	C3'-C4'-O1B-C1B
26	A	410[B]	SQD	C15-C16-C17-C18
33	C	501	LMG	C17-C18-C19-C20
32	m	103	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
32	I	101	LMT	C3-C4-C5-C6
33	m	101	LMG	C35-C36-C37-C38
34	B	623	HTG	C3'-C4'-C5'-C6'
35	c	517[A]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	C9A-CAA-CBA-CCA
35	c	517[B]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	C9A-CAA-CBA-CCA
35	c	518[B]	DGD	CBA-CCA-CDA-CEA
37	L	101[A]	LHG	C15-C16-C17-C18
37	L	101[A]	LHG	C17-C18-C19-C20
37	L	101[B]	LHG	C25-C26-C27-C28
23	B	603	CLA	C16-C17-C18-C20
23	B	615	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C19
26	F	101	SQD	C30-C31-C32-C33
35	c	518[B]	DGD	C9A-CAA-CBA-CCA
37	L	101[B]	LHG	C13-C14-C15-C16
37	d	711[A]	LHG	C16-C17-C18-C19
33	B	621	LMG	O9-C10-O7-C8
32	D	404	LMT	C5-C6-C7-C8
35	c	517[B]	DGD	C5A-C6A-C7A-C8A
33	D	415	LMG	C19-C20-C21-C22
35	C	517[A]	DGD	C5B-C6B-C7B-C8B
35	C	518[B]	DGD	CCB-CDB-CEB-CFB
37	D	410[A]	LHG	C16-C17-C18-C19
37	d	711[A]	LHG	C32-C33-C34-C35
37	E	101[B]	LHG	O2-C2-C3-O3
26	f	102	SQD	C32-C33-C34-C35
32	A	359	LMT	O1'-C1-C2-C3
32	b	627	LMT	C7-C8-C9-C10
35	c	517[A]	DGD	C5A-C6A-C7A-C8A
35	c	518[A]	DGD	CBA-CCA-CDA-CEA
37	L	101[B]	LHG	C12-C13-C14-C15
37	e	101[A]	LHG	C26-C27-C28-C29
37	l	101[B]	LHG	C14-C15-C16-C17
26	A	412	SQD	C2-C1-O6-C44
32	e	102	LMT	C2'-C1'-O1'-C1
35	C	518[A]	DGD	C2E-C1E-O5D-C6D
35	C	518[B]	DGD	C2E-C1E-O5D-C6D
26	A	412	SQD	C17-C18-C19-C20
32	t	101	LMT	C3-C4-C5-C6
32	t	102	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
32	t	102	LMT	C4-C5-C6-C7
35	C	517[A]	DGD	C4B-C5B-C6B-C7B
35	c	517[A]	DGD	C2B-C3B-C4B-C5B
35	c	518[A]	DGD	CAA-CBA-CCA-CDA
35	c	519	DGD	CBB-CCB-CDB-CEB
37	D	411[B]	LHG	C32-C33-C34-C35
23	c	510	CLA	O1A-CGA-O2A-C1
23	b	602	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C20
23	c	510	CLA	C16-C17-C18-C20
26	a	413	SQD	C16-C17-C18-C19
34	b	622	HTG	C2'-C3'-C4'-C5'
35	H	102	DGD	CCB-CDB-CEB-CFB
37	L	101[A]	LHG	C13-C14-C15-C16
37	e	101[B]	LHG	C26-C27-C28-C29
37	l	101[B]	LHG	C16-C17-C18-C19
23	a	407[A]	CLA	C11-C12-C13-C14
23	a	407[B]	CLA	C11-C12-C13-C14
23	b	606	CLA	C14-C13-C15-C16
23	c	505	CLA	C14-C13-C15-C16
23	D	406	CLA	O1D-CGD-O2D-CED
26	A	410[A]	SQD	C15-C16-C17-C18
33	C	501	LMG	C12-C13-C14-C15
33	D	415	LMG	C35-C36-C37-C38
35	C	518[A]	DGD	CCB-CDB-CEB-CFB
37	D	410[B]	LHG	C16-C17-C18-C19
23	c	507	CLA	C15-C16-C17-C18
23	B	610	CLA	C2A-CAA-CBA-CGA
23	b	610	CLA	C2A-CAA-CBA-CGA
23	c	508	CLA	C2A-CAA-CBA-CGA
23	a	409	CLA	O1A-CGA-O2A-C1
25	b	619	BCR	C7-C8-C9-C34
26	B	620	SQD	C30-C31-C32-C33
32	e	102	LMT	C4-C5-C6-C7
32	t	101	LMT	C11-C10-C9-C8
33	C	521	LMG	C19-C20-C21-C22
37	d	711[B]	LHG	C16-C17-C18-C19
27	B	624	GOL	O1-C1-C2-C3
27	a	701	GOL	O1-C1-C2-C3
27	d	801[B]	GOL	O1-C1-C2-C3
27	v	401[A]	GOL	O1-C1-C2-C3
27	v	401[B]	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
37	D	409[B]	LHG	O1-C1-C2-C3
25	b	619	BCR	C7-C8-C9-C10
23	C	513	CLA	C10-C11-C12-C13
33	B	621	LMG	C11-C10-O7-C8
33	m	101	LMG	C11-C10-O7-C8
32	e	102	LMT	C5-C6-C7-C8
32	t	101	LMT	C4-C5-C6-C7
33	a	419	LMG	C34-C35-C36-C37
35	h	102	DGD	CAA-CBA-CCA-CDA
37	D	411[A]	LHG	C32-C33-C34-C35
37	L	101[B]	LHG	C15-C16-C17-C18
37	l	101[A]	LHG	C14-C15-C16-C17
26	F	101	SQD	C29-C30-C31-C32
32	a	414	LMT	C2-C3-C4-C5
32	m	103	LMT	C7-C8-C9-C10
33	B	621	LMG	C34-C35-C36-C37
33	C	501	LMG	C19-C20-C21-C22
33	C	521	LMG	C18-C19-C20-C21
33	D	415	LMG	C30-C31-C32-C33
35	c	518[B]	DGD	CAA-CBA-CCA-CDA
37	L	101[A]	LHG	C12-C13-C14-C15
37	d	711[A]	LHG	C29-C30-C31-C32
32	I	101	LMT	C1-C2-C3-C4
33	Z	101	LMG	O6-C5-C6-O5
34	b	622	HTG	O5-C5-C6-O6
23	D	405[B]	CLA	C4B-C3B-CAB-CBB
23	b	604	CLA	C4B-C3B-CAB-CBB
23	B	603	CLA	C16-C17-C18-C19
23	a	409	CLA	C16-C17-C18-C20
23	b	602	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C20
23	d	402[A]	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C20
23	A	405[A]	CLA	C15-C16-C17-C18
26	a	413	SQD	C25-C26-C27-C28
33	C	501	LMG	C36-C37-C38-C39
33	C	521	LMG	C17-C18-C19-C20
33	a	419	LMG	C30-C31-C32-C33
33	m	101	LMG	C39-C40-C41-C42
35	C	517[B]	DGD	C4B-C5B-C6B-C7B
35	C	519	DGD	C2B-C3B-C4B-C5B
37	l	101[A]	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	b	613	CLA	CBD-CGD-O2D-CED
23	C	502	CLA	O1D-CGD-O2D-CED
33	B	621	LMG	C17-C18-C19-C20
33	C	520	LMG	C17-C18-C19-C20
33	c	520	LMG	C31-C32-C33-C34
33	d	412	LMG	C29-C30-C31-C32
37	d	407[B]	LHG	C34-C35-C36-C37
33	C	501	LMG	C10-C11-C12-C13
33	a	419	LMG	C10-C11-C12-C13
26	F	101	SQD	C24-C25-C26-C27
33	C	521	LMG	C13-C14-C15-C16
35	h	102	DGD	C9A-CAA-CBA-CCA
32	M	103	LMT	C7-C8-C9-C10
33	D	415	LMG	C36-C37-C38-C39
35	C	517[A]	DGD	C9A-CAA-CBA-CCA
35	H	102	DGD	CAB-CBB-CCB-CDB
37	d	408[A]	LHG	C27-C28-C29-C30
40	v	202	HEC	C4C-C3C-CAC-CBC
23	B	614	CLA	C5-C6-C7-C8
32	E	102	LMT	C2-C1-O1'-C1'
32	M	101	LMT	C3-C4-C5-C6
35	C	519	DGD	C6B-C7B-C8B-C9B
37	E	101[A]	LHG	C24-C25-C26-C27
23	c	514	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	C16-C17-C18-C20
23	b	614	CLA	C16-C17-C18-C19
23	b	615	CLA	C16-C17-C18-C19
23	c	510	CLA	C16-C17-C18-C19
33	C	520	LMG	C16-C17-C18-C19
37	L	101[A]	LHG	C25-C26-C27-C28
37	d	711[B]	LHG	C32-C33-C34-C35
37	l	101[B]	LHG	C27-C28-C29-C30
26	B	620	SQD	C34-C35-C36-C37
37	E	101[B]	LHG	C24-C25-C26-C27
37	l	101[A]	LHG	C27-C28-C29-C30
35	c	517[A]	DGD	O6D-C5D-C6D-O5D
35	c	517[B]	DGD	O6D-C5D-C6D-O5D
26	B	620	SQD	C11-C10-C9-C8
32	t	101	LMT	O1'-C1-C2-C3
35	H	102	DGD	C9B-CAB-CBB-CCB
29	d	405[B]	PL9	C15-C14-C16-C17
29	A	414[A]	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
29	A	414[B]	PL9	C12-C11-C9-C8
29	D	408[A]	PL9	C13-C14-C16-C17
29	d	405[B]	PL9	C13-C14-C16-C17
27	A	701	GOL	O1-C1-C2-O2
27	B	624	GOL	O2-C2-C3-O3
27	D	701	GOL	O1-C1-C2-O2
27	D	701	GOL	O2-C2-C3-O3
27	O	501	GOL	O1-C1-C2-O2
27	V	401[A]	GOL	O2-C2-C3-O3
27	a	412	GOL	O1-C1-C2-O2
27	a	412	GOL	O2-C2-C3-O3
27	a	701	GOL	O1-C1-C2-O2
27	b	624	GOL	O2-C2-C3-O3
27	c	743	GOL	O2-C2-C3-O3
27	o	501	GOL	O2-C2-C3-O3
33	a	419	LMG	C21-C22-C23-C24
35	C	517[B]	DGD	C5B-C6B-C7B-C8B
35	h	102	DGD	C7B-C8B-C9B-CAB
37	d	711[A]	LHG	C24-C25-C26-C27
32	M	101	LMT	O5'-C5'-C6'-O6'
32	b	627	LMT	C3-C4-C5-C6
33	C	501	LMG	C39-C40-C41-C42
32	a	420	LMT	C1-C2-C3-C4
23	D	405[B]	CLA	C2B-C3B-CAB-CBB
23	b	604	CLA	C2B-C3B-CAB-CBB
37	E	101[A]	LHG	O2-C2-C3-O3
33	B	621	LMG	C15-C16-C17-C18
37	D	410[A]	LHG	C12-C13-C14-C15
35	H	102	DGD	C5B-C6B-C7B-C8B
33	m	101	LMG	O9-C10-O7-C8
23	B	616	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C1-O2A-CGA
35	C	517[A]	DGD	O6D-C5D-C6D-O5D
26	a	413	SQD	C31-C32-C33-C34
26	f	102	SQD	C25-C26-C27-C28
32	b	621	LMT	C11-C10-C9-C8
23	A	404[B]	CLA	C13-C15-C16-C17
23	B	603	CLA	C13-C15-C16-C17
23	B	615	CLA	C10-C11-C12-C13
37	D	409[A]	LHG	C34-C35-C36-C37
23	B	610	CLA	C16-C17-C18-C19
25	D	407	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
25	Y	101	BCR	C1-C6-C7-C8
25	b	617	BCR	C1-C6-C7-C8
25	b	617	BCR	C5-C6-C7-C8
25	b	619	BCR	C5-C6-C7-C8
25	d	404	BCR	C23-C24-C25-C26
25	y	101	BCR	C1-C6-C7-C8
35	c	517[A]	DGD	C7A-C8A-C9A-CAA
23	C	513	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C27-C28-C29-C30
37	d	408[A]	LHG	C29-C30-C31-C32
37	d	711[B]	LHG	C29-C30-C31-C32
35	c	518[A]	DGD	C6A-C7A-C8A-C9A
37	d	407[A]	LHG	C34-C35-C36-C37
23	c	506	CLA	C4-C3-C5-C6
24	a	408[B]	PHO	C4-C3-C5-C6
29	A	414[A]	PL9	C45-C44-C46-C47
29	D	408[B]	PL9	C15-C14-C16-C17
29	a	416[A]	PL9	C12-C11-C9-C10
23	B	602	CLA	C11-C12-C13-C15
23	B	613	CLA	C11-C10-C8-C7
23	B	614	CLA	C11-C10-C8-C7
23	C	506	CLA	C2-C3-C5-C6
23	C	511	CLA	C2-C3-C5-C6
23	C	511	CLA	C11-C12-C13-C15
23	D	406	CLA	C11-C10-C8-C7
23	a	407[A]	CLA	C11-C12-C13-C15
23	a	407[B]	CLA	C11-C12-C13-C15
23	c	506	CLA	C2-C3-C5-C6
24	a	408[B]	PHO	C2-C3-C5-C6
29	d	405[A]	PL9	C13-C14-C16-C17
35	c	518[A]	DGD	C4A-C5A-C6A-C7A
37	D	409[A]	LHG	C12-C13-C14-C15
23	d	402[B]	CLA	C16-C17-C18-C20
23	d	403	CLA	C16-C17-C18-C19
23	c	513	CLA	CBA-CGA-O2A-C1
35	c	517[B]	DGD	C2A-C1A-O1G-C1G
32	e	102	LMT	C1-C2-C3-C4
26	b	620	SQD	C27-C28-C29-C30
26	b	620	SQD	C28-C29-C30-C31
32	e	102	LMT	O5B-C5B-C6B-O6B
33	D	415	LMG	C12-C13-C14-C15
26	A	410[B]	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
32	D	404	LMT	C5'-C4'-O1B-C1B
37	d	408[A]	LHG	C25-C26-C27-C28
23	c	513	CLA	O1D-CGD-O2D-CED
23	A	406[B]	CLA	C13-C15-C16-C17
26	A	412	SQD	C26-C27-C28-C29
35	c	517[A]	DGD	CAA-CBA-CCA-CDA
37	D	409[B]	LHG	C26-C27-C28-C29
37	D	411[A]	LHG	C13-C14-C15-C16
32	D	404	LMT	C1-C2-C3-C4
26	A	410[B]	SQD	C11-C10-C9-C8
35	c	517[B]	DGD	CAA-CBA-CCA-CDA
35	c	517[B]	DGD	C4D-C5D-C6D-O5D
23	B	608	CLA	C16-C17-C18-C20
33	c	520	LMG	C4-C5-C6-O5
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
32	b	627	LMT	C5-C6-C7-C8
33	a	419	LMG	C29-C30-C31-C32
35	C	517[B]	DGD	C9A-CAA-CBA-CCA
37	D	411[A]	LHG	C15-C16-C17-C18
33	c	520	LMG	C33-C34-C35-C36
37	D	411[B]	LHG	C29-C30-C31-C32
37	d	408[B]	LHG	C34-C35-C36-C37
23	C	503	CLA	C15-C16-C17-C18
35	H	102	DGD	C7A-C8A-C9A-CAA
32	a	414	LMT	C5-C6-C7-C8
33	z	101	LMG	C14-C15-C16-C17
37	L	101[B]	LHG	C27-C28-C29-C30
40	v	202	HEC	C2B-C3B-CAB-CBB
26	A	410[A]	SQD	O6-C44-C45-O47
26	A	410[B]	SQD	O6-C44-C45-O47
33	m	101	LMG	C38-C39-C40-C41
35	c	517[B]	DGD	C7A-C8A-C9A-CAA
37	d	408[A]	LHG	C34-C35-C36-C37
37	d	711[A]	LHG	C25-C26-C27-C28
32	a	414	LMT	C6-C7-C8-C9
37	d	711[B]	LHG	C25-C26-C27-C28
29	a	416[B]	PL9	C12-C11-C9-C10
33	C	520	LMG	C37-C38-C39-C40
23	B	602	CLA	C11-C12-C13-C14
23	B	606	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C11-C12-C13-C14
23	D	406	CLA	C11-C10-C8-C9
23	D	406	CLA	C14-C13-C15-C16
23	b	606	CLA	C11-C10-C8-C9
23	C	509	CLA	CBD-CGD-O2D-CED
35	c	518[A]	DGD	C2B-C3B-C4B-C5B
26	b	620	SQD	C26-C27-C28-C29
35	C	517[B]	DGD	O6E-C5E-C6E-O5E
23	A	406[A]	CLA	C13-C15-C16-C17
23	B	615	CLA	C13-C15-C16-C17
37	D	411[B]	LHG	C13-C14-C15-C16
23	C	513	CLA	O1A-CGA-O2A-C1
23	A	405[B]	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	B	611	CLA	C1A-C2A-CAA-CBA
33	D	415	LMG	O6-C5-C6-O5
23	B	610	CLA	C16-C17-C18-C20
23	b	606	CLA	C16-C17-C18-C20
26	F	101	SQD	C34-C35-C36-C37
26	a	411[A]	SQD	C9-C10-C11-C12
26	b	620	SQD	C30-C31-C32-C33
32	t	102	LMT	C7-C8-C9-C10
37	D	409[A]	LHG	C26-C27-C28-C29
23	B	615	CLA	C5-C6-C7-C8
37	D	410[A]	LHG	C4-O6-P-O3
37	d	407[B]	LHG	C4-O6-P-O3
37	D	411[B]	LHG	C15-C16-C17-C18
37	L	101[B]	LHG	C17-C18-C19-C20
23	A	405[B]	CLA	C15-C16-C17-C18
37	d	407[B]	LHG	C11-C10-C9-C8
33	c	520	LMG	C10-C11-C12-C13
35	c	518[B]	DGD	C2B-C3B-C4B-C5B
37	D	410[B]	LHG	C13-C14-C15-C16
37	d	408[A]	LHG	C28-C29-C30-C31
35	c	517[B]	DGD	O6E-C5E-C6E-O5E
32	I	101	LMT	C3'-C4'-O1B-C1B
34	B	622	HTG	C2'-C3'-C4'-C5'
23	B	608	CLA	C13-C15-C16-C17
35	C	517[A]	DGD	C8A-C9A-CAA-CBA
35	c	517[A]	DGD	C4D-C5D-C6D-O5D
23	C	506	CLA	C4-C3-C5-C6
33	d	412	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
33	Z	101	LMG	C19-C20-C21-C22
35	c	519	DGD	CBA-CCA-CDA-CEA
37	l	101[B]	LHG	C13-C14-C15-C16
23	b	601	CLA	C8-C10-C11-C12
32	A	359	LMT	O5B-C5B-C6B-O6B
26	a	411[B]	SQD	C9-C10-C11-C12
33	m	101	LMG	C14-C15-C16-C17
33	c	520	LMG	C30-C31-C32-C33
37	D	410[A]	LHG	C10-C11-C12-C13
23	B	608	CLA	C16-C17-C18-C19
23	c	509	CLA	C16-C17-C18-C20
23	d	402[A]	CLA	C16-C17-C18-C19
23	C	512	CLA	C3-C5-C6-C7
26	A	412	SQD	O6-C44-C45-C46
26	a	411[A]	SQD	O6-C44-C45-C46
26	a	411[B]	SQD	O6-C44-C45-C46
26	f	102	SQD	C44-C45-C46-O48
35	C	518[A]	DGD	CDA-CEA-CFA-CGA
35	c	518[B]	DGD	C4A-C5A-C6A-C7A
37	E	101[A]	LHG	C4-C5-C6-O8
37	E	101[B]	LHG	C4-C5-C6-O8
37	d	408[B]	LHG	C27-C28-C29-C30
23	C	511	CLA	C10-C11-C12-C13
33	a	419	LMG	C4-C5-C6-O5
35	C	518[A]	DGD	C2G-C3G-O3G-C1D
35	C	518[B]	DGD	C5D-C6D-O5D-C1E
35	c	518[A]	DGD	C2G-C3G-O3G-C1D
35	c	518[A]	DGD	C5D-C6D-O5D-C1E
35	c	518[B]	DGD	C2G-C3G-O3G-C1D
35	c	518[B]	DGD	C5D-C6D-O5D-C1E
37	D	409[B]	LHG	C12-C13-C14-C15
37	D	409[B]	LHG	C34-C35-C36-C37
37	l	101[A]	LHG	C9-C10-C11-C12
33	d	412	LMG	O6-C5-C6-O5
34	b	623	HTG	O5-C5-C6-O6
37	D	411[A]	LHG	C29-C30-C31-C32
35	C	518[B]	DGD	CDA-CEA-CFA-CGA
37	d	711[A]	LHG	C33-C34-C35-C36
27	o	601	GOL	O2-C2-C3-O3
37	D	411[B]	LHG	C17-C18-C19-C20
35	H	102	DGD	C4E-C5E-C6E-O5E
35	c	517[B]	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
35	h	102	DGD	CAB-CBB-CCB-CDB
35	C	517[A]	DGD	O6E-C5E-C6E-O5E
35	c	517[A]	DGD	O6E-C5E-C6E-O5E
32	a	420	LMT	C9-C10-C11-C12
23	c	503	CLA	C16-C17-C18-C19
23	d	402[B]	CLA	C16-C17-C18-C19
33	c	521	LMG	C29-C28-O8-C9
23	c	512	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	C5-C6-C7-C8
23	a	406[A]	CLA	C2C-C3C-CAC-CBC
35	c	519	DGD	C2B-C3B-C4B-C5B
37	l	101[B]	LHG	C17-C18-C19-C20
26	B	620	SQD	C46-C45-O47-C7
26	b	620	SQD	C46-C45-O47-C7
23	b	610	CLA	C15-C16-C17-C18
23	A	408	CLA	C2-C1-O2A-CGA
26	a	411[A]	SQD	C12-C13-C14-C15
35	h	102	DGD	CDB-CEB-CFB-CGB
37	D	410[B]	LHG	C12-C13-C14-C15
33	a	419	LMG	C35-C36-C37-C38
35	c	517[A]	DGD	C2A-C1A-O1G-C1G
23	C	514	CLA	O1D-CGD-O2D-CED
33	c	520	LMG	C34-C35-C36-C37
35	c	518[B]	DGD	C6A-C7A-C8A-C9A
37	D	411[A]	LHG	C17-C18-C19-C20
35	C	517[B]	DGD	O6D-C5D-C6D-O5D
26	A	410[A]	SQD	C11-C10-C9-C8
32	e	102	LMT	C9-C10-C11-C12
35	C	517[B]	DGD	C8A-C9A-CAA-CBA
35	C	519	DGD	C7B-C8B-C9B-CAB
37	D	409[A]	LHG	O2-C2-C3-O3
23	C	504	CLA	O1D-CGD-O2D-CED
33	C	520	LMG	C11-C12-C13-C14
35	c	518[B]	DGD	CBB-CCB-CDB-CEB
23	B	610	CLA	C13-C15-C16-C17
23	C	512	CLA	C8-C10-C11-C12
35	c	518[B]	DGD	C2E-C1E-O5D-C6D
37	E	101[A]	LHG	C25-C26-C27-C28
37	d	408[A]	LHG	C33-C34-C35-C36
26	a	411[B]	SQD	O6-C44-C45-O47
26	b	620	SQD	C11-C10-C9-C8
32	a	420	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
32	b	621	LMT	C7-C8-C9-C10
37	E	101[A]	LHG	C13-C14-C15-C16
23	A	404[A]	CLA	C13-C15-C16-C17
33	C	521	LMG	C35-C36-C37-C38
23	C	514	CLA	C11-C10-C8-C7
23	C	514	CLA	C11-C12-C13-C15
23	D	406	CLA	C12-C13-C15-C16
23	b	604	CLA	C6-C7-C8-C10
23	b	606	CLA	C11-C10-C8-C7
23	b	614	CLA	C12-C13-C15-C16
23	b	616	CLA	C6-C7-C8-C10
23	c	506	CLA	C11-C12-C13-C15
23	c	507	CLA	C11-C10-C8-C7
29	d	405[B]	PL9	C28-C29-C31-C32
23	b	601	CLA	CAA-CBA-CGA-O2A
23	C	505	CLA	C14-C13-C15-C16
23	C	506	CLA	C11-C12-C13-C14
23	C	507	CLA	C6-C7-C8-C9
23	C	514	CLA	C11-C10-C8-C9
23	c	506	CLA	C11-C12-C13-C14
33	z	101	LMG	C13-C14-C15-C16
37	d	408[B]	LHG	C29-C30-C31-C32
26	b	620	SQD	C24-C23-O48-C46
32	a	414	LMT	C3-C4-C5-C6
40	V	202	HEC	C2B-C3B-CAB-CBB
37	L	101[B]	LHG	C24-C25-C26-C27
27	d	801[A]	GOL	O1-C1-C2-C3
32	b	627	LMT	C1-C2-C3-C4
23	C	513	CLA	C3-C5-C6-C7
32	I	101	LMT	C5-C6-C7-C8
23	B	601	CLA	CBA-CGA-O2A-C1
33	C	520	LMG	C34-C35-C36-C37
37	e	101[A]	LHG	C23-C24-C25-C26
23	B	613	CLA	C13-C15-C16-C17
23	c	513	CLA	C10-C11-C12-C13
26	b	620	SQD	C13-C14-C15-C16
35	C	517[B]	DGD	C7A-C8A-C9A-CAA
37	d	711[B]	LHG	C24-C25-C26-C27
23	C	510	CLA	CBD-CGD-O2D-CED
23	a	406[B]	CLA	C2C-C3C-CAC-CBC
23	B	602	CLA	C4B-C3B-CAB-CBB
23	C	505	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	a	407[A]	CLA	C4B-C3B-CAB-CBB
23	B	612	CLA	C10-C11-C12-C13
29	A	414[A]	PL9	C39-C41-C42-C43
29	A	414[B]	PL9	C39-C41-C42-C43
32	D	404	LMT	C3'-C4'-O1B-C1B
32	a	420	LMT	C2-C3-C4-C5
35	h	102	DGD	C9B-CAB-CBB-CCB
35	c	519	DGD	C2A-C1A-O1G-C1G
29	D	408[A]	PL9	C45-C44-C46-C47
29	D	408[B]	PL9	C13-C14-C16-C17
37	D	410[B]	LHG	O2-C2-C3-O3
35	c	518[A]	DGD	CBB-CCB-CDB-CEB
35	C	519	DGD	CDB-CEB-CFB-CGB
37	E	101[B]	LHG	C25-C26-C27-C28
35	C	517[A]	DGD	CCA-CDA-CEA-CFA
33	c	521	LMG	O10-C28-O8-C9
37	E	101[B]	LHG	C13-C14-C15-C16
37	e	101[A]	LHG	C10-C11-C12-C13
32	b	627	LMT	C2-C1-O1'-C1'
32	e	102	LMT	C2-C1-O1'-C1'
32	m	103	LMT	C2-C1-O1'-C1'
33	z	101	LMG	C20-C21-C22-C23
37	D	410[B]	LHG	C10-C11-C12-C13
37	d	407[B]	LHG	C16-C17-C18-C19
23	B	606	CLA	C8-C10-C11-C12
23	c	513	CLA	O1A-CGA-O2A-C1
37	d	408[B]	LHG	C24-C23-O8-C6
26	a	413	SQD	C15-C16-C17-C18
33	C	521	LMG	C38-C39-C40-C41
26	A	410[A]	SQD	O6-C44-C45-C46
26	A	410[B]	SQD	O6-C44-C45-C46
26	B	620	SQD	C44-C45-C46-O48
37	e	101[A]	LHG	C4-C5-C6-O8
37	e	101[B]	LHG	C4-C5-C6-O8
37	L	101[A]	LHG	C27-C28-C29-C30
35	C	517[A]	DGD	C1B-C2B-C3B-C4B
35	h	102	DGD	CBA-CCA-CDA-CEA
37	D	409[B]	LHG	C32-C33-C34-C35
37	d	407[B]	LHG	C13-C14-C15-C16
23	b	607	CLA	C3-C5-C6-C7
35	h	102	DGD	C2B-C3B-C4B-C5B
35	c	517[A]	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
29	D	408[A]	PL9	C15-C14-C16-C17
29	D	408[A]	PL9	C43-C44-C46-C47
35	C	517[A]	DGD	C4D-C5D-C6D-O5D
35	C	517[A]	DGD	C7A-C8A-C9A-CAA
35	C	519	DGD	CAB-CBB-CCB-CDB
37	e	101[B]	LHG	C10-C11-C12-C13
37	d	711[A]	LHG	C3-O3-P-O6
26	F	101	SQD	C7-C8-C9-C10
34	B	626	HTG	C2'-C3'-C4'-C5'
27	v	401[A]	GOL	O1-C1-C2-O2
35	C	517[A]	DGD	C3B-C4B-C5B-C6B
37	d	711[B]	LHG	C33-C34-C35-C36
35	C	517[B]	DGD	C4D-C5D-C6D-O5D
23	C	512	CLA	CBA-CGA-O2A-C1
23	c	512	CLA	CBA-CGA-O2A-C1
32	b	627	LMT	C6-C7-C8-C9
37	d	408[B]	LHG	C9-C10-C11-C12
37	d	408[B]	LHG	C28-C29-C30-C31
23	A	406[A]	CLA	C16-C17-C18-C20
23	B	605	CLA	C5-C6-C7-C8
26	a	413	SQD	C18-C19-C20-C21
23	B	602	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB
23	a	407[A]	CLA	C2B-C3B-CAB-CBB
23	a	406[B]	CLA	C15-C16-C17-C18
23	B	601	CLA	O1A-CGA-O2A-C1
26	B	620	SQD	O47-C45-C46-O48
26	a	411[A]	SQD	O6-C44-C45-O47
26	b	620	SQD	O47-C45-C46-O48
26	f	102	SQD	O47-C45-C46-O48
37	D	411[B]	LHG	C24-C23-O8-C6
26	a	411[B]	SQD	C12-C13-C14-C15
23	b	606	CLA	C16-C17-C18-C19
35	c	517[A]	DGD	O6E-C1E-O5D-C6D
35	c	518[B]	DGD	O6E-C1E-O5D-C6D
29	a	416[A]	PL9	C24-C26-C27-C28
37	D	409[A]	LHG	C1-C2-C3-O3
26	a	411[B]	SQD	C34-C35-C36-C37
23	A	404[B]	CLA	C2-C1-O2A-CGA
23	b	608	CLA	C2-C1-O2A-CGA
23	b	613	CLA	C2-C1-O2A-CGA
29	a	416[B]	PL9	C12-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C6-C7-C8-C9
23	B	610	CLA	C14-C13-C15-C16
23	B	614	CLA	C14-C13-C15-C16
23	C	511	CLA	C14-C13-C15-C16
23	C	513	CLA	C6-C7-C8-C9
23	b	601	CLA	C6-C7-C8-C9
23	c	513	CLA	C6-C7-C8-C9
23	c	514	CLA	C6-C7-C8-C9
23	d	403	CLA	C11-C12-C13-C14
32	E	102	LMT	C4-C5-C6-C7
33	m	101	LMG	C37-C38-C39-C40
37	d	408[B]	LHG	C2-C3-O3-P
37	D	411[A]	LHG	C27-C28-C29-C30
37	L	101[B]	LHG	C10-C11-C12-C13
37	l	101[A]	LHG	C34-C35-C36-C37
23	c	503	CLA	C16-C17-C18-C20
25	H	101	BCR	C23-C24-C25-C26
25	H	101	BCR	C23-C24-C25-C30
25	a	410	BCR	C23-C24-C25-C26
25	b	619	BCR	C1-C6-C7-C8
25	h	101	BCR	C23-C24-C25-C26
23	b	602	CLA	C10-C11-C12-C13
23	b	613	CLA	O1D-CGD-O2D-CED
26	a	411[B]	SQD	C27-C28-C29-C30
37	L	101[A]	LHG	C11-C10-C9-C8
23	B	602	CLA	C15-C16-C17-C18
26	A	410[A]	SQD	C18-C19-C20-C21
23	c	507	CLA	CBD-CGD-O2D-CED
37	e	101[A]	LHG	C7-C8-C9-C10
35	C	518[A]	DGD	C5B-C6B-C7B-C8B
26	b	620	SQD	O10-C23-O48-C46
33	C	520	LMG	C36-C37-C38-C39
37	l	101[A]	LHG	C13-C14-C15-C16
23	B	601	CLA	C15-C16-C17-C18
37	D	410[B]	LHG	O6-C4-C5-C6
37	L	101[A]	LHG	O6-C4-C5-C6
33	B	621	LMG	C18-C19-C20-C21
35	C	518[A]	DGD	C8B-C9B-CAB-CBB
23	B	610	CLA	C12-C13-C15-C16
23	B	614	CLA	C12-C13-C15-C16
23	C	503	CLA	C12-C13-C15-C16
23	C	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	C	506	CLA	C11-C12-C13-C15
23	C	507	CLA	C6-C7-C8-C10
23	C	511	CLA	C12-C13-C15-C16
23	a	409	CLA	C11-C10-C8-C7
23	b	601	CLA	C6-C7-C8-C10
23	b	601	CLA	C11-C10-C8-C7
23	c	505	CLA	C11-C12-C13-C15
23	c	505	CLA	C12-C13-C15-C16
23	c	510	CLA	C6-C7-C8-C10
23	d	402[B]	CLA	C11-C12-C13-C15
29	a	416[A]	PL9	C12-C11-C9-C8
34	B	626	HTG	S1-C1'-C2'-C3'
35	c	517[A]	DGD	CCB-CDB-CEB-CFB
37	D	410[A]	LHG	C11-C10-C9-C8
26	a	411[A]	SQD	C27-C28-C29-C30
37	L	101[A]	LHG	C24-C25-C26-C27
37	D	411[A]	LHG	C10-C11-C12-C13
37	d	407[A]	LHG	C13-C14-C15-C16
23	C	513	CLA	O1D-CGD-O2D-CED
23	C	508	CLA	C13-C15-C16-C17
23	b	615	CLA	C5-C6-C7-C8
23	B	601	CLA	C2A-CAA-CBA-CGA
35	C	518[A]	DGD	C7A-C8A-C9A-CAA
34	c	522	HTG	C2'-C1'-S1-C1
34	b	622	HTG	C1'-C2'-C3'-C4'
32	I	101	LMT	C4-C5-C6-C7
32	a	420	LMT	O5'-C5'-C6'-O6'
23	b	601	CLA	CBA-CGA-O2A-C1
37	d	407[B]	LHG	C24-C23-O8-C6
32	b	621	LMT	C3-C4-C5-C6
33	C	501	LMG	C13-C14-C15-C16
37	D	410[B]	LHG	C11-C10-C9-C8
37	d	711[B]	LHG	C17-C18-C19-C20
32	e	102	LMT	C3-C4-C5-C6
23	A	404[B]	CLA	CAD-CBD-CGD-O2D
23	B	616	CLA	CAD-CBD-CGD-O2D
23	b	604	CLA	CAD-CBD-CGD-O2D
23	b	612	CLA	CAD-CBD-CGD-O2D
23	b	616	CLA	CAD-CBD-CGD-O2D
23	c	511	CLA	CAD-CBD-CGD-O2D
24	A	407[B]	PHO	CAD-CBD-CGD-O2D
24	a	408[A]	PHO	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	a	408[B]	PHO	CAD-CBD-CGD-O2D
38	e	87	HEM	C2C-C3C-CAC-CBC
37	l	101[B]	LHG	C9-C10-C11-C12
23	b	605	CLA	C5-C6-C7-C8
37	e	101[B]	LHG	C23-C24-C25-C26
23	B	601	CLA	CAA-CBA-CGA-O2A
33	c	520	LMG	C32-C33-C34-C35
33	z	101	LMG	C19-C20-C21-C22
23	C	507	CLA	C4-C3-C5-C6
29	d	405[A]	PL9	C45-C44-C46-C47
23	A	406[B]	CLA	C16-C17-C18-C20
26	a	411[A]	SQD	C34-C35-C36-C37
33	a	419	LMG	C33-C34-C35-C36
35	c	517[B]	DGD	O6E-C1E-O5D-C6D
35	c	518[A]	DGD	O6E-C1E-O5D-C6D
26	a	413	SQD	O6-C44-C45-C46
26	b	620	SQD	C44-C45-C46-O48
26	f	102	SQD	O6-C44-C45-C46
35	c	519	DGD	O1A-C1A-O1G-C1G
35	C	517[B]	DGD	CCA-CDA-CEA-CFA
37	D	410[B]	LHG	O6-C4-C5-O7
37	E	101[A]	LHG	O6-C4-C5-O7
37	L	101[A]	LHG	O6-C4-C5-O7
23	b	612	CLA	C10-C11-C12-C13
23	d	403	CLA	CBA-CGA-O2A-C1
34	B	626	HTG	C4'-C5'-C6'-C7'
23	B	601	CLA	CHA-CBD-CGD-O2D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O1D
23	c	503	CLA	CHA-CBD-CGD-O1D
23	C	512	CLA	O1A-CGA-O2A-C1
23	c	512	CLA	O1A-CGA-O2A-C1
23	d	403	CLA	O1A-CGA-O2A-C1
37	D	411[B]	LHG	O10-C23-O8-C6
37	d	408[B]	LHG	O10-C23-O8-C6
32	D	404	LMT	C7-C8-C9-C10
35	c	517[A]	DGD	C2E-C1E-O5D-C6D
35	c	518[A]	DGD	C2E-C1E-O5D-C6D
32	E	102	LMT	C2-C3-C4-C5
33	C	501	LMG	C11-C12-C13-C14
37	D	409[A]	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
37	e	101[A]	LHG	O7-C5-C6-O8
37	e	101[B]	LHG	O7-C5-C6-O8
26	A	410[A]	SQD	C34-C35-C36-C37
26	B	620	SQD	C29-C30-C31-C32
26	b	620	SQD	C14-C15-C16-C17
33	d	412	LMG	C18-C19-C20-C21
37	d	407[B]	LHG	O10-C23-O8-C6
33	c	520	LMG	C29-C30-C31-C32
27	B	624	GOL	O1-C1-C2-O2
27	c	743	GOL	O1-C1-C2-O2
37	d	407[A]	LHG	C11-C10-C9-C8
37	d	408[A]	LHG	C9-C10-C11-C12
23	c	510	CLA	C10-C11-C12-C13
29	D	408[B]	PL9	C4-C3-C7-C8
37	D	410[B]	LHG	C28-C29-C30-C31
23	b	615	CLA	C13-C15-C16-C17
23	c	507	CLA	C10-C11-C12-C13
23	C	514	CLA	C6-C7-C8-C9
23	c	510	CLA	C6-C7-C8-C9
23	c	511	CLA	CBD-CGD-O2D-CED
35	c	517[B]	DGD	CCB-CDB-CEB-CFB
23	c	507	CLA	C13-C15-C16-C17
33	C	521	LMG	C4-C5-C6-O5
23	b	605	CLA	C3-C5-C6-C7
26	a	413	SQD	C24-C25-C26-C27
33	C	520	LMG	C31-C32-C33-C34
23	b	601	CLA	O1A-CGA-O2A-C1
33	d	412	LMG	C28-C29-C30-C31
33	C	501	LMG	C18-C19-C20-C21
27	o	601	GOL	O1-C1-C2-C3
25	y	101	BCR	C21-C22-C23-C24
37	d	711[A]	LHG	C18-C19-C20-C21
23	a	406[A]	CLA	C1A-C2A-CAA-CBA
23	c	509	CLA	C1A-C2A-CAA-CBA
23	c	514	CLA	C1A-C2A-CAA-CBA
37	d	407[A]	LHG	C16-C17-C18-C19
26	A	412	SQD	C24-C23-O48-C46
35	C	518[B]	DGD	C8B-C9B-CAB-CBB
26	a	411[A]	SQD	C35-C36-C37-C38
37	D	411[A]	LHG	C2-C3-O3-P
37	D	411[B]	LHG	C2-C3-O3-P
26	A	412	SQD	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
33	C	501	LMG	C20-C21-C22-C23
35	C	518[B]	DGD	C7A-C8A-C9A-CAA
23	a	407[B]	CLA	C4B-C3B-CAB-CBB
23	b	606	CLA	C4B-C3B-CAB-CBB
37	D	410[A]	LHG	C4-O6-P-O5
37	E	101[A]	LHG	C4-O6-P-O5
37	d	407[B]	LHG	C3-O3-P-O5
37	d	407[B]	LHG	C4-O6-P-O5
37	e	101[A]	LHG	C4-O6-P-O4
37	e	101[B]	LHG	C4-O6-P-O4
23	b	608	CLA	C16-C17-C18-C20
32	M	101	LMT	C2-C3-C4-C5
23	C	511	CLA	C13-C15-C16-C17
23	b	610	CLA	C13-C15-C16-C17
37	E	101[A]	LHG	O6-C4-C5-C6
32	D	404	LMT	C9-C10-C11-C12
33	d	412	LMG	C35-C36-C37-C38
34	c	522	HTG	C4'-C5'-C6'-C7'
33	B	621	LMG	C29-C30-C31-C32
23	c	513	CLA	C13-C15-C16-C17
33	B	621	LMG	C32-C33-C34-C35
37	L	101[A]	LHG	C26-C27-C28-C29
35	c	518[A]	DGD	C7B-C8B-C9B-CAB
23	B	601	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	b	601	CLA	CAD-CBD-CGD-O1D
23	c	503	CLA	CAD-CBD-CGD-O1D
23	c	512	CLA	C8-C10-C11-C12
35	C	517[A]	DGD	C6A-C7A-C8A-C9A
26	f	102	SQD	C23-C24-C25-C26
23	C	511	CLA	CBA-CGA-O2A-C1
32	t	102	LMT	C11-C10-C9-C8
23	C	507	CLA	C16-C17-C18-C20
23	A	406[A]	CLA	C12-C13-C15-C16
23	A	406[B]	CLA	C12-C13-C15-C16
23	b	608	CLA	C12-C13-C15-C16
23	b	615	CLA	C12-C13-C15-C16
23	c	506	CLA	C12-C13-C15-C16
23	c	510	CLA	C11-C10-C8-C7
23	c	511	CLA	C11-C10-C8-C7
23	c	511	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
23	c	513	CLA	C12-C13-C15-C16
23	d	402[A]	CLA	C11-C12-C13-C15
26	A	410[A]	SQD	C13-C14-C15-C16
23	C	510	CLA	C3-C5-C6-C7
37	D	410[B]	LHG	C34-C35-C36-C37
37	D	410[A]	LHG	C34-C35-C36-C37
35	c	518[B]	DGD	C5A-C6A-C7A-C8A
23	C	511	CLA	O1A-CGA-O2A-C1
35	c	518[A]	DGD	C5A-C6A-C7A-C8A
35	h	102	DGD	C5B-C6B-C7B-C8B
35	C	517[B]	DGD	C1B-C2B-C3B-C4B
26	F	101	SQD	O47-C45-C46-O48
37	E	101[A]	LHG	O7-C5-C6-O8
37	E	101[B]	LHG	O7-C5-C6-O8
35	C	518[A]	DGD	C8A-C9A-CAA-CBA
37	D	411[B]	LHG	C27-C28-C29-C30
37	d	408[A]	LHG	C32-C33-C34-C35
35	C	518[A]	DGD	C5D-C6D-O5D-C1E
35	C	518[B]	DGD	C2G-C3G-O3G-C1D
35	H	102	DGD	O2G-C1B-C2B-C3B
23	B	601	CLA	C13-C15-C16-C17
23	c	504	CLA	C8-C10-C11-C12
37	d	408[A]	LHG	C2-C3-O3-P
26	A	412	SQD	O10-C23-O48-C46
35	C	519	DGD	C7A-C8A-C9A-CAA
37	d	711[A]	LHG	C34-C35-C36-C37
23	a	409	CLA	C11-C10-C8-C9
37	D	410[A]	LHG	C26-C27-C28-C29
29	a	416[B]	PL9	C24-C26-C27-C28
32	E	102	LMT	C6-C7-C8-C9
37	l	101[B]	LHG	C34-C35-C36-C37
27	O	601	GOL	O1-C1-C2-O2
27	o	601	GOL	O1-C1-C2-O2
35	C	518[A]	DGD	C7B-C8B-C9B-CAB
37	d	711[A]	LHG	C11-C12-C13-C14
32	b	627	LMT	O1'-C1-C2-C3
37	D	410[B]	LHG	C26-C27-C28-C29
23	C	511	CLA	C8-C10-C11-C12
35	C	517[B]	DGD	C2A-C3A-C4A-C5A
35	C	518[B]	DGD	C5B-C6B-C7B-C8B
23	D	405[A]	CLA	C2B-C3B-CAB-CBB
23	a	407[B]	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	b	606	CLA	C2B-C3B-CAB-CBB
23	c	503	CLA	C2B-C3B-CAB-CBB
35	C	517[B]	DGD	C3B-C4B-C5B-C6B
33	c	521	LMG	C32-C33-C34-C35
23	C	509	CLA	O1D-CGD-O2D-CED
29	a	416[A]	PL9	C43-C44-C46-C47
37	L	101[A]	LHG	C23-C24-C25-C26
33	Z	101	LMG	C11-C12-C13-C14
37	D	410[A]	LHG	C13-C14-C15-C16
37	l	101[B]	LHG	C12-C13-C14-C15
35	C	519	DGD	CBA-CCA-CDA-CEA
37	l	101[A]	LHG	C28-C29-C30-C31
23	B	613	CLA	C2-C1-O2A-CGA
23	C	507	CLA	C2-C1-O2A-CGA
23	b	614	CLA	C2-C1-O2A-CGA
35	C	517[B]	DGD	C6A-C7A-C8A-C9A
32	A	359	LMT	C9-C10-C11-C12
35	C	519	DGD	C9A-CAA-CBA-CCA
35	H	102	DGD	CCA-CDA-CEA-CFA
37	d	408[B]	LHG	C32-C33-C34-C35
35	C	519	DGD	CDA-CEA-CFA-CGA
35	H	102	DGD	C8A-C9A-CAA-CBA
34	d	411	HTG	S1-C1'-C2'-C3'
23	D	406	CLA	O1A-CGA-O2A-C1
37	L	101[B]	LHG	O6-C4-C5-O7
32	e	102	LMT	O1'-C1-C2-C3
25	h	101	BCR	C23-C24-C25-C30
29	A	414[A]	PL9	C28-C29-C31-C32
26	b	620	SQD	C16-C17-C18-C19
37	d	408[A]	LHG	C10-C11-C12-C13
23	c	507	CLA	O1D-CGD-O2D-CED
23	B	606	CLA	C15-C16-C17-C18
33	C	521	LMG	C20-C21-C22-C23
32	M	101	LMT	O5'-C1'-O1'-C1
32	a	420	LMT	O5'-C1'-O1'-C1
32	e	102	LMT	C2-C3-C4-C5
33	m	101	LMG	C2-C1-O1-C7
35	c	517[B]	DGD	C2E-C1E-O5D-C6D
33	d	412	LMG	C16-C17-C18-C19
37	d	711[B]	LHG	C3-O3-P-O6
37	e	101[B]	LHG	C7-C8-C9-C10
35	c	519	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	C	521	LMG	C12-C13-C14-C15
26	A	410[A]	SQD	C16-C17-C18-C19
40	v	202	HEC	C4B-C3B-CAB-CBB
33	a	419	LMG	C7-C8-C9-O8
23	c	511	CLA	C4-C3-C5-C6
29	d	405[B]	PL9	C45-C44-C46-C47
23	B	613	CLA	C11-C12-C13-C15
23	B	616	CLA	C12-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C15
35	h	102	DGD	O2G-C1B-C2B-C3B
23	B	607	CLA	C3-C5-C6-C7
23	a	406[A]	CLA	C4C-C3C-CAC-CBC
23	A	406[A]	CLA	C14-C13-C15-C16
23	A	406[B]	CLA	C14-C13-C15-C16
23	B	614	CLA	C11-C10-C8-C9
23	b	615	CLA	C14-C13-C15-C16
23	c	506	CLA	C14-C13-C15-C16
23	c	507	CLA	C11-C10-C8-C9
23	c	511	CLA	C11-C10-C8-C9
23	d	402[A]	CLA	C11-C12-C13-C14
23	d	402[B]	CLA	C11-C12-C13-C14
37	D	410[A]	LHG	C28-C29-C30-C31
24	a	408[A]	PHO	C2C-C3C-CAC-CBC
37	L	101[B]	LHG	C23-C24-C25-C26
37	d	407[B]	LHG	C25-C26-C27-C28
23	c	510	CLA	C8-C10-C11-C12
32	m	103	LMT	C9-C10-C11-C12
34	B	623	HTG	C4'-C5'-C6'-C7'
35	C	518[B]	DGD	C8A-C9A-CAA-CBA
37	l	101[B]	LHG	C10-C11-C12-C13
37	D	409[A]	LHG	O1-C1-C2-C3
37	D	409[B]	LHG	C17-C18-C19-C20
23	a	406[A]	CLA	C15-C16-C17-C18
35	c	518[B]	DGD	C1A-C2A-C3A-C4A
27	d	801[B]	GOL	O1-C1-C2-O2
27	v	401[B]	GOL	O1-C1-C2-O2
29	A	414[B]	PL9	C28-C29-C31-C32
23	b	608	CLA	C16-C17-C18-C19
38	E	103	HEM	CAD-CBD-CGD-O1D
26	a	411[A]	SQD	C11-C12-C13-C14
35	c	517[B]	DGD	CBA-CCA-CDA-CEA
23	a	406[B]	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
23	B	602	CLA	C8-C10-C11-C12
37	D	411[A]	LHG	O10-C23-O8-C6
37	D	411[A]	LHG	C24-C23-O8-C6
23	D	405[A]	CLA	C4B-C3B-CAB-CBB
23	c	503	CLA	C4B-C3B-CAB-CBB
23	b	612	CLA	C8-C10-C11-C12
37	L	101[B]	LHG	O6-C4-C5-C6
23	C	503	CLA	C3-C5-C6-C7
23	b	601	CLA	C3-C5-C6-C7
35	C	519	DGD	O1A-C1A-O1G-C1G
33	z	101	LMG	O7-C10-C11-C12
23	b	616	CLA	C5-C6-C7-C8
23	a	405[B]	CLA	C2C-C3C-CAC-CBC
23	a	405[B]	CLA	C4C-C3C-CAC-CBC
33	Z	101	LMG	C29-C28-O8-C9
26	F	101	SQD	C32-C33-C34-C35
35	c	518[B]	DGD	C7B-C8B-C9B-CAB
33	d	412	LMG	C10-C11-C12-C13
38	e	87	HEM	C4C-C3C-CAC-CBC
34	b	623	HTG	S1-C1'-C2'-C3'
24	a	408[A]	PHO	C4-C3-C5-C6
23	B	611	CLA	C8-C10-C11-C12
33	C	501	LMG	C29-C30-C31-C32
23	c	512	CLA	O1D-CGD-O2D-CED
24	a	408[A]	PHO	C2-C3-C5-C6
37	d	408[B]	LHG	C25-C26-C27-C28
23	b	601	CLA	C13-C15-C16-C17
35	C	519	DGD	C3B-C4B-C5B-C6B
23	d	402[B]	CLA	C2-C1-O2A-CGA
26	a	411[B]	SQD	C35-C36-C37-C38
23	c	510	CLA	C15-C16-C17-C18
23	A	404[B]	CLA	C2A-CAA-CBA-CGA
23	C	502	CLA	C2A-CAA-CBA-CGA
35	c	517[A]	DGD	C4B-C5B-C6B-C7B
37	D	409[B]	LHG	C18-C19-C20-C21
23	c	502	CLA	CBD-CGD-O2D-CED
37	d	407[A]	LHG	C9-C10-C11-C12
35	c	518[B]	DGD	C9B-CAB-CBB-CCB
37	D	410[A]	LHG	C17-C18-C19-C20
23	b	601	CLA	C4-C3-C5-C6
33	C	520	LMG	C29-C30-C31-C32
29	A	414[B]	PL9	C4-C3-C7-C8

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Mol	Chain	Res	Type	Atoms
29	a	416[A]	PL9	C4-C3-C7-C8
29	a	416[B]	PL9	C4-C3-C7-C8
23	A	408	CLA	C11-C12-C13-C14
23	B	610	CLA	C11-C12-C13-C14
23	a	407[A]	CLA	C14-C13-C15-C16
23	b	614	CLA	C11-C12-C13-C14
23	c	511	CLA	C11-C12-C13-C14
35	C	519	DGD	C8B-C9B-CAB-CBB
37	l	101[A]	LHG	C10-C11-C12-C13
23	C	507	CLA	C15-C16-C17-C18
23	b	604	CLA	C10-C11-C12-C13
33	C	501	LMG	C7-C8-C9-O8
35	H	102	DGD	O1G-C1G-C2G-C3G
37	d	711[A]	LHG	C1-C2-C3-O3
26	a	411[A]	SQD	C10-C11-C12-C13
32	a	414	LMT	C7-C8-C9-C10
37	E	101[A]	LHG	C12-C13-C14-C15
24	A	407[A]	PHO	O2A-C1-C2-C3
24	a	408[A]	PHO	O2A-C1-C2-C3
24	a	408[B]	PHO	O2A-C1-C2-C3
23	D	406	CLA	CBA-CGA-O2A-C1
24	A	353[A]	PHO	C2C-C3C-CAC-CBC
33	B	621	LMG	O6-C1-O1-C7
35	c	517[A]	DGD	CBA-CCA-CDA-CEA
26	A	410[B]	SQD	C34-C35-C36-C37
23	a	409	CLA	C15-C16-C17-C18
29	a	416[A]	PL9	C45-C44-C46-C47
23	C	502	CLA	C1A-C2A-CAA-CBA
23	a	407[A]	CLA	C1A-C2A-CAA-CBA
23	c	512	CLA	C1A-C2A-CAA-CBA
23	A	408	CLA	C16-C17-C18-C19
23	B	615	CLA	C12-C13-C15-C16
23	C	506	CLA	C12-C13-C15-C16
23	C	507	CLA	C12-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C15
23	b	615	CLA	C11-C12-C13-C15
23	c	514	CLA	C12-C13-C15-C16
32	M	103	LMT	C3-C4-C5-C6
38	e	87	HEM	CAD-CBD-CGD-O1D
33	a	419	LMG	C31-C32-C33-C34
37	D	409[A]	LHG	C29-C30-C31-C32
37	L	101[A]	LHG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
37	L	101[B]	LHG	C26-C27-C28-C29
23	b	605	CLA	C13-C15-C16-C17
27	B	901	GOL	O1-C1-C2-O2
37	e	101[B]	LHG	C24-C25-C26-C27
35	C	519	DGD	C2A-C1A-O1G-C1G
26	A	410[B]	SQD	C16-C17-C18-C19
37	l	101[B]	LHG	O6-C4-C5-C6
33	m	101	LMG	C32-C33-C34-C35
37	l	101[B]	LHG	C28-C29-C30-C31
35	C	519	DGD	C5B-C6B-C7B-C8B
29	a	416[B]	PL9	C45-C44-C46-C47
26	b	620	SQD	C15-C16-C17-C18
23	c	508	CLA	C8-C10-C11-C12
29	a	416[B]	PL9	C43-C44-C46-C47
23	C	513	CLA	C2B-C3B-CAB-CBB
23	C	509	CLA	C5-C6-C7-C8
32	a	420	LMT	C2'-C1'-O1'-C1
38	E	103	HEM	CAD-CBD-CGD-O2D
40	V	202	HEC	CAD-CBD-CGD-O1D
37	L	101[B]	LHG	C11-C10-C9-C8
33	c	521	LMG	O1-C7-C8-O7
26	f	102	SQD	C34-C35-C36-C37
23	c	512	CLA	C3-C5-C6-C7
37	d	711[A]	LHG	C27-C28-C29-C30
37	e	101[A]	LHG	C24-C25-C26-C27
33	z	101	LMG	C10-C11-C12-C13
23	A	406[A]	CLA	C16-C17-C18-C19
37	d	711[A]	LHG	C17-C18-C19-C20
33	m	101	LMG	O6-C1-O1-C7
23	b	603	CLA	C5-C6-C7-C8
33	c	520	LMG	O6-C5-C6-O5
32	A	359	LMT	C2B-C1B-O1B-C4'
35	c	519	DGD	C2A-C3A-C4A-C5A
37	d	407[A]	LHG	C25-C26-C27-C28
23	a	405[A]	CLA	C2-C1-O2A-CGA
23	a	405[B]	CLA	C2-C1-O2A-CGA
23	c	514	CLA	C2-C1-O2A-CGA
23	b	601	CLA	C2-C3-C5-C6
29	d	405[A]	PL9	C43-C44-C46-C47
29	d	405[B]	PL9	C43-C44-C46-C47
35	c	519	DGD	C1A-C2A-C3A-C4A
23	B	614	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C11-C12-C13-C14
23	D	406	CLA	C6-C7-C8-C9
33	a	419	LMG	O8-C28-C29-C30
26	a	411[B]	SQD	C11-C12-C13-C14
34	b	622	HTG	C3'-C4'-C5'-C6'
37	D	411[B]	LHG	C28-C29-C30-C31
40	V	202	HEC	CAD-CBD-CGD-O2D
32	A	359	LMT	C7-C8-C9-C10
25	B	617	BCR	C1-C6-C7-C8
25	a	410	BCR	C1-C6-C7-C8
25	a	410	BCR	C23-C24-C25-C30
25	c	515	BCR	C23-C24-C25-C30
25	y	101	BCR	C23-C24-C25-C30
37	D	411[B]	LHG	C10-C11-C12-C13
27	d	701	GOL	O1-C1-C2-C3
37	L	101[B]	LHG	C11-C12-C13-C14
25	K	102	BCR	C19-C20-C21-C22
23	b	616	CLA	C4-C3-C5-C6
37	d	711[A]	LHG	C9-C10-C11-C12
23	c	511	CLA	C2-C3-C5-C6
29	A	414[A]	PL9	C43-C44-C46-C47
32	M	101	LMT	O1'-C1-C2-C3
35	c	517[B]	DGD	C5D-C6D-O5D-C1E
37	D	409[A]	LHG	C17-C18-C19-C20
23	b	601	CLA	CAA-CBA-CGA-O1A
23	A	404[B]	CLA	C2C-C3C-CAC-CBC
23	C	502	CLA	C16-C17-C18-C20
23	A	404[B]	CLA	C4C-C3C-CAC-CBC
35	c	517[A]	DGD	CDB-CEB-CFB-CGB
23	a	409	CLA	C4B-C3B-CAB-CBB
23	b	603	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	C16-C17-C18-C19
35	c	518[A]	DGD	C1A-C2A-C3A-C4A
23	B	612	CLA	O1A-CGA-O2A-C1
23	b	616	CLA	O1A-CGA-O2A-C1
29	D	408[A]	PL9	C35-C34-C36-C37
29	D	408[B]	PL9	C20-C19-C21-C22
29	D	408[B]	PL9	C45-C44-C46-C47
23	B	601	CLA	C11-C12-C13-C15
23	b	607	CLA	C12-C13-C15-C16
23	b	616	CLA	C2-C3-C5-C6
29	D	408[B]	PL9	C18-C19-C21-C22

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Mol	Chain	Res	Type	Atoms
29	D	408[B]	PL9	C28-C29-C31-C32
23	B	613	CLA	C15-C16-C17-C18
23	b	612	CLA	C13-C15-C16-C17
33	B	621	LMG	C2-C1-O1-C7
33	Z	101	LMG	C2-C1-O1-C7
37	l	101[A]	LHG	C25-C26-C27-C28
23	b	616	CLA	CBA-CGA-O2A-C1
26	a	413	SQD	C26-C27-C28-C29
33	B	621	LMG	C14-C15-C16-C17
33	C	501	LMG	C22-C23-C24-C25
37	D	409[A]	LHG	O8-C23-C24-C25
23	C	507	CLA	C16-C17-C18-C19
38	e	87	HEM	CAA-CBA-CGA-O2A
40	v	202	HEC	CAD-CBD-CGD-O2D
24	a	408[B]	PHO	C2C-C3C-CAC-CBC
34	b	623	HTG	O5-C1-S1-C1'
23	c	505	CLA	C4-C3-C5-C6
29	A	414[A]	PL9	C25-C24-C26-C27
23	b	615	CLA	C10-C11-C12-C13
37	d	408[B]	LHG	C10-C11-C12-C13
23	c	502	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	CAA-CBA-CGA-O2A
23	B	615	CLA	C14-C13-C15-C16
23	C	506	CLA	C14-C13-C15-C16
23	C	508	CLA	C11-C12-C13-C14
23	C	510	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	a	407[A]	CLA	C6-C7-C8-C9
23	a	407[B]	CLA	C14-C13-C15-C16
23	b	601	CLA	C11-C12-C13-C14
23	b	603	CLA	C11-C10-C8-C9
23	b	607	CLA	C14-C13-C15-C16
38	e	87	HEM	CAD-CBD-CGD-O2D
32	a	420	LMT	C4'-C5'-C6'-O6'
23	C	507	CLA	C3A-C2A-CAA-CBA
23	c	511	CLA	O1A-CGA-O2A-C1
33	B	621	LMG	O8-C28-C29-C30
37	e	101[A]	LHG	O8-C23-C24-C25
37	e	101[B]	LHG	O8-C23-C24-C25
35	c	517[B]	DGD	C4B-C5B-C6B-C7B
37	d	408[B]	LHG	C11-C10-C9-C8
23	B	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	B	604	CLA	CAD-CBD-CGD-O2D
23	B	610	CLA	CAD-CBD-CGD-O2D
23	C	513	CLA	CAD-CBD-CGD-O2D
23	b	603	CLA	CAD-CBD-CGD-O2D
23	b	610	CLA	CAD-CBD-CGD-O2D
23	c	502	CLA	CAD-CBD-CGD-O2D
23	c	506	CLA	CAD-CBD-CGD-O2D
24	A	407[A]	PHO	CAD-CBD-CGD-O2D
38	E	103	HEM	C2B-C3B-CAB-CBB
38	e	87	HEM	C2B-C3B-CAB-CBB
35	H	102	DGD	O6E-C5E-C6E-O5E
35	C	519	DGD	CAA-CBA-CCA-CDA
33	C	521	LMG	C11-C12-C13-C14
33	c	521	LMG	C39-C40-C41-C42
37	L	101[A]	LHG	C11-C12-C13-C14
23	C	513	CLA	CAA-CBA-CGA-O2A
37	L	101[A]	LHG	O7-C7-C8-C9
33	B	621	LMG	C37-C38-C39-C40
29	D	408[B]	PL9	C43-C44-C46-C47
33	Z	101	LMG	O7-C10-C11-C12
37	E	101[B]	LHG	O7-C7-C8-C9
37	l	101[A]	LHG	O7-C7-C8-C9
35	C	519	DGD	C6A-C7A-C8A-C9A
23	D	406	CLA	C8-C10-C11-C12
37	l	101[B]	LHG	O7-C7-C8-C9
23	B	602	CLA	O2A-C1-C2-C3
23	D	405[B]	CLA	O2A-C1-C2-C3
23	b	613	CLA	O2A-C1-C2-C3
24	A	407[B]	PHO	O2A-C1-C2-C3
23	b	612	CLA	O1A-CGA-O2A-C1
35	h	102	DGD	C6A-C7A-C8A-C9A
38	E	103	HEM	C4B-C3B-CAB-CBB
38	e	87	HEM	C4B-C3B-CAB-CBB
32	a	414	LMT	C1-C2-C3-C4
37	D	409[B]	LHG	C7-C8-C9-C10
37	D	409[B]	LHG	O8-C23-C24-C25
40	v	202	HEC	CAD-CBD-CGD-O1D
23	a	405[A]	CLA	C2C-C3C-CAC-CBC
33	m	101	LMG	C40-C41-C42-C43
23	A	404[A]	CLA	C2C-C3C-CAC-CBC
35	h	102	DGD	CCB-CDB-CEB-CFB
23	A	405[A]	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
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	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	a	406[A]	CLA	CHA-CBD-CGD-O1D
23	a	406[A]	CLA	CHA-CBD-CGD-O2D
23	b	601	CLA	CHA-CBD-CGD-O2D
23	b	606	CLA	CHA-CBD-CGD-O1D
23	b	606	CLA	CHA-CBD-CGD-O2D
23	c	503	CLA	CHA-CBD-CGD-O2D
23	c	508	CLA	CHA-CBD-CGD-O1D
23	c	508	CLA	CHA-CBD-CGD-O2D
23	c	510	CLA	CHA-CBD-CGD-O1D
38	e	87	HEM	CAA-CBA-CGA-O1A
29	D	408[B]	PL9	C35-C34-C36-C37
35	C	519	DGD	C2A-C3A-C4A-C5A
37	D	409[B]	LHG	C11-C12-C13-C14
23	C	503	CLA	C16-C17-C18-C20
33	c	520	LMG	O7-C10-C11-C12
37	L	101[B]	LHG	O7-C7-C8-C9
35	c	517[B]	DGD	C8B-C9B-CAB-CBB
35	H	102	DGD	O1G-C1G-C2G-O2G
23	b	608	CLA	C13-C15-C16-C17
35	h	102	DGD	CCA-CDA-CEA-CFA
23	c	511	CLA	CAA-CBA-CGA-O2A
32	e	102	LMT	C2B-C1B-O1B-C4'
24	A	407[A]	PHO	CHA-CBD-CGD-O2D
24	A	407[B]	PHO	CHA-CBD-CGD-O1D
24	a	408[A]	PHO	CHA-CBD-CGD-O1D
24	a	353[B]	PHO	CHA-CBD-CGD-O1D
24	a	353[B]	PHO	CHA-CBD-CGD-O2D
37	D	409[A]	LHG	O1-C1-C2-O2
37	D	409[B]	LHG	O1-C1-C2-O2
35	c	517[B]	DGD	CDB-CEB-CFB-CGB
26	F	101	SQD	C24-C23-O48-C46
23	B	614	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C2-C3-C5-C6
23	a	406[A]	CLA	C11-C12-C13-C15
23	b	604	CLA	C11-C12-C13-C15
23	D	405[B]	CLA	C16-C17-C18-C20
23	b	610	CLA	C16-C17-C18-C19
29	A	414[A]	PL9	C4-C3-C7-C8
24	a	353[A]	PHO	C2C-C3C-CAC-CBC
23	b	613	CLA	CAA-CBA-CGA-O2A
37	d	711[A]	LHG	C30-C31-C32-C33
23	A	408	CLA	C14-C13-C15-C16
23	a	407[B]	CLA	C6-C7-C8-C9
23	b	604	CLA	C11-C12-C13-C14
23	b	608	CLA	C14-C13-C15-C16
23	b	614	CLA	C14-C13-C15-C16
23	c	514	CLA	C14-C13-C15-C16
29	d	405[A]	PL9	C34-C36-C37-C38
37	E	101[B]	LHG	C11-C10-C9-C8
33	C	521	LMG	C10-C11-C12-C13
35	C	518[B]	DGD	C1A-C2A-C3A-C4A
33	C	520	LMG	O7-C10-C11-C12
23	a	405[A]	CLA	C4C-C3C-CAC-CBC
34	b	623	HTG	C4'-C5'-C6'-C7'
29	d	405[B]	PL9	C11-C12-C13-C14
23	B	613	CLA	CAA-CBA-CGA-O2A
23	b	604	CLA	C13-C15-C16-C17
35	H	102	DGD	CDB-CEB-CFB-CGB
25	y	101	BCR	C37-C22-C23-C24
37	E	101[B]	LHG	O9-C7-C8-C9
23	D	405[B]	CLA	C16-C17-C18-C19
35	c	517[B]	DGD	C7B-C8B-C9B-CAB
27	c	743	GOL	O1-C1-C2-C3
27	d	701	GOL	C1-C2-C3-O3
26	f	102	SQD	C31-C32-C33-C34
37	l	101[B]	LHG	C32-C33-C34-C35
35	c	519	DGD	CDA-CEA-CFA-CGA
23	B	605	CLA	C16-C17-C18-C19
23	C	511	CLA	CAA-CBA-CGA-O1A
37	l	101[A]	LHG	O9-C7-C8-C9
23	C	510	CLA	O1D-CGD-O2D-CED
23	A	404[A]	CLA	C4C-C3C-CAC-CBC
26	A	412	SQD	C15-C16-C17-C18
33	Z	101	LMG	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
37	D	409[A]	LHG	O10-C23-C24-C25
37	L	101[A]	LHG	O9-C7-C8-C9
37	e	101[A]	LHG	O10-C23-C24-C25
35	C	517[A]	DGD	C3A-C4A-C5A-C6A
37	L	101[B]	LHG	C14-C15-C16-C17
26	F	101	SQD	C44-C45-C46-O48
33	B	621	LMG	O1-C7-C8-C9
33	C	520	LMG	O1-C7-C8-C9
26	A	412	SQD	O48-C23-C24-C25
37	E	101[A]	LHG	O7-C7-C8-C9
40	V	202	HEC	C4B-C3B-CAB-CBB
23	B	603	CLA	C2A-CAA-CBA-CGA
23	B	614	CLA	C2A-CAA-CBA-CGA
23	c	502	CLA	C2A-CAA-CBA-CGA
23	a	409	CLA	C8-C10-C11-C12
23	c	513	CLA	CAA-CBA-CGA-O2A
33	D	415	LMG	O7-C10-C11-C12
23	C	513	CLA	CAA-CBA-CGA-O1A
26	f	102	SQD	C28-C29-C30-C31
35	H	102	DGD	C3B-C4B-C5B-C6B
33	C	521	LMG	C33-C34-C35-C36
23	B	610	CLA	C4B-C3B-CAB-CBB
23	C	513	CLA	C4B-C3B-CAB-CBB
37	d	407[A]	LHG	C4-O6-P-O5
37	d	408[B]	LHG	C4-O6-P-O5
33	B	621	LMG	C36-C37-C38-C39
33	Z	101	LMG	O9-C10-C11-C12
37	D	409[B]	LHG	O10-C23-C24-C25
37	L	101[B]	LHG	O9-C7-C8-C9
37	e	101[B]	LHG	O10-C23-C24-C25
23	C	506	CLA	CAA-CBA-CGA-O2A
37	d	711[B]	LHG	C27-C28-C29-C30
23	b	611	CLA	C13-C15-C16-C17
23	c	508	CLA	C5-C6-C7-C8
35	C	519	DGD	CCB-CDB-CEB-CFB
37	D	409[B]	LHG	C29-C30-C31-C32
23	c	502	CLA	CAA-CBA-CGA-O2A
23	B	616	CLA	C16-C17-C18-C20
23	C	508	CLA	C2A-CAA-CBA-CGA
23	b	603	CLA	C2A-CAA-CBA-CGA
26	F	101	SQD	O10-C23-O48-C46
37	d	408[A]	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
23	B	615	CLA	C8-C10-C11-C12
37	D	409[A]	LHG	C18-C19-C20-C21
37	d	408[B]	LHG	C33-C34-C35-C36
37	l	101[B]	LHG	O9-C7-C8-C9
23	b	604	CLA	C4-C3-C5-C6
29	d	405[A]	PL9	C15-C14-C16-C17
37	d	408[A]	LHG	C30-C31-C32-C33
29	d	405[A]	PL9	C11-C12-C13-C14
23	A	405[B]	CLA	C2C-C3C-CAC-CBC
35	c	518[A]	DGD	CDA-CEA-CFA-CGA
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	607	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	b	605	CLA	CAD-CBD-CGD-O1D
23	b	607	CLA	CAD-CBD-CGD-O1D
23	b	609	CLA	CAD-CBD-CGD-O1D
23	c	505	CLA	CAD-CBD-CGD-O1D
23	c	507	CLA	CAD-CBD-CGD-O1D
23	c	513	CLA	CAA-CBA-CGA-O1A
26	a	413	SQD	C28-C29-C30-C31
35	C	518[A]	DGD	O2G-C1B-C2B-C3B
37	E	101[A]	LHG	O8-C23-C24-C25
23	A	405[B]	CLA	C13-C15-C16-C17
35	C	519	DGD	O6D-C5D-C6D-O5D
23	B	601	CLA	C11-C12-C13-C14
23	B	605	CLA	C11-C12-C13-C14
23	B	612	CLA	C11-C10-C8-C9
23	B	616	CLA	C14-C13-C15-C16
23	a	406[A]	CLA	C11-C12-C13-C14
35	c	519	DGD	C3A-C4A-C5A-C6A
37	D	409[A]	LHG	C30-C31-C32-C33
37	D	411[A]	LHG	C28-C29-C30-C31
23	B	612	CLA	CBA-CGA-O2A-C1
26	a	413	SQD	O48-C23-C24-C25
33	c	521	LMG	O7-C10-C11-C12
37	D	411[B]	LHG	O8-C23-C24-C25
37	E	101[B]	LHG	O8-C23-C24-C25
34	B	622	HTG	C3'-C4'-C5'-C6'
35	C	517[A]	DGD	CBA-CCA-CDA-CEA
37	L	101[A]	LHG	C32-C33-C34-C35
23	B	612	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
37	D	411[A]	LHG	O8-C23-C24-C25
26	A	412	SQD	O10-C23-C24-C25
23	c	514	CLA	C4-C3-C5-C6
23	B	616	CLA	C11-C12-C13-C15
23	C	504	CLA	C6-C7-C8-C10
23	a	407[A]	CLA	C6-C7-C8-C10
23	a	407[B]	CLA	C6-C7-C8-C10
23	b	603	CLA	C11-C10-C8-C7
23	b	610	CLA	C11-C12-C13-C15
33	c	520	LMG	O9-C10-C11-C12
33	c	521	LMG	O9-C10-C11-C12
37	E	101[A]	LHG	O9-C7-C8-C9
37	E	101[A]	LHG	O10-C23-C24-C25
35	C	518[B]	DGD	O2G-C1B-C2B-C3B
35	c	517[A]	DGD	O2G-C1B-C2B-C3B
32	A	359	LMT	O5B-C1B-O1B-C4'
25	K	102	BCR	C7-C8-C9-C10
25	Y	101	BCR	C21-C22-C23-C24
35	c	517[A]	DGD	O1B-C1B-C2B-C3B
37	D	411[A]	LHG	O10-C23-C24-C25
37	E	101[B]	LHG	O10-C23-C24-C25
35	c	517[B]	DGD	O2G-C1B-C2B-C3B
33	d	412	LMG	C40-C41-C42-C43
23	b	613	CLA	CAA-CBA-CGA-O1A
23	c	502	CLA	CAA-CBA-CGA-O1A
23	c	511	CLA	CAA-CBA-CGA-O1A
33	C	520	LMG	O9-C10-C11-C12
35	C	518[A]	DGD	O1B-C1B-C2B-C3B
35	C	518[B]	DGD	O1B-C1B-C2B-C3B
38	E	103	HEM	CAA-CBA-CGA-O2A
37	d	711[A]	LHG	C31-C32-C33-C34
23	B	613	CLA	CAA-CBA-CGA-O1A
37	D	411[B]	LHG	O10-C23-C24-C25
38	E	103	HEM	CAA-CBA-CGA-O1A
37	D	409[B]	LHG	C25-C26-C27-C28
33	D	415	LMG	O9-C10-C11-C12
26	A	410[B]	SQD	C13-C14-C15-C16
37	E	101[A]	LHG	C11-C10-C9-C8
37	d	408[A]	LHG	O8-C23-C24-C25
37	d	408[B]	LHG	O8-C23-C24-C25

There are no ring outliers.

170 monomers are involved in 360 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	d	403	CLA	2	0
25	b	619	BCR	4	0
25	c	516	BCR	1	0
23	c	503	CLA	2	0
23	c	511	CLA	1	0
23	C	514	CLA	2	0
25	k	101	BCR	2	0
33	c	521	LMG	1	0
34	B	622	HTG	1	0
23	b	613	CLA	1	0
23	b	604	CLA	2	0
29	a	416[B]	PL9	5	0
27	A	701	GOL	6	0
23	c	512	CLA	6	0
25	C	515	BCR	1	0
23	c	514	CLA	2	0
32	a	420	LMT	1	0
35	c	517[B]	DGD	2	0
26	B	620	SQD	1	0
35	C	517[B]	DGD	1	0
23	B	601	CLA	3	0
23	D	405[B]	CLA	5	0
23	b	614	CLA	2	0
35	c	517[A]	DGD	1	0
38	E	103	HEM	2	0
35	C	517[A]	DGD	1	0
34	b	622	HTG	2	0
25	b	617	BCR	1	0
23	C	504	CLA	4	0
23	c	509	CLA	3	0
27	B	624	GOL	2	0
26	A	410[B]	SQD	2	0
32	M	101	LMT	2	0
32	b	621	LMT	1	0
23	b	611	CLA	1	0
23	b	610	CLA	1	0
23	b	606	CLA	2	0
23	c	504	CLA	3	0
23	C	511	CLA	5	0
23	a	406[B]	CLA	1	0
23	C	508	CLA	2	0
34	B	626	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	410[A]	SQD	1	0
32	e	102	LMT	1	0
29	A	414[B]	PL9	9	0
23	C	505	CLA	1	0
23	B	604	CLA	2	0
27	O	501	GOL	1	0
23	A	408	CLA	3	0
37	d	711[B]	LHG	2	0
24	A	353[B]	PHO	3	0
23	a	406[A]	CLA	3	0
25	a	410	BCR	1	0
25	K	102	BCR	2	0
37	D	411[B]	LHG	5	0
23	b	612	CLA	1	0
23	B	609	CLA	2	0
26	b	620	SQD	4	0
24	A	353[A]	PHO	1	0
29	a	416[A]	PL9	5	0
23	B	614	CLA	2	0
23	c	508	CLA	3	0
37	D	411[A]	LHG	4	0
35	c	518[B]	DGD	2	0
23	c	505	CLA	2	0
27	d	801[A]	GOL	1	0
27	D	701	GOL	3	0
23	B	612	CLA	2	0
23	a	405[B]	CLA	4	0
23	C	503	CLA	4	0
23	B	605	CLA	3	0
23	D	405[A]	CLA	3	0
32	m	103	LMT	1	0
23	A	406[B]	CLA	2	0
23	a	405[A]	CLA	2	0
23	b	605	CLA	3	0
27	a	801	GOL	4	0
26	a	413	SQD	1	0
23	C	506	CLA	5	0
32	t	101	LMT	1	0
37	D	409[B]	LHG	2	0
34	D	414	HTG	1	0
23	A	406[A]	CLA	1	0
23	A	404[B]	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	D	407	BCR	1	0
23	C	512	CLA	3	0
23	c	510	CLA	4	0
23	B	616	CLA	4	0
24	A	407[B]	PHO	1	0
24	a	353[B]	PHO	1	0
24	a	408[B]	PHO	3	0
25	T	101	BCR	7	0
26	a	411[B]	SQD	3	0
23	d	402[B]	CLA	4	0
34	b	625	HTG	1	0
27	a	701	GOL	2	0
23	B	602	CLA	1	0
37	e	101[B]	LHG	4	0
34	d	411	HTG	1	0
23	A	405[B]	CLA	5	0
27	A	411	GOL	1	0
29	A	414[A]	PL9	11	0
23	a	407[B]	CLA	3	0
25	Y	101	BCR	1	0
23	b	601	CLA	2	0
24	A	407[A]	PHO	1	0
24	a	353[A]	PHO	1	0
29	D	408[A]	PL9	1	0
26	a	411[A]	SQD	3	0
35	C	518[A]	DGD	1	0
34	B	623	HTG	1	0
27	v	401[B]	GOL	2	0
35	C	519	DGD	1	0
23	A	405[A]	CLA	1	0
23	c	507	CLA	3	0
25	b	618	BCR	2	0
23	a	407[A]	CLA	2	0
25	H	101	BCR	2	0
33	z	101	LMG	2	0
26	F	101	SQD	2	0
27	O	601	GOL	1	0
34	c	522	HTG	1	0
25	h	101	BCR	5	0
23	c	513	CLA	7	0
27	v	401[A]	GOL	1	0
25	B	618	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	c	518[A]	DGD	3	0
33	d	412	LMG	3	0
27	C	523[B]	GOL	1	0
37	d	407[B]	LHG	3	0
23	b	616	CLA	3	0
23	c	502	CLA	3	0
37	d	408[B]	LHG	10	0
23	C	502	CLA	4	0
37	E	101[B]	LHG	3	0
23	a	409	CLA	5	0
35	H	102	DGD	1	0
23	B	615	CLA	4	0
25	y	101	BCR	2	0
23	B	606	CLA	2	0
23	C	513	CLA	3	0
37	d	407[A]	LHG	2	0
27	c	742[B]	GOL	1	0
37	d	408[A]	LHG	11	0
23	c	506	CLA	4	0
37	D	410[B]	LHG	3	0
37	E	101[A]	LHG	3	0
23	b	615	CLA	4	0
35	c	519	DGD	4	0
33	C	521	LMG	2	0
37	D	409[A]	LHG	2	0
23	B	613	CLA	6	0
25	t	103	BCR	5	0
23	A	404[A]	CLA	2	0
23	C	507	CLA	4	0
33	Z	101	LMG	1	0
37	D	410[A]	LHG	2	0
32	a	414	LMT	1	0
27	b	901	GOL	1	0
37	e	101[A]	LHG	5	0
23	d	402[A]	CLA	1	0
25	d	404	BCR	2	0
25	c	515	BCR	3	0
25	A	409	BCR	3	0
23	C	509	CLA	3	0
23	b	607	CLA	1	0
23	C	510	CLA	4	0
23	b	609	CLA	6	0

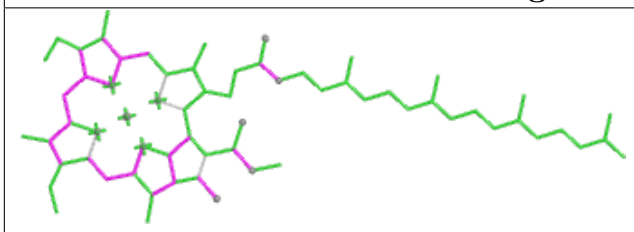
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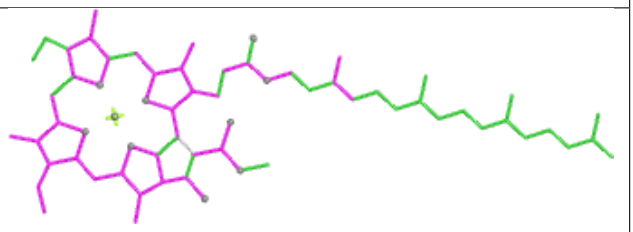
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	I	101	LMT	1	0
32	t	102	LMT	2	0

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.

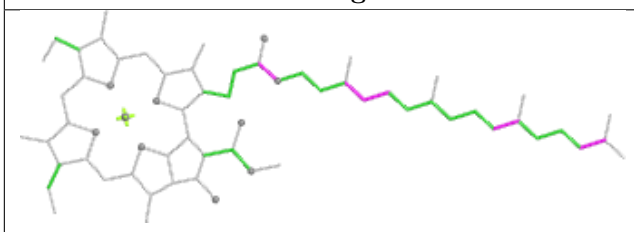
Ligand CLA d 403



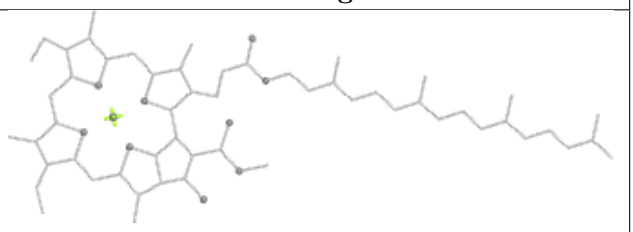
Bond lengths



Bond angles



Torsions

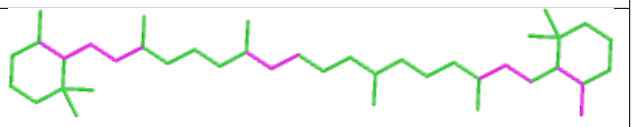


Rings

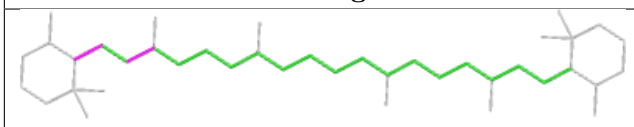
Ligand BCR b 619



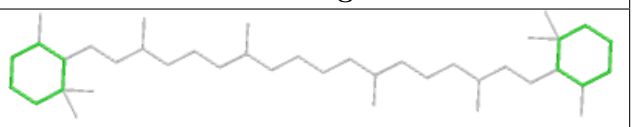
Bond lengths



Bond angles

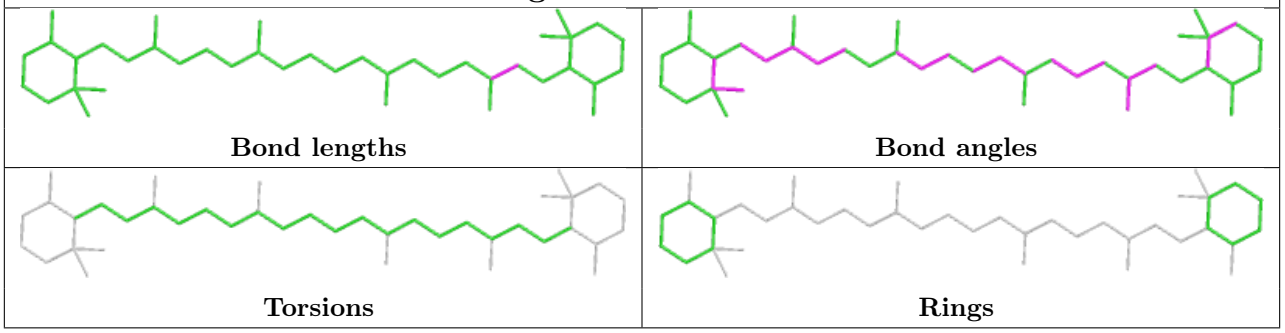


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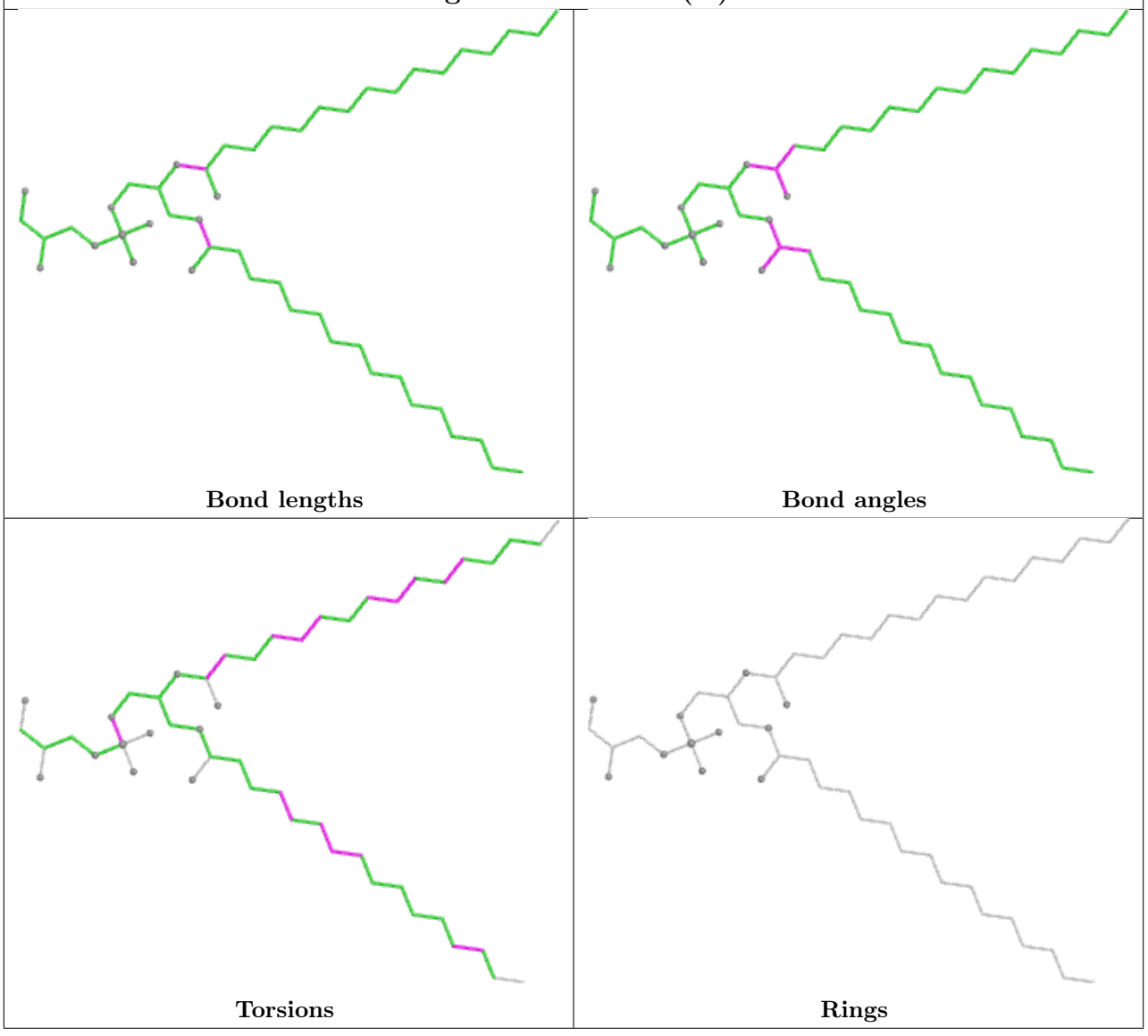


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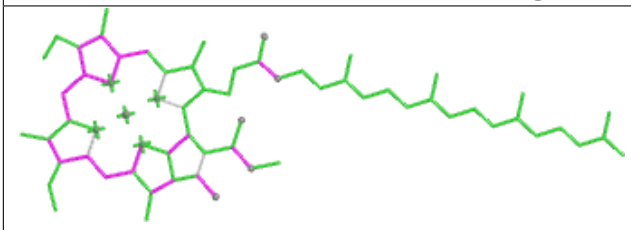
Ligand BCR c 516



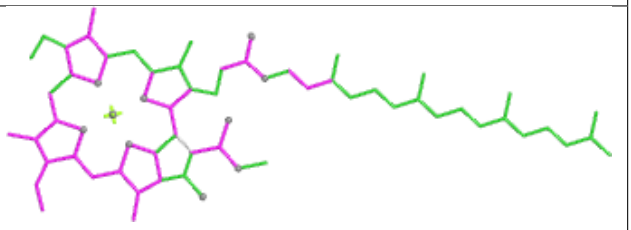
Ligand LHG l 101 (A)



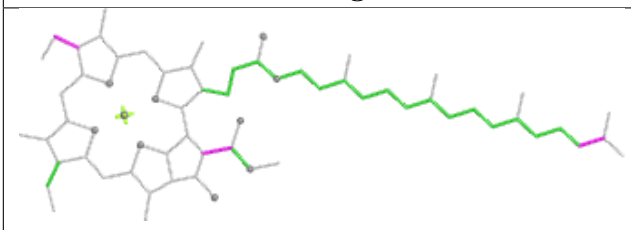
Ligand CLA c 503



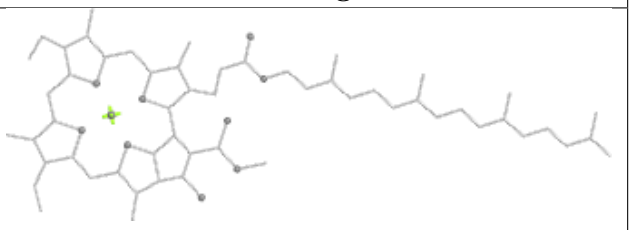
Bond lengths



Bond angles

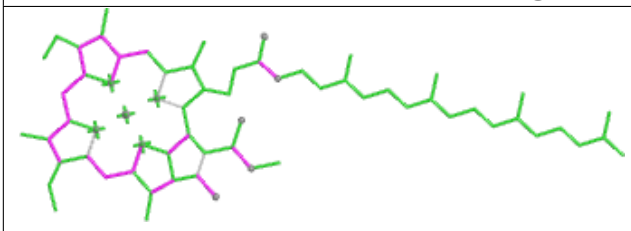


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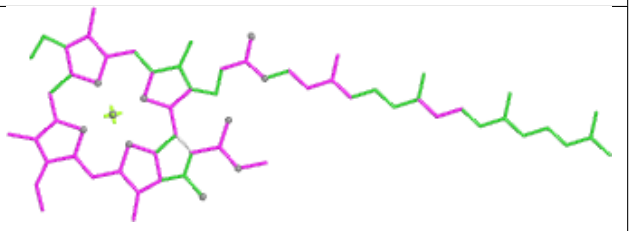


Rings

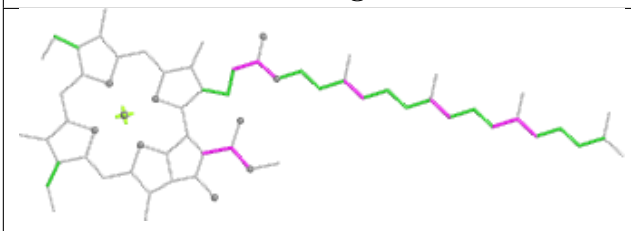
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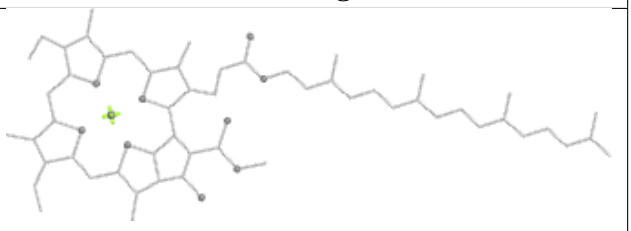
Bond lengths



Bond angles

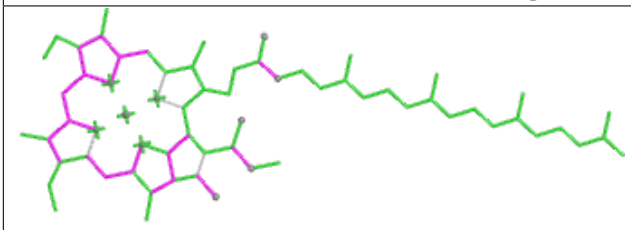


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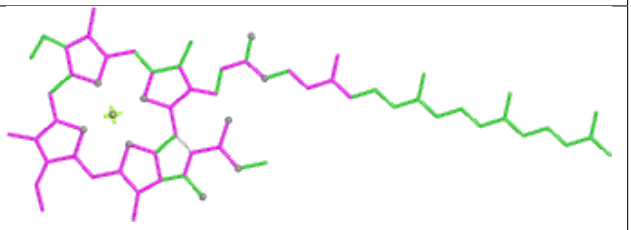


Rings

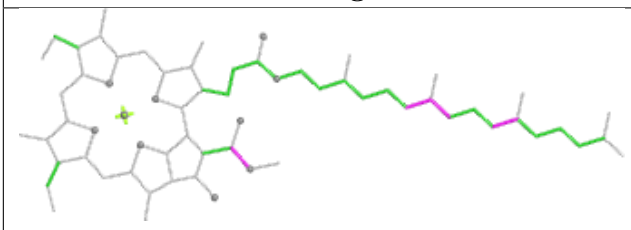
Ligand CLA C 514



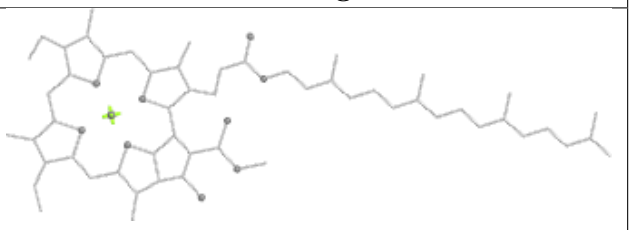
Bond lengths



Bond angles

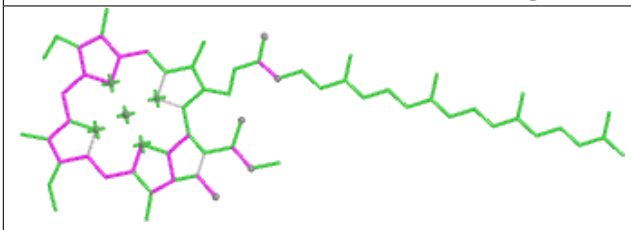


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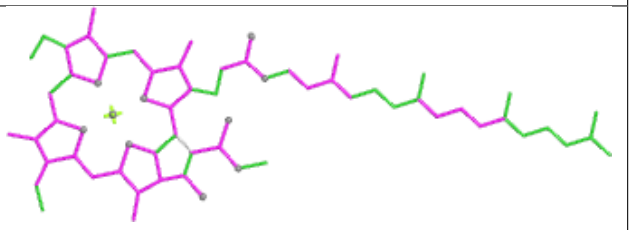


Rings

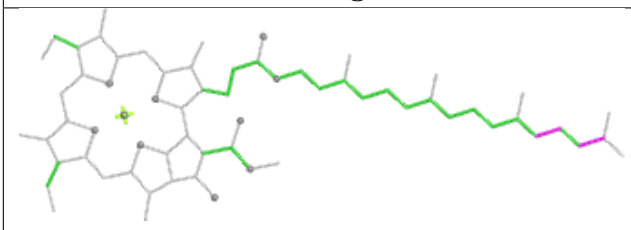
Ligand CLA B 608



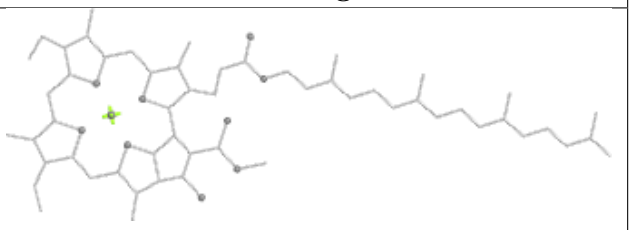
Bond lengths



Bond angles

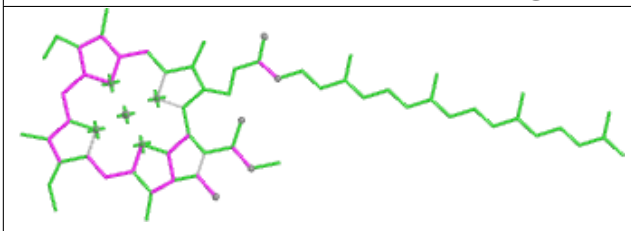


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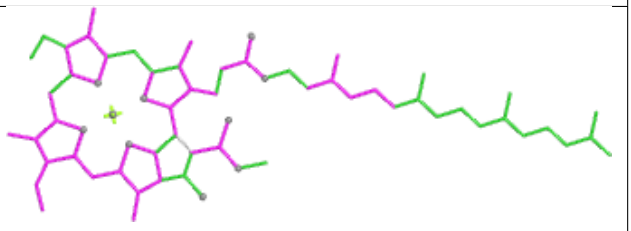


Rings

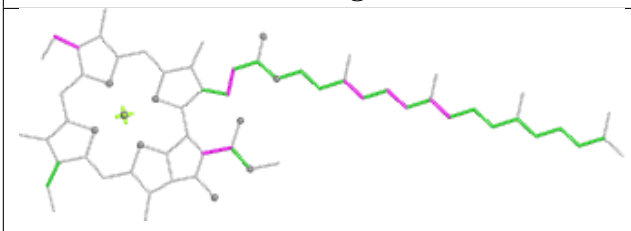
Ligand CLA b 603



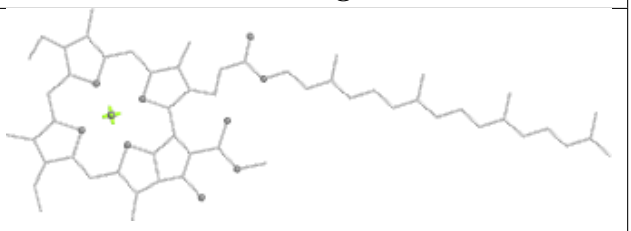
Bond lengths



Bond angles

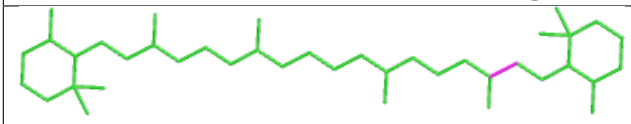


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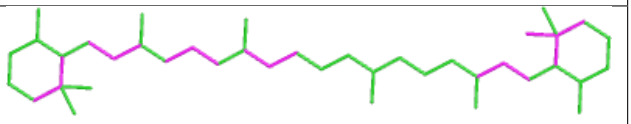


Rings

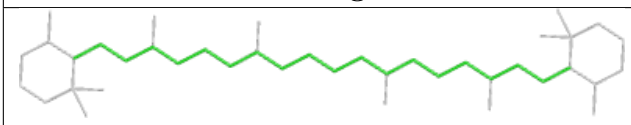
Ligand BCR k 101



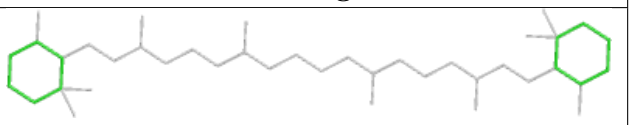
Bond lengths



Bond angles

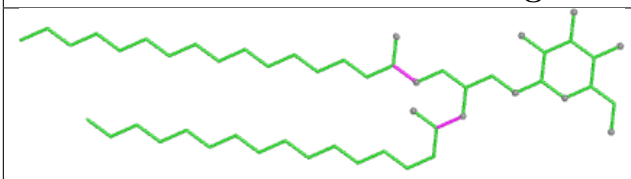


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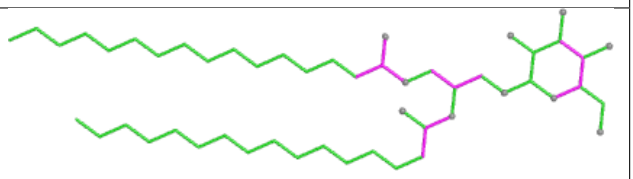


Rings

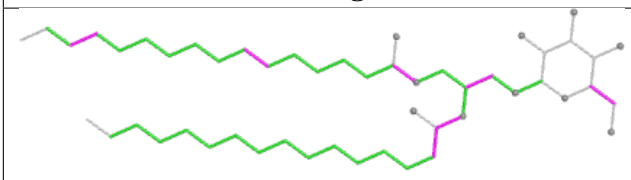
Ligand LMG c 521



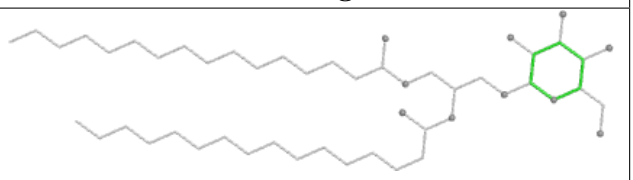
Bond lengths



Bond angles

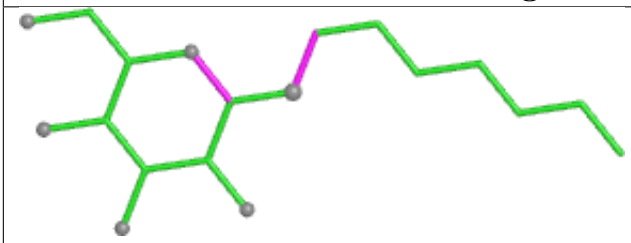


Torsions

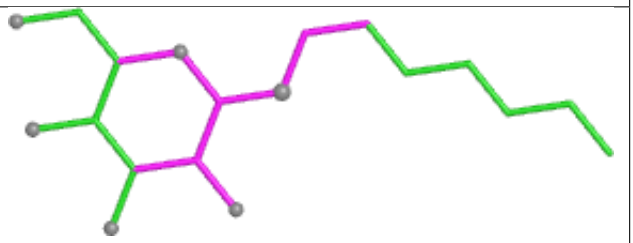


Rings

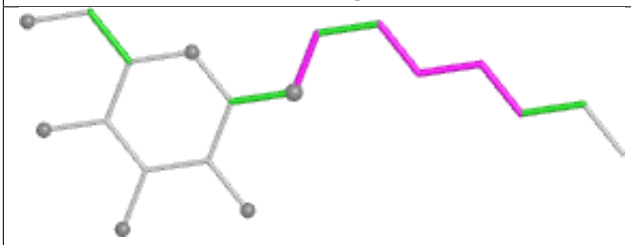
Ligand HTG B 622



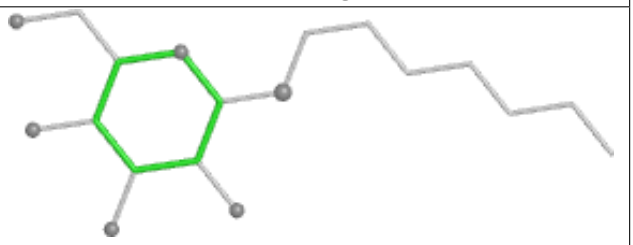
Bond lengths



Bond angles

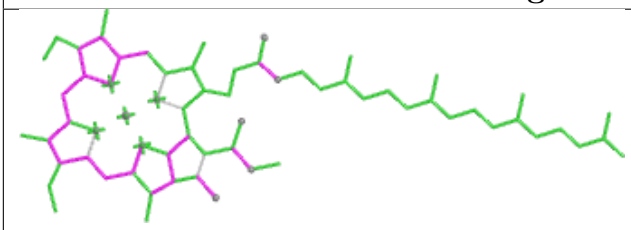


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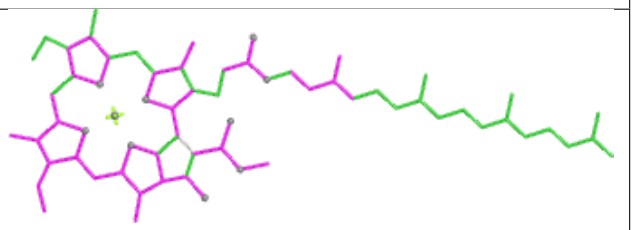


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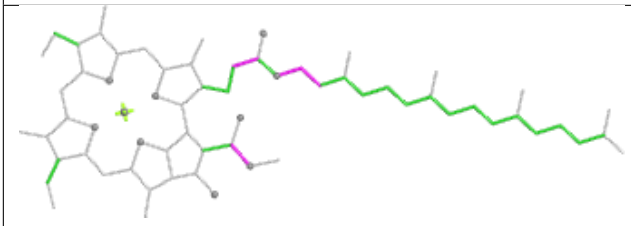
Ligand CLA b 613



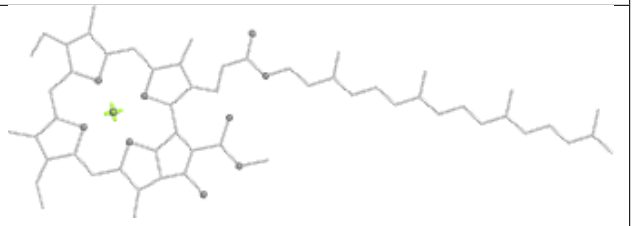
Bond lengths



Bond angles

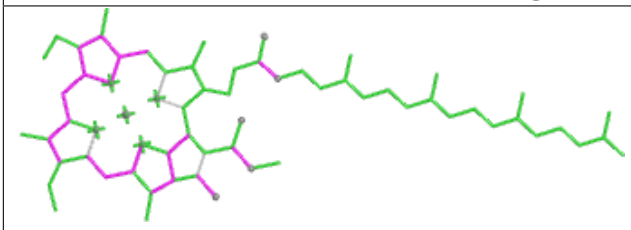


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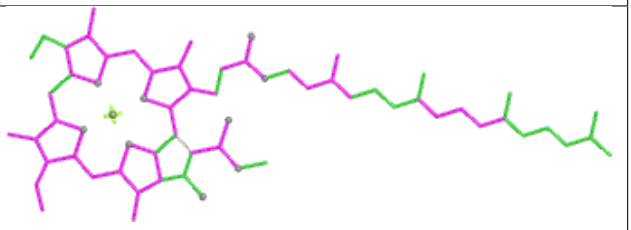


Rings

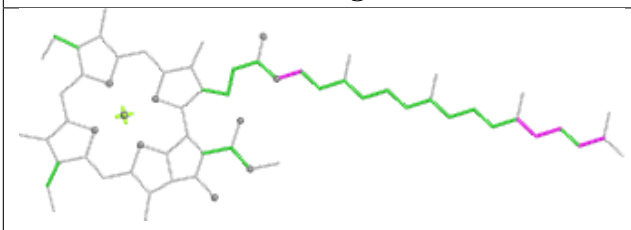
Ligand CLA b 608



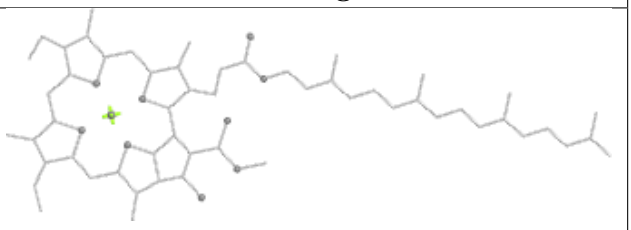
Bond lengths



Bond angles

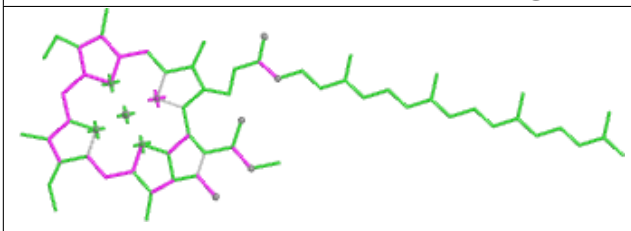


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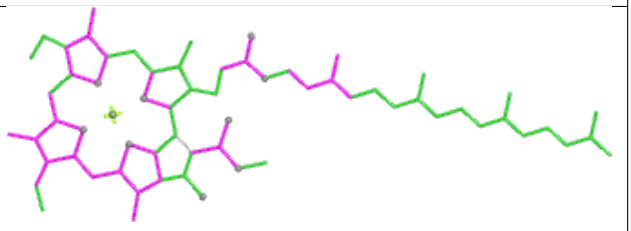


Rings

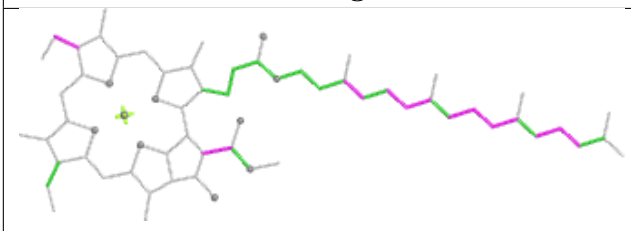
Ligand CLA b 604



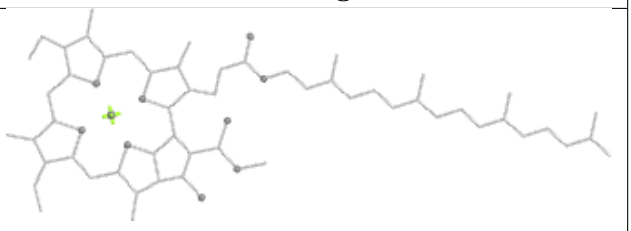
Bond lengths



Bond angles

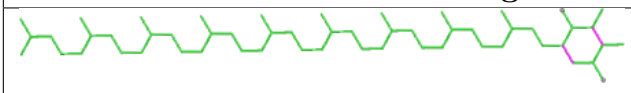


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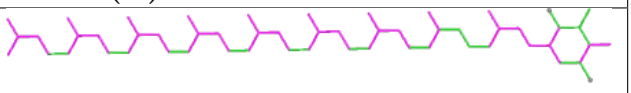


Rings

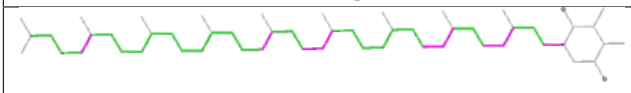
Ligand PL9 a 416 (B)



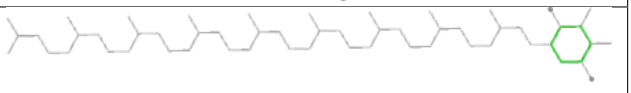
Bond lengths



Bond angles

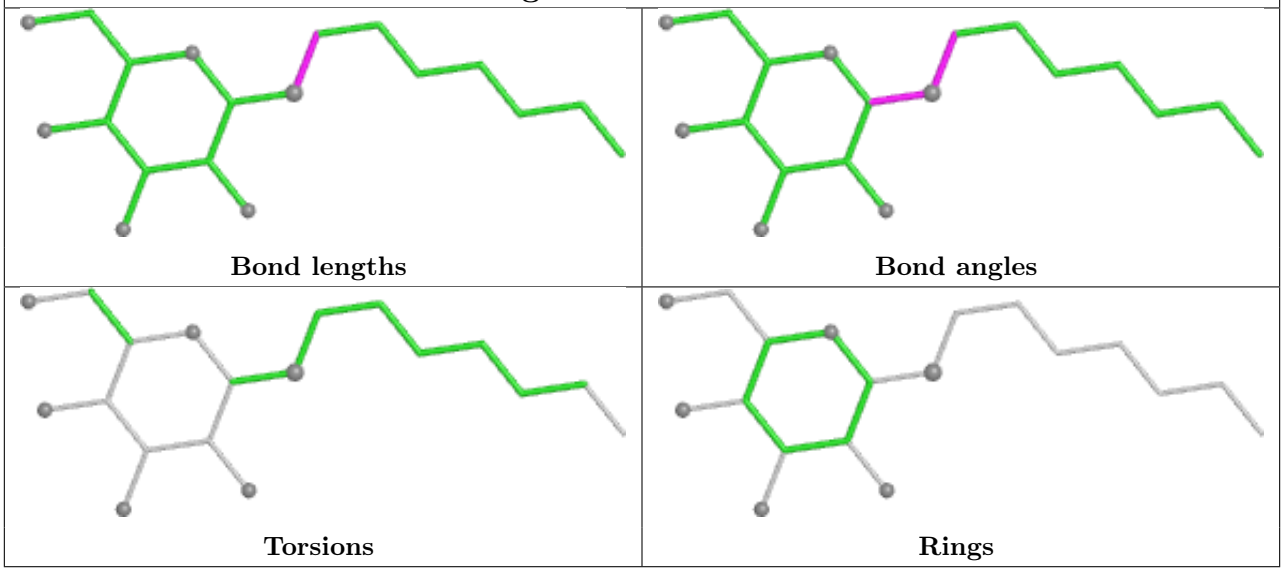


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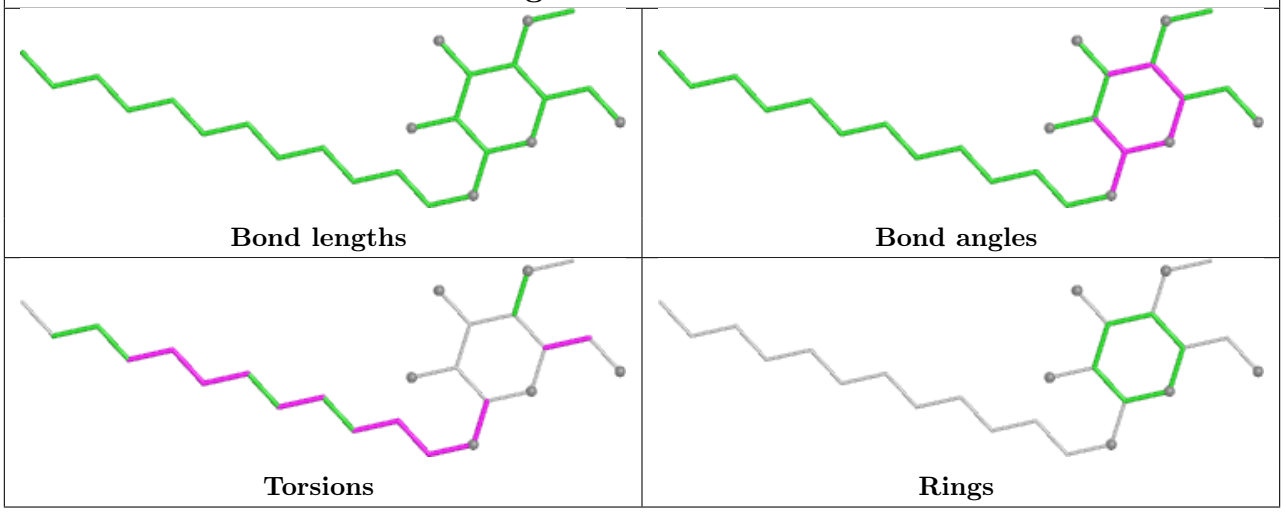


Rings

Ligand HTG C 522



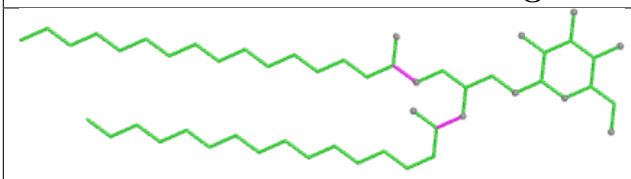
Ligand LMT b 627



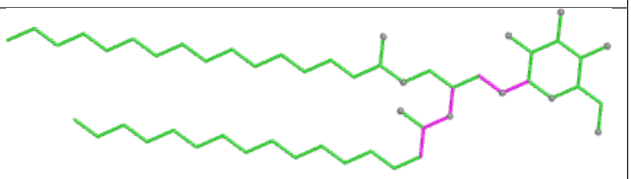
Ligand PL9 d 405 (A)



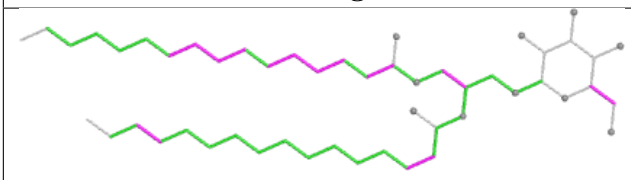
Ligand LMG a 419



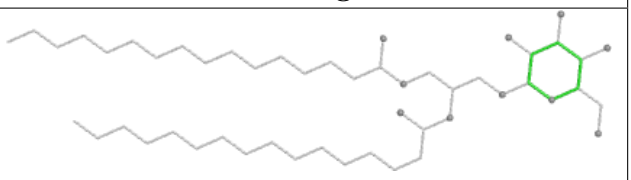
Bond lengths



Bond angles

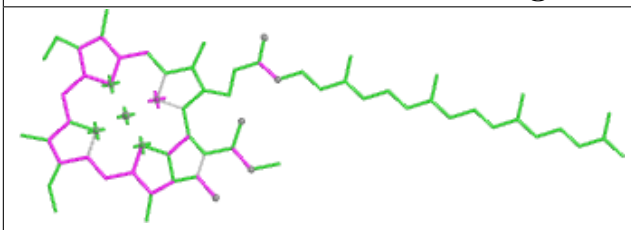


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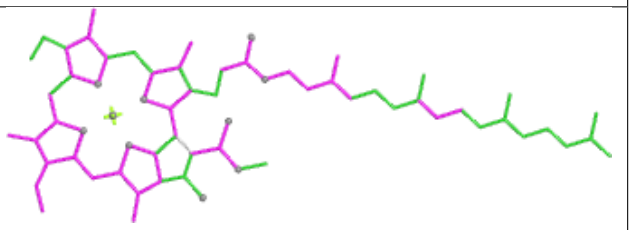


Rings

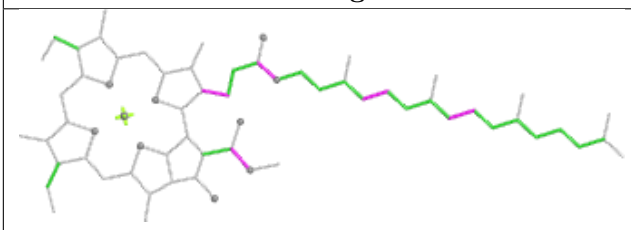
Ligand CLA c 512



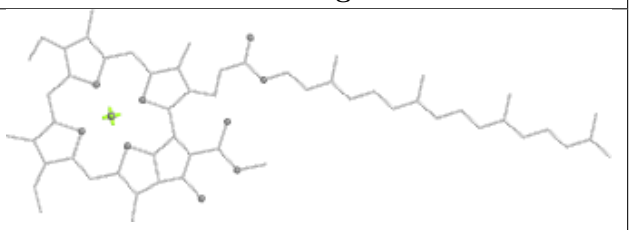
Bond lengths



Bond angles

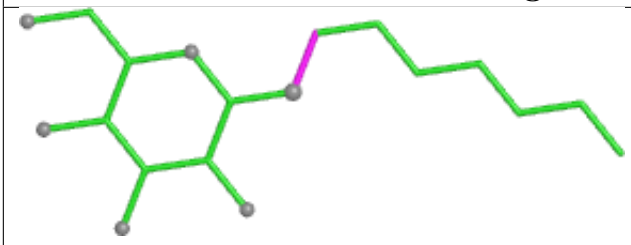


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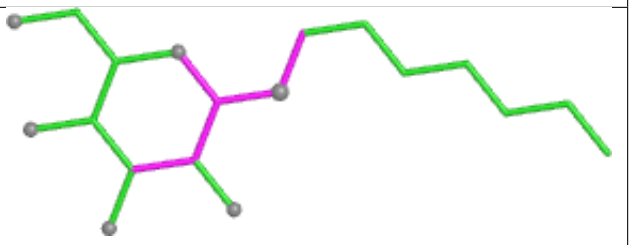


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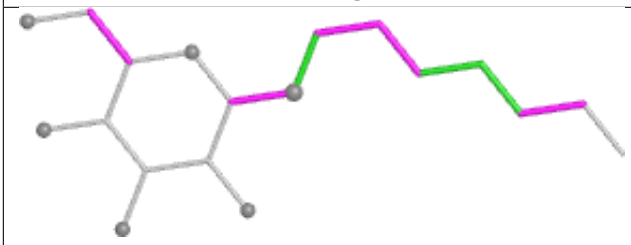
Ligand HTG b 623



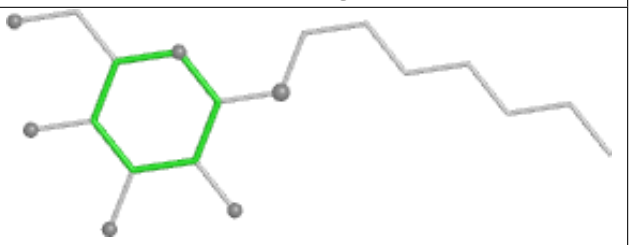
Bond lengths



Bond angles

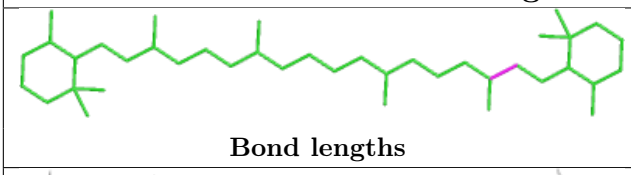


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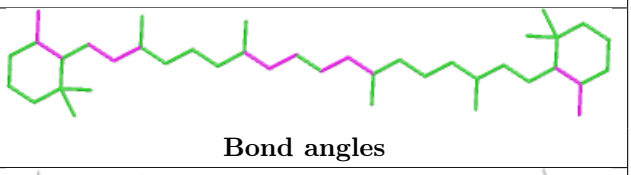


