Full wwPDB X-ray Structure Validation Report (i)

Mar 12, 2026 – 01:54 PM UTC

PDB ID	:	6JLN / pdb_00006jln
Title	:	XFEL structure of cyanobacterial photosystem II (1F state, dataset2)
Authors	:	Suga, M.; Shen, J.R.
Deposited on	:	2019-03-06
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

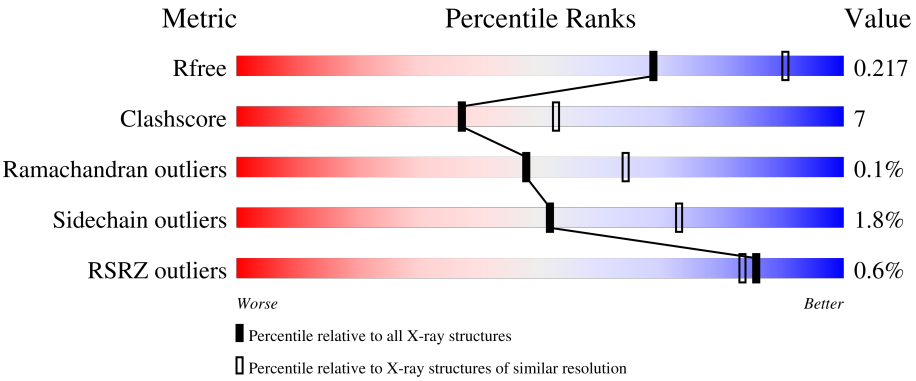
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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.



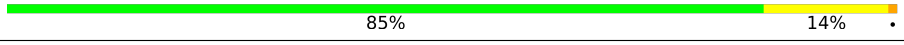
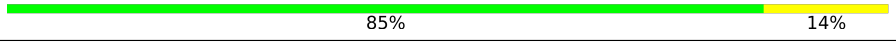
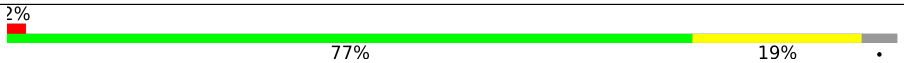
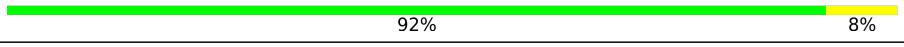
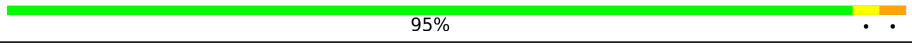
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	84% 13% .
1	a	344	84% 13% .
2	B	505	84% 16%
2	b	505	% 86% 14%
3	C	455	86% 13% .

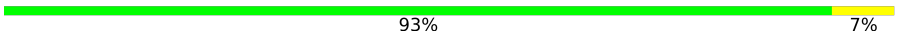
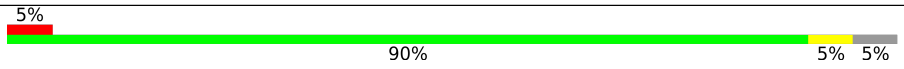
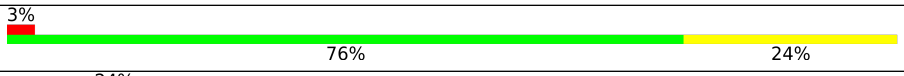
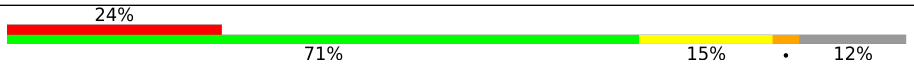
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Mol	Chain	Length	Quality of chain
3	c	455	
4	D	342	
4	d	342	
5	E	84	
5	e	84	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	39	
9	j	39	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u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

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	
20	R	34	

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
24	CLA	A	405	X	-	-	-
24	CLA	A	406	X	-	-	-
24	CLA	B	602	X	-	-	-
24	CLA	B	603	X	-	-	-
24	CLA	B	604	X	-	-	-
24	CLA	B	605	X	-	-	-
24	CLA	B	606	X	-	-	-
24	CLA	B	607	X	-	-	-
24	CLA	B	608	X	-	-	-
24	CLA	B	610	X	-	-	-
24	CLA	B	611	X	-	-	-
24	CLA	B	612	X	-	-	-
24	CLA	B	613	X	-	-	-
24	CLA	B	614	X	-	-	-
24	CLA	B	615	X	-	-	-
24	CLA	B	616	X	-	-	-
24	CLA	B	617	X	-	-	-
24	CLA	C	501	X	-	-	-
24	CLA	C	502	X	-	-	-
24	CLA	C	503	X	-	-	-
24	CLA	C	504	X	-	-	-
24	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CLA	C	506	X	-	-	-
24	CLA	C	507	X	-	-	-
24	CLA	C	508	X	-	-	-
24	CLA	C	509	X	-	-	-
24	CLA	C	510	X	-	-	-
24	CLA	C	512	X	-	-	-
24	CLA	C	513	X	-	-	-
24	CLA	D	404	X	-	-	-
24	CLA	D	405	X	-	-	-
24	CLA	a	409	X	-	-	-
24	CLA	a	412	X	-	-	-
24	CLA	b	610	X	-	-	-
24	CLA	b	611	X	-	-	-
24	CLA	b	612	X	-	-	-
24	CLA	b	613	X	-	-	-
24	CLA	b	614	X	-	-	-
24	CLA	b	615	X	-	-	-
24	CLA	b	616	X	-	-	-
24	CLA	b	618	X	-	-	-
24	CLA	b	619	X	-	-	-
24	CLA	b	620	X	-	-	-
24	CLA	b	621	X	-	-	-
24	CLA	b	622	X	-	-	-
24	CLA	b	623	X	-	-	-
24	CLA	b	624	X	-	-	-
24	CLA	b	625	X	-	-	-
24	CLA	c	505	X	-	-	-
24	CLA	c	506	X	-	-	-
24	CLA	c	507	X	-	-	-
24	CLA	c	508	X	-	-	-
24	CLA	c	509	X	-	-	-
24	CLA	c	510	X	-	-	-
24	CLA	c	511	X	-	-	-
24	CLA	c	512	X	-	-	-
24	CLA	c	513	X	-	-	-
24	CLA	c	514	X	-	-	-
24	CLA	c	515	X	-	-	-
24	CLA	c	516	X	-	-	-
24	CLA	d	403	X	-	-	-
24	CLA	d	404	X	-	-	-
24	CLA	d	405	X	-	-	-

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 55631 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	53	0
			3019	1966	498	537	18			
1	a	334	Total	C	N	O	S	0	55	0
			3027	1973	498	538	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	See sequence details	UNP P51765
a	279	PRO	ARG	See sequence details	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	10	0
			4021	2639	667	702	13			
2	b	503	Total	C	N	O	S	0	12	0
			4022	2644	664	701	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	7	0
			3518	2300	587	618	13			
3	c	455	Total	C	N	O	S	0	13	0
			3598	2356	599	629	14			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	See sequence details	UNP D0VWR7
C	20	SER	-	See sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	See sequence details	UNP D0VWR7
C	22	PHE	-	See sequence details	UNP D0VWR7
c	19	ASN	-	See sequence details	UNP D0VWR7
c	20	SER	-	See sequence details	UNP D0VWR7
c	21	ILE	-	See sequence details	UNP D0VWR7
c	22	PHE	-	See sequence details	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			
4	d	341	Total	C	N	O	S	0	16	0
			2849	1884	469	483	13			

- 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	2	0
			668	436	107	125			
5	e	81	Total	C	N	O	0	2	0
			670	439	107	124			

- 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	32	Total	C	N	O	S	0	0	0
			257	175	43	38	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	65	Total	C	N	O	S	0	1	0
			519	346	85	86	2			
7	h	65	Total	C	N	O	S	0	0	0
			511	341	82	86	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
			280	187	43	48	2			

- 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	See sequence details	UNP P19054
K	39	TRP	VAL	See sequence details	UNP P19054
k	33	LEU	PHE	See sequence details	UNP P19054
k	39	TRP	VAL	See sequence details	UNP P19054

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			274	184	40	49	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	0	0
			269	179	40	49	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	See sequence details	UNP P12312
m	8	LEU	PHE	See sequence details	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	8	0
			1903	1191	315	392	5			
13	o	243	Total	C	N	O	S	0	5	0
			1891	1183	315	388	5			

- 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	1	0
			264	185	36	41	2			
14	t	30	Total	C	N	O	S	0	1	0
			264	185	36	41	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O	0	0	0
			774	491	129	154			
15	u	97	Total	C	N	O	0	0	0
			774	491	129	154			

- 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	2	0
			1085	689	181	211	4			
16	v	137	Total	C	N	O	S	0	1	0
			1077	684	178	211	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	X	39	Total	C	N	O	0	0	0
			287	191	46	50			
18	x	38	Total	C	N	O	0	0	0
			281	188	45	48			

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	30	Total	C	N	O	98	0	0
			239	163	41	35			

- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 22 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

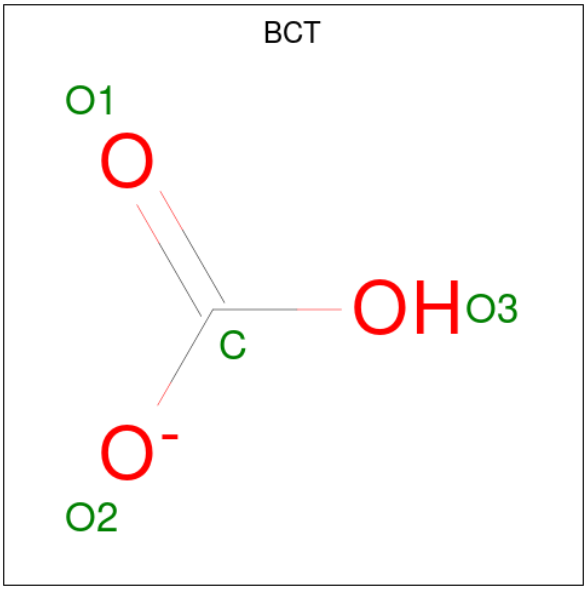
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	2
			4	4		
22	U	1	Total	Cl	0	0
			1	1		

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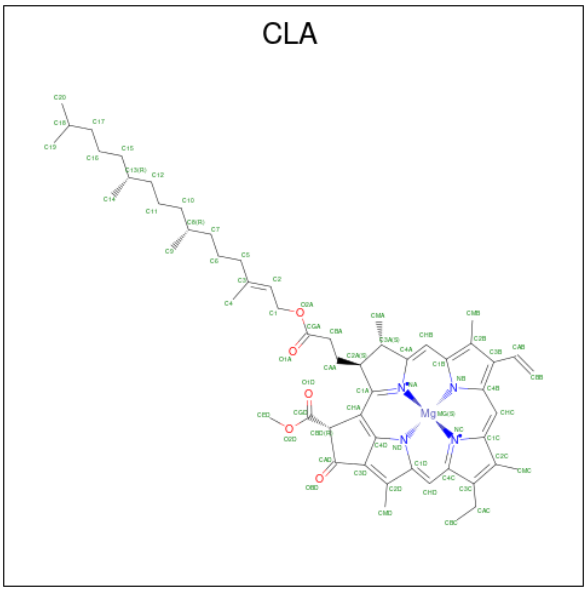
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	a	2	Total Cl 4 4	0	2
22	v	1	Total Cl 1 1	0	0

- Molecule 23 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 8 2 6	0	1
23	d	1	Total C O 8 2 6	0	1

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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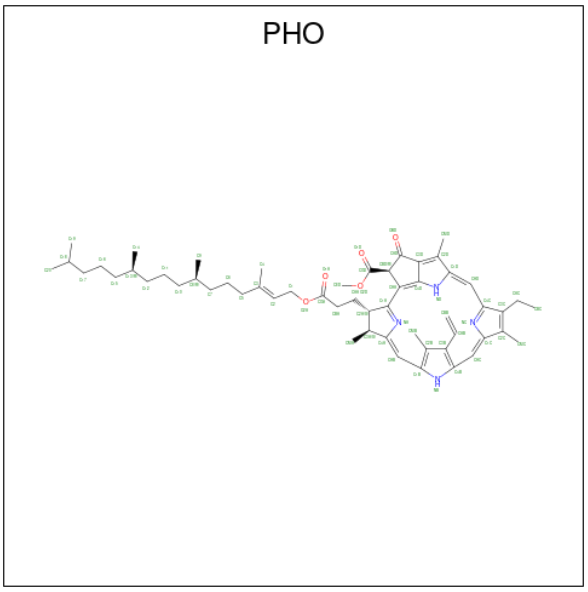
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

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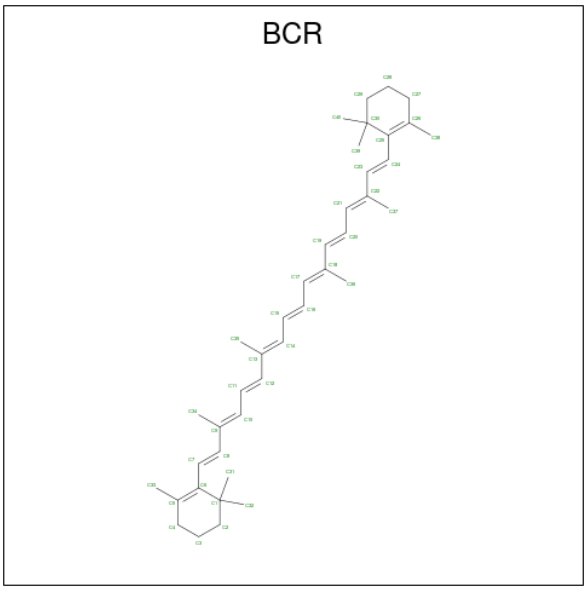
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5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

- Molecule 25 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



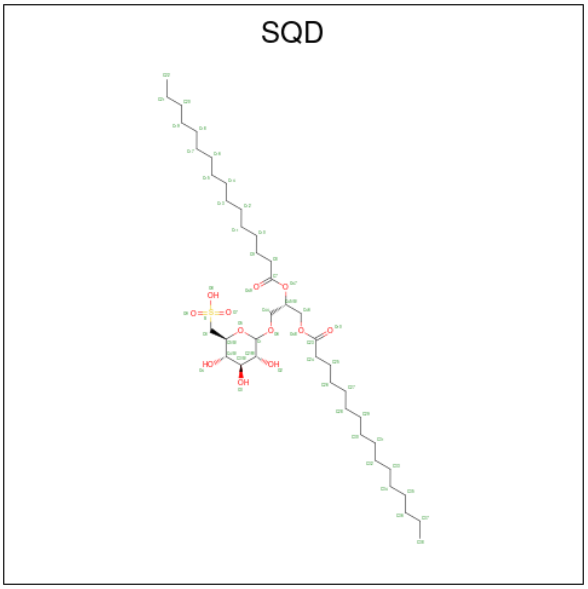
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C N O 64 55 4 5	0	0
25	D	1	Total C N O 128 110 8 10	0	1
25	a	1	Total C N O 64 55 4 5	0	0
25	d	1	Total C N O 128 110 8 10	0	1

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



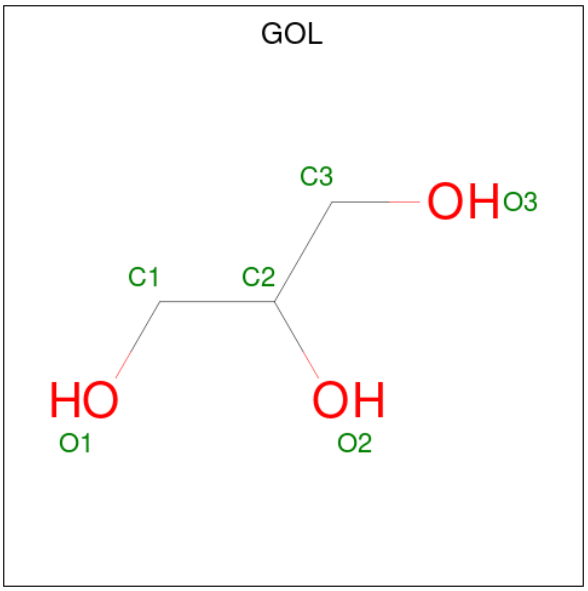
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	Y	1	Total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

- Molecule 27 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
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	A	1	Total	C	O	S	0	0
			54	41	12	1		
27	B	1	Total	C	O	S	0	0
			54	41	12	1		
27	F	1	Total	C	O	S	0	0
			43	30	12	1		
27	L	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	a	1	Total	C	O	S	0	0
			54	41	12	1		
27	f	1	Total	C	O	S	0	0
			43	30	12	1		

- Molecule 28 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



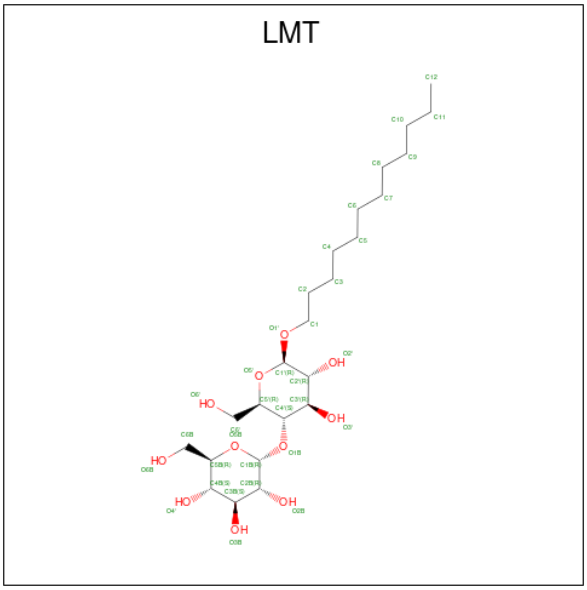
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
28	A	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	B	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	C	1	Total C O 6 3 3	0	0
28	D	1	Total C O 6 3 3	0	0
28	F	1	Total C O 6 3 3	0	0
28	O	1	Total C O 6 3 3	0	0
28	T	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	T	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	V	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	a	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	b	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	c	1	Total	C	O	0	0
			6	3	3		
28	o	1	Total	C	O	0	0
			6	3	3		
28	t	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		
28	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



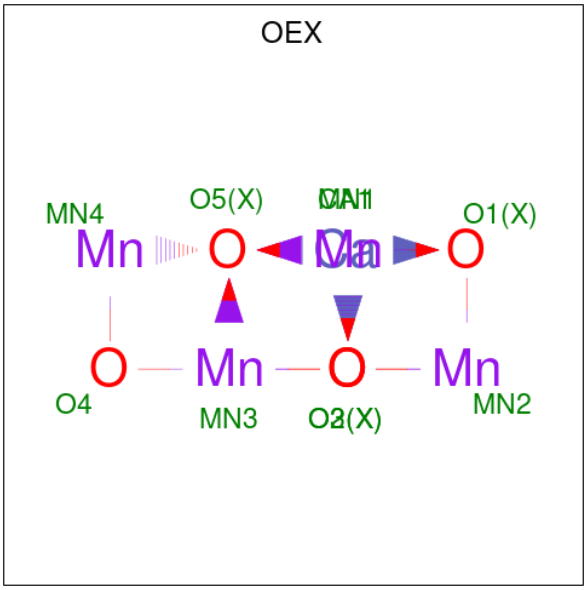
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 35 24 11	0	0
29	C	1	Total C O 35 24 11	0	0
29	D	1	Total C O 35 24 11	0	0
29	E	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	M	1	Total C O 35 24 11	0	0
29	T	1	Total C O 25 19 6	0	0
29	a	1	Total C O 35 24 11	0	0
29	a	1	Total C O 35 24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

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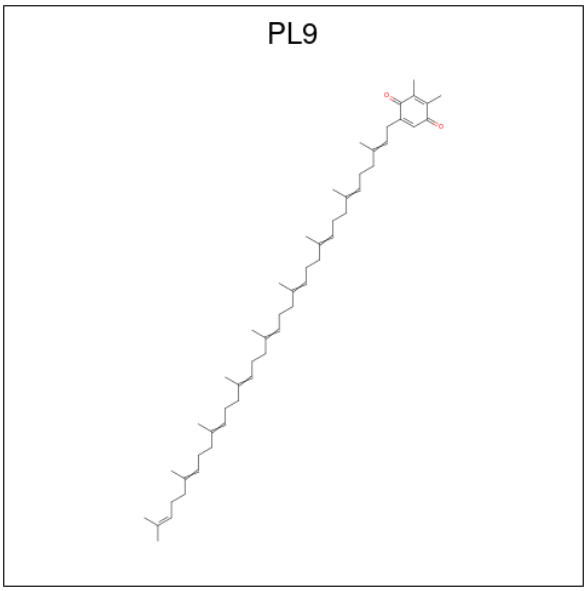
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
29	t	1	Total	C	O	0	0
			25	19	6		

- Molecule 30 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	A	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		
30	a	1	Total	Ca	Mn	O	0	1
			10	1	4	5		

- Molecule 31 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: $C_{53}H_{80}O_2$).



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

- Molecule 32 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

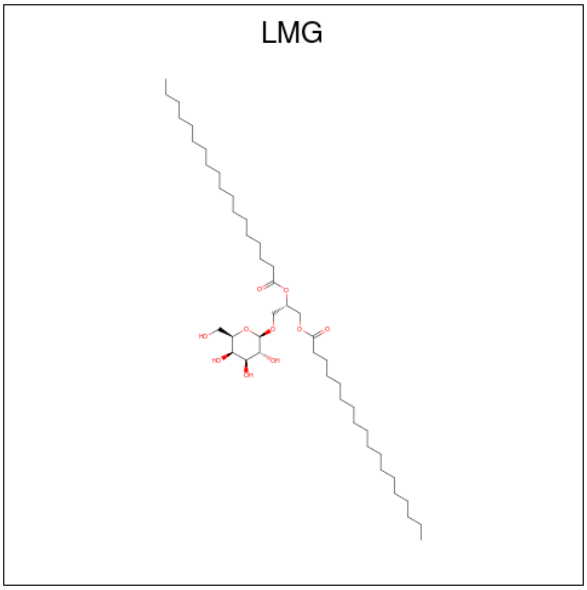
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	1	Total C O 28 23 5	0	0
32	B	1	Total C O 33 28 5	0	0
32	C	1	Total C O 34 29 5	0	0
32	D	2	Total C O 57 51 6	0	0
32	I	1	Total C O 40 35 5	0	0
32	J	1	Total C 10 10	0	0
32	M	1	Total C 10 10	0	0
32	X	1	Total C O 18 16 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	a	1	Total C O 30 25 5	0	0
32	b	1	Total C O 33 28 5	0	0
32	c	1	Total C O 32 27 5	0	0
32	d	3	Total C O 71 63 8	0	0
32	i	1	Total C O 40 35 5	0	0
32	j	1	Total C 10 10	0	0
32	m	1	Total C 10 10	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	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

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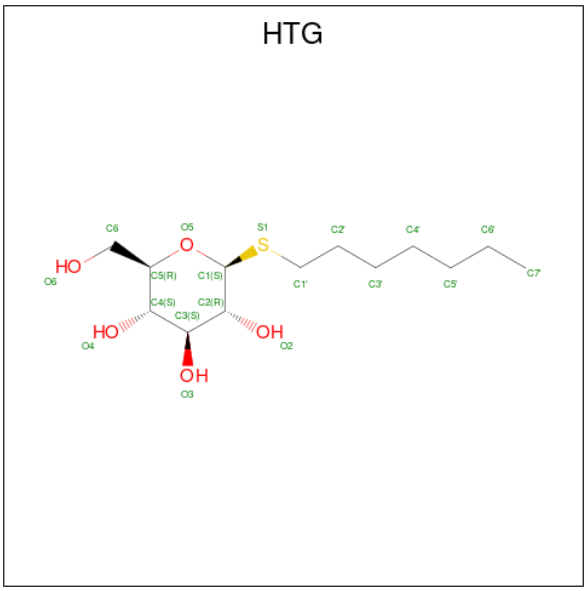
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	M	1	Total C O 51 41 10	0	0
33	Z	1	Total C O 37 27 10	0	0
33	a	1	Total C O 51 41 10	0	0
33	b	1	Total C O 51 41 10	0	0
33	c	1	Total C O 51 41 10	0	0
33	d	1	Total C O 51 41 10	0	0
33	k	1	Total C O 51 41 10	0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

- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 35 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



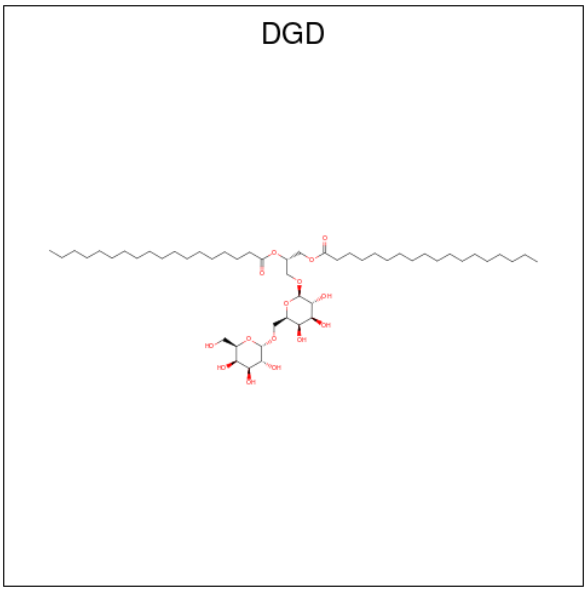
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19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