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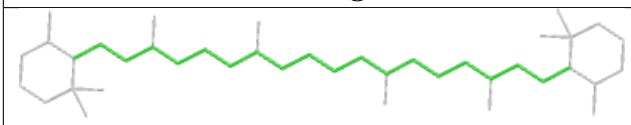
Ligand BCR C 515



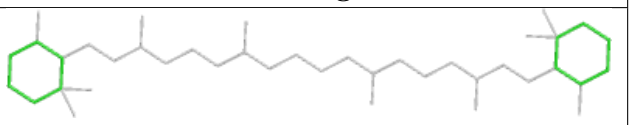
Bond lengths



Bond angles

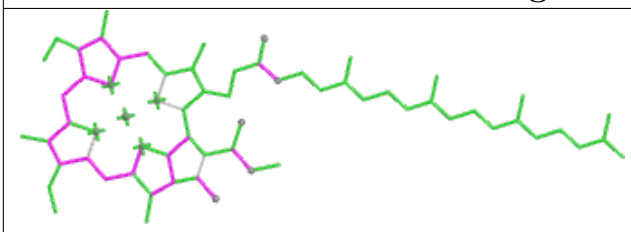


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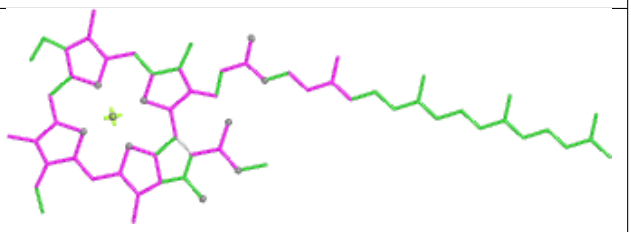


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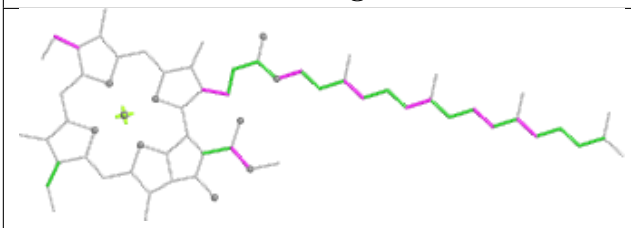
Ligand CLA c 514



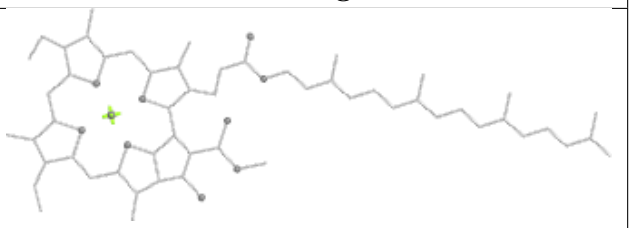
Bond lengths



Bond angles

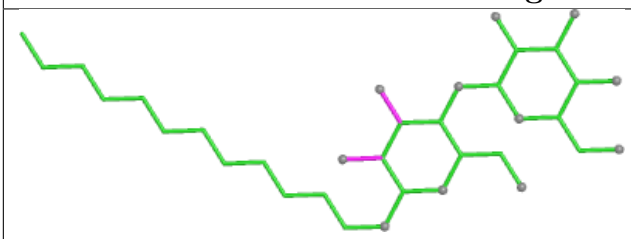


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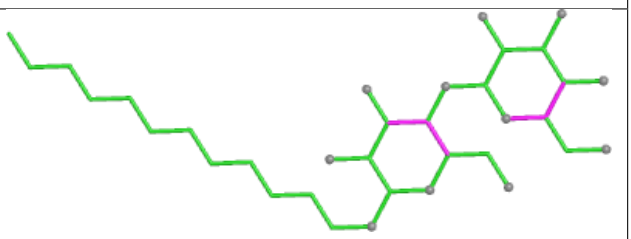


Rings

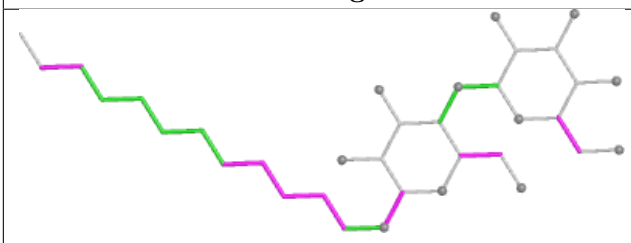
Ligand LMT a 420



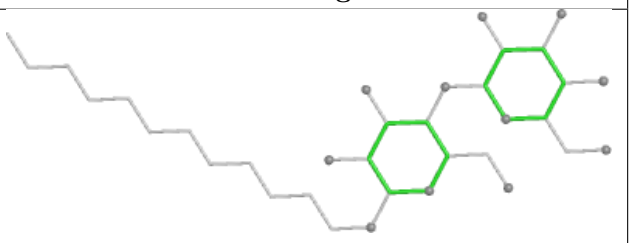
Bond lengths



Bond angles

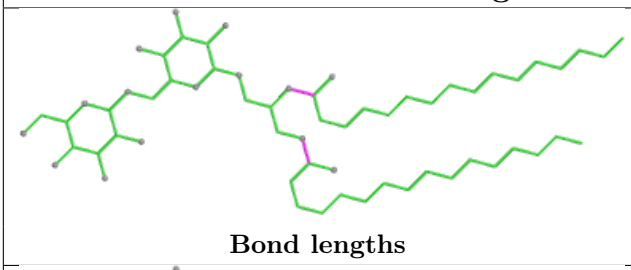


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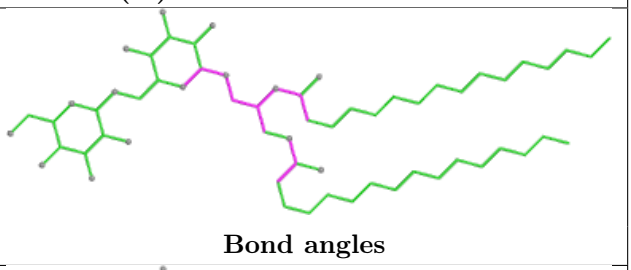


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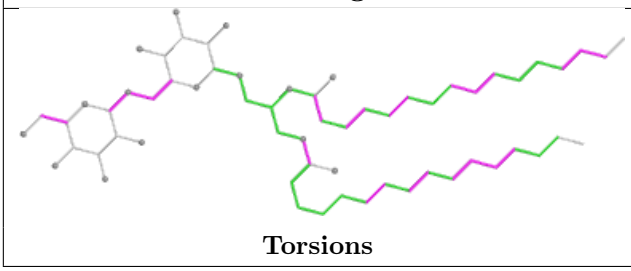
Ligand DGD c 517 (B)



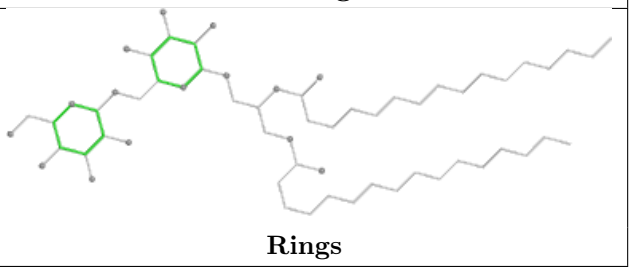
Bond lengths



Bond angles

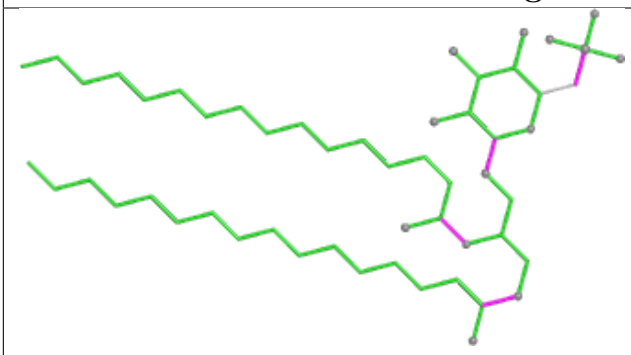


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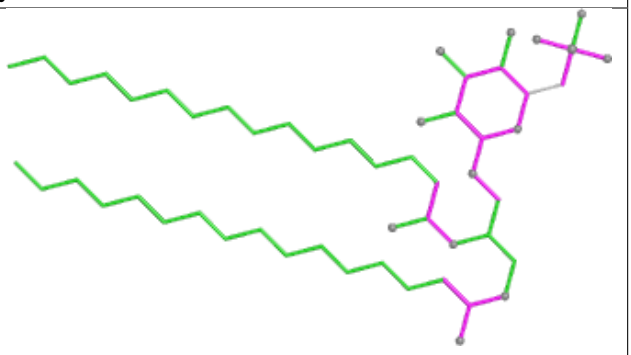


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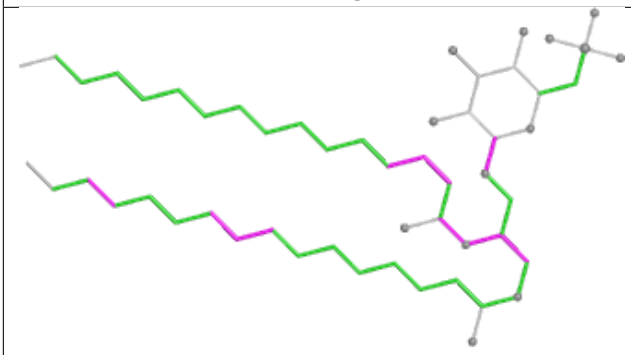
Ligand SQD B 620



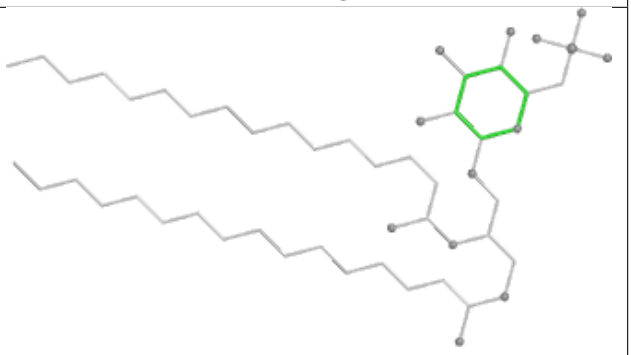
Bond lengths



Bond angles

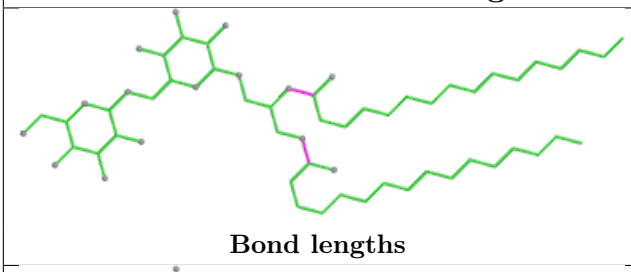


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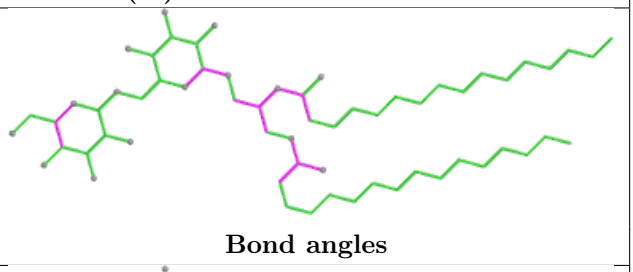


Rings

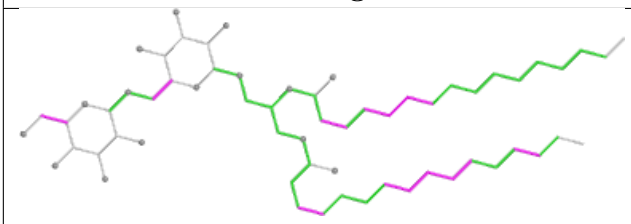
Ligand DGD C 517 (B)



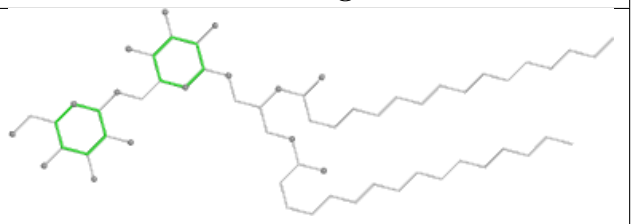
Bond lengths



Bond angles

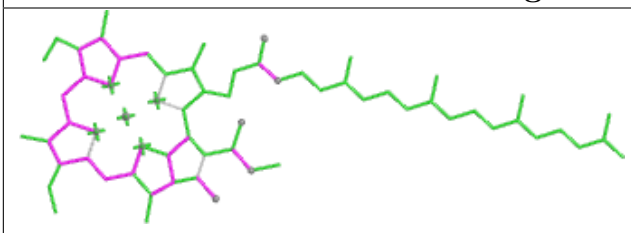


Torsions

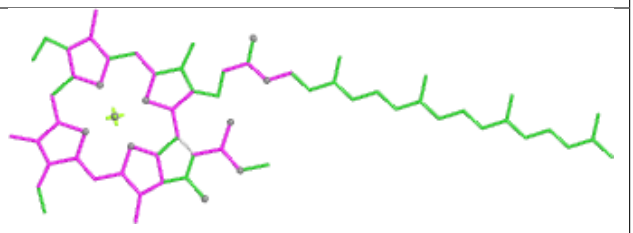


Rings

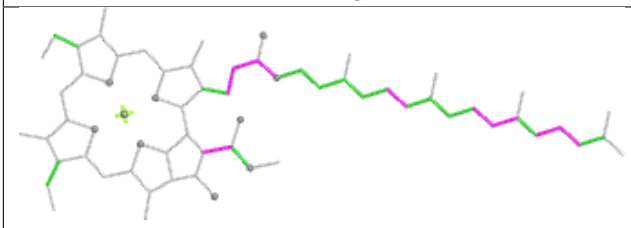
Ligand CLA B 601



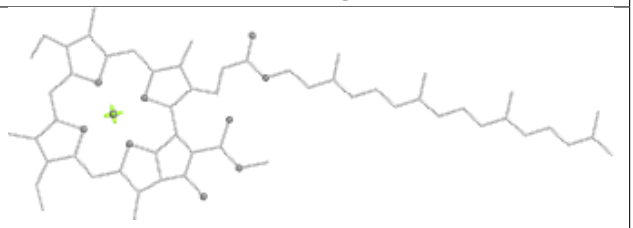
Bond lengths



Bond angles

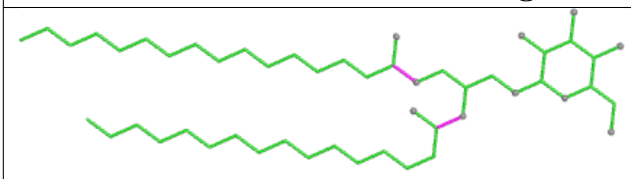


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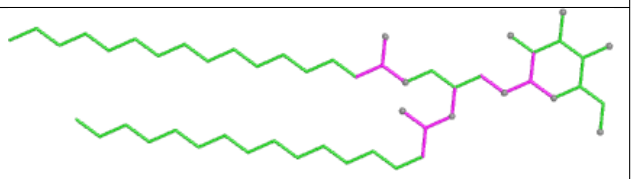


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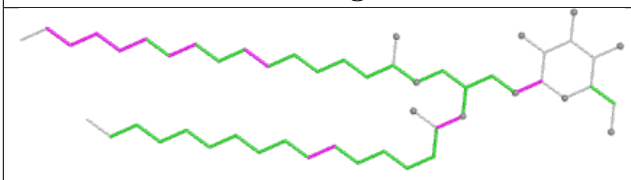
Ligand LMG m 101



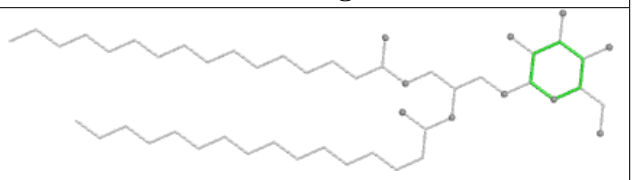
Bond lengths



Bond angles

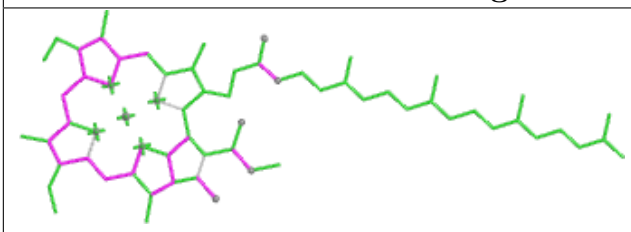


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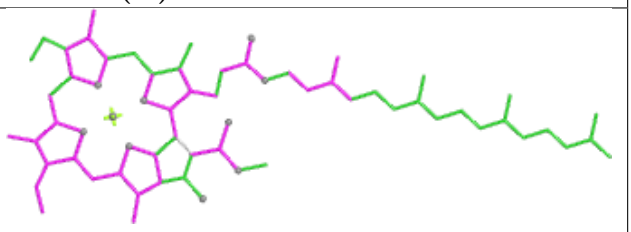


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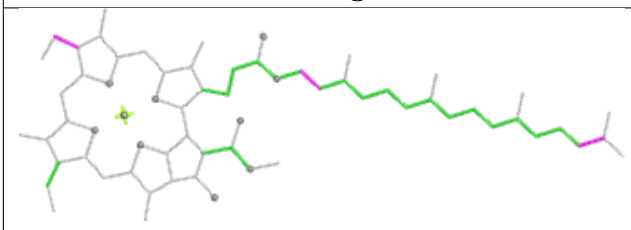
Ligand CLA D 405 (B)



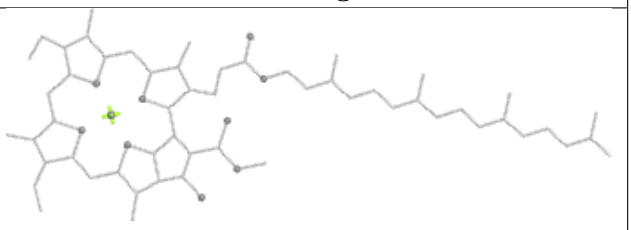
Bond lengths



Bond angles

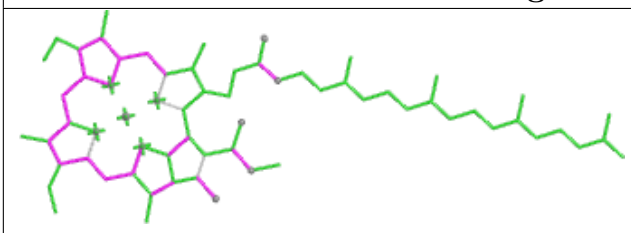


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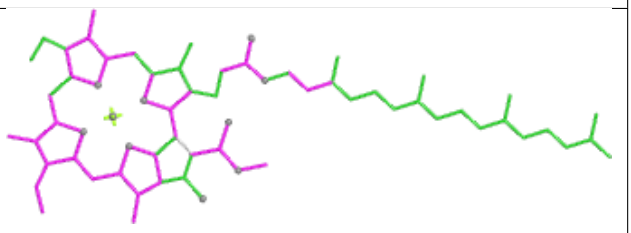


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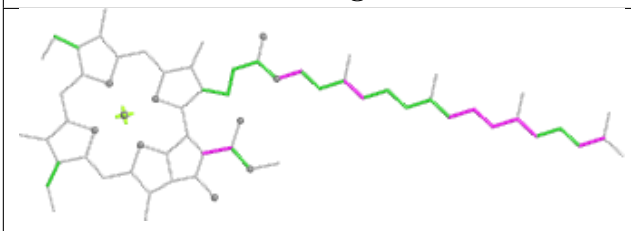
Ligand CLA b 614



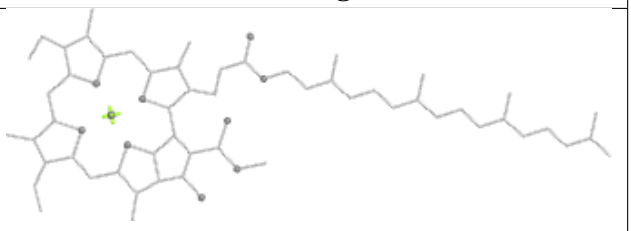
Bond lengths



Bond angles

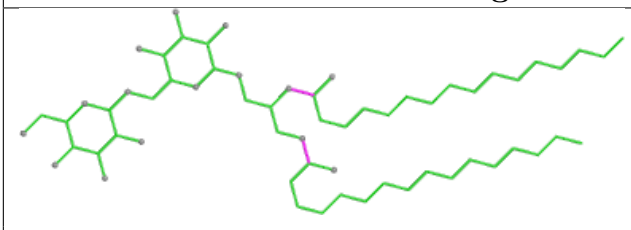


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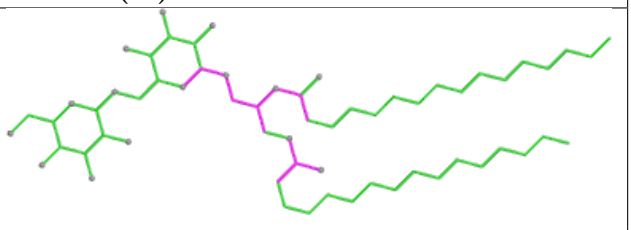


Rings

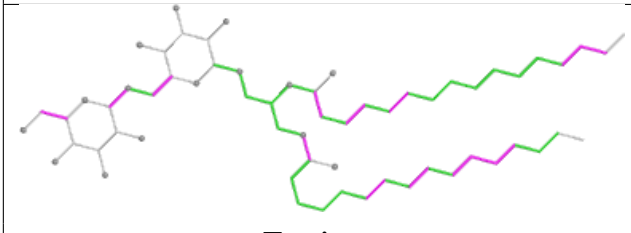
Ligand DGD c 517 (A)



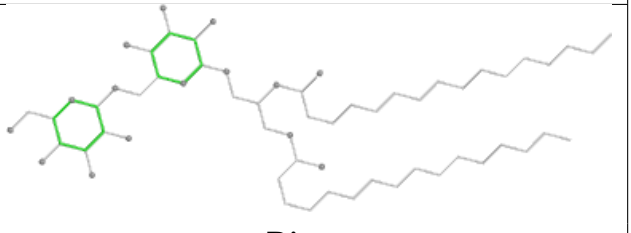
Bond lengths



Bond angles

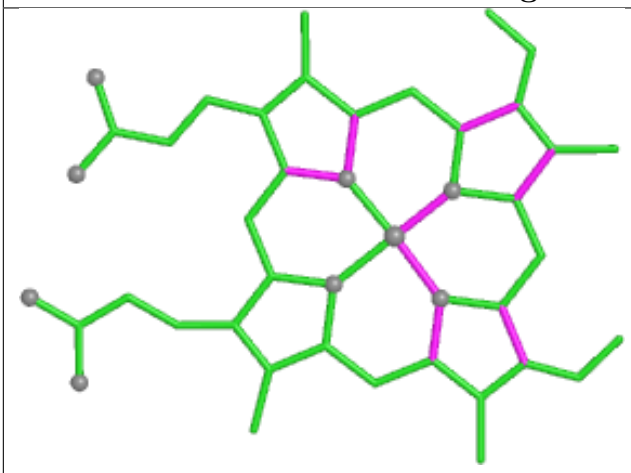


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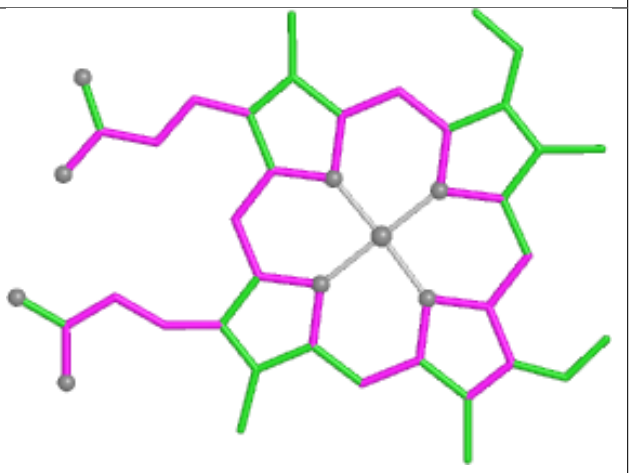


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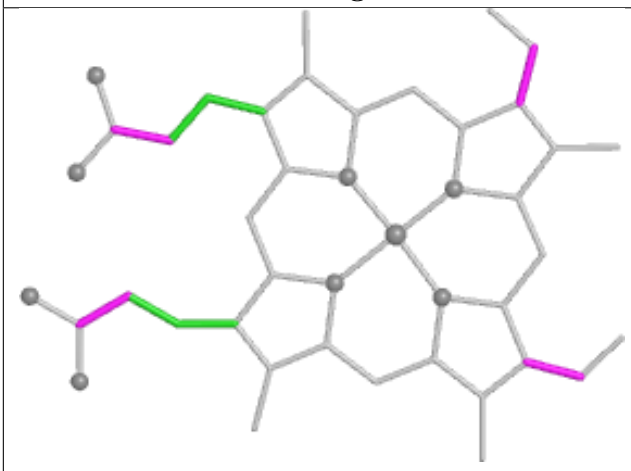
Ligand HEM E 103



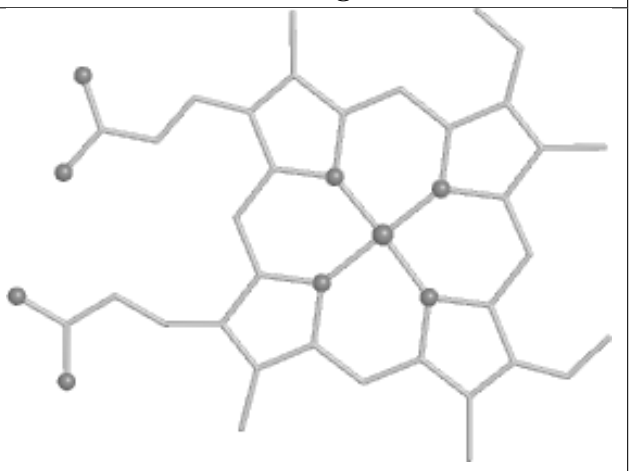
Bond lengths



Bond angles

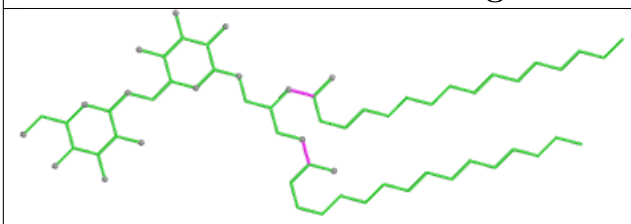


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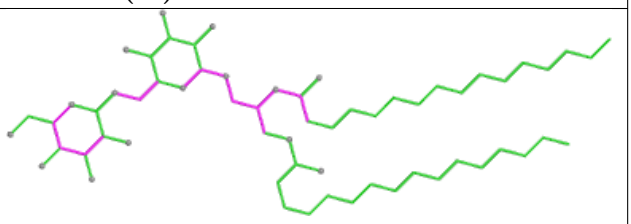


Rings

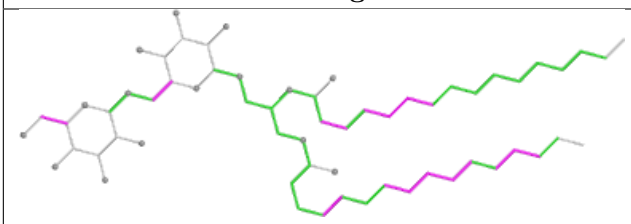
Ligand DGD C 517 (A)



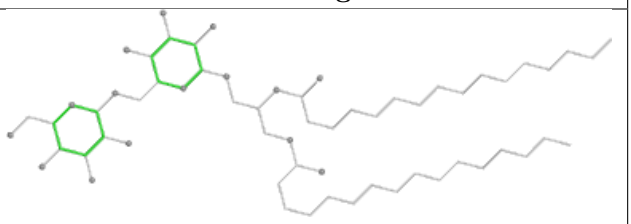
Bond lengths



Bond angles

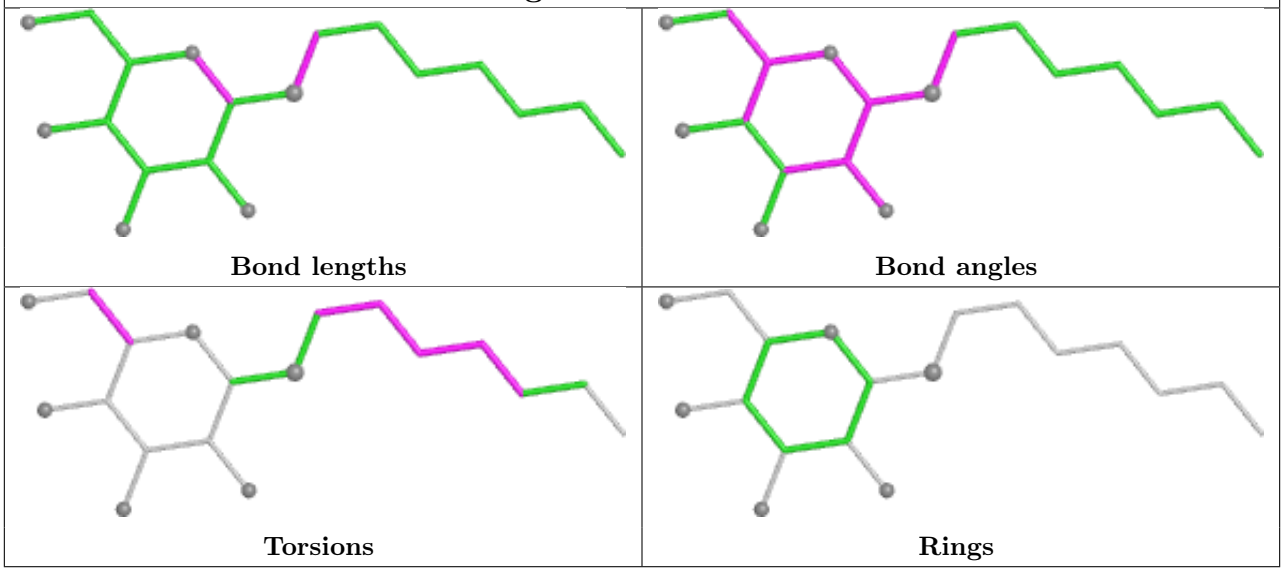


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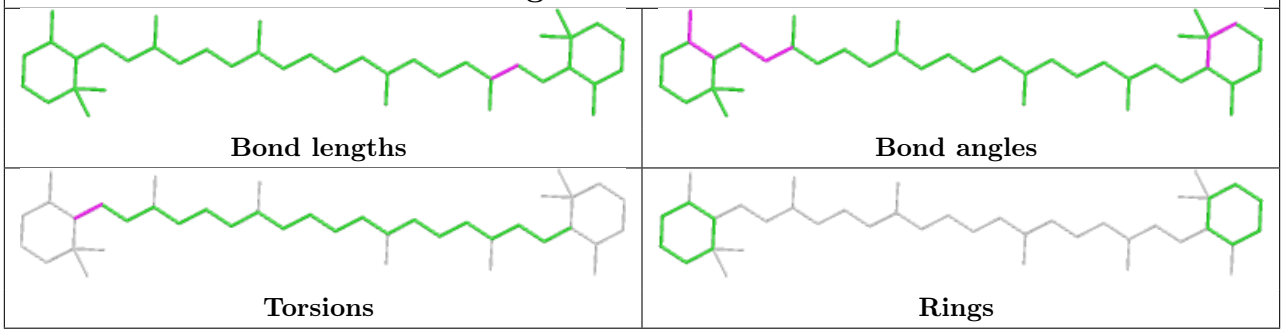


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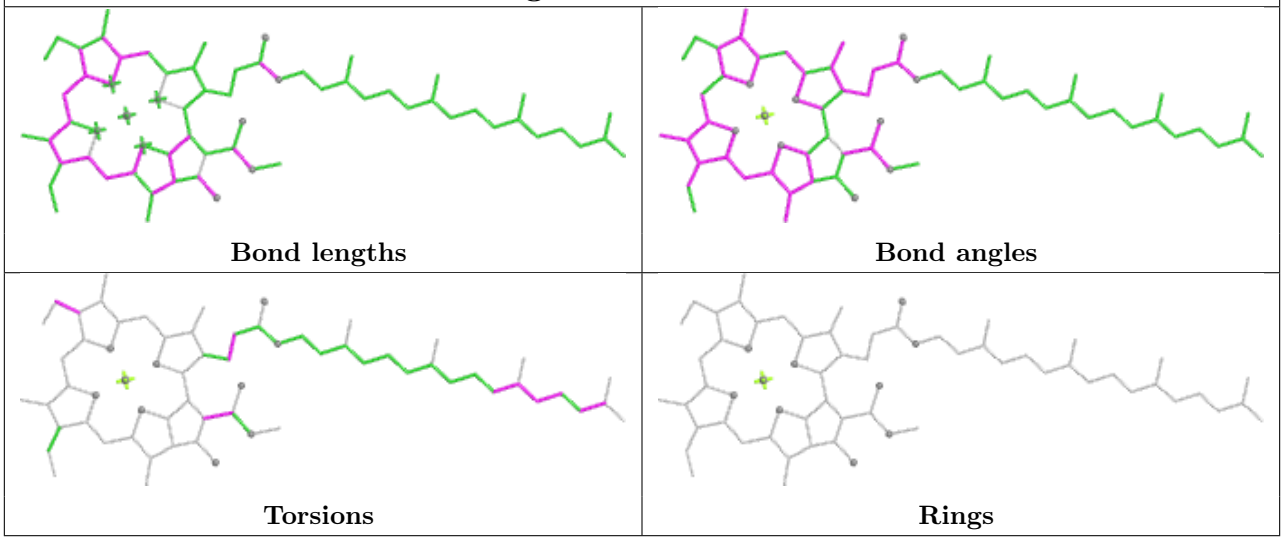
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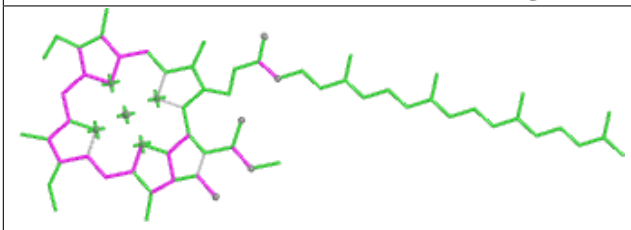
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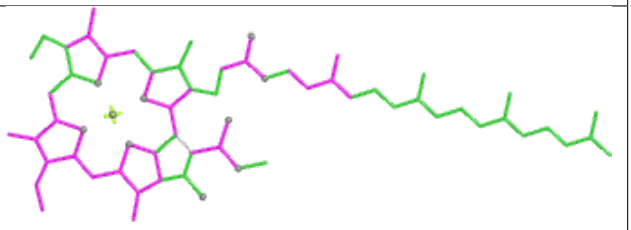
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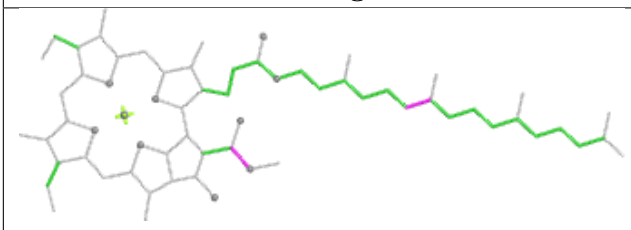
Ligand CLA C 504



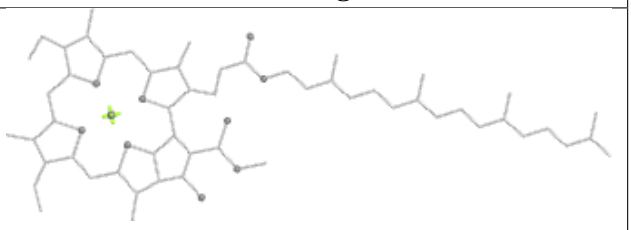
Bond lengths



Bond angles

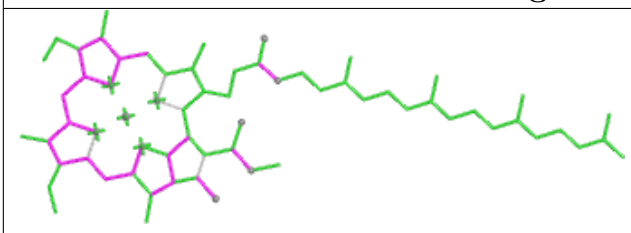


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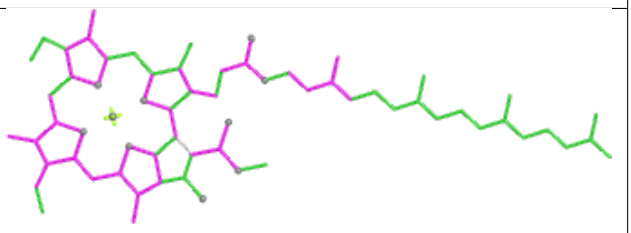


Rings

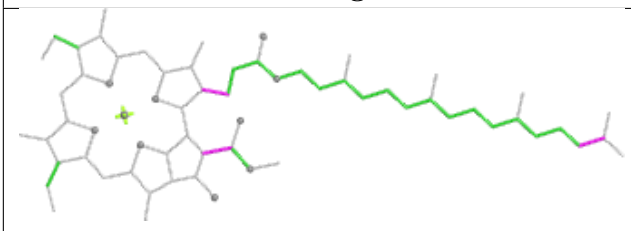
Ligand CLA c 509



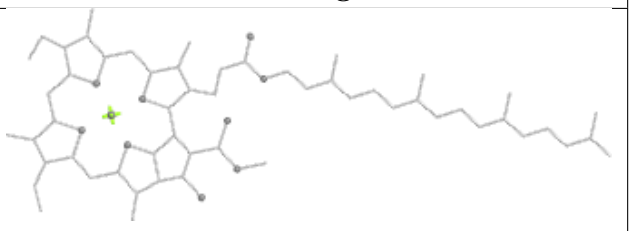
Bond lengths



Bond angles

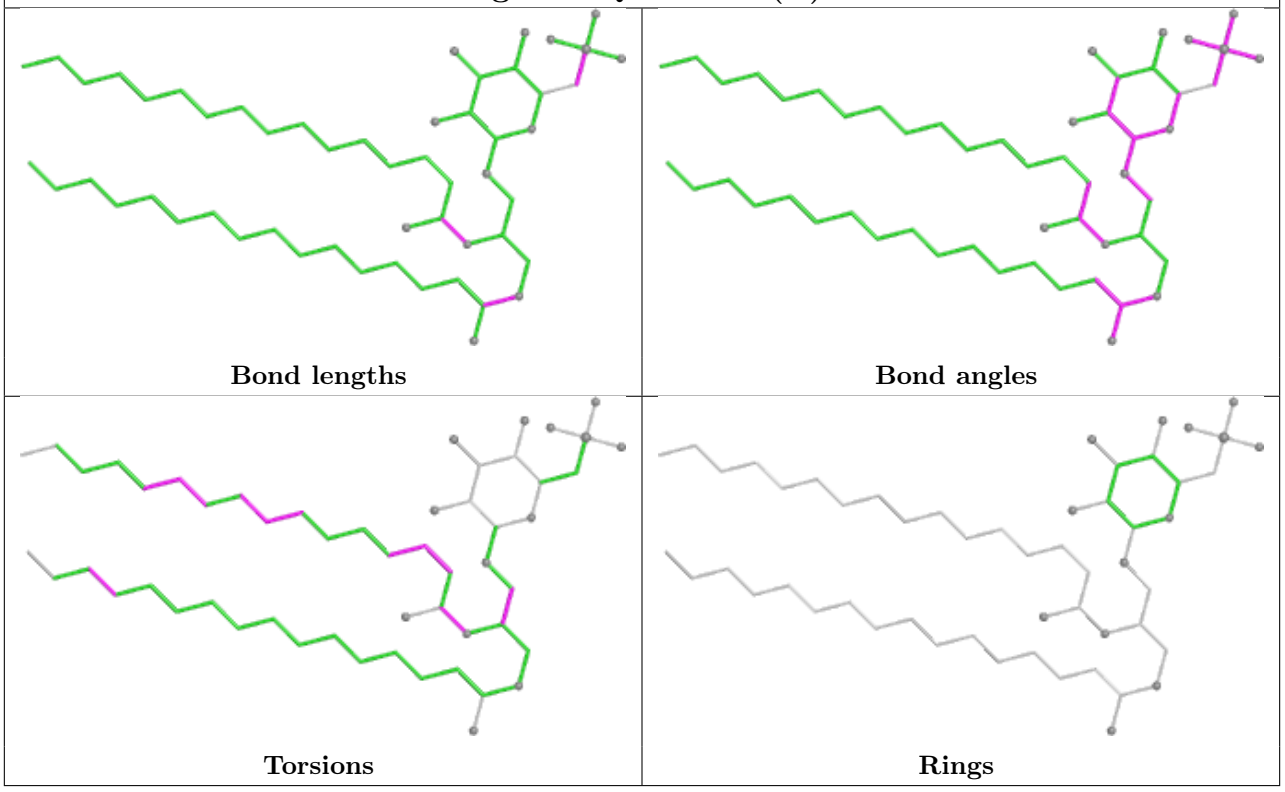


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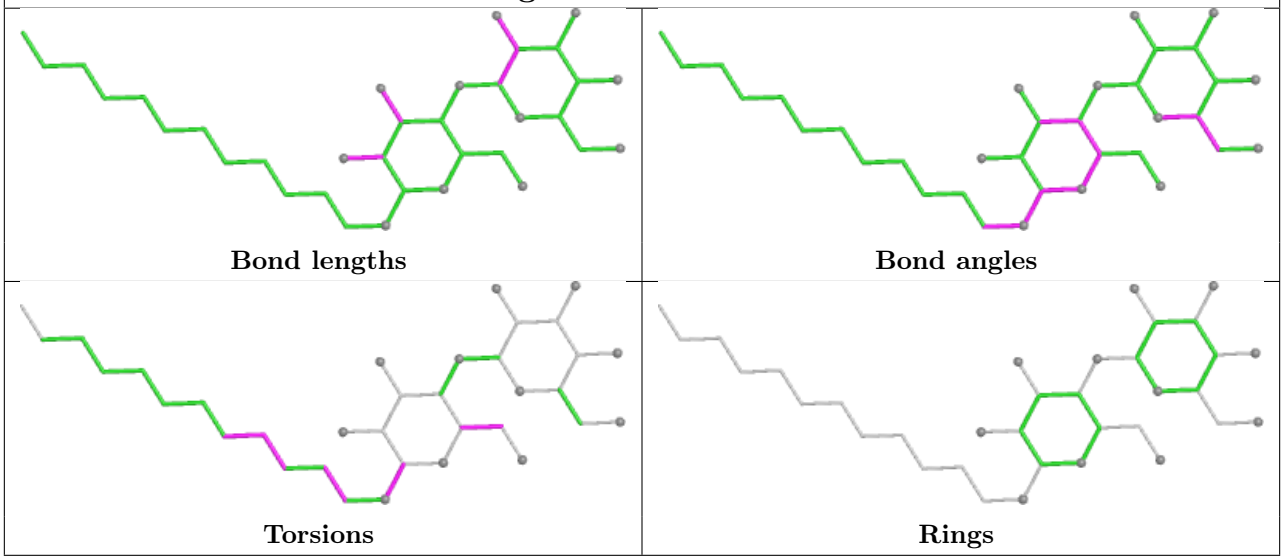


Rings

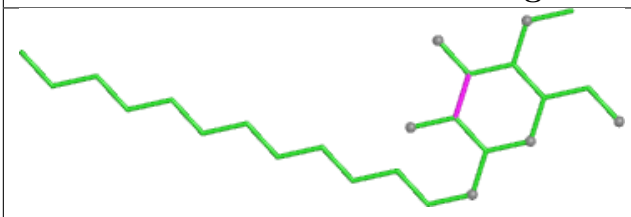
Ligand SQD A 410 (B)



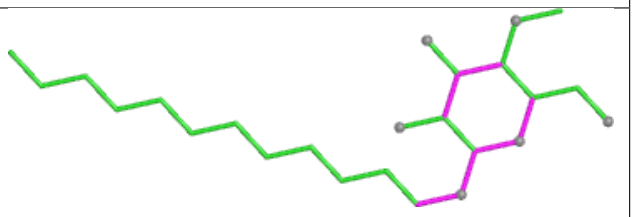
Ligand LMT M 101



Ligand LMT b 621



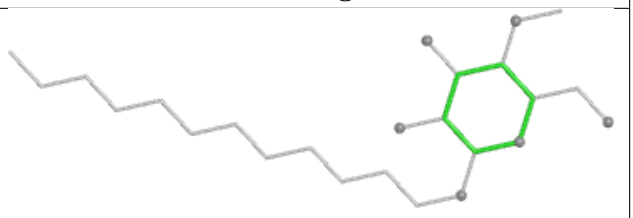
Bond lengths



Bond angles

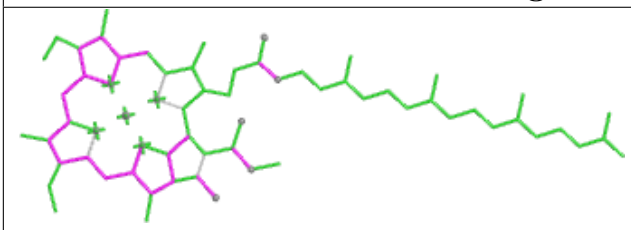


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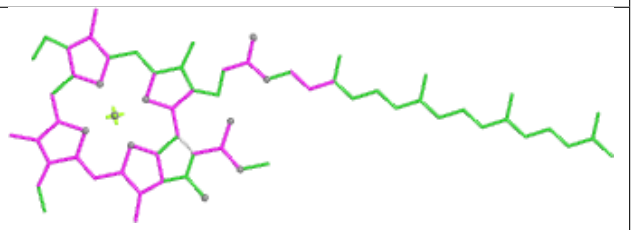


Rings

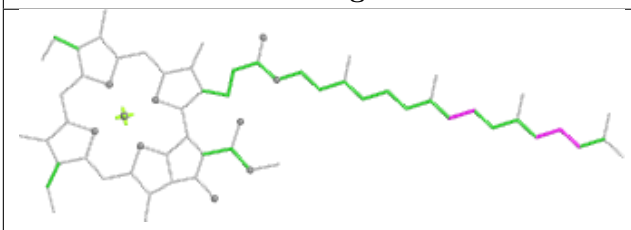
Ligand CLA b 611



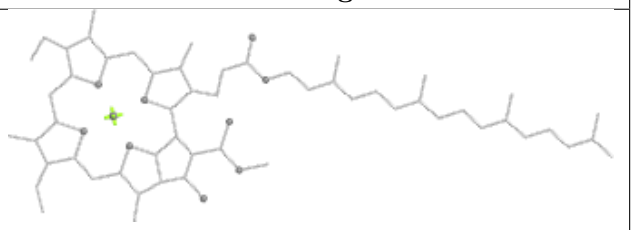
Bond lengths



Bond angles

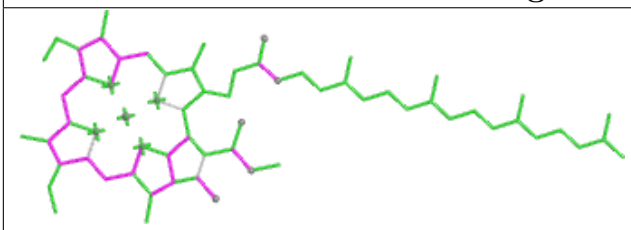


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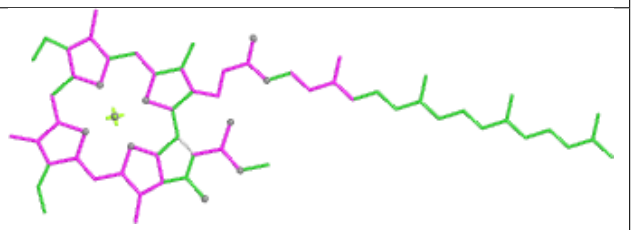


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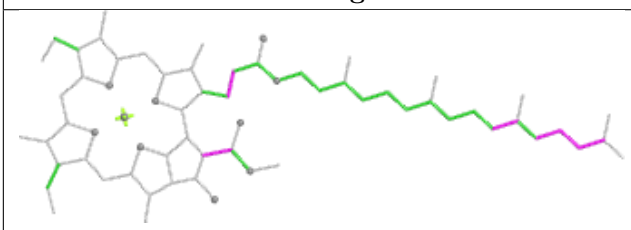
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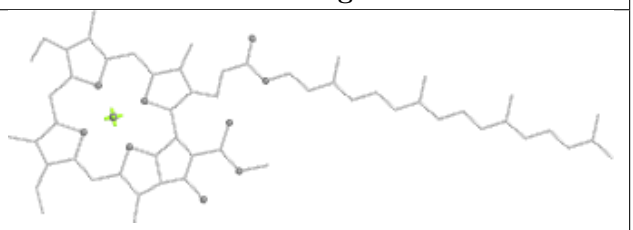
Bond lengths



Bond angles

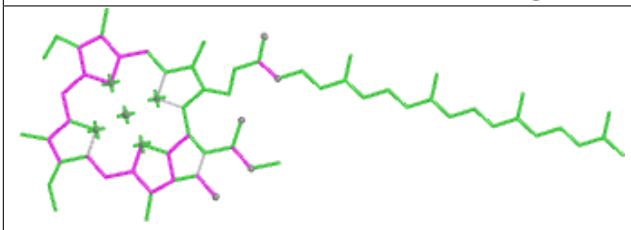


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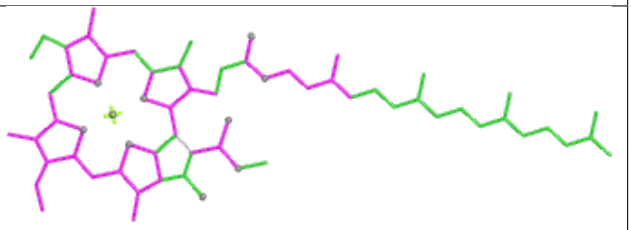


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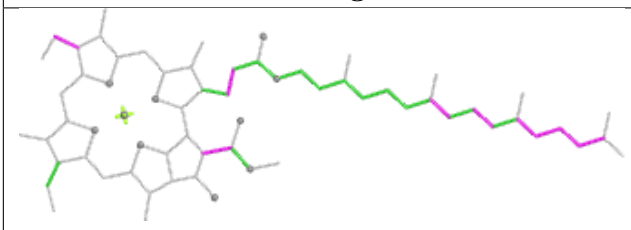
Ligand CLA b 606



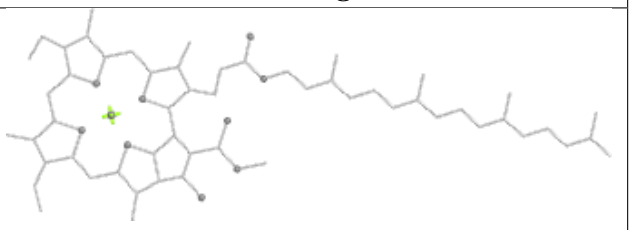
Bond lengths



Bond angles

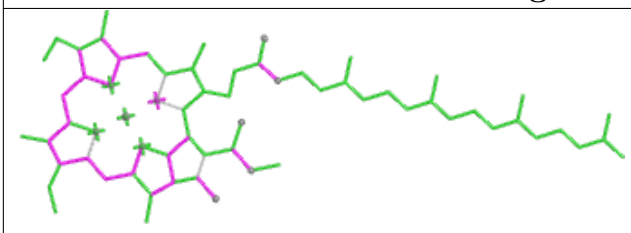


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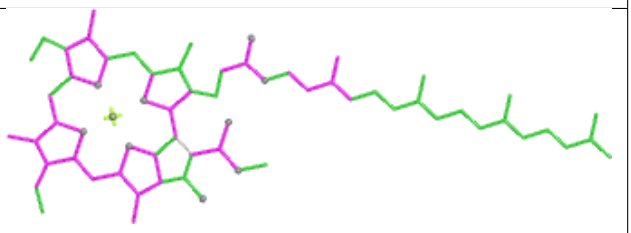


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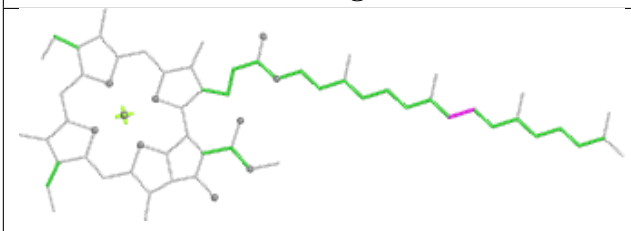
Ligand CLA c 504



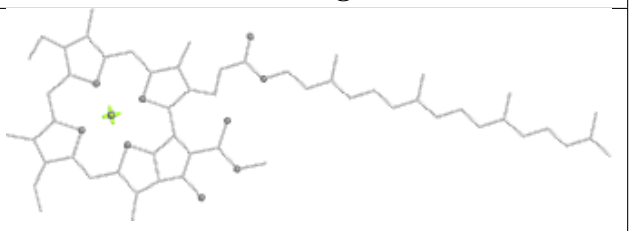
Bond lengths



Bond angles

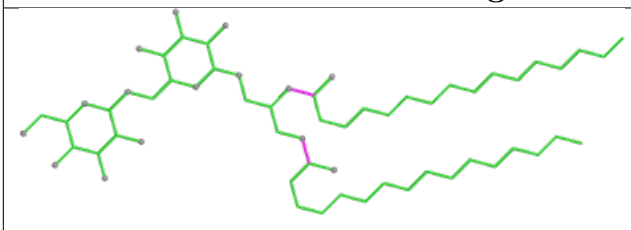


Torsions

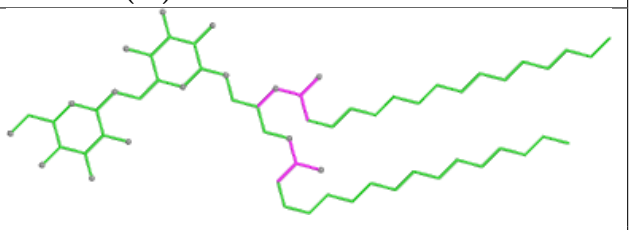


Rings

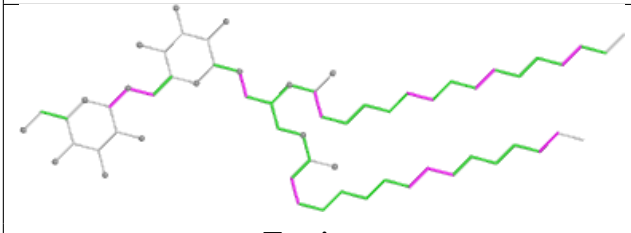
Ligand DGD C 518 (B)



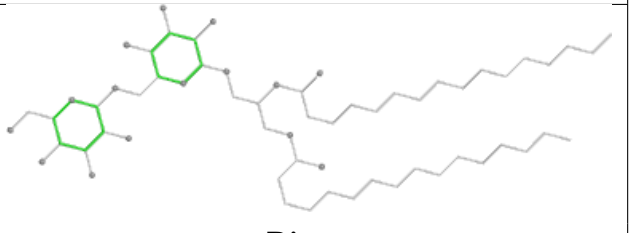
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Bond angles

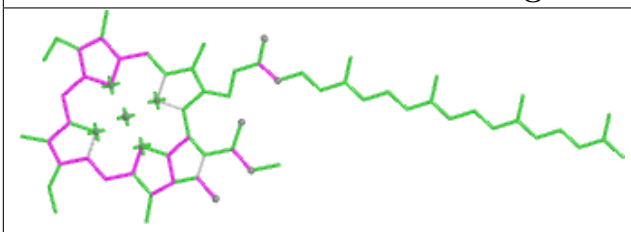


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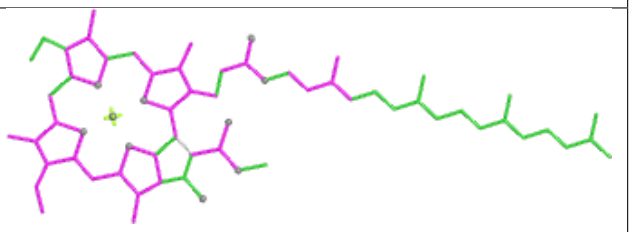


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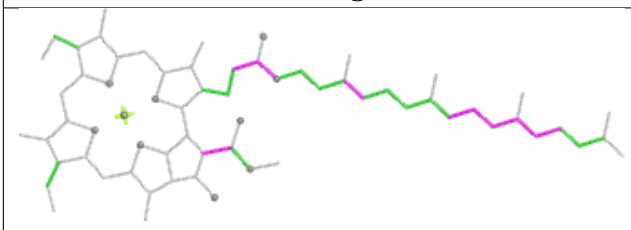
Ligand CLA C 511



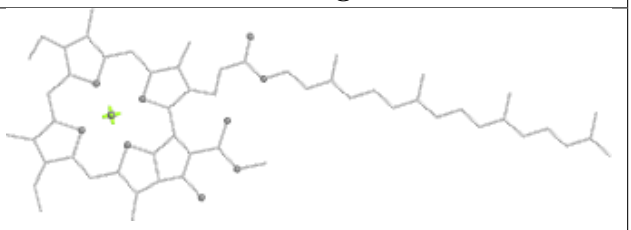
Bond lengths



Bond angles

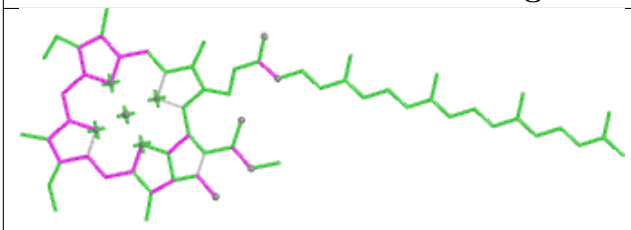


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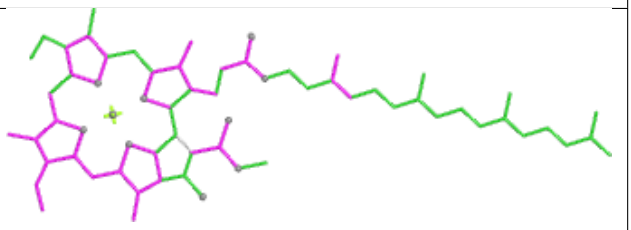


Rings

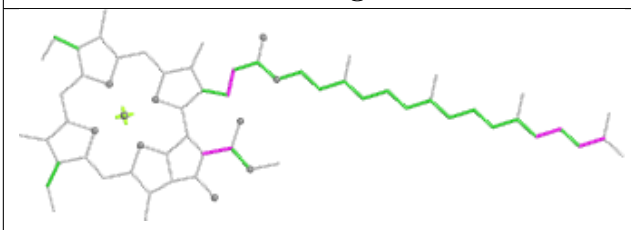
Ligand CLA B 603



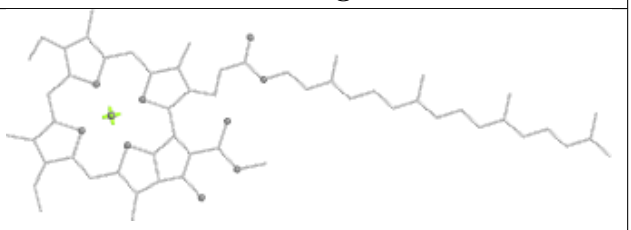
Bond lengths



Bond angles

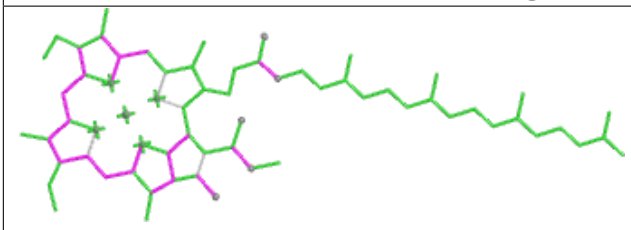


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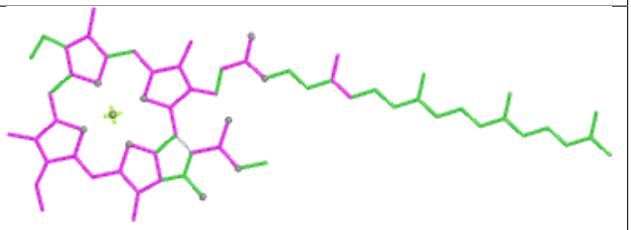


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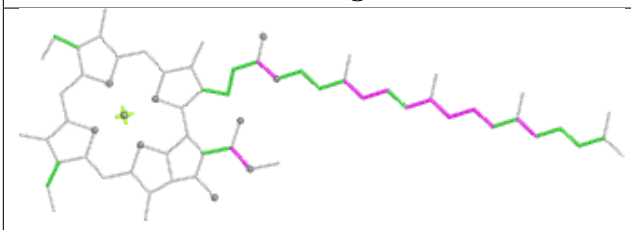
Ligand CLA D 406



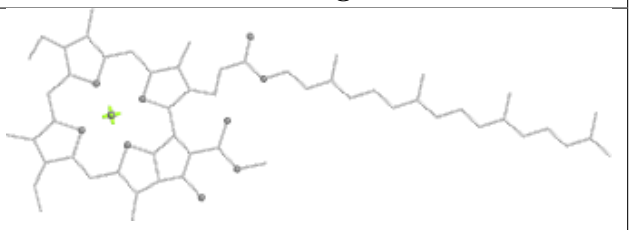
Bond lengths



Bond angles

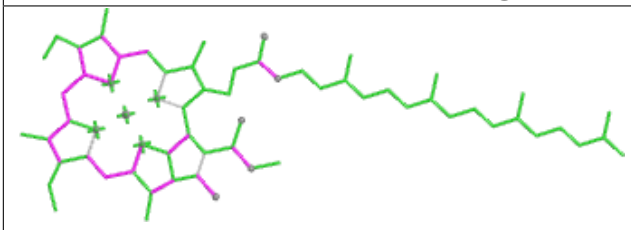


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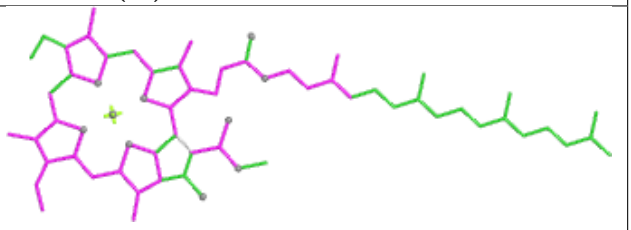


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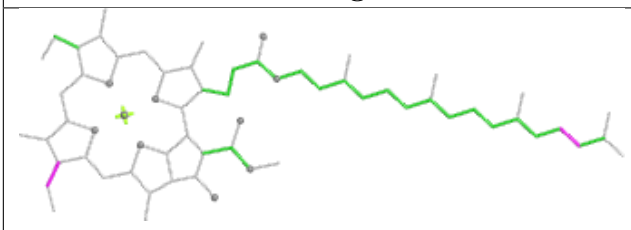
Ligand CLA a 406 (B)



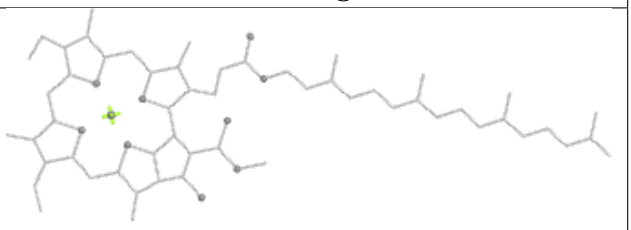
Bond lengths



Bond angles

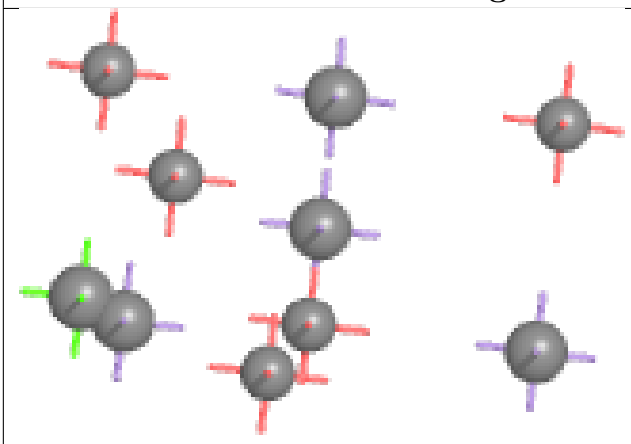


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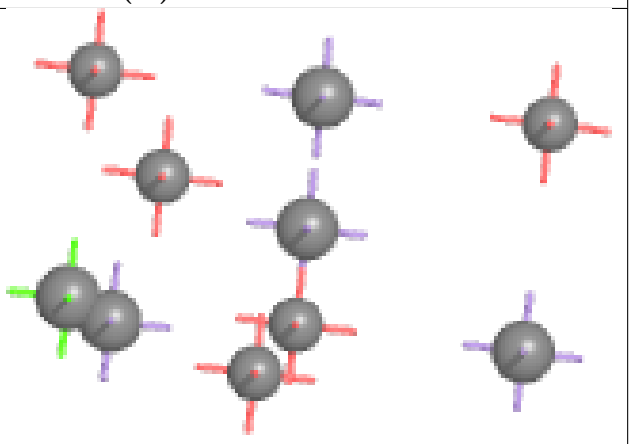


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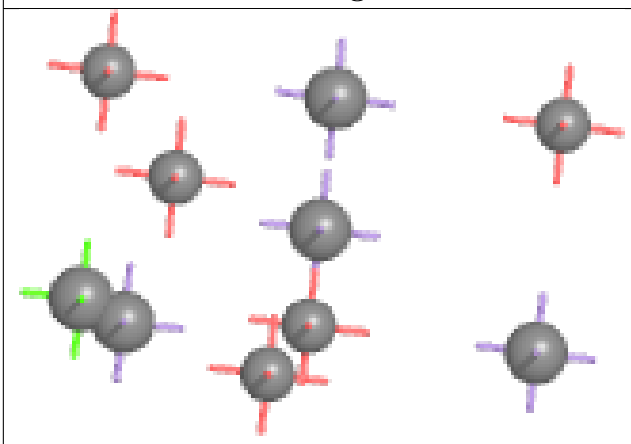
Ligand OEX A 413 (B)



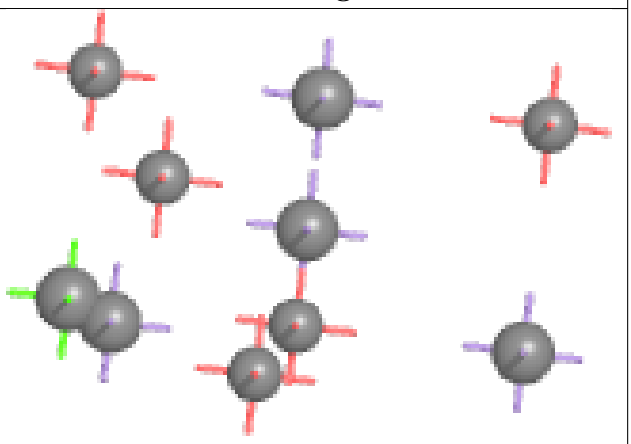
Bond lengths



Bond angles

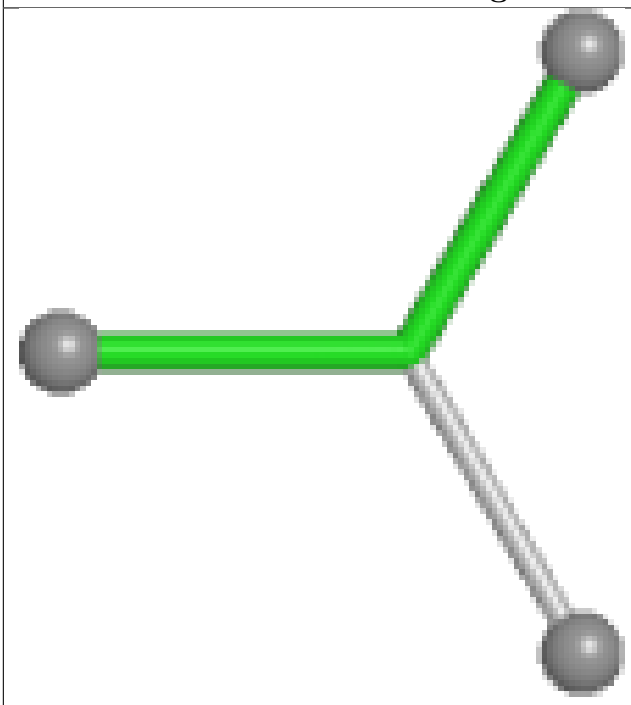


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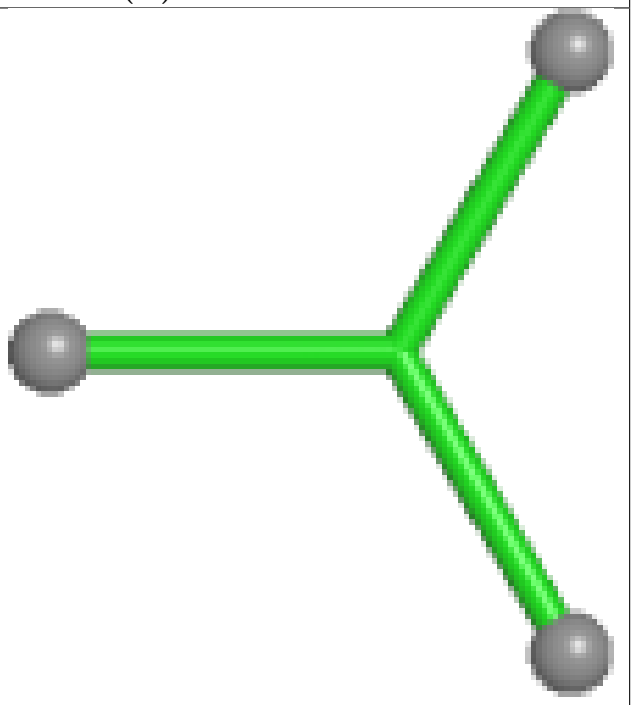


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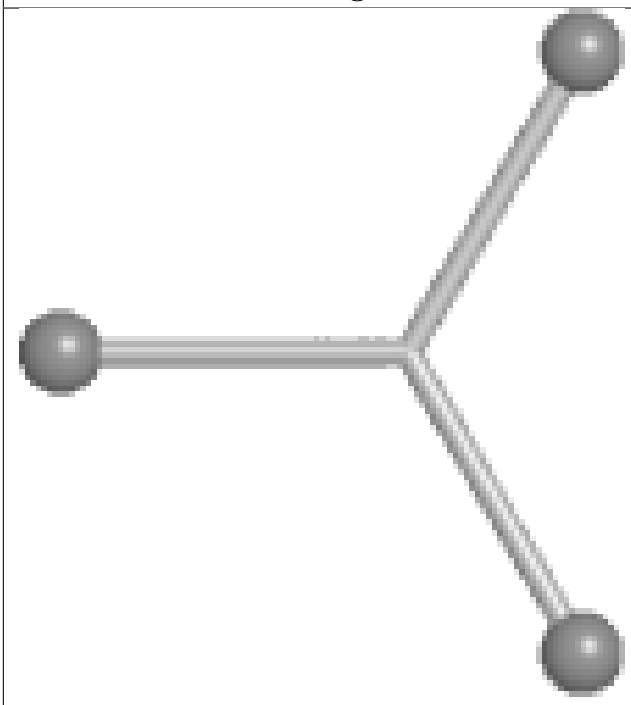
Ligand BCT A 348 (B)



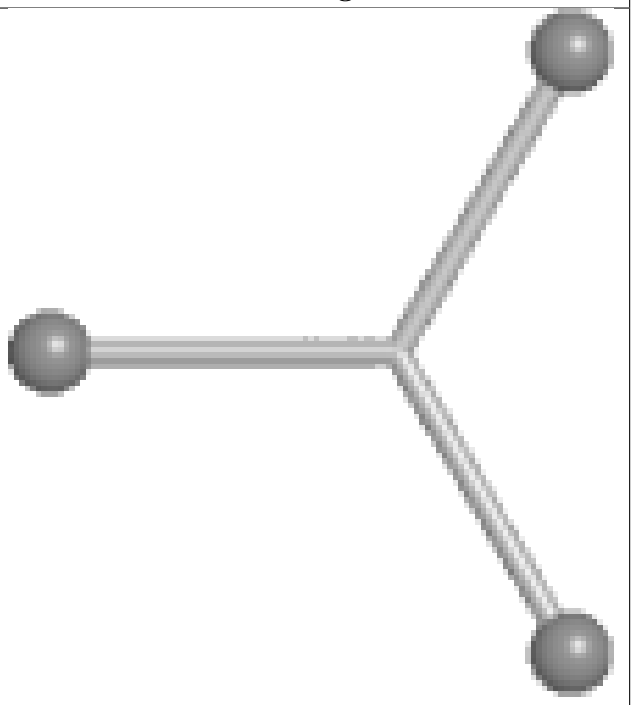
Bond lengths



Bond angles

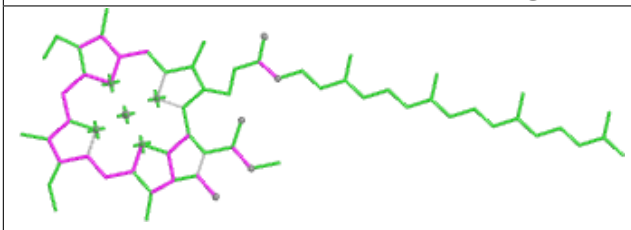


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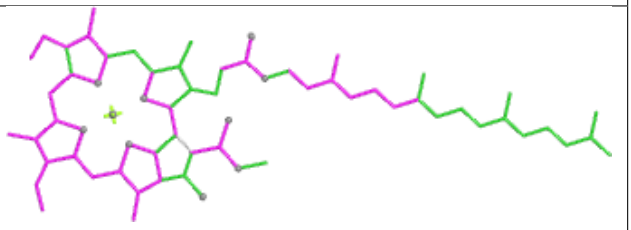


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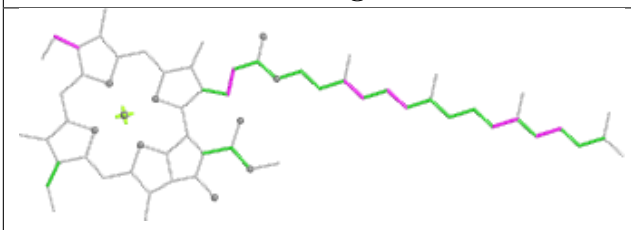
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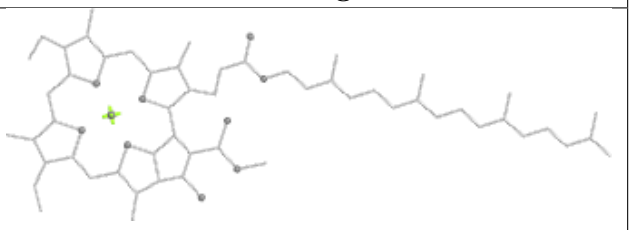
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Bond angles

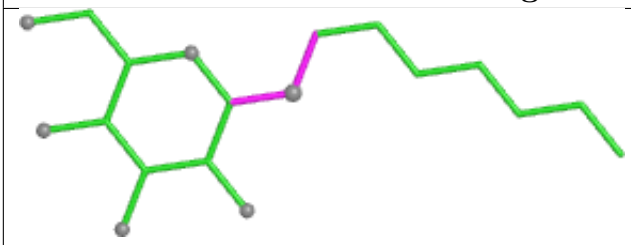


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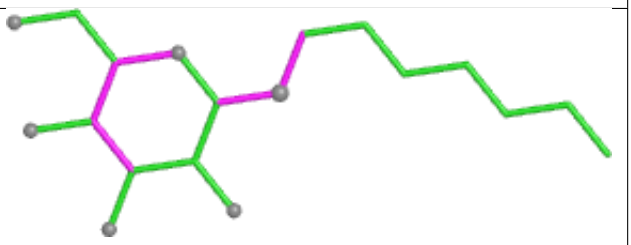


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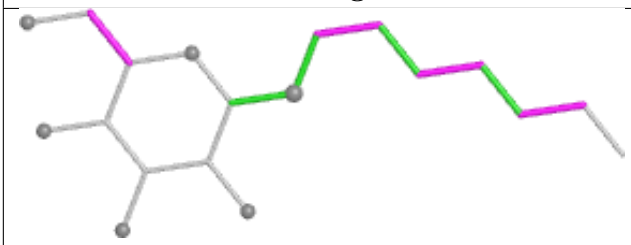
Ligand HTG B 626



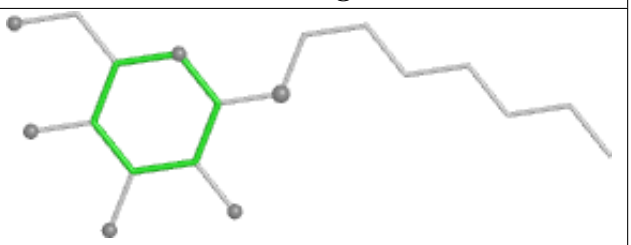
Bond lengths



Bond angles

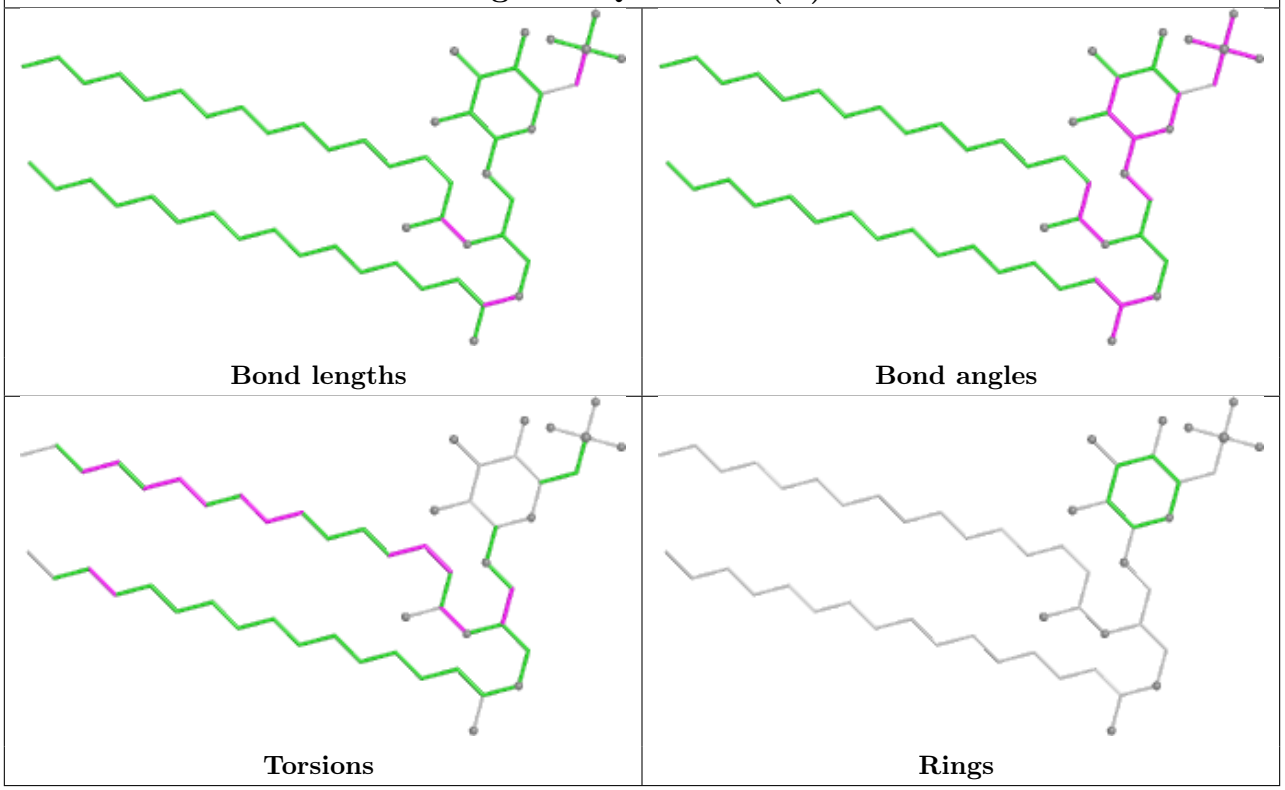


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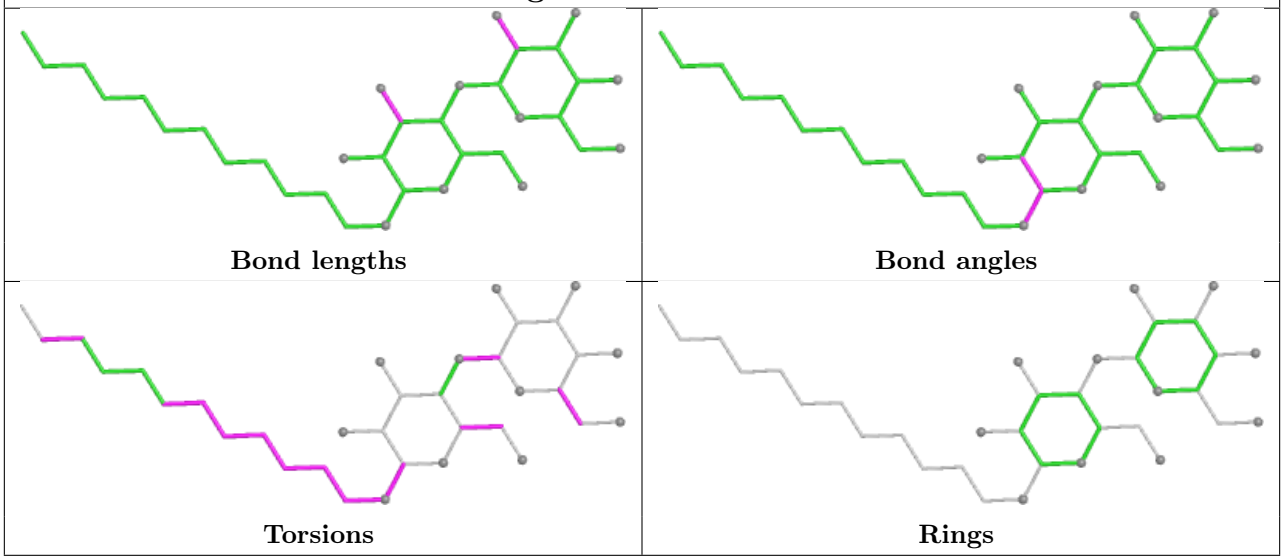


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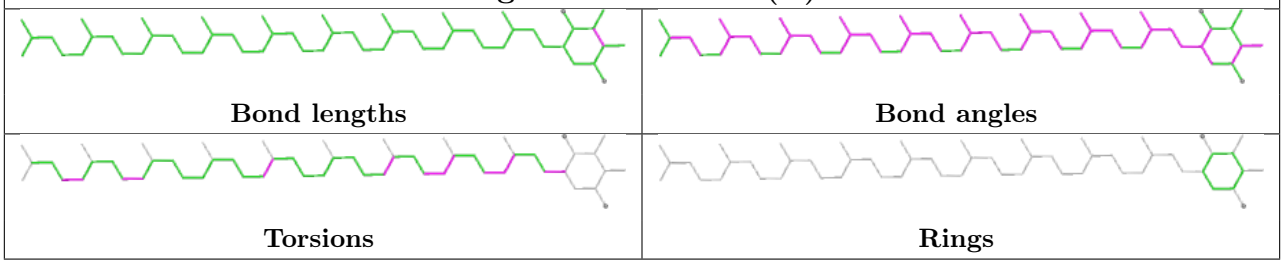
Ligand SQD A 410 (A)



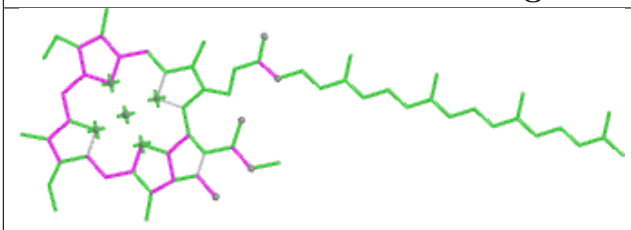
Ligand LMT e 102



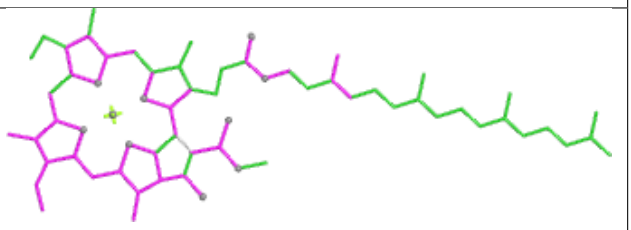
Ligand PL9 A 414 (B)



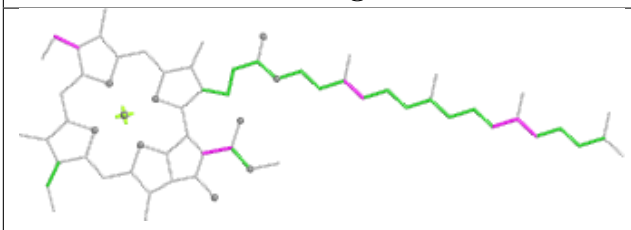
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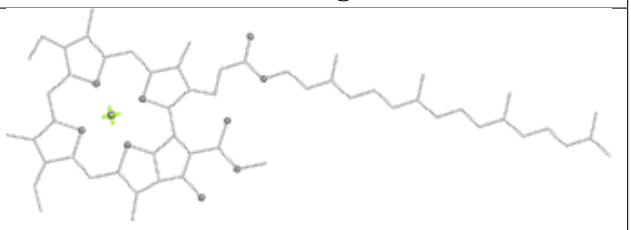
Bond lengths



Bond angles

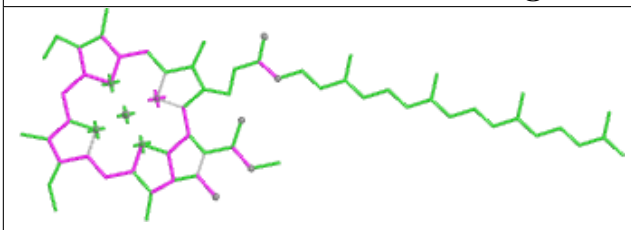


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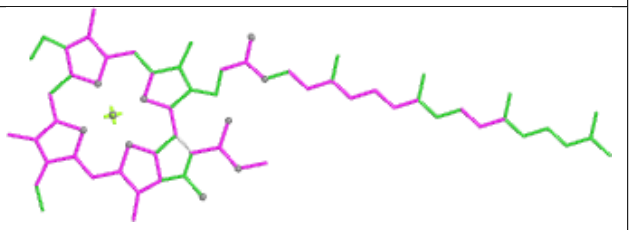


Rings

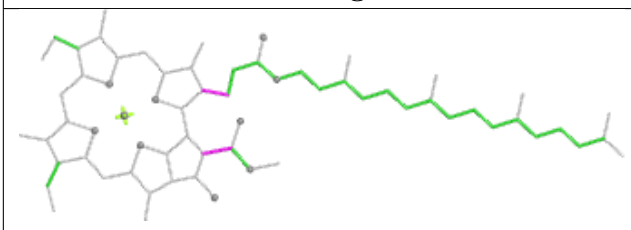
Ligand CLA B 604



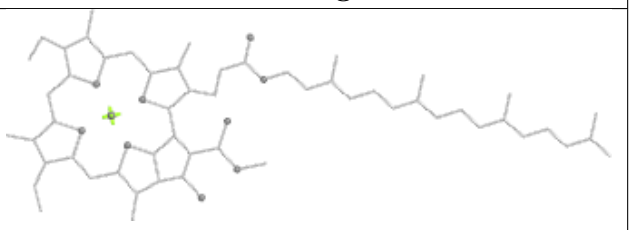
Bond lengths



Bond angles

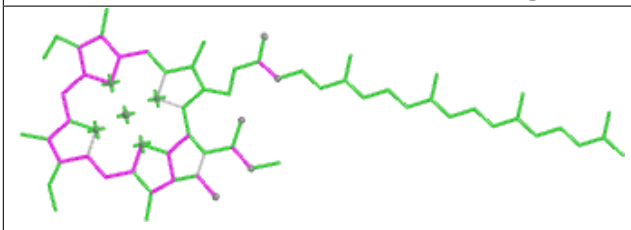


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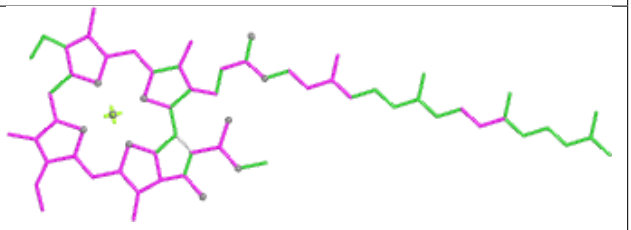


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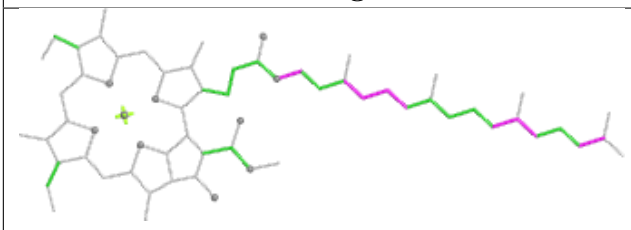
Ligand CLA A 408



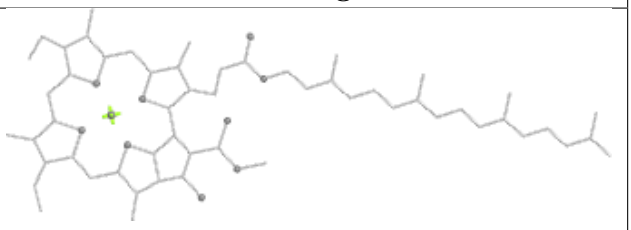
Bond lengths



Bond angles

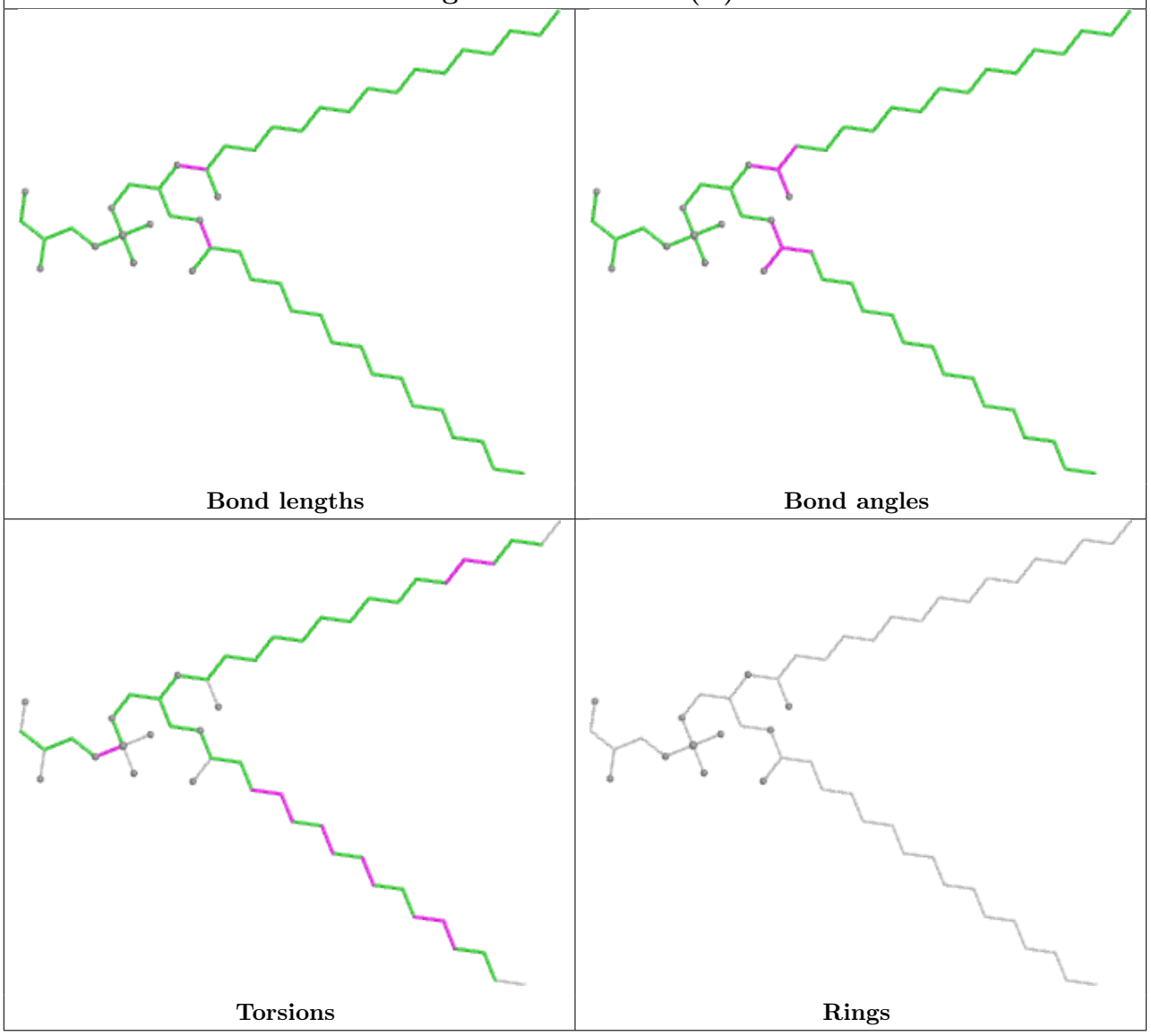


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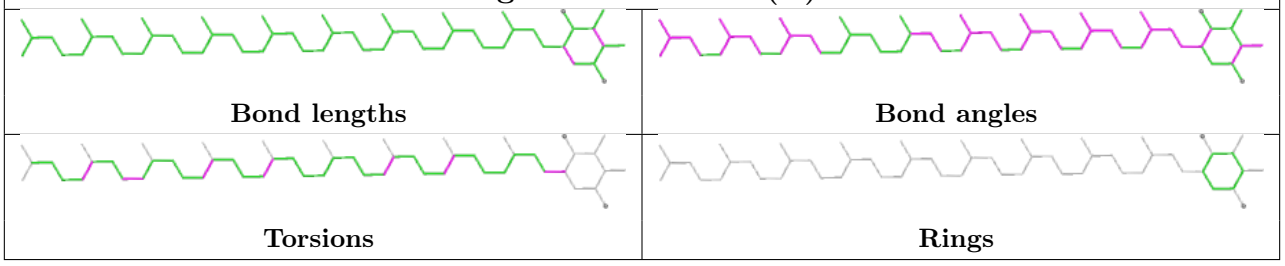


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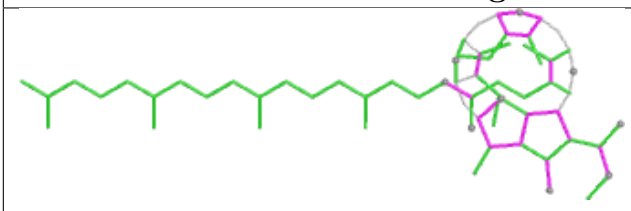
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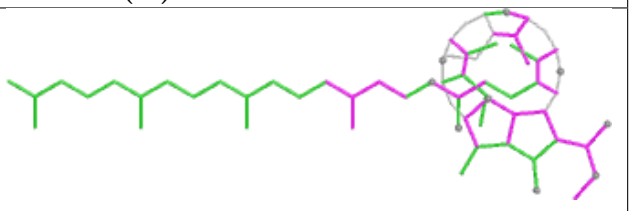
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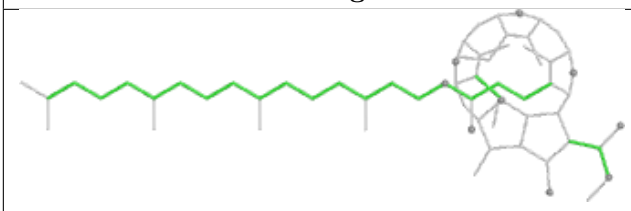
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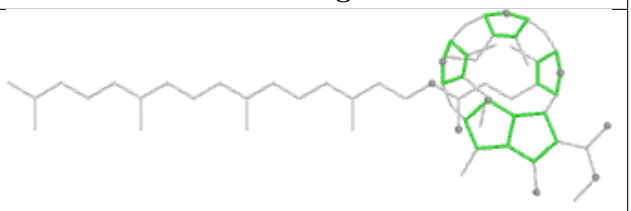
Bond lengths



Bond angles

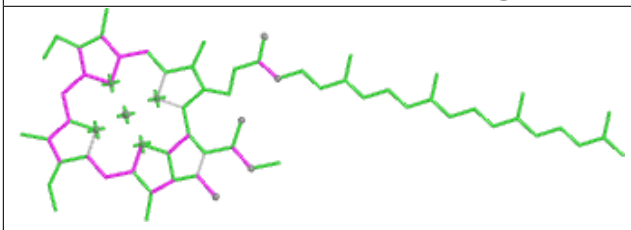


Torsions

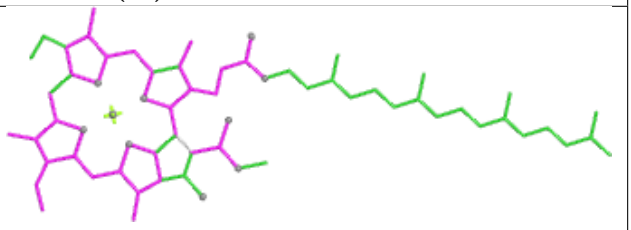


Rings

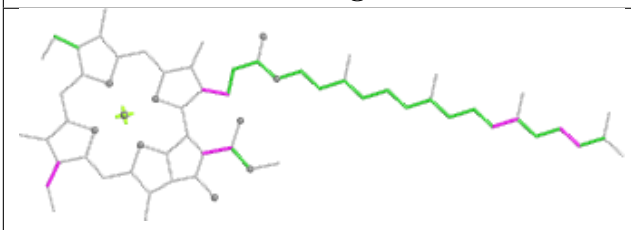
Ligand CLA a 406 (A)



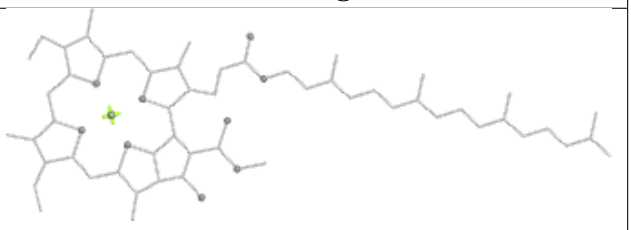
Bond lengths



Bond angles

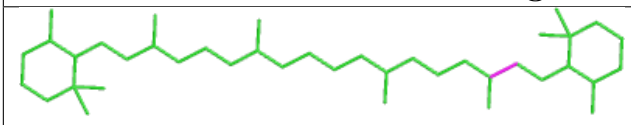


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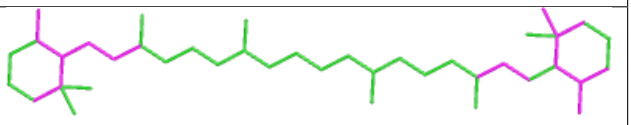


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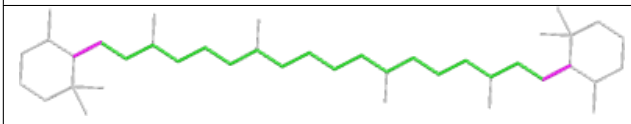
Ligand BCR a 410



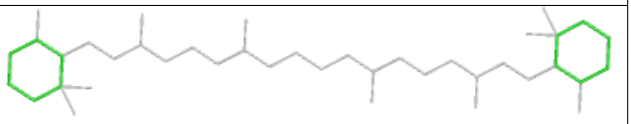
Bond lengths



Bond angles

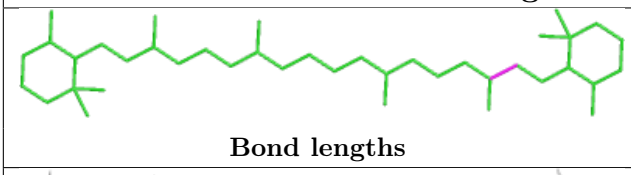


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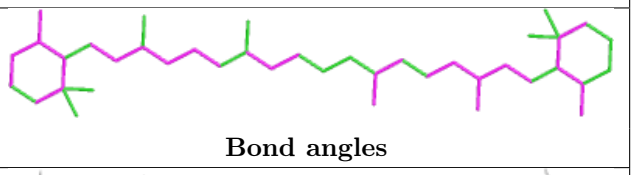


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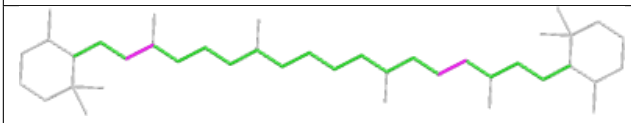
Ligand BCR K 102



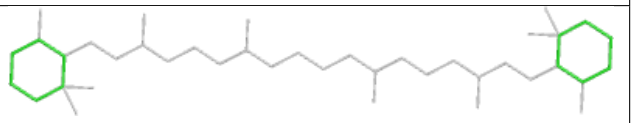
Bond lengths



Bond angles

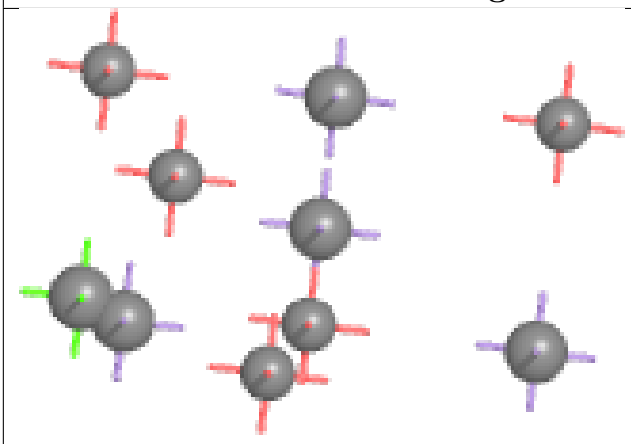


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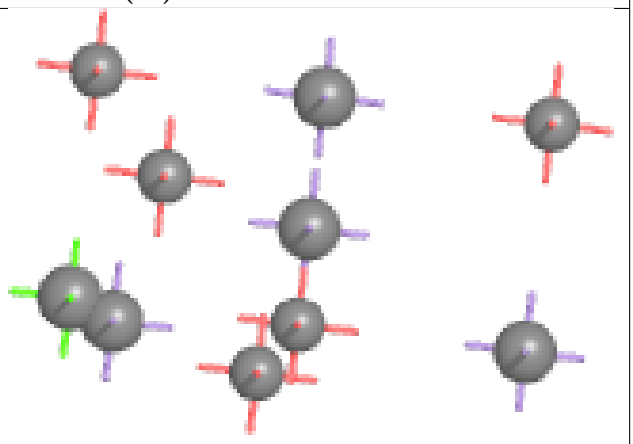


Rings

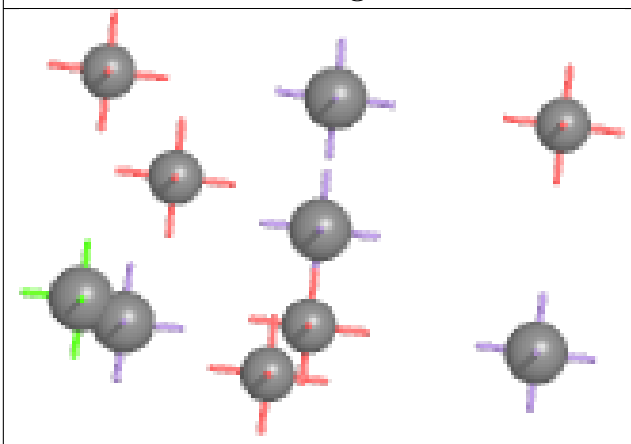
Ligand OEX A 413 (A)



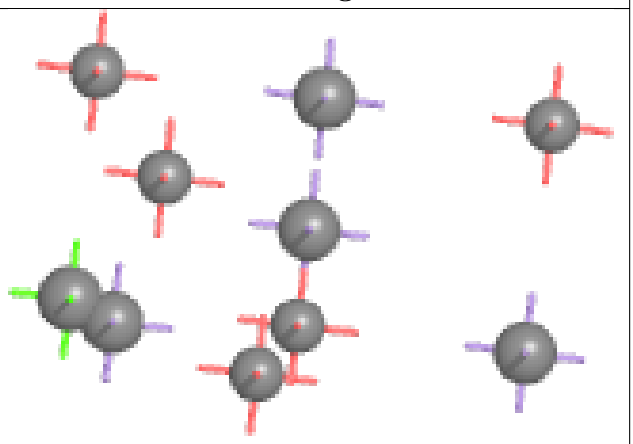
Bond lengths



Bond angles

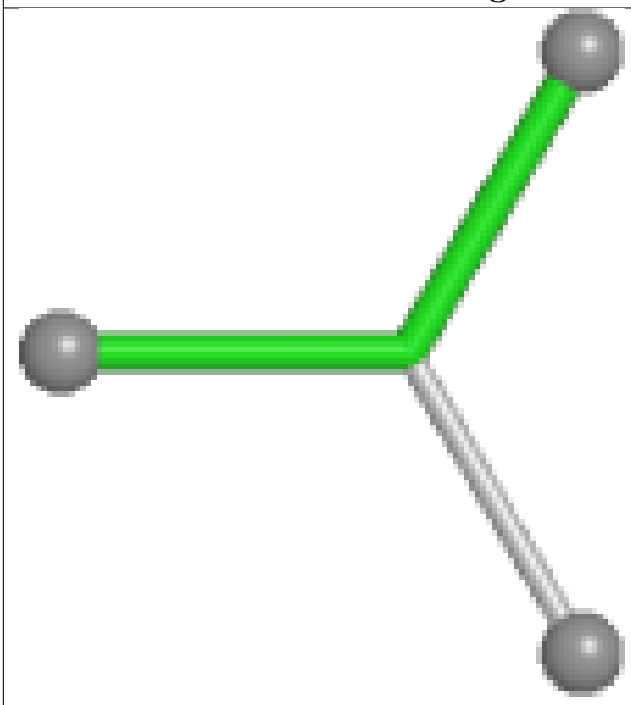


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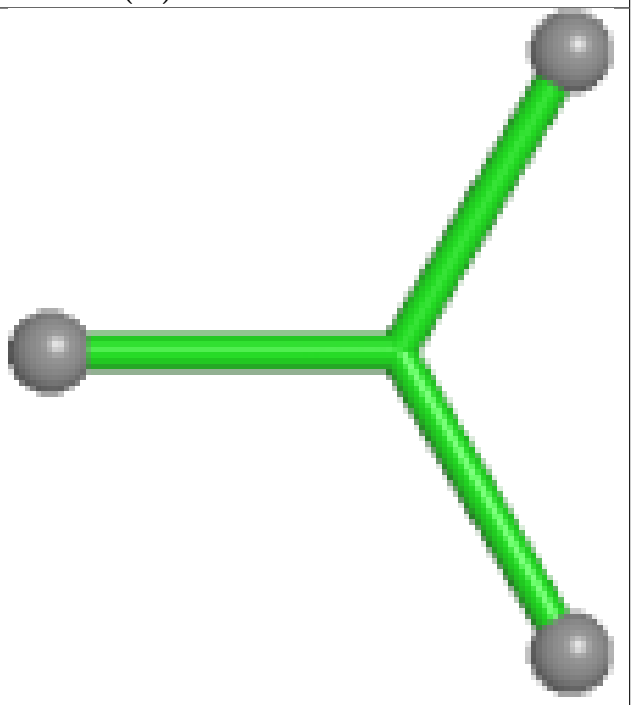


Rings

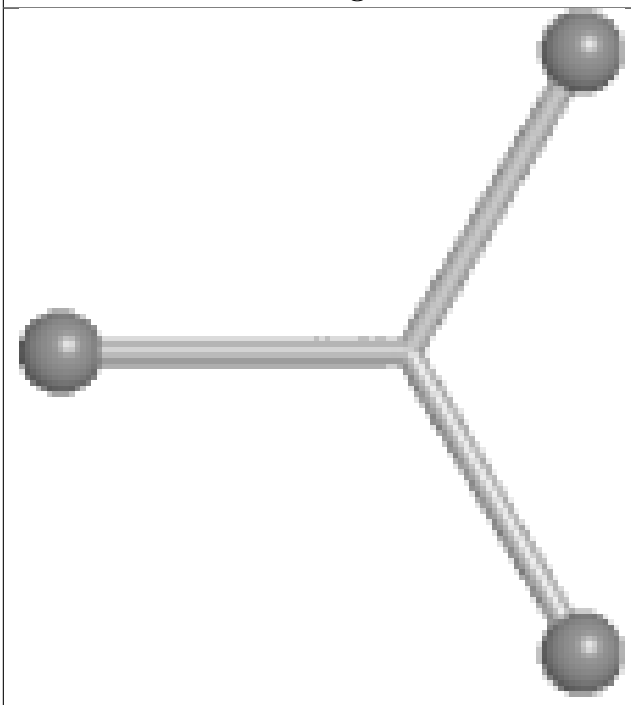
Ligand BCT A 348 (A)



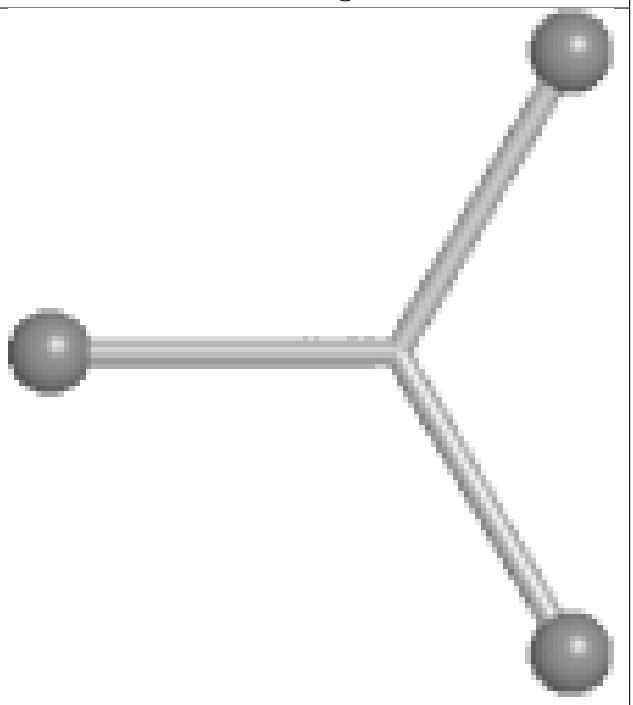
Bond lengths



Bond angles

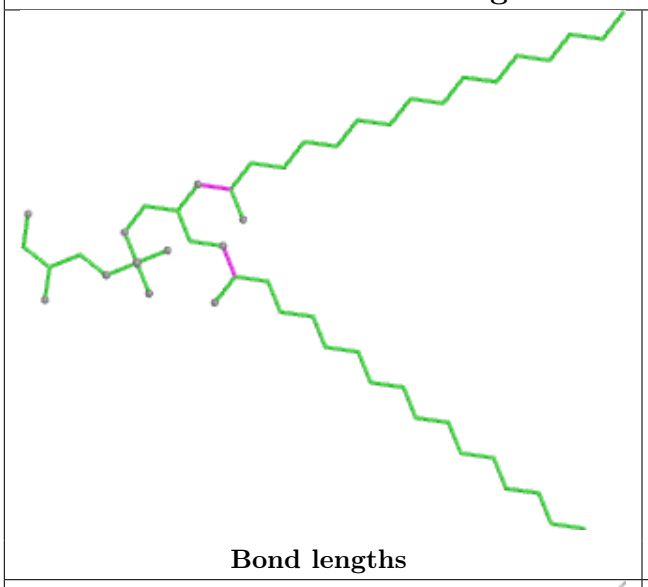


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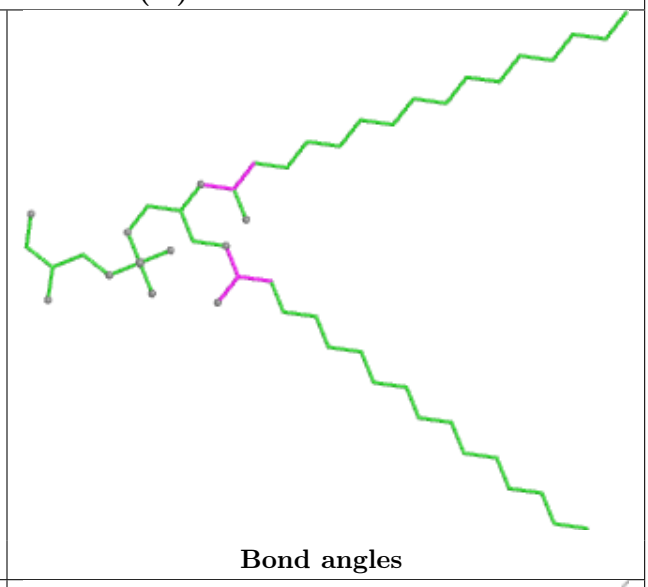


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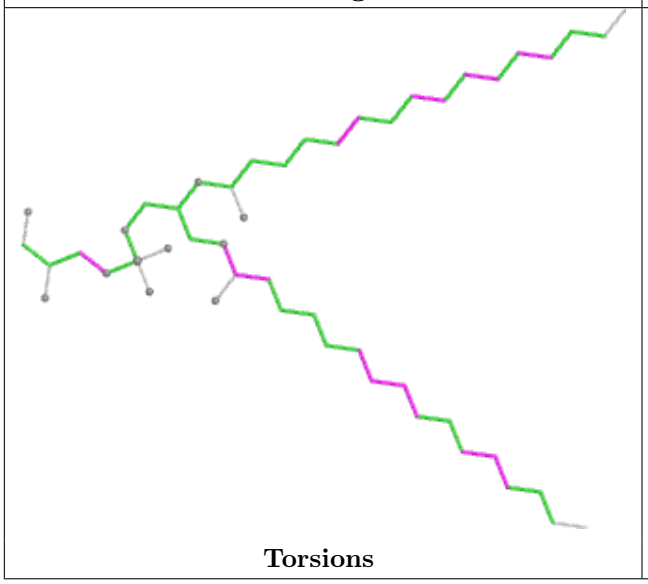
Ligand LHG D 411 (B)



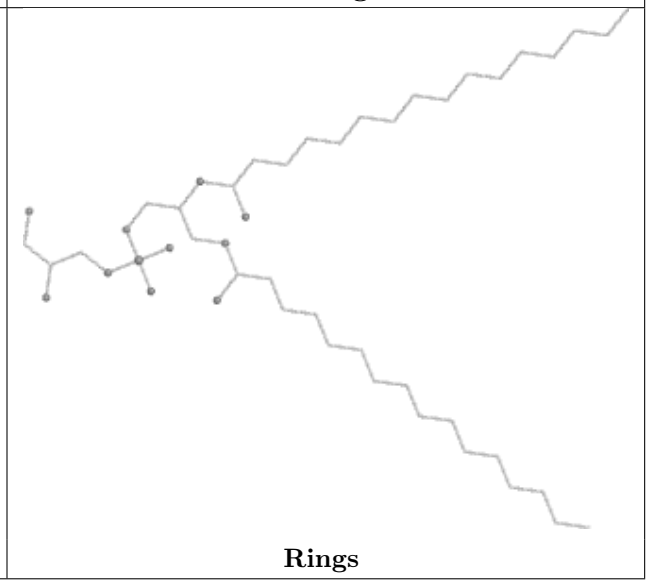
Bond lengths



Bond angles

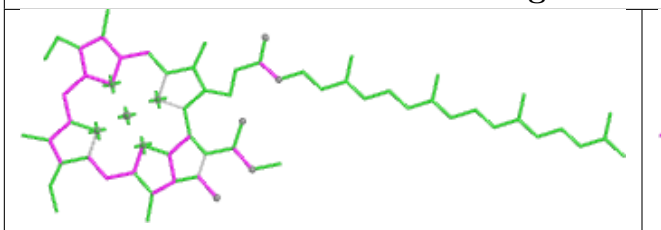


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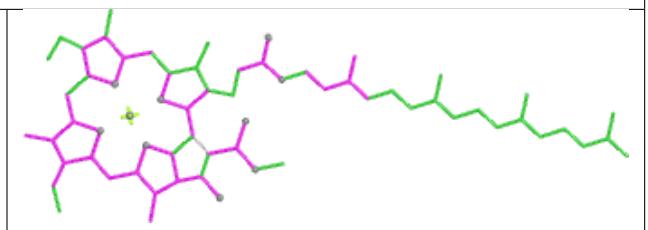


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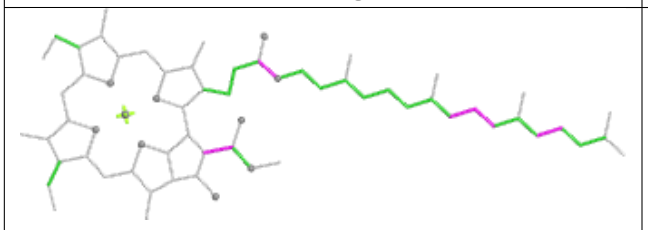
Ligand CLA b 612



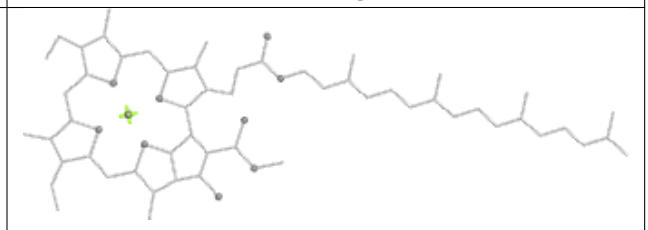
Bond lengths



Bond angles

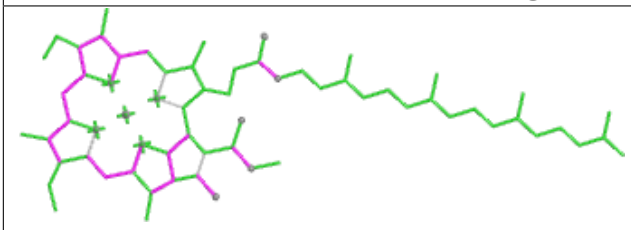


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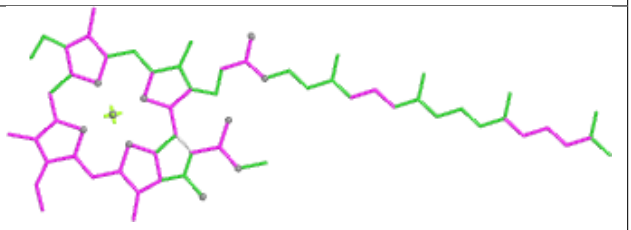


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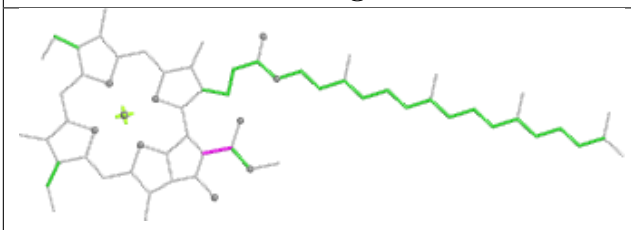
Ligand CLA B 609



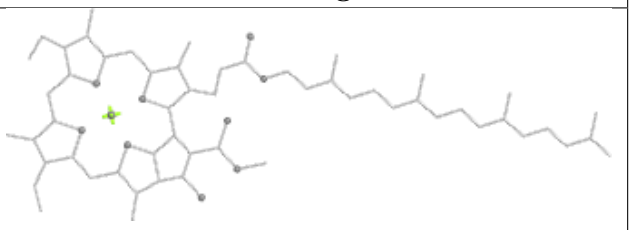
Bond lengths



Bond angles

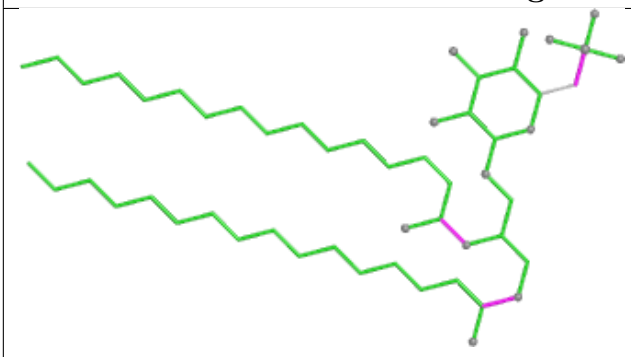


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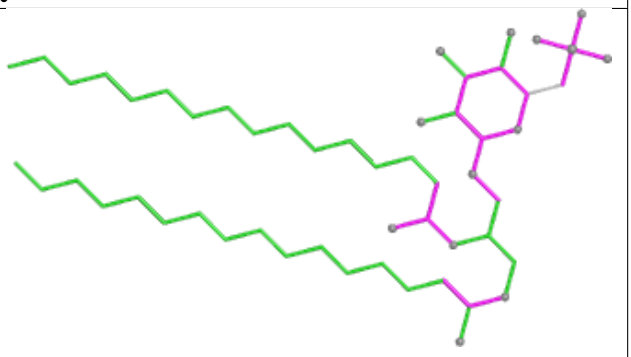


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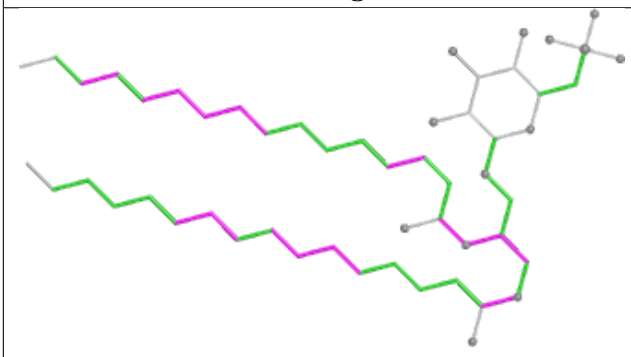
Ligand SQD b 620