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

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



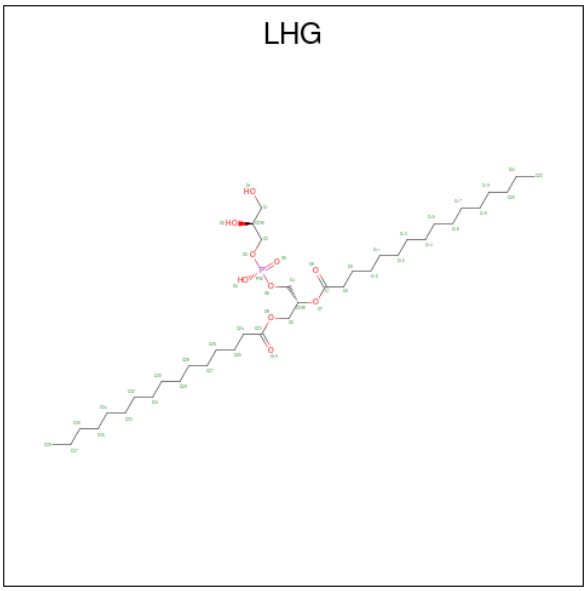
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	C	1	Total C O 62 47 15	0	0
36	D	1	Total C O 52 42 10	0	0
36	H	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0
36	c	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	e	1	Total C O 62 47 15	0	0
36	h	1	Total C O 62 47 15	0	0

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



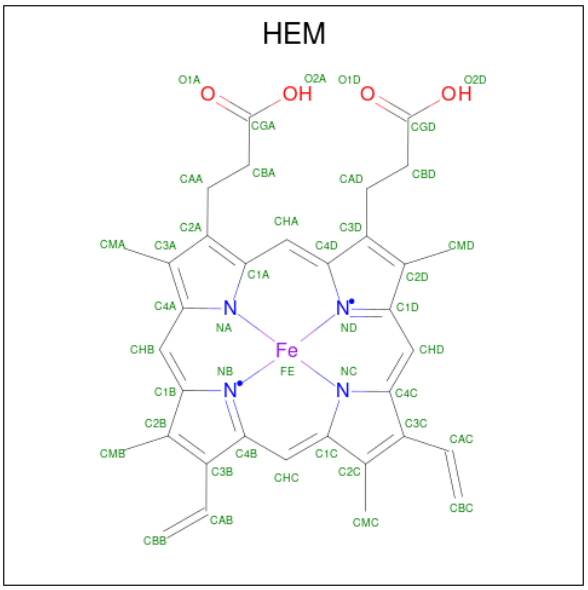
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	D	1	Total C O P 49 38 10 1	0	0
37	E	1	Total C O P 42 31 10 1	0	0
37	L	1	Total C O P 49 38 10 1	0	0
37	a	1	Total C O P 42 31 10 1	0	0
37	b	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0
37	d	1	Total C O P 49 38 10 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	d	1	Total C O P 49 38 10 1	0	0

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

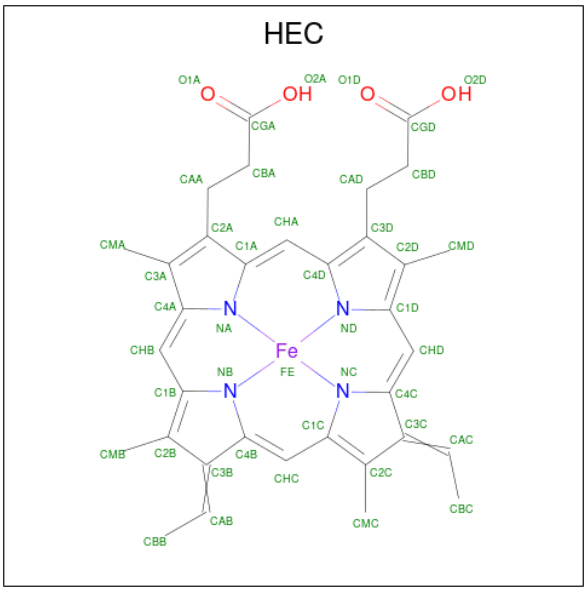


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	E	1	Total C Fe N O 43 34 1 4 4	0	0
38	f	1	Total C Fe N O 43 34 1 4 4	0	0

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



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

- Molecule 41 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
41	A	162	Total	O	0	15
			175	175		
41	B	284	Total	O	0	4
			288	288		
41	C	232	Total	O	0	6
			236	236		
41	D	144	Total	O	0	5
			149	149		
41	E	36	Total	O	0	1
			37	37		
41	F	7	Total	O	0	0
			7	7		
41	H	41	Total	O	0	0
			41	41		
41	I	4	Total	O	0	0
			4	4		
41	J	10	Total	O	0	0
			10	10		
41	K	8	Total	O	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	L	16	Total O 17 17	0	1
41	M	23	Total O 23 23	0	0
41	O	177	Total O 179 179	0	2
41	T	15	Total O 16 16	0	1
41	U	83	Total O 83 83	0	0
41	V	114	Total O 116 116	0	2
41	Y	4	Total O 4 4	0	0
41	X	8	Total O 8 8	0	0
41	Z	1	Total O 1 1	0	0
41	a	157	Total O 168 168	0	13
41	b	261	Total O 264 264	0	3
41	c	200	Total O 206 206	0	8
41	d	134	Total O 137 137	0	3
41	e	20	Total O 20 20	0	0
41	f	6	Total O 6 6	0	0
41	h	42	Total O 42 42	0	0
41	i	5	Total O 5 5	0	0
41	j	7	Total O 7 7	0	0
41	k	8	Total O 8 8	0	0
41	l	7	Total O 7 7	0	0
41	m	15	Total O 15 15	0	0

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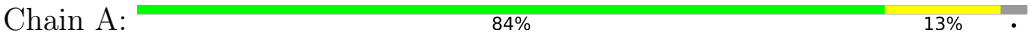
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
41	o	152	Total O 152 152	0	0
41	t	14	Total O 14 14	0	0
41	u	95	Total O 95 95	0	0
41	v	85	Total O 86 86	0	1
41	y	2	Total O 2 2	0	0
41	x	6	Total O 6 6	0	0

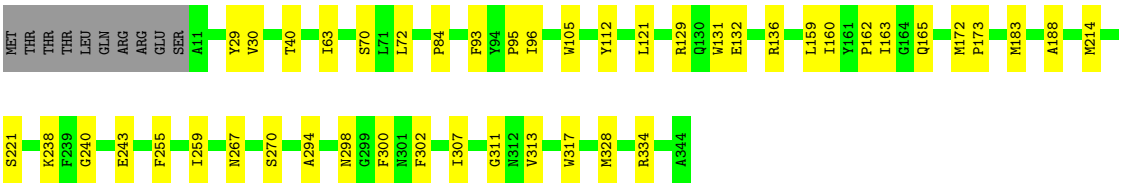
3 Residue-property plots (i)

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

• Molecule 1: Photosystem II protein D1

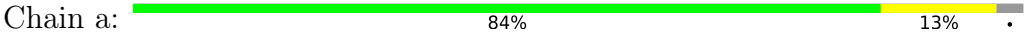
Chain A:

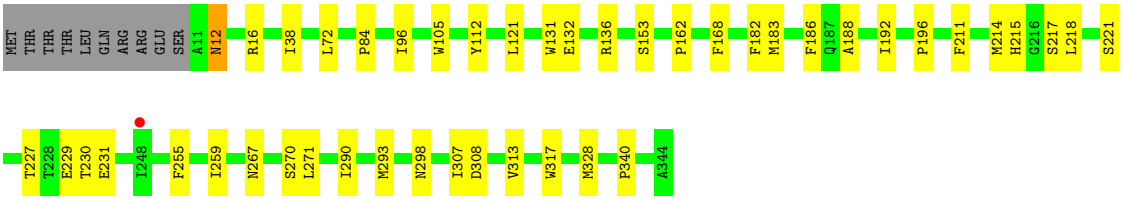




• Molecule 1: Photosystem II protein D1

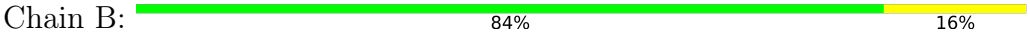
Chain a:





• Molecule 2: Photosystem II CP47 reaction center protein

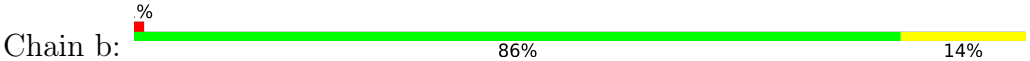
Chain B:

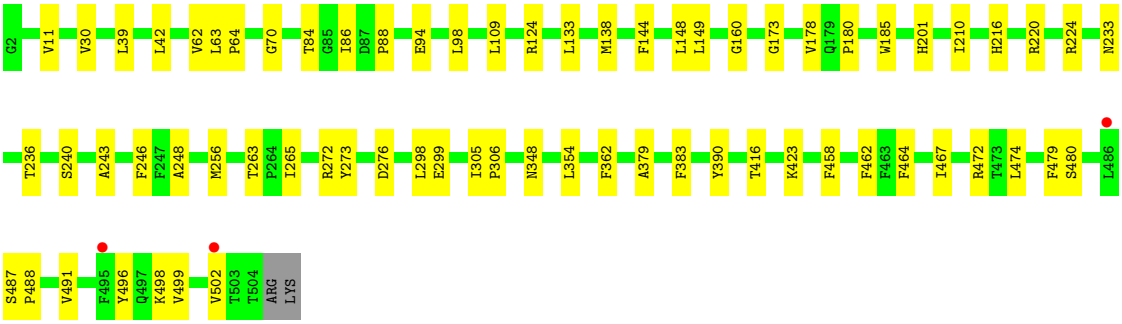




• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:

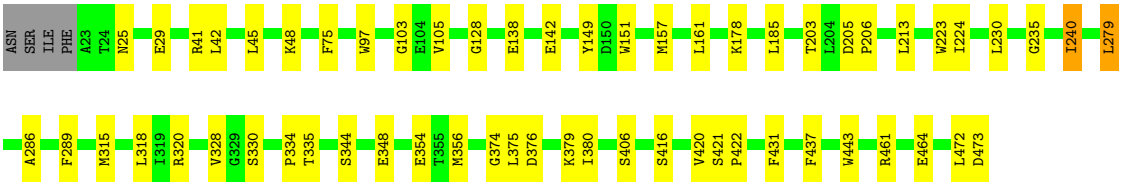




• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:





• Molecule 3: Photosystem II CP43 reaction center protein

Chain c:

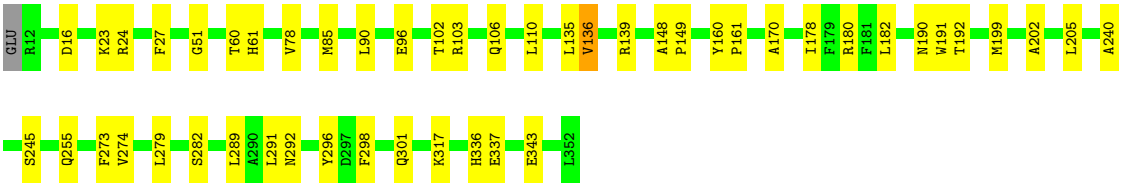




• Molecule 4: Photosystem II D2 protein

Chain D:





• Molecule 4: Photosystem II D2 protein

Chain d:



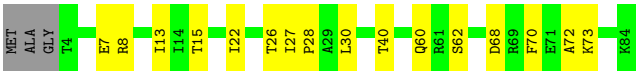




• Molecule 5: Cytochrome b559 subunit alpha

Chain E:





• Molecule 5: Cytochrome b559 subunit alpha

Chain e:

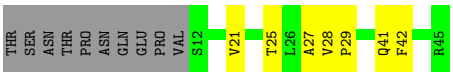




• Molecule 6: Cytochrome b559 subunit beta

Chain F:

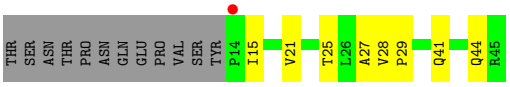




• Molecule 6: Cytochrome b559 subunit beta

Chain f:





• Molecule 7: Photosystem II reaction center protein H

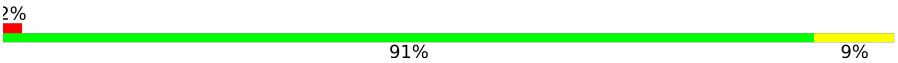
Chain H:

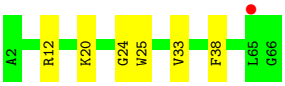




• Molecule 7: Photosystem II reaction center protein H

Chain h:

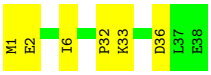




• Molecule 8: Photosystem II reaction center protein I

Chain I:

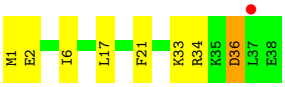




• Molecule 8: Photosystem II reaction center protein I

Chain i:





• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:

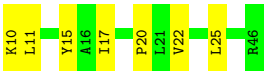




• Molecule 10: Photosystem II reaction center protein K

Chain K:

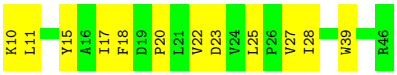




• Molecule 10: Photosystem II reaction center protein K

Chain k:

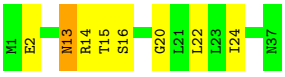




• Molecule 11: Photosystem II reaction center protein L

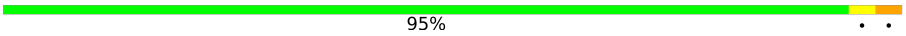
Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:





• Molecule 12: Photosystem II reaction center protein M

Chain M:

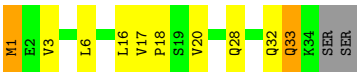




• Molecule 12: Photosystem II reaction center protein M

Chain m:

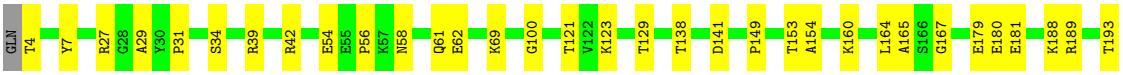


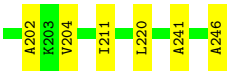


• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:



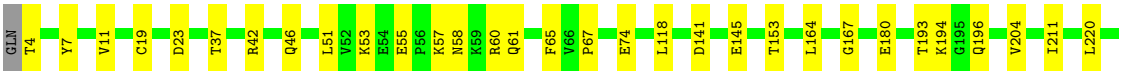




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:







• Molecule 14: Photosystem II reaction center protein T

Chain T:

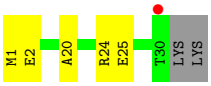




• Molecule 14: Photosystem II reaction center protein T

Chain t:

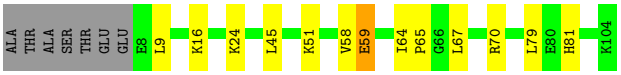




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:

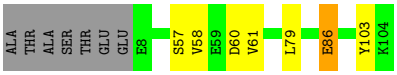




• Molecule 15: Photosystem II 12 kDa extrinsic protein

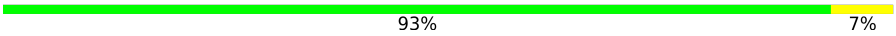
Chain u:

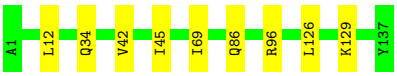




• Molecule 16: Cytochrome c-550

Chain V:

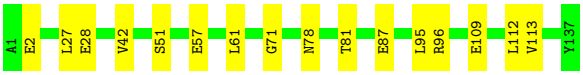




• Molecule 16: Cytochrome c-550

Chain v:





• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:





• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

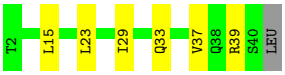




• Molecule 18: Photosystem II reaction center protein X

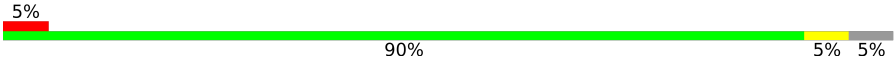
Chain X:

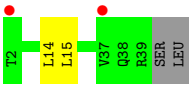




• Molecule 18: Photosystem II reaction center protein X

Chain x:

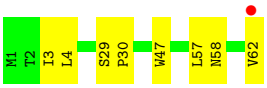




• Molecule 19: Photosystem II reaction center protein Z

Chain Z:

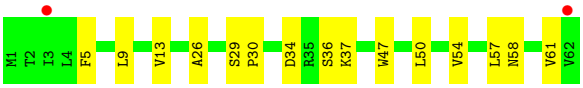




• Molecule 19: Photosystem II reaction center protein Z

Chain z:

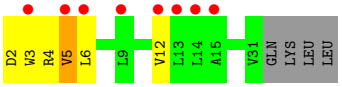




• Molecule 20: Photosystem II protein Y

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	122.04Å 228.84Å 286.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.40 19.99 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-2.40) 99.7 (19.99-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.154 , 0.212 0.161 , 0.217	Depositor DCC
R_{free} test set	17838 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å^2)	47.9	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 89.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	55631	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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: HEC, GOL, LMT, MG, OEX, BCT, DGD, HEM, PL9, LHG, UNL, PHO, FE2, LMG, CL, CA, HTG, BCR, SQD, CLA, FME

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	0.52	0/3121	0.81	2/4250 (0.0%)
1	a	0.53	0/3135	0.81	0/4269
2	B	0.52	0/4191	0.83	1/5709 (0.0%)
2	b	0.51	0/4198	0.82	0/5720
3	C	0.47	0/3643	0.81	0/4958
3	c	0.47	0/3731	0.82	2/5076 (0.0%)
4	D	0.55	0/2952	0.81	2/4021 (0.0%)
4	d	0.55	1/2952 (0.0%)	0.83	3/4021 (0.1%)
5	E	0.48	0/693	0.80	0/944
5	e	0.42	0/695	0.83	2/948 (0.2%)
6	F	0.53	0/284	0.85	0/387
6	f	0.50	0/265	0.78	0/360
7	H	0.48	0/535	0.82	0/728
7	h	0.43	0/524	0.79	0/713
8	I	0.46	0/311	0.86	1/419 (0.2%)
8	i	0.49	0/311	0.85	0/419
9	J	0.50	0/278	0.71	0/376
9	j	0.44	0/286	0.78	0/386
10	K	0.45	0/303	0.85	0/416
10	k	0.48	0/303	0.78	0/416
11	L	0.57	0/319	0.73	0/433
11	l	0.49	0/319	0.74	0/433
12	M	0.63	0/270	0.88	0/368
12	m	0.56	0/262	0.98	2/357 (0.6%)
13	O	0.47	0/1958	0.78	0/2654
13	o	0.46	0/1937	0.79	2/2625 (0.1%)
14	T	0.51	0/266	0.77	0/362
14	t	0.60	0/266	0.76	0/362
15	U	0.47	0/785	0.77	0/1064
15	u	0.48	0/785	0.76	0/1064
16	V	0.49	0/1109	0.76	0/1502

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	0.46	0/1098	0.81	0/1488
17	Y	0.50	0/216	0.90	2/289 (0.7%)
17	y	0.46	0/216	0.80	0/289
18	X	0.44	0/290	0.77	0/392
18	x	0.44	0/284	0.80	0/384
19	Z	0.38	0/490	0.79	0/669
19	z	0.39	0/490	0.83	0/669
20	R	0.37	0/245	0.70	0/338
All	All	0.50	1/44316 (0.0%)	0.81	19/60278 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	274	VAL	CA-C	5.12	1.58	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	170	ALA	CA-C-N	-7.10	112.68	119.85
4	d	170	ALA	C-N-CA	-7.10	112.68	119.85
1	A	334	ARG	N-CA-C	6.16	119.23	111.84
12	m	17	VAL	CA-C-N	-5.82	112.56	119.84
12	m	17	VAL	C-N-CA	-5.82	112.56	119.84
4	d	262	SER	N-CA-C	-5.82	107.17	114.56
3	c	367	GLU	CA-C-N	-5.71	113.79	119.56
3	c	367	GLU	C-N-CA	-5.71	113.79	119.56
13	o	55	GLU	CA-C-N	5.32	126.49	119.84
13	o	55	GLU	C-N-CA	5.32	126.49	119.84
4	D	160	TYR	CA-C-N	-5.11	113.78	119.19
4	D	160	TYR	C-N-CA	-5.11	113.78	119.19
5	e	8	ARG	CA-C-N	5.07	125.36	119.93
5	e	8	ARG	C-N-CA	5.07	125.36	119.93
1	A	70	SER	N-CA-C	5.06	117.38	110.55
8	I	33	LYS	CB-CA-C	-5.04	109.81	117.07
17	Y	32	GLY	CA-C-N	5.04	124.70	119.56
17	Y	32	GLY	C-N-CA	5.04	124.70	119.56
2	B	77	GLY	N-CA-C	5.02	120.70	114.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3019	0	2872	32	0
1	a	3027	0	2888	39	0
2	B	4021	0	3898	64	0
2	b	4022	0	3908	53	0
3	C	3518	0	3439	44	0
3	c	3598	0	3529	48	0
4	D	2849	0	2741	39	0
4	d	2849	0	2741	33	0
5	E	668	0	658	14	0
5	e	670	0	664	12	0
6	F	275	0	282	5	0
6	f	257	0	269	5	0
7	H	519	0	545	12	0
7	h	511	0	532	9	0
8	I	314	0	328	2	0
8	i	314	0	328	4	0
9	J	272	0	279	3	0
9	j	280	0	291	2	0
10	K	293	0	305	6	0
10	k	293	0	305	10	0
11	L	309	0	327	6	0
11	l	309	0	327	2	0
12	M	274	0	299	12	0
12	m	269	0	288	9	0
13	O	1903	0	1886	23	0
13	o	1891	0	1870	17	0
14	T	264	0	267	6	0
14	t	264	0	267	3	0
15	U	774	0	773	9	0
15	u	774	0	773	4	0
16	V	1085	0	1095	6	0
16	v	1077	0	1082	9	0
17	Y	215	0	246	6	0
17	y	215	0	246	5	0
18	X	287	0	317	5	0
18	x	281	0	312	2	0
19	Z	479	0	516	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	z	479	0	516	10	0
20	R	239	0	262	4	0
21	A	2	0	0	0	0
21	a	2	0	0	0	0
22	A	4	0	0	0	0
22	U	1	0	0	1	0
22	a	4	0	0	0	0
22	v	1	0	0	0	0
23	A	8	0	0	0	0
23	d	8	0	0	0	0
24	A	260	0	288	11	0
24	B	1040	0	1152	48	0
24	C	845	0	936	41	0
24	D	130	0	144	4	0
24	a	195	0	216	12	0
24	b	1040	0	1152	39	0
24	c	845	0	936	42	0
24	d	195	0	216	12	0
25	A	64	0	74	1	0
25	D	128	0	148	3	0
25	a	64	0	74	2	0
25	d	128	0	148	5	0
26	A	40	0	56	1	0
26	B	120	0	168	11	0
26	C	80	0	112	3	0
26	D	40	0	56	2	0
26	H	40	0	56	5	0
26	K	40	0	56	3	0
26	T	40	0	56	6	0
26	Y	40	0	56	6	0
26	a	40	0	56	1	0
26	b	120	0	168	6	0
26	c	80	0	112	6	0
26	d	40	0	56	1	0
26	h	40	0	56	5	0
26	k	40	0	56	1	0
26	t	40	0	56	6	0
26	y	40	0	56	2	0
27	A	108	0	156	4	0
27	B	54	0	78	1	0
27	F	43	0	53	0	0
27	L	54	0	78	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	a	108	0	156	4	0
27	f	43	0	53	3	0
28	A	6	0	8	0	0
28	B	42	0	56	2	0
28	C	12	0	16	2	0
28	D	6	0	8	2	0
28	F	6	0	8	0	0
28	O	6	0	8	0	0
28	T	12	0	16	4	0
28	V	24	0	32	0	0
28	a	18	0	24	3	0
28	b	30	0	40	1	0
28	c	12	0	16	1	0
28	o	6	0	8	0	0
28	t	6	0	8	0	0
28	v	24	0	32	2	0
29	A	35	0	46	3	0
29	C	35	0	46	2	0
29	D	35	0	46	1	0
29	E	35	0	46	1	0
29	M	70	0	92	3	0
29	T	25	0	35	1	0
29	a	70	0	92	1	0
29	b	25	0	35	0	0
29	e	35	0	46	1	0
29	m	70	0	92	3	0
29	t	25	0	35	0	0
30	A	20	0	0	0	0
30	a	20	0	0	1	0
31	A	110	0	160	8	0
31	D	110	0	160	3	0
31	a	110	0	160	19	0
31	d	110	0	160	0	0
32	A	28	0	0	0	0
32	B	33	0	0	0	0
32	C	34	0	0	0	0
32	D	57	0	0	0	0
32	I	40	0	0	0	0
32	J	10	0	0	0	0
32	M	10	0	0	0	0
32	X	18	0	0	0	0
32	a	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	b	33	0	0	0	0
32	c	32	0	0	0	0
32	d	71	0	0	0	0
32	i	40	0	0	0	0
32	j	10	0	0	0	0
32	m	10	0	0	0	0
33	A	51	0	72	3	0
33	C	102	0	144	4	0
33	D	51	0	72	1	0
33	M	51	0	72	3	0
33	Z	37	0	44	2	0
33	a	51	0	72	5	0
33	b	51	0	72	3	0
33	c	51	0	72	5	0
33	d	51	0	72	4	0
33	k	51	0	72	2	0
33	z	39	0	48	6	0
34	B	1	0	0	0	0
34	C	1	0	0	0	0
34	F	1	0	0	0	0
34	O	1	0	0	0	0
34	b	1	0	0	0	0
34	c	2	0	0	0	0
34	f	1	0	0	0	0
34	o	1	0	0	0	0
35	B	95	0	130	1	0
35	C	38	0	52	1	0
35	D	16	0	17	2	0
35	V	19	0	26	1	0
35	b	95	0	130	5	0
35	c	38	0	52	1	0
35	d	16	0	17	3	0
36	C	186	0	246	6	0
36	D	52	0	71	2	0
36	H	62	0	82	2	0
36	c	186	0	246	8	0
36	e	62	0	82	7	0
36	h	62	0	82	1	0
37	D	147	0	222	12	0
37	E	42	0	57	2	0
37	L	49	0	74	2	0
37	a	42	0	57	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	b	49	0	74	4	0
37	d	147	0	222	14	0
38	E	43	0	30	2	0
38	f	43	0	30	4	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	175	0	0	2	0
41	B	288	0	0	5	0
41	C	236	0	0	4	0
41	D	149	0	0	3	0
41	E	37	0	0	0	0
41	F	7	0	0	0	0
41	H	41	0	0	0	0
41	I	4	0	0	0	0
41	J	10	0	0	0	0
41	K	8	0	0	1	0
41	L	17	0	0	1	0
41	M	23	0	0	0	0
41	O	179	0	0	3	0
41	T	16	0	0	1	0
41	U	83	0	0	3	0
41	V	116	0	0	1	0
41	X	8	0	0	0	0
41	Y	4	0	0	0	0
41	Z	1	0	0	0	0
41	a	168	0	0	3	0
41	b	264	0	0	4	0
41	c	206	0	0	3	0
41	d	137	0	0	2	0
41	e	20	0	0	1	0
41	f	6	0	0	0	0
41	h	42	0	0	1	0
41	i	5	0	0	0	0
41	j	7	0	0	0	0
41	k	8	0	0	0	0
41	l	7	0	0	0	0
41	m	15	0	0	0	0
41	o	152	0	0	1	0
41	t	14	0	0	0	0
41	u	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	v	86	0	0	1	0
41	x	6	0	0	0	0
41	y	2	0	0	0	0
All	All	55631	0	54163	754	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 7.