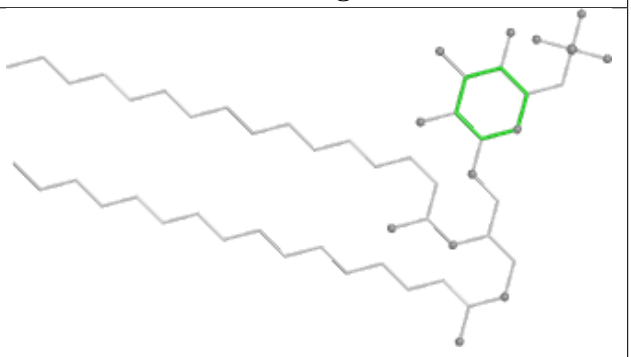
Bond lengths



Bond angles

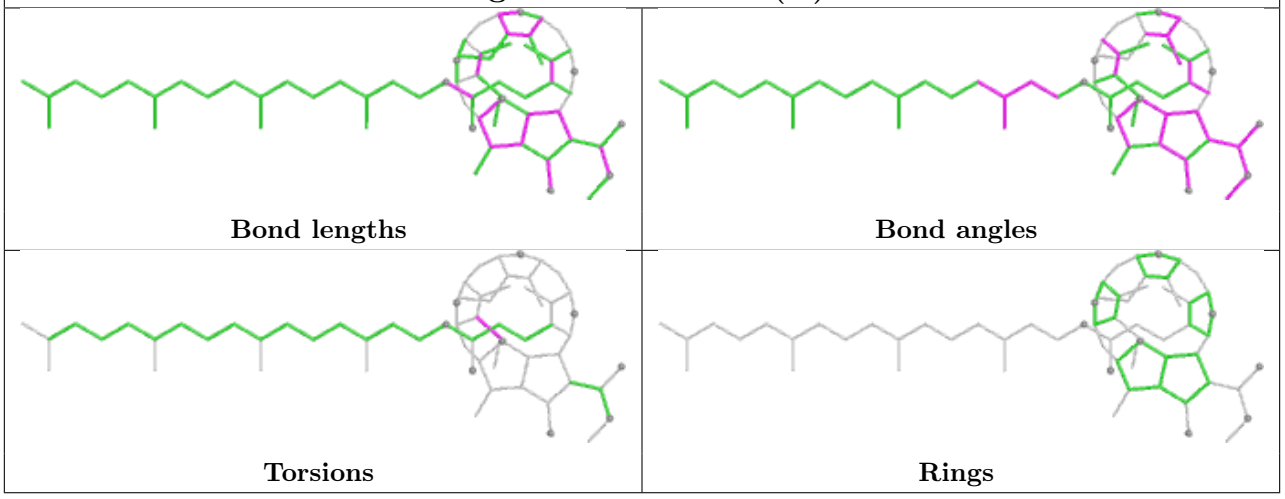


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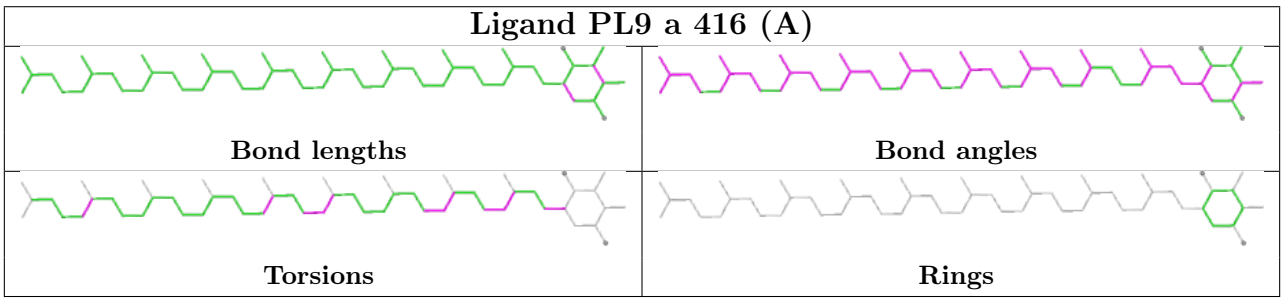


Rings

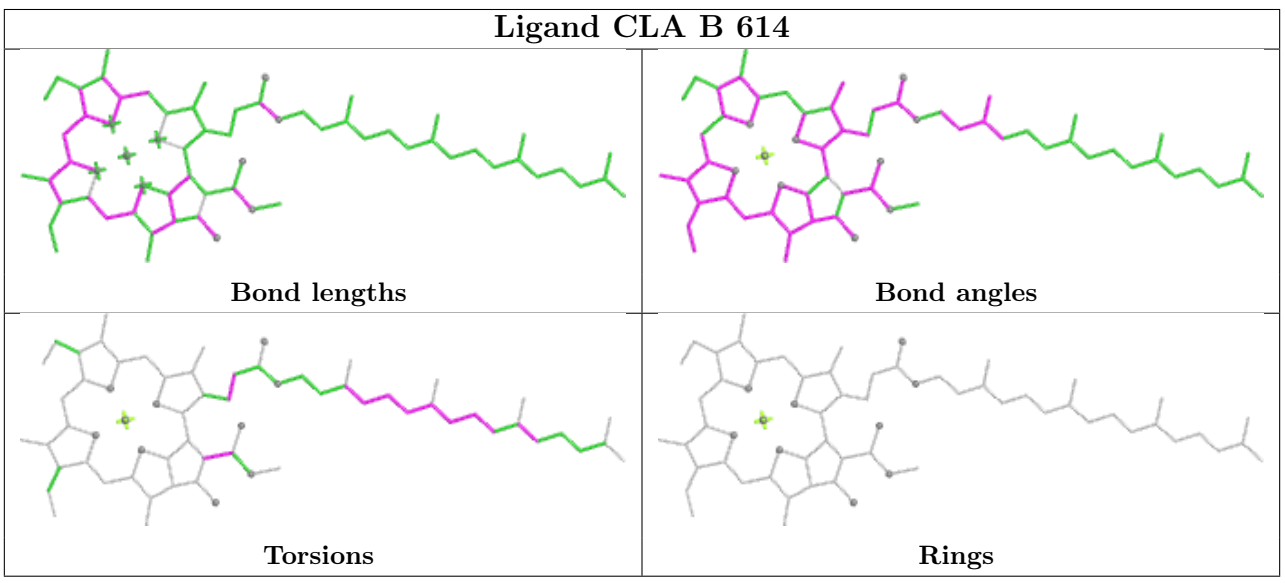
Ligand PHO A 353 (A)



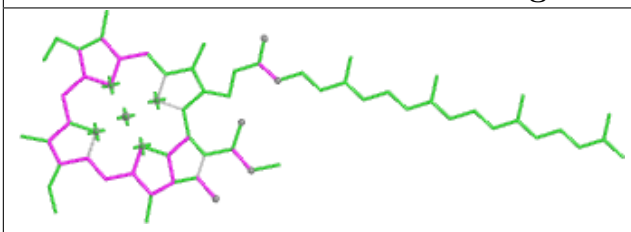
Ligand PL9 a 416 (A)



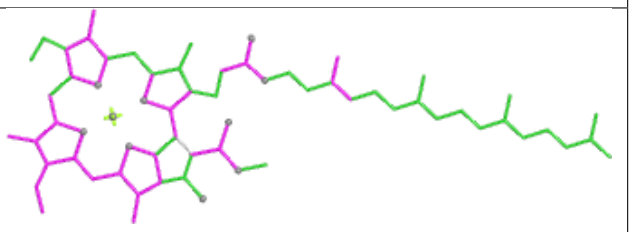
Ligand CLA B 614



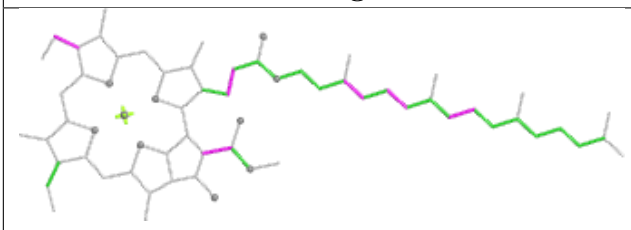
Ligand CLA c 508



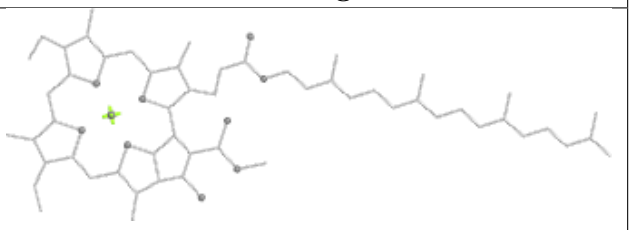
Bond lengths



Bond angles

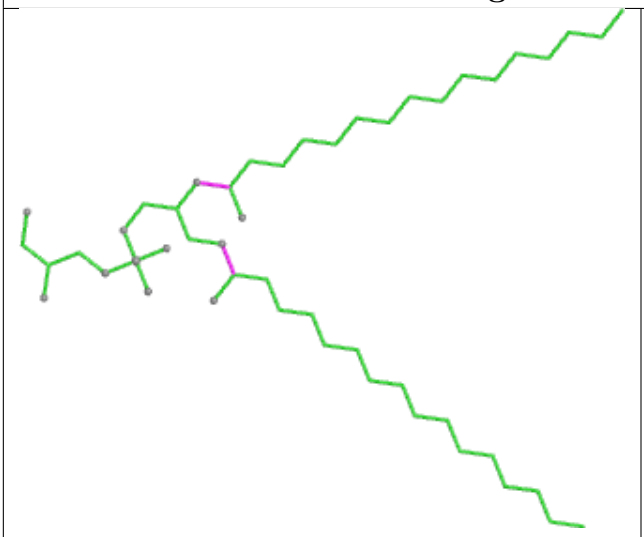


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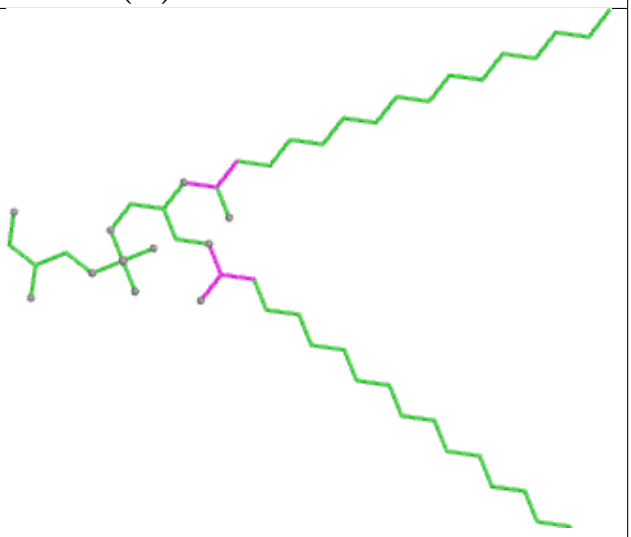


Rings

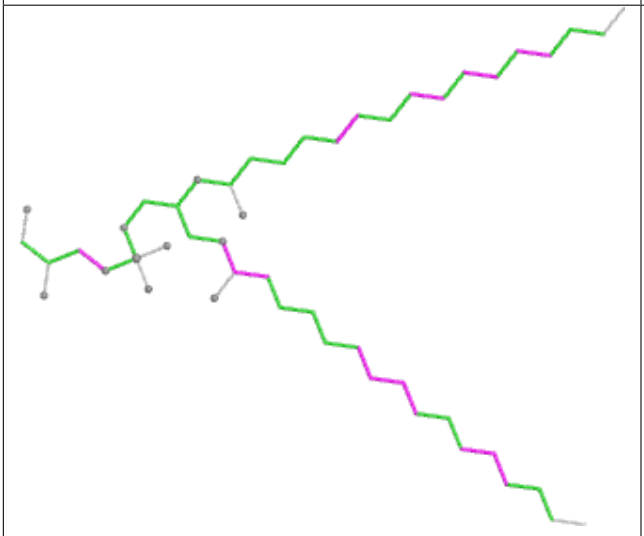
Ligand LHG D 411 (A)



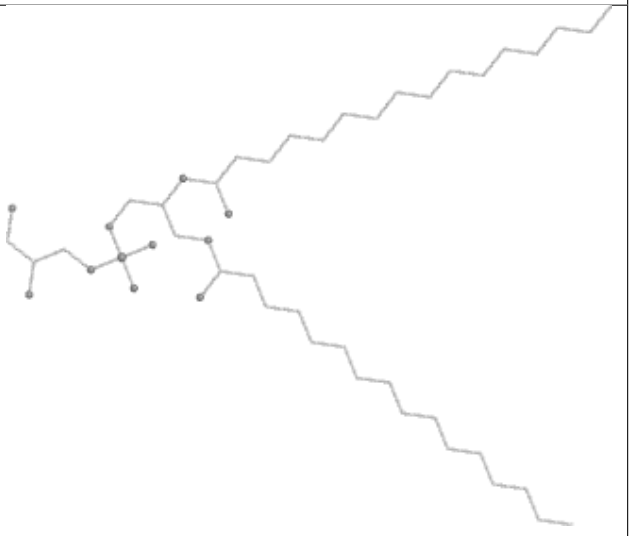
Bond lengths



Bond angles

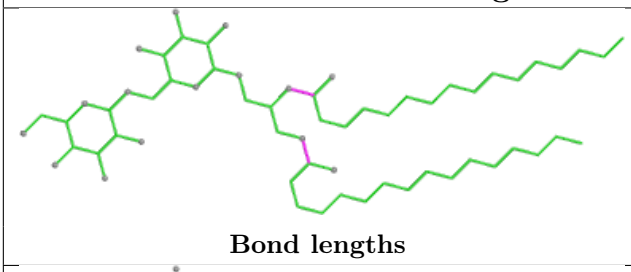


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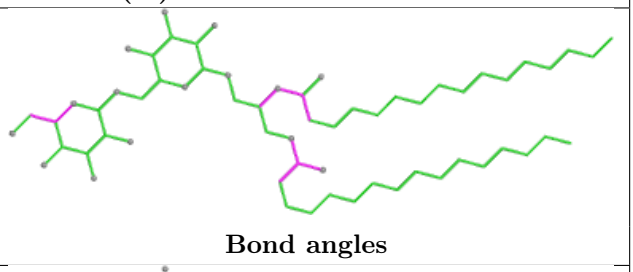


Rings

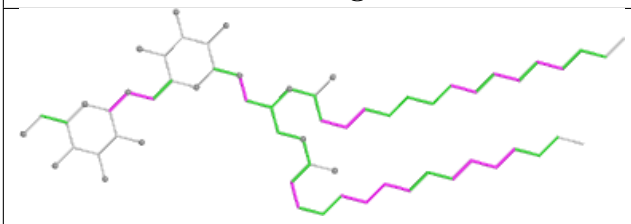
Ligand DGD c 518 (B)



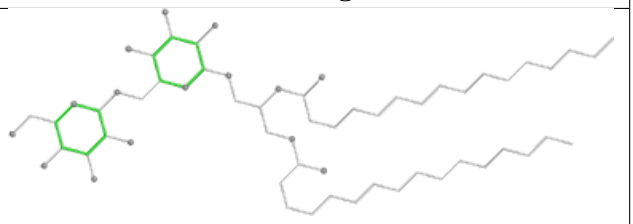
Bond lengths



Bond angles

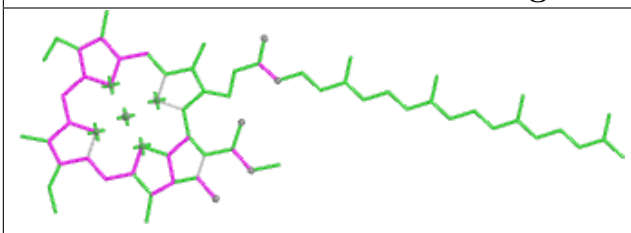


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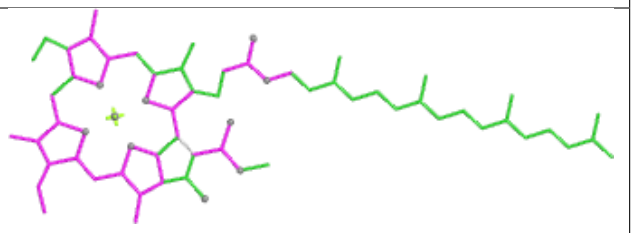


Rings

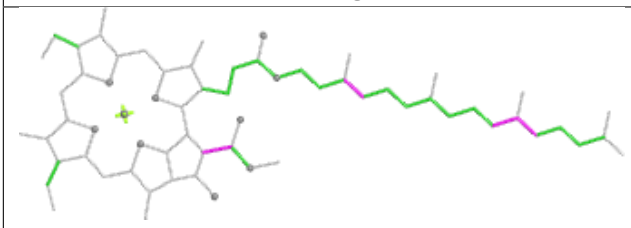
Ligand CLA c 505



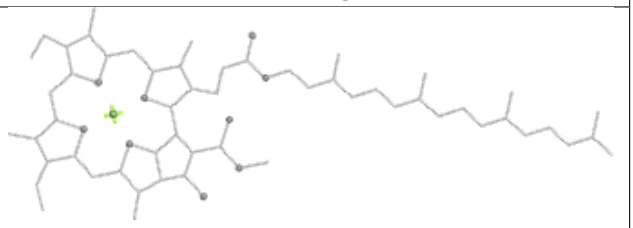
Bond lengths



Bond angles

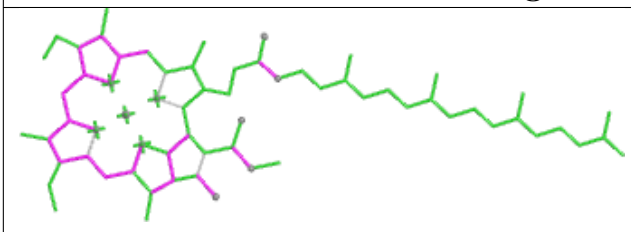


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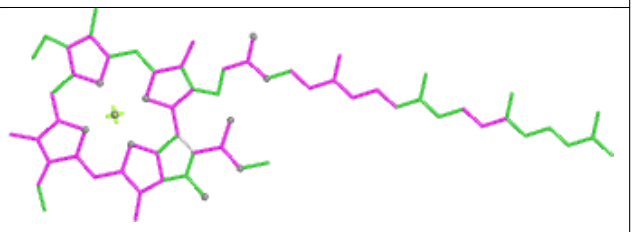


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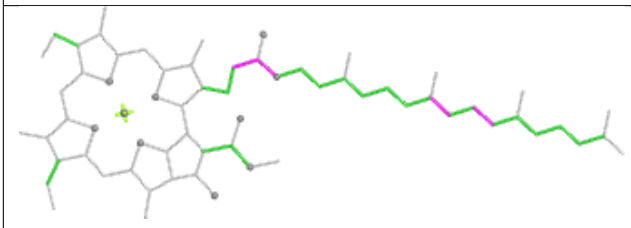
Ligand CLA B 612



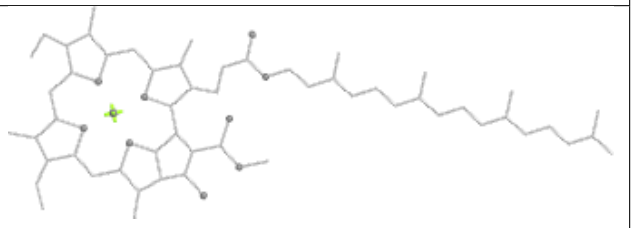
Bond lengths



Bond angles

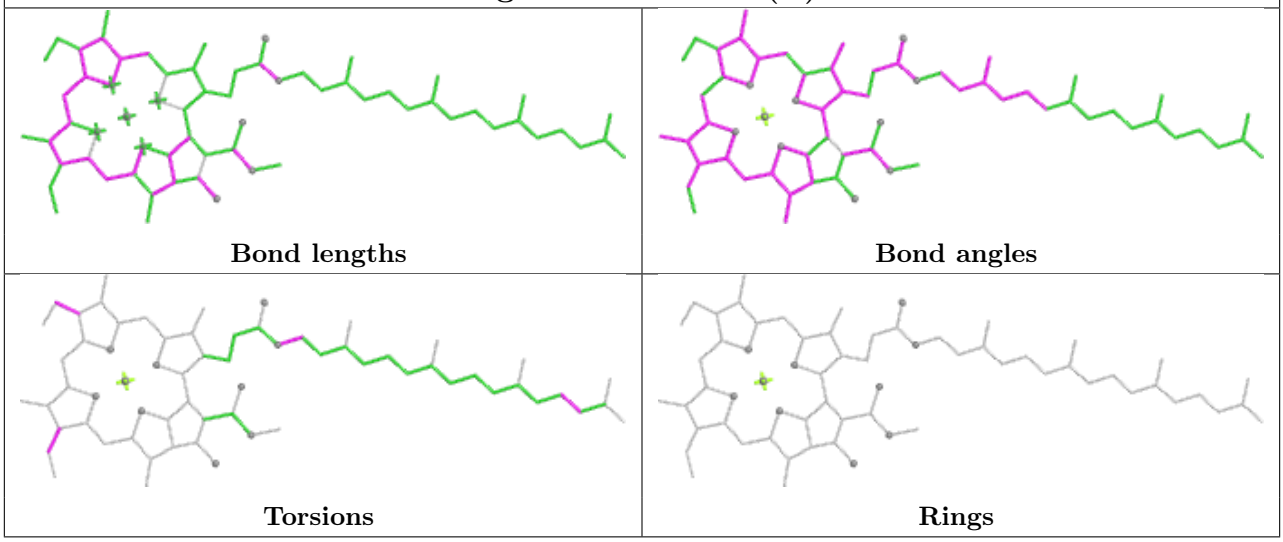


Torsions

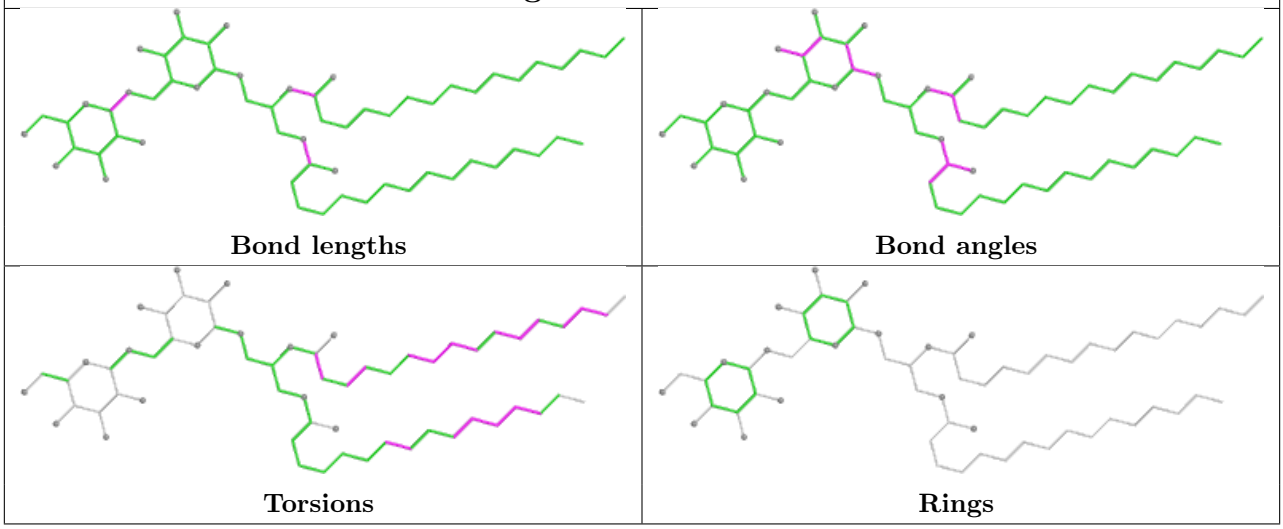


Rings

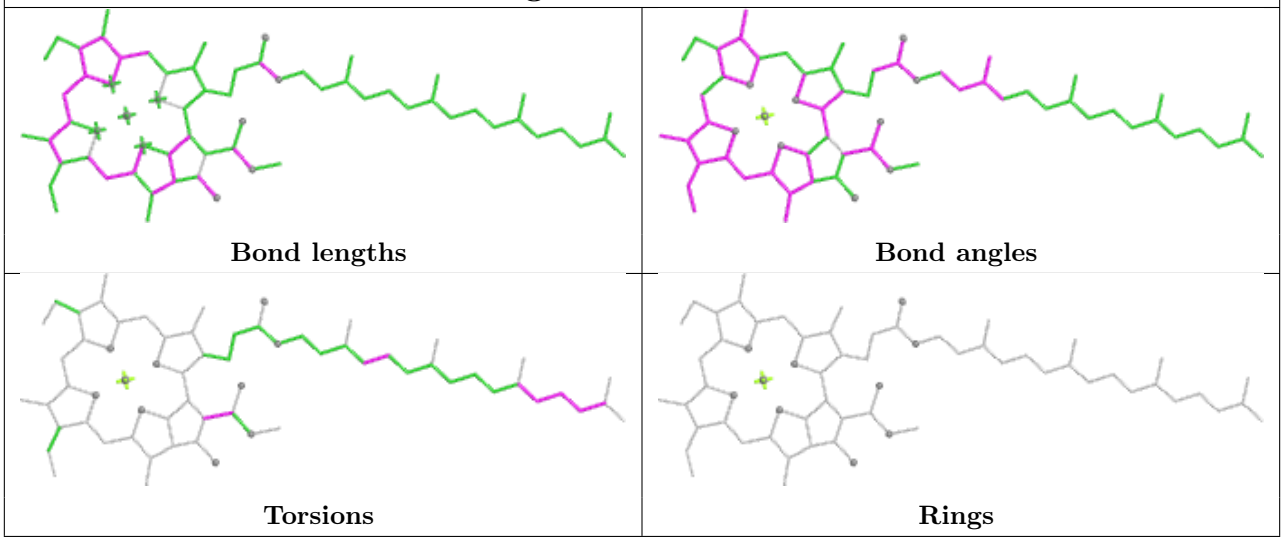
Ligand CLA a 405 (B)



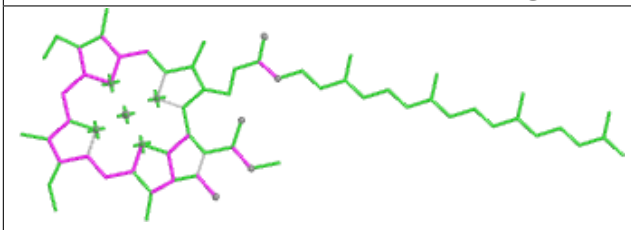
Ligand DGD h 102



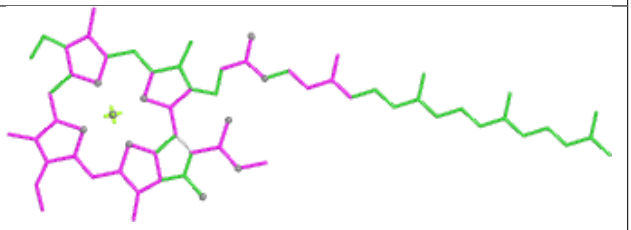
Ligand CLA C 503



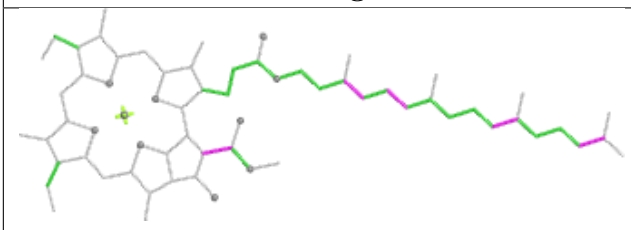
Ligand CLA B 605



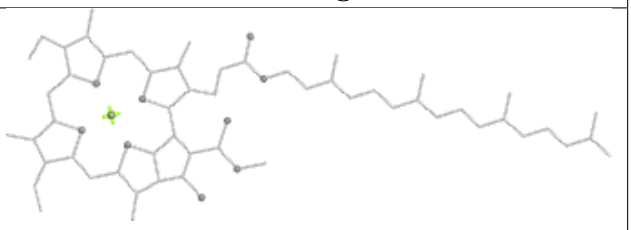
Bond lengths



Bond angles

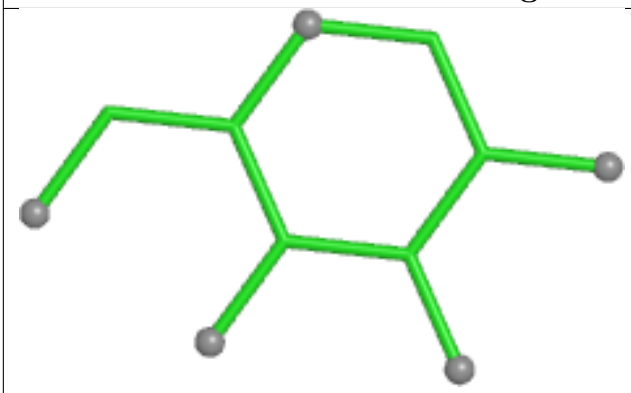


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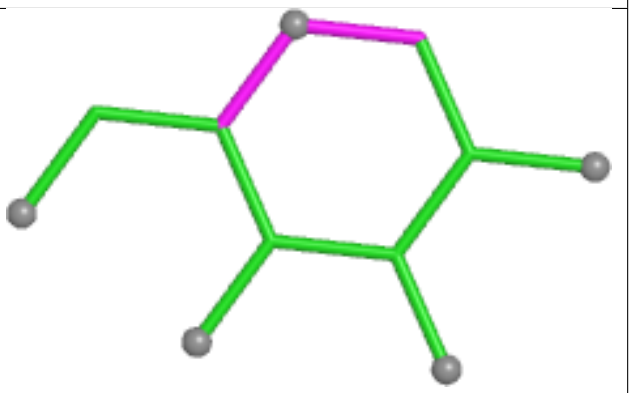


Rings

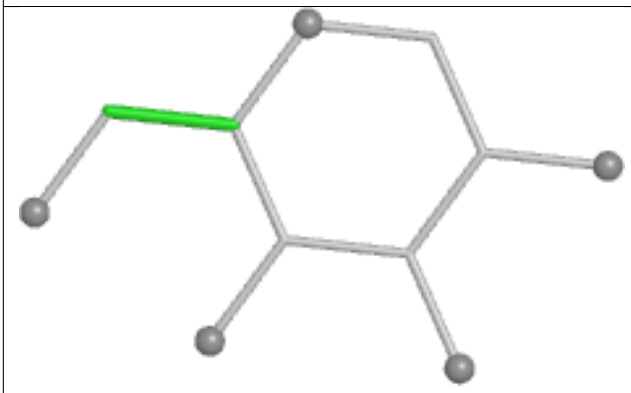
Ligand HTG V 203



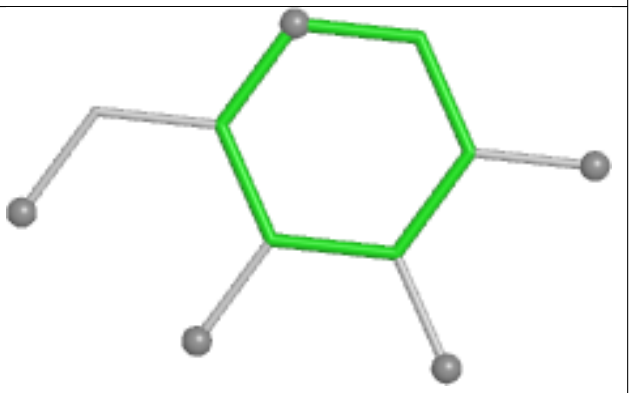
Bond lengths



Bond angles

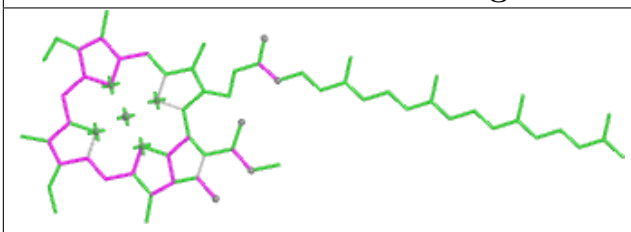


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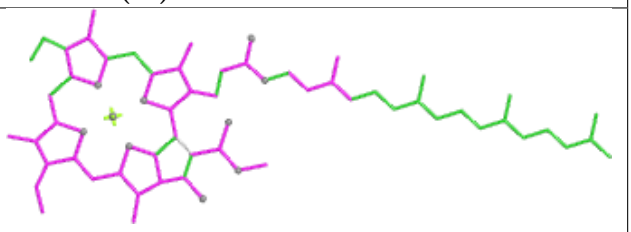


Rings

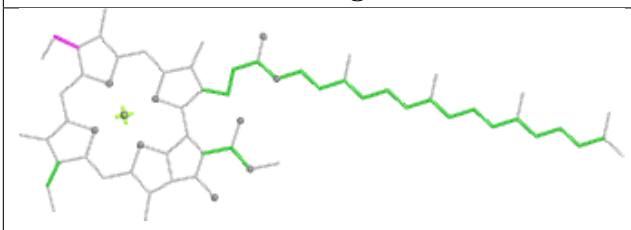
Ligand CLA D 405 (A)



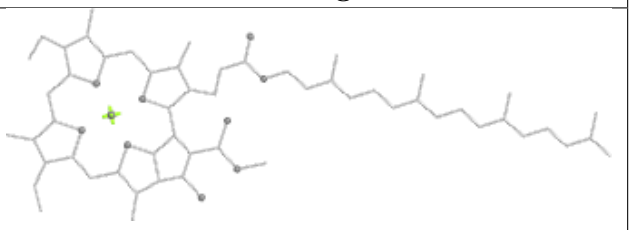
Bond lengths



Bond angles

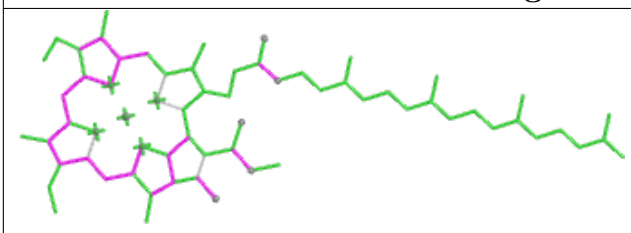


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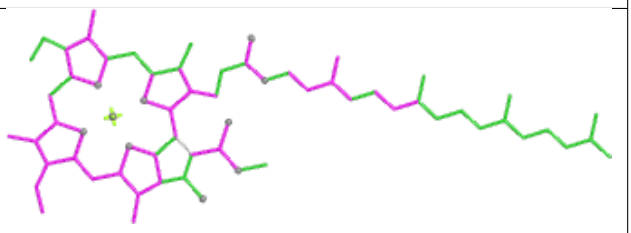


Rings

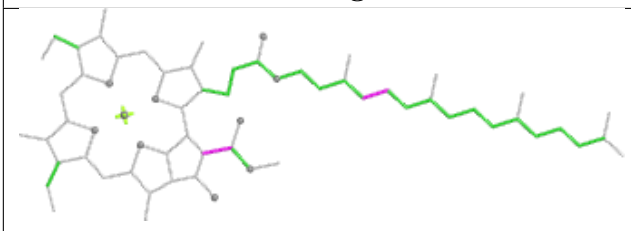
Ligand CLA B 607



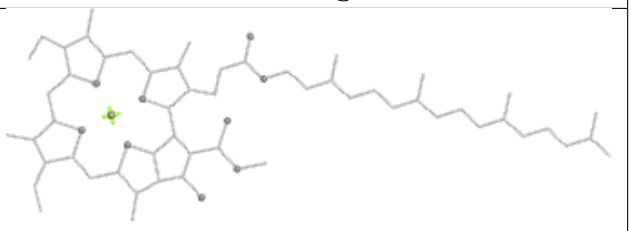
Bond lengths



Bond angles

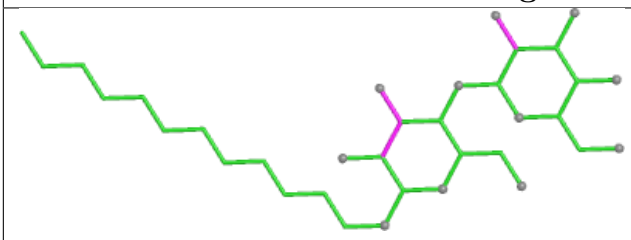


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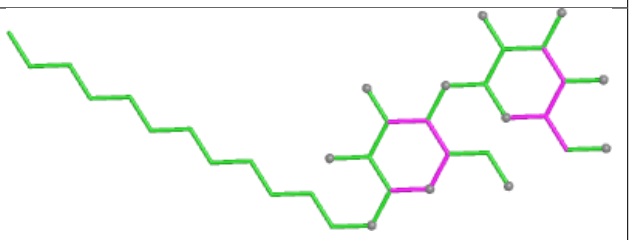


Rings

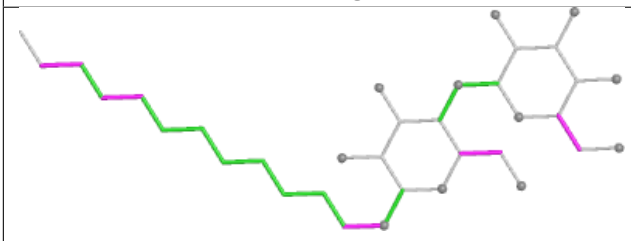
Ligand LMT m 103



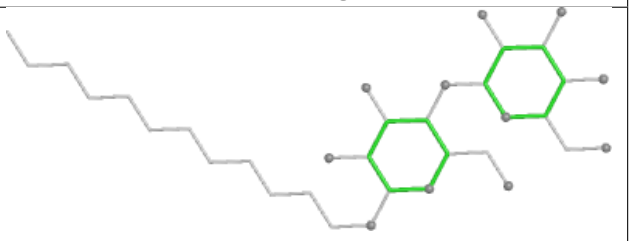
Bond lengths



Bond angles

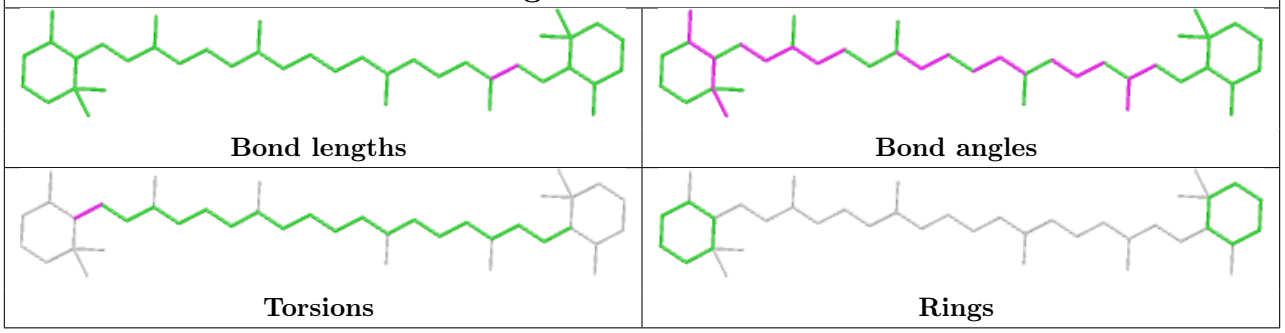


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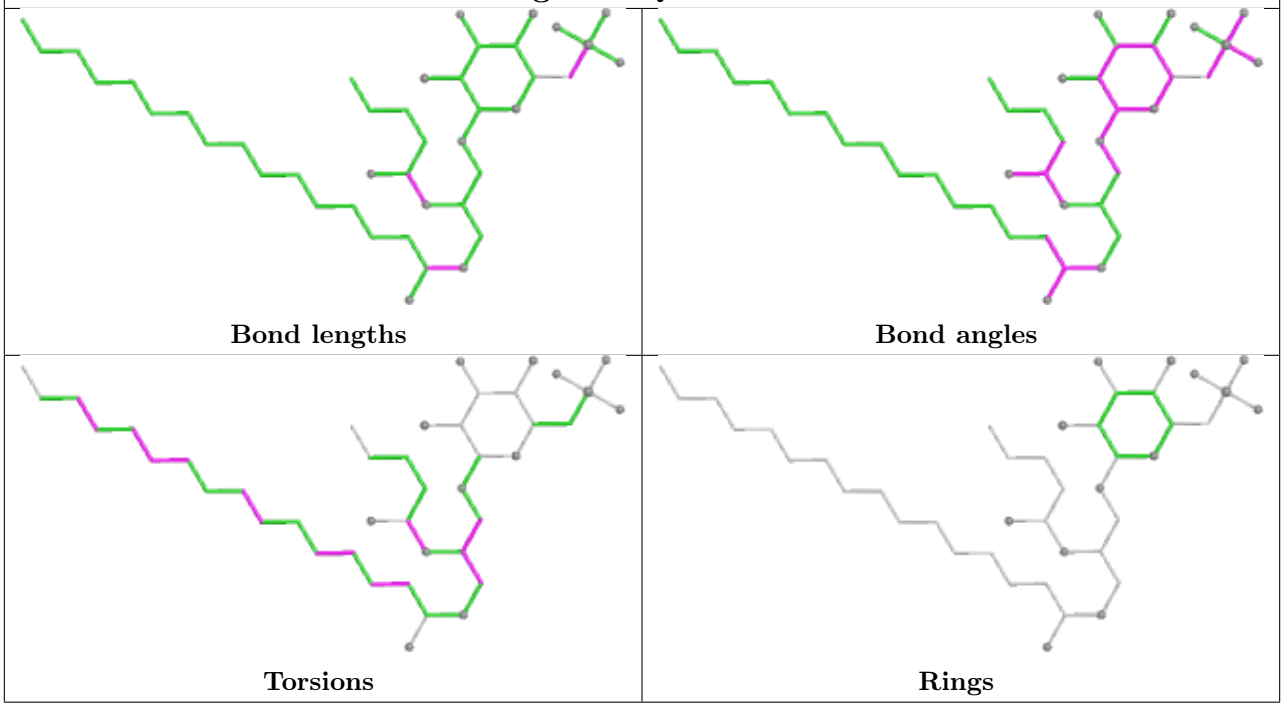


Rings

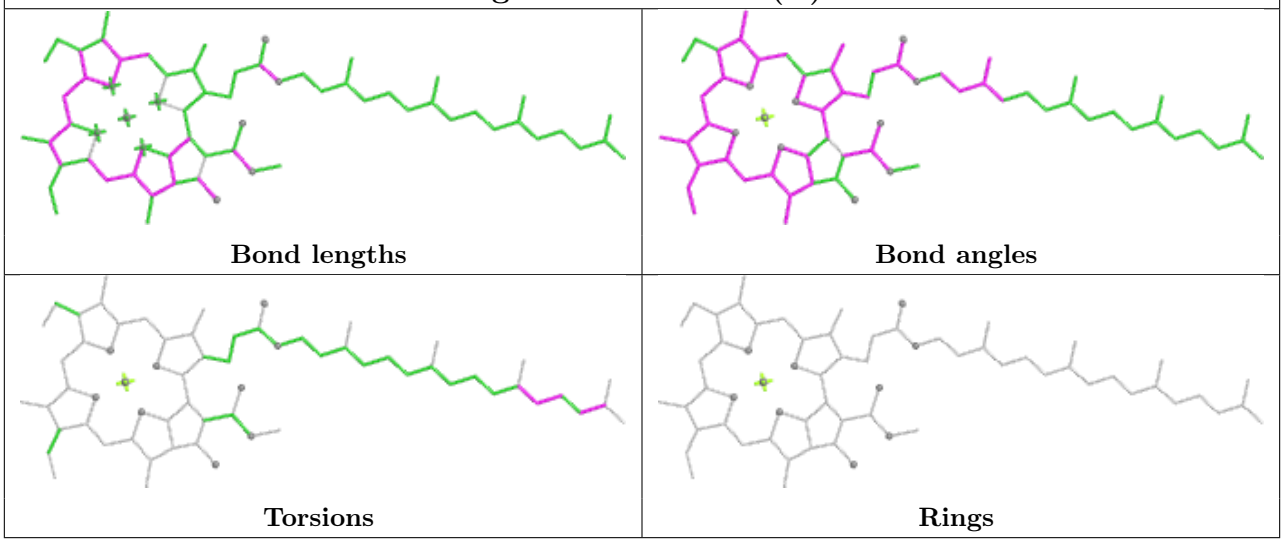
Ligand BCR B 617



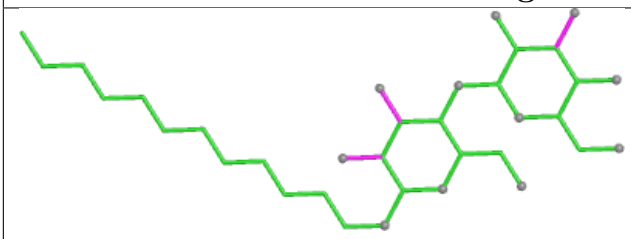
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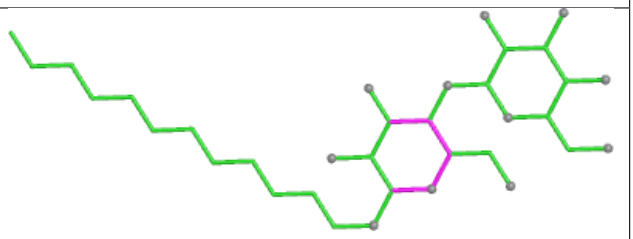
Ligand CLA A 406 (B)



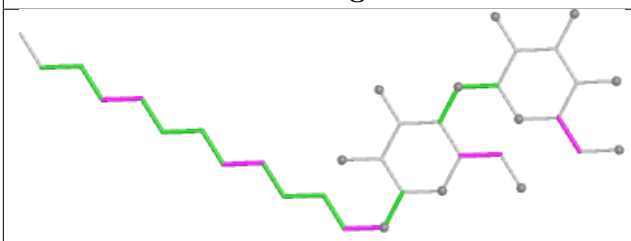
Ligand LMT M 103



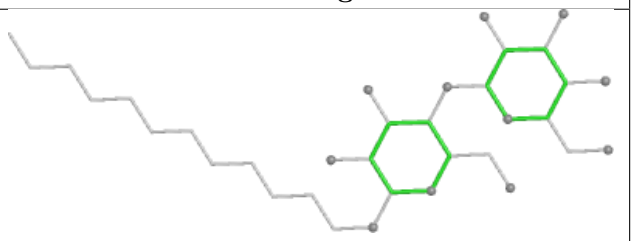
Bond lengths



Bond angles

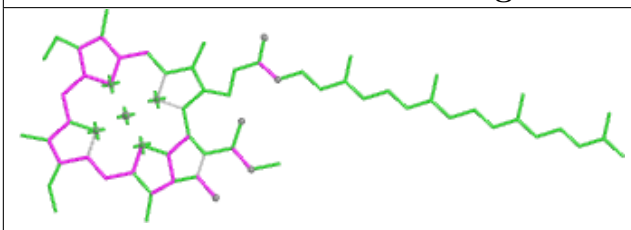


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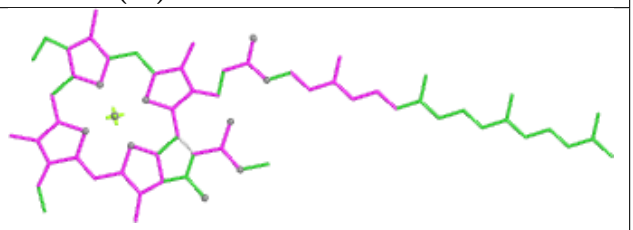


Rings

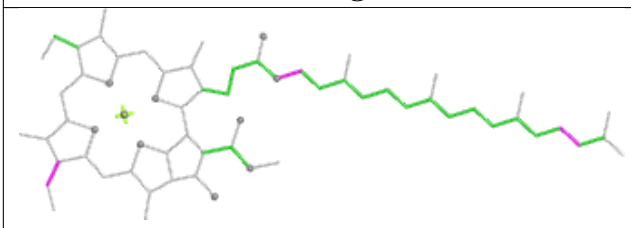
Ligand CLA a 405 (A)



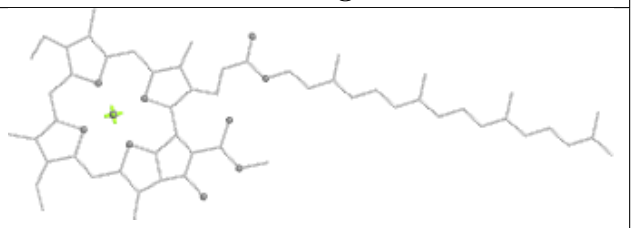
Bond lengths



Bond angles

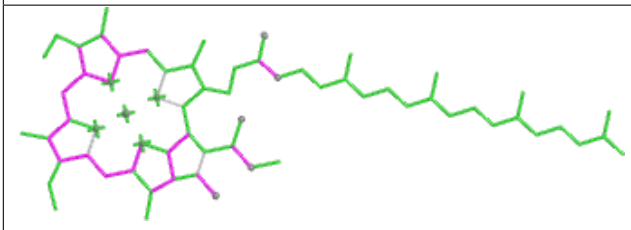


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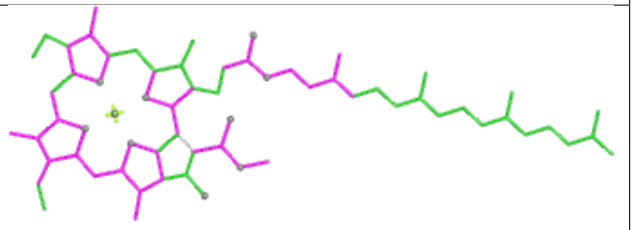


Rings

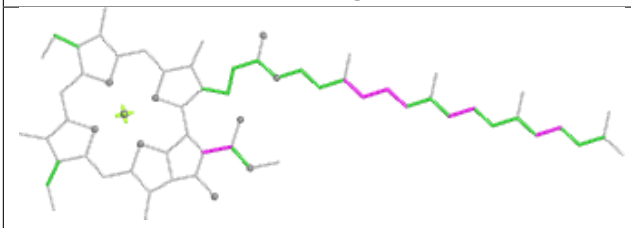
Ligand CLA b 605



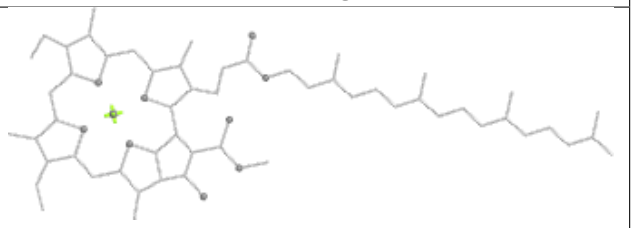
Bond lengths



Bond angles

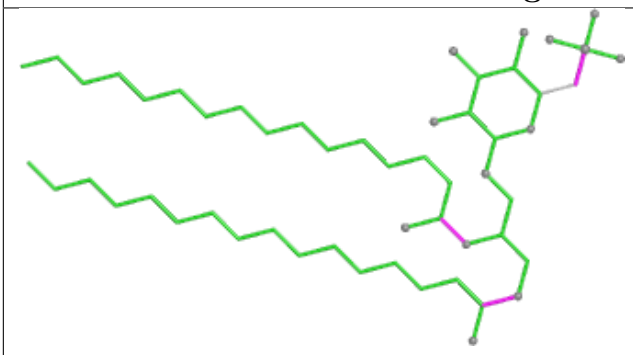


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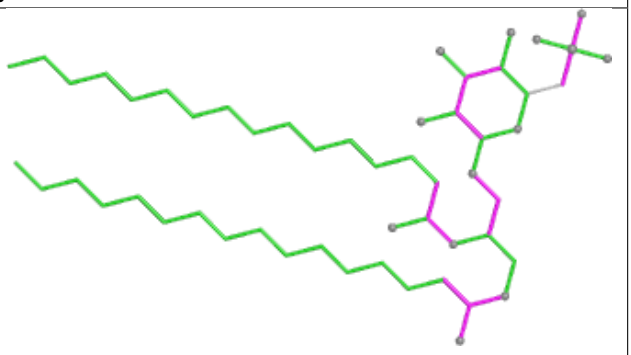


Rings

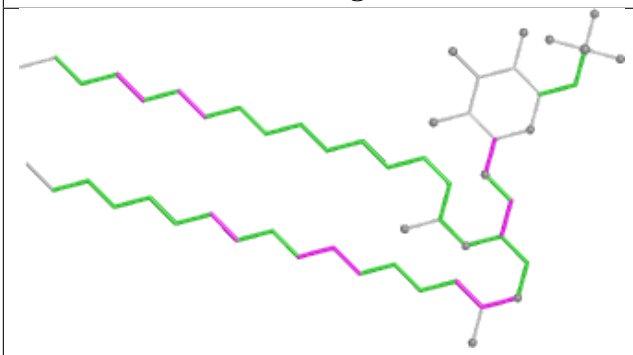
Ligand SQD A 412



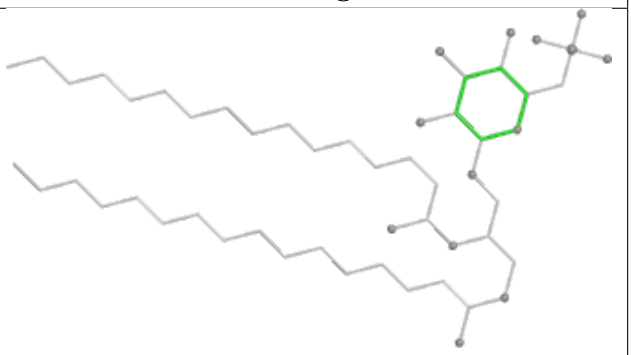
Bond lengths



Bond angles

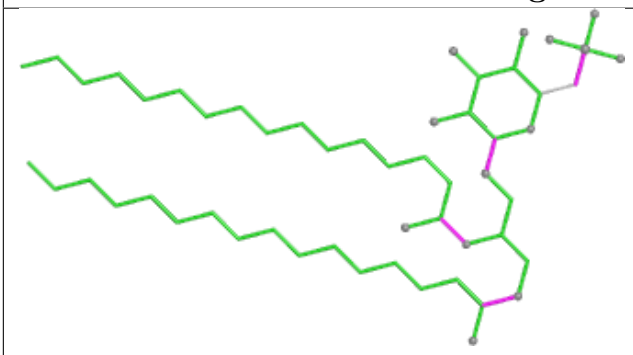


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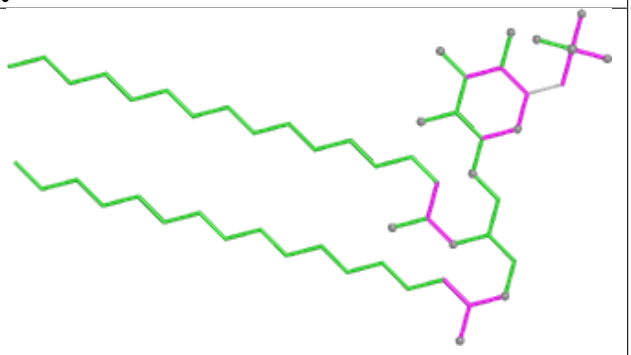


Rings

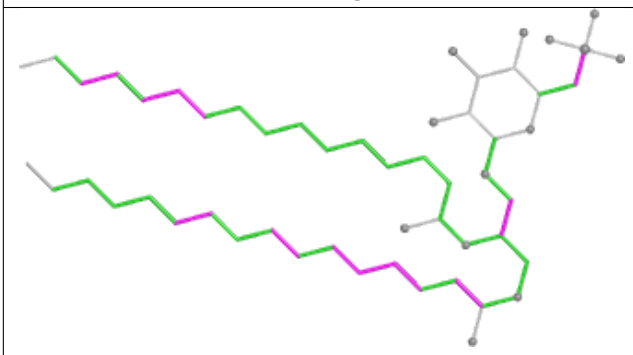
Ligand SQD a 413



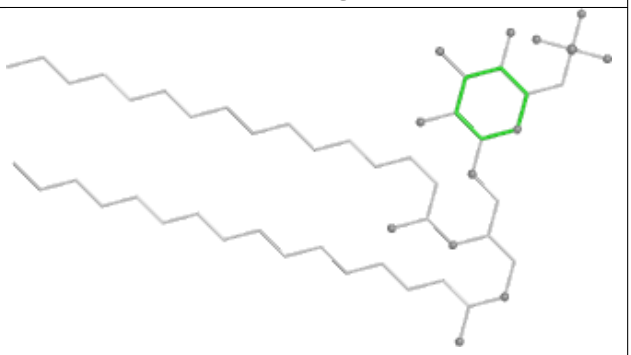
Bond lengths



Bond angles

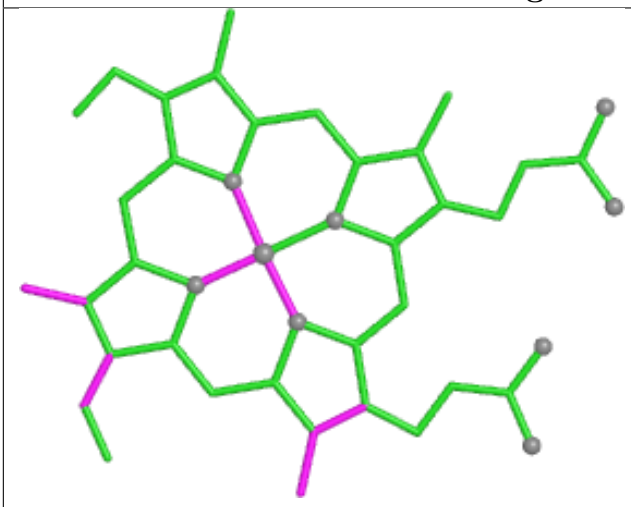


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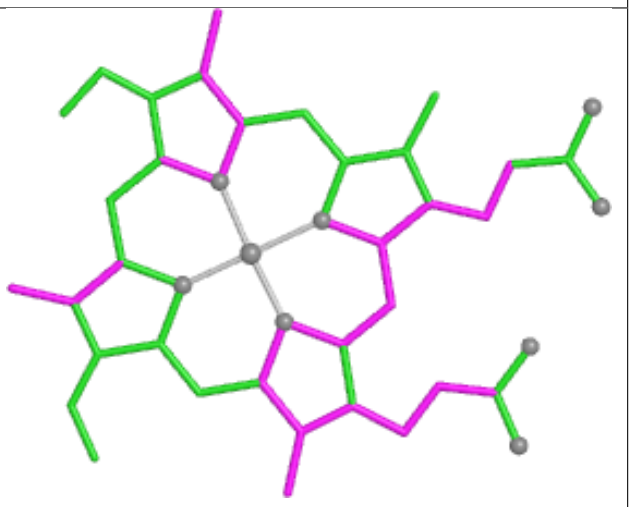


Rings

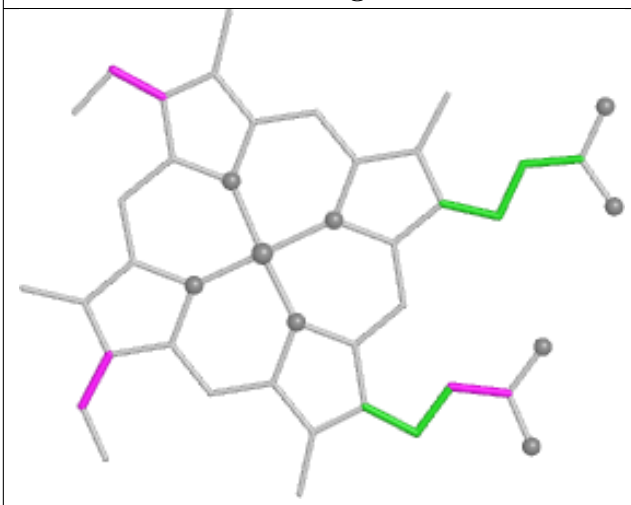
Ligand HEC v 202



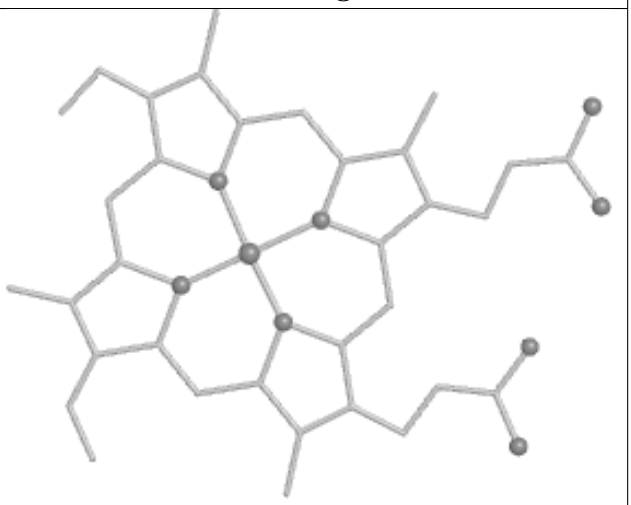
Bond lengths



Bond angles

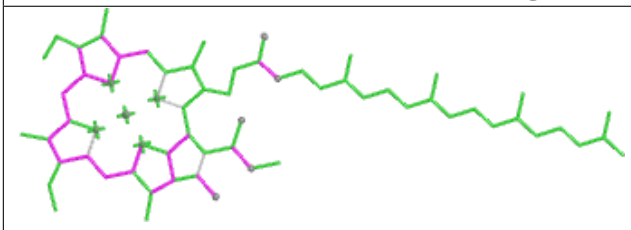


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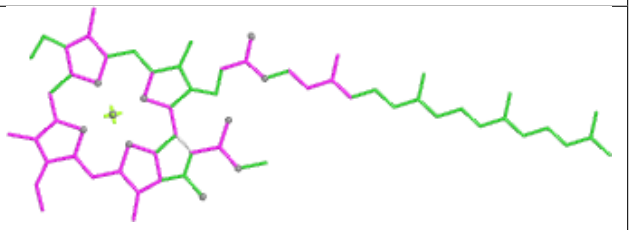


Rings

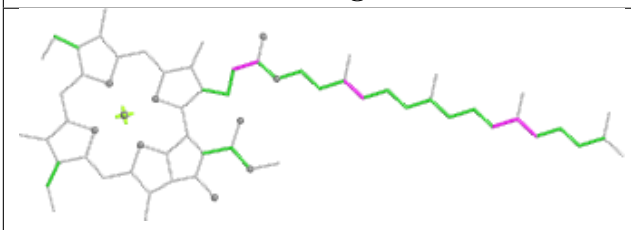
Ligand CLA C 506



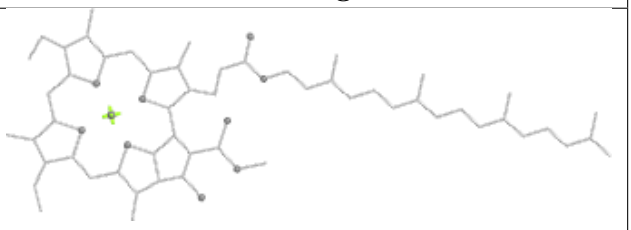
Bond lengths



Bond angles

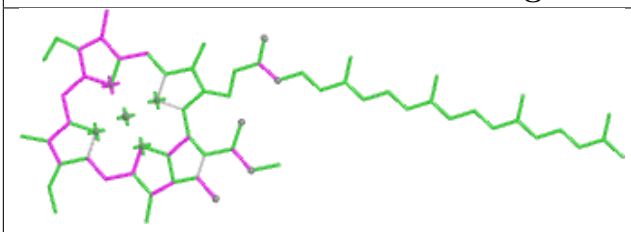


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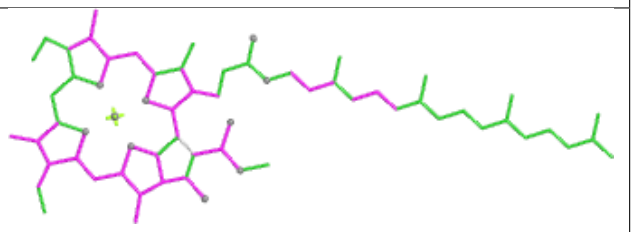


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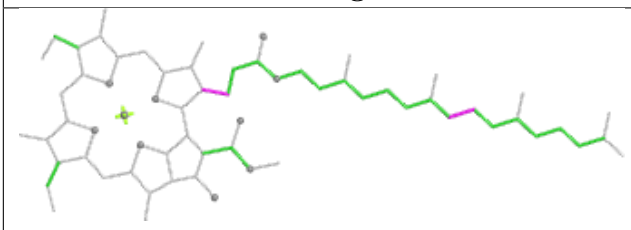
Ligand CLA B 611



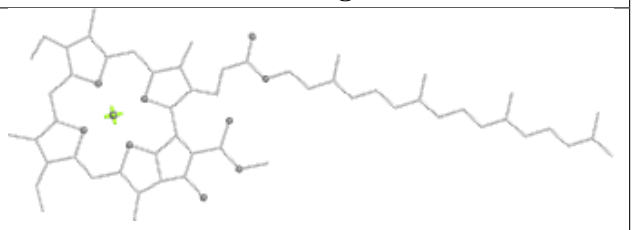
Bond lengths



Bond angles



Torsions



Rings

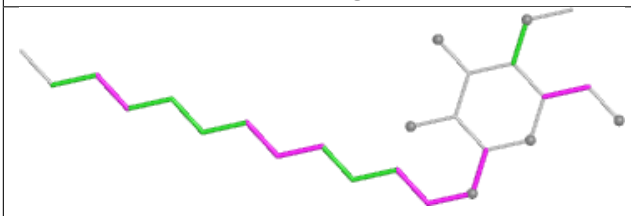
Ligand LMT t 101



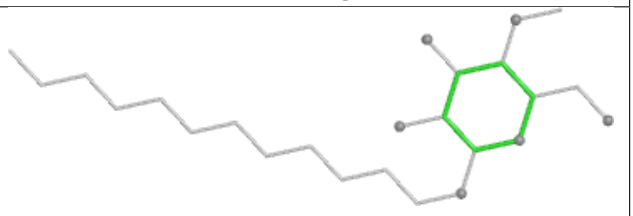
Bond lengths



Bond angles

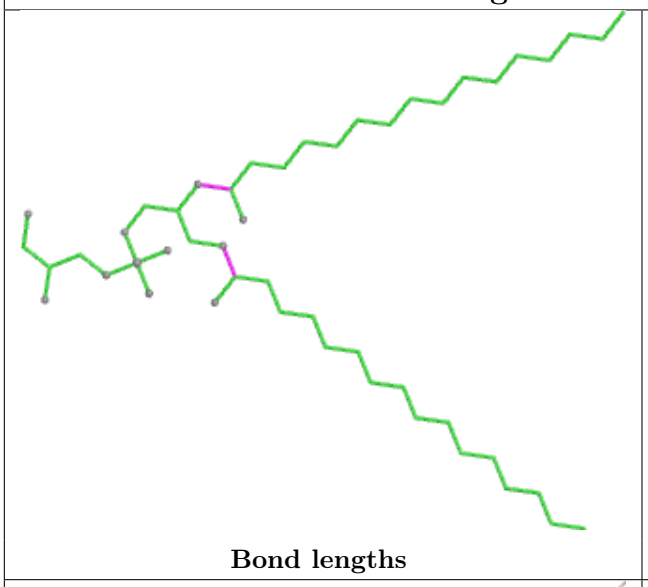


Torsions

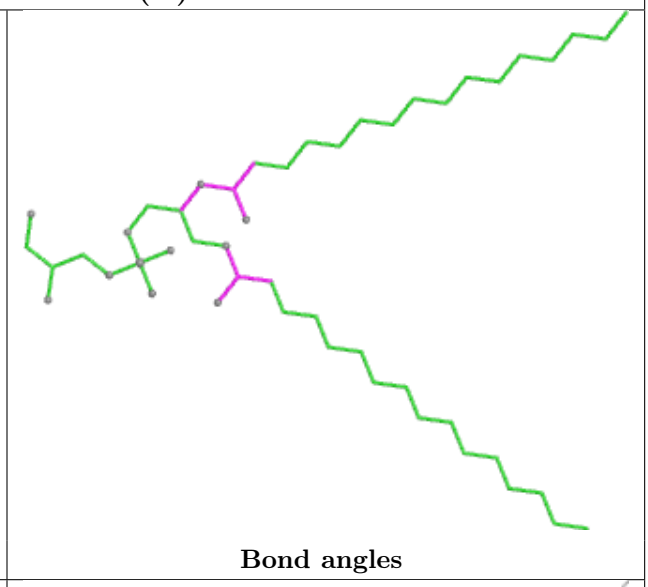


Rings

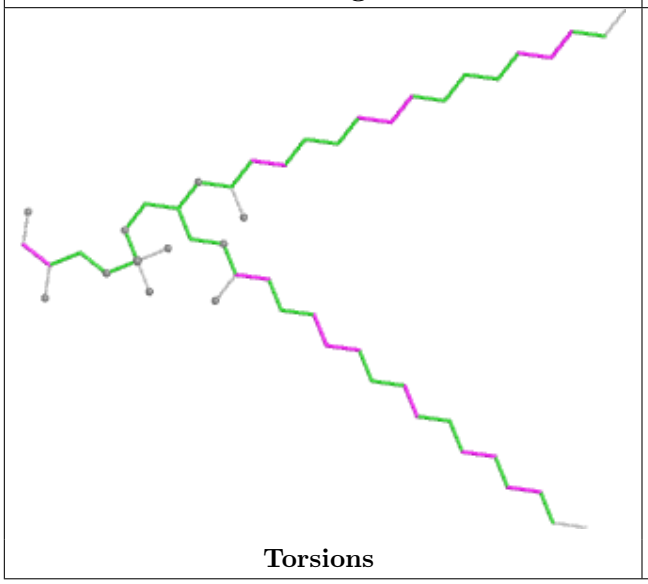
Ligand LHG D 409 (B)



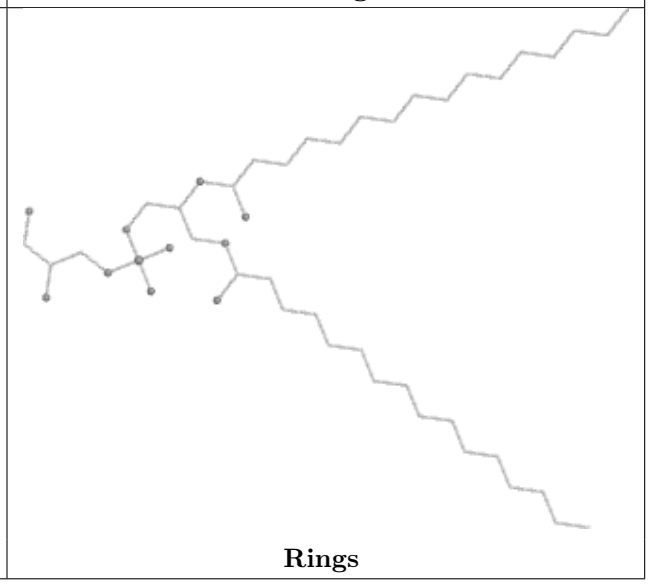
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Bond angles

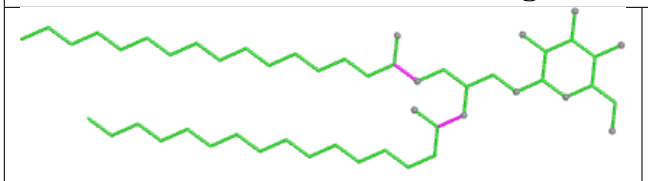


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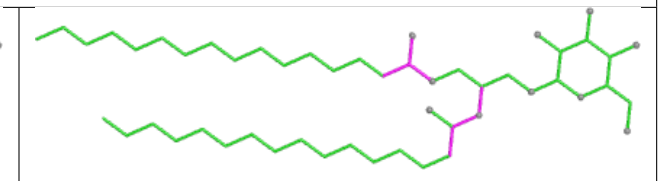


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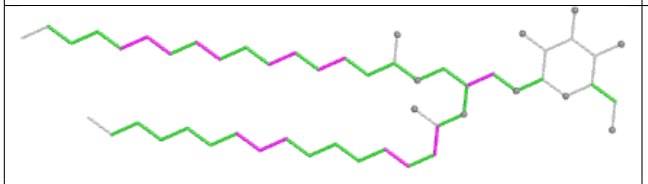
Ligand LMG C 520



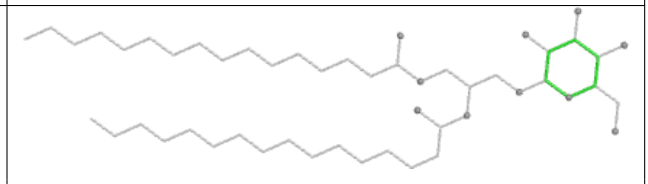
Bond lengths



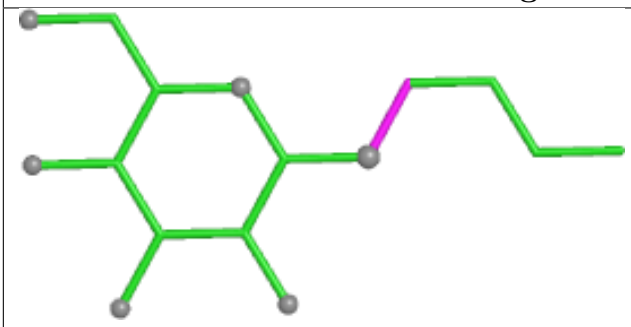
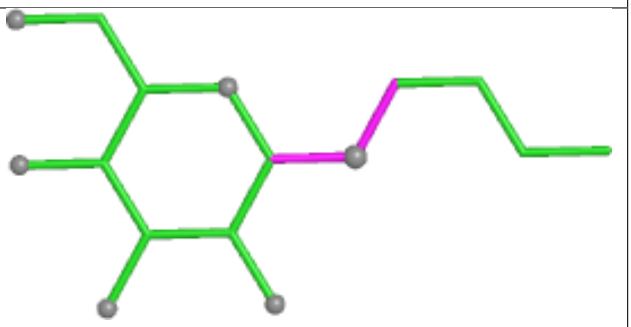
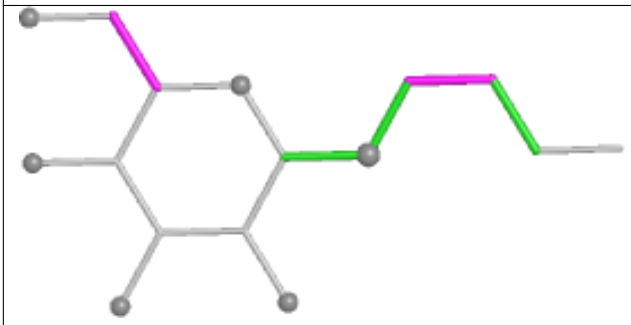
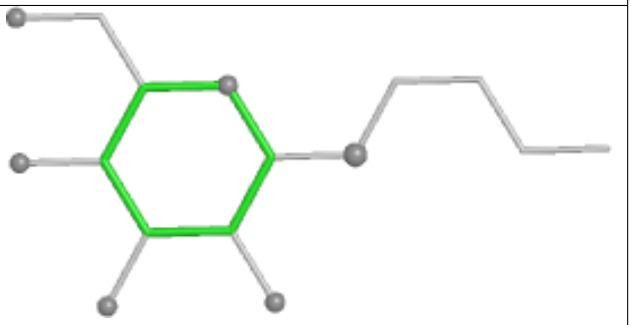
Bond angles

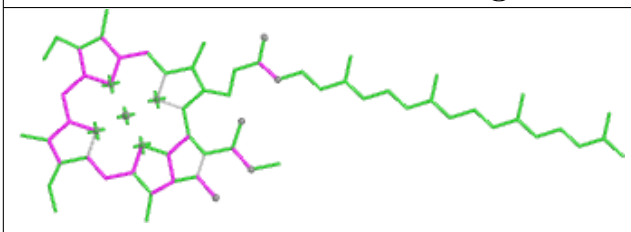
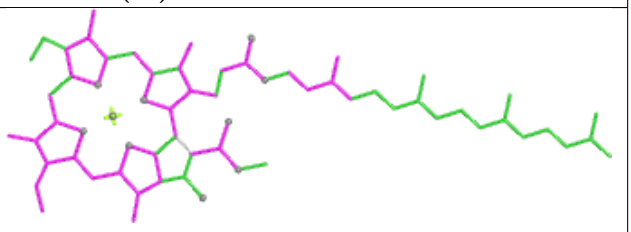
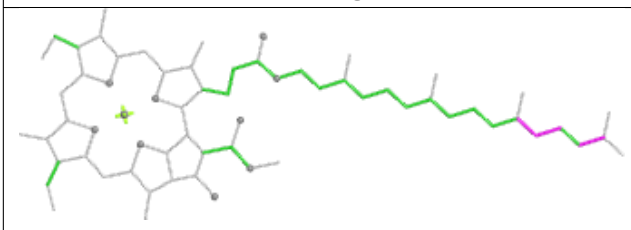
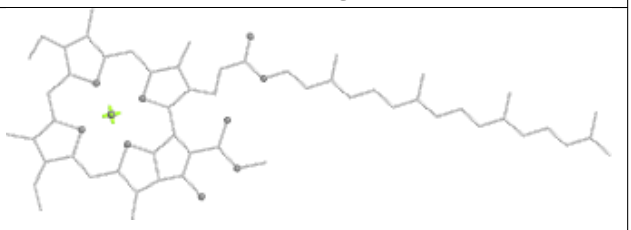


Torsions

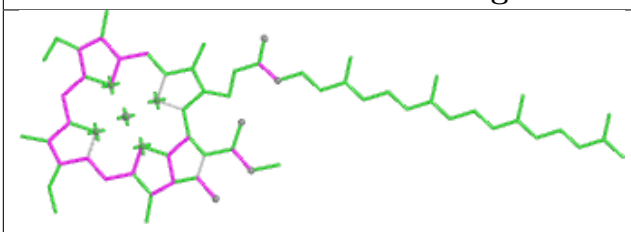


Rings

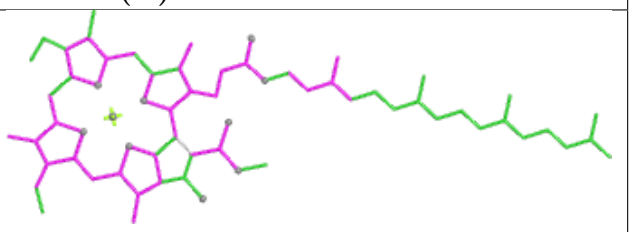
Ligand HTG D 414	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 406 (A)	
	
Bond lengths	Bond angles
	
Torsions	Rings

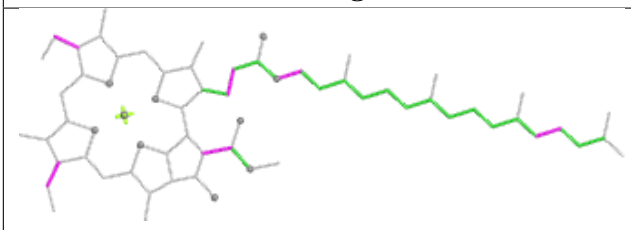
Ligand CLA A 404 (B)



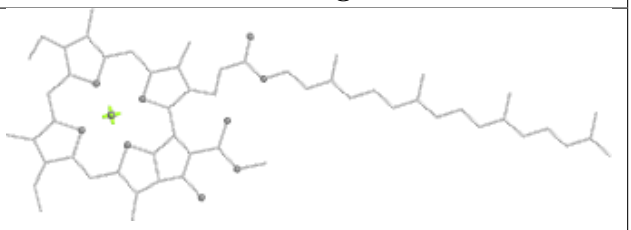
Bond lengths



Bond angles

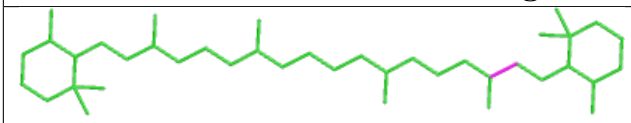


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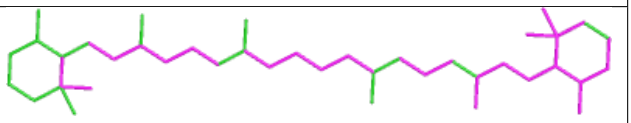


Rings

Ligand BCR D 407



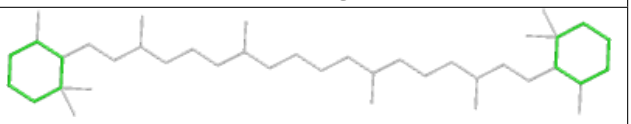
Bond lengths



Bond angles

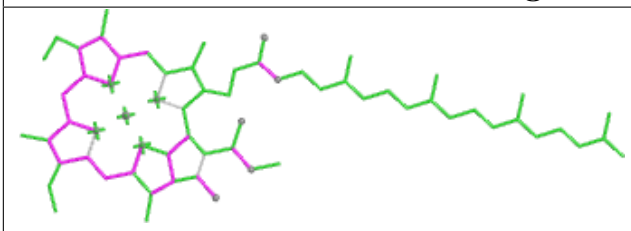


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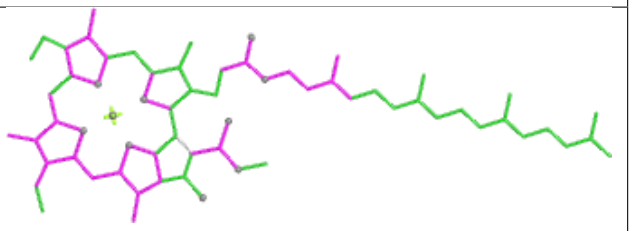


Rings

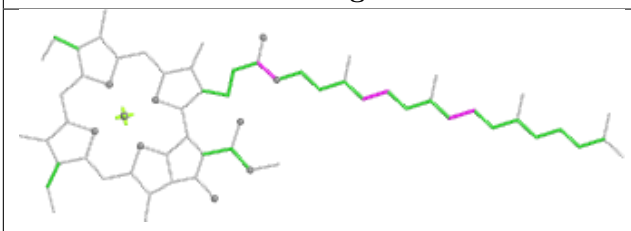
Ligand CLA C 512



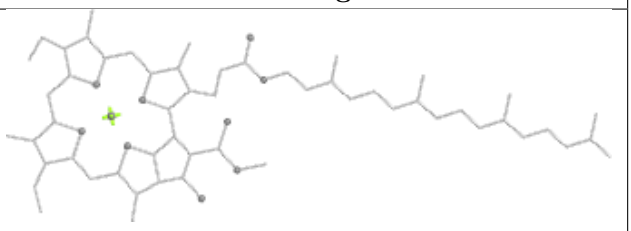
Bond lengths



Bond angles

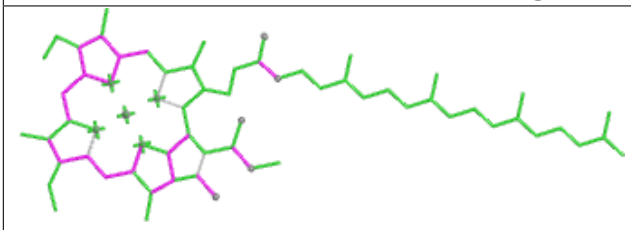


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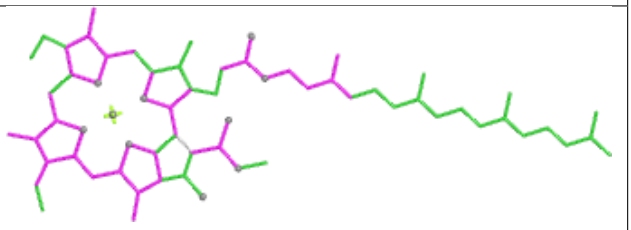


Rings

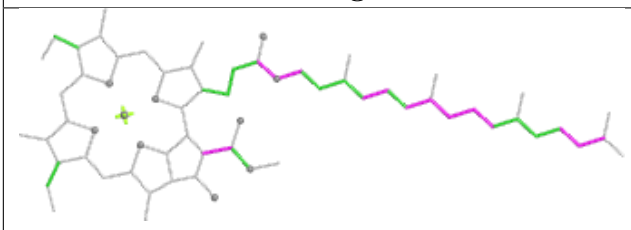
Ligand CLA c 510



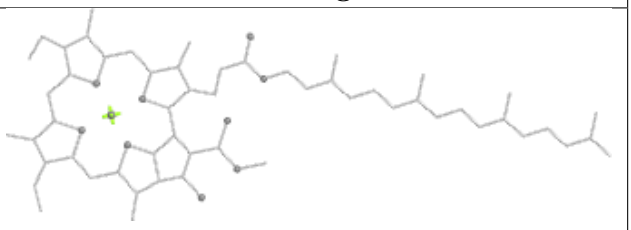
Bond lengths



Bond angles

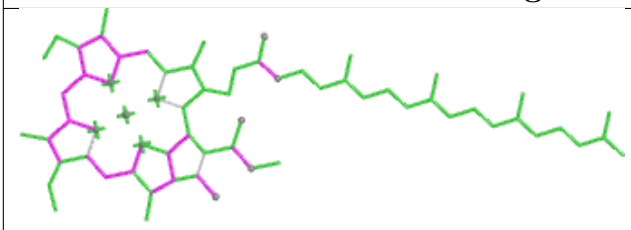


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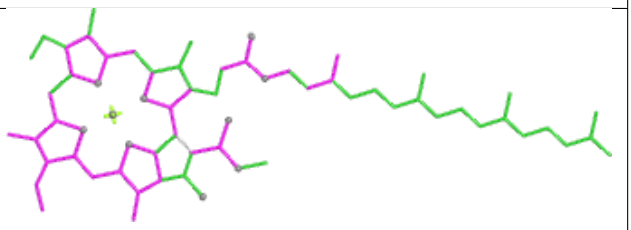


Rings

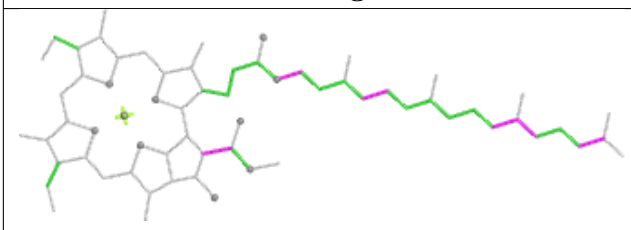
Ligand CLA B 616



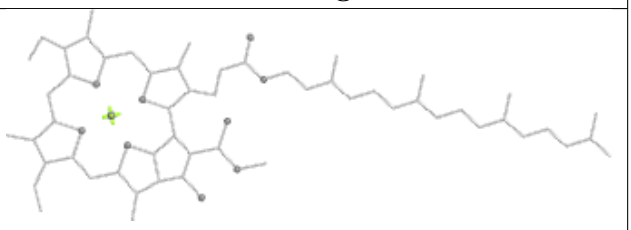
Bond lengths



Bond angles

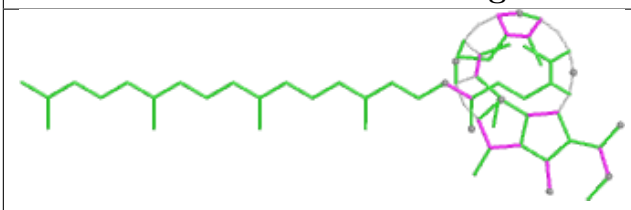


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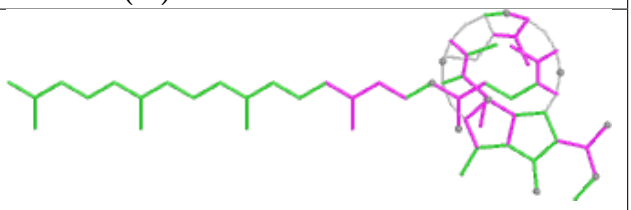


Rings

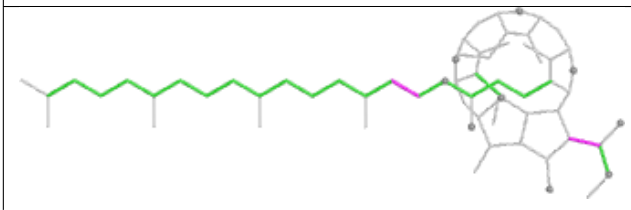
Ligand PHO A 407 (B)



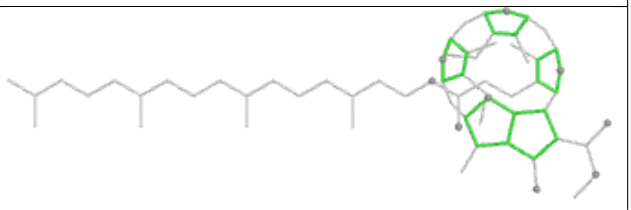
Bond lengths



Bond angles

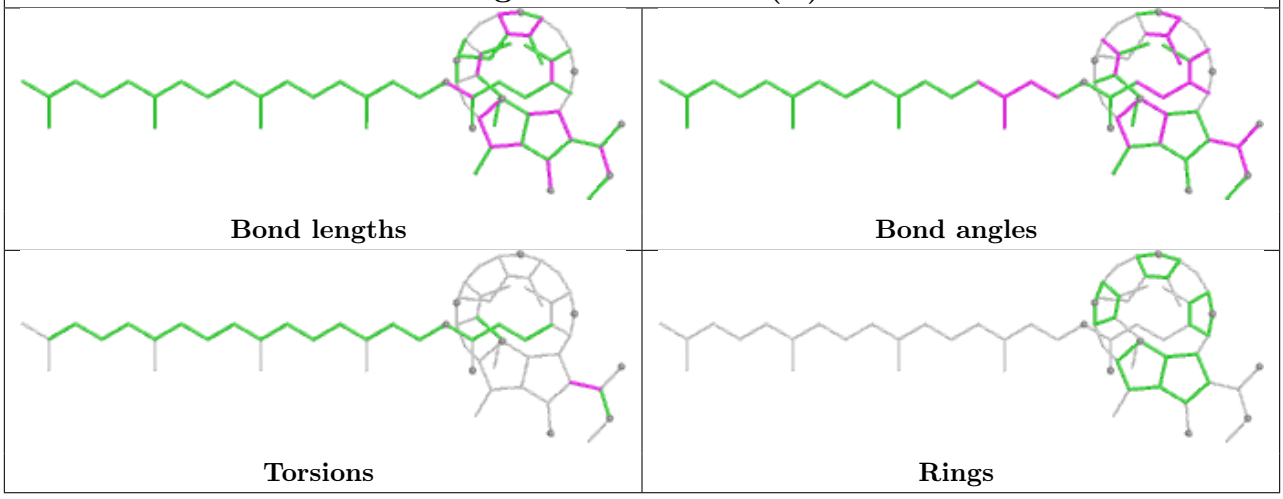


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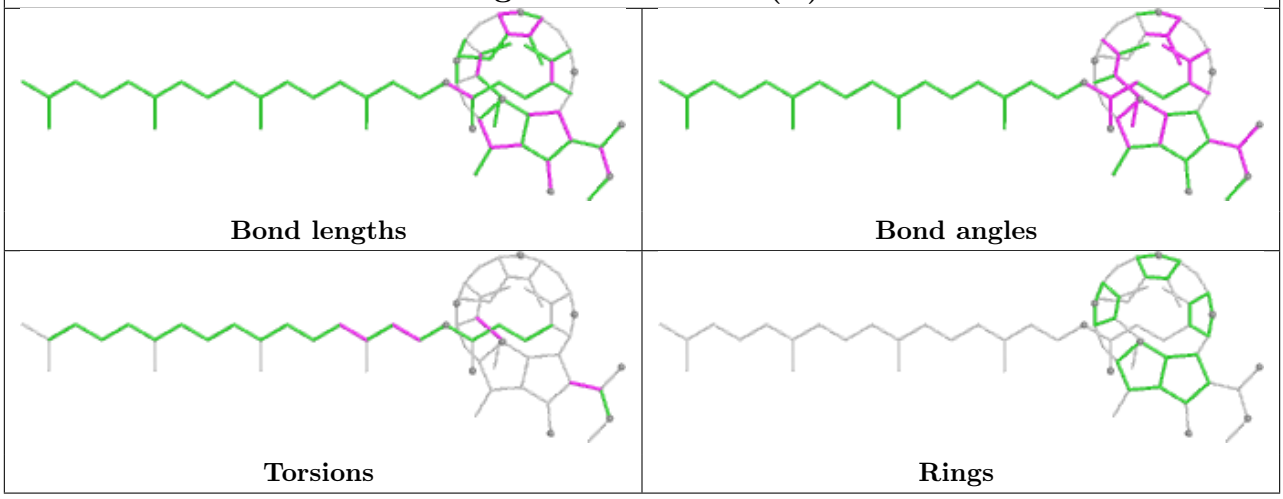


Rings

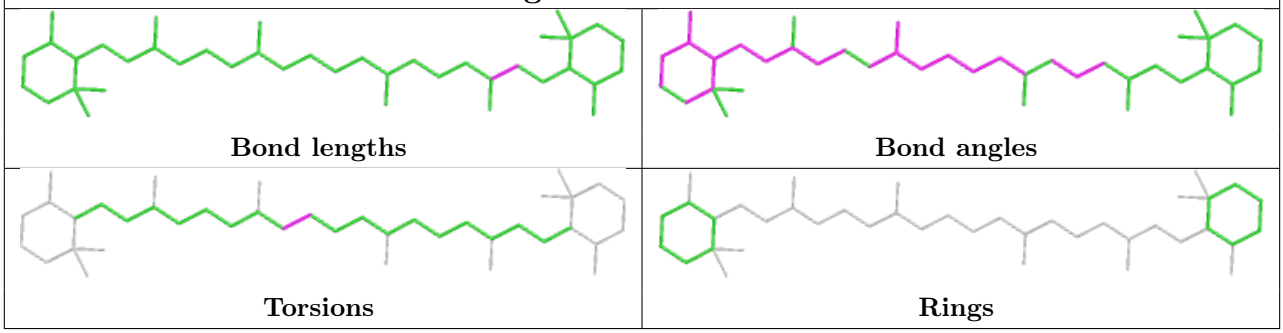
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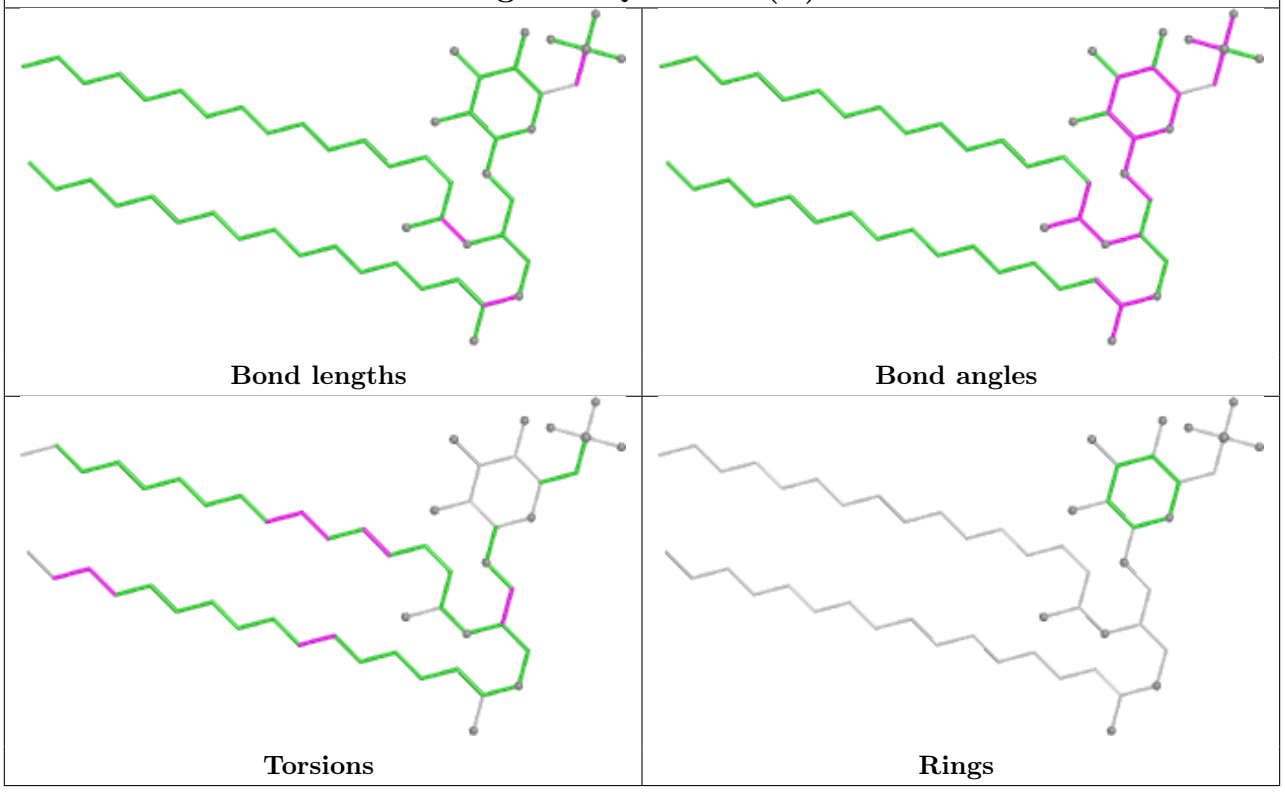
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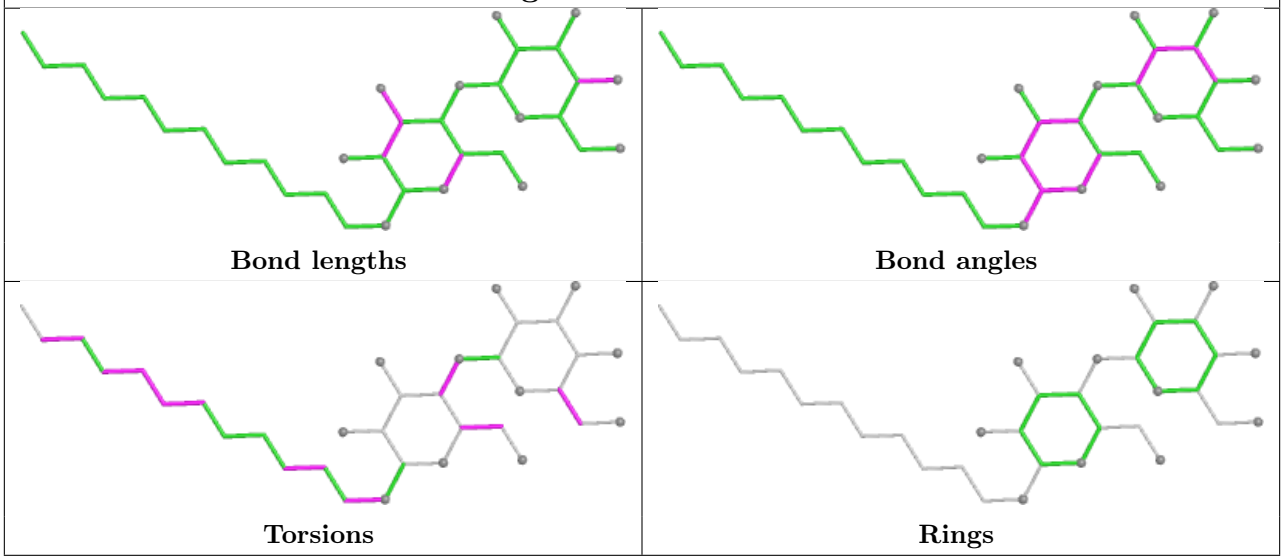
Ligand BCR T 101



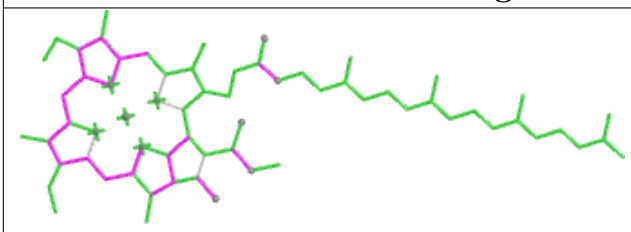
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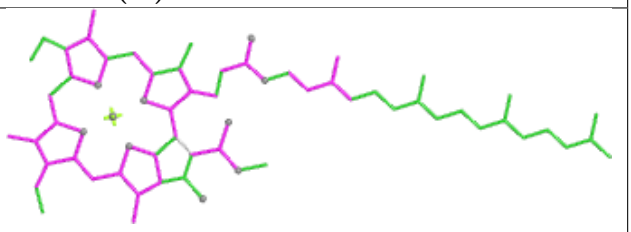
Ligand LMT D 404



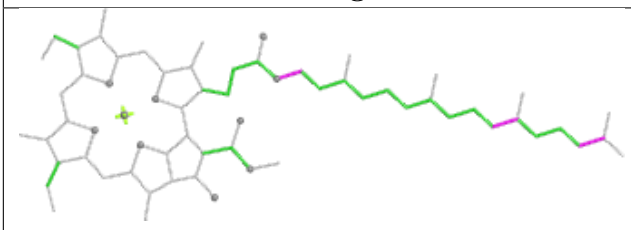
Ligand CLA d 402 (B)



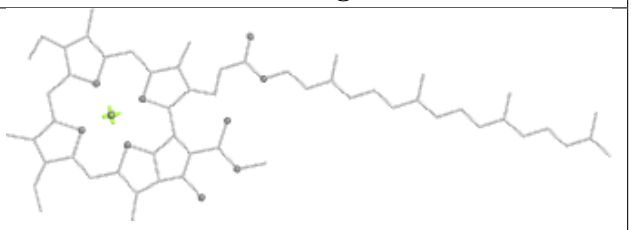
Bond lengths



Bond angles

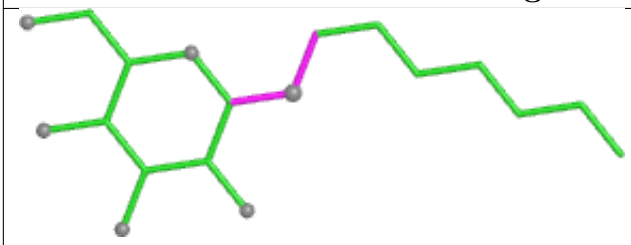


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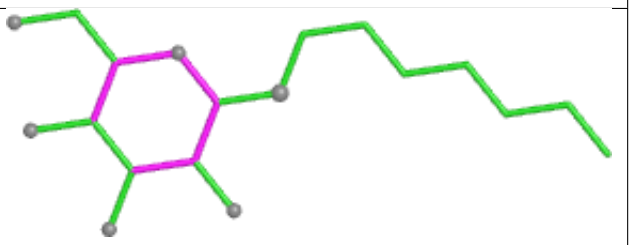


Rings

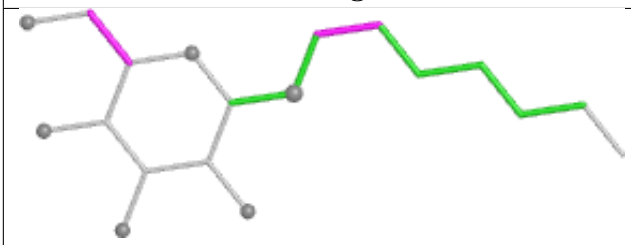
Ligand HTG b 625



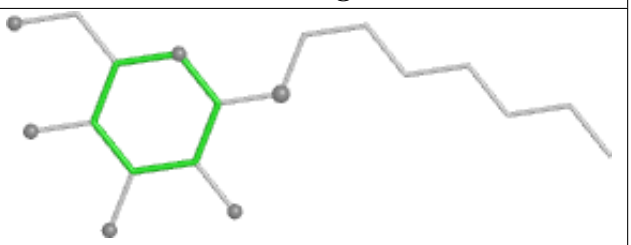
Bond lengths



Bond angles

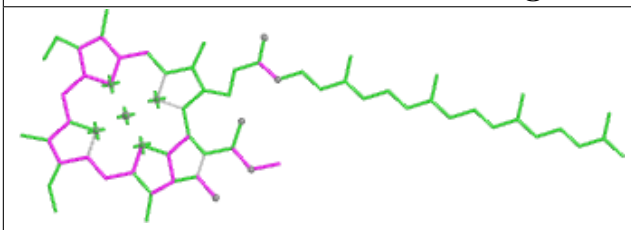


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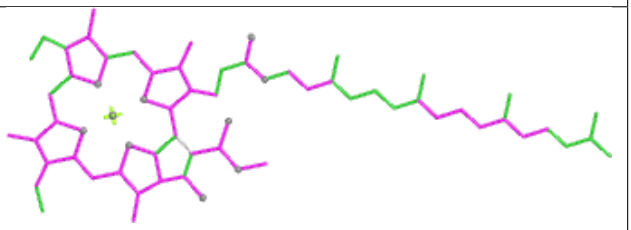


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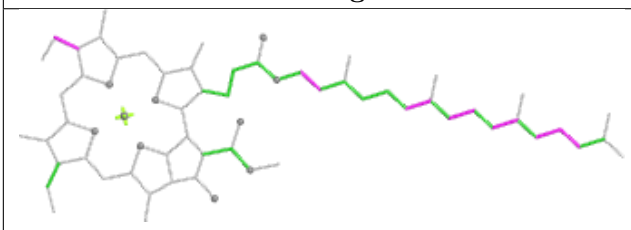
Ligand CLA B 602



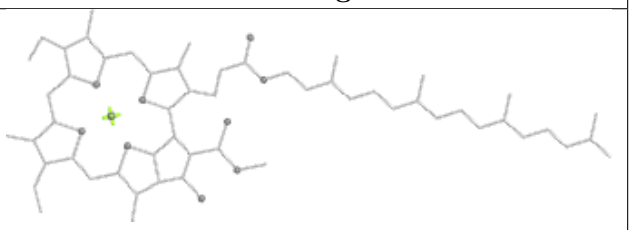
Bond lengths



Bond angles

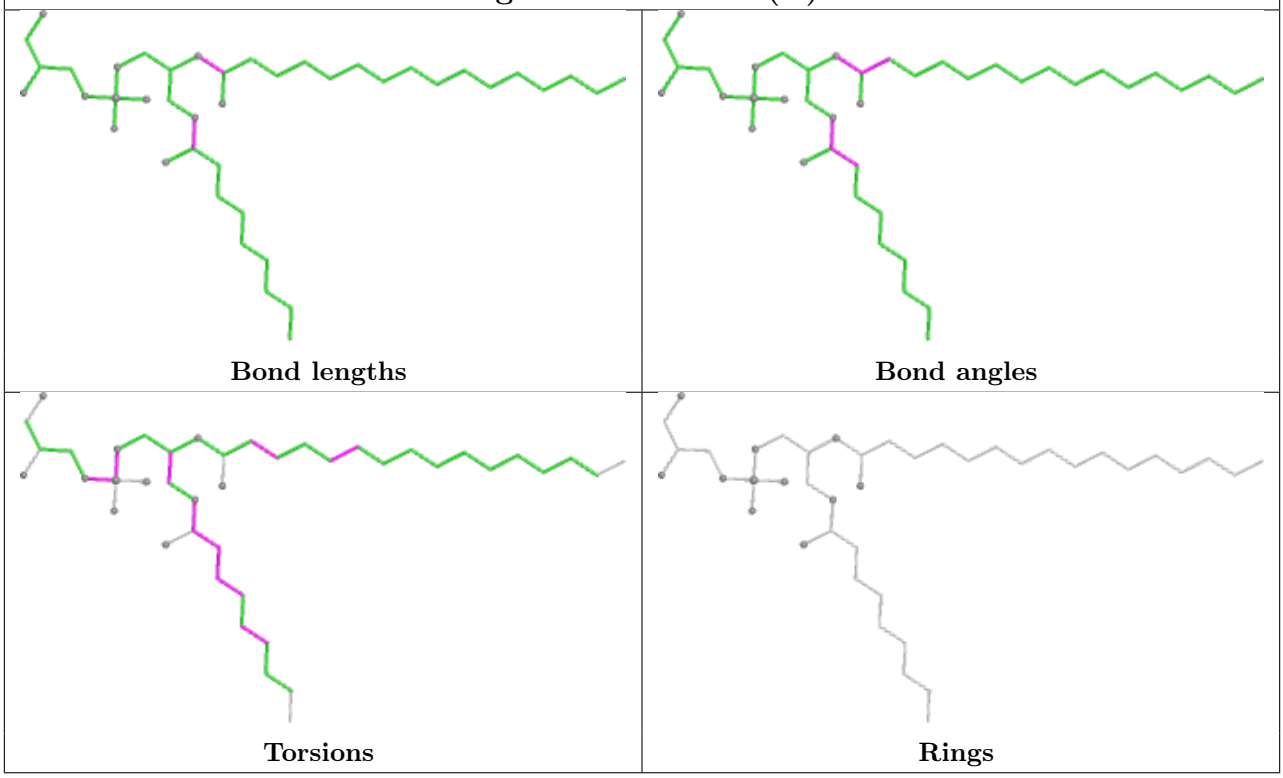


Torsions

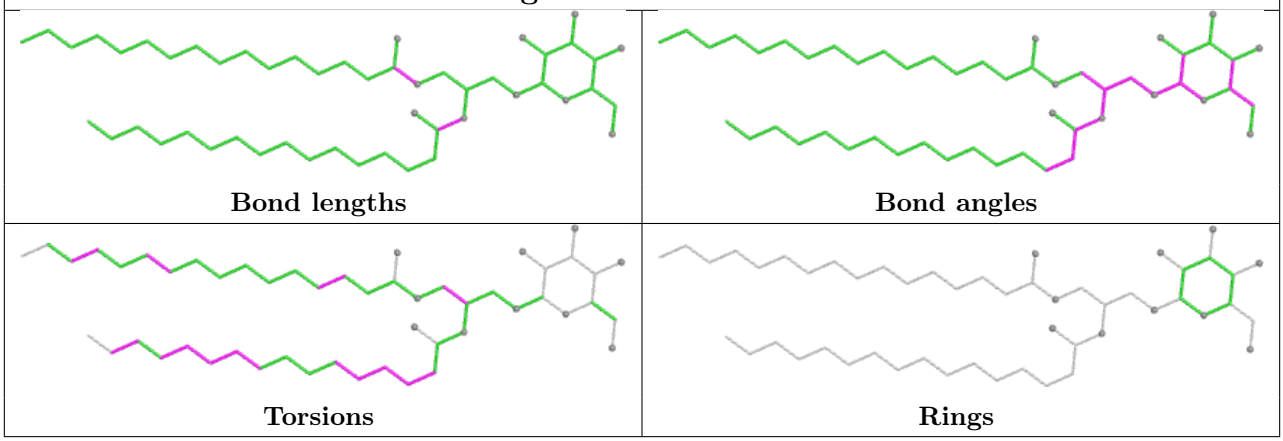


Rings

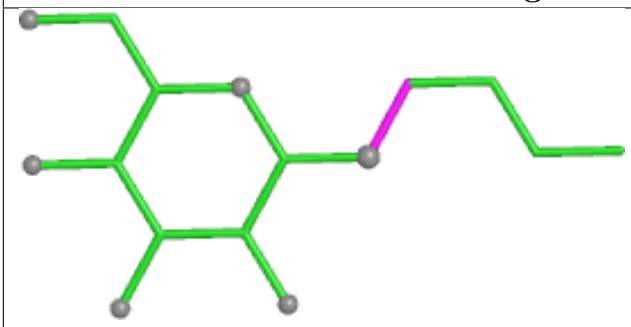
Ligand LHG e 101 (B)



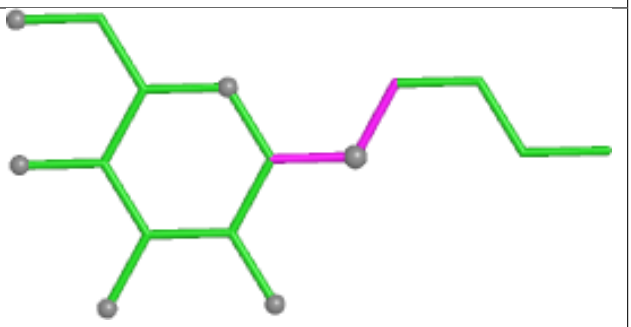
Ligand LMG C 501



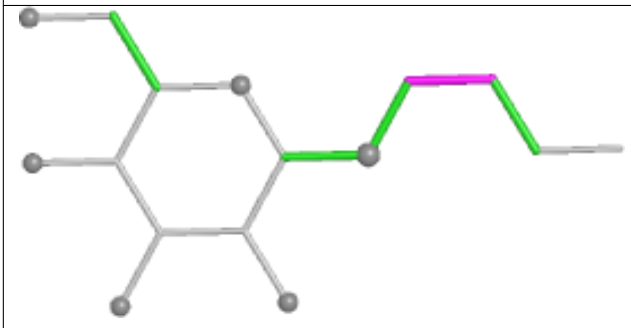
Ligand HTG d 411



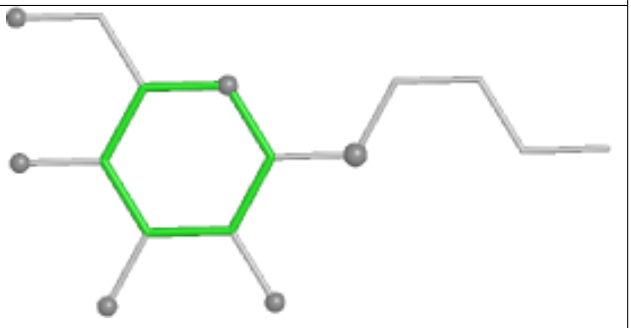
Bond lengths



Bond angles

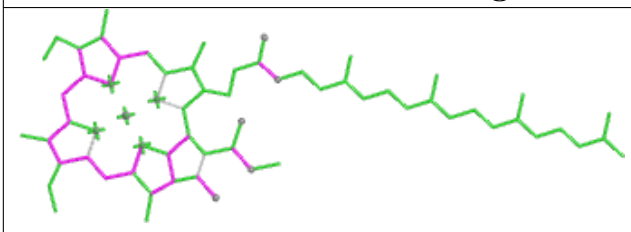


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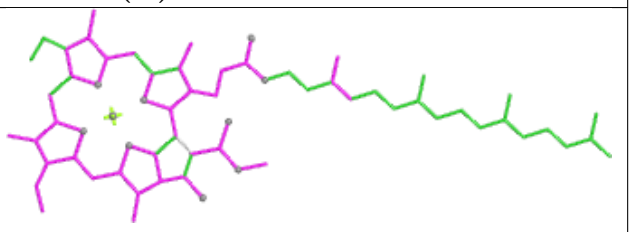


Rings

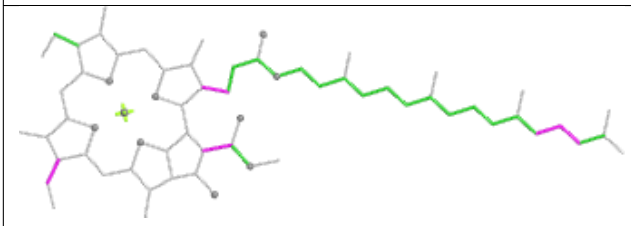
Ligand CLA A 405 (B)



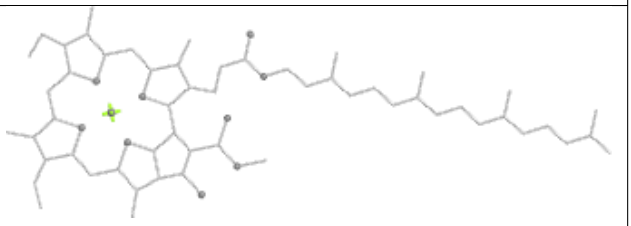
Bond lengths



Bond angles

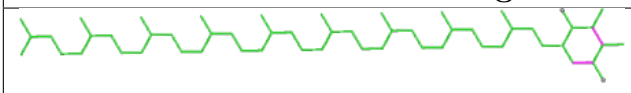


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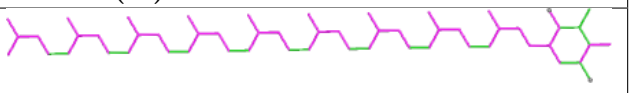


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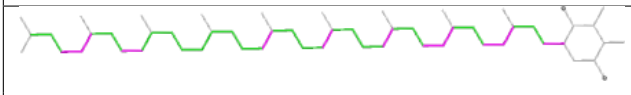
Ligand PL9 A 414 (A)



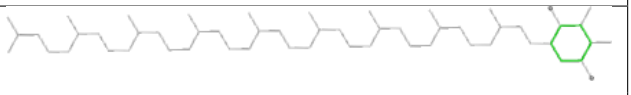
Bond lengths



Bond angles

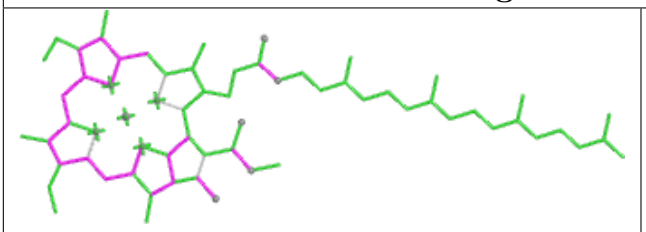


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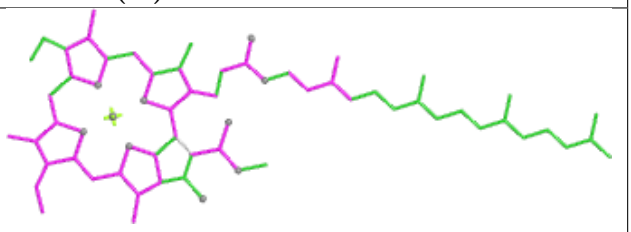


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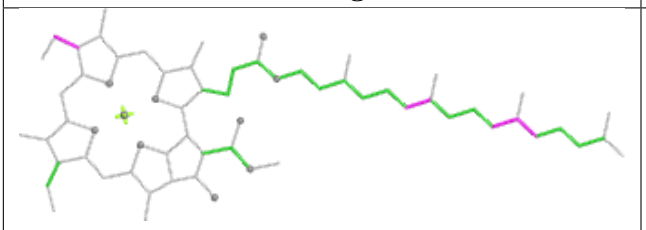
Ligand CLA a 407 (B)



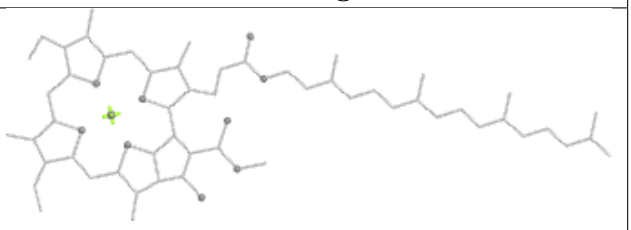
Bond lengths



Bond angles

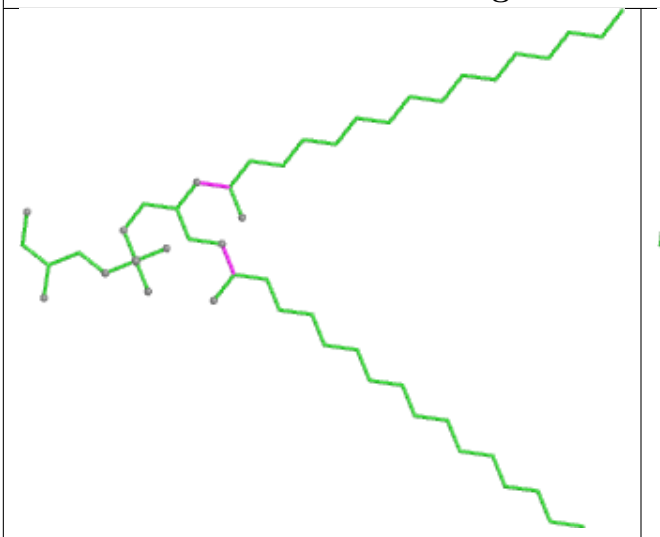


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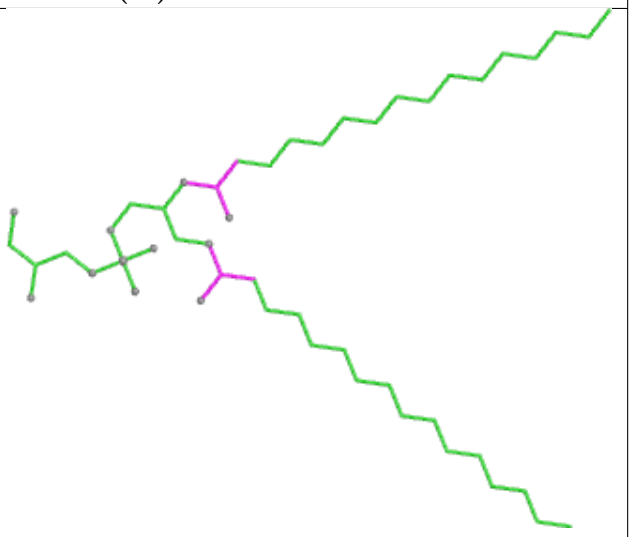


Rings

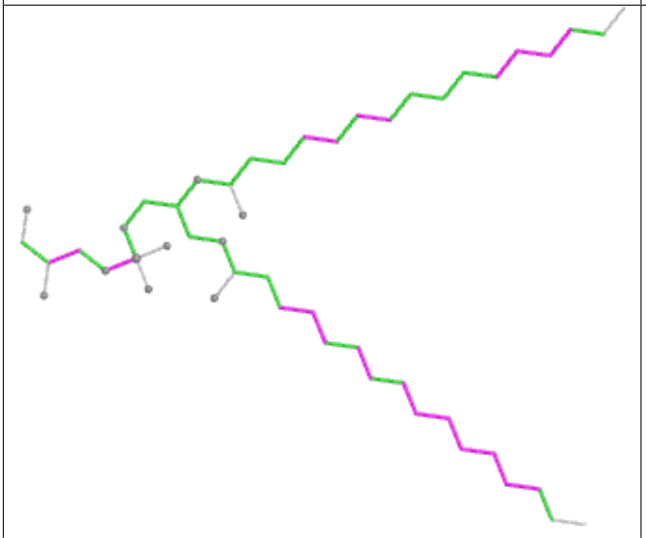
Ligand LHG d 711 (A)



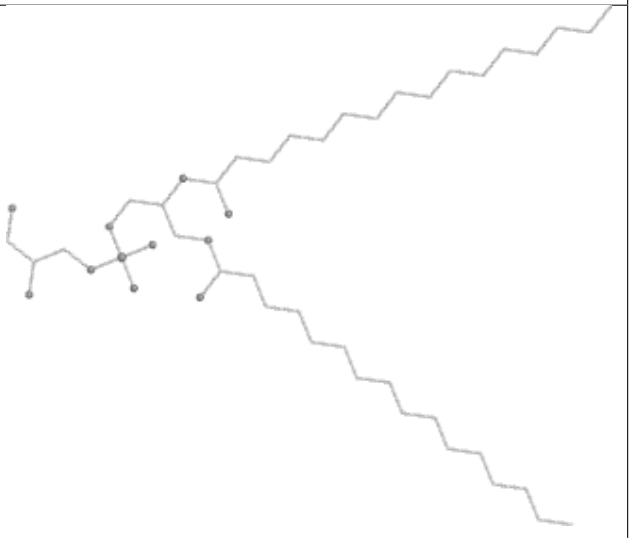
Bond lengths



Bond angles

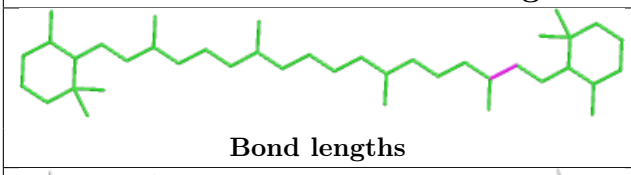


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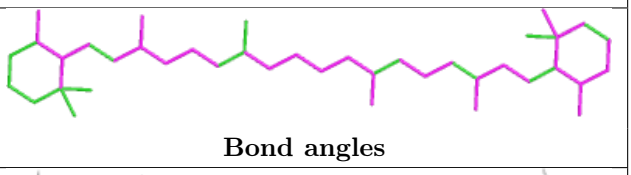


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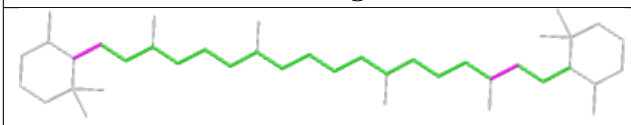
Ligand BCR Y 101



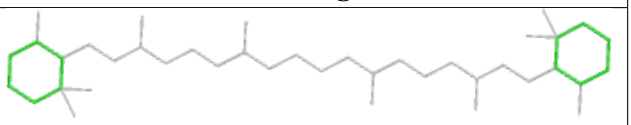
Bond lengths



Bond angles

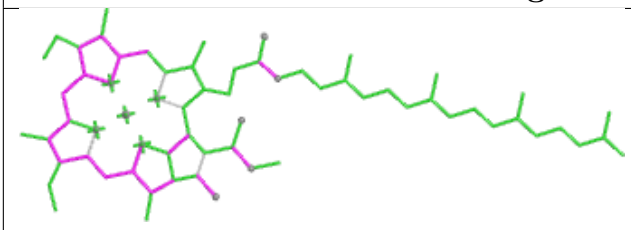


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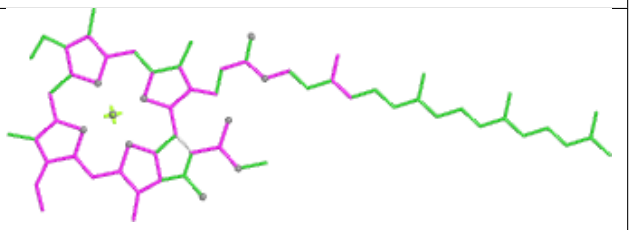


Rings

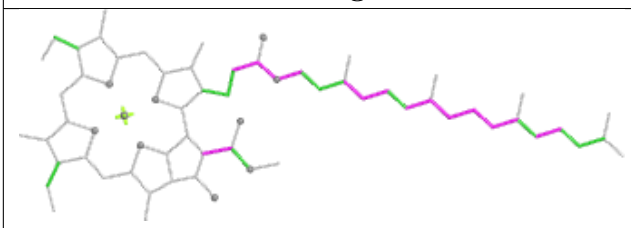
Ligand CLA b 601



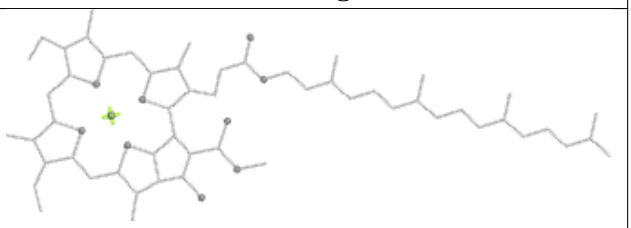
Bond lengths



Bond angles

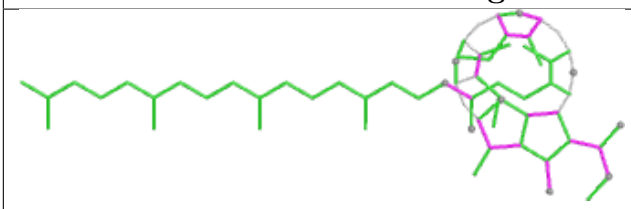


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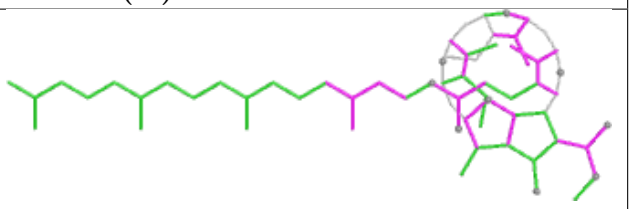


Rings

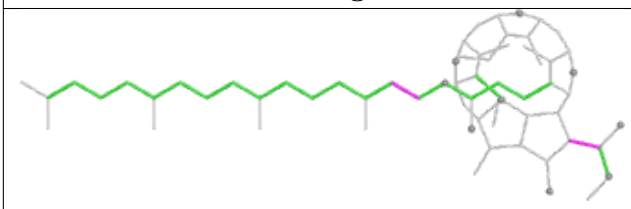
Ligand PHO A 407 (A)



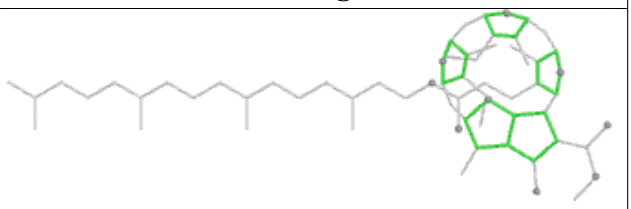
Bond lengths



Bond angles

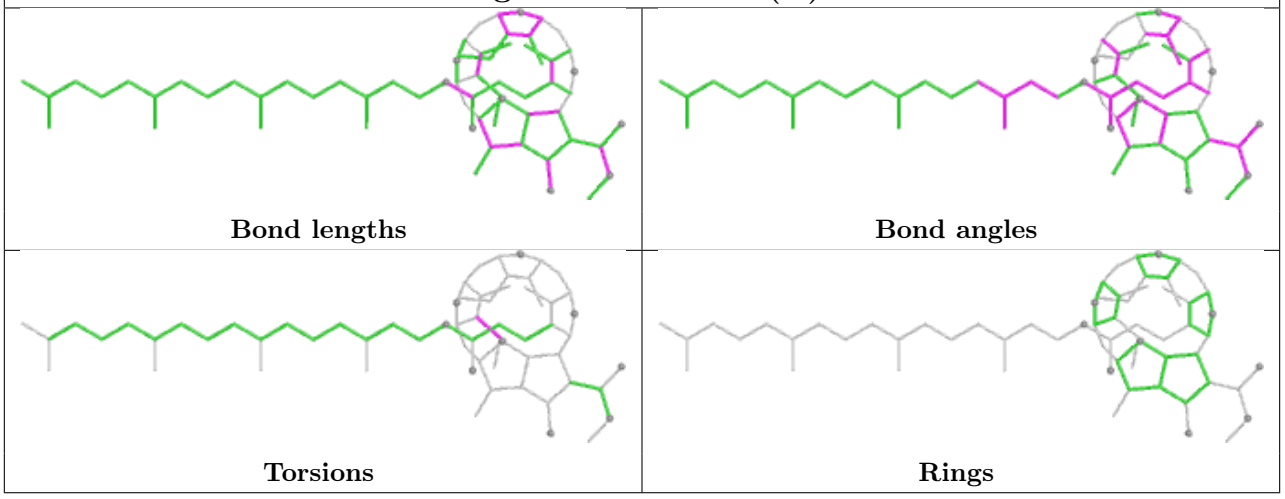


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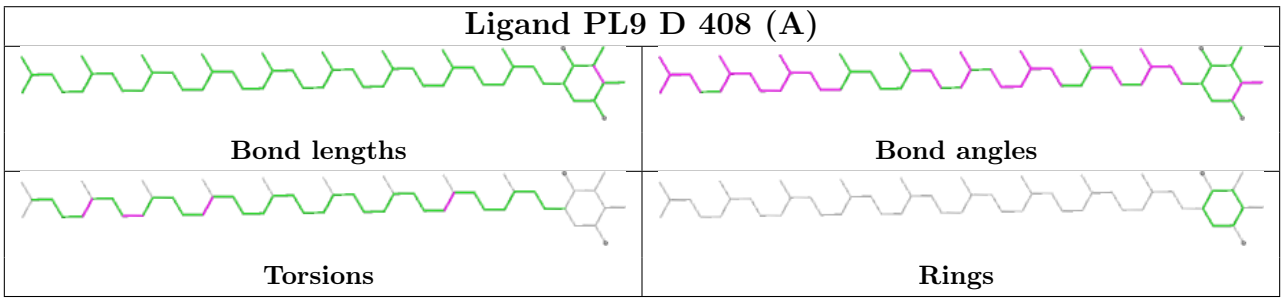


Rings

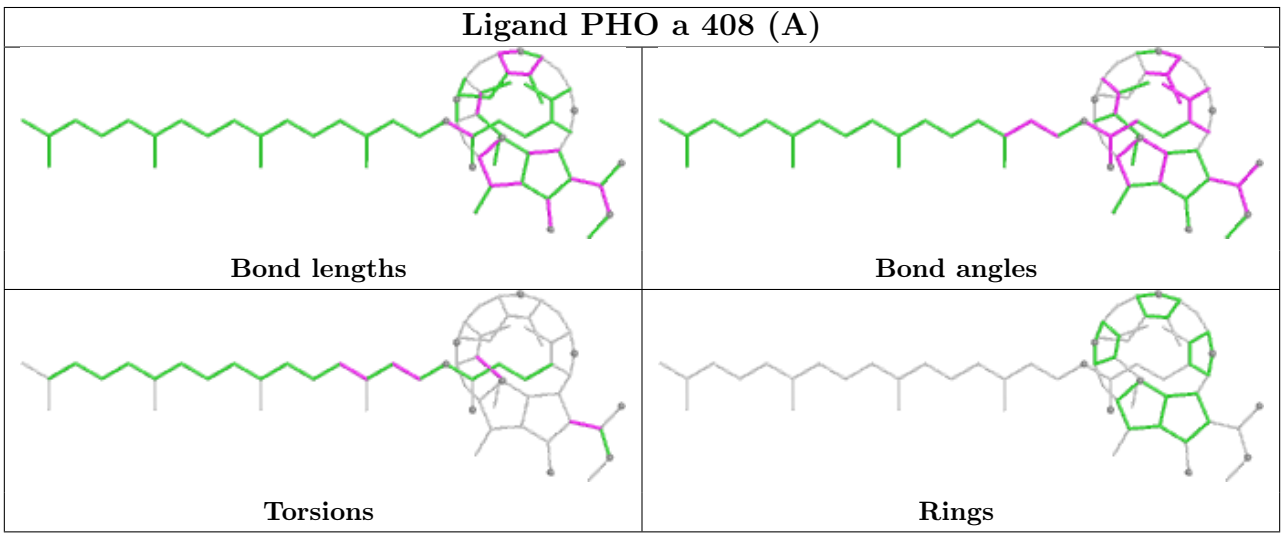
Ligand PHO a 353 (A)



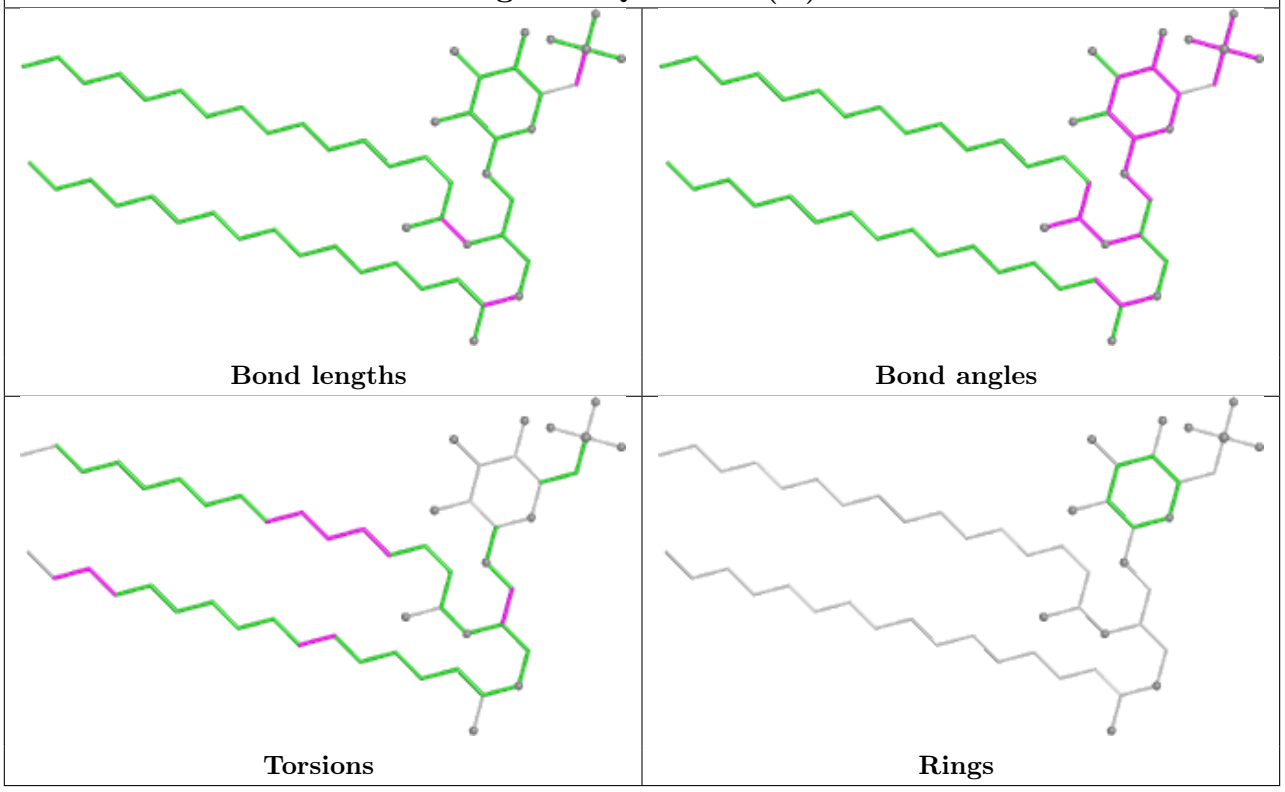
Ligand PL9 D 408 (A)



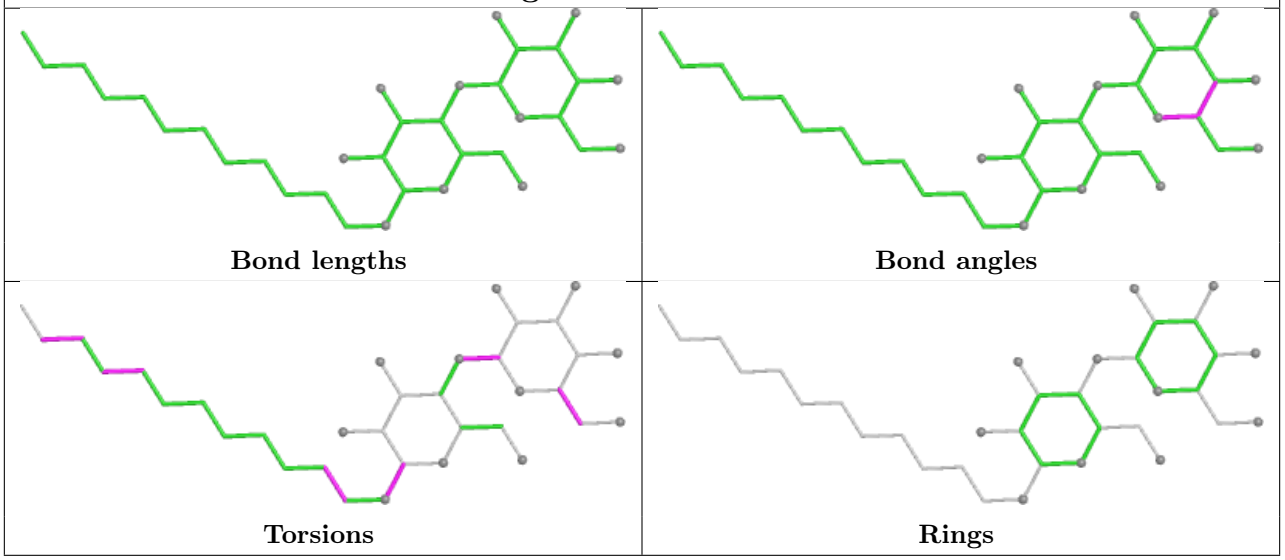
Ligand PHO a 408 (A)



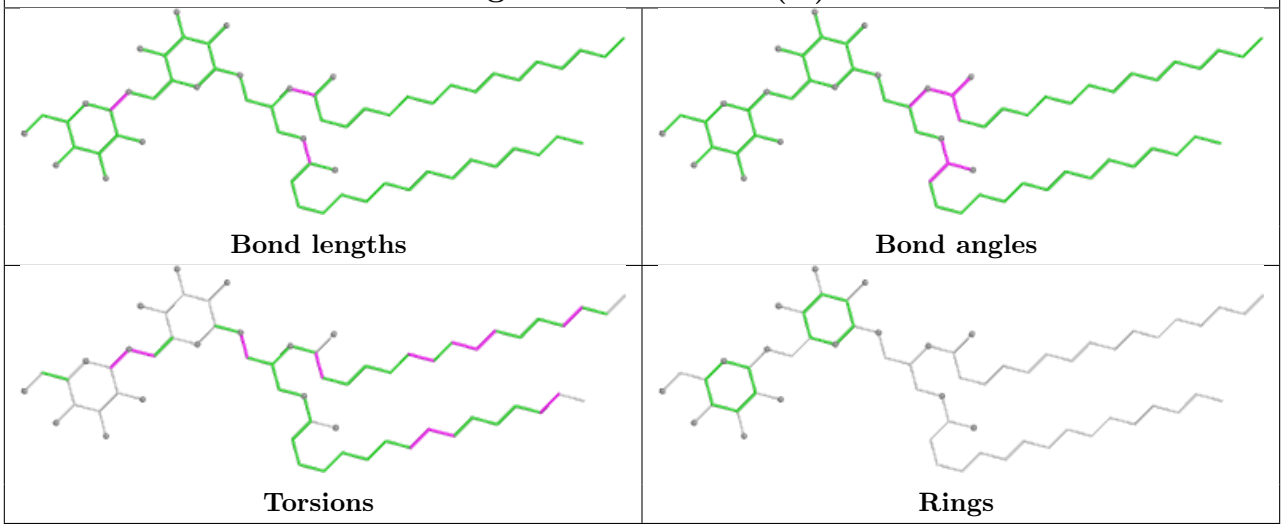
Ligand SQD a 411 (A)



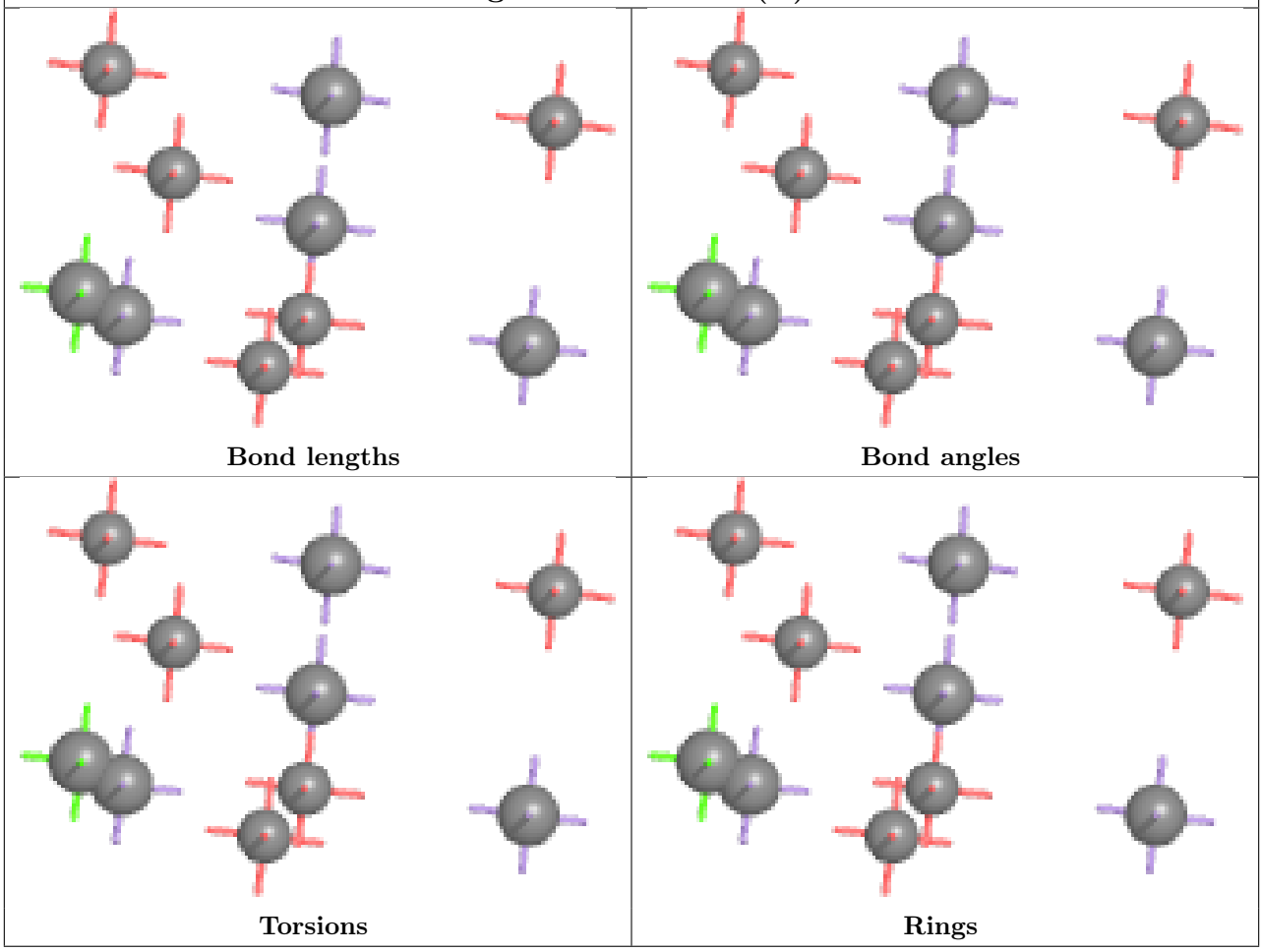
Ligand LMT A 359



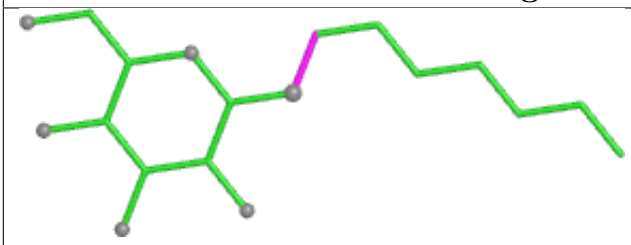
Ligand DGD C 518 (A)



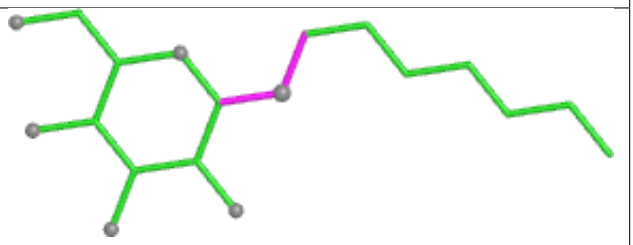
Ligand OEX a 415 (B)



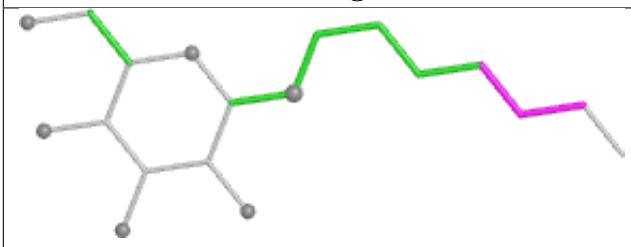
Ligand HTG B 623



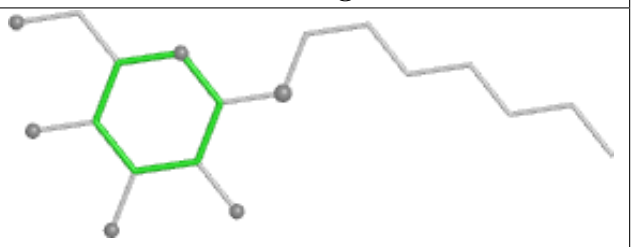
Bond lengths



Bond angles

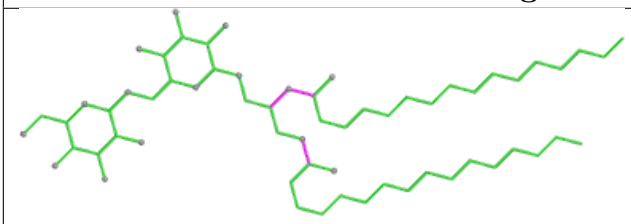


Torsions

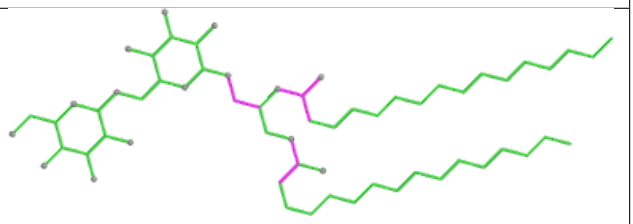


Rings

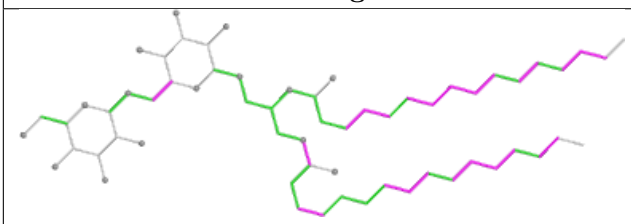
Ligand DGD C 519



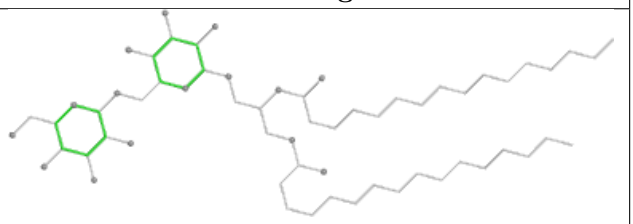
Bond lengths



Bond angles

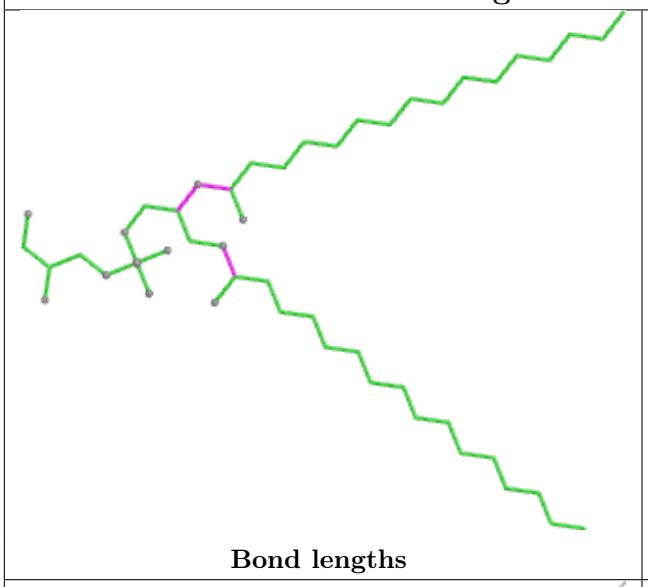


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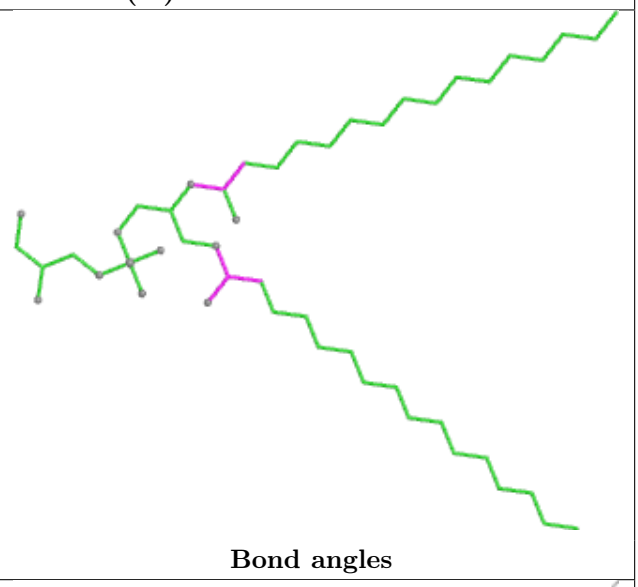


Rings

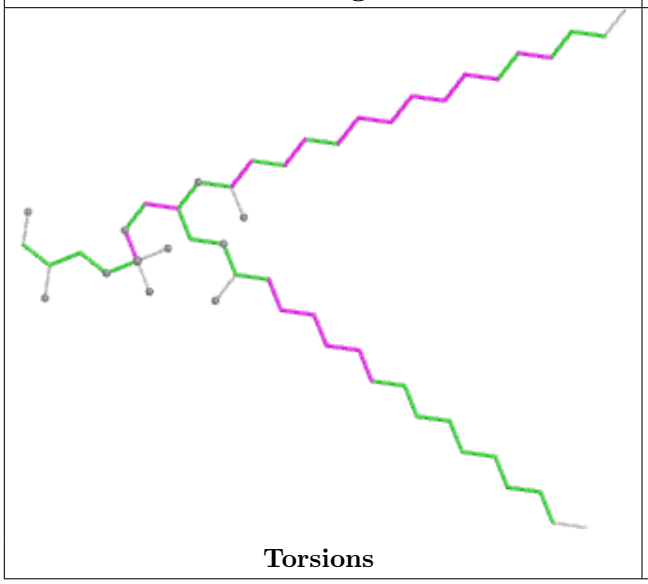
Ligand LHG L 101 (B)



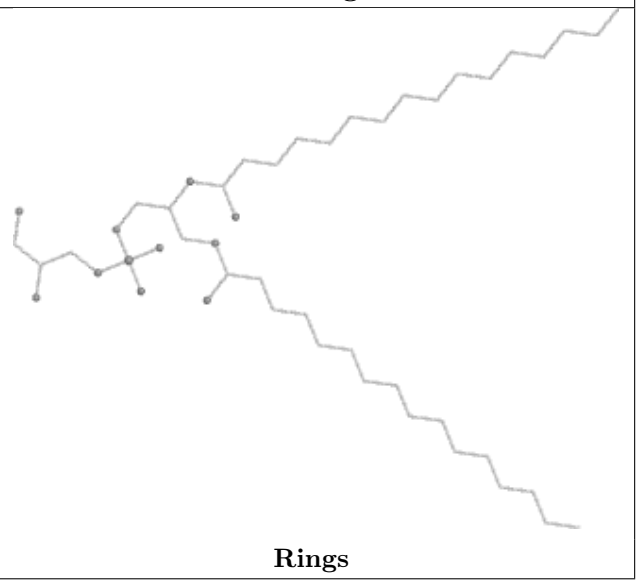
Bond lengths



Bond angles

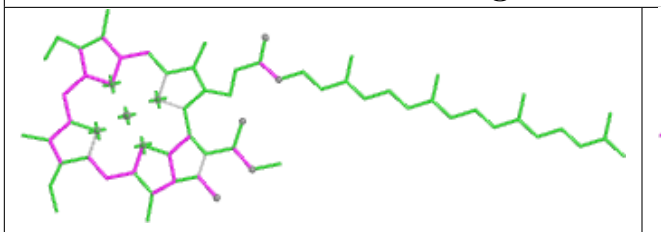


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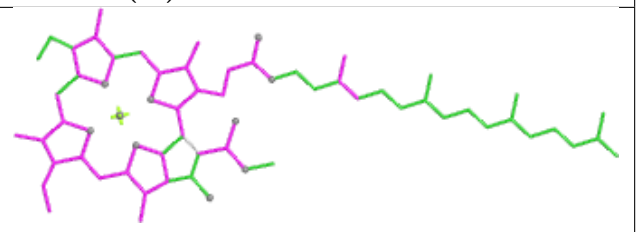


Rings

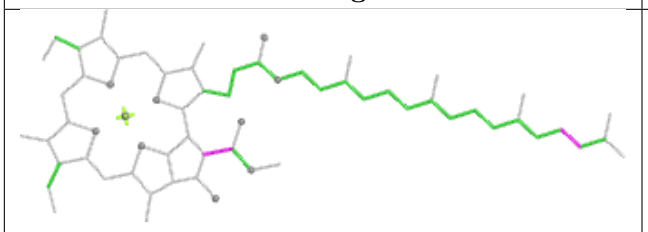
Ligand CLA A 405 (A)



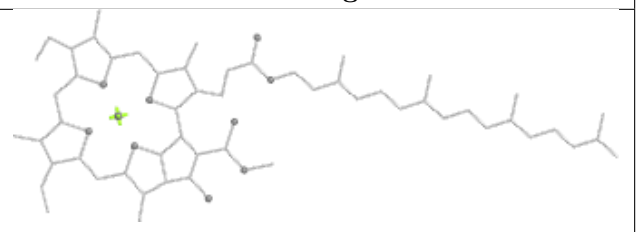
Bond lengths



Bond angles

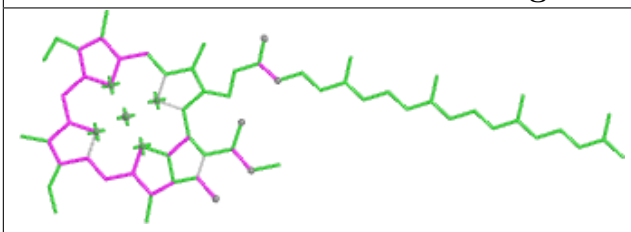


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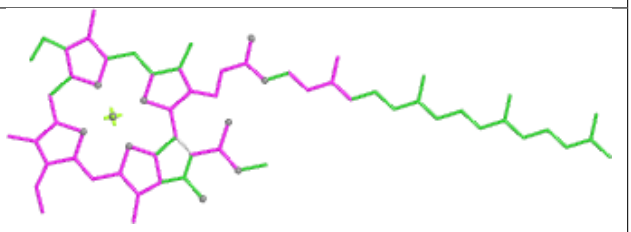


Rings

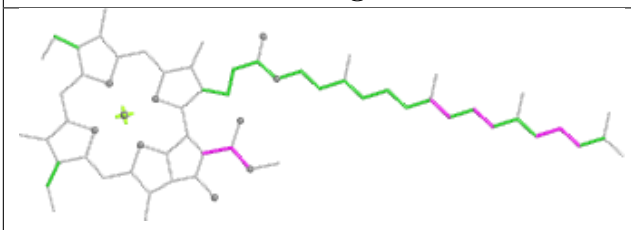
Ligand CLA c 507



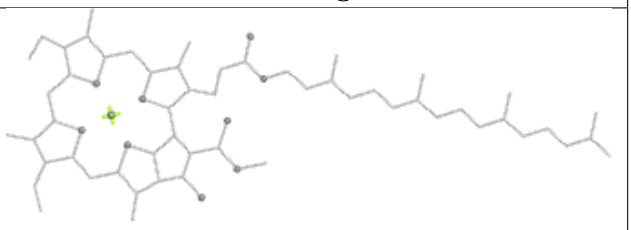
Bond lengths



Bond angles



Torsions

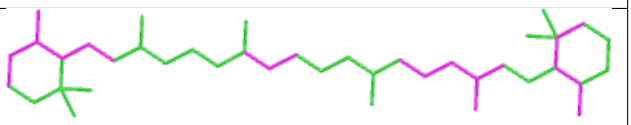


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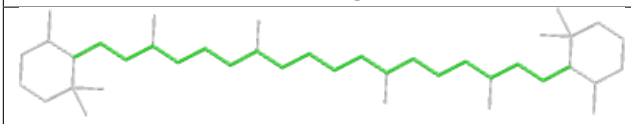
Ligand BCR b 618



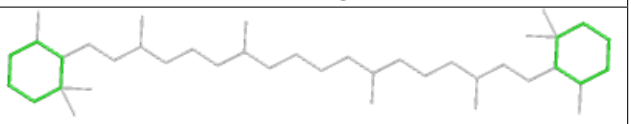
Bond lengths



Bond angles

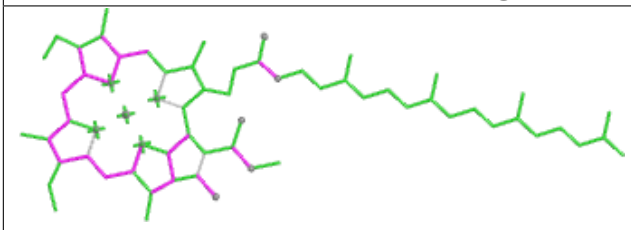


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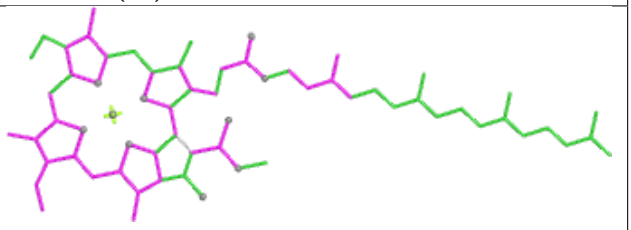


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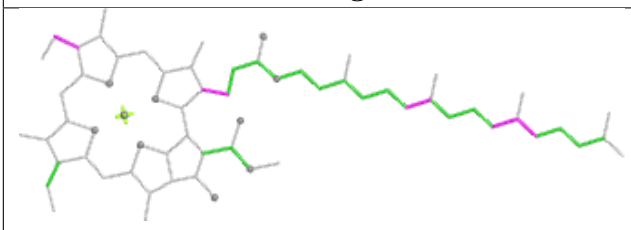
Ligand CLA a 407 (A)



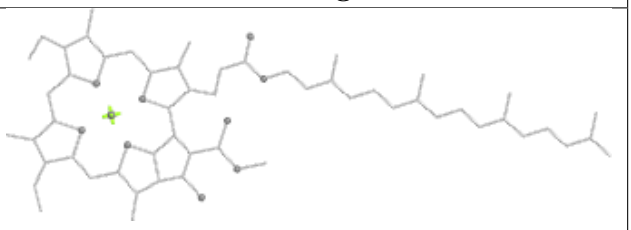
Bond lengths



Bond angles

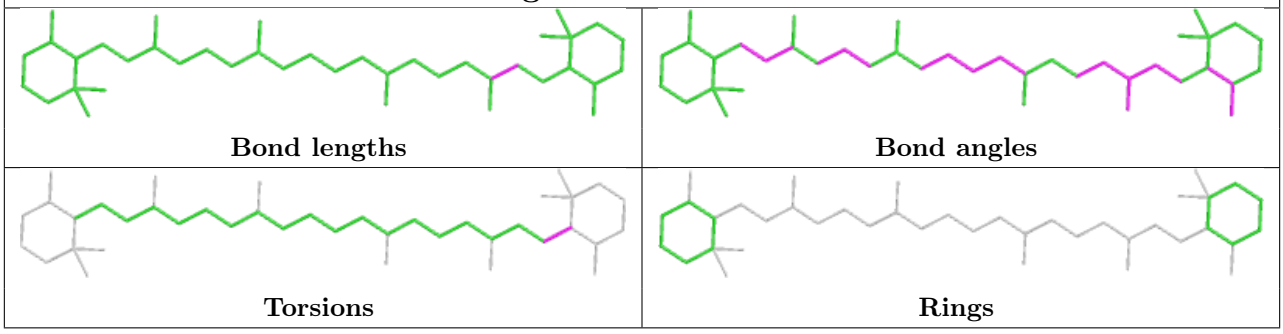


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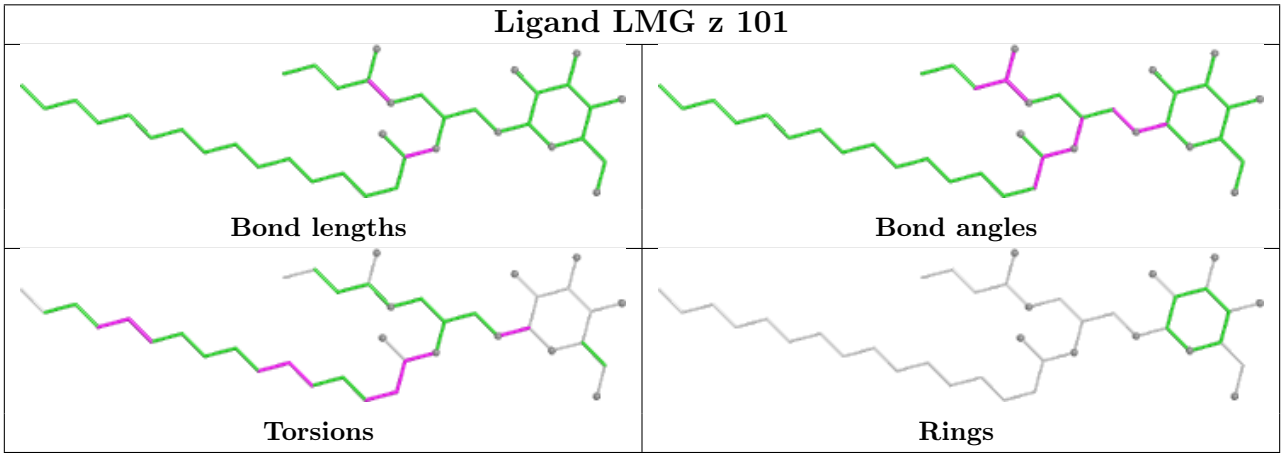


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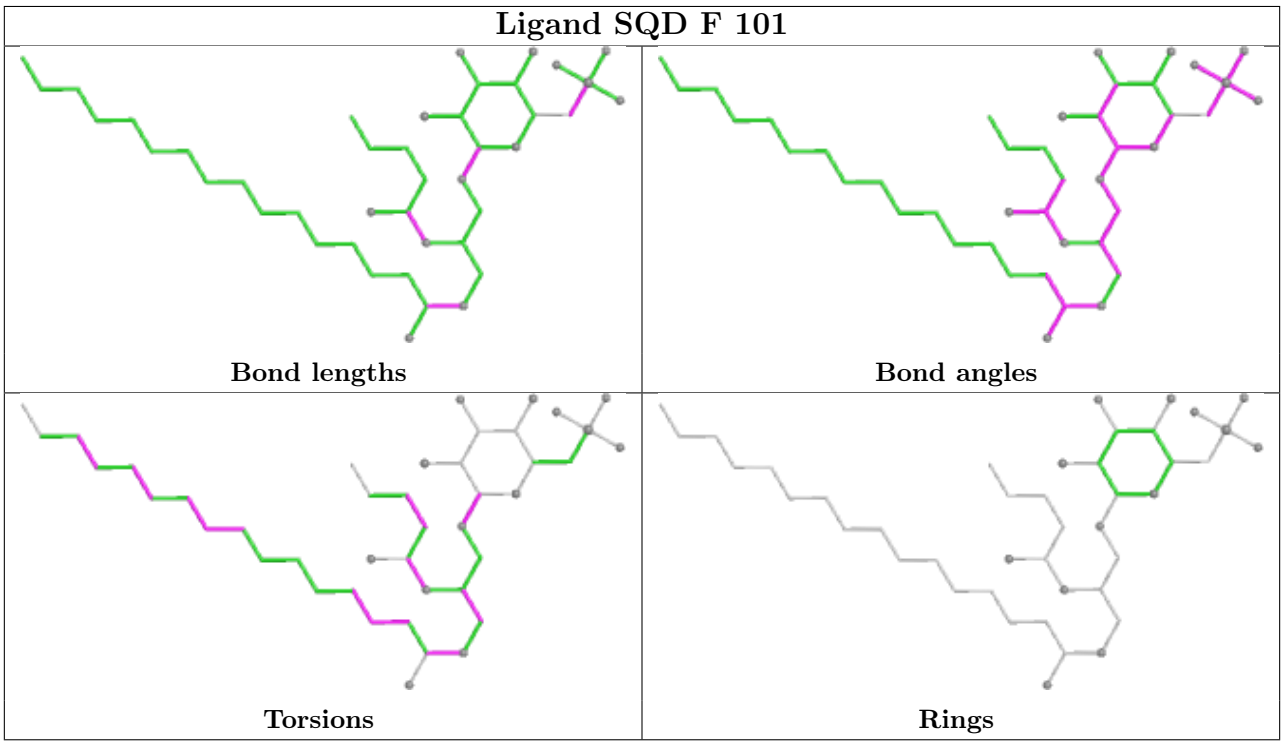
Ligand BCR H 101



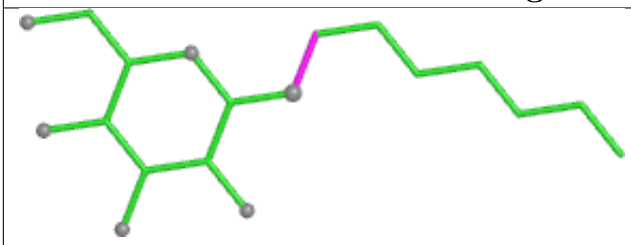
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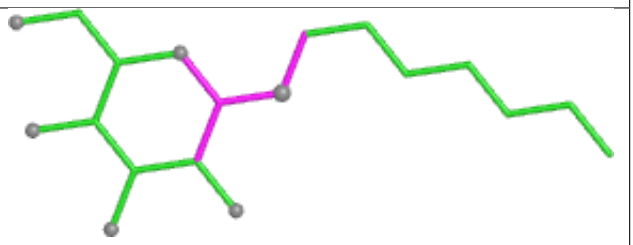
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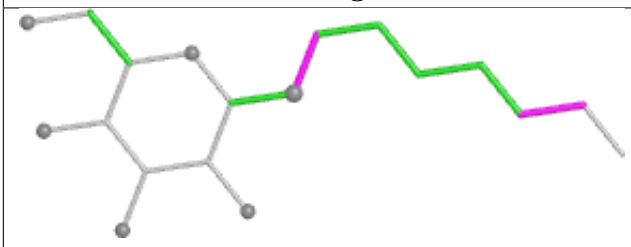
Ligand HTG c 522



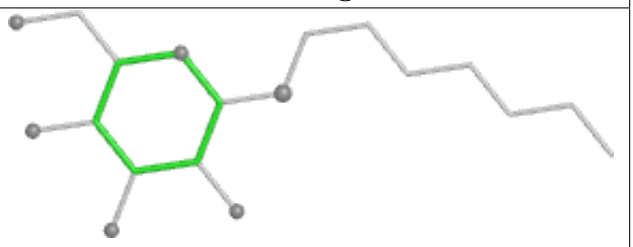
Bond lengths



Bond angles



Torsions

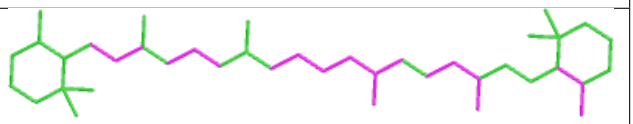


Rings

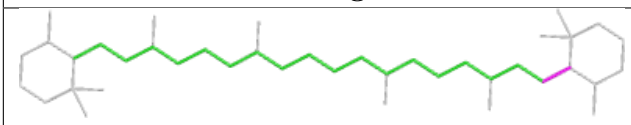
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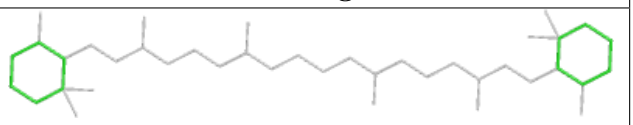
Bond lengths



Bond angles

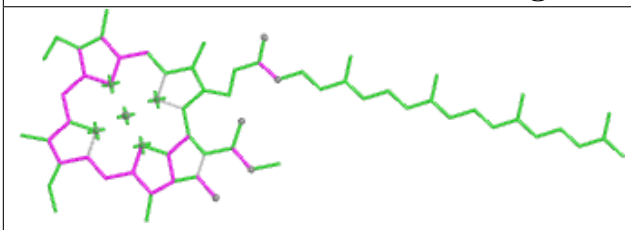


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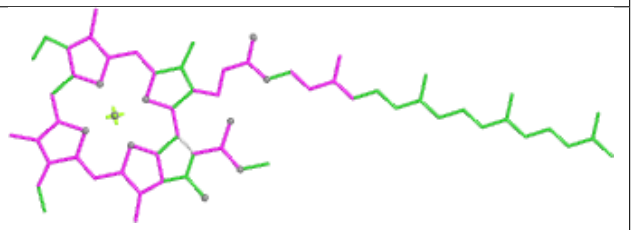


Rings

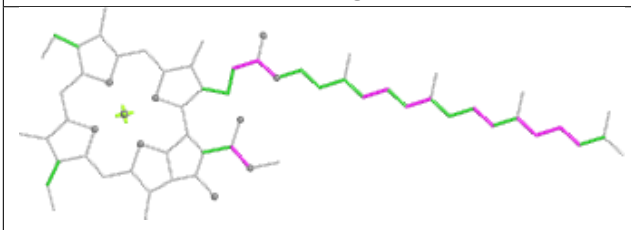
Ligand CLA c 513



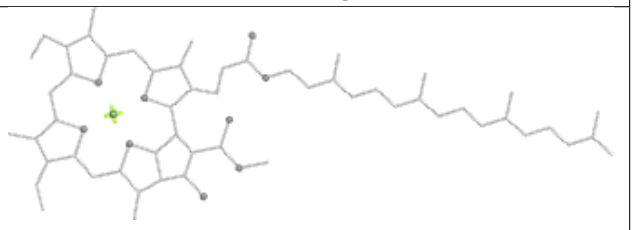
Bond lengths



Bond angles

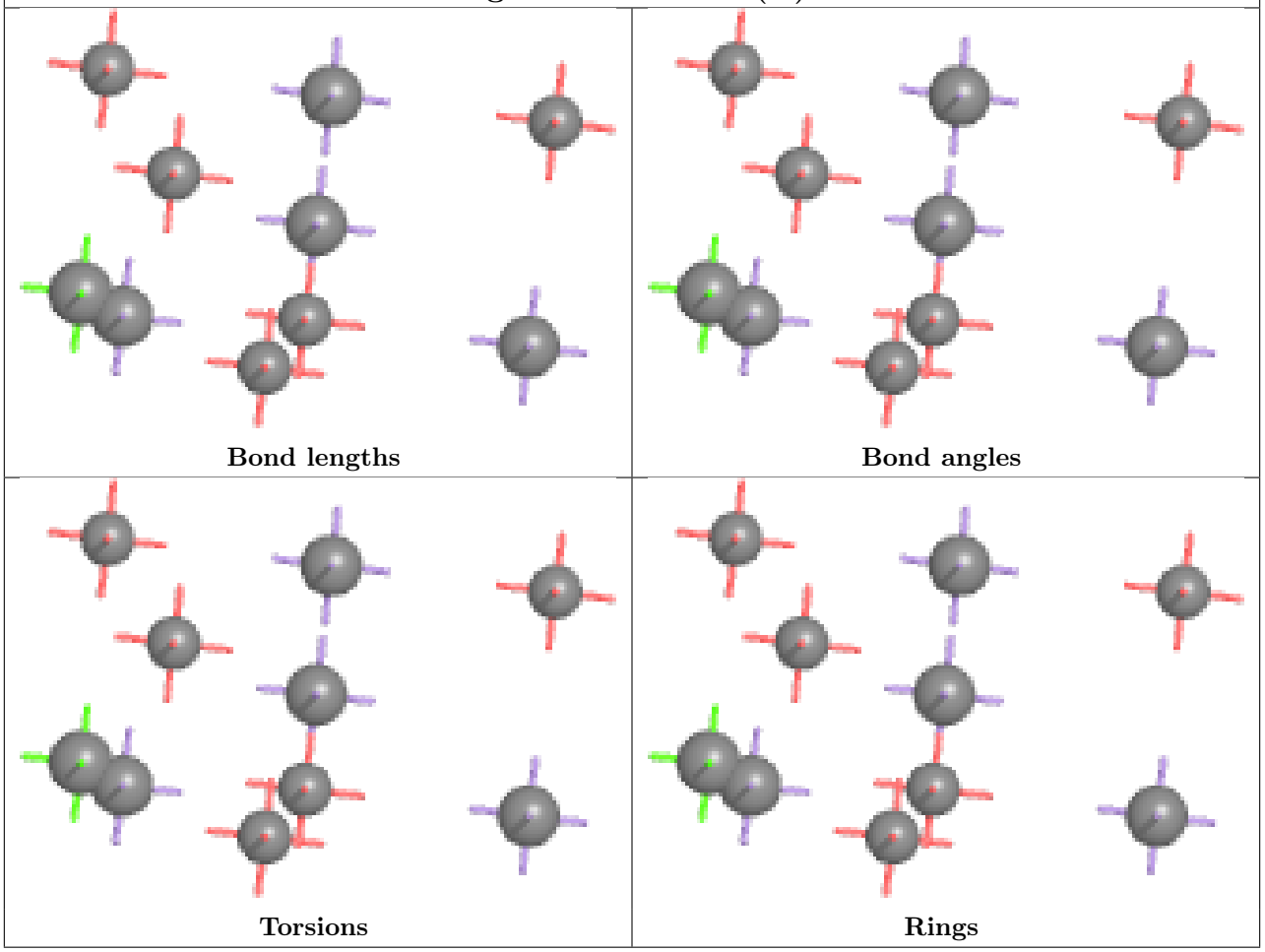


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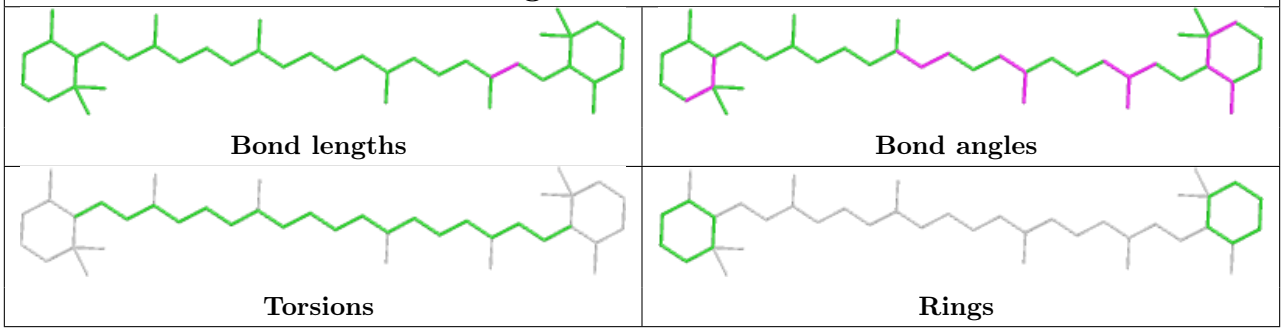


Rings

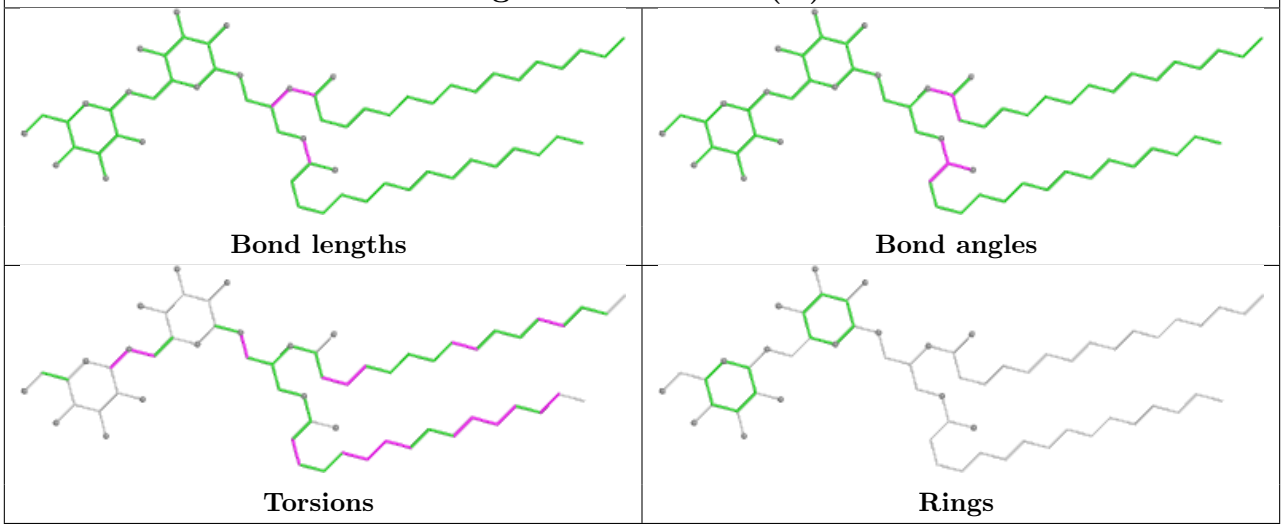
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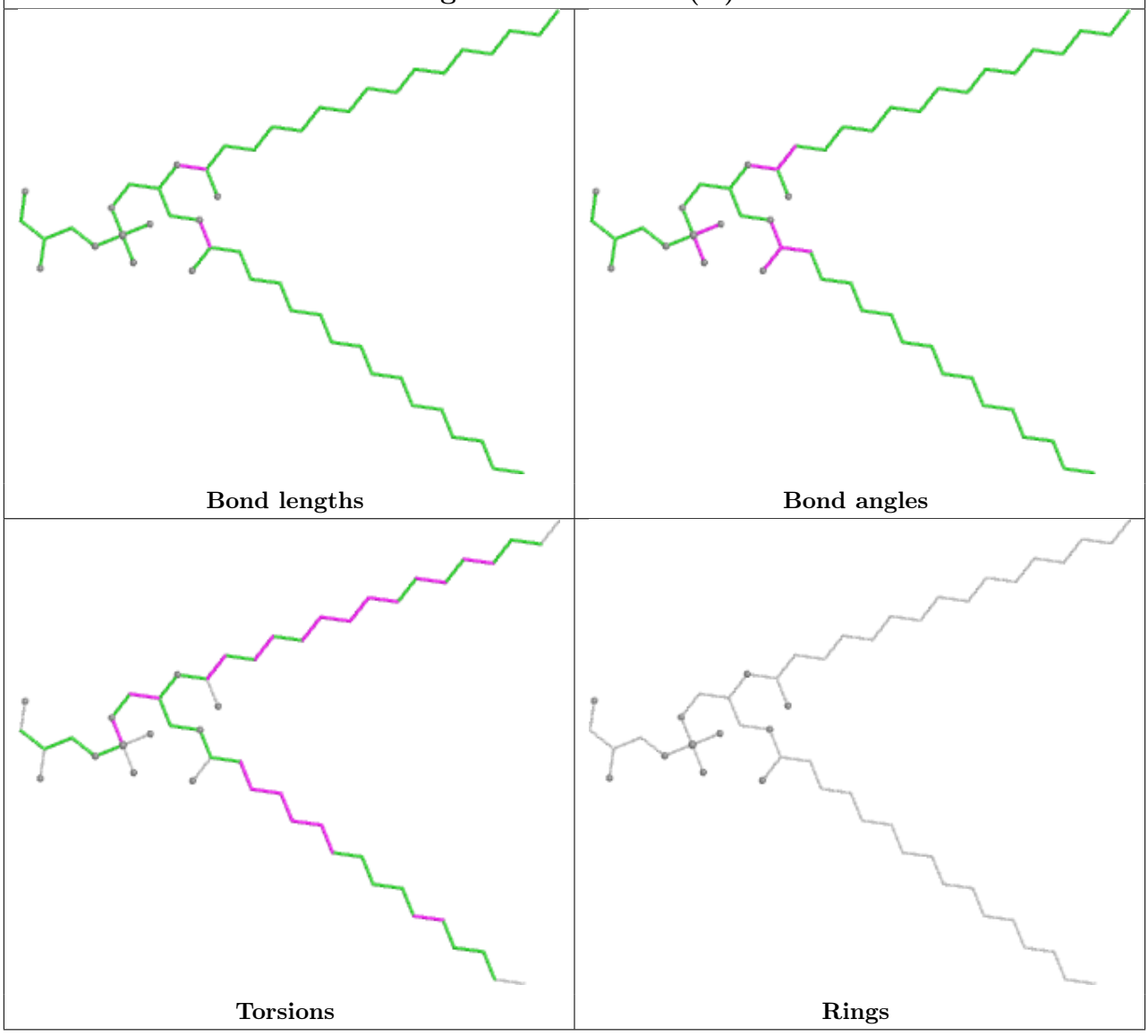
Ligand BCR B 618



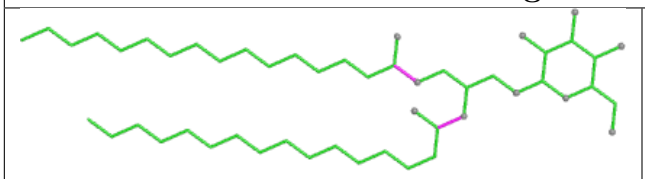
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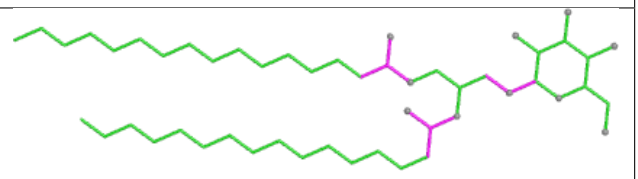
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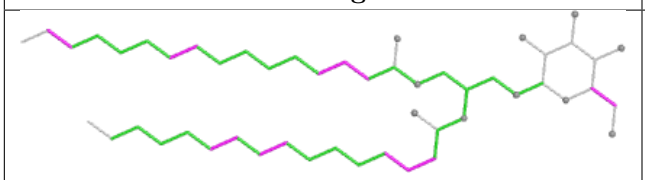
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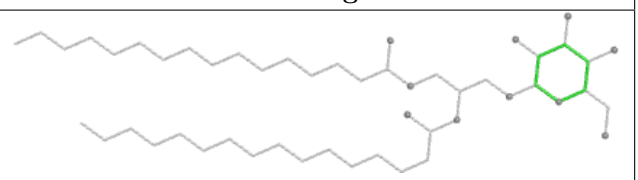
Bond lengths



Bond angles

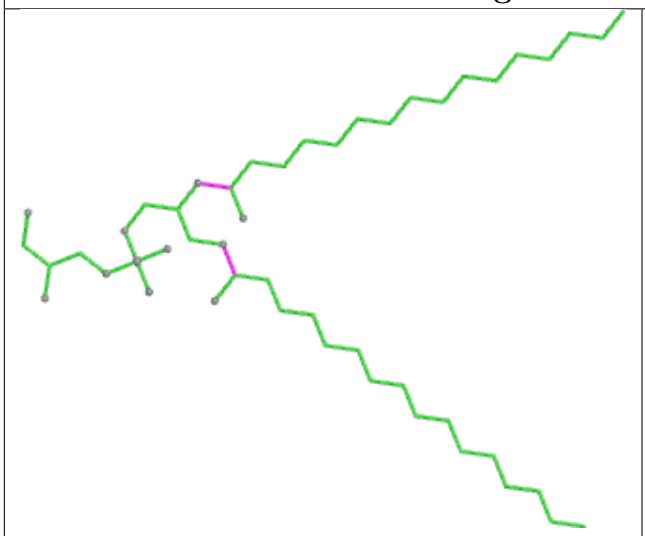


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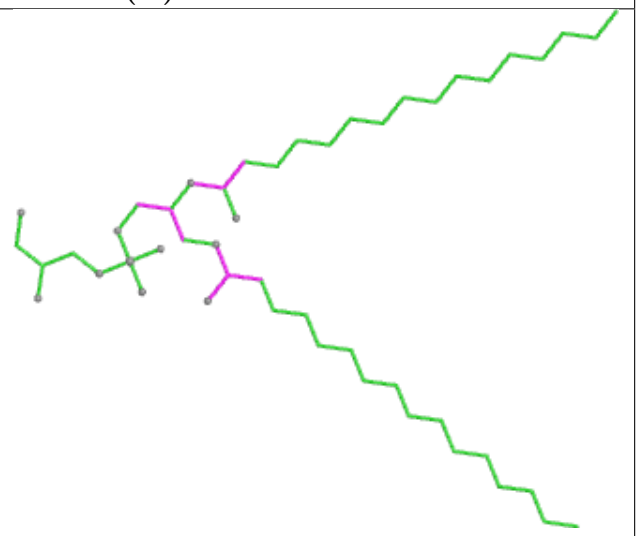


Rings

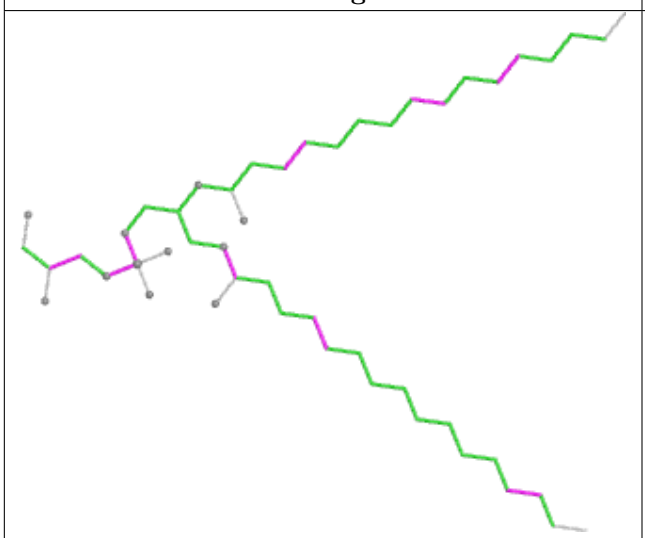
Ligand LHG d 407 (B)



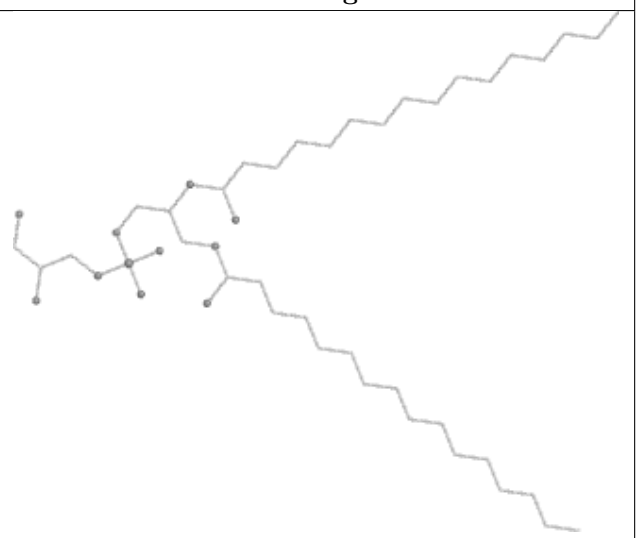
Bond lengths



Bond angles

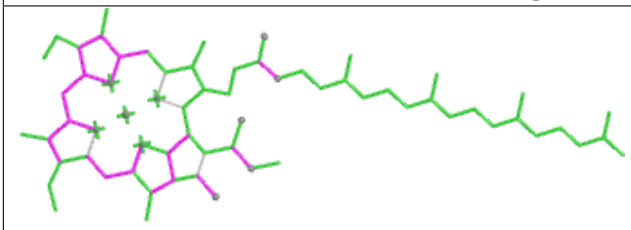


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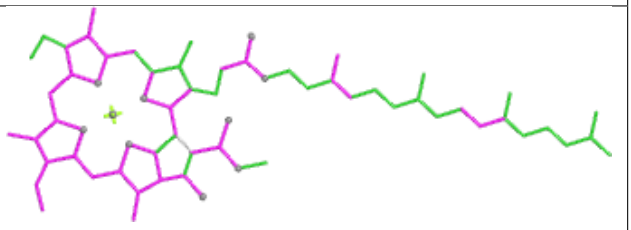


Rings

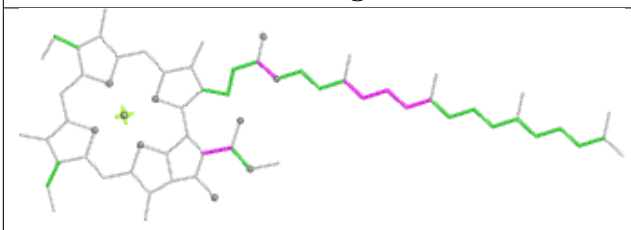
Ligand CLA b 616



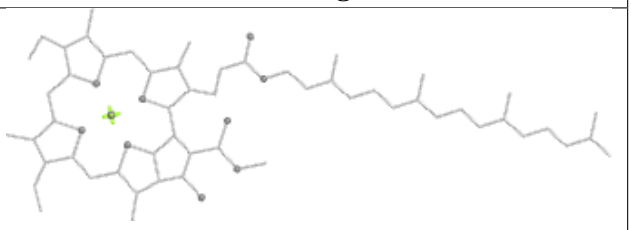
Bond lengths



Bond angles

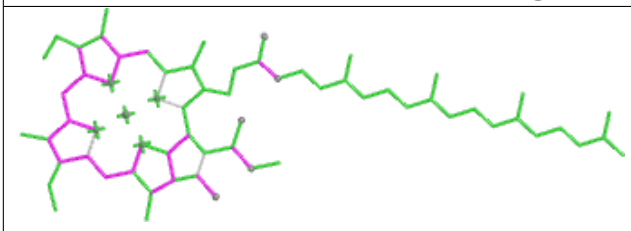


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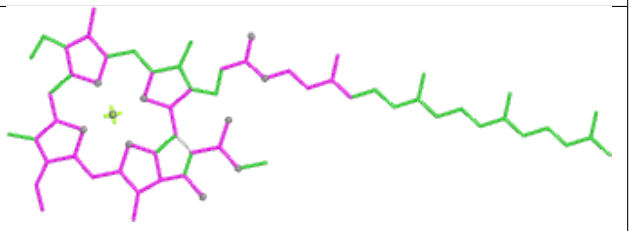


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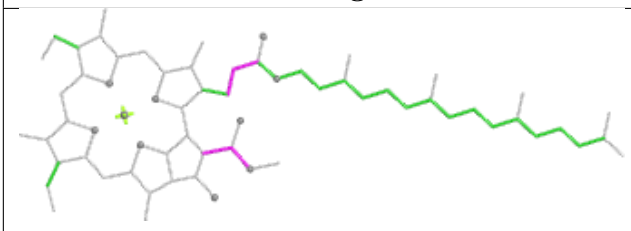
Ligand CLA c 502



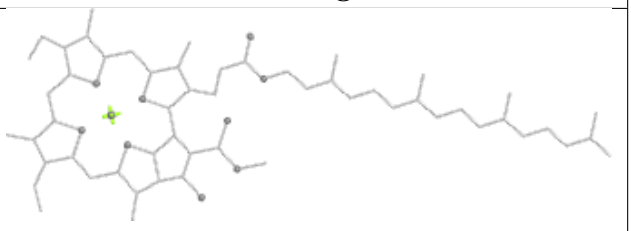
Bond lengths



Bond angles

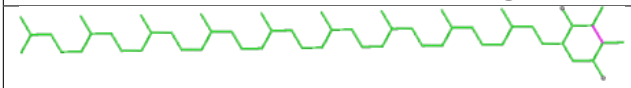


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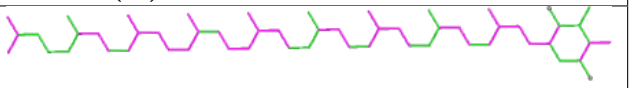


Rings

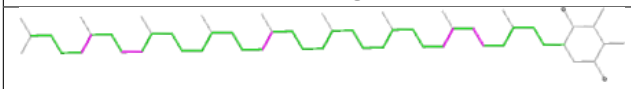
Ligand PL9 d 405 (B)



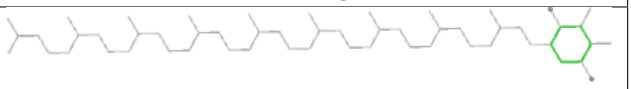
Bond lengths



Bond angles

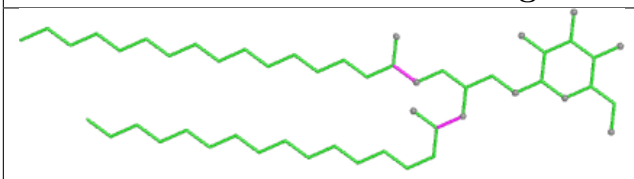


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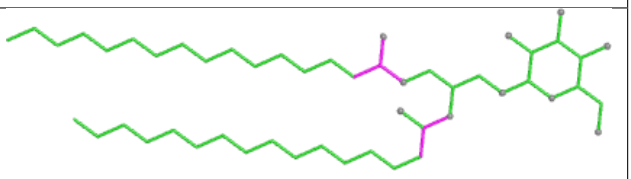


Rings

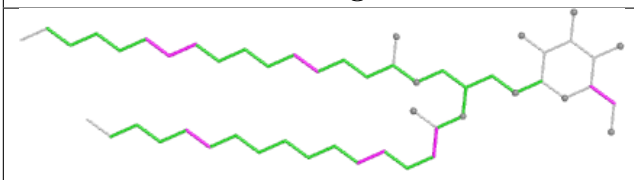
Ligand LMG D 415



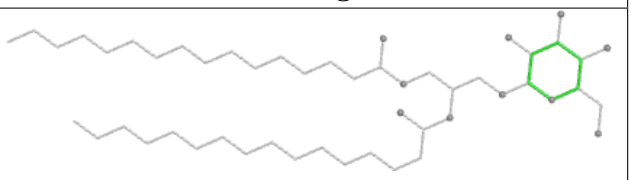
Bond lengths



Bond angles

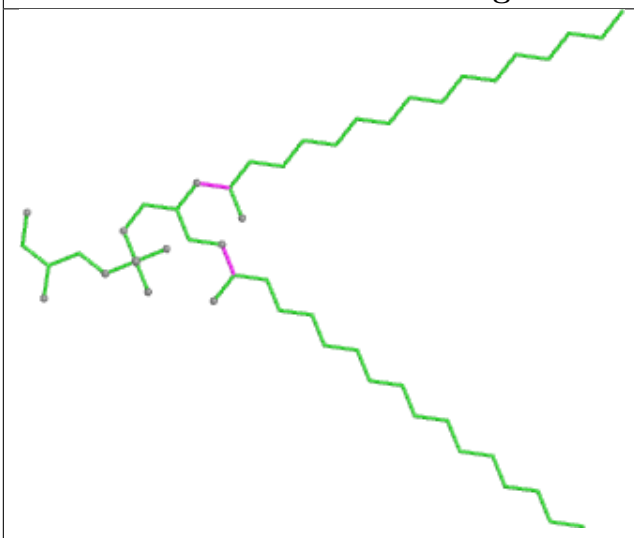


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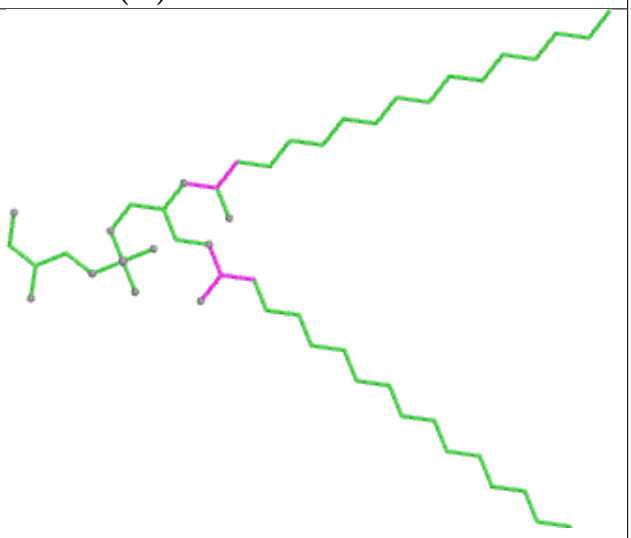


Rings

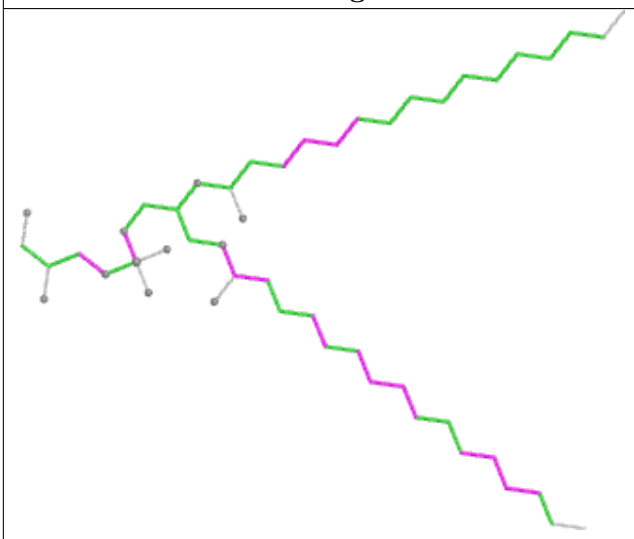
Ligand LHG d 408 (B)



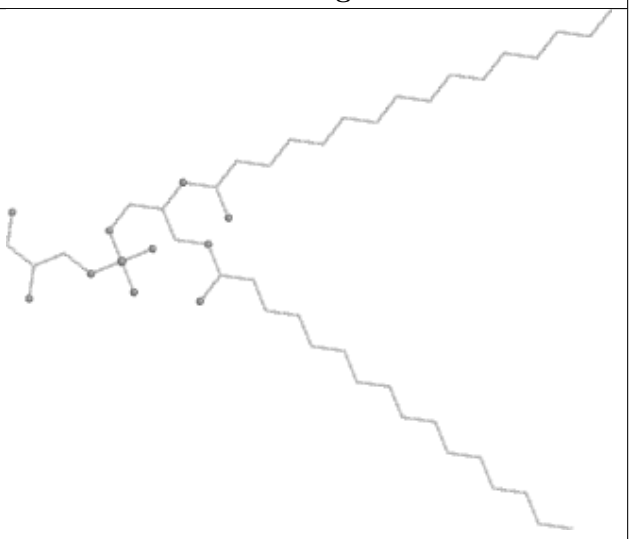
Bond lengths



Bond angles

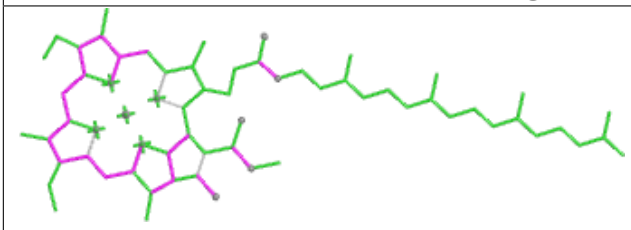


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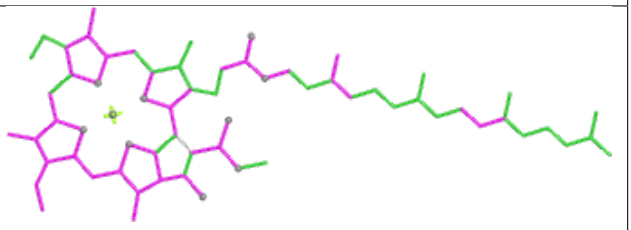


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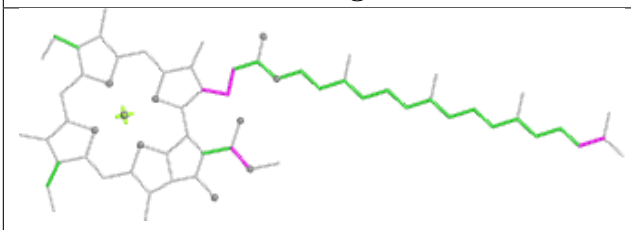
Ligand CLA C 502



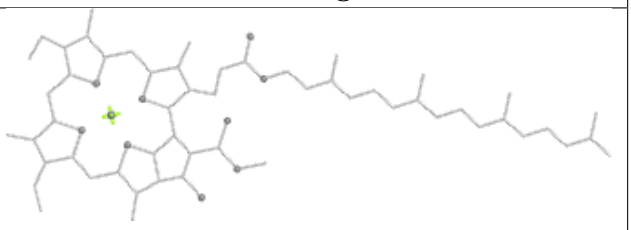
Bond lengths



Bond angles

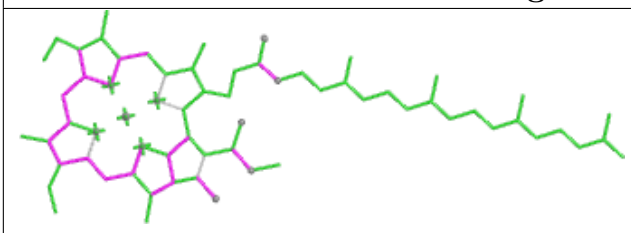


Torsions

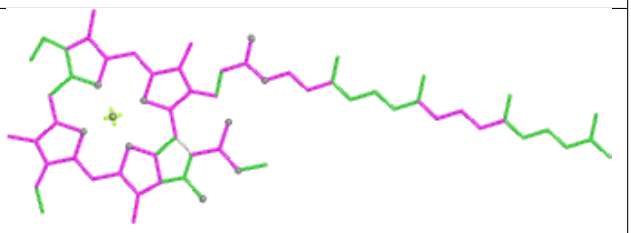


Rings

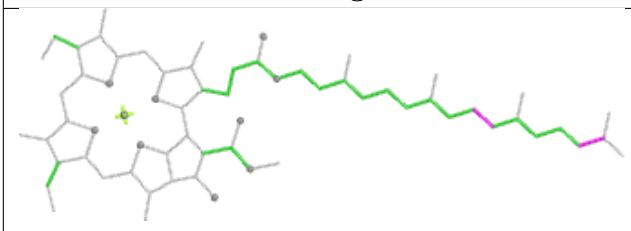
Ligand CLA b 602



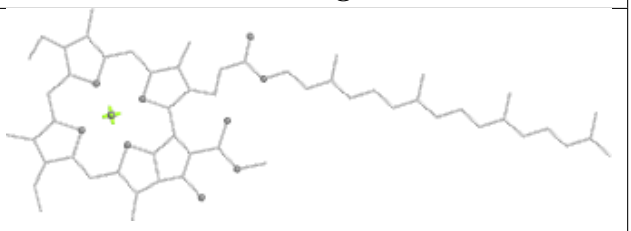
Bond lengths



Bond angles

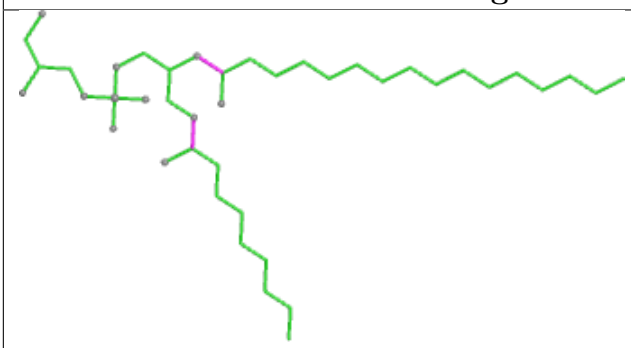


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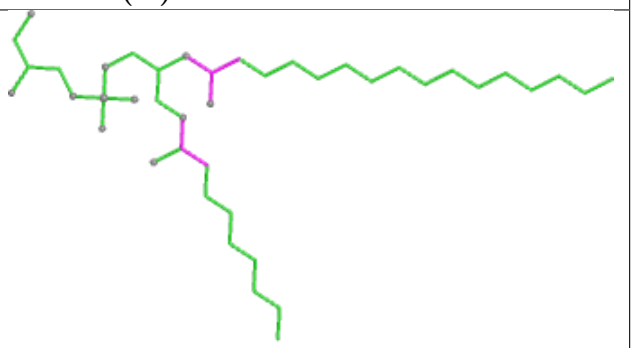


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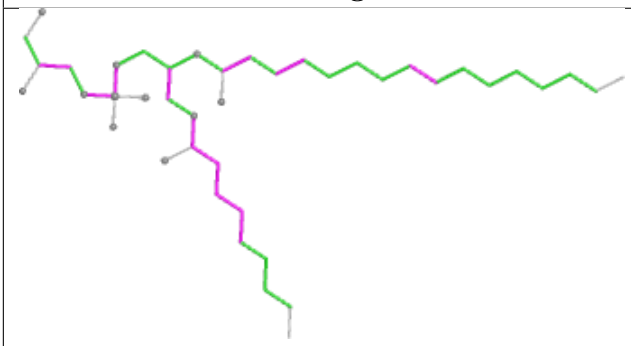
Ligand LHG E 101 (B)



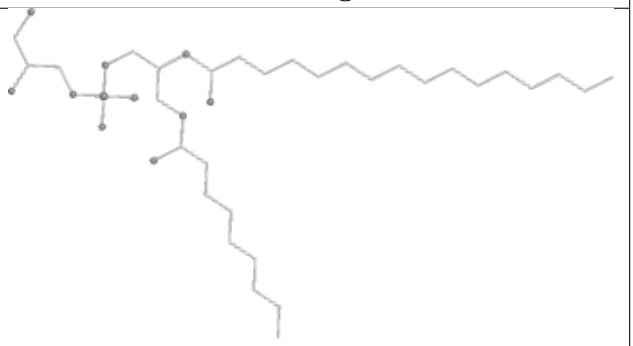
Bond lengths



Bond angles

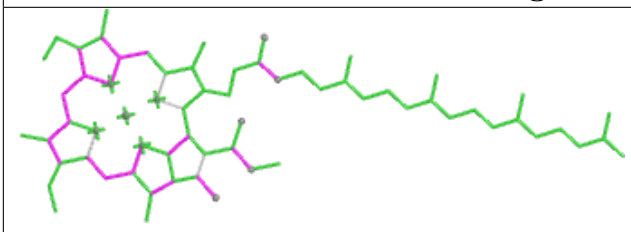


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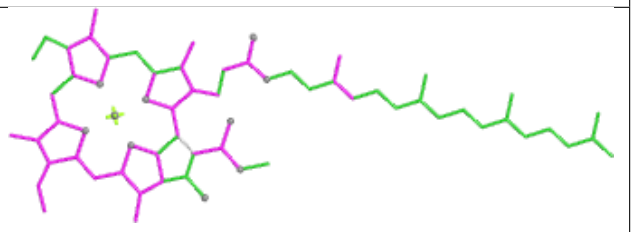


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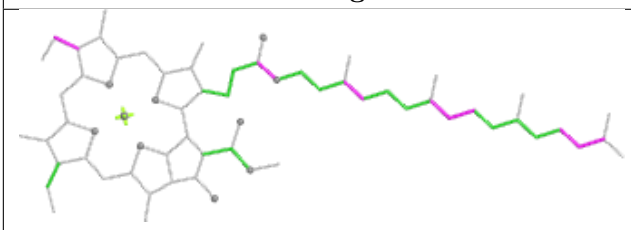
Ligand CLA a 409



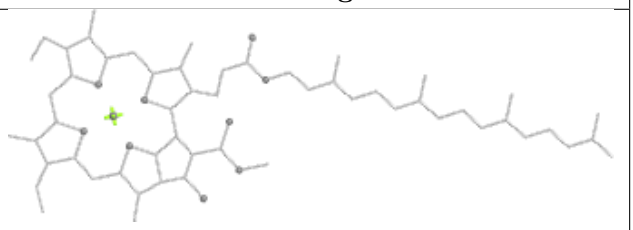
Bond lengths



Bond angles

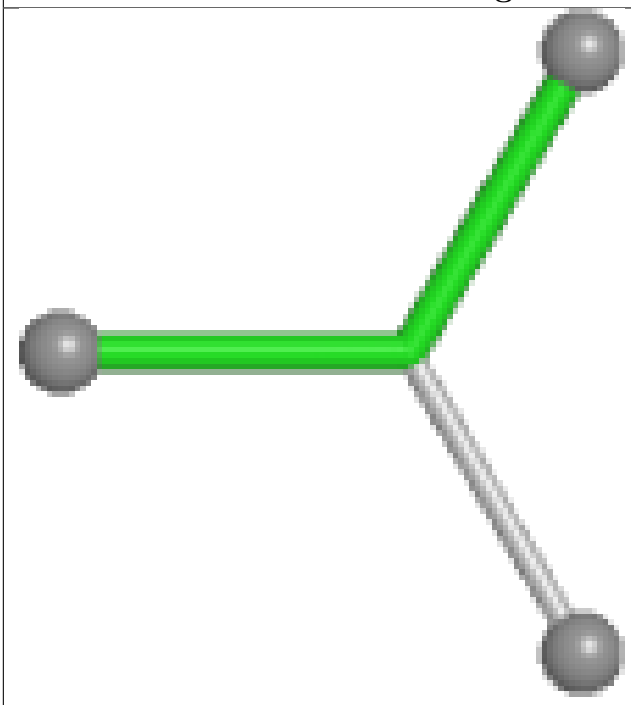


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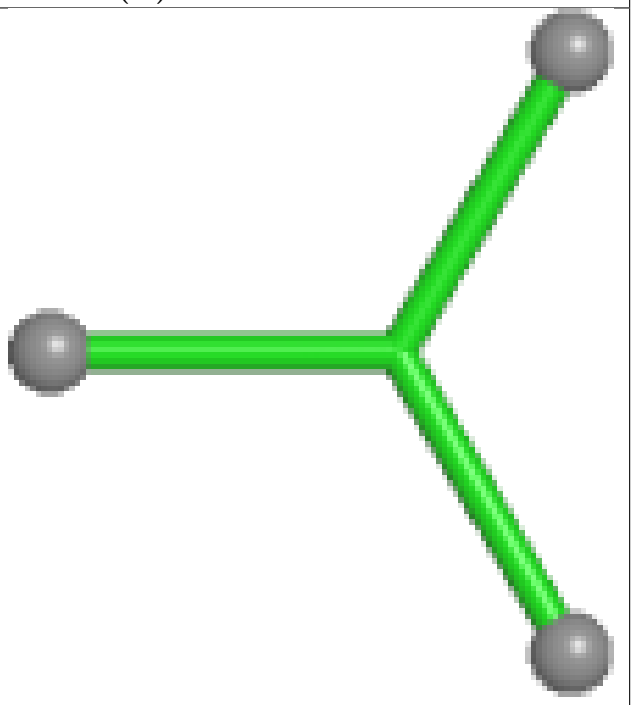


Rings

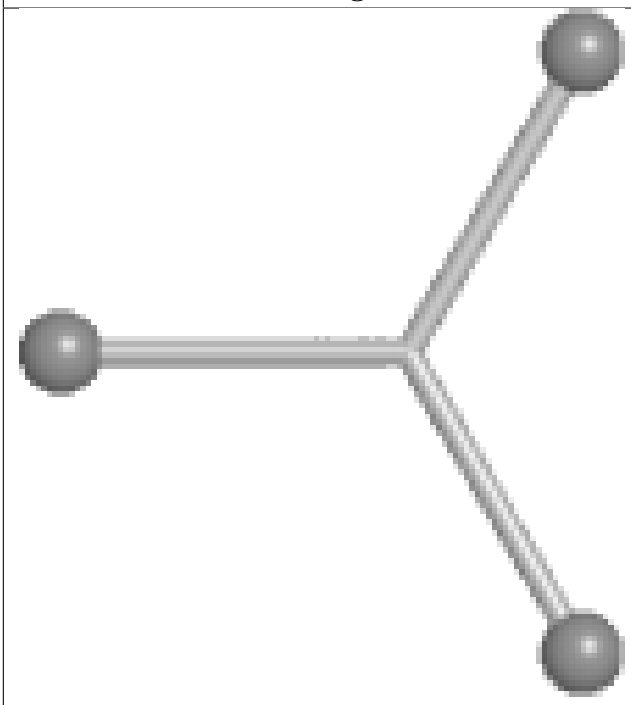
Ligand BCT a 404 (B)



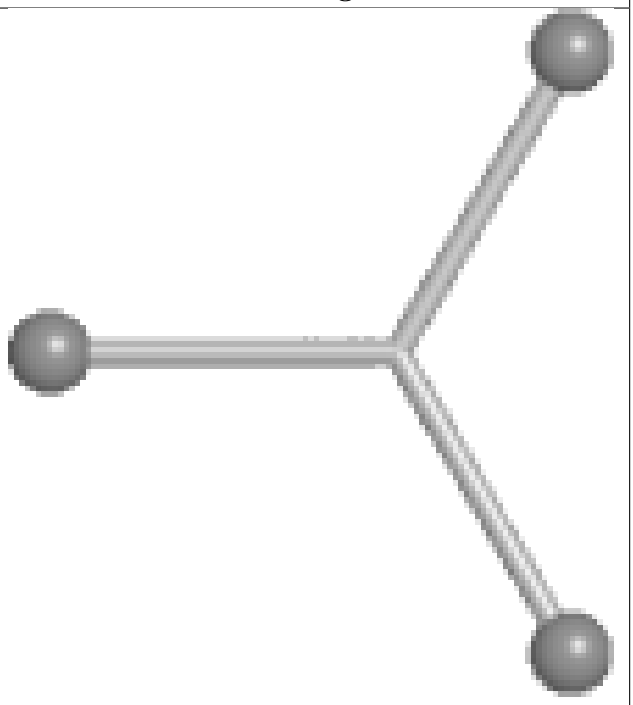
Bond lengths



Bond angles

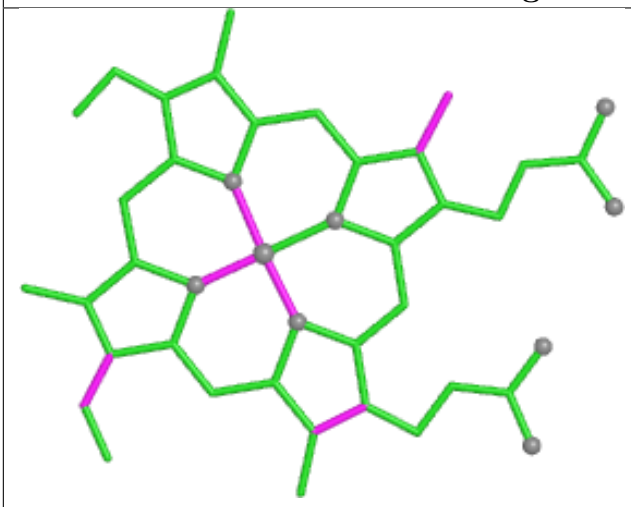


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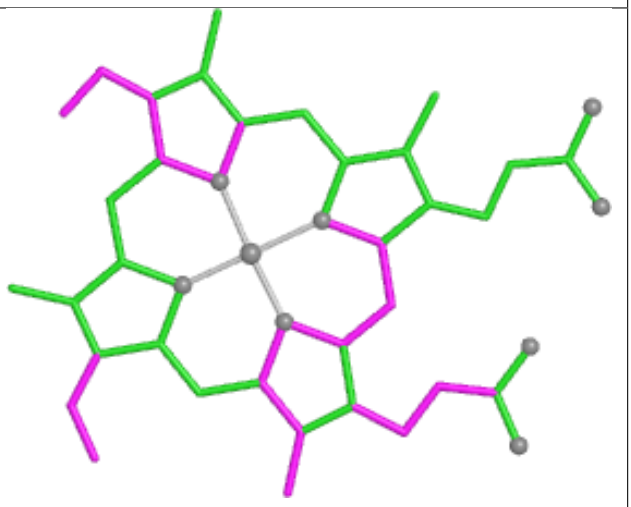


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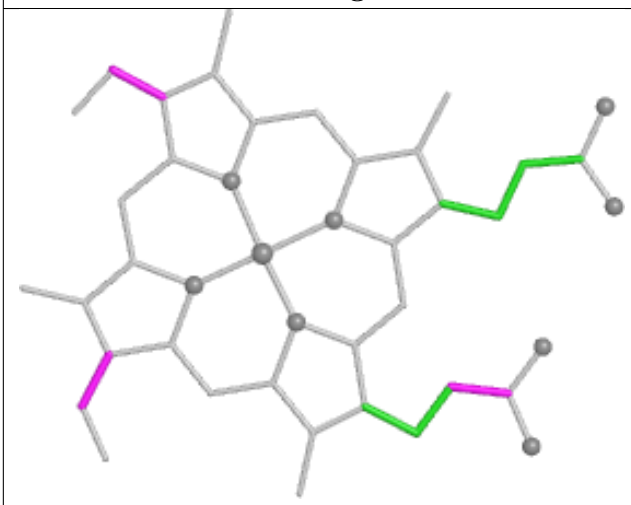
Ligand HEC V 202



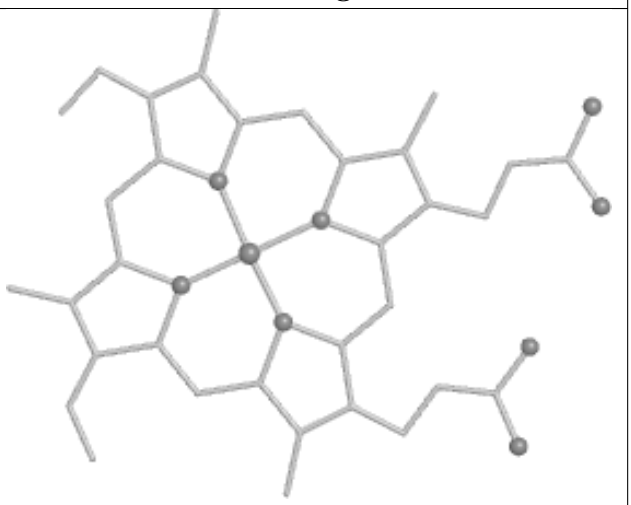
Bond lengths



Bond angles

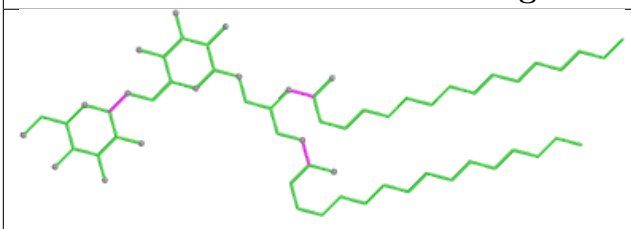


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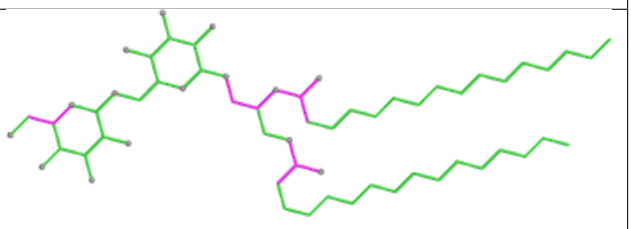


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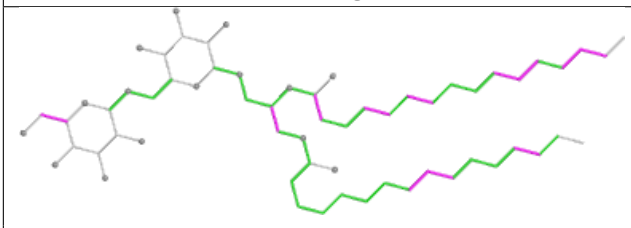
Ligand DGD H 102



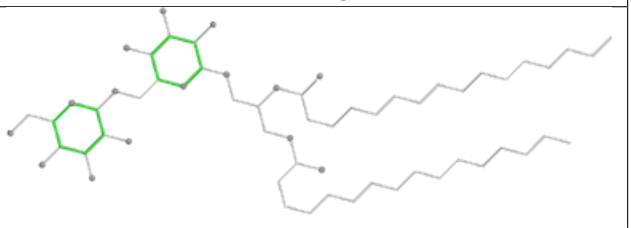
Bond lengths



Bond angles

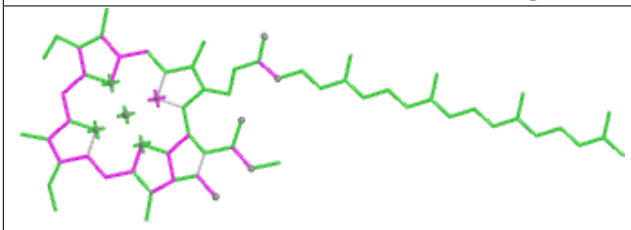


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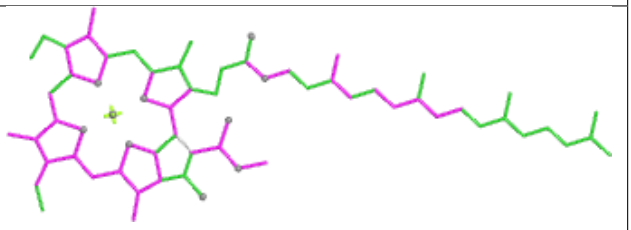


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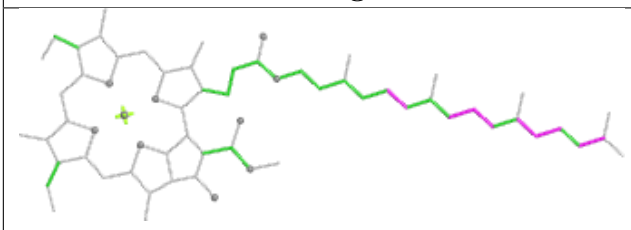
Ligand CLA B 615



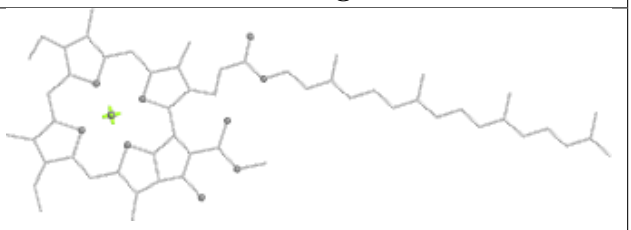
Bond lengths



Bond angles



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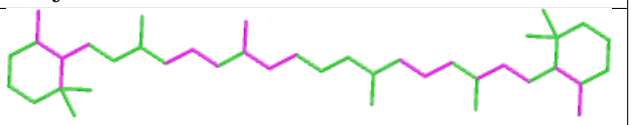


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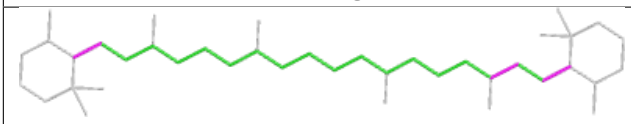
Ligand BCR y 101



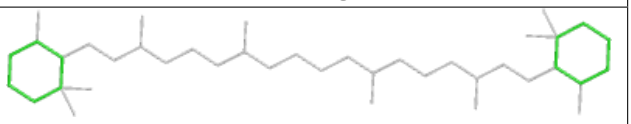
Bond lengths



Bond angles

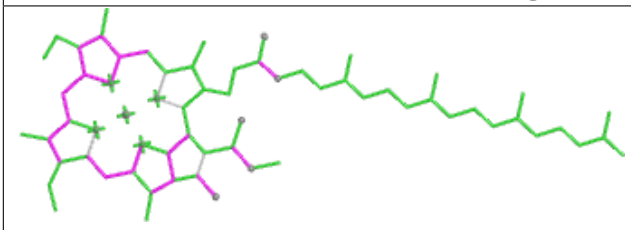


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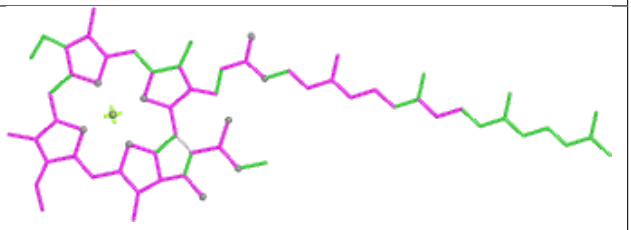


Rings

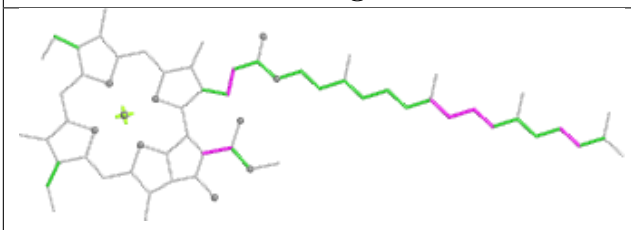
Ligand CLA B 606



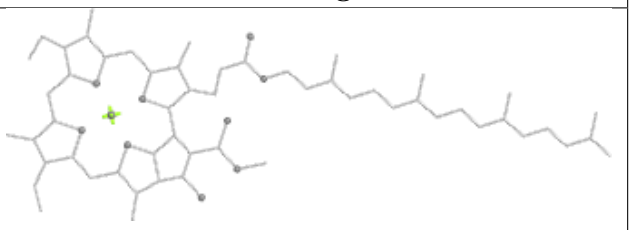
Bond lengths



Bond angles

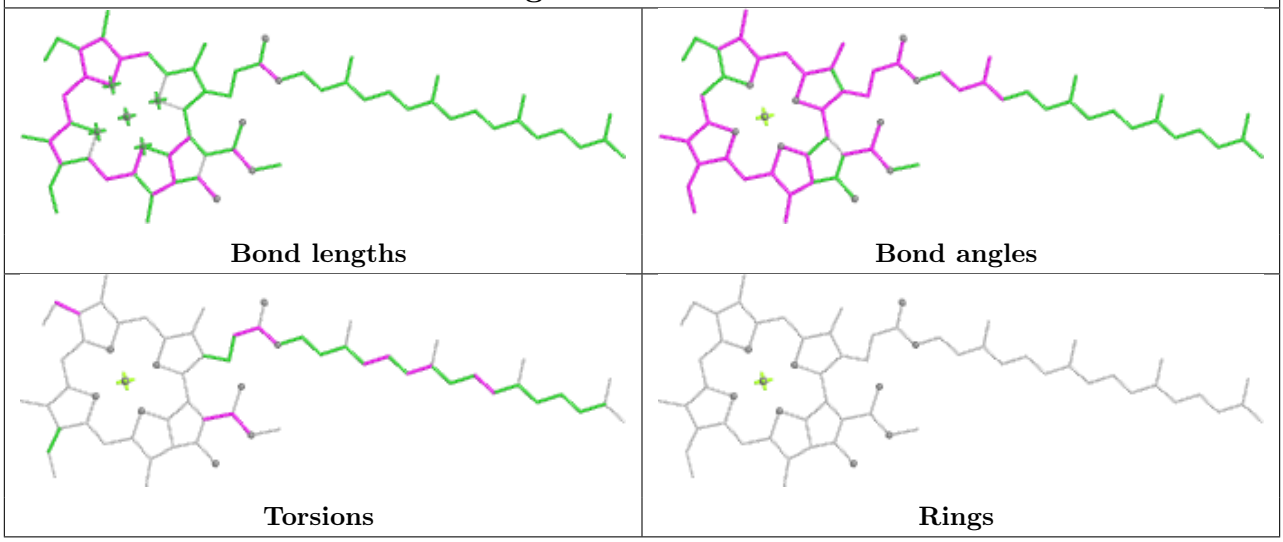


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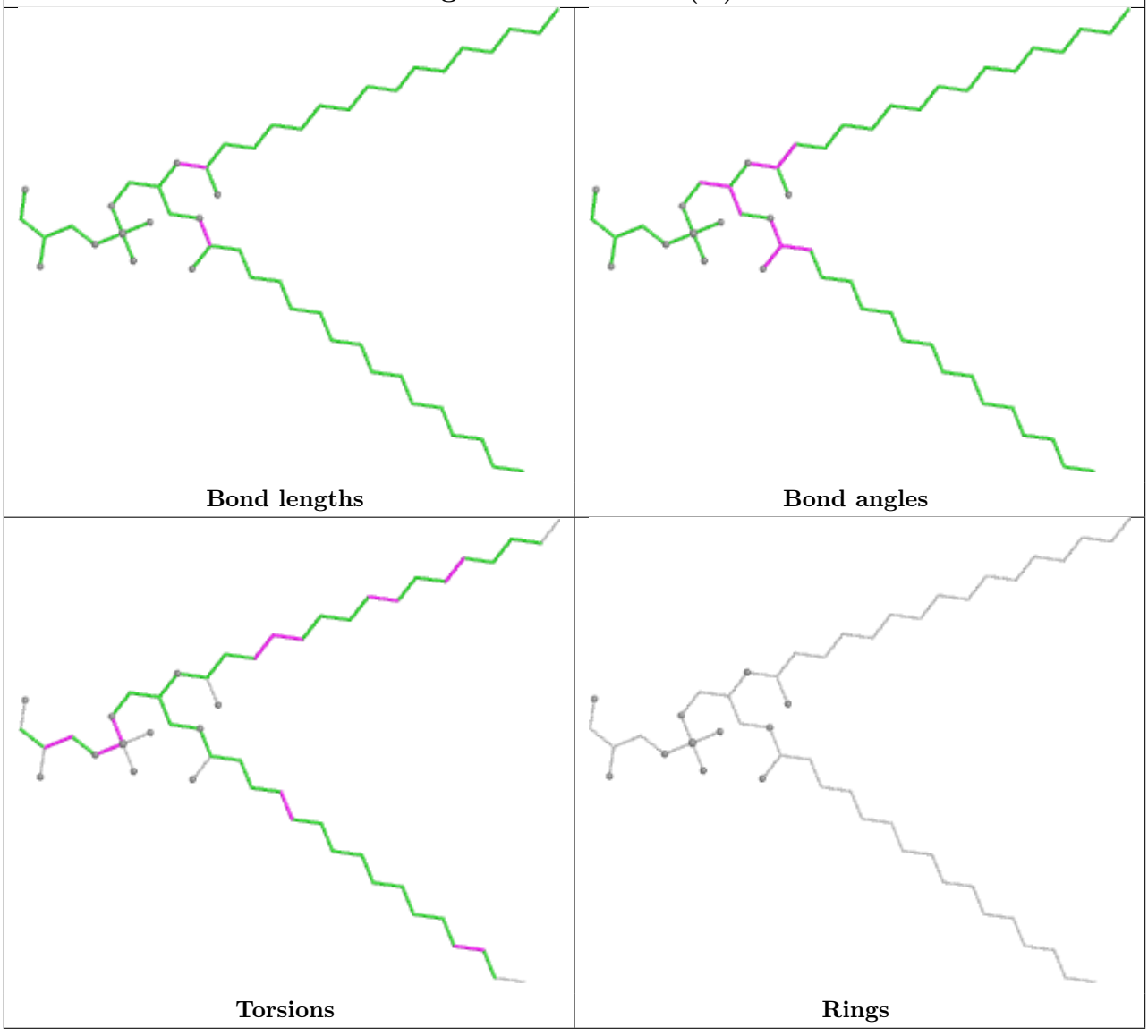


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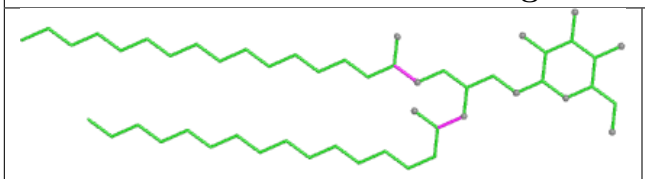
Ligand CLA C 513



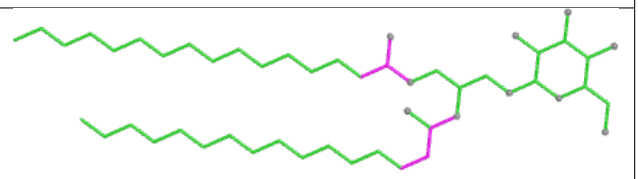
Ligand LHG d 407 (A)



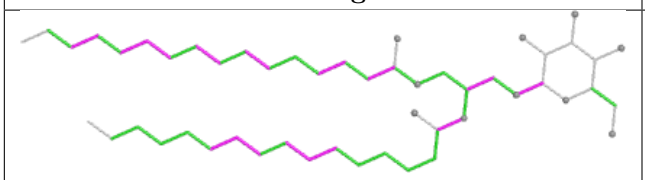
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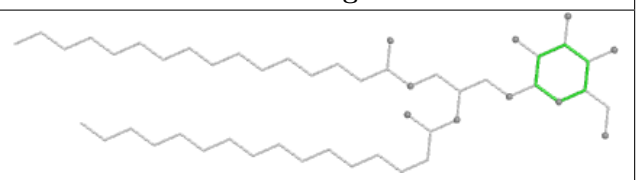
Bond lengths



Bond angles

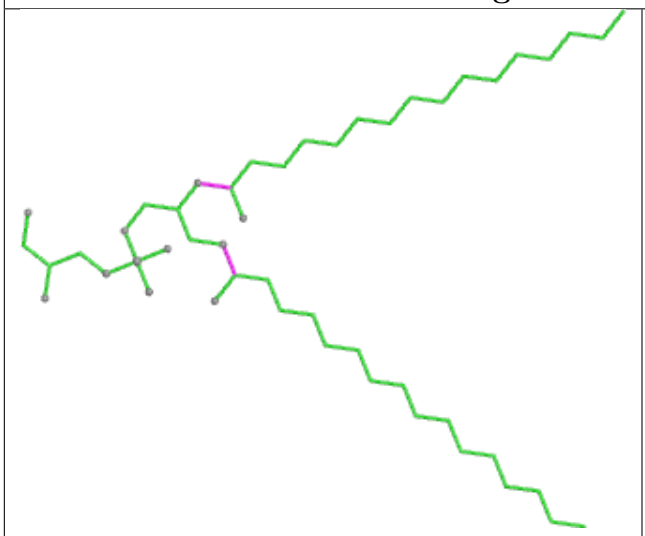


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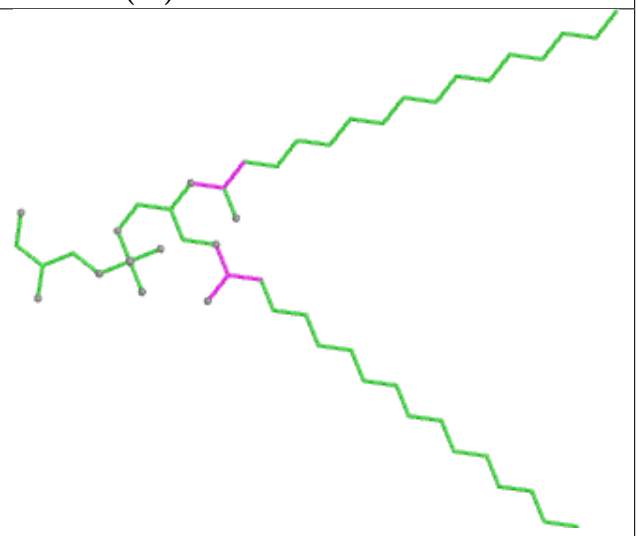


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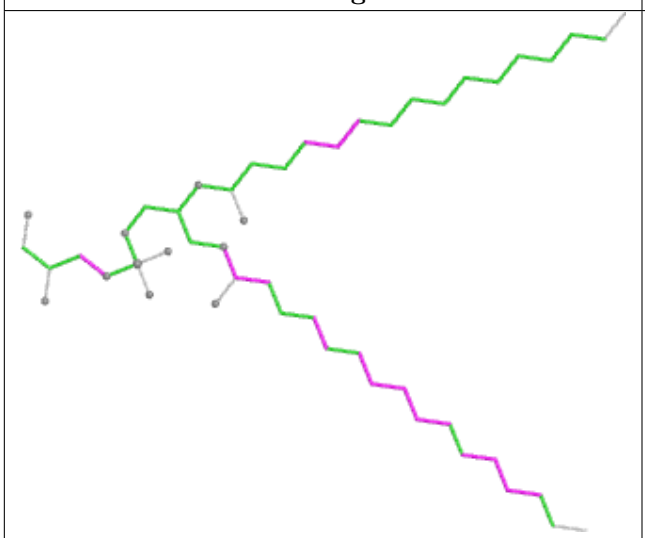
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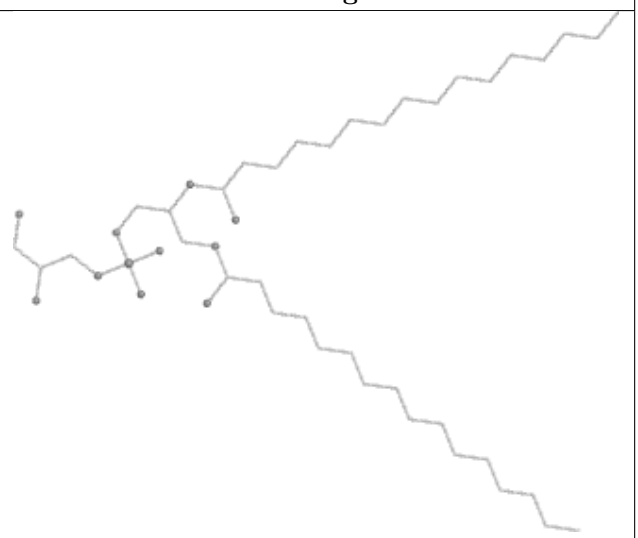
Bond lengths



Bond angles

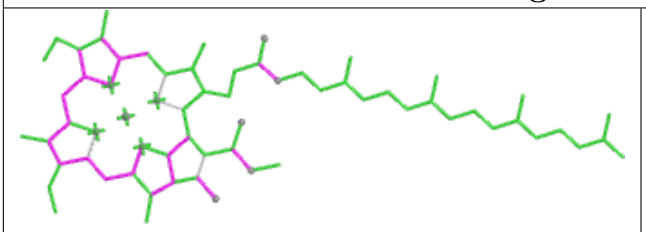


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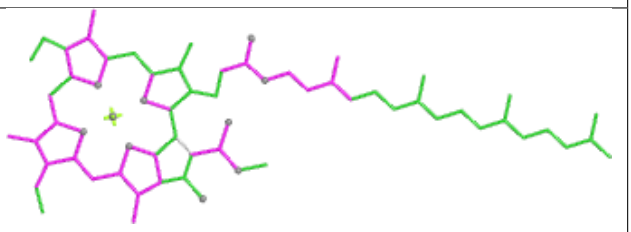


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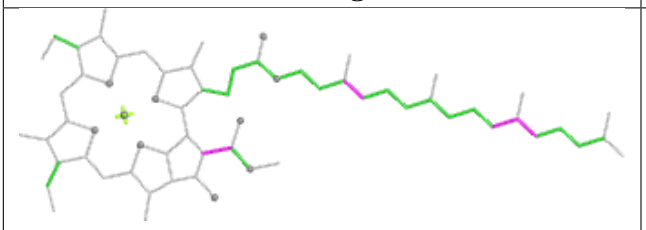
Ligand CLA c 506



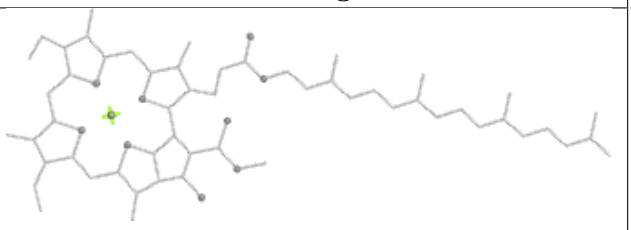
Bond lengths



Bond angles

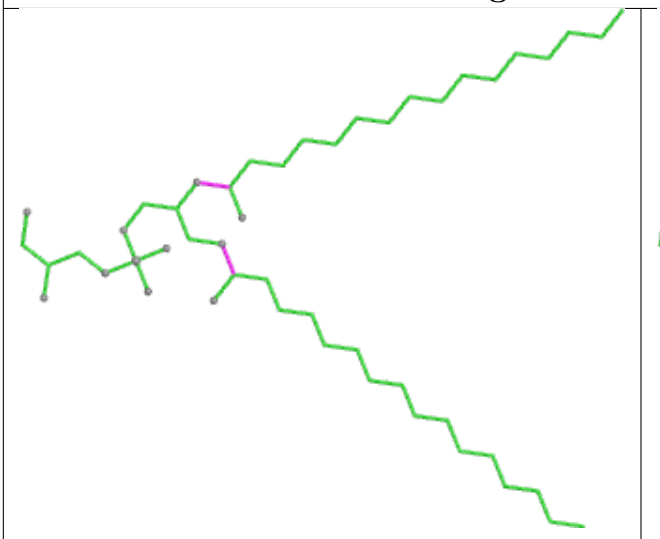


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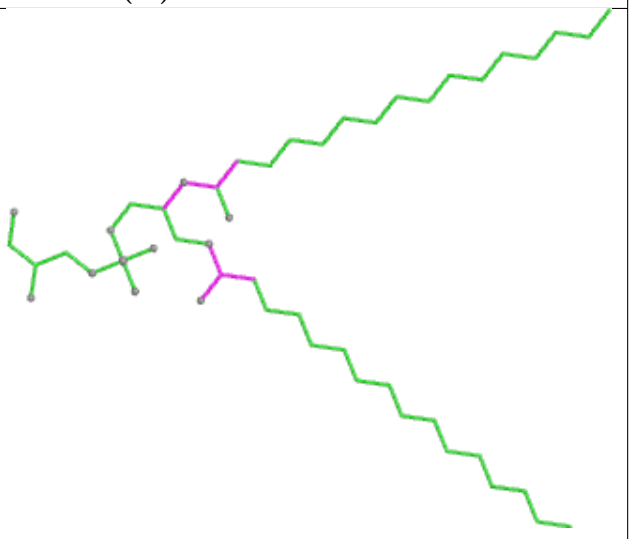


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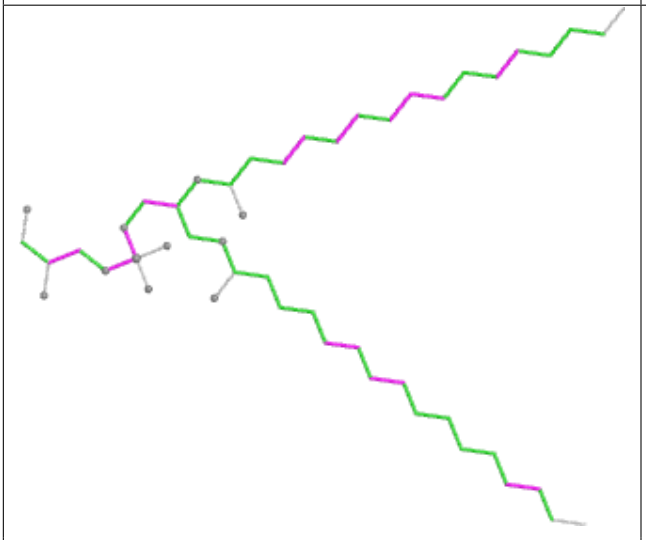
Ligand LHG D 410 (B)