All (754) 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)
24:C:503:CLA:HBB1	24:C:512:CLA:H41	1.50	0.93
1:A:214[A]:MET:HG2	31:A:417[A]:PL9:H102	1.50	0.92
1:A:214[B]:MET:HG2	31:A:417[B]:PL9:H102	1.54	0.89
4:d:192:THR:HG23	24:d:404:CLA:HBC2	1.59	0.84
24:B:616:CLA:H71	24:B:617:CLA:H192	1.62	0.82
28:D:402:GOL:H11	12:M:1:FME:HG2	1.62	0.82
24:B:615:CLA:H18	33:M:101:LMG:H421	1.61	0.80
4:D:192:THR:HG23	24:D:404:CLA:HBC2	1.63	0.79
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.65	0.79
3:c:279:LEU:HD22	24:c:513:CLA:HED2	1.67	0.77
1:a:214[A]:MET:HG2	31:a:416[A]:PL9:H102	1.68	0.73
13:o:74[B]:GLU:OE1	41:o:401:HOH:O	2.05	0.73
24:c:507:CLA:HBB1	33:c:522:LMG:H231	1.71	0.73
24:c:505:CLA:H202	24:c:511:CLA:HBB1	1.71	0.72
1:a:298:ASN:ND2	41:a:501[A]:HOH:O	2.20	0.72
31:a:416[A]:PL9:H28	37:a:420:LHG:H222	1.73	0.71
3:C:335:THR:OG1	41:C:601[A]:HOH:O	2.07	0.71
1:a:214[B]:MET:HG2	31:a:416[B]:PL9:H102	1.73	0.70
24:b:624:CLA:H2	24:b:625:CLA:HBB2	1.75	0.69
16:v:78:ASN:OD1	16:v:96:ARG:NH1	2.25	0.69
24:c:509:CLA:HHC	24:c:509:CLA:HBB1	1.75	0.67
10:k:27:VAL:HG11	33:k:101:LMG:H181	1.76	0.67
1:A:121[B]:LEU:HD11	24:C:505:CLA:H122	1.74	0.67
24:C:505:CLA:CMD	24:C:507:CLA:HAB	2.25	0.67
31:A:417[B]:PL9:H261	37:E:101:LHG:H223	1.75	0.67
24:B:607:CLA:H191	26:B:620:BCR:H363	1.76	0.66
2:b:86[A]:ILE:HD12	2:b:88:PRO:HD3	1.77	0.66
28:a:421:GOL:H11	16:v:27:LEU:HD21	1.76	0.66
4:D:103:ARG:HG3	5:E:73:LYS:HE2	1.78	0.66
24:c:512:CLA:H191	33:k:101:LMG:H232	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ASN:ND2	41:A:501[A]:HOH:O	2.29	0.65
13:O:27:ARG:NH1	13:O:202:ALA:O	2.29	0.65
1:a:183:MET:HA	24:a:409:CLA:HMD1	1.78	0.65
19:z:37:LYS:HZ2	33:z:101:LMG:HC4	1.62	0.65
14:T:25[A]:GLU:HG3	28:T:101:GOL:H2	1.77	0.65
37:a:420:LHG:HC31	5:e:9:PRO:HA	1.78	0.65
3:C:286:ALA:HB2	24:C:502:CLA:HMD1	1.78	0.64
1:a:215[A]:HIS:ND1	31:a:416[A]:PL9:O1	2.28	0.64
41:B:981:HOH:O	22:U:201:CL:CL	2.52	0.64
12:m:6:LEU:HD11	29:m:103:LMT:H11	1.79	0.64
26:d:406:BCR:H313	36:e:101:DGD:HA91	1.80	0.64
10:K:15:TYR:OH	19:Z:58:ASN:ND2	2.32	0.63
27:a:414:SQD:H271	37:d:410:LHG:H141	1.79	0.63
4:D:103:ARG:NH1	4:D:106:GLN:OE1	2.31	0.63
24:b:622:CLA:H18	37:d:408:LHG:H202	1.81	0.63
4:d:123:ILE:HD11	36:h:102:DGD:HAH1	1.79	0.63
2:B:472:ARG:NH2	41:B:706:HOH:O	2.31	0.63
3:C:161:LEU:HD11	24:C:506:CLA:HBB1	1.80	0.63
24:B:616:CLA:H61	24:B:617:CLA:HBB1	1.80	0.62
31:a:416[B]:PL9:H28	37:a:420:LHG:H222	1.81	0.62
37:d:410:LHG:H342	37:d:410:LHG:H151	1.81	0.62
13:O:204:VAL:HG22	13:O:211:ILE:HG22	1.82	0.62
3:c:320:ARG:HB2	28:c:502:GOL:H32	1.82	0.62
24:B:617:CLA:HED2	24:B:617:CLA:H43	1.81	0.62
24:C:513:CLA:H171	26:C:514:BCR:H373	1.81	0.61
26:H:101:BCR:HC8	26:H:101:BCR:H331	1.81	0.61
2:b:248:ALA:HA	24:b:612:CLA:H42	1.82	0.61
24:c:517:CLA:H171	26:c:526:BCR:H373	1.81	0.61
6:f:41:GLN:OE1	9:j:30:GLY:HA3	1.99	0.61
2:B:124:ARG:O	7:H:12[A]:ARG:NH1	2.32	0.60
4:D:279:LEU:HD22	25:D:401[A]:PHO:HBC3	1.83	0.60
1:a:271:LEU:HD11	31:a:416[B]:PL9:HC8	1.83	0.60
3:C:45:LEU:HD22	3:C:138:GLU:HG2	1.81	0.60
24:b:617:CLA:HAB	4:d:123:ILE:HG12	1.84	0.59
2:b:62:VAL:HB	24:b:614:CLA:HED3	1.84	0.59
2:B:341:LYS:HA	2:B:405[A]:GLU:HG2	1.83	0.59
13:o:204:VAL:HG22	13:o:211:ILE:HG22	1.83	0.59
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.38	0.59
24:c:505:CLA:C4D	24:c:507:CLA:H2	2.32	0.58
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.85	0.58
19:z:37:LYS:NZ	33:z:101:LMG:HC4	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:16:LYS:NZ	41:U:304:HOH:O	2.36	0.58
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.38	0.58
24:c:506:CLA:H61	24:c:516:CLA:H42	1.85	0.58
24:c:510:CLA:HMC2	24:c:511:CLA:H102	1.84	0.58
2:B:256:MET:HA	2:B:263:THR:HG21	1.86	0.58
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.16	0.58
8:I:2:GLU:O	8:I:6:ILE:HG12	2.04	0.58
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.39	0.58
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.39	0.58
1:A:183:MET:HA	24:A:405:CLA:HMD1	1.86	0.57
4:D:279:LEU:HD22	25:D:401[B]:PHO:HBC3	1.86	0.57
27:L:102:SQD:H1	27:L:102:SQD:H462	1.86	0.57
13:o:58:ASN:HD21	13:o:61:GLN:HB2	1.69	0.57
24:C:510:CLA:H43	37:D:411:LHG:H383	1.86	0.57
10:k:11:LEU:HD11	10:k:22:VAL:HG21	1.86	0.57
24:B:613:CLA:CMB	24:B:615:CLA:HBB1	2.34	0.57
12:M:4:ASN:ND2	33:M:101:LMG:O10	2.34	0.57
24:c:514:CLA:HED2	24:c:514:CLA:H2	1.86	0.57
13:o:145:GLU:HG2	13:o:196:GLN:HG3	1.86	0.57
19:z:9:LEU:HD13	19:z:54:VAL:HG11	1.87	0.56
24:A:407:CLA:HMD3	4:D:182:LEU:HD11	1.87	0.56
27:A:411:SQD:H251	37:D:411:LHG:H131	1.87	0.56
2:B:195:PRO:HD2	7:H:65:LEU:HD11	1.87	0.56
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.41	0.56
1:a:72:LEU:HD11	29:a:404:LMT:H52	1.87	0.56
1:a:121[A]:LEU:HD11	24:c:509:CLA:H152	1.87	0.56
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.88	0.56
3:c:213[A]:LEU:HG	24:c:510:CLA:H202	1.88	0.56
1:A:240:GLY:HA3	14:T:29:ILE:HG23	1.87	0.56
5:e:7:GLU:OE2	41:e:201:HOH:O	2.18	0.56
11:L:13:ASN:ND2	11:L:16:SER:H	2.04	0.56
33:b:629:LMG:H421	37:b:634:LHG:H372	1.88	0.56
24:C:512:CLA:H101	24:C:513:CLA:H141	1.87	0.56
1:a:307[B]:ILE:HG22	1:a:313:VAL:HA	1.88	0.56
24:a:410:CLA:H203	33:d:415:LMG:H412	1.88	0.56
26:b:626:BCR:H12C	33:b:629:LMG:C43	2.35	0.56
17:Y:22:LEU:HA	17:Y:25:ILE:HG22	1.88	0.56
8:i:36:ASP:OD1	8:i:36:ASP:N	2.36	0.56
37:D:411:LHG:H132	37:D:411:LHG:H372	1.88	0.55
26:T:103:BCR:H321	26:T:103:BCR:HC8	1.89	0.55
11:L:13:ASN:HD22	11:L:16:SER:H	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:213[B]:LEU:HD11	26:c:518:BCR:H373	1.87	0.55
24:c:512:CLA:HBC3	24:c:514:CLA:H71	1.89	0.55
4:D:343:GLU:O	41:D:545[B]:HOH:O	2.18	0.55
37:d:409:LHG:HC62	11:l:15:THR:HG23	1.88	0.55
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.42	0.55
24:a:410:CLA:HMB2	24:d:404:CLA:H122	1.88	0.55
1:a:271:LEU:HD11	31:a:416[A]:PL9:HC8	1.89	0.55
30:a:418[B]:OEX:O4	41:a:506[B]:HOH:O	2.18	0.55
16:v:71:GLY:HA2	28:v:202:GOL:H31	1.88	0.55
24:C:506:CLA:H62	29:C:521:LMT:H92	1.89	0.54
1:A:84:PRO:HA	1:A:112:TYR:CG	2.42	0.54
3:C:149:TYR:HB2	3:C:157:MET:HE1	1.89	0.54
31:a:416[B]:PL9:H512	27:f:102:SQD:H302	1.89	0.54
24:c:517:CLA:HHC	24:c:517:CLA:HBB1	1.89	0.54
10:K:25:LEU:HD22	26:Y:101:BCR:H332	1.88	0.54
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.90	0.54
2:B:162:PHE:O	24:B:607:CLA:HHD	2.08	0.54
31:a:416[A]:PL9:HC2	31:a:416[A]:PL9:H103	1.90	0.54
2:b:216:HIS:HE1	24:b:618:CLA:C1A	2.21	0.54
37:d:410:LHG:H381	37:d:410:LHG:H122	1.90	0.54
12:M:33:GLN:HB2	12:m:33:GLN:HB2	1.89	0.54
9:J:17:GLY:HA3	26:Y:101:BCR:H371	1.90	0.54
33:a:415:LMG:H221	36:c:519:DGD:HA81	1.90	0.54
24:b:613:CLA:H43	24:b:614:CLA:H2	1.90	0.54
36:e:101:DGD:HE3	36:e:101:DGD:HD4	1.89	0.54
26:y:101:BCR:H321	26:y:101:BCR:HC8	1.90	0.54
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
3:c:286:ALA:HB2	24:c:506:CLA:HMD1	1.89	0.53
4:D:199:MET:HG2	31:D:407[B]:PL9:H321	1.91	0.53
37:D:411:LHG:H382	37:D:411:LHG:H112	1.90	0.53
4:d:139:ARG:NH2	41:d:502:HOH:O	2.34	0.53
2:B:248:ALA:HA	24:B:604:CLA:H42	1.91	0.53
3:c:348:GLU:OE1	13:o:11:VAL:HA	2.07	0.53
1:A:40:THR:HG23	24:A:409:CLA:HBB1	1.90	0.53
1:A:267[B]:ASN:HB3	1:A:270:SER:HB3	1.90	0.53
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.43	0.53
24:c:516:CLA:O2D	24:c:517:CLA:HBB2	2.09	0.53
24:B:608:CLA:C4A	24:B:608:CLA:HBA2	2.39	0.53
36:e:101:DGD:HB71	36:e:101:DGD:HBW2	1.91	0.53
33:A:419:LMG:H382	36:C:516:DGD:HB42	1.89	0.52
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ILE:HB	3:C:335:THR:HG21	1.91	0.52
24:A:407:CLA:H122	31:A:417[A]:PL9:H252	1.91	0.52
11:L:2:GLU:O	41:L:201:HOH:O	2.19	0.52
13:o:53:LYS:HE3	13:o:65:PHE:CE1	2.44	0.52
29:M:102:LMT:H6'2	11:l:9:PRO:HB3	1.90	0.52
33:a:415:LMG:H242	24:c:509:CLA:H92	1.90	0.52
31:A:417[A]:PL9:H261	37:E:101:LHG:H223	1.90	0.52
3:c:225:VAL:HG13	3:c:289:PHE:HA	1.90	0.52
1:A:238[A]:LYS:HG2	14:T:30:THR:HG21	1.90	0.52
2:b:379:ALA:HA	2:b:390:TYR:HB3	1.91	0.52
3:c:210:PHE:HA	3:c:213[B]:LEU:HG	1.91	0.52
26:t:102:BCR:HC8	26:t:102:BCR:H311	1.92	0.52
6:F:21:VAL:O	6:F:25:THR:HG23	2.09	0.52
24:a:410:CLA:H141	33:d:415:LMG:H361	1.90	0.52
4:d:40:CYS:HB3	4:d:117:HIS:O	2.09	0.52
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.08	0.52
24:B:607:CLA:H151	24:B:617:CLA:H142	1.92	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
6:f:27:ALA:HB1	38:f:101:HEM:CAC	2.39	0.52
3:C:103:GLY:O	41:C:602:HOH:O	2.19	0.52
4:D:102:THR:OG1	36:D:408:DGD:HG31	2.10	0.52
2:b:458:PHE:HB3	24:b:613:CLA:HBC2	1.91	0.51
3:C:213:LEU:HD21	26:C:515:BCR:C20	2.40	0.51
37:b:634:LHG:H111	4:d:273:PHE:CZ	2.46	0.51
26:H:101:BCR:H331	26:H:101:BCR:C8	2.38	0.51
2:B:116:VAL:HG21	26:B:620:BCR:H292	1.92	0.51
2:B:405[B]:GLU:OE1	13:o:60:ARG:HD3	2.11	0.51
10:k:15:TYR:OH	19:z:58:ASN:ND2	2.39	0.51
2:B:50:PRO:HB2	28:B:629:GOL:H12	1.93	0.51
24:C:501:CLA:C4D	24:C:503:CLA:H2	2.41	0.51
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.91	0.51
10:K:20:PRO:HB3	17:Y:21:GLN:HG3	1.93	0.51
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.92	0.51
1:a:153:SER:HB2	24:a:409:CLA:H43	1.93	0.51
3:c:377:LEU:HG	3:c:381:LYS:HE3	1.93	0.51
5:e:10:PHE:HE2	38:f:101:HEM:HBD2	1.76	0.51
31:A:417[A]:PL9:H221	25:D:401[A]:PHO:HMA2	1.93	0.51
3:C:330:SER:HB3	13:O:100:GLY:O	2.11	0.51
26:t:102:BCR:H382	26:t:102:BCR:H23C	1.91	0.51
2:B:482:ILE:HD12	2:B:486:LEU:HD22	1.92	0.51
10:K:10:LYS:HD2	10:K:10:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:610:CLA:HBA2	24:b:610:CLA:H101	1.93	0.50
3:c:84:GLN:OE1	41:c:1101:HOH:O	2.19	0.50
3:c:334:PRO:HA	13:o:153:THR:OG1	2.10	0.50
13:o:193:THR:HG21	13:o:220:LEU:HD12	1.92	0.50
24:C:513:CLA:HHC	24:C:513:CLA:HBB1	1.92	0.50
1:a:214[A]:MET:HE2	1:a:255:PHE:CE1	2.47	0.50
6:f:27:ALA:HB1	38:f:101:HEM:HAC	1.92	0.50
24:B:605:CLA:H43	24:B:606:CLA:H2	1.93	0.50
4:D:273:PHE:CZ	37:L:101:LHG:H112	2.46	0.50
28:T:102:GOL:H2	29:m:103:LMT:H6D	1.93	0.50
1:a:215[B]:HIS:ND1	31:a:416[B]:PL9:O1	2.37	0.50
3:c:472:LEU:HD11	4:d:255:GLN:HG3	1.94	0.50
24:d:405:CLA:H2	18:x:14:LEU:HA	1.92	0.50
1:a:317:TRP:CZ3	4:d:180:ARG:HD2	2.46	0.50
3:c:406:SER:HA	3:c:420:VAL:HG23	1.94	0.50
15:u:86:GLU:HG2	41:u:291:HOH:O	2.12	0.50
29:A:414:LMT:H71	2:b:39:LEU:HD13	1.93	0.50
2:B:422:ARG:O	2:B:425:ILE:HG12	2.12	0.50
3:C:223:TRP:CG	3:C:224:ILE:H	2.30	0.50
28:D:402:GOL:O2	41:D:501:HOH:O	2.04	0.50
13:O:189:ARG:HD3	15:U:9:LEU:HD22	1.93	0.50
26:T:103:BCR:H19C	26:b:627:BCR:H363	1.94	0.50
2:B:458:PHE:HB3	24:B:605:CLA:HBC2	1.94	0.50
3:C:473:ASP:OXT	14:T:28:ARG:NH2	2.40	0.50
24:C:510:CLA:HBC3	24:C:510:CLA:H192	1.92	0.50
27:a:414:SQD:H301	24:c:512:CLA:H71	1.93	0.50
24:b:610:CLA:H193	26:h:101:BCR:H353	1.94	0.50
24:b:614:CLA:HHC	24:b:614:CLA:HBB1	1.94	0.50
35:d:413:HTG:H1	7:h:25:TRP:CD1	2.46	0.50
33:c:522:LMG:H232	33:c:522:LMG:H391	1.94	0.49
16:v:95:LEU:HD11	16:v:112:LEU:HD11	1.94	0.49
2:B:121:GLU:HA	7:H:2:ALA:HB1	1.95	0.49
2:b:201:HIS:HB2	24:b:611:CLA:CHB	2.42	0.49
3:C:443:TRP:CZ2	24:C:508:CLA:HMD1	2.46	0.49
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.93	0.49
38:E:103:HEM:HAC	6:F:27:ALA:HB1	1.94	0.49
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.92	0.49
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.94	0.49
37:D:411:LHG:H132	37:D:411:LHG:H352	1.94	0.49
3:c:363:GLY:O	3:c:367:GLU:HG2	2.12	0.49
3:c:443:TRP:CE2	24:c:512:CLA:HMD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:3:VAL:HG11	14:t:2:GLU:HG2	1.94	0.49
1:A:132:GLU:O	1:A:136:ARG:HG2	2.13	0.49
2:B:379:ALA:HA	2:B:390:TYR:HB3	1.95	0.49
24:C:506:CLA:HBA2	24:C:507:CLA:H202	1.95	0.49
1:a:153:SER:CB	24:a:409:CLA:H43	2.43	0.49
1:a:192:ILE:HG13	1:a:293:MET:HE1	1.94	0.49
2:b:464:PHE:CZ	37:d:408:LHG:H252	2.48	0.49
24:B:613:CLA:HMB1	24:B:615:CLA:HBB1	1.94	0.49
4:D:317:LYS:NZ	41:D:550[B]:HOH:O	2.45	0.49
2:b:220:ARG:NH1	41:b:710:HOH:O	2.42	0.49
2:B:499:VAL:HG12	4:D:135:LEU:HB3	1.94	0.49
3:c:163:PHE:O	3:c:167:VAL:HG23	2.13	0.49
10:K:11:LEU:HD11	10:K:22:VAL:HG21	1.93	0.49
1:a:162:PRO:HB3	1:a:168[B]:PHE:HA	1.95	0.49
1:a:229:GLU:HG3	1:a:230:THR:HG23	1.94	0.49
13:O:180:GLU:CD	13:O:180:GLU:H	2.21	0.48
24:B:607:CLA:H201	27:a:405:SQD:H282	1.95	0.48
12:M:18:PRO:O	12:M:21:PHE:HB3	2.13	0.48
16:V:96:ARG:HH21	35:V:206:HTG:H6'1	1.77	0.48
5:e:60:GLN:HG2	5:e:61:ARG:N	2.27	0.48
1:A:221[B]:SER:HB2	4:D:139:ARG:O	2.12	0.48
2:B:171:PRO:HD3	7:H:66:GLY:HA2	1.95	0.48
2:B:461:LEU:HD22	37:D:409:LHG:H301	1.95	0.48
1:a:214[B]:MET:HE2	1:a:255:PHE:CE1	2.48	0.48
2:b:256:MET:HA	2:b:263:THR:HG21	1.95	0.48
16:v:57:GLU:OE1	16:v:57:GLU:N	2.40	0.48
24:c:509:CLA:HAA1	24:c:509:CLA:HBD	1.96	0.48
3:C:437:PHE:CZ	24:C:510:CLA:HMB2	2.49	0.48
13:o:42:ARG:O	13:o:241:ALA:HA	2.14	0.48
3:C:376:ASP:HB3	3:C:379:LYS:HB2	1.95	0.48
33:b:629:LMG:O2	41:b:701:HOH:O	2.20	0.48
1:A:238[A]:LYS:NZ	41:A:507:HOH:O	2.46	0.48
26:B:619:BCR:H363	26:t:102:BCR:H19C	1.95	0.48
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.49	0.48
24:C:508:CLA:HBC3	24:C:510:CLA:H71	1.96	0.48
3:C:185:LEU:HB2	3:C:230:LEU:HD13	1.96	0.48
3:C:223:TRP:CE3	3:C:224:ILE:HG12	2.49	0.48
35:b:607:HTG:O2	35:b:608:HTG:S1	2.68	0.48
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.96	0.48
33:A:419:LMG:H221	36:C:516:DGD:HAE1	1.96	0.47
24:B:602:CLA:H91	26:H:101:BCR:H21C	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:182:PHE:HA	35:c:523:HTG:H61	1.96	0.47
36:c:520:DGD:HAT1	36:c:521:DGD:HBF2	1.96	0.47
2:B:12:LEU:HB2	24:B:613:CLA:HMC2	1.96	0.47
24:b:612:CLA:H3A	24:b:612:CLA:CGA	2.44	0.47
3:c:175:LEU:HD23	3:c:237:HIS:CG	2.49	0.47
41:U:302:HOH:O	16:V:86:GLN:NE2	2.46	0.47
4:d:136:VAL:HG12	4:d:138:VAL:HG13	1.96	0.47
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.97	0.47
5:e:37:PHE:HD1	5:e:42:LEU:HD23	1.80	0.47
27:B:621:SQD:H223	26:t:102:BCR:H351	1.96	0.47
24:C:505:CLA:HAA1	24:C:505:CLA:HBD	1.97	0.47
24:D:405:CLA:H171	18:X:15:LEU:HD13	1.97	0.47
31:a:416[A]:PL9:H201	31:a:416[A]:PL9:H221	1.68	0.47
24:b:622:CLA:H191	37:d:408:LHG:H223	1.97	0.47
24:c:512:CLA:H141	24:c:514:CLA:H203	1.96	0.47
36:c:520:DGD:HB32	36:c:520:DGD:HB61	1.58	0.47
26:h:101:BCR:H331	26:h:101:BCR:C8	2.44	0.47
35:D:414:HTG:H1'2	7:H:25:TRP:CD2	2.49	0.47
2:b:30:VAL:HG12	24:b:614:CLA:HHD	1.95	0.47
3:c:113:VAL:HG12	33:c:522:LMG:H161	1.96	0.47
2:B:476:ARG:NE	41:B:715:HOH:O	2.42	0.47
15:U:51:LYS:NZ	41:U:301:HOH:O	2.29	0.47
25:a:411:PHO:HAB	4:d:205:LEU:HD13	1.97	0.47
2:b:348:ASN:HB3	2:b:354:LEU:HD11	1.96	0.47
5:e:17:VAL:O	5:e:21:VAL:HG23	2.15	0.47
16:v:109:GLU:O	16:v:113:VAL:HG23	2.14	0.47
19:z:26:ALA:HB1	19:z:36:SER:HB3	1.97	0.47
2:B:24:LEU:HD21	24:B:617:CLA:CAB	2.45	0.47
24:C:513:CLA:H202	33:C:520:LMG:H402	1.97	0.47
2:b:148[B]:LEU:HD23	24:b:613:CLA:H191	1.97	0.47
4:d:279:LEU:HD22	25:d:402[A]:PHO:HBC3	1.96	0.47
24:d:405:CLA:H162	7:h:33:VAL:HG13	1.97	0.47
37:d:410:LHG:H251	37:d:410:LHG:H281	1.60	0.47
29:e:102:LMT:O3'	29:e:102:LMT:O2B	2.29	0.47
28:T:102:GOL:O1	41:T:201:HOH:O	2.20	0.46
31:a:416[B]:PL9:H151	31:a:416[B]:PL9:H171	1.70	0.46
24:c:517:CLA:H61	26:c:526:BCR:H281	1.96	0.46
4:d:101:PHE:HB3	36:e:101:DGD:HG2	1.95	0.46
24:B:615:CLA:H93	29:m:102:LMT:H112	1.96	0.46
17:Y:32:GLY:HA3	26:Y:101:BCR:C15	2.45	0.46
3:c:223:TRP:CG	3:c:224:ILE:H	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:HG12	24:B:606:CLA:HHD	1.97	0.46
2:B:149:LEU:HD21	24:B:607:CLA:HBB2	1.96	0.46
2:B:480[A]:SER:OG	41:B:701:HOH:O	2.21	0.46
24:c:505:CLA:H101	26:c:518:BCR:H17C	1.98	0.46
24:C:512:CLA:HMB2	24:C:512:CLA:H202	1.96	0.46
3:c:162:GLY:HA2	3:c:248:GLY:HA2	1.96	0.46
24:c:512:CLA:H162	36:c:521:DGD:HBN2	1.98	0.46
6:f:21:VAL:O	6:f:25:THR:HG23	2.15	0.46
24:A:407:CLA:H122	31:A:417[B]:PL9:H252	1.98	0.46
2:B:450:TRP:CD1	24:B:608:CLA:HBA1	2.51	0.46
26:B:620:BCR:H331	26:B:620:BCR:C8	2.44	0.46
3:C:203:THR:O	3:C:235:GLY:HA3	2.16	0.46
4:D:282:SER:OG	24:D:404:CLA:HED3	2.15	0.46
13:O:149:PRO:HB2	41:O:481:HOH:O	2.14	0.46
1:a:217[B]:SER:O	1:a:221[B]:SER:HB3	2.15	0.46
2:b:98:LEU:HD13	35:b:602:HTG:H7'1	1.97	0.46
4:D:51:GLY:HA3	4:D:78:VAL:HG22	1.97	0.46
3:c:178:LYS:HB2	24:c:506:CLA:H162	1.98	0.46
12:M:27:VAL:HG12	12:m:28:GLN:HB3	1.97	0.46
17:Y:23:THR:HB	17:Y:24:MET:HE2	1.97	0.46
2:b:272:ARG:HG3	2:b:273:TYR:N	2.30	0.46
3:c:53:HIS:CB	24:c:516:CLA:HMD1	2.45	0.46
4:D:336:HIS:CD2	4:D:337:GLU:HG2	2.51	0.46
2:b:173:GLY:HA3	2:b:265:ILE:HD11	1.97	0.46
3:c:48:LYS:NZ	41:c:1117:HOH:O	2.49	0.46
26:A:410:BCR:H24C	26:A:410:BCR:H371	1.74	0.46
24:C:503:CLA:H72	24:C:503:CLA:H112	1.68	0.46
41:K:204:HOH:O	19:Z:62:VAL:HG22	2.15	0.46
20:R:2:ASP:HB3	20:R:5:VAL:HG23	1.97	0.46
3:c:210:PHE:HD2	3:c:213[B]:LEU:HD12	1.81	0.46
17:y:22:LEU:HA	17:y:25:ILE:HG22	1.98	0.46
1:A:72:LEU:HD13	29:A:414:LMT:H11	1.97	0.46
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.98	0.46
36:C:517:DGD:HBF2	36:C:517:DGD:HBE2	1.53	0.46
24:b:624:CLA:H2	24:b:625:CLA:CBB	2.45	0.46
4:d:83:ASN:ND2	4:d:166:SER:OG	2.49	0.46
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.51	0.45
2:B:419:SER:HG	13:O:179[A]:GLU:CD	2.24	0.45
24:C:509:CLA:H141	24:C:509:CLA:H161	1.76	0.45
26:Y:101:BCR:H321	26:Y:101:BCR:HC8	1.97	0.45
27:A:411:SQD:H152	27:A:411:SQD:H122	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:614:CLA:H121	24:B:614:CLA:H162	1.68	0.45
3:C:42:LEU:HD21	24:C:511:CLA:H2A	1.96	0.45
3:C:128:GLY:HA3	24:C:513:CLA:C3C	2.47	0.45
3:C:334:PRO:HA	13:O:153:THR:OG1	2.16	0.45
7:H:43:LEU:O	7:H:47:GLU:HG3	2.16	0.45
15:U:59:GLU:H	15:U:59:GLU:CD	2.23	0.45
3:c:241:GLY:O	3:c:245:ILE:HG13	2.16	0.45
4:d:85:MET:HE1	4:d:96:GLU:HG2	1.97	0.45
35:d:413:HTG:H1	7:h:25:TRP:CG	2.51	0.45
24:A:407:CLA:HED1	36:C:518:DGD:HAE2	1.98	0.45
13:O:61:GLN:HG2	13:O:62:GLU:N	2.31	0.45
1:a:131:TRP:CH2	24:c:509:CLA:HAA2	2.51	0.45
3:c:75:PHE:CZ	3:c:105:VAL:HG21	2.50	0.45
24:c:516:CLA:H192	24:c:516:CLA:H161	1.80	0.45
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.83	0.45
24:B:614:CLA:H18	37:D:409:LHG:H202	1.98	0.45
3:C:472:LEU:HD11	4:D:255:GLN:HG3	1.99	0.45
36:C:517:DGD:HA31	36:C:517:DGD:HA62	1.69	0.45
4:D:202:ALA:HB2	31:D:407[B]:PL9:H353	1.97	0.45
3:c:185:LEU:HB2	3:c:230:LEU:HD13	1.99	0.45
10:k:10:LYS:HD2	10:k:10:LYS:N	2.31	0.45
2:B:454:ALA:HB2	33:M:101:LMG:H172	1.98	0.45
26:a:413:BCR:H15C	26:a:413:BCR:H351	1.83	0.45
3:c:148:GLY:O	3:c:156:LYS:NZ	2.35	0.45
7:h:20:LYS:HG3	41:h:231:HOH:O	2.17	0.45
1:A:159:LEU:C	1:A:162:PRO:HD2	2.42	0.45
2:B:154:GLY:O	2:B:159:THR:HG23	2.17	0.45
3:c:429:SER:HA	36:c:520:DGD:HBW1	1.98	0.45
4:D:161:PRO:HG3	4:D:170:ALA:HB2	1.99	0.45
11:L:20:GLY:O	11:L:24[B]:ILE:HG13	2.16	0.45
2:B:237:VAL:HG12	24:B:613:CLA:HMD1	1.98	0.45
35:D:414:HTG:H1	7:H:25:TRP:CD1	2.52	0.45