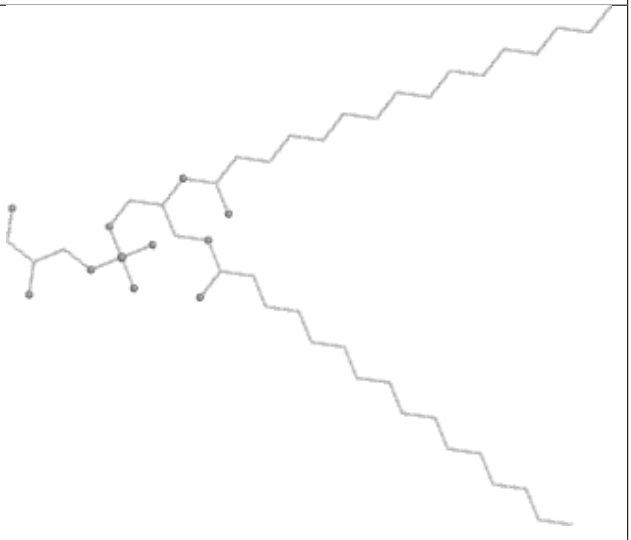
Bond lengths



Bond angles

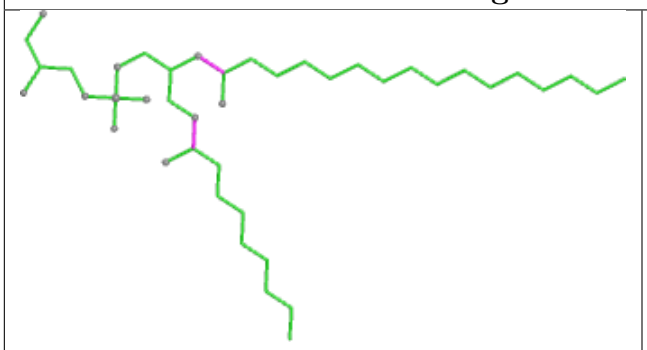


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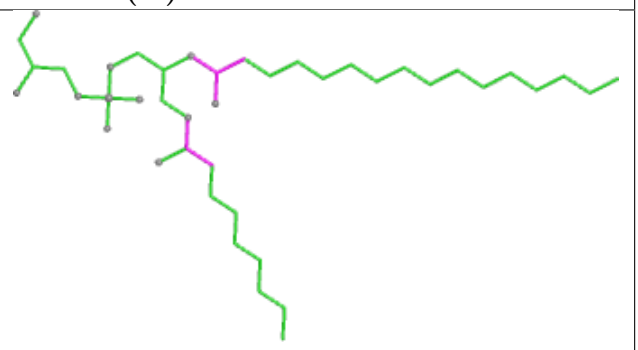


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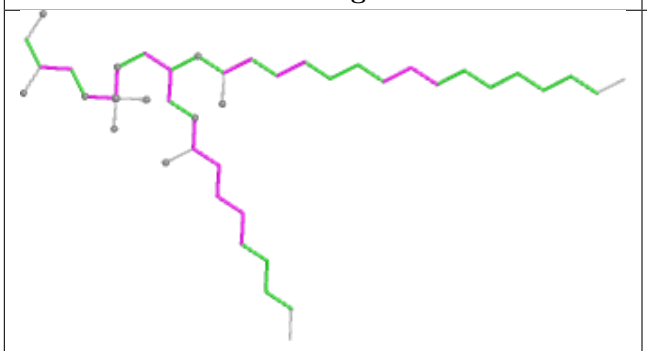
Ligand LHG E 101 (A)



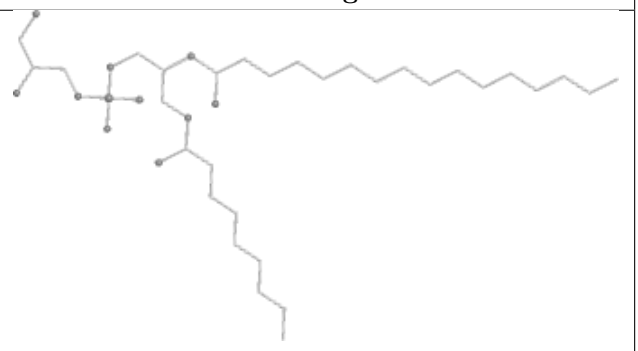
Bond lengths



Bond angles

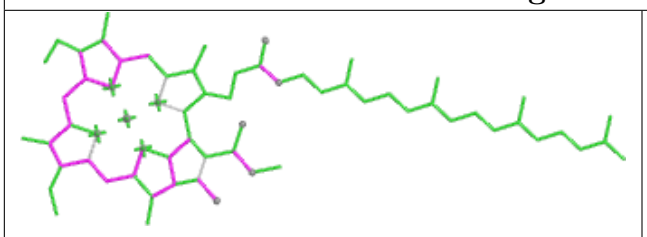


Torsions

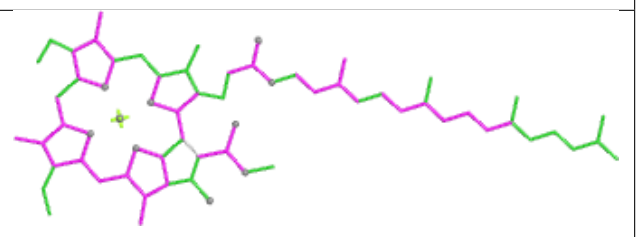


Rings

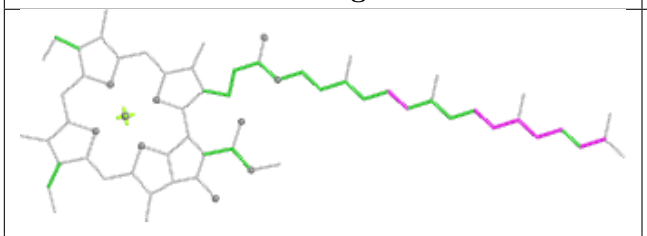
Ligand CLA b 615



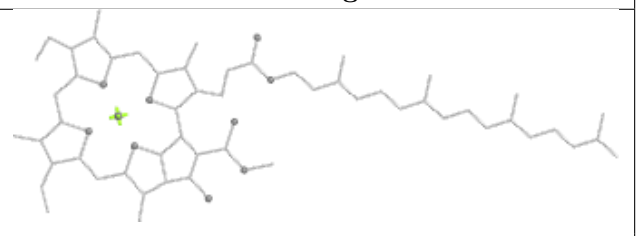
Bond lengths



Bond angles

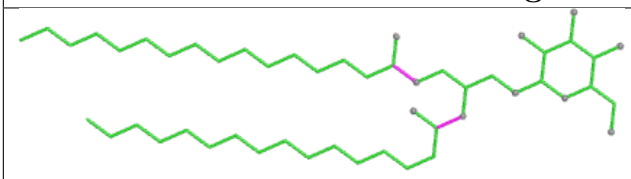


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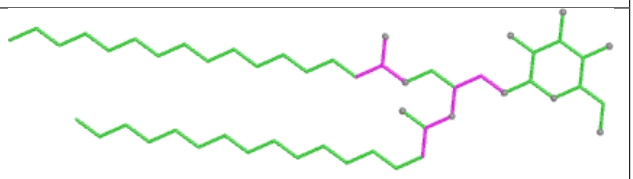


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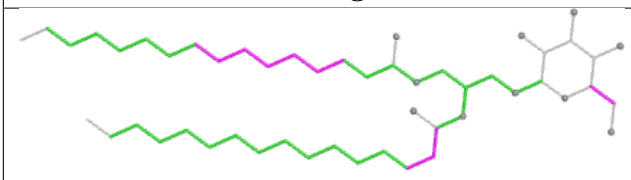
Ligand LMG c 520



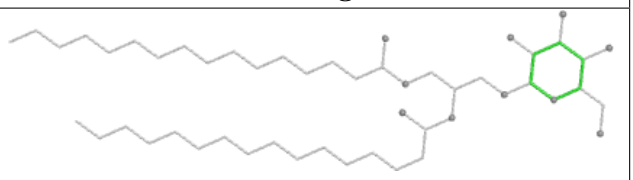
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Bond angles

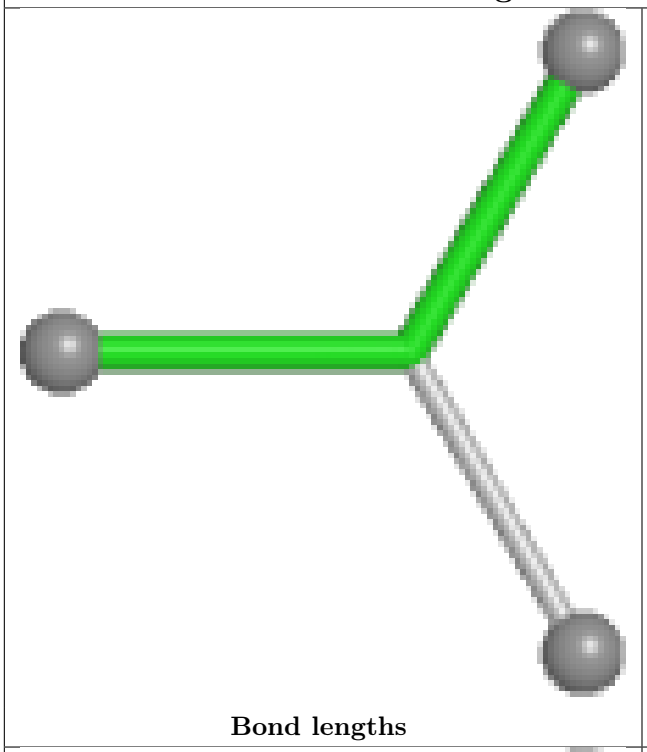


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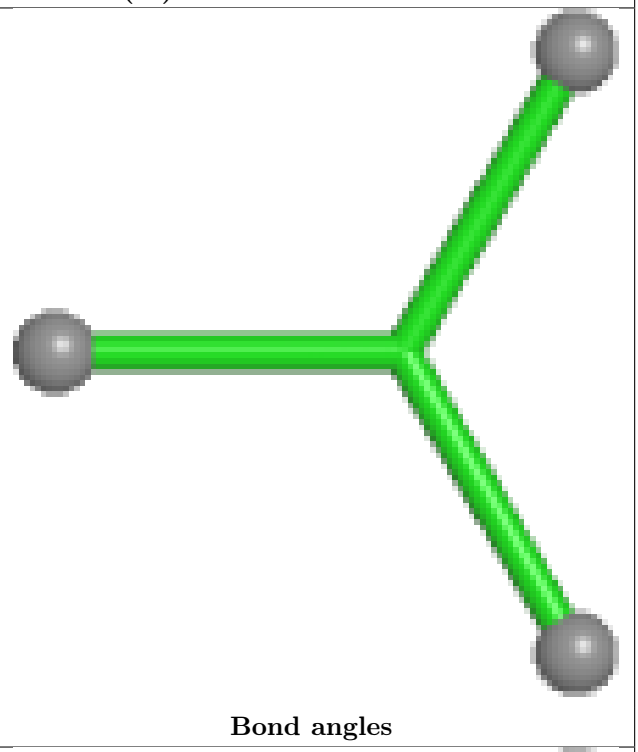


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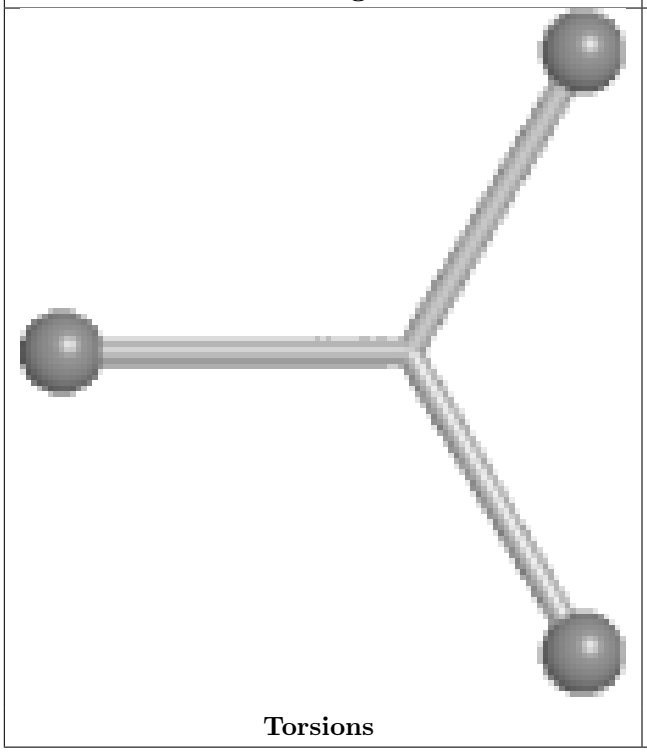
Ligand BCT a 404 (A)



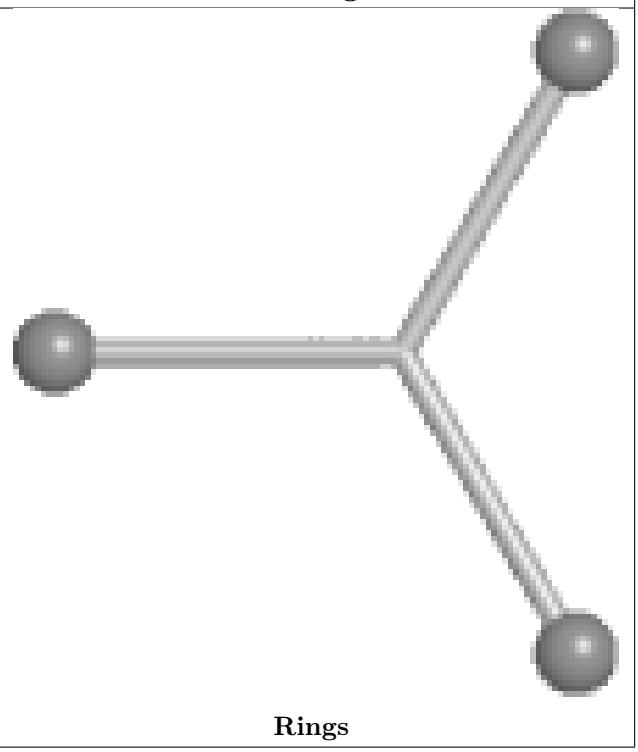
Bond lengths



Bond angles

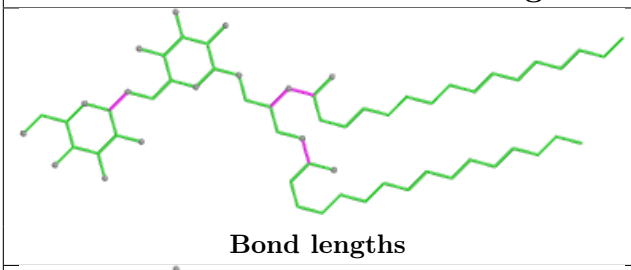


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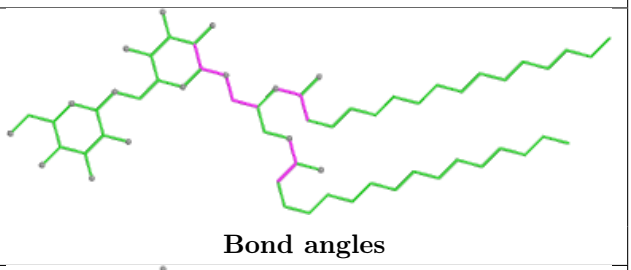


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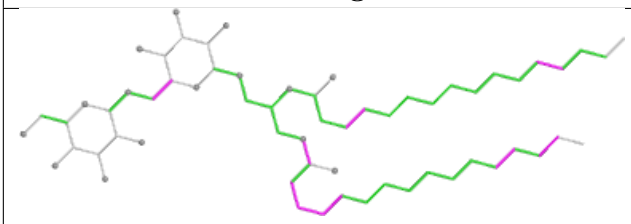
Ligand DGD c 519



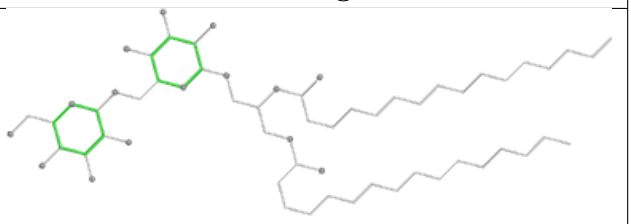
Bond lengths



Bond angles

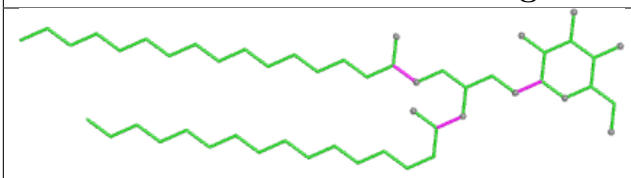


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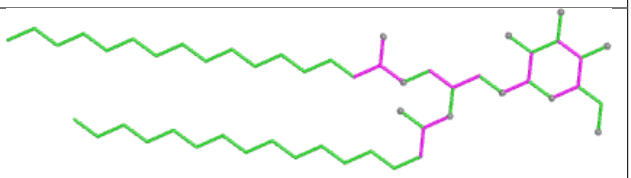


Rings

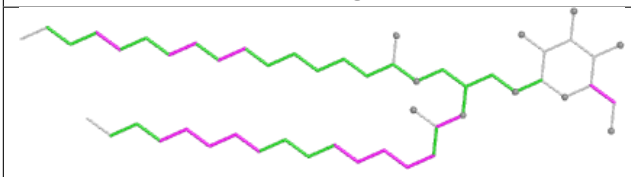
Ligand LMG C 521



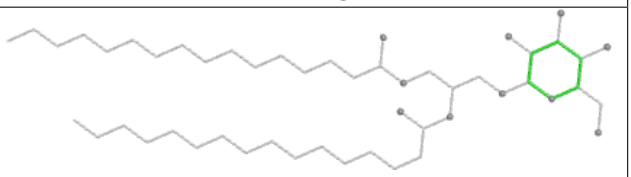
Bond lengths



Bond angles

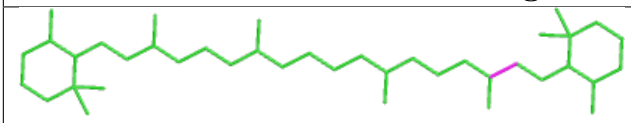


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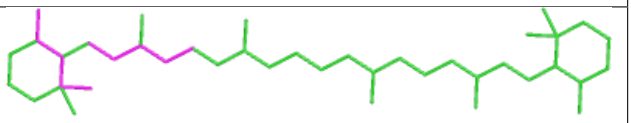


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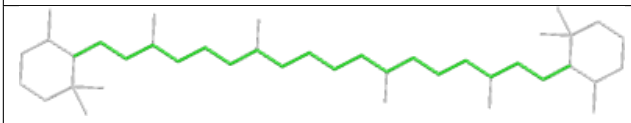
Ligand BCR C 516



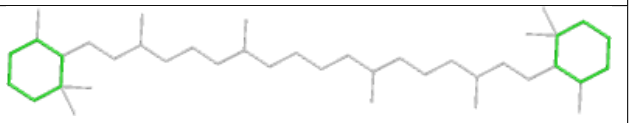
Bond lengths



Bond angles

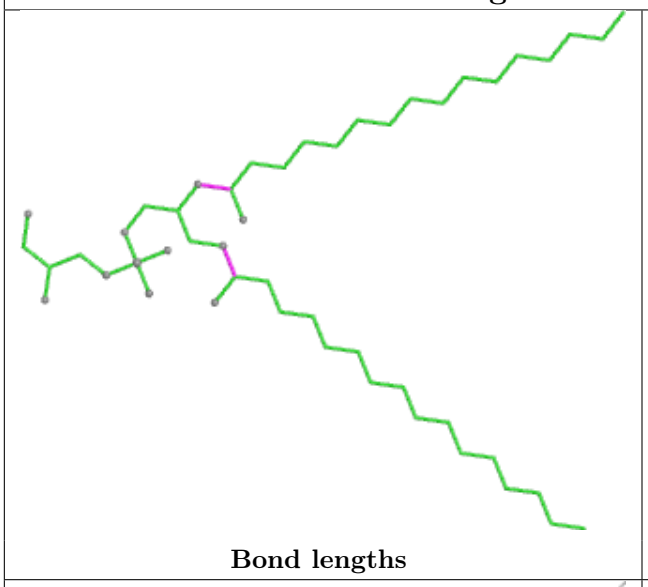


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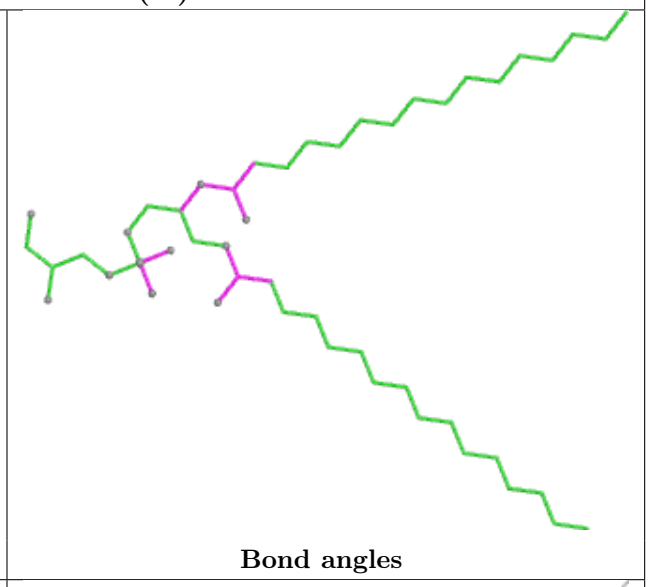


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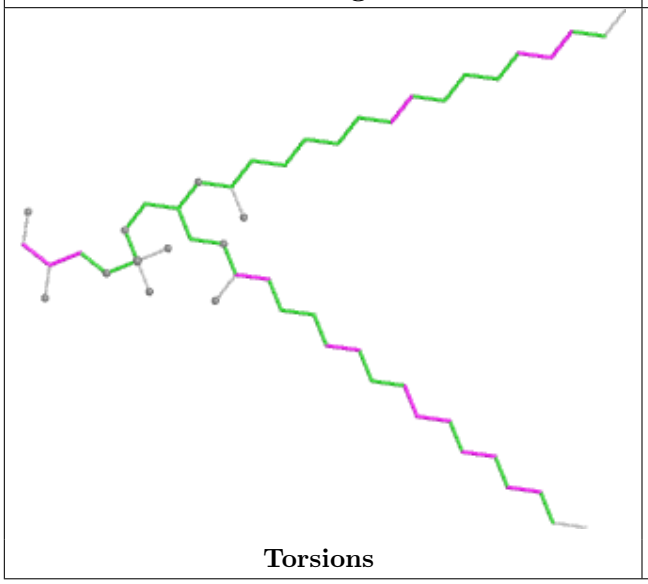
Ligand LHG D 409 (A)



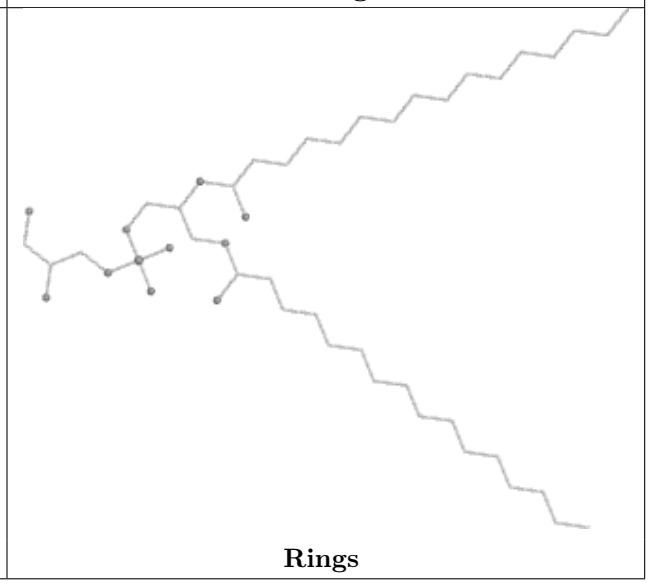
Bond lengths



Bond angles

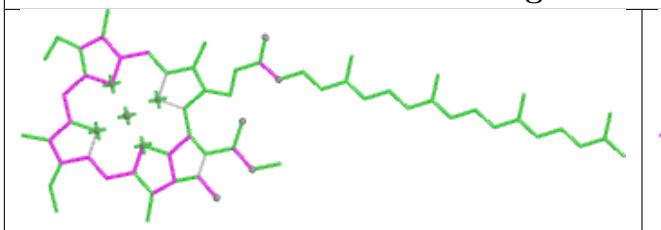


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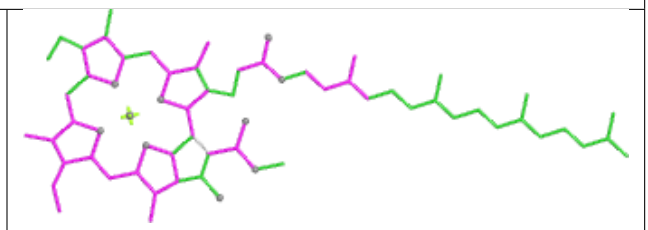


Rings

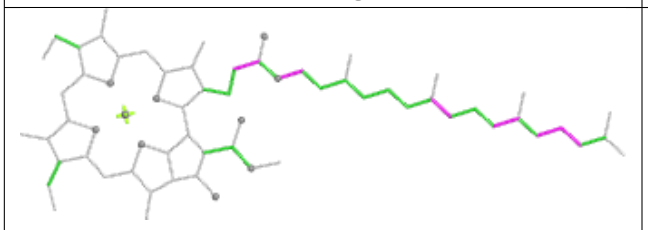
Ligand CLA B 613



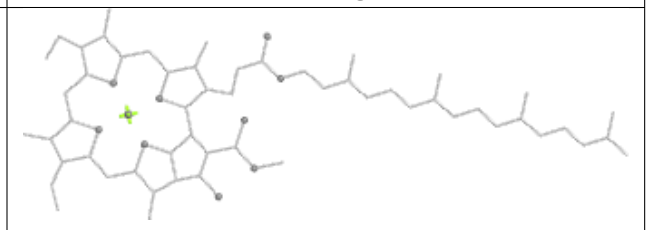
Bond lengths



Bond angles

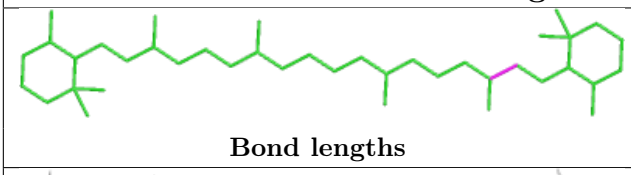


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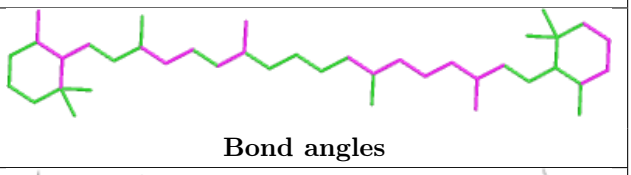


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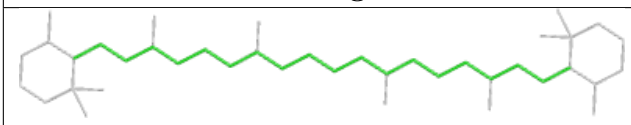
Ligand BCR t 103



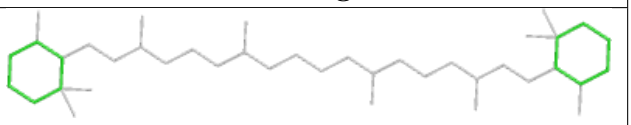
Bond lengths



Bond angles

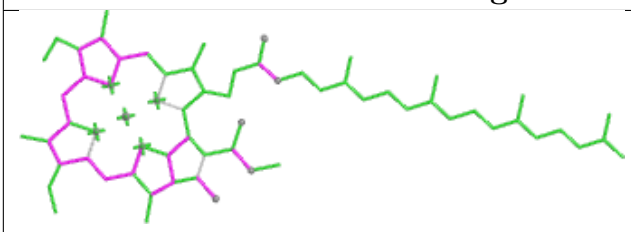


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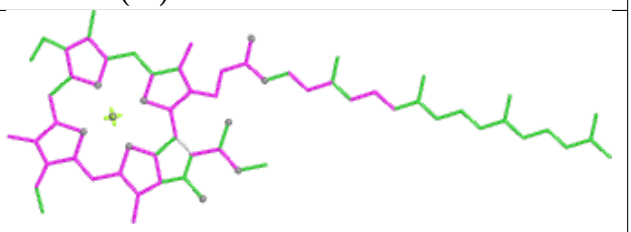


Rings

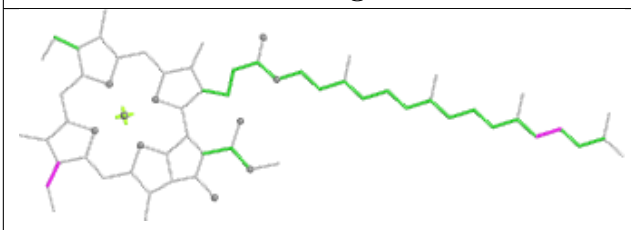
Ligand CLA A 404 (A)



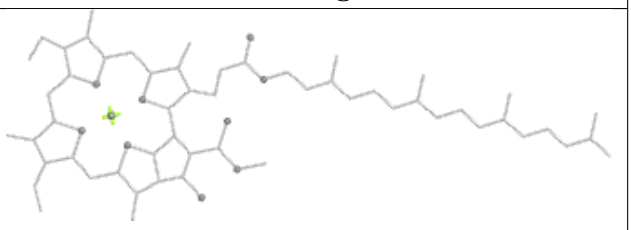
Bond lengths



Bond angles

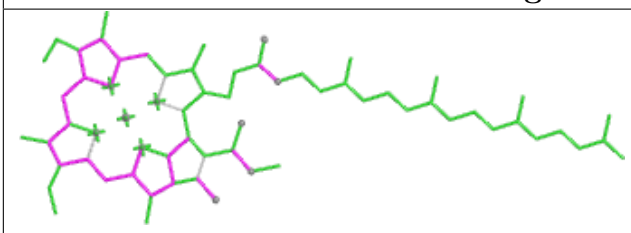


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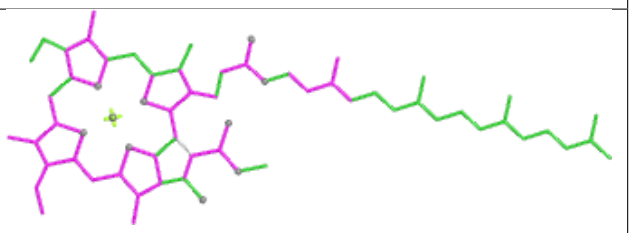


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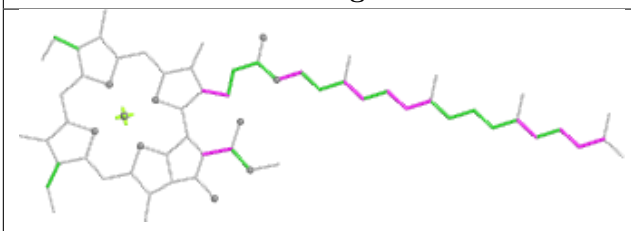
Ligand CLA C 507



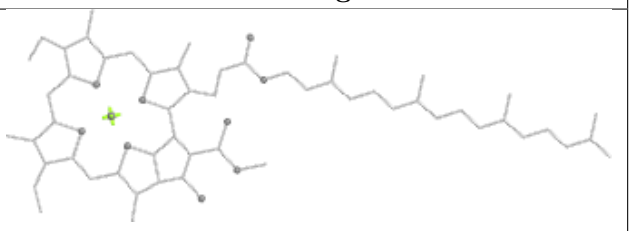
Bond lengths



Bond angles

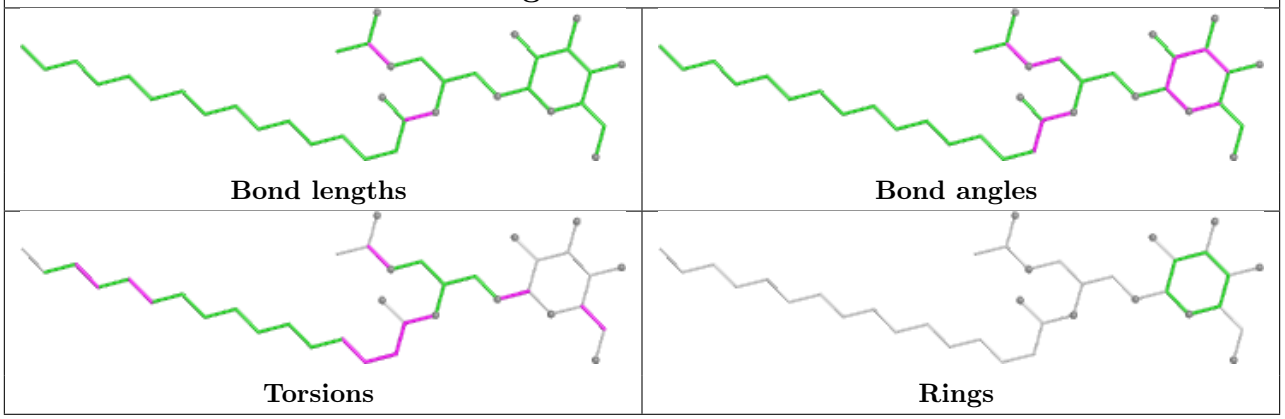


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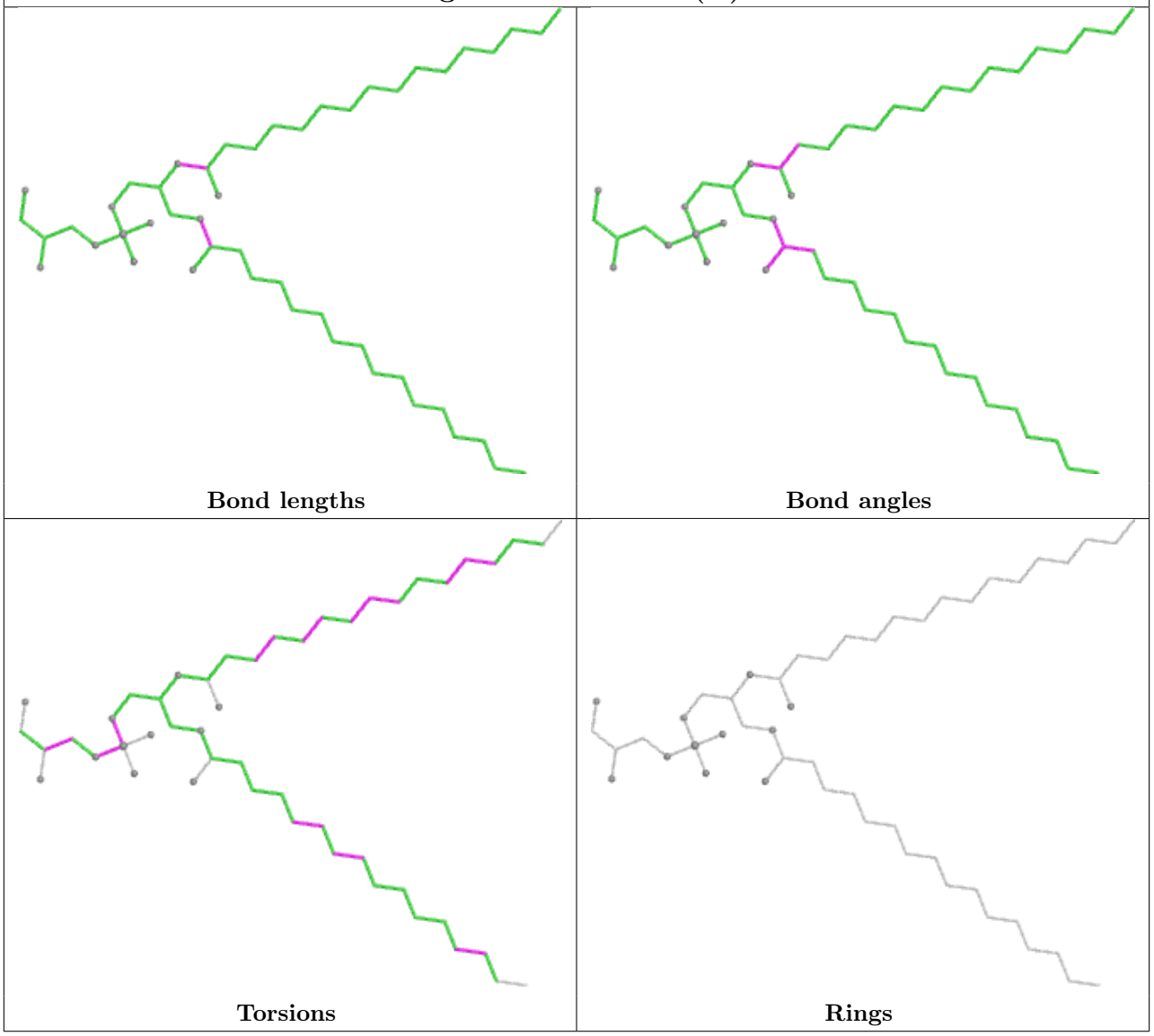


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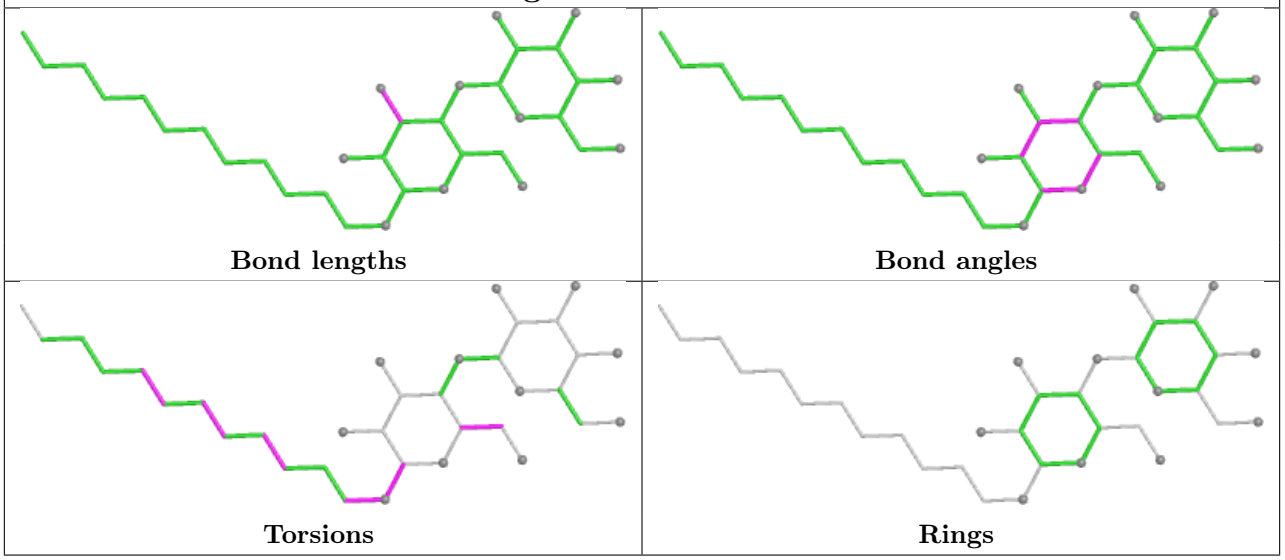
Ligand LMG Z 101



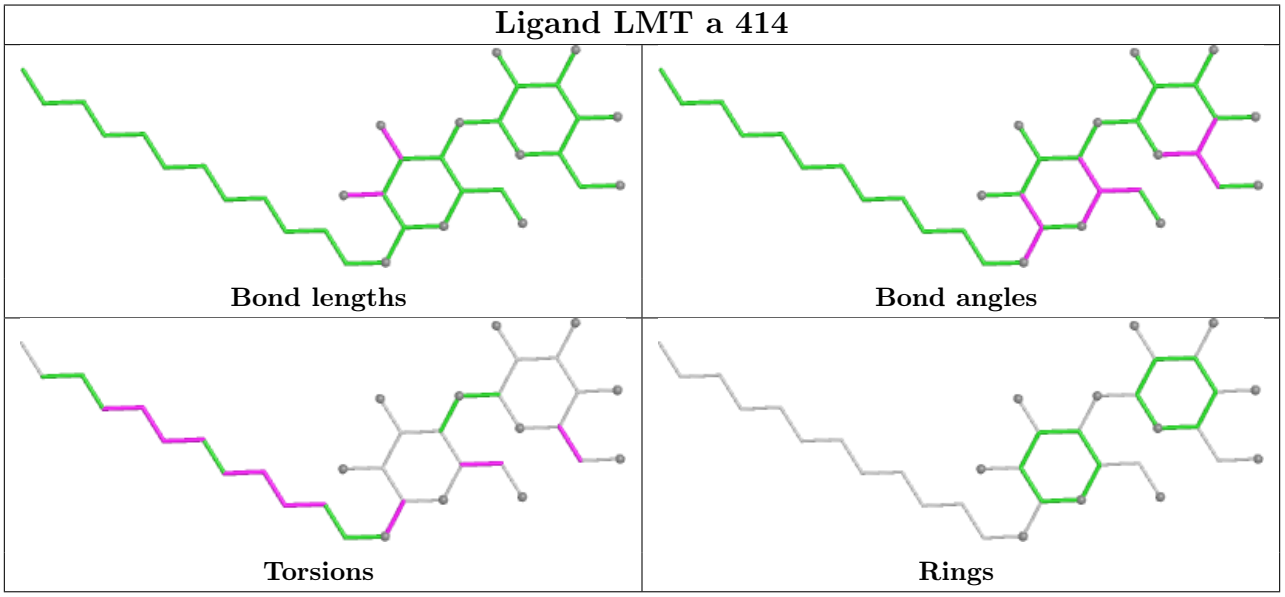
Ligand LHG D 410 (A)



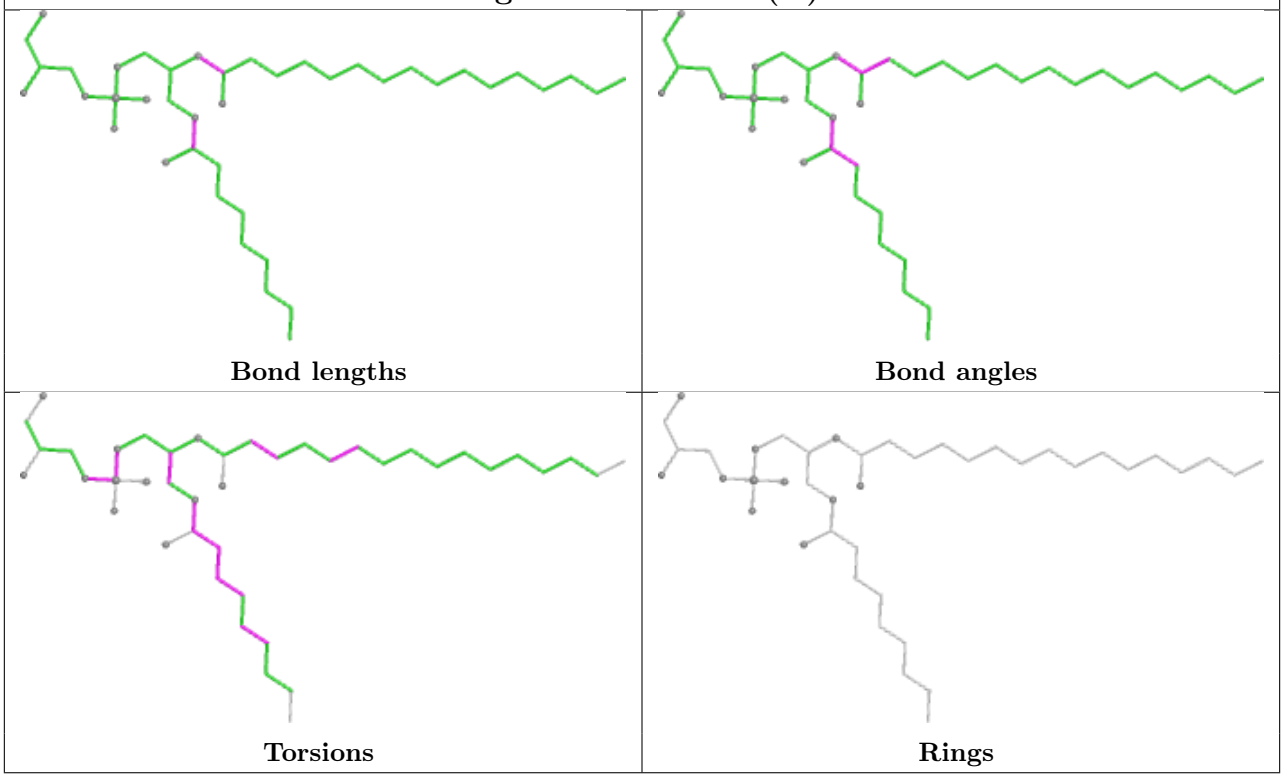
Ligand LMT E 102



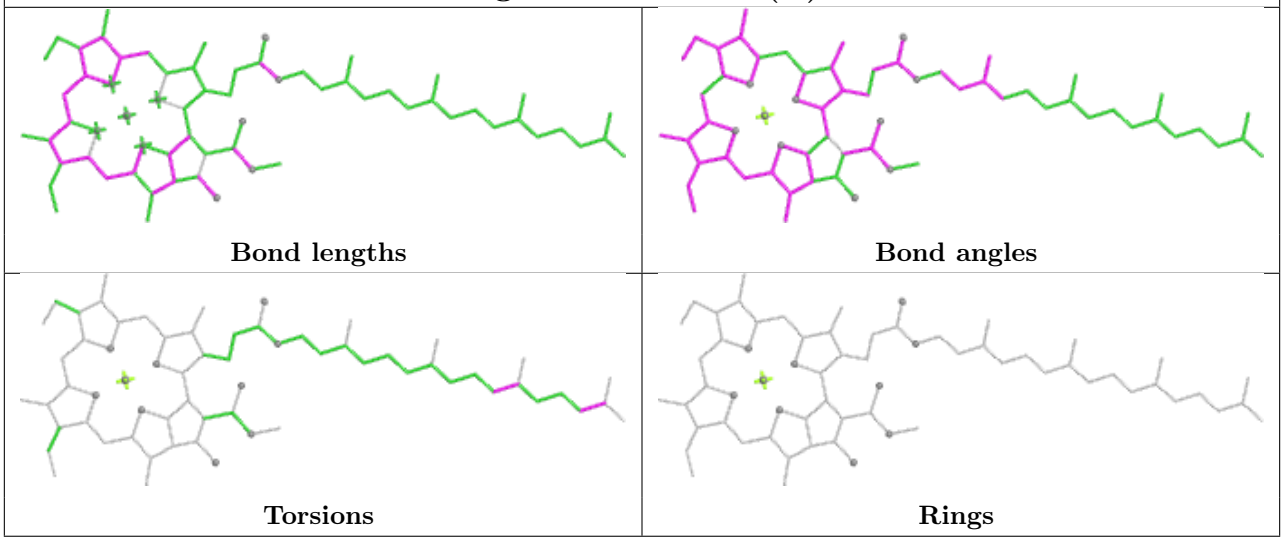
Ligand LMT a 414



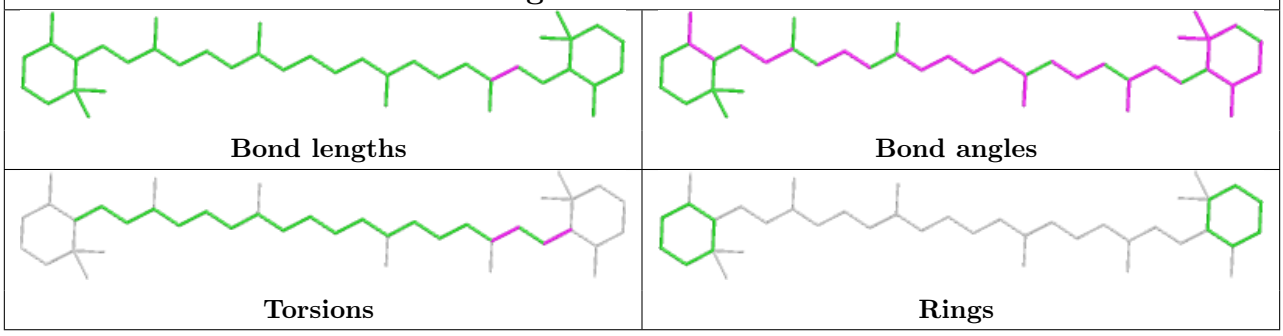
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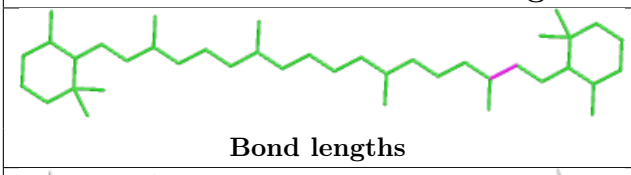
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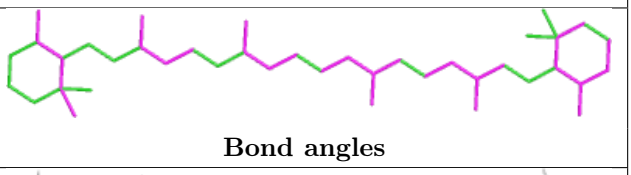


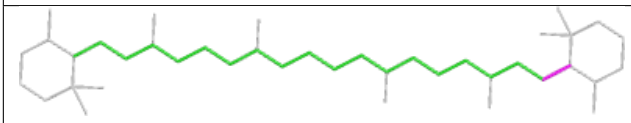
Ligand BCR d 404

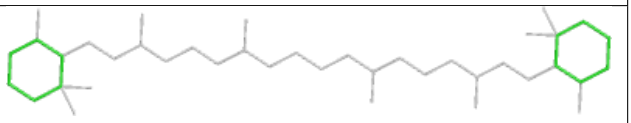


Ligand BCR c 515


Bond lengths

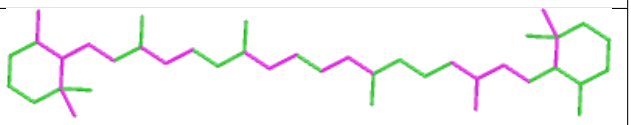

Bond angles

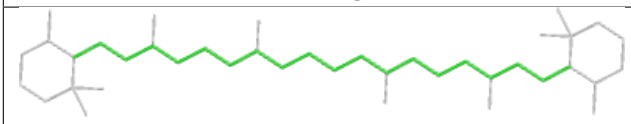

Torsions

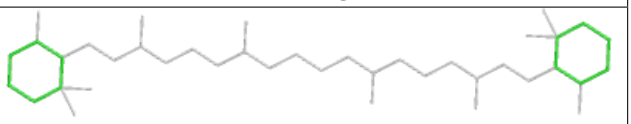

Rings

Ligand BCR A 409

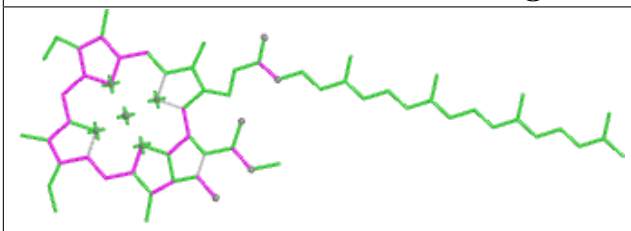

Bond lengths

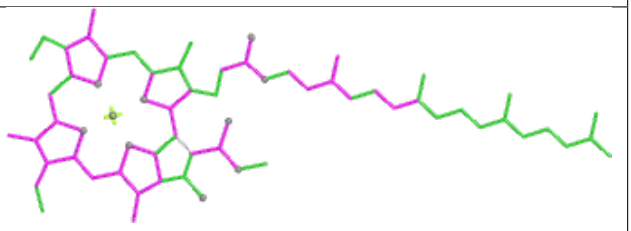

Bond angles

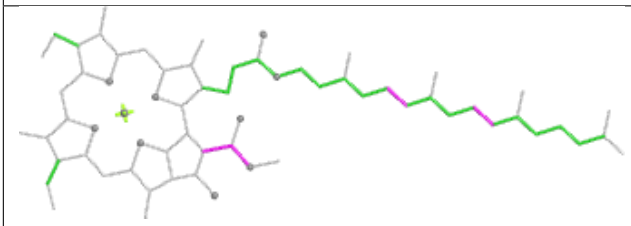

Torsions

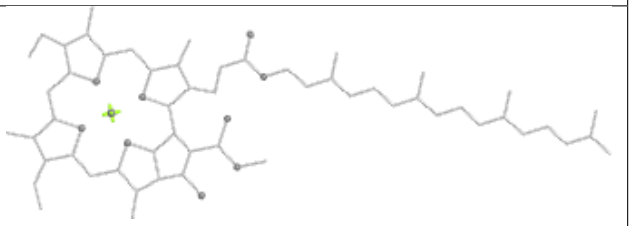

Rings

Ligand CLA C 509

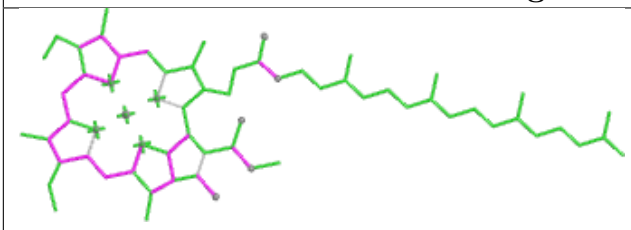

Bond lengths


Bond angles

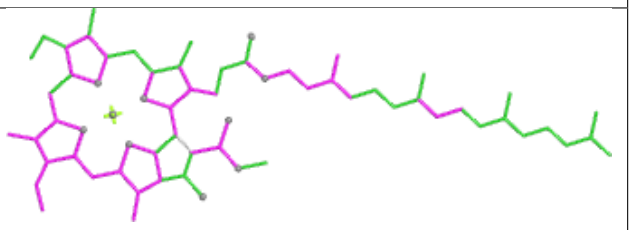

Torsions


Rings

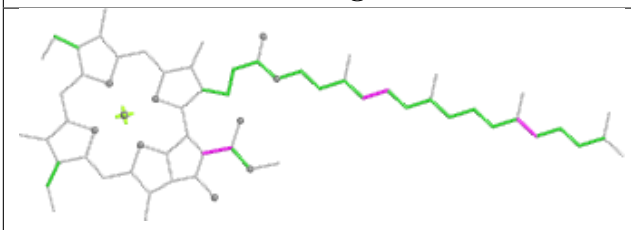
Ligand CLA b 607



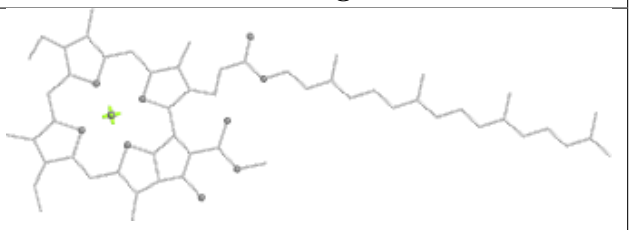
Bond lengths



Bond angles

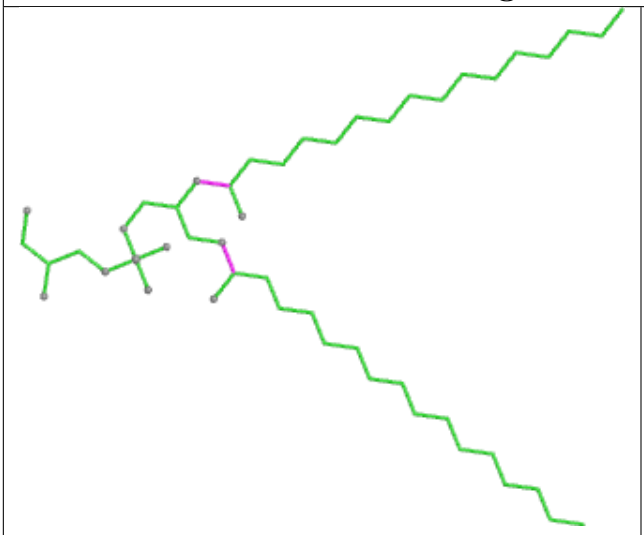


Torsions

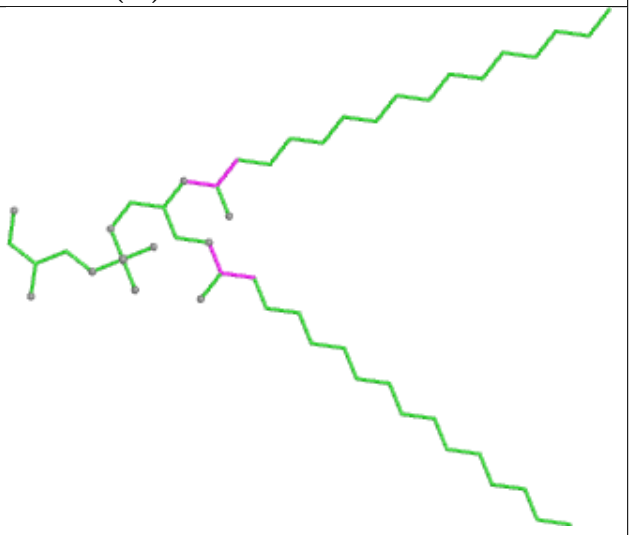


Rings

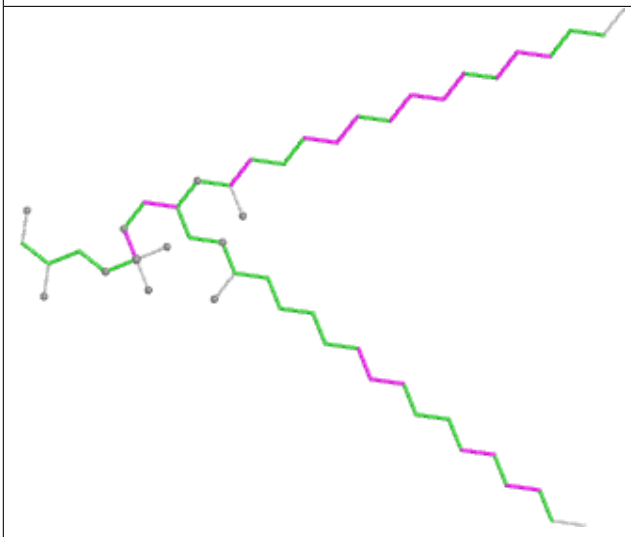
Ligand LHG l 101 (B)



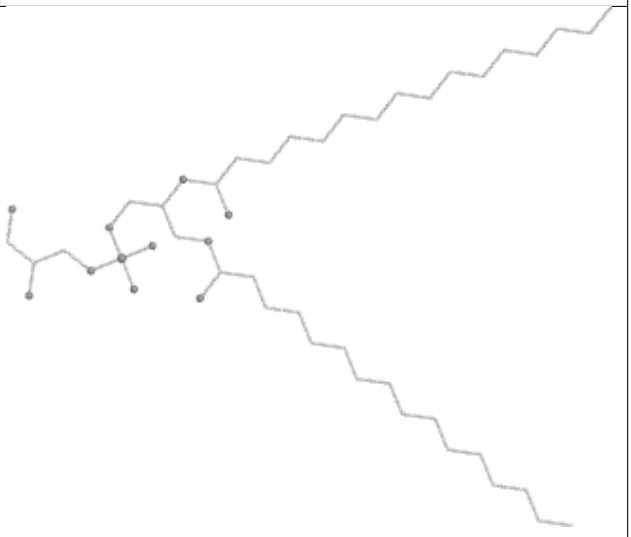
Bond lengths



Bond angles

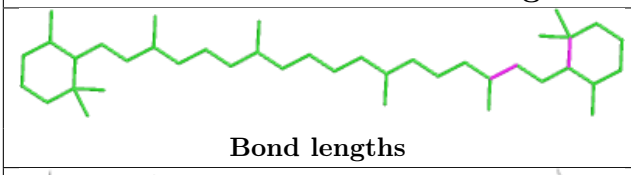


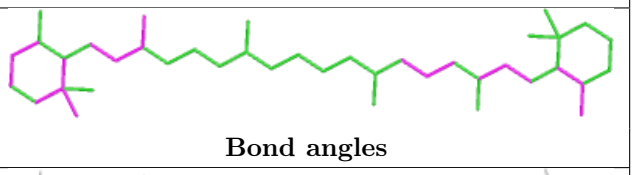
Torsions

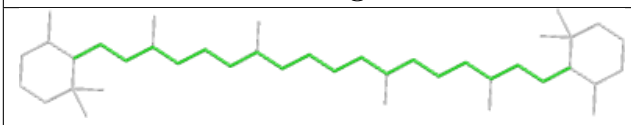


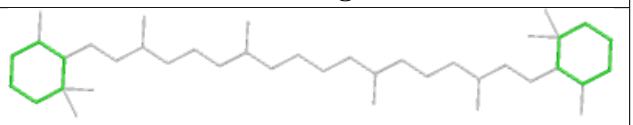
Rings

Ligand BCR B 619

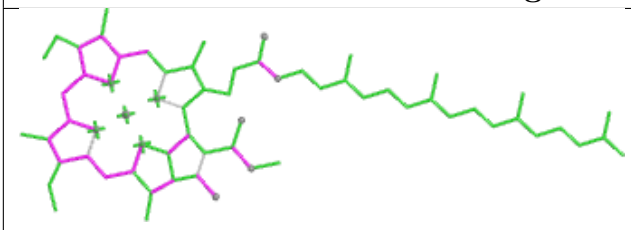

Bond lengths

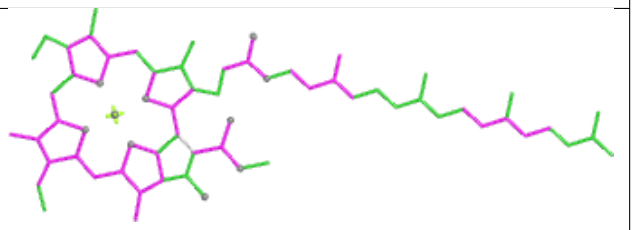

Bond angles

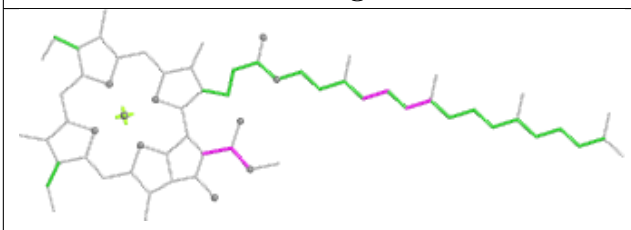

Torsions

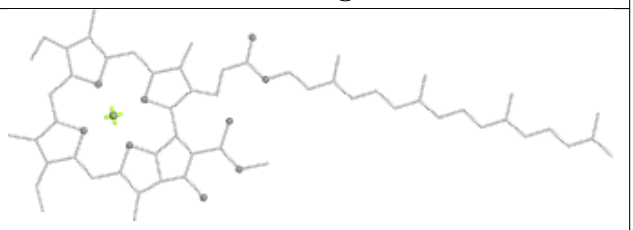

Rings

Ligand CLA C 510

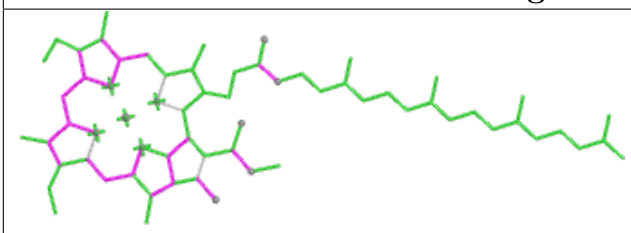

Bond lengths

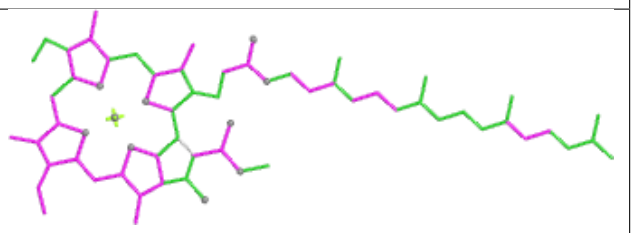

Bond angles

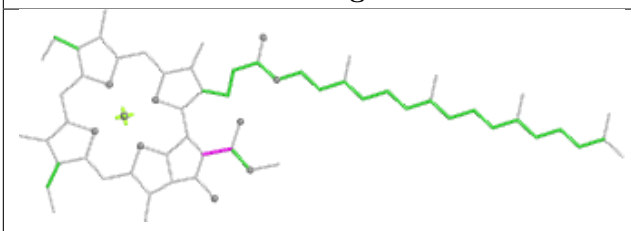

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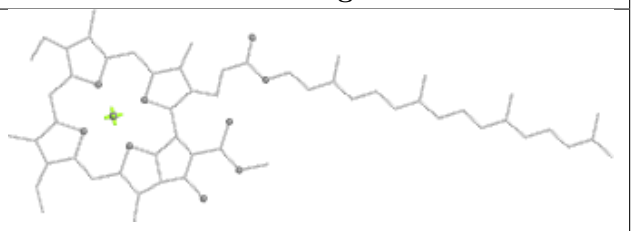

Rings

Ligand CLA b 609

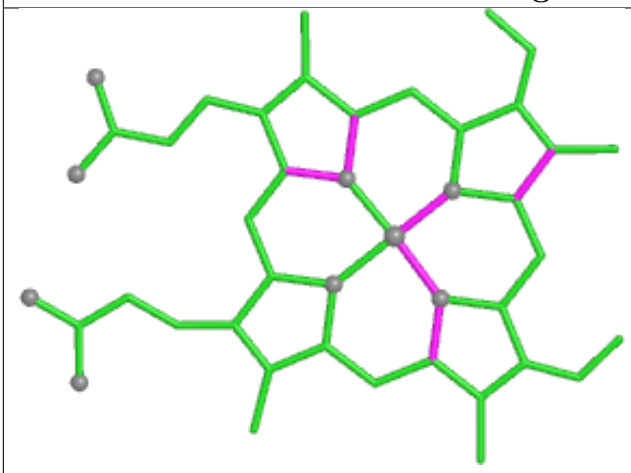

Bond lengths


Bond angles

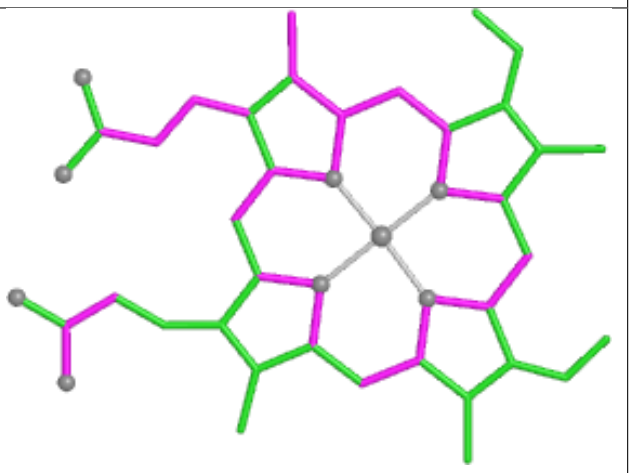

Torsions


Rings

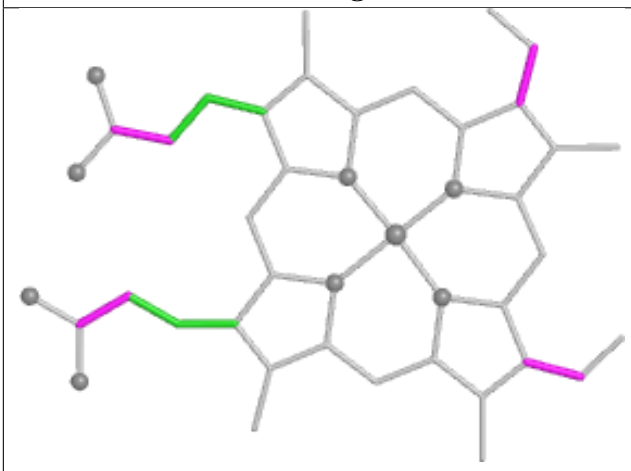
Ligand HEM e 87



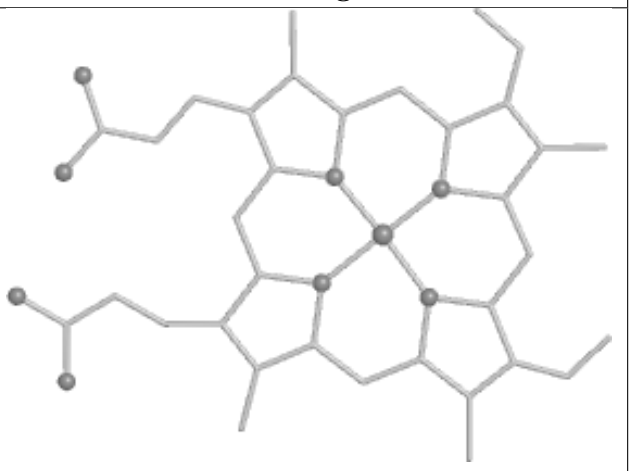
Bond lengths



Bond angles

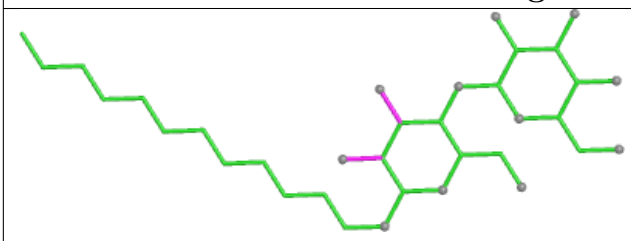


Torsions

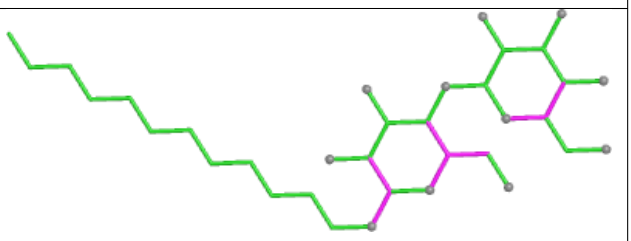


Rings

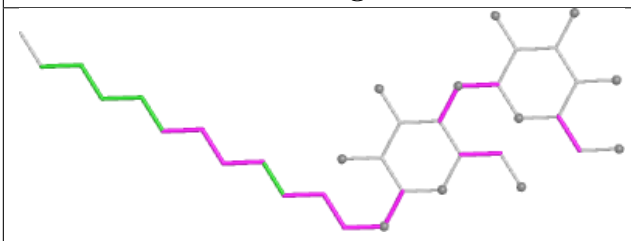
Ligand LMT I 101



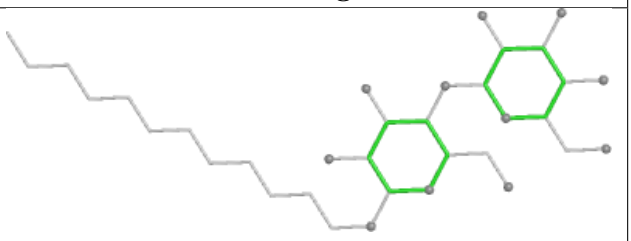
Bond lengths



Bond angles

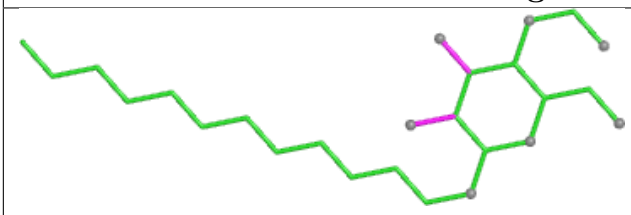


Torsions

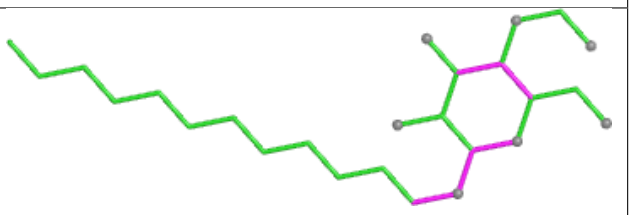


Rings

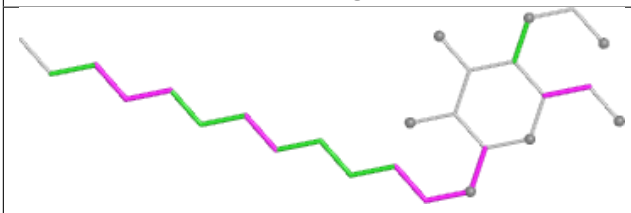
Ligand LMT t 102



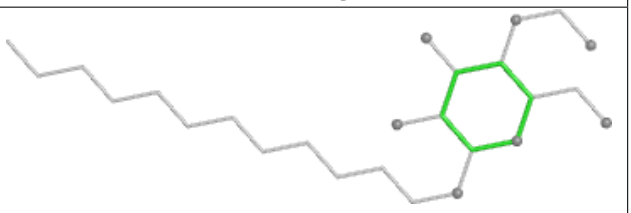
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.68	0 100 100	19, 25, 60, 122	222 (66%)
1	a	334/344 (97%)	-0.65	1 (0%) 90 90	20, 28, 63, 128	221 (66%)
2	B	504/505 (99%)	-0.58	1 (0%) 91 92	22, 52, 83, 114	20 (3%)
2	b	504/505 (99%)	-0.48	1 (0%) 91 92	24, 57, 100, 152	19 (3%)
3	C	451/455 (99%)	-0.58	0 100 100	21, 59, 82, 133	97 (21%)
3	c	455/455 (100%)	-0.53	1 (0%) 91 92	24, 65, 88, 127	100 (21%)
4	D	342/342 (100%)	-0.70	0 100 100	18, 44, 64, 129	114 (33%)
4	d	341/342 (99%)	-0.70	0 100 100	21, 49, 75, 127	116 (34%)
5	E	81/84 (96%)	-0.41	1 (1%) 76 77	52, 69, 97, 148	0
5	e	79/84 (94%)	-0.40	1 (1%) 75 76	33, 77, 120, 141	2 (2%)
6	F	34/44 (77%)	-0.63	0 100 100	54, 61, 91, 116	0
6	f	31/44 (70%)	-0.40	1 (3%) 50 50	54, 67, 96, 137	1 (3%)
7	H	64/65 (98%)	-0.31	1 (1%) 70 71	52, 63, 88, 112	0
7	h	64/65 (98%)	-0.37	0 100 100	40, 73, 95, 105	1 (1%)
8	I	37/38 (97%)	-0.21	0 100 100	56, 65, 121, 145	0
8	i	37/38 (97%)	-0.32	1 (2%) 56 57	55, 64, 116, 133	0
9	J	38/39 (97%)	-0.42	0 100 100	49, 67, 117, 155	0
9	j	39/39 (100%)	-0.37	0 100 100	57, 76, 132, 157	0
10	K	37/37 (100%)	-0.68	0 100 100	56, 67, 86, 103	0
10	k	37/37 (100%)	-0.53	0 100 100	64, 75, 99, 111	0
11	L	36/37 (97%)	-0.66	0 100 100	22, 44, 109, 130	2 (5%)
11	l	36/37 (97%)	-0.66	0 100 100	23, 46, 108, 119	2 (5%)
12	M	32/36 (88%)	-0.62	0 100 100	26, 47, 78, 123	1 (3%)
12	m	33/36 (91%)	-0.60	0 100 100	24, 47, 70, 137	2 (6%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.54	0	100	100	21, 65, 118, 161	10 (4%)
13	o	243/244 (99%)	-0.51	0	100	100	22, 69, 122, 155	8 (3%)
14	T	29/32 (90%)	-0.65	0	100	100	26, 46, 55, 67	6 (20%)
14	t	29/32 (90%)	-0.63	0	100	100	27, 47, 60, 71	5 (17%)
15	U	96/104 (92%)	-0.64	0	100	100	25, 57, 88, 100	4 (4%)
15	u	97/104 (93%)	-0.70	0	100	100	28, 61, 80, 124	4 (4%)
16	V	137/137 (100%)	-0.69	0	100	100	23, 56, 83, 107	6 (4%)
16	v	137/137 (100%)	-0.60	0	100	100	26, 71, 101, 132	6 (4%)
17	X	38/40 (95%)	-0.29	0	100	100	34, 73, 93, 114	1 (2%)
17	x	38/40 (95%)	-0.10	0	100	100	67, 80, 123, 152	0
18	Y	29/30 (96%)	-0.14	1 (3%)	48	48	68, 83, 122, 124	0
18	y	29/30 (96%)	-0.23	0	100	100	74, 91, 113, 115	0
19	Z	62/62 (100%)	-0.32	0	100	100	67, 80, 132, 148	0
19	z	62/62 (100%)	0.08	0	100	100	81, 95, 140, 165	0
20	R	34/34 (100%)	0.46	1 (2%)	53	54	87, 114, 135, 147	0
All	All	5283/5384 (98%)	-0.55	11 (0%)	91	92	18, 57, 101, 165	970 (18%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	H	65	LEU	4.1
5	e	79[A]	PHE	3.6
6	f	16[A]	PHE	2.9
1	a	11	ALA	2.7
3	c	245[A]	ILE	2.6
8	i	37	LEU	2.5
2	B	494	GLY	2.3
18	Y	18	VAL	2.3
2	b	499	VAL	2.2
5	E	4	THR	2.1
20	R	35	LEU	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	T	1	10/11	0.95	0.08	42,50,63,69	0
8	FME	I	1	10/11	0.96	0.07	61,69,83,84	0
14	FME	t	1	10/11	0.96	0.07	42,47,56,74	0
8	FME	i	1	10/11	0.97	0.07	59,70,80,86	0
12	FME	M	1	10/11	0.97	0.07	46,58,100,100	0
12	FME	m	1	10/11	0.98	0.07	52,61,91,116	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LMT	E	102	35/35	0.65	0.15	91,128,168,171	0
30	UNL	A	415	28/-	0.70	0.13	80,104,125,143	0
30	UNL	a	417	30/-	0.70	0.12	85,108,137,149	0
27	GOL	a	701	6/6	0.70	0.16	76,98,100,110	0
30	UNL	m	102	10/-	0.71	0.19	68,73,88,96	0
30	UNL	j	101	10/-	0.71	0.17	75,87,105,106	0
30	UNL	K	101[A]	34/-	0.72	0.14	77,99,112,119	34
30	UNL	K	101[B]	34/-	0.72	0.14	77,99,112,119	34
30	UNL	J	101	10/-	0.72	0.24	70,81,89,93	0
32	LMT	I	101	35/35	0.72	0.12	89,124,145,158	0
32	LMT	a	420	35/35	0.72	0.13	102,128,153,158	0
32	LMT	e	102	35/35	0.72	0.14	105,142,178,187	0
30	UNL	I	102	40/-	0.73	0.15	75,100,151,158	0
32	LMT	a	414	35/35	0.73	0.14	63,118,143,159	0
37	LHG	e	101[A]	42/49	0.74	0.12	87,125,143,156	42
37	LHG	e	101[B]	42/49	0.74	0.12	87,125,143,157	42
26	SQD	f	102	43/54	0.75	0.12	96,127,172,187	0
34	HTG	C	522	19/19	0.75	0.12	98,125,139,139	0
30	UNL	M	102	10/-	0.76	0.16	65,74,86,91	0
27	GOL	o	501	6/6	0.77	0.18	87,100,112,126	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LMT	A	359	35/35	0.77	0.12	58,115,139,142	0
30	UNL	i	101	40/-	0.78	0.13	74,103,146,164	0
27	GOL	O	601	6/6	0.78	0.15	74,91,94,104	0
30	UNL	c	525[A]	32/-	0.78	0.14	86,103,117,128	32
30	UNL	c	525[B]	32/-	0.78	0.14	86,103,117,128	32
30	UNL	b	626	33/-	0.79	0.12	67,95,148,162	0
34	HTG	D	414	16/19	0.79	0.12	89,105,139,149	0
33	LMG	C	521	51/55	0.79	0.11	59,112,155,180	0
34	HTG	B	623	19/19	0.79	0.15	64,98,120,127	0
27	GOL	o	601	6/6	0.80	0.14	79,90,95,95	0
32	LMT	b	621	25/35	0.80	0.12	80,106,154,170	0
27	GOL	d	701	6/6	0.80	0.22	49,68,78,91	0
30	UNL	D	413	40/-	0.81	0.12	64,84,131,145	0
34	HTG	b	623	19/19	0.82	0.11	85,131,161,163	0
27	GOL	B	901	6/6	0.82	0.14	63,92,105,111	0
32	LMT	M	103	35/35	0.82	0.10	64,121,173,173	0
29	PL9	a	416[A]	55/55	0.83	0.14	76,95,109,113	55
30	UNL	d	410	36/-	0.83	0.11	65,96,126,137	0
29	PL9	a	416[B]	55/55	0.83	0.14	76,95,109,113	55
34	HTG	c	522	19/19	0.83	0.09	101,122,142,144	0
36	CA	F	102	1/1	0.83	0.21	124,124,124,124	0
27	GOL	d	801[A]	6/6	0.83	0.18	63,95,101,101	6
27	GOL	d	801[B]	6/6	0.83	0.18	62,95,101,101	6
40	HEC	V	202	43/43	0.83	0.10	36,52,73,160	0
29	PL9	A	414[A]	55/55	0.84	0.13	62,86,100,105	55
34	HTG	V	203	11/19	0.84	0.10	80,115,125,142	0
29	PL9	A	414[B]	55/55	0.84	0.13	62,86,100,105	55
27	GOL	A	411	6/6	0.84	0.12	63,80,84,85	0
32	LMT	D	404	35/35	0.85	0.11	66,111,146,151	0
26	SQD	a	413	54/54	0.85	0.09	66,92,138,151	0
32	LMT	t	102	26/35	0.85	0.11	68,101,136,149	0
34	HTG	d	411	16/19	0.85	0.10	88,119,142,147	0
27	GOL	v	401[A]	6/6	0.85	0.13	64,80,82,84	6
27	GOL	v	401[B]	6/6	0.85	0.13	64,80,82,84	6
27	GOL	O	501	6/6	0.85	0.09	77,92,105,105	0
30	UNL	B	627	33/-	0.85	0.13	53,105,143,149	0
26	SQD	A	412	54/54	0.86	0.10	61,86,126,153	0
27	GOL	b	624	6/6	0.86	0.14	87,95,105,108	0
33	LMG	c	521	51/55	0.86	0.10	77,128,157,190	0
32	LMT	b	627	25/35	0.86	0.12	54,96,143,150	0
27	GOL	c	743	6/6	0.86	0.16	99,103,109,114	0
32	LMT	m	103	35/35	0.86	0.11	61,93,108,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	LMT	t	101	25/35	0.86	0.12	58,84,141,151	0
33	LMG	z	101	39/55	0.87	0.11	74,123,146,161	0
33	LMG	Z	101	37/55	0.87	0.12	68,117,149,168	0
27	GOL	a	801	6/6	0.88	0.26	52,76,81,87	0
34	HTG	b	622	19/19	0.88	0.11	59,85,118,122	0
32	LMT	M	101	35/35	0.88	0.10	58,103,129,138	0
37	LHG	E	101[A]	42/49	0.89	0.10	71,98,113,121	42
37	LHG	E	101[B]	42/49	0.89	0.10	71,98,113,121	42
26	SQD	F	101	43/54	0.89	0.11	69,103,128,137	0
26	SQD	B	620	54/54	0.89	0.09	60,89,130,150	0
26	SQD	b	620	54/54	0.89	0.09	59,92,120,132	0
23	CLA	b	601	65/65	0.90	0.09	64,87,123,160	0
34	HTG	B	622	19/19	0.90	0.11	63,81,124,126	0
30	UNL	D	412	17/-	0.90	0.10	58,77,99,114	0
27	GOL	a	412	6/6	0.90	0.11	75,77,87,92	0
36	CA	o	301	1/1	0.91	0.07	116,116,116,116	0
23	CLA	B	601	65/65	0.91	0.09	55,79,111,156	0
27	GOL	A	701	6/6	0.91	0.25	49,73,80,83	0
33	LMG	C	501	51/55	0.91	0.09	64,89,115,129	0
34	HTG	B	626	19/19	0.91	0.07	67,81,97,106	0
36	CA	f	103	1/1	0.91	0.12	124,124,124,124	0
33	LMG	a	419	51/55	0.92	0.08	67,94,110,121	0
33	LMG	c	520	51/55	0.92	0.09	59,90,130,156	0
27	GOL	V	401[B]	6/6	0.92	0.12	59,67,73,77	6
33	LMG	m	101	51/55	0.92	0.08	47,73,96,109	0
23	CLA	c	514	65/65	0.92	0.09	69,95,119,147	0
33	LMG	B	621	51/55	0.92	0.08	47,68,91,111	0
27	GOL	V	401[A]	6/6	0.92	0.12	59,67,73,76	6
30	UNL	d	409	17/-	0.92	0.09	64,79,116,123	0
33	LMG	C	520	51/55	0.93	0.09	54,84,115,125	0
35	DGD	C	518[A]	62/66	0.93	0.08	48,63,108,112	62
35	DGD	C	518[B]	62/66	0.93	0.08	48,63,108,112	62
27	GOL	C	523[B]	6/6	0.93	0.09	57,62,65,66	6
33	LMG	D	415	51/55	0.93	0.09	49,66,117,139	0
27	GOL	D	701	6/6	0.93	0.15	45,60,70,92	0
23	CLA	C	514	65/65	0.93	0.08	62,88,111,123	0
25	BCR	T	101	40/40	0.93	0.07	43,58,69,69	0
27	GOL	B	624	6/6	0.93	0.08	65,73,81,84	0
25	BCR	d	404	40/40	0.93	0.08	48,65,105,108	0
27	GOL	C	523[A]	6/6	0.93	0.09	58,61,64,67	6
23	CLA	C	507	65/65	0.94	0.08	54,70,121,141	0
25	BCR	C	515	40/40	0.94	0.08	53,77,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	D	407	40/40	0.94	0.08	43,58,100,103	0
26	SQD	a	411[A]	54/54	0.94	0.09	56,80,112,121	54
34	HTG	b	625	19/19	0.94	0.07	62,76,93,109	0
26	SQD	a	411[B]	54/54	0.94	0.09	56,80,112,121	54
23	CLA	b	616	65/65	0.94	0.08	48,63,124,134	0
30	UNL	X	101	18/-	0.94	0.10	56,71,105,107	0
25	BCR	Y	101	40/40	0.94	0.08	52,64,83,87	0
35	DGD	c	518[A]	62/66	0.94	0.07	54,67,113,129	62
35	DGD	c	518[B]	62/66	0.94	0.07	54,67,113,129	62
33	LMG	d	412	51/55	0.94	0.08	53,73,117,144	0
25	BCR	c	515	40/40	0.94	0.08	69,84,96,97	0
23	CLA	c	513	65/65	0.94	0.09	59,82,121,133	0
37	LHG	D	409[A]	49/49	0.94	0.08	46,61,83,87	49
37	LHG	D	409[B]	49/49	0.94	0.08	46,61,83,87	49
37	LHG	D	411[A]	49/49	0.94	0.09	47,61,105,108	49
37	LHG	D	411[B]	49/49	0.94	0.09	47,60,105,108	49
25	BCR	t	103	40/40	0.94	0.06	43,58,77,81	0
26	SQD	A	410[A]	54/54	0.94	0.08	57,78,112,116	54
27	GOL	c	742[A]	6/6	0.94	0.07	64,66,75,76	6
27	GOL	c	742[B]	6/6	0.94	0.07	65,66,75,76	6
26	SQD	A	410[B]	54/54	0.94	0.08	57,78,112,116	54
23	CLA	c	508	65/65	0.95	0.08	56,69,85,90	0
23	CLA	C	505	65/65	0.95	0.07	40,55,102,129	0
23	CLA	A	408	65/65	0.95	0.08	38,52,127,140	0
23	CLA	d	403	65/65	0.95	0.08	50,68,116,148	0
25	BCR	A	409	40/40	0.95	0.07	37,50,63,66	0
25	BCR	B	618	40/40	0.95	0.05	40,52,67,75	0
25	BCR	B	619	40/40	0.95	0.07	48,58,88,99	0
23	CLA	C	509	65/65	0.95	0.07	47,56,116,149	0
29	PL9	D	408[A]	55/55	0.95	0.06	37,47,59,70	55
29	PL9	D	408[B]	55/55	0.95	0.06	37,47,59,71	55
23	CLA	C	513	65/65	0.95	0.08	59,78,111,125	0
25	BCR	H	101	40/40	0.95	0.08	52,66,86,89	0
25	BCR	K	102	40/40	0.95	0.08	57,66,83,86	0
23	CLA	B	606	65/65	0.95	0.07	41,55,101,128	0
35	DGD	C	519	62/66	0.95	0.07	42,58,93,111	0
35	DGD	H	102	62/66	0.95	0.08	42,61,79,101	0
35	DGD	c	517[A]	62/66	0.95	0.07	50,65,99,106	62
35	DGD	c	517[B]	62/66	0.95	0.07	50,65,99,106	62
23	CLA	a	407[A]	65/65	0.95	0.07	38,51,119,128	65
25	BCR	a	410	40/40	0.95	0.07	44,54,61,69	0
35	DGD	c	519	62/66	0.95	0.07	49,64,99,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
25	BCR	b	619	40/40	0.95	0.07	51,62,88,91	0
23	CLA	a	407[B]	65/65	0.95	0.07	38,51,119,128	65
23	CLA	a	409	65/65	0.95	0.09	44,57,138,156	0
25	BCR	h	101	40/40	0.95	0.09	59,73,94,96	0
25	BCR	k	101	40/40	0.95	0.09	60,73,90,92	0
23	CLA	B	614	65/65	0.95	0.07	36,48,103,127	0
25	BCR	y	101	40/40	0.95	0.07	58,70,85,97	0
27	GOL	b	901	6/6	0.95	0.07	78,79,83,88	0
23	CLA	b	614	65/65	0.95	0.07	40,51,102,120	0
37	LHG	d	408[A]	49/49	0.95	0.08	50,62,109,125	49
37	LHG	d	408[B]	49/49	0.95	0.08	50,62,109,125	49
37	LHG	d	711[A]	49/49	0.95	0.08	46,67,80,89	49
37	LHG	d	711[B]	49/49	0.95	0.08	45,67,80,89	49
23	CLA	B	616	65/65	0.95	0.08	41,58,131,139	0
23	CLA	c	505	65/65	0.95	0.07	50,63,108,146	0
37	LHG	l	101[A]	49/49	0.95	0.08	48,58,72,93	49
37	LHG	l	101[B]	49/49	0.95	0.08	48,57,72,93	49
23	CLA	c	507	65/65	0.95	0.08	51,68,125,135	0
23	CLA	A	406[B]	65/65	0.96	0.06	38,47,110,122	65
25	BCR	B	617	40/40	0.96	0.06	40,49,62,66	0
23	CLA	A	404[A]	65/65	0.96	0.06	35,41,58,68	65
23	CLA	C	502	65/65	0.96	0.07	47,61,74,84	0
35	DGD	C	517[A]	62/66	0.96	0.06	44,58,99,101	62
35	DGD	C	517[B]	62/66	0.96	0.06	44,58,99,101	62
23	CLA	b	602	65/65	0.96	0.07	50,60,82,92	0
23	CLA	b	604	65/65	0.96	0.07	41,52,96,119	0
23	CLA	b	606	65/65	0.96	0.07	44,61,120,133	0
29	PL9	d	405[A]	55/55	0.96	0.06	37,49,61,72	55
29	PL9	d	405[B]	55/55	0.96	0.06	36,49,61,72	55
23	CLA	b	607	65/65	0.96	0.06	37,46,79,94	0
23	CLA	b	611	65/65	0.96	0.06	37,48,71,81	0
23	CLA	b	612	65/65	0.96	0.07	44,53,68,81	0
23	CLA	A	404[B]	65/65	0.96	0.06	35,42,60,68	65
35	DGD	h	102	62/66	0.96	0.07	51,66,81,95	0
25	BCR	b	617	40/40	0.96	0.05	45,52,61,70	0
36	CA	O	301	1/1	0.96	0.05	105,105,105,105	0
25	BCR	b	618	40/40	0.96	0.06	44,58,75,87	0
23	CLA	B	602	65/65	0.96	0.07	46,58,75,94	0
23	CLA	c	502	65/65	0.96	0.07	56,67,80,86	0
25	BCR	c	516	40/40	0.96	0.06	57,67,80,96	0
37	LHG	D	410[A]	49/49	0.96	0.07	43,54,67,76	49
37	LHG	D	410[B]	49/49	0.96	0.07	43,54,66,76	49

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	c	504	65/65	0.96	0.07	48,70,86,92	0
23	CLA	C	508	65/65	0.96	0.08	50,63,82,93	0
23	CLA	c	506	65/65	0.96	0.07	50,64,92,101	0
23	CLA	B	603	65/65	0.96	0.07	40,53,74,81	0
37	LHG	d	407[A]	49/49	0.96	0.07	45,55,67,79	49
37	LHG	d	407[B]	49/49	0.96	0.07	45,56,68,79	49
23	CLA	A	406[A]	65/65	0.96	0.06	38,47,110,122	65
23	CLA	c	509	65/65	0.96	0.07	46,63,125,155	0
23	CLA	c	512	65/65	0.96	0.07	56,70,89,101	0
23	CLA	B	609	65/65	0.96	0.07	50,59,72,83	0
23	CLA	D	406	65/65	0.96	0.07	46,59,123,146	0
23	CLA	B	611	65/65	0.96	0.07	34,44,64,73	0
30	UNL	x	101	18/-	0.96	0.10	70,76,127,129	0
24	PHO	a	353[A]	64/64	0.96	0.06	43,54,61,66	64
24	PHO	a	353[B]	64/64	0.96	0.06	43,54,61,66	64
24	PHO	A	353[A]	64/64	0.97	0.05	38,48,54,62	64
24	PHO	A	353[B]	64/64	0.97	0.05	38,48,54,61	64
24	PHO	a	408[A]	64/64	0.97	0.05	38,47,55,57	64
24	PHO	a	408[B]	64/64	0.97	0.05	38,47,55,57	64
23	CLA	A	405[A]	65/65	0.97	0.05	32,42,54,71	65
23	CLA	B	607	65/65	0.97	0.06	36,45,72,86	0
23	CLA	C	503	65/65	0.97	0.06	44,54,80,92	0
23	CLA	C	504	65/65	0.97	0.06	48,61,73,79	0
23	CLA	b	603	65/65	0.97	0.06	43,56,81,93	0
23	CLA	B	608	65/65	0.97	0.05	37,48,69,74	0
23	CLA	b	605	65/65	0.97	0.06	38,50,77,79	0
25	BCR	C	516	40/40	0.97	0.06	52,66,77,90	0
31	BCT	A	348[A]	4/4	0.97	0.06	51,52,58,68	4
31	BCT	A	348[B]	4/4	0.97	0.06	51,52,58,69	4
31	BCT	a	404[A]	4/4	0.97	0.06	55,58,67,76	4
31	BCT	a	404[B]	4/4	0.97	0.06	55,58,67,76	4
23	CLA	C	506	65/65	0.97	0.06	45,61,88,104	0
23	CLA	A	405[B]	65/65	0.97	0.05	33,42,54,71	65
23	CLA	b	609	65/65	0.97	0.06	52,66,84,94	0
23	CLA	b	610	65/65	0.97	0.07	47,58,69,74	0
23	CLA	B	610	65/65	0.97	0.07	39,54,66,83	0
36	CA	C	524	1/1	0.97	0.05	77,77,77,77	0
23	CLA	B	604	65/65	0.97	0.06	36,47,112,136	0
23	CLA	b	613	65/65	0.97	0.05	39,50,88,105	0
36	CA	c	523	1/1	0.97	0.08	78,78,78,78	0
23	CLA	C	510	65/65	0.97	0.07	45,58,82,88	0
23	CLA	b	615	65/65	0.97	0.06	52,62,83,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
23	CLA	C	511	65/65	0.97	0.06	48,57,79,89	0
23	CLA	C	512	65/65	0.97	0.07	51,62,81,87	0
23	CLA	c	503	65/65	0.97	0.06	44,59,90,102	0
23	CLA	B	612	65/65	0.97	0.06	34,49,60,66	0
23	CLA	B	613	65/65	0.97	0.06	36,45,98,113	0
23	CLA	D	405[A]	65/65	0.97	0.06	32,43,68,76	65
23	CLA	D	405[B]	65/65	0.97	0.06	32,43,68,76	65
23	CLA	B	605	65/65	0.97	0.06	39,48,67,83	0
37	LHG	L	101[A]	49/49	0.97	0.06	45,55,66,88	49
37	LHG	L	101[B]	49/49	0.97	0.06	45,55,66,88	49
23	CLA	a	405[A]	65/65	0.97	0.06	33,44,60,74	65
23	CLA	c	510	65/65	0.97	0.07	46,61,90,95	0
23	CLA	c	511	65/65	0.97	0.06	47,63,79,93	0
23	CLA	a	405[B]	65/65	0.97	0.06	38,44,62,74	65
23	CLA	a	406[A]	65/65	0.97	0.05	36,43,59,68	65
23	CLA	a	406[B]	65/65	0.97	0.05	36,43,59,68	65
23	CLA	d	402[A]	65/65	0.97	0.06	36,45,72,89	65
23	CLA	d	402[B]	65/65	0.97	0.06	36,45,72,89	65
23	CLA	B	615	65/65	0.97	0.06	42,54,79,90	0
24	PHO	A	407[A]	64/64	0.97	0.04	35,45,50,56	64
24	PHO	A	407[B]	64/64	0.97	0.04	35,45,50,56	64
22	CL	A	403[B]	1/1	0.98	0.04	45,45,45,45	1
22	CL	A	403[A]	1/1	0.98	0.04	46,46,46,46	1
38	HEM	E	103	43/43	0.98	0.06	52,70,83,95	0
38	HEM	e	87	43/43	0.98	0.08	63,85,118,137	0
23	CLA	b	608	65/65	0.98	0.05	42,54,78,91	0
40	HEC	v	202	43/43	0.98	0.07	51,63,70,77	0
36	CA	c	524	1/1	0.99	0.05	78,78,78,78	0
22	CL	a	403[B]	1/1	0.99	0.07	53,53,53,53	1
28	OEX	A	413[A]	10/10	0.99	0.03	37,45,50,50	10
28	OEX	A	413[B]	10/10	0.99	0.03	37,45,49,50	10
22	CL	A	402[A]	1/1	0.99	0.07	41,41,41,41	1
22	CL	A	402[B]	1/1	0.99	0.07	41,41,41,41	1
22	CL	a	402[A]	1/1	0.99	0.06	48,48,48,48	1
39	MG	J	102	1/1	0.99	0.03	57,57,57,57	0
39	MG	j	102	1/1	0.99	0.03	65,65,65,65	0
22	CL	a	402[B]	1/1	0.99	0.06	48,48,48,48	1
22	CL	a	403[A]	1/1	0.99	0.07	53,53,53,53	1
21	FE2	a	401[A]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	a	401[B]	1/1	1.00	0.01	52,52,52,52	1
21	FE2	A	401[A]	1/1	1.00	0.01	50,50,50,50	1
21	FE2	A	401[B]	1/1	1.00	0.01	50,50,50,50	1

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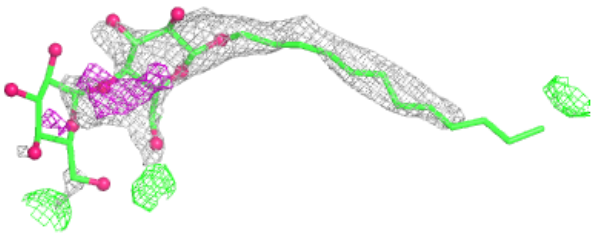
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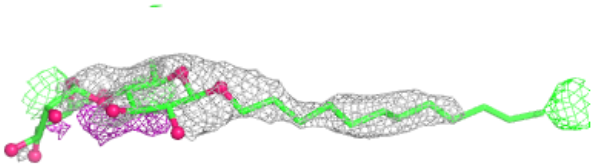
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	OEX	a	415[A]	10/10	1.00	0.03	47,49,55,56	10
28	OEX	a	415[B]	10/10	1.00	0.03	47,49,55,56	10

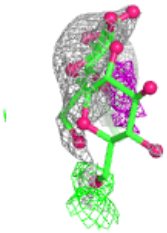
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

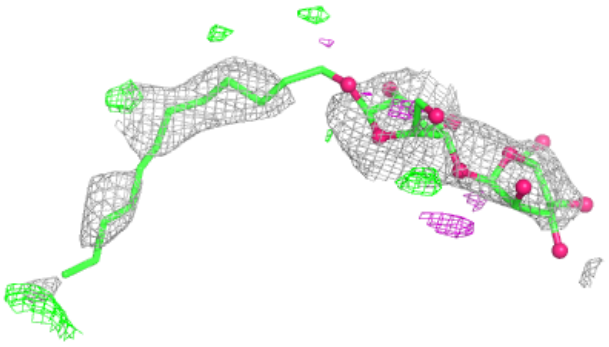


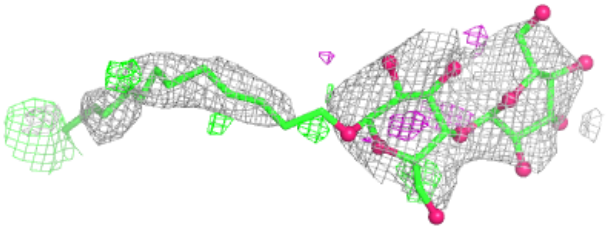


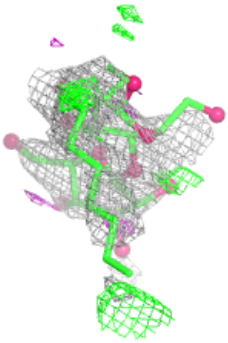


Electron density around LMT I 101:

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

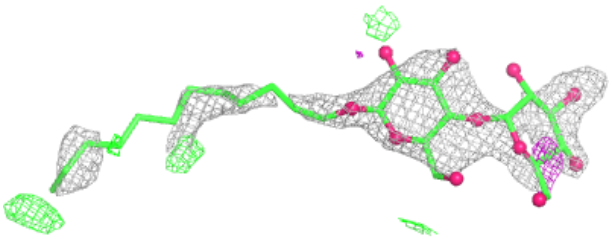


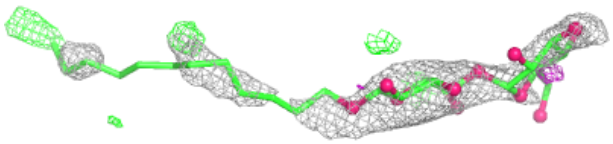


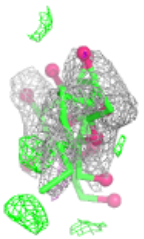


Electron density around LMT a 420:

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

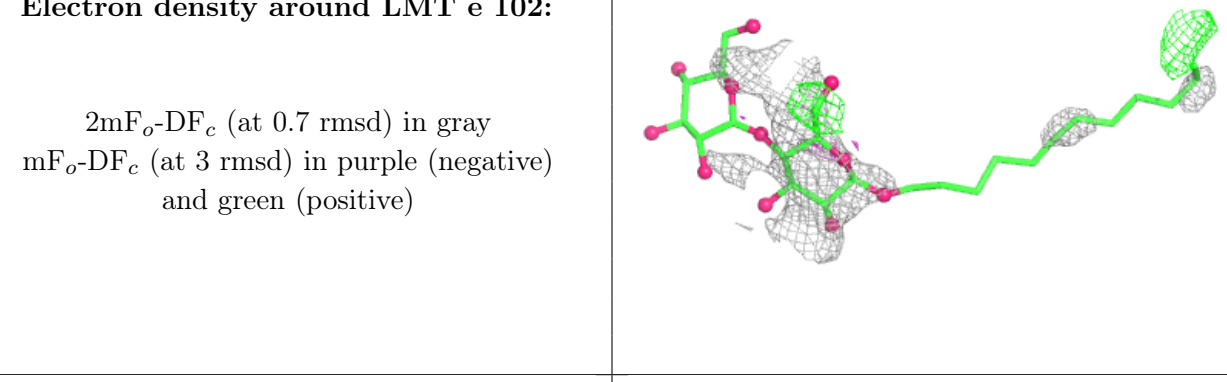






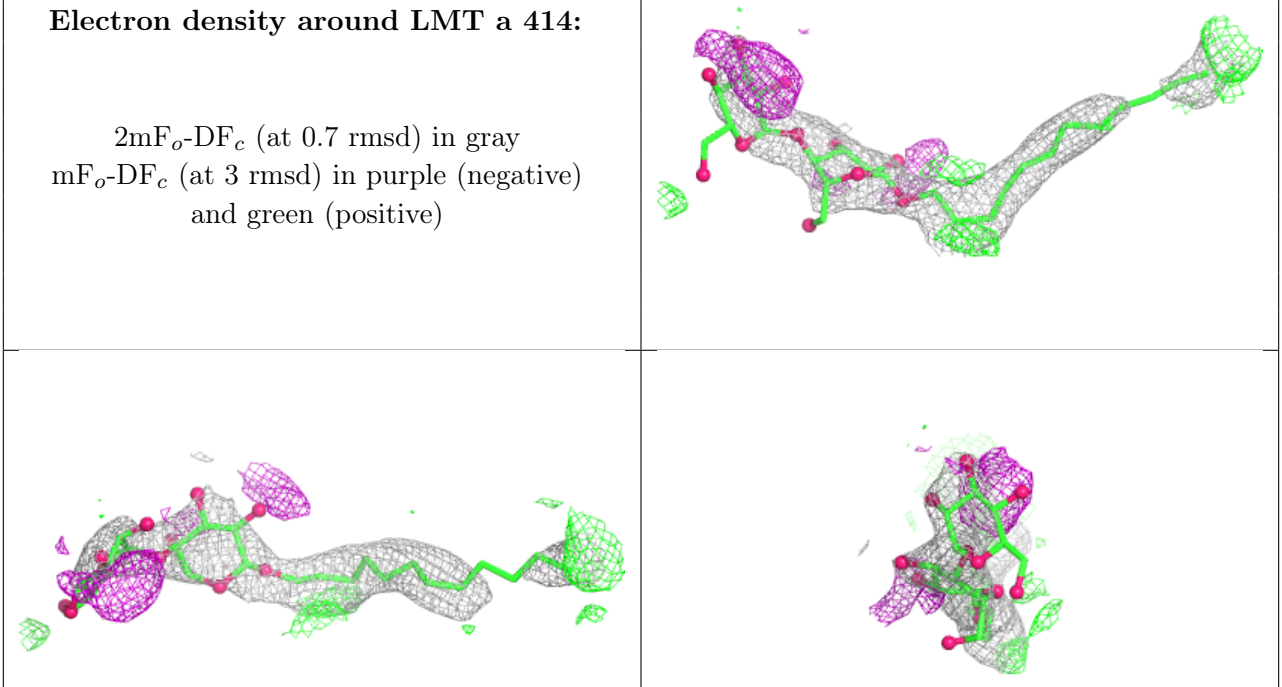
Electron density around LMT e 102:

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



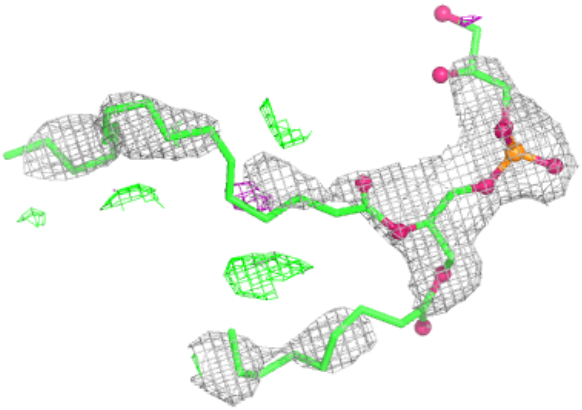
Electron density around LMT a 414:

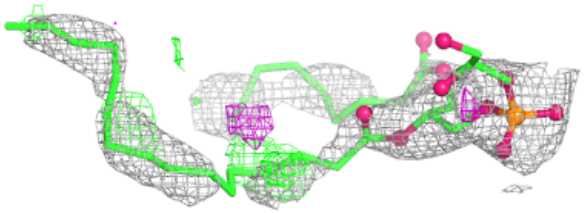
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

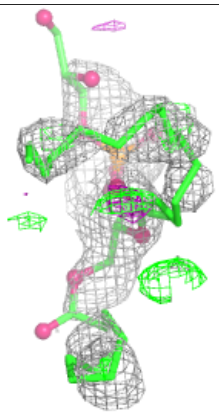


Electron density around LHG e 101 (A):

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

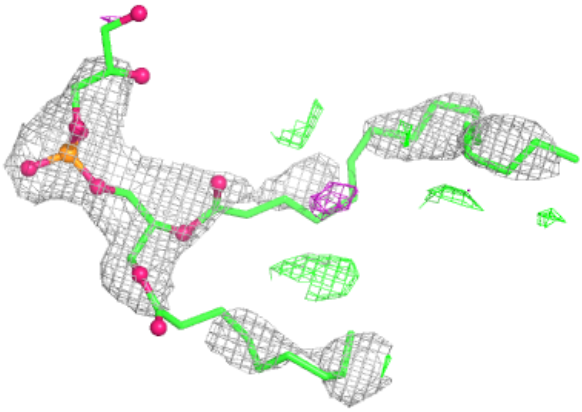


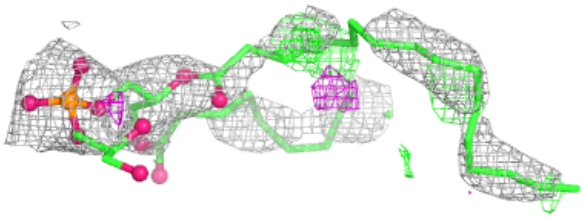


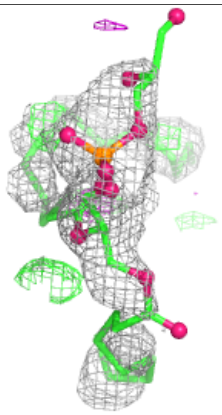


Electron density around LHG e 101 (B):

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

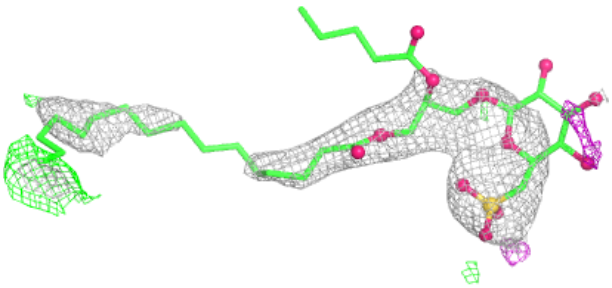


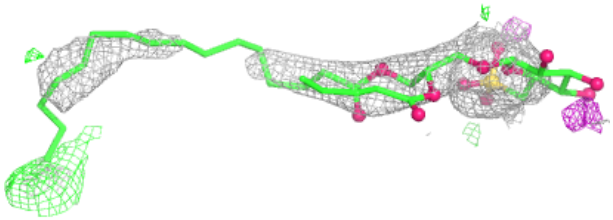


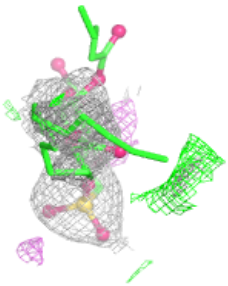


Electron density around SQD f 102:

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

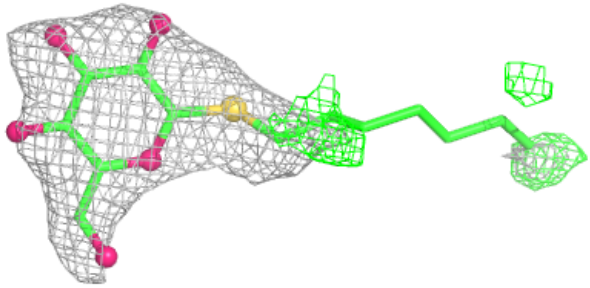


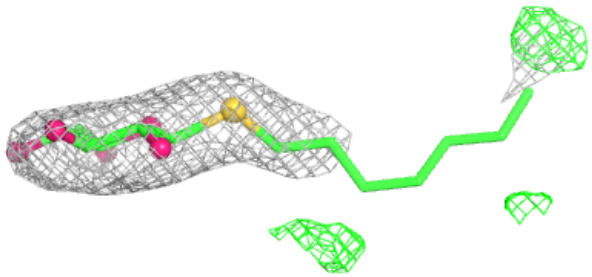


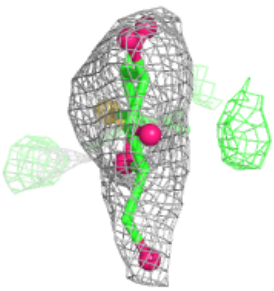


Electron density around HTG C 522:

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

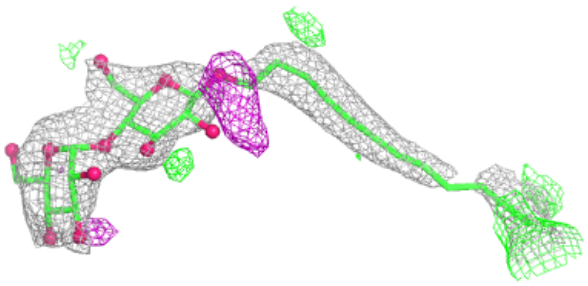


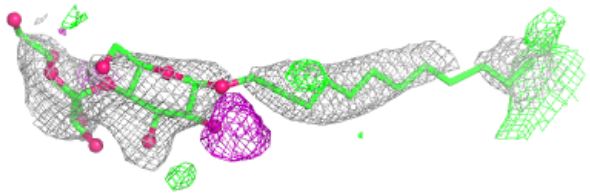


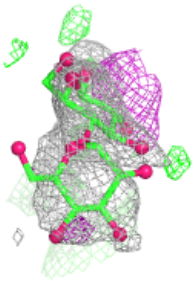


Electron density around LMT A 359:

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

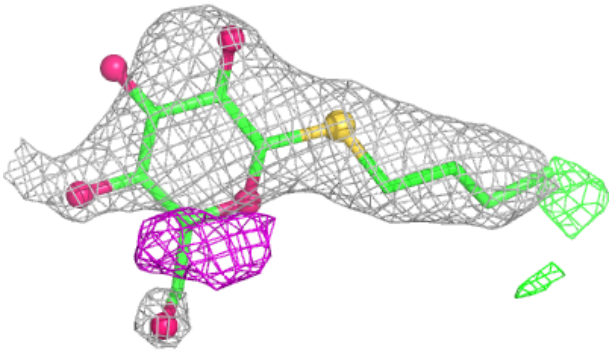


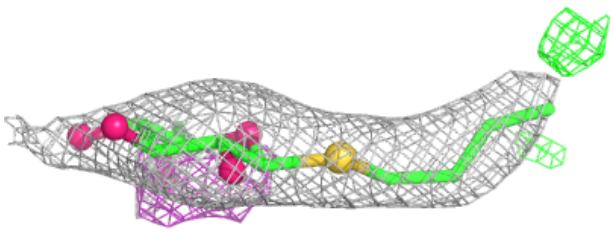


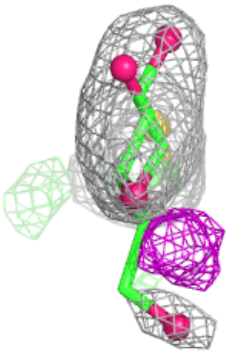


Electron density around HTG D 414:

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

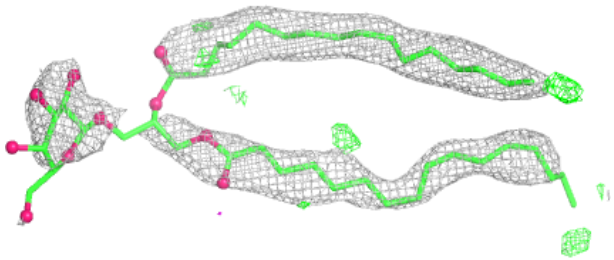


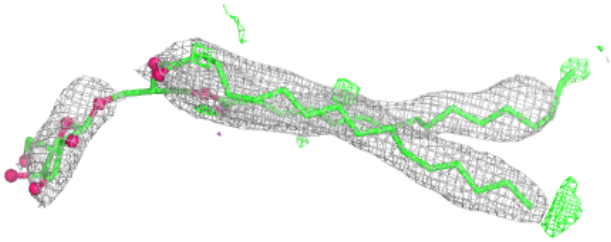


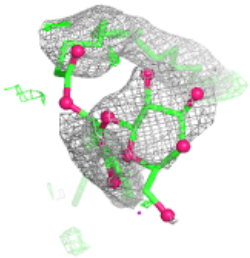


Electron density around LMG C 521:

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

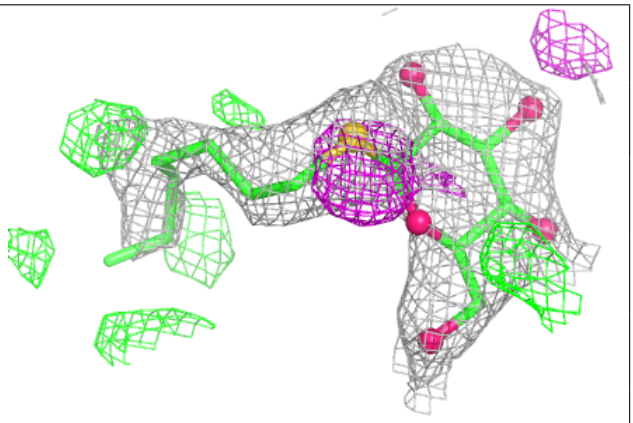


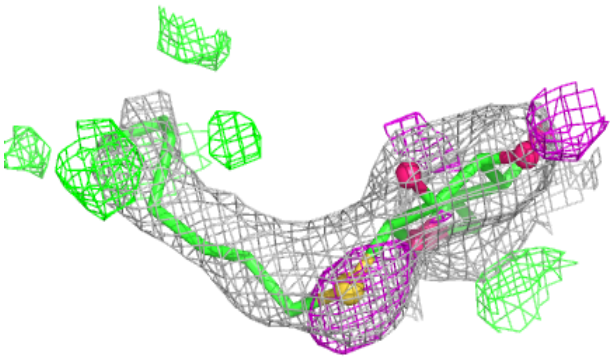


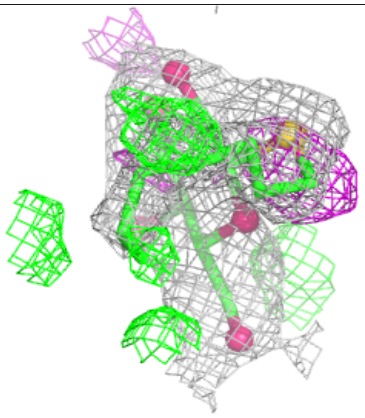


Electron density around HTG B 623:

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

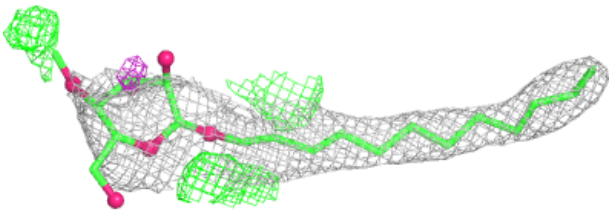


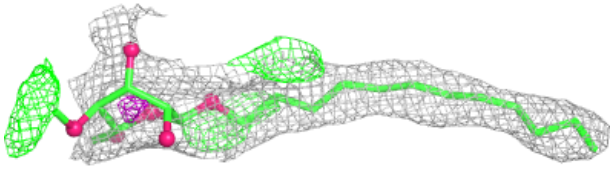


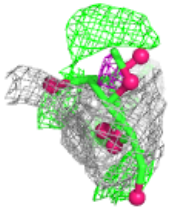


Electron density around LMT b 621:

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

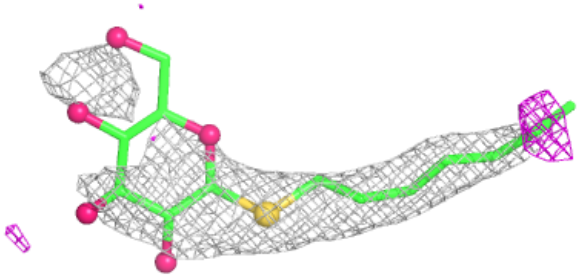


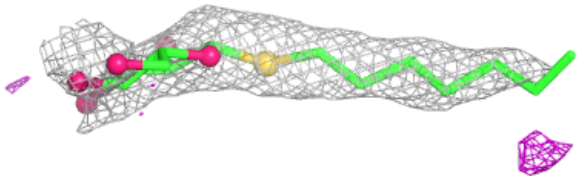


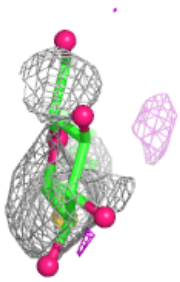


Electron density around HTG b 623:

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

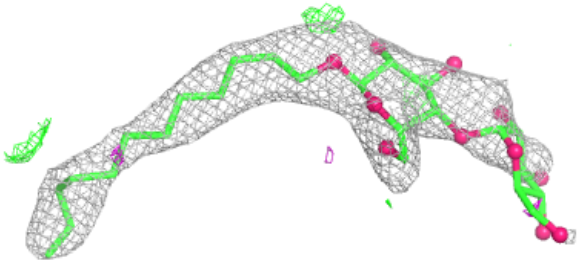


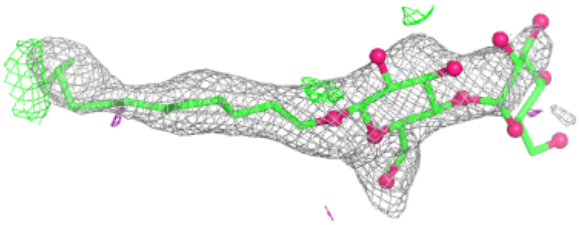


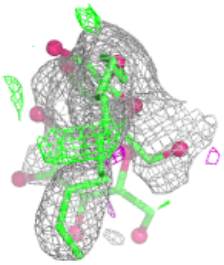


Electron density around LMT M 103:

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

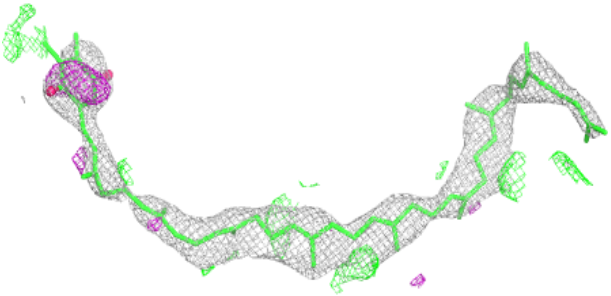


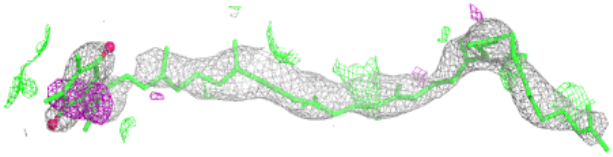


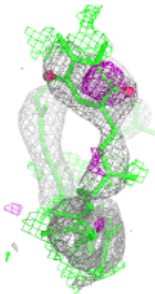


Electron density around PL9 a 416 (A):

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

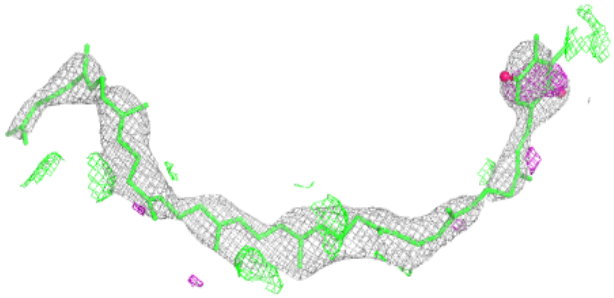


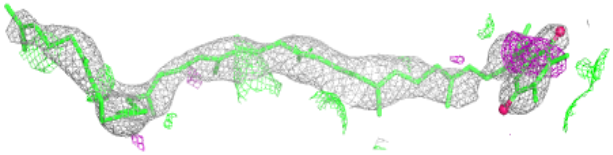


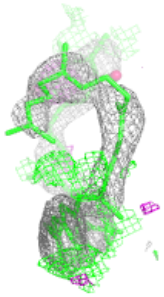


Electron density around PL9 a 416 (B):