13:O:42:ARG:O	13:O:241:ALA:HA	2.17	0.45
24:b:620:CLA:H142	37:b:634:LHG:H362	1.99	0.45
37:d:408:LHG:H212	12:m:18:PRO:HG3	1.98	0.45
10:k:28:ILE:HD11	17:y:28:ILE:HD13	1.98	0.45
2:B:266:GLU:HB3	28:B:629:GOL:H31	1.98	0.45
24:C:510:CLA:HED2	24:C:510:CLA:H2	1.98	0.45
2:b:467:ILE:HG13	4:d:126:MET:HE1	1.99	0.45
24:b:614:CLA:H62	24:b:614:CLA:H41	1.69	0.45
17:y:26:ALA:O	17:y:30:ILE:HB	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TYR:O	1:A:129:ARG:NH2	2.39	0.44
2:B:243:ALA:HA	2:B:246:PHE:CD2	2.52	0.44
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.52	0.44
4:D:27:PHE:HB2	5:E:7:GLU:OE1	2.17	0.44
1:a:188:ALA:HB2	1:a:328:MET:HB2	1.98	0.44
3:c:127:PHE:CE1	33:z:101:LMG:H152	2.52	0.44
4:d:78:VAL:HG11	4:d:114:ILE:HD12	1.98	0.44
24:d:403:CLA:H203	24:d:403:CLA:H162	1.75	0.44
2:B:224:ARG:NH1	4:D:16:ASP:OD2	2.51	0.44
2:B:414:PRO:HB2	2:B:415:PRO:HD3	2.00	0.44
4:D:273:PHE:CE2	37:L:101:LHG:H112	2.51	0.44
5:E:15:THR:HB	9:J:7:ILE:O	2.17	0.44
36:H:102:DGD:HB61	36:H:102:DGD:HB91	1.91	0.44
15:U:58:VAL:HG12	15:U:79:LEU:HD22	1.99	0.44
1:a:215[B]:HIS:HA	31:a:416[B]:PL9:HC71	1.99	0.44
13:o:51:LEU:HD23	13:o:67:PRO:HA	1.99	0.44
16:v:87:GLU:CD	16:v:96:ARG:HH12	2.25	0.44
24:B:615:CLA:H92	24:B:615:CLA:H61	1.74	0.44
3:C:406:SER:HA	3:C:420:VAL:HG23	1.99	0.44
1:a:308:ASP:HA	41:a:546:HOH:O	2.17	0.44
28:a:402:GOL:H2	5:e:63[A]:ILE:HD11	1.99	0.44
24:a:410:CLA:H13	33:d:415:LMG:H242	1.99	0.44
24:B:606:CLA:HAA1	24:B:606:CLA:HBD	1.98	0.44
37:D:411:LHG:H352	37:D:411:LHG:H151	1.99	0.44
15:U:24:LYS:HB3	15:U:81:HIS:O	2.17	0.44
26:B:619:BCR:H24C	26:B:619:BCR:H371	1.74	0.44
2:b:138:MET:HE3	24:b:624:CLA:CHD	2.47	0.44
24:b:622:CLA:H43	37:d:408:LHG:H372	1.99	0.44
26:b:626:BCR:H15C	26:b:626:BCR:H351	1.82	0.44
33:d:415:LMG:H392	33:d:415:LMG:H362	1.90	0.44
2:B:71:VAL:HG22	24:B:607:CLA:HED1	1.99	0.44
24:C:501:CLA:H201	24:C:507:CLA:H13	2.00	0.44
10:K:20:PRO:HG2	17:Y:20:ALA:HB3	2.00	0.44
26:T:103:BCR:H331	26:T:103:BCR:HC7	1.51	0.44
2:b:149:LEU:HB2	24:b:613:CLA:H171	2.00	0.44
24:b:624:CLA:HHC	24:b:624:CLA:HBB1	2.00	0.44
4:d:14:TRP:CD1	35:d:413:HTG:H61	2.53	0.44
26:k:102:BCR:H24C	26:k:102:BCR:H371	1.67	0.44
12:m:28:GLN:O	12:m:32:GLN:HG3	2.18	0.44
25:A:408:PHO:HAB	4:D:205:LEU:HD13	2.00	0.44
2:B:224:ARG:HH11	29:D:403:LMT:H2'	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B:605:CLA:H192	24:B:605:CLA:H162	1.88	0.44
24:B:616:CLA:H112	24:B:616:CLA:H152	1.48	0.44
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.78	0.44
26:B:620:BCR:H15C	26:B:620:BCR:H351	1.81	0.44
4:D:298:PHE:O	4:D:301:GLN:HB2	2.17	0.44
37:D:410:LHG:H141	11:L:22:LEU:HD21	2.00	0.44
5:E:30:LEU:HD23	20:R:12:VAL:HG22	1.99	0.44
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.53	0.44
24:b:622:CLA:OBD	24:b:623:CLA:HHC	2.18	0.44
3:c:230:LEU:O	3:c:234:VAL:HG23	2.17	0.44
24:C:508:CLA:H111	24:C:508:CLA:H142	1.78	0.44
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.99	0.44
11:L:14:ARG:HH12	27:L:102:SQD:H3	1.83	0.44
26:T:103:BCR:H382	26:T:103:BCR:H23C	2.00	0.44
19:Z:57:LEU:HD23	19:Z:57:LEU:HA	1.83	0.44
25:d:402[A]:PHO:ND	25:d:402[A]:PHO:NC	2.66	0.44
31:A:417[A]:PL9:H421	31:A:417[A]:PL9:H401	1.79	0.44
24:a:409:CLA:CBD	24:d:403:CLA:HAC2	2.48	0.44
24:b:618:CLA:C3B	26:h:101:BCR:H323	2.48	0.44
4:d:293:LEU:HD12	4:d:293:LEU:HA	1.79	0.44
3:C:151:TRP:HH2	24:C:509:CLA:H193	1.83	0.43
3:C:464:GLU:OE2	4:D:245:SER:OG	2.31	0.43
24:C:505:CLA:H93	24:C:505:CLA:H111	1.80	0.43
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.99	0.43
16:V:12:LEU:HD12	16:V:69:ILE:HB	1.99	0.43
2:b:42:LEU:HD13	2:b:94:GLU:HG3	1.98	0.43
26:b:628:BCR:H15C	26:b:628:BCR:H351	1.89	0.43
24:A:405:CLA:H202	37:D:410:LHG:H161	2.00	0.43
2:B:423:LYS:HA	2:B:423:LYS:HD3	1.82	0.43
3:C:48:LYS:HG3	3:C:138:GLU:HG3	1.99	0.43
5:E:60:GLN:HG2	5:E:62[A]:SER:H	1.82	0.43
3:c:60:ILE:HG22	24:c:507:CLA:HHD	2.00	0.43
3:c:461:ARG:HG2	4:d:223:PHE:CD1	2.53	0.43
8:i:33:LYS:HB3	8:i:34:ARG:H	1.59	0.43
24:B:610:CLA:HMA3	24:B:611:CLA:C1C	2.48	0.43
24:C:506:CLA:HMC2	24:C:507:CLA:H102	2.00	0.43
4:D:60:THR:OG1	4:D:61:HIS:HD2	2.01	0.43
33:D:415:LMG:H292	33:D:415:LMG:H152	2.01	0.43
1:a:290:ILE:CG1	24:a:409:CLA:HED2	2.48	0.43
37:a:420:LHG:H181	37:a:420:LHG:H151	1.88	0.43
2:b:299:GLU:HG3	41:b:924:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:512:CLA:H162	24:c:512:CLA:H122	1.77	0.43
2:B:487:SER:HA	2:B:488:PRO:HD3	1.89	0.43
3:C:344:SER:OG	3:C:348:GLU:OE2	2.35	0.43
36:C:517:DGD:HB51	33:C:519:LMG:H392	2.01	0.43
31:a:416[B]:PL9:H272	31:a:416[B]:PL9:H251	1.86	0.43
2:b:499:VAL:HB	4:d:135:LEU:HD13	2.00	0.43
3:c:240:ILE:HD13	3:c:240:ILE:HA	1.88	0.43
19:z:47:TRP:CE2	33:z:101:LMG:H241	2.53	0.43
3:C:461:ARG:NH2	41:C:618:HOH:O	2.49	0.43
5:E:60:GLN:HG2	5:E:62[B]:SER:H	1.82	0.43
13:O:58:ASN:HB3	41:b:889[B]:HOH:O	2.18	0.43
19:Z:47:TRP:CD2	33:Z:101:LMG:H231	2.53	0.43
31:a:416[A]:PL9:H171	31:a:416[A]:PL9:H151	1.75	0.43
24:c:512:CLA:HED2	37:d:410:LHG:HC12	1.99	0.43
13:o:19:CYS:SG	13:o:46:GLN:HB2	2.57	0.43
18:x:15:LEU:HD12	18:x:15:LEU:HA	1.75	0.43
1:A:307:ILE:HD13	1:A:313:VAL:HA	2.00	0.43
33:A:419:LMG:H161	33:A:419:LMG:H191	1.72	0.43
3:C:151:TRP:CH2	24:C:509:CLA:H193	2.54	0.43
33:C:520:LMG:H411	33:C:520:LMG:H381	1.74	0.43
1:a:196:PRO:HB3	36:c:521:DGD:HA82	2.01	0.43
2:b:138:MET:HE1	24:b:619:CLA:H192	2.00	0.43
2:b:498:LYS:HA	4:d:24:ARG:HA	2.01	0.43
24:b:624:CLA:H92	24:b:625:CLA:HBB1	2.00	0.43
4:d:160:TYR:HA	4:d:290:ALA:HB2	2.01	0.43
10:k:20:PRO:HB3	17:y:21:GLN:HG3	2.00	0.43
13:O:160:LYS:NZ	41:O:427:HOH:O	2.51	0.43
16:V:34:GLN:OE1	41:V:301:HOH:O	2.21	0.43
2:b:144:PHE:CE1	2:b:210:ILE:HG23	2.53	0.43
24:b:620:CLA:H71	37:b:634:LHG:H311	2.00	0.43
24:b:624:CLA:H91	24:b:624:CLA:H112	1.76	0.43
3:c:343:ARG:NH1	3:c:347:GLY:O	2.49	0.43
4:d:39:PRO:HG2	24:d:405:CLA:HAB	2.00	0.43
36:e:101:DGD:HG2	36:e:101:DGD:HB21	1.87	0.43
8:i:17:LEU:HD22	8:i:21:PHE:HE2	1.83	0.43
26:t:102:BCR:HC7	26:t:102:BCR:H331	1.67	0.43
24:B:607:CLA:H193	24:B:617:CLA:H71	2.01	0.43
26:H:101:BCR:H24C	26:H:101:BCR:H371	1.70	0.43
1:a:182:PHE:O	1:a:186:PHE:HB2	2.19	0.43
28:a:401:GOL:H11	12:m:1:FME:HB3	2.01	0.43
2:b:276:ASP:O	28:b:603:GOL:O2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:b:623:CLA:HAA1	24:b:623:CLA:HBD	2.01	0.43
3:c:95:LEU:HD21	24:c:505:CLA:OBD	2.18	0.43
24:c:512:CLA:H203	24:c:512:CLA:H161	1.81	0.43
2:B:58:GLN:C	2:B:329:PRO:HB3	2.44	0.43
2:B:61:PHE:CZ	24:B:608:CLA:HBB1	2.54	0.43
2:B:480[B]:SER:OG	41:B:702:HOH:O	2.21	0.43
24:B:602:CLA:CGA	24:B:602:CLA:H72	2.49	0.43
3:C:437:PHE:CE1	24:C:510:CLA:HMB2	2.54	0.43
24:C:511:CLA:HMB1	26:K:101:BCR:H382	2.01	0.43
12:M:13:LEU:HD23	12:M:13:LEU:HA	1.86	0.43
2:b:133:LEU:HB3	2:b:138:MET:SD	2.59	0.43
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.52	0.43
1:A:214[B]:MET:HE2	1:A:255:PHE:CE1	2.54	0.42
2:B:451:PHE:CE1	2:B:455:HIS:CE1	3.06	0.42
4:D:23:LYS:HG2	4:D:135:LEU:HD11	2.00	0.42
4:D:190:ASN:HB2	4:D:296:TYR:CD1	2.54	0.42
6:F:41:GLN:OE1	9:J:30:GLY:HA3	2.19	0.42
1:a:267[B]:ASN:HB3	1:a:270[B]:SER:OG	2.19	0.42
2:b:243:ALA:HA	2:b:246:PHE:CD2	2.54	0.42
3:c:180:MET:HE2	3:c:180:MET:HB3	1.92	0.42
33:c:522:LMG:H412	33:c:522:LMG:H381	1.86	0.42
24:a:412:CLA:HBA1	24:a:412:CLA:H3A	1.72	0.42
1:A:160:ILE:HD12	3:C:431:PHE:HE1	1.84	0.42
13:O:54:GLU:O	13:O:56:PRO:HD3	2.19	0.42
18:X:29:ILE:O	18:X:33:GLN:HG2	2.19	0.42
2:b:298:LEU:HD12	2:b:298:LEU:HA	1.90	0.42
2:b:416:THR:HG23	35:b:631:HTG:H5'1	2.01	0.42
24:b:613:CLA:HMD1	24:b:621:CLA:H203	2.01	0.42
24:b:622:CLA:H72	24:b:622:CLA:H111	1.71	0.42
3:c:348:GLU:HG2	13:o:7:TYR:CE2	2.55	0.42
24:C:502:CLA:H61	24:C:512:CLA:H42	2.00	0.42
29:C:521:LMT:H32	29:C:521:LMT:H61	1.66	0.42
13:O:39:ARG:HB2	13:O:246:ALA:HB2	2.01	0.42
19:Z:29:SER:HA	19:Z:30:PRO:HD3	1.85	0.42
2:b:11:VAL:HG11	24:b:623:CLA:HED2	2.00	0.42
24:c:517:CLA:H202	33:c:522:LMG:H402	2.02	0.42
36:e:101:DGD:HAW1	27:f:102:SQD:H382	2.00	0.42
7:h:38:PHE:HB2	26:h:101:BCR:C10	2.49	0.42
24:A:405:CLA:CBD	24:A:406:CLA:HAC2	2.49	0.42
2:B:144:PHE:CE1	2:B:210:ILE:HG23	2.55	0.42
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:D:409:LHG:H212	12:M:18:PRO:HD3	2.02	0.42
26:h:101:BCR:H371	26:h:101:BCR:H24C	1.78	0.42
14:t:20:ALA:O	14:t:24:ARG:HB3	2.19	0.42
1:A:136:ARG:O	8:I:32:PRO:HD3	2.19	0.42
1:A:165:GLN:NE2	1:A:294:ALA:O	2.52	0.42
1:A:300:PHE:HB3	1:A:302:PHE:CE1	2.54	0.42
17:Y:28:ILE:HG23	26:Y:101:BCR:H10C	2.02	0.42
1:a:227:THR:HB	1:a:231:GLU:HG3	2.01	0.42
24:b:625:CLA:H91	24:b:625:CLA:H112	1.81	0.42
26:c:526:BCR:H351	26:c:526:BCR:H15C	1.80	0.42
12:m:16:LEU:HD23	12:m:16:LEU:HA	1.85	0.42
14:t:2:GLU:H	14:t:2:GLU:CD	2.26	0.42
1:A:243[B]:GLU:OE2	4:D:240[B]:ALA:HB1	2.19	0.42
5:E:26:THR:HB	38:E:103:HEM:HAB	2.02	0.42
13:O:138:THR:HG23	41:O:415:HOH:O	2.19	0.42
16:V:126:LEU:HB3	16:V:129:LYS:HB2	2.02	0.42
33:Z:101:LMG:HC8	33:Z:101:LMG:H111	1.63	0.42
3:c:321:ASP:OD2	3:c:340:TYR:OH	2.35	0.42
36:c:519:DGD:HA21	36:c:519:DGD:HA52	1.89	0.42
4:d:148:ALA:HB3	4:d:149:PRO:HD3	2.02	0.42
25:d:402[B]:PHO:ND	25:d:402[B]:PHO:NC	2.67	0.42
8:i:2:GLU:O	8:i:6:ILE:HG12	2.19	0.42
33:z:101:LMG:H302	33:z:101:LMG:H151	2.02	0.42
1:A:159:LEU:O	1:A:163:ILE:HG13	2.19	0.42
24:A:407:CLA:H142	24:A:407:CLA:H112	1.87	0.42
13:O:164:LEU:HB2	13:O:188:LYS:HB2	2.02	0.42
1:a:38:ILE:HG12	27:a:405:SQD:H131	2.01	0.42
26:b:628:BCR:C8	26:b:628:BCR:H331	2.50	0.42
37:d:410:LHG:H302	37:d:410:LHG:H332	1.48	0.42
24:B:609:CLA:HBB1	24:B:609:CLA:HMB1	2.01	0.42
4:D:291:LEU:O	4:D:292:ASN:HB2	2.19	0.42
26:b:628:BCR:H24C	26:b:628:BCR:H371	1.76	0.42
3:c:130:VAL:HG22	24:c:515:CLA:H91	2.01	0.42
4:d:88:SER:HB2	5:e:69:ARG:CZ	2.50	0.42
1:A:172[A]:MET:HA	1:A:173:PRO:HD3	1.92	0.42
27:A:413:SQD:H272	2:b:109:LEU:HD13	2.01	0.42
2:B:172:TYR:CE1	2:B:283:GLU:HB2	2.55	0.42
3:C:240:ILE:HA	3:C:240:ILE:HD13	1.75	0.42
5:E:40:THR:HB	20:R:4:ARG:HG2	2.02	0.42
7:H:7:LEU:HA	7:H:10:ILE:HD12	2.02	0.42
12:M:20:VAL:HG11	12:m:20:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:216:HIS:CE1	24:b:618:CLA:NA	2.87	0.42
19:z:5:PHE:HD2	19:z:57:LEU:HB3	1.85	0.42
2:B:69:LEU:HD12	24:B:606:CLA:HBA1	2.02	0.41
24:B:606:CLA:C14	24:B:611:CLA:HED2	2.50	0.41
13:O:154:ALA:HB1	13:O:165:ALA:HB2	2.02	0.41
1:a:218[B]:LEU:HD12	31:a:416[B]:PL9:C3	2.50	0.41
2:b:63:LEU:N	2:b:64:PRO:HD2	2.34	0.41
2:b:423:LYS:HA	2:b:423:LYS:HD3	1.75	0.41
24:b:622:CLA:HBB1	24:b:622:CLA:HMB1	2.02	0.41
4:d:110:LEU:HB2	41:d:590:HOH:O	2.19	0.41
1:A:307:ILE:CG2	1:A:311:GLY:HA2	2.49	0.41
24:B:606:CLA:H62	24:B:606:CLA:H41	1.83	0.41
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.92	0.41
3:C:320:ARG:HB2	28:C:524:GOL:H32	2.01	0.41
3:C:375:LEU:HD23	3:C:375:LEU:HA	1.85	0.41
5:E:70:PHE:CE1	7:H:54:ILE:HD11	2.55	0.41
12:M:34:LYS:HG2	29:M:102:LMT:O3B	2.20	0.41
1:a:221[A]:SER:HB2	4:d:139:ARG:O	2.20	0.41
2:b:233:ASN:O	2:b:236:THR:HG22	2.20	0.41
2:b:474:LEU:O	4:d:134:ARG:NH1	2.53	0.41
24:d:404:CLA:HBD	24:d:404:CLA:HAA2	2.02	0.41
3:C:97:TRP:CE2	3:C:178:LYS:HE2	2.56	0.41
4:D:148:ALA:HB3	4:D:149:PRO:HD3	2.03	0.41
26:D:406:BCR:HC22	36:D:408:DGD:HA92	2.01	0.41
26:T:103:BCR:H11C	26:T:103:BCR:H341	1.77	0.41
15:U:64:ILE:O	15:U:67:LEU:HG	2.19	0.41
1:a:12:ASN:O	1:a:16:ARG:HG3	2.20	0.41
33:a:415:LMG:H211	33:a:415:LMG:H241	1.91	0.41
13:o:180:GLU:H	13:o:180:GLU:CD	2.29	0.41
27:A:411:SQD:H291	24:C:508:CLA:H71	2.02	0.41
3:C:374:GLY:HA2	13:O:7:TYR:CE2	2.55	0.41
24:C:501:CLA:H192	24:C:506:CLA:C1B	2.50	0.41
24:C:503:CLA:HBD	24:C:503:CLA:HAA1	2.02	0.41
4:D:178:ILE:HD13	4:D:178:ILE:HA	1.92	0.41
1:a:211[B]:PHE:CE2	31:a:416[B]:PL9:H13	2.54	0.41
31:a:416[B]:PL9:HC2	31:a:416[B]:PL9:H103	2.03	0.41
2:b:216:HIS:CE1	24:b:618:CLA:C1A	3.03	0.41
24:c:505:CLA:C3D	24:c:507:CLA:H2	2.49	0.41
24:c:515:CLA:C4D	10:k:39:TRP:HH2	2.34	0.41
4:d:85:MET:CE	4:d:96:GLU:HG2	2.50	0.41
4:D:274:VAL:HG22	31:D:407[B]:PL9:H222	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:412:CLA:H102	24:a:412:CLA:H61	1.88	0.41
2:b:496:TYR:OH	2:b:502:VAL:HG13	2.20	0.41
24:A:405:CLA:H192	24:A:405:CLA:H161	1.75	0.41
2:B:25:MET:HG2	26:B:618:BCR:H23C	2.02	0.41
4:D:85:MET:CE	4:D:96:GLU:HG2	2.51	0.41
26:D:406:BCR:H15C	26:D:406:BCR:H351	1.87	0.41
24:a:409:CLA:CAD	24:d:403:CLA:HAC2	2.51	0.41
2:b:462:PHE:CE1	24:b:622:CLA:HMB3	2.56	0.41
3:c:203:THR:HG21	3:c:208:VAL:HG11	2.03	0.41
19:z:47:TRP:CE3	33:z:101:LMG:H221	2.55	0.41
2:B:49:ASP:OD1	13:o:57:LYS:NZ	2.38	0.41
2:B:491:VAL:HG12	4:D:136:VAL:HG13	2.02	0.41
3:C:354[A]:GLU:C	3:C:356:MET:N	2.79	0.41
28:C:524:GOL:H2	41:C:630:HOH:O	2.20	0.41
29:E:102:LMT:H32	6:F:42:PHE:CZ	2.56	0.41
26:H:101:BCR:HC7	26:H:101:BCR:H321	1.82	0.41
31:a:416[A]:PL9:H512	27:f:102:SQD:H302	2.02	0.41
2:b:124:ARG:O	7:h:12:ARG:NH2	2.50	0.41
24:c:511:CLA:H61	24:c:511:CLA:H92	1.84	0.41
24:c:517:CLA:C4B	26:c:526:BCR:H383	2.50	0.41
24:B:614:CLA:OBD	24:B:615:CLA:HHC	2.21	0.41
24:B:615:CLA:H112	24:B:615:CLA:H71	1.78	0.41
3:C:421:SER:HA	3:C:422:PRO:HD3	1.93	0.41
24:C:502:CLA:H193	35:C:522:HTG:H2'2	2.01	0.41
12:M:27:VAL:HG13	29:M:102:LMT:H11	2.02	0.41
13:O:29:ALA:O	13:O:31:PRO:HD3	2.21	0.41
26:Y:101:BCR:H15C	26:Y:101:BCR:H351	1.82	0.41
20:R:3:TRP:CD2	20:R:4:ARG:HG3	2.55	0.41
1:a:340[B]:PRO:HD3	15:u:103:TYR:CZ	2.55	0.41
2:b:185:TRP:CZ2	35:b:632:HTG:H2'1	2.56	0.41
3:c:63:TRP:HB2	24:c:514:CLA:HAC2	2.03	0.41
4:d:286:VAL:HG21	24:d:404:CLA:HED2	2.02	0.41
13:o:51:LEU:HB3	13:o:65:PHE:HB3	2.02	0.41
19:z:50:LEU:O	19:z:54:VAL:HG23	2.21	0.41
1:A:131:TRP:CH2	24:C:505:CLA:HAA2	2.56	0.41
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.02	0.41
24:B:603:CLA:H41	7:H:46:LEU:HA	2.03	0.41
24:B:615:CLA:H41	24:B:615:CLA:H62	1.77	0.41
3:C:354[A]:GLU:C	3:C:356:MET:H	2.29	0.41
5:E:8:ARG:HD3	5:E:13:ILE:HG12	2.03	0.41
12:M:25:LEU:HD23	12:M:25:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:23:LEU:HD23	18:X:23:LEU:HA	1.94	0.41
1:a:121[B]:LEU:HD23	1:a:121[B]:LEU:HA	1.96	0.41
33:a:415:LMG:H152	33:a:415:LMG:H182	1.90	0.41
2:b:224:ARG:HG3	7:h:24:GLY:O	2.20	0.41
3:c:229:ASN:HB2	41:c:1257:HOH:O	2.20	0.41
3:c:443:TRP:CD2	24:c:512:CLA:HMD2	2.56	0.41
24:c:508:CLA:H191	37:d:410:LHG:H362	2.03	0.41
24:d:403:CLA:HBA1	24:d:403:CLA:C4A	2.51	0.41
5:e:23:HIS:CD2	38:f:101:HEM:NC	2.89	0.41
5:e:47:PHE:HZ	36:e:101:DGD:HBT2	1.86	0.41
16:v:51:SER:HA	28:v:201:GOL:H11	2.03	0.41
2:B:288:VAL:HG23	2:B:305:ILE:HD11	2.03	0.41
2:B:503:THR:O	18:X:39:ARG:HG2	2.21	0.41
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.56	0.41
15:U:45:LEU:HD23	15:U:45:LEU:HA	1.88	0.41
16:V:45:ILE:H	16:V:45:ILE:HG13	1.76	0.41
1:a:132:GLU:O	1:a:136:ARG:HG2	2.20	0.41
5:e:37:PHE:CD1	5:e:42:LEU:HD23	2.56	0.41
16:v:61:LEU:O	41:v:301:HOH:O	2.22	0.41
3:C:25:ASN:O	3:C:41:ARG:HD3	2.21	0.40
37:D:411:LHG:H112	37:D:411:LHG:C38	2.49	0.40
26:K:101:BCR:H371	26:K:101:BCR:H24C	1.64	0.40
26:T:103:BCR:H371	26:T:103:BCR:H24C	1.89	0.40
33:a:415:LMG:HC71	3:c:216:SER:HB2	2.04	0.40
25:d:402[B]:PHO:HHD	25:d:402[B]:PHO:HBC2	2.03	0.40
9:j:6:ARG:HA	9:j:6:ARG:NH2	2.36	0.40
10:k:18:PHE:HE1	19:z:13:VAL:HG21	1.86	0.40
24:A:409:CLA:H162	24:A:409:CLA:H122	1.71	0.40
2:B:138:MET:HE3	24:B:616:CLA:CHD	2.52	0.40
24:B:603:CLA:H171	36:H:102:DGD:HA72	2.03	0.40
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.56	0.40
26:C:515:BCR:H11C	26:C:515:BCR:H341	1.90	0.40
13:O:121:THR:OG1	13:O:123:LYS:HG3	2.21	0.40
28:T:102:GOL:O2	29:T:104:LMT:O1'	2.38	0.40
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.57	0.40
2:b:487:SER:HA	2:b:488:PRO:HD3	1.82	0.40
24:b:612:CLA:HBB2	24:b:612:CLA:H92	2.04	0.40
3:c:150:ASP:O	3:c:157:MET:HE3	2.21	0.40
3:c:288:CYS:SG	36:c:519:DGD:HB52	2.62	0.40
4:d:125:PHE:CE1	25:d:402[B]:PHO:HBD	2.56	0.40
37:d:410:LHG:H331	37:d:410:LHG:H361	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:LEU:N	2:B:64:PRO:HD2	2.36	0.40
2:B:477:ASP:N	2:B:477:ASP:OD1	2.54	0.40
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	2.03	0.40
26:B:619:BCR:H381	26:t:102:BCR:H341	2.02	0.40
33:C:519:LMG:H331	33:C:519:LMG:H212	2.03	0.40
5:E:22:ILE:O	5:E:26:THR:HG23	2.21	0.40
25:a:411:PHO:H61	25:a:411:PHO:H2	1.87	0.40
2:b:305:ILE:HA	2:b:306:PRO:HD3	1.95	0.40
4:d:87:HIS:CD2	4:d:162:LEU:HA	2.57	0.40
24:d:405:CLA:H3A	24:d:405:CLA:HBA1	1.77	0.40
15:u:57:SER:O	15:u:60:ASP:HB2	2.21	0.40
29:A:414:LMT:H6E	35:b:602:HTG:O4	2.22	0.40
2:B:102:VAL:HA	26:B:619:BCR:H402	2.04	0.40
2:B:185:TRP:CZ2	35:B:624:HTG:H2'2	2.56	0.40
3:C:318:LEU:HD21	3:C:380:ILE:HG23	2.04	0.40
10:k:25:LEU:HD22	26:y:101:BCR:H332	2.02	0.40
24:B:610:CLA:HAA1	24:B:610:CLA:HBD	2.03	0.40
24:B:611:CLA:HBB1	24:B:611:CLA:HHC	2.04	0.40
24:C:506:CLA:C4A	24:C:506:CLA:HBA1	2.51	0.40
24:D:404:CLA:HAA2	24:D:404:CLA:HBD	2.04	0.40
5:E:68:ASP:O	5:E:72:ALA:HB2	2.21	0.40
26:K:101:BCR:H15C	26:K:101:BCR:H351	1.96	0.40
13:O:129:THR:HA	13:O:141:ASP:O	2.22	0.40
14:T:20:ALA:O	14:T:24:ARG:HB3	2.22	0.40
15:U:64:ILE:HA	15:U:65:PRO:HD3	1.89	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	384/344 (112%)	377 (98%)	5 (1%)	2 (0%)	24	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	386/344 (112%)	378 (98%)	7 (2%)	1 (0%)	36	50
2	B	512/505 (101%)	505 (99%)	7 (1%)	0	100	100
2	b	513/505 (102%)	503 (98%)	10 (2%)	0	100	100
3	C	456/455 (100%)	446 (98%)	8 (2%)	2 (0%)	30	43
3	c	466/455 (102%)	450 (97%)	14 (3%)	2 (0%)	30	43
4	D	355/342 (104%)	343 (97%)	12 (3%)	0	100	100
4	d	355/342 (104%)	346 (98%)	9 (2%)	0	100	100
5	E	81/84 (96%)	80 (99%)	1 (1%)	0	100	100
5	e	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
6	F	32/44 (73%)	30 (94%)	2 (6%)	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	64/65 (98%)	58 (91%)	6 (9%)	0	100	100
7	h	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
8	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	36/39 (92%)	36 (100%)	0	0	100	100
9	j	37/39 (95%)	34 (92%)	3 (8%)	0	100	100
10	K	35/37 (95%)	35 (100%)	0	0	100	100
10	k	35/37 (95%)	35 (100%)	0	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	33/36 (92%)	33 (100%)	0	0	100	100
12	m	32/36 (89%)	32 (100%)	0	0	100	100
13	O	249/244 (102%)	241 (97%)	8 (3%)	0	100	100
13	o	246/244 (101%)	235 (96%)	11 (4%)	0	100	100
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	136/137 (99%)	130 (96%)	6 (4%)	0	100	100
16	v	135/137 (98%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	Y	27/30 (90%)	25 (93%)	2 (7%)	0	100 100
17	y	27/30 (90%)	25 (93%)	2 (7%)	0	100 100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100 100
18	x	36/40 (90%)	34 (94%)	2 (6%)	0	100 100
19	Z	60/62 (97%)	58 (97%)	2 (3%)	0	100 100
19	z	60/62 (97%)	57 (95%)	1 (2%)	2 (3%)	3 2
20	R	28/34 (82%)	28 (100%)	0	0	100 100
All	All	5419/5384 (101%)	5272 (97%)	138 (2%)	9 (0%)	48 58

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	416[A]	SER
3	C	416[B]	SER
3	c	416[A]	SER
3	c	416[B]	SER
1	a	259	ILE
19	z	30	PRO
1	A	259	ILE
1	A	30	VAL
19	z	61	VAL

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	312/279 (112%)	312 (100%)	0	100 100
1	a	314/279 (112%)	313 (100%)	1 (0%)	86 93
2	B	412/403 (102%)	408 (99%)	4 (1%)	68 84
2	b	413/403 (102%)	407 (98%)	6 (2%)	57 77
3	C	357/356 (100%)	351 (98%)	6 (2%)	53 74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	c	367/356 (103%)	357 (97%)	10 (3%)	39 62
4	D	290/277 (105%)	288 (99%)	2 (1%)	76 88
4	d	290/277 (105%)	287 (99%)	3 (1%)	68 84
5	E	74/73 (101%)	74 (100%)	0	100 100
5	e	74/73 (101%)	72 (97%)	2 (3%)	39 62
6	F	28/38 (74%)	28 (100%)	0	100 100
6	f	26/38 (68%)	24 (92%)	2 (8%)	12 20
7	H	55/54 (102%)	54 (98%)	1 (2%)	51 73
7	h	54/54 (100%)	54 (100%)	0	100 100
8	I	34/34 (100%)	33 (97%)	1 (3%)	37 60
8	i	34/34 (100%)	33 (97%)	1 (3%)	37 60
9	J	26/27 (96%)	26 (100%)	0	100 100
9	j	27/27 (100%)	26 (96%)	1 (4%)	30 51
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 55
10	k	30/30 (100%)	29 (97%)	1 (3%)	33 55
11	L	36/35 (103%)	34 (94%)	2 (6%)	19 33
11	l	36/35 (103%)	35 (97%)	1 (3%)	38 60
12	M	31/32 (97%)	30 (97%)	1 (3%)	34 56
12	m	30/32 (94%)	29 (97%)	1 (3%)	33 55
13	O	214/207 (103%)	209 (98%)	5 (2%)	44 66
13	o	211/207 (102%)	204 (97%)	7 (3%)	33 55
14	T	27/28 (96%)	25 (93%)	2 (7%)	13 22
14	t	27/28 (96%)	25 (93%)	2 (7%)	13 22
15	U	84/89 (94%)	82 (98%)	2 (2%)	43 65
15	u	84/89 (94%)	82 (98%)	2 (2%)	43 65
16	V	119/117 (102%)	118 (99%)	1 (1%)	73 86
16	v	118/117 (101%)	114 (97%)	4 (3%)	32 54
17	Y	22/23 (96%)	19 (86%)	3 (14%)	3 5
17	y	22/23 (96%)	19 (86%)	3 (14%)	3 5
18	X	32/33 (97%)	32 (100%)	0	100 100
18	x	31/33 (94%)	31 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29 49
19	z	52/52 (100%)	50 (96%)	2 (4%)	29 49
20	R	25/29 (86%)	23 (92%)	2 (8%)	11 19
All	All	4500/4403 (102%)	4416 (98%)	84 (2%)	51 71

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	86	ILE
2	B	240	SER
2	B	492	GLU
2	B	505	ARG
3	C	29	GLU
3	C	142	GLU
3	C	240	ILE
3	C	279	LEU
3	C	289	PHE
3	C	315	MET
4	D	90	LEU
4	D	136	VAL
7	H	65	LEU
8	I	36	ASP
10	K	17	ILE
11	L	13	ASN
11	L	15	THR
12	M	5	GLN
13	O	4	THR
13	O	34	SER
13	O	69	LYS
13	O	181[A]	GLU
13	O	181[B]	GLU
14	T	25[A]	GLU
14	T	25[B]	GLU
15	U	59	GLU
15	U	70	ARG
16	V	42	VAL
17	Y	18	VAL
17	Y	24	MET
17	Y	30	ILE
19	Z	3	ILE
19	Z	4	LEU

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Mol	Chain	Res	Type
20	R	5	VAL
20	R	6	LEU
1	a	12	ASN
2	b	84	THR
2	b	240	SER
2	b	362	PHE
2	b	472	ARG
2	b	479	PHE
2	b	480	SER
3	c	19	ASN
3	c	21	ILE
3	c	142	GLU
3	c	255	THR
3	c	279	LEU
3	c	289	PHE
3	c	416[A]	SER
3	c	416[B]	SER
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	136	VAL
4	d	150	ILE
4	d	329	MET
5	e	11	SER
5	e	16	SER
6	f	15	ILE
6	f	44	GLN
8	i	36	ASP
9	j	1	MET
10	k	17	ILE
11	l	15	THR
12	m	33	GLN
13	o	4	THR
13	o	23	ASP
13	o	37	THR
13	o	118	LEU
13	o	141	ASP
13	o	164	LEU
13	o	194	LYS
14	t	25[A]	GLU
14	t	25[B]	GLU
15	u	61	VAL
15	u	86	GLU

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Mol	Chain	Res	Type
16	v	2	GLU
16	v	28	GLU
16	v	42	VAL
16	v	81	THR
17	y	18	VAL
17	y	24	MET
17	y	30	ILE
19	z	29	SER
19	z	34	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	296	ASN
2	B	53	ASN
2	B	497	GLN
3	C	44	ASN
4	D	61	HIS
4	D	83	ASN
4	D	255	GLN
4	D	301	GLN
4	D	332	GLN
5	E	74	GLN
11	L	13	ASN
13	O	124	ASN
13	O	147	ASN
13	O	231	HIS
15	U	81	HIS
19	Z	58	ASN
1	a	12	ASN
1	a	75	ASN
1	a	165	GLN
2	b	53	ASN
2	b	331	ASN
2	b	490	GLN
3	c	44	ASN
3	c	155	ASN
3	c	201	ASN
3	c	373	ASN
4	d	83	ASN

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Mol	Chain	Res	Type
4	d	186	GLN
4	d	301	GLN
4	d	332	GLN
13	o	124	ASN
13	o	147	ASN
15	u	78	ASN
15	u	81	HIS
16	v	86	GLN
16	v	118	HIS
19	z	58	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	FME	M	1	12	8,9,10	0.74	0	8,9,11	1.29	2 (25%)
12	FME	m	1	12	8,9,10	0.64	0	8,9,11	1.27	1 (12%)
14	FME	t	1	14	8,9,10	0.82	0	8,9,11	1.90	3 (37%)
8	FME	I	1	8	8,9,10	0.75	0	8,9,11	1.35	2 (25%)
14	FME	T	1	14	8,9,10	0.74	0	8,9,11	1.25	1 (12%)
8	FME	i	1	8	8,9,10	0.70	0	8,9,11	1.13	1 (12%)

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

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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	t	1	FME	C-CA-N	3.16	115.61	109.50
14	t	1	FME	CA-N-CN	-2.77	118.57	122.82
8	I	1	FME	CA-N-CN	-2.50	118.97	122.82
14	T	1	FME	O-C-CA	-2.46	118.45	124.77
14	t	1	FME	O-C-CA	-2.41	118.57	124.77
12	M	1	FME	CA-N-CN	-2.32	119.25	122.82
8	i	1	FME	O-C-CA	-2.23	119.04	124.77
12	M	1	FME	O-C-CA	-2.13	119.30	124.77
8	I	1	FME	O-C-CA	-2.12	119.33	124.77
12	m	1	FME	CA-N-CN	-2.04	119.69	122.82