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

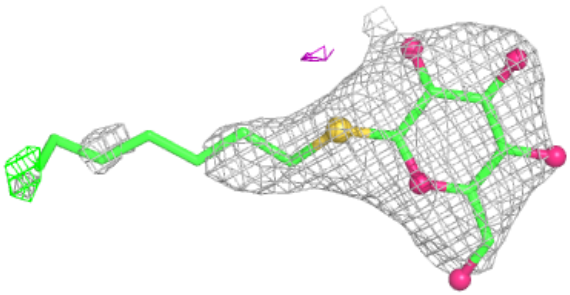


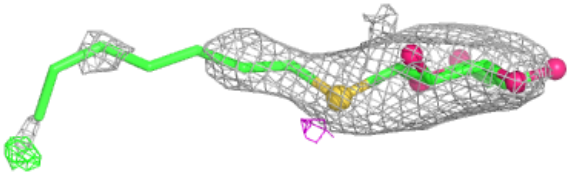


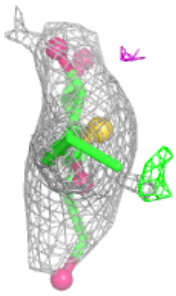


Electron density around HTG c 522:

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

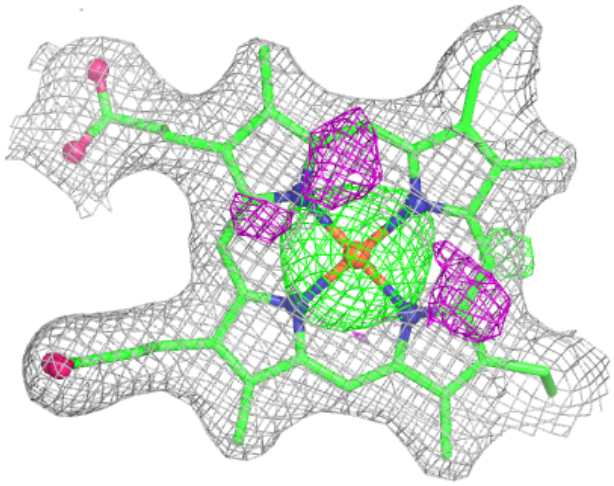


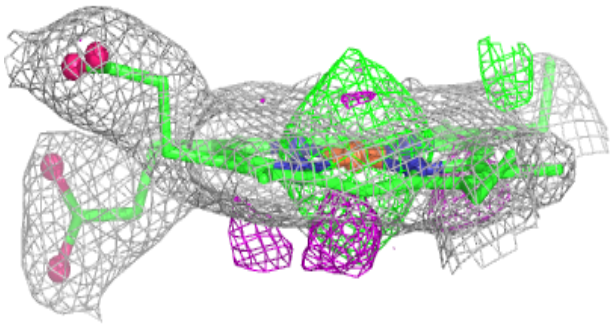


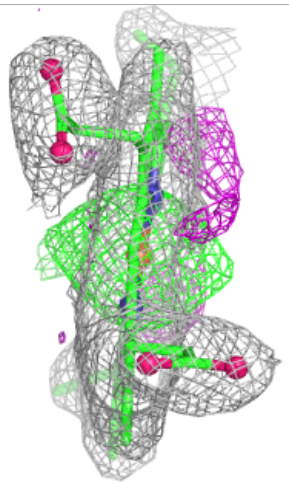


Electron density around HEC V 202:

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

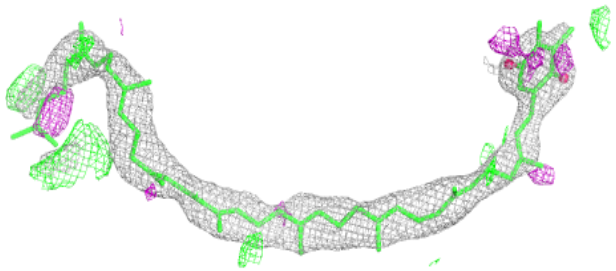


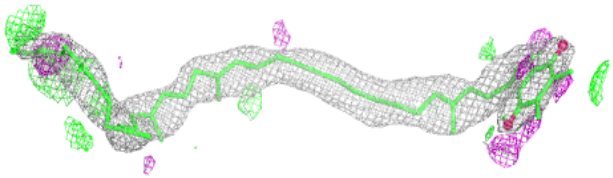


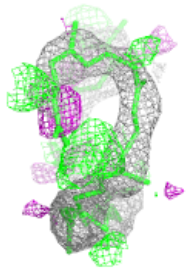


Electron density around PL9 A 414 (A):

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

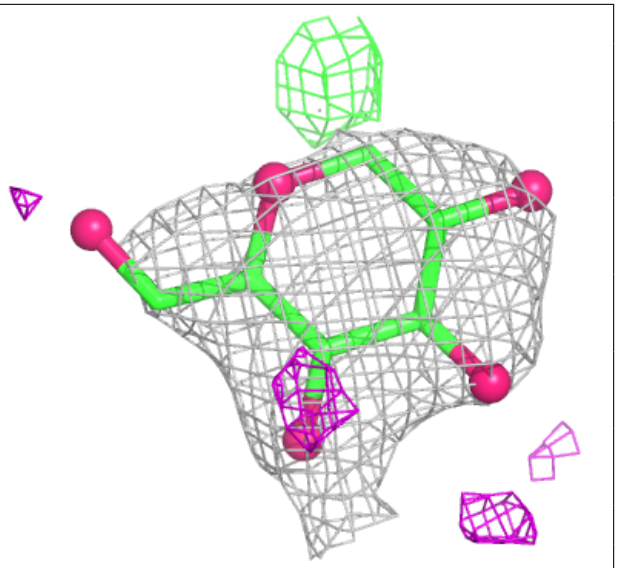


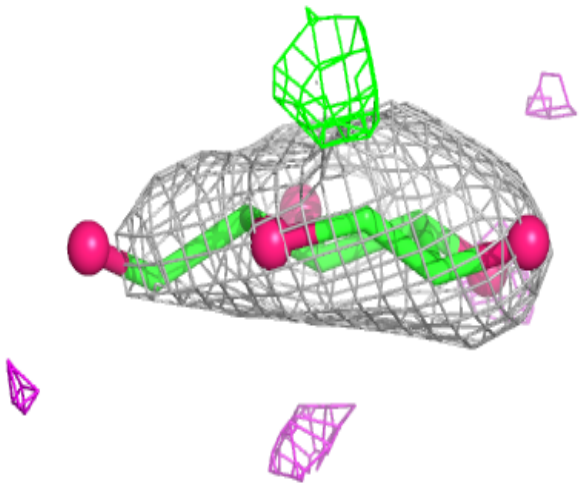


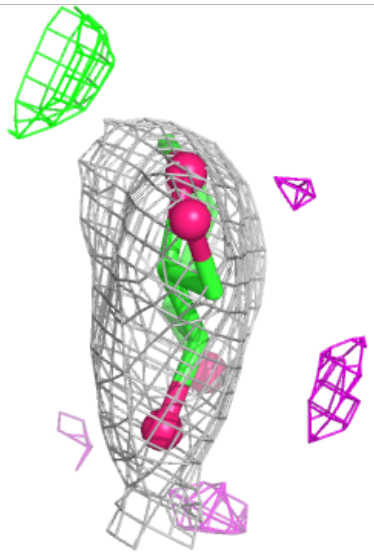


Electron density around HTG V 203:

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

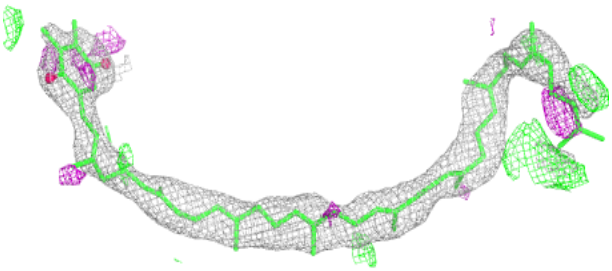


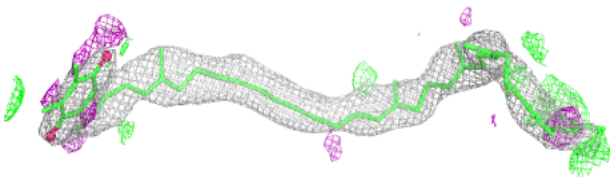


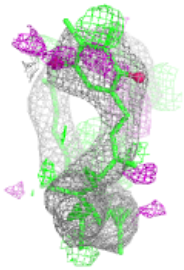


Electron density around PL9 A 414 (B):

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

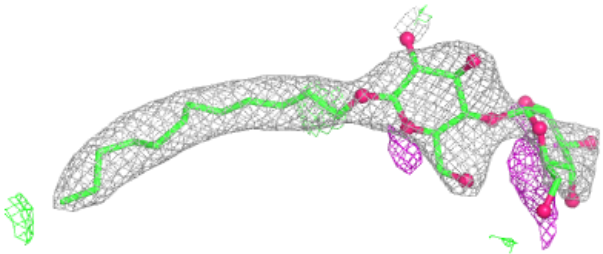


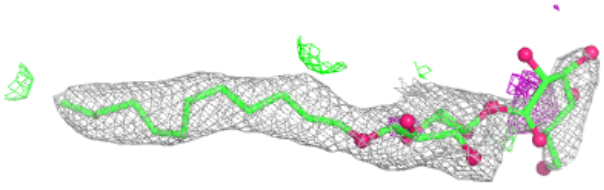


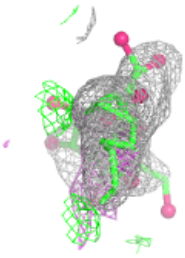


Electron density around LMT D 404:

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

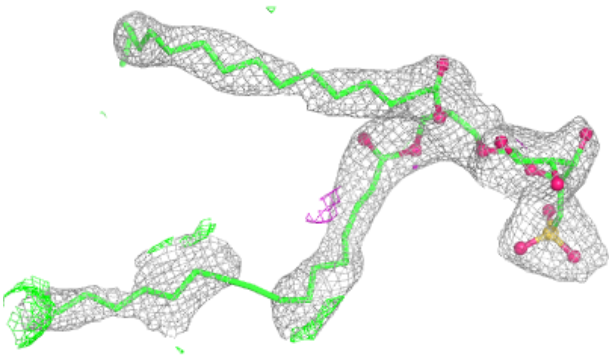


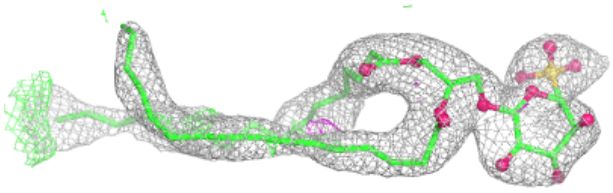


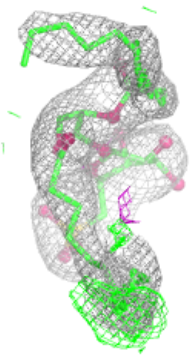


Electron density around SQD a 413:

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

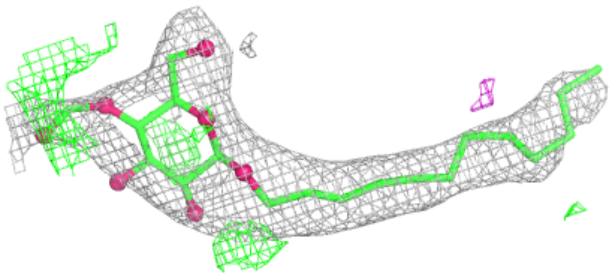


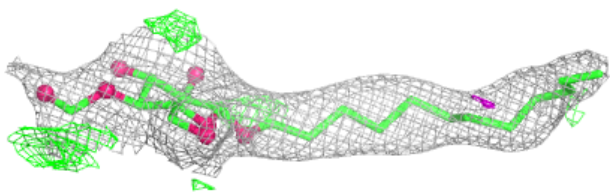


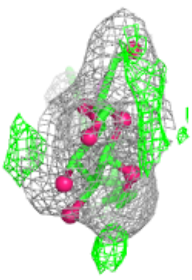


Electron density around LMT t 102:

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

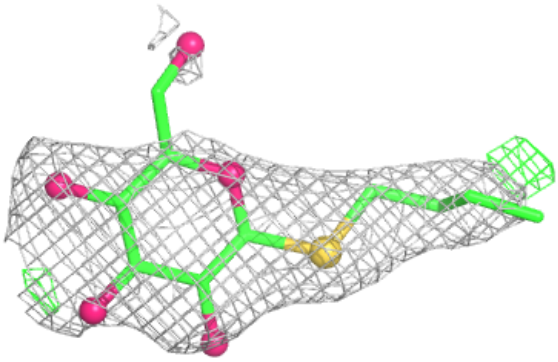


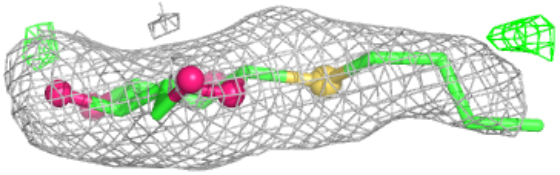


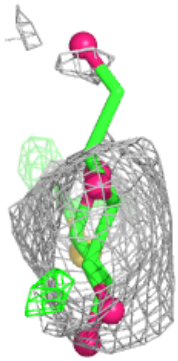


Electron density around HTG d 411:

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

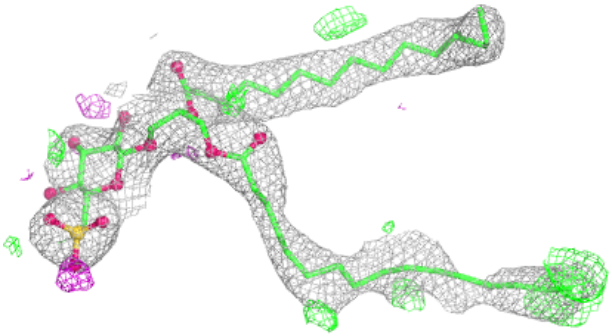


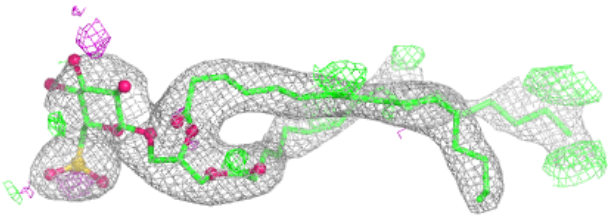


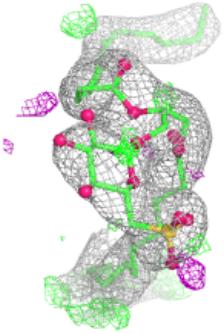


Electron density around SQD A 412:

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

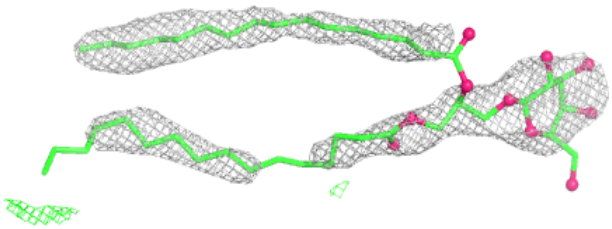


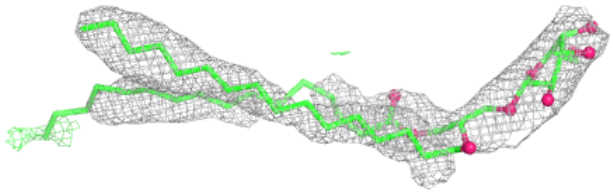


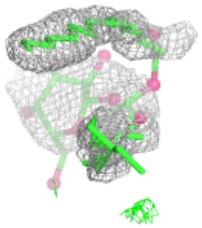


Electron density around LMG c 521:

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

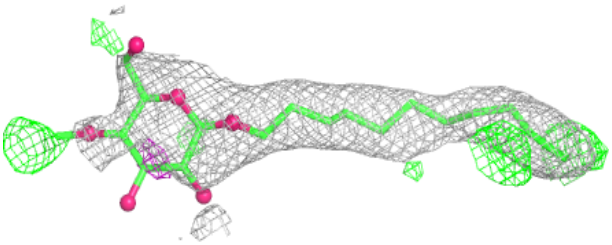


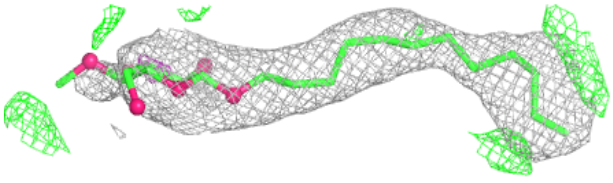


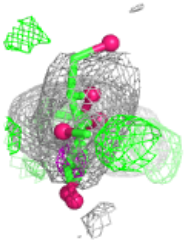


Electron density around LMT b 627:

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

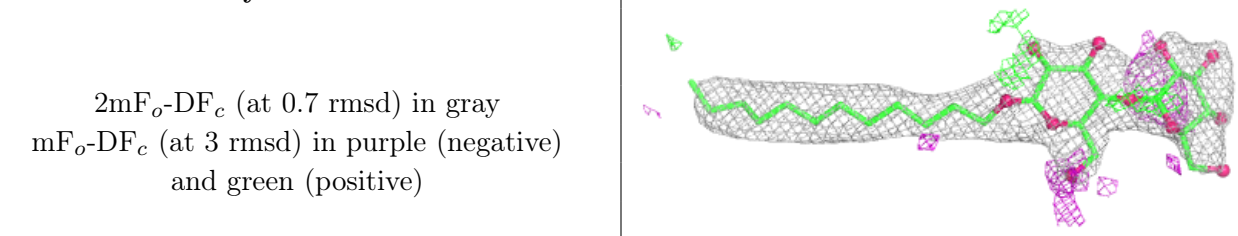


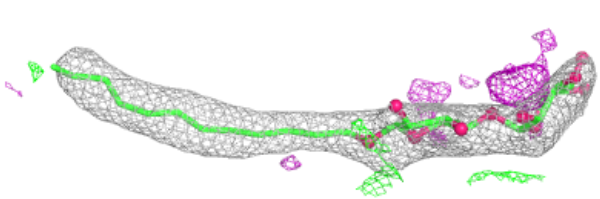


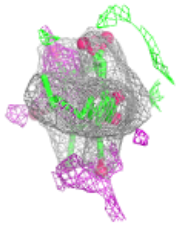


Electron density around LMT m 103:

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

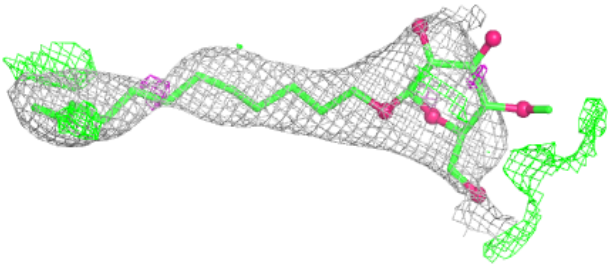


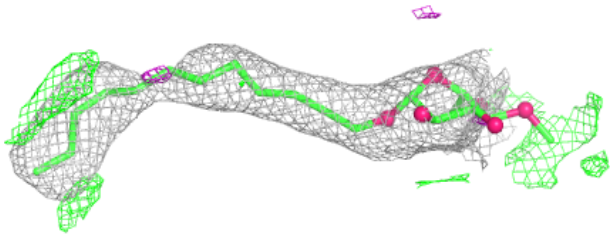


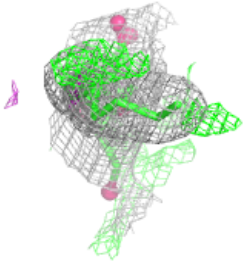


Electron density around LMT t 101:

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

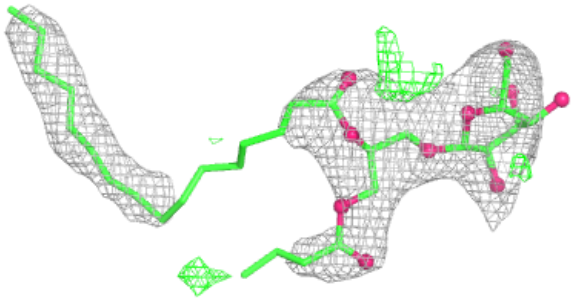


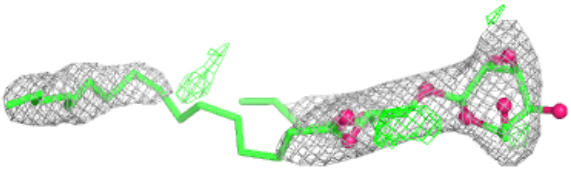


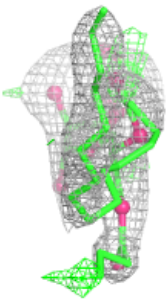


Electron density around LMG z 101:

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

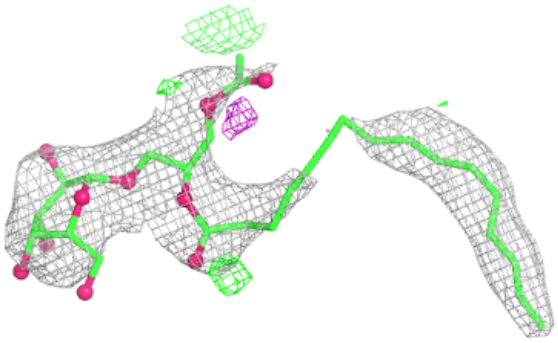


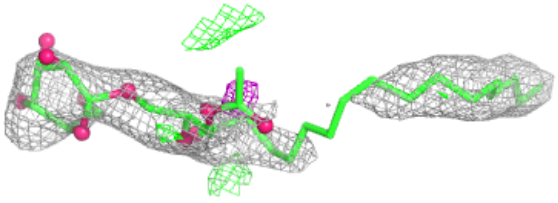


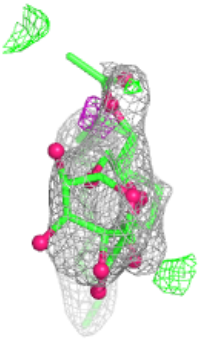


Electron density around LMG Z 101:

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

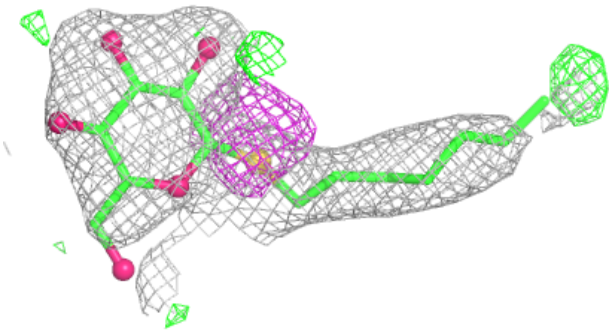


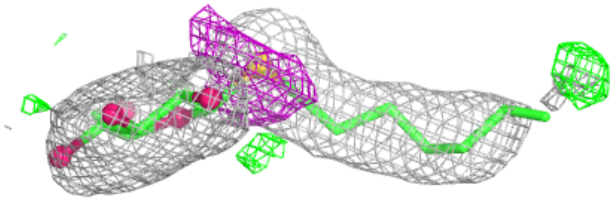


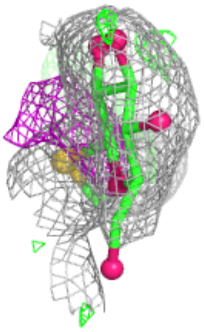


Electron density around HTG b 622:

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

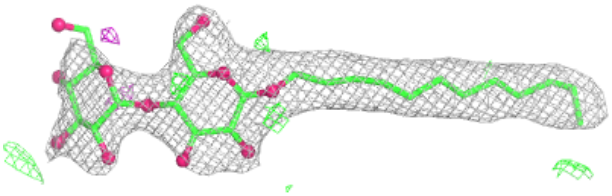


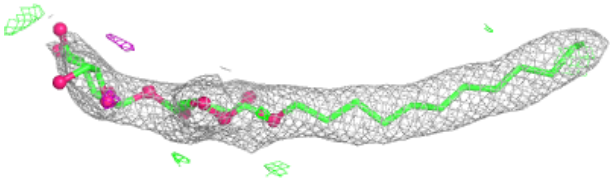


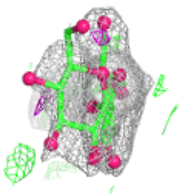


Electron density around LMT M 101:

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

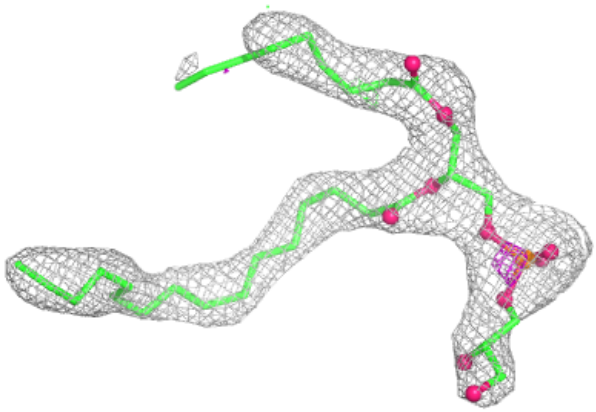


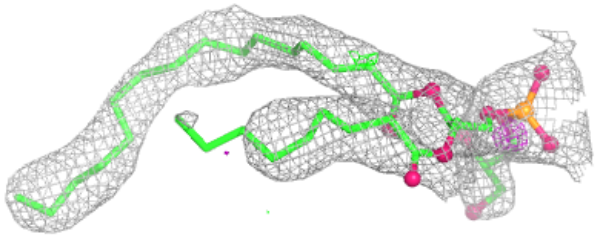


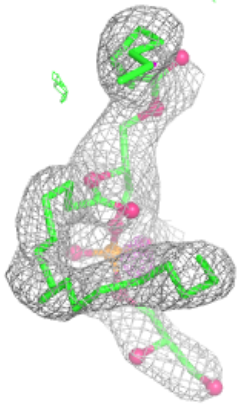


Electron density around LHG E 101 (A):

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

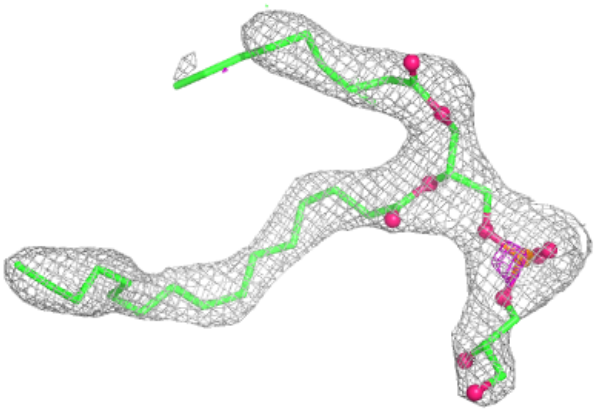


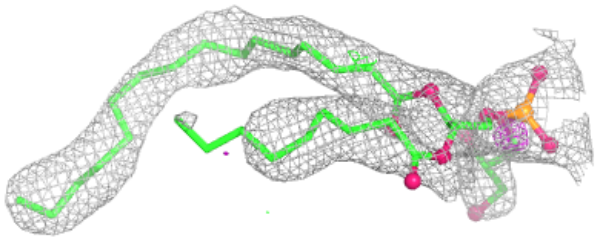


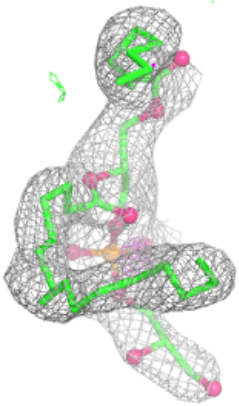


Electron density around LHG E 101 (B):

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

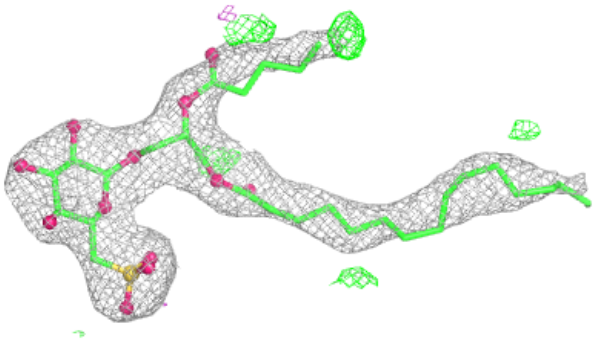


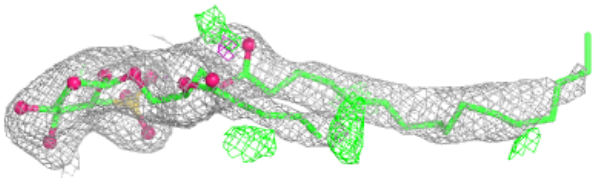


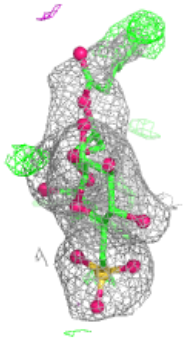


Electron density around SQD F 101:

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

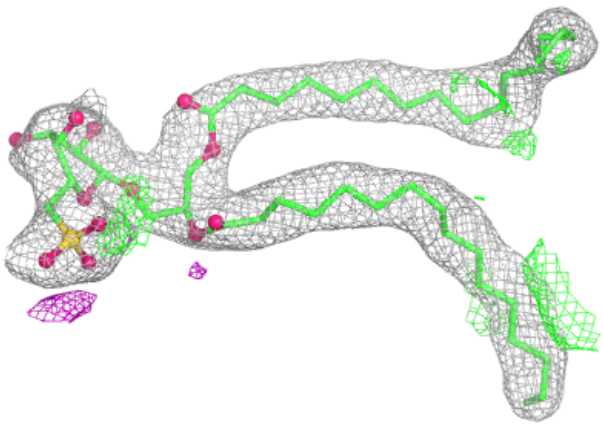


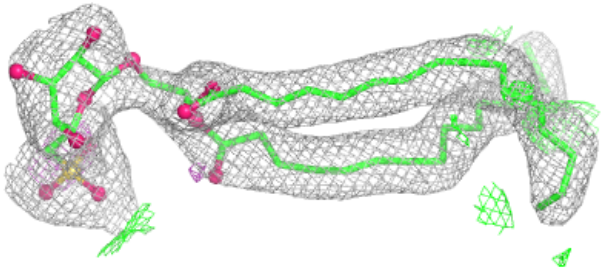


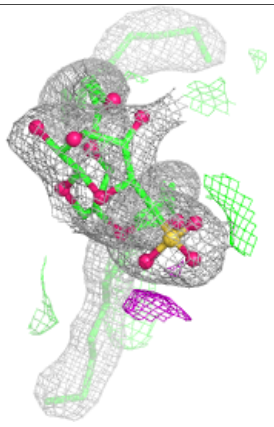


Electron density around SQD B 620:

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

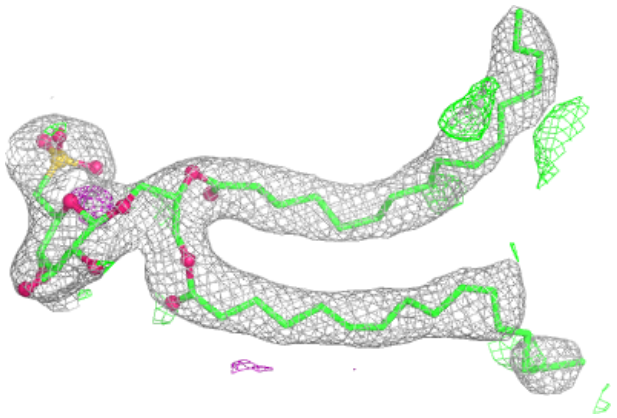


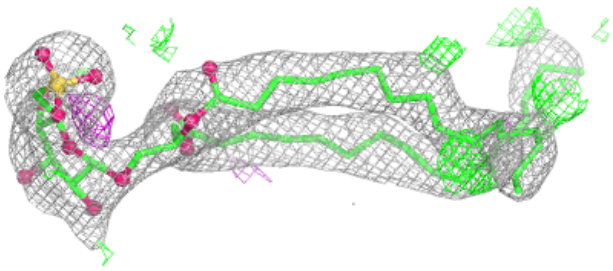


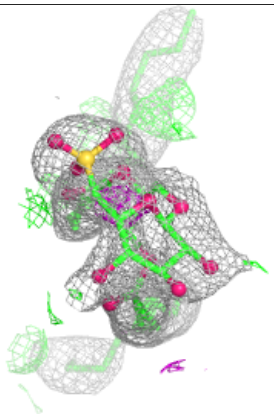


Electron density around SQD b 620:

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

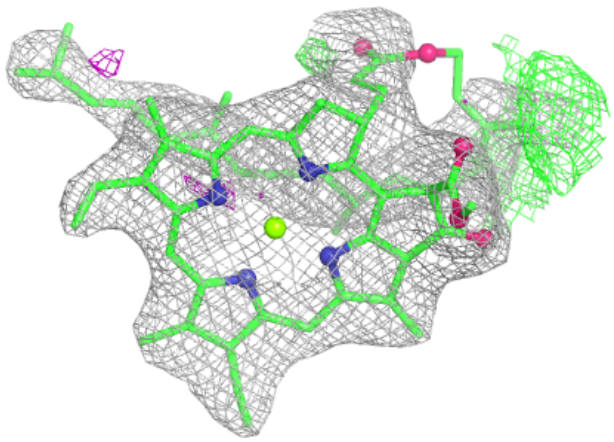


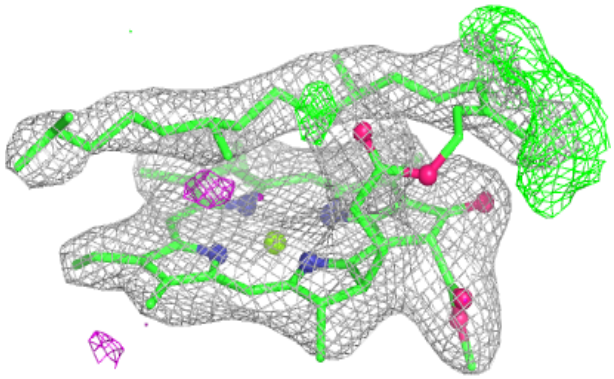


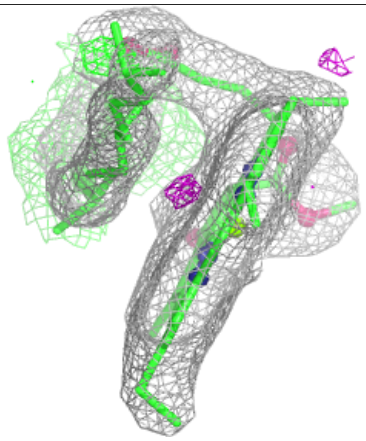


Electron density around CLA b 601:

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

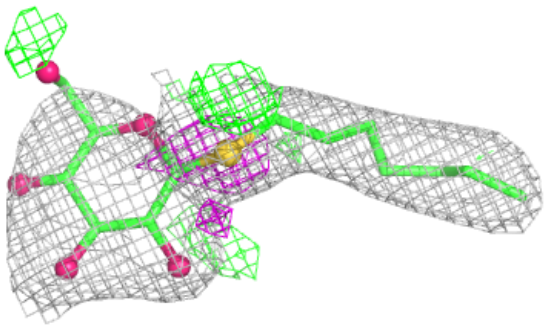


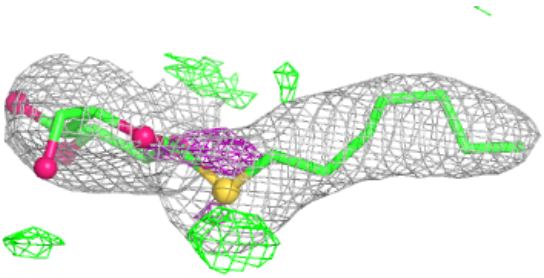


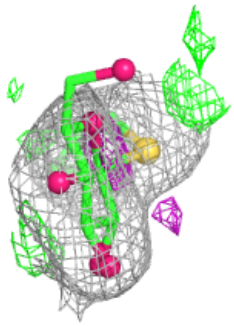


Electron density around HTG B 622:

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

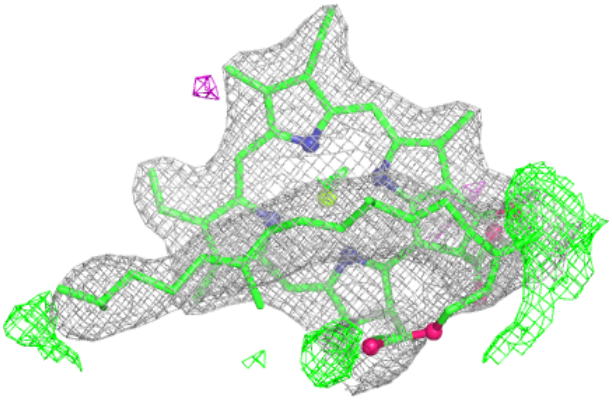


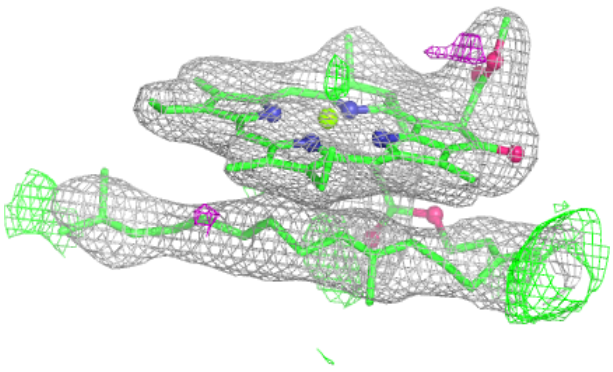


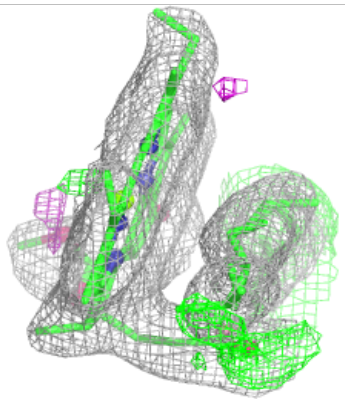


Electron density around CLA B 601:

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

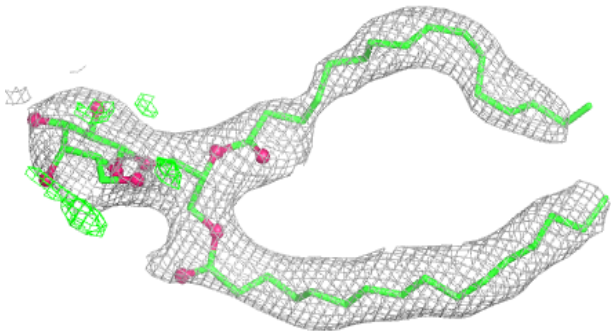


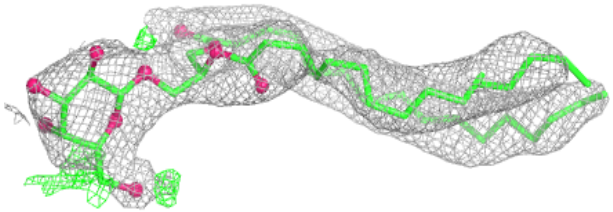


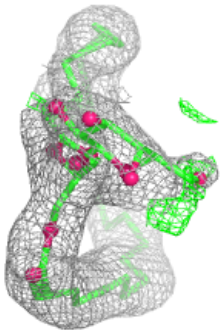


Electron density around LMG C 501:

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

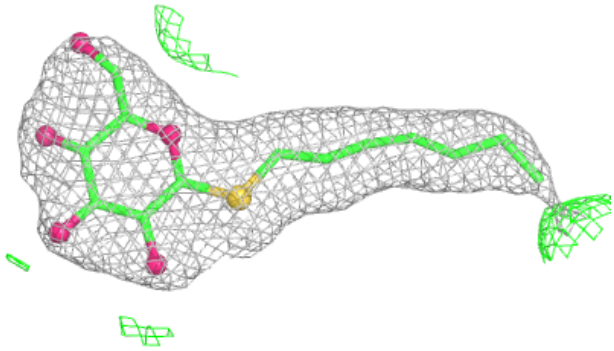


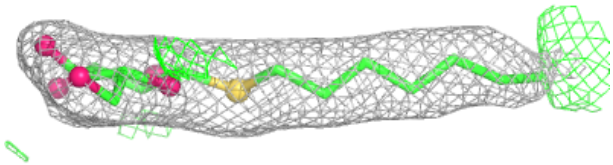


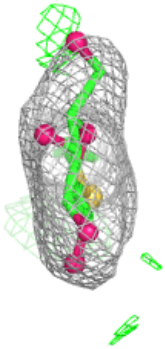


Electron density around HTG B 626:

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

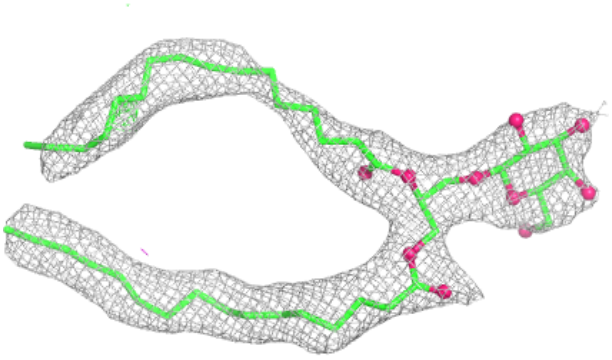


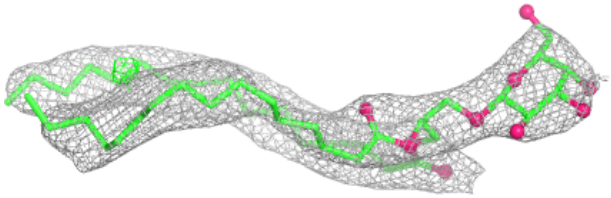


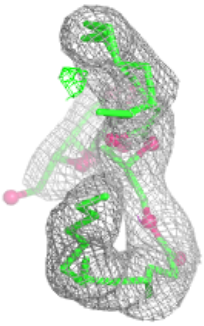


Electron density around LMG a 419:

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

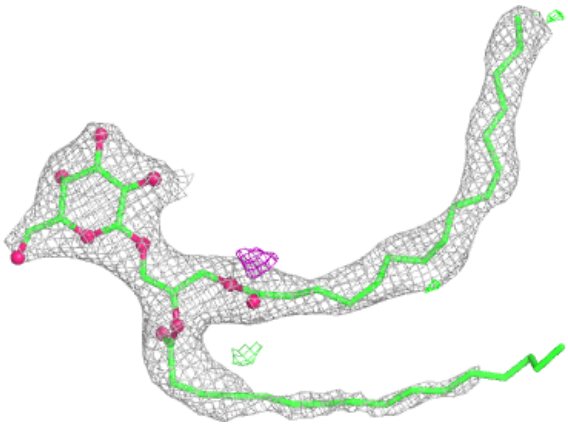


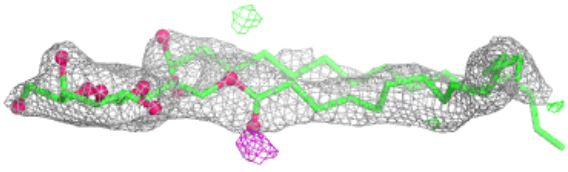


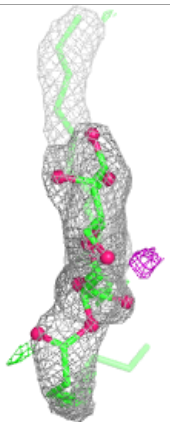


Electron density around LMG c 520:

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

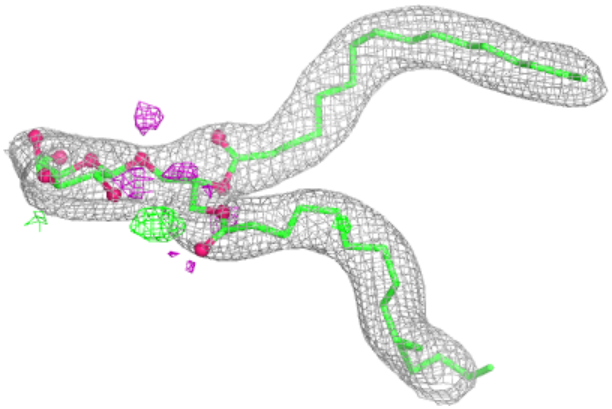


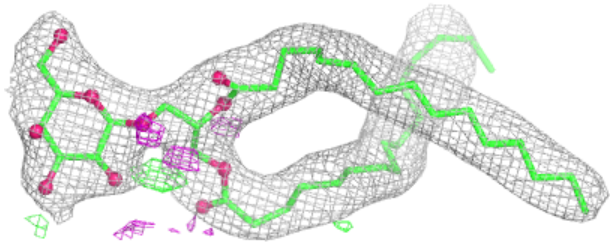


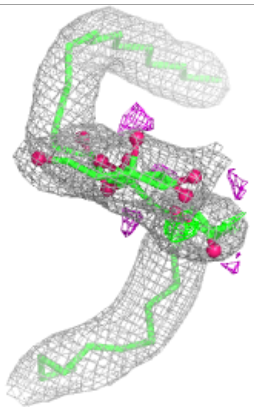


Electron density around LMG m 101:

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

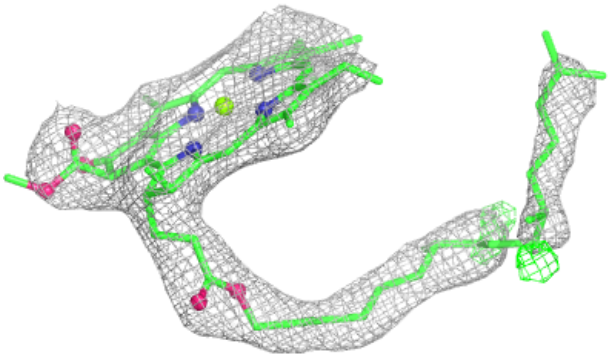


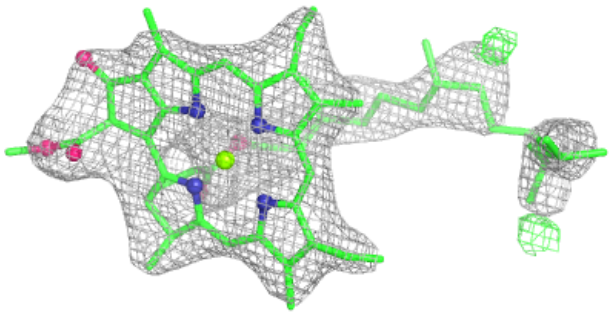


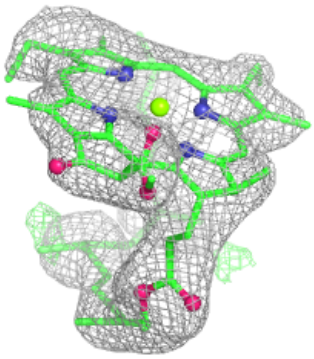


Electron density around CLA c 514:

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

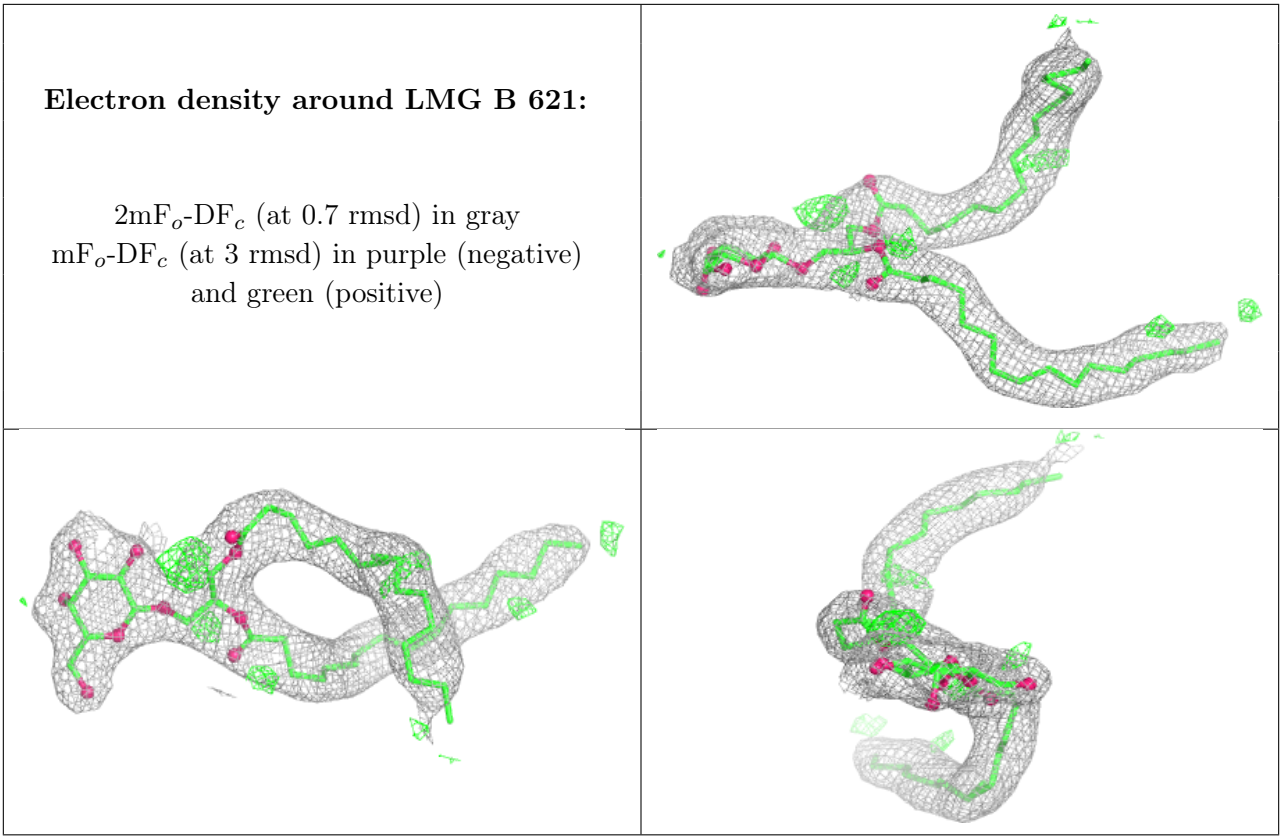






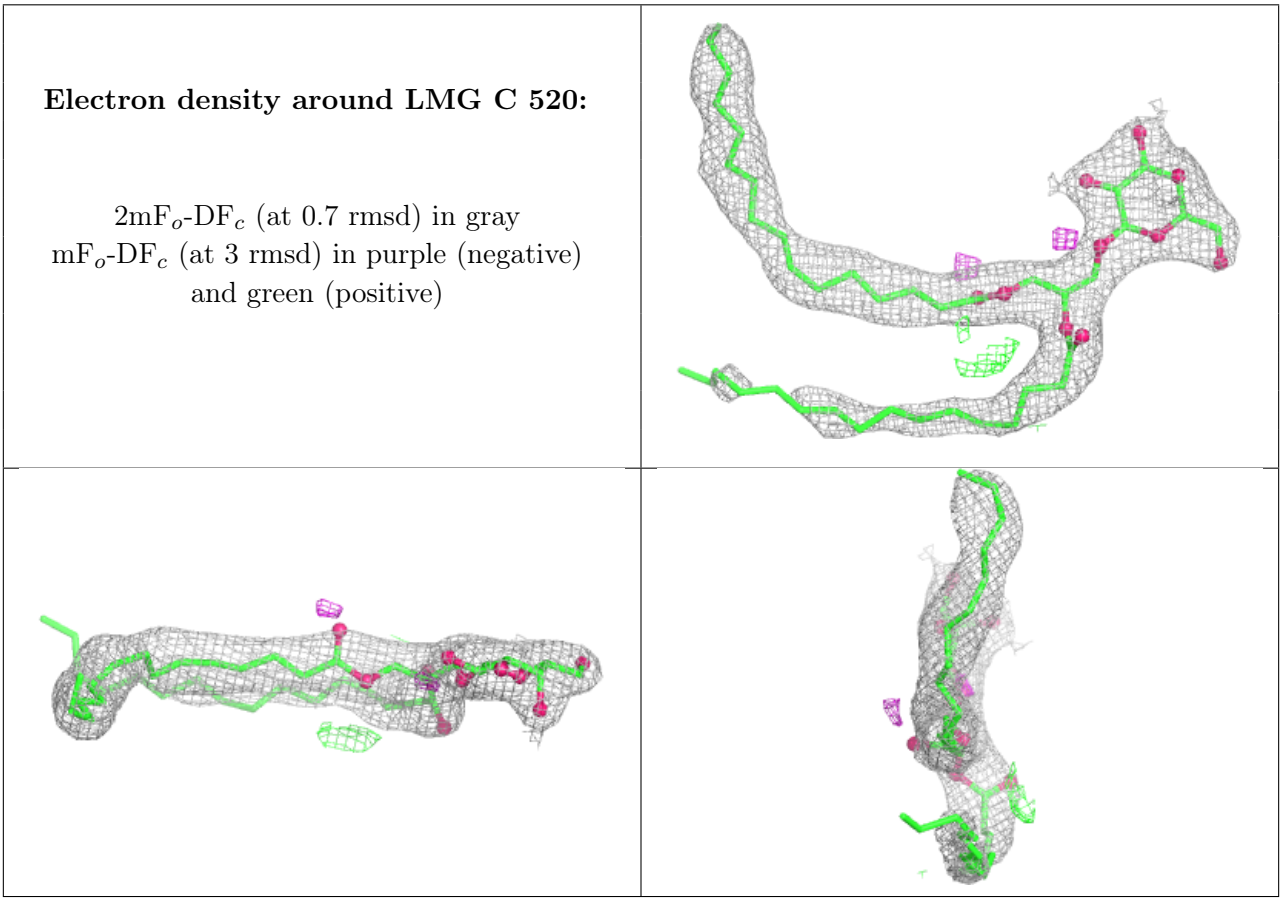
Electron density around LMG B 621:

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



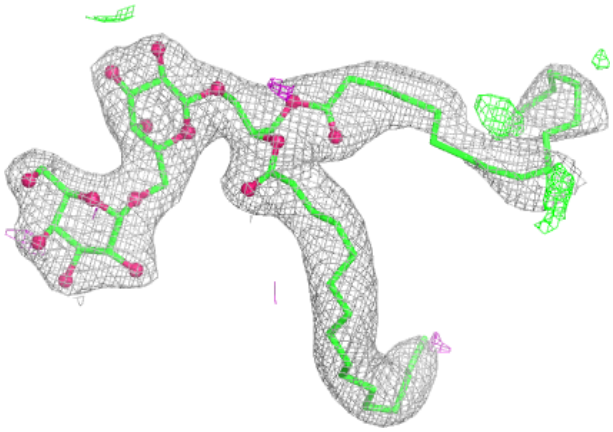
Electron density around LMG C 520:

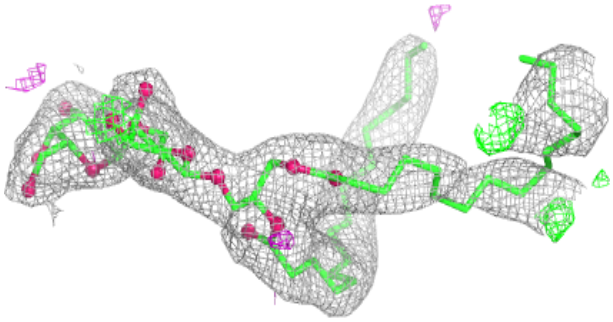
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

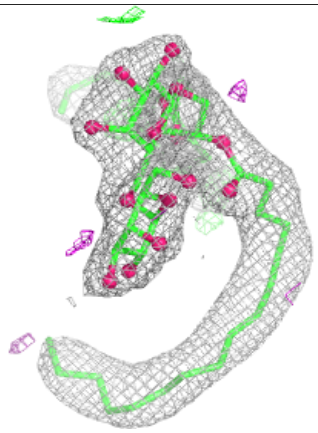


Electron density around DGD C 518 (A):

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

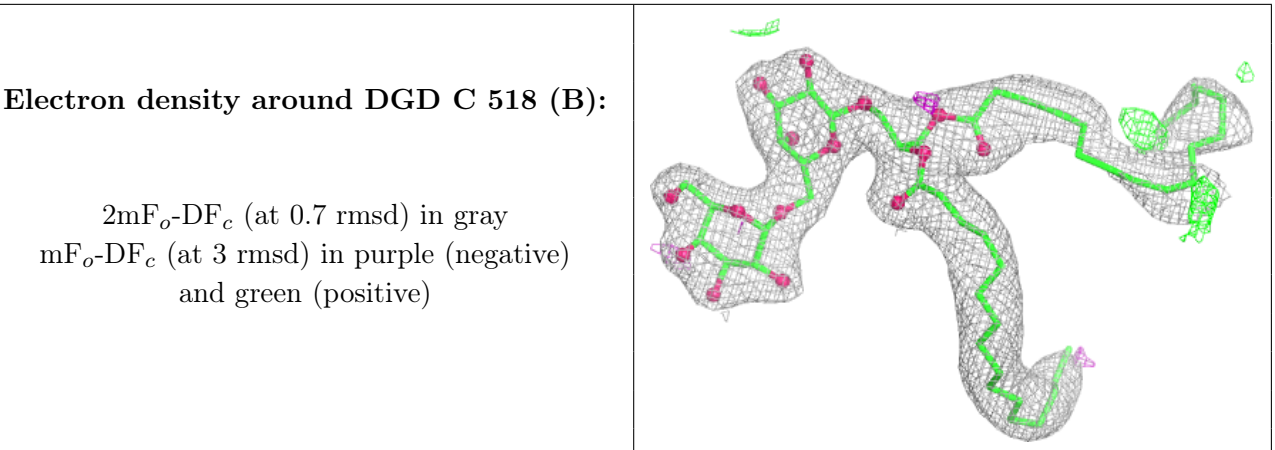






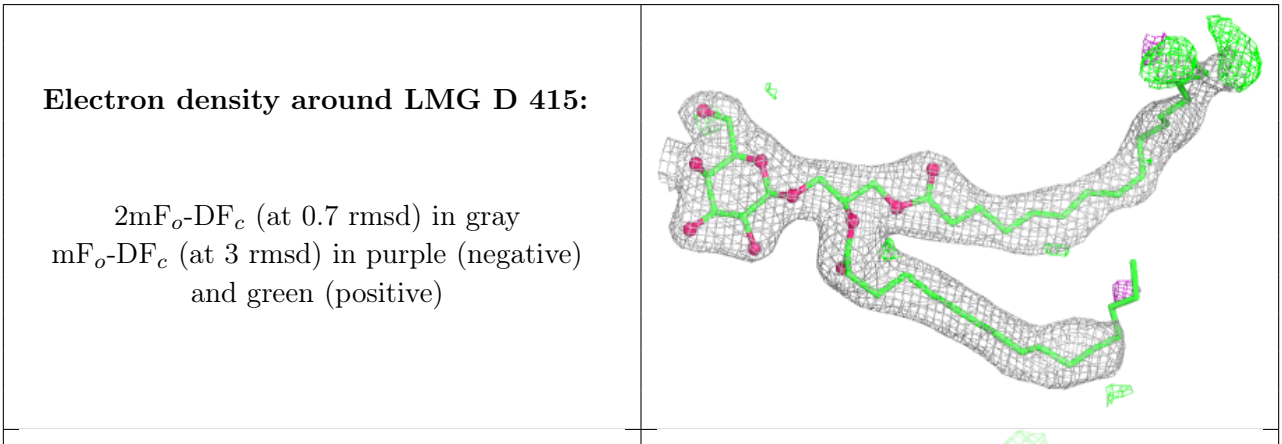
Electron density around DGD C 518 (B):

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



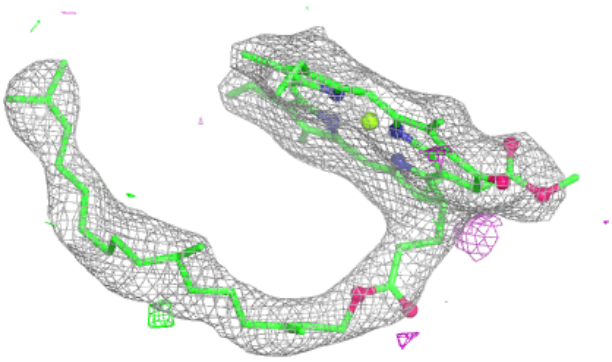
Electron density around LMG D 415:

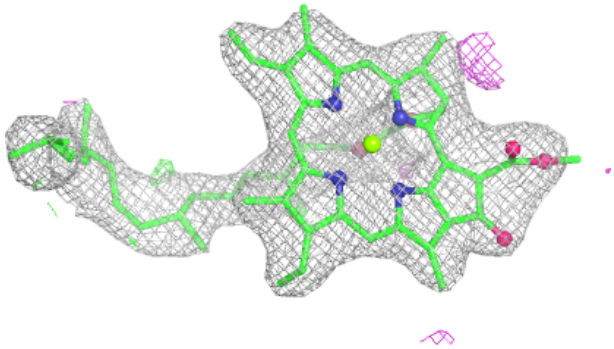
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

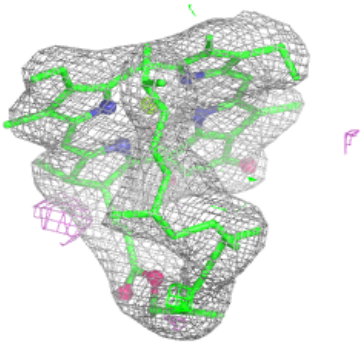


Electron density around CLA C 514:

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

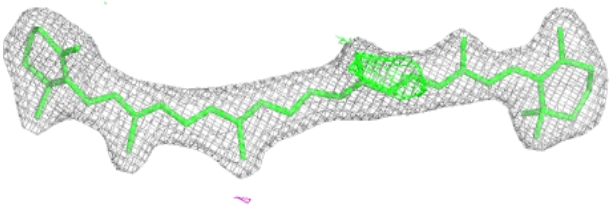


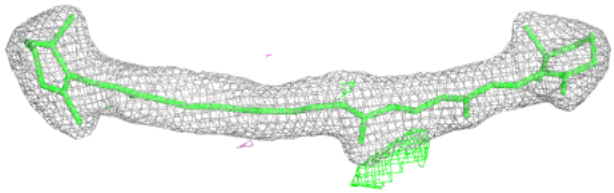


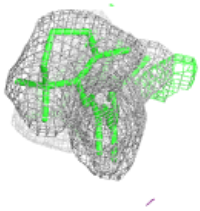


Electron density around BCR T 101:

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

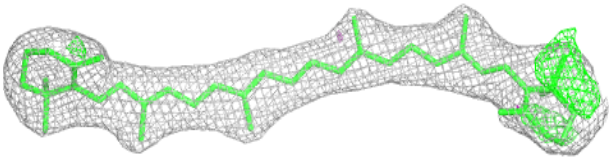


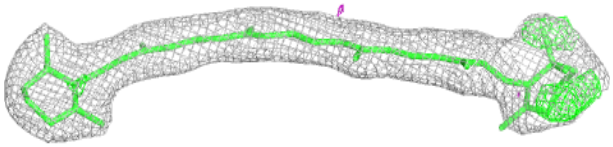


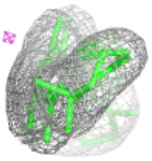


Electron density around BCR d 404:

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

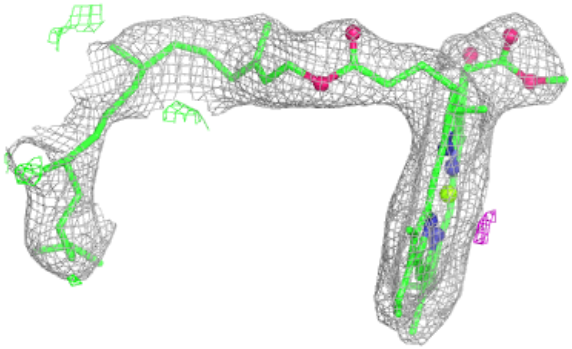


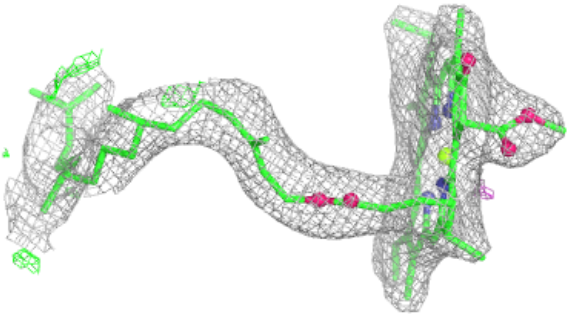


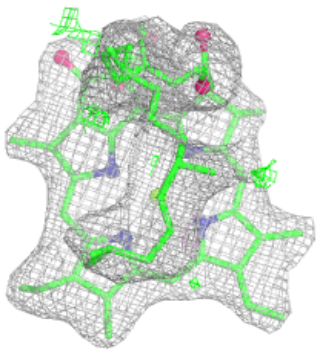


Electron density around CLA C 507:

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

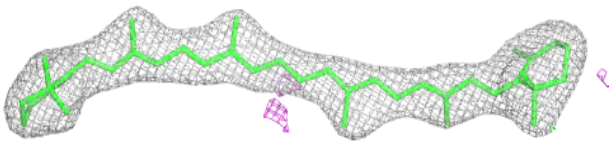


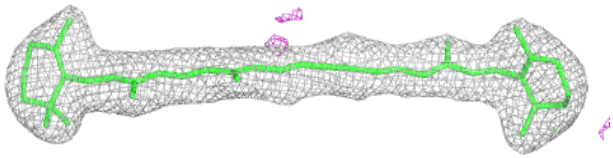


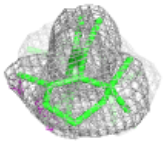


Electron density around BCR C 515:

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

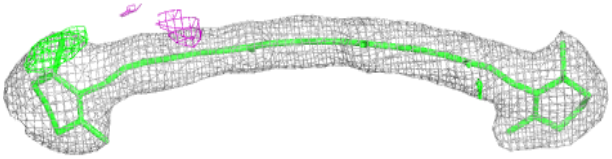


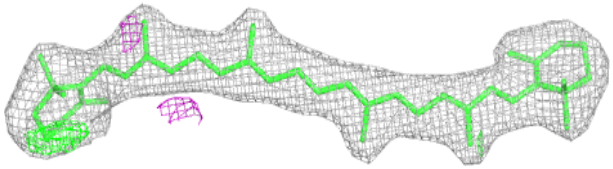


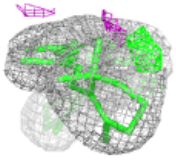


Electron density around BCR D 407:

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

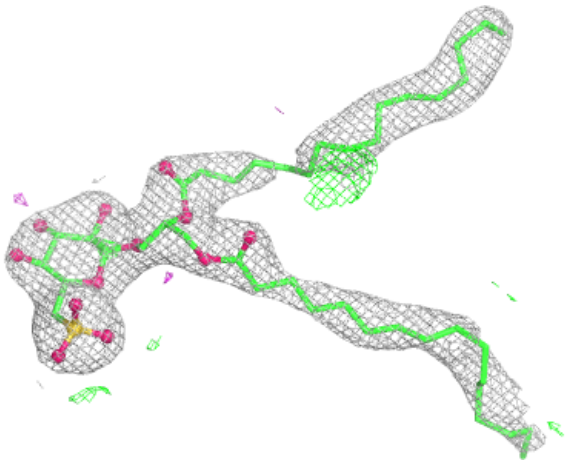


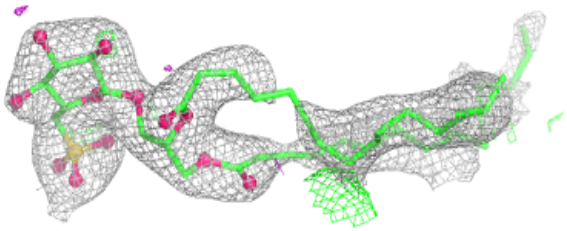


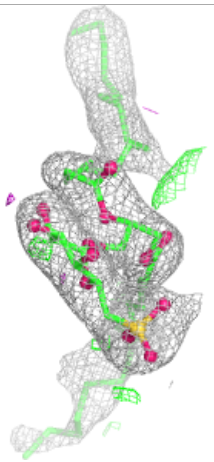


Electron density around SQD a 411 (A):

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

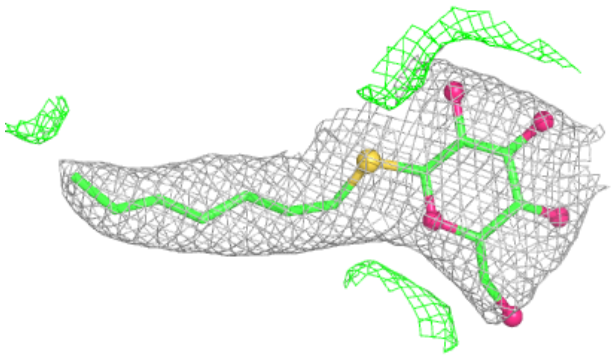


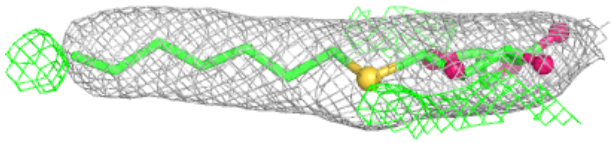


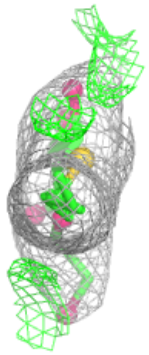


Electron density around HTG b 625:

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

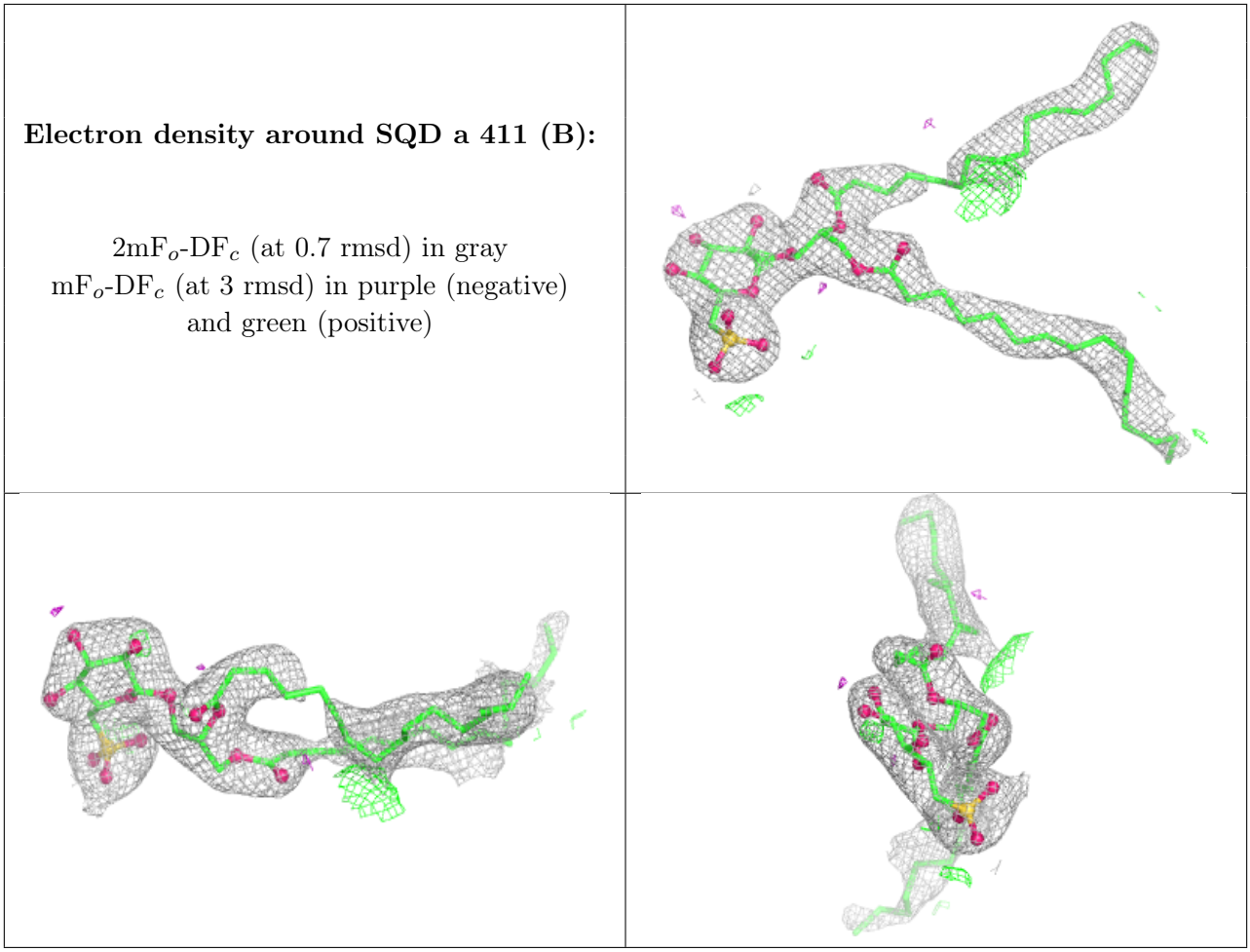






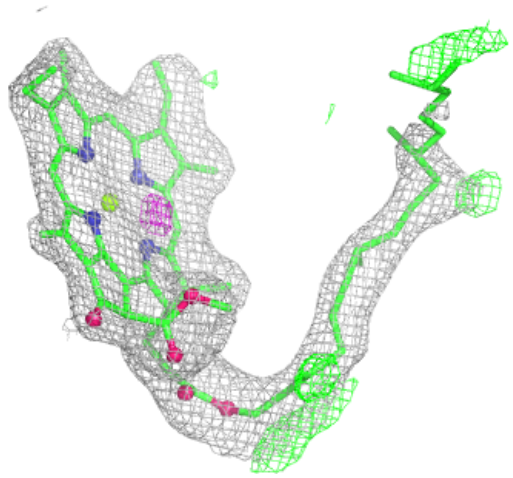
Electron density around SQD a 411 (B):

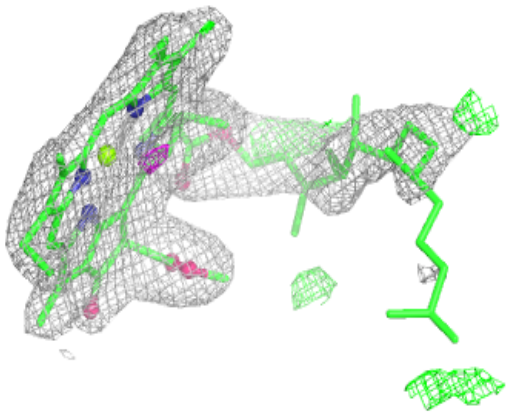
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

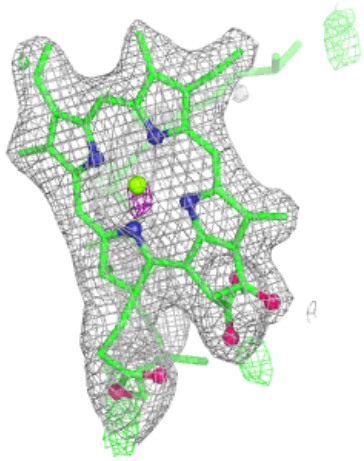


Electron density around CLA b 616:

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

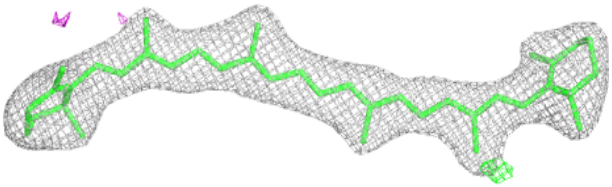


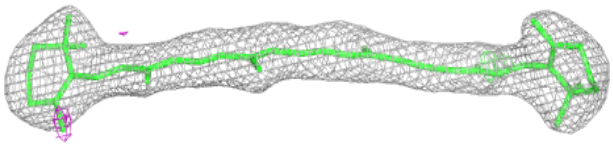


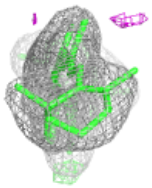


Electron density around BCR Y 101:

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

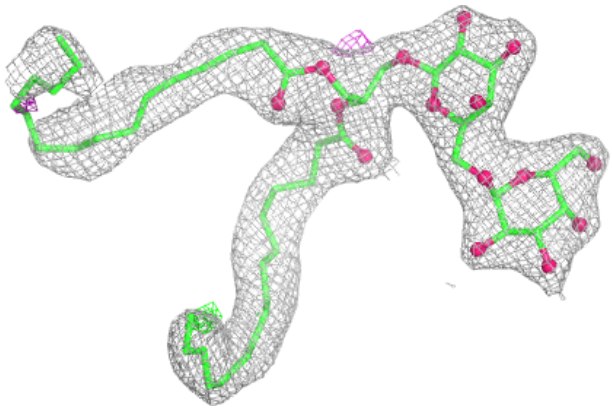


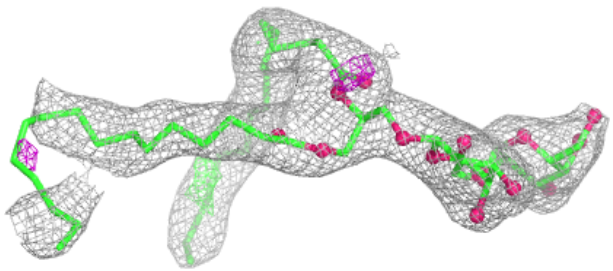


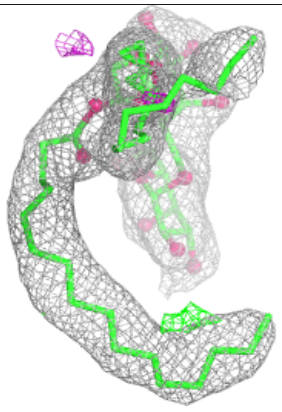


Electron density around DGD c 518 (A):

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

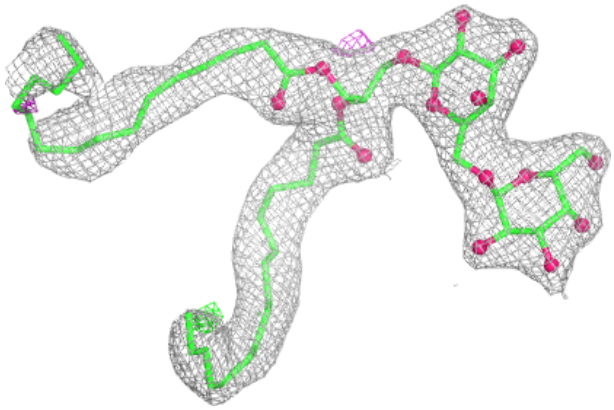


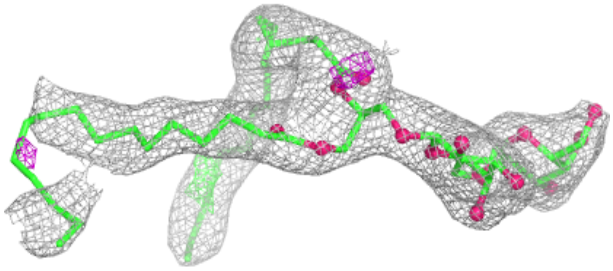


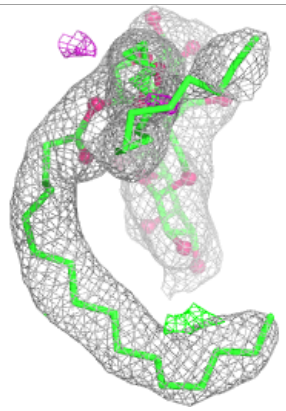


Electron density around DGD c 518 (B):

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

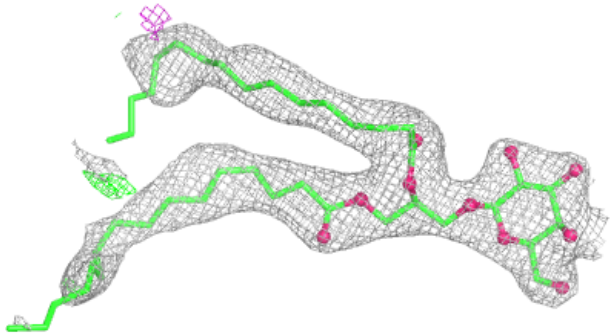


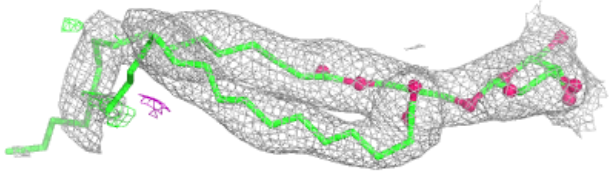


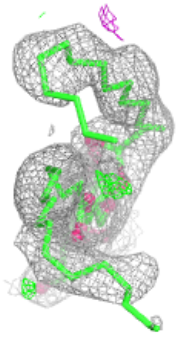


Electron density around LMG d 412:

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

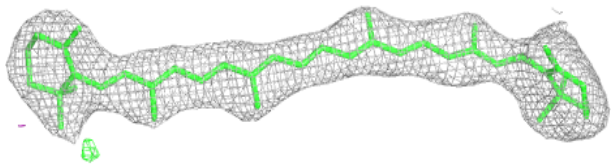


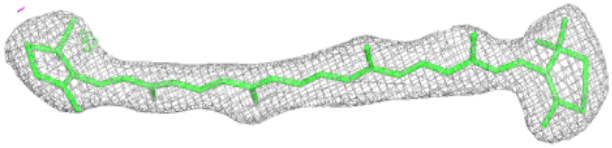


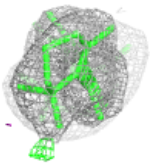


Electron density around BCR c 515:

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

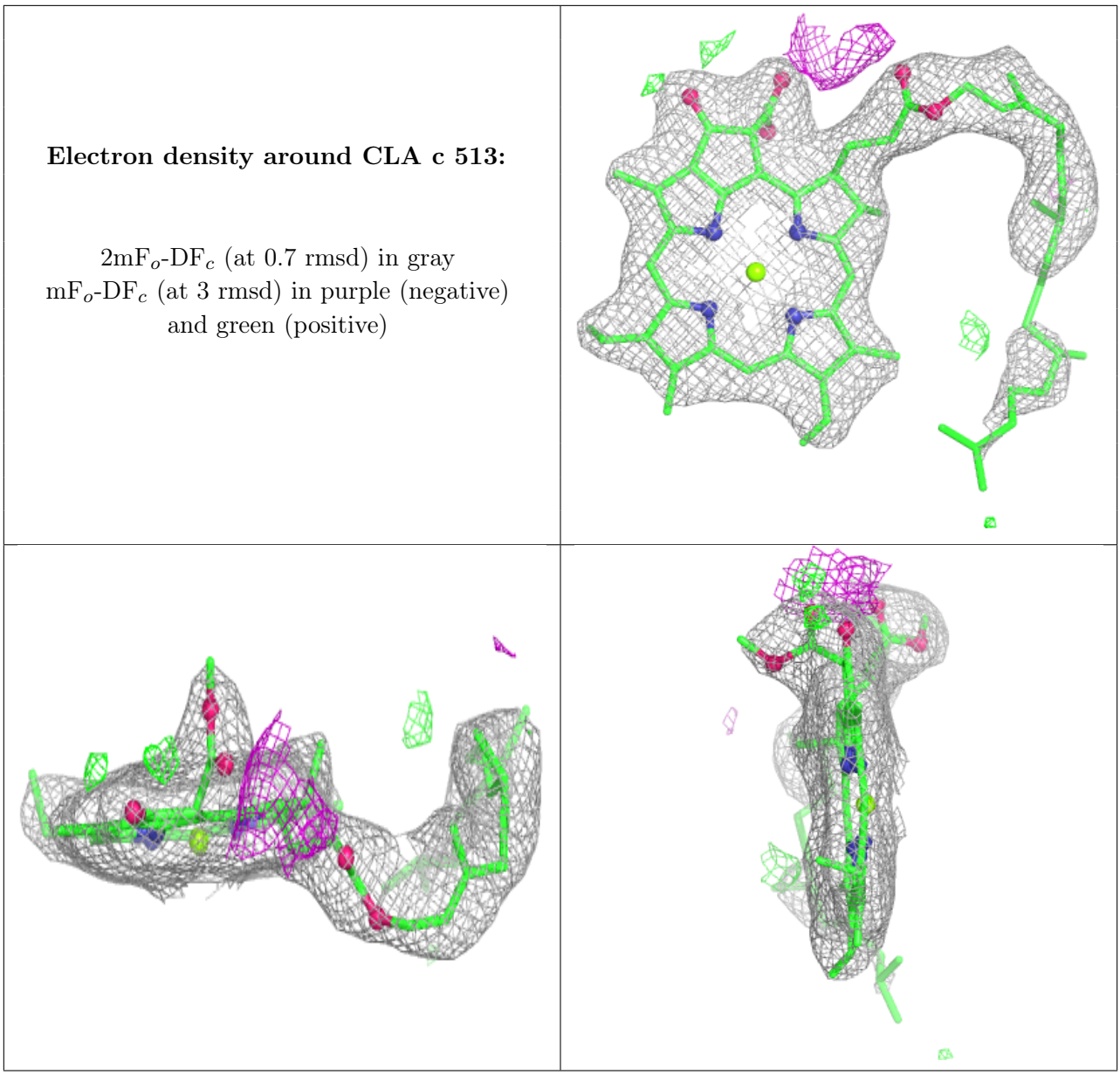






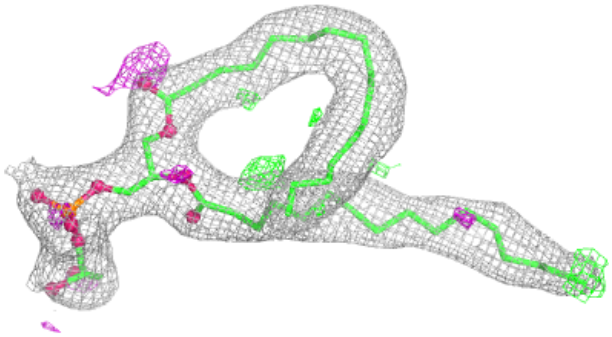
Electron density around CLA c 513:

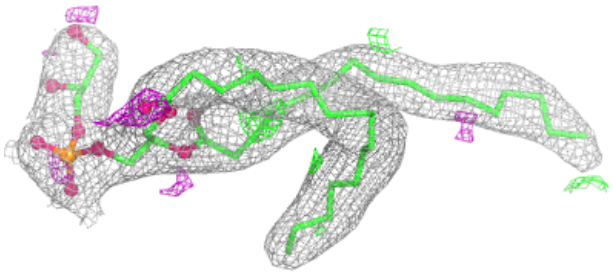
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LHG D 409 (A):

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

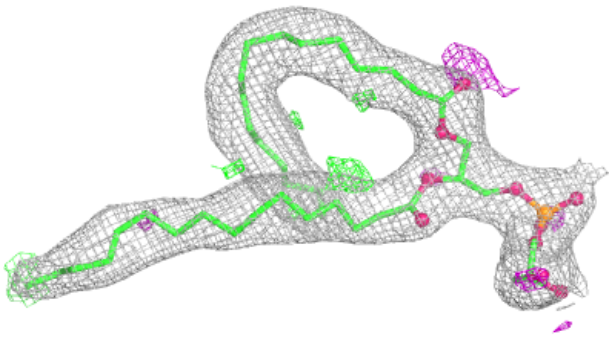


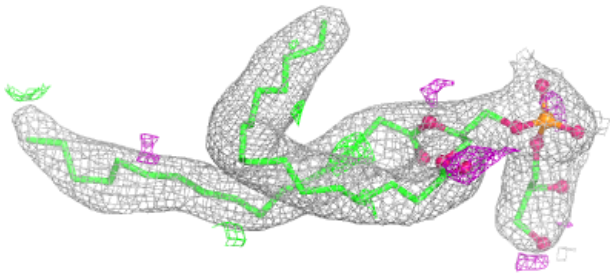


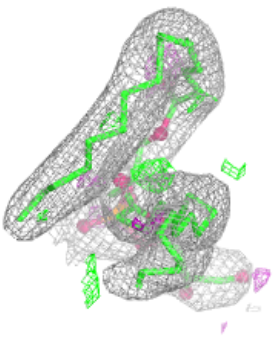


Electron density around LHG D 409 (B):

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

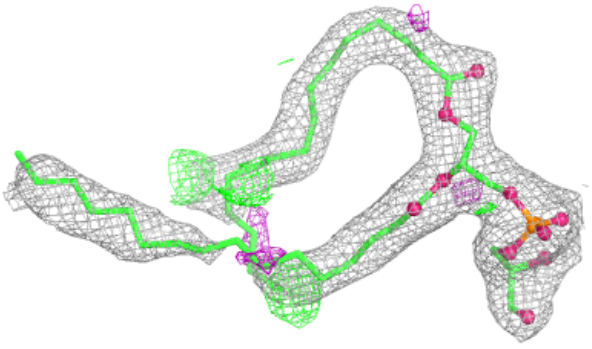


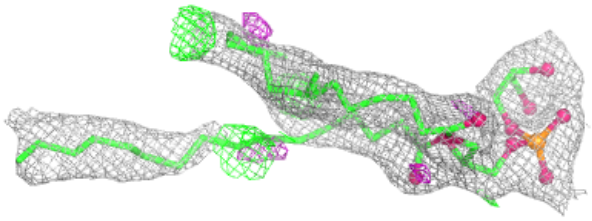


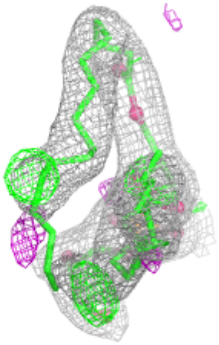


Electron density around LHG D 411 (A):

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

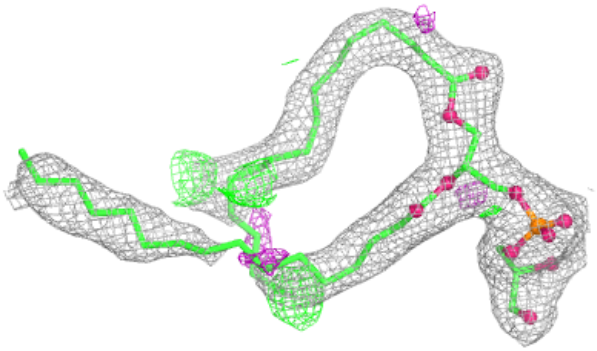


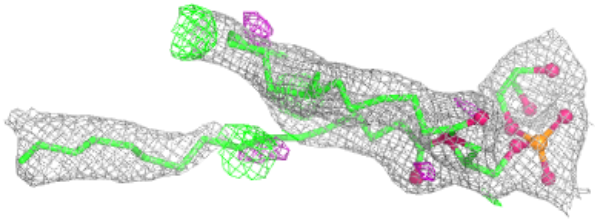


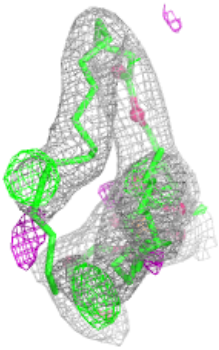


Electron density around LHG D 411 (B):

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

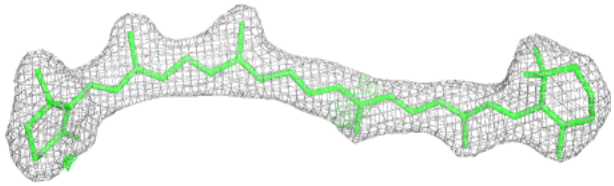


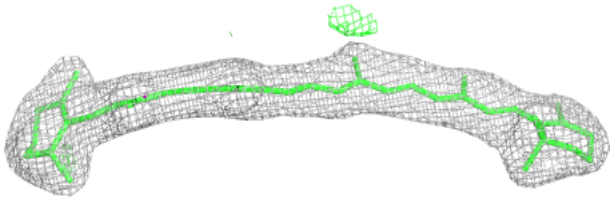


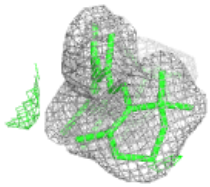


Electron density around BCR t 103:

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

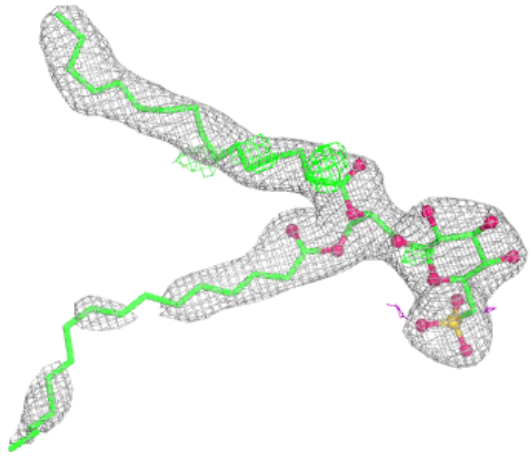


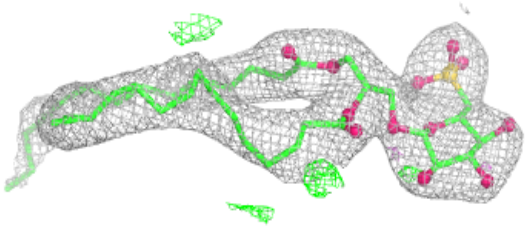


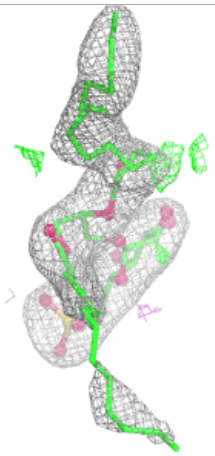


Electron density around SQD A 410 (A):

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

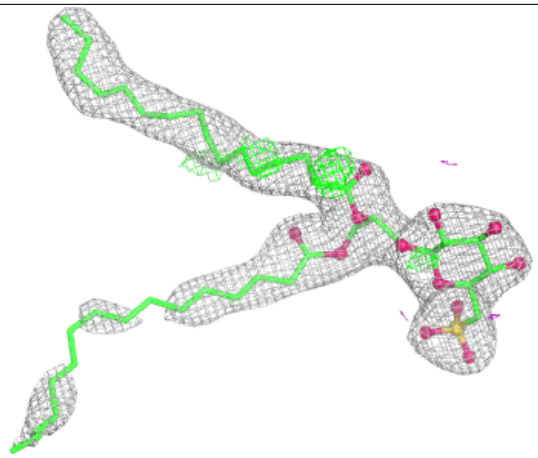


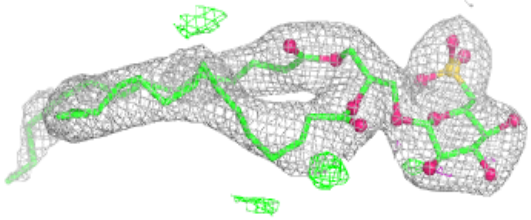


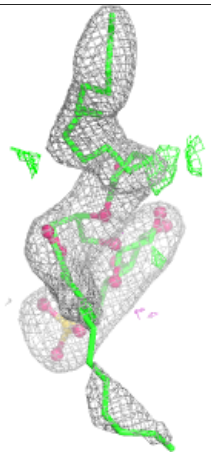


Electron density around SQD A 410 (B):

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

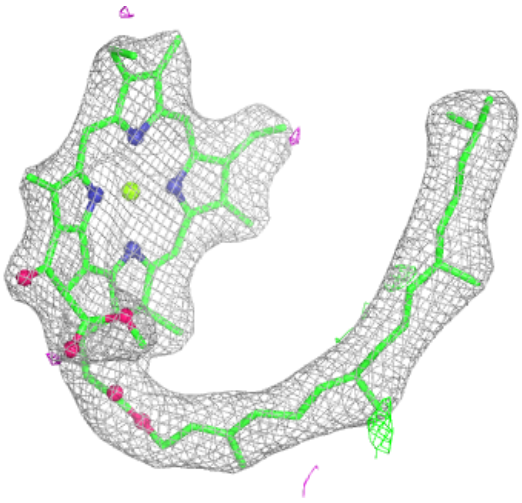


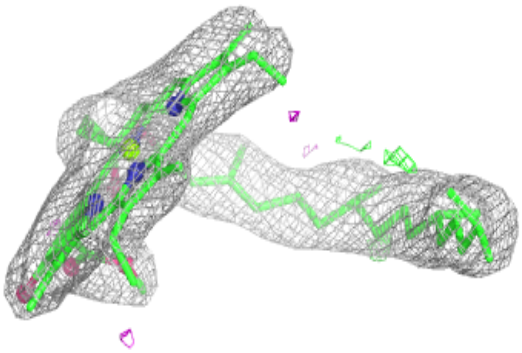


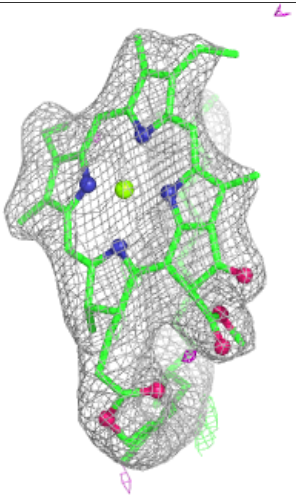


Electron density around CLA c 508:

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

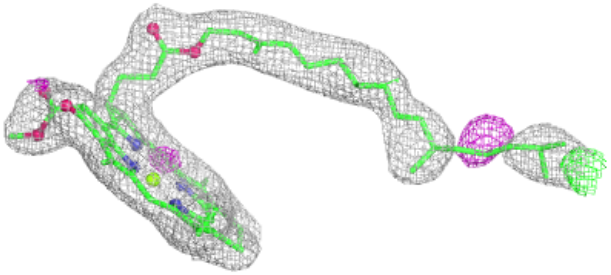


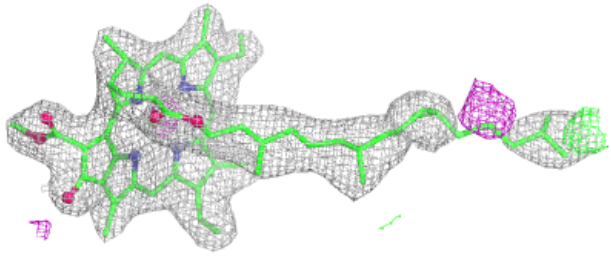


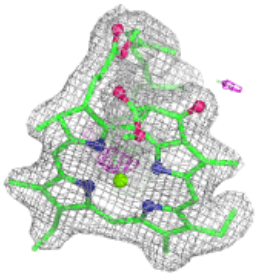


Electron density around CLA C 505:

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

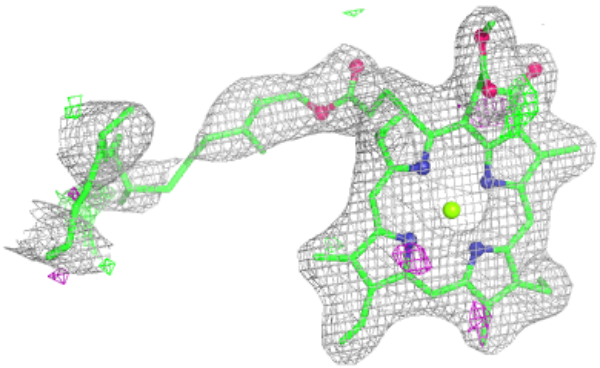


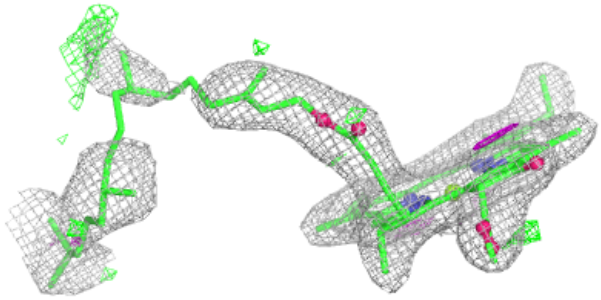


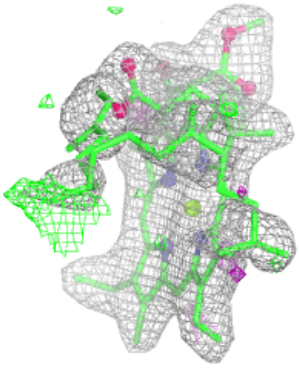


Electron density around CLA A 408:

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

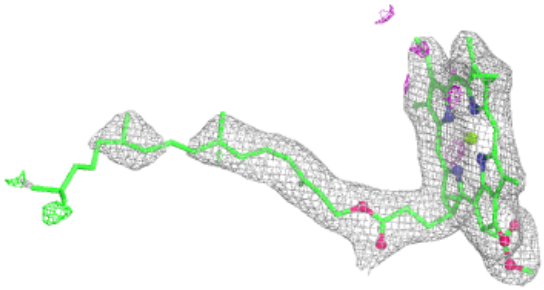


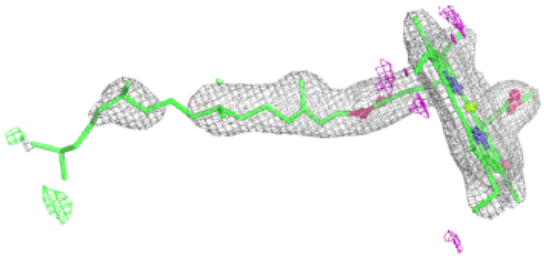


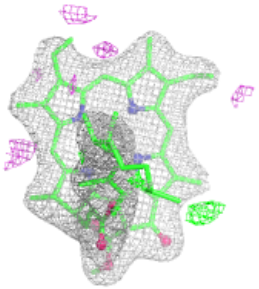


Electron density around CLA d 403:

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

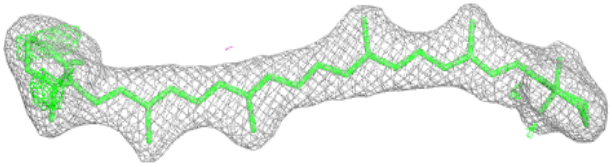


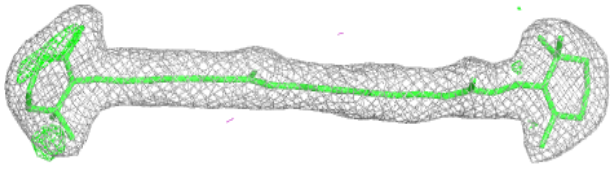


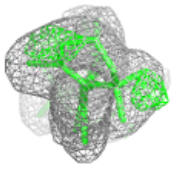


Electron density around BCR A 409:

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

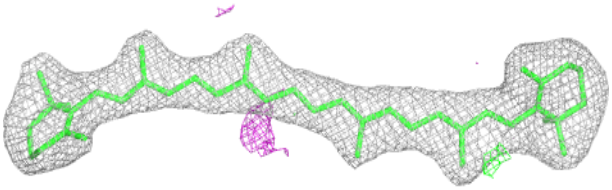


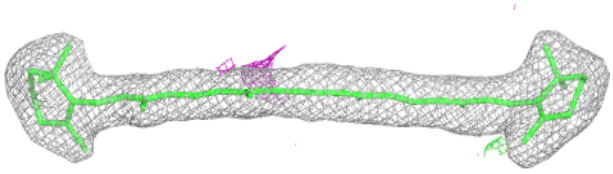


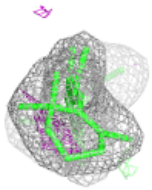


Electron density around BCR B 618:

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

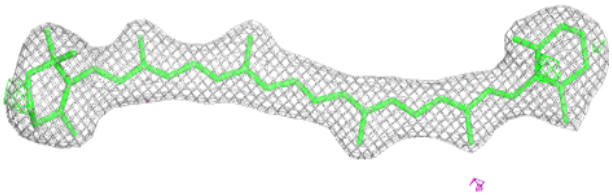


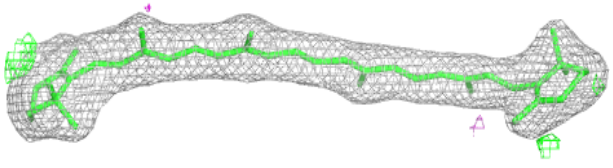


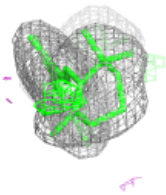


Electron density around BCR B 619:

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

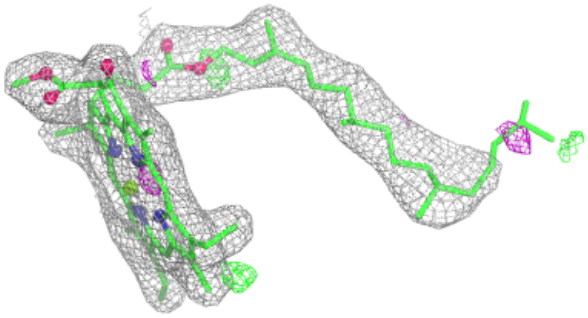


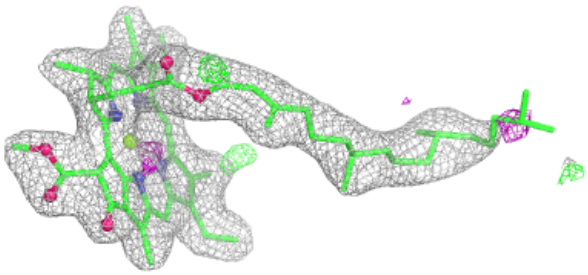


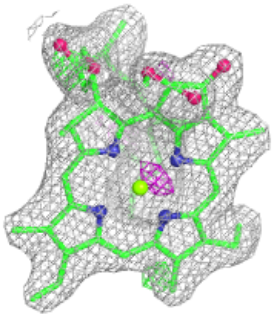


Electron density around CLA C 509:

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

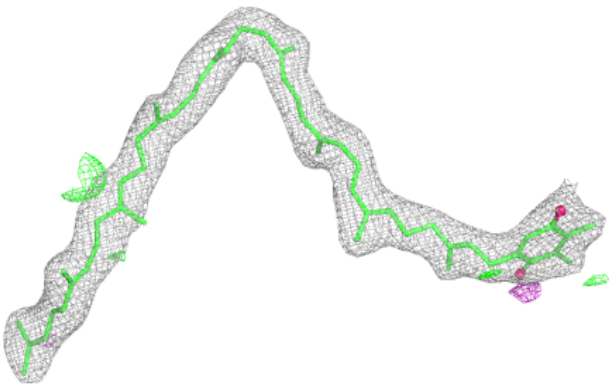


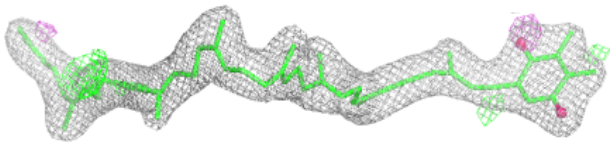


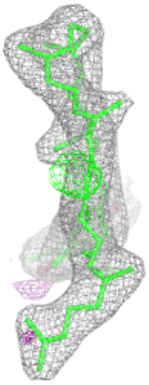


Electron density around PL9 D 408 (A):

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

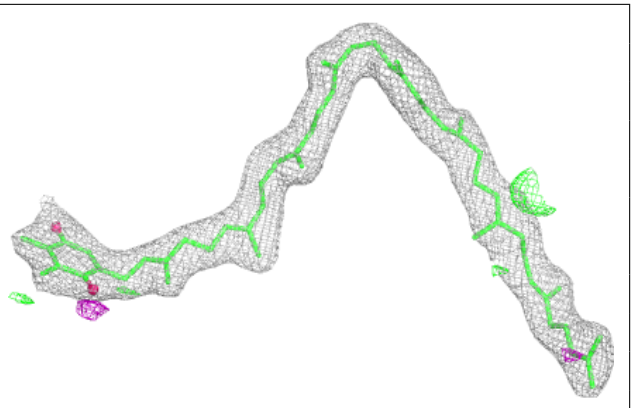


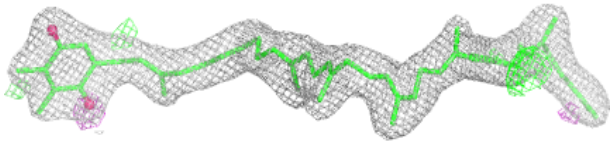




Electron density around PL9 D 408 (B):

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

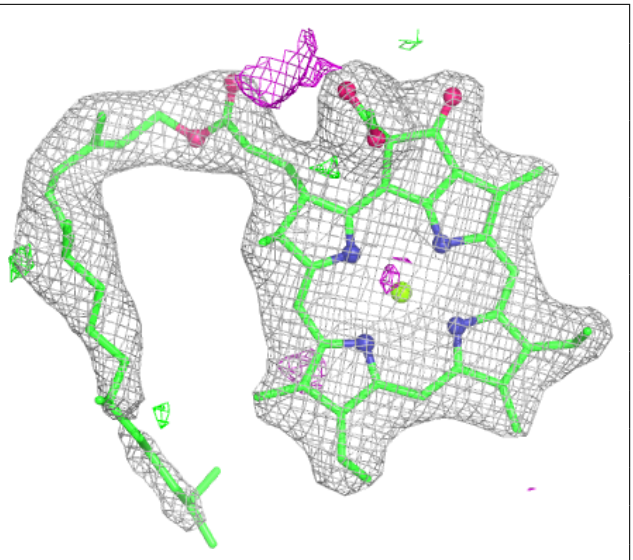


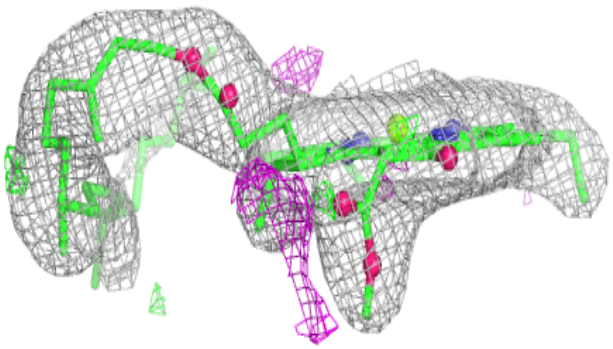


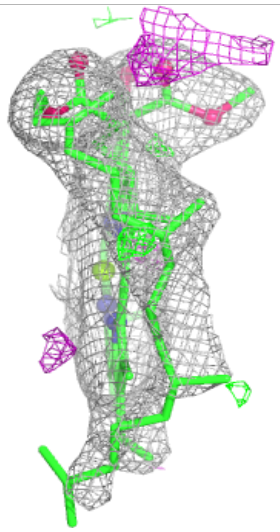


Electron density around CLA C 513:

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

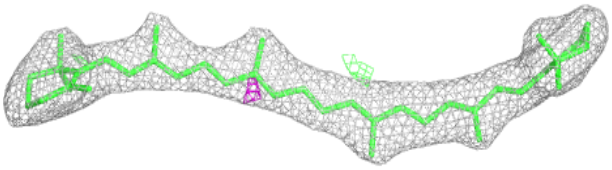


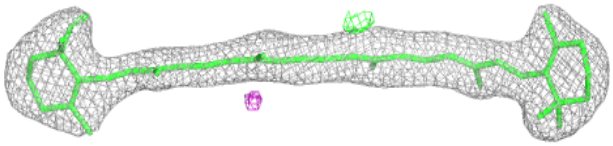


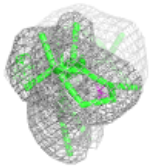


Electron density around BCR H 101:

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

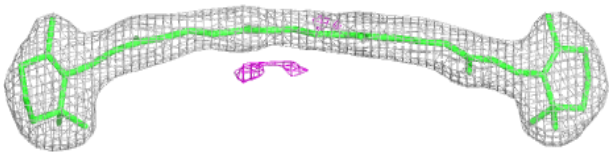


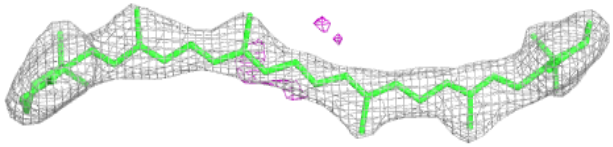


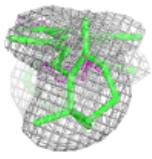


Electron density around BCR K 102:

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

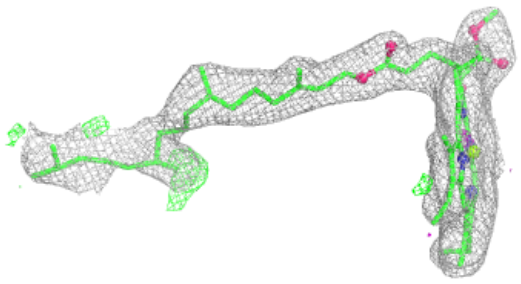


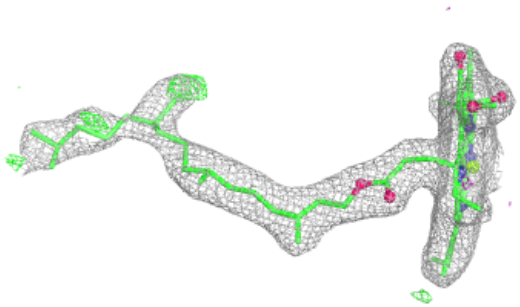


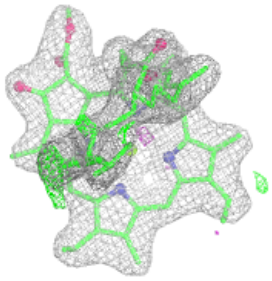


Electron density around CLA B 606:

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

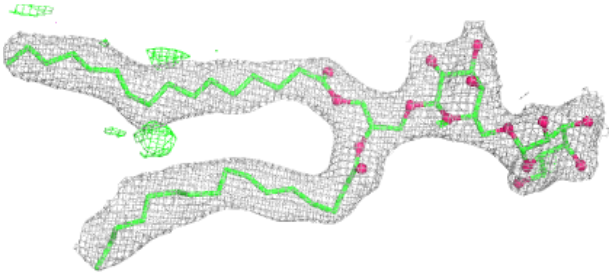


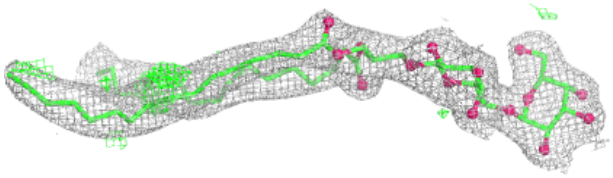


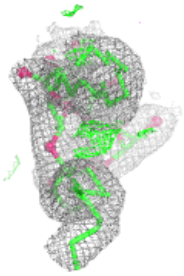


Electron density around DGD C 519:

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

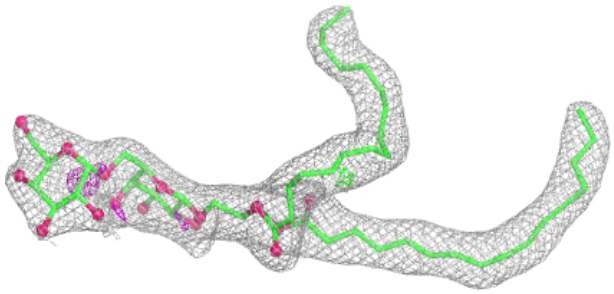


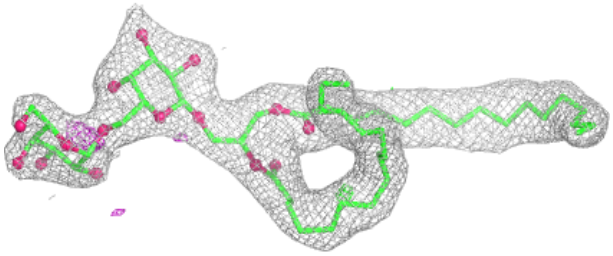


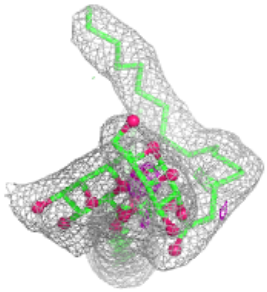


Electron density around DGD H 102:

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

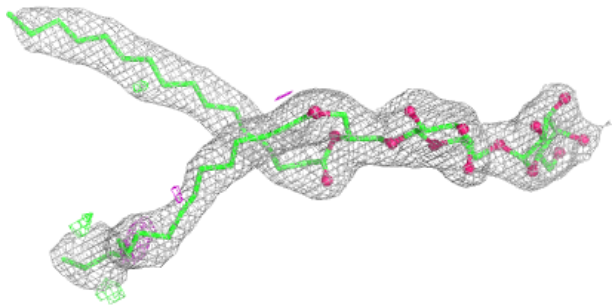


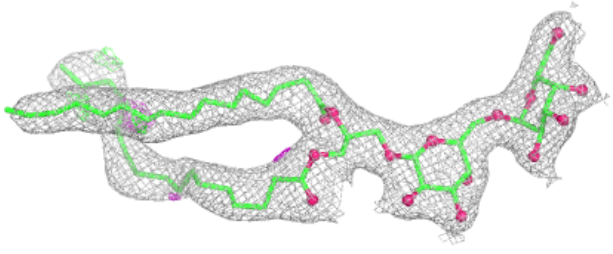


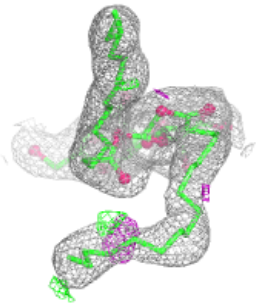


Electron density around DGD c 517 (A):

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

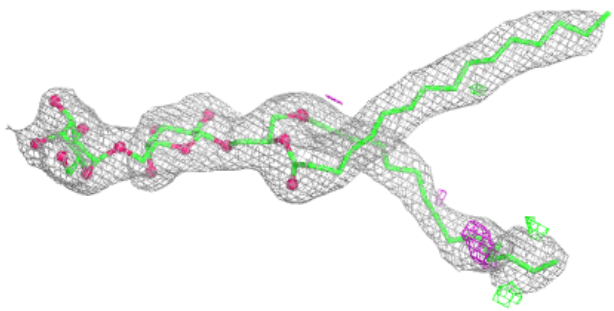


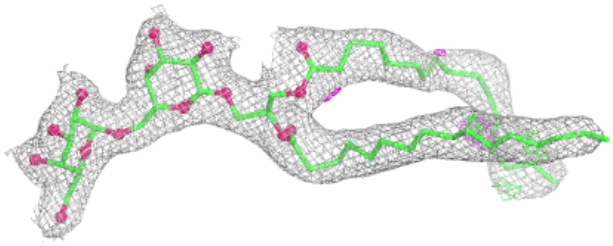


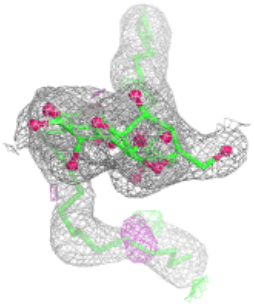


Electron density around DGD c 517 (B):

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

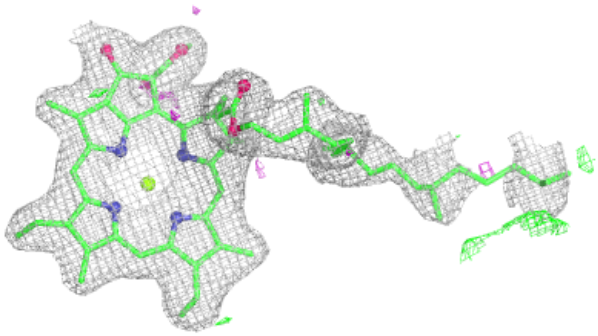


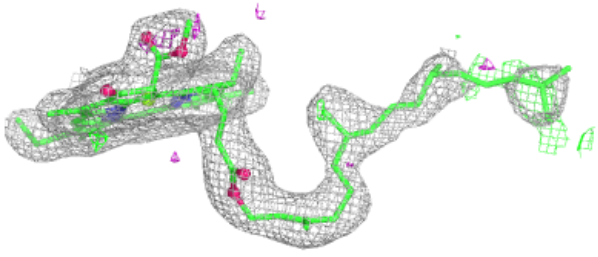


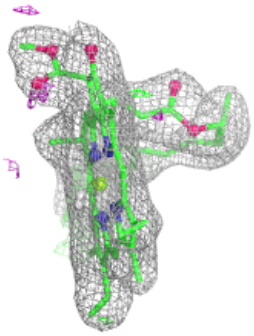


Electron density around CLA a 407 (A):

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

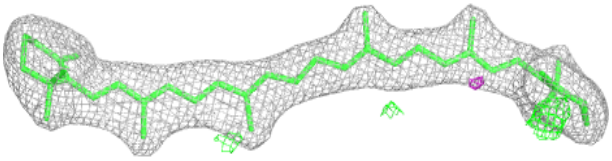


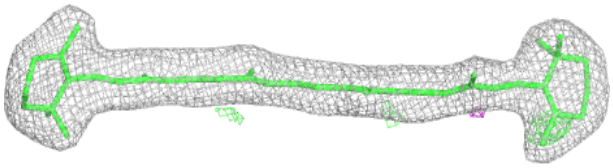


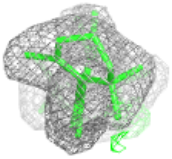


Electron density around BCR a 410:

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

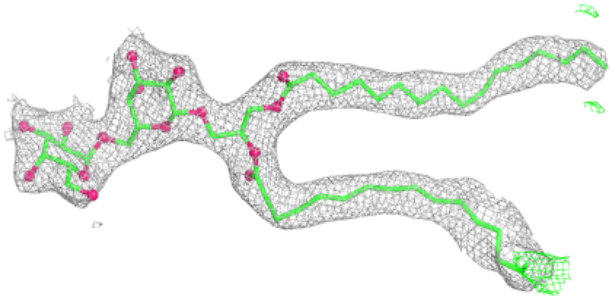


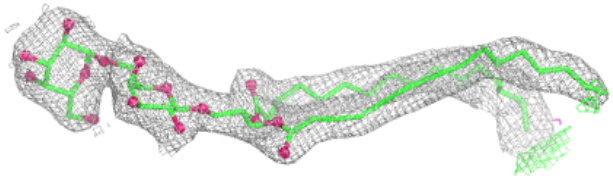




Electron density around DGD c 519:

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

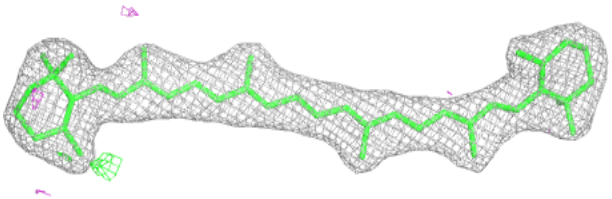


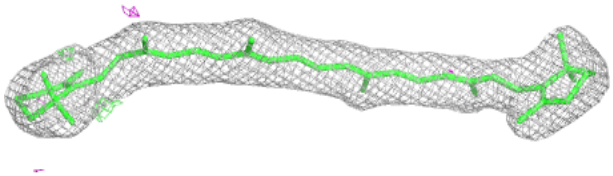


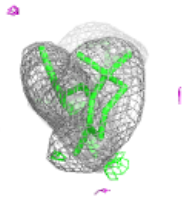


Electron density around BCR b 619:

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

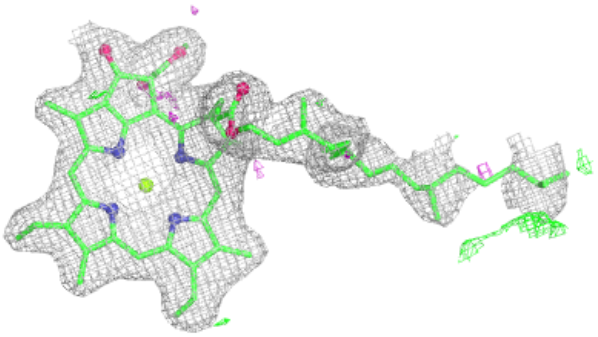


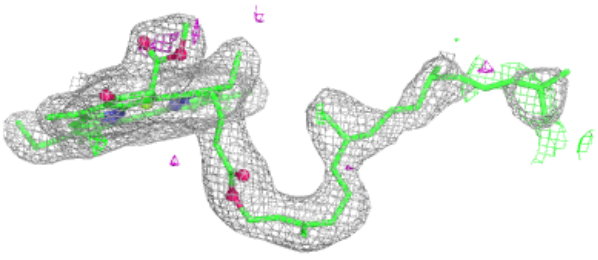


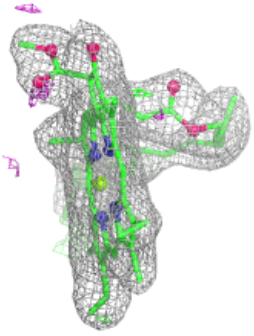


Electron density around CLA a 407 (B):

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

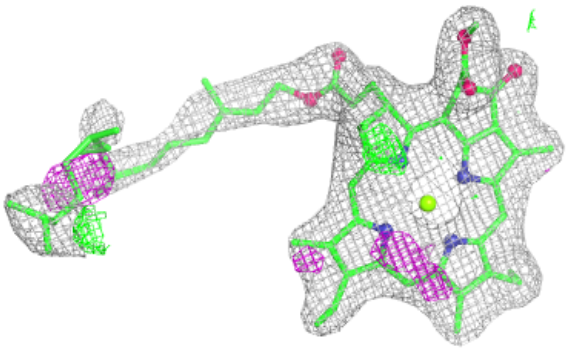


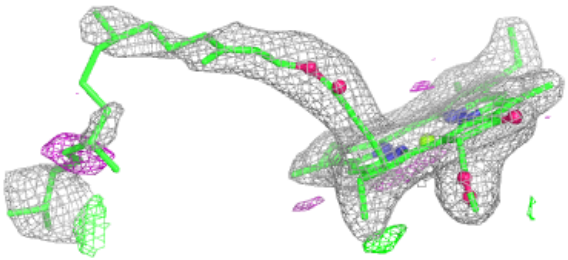


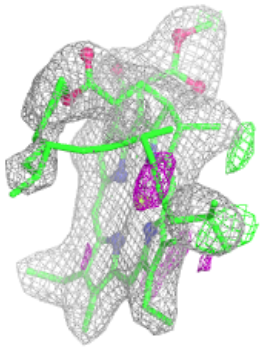


Electron density around CLA a 409:

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

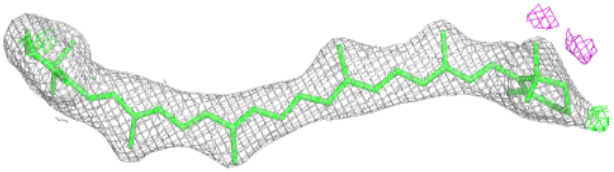


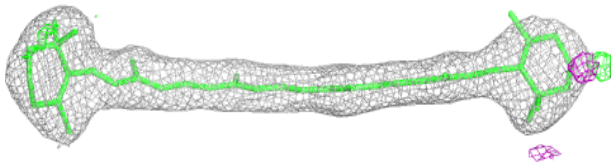


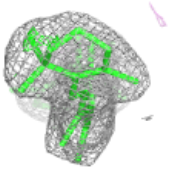


Electron density around BCR h 101:

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

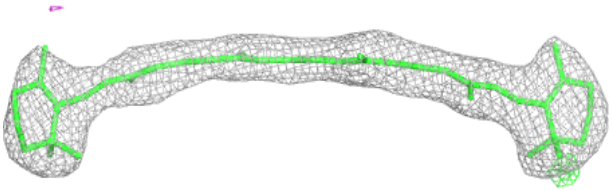


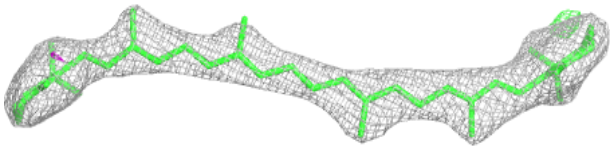


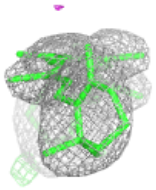


Electron density around BCR k 101:

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

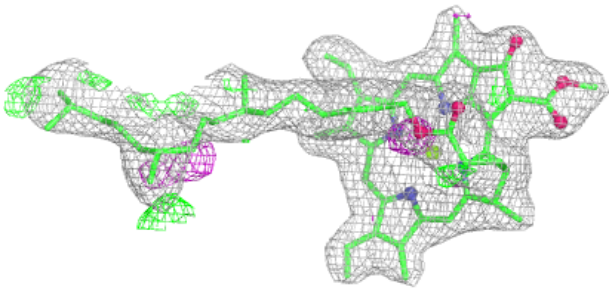


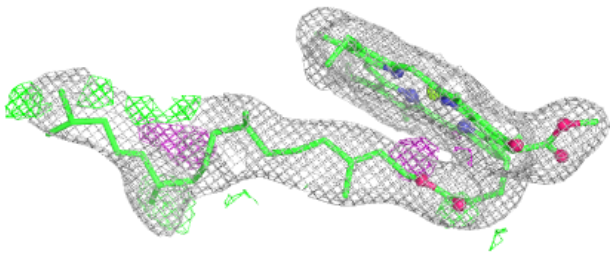


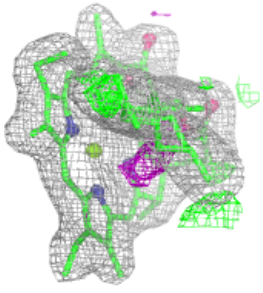


Electron density around CLA B 614:

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

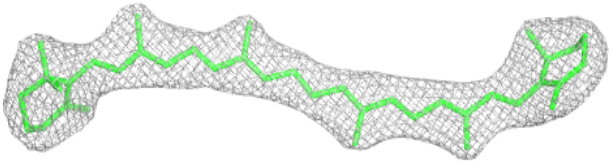


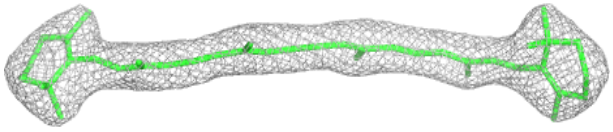


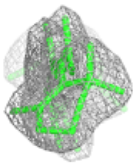


Electron density around BCR y 101:

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

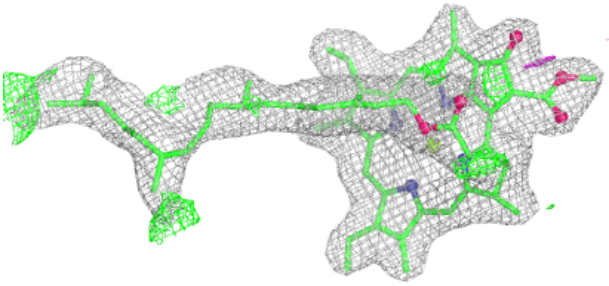


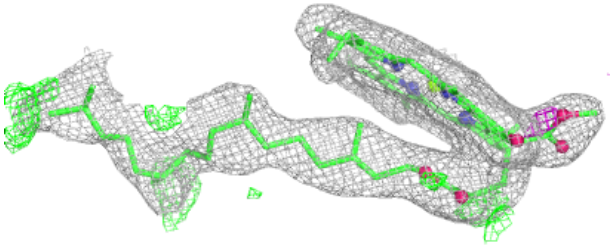


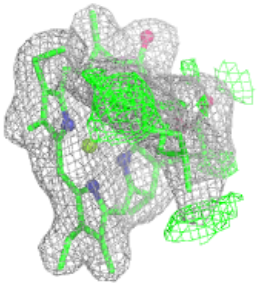


Electron density around CLA b 614:

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

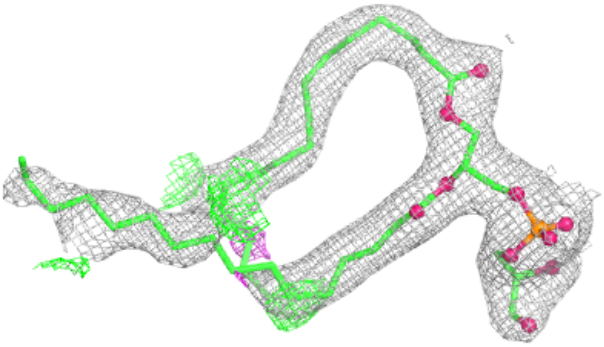


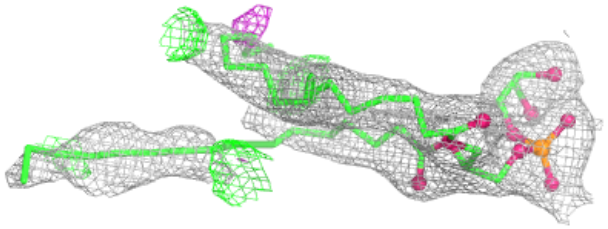


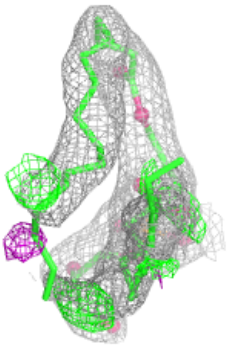


Electron density around LHG d 408 (A):

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

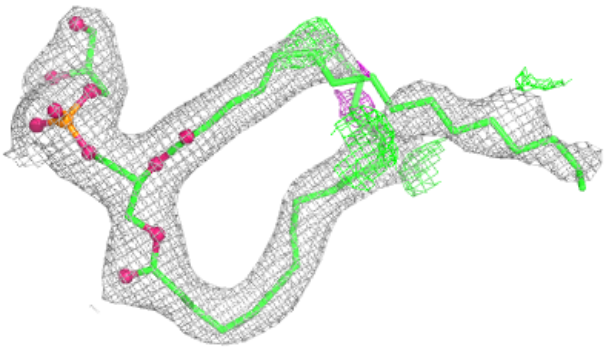


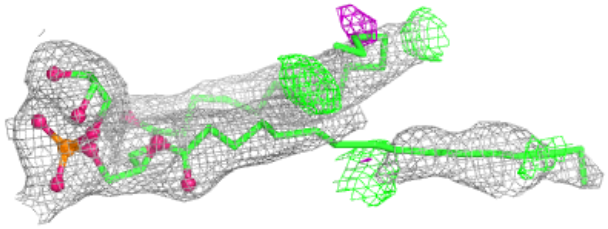


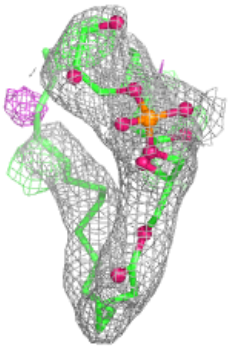


Electron density around LHG d 408 (B):

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

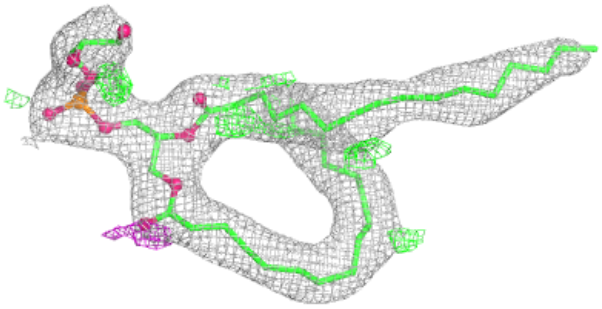


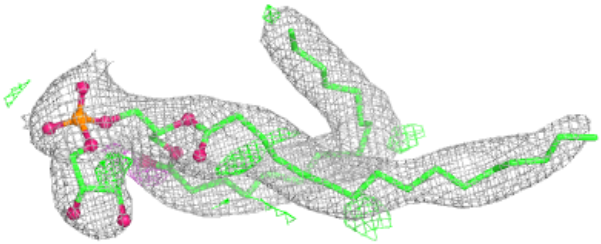


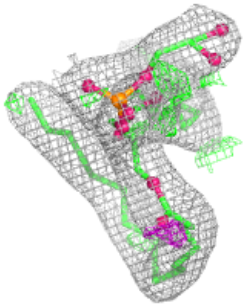


Electron density around LHG d 711 (A):

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

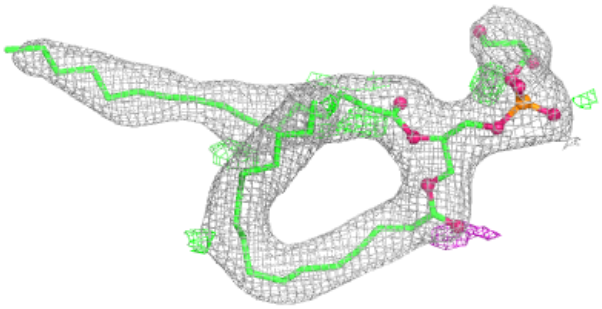


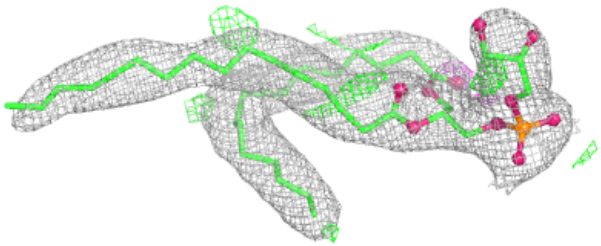


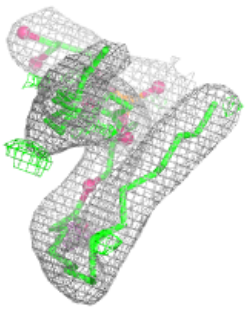


Electron density around LHG d 711 (B):

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

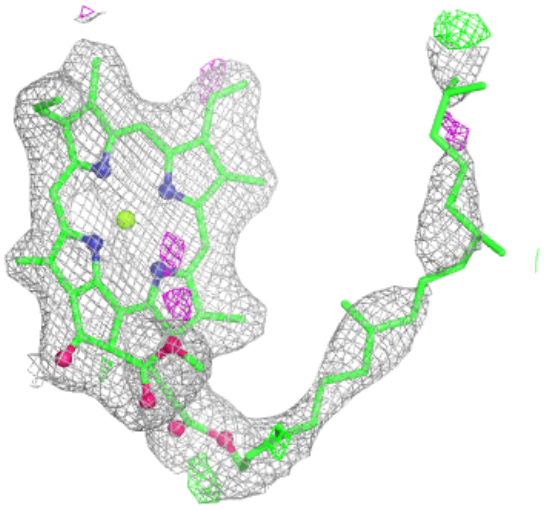


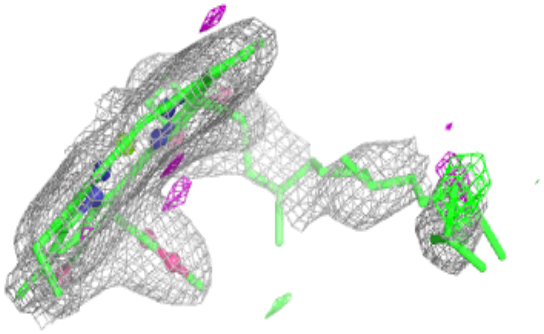


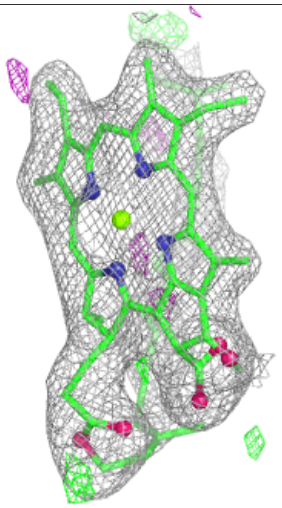


Electron density around CLA B 616:

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

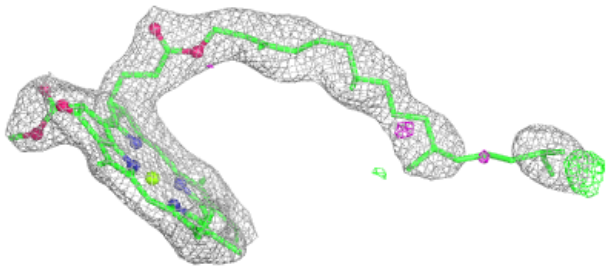


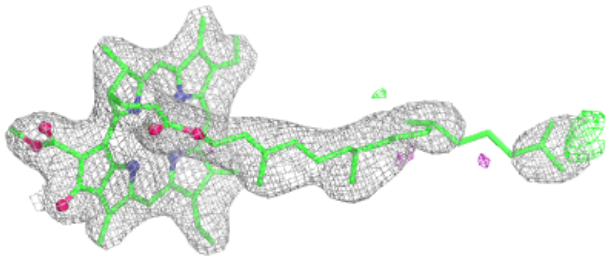


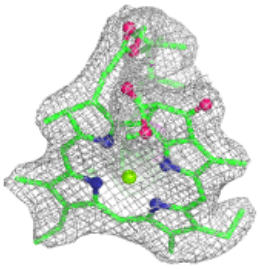


Electron density around CLA c 505:

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

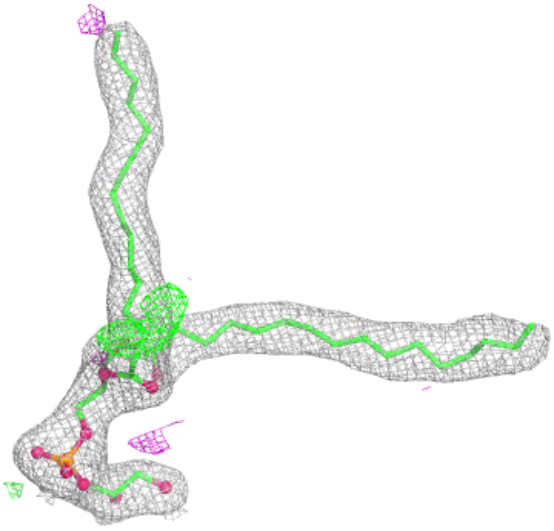


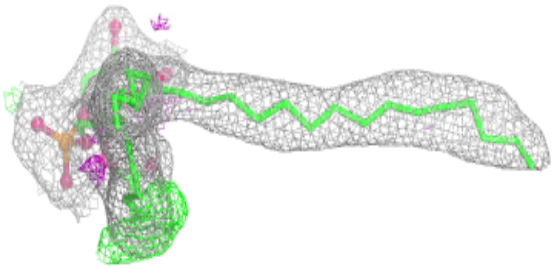


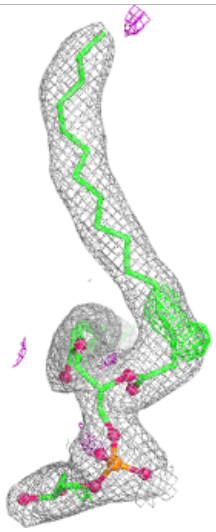


Electron density around LHG l 101 (A):

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

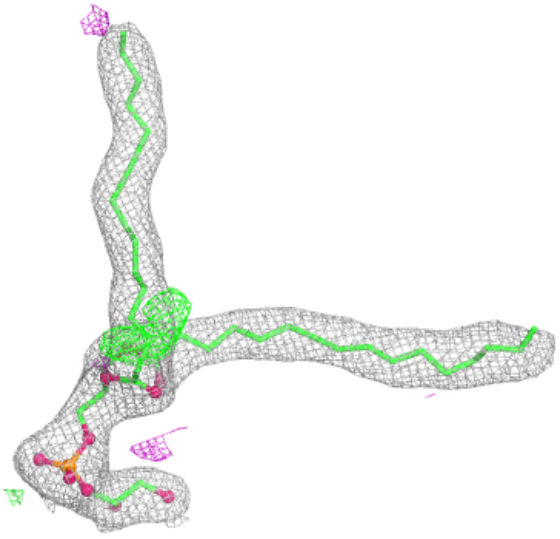


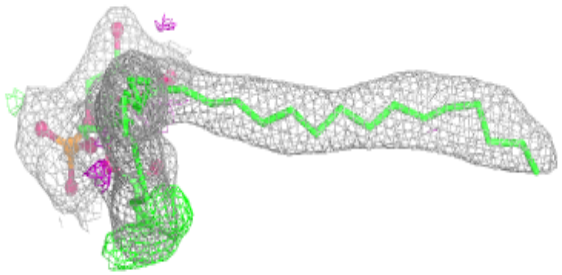


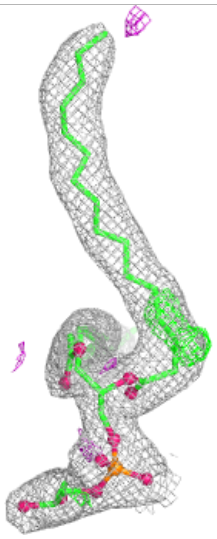


Electron density around LHG l 101 (B):

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

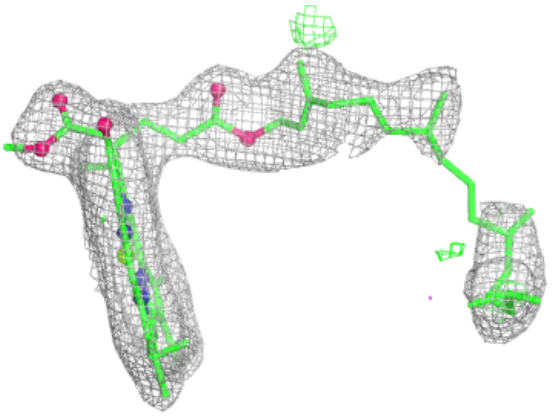


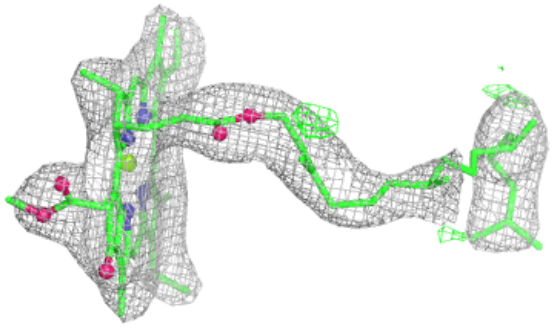


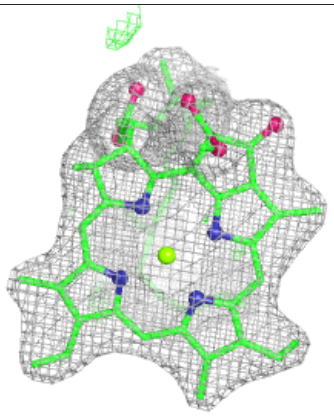


Electron density around CLA c 507:

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

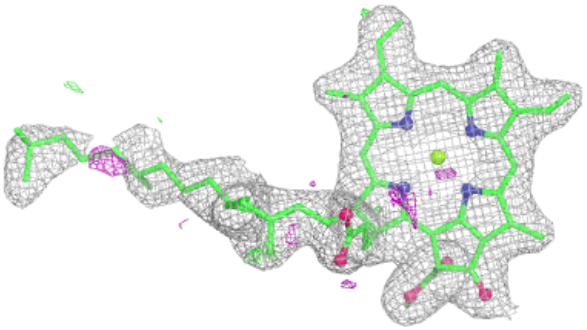


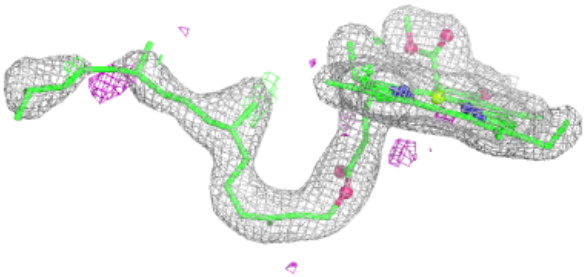


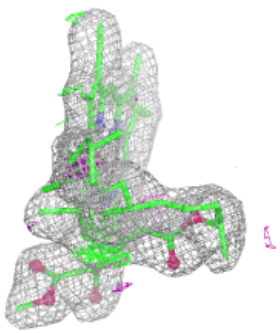


Electron density around CLA A 406 (B):

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

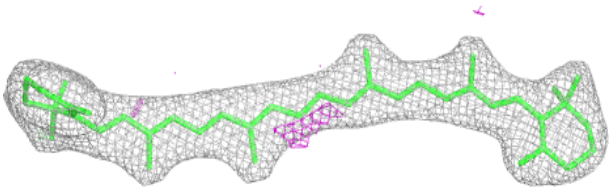


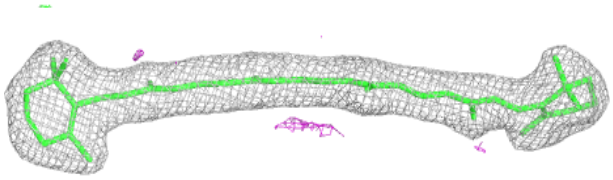


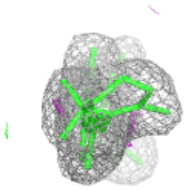


Electron density around BCR B 617:

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

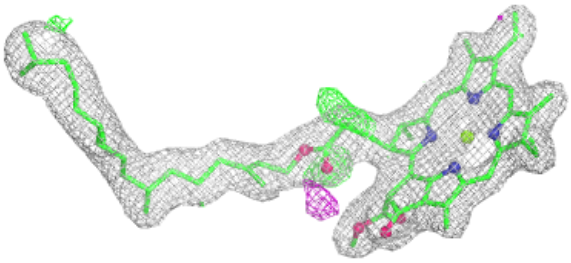


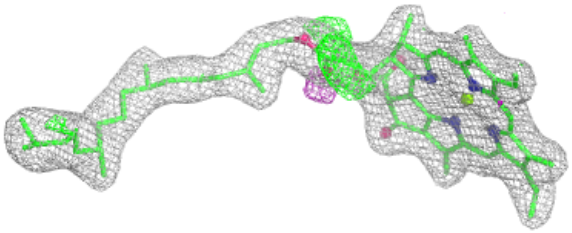


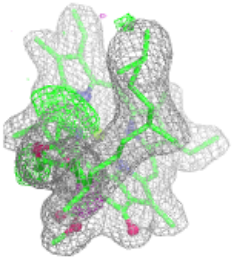


Electron density around CLA A 404 (A):

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

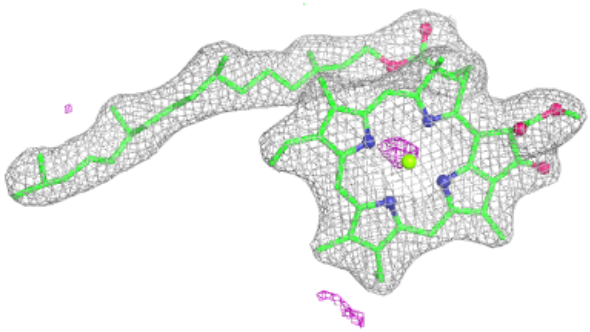


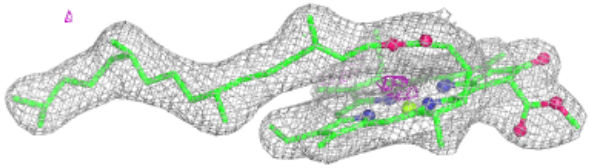


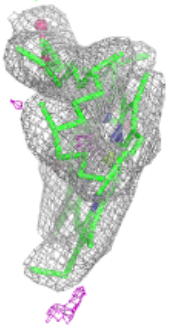


Electron density around CLA C 502:

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

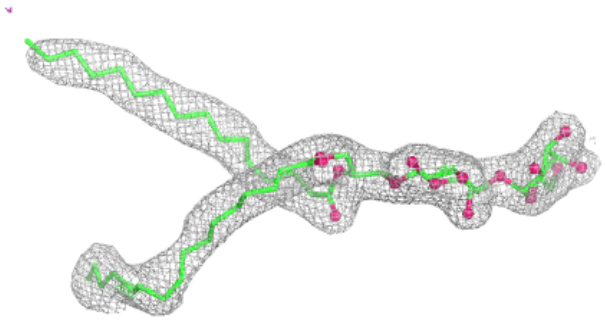


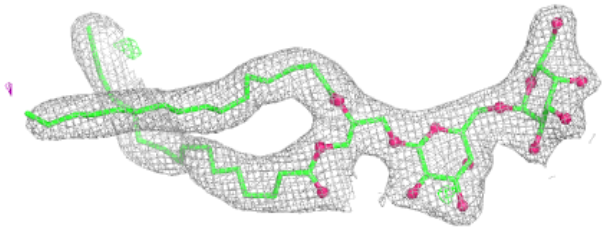


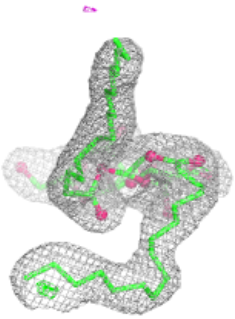


Electron density around DGD C 517 (A):

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

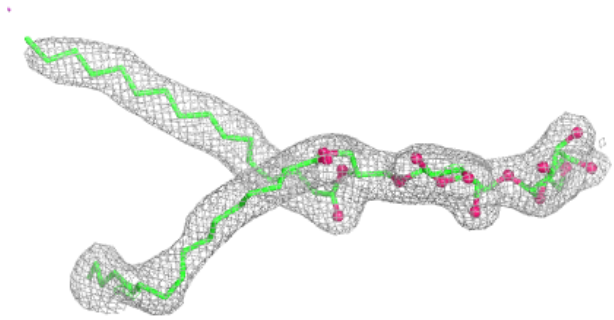


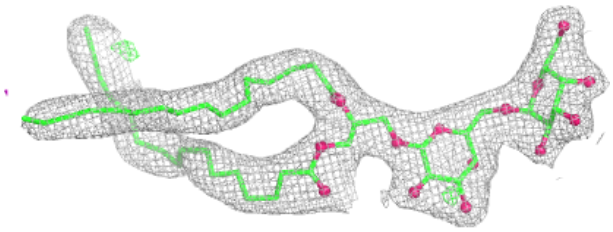


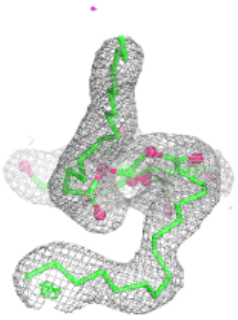


Electron density around DGD C 517 (B):

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

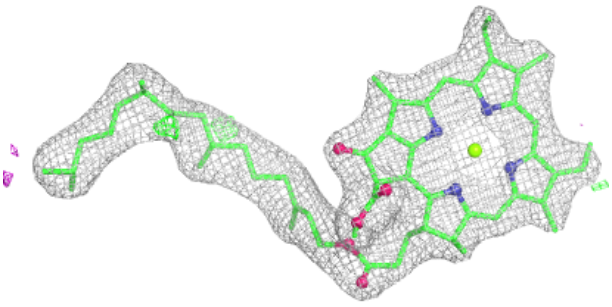


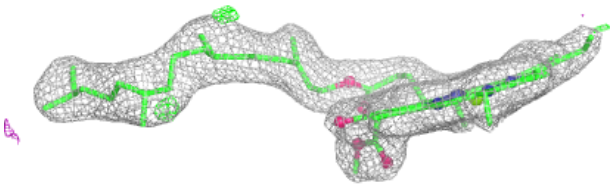


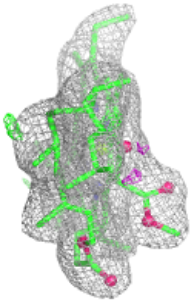


Electron density around CLA b 602:

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

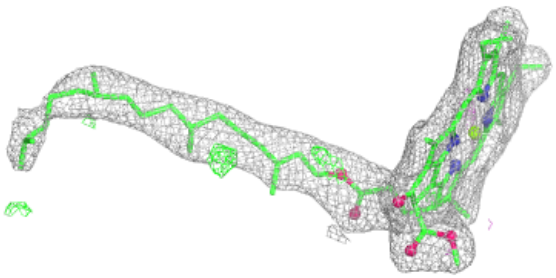


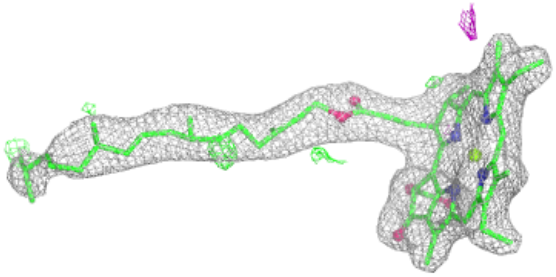


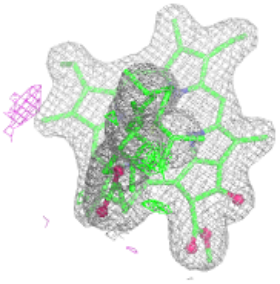


Electron density around CLA b 604:

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

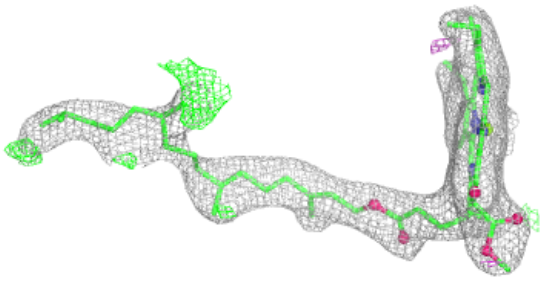


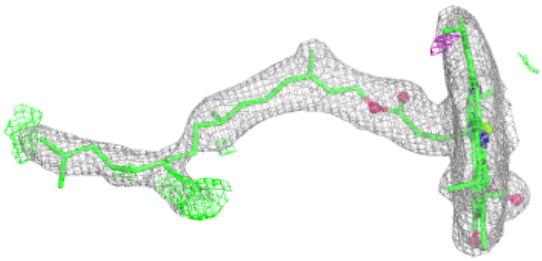


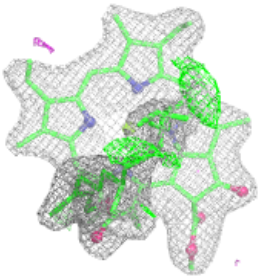


Electron density around CLA b 606:

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

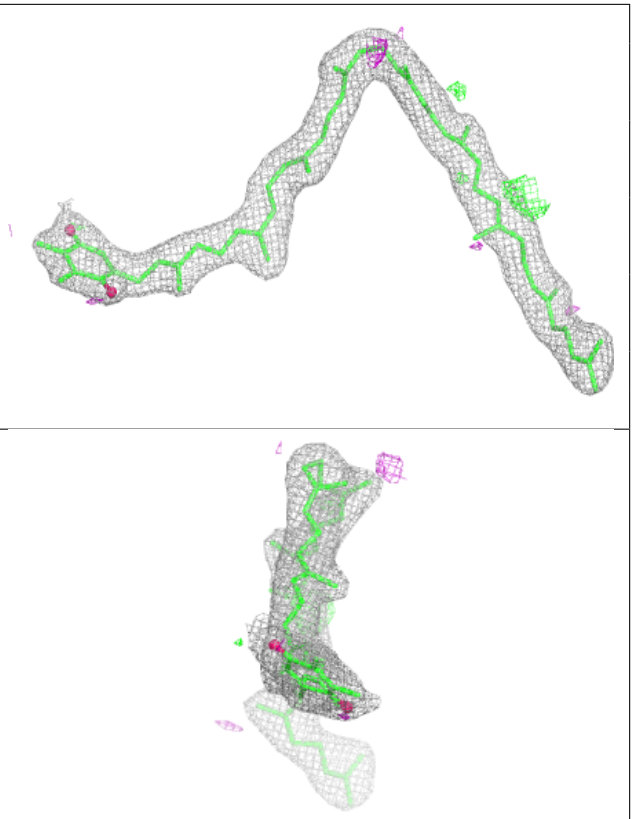






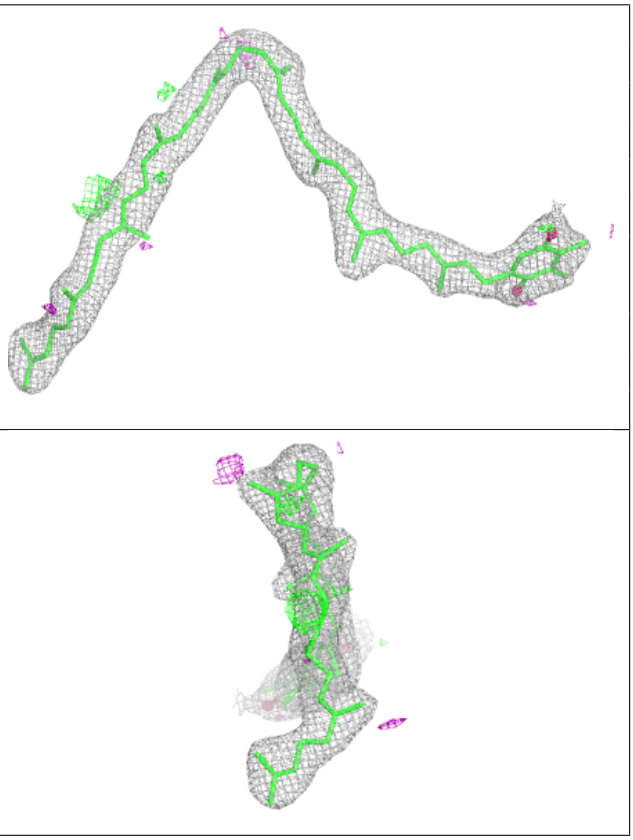
Electron density around PL9 d 405 (A):

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



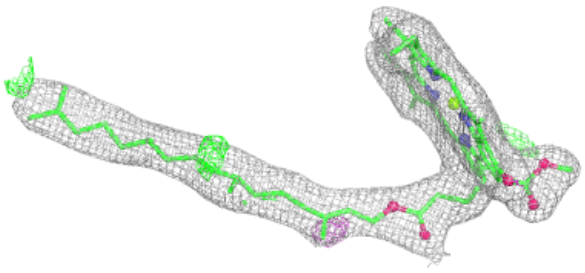
Electron density around PL9 d 405 (B):

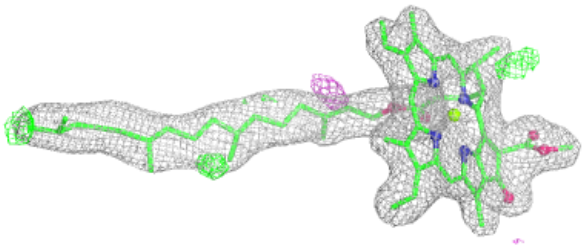
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

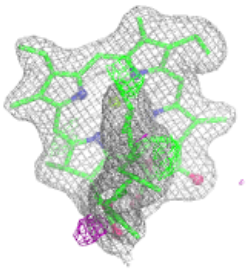


Electron density around CLA b 607:

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

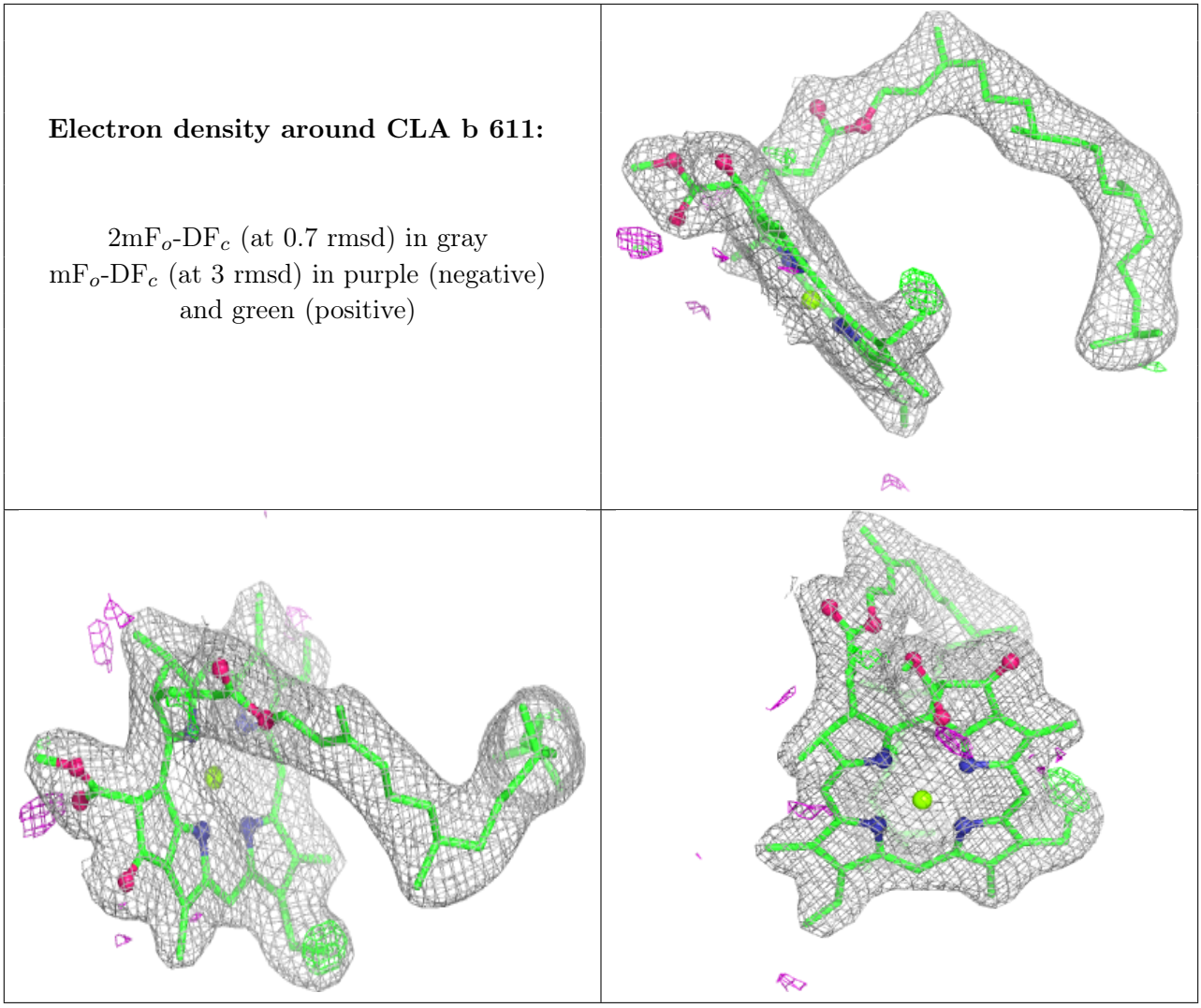






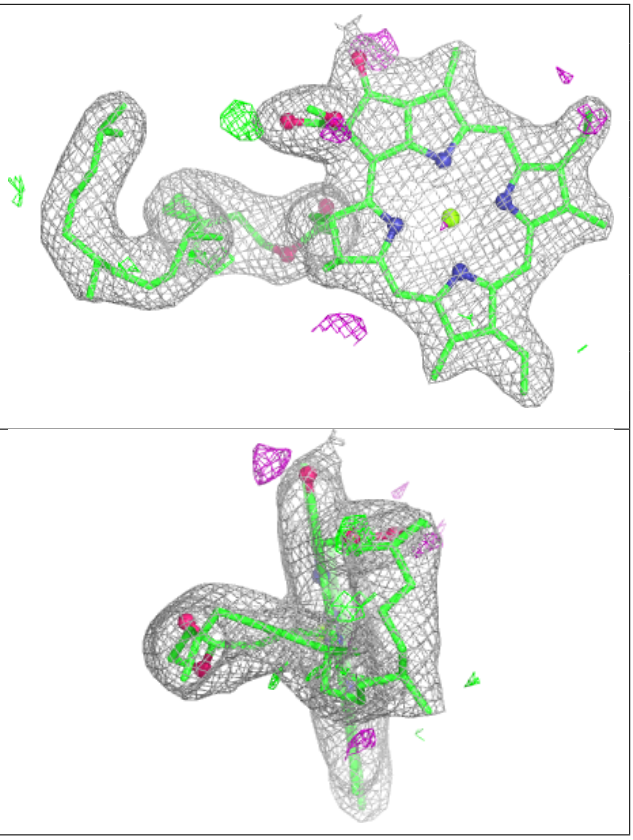
Electron density around CLA b 611:

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



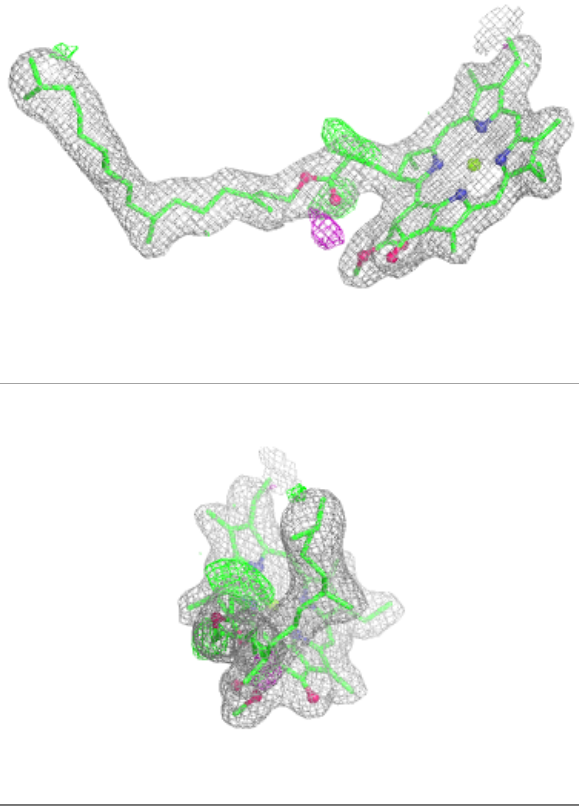
Electron density around CLA b 612:

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



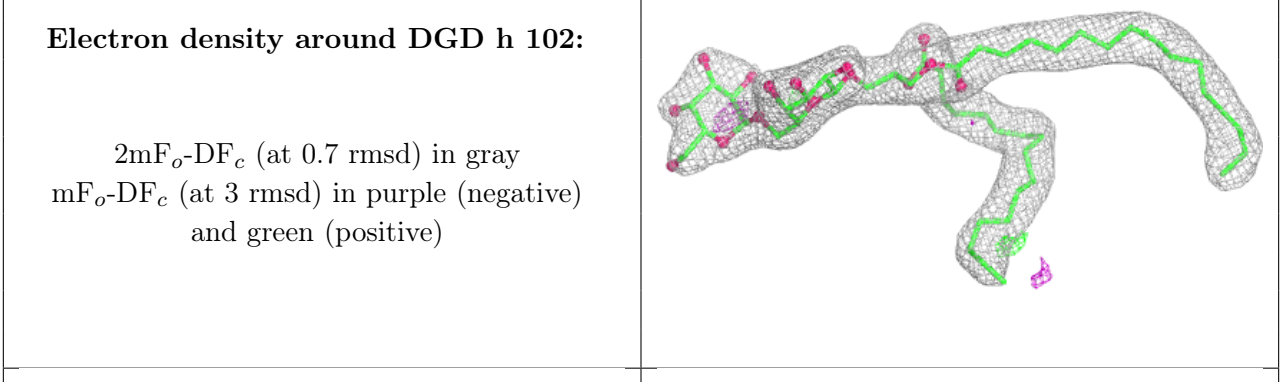
Electron density around CLA A 404 (B):

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



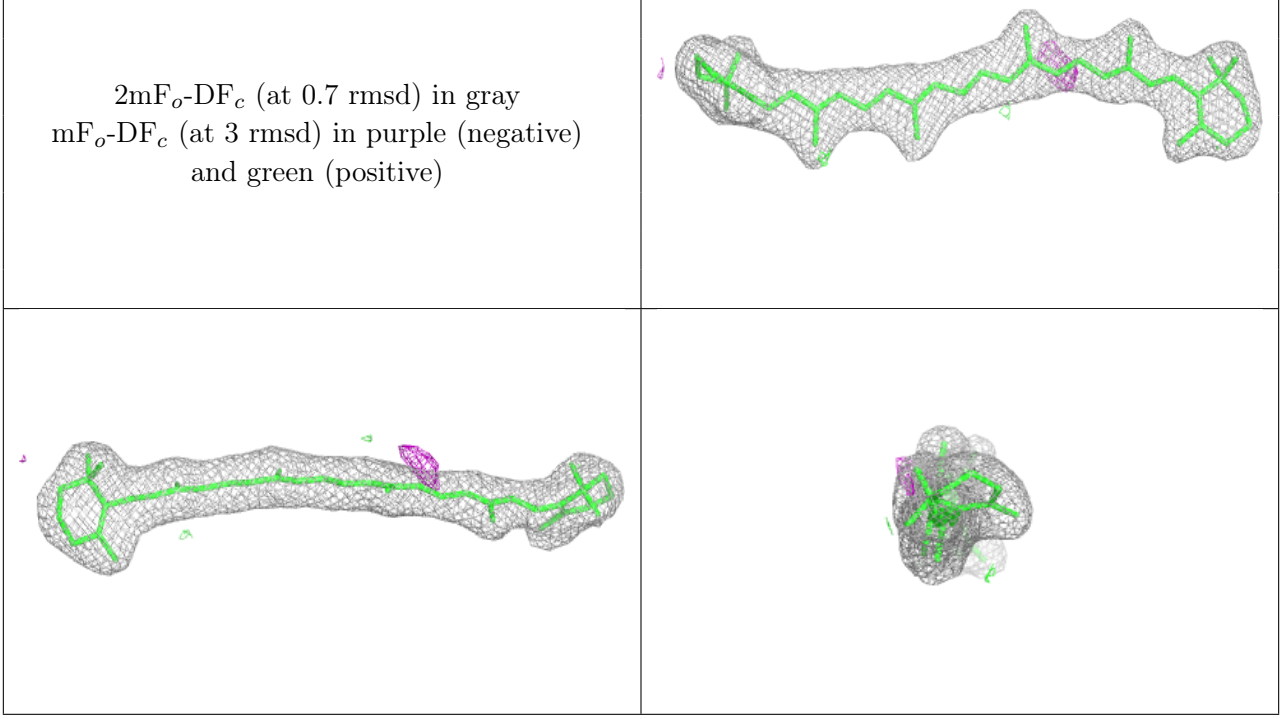
Electron density around DGD h 102:

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



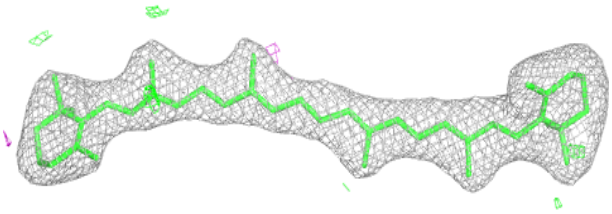
Electron density around BCR b 617:

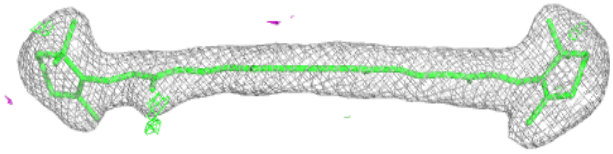
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

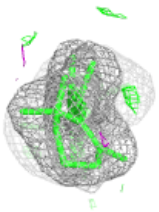


Electron density around BCR b 618:

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

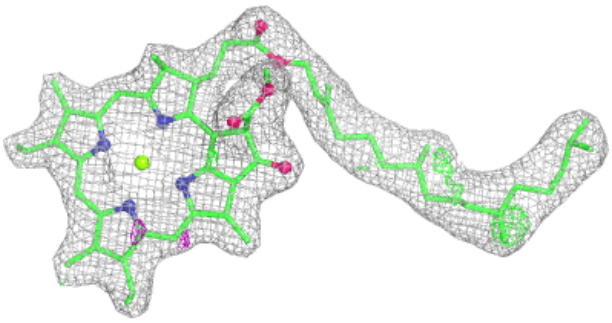


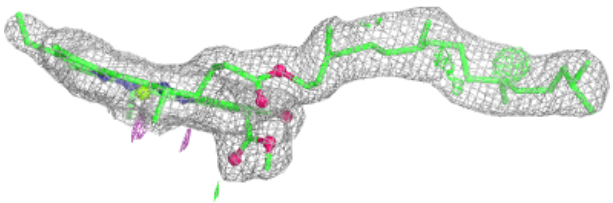


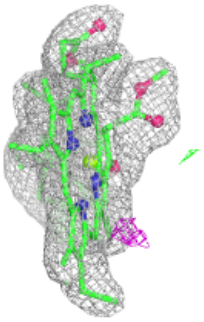


Electron density around CLA B 602:

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

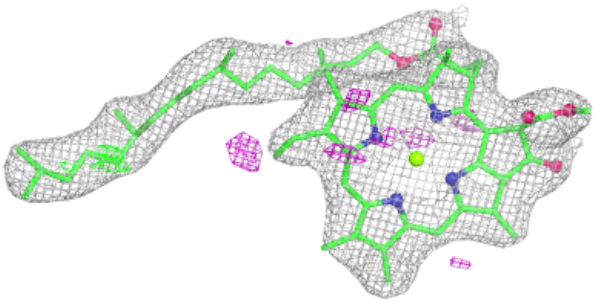


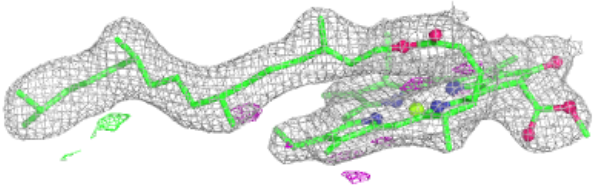


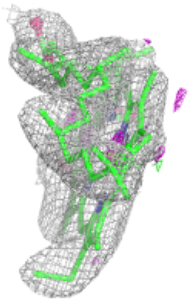


Electron density around CLA c 502:

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

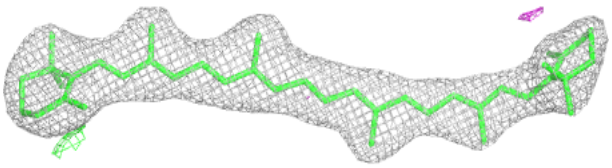


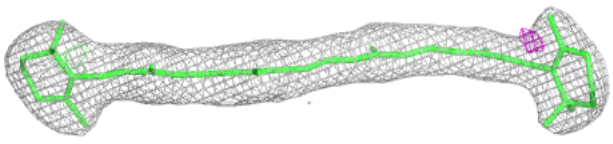


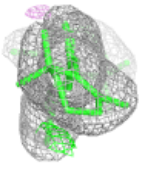


Electron density around BCR c 516:

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

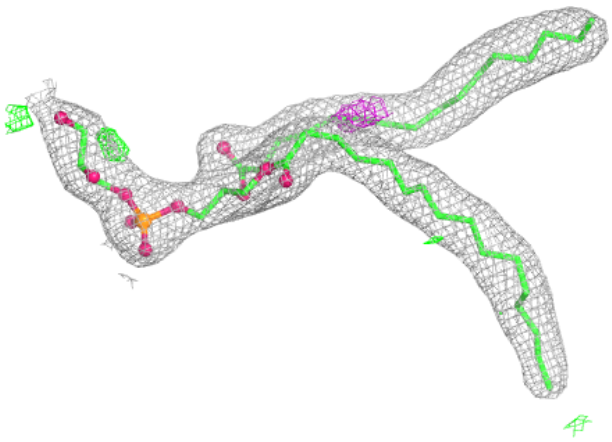


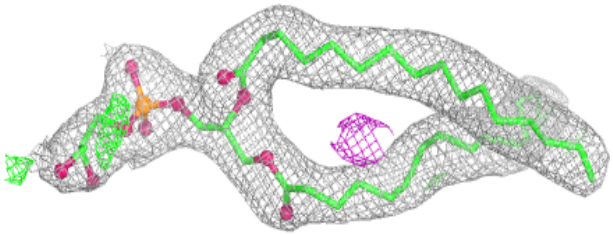


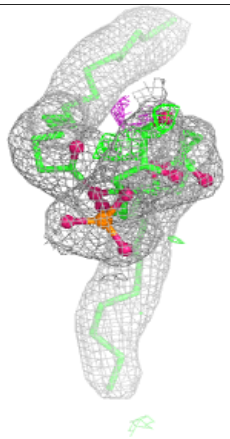


Electron density around LHG D 410 (A):

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

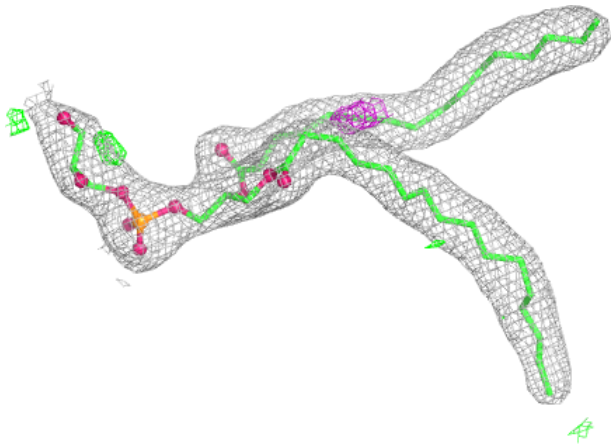


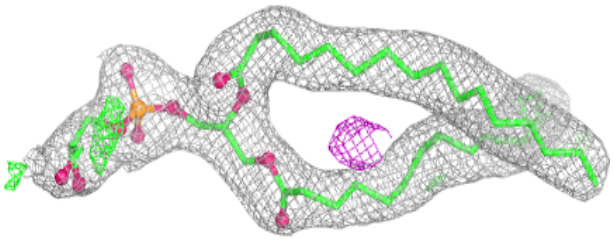




Electron density around LHG D 410 (B):

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

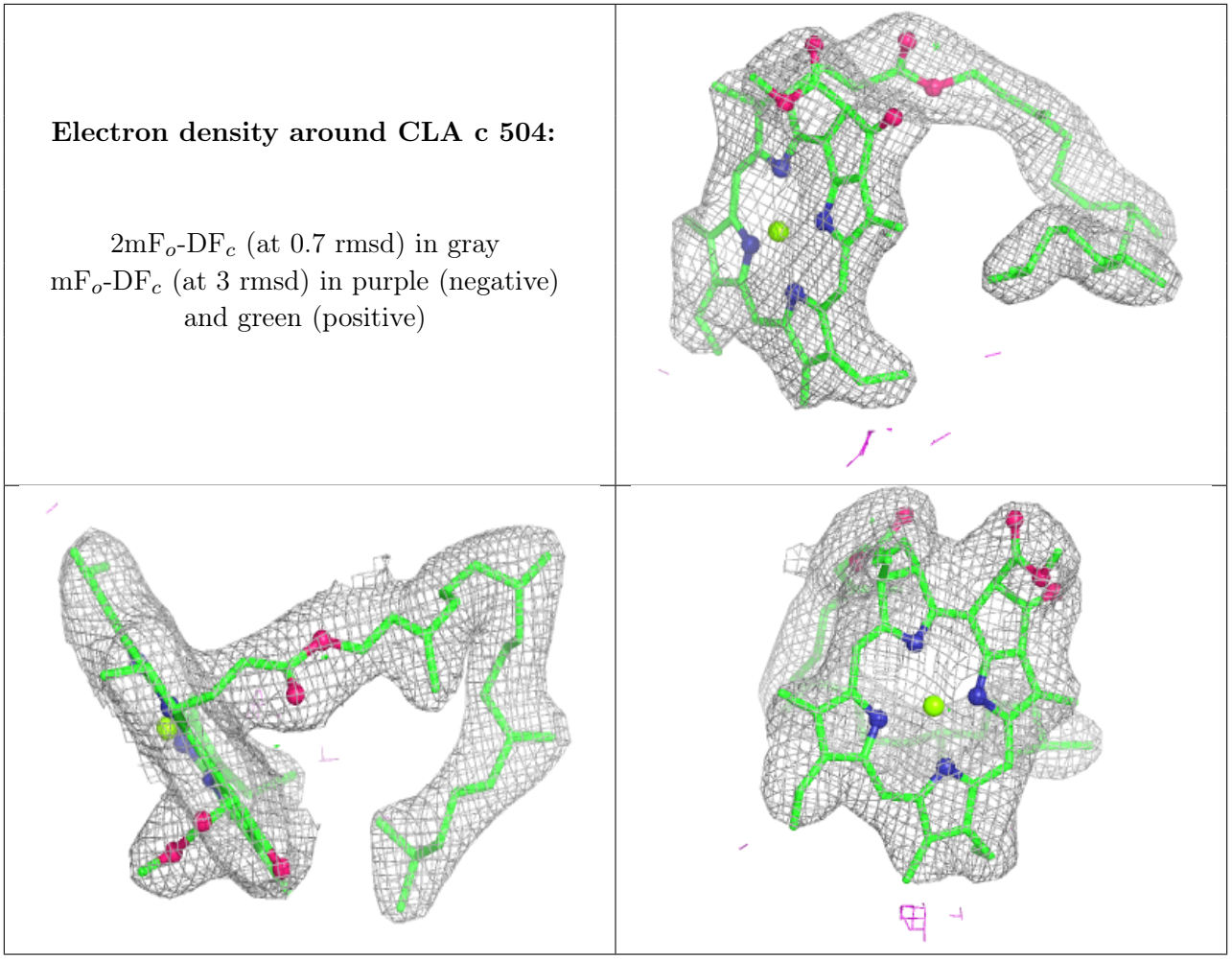






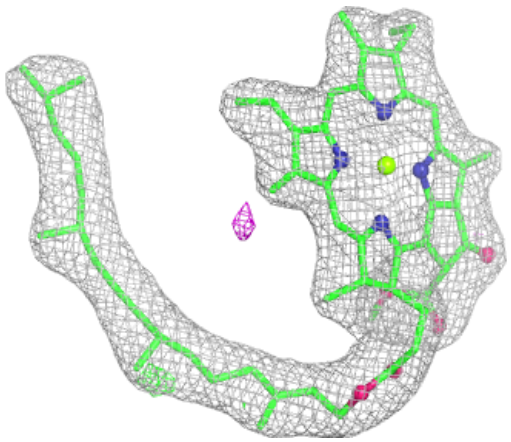
Electron density around CLA c 504:

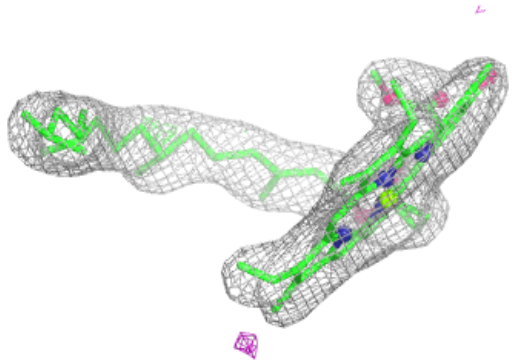
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

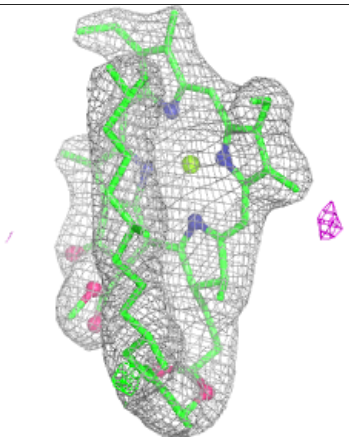


Electron density around CLA C 508:

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

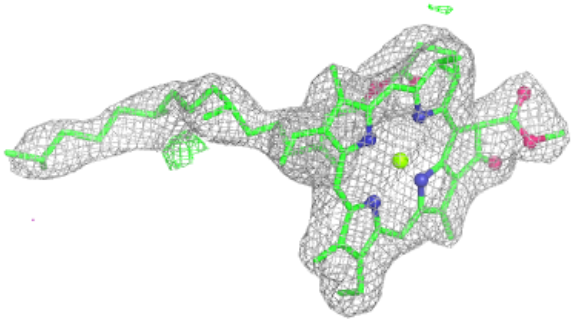


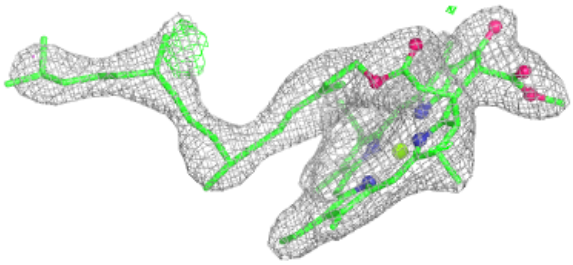


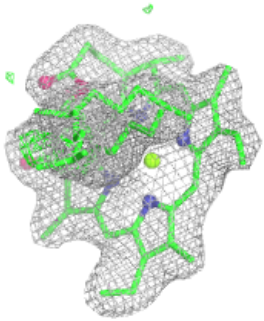


Electron density around CLA c 506:

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

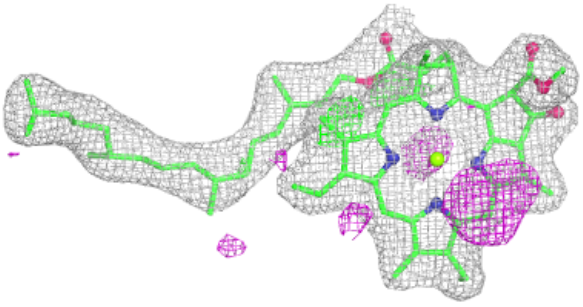


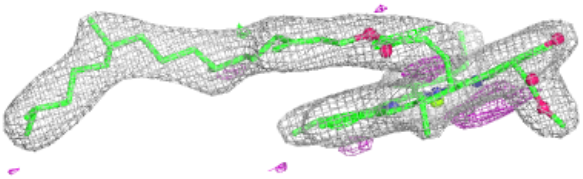


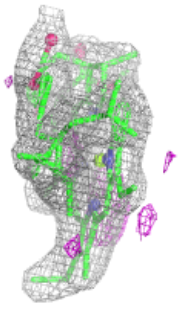


Electron density around CLA B 603:

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

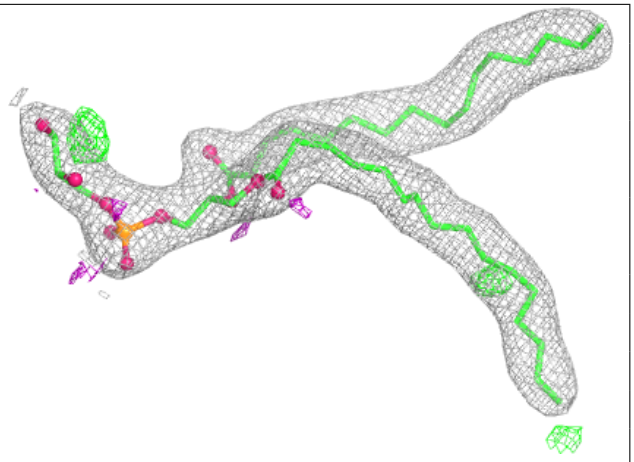


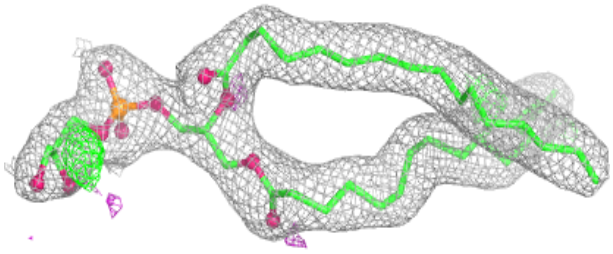




Electron density around LHG d 407 (A):

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

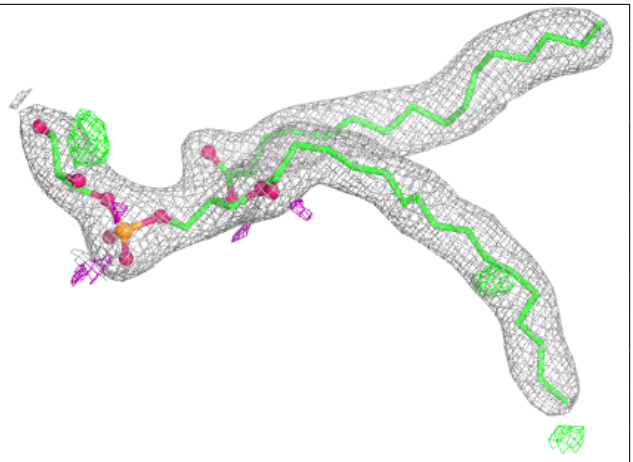


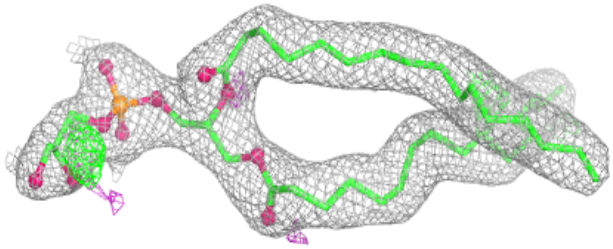




Electron density around LHG d 407 (B):

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

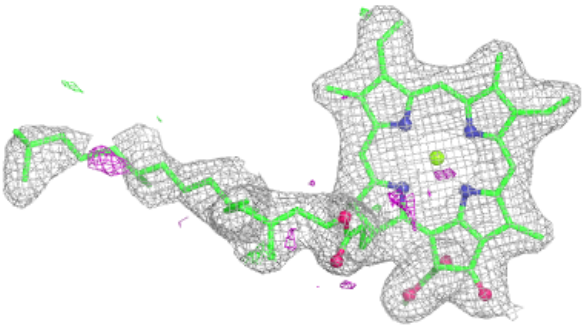


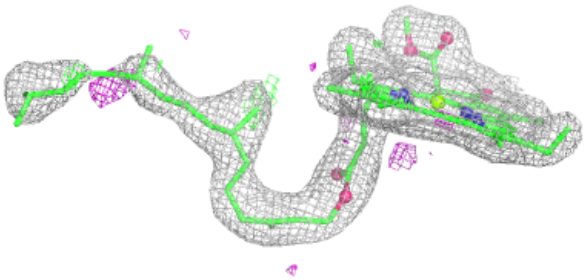


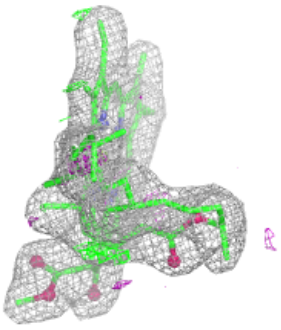


Electron density around CLA A 406 (A):

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

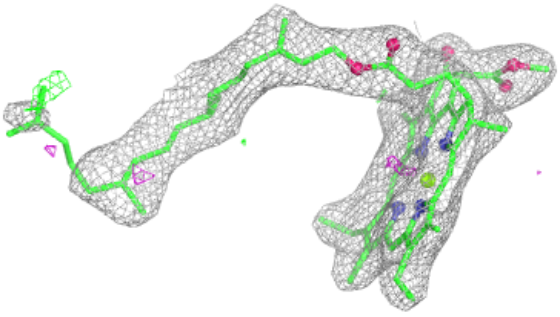


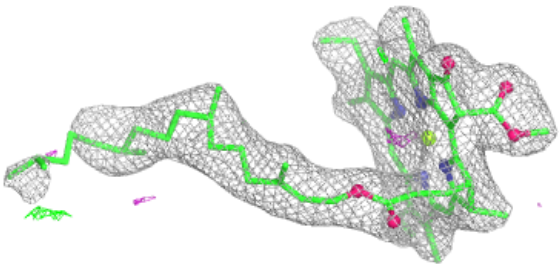


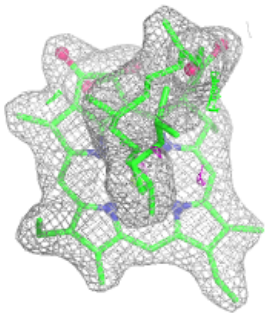


Electron density around CLA c 509:

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

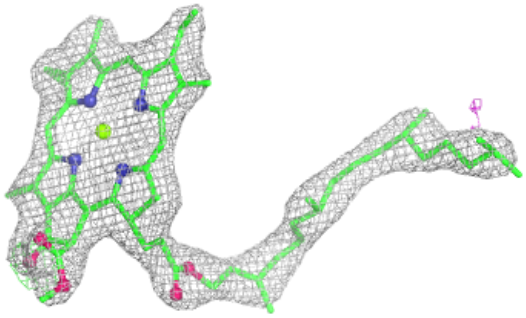


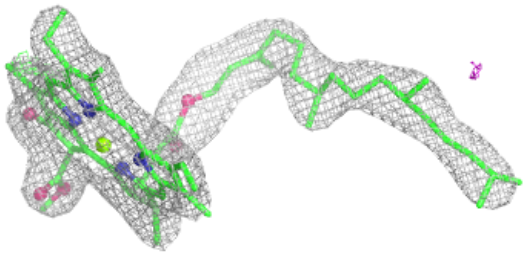


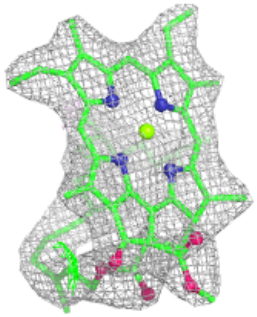


Electron density around CLA c 512:

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

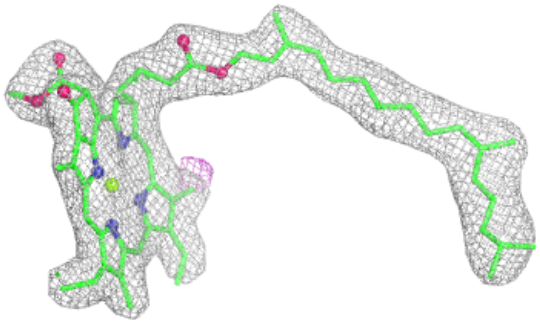


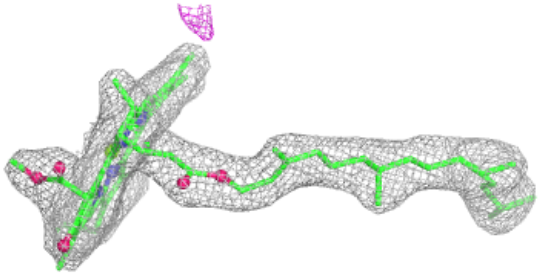


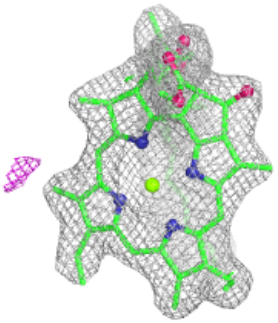


Electron density around CLA B 609:

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

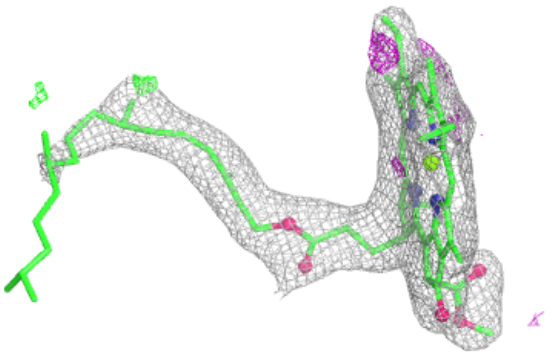


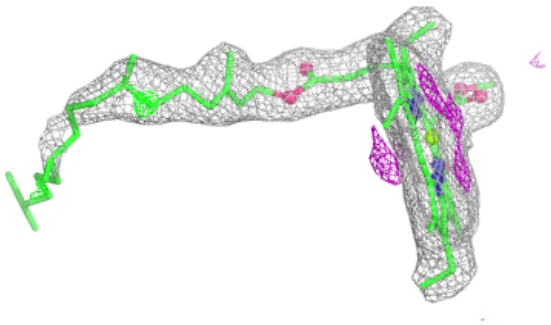


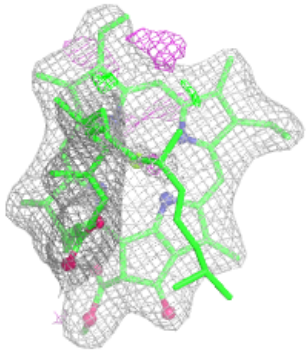


Electron density around CLA D 406:

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

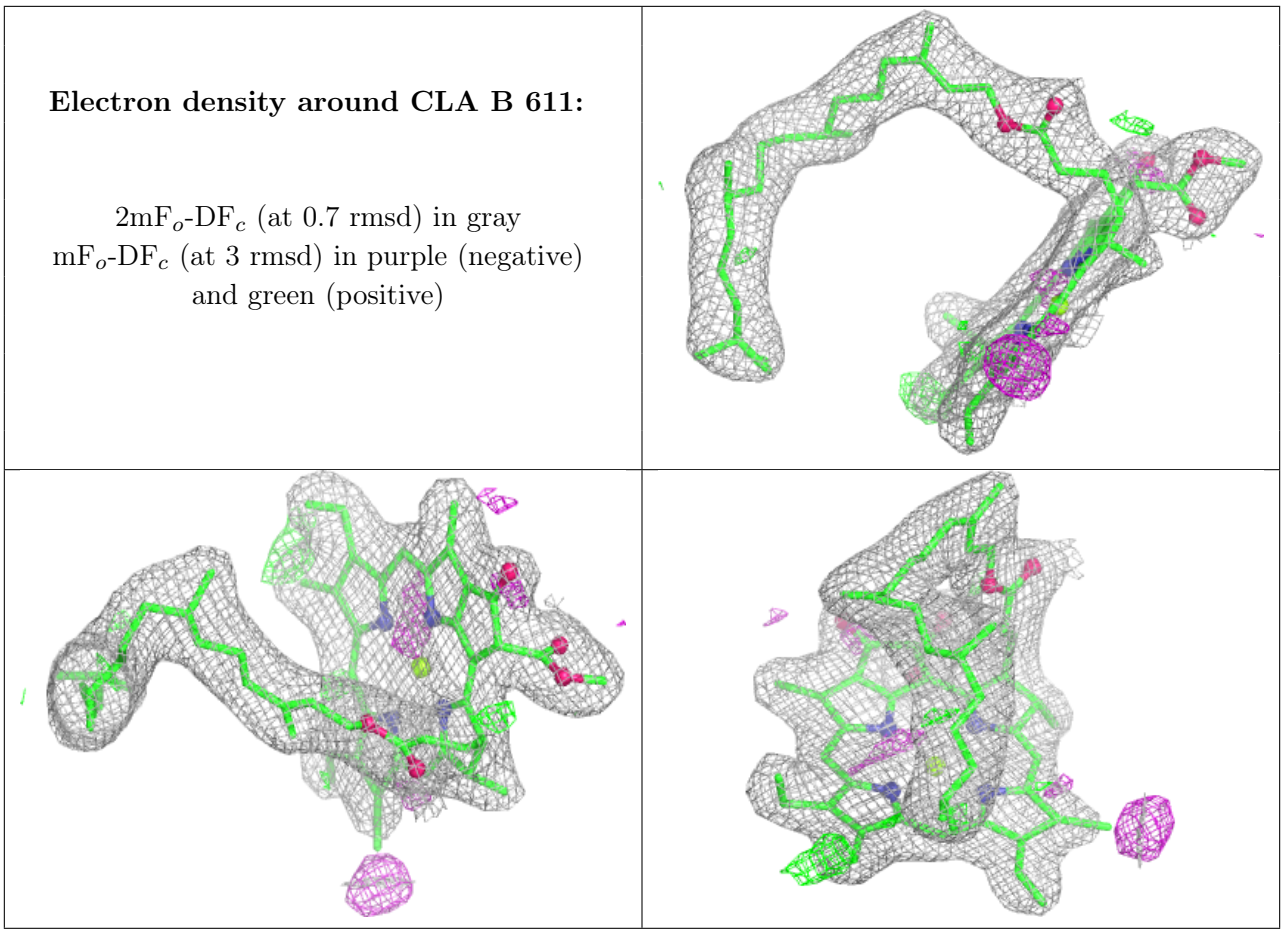






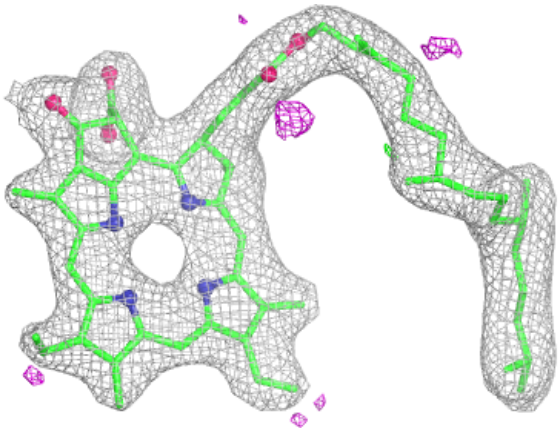
Electron density around CLA B 611:

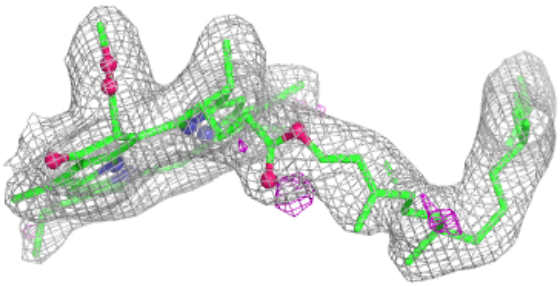
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around PHO a 353 (A):

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

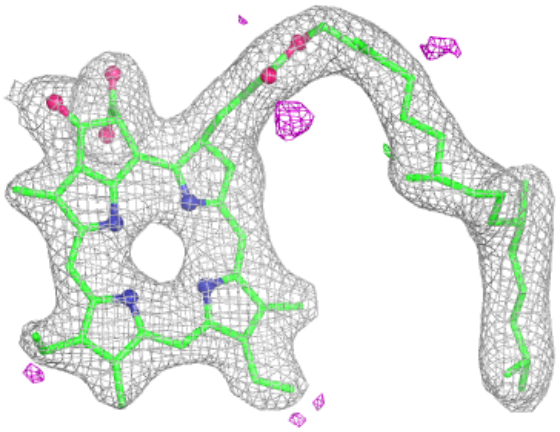


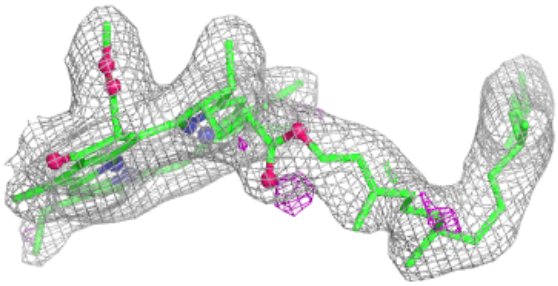




Electron density around PHO a 353 (B):

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

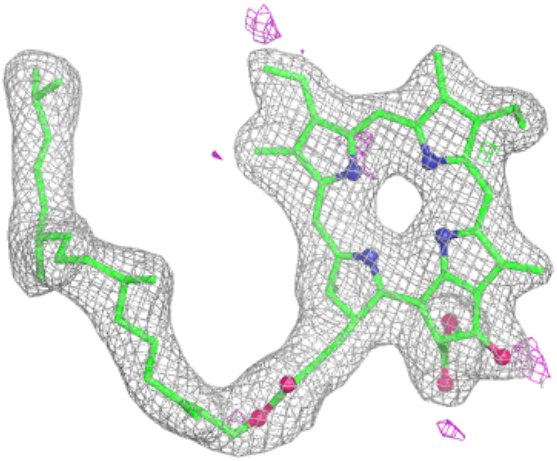


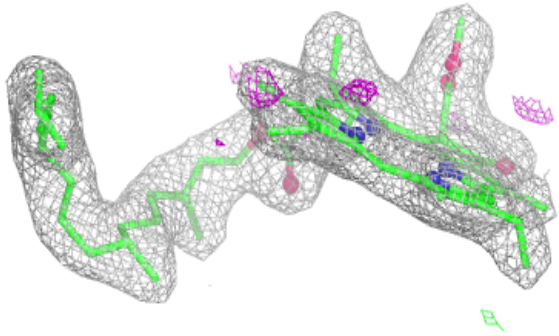


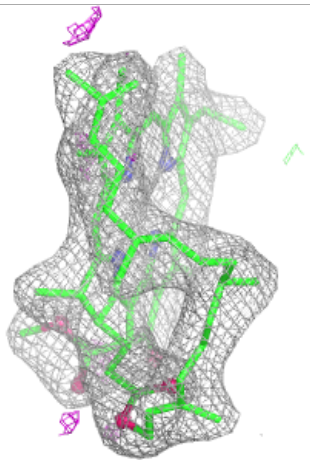


Electron density around PHO A 353 (A):

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

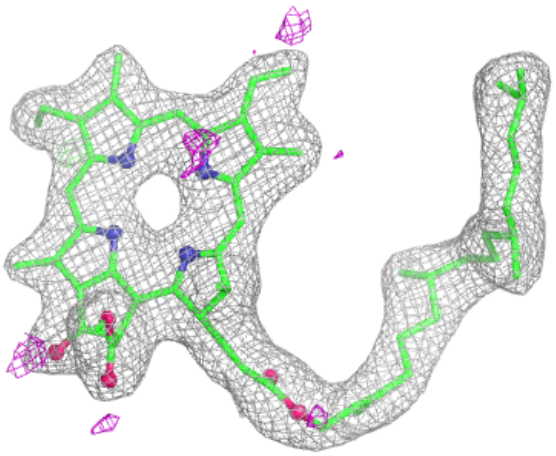


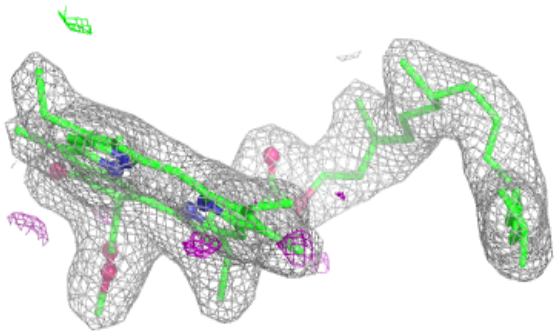


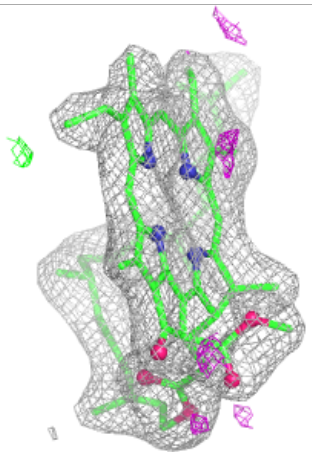


Electron density around PHO A 353 (B):

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

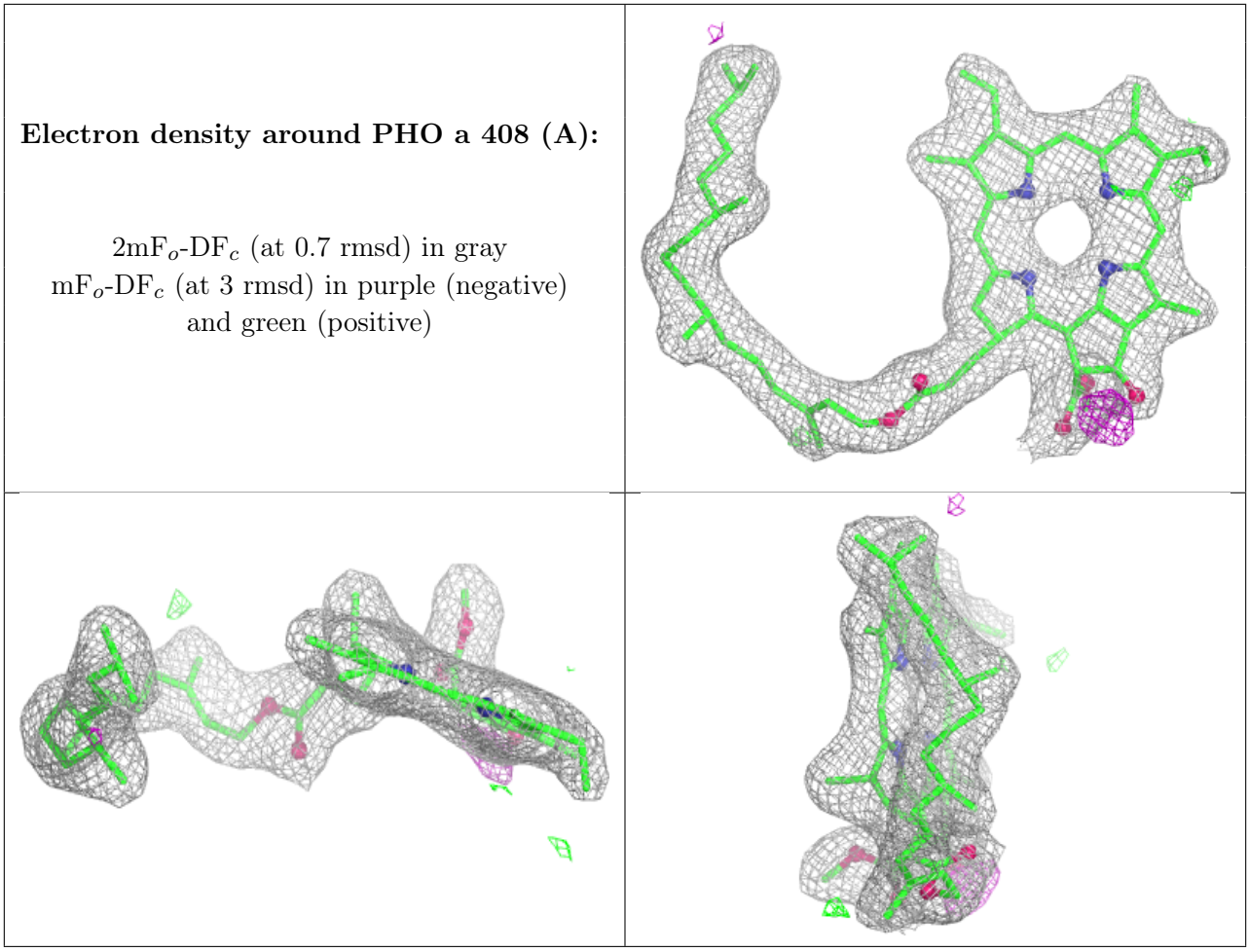






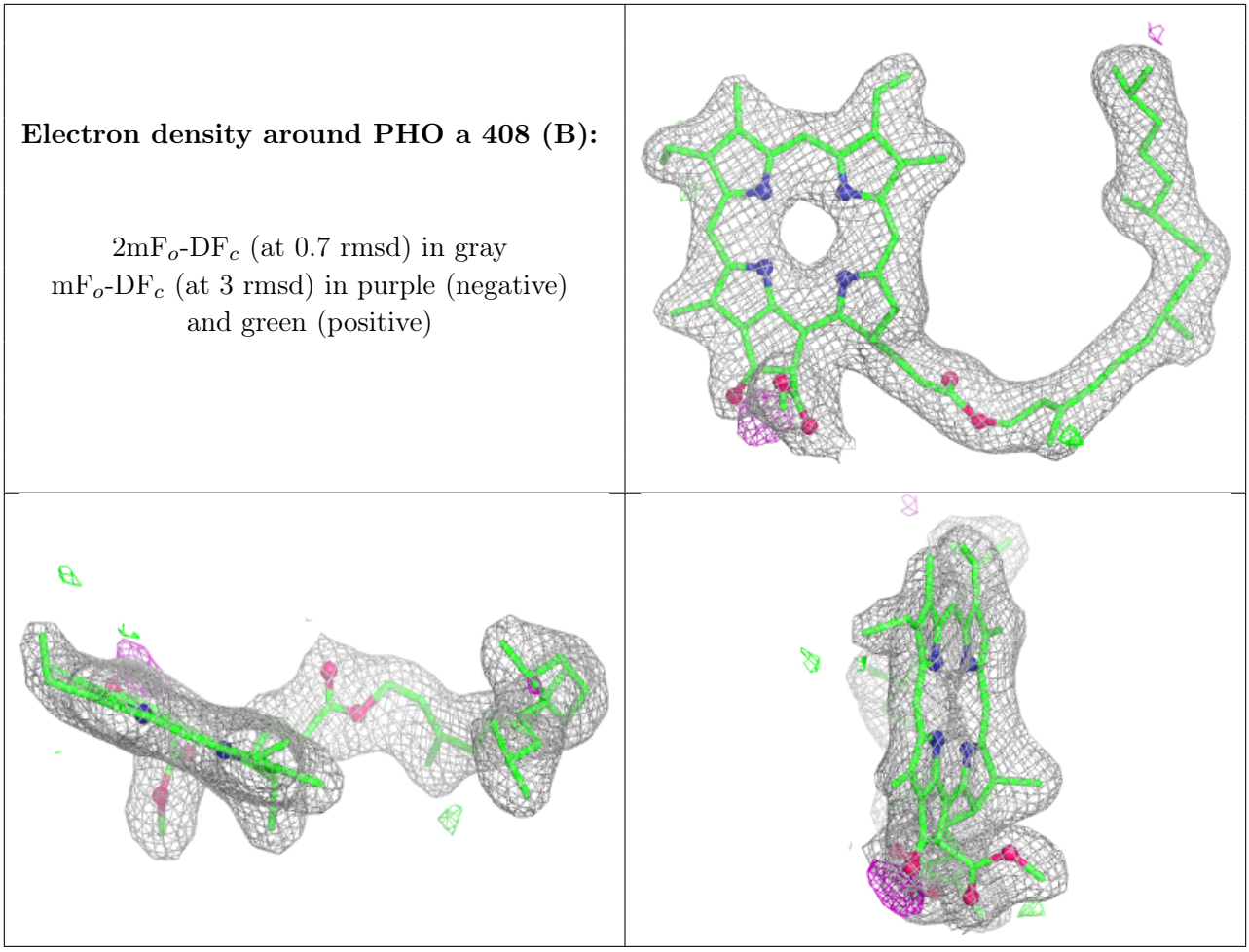
Electron density around PHO a 408 (A):

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



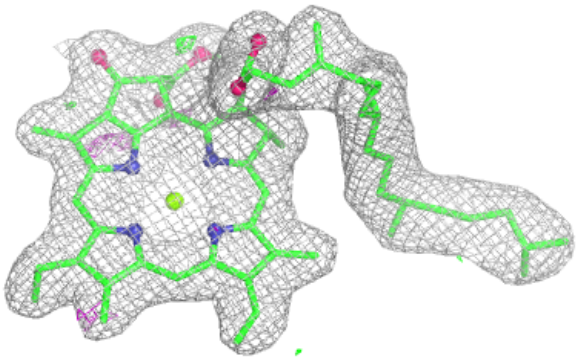
Electron density around PHO a 408 (B):

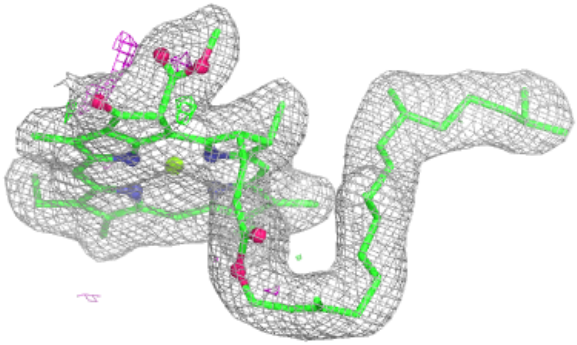
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

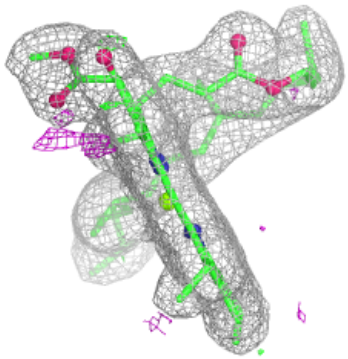


Electron density around CLA A 405 (A):

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

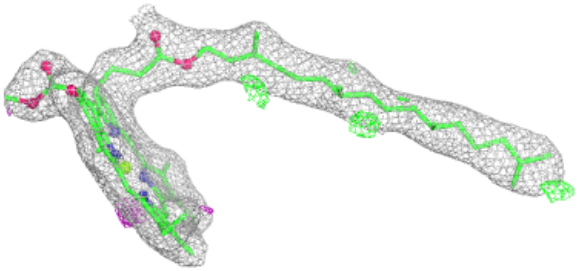


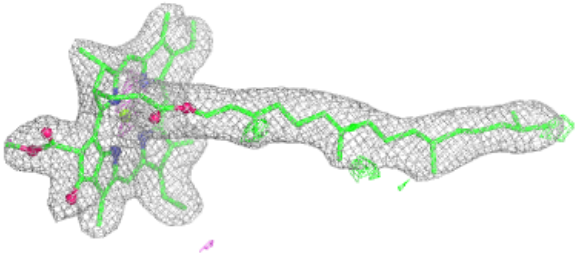


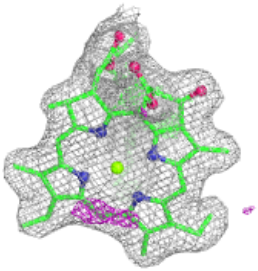


Electron density around CLA B 607:

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

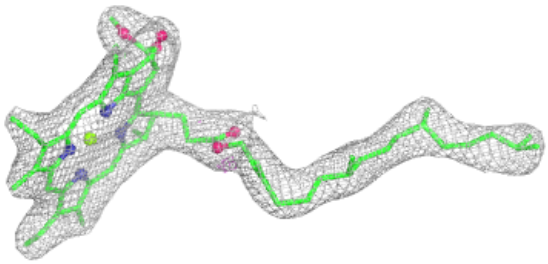


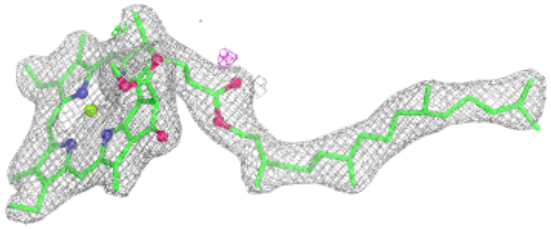


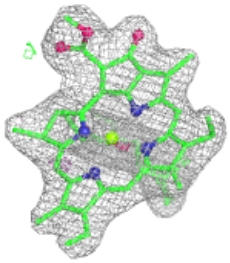


Electron density around CLA C 503:

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

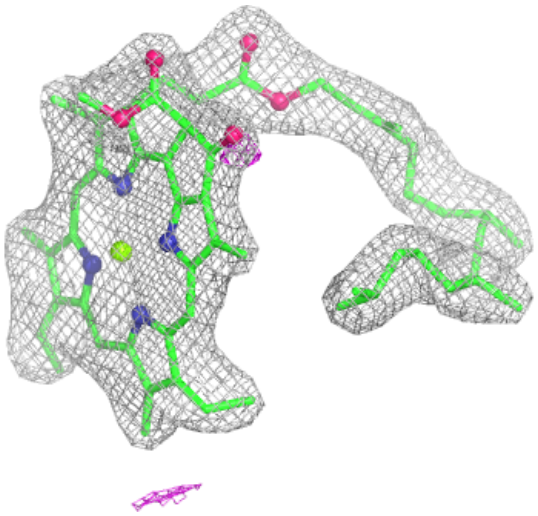


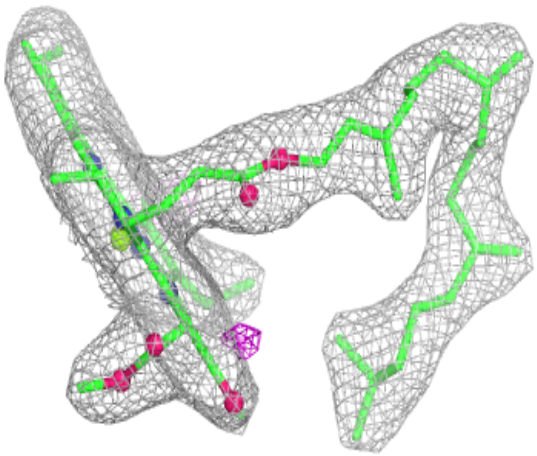


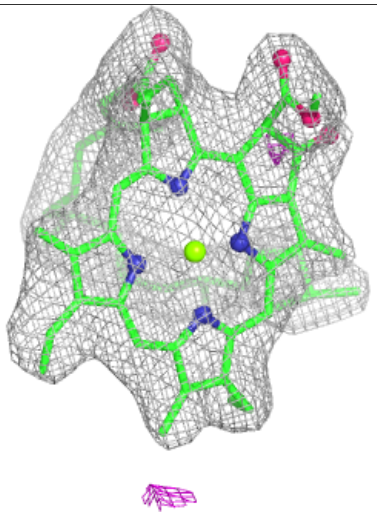


Electron density around CLA C 504:

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

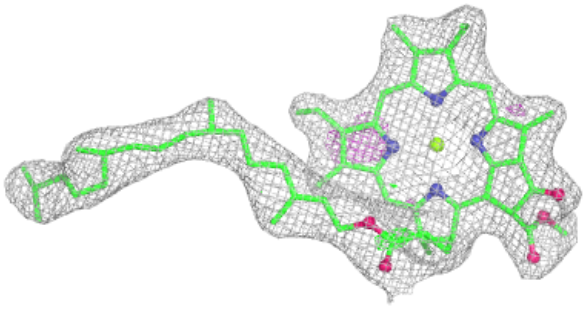


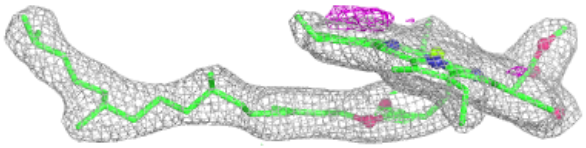


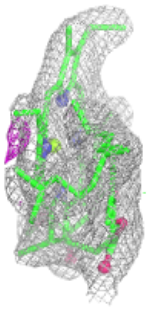


Electron density around CLA b 603:

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

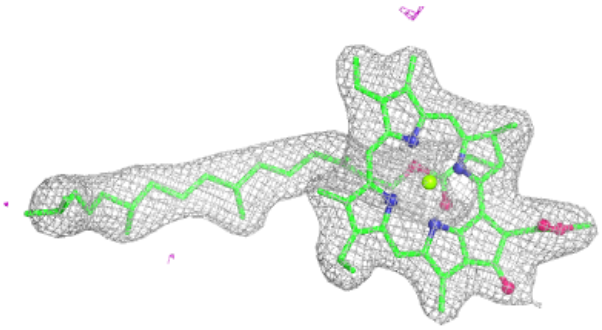


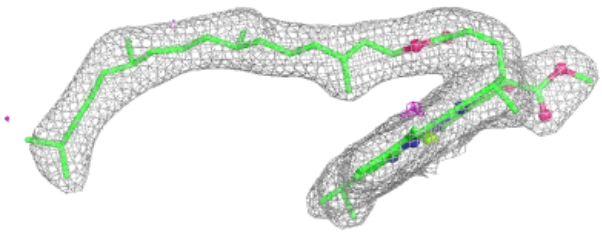


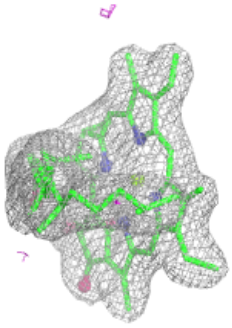


Electron density around CLA B 608:

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

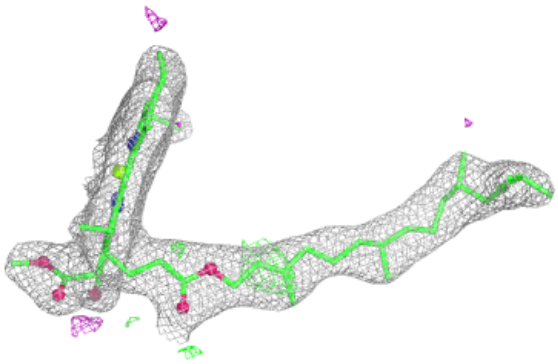


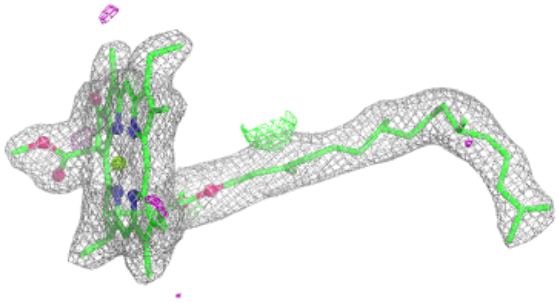


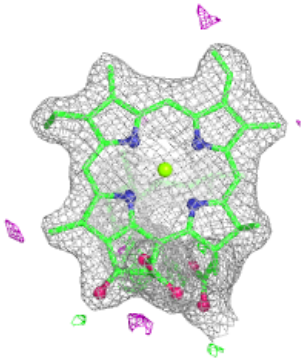


Electron density around CLA b 605:

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

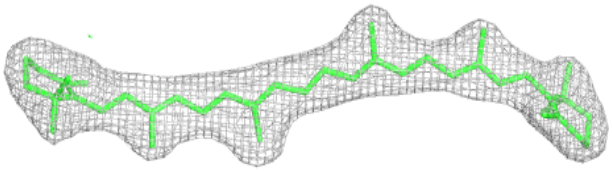


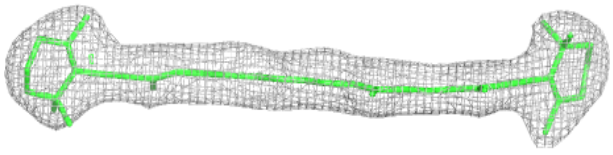


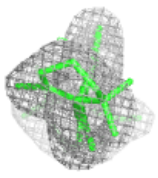


Electron density around BCR C 516:

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

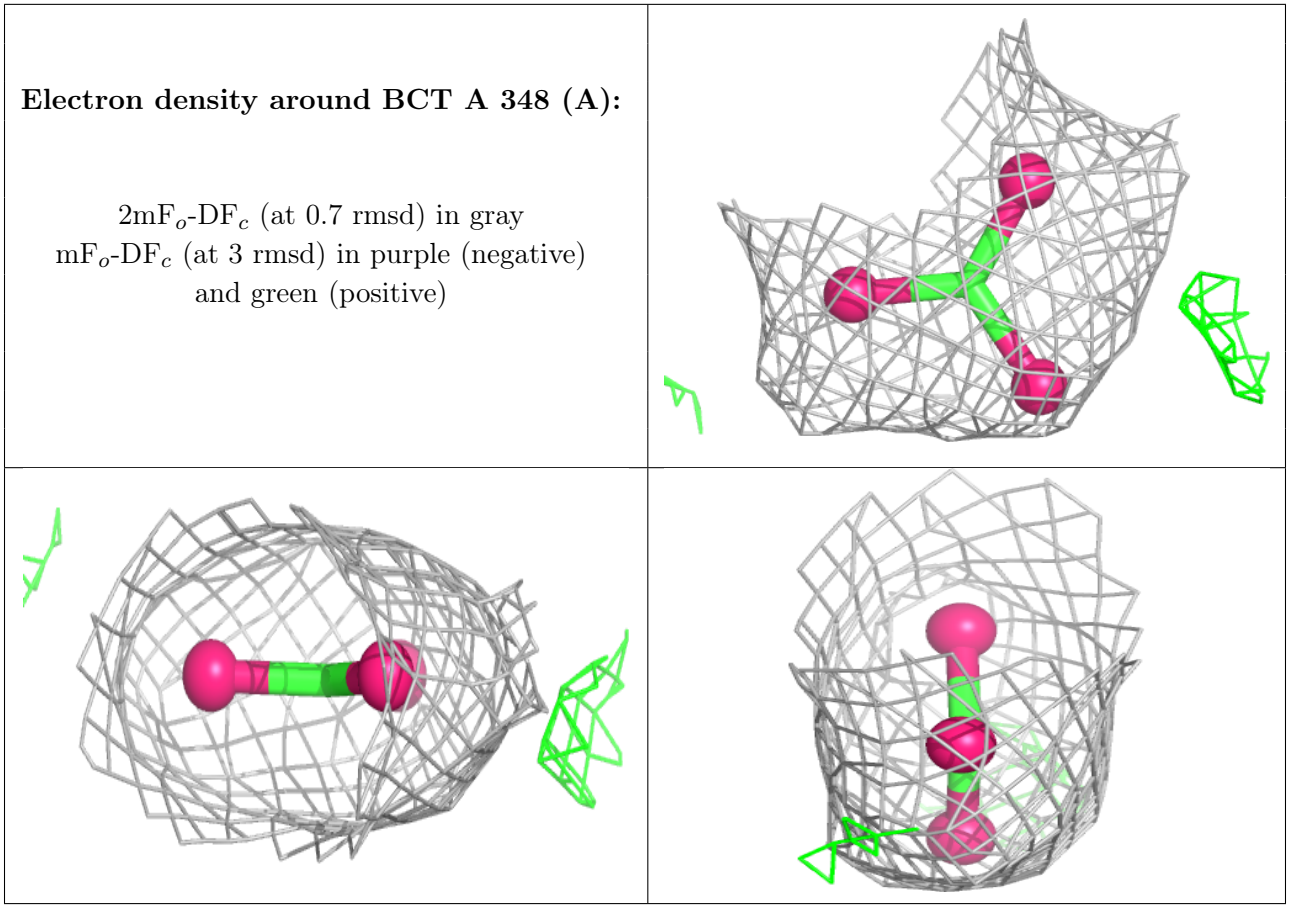






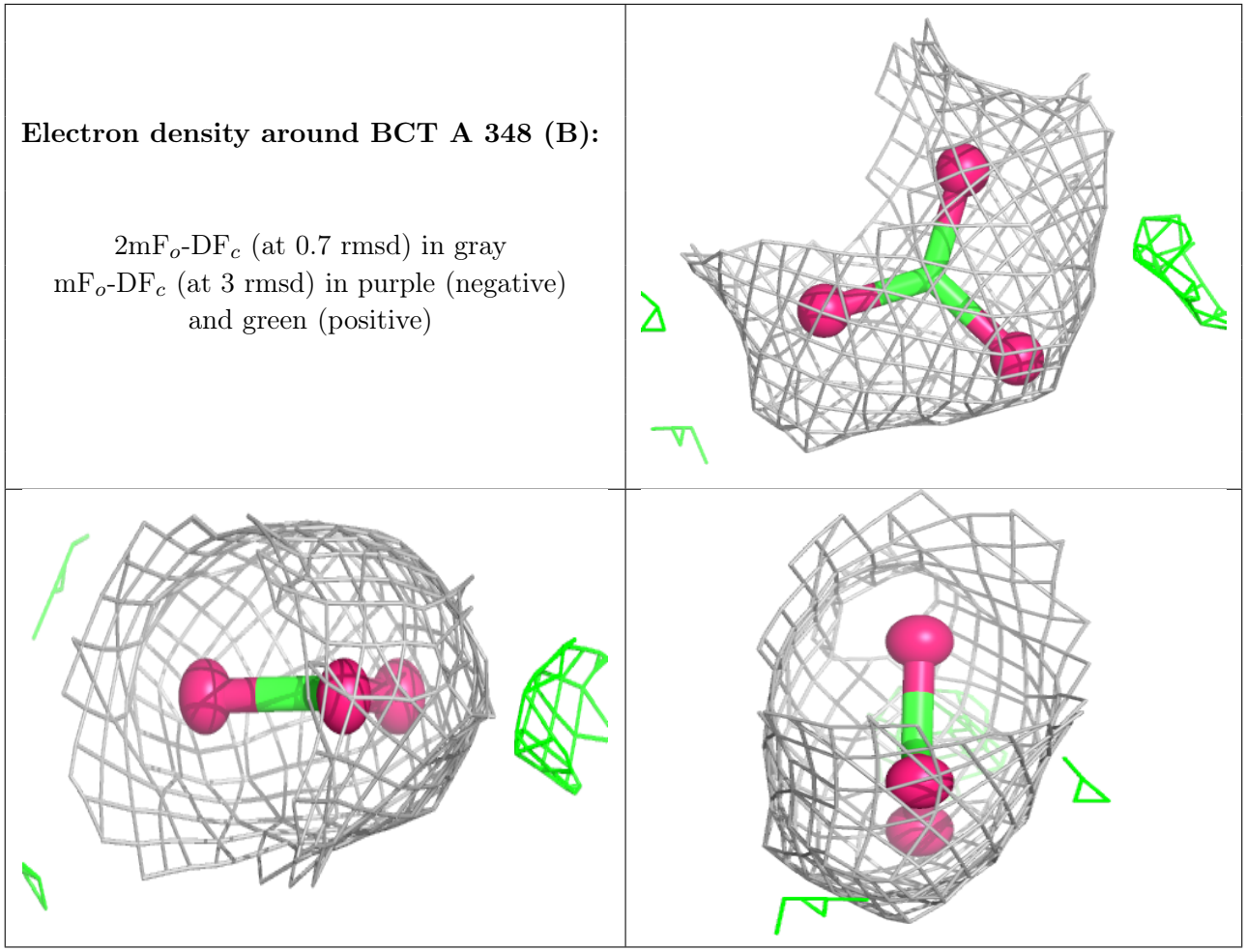
Electron density around BCT A 348 (A):

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



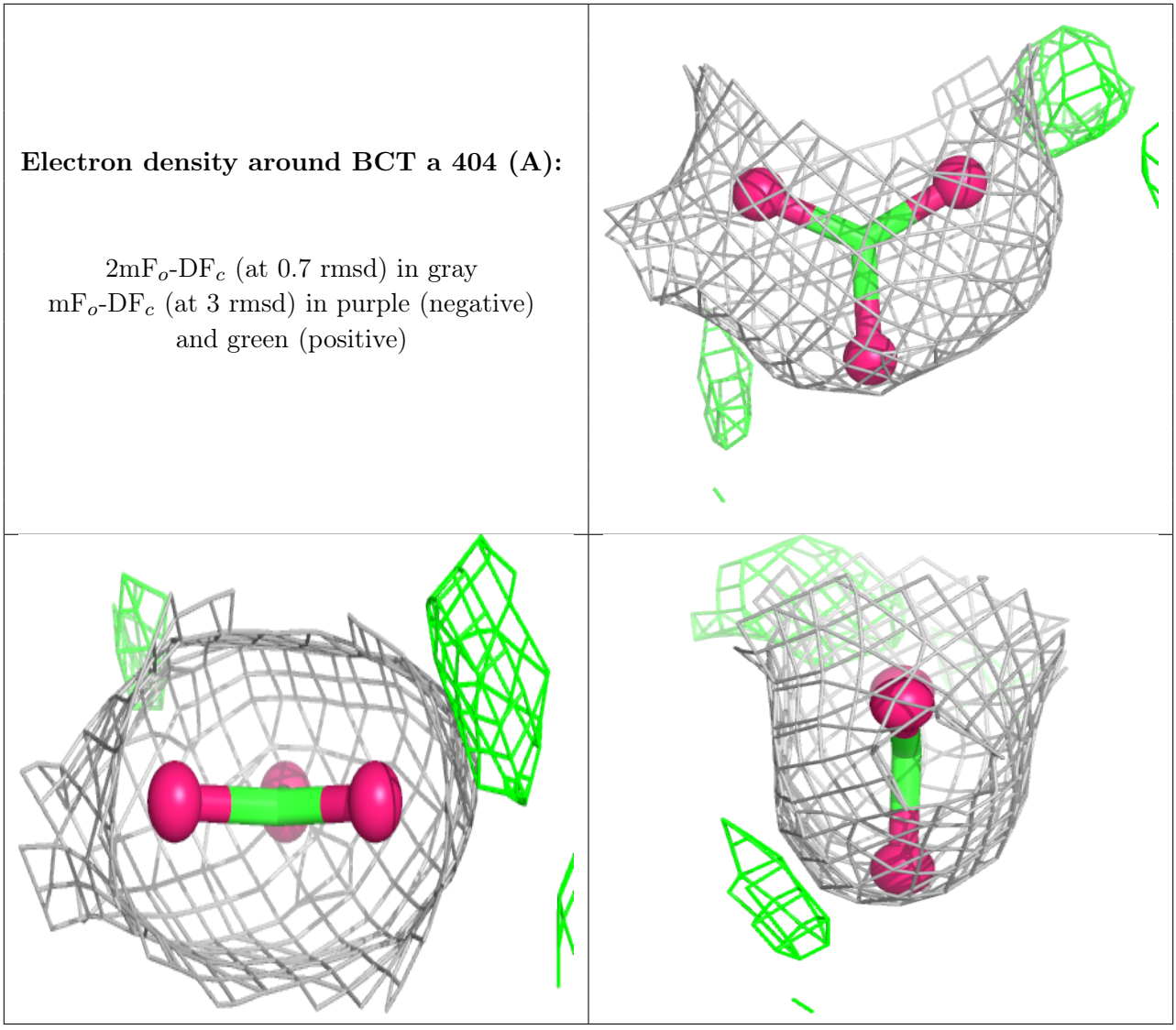
Electron density around BCT A 348 (B):

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



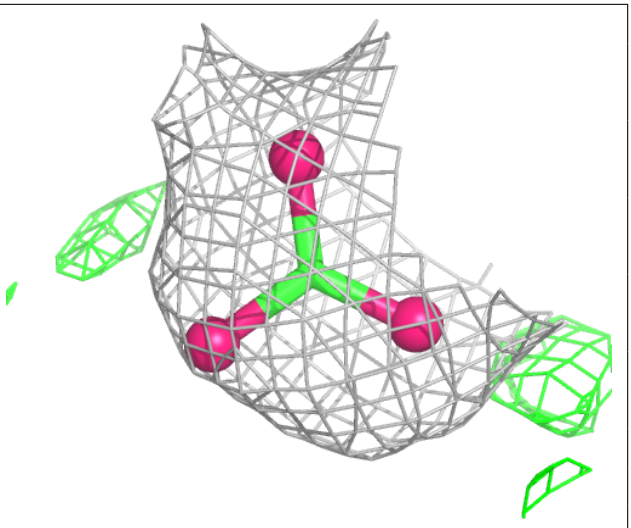
Electron density around BCT a 404 (A):

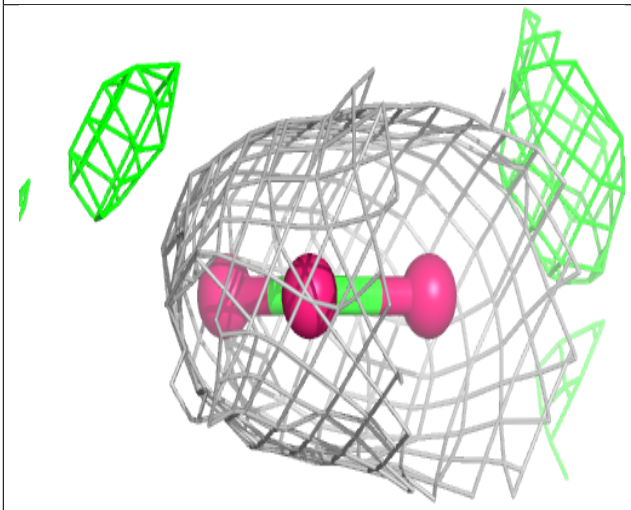
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

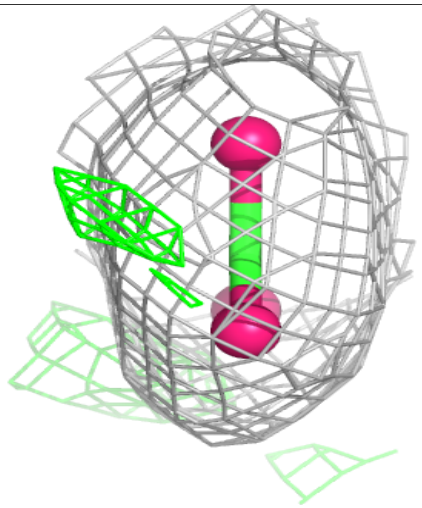


Electron density around BCT a 404 (B):

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

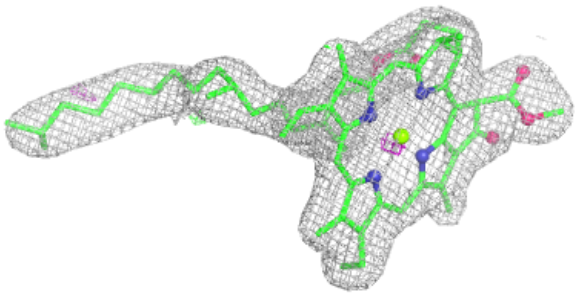


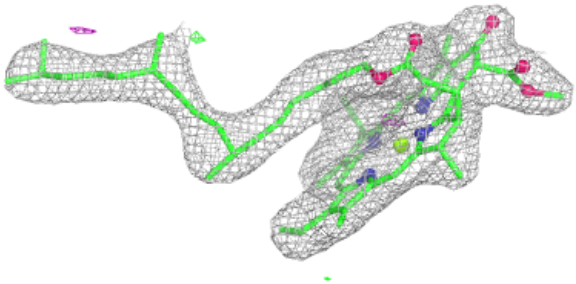


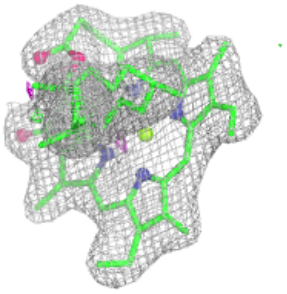


Electron density around CLA C 506:

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

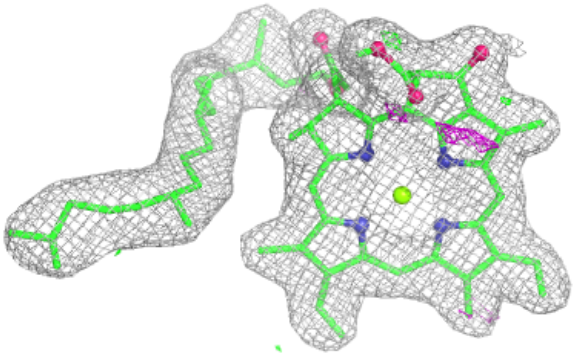


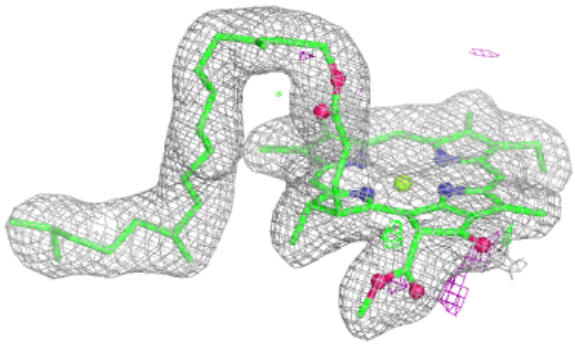


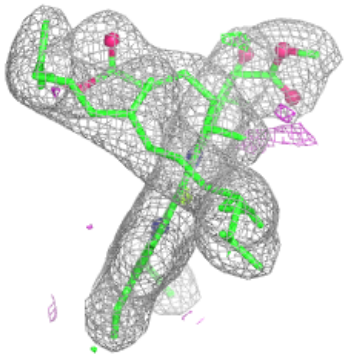


Electron density around CLA A 405 (B):

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

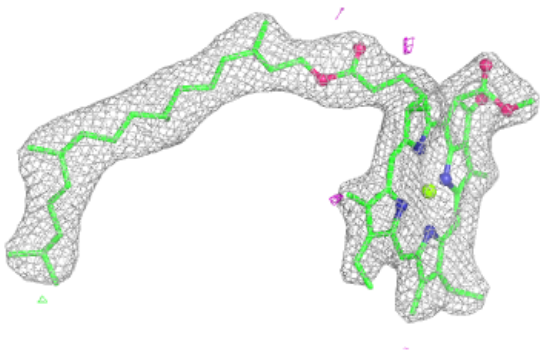


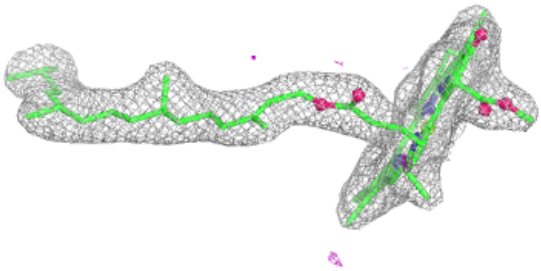


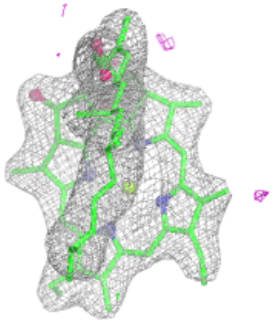


Electron density around CLA b 609:

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

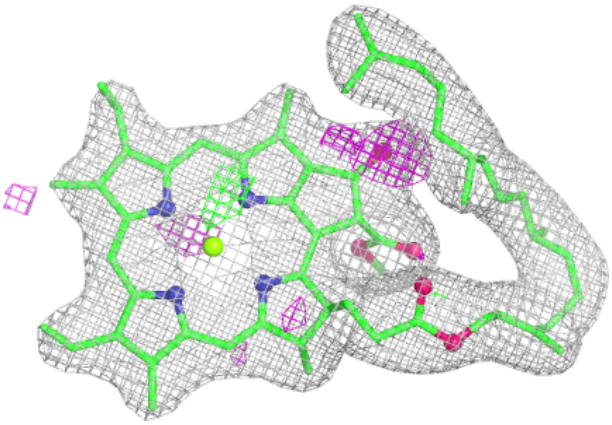


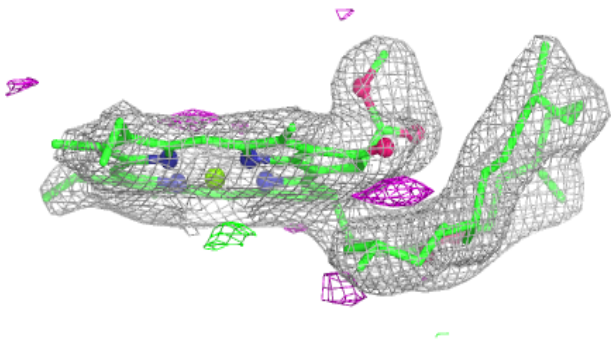


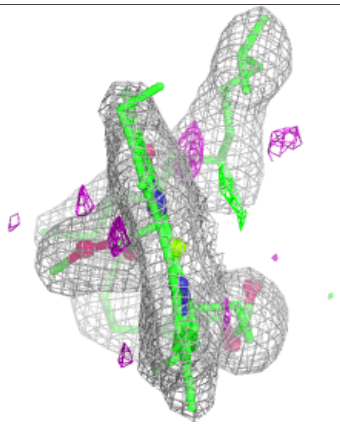


Electron density around CLA b 610:

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

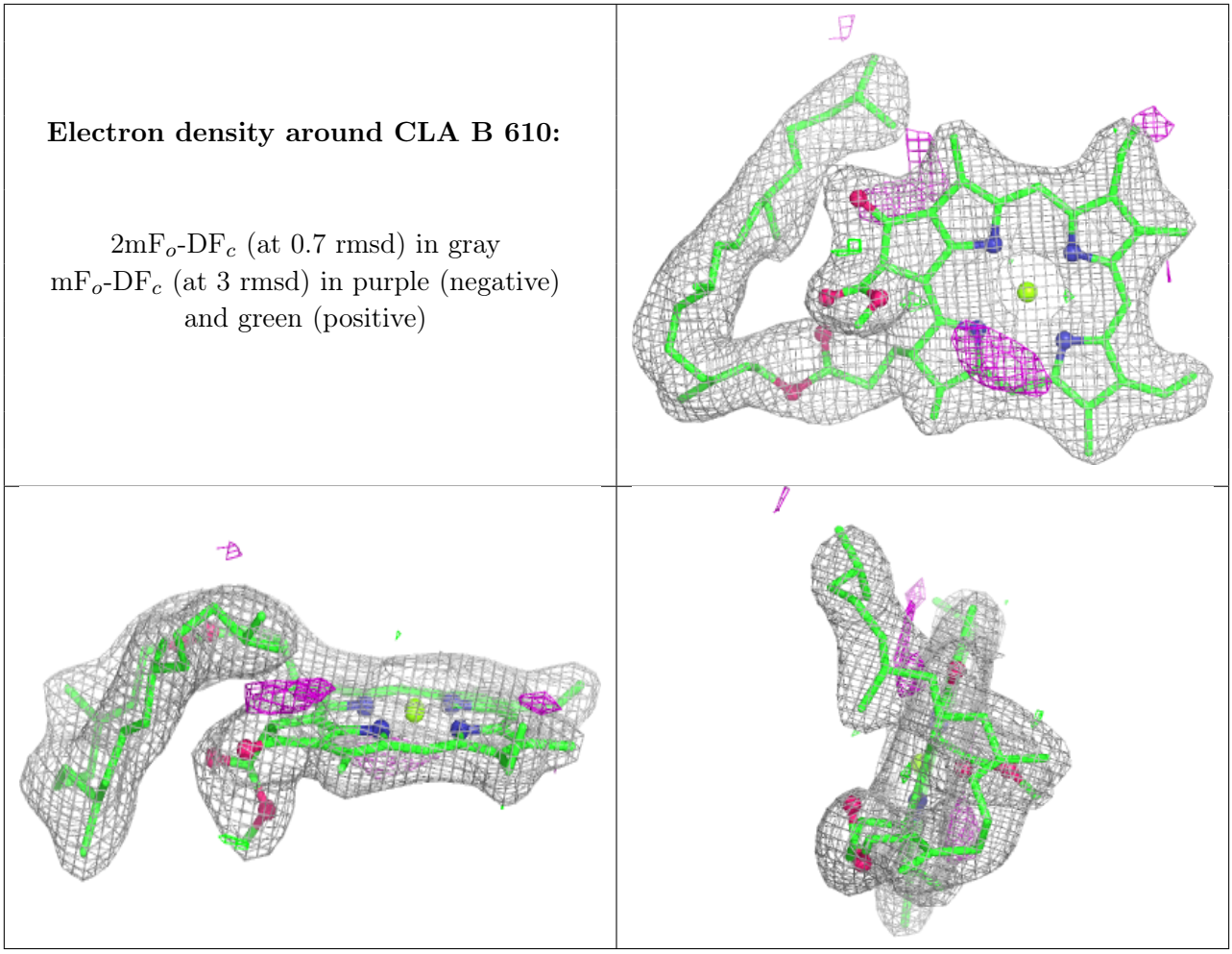






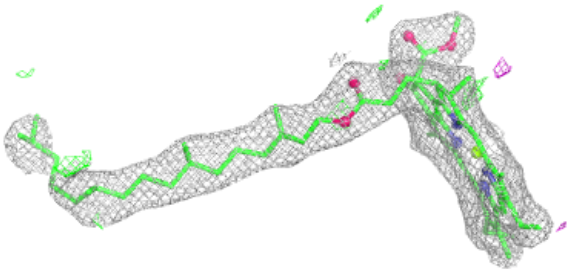
Electron density around CLA B 610:

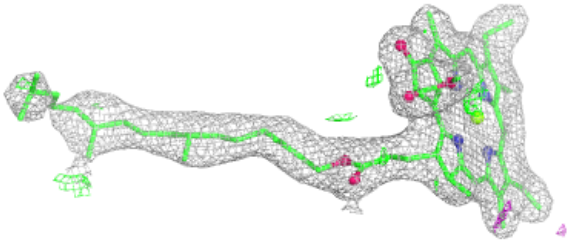
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

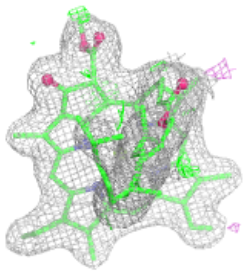


Electron density around CLA B 604:

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

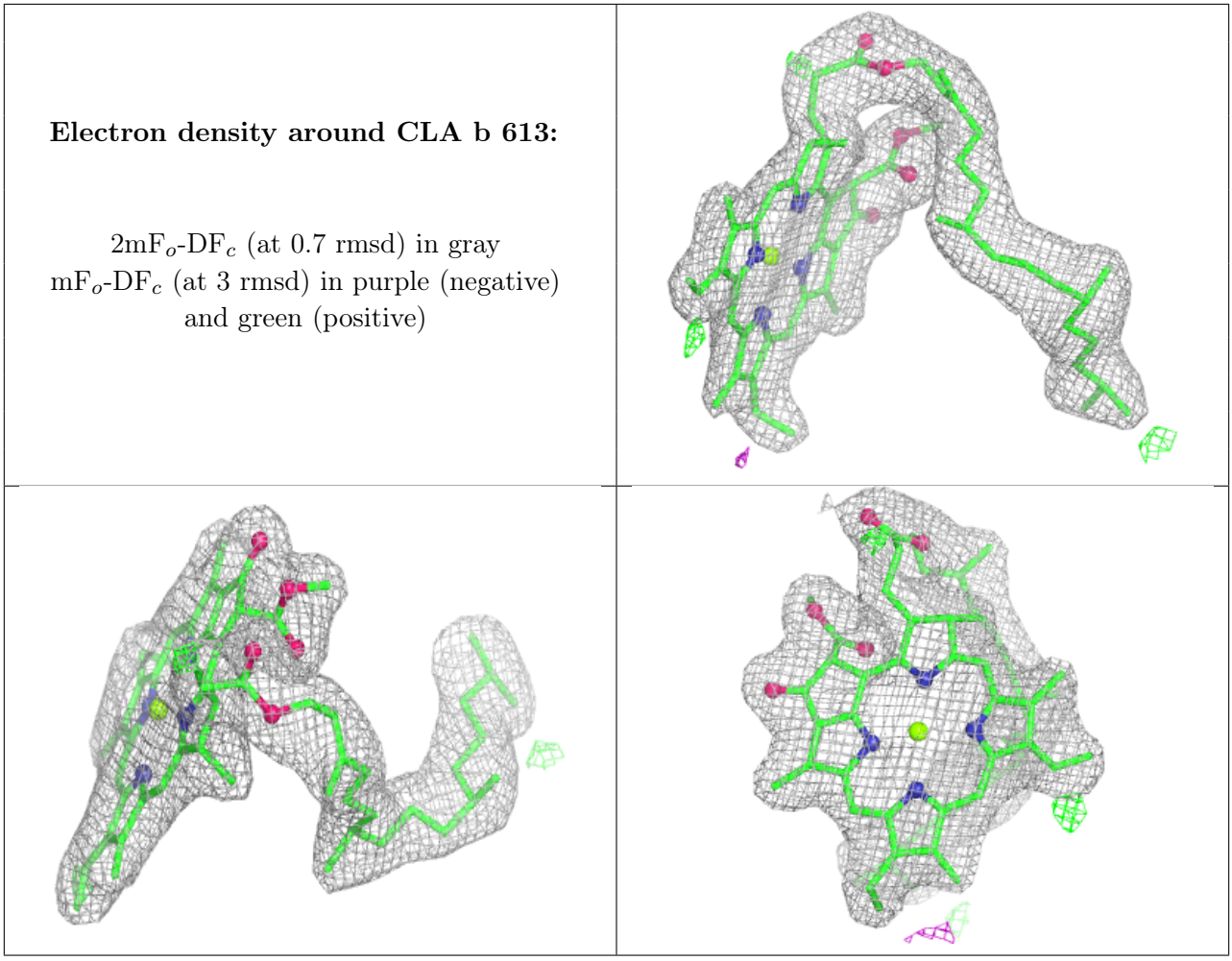






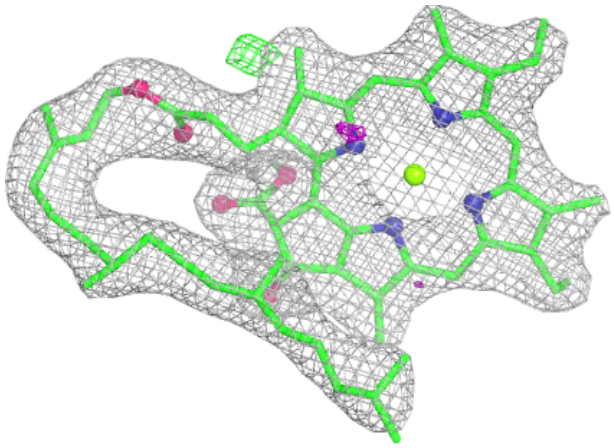
Electron density around CLA b 613:

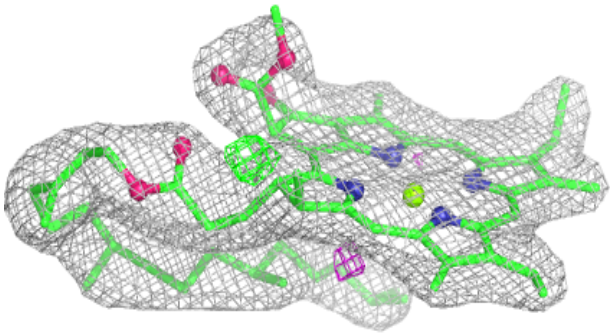
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

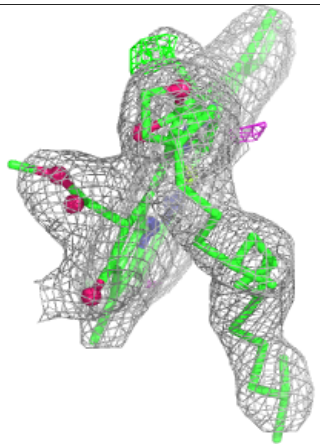


Electron density around CLA C 510:

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

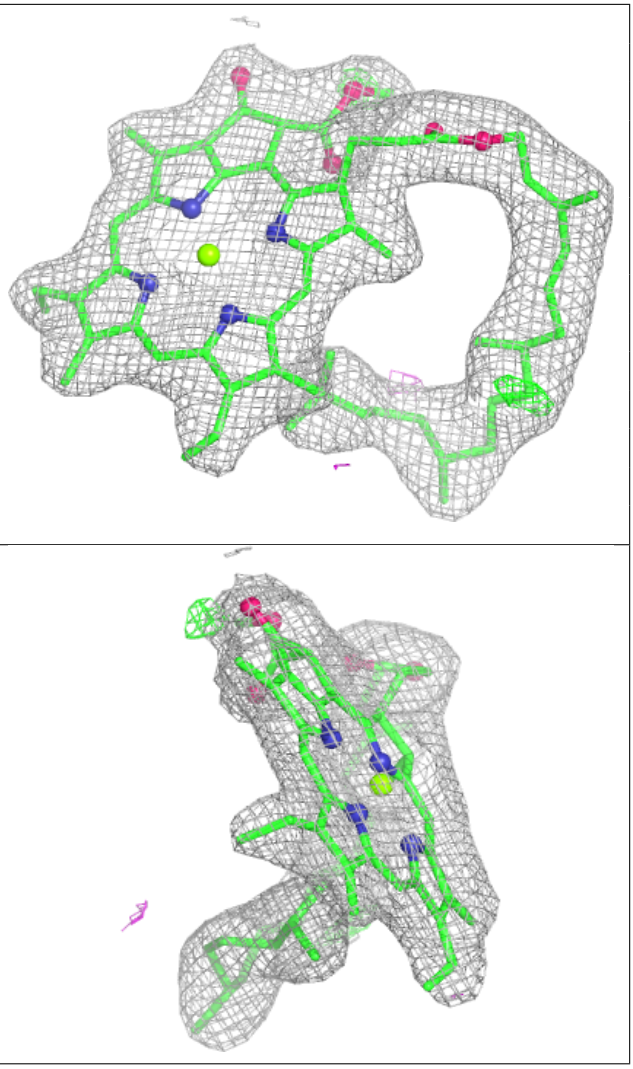






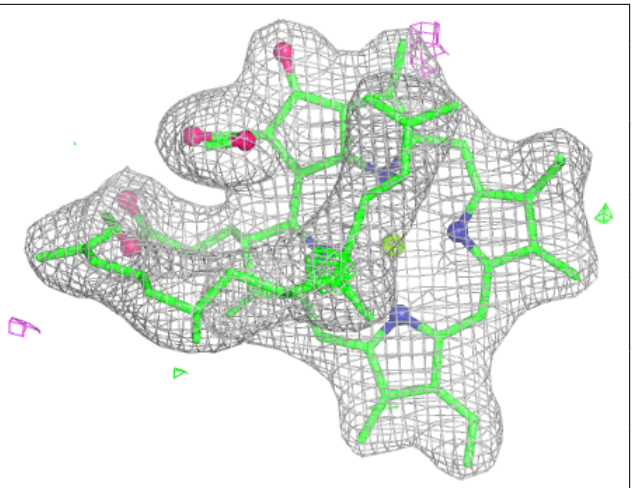
Electron density around CLA b 615:

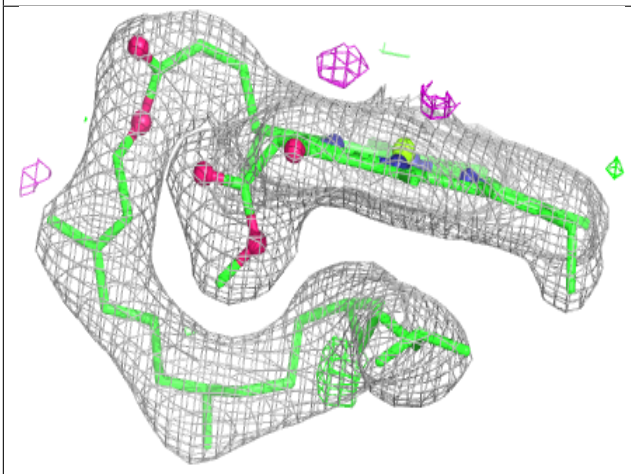
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

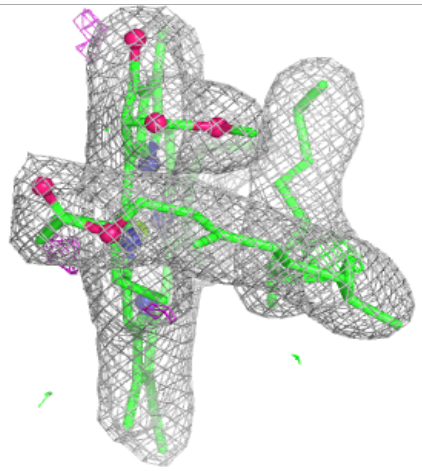


Electron density around CLA C 511:

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

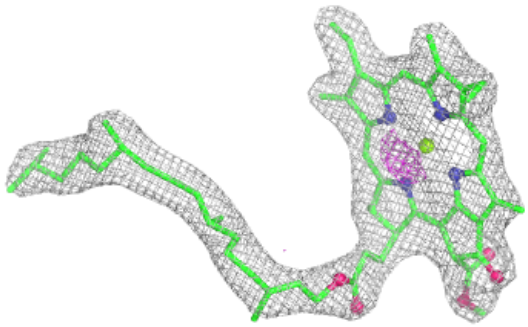


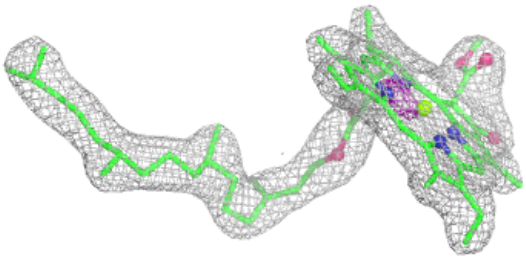


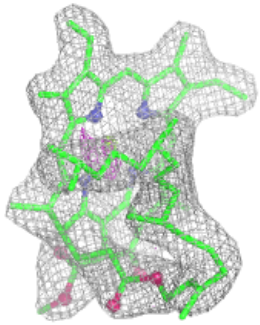


Electron density around CLA C 512:

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

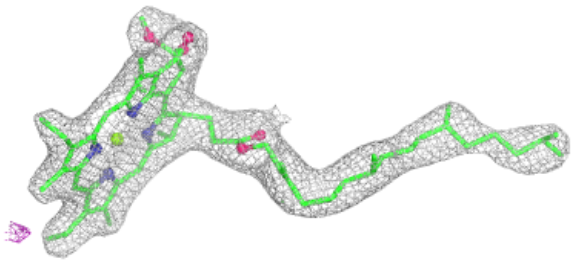


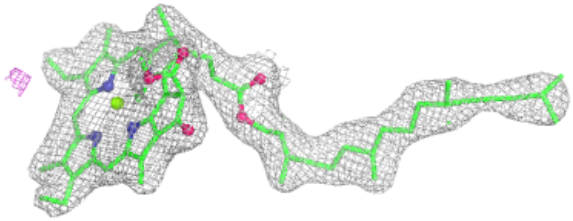


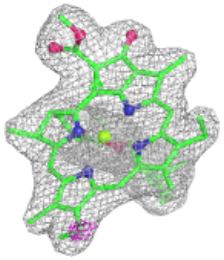


Electron density around CLA c 503:

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

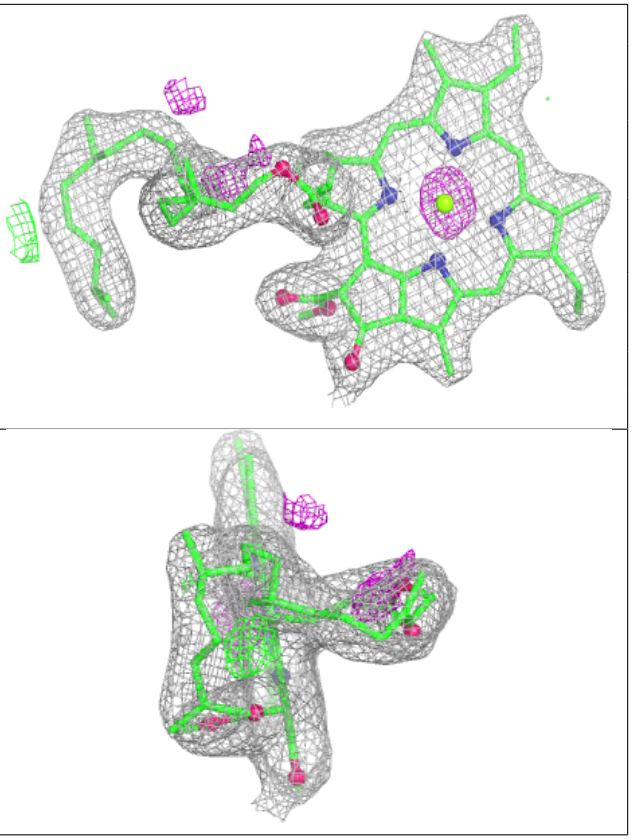


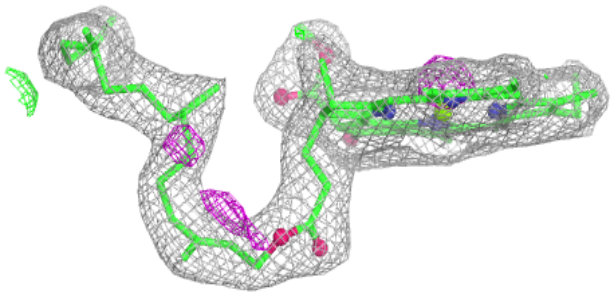




Electron density around CLA B 612:

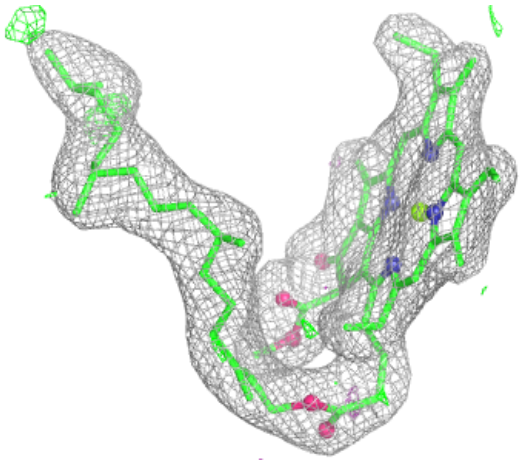
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

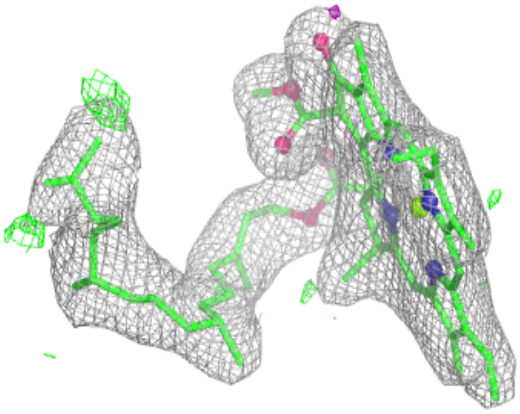


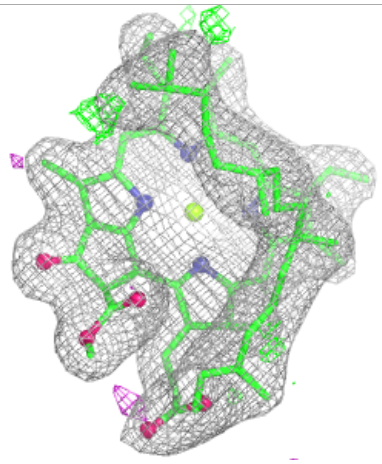


Electron density around CLA B 613:

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

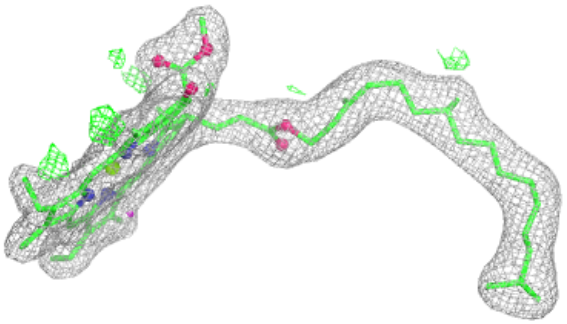


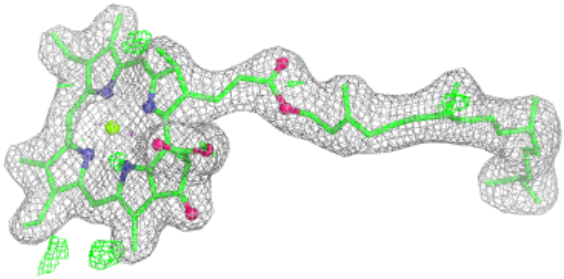


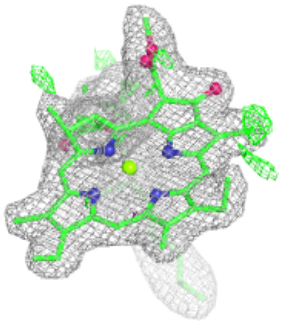


Electron density around CLA D 405 (A):

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

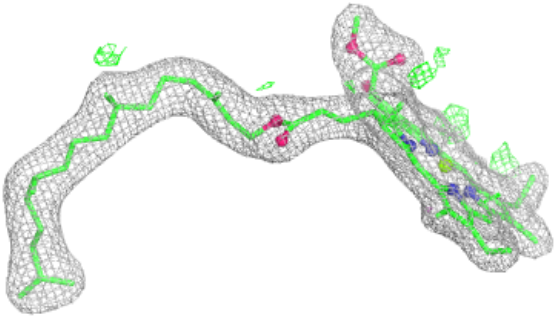


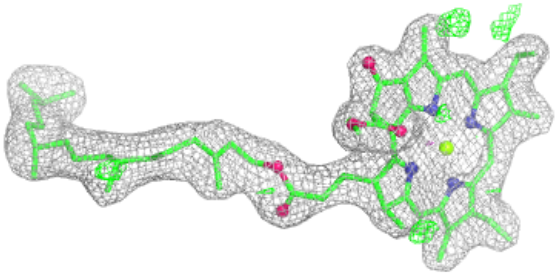


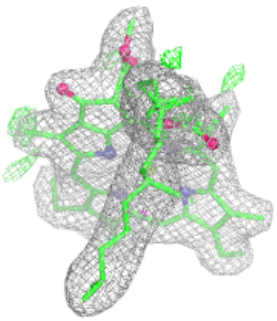


Electron density around CLA D 405 (B):

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

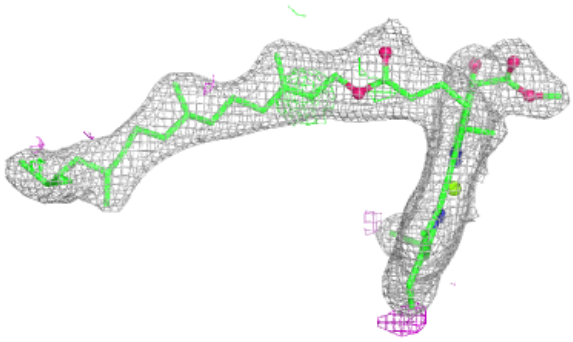


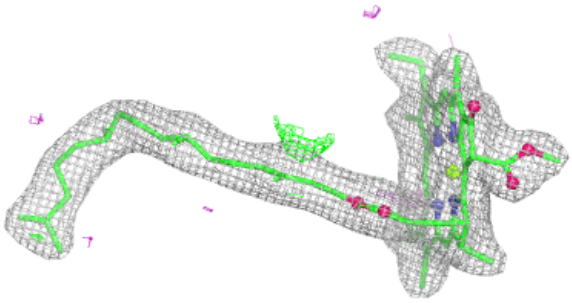


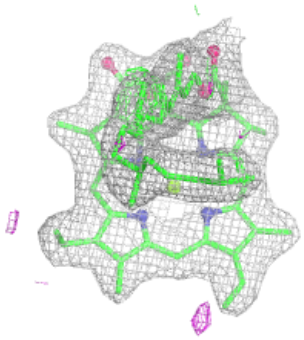


Electron density around CLA B 605:

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

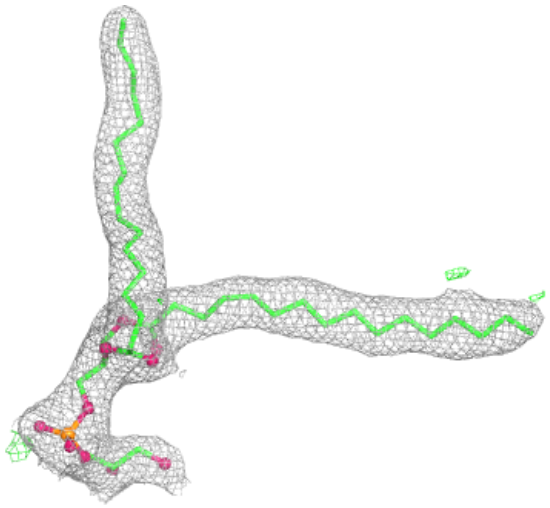


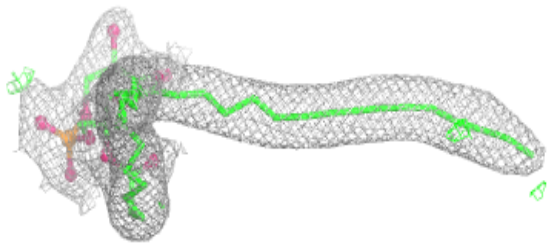


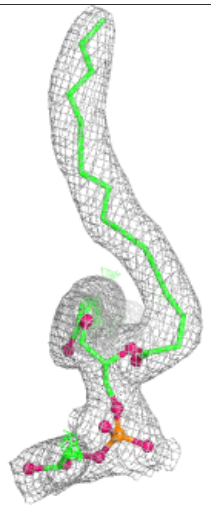


Electron density around LHG L 101 (A):

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



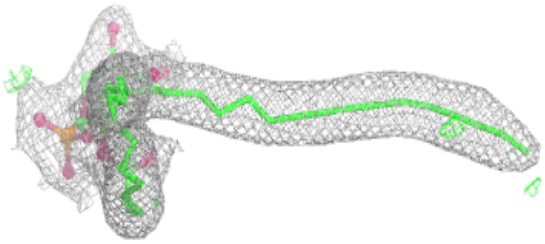


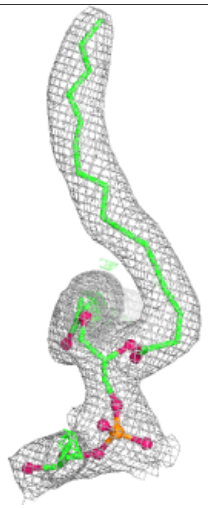


Electron density around LHG L 101 (B):

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

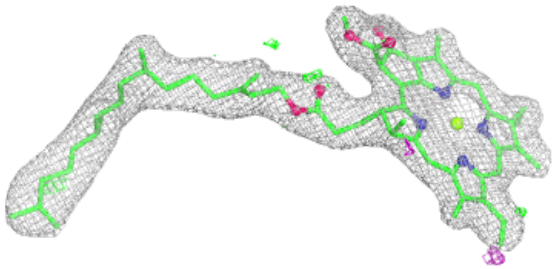


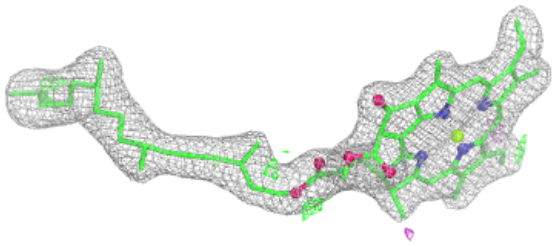


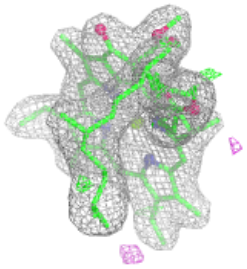


Electron density around CLA a 405 (A):

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

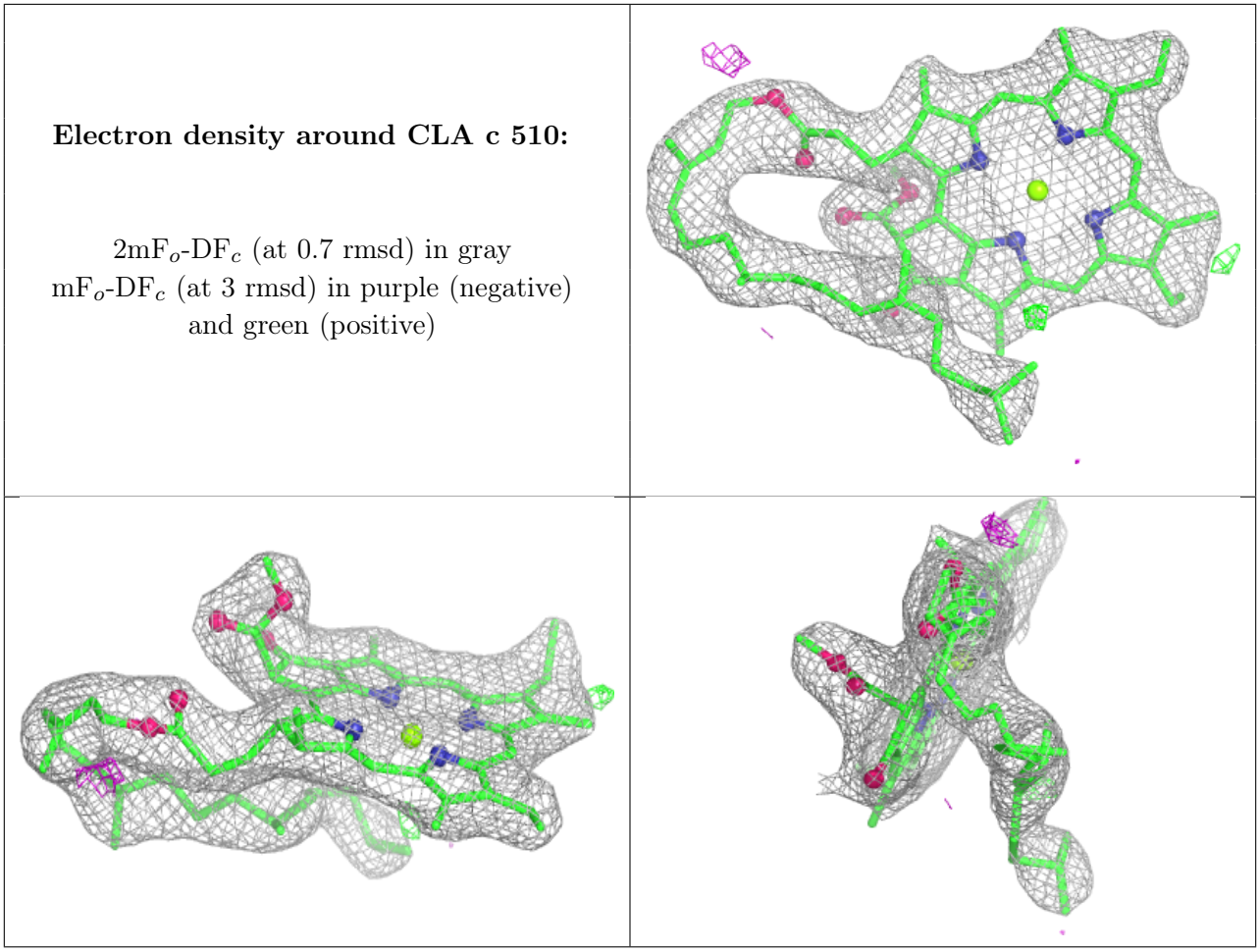






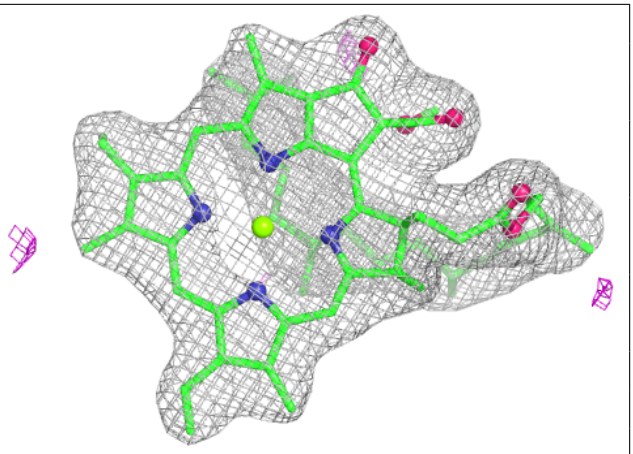
Electron density around CLA c 510:

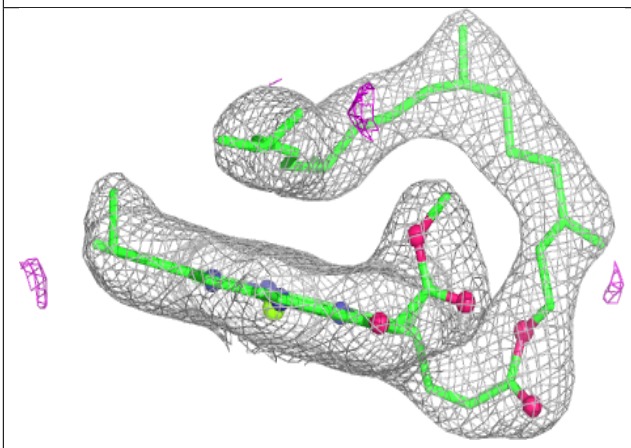
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

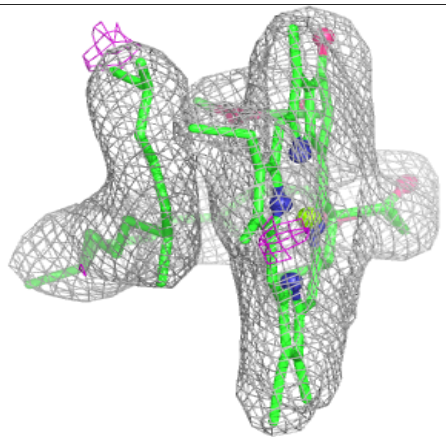


Electron density around CLA c 511:

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

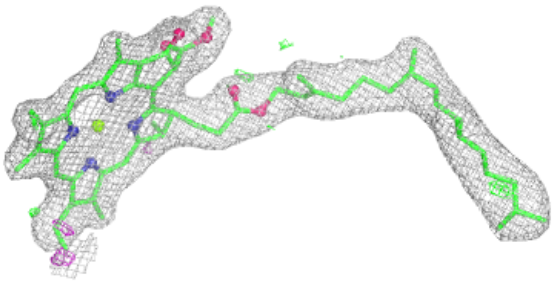


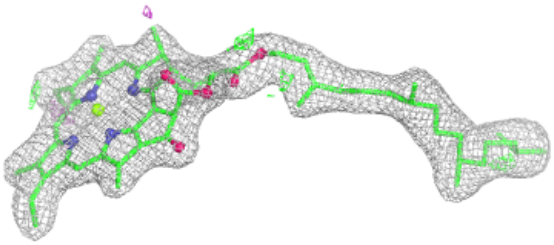


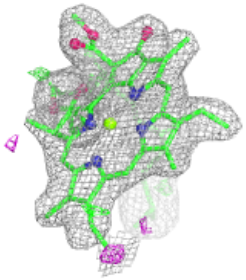


Electron density around CLA a 405 (B):

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

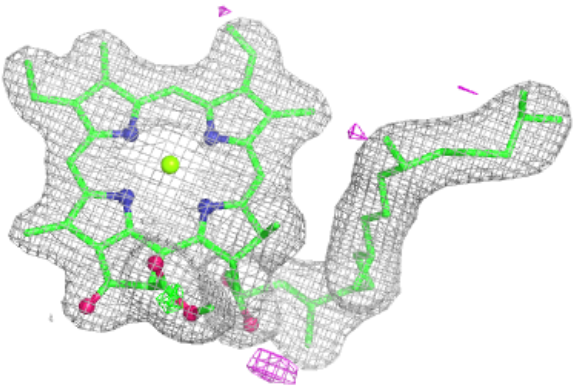


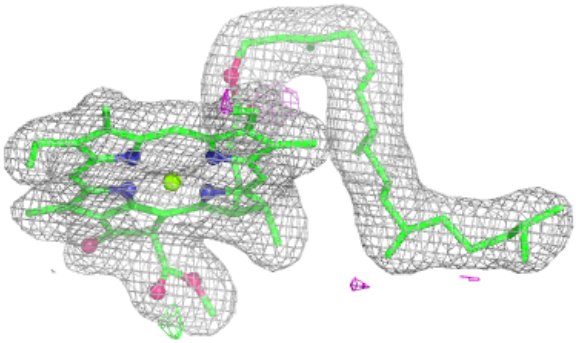


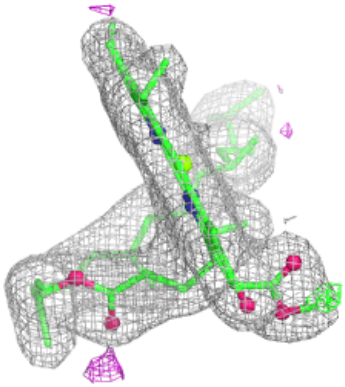


Electron density around CLA a 406 (A):

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

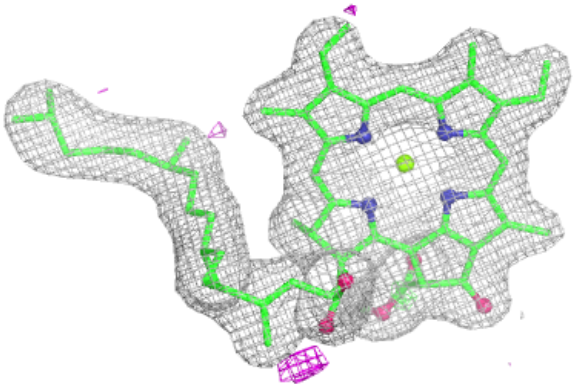


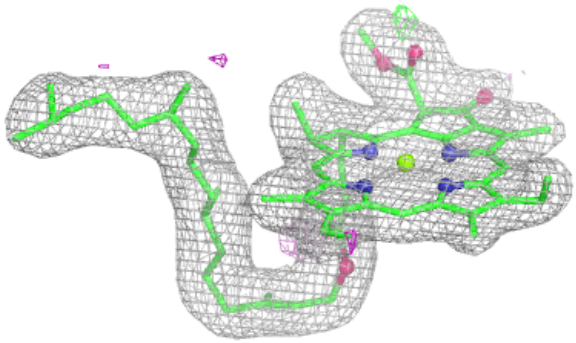


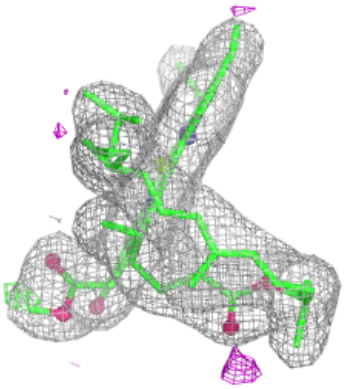


Electron density around CLA a 406 (B):

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

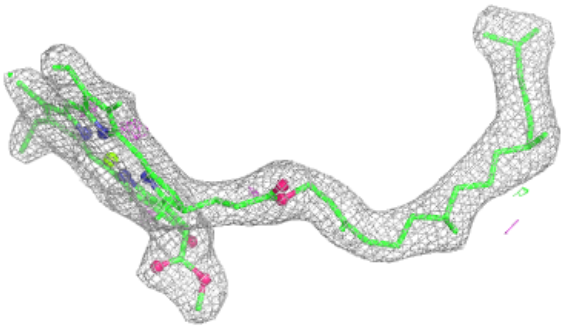


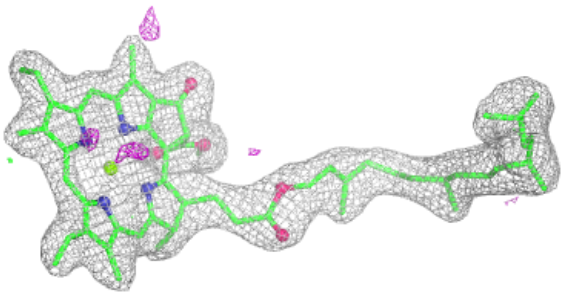


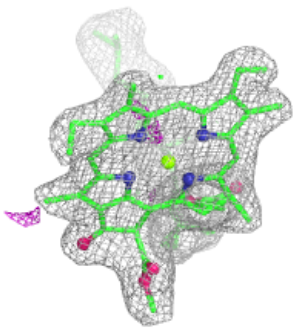


Electron density around CLA d 402 (A):

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

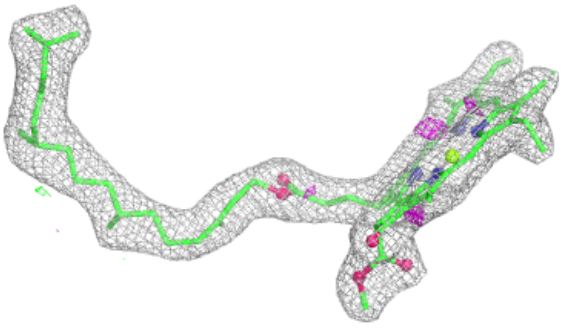


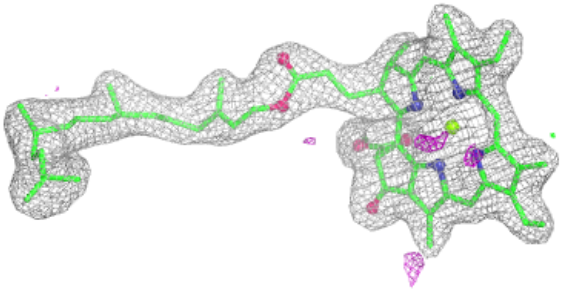


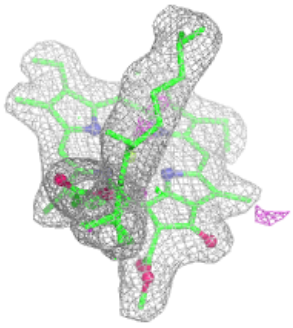


Electron density around CLA d 402 (B):

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

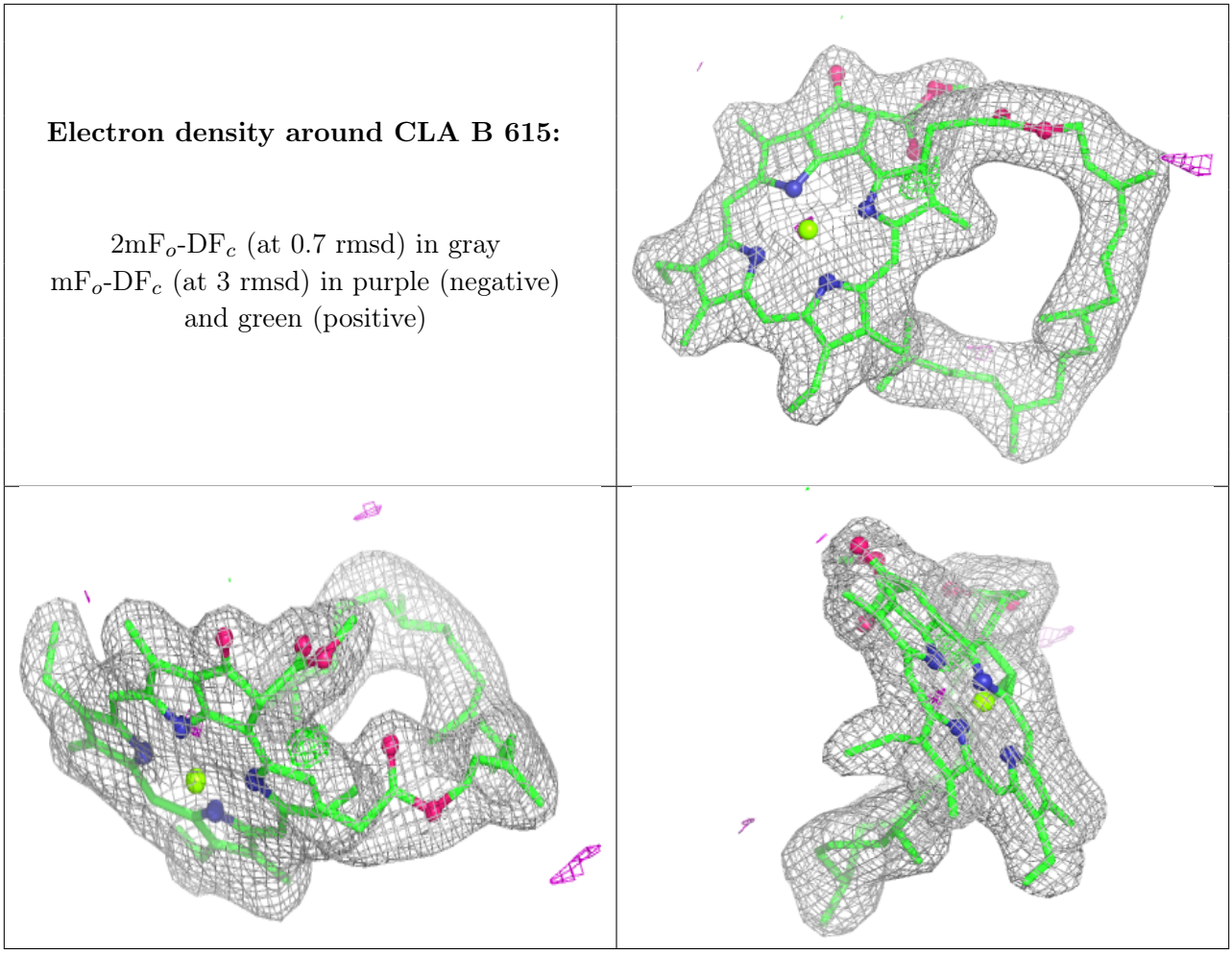






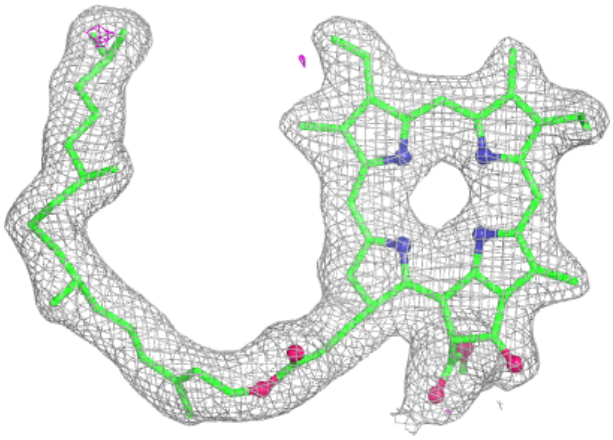
Electron density around CLA B 615:

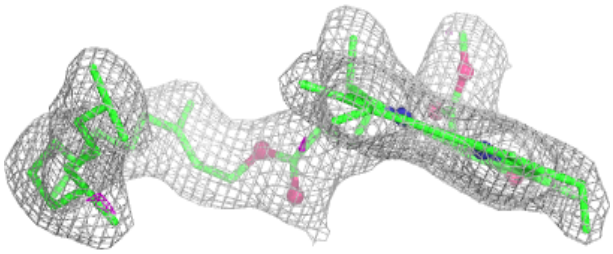
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

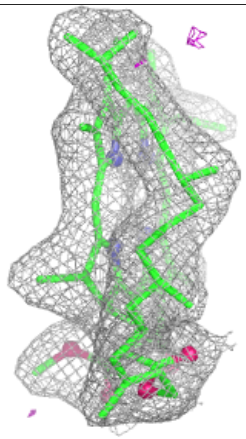


Electron density around PHO A 407 (A):

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

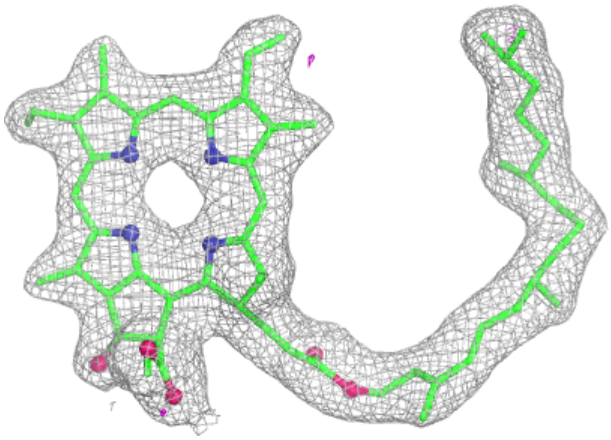


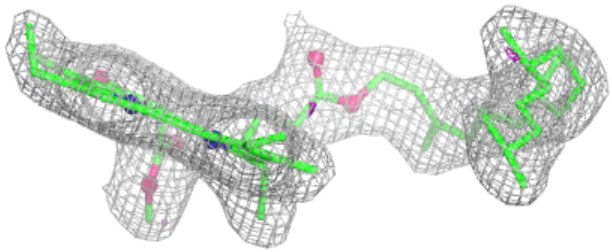


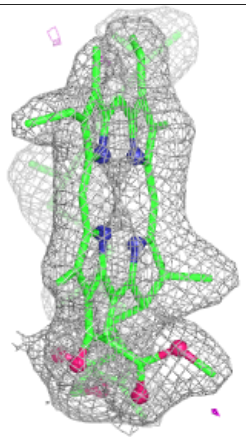


Electron density around PHO A 407 (B):

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

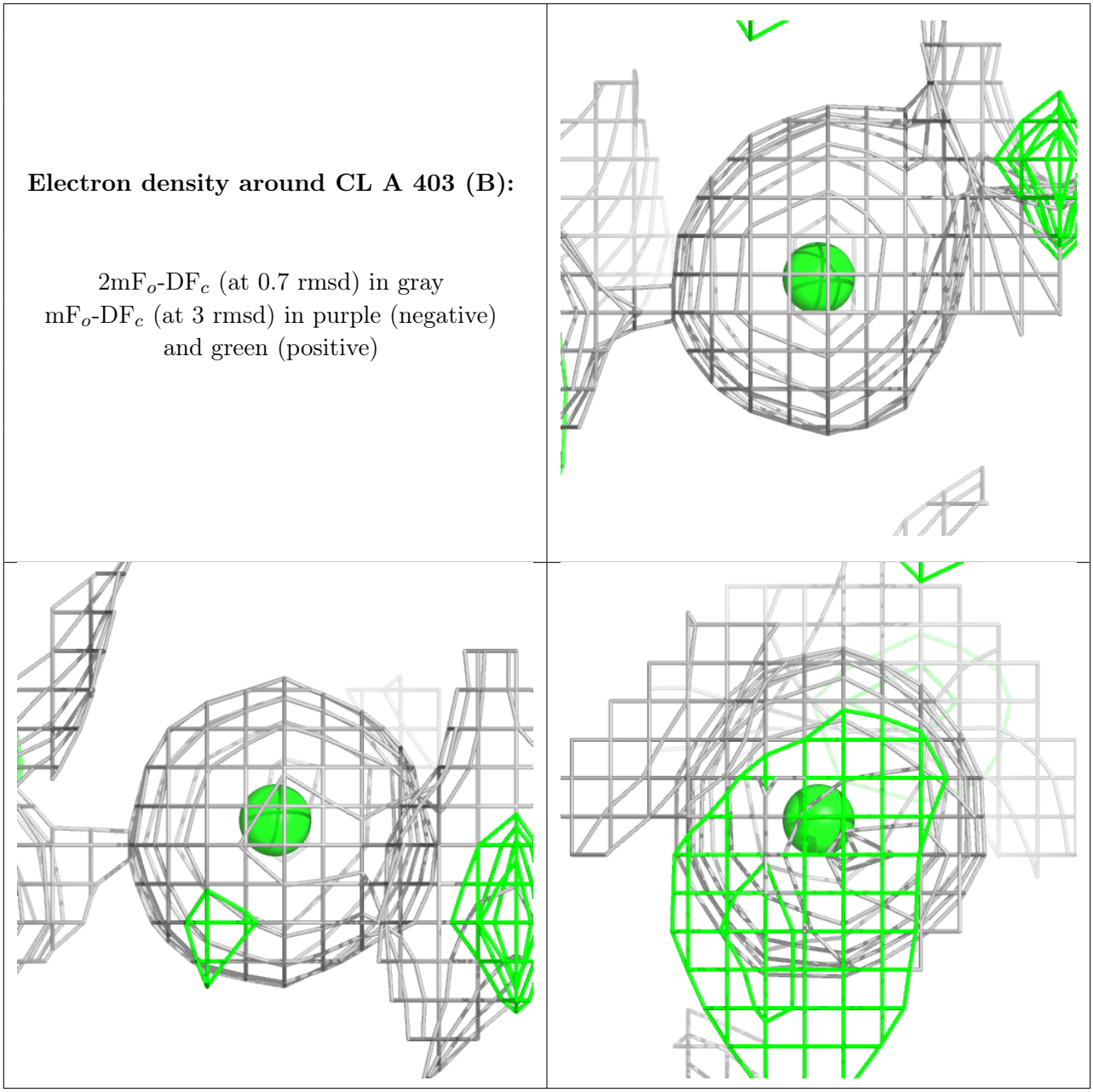






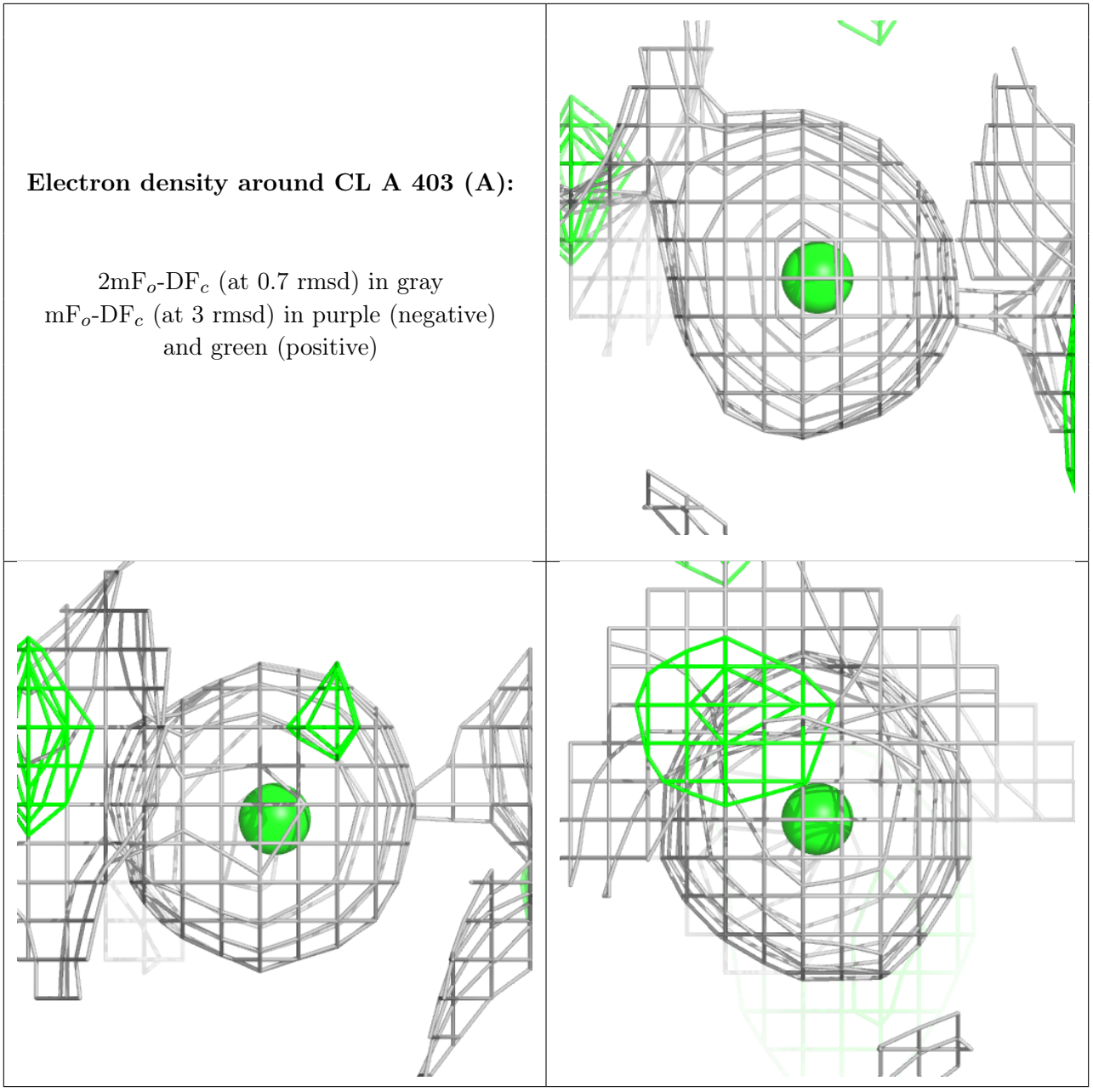
Electron density around CL A 403 (B):

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



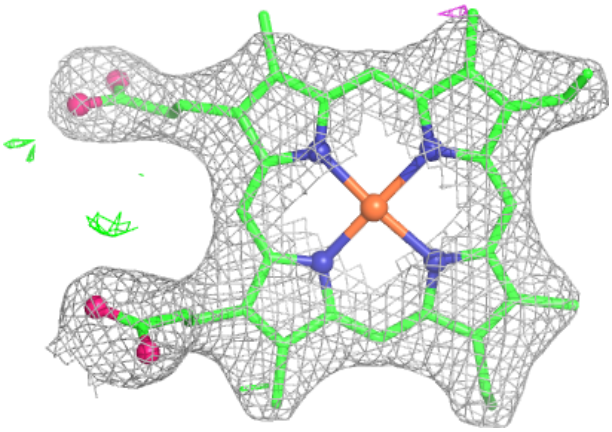
Electron density around CL A 403 (A):

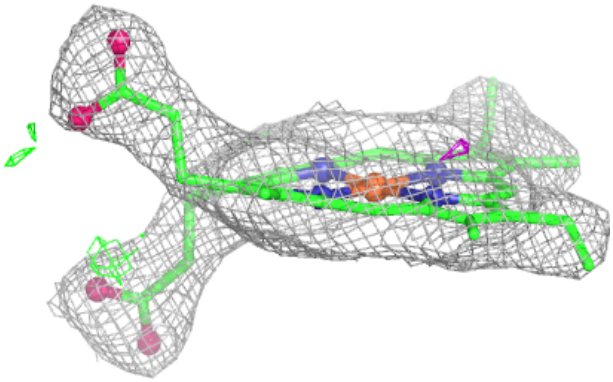
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

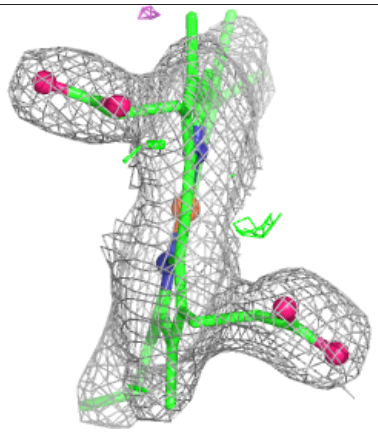


Electron density around HEM E 103:

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

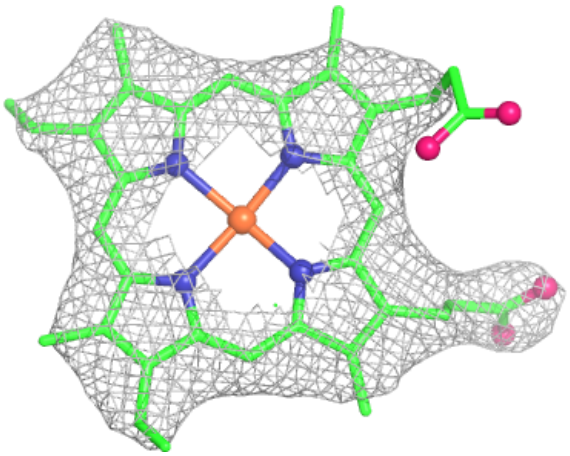


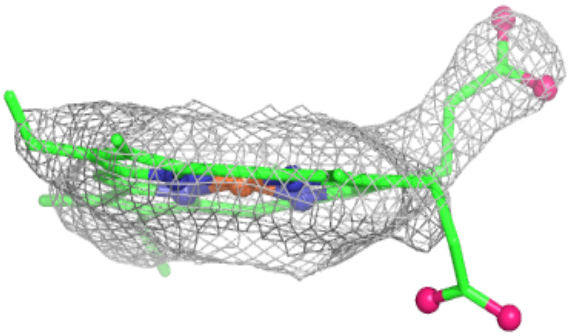


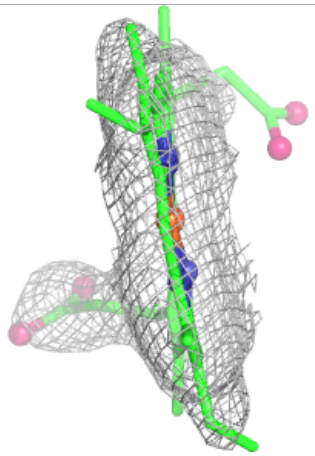


Electron density around HEM e 87:

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

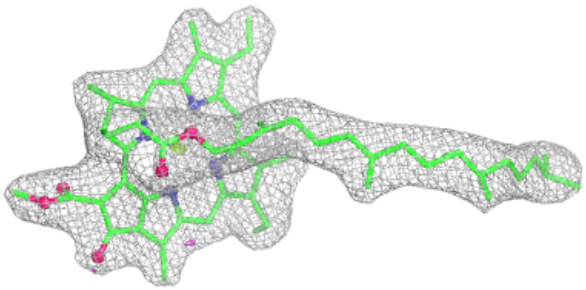


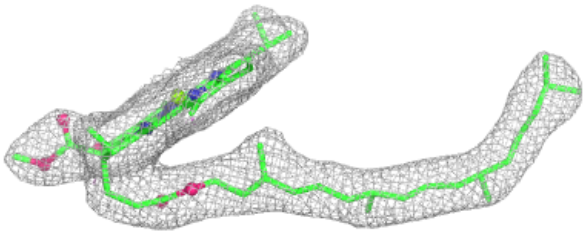


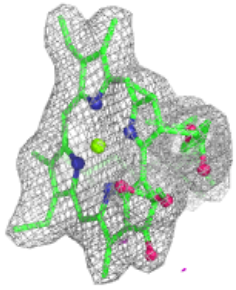


Electron density around CLA b 608:

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

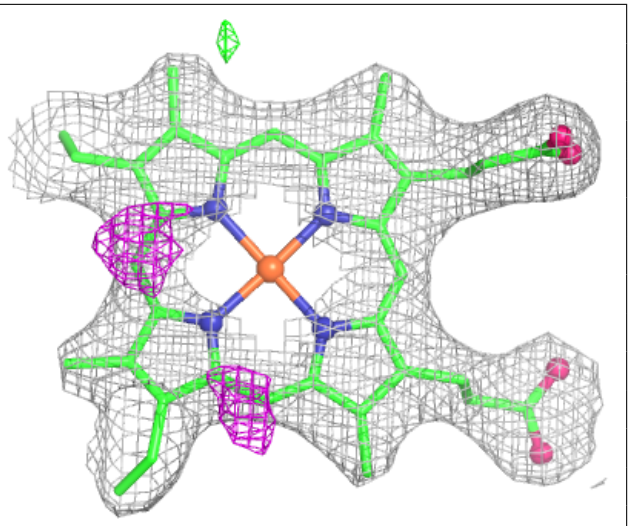


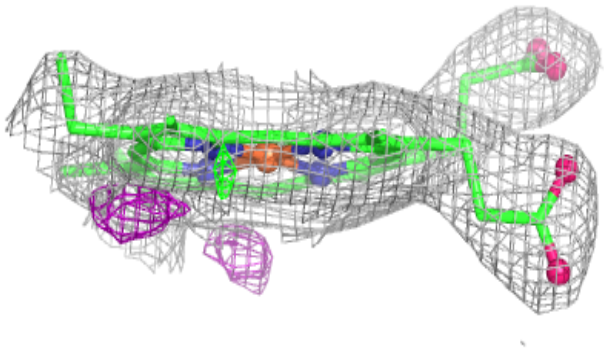


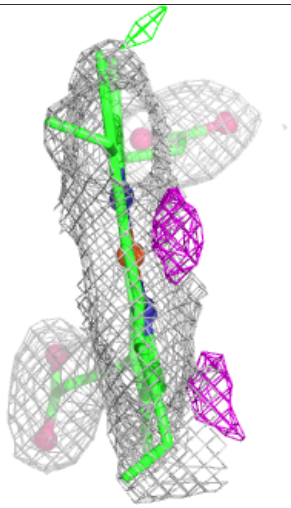


Electron density around HEC v 202:

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

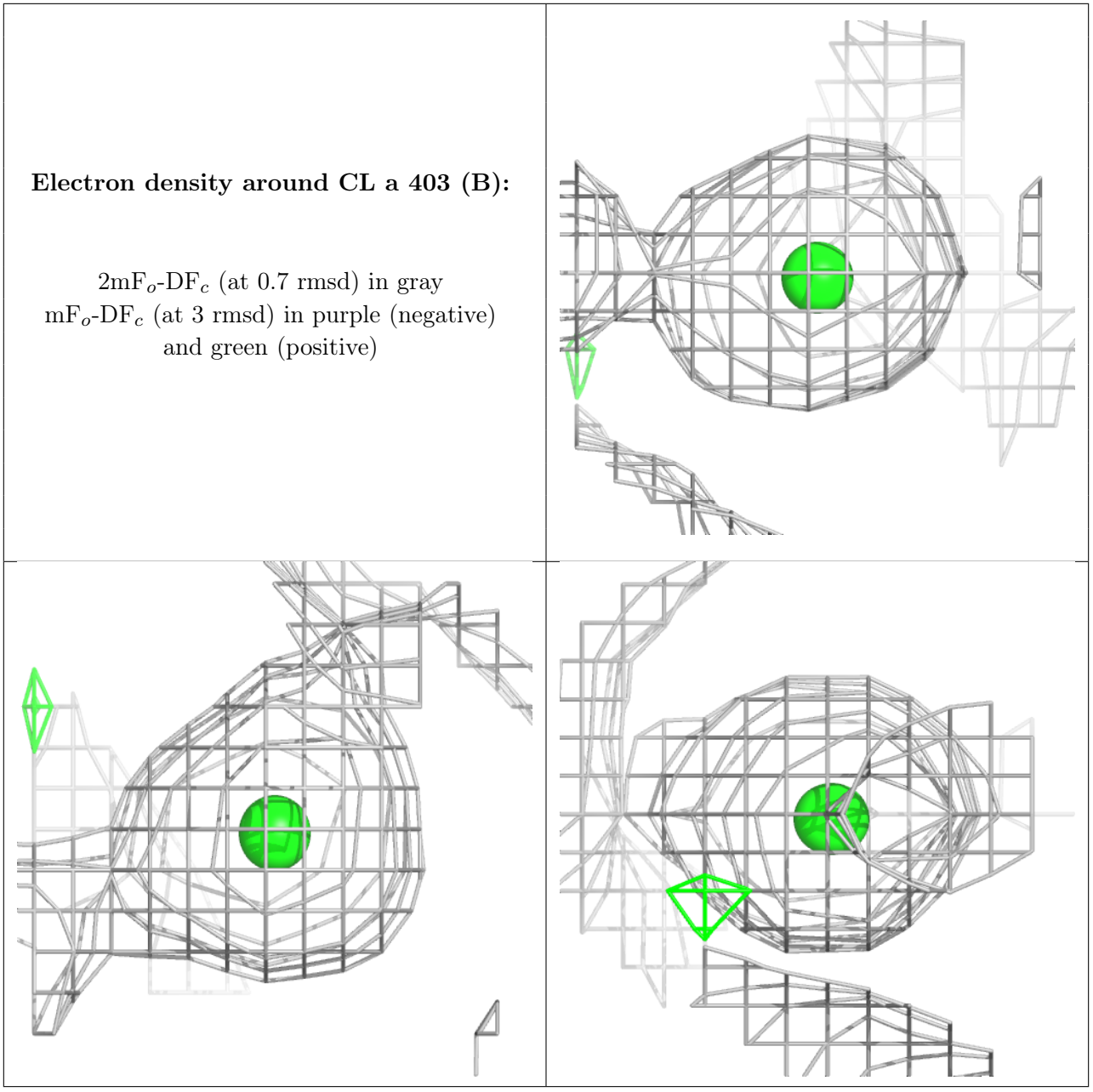






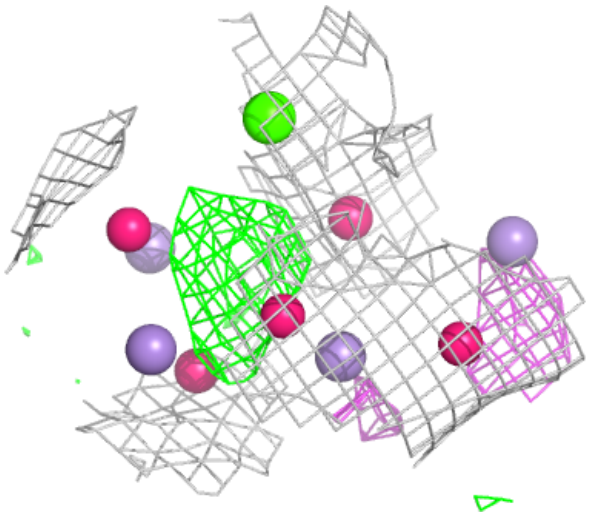
Electron density around CL a 403 (B):

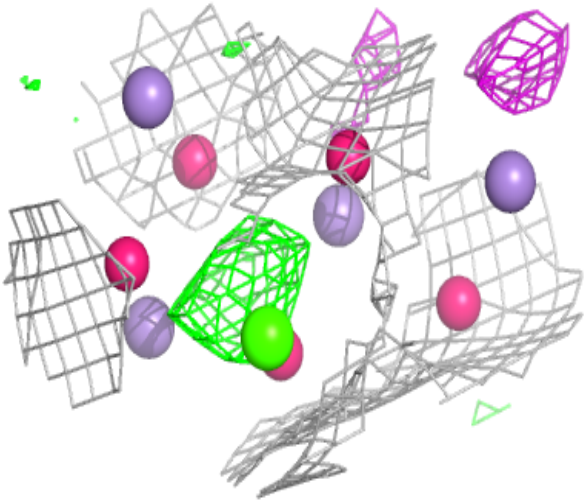
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

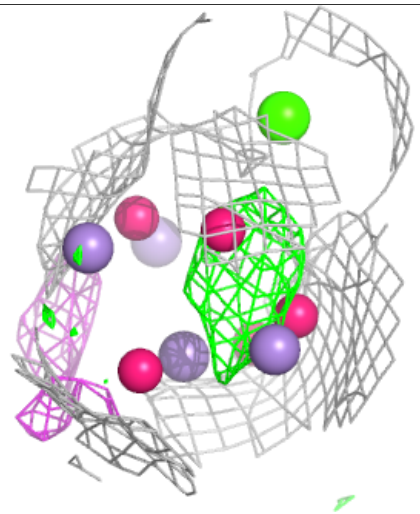


Electron density around OEX A 413 (A):

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

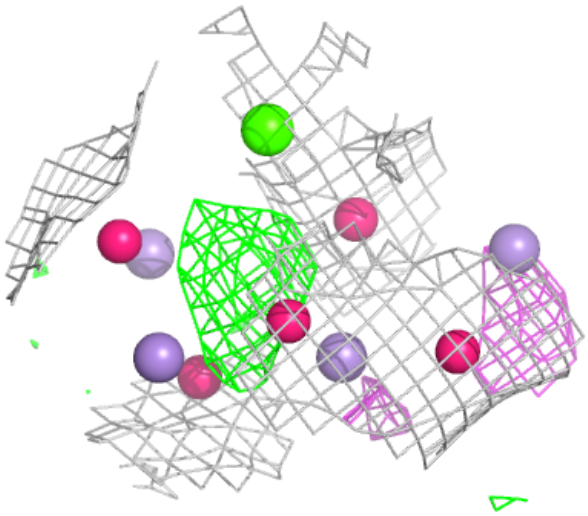


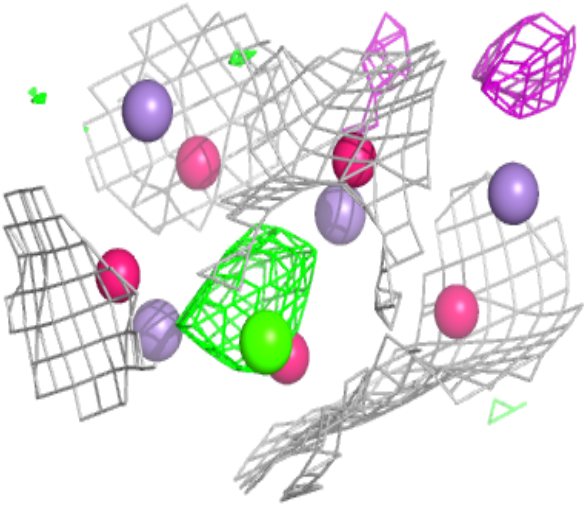


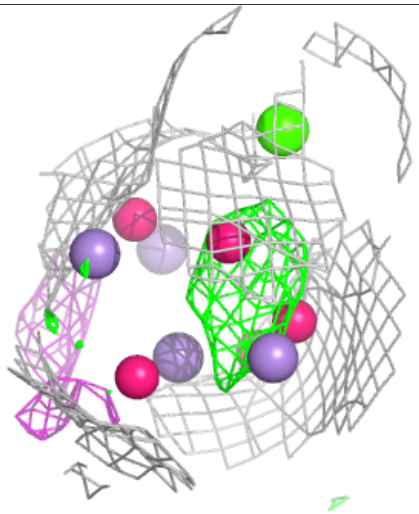


Electron density around OEX A 413 (B):

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

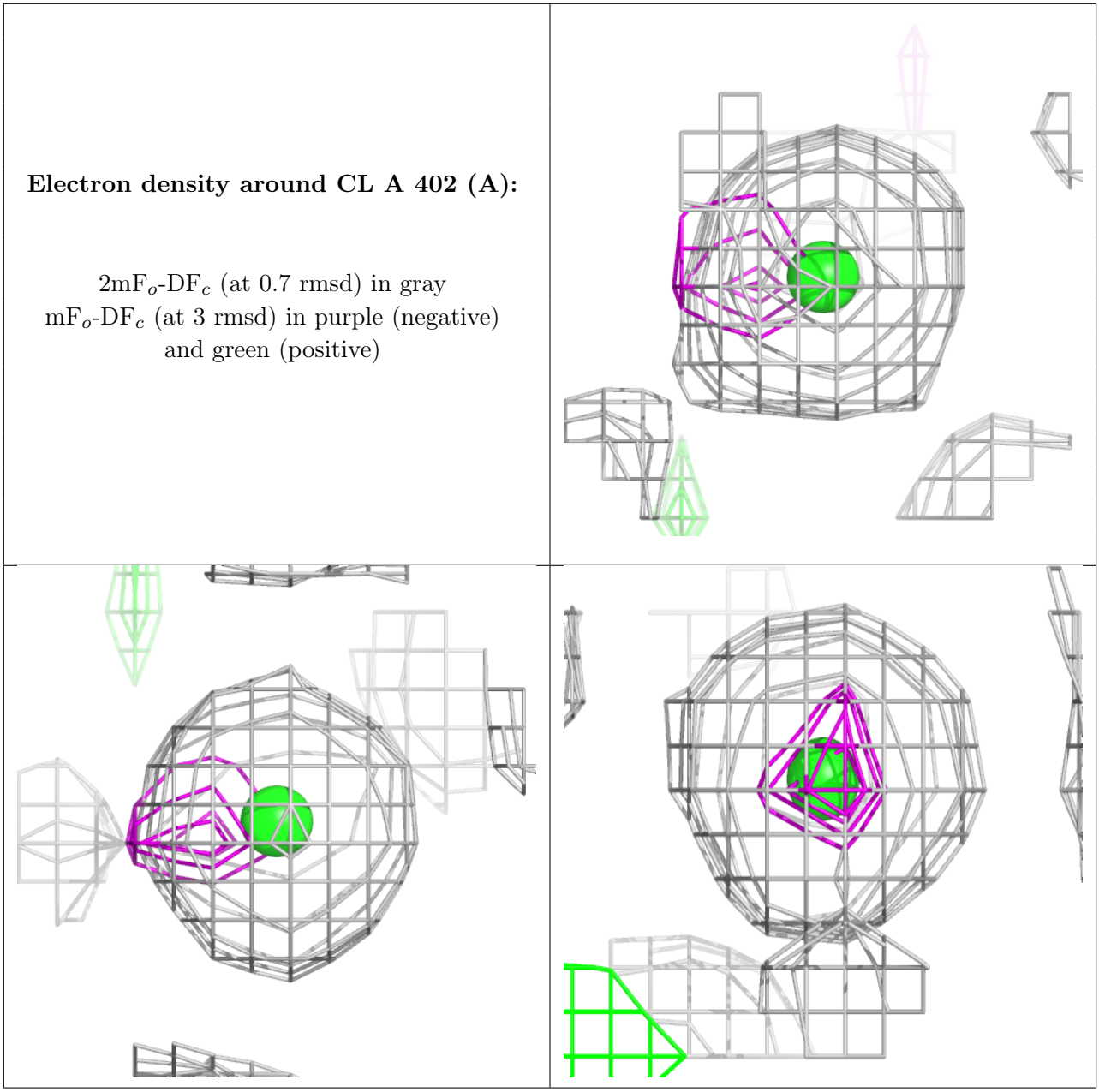






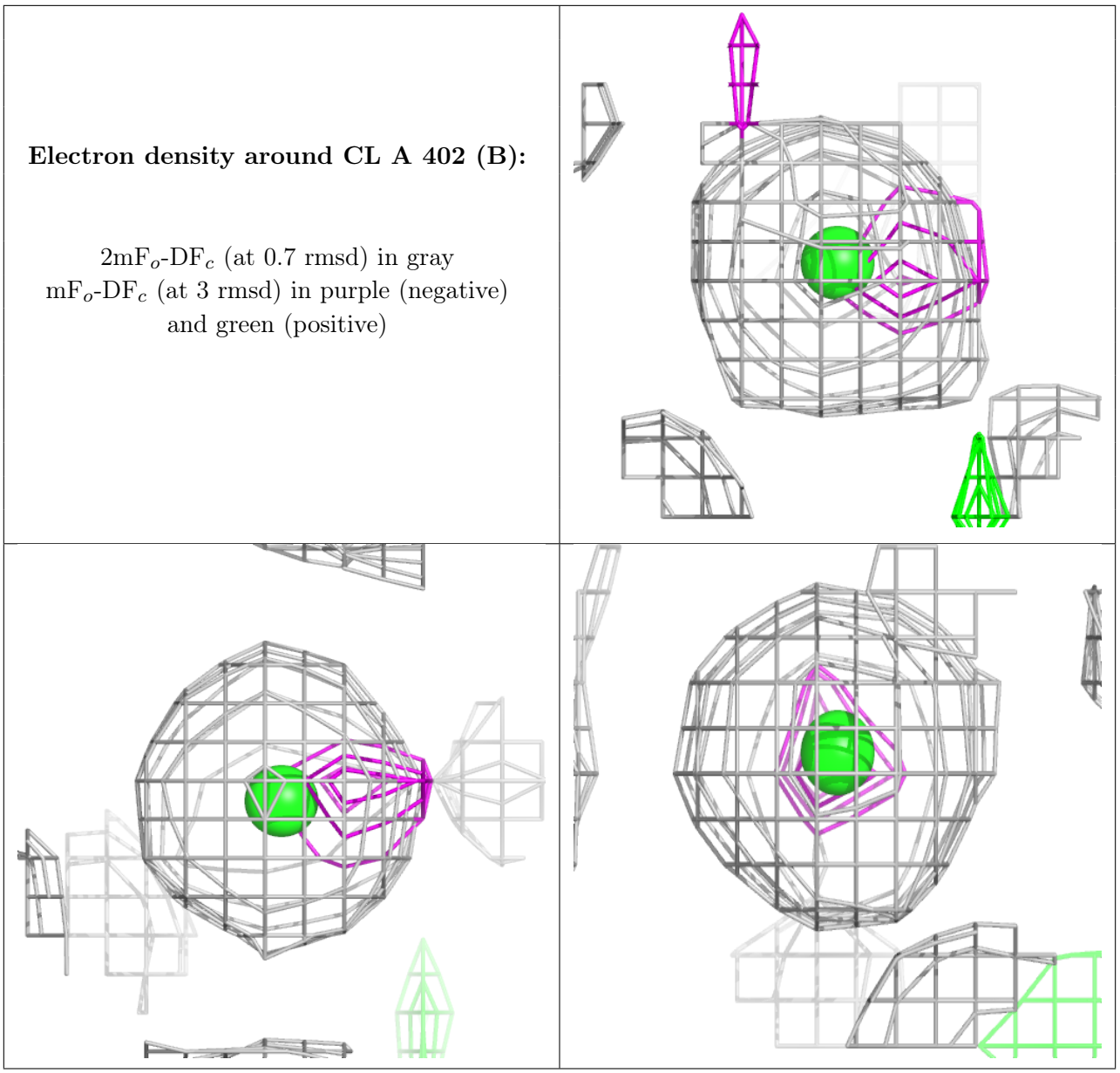
Electron density around CL A 402 (A):

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



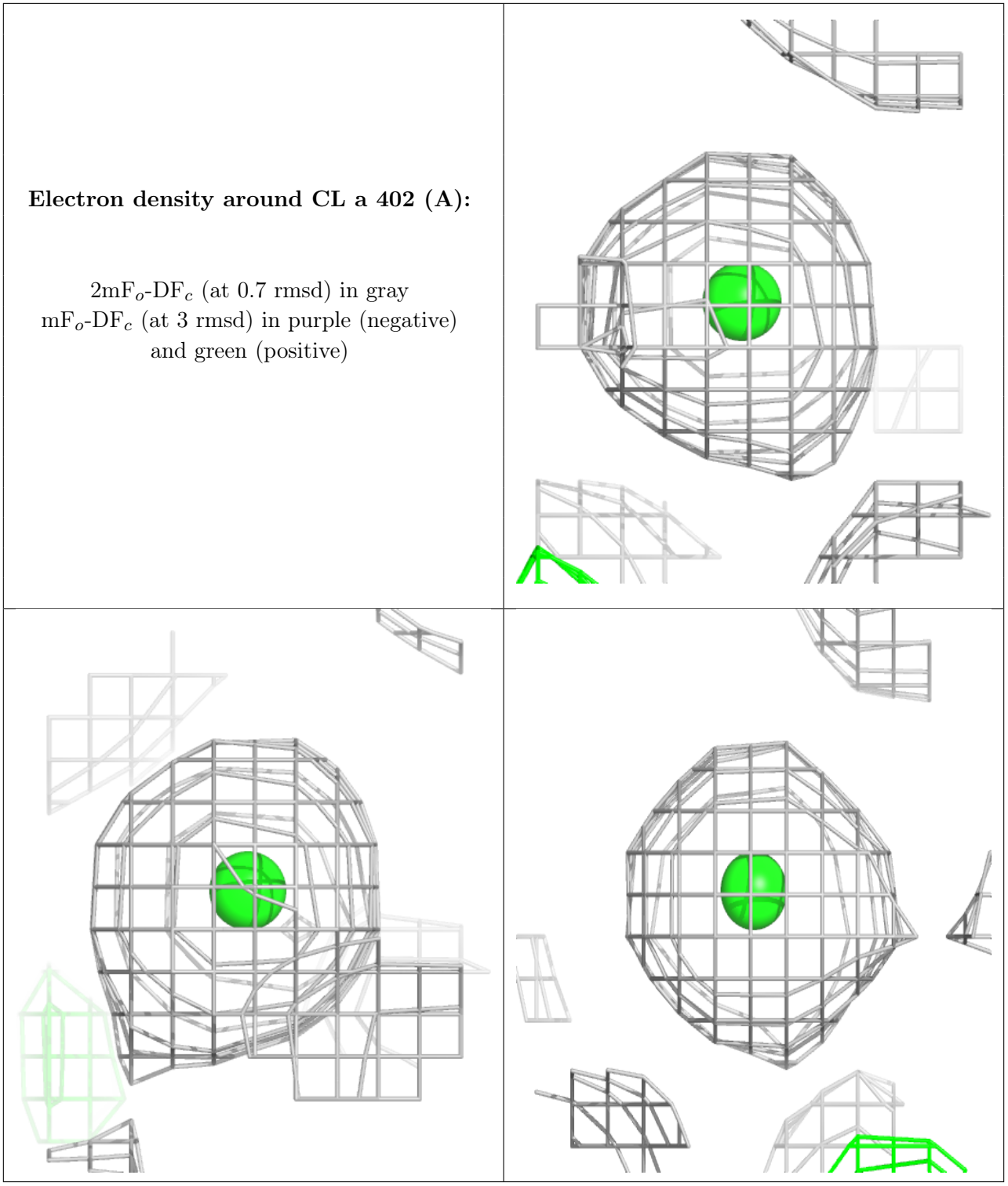
Electron density around CL A 402 (B):

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



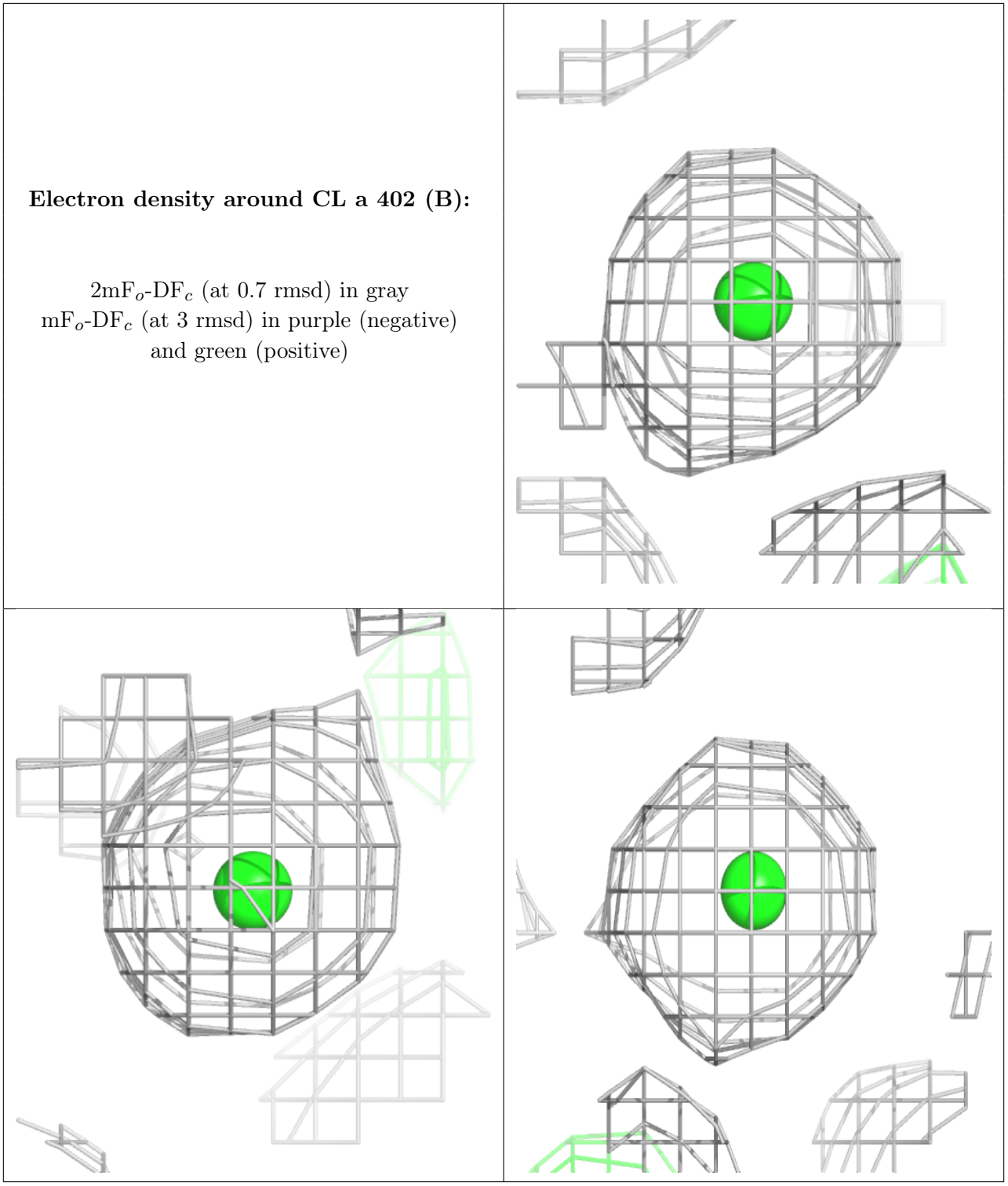
Electron density around CL a 402 (A):

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



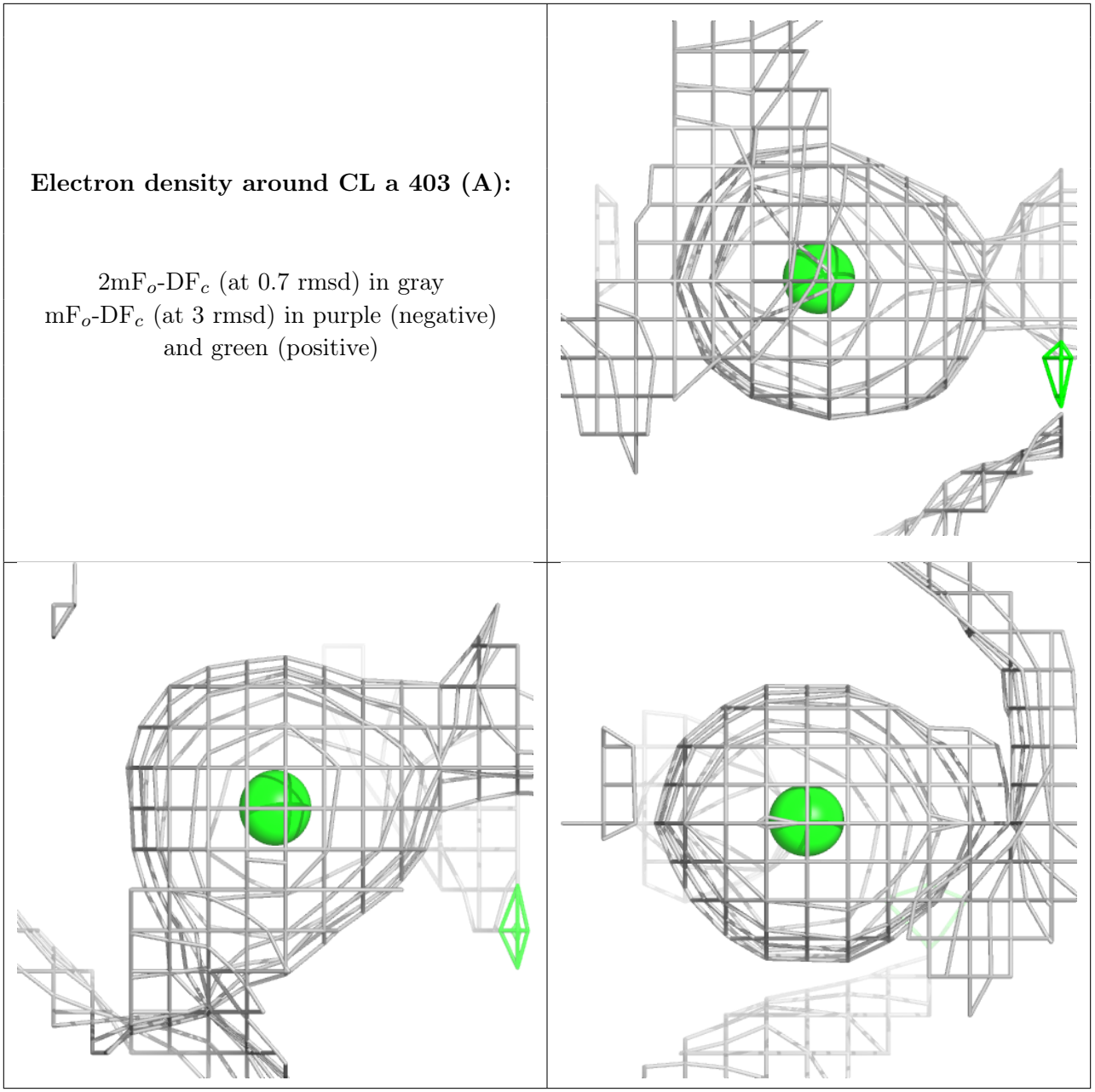
Electron density around CL a 402 (B):

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



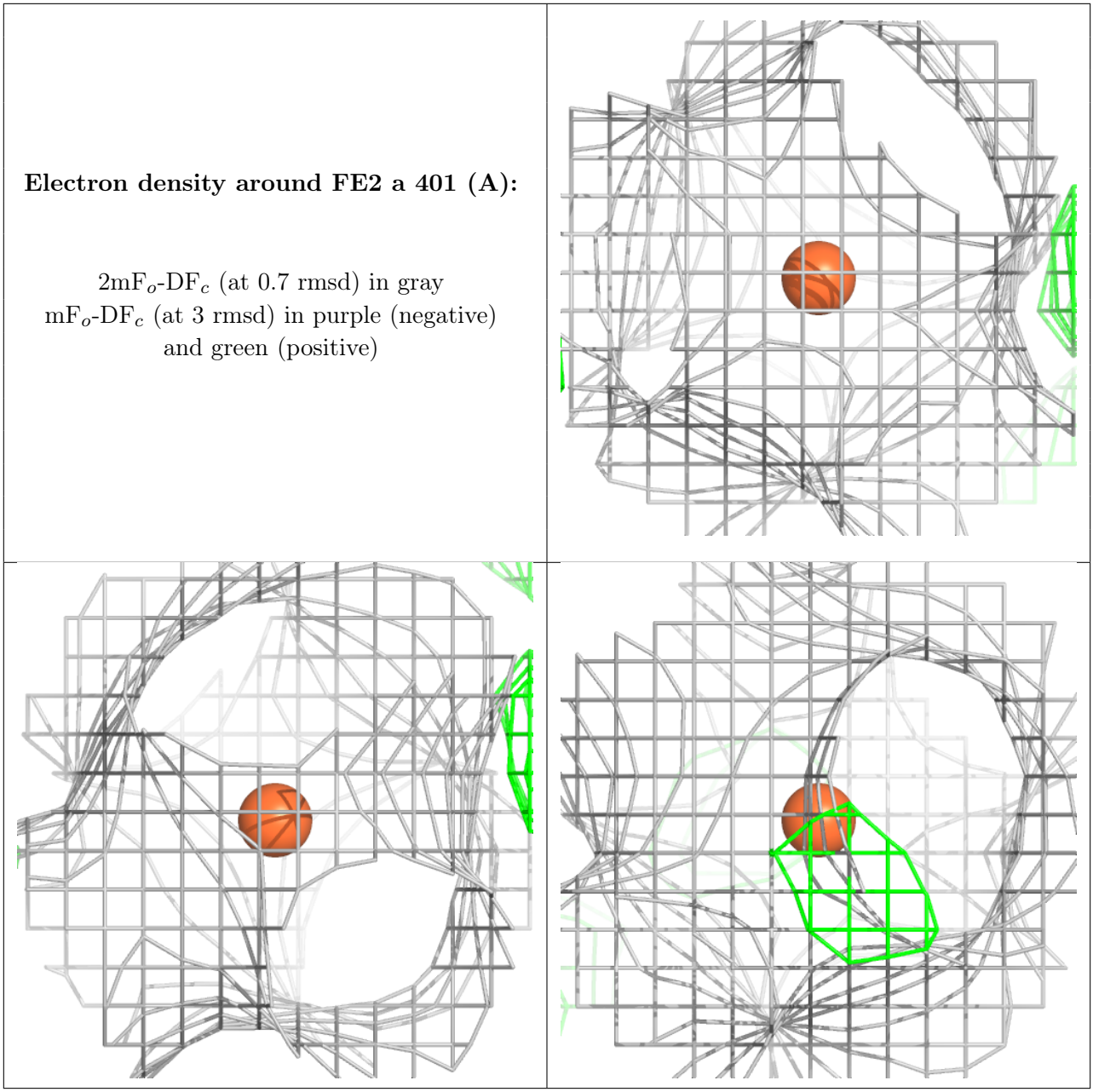
Electron density around CL a 403 (A):

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



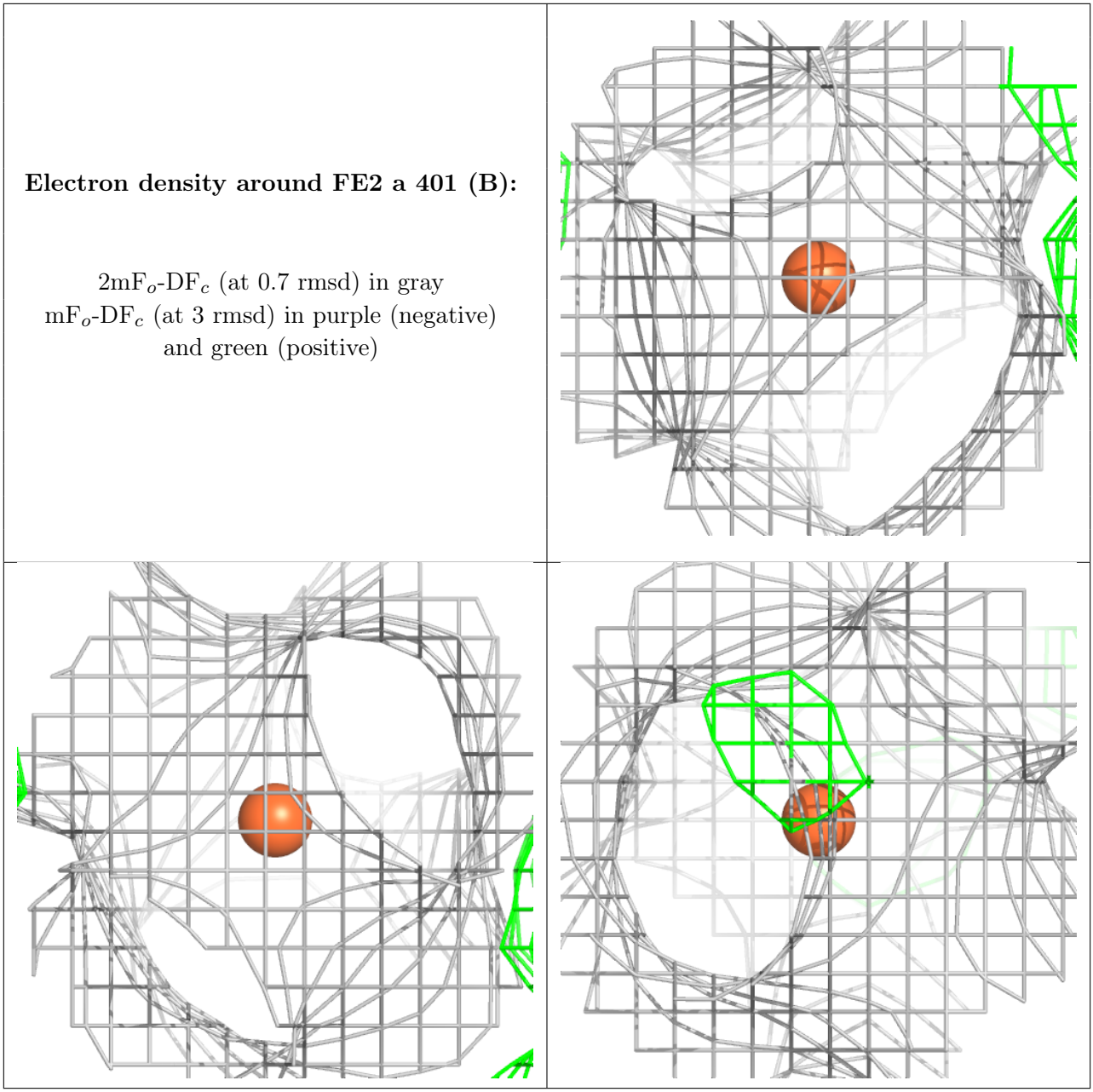
Electron density around FE2 a 401 (A):

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



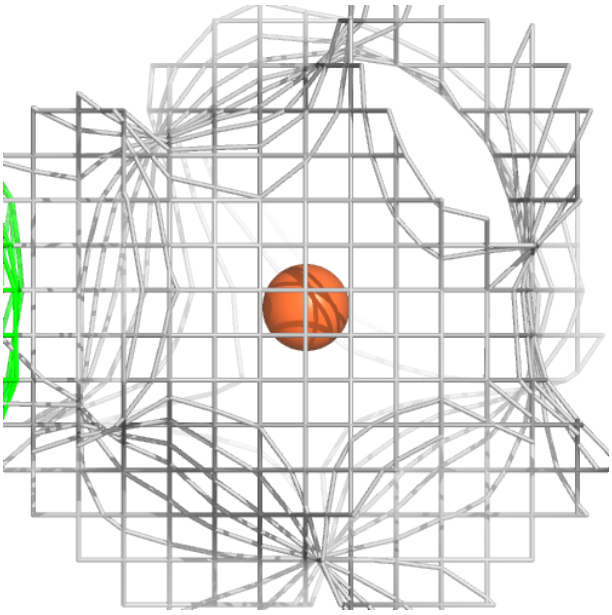
Electron density around FE2 a 401 (B):

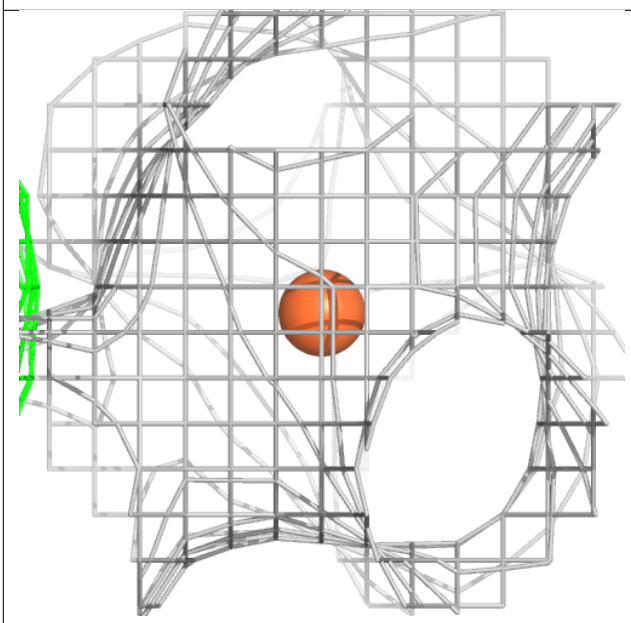
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

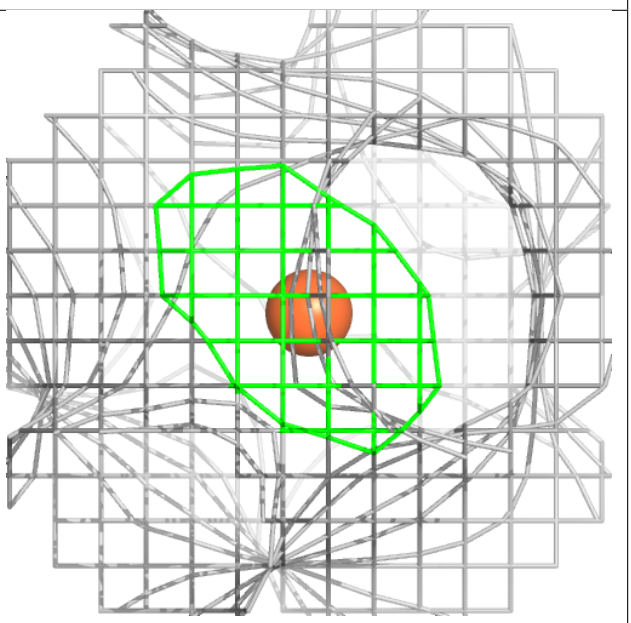


Electron density around FE2 A 401 (A):

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

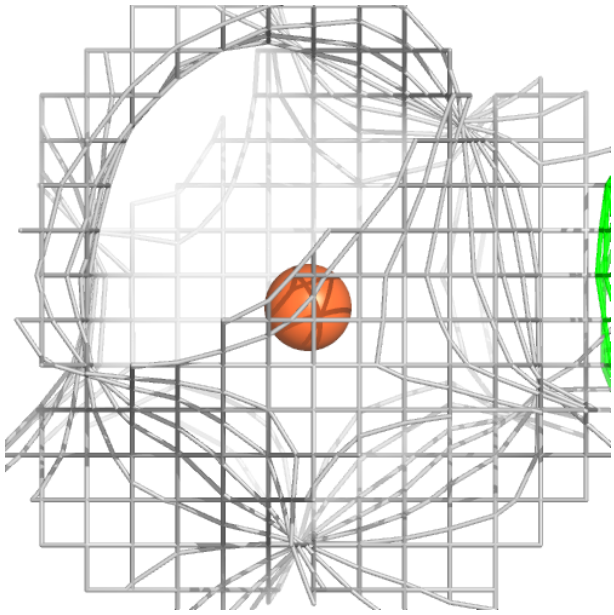


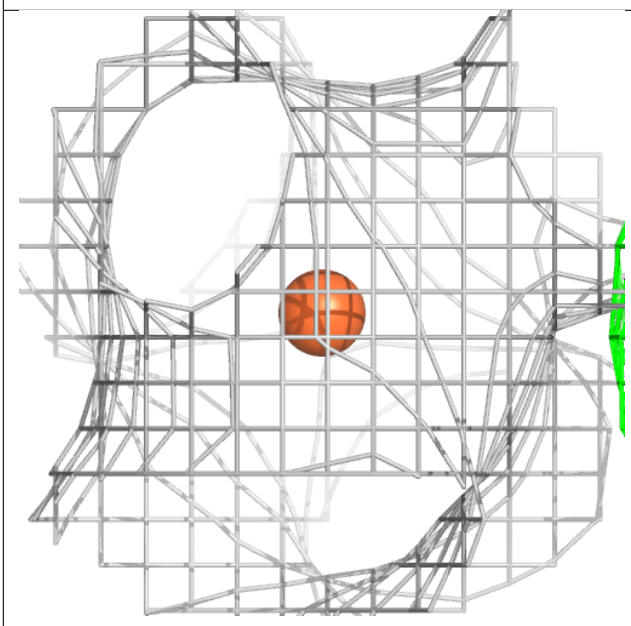


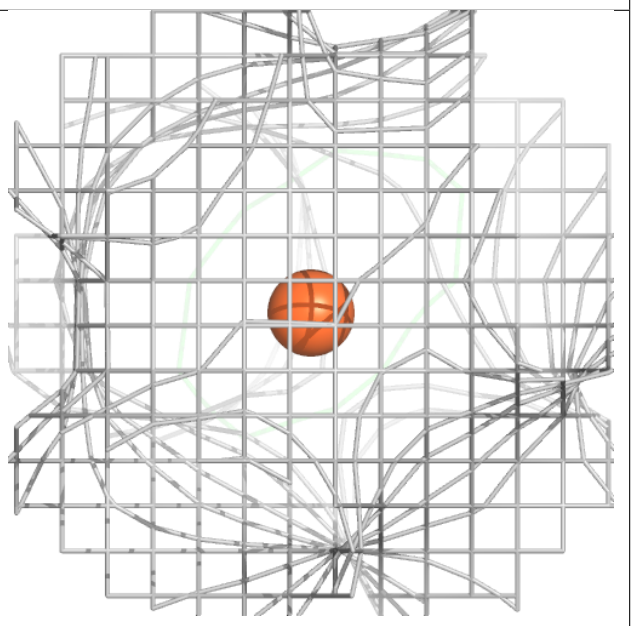


Electron density around FE2 A 401 (B):

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

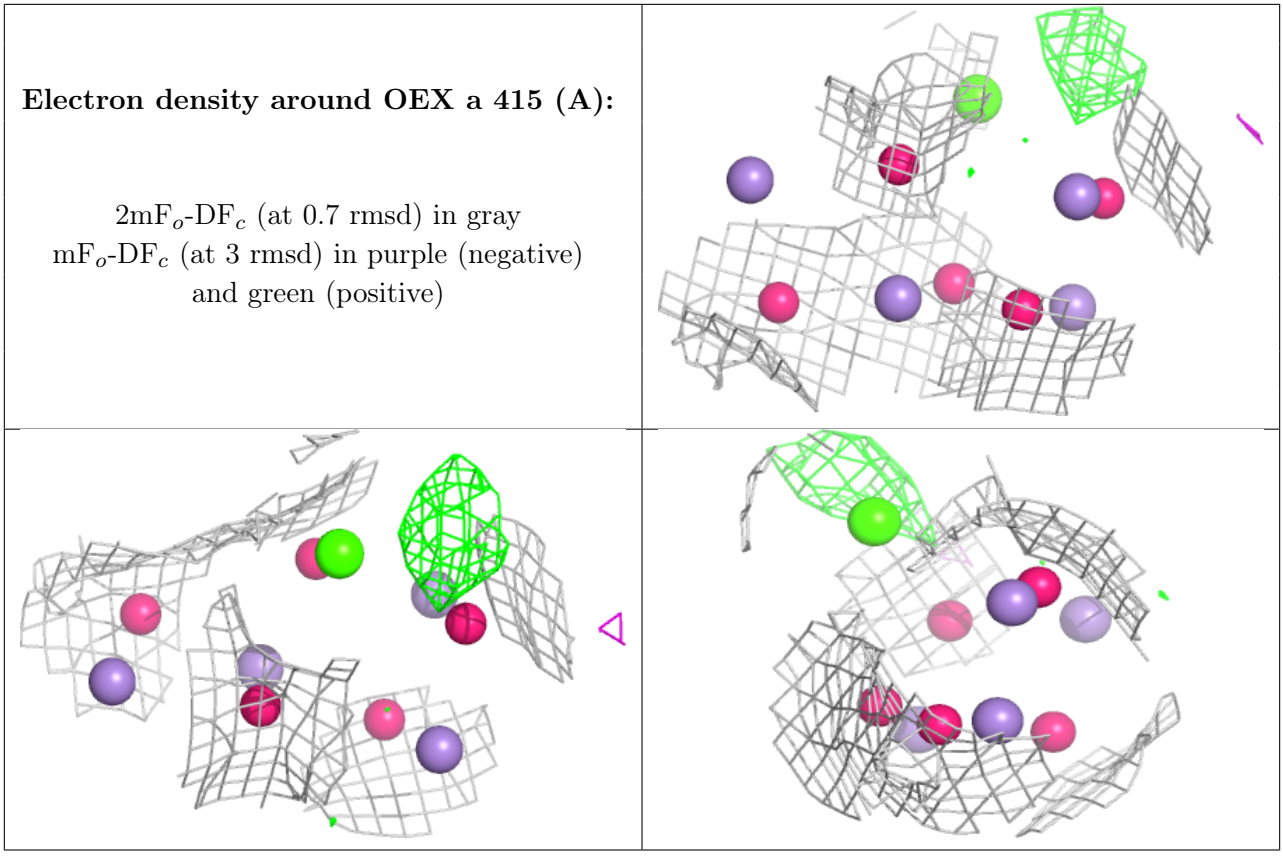






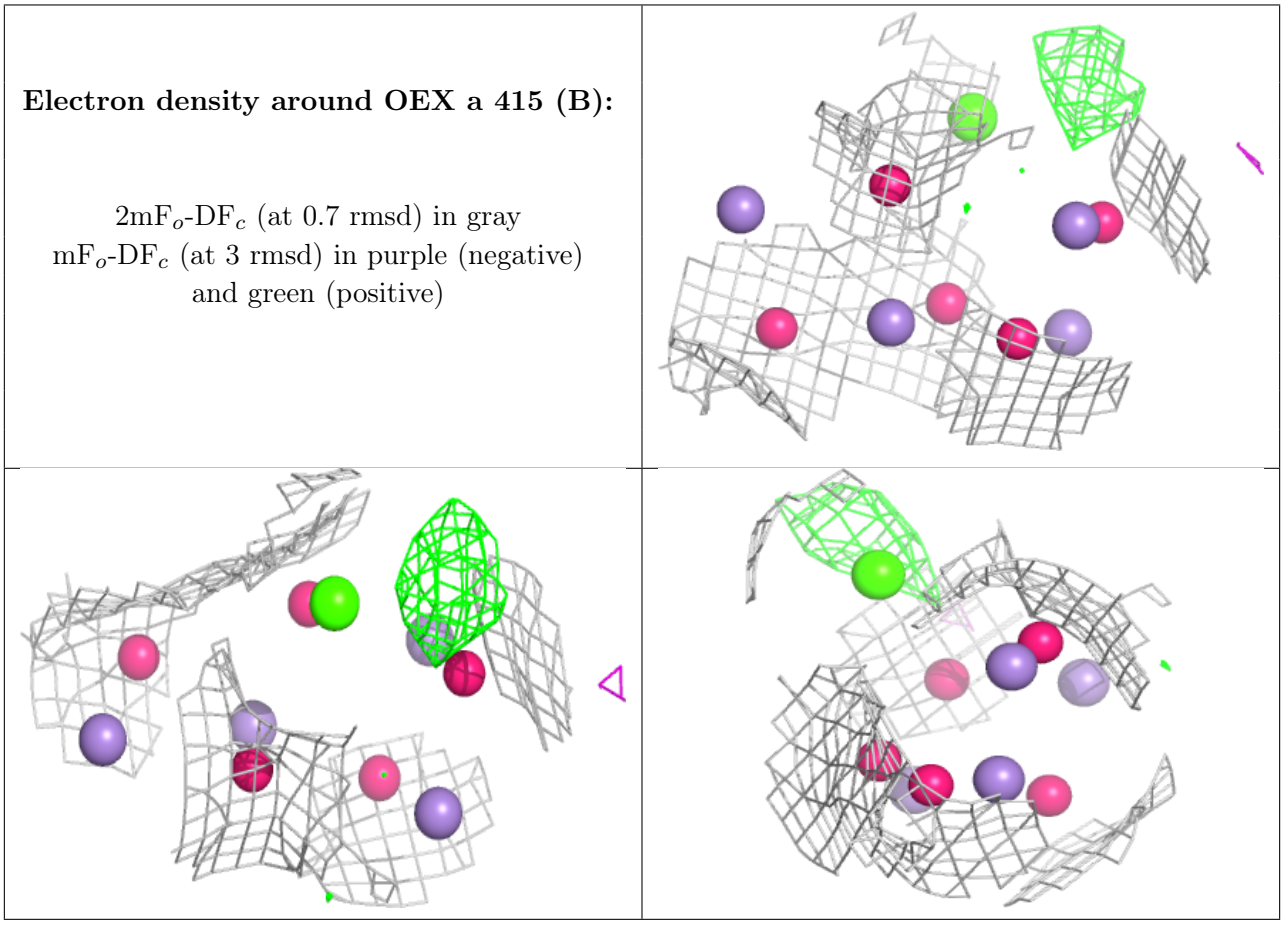
Electron density around OEX a 415 (A):

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



Electron density around OEX a 415 (B):

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



6.5 Other polymers (i)

There are no such residues in this entry.