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	t	1	FME	O1-CN-N-CA
12	M	1	FME	CA-CB-CG-SD
14	t	1	FME	CB-CA-N-CN
8	I	1	FME	CA-CB-CG-SD
12	m	1	FME	CA-CB-CG-SD
12	M	1	FME	N-CA-CB-CG
12	m	1	FME	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 267 ligands modelled in this entry, 25 are monoatomic and 18 are unknown - leaving 224 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	$\#\|Z\| > 2$
28	GOL	c	501	-	5,5,5	0.40	0	5,5,5	0.25	0
24	CLA	B	615	-	69,73,73	2.00	20 (28%)	82,113,113	2.75	33 (40%)
25	PHO	a	411	-	58,69,69	2.85	14 (24%)	55,99,99	2.82	17 (30%)
26	BCR	K	101	-	41,41,41	1.03	1 (2%)	56,56,56	1.58	13 (23%)
28	GOL	T	102	-	5,5,5	0.41	0	5,5,5	0.33	0
35	HTG	B	631	-	19,19,19	0.94	1 (5%)	23,24,24	1.23	2 (8%)
24	CLA	b	610	41	69,73,73	2.07	19 (27%)	82,113,113	2.64	31 (37%)
37	LHG	E	101	-	41,41,48	1.04	2 (4%)	44,47,54	1.17	4 (9%)
29	LMT	a	419	-	36,36,36	0.43	0	47,47,47	0.80	1 (2%)
37	LHG	d	408	-	48,48,48	0.91	3 (6%)	51,54,54	1.08	5 (9%)
33	LMG	a	415	-	51,51,55	0.91	2 (3%)	59,59,63	1.19	5 (8%)
37	LHG	d	409	-	48,48,48	0.89	2 (4%)	51,54,54	1.02	5 (9%)
29	LMT	m	102	-	36,36,36	0.46	0	47,47,47	0.88	0
24	CLA	D	404	-	69,73,73	1.94	19 (27%)	82,113,113	2.76	30 (36%)
31	PL9	a	416[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.86	20 (29%)
24	CLA	c	507	-	69,73,73	2.02	20 (28%)	82,113,113	2.64	31 (37%)
29	LMT	M	104	-	36,36,36	0.54	1 (2%)	47,47,47	1.15	6 (12%)
24	CLA	B	605	-	69,73,73	1.94	20 (28%)	82,113,113	2.65	30 (36%)
28	GOL	b	604	-	5,5,5	0.34	0	5,5,5	0.29	0
24	CLA	b	625	-	69,73,73	2.04	19 (27%)	82,113,113	2.65	32 (39%)
31	PL9	D	407[B]	-	55,55,55	0.65	2 (3%)	68,69,69	1.82	23 (33%)
24	CLA	a	412	-	69,73,73	2.00	20 (28%)	82,113,113	2.73	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
28	GOL	O	301	-	5,5,5	0.36	0	5,5,5	0.38	0
31	PL9	d	407[A]	-	55,55,55	0.71	2 (3%)	68,69,69	1.52	15 (22%)
35	HTG	c	523	-	19,19,19	0.90	2 (10%)	23,24,24	1.32	2 (8%)
36	DGD	H	102	-	63,63,67	0.91	2 (3%)	77,77,81	1.03	6 (7%)
28	GOL	b	606	-	5,5,5	0.39	0	5,5,5	0.24	0
29	LMT	D	403	-	36,36,36	0.43	0	47,47,47	1.02	1 (2%)
24	CLA	c	512	-	69,73,73	2.01	20 (28%)	82,113,113	2.62	30 (36%)
28	GOL	B	630	-	5,5,5	0.37	0	5,5,5	0.32	0
23	BCT	A	404[B]	21	3,3,3	0.53	0	2,3,3	0.99	0
24	CLA	b	616	41	69,73,73	2.02	18 (26%)	82,113,113	2.64	31 (37%)
25	PHO	D	401[A]	-	58,69,69	2.83	14 (24%)	55,99,99	2.86	13 (23%)
35	HTG	b	631	-	19,19,19	0.75	1 (5%)	23,24,24	1.22	1 (4%)
37	LHG	D	410	-	48,48,48	0.93	2 (4%)	51,54,54	0.74	2 (3%)
26	BCR	C	514	-	41,41,41	1.08	1 (2%)	56,56,56	1.42	8 (14%)
24	CLA	d	403	41	69,73,73	2.00	19 (27%)	82,113,113	2.76	32 (39%)
36	DGD	C	517	-	63,63,67	0.89	2 (3%)	77,77,81	1.06	9 (11%)
30	OEX	A	416[B]	41,3,1	0,15,15	-	-	-		
28	GOL	B	629	-	5,5,5	0.45	0	5,5,5	0.29	0
35	HTG	B	623	-	19,19,19	0.78	1 (5%)	23,24,24	1.33	2 (8%)
35	HTG	b	602	-	19,19,19	0.88	1 (5%)	23,24,24	1.02	1 (4%)
26	BCR	c	526	-	41,41,41	1.07	1 (2%)	56,56,56	1.57	8 (14%)
38	HEM	f	101	6,5	50,50,50	1.53	7 (14%)	67,82,82	1.60	12 (17%)
24	CLA	B	611	41	69,73,73	2.10	20 (28%)	82,113,113	2.74	34 (41%)
24	CLA	c	515	3	69,73,73	1.97	20 (28%)	82,113,113	2.65	30 (36%)
26	BCR	y	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.60	10 (17%)
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	0.96	3 (3%)
24	CLA	b	619	41	69,73,73	2.04	21 (30%)	82,113,113	2.70	33 (40%)
26	BCR	b	628	-	41,41,41	1.07	2 (4%)	56,56,56	1.43	10 (17%)
28	GOL	a	421	34	5,5,5	0.34	0	5,5,5	0.46	0
27	SQD	F	101	-	41,43,54	1.10	2 (4%)	51,54,65	1.68	11 (21%)
28	GOL	t	103	-	5,5,5	0.42	0	5,5,5	0.23	0
31	PL9	a	416[A]	-	55,55,55	0.65	2 (3%)	68,69,69	1.92	20 (29%)
37	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.11	5 (9%)
28	GOL	D	402	-	5,5,5	0.43	0	5,5,5	0.32	0
28	GOL	b	603	-	5,5,5	0.41	0	5,5,5	0.41	0
24	CLA	B	606	-	69,73,73	2.05	20 (28%)	82,113,113	2.70	29 (35%)
24	CLA	B	616	-	69,73,73	2.02	18 (26%)	82,113,113	2.62	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	d	405	-	69,73,73	2.02	19 (27%)	82,113,113	2.66	31 (37%)
24	CLA	B	607	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	32 (39%)
24	CLA	B	612	-	69,73,73	1.98	19 (27%)	82,113,113	2.66	32 (39%)
24	CLA	C	504	41	69,73,73	2.05	20 (28%)	82,113,113	2.71	29 (35%)
31	PL9	D	407[A]	-	55,55,55	0.68	2 (3%)	68,69,69	1.74	22 (32%)
33	LMG	d	415	39	51,51,55	0.94	2 (3%)	59,59,63	1.12	7 (11%)
24	CLA	a	409	-	69,73,73	2.04	19 (27%)	82,113,113	2.68	32 (39%)
24	CLA	A	409	-	69,73,73	2.05	20 (28%)	82,113,113	2.62	33 (40%)
23	BCT	A	404[A]	21	3,3,3	0.50	0	2,3,3	1.27	0
24	CLA	c	513	-	69,73,73	2.07	19 (27%)	82,113,113	2.62	31 (37%)
29	LMT	E	102	-	36,36,36	0.49	0	47,47,47	0.95	1 (2%)
24	CLA	A	407	41	69,73,73	1.99	20 (28%)	82,113,113	2.73	33 (40%)
24	CLA	A	405	-	69,73,73	2.08	20 (28%)	82,113,113	2.66	32 (39%)
26	BCR	B	619	-	41,41,41	1.03	1 (2%)	56,56,56	1.37	10 (17%)
27	SQD	f	102	-	41,43,54	1.12	2 (4%)	51,54,65	1.42	6 (11%)
27	SQD	a	414	-	52,54,54	0.89	2 (3%)	62,65,65	1.54	11 (17%)
24	CLA	B	602	41	69,73,73	2.08	22 (31%)	82,113,113	2.66	28 (34%)
35	HTG	C	523	-	19,19,19	0.89	1 (5%)	23,24,24	1.64	4 (17%)
28	GOL	V	204	-	5,5,5	0.36	0	5,5,5	0.31	0
28	GOL	a	402	-	5,5,5	0.39	0	5,5,5	0.35	0
26	BCR	d	406	-	41,41,41	1.10	1 (2%)	56,56,56	1.68	13 (23%)
26	BCR	A	410	-	41,41,41	1.09	1 (2%)	56,56,56	1.16	4 (7%)
24	CLA	C	509	-	69,73,73	2.06	20 (28%)	82,113,113	2.67	31 (37%)
28	GOL	A	412	-	5,5,5	0.41	0	5,5,5	0.16	0
24	CLA	b	615	-	69,73,73	2.02	20 (28%)	82,113,113	2.66	30 (36%)
36	DGD	e	101	-	63,63,67	0.95	3 (4%)	77,77,81	1.28	7 (9%)
27	SQD	L	102	-	52,54,54	1.00	2 (3%)	62,65,65	1.58	11 (17%)
24	CLA	C	501	-	69,73,73	2.03	20 (28%)	82,113,113	2.68	30 (36%)
26	BCR	T	103	-	41,41,41	1.01	1 (2%)	56,56,56	1.79	13 (23%)
24	CLA	C	505	-	69,73,73	2.01	20 (28%)	82,113,113	2.59	29 (35%)
26	BCR	b	626	-	41,41,41	1.03	1 (2%)	56,56,56	1.59	10 (17%)
26	BCR	t	102	-	41,41,41	1.05	1 (2%)	56,56,56	1.72	15 (26%)
27	SQD	B	621	-	52,54,54	0.96	2 (3%)	62,65,65	1.36	5 (8%)
28	GOL	V	203	-	5,5,5	0.43	0	5,5,5	0.27	0
35	HTG	B	632	-	19,19,19	0.96	1 (5%)	23,24,24	1.29	2 (8%)
23	BCT	d	401[A]	21	3,3,3	0.52	0	2,3,3	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	D	406	-	41,41,41	1.07	1 (2%)	56,56,56	1.78	14 (25%)
37	LHG	D	411	-	48,48,48	0.99	2 (4%)	51,54,54	1.13	3 (5%)
38	HEM	E	103	6,5	50,50,50	1.50	5 (10%)	67,82,82	1.74	15 (22%)
33	LMG	A	419	-	51,51,55	0.92	2 (3%)	59,59,63	1.08	3 (5%)
28	GOL	b	605	-	5,5,5	0.38	0	5,5,5	0.35	0
30	OEX	a	417[A]	41,3,1	0,15,15	-	-	-		
30	OEX	a	418[B]	41,3,1	0,15,15	-	-	-		
25	PHO	A	408	-	58,69,69	2.76	12 (20%)	55,99,99	2.96	18 (32%)
31	PL9	A	417[B]	-	55,55,55	0.66	2 (3%)	68,69,69	1.83	22 (32%)
29	LMT	M	102	-	36,36,36	0.42	0	47,47,47	0.88	1 (2%)
28	GOL	T	101	-	5,5,5	0.40	0	5,5,5	0.29	0
29	LMT	a	404	-	36,36,36	0.48	1 (2%)	47,47,47	1.19	3 (6%)
24	CLA	c	510	-	69,73,73	2.03	19 (27%)	82,113,113	2.62	29 (35%)
24	CLA	B	609	-	69,73,73	2.01	20 (28%)	82,113,113	2.60	30 (36%)
40	HEC	V	205	16	46,50,50	1.79	12 (26%)	58,82,82	1.65	14 (24%)
24	CLA	b	611	-	69,73,73	2.04	21 (30%)	82,113,113	2.78	34 (41%)
24	CLA	c	505	-	69,73,73	2.00	19 (27%)	82,113,113	2.63	31 (37%)
36	DGD	c	520	-	63,63,67	0.89	3 (4%)	77,77,81	1.04	6 (7%)
28	GOL	v	202	-	5,5,5	0.37	0	5,5,5	0.32	0
24	CLA	C	508	-	69,73,73	2.05	20 (28%)	82,113,113	2.65	33 (40%)
28	GOL	V	202	-	5,5,5	0.34	0	5,5,5	0.39	0
28	GOL	v	203	-	5,5,5	0.34	0	5,5,5	0.52	0
28	GOL	C	525	-	5,5,5	0.43	0	5,5,5	0.43	0
24	CLA	C	511	3	69,73,73	2.06	20 (28%)	82,113,113	2.65	30 (36%)
23	BCT	d	401[B]	21	3,3,3	0.52	0	2,3,3	0.77	0
27	SQD	A	411	-	52,54,54	0.92	2 (3%)	62,65,65	1.51	11 (17%)
33	LMG	c	522	-	51,51,55	0.96	2 (3%)	59,59,63	1.18	7 (11%)
36	DGD	D	408	-	52,52,67	1.04	3 (5%)	60,60,81	1.20	5 (8%)
24	CLA	b	612	-	69,73,73	1.98	20 (28%)	82,113,113	2.72	30 (36%)
24	CLA	b	618	-	69,73,73	2.03	19 (27%)	82,113,113	2.69	32 (39%)
28	GOL	F	103	34	5,5,5	0.36	0	5,5,5	0.27	0
37	LHG	b	634	-	48,48,48	0.94	2 (4%)	51,54,54	0.98	3 (5%)
27	SQD	A	413	-	52,54,54	0.96	2 (3%)	62,65,65	1.13	5 (8%)
27	SQD	a	405	-	52,54,54	1.02	2 (3%)	62,65,65	1.15	4 (6%)
26	BCR	B	618	-	41,41,41	1.06	1 (2%)	56,56,56	1.38	8 (14%)
26	BCR	a	413	-	41,41,41	1.05	1 (2%)	56,56,56	1.47	10 (17%)
24	CLA	b	614	-	69,73,73	1.99	20 (28%)	82,113,113	2.76	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	LMG	z	101	-	39,39,55	1.09	2 (5%)	47,47,63	1.14	4 (8%)
24	CLA	d	404	-	69,73,73	1.98	19 (27%)	82,113,113	2.67	31 (37%)
29	LMT	b	630	-	25,25,36	0.50	0	30,30,47	0.66	0
28	GOL	B	627	-	5,5,5	0.37	0	5,5,5	0.55	0
24	CLA	B	617	-	69,73,73	2.02	19 (27%)	82,113,113	2.63	29 (35%)
26	BCR	h	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.34	7 (12%)
24	CLA	B	604	-	69,73,73	2.04	20 (28%)	82,113,113	2.66	30 (36%)
26	BCR	Y	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.78	12 (21%)
26	BCR	c	518	-	41,41,41	1.05	1 (2%)	56,56,56	1.60	10 (17%)
31	PL9	A	417[A]	-	55,55,55	0.66	2 (3%)	68,69,69	1.80	22 (32%)
24	CLA	c	506	-	69,73,73	2.03	20 (28%)	82,113,113	2.56	25 (30%)
33	LMG	C	519	-	51,51,55	0.95	2 (3%)	59,59,63	1.03	5 (8%)
24	CLA	C	506	-	69,73,73	2.00	19 (27%)	82,113,113	2.56	31 (37%)
35	HTG	B	622	-	19,19,19	1.02	1 (5%)	23,24,24	1.23	1 (4%)
28	GOL	b	601	-	5,5,5	0.39	0	5,5,5	0.47	0
37	LHG	d	410	-	48,48,48	0.91	2 (4%)	51,54,54	1.08	3 (5%)
24	CLA	B	614	-	69,73,73	2.03	18 (26%)	82,113,113	2.61	30 (36%)
28	GOL	c	502	-	5,5,5	0.40	0	5,5,5	0.40	0
24	CLA	b	624	-	69,73,73	2.03	18 (26%)	82,113,113	2.60	27 (32%)
35	HTG	B	624	-	19,19,19	0.97	1 (5%)	23,24,24	1.90	4 (17%)
24	CLA	B	610	-	69,73,73	2.00	18 (26%)	82,113,113	2.65	30 (36%)
33	LMG	D	415	39	51,51,55	0.90	2 (3%)	59,59,63	0.96	3 (5%)
35	HTG	b	607	-	19,19,19	0.92	1 (5%)	23,24,24	1.29	3 (13%)
36	DGD	C	518	-	63,63,67	0.90	2 (3%)	77,77,81	0.99	4 (5%)
24	CLA	C	512	-	69,73,73	2.04	20 (28%)	82,113,113	2.65	31 (37%)
29	LMT	A	414	-	36,36,36	0.58	1 (2%)	47,47,47	1.29	4 (8%)
30	OEX	A	415[A]	41,3,1	0,15,15	-	-	-		
24	CLA	B	608	41	69,73,73	2.05	20 (28%)	82,113,113	2.62	30 (36%)
24	CLA	a	410	41	69,73,73	2.00	20 (28%)	82,113,113	2.72	32 (39%)
37	LHG	a	420	-	41,41,48	1.04	2 (4%)	44,47,54	0.95	2 (4%)
24	CLA	c	511	41	69,73,73	2.00	19 (27%)	82,113,113	2.66	30 (36%)
24	CLA	b	617	-	69,73,73	2.03	20 (28%)	82,113,113	2.62	33 (40%)
24	CLA	A	406	41	69,73,73	2.03	20 (28%)	82,113,113	2.80	32 (39%)
24	CLA	C	503	-	69,73,73	2.07	20 (28%)	82,113,113	2.71	29 (35%)
24	CLA	c	509	-	69,73,73	2.02	20 (28%)	82,113,113	2.62	29 (35%)
24	CLA	C	502	-	69,73,73	2.03	20 (28%)	82,113,113	2.63	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMT	e	102	-	36,36,36	0.49	1 (2%)	47,47,47	0.86	1 (2%)
33	LMG	b	629	-	51,51,55	0.91	3 (5%)	59,59,63	1.07	5 (8%)
24	CLA	B	603	-	69,73,73	2.04	20 (28%)	82,113,113	2.72	32 (39%)
26	BCR	B	620	-	41,41,41	1.00	1 (2%)	56,56,56	1.59	11 (19%)
24	CLA	b	613	-	69,73,73	2.00	19 (27%)	82,113,113	2.65	29 (35%)
25	PHO	d	402[B]	-	58,69,69	2.76	14 (24%)	55,99,99	3.04	16 (29%)
37	LHG	D	409	-	48,48,48	0.86	2 (4%)	51,54,54	1.02	4 (7%)
33	LMG	k	101	-	51,51,55	0.89	2 (3%)	59,59,63	1.09	5 (8%)
28	GOL	B	625	-	5,5,5	0.41	0	5,5,5	0.18	0
33	LMG	Z	101	-	37,37,55	0.99	3 (8%)	45,45,63	1.37	7 (15%)
24	CLA	D	405	-	69,73,73	2.01	20 (28%)	82,113,113	2.68	30 (36%)
29	LMT	t	101	-	25,25,36	0.53	0	30,30,47	0.77	1 (3%)
40	HEC	v	206	16	46,50,50	1.71	9 (19%)	58,82,82	1.70	16 (27%)
24	CLA	c	514	-	69,73,73	2.05	20 (28%)	82,113,113	2.66	32 (39%)
36	DGD	C	516	-	63,63,67	0.87	2 (3%)	77,77,81	1.09	6 (7%)
24	CLA	b	621	-	69,73,73	2.01	20 (28%)	82,113,113	2.74	32 (39%)
36	DGD	c	521	-	63,63,67	0.86	2 (3%)	77,77,81	1.03	4 (5%)
24	CLA	b	623	-	69,73,73	2.01	19 (27%)	82,113,113	2.72	31 (37%)
33	LMG	M	101	-	51,51,55	0.94	2 (3%)	59,59,63	0.97	3 (5%)
28	GOL	B	626	-	5,5,5	0.33	0	5,5,5	0.41	0
24	CLA	B	613	-	69,73,73	1.92	17 (24%)	82,113,113	2.68	29 (35%)
28	GOL	v	204	-	5,5,5	0.38	0	5,5,5	0.27	0
35	HTG	b	608	-	19,19,19	0.96	2 (10%)	23,24,24	1.02	3 (13%)
24	CLA	b	622	-	69,73,73	2.04	20 (28%)	82,113,113	2.65	30 (36%)
28	GOL	o	301	-	5,5,5	0.42	0	5,5,5	0.37	0
28	GOL	B	628	-	5,5,5	0.35	0	5,5,5	0.42	0
26	BCR	H	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.58	9 (16%)
24	CLA	C	507	41	69,73,73	2.02	20 (28%)	82,113,113	2.56	27 (32%)
26	BCR	k	102	-	41,41,41	1.06	1 (2%)	56,56,56	1.53	10 (17%)
33	LMG	C	520	-	51,51,55	0.96	2 (3%)	59,59,63	1.13	5 (8%)
35	HTG	c	524	-	19,19,19	0.94	2 (10%)	23,24,24	1.38	2 (8%)
29	LMT	T	104	-	25,25,36	0.56	1 (4%)	30,30,47	1.08	2 (6%)
35	HTG	C	522	-	19,19,19	0.95	2 (10%)	23,24,24	1.47	1 (4%)
36	DGD	c	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.05	6 (7%)
29	LMT	C	521	-	36,36,36	0.49	0	47,47,47	1.13	3 (6%)
35	HTG	d	413	-	16,16,19	1.13	2 (12%)	20,21,24	1.60	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	HTG	D	414	-	16,16,19	0.98	2 (12%)	20,21,24	1.17	1 (5%)
24	CLA	C	513	-	69,73,73	2.04	20 (28%)	82,113,113	2.61	30 (36%)
31	PL9	d	407[B]	-	55,55,55	0.69	2 (3%)	68,69,69	1.63	17 (25%)
24	CLA	c	517	-	69,73,73	2.04	20 (28%)	82,113,113	2.66	31 (37%)
25	PHO	d	402[A]	-	58,69,69	2.78	13 (22%)	55,99,99	3.07	15 (27%)
24	CLA	b	620	-	69,73,73	1.94	18 (26%)	82,113,113	2.57	31 (37%)
26	BCR	b	627	-	41,41,41	1.01	1 (2%)	56,56,56	1.41	7 (12%)
28	GOL	B	634	-	5,5,5	0.46	0	5,5,5	0.49	0
28	GOL	C	524	-	5,5,5	0.37	0	5,5,5	0.80	0
24	CLA	c	508	41	69,73,73	1.99	19 (27%)	82,113,113	2.67	31 (37%)
28	GOL	v	201	-	5,5,5	0.33	0	5,5,5	0.35	0
29	LMT	m	103	-	36,36,36	0.51	0	47,47,47	1.08	4 (8%)
25	PHO	D	401[B]	-	58,69,69	2.82	15 (25%)	55,99,99	2.80	14 (25%)
35	HTG	V	206	-	19,19,19	0.93	2 (10%)	23,24,24	1.33	5 (21%)
35	HTG	b	632	-	19,19,19	1.09	2 (10%)	23,24,24	1.53	3 (13%)
24	CLA	C	510	-	69,73,73	2.07	19 (27%)	82,113,113	2.60	34 (41%)
24	CLA	c	516	-	69,73,73	2.05	20 (28%)	82,113,113	2.74	33 (40%)
26	BCR	C	515	-	41,41,41	1.05	1 (2%)	56,56,56	1.55	10 (17%)
28	GOL	V	201	-	5,5,5	0.38	0	5,5,5	0.34	0
28	GOL	a	401	-	5,5,5	0.40	0	5,5,5	0.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	c	501	-	-	0/4/4/4	-
24	CLA	B	615	-	1/1/15/20	16/39/115/115	-
25	PHO	a	411	-	-	3/37/103/103	0/5/6/6
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
28	GOL	T	102	-	-	2/4/4/4	-
35	HTG	B	631	-	-	1/10/30/30	0/1/1/1
24	CLA	b	610	41	1/1/15/20	14/39/115/115	-
37	LHG	E	101	-	-	22/46/46/53	-
29	LMT	a	419	-	-	4/21/61/61	0/2/2/2
37	LHG	d	408	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	LMG	a	415	-	-	17/46/66/70	0/1/1/1
29	LMT	m	102	-	-	8/21/61/61	0/2/2/2
24	CLA	D	404	-	1/1/15/20	2/39/115/115	-
31	PL9	a	416[B]	-	-	15/53/73/73	0/1/1/1
24	CLA	c	507	-	1/1/15/20	5/39/115/115	-
29	LMT	M	104	-	-	10/21/61/61	0/2/2/2
24	CLA	B	605	-	1/1/15/20	3/39/115/115	-
28	GOL	b	604	-	-	2/4/4/4	-
24	CLA	b	625	-	1/1/15/20	12/39/115/115	-
31	PL9	D	407[B]	-	-	9/53/73/73	0/1/1/1
24	CLA	a	412	-	1/1/15/20	12/39/115/115	-
28	GOL	O	301	-	-	2/4/4/4	-
31	PL9	d	407[A]	-	-	5/53/73/73	0/1/1/1
35	HTG	c	523	-	-	3/10/30/30	0/1/1/1
36	DGD	H	102	-	-	9/51/91/95	0/2/2/2
28	GOL	b	606	-	-	2/4/4/4	-
29	LMT	D	403	-	-	9/21/61/61	0/2/2/2
24	CLA	c	512	-	1/1/15/20	2/39/115/115	-
28	GOL	B	630	-	-	0/4/4/4	-
24	CLA	b	616	41	1/1/15/20	2/39/115/115	-
25	PHO	D	401[A]	-	-	0/37/103/103	0/5/6/6
35	HTG	b	631	-	-	2/10/30/30	0/1/1/1
37	LHG	D	410	-	-	5/53/53/53	-
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
24	CLA	d	403	41	1/1/15/20	6/39/115/115	-
36	DGD	C	517	-	-	20/51/91/95	0/2/2/2
28	GOL	B	629	-	-	4/4/4/4	-
35	HTG	B	623	-	-	6/10/30/30	0/1/1/1
35	HTG	b	602	-	-	3/10/30/30	0/1/1/1
26	BCR	c	526	-	-	0/29/63/63	0/2/2/2
38	HEM	f	101	6,5	-	10/14/54/54	-
24	CLA	B	611	41	1/1/15/20	3/39/115/115	-
24	CLA	c	515	3	1/1/15/20	6/39/115/115	-
26	BCR	y	101	-	-	2/29/63/63	0/2/2/2
36	DGD	h	102	-	-	11/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	b	619	41	1/1/15/20	6/39/115/115	-
26	BCR	b	628	-	-	2/29/63/63	0/2/2/2
28	GOL	a	421	34	-	2/4/4/4	-
27	SQD	F	101	-	-	14/38/58/69	0/1/1/1
28	GOL	t	103	-	-	0/4/4/4	-
31	PL9	a	416[A]	-	-	17/53/73/73	0/1/1/1
37	LHG	L	101	-	-	13/53/53/53	-
28	GOL	D	402	-	-	3/4/4/4	-
28	GOL	b	603	-	-	0/4/4/4	-
24	CLA	B	606	-	1/1/15/20	7/39/115/115	-
24	CLA	B	616	-	1/1/15/20	9/39/115/115	-
24	CLA	d	405	-	1/1/15/20	7/39/115/115	-
24	CLA	B	607	-	1/1/15/20	5/39/115/115	-
24	CLA	B	612	-	1/1/15/20	1/39/115/115	-
24	CLA	C	504	41	1/1/15/20	6/39/115/115	-
31	PL9	D	407[A]	-	-	7/53/73/73	0/1/1/1
33	LMG	d	415	39	-	10/46/66/70	0/1/1/1
24	CLA	a	409	-	1/1/15/20	6/39/115/115	-
24	CLA	A	409	-	-	12/39/115/115	-
24	CLA	c	513	-	1/1/15/20	15/39/115/115	-
29	LMT	E	102	-	-	4/21/61/61	0/2/2/2
24	CLA	A	407	41	-	7/39/115/115	-
24	CLA	A	405	-	1/1/15/20	4/39/115/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
27	SQD	f	102	-	-	15/38/58/69	0/1/1/1
27	SQD	a	414	-	-	14/49/69/69	0/1/1/1
24	CLA	B	602	41	1/1/15/20	13/39/115/115	-
35	HTG	C	523	-	-	3/10/30/30	0/1/1/1
28	GOL	V	204	-	-	4/4/4/4	-
28	GOL	a	402	-	-	2/4/4/4	-
26	BCR	d	406	-	-	4/29/63/63	0/2/2/2
26	BCR	A	410	-	-	0/29/63/63	0/2/2/2
24	CLA	C	509	-	1/1/15/20	14/39/115/115	-
28	GOL	A	412	-	-	0/4/4/4	-
24	CLA	b	615	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	DGD	e	101	-	-	26/51/91/95	0/2/2/2
27	SQD	L	102	-	-	20/49/69/69	0/1/1/1
24	CLA	C	501	-	1/1/15/20	11/39/115/115	-
26	BCR	T	103	-	-	1/29/63/63	0/2/2/2
24	CLA	C	505	-	1/1/15/20	6/39/115/115	-
26	BCR	b	626	-	-	2/29/63/63	0/2/2/2
26	BCR	t	102	-	-	7/29/63/63	0/2/2/2
27	SQD	B	621	-	-	22/49/69/69	0/1/1/1
28	GOL	V	203	-	-	0/4/4/4	-
35	HTG	B	632	-	-	0/10/30/30	0/1/1/1
37	LHG	D	411	-	-	10/53/53/53	-
26	BCR	D	406	-	-	6/29/63/63	0/2/2/2
38	HEM	E	103	6,5	-	6/14/54/54	-
33	LMG	A	419	-	-	19/46/66/70	0/1/1/1
28	GOL	b	605	-	-	2/4/4/4	-
31	PL9	A	417[B]	-	-	10/53/73/73	0/1/1/1
25	PHO	A	408	-	-	2/37/103/103	0/5/6/6
29	LMT	M	102	-	-	10/21/61/61	0/2/2/2
28	GOL	T	101	-	-	0/4/4/4	-
29	LMT	a	404	-	-	7/21/61/61	0/2/2/2
24	CLA	c	510	-	1/1/15/20	13/39/115/115	-
24	CLA	B	609	-	-	0/39/115/115	-
40	HEC	V	205	16	-	6/14/54/54	-
24	CLA	b	611	-	1/1/15/20	4/39/115/115	-
24	CLA	c	505	-	1/1/15/20	5/39/115/115	-
36	DGD	c	520	-	-	18/51/91/95	0/2/2/2
28	GOL	v	202	-	-	2/4/4/4	-
24	CLA	C	508	-	1/1/15/20	4/39/115/115	-
28	GOL	V	202	-	-	2/4/4/4	-
28	GOL	v	203	-	-	2/4/4/4	-
28	GOL	C	525	-	-	1/4/4/4	-
24	CLA	C	511	3	-	2/39/115/115	-
27	SQD	A	411	-	-	13/49/69/69	0/1/1/1
33	LMG	c	522	-	-	7/46/66/70	0/1/1/1
36	DGD	D	408	-	-	22/47/67/95	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LHG	d	409	-	-	9/53/53/53	-
24	CLA	b	612	-	1/1/15/20	9/39/115/115	-
24	CLA	b	618	-	1/1/15/20	2/39/115/115	-
28	GOL	F	103	34	-	0/4/4/4	-
37	LHG	b	634	-	-	14/53/53/53	-
27	SQD	A	413	-	-	17/49/69/69	0/1/1/1
27	SQD	a	405	-	-	12/49/69/69	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	BCR	a	413	-	-	0/29/63/63	0/2/2/2
24	CLA	b	614	-	1/1/15/20	8/39/115/115	-
33	LMG	z	101	-	-	13/34/54/70	0/1/1/1
24	CLA	d	404	-	1/1/15/20	6/39/115/115	-
29	LMT	b	630	-	-	4/17/37/61	0/1/1/2
28	GOL	B	627	-	-	2/4/4/4	-
24	CLA	B	617	-	1/1/15/20	7/39/115/115	-
26	BCR	h	101	-	-	1/29/63/63	0/2/2/2
24	CLA	B	604	-	1/1/15/20	6/39/115/115	-
26	BCR	Y	101	-	-	4/29/63/63	0/2/2/2
26	BCR	c	518	-	-	4/29/63/63	0/2/2/2
31	PL9	A	417[A]	-	-	14/53/73/73	0/1/1/1
24	CLA	c	506	-	1/1/15/20	6/39/115/115	-
33	LMG	C	519	-	-	9/46/66/70	0/1/1/1
24	CLA	C	506	-	1/1/15/20	11/39/115/115	-
35	HTG	B	622	-	-	2/10/30/30	0/1/1/1
28	GOL	b	601	-	-	0/4/4/4	-
37	LHG	d	410	-	-	15/53/53/53	-
24	CLA	B	614	-	1/1/15/20	6/39/115/115	-
28	GOL	c	502	-	-	2/4/4/4	-
24	CLA	b	624	-	1/1/15/20	6/39/115/115	-
35	HTG	B	624	-	-	4/10/30/30	0/1/1/1
24	CLA	B	610	-	1/1/15/20	7/39/115/115	-
33	LMG	D	415	39	-	8/46/66/70	0/1/1/1
35	HTG	b	607	-	-	3/10/30/30	0/1/1/1
36	DGD	C	518	-	-	12/51/91/95	0/2/2/2
24	CLA	C	512	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LMT	A	414	-	-	6/21/61/61	0/2/2/2
24	CLA	B	608	41	1/1/15/20	6/39/115/115	-
24	CLA	a	410	41	-	8/39/115/115	-
37	LHG	a	420	-	-	16/46/46/53	-
24	CLA	c	511	41	1/1/15/20	5/39/115/115	-
24	CLA	b	617	-	-	1/39/115/115	-
24	CLA	A	406	41	1/1/15/20	3/39/115/115	-
24	CLA	C	503	-	1/1/15/20	3/39/115/115	-
24	CLA	c	509	-	1/1/15/20	0/39/115/115	-
24	CLA	C	502	-	1/1/15/20	6/39/115/115	-
29	LMT	e	102	-	-	10/21/61/61	0/2/2/2
33	LMG	b	629	-	-	11/46/66/70	0/1/1/1
24	CLA	B	603	-	1/1/15/20	1/39/115/115	-
26	BCR	B	620	-	-	0/29/63/63	0/2/2/2
24	CLA	b	613	-	1/1/15/20	3/39/115/115	-
25	PHO	d	402[B]	-	-	2/37/103/103	0/5/6/6
37	LHG	D	409	-	-	13/53/53/53	-
33	LMG	k	101	-	-	14/46/66/70	0/1/1/1
28	GOL	B	625	-	-	0/4/4/4	-
33	LMG	Z	101	-	-	14/31/51/70	0/1/1/1
24	CLA	D	405	-	1/1/15/20	4/39/115/115	-
29	LMT	t	101	-	-	7/17/37/61	0/1/1/2
40	HEC	v	206	16	-	6/14/54/54	-
24	CLA	c	514	-	1/1/15/20	7/39/115/115	-
36	DGD	C	516	-	-	15/51/91/95	0/2/2/2
24	CLA	b	621	-	1/1/15/20	0/39/115/115	-
36	DGD	c	521	-	-	14/51/91/95	0/2/2/2
24	CLA	b	623	-	1/1/15/20	20/39/115/115	-
33	LMG	M	101	-	-	12/46/66/70	0/1/1/1
28	GOL	B	626	-	-	2/4/4/4	-
24	CLA	B	613	-	1/1/15/20	3/39/115/115	-
28	GOL	v	204	-	-	2/4/4/4	-
35	HTG	b	608	-	-	0/10/30/30	0/1/1/1
24	CLA	b	622	-	1/1/15/20	9/39/115/115	-
28	GOL	o	301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	GOL	B	628	-	-	2/4/4/4	-
26	BCR	H	101	-	-	4/29/63/63	0/2/2/2
24	CLA	C	507	41	1/1/15/20	6/39/115/115	-
26	BCR	k	102	-	-	1/29/63/63	0/2/2/2
33	LMG	C	520	-	-	12/46/66/70	0/1/1/1
35	HTG	c	524	-	-	2/10/30/30	0/1/1/1
29	LMT	T	104	-	-	9/17/37/61	0/1/1/2
35	HTG	C	522	-	-	1/10/30/30	0/1/1/1
36	DGD	c	519	-	-	15/51/91/95	0/2/2/2
29	LMT	C	521	-	-	10/21/61/61	0/2/2/2
35	HTG	d	413	-	-	1/7/27/30	0/1/1/1
35	HTG	D	414	-	-	0/7/27/30	0/1/1/1
24	CLA	C	513	-	1/1/15/20	7/39/115/115	-
31	PL9	d	407[B]	-	-	7/53/73/73	0/1/1/1
24	CLA	c	517	-	-	5/39/115/115	-
25	PHO	d	402[A]	-	-	0/37/103/103	0/5/6/6
24	CLA	b	620	-	1/1/15/20	6/39/115/115	-
26	BCR	b	627	-	-	0/29/63/63	0/2/2/2
28	GOL	B	634	-	-	0/4/4/4	-
28	GOL	C	524	-	-	1/4/4/4	-
24	CLA	c	508	41	1/1/15/20	8/39/115/115	-
28	GOL	v	201	-	-	1/4/4/4	-
29	LMT	m	103	-	-	7/21/61/61	0/2/2/2
25	PHO	D	401[B]	-	-	0/37/103/103	0/5/6/6
35	HTG	V	206	-	-	3/10/30/30	0/1/1/1
35	HTG	b	632	-	-	4/10/30/30	0/1/1/1
24	CLA	C	510	-	1/1/15/20	9/39/115/115	-
24	CLA	c	516	-	1/1/15/20	8/39/115/115	-
26	BCR	C	515	-	-	6/29/63/63	0/2/2/2
28	GOL	V	201	-	-	2/4/4/4	-
28	GOL	a	401	-	-	2/4/4/4	-

All (1642) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	a	411	PHO	C1B-C2B	9.46	1.49	1.39
25	D	401[B]	PHO	C1B-C2B	9.43	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	402[A]	PHO	C1B-C2B	9.38	1.49	1.39
25	d	402[B]	PHO	C1B-C2B	9.23	1.49	1.39
25	D	401[A]	PHO	C1D-C2D	9.11	1.49	1.39
25	A	408	PHO	C1D-C2D	9.02	1.49	1.39
25	d	402[A]	PHO	C1D-C2D	8.83	1.49	1.39
25	A	408	PHO	C1B-C2B	8.81	1.49	1.39
25	a	411	PHO	C1D-C2D	8.75	1.49	1.39
25	D	401[B]	PHO	C1D-C2D	8.75	1.49	1.39
25	D	401[A]	PHO	C1B-C2B	8.63	1.49	1.39
25	d	402[B]	PHO	C1D-C2D	8.59	1.48	1.39
25	D	401[A]	PHO	C3B-C4B	8.23	1.49	1.41
25	d	402[A]	PHO	C3B-C4B	8.14	1.49	1.41
25	D	401[B]	PHO	C3B-C4B	7.96	1.49	1.41
25	A	408	PHO	C3B-C4B	7.92	1.49	1.41
25	a	411	PHO	C3B-C4B	7.70	1.49	1.41
25	d	402[B]	PHO	C3B-C4B	7.59	1.49	1.41
25	D	401[A]	PHO	C4D-CHA	7.24	1.50	1.39
25	A	408	PHO	C4D-CHA	7.00	1.50	1.39
25	a	411	PHO	C4D-CHA	6.91	1.49	1.39
25	D	401[B]	PHO	C4D-CHA	6.77	1.49	1.39
25	d	402[B]	PHO	C4D-CHA	6.61	1.49	1.39
25	d	402[A]	PHO	C4D-CHA	6.60	1.49	1.39
25	d	402[B]	PHO	C3B-C2B	6.60	1.49	1.40
25	D	401[A]	PHO	C3B-C2B	6.47	1.49	1.40
25	A	408	PHO	C3B-C2B	6.42	1.49	1.40
25	D	401[B]	PHO	C3B-C2B	6.34	1.49	1.40
25	a	411	PHO	C3B-C2B	6.18	1.48	1.40
25	D	401[A]	PHO	C3D-C2D	5.89	1.49	1.39
25	a	411	PHO	C3D-C2D	5.87	1.49	1.39
25	d	402[A]	PHO	C3D-C2D	5.84	1.49	1.39
25	d	402[A]	PHO	C3B-C2B	5.84	1.48	1.40
25	a	411	PHO	OBD-CAD	5.83	1.30	1.22
24	B	603	CLA	C3C-C2C	5.66	1.49	1.36
24	B	611	CLA	C3C-C2C	5.66	1.49	1.36
24	B	604	CLA	C3C-C2C	5.59	1.48	1.36
24	b	624	CLA	C1D-ND	5.59	1.45	1.37
24	C	508	CLA	C3C-C2C	5.55	1.48	1.36
24	b	610	CLA	C3C-C2C	5.54	1.48	1.36
25	A	408	PHO	C3D-C2D	5.49	1.49	1.39
24	B	602	CLA	C3C-C2C	5.45	1.48	1.36
25	D	401[B]	PHO	C3D-C2D	5.42	1.48	1.39
24	A	406	CLA	C3C-C2C	5.38	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	516	CLA	C3C-C2C	5.38	1.48	1.36
24	C	512	CLA	C3C-C2C	5.36	1.48	1.36
24	B	616	CLA	O2D-CGD	5.36	1.46	1.33
24	C	510	CLA	C3C-C2C	5.36	1.48	1.36
24	b	611	CLA	C3C-C2C	5.35	1.48	1.36
38	f	101	HEM	FE-NB	5.35	2.11	1.94
24	C	503	CLA	C3C-C2C	5.33	1.48	1.36
24	A	405	CLA	C3C-C2C	5.31	1.48	1.36
24	c	517	CLA	C3C-C2C	5.30	1.48	1.36
24	B	614	CLA	C1D-ND	5.30	1.44	1.37
24	b	621	CLA	C3C-C2C	5.29	1.48	1.36
24	B	606	CLA	O2D-CGD	5.29	1.46	1.33
24	B	607	CLA	C3C-C2C	5.29	1.48	1.36
24	c	514	CLA	C3C-C2C	5.29	1.48	1.36
24	B	615	CLA	C3C-C2C	5.29	1.48	1.36
24	c	507	CLA	C1D-ND	5.28	1.44	1.37
24	C	501	CLA	C3C-C2C	5.28	1.48	1.36
24	C	507	CLA	C3C-C2C	5.28	1.48	1.36
24	b	615	CLA	C3C-C2C	5.28	1.48	1.36
24	a	412	CLA	C3C-C2C	5.28	1.48	1.36
24	a	409	CLA	C3C-C2C	5.27	1.48	1.36
26	C	514	BCR	C23-C22	-5.26	1.34	1.46
24	c	507	CLA	C3C-C2C	5.26	1.48	1.36
25	a	411	PHO	O2D-CGD	5.25	1.46	1.33
26	k	102	BCR	C23-C22	-5.24	1.34	1.46
24	a	412	CLA	O2D-CGD	5.24	1.46	1.33
24	B	617	CLA	C3C-C2C	5.24	1.48	1.36
24	C	503	CLA	CHC-C1C	5.24	1.49	1.38
24	b	619	CLA	C3C-C2C	5.23	1.48	1.36
24	b	618	CLA	O2D-CGD	5.23	1.46	1.33
24	b	622	CLA	C3C-C2C	5.23	1.48	1.36
24	C	513	CLA	C3C-C2C	5.21	1.48	1.36
24	D	404	CLA	C3C-C2C	5.21	1.48	1.36
24	B	615	CLA	O2D-CGD	5.20	1.46	1.33
24	b	617	CLA	C3C-C2C	5.19	1.48	1.36
24	b	622	CLA	O2D-CGD	5.19	1.46	1.33
24	b	620	CLA	O2D-CGD	5.19	1.46	1.33
24	b	624	CLA	C3C-C2C	5.18	1.47	1.36
24	C	509	CLA	C3C-C2C	5.18	1.47	1.36
24	A	407	CLA	C3C-C2C	5.17	1.47	1.36
24	c	506	CLA	C3C-C2C	5.17	1.47	1.36
24	c	506	CLA	O2D-CGD	5.16	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	405	CLA	C3C-C2C	5.16	1.47	1.36
24	d	403	CLA	C3C-C2C	5.16	1.47	1.36
24	c	513	CLA	C3C-C2C	5.15	1.47	1.36
24	C	501	CLA	CHC-C1C	5.15	1.48	1.38
24	d	405	CLA	O2D-CGD	5.15	1.45	1.33
24	c	510	CLA	O2D-CGD	5.15	1.45	1.33
24	B	602	CLA	O2D-CGD	5.15	1.45	1.33
24	C	505	CLA	C3C-C2C	5.14	1.47	1.36
26	Y	101	BCR	C23-C22	-5.14	1.35	1.46
24	c	509	CLA	C3C-C2C	5.13	1.47	1.36
24	C	504	CLA	C1D-ND	5.13	1.44	1.37
24	A	405	CLA	CHC-C1C	5.13	1.48	1.38
25	D	401[B]	PHO	O2D-CGD	5.13	1.45	1.33
24	B	607	CLA	O2D-CGD	5.13	1.45	1.33
24	b	614	CLA	C3C-C2C	5.13	1.47	1.36
24	B	610	CLA	C3C-C2C	5.11	1.47	1.36
24	B	612	CLA	C3C-C2C	5.11	1.47	1.36
24	c	516	CLA	CHC-C1C	5.09	1.48	1.38
24	B	609	CLA	C3C-C2C	5.09	1.47	1.36
24	B	617	CLA	O2D-CGD	5.09	1.45	1.33
24	c	512	CLA	C3C-C2C	5.08	1.47	1.36
24	C	504	CLA	C3C-C2C	5.08	1.47	1.36
24	b	616	CLA	O2D-CGD	5.08	1.45	1.33
24	B	616	CLA	CHC-C1C	5.06	1.48	1.38
26	t	102	BCR	C23-C22	-5.06	1.35	1.46
26	h	101	BCR	C23-C22	-5.05	1.35	1.46
24	B	614	CLA	O2D-CGD	5.05	1.45	1.33
24	A	409	CLA	O2D-CGD	5.04	1.45	1.33
24	A	405	CLA	C1D-ND	5.04	1.44	1.37
24	B	611	CLA	CHC-C1C	5.04	1.48	1.38
26	b	628	BCR	C23-C22	-5.04	1.35	1.46
24	B	611	CLA	C1D-ND	5.03	1.44	1.37
24	C	508	CLA	O2D-CGD	5.03	1.45	1.33
24	B	610	CLA	O2D-CGD	5.03	1.45	1.33
26	A	410	BCR	C23-C22	-5.03	1.35	1.46
26	K	101	BCR	C23-C22	-5.03	1.35	1.46
24	C	511	CLA	C1D-ND	5.03	1.44	1.37
24	b	621	CLA	O2D-CGD	5.02	1.45	1.33
24	C	510	CLA	O2D-CGD	5.02	1.45	1.33
24	c	511	CLA	CHC-C1C	5.02	1.48	1.38
24	B	608	CLA	CHC-C1C	5.02	1.48	1.38
24	C	504	CLA	CHC-C1C	5.02	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	405	CLA	C3C-C2C	5.01	1.47	1.36
24	b	617	CLA	CHC-C1C	5.00	1.48	1.38
24	b	617	CLA	O2D-CGD	5.00	1.45	1.33
24	d	404	CLA	C3C-C2C	5.00	1.47	1.36
24	c	507	CLA	O2D-CGD	4.99	1.45	1.33
24	C	503	CLA	C1D-ND	4.99	1.44	1.37
24	C	502	CLA	O2D-CGD	4.99	1.45	1.33
24	b	623	CLA	O2D-CGD	4.99	1.45	1.33
24	C	511	CLA	O2D-CGD	4.99	1.45	1.33
25	d	402[B]	PHO	O2D-CGD	4.98	1.45	1.33
25	D	401[B]	PHO	OBD-CAD	4.98	1.28	1.22
24	c	510	CLA	C3C-C2C	4.98	1.47	1.36
24	b	610	CLA	C1D-ND	4.98	1.44	1.37
25	D	401[A]	PHO	O2D-CGD	4.98	1.45	1.33
24	C	509	CLA	C1D-ND	4.98	1.44	1.37
24	B	606	CLA	C3C-C2C	4.98	1.47	1.36
24	C	509	CLA	O2D-CGD	4.97	1.45	1.33
24	c	505	CLA	O2D-CGD	4.97	1.45	1.33
24	c	505	CLA	C3C-C2C	4.97	1.47	1.36
24	b	612	CLA	C3C-C2C	4.97	1.47	1.36
24	b	625	CLA	CHC-C1C	4.97	1.48	1.38
24	b	623	CLA	C1D-ND	4.97	1.44	1.37
24	b	625	CLA	O2D-CGD	4.96	1.45	1.33
24	C	512	CLA	CHC-C1C	4.96	1.48	1.38
24	c	514	CLA	C1D-ND	4.96	1.44	1.37
24	C	511	CLA	C3C-C2C	4.96	1.47	1.36
24	c	511	CLA	C3C-C2C	4.96	1.47	1.36
25	d	402[B]	PHO	C3D-C2D	4.96	1.48	1.39
24	b	614	CLA	O2D-CGD	4.96	1.45	1.33
24	C	504	CLA	O2D-CGD	4.95	1.45	1.33
24	b	611	CLA	CHC-C1C	4.95	1.48	1.38
24	B	605	CLA	C3C-C2C	4.95	1.47	1.36
24	c	515	CLA	C3C-C2C	4.95	1.47	1.36
26	c	526	BCR	C23-C22	-4.95	1.35	1.46
24	a	410	CLA	C3C-C2C	4.95	1.47	1.36
24	B	613	CLA	CHC-C1C	4.95	1.48	1.38
24	C	512	CLA	O2D-CGD	4.95	1.45	1.33
24	C	506	CLA	O2D-CGD	4.95	1.45	1.33
24	b	623	CLA	C3C-C2C	4.94	1.47	1.36
24	b	613	CLA	C1D-ND	4.94	1.44	1.37
24	b	610	CLA	O2D-CGD	4.94	1.45	1.33
24	a	409	CLA	C1D-ND	4.94	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	515	BCR	C23-C22	-4.94	1.35	1.46
24	c	513	CLA	O2D-CGD	4.94	1.45	1.33
38	E	103	HEM	FE-NB	4.94	2.10	1.94
24	A	409	CLA	C3C-C2C	4.93	1.47	1.36
24	b	625	CLA	C3C-C2C	4.93	1.47	1.36
24	c	509	CLA	CHC-C1C	4.93	1.48	1.38
24	A	405	CLA	O2D-CGD	4.93	1.45	1.33
25	d	402[B]	PHO	OBD-CAD	4.93	1.28	1.22
24	c	508	CLA	O2D-CGD	4.92	1.45	1.33
24	C	502	CLA	C1D-ND	4.92	1.44	1.37
24	b	611	CLA	C1D-ND	4.92	1.44	1.37
24	b	612	CLA	O2D-CGD	4.92	1.45	1.33
24	b	622	CLA	C1D-ND	4.91	1.44	1.37
24	b	615	CLA	O2D-CGD	4.91	1.45	1.33
24	d	405	CLA	CHC-C1C	4.91	1.48	1.38
24	A	407	CLA	O2D-CGD	4.91	1.45	1.33
24	c	517	CLA	O2D-CGD	4.90	1.45	1.33
24	A	409	CLA	CHD-C1D	4.90	1.48	1.38
24	C	502	CLA	C3C-C2C	4.90	1.47	1.36
24	B	613	CLA	C3C-C2C	4.90	1.47	1.36
24	A	407	CLA	CHC-C1C	4.90	1.48	1.38
24	B	603	CLA	CHC-C1C	4.90	1.48	1.38
26	c	518	BCR	C23-C22	-4.88	1.35	1.46
25	A	408	PHO	O2D-CGD	4.88	1.45	1.33
26	y	101	BCR	C23-C22	-4.88	1.35	1.46
24	B	607	CLA	CHC-C1C	4.88	1.48	1.38
26	D	406	BCR	C23-C22	-4.87	1.35	1.46
24	C	510	CLA	C1D-ND	4.87	1.44	1.37
24	B	612	CLA	O2D-CGD	4.86	1.45	1.33
24	b	619	CLA	O2D-CGD	4.86	1.45	1.33
24	c	516	CLA	O2D-CGD	4.86	1.45	1.33
24	B	606	CLA	C1D-ND	4.86	1.44	1.37
24	b	620	CLA	C3C-C2C	4.86	1.47	1.36
24	B	614	CLA	C3C-C2C	4.86	1.47	1.36
24	B	609	CLA	O2D-CGD	4.85	1.45	1.33
24	C	513	CLA	O2D-CGD	4.85	1.45	1.33
26	H	101	BCR	C23-C22	-4.85	1.35	1.46
24	B	608	CLA	C1D-ND	4.85	1.44	1.37
24	C	505	CLA	CHC-C1C	4.85	1.48	1.38
24	b	610	CLA	CHC-C1C	4.84	1.48	1.38
24	c	512	CLA	CHC-C1C	4.84	1.48	1.38
26	T	103	BCR	C23-C22	-4.84	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	608	CLA	C3C-C2C	4.84	1.47	1.36
24	C	513	CLA	C1D-ND	4.84	1.44	1.37
26	d	406	BCR	C23-C22	-4.83	1.35	1.46
24	B	604	CLA	CHC-C1C	4.83	1.48	1.38
24	B	602	CLA	C1D-ND	4.83	1.44	1.37
24	B	602	CLA	O2A-CGA	4.82	1.47	1.33
24	c	507	CLA	CHC-C1C	4.81	1.48	1.38
24	d	403	CLA	C1D-ND	4.81	1.44	1.37
24	c	508	CLA	C3C-C2C	4.81	1.47	1.36
24	b	613	CLA	C3C-C2C	4.81	1.47	1.36
24	C	505	CLA	O2D-CGD	4.80	1.45	1.33
24	C	507	CLA	CHC-C1C	4.80	1.48	1.38
24	b	618	CLA	C3C-C2C	4.80	1.47	1.36
24	A	409	CLA	CHC-C1C	4.80	1.48	1.38
24	c	517	CLA	C1D-ND	4.79	1.44	1.37
24	B	605	CLA	C1D-ND	4.79	1.44	1.37
24	B	608	CLA	O2D-CGD	4.79	1.45	1.33
24	B	602	CLA	CHC-C1C	4.78	1.48	1.38
24	C	506	CLA	C3C-C2C	4.78	1.47	1.36
24	C	508	CLA	CHC-C1C	4.78	1.48	1.38
24	b	618	CLA	CHC-C1C	4.78	1.48	1.38
24	d	405	CLA	C1D-ND	4.77	1.44	1.37
24	b	616	CLA	CHC-C1C	4.77	1.48	1.38
24	A	406	CLA	C1D-ND	4.77	1.44	1.37
24	c	513	CLA	C1D-ND	4.77	1.44	1.37
24	c	512	CLA	O2D-CGD	4.76	1.44	1.33
24	b	616	CLA	C3C-C2C	4.76	1.47	1.36
24	c	511	CLA	O2D-CGD	4.76	1.44	1.33
26	B	620	BCR	C23-C22	-4.76	1.35	1.46
24	c	509	CLA	O2D-CGD	4.76	1.44	1.33
24	B	616	CLA	C3C-C2C	4.76	1.47	1.36
24	b	615	CLA	C1D-ND	4.76	1.44	1.37
24	b	618	CLA	C1D-ND	4.75	1.44	1.37
24	B	603	CLA	O2D-CGD	4.75	1.44	1.33
24	c	514	CLA	O2D-CGD	4.75	1.44	1.33
24	a	410	CLA	CHC-C1C	4.74	1.48	1.38
24	D	405	CLA	C1D-ND	4.74	1.44	1.37
24	d	403	CLA	O2D-CGD	4.74	1.44	1.33
24	C	502	CLA	CHC-C1C	4.74	1.48	1.38
24	d	404	CLA	O2D-CGD	4.74	1.44	1.33
25	d	402[A]	PHO	O2D-CGD	4.73	1.44	1.33
24	B	617	CLA	CHC-C1C	4.73	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	406	CLA	O2D-CGD	4.73	1.44	1.33
24	b	611	CLA	O2D-CGD	4.73	1.44	1.33
24	c	510	CLA	C1D-ND	4.72	1.44	1.37
26	B	618	BCR	C23-C22	-4.72	1.35	1.46
24	B	604	CLA	O2D-CGD	4.70	1.44	1.33
24	b	619	CLA	CHC-C1C	4.70	1.47	1.38
24	c	513	CLA	CHC-C1C	4.70	1.47	1.38
24	C	511	CLA	CHC-C1C	4.69	1.47	1.38
24	D	405	CLA	O2D-CGD	4.69	1.44	1.33
24	b	614	CLA	CHC-C1C	4.69	1.47	1.38
24	C	507	CLA	C1D-ND	4.69	1.44	1.37
24	C	513	CLA	CHC-C1C	4.69	1.47	1.38
24	B	613	CLA	O2D-CGD	4.69	1.44	1.33
24	b	623	CLA	CHC-C1C	4.68	1.47	1.38
24	C	512	CLA	C1D-ND	4.68	1.44	1.37
24	B	611	CLA	O2D-CGD	4.67	1.44	1.33
24	C	509	CLA	CHC-C1C	4.67	1.47	1.38
24	c	508	CLA	CHC-C1C	4.66	1.47	1.38
24	C	501	CLA	O2D-CGD	4.66	1.44	1.33
24	b	613	CLA	O2D-CGD	4.65	1.44	1.33
24	b	625	CLA	C1D-ND	4.65	1.44	1.37
24	C	508	CLA	CHD-C1D	4.65	1.47	1.38
24	c	517	CLA	CHC-C1C	4.64	1.47	1.38
24	c	505	CLA	CHC-C1C	4.64	1.47	1.38
24	C	501	CLA	C1D-ND	4.64	1.44	1.37
24	b	624	CLA	O2D-CGD	4.64	1.44	1.33
24	b	619	CLA	C1D-ND	4.63	1.43	1.37
24	C	508	CLA	C1D-ND	4.63	1.43	1.37
24	c	515	CLA	CHC-C1C	4.63	1.47	1.38
24	c	515	CLA	C1D-ND	4.63	1.43	1.37
24	c	515	CLA	O2D-CGD	4.62	1.44	1.33
26	b	627	BCR	C23-C22	-4.61	1.36	1.46
24	b	612	CLA	CHC-C1C	4.61	1.47	1.38
24	c	514	CLA	CHC-C1C	4.61	1.47	1.38
24	a	409	CLA	O2D-CGD	4.61	1.44	1.33
24	b	624	CLA	CHC-C1C	4.61	1.47	1.38
24	a	412	CLA	CHC-C1C	4.61	1.47	1.38
24	c	505	CLA	C1D-ND	4.60	1.43	1.37
24	c	513	CLA	CHD-C1D	4.60	1.47	1.38
24	B	615	CLA	CHC-C1C	4.59	1.47	1.38
24	B	609	CLA	C1D-ND	4.59	1.43	1.37
24	a	410	CLA	O2D-CGD	4.59	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	CHC-C1C	4.59	1.47	1.38
24	c	506	CLA	C1D-ND	4.59	1.43	1.37
24	B	608	CLA	CHD-C1D	4.58	1.47	1.38
24	B	616	CLA	C1D-ND	4.58	1.43	1.37
26	a	413	BCR	C23-C22	-4.58	1.36	1.46
24	c	512	CLA	C1D-ND	4.58	1.43	1.37
24	B	617	CLA	C1D-ND	4.56	1.43	1.37
24	a	409	CLA	CHC-C1C	4.56	1.47	1.38
26	b	626	BCR	C23-C22	-4.55	1.36	1.46
24	B	614	CLA	CHC-C1C	4.55	1.47	1.38
27	f	102	SQD	O47-C7	4.55	1.47	1.34
24	b	614	CLA	C1D-ND	4.55	1.43	1.37
24	b	616	CLA	O2A-CGA	4.54	1.46	1.33
36	D	408	DGD	O1G-C1A	4.54	1.46	1.33
33	z	101	LMG	O8-C28	4.54	1.46	1.33
24	B	606	CLA	CHC-C1C	4.54	1.47	1.38
24	C	506	CLA	CHC-C1C	4.53	1.47	1.38
27	a	405	SQD	O48-C23	4.52	1.46	1.33
24	B	604	CLA	C1D-ND	4.52	1.43	1.37
24	a	410	CLA	C1D-ND	4.52	1.43	1.37
24	C	506	CLA	C1D-ND	4.51	1.43	1.37
24	D	405	CLA	CHC-C1C	4.51	1.47	1.38
24	C	507	CLA	O2D-CGD	4.51	1.44	1.33
24	b	615	CLA	CHC-C1C	4.50	1.47	1.38
25	D	401[A]	PHO	OBD-CAD	4.50	1.28	1.22
24	b	610	CLA	O2A-CGA	4.50	1.46	1.33
24	b	613	CLA	CHC-C1C	4.49	1.47	1.38
24	A	409	CLA	C1D-ND	4.49	1.43	1.37
27	A	413	SQD	O48-C23	4.49	1.46	1.33
24	C	508	CLA	O2A-CGA	4.48	1.46	1.33
24	b	622	CLA	CHD-C1D	4.48	1.47	1.38
24	c	514	CLA	CHD-C1D	4.48	1.47	1.38
24	B	615	CLA	C1D-ND	4.48	1.43	1.37
24	c	511	CLA	C1D-ND	4.48	1.43	1.37
24	b	610	CLA	CHD-C1D	4.47	1.47	1.38
24	B	611	CLA	CHD-C1D	4.47	1.47	1.38
24	b	621	CLA	CHC-C1C	4.46	1.47	1.38
24	C	510	CLA	CHC-C1C	4.46	1.47	1.38
24	c	506	CLA	CHD-C1D	4.46	1.47	1.38
24	c	506	CLA	CHC-C1C	4.46	1.47	1.38
24	C	509	CLA	O2A-CGA	4.46	1.46	1.33
36	e	101	DGD	O2G-C1B	4.46	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	619	BCR	C23-C22	-4.46	1.36	1.46
24	b	623	CLA	CHD-C1D	4.45	1.47	1.38
24	B	610	CLA	CHD-C1D	4.45	1.47	1.38
24	C	503	CLA	O2D-CGD	4.45	1.44	1.33
27	F	101	SQD	O47-C7	4.45	1.46	1.34
24	c	512	CLA	O2A-CGA	4.45	1.46	1.33
24	c	510	CLA	CHD-C1D	4.44	1.47	1.38
24	d	405	CLA	O2A-CGA	4.44	1.46	1.33
24	C	513	CLA	CHD-C1D	4.44	1.47	1.38
24	c	513	CLA	O2A-CGA	4.43	1.46	1.33
24	c	508	CLA	C1D-ND	4.43	1.43	1.37
24	B	610	CLA	CHC-C1C	4.43	1.47	1.38
24	d	403	CLA	O2A-CGA	4.42	1.46	1.33
27	a	405	SQD	O47-C7	4.42	1.46	1.34
24	b	611	CLA	CHD-C1D	4.41	1.47	1.38
24	c	510	CLA	CHC-C1C	4.41	1.47	1.38
24	C	509	CLA	CHD-C1D	4.41	1.47	1.38
24	b	624	CLA	CHD-C1D	4.40	1.47	1.38
24	B	605	CLA	CHC-C1C	4.40	1.47	1.38
24	C	510	CLA	CHD-C1D	4.39	1.47	1.38
37	D	411	LHG	O7-C7	4.39	1.46	1.34
36	D	408	DGD	O2G-C1B	4.39	1.46	1.34
33	C	519	LMG	O8-C28	4.39	1.46	1.33
24	b	624	CLA	O2A-CGA	4.39	1.46	1.33
24	C	506	CLA	CHD-C1D	4.38	1.47	1.38
24	c	516	CLA	CHD-C1D	4.38	1.47	1.38
24	B	615	CLA	O2A-CGA	4.37	1.46	1.33
24	b	621	CLA	C1D-ND	4.36	1.43	1.37
24	B	604	CLA	O2A-CGA	4.36	1.46	1.33
24	B	610	CLA	C1D-ND	4.36	1.43	1.37
24	B	606	CLA	CHD-C1D	4.35	1.46	1.38
24	a	410	CLA	O2A-CGA	4.35	1.46	1.33
24	B	603	CLA	CHD-C1D	4.35	1.46	1.38
24	D	404	CLA	O2A-CGA	4.35	1.46	1.33
37	a	420	LHG	O8-C23	4.35	1.46	1.33
24	b	615	CLA	O2A-CGA	4.35	1.46	1.33
37	D	411	LHG	O8-C23	4.35	1.46	1.33
24	b	622	CLA	CHC-C1C	4.34	1.47	1.38
37	E	101	LHG	O8-C23	4.34	1.46	1.33
24	D	404	CLA	O2D-CGD	4.34	1.43	1.33
36	e	101	DGD	O1G-C1A	4.34	1.46	1.33
24	b	616	CLA	C1D-ND	4.33	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	CHD-C1D	4.33	1.46	1.38
33	C	520	LMG	O7-C10	4.33	1.46	1.34
36	C	518	DGD	O1G-C1A	4.32	1.45	1.33
24	A	405	CLA	CHD-C1D	4.32	1.46	1.38
24	B	607	CLA	O2A-CGA	4.32	1.45	1.33
24	b	612	CLA	C1D-ND	4.32	1.43	1.37
24	C	511	CLA	CHD-C4C	4.32	1.49	1.39
40	v	206	HEC	CAC-C3C	4.32	1.49	1.35
24	C	504	CLA	CHD-C1D	4.31	1.46	1.38
24	b	625	CLA	CHD-C1D	4.31	1.46	1.38
24	b	621	CLA	CHB-C1B	4.31	1.49	1.39
27	f	102	SQD	O48-C23	4.30	1.45	1.33
24	B	606	CLA	O2A-CGA	4.30	1.45	1.33
36	c	521	DGD	O1G-C1A	4.30	1.45	1.33
24	b	620	CLA	O2A-CGA	4.30	1.45	1.33
24	c	516	CLA	C1D-ND	4.30	1.43	1.37
24	a	409	CLA	CHD-C1D	4.30	1.46	1.38
24	b	625	CLA	O2A-CGA	4.30	1.45	1.33
24	B	609	CLA	O2A-CGA	4.29	1.45	1.33
24	B	616	CLA	C3D-C2D	4.29	1.50	1.39
24	B	617	CLA	O2A-CGA	4.29	1.45	1.33
24	C	506	CLA	O2A-CGA	4.29	1.45	1.33
24	c	511	CLA	O2A-CGA	4.28	1.45	1.33
24	C	512	CLA	O2A-CGA	4.28	1.45	1.33
27	B	621	SQD	O47-C7	4.28	1.46	1.34
24	b	617	CLA	CHD-C1D	4.28	1.46	1.38
27	L	102	SQD	O47-C7	4.28	1.46	1.34
24	C	510	CLA	O2A-CGA	4.28	1.45	1.33
24	c	517	CLA	O2A-CGA	4.27	1.45	1.33
24	C	513	CLA	CHD-C4C	4.27	1.48	1.39
24	d	403	CLA	CHD-C4C	4.27	1.48	1.39
24	C	502	CLA	CHD-C1D	4.27	1.46	1.38
24	C	507	CLA	CHD-C1D	4.27	1.46	1.38
40	V	205	HEC	CBC-CAC	-4.27	1.33	1.49
24	A	407	CLA	CHD-C1D	4.27	1.46	1.38
33	d	415	LMG	O8-C28	4.27	1.45	1.33
24	B	616	CLA	CHC-C4B	4.26	1.49	1.39
40	v	206	HEC	CBC-CAC	-4.26	1.33	1.49
24	B	605	CLA	O2D-CGD	4.26	1.43	1.33
24	A	406	CLA	O2A-CGA	4.26	1.45	1.33
24	C	507	CLA	O2A-CGA	4.25	1.45	1.33
38	E	103	HEM	FE-NC	4.25	2.09	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C1D-ND	4.25	1.43	1.37
25	A	408	PHO	OBD-CAD	4.25	1.27	1.22
24	D	404	CLA	C1D-ND	4.25	1.43	1.37
25	d	402[B]	PHO	O2A-CGA	4.25	1.45	1.33
36	H	102	DGD	O1G-C1A	4.24	1.45	1.33
33	M	101	LMG	O8-C28	4.24	1.45	1.33
24	C	501	CLA	CHD-C1D	4.24	1.46	1.38
24	C	503	CLA	O2A-CGA	4.24	1.45	1.33
24	B	610	CLA	O2A-CGA	4.24	1.45	1.33
24	b	610	CLA	C3D-C2D	4.24	1.50	1.39
24	B	611	CLA	CHD-C4C	4.24	1.48	1.39
24	d	403	CLA	CHC-C1C	4.24	1.47	1.38
24	d	404	CLA	O2A-CGA	4.23	1.45	1.33
24	c	516	CLA	O2A-CGA	4.23	1.45	1.33
24	b	613	CLA	CHD-C1D	4.23	1.46	1.38
24	B	607	CLA	C1D-ND	4.23	1.43	1.37
33	c	522	LMG	O8-C28	4.23	1.45	1.33
24	C	511	CLA	CHD-C1D	4.23	1.46	1.38
24	c	516	CLA	CHD-C4C	4.23	1.48	1.39
24	b	623	CLA	CHD-C4C	4.23	1.48	1.39
24	c	515	CLA	O2A-CGA	4.23	1.45	1.33
24	b	612	CLA	O2A-CGA	4.22	1.45	1.33
27	L	102	SQD	O48-C23	4.22	1.45	1.33
24	a	412	CLA	C1D-ND	4.22	1.43	1.37
24	b	620	CLA	CHD-C1D	4.22	1.46	1.38
24	b	618	CLA	O2A-CGA	4.22	1.45	1.33
24	c	509	CLA	O2A-CGA	4.21	1.45	1.33
40	V	205	HEC	CAB-C3B	4.21	1.48	1.35
24	C	503	CLA	CHD-C1D	4.21	1.46	1.38
24	B	608	CLA	O2A-CGA	4.21	1.45	1.33
24	D	405	CLA	CHD-C1D	4.21	1.46	1.38
24	c	507	CLA	CHD-C1D	4.21	1.46	1.38
33	A	419	LMG	O7-C10	4.21	1.46	1.34
24	C	510	CLA	CHD-C4C	4.21	1.48	1.39
24	C	511	CLA	C3D-C2D	4.21	1.50	1.39
40	V	205	HEC	CAC-C3C	4.20	1.48	1.35
24	b	622	CLA	CHD-C4C	4.20	1.48	1.39
37	E	101	LHG	O7-C7	4.20	1.46	1.34
24	B	602	CLA	CHD-C1D	4.20	1.46	1.38
24	C	501	CLA	O2A-CGA	4.19	1.45	1.33
24	C	504	CLA	CHD-C4C	4.19	1.48	1.39
24	c	506	CLA	O2A-CGA	4.19	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	607	CLA	CHD-C1D	4.19	1.46	1.38
33	A	419	LMG	O8-C28	4.19	1.45	1.33
24	B	617	CLA	CHD-C1D	4.19	1.46	1.38
24	B	612	CLA	CHC-C1C	4.18	1.46	1.38
24	C	512	CLA	CHD-C1D	4.18	1.46	1.38
33	a	415	LMG	O8-C28	4.18	1.45	1.33
36	C	518	DGD	O2G-C1B	4.18	1.46	1.34
24	D	405	CLA	O2A-CGA	4.18	1.45	1.33
24	b	619	CLA	CHD-C1D	4.18	1.46	1.38
24	B	603	CLA	C1D-ND	4.18	1.43	1.37
36	H	102	DGD	O2G-C1B	4.17	1.46	1.34
24	b	618	CLA	OBD-CAD	4.17	1.29	1.22
37	L	101	LHG	O8-C23	4.17	1.45	1.33
24	a	412	CLA	O2A-CGA	4.17	1.45	1.33
24	b	624	CLA	C3D-C2D	4.17	1.50	1.39
24	A	405	CLA	C3D-C2D	4.17	1.50	1.39
24	C	512	CLA	C3D-C2D	4.17	1.50	1.39
40	V	205	HEC	CBB-CAB	-4.16	1.34	1.49
24	c	514	CLA	CHD-C4C	4.16	1.48	1.39
38	f	101	HEM	FE-NC	4.16	2.08	1.95
24	a	409	CLA	CHD-C4C	4.16	1.48	1.39
37	a	420	LHG	O7-C7	4.16	1.46	1.34
33	C	520	LMG	O8-C28	4.15	1.45	1.33
33	c	522	LMG	O7-C10	4.15	1.46	1.34
24	B	614	CLA	C3D-C2D	4.15	1.50	1.39
24	A	405	CLA	CHD-C4C	4.15	1.48	1.39
24	C	504	CLA	O2A-CGA	4.15	1.45	1.33
24	c	510	CLA	CHD-C4C	4.15	1.48	1.39
24	A	406	CLA	CHC-C1C	4.15	1.46	1.38
24	C	504	CLA	C3D-C2D	4.14	1.50	1.39
24	b	610	CLA	CHD-C4C	4.14	1.48	1.39
24	C	513	CLA	O2A-CGA	4.14	1.45	1.33
33	d	415	LMG	O7-C10	4.14	1.46	1.34
24	c	510	CLA	O2A-CGA	4.14	1.45	1.33
24	C	505	CLA	CHD-C1D	4.14	1.46	1.38
24	c	516	CLA	C3D-C2D	4.14	1.50	1.39
24	C	503	CLA	CHC-C4B	4.14	1.48	1.39
24	B	603	CLA	OBD-CAD	4.14	1.29	1.22
25	d	402[A]	PHO	OBD-CAD	4.14	1.27	1.22
24	d	405	CLA	CHD-C1D	4.14	1.46	1.38
36	c	520	DGD	O1G-C1A	4.14	1.45	1.33
24	A	407	CLA	C1D-ND	4.13	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	CHC-C1C	4.13	1.46	1.38
24	c	509	CLA	C1D-ND	4.13	1.43	1.37
25	d	402[A]	PHO	O2A-CGA	4.13	1.45	1.33
24	B	609	CLA	CHD-C1D	4.12	1.46	1.38
24	C	503	CLA	CHD-C4C	4.12	1.48	1.39
27	F	101	SQD	O48-C23	4.12	1.45	1.33
24	c	514	CLA	CHB-C1B	4.12	1.48	1.39
24	c	505	CLA	O2A-CGA	4.12	1.45	1.33
24	a	410	CLA	CHD-C1D	4.12	1.46	1.38
24	B	608	CLA	CHD-C4C	4.12	1.48	1.39
24	c	513	CLA	CHD-C4C	4.11	1.48	1.39
40	v	206	HEC	CBB-CAB	-4.11	1.34	1.49
24	d	405	CLA	C3D-C2D	4.11	1.50	1.39
24	d	403	CLA	CHD-C1D	4.11	1.46	1.38
33	z	101	LMG	O7-C10	4.11	1.45	1.34
24	b	613	CLA	O2A-CGA	4.11	1.45	1.33
24	b	623	CLA	O2A-CGA	4.11	1.45	1.33
36	h	102	DGD	O2G-C1B	4.11	1.45	1.34
24	B	611	CLA	CHC-C4B	4.10	1.48	1.39
24	B	604	CLA	CHD-C1D	4.10	1.46	1.38
37	b	634	LHG	O7-C7	4.10	1.45	1.34
24	c	505	CLA	CHD-C1D	4.09	1.46	1.38
24	C	502	CLA	C3D-C2D	4.09	1.50	1.39
24	B	612	CLA	CHD-C1D	4.09	1.46	1.38
25	D	401[B]	PHO	O2A-CGA	4.09	1.45	1.33
33	M	101	LMG	O7-C10	4.09	1.45	1.34
24	C	511	CLA	O2A-CGA	4.09	1.45	1.33
24	d	404	CLA	CHD-C1D	4.08	1.46	1.38
24	b	617	CLA	O2A-CGA	4.08	1.45	1.33
24	C	509	CLA	CHD-C4C	4.08	1.48	1.39
24	b	611	CLA	O2A-CGA	4.08	1.45	1.33
24	B	605	CLA	CHD-C1D	4.08	1.46	1.38
33	Z	101	LMG	O7-C10	4.08	1.45	1.34
37	D	409	LHG	O8-C23	4.08	1.45	1.33
24	b	616	CLA	CHD-C1D	4.07	1.46	1.38
24	A	409	CLA	O2A-CGA	4.07	1.45	1.33
24	B	612	CLA	O2A-CGA	4.07	1.45	1.33
24	b	621	CLA	OBD-CAD	4.06	1.29	1.22
24	C	506	CLA	C3D-C2D	4.06	1.50	1.39
24	B	612	CLA	C1D-ND	4.06	1.43	1.37
37	b	634	LHG	O8-C23	4.06	1.45	1.33
24	c	517	CLA	CHD-C1D	4.05	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	514	CLA	O2A-CGA	4.04	1.45	1.33
24	A	409	CLA	CHD-C4C	4.04	1.48	1.39
24	c	515	CLA	CHD-C4C	4.04	1.48	1.39
24	b	619	CLA	CHD-C4C	4.04	1.48	1.39
33	k	101	LMG	O8-C28	4.03	1.45	1.33
24	B	609	CLA	CHD-C4C	4.03	1.48	1.39
24	b	618	CLA	CHB-C1B	4.03	1.48	1.39
24	C	502	CLA	O2A-CGA	4.03	1.45	1.33
27	A	411	SQD	O48-C23	4.03	1.45	1.33
24	A	407	CLA	CHD-C4C	4.03	1.48	1.39
36	C	517	DGD	O1G-C1A	4.02	1.45	1.33
37	d	410	LHG	O7-C7	4.02	1.45	1.34
24	c	512	CLA	C3D-C2D	4.02	1.50	1.39
24	b	617	CLA	CHC-C4B	4.02	1.48	1.39
24	C	507	CLA	CHD-C4C	4.02	1.48	1.39
27	a	414	SQD	O48-C23	4.02	1.45	1.33
24	A	406	CLA	C3D-C2D	4.02	1.50	1.39
24	b	617	CLA	C3D-C2D	4.02	1.50	1.39
24	c	505	CLA	CHD-C4C	4.02	1.48	1.39
24	c	517	CLA	CHD-C4C	4.02	1.48	1.39
24	c	508	CLA	O2A-CGA	4.01	1.45	1.33
24	B	616	CLA	O2A-CGA	4.01	1.45	1.33
37	D	410	LHG	O7-C7	4.01	1.45	1.34
24	a	410	CLA	OBD-CAD	4.01	1.29	1.22
24	B	612	CLA	C3D-C2D	4.01	1.49	1.39
24	b	618	CLA	CHD-C4C	4.01	1.48	1.39
27	B	621	SQD	O48-C23	4.01	1.45	1.33
24	b	611	CLA	CHD-C4C	4.00	1.48	1.39
36	h	102	DGD	O1G-C1A	4.00	1.45	1.33
24	C	508	CLA	CHD-C4C	4.00	1.48	1.39
24	c	509	CLA	CHD-C1D	4.00	1.46	1.38
24	C	501	CLA	CHC-C4B	4.00	1.48	1.39
27	A	413	SQD	O47-C7	4.00	1.45	1.34
36	C	516	DGD	O2G-C1B	3.99	1.45	1.34
33	D	415	LMG	O7-C10	3.99	1.45	1.34
40	v	206	HEC	CAB-C3B	3.99	1.48	1.35
24	B	606	CLA	CHD-C4C	3.99	1.48	1.39
24	c	508	CLA	CHD-C1D	3.99	1.46	1.38
24	c	506	CLA	CHD-C4C	3.99	1.48	1.39
33	b	629	LMG	O7-C10	3.99	1.45	1.34
37	d	409	LHG	O7-C7	3.99	1.45	1.34
24	C	511	CLA	CHB-C1B	3.99	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	615	CLA	C3D-C2D	3.99	1.49	1.39
24	c	509	CLA	CHB-C1B	3.99	1.48	1.39
24	A	405	CLA	O2A-CGA	3.99	1.45	1.33
24	B	614	CLA	CHD-C4C	3.99	1.48	1.39
37	d	410	LHG	O8-C23	3.98	1.45	1.33
24	C	507	CLA	CHC-C4B	3.98	1.48	1.39
24	b	611	CLA	OBD-CAD	3.98	1.29	1.22
24	a	409	CLA	C3D-C2D	3.98	1.49	1.39
24	b	625	CLA	C3D-C2D	3.98	1.49	1.39
37	D	410	LHG	O8-C23	3.98	1.44	1.33
24	B	603	CLA	O2A-CGA	3.98	1.44	1.33
24	b	613	CLA	C3D-C2D	3.98	1.49	1.39
24	c	507	CLA	O2A-CGA	3.98	1.44	1.33
24	C	505	CLA	C1D-ND	3.97	1.43	1.37
24	b	624	CLA	CHD-C4C	3.97	1.48	1.39
24	b	622	CLA	CHB-C1B	3.97	1.48	1.39
24	b	621	CLA	O2A-CGA	3.97	1.44	1.33
24	d	404	CLA	C3D-C2D	3.97	1.49	1.39
24	c	515	CLA	CHD-C1D	3.97	1.46	1.38
24	C	503	CLA	C3D-C2D	3.97	1.49	1.39
24	C	510	CLA	C3D-C2D	3.96	1.49	1.39
24	B	602	CLA	CHD-C4C	3.96	1.48	1.39
24	B	610	CLA	C3D-C2D	3.96	1.49	1.39
25	D	401[A]	PHO	O2A-CGA	3.96	1.44	1.33
24	a	412	CLA	CHD-C4C	3.96	1.48	1.39
35	B	622	HTG	C1'-S1	-3.95	1.75	1.81
24	c	506	CLA	C3D-C2D	3.95	1.49	1.39
24	B	614	CLA	OBD-CAD	3.95	1.29	1.22
24	b	615	CLA	CHD-C1D	3.95	1.46	1.38
27	A	411	SQD	O47-C7	3.95	1.45	1.34
24	B	604	CLA	CHD-C4C	3.95	1.48	1.39
24	B	614	CLA	CHD-C1D	3.95	1.46	1.38
24	b	625	CLA	CHD-C4C	3.94	1.48	1.39
24	B	611	CLA	OBD-CAD	3.94	1.29	1.22
24	c	508	CLA	CHD-C4C	3.94	1.48	1.39
36	c	519	DGD	O2G-C1B	3.94	1.45	1.34
24	B	609	CLA	CHC-C1C	3.94	1.46	1.38
24	C	501	CLA	C3D-C2D	3.94	1.49	1.39
24	B	614	CLA	O2A-CGA	3.94	1.44	1.33
24	b	621	CLA	CHD-C1D	3.93	1.46	1.38
24	B	613	CLA	O2A-CGA	3.93	1.44	1.33
24	c	511	CLA	CHD-C1D	3.93	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	CHD-C4C	3.93	1.48	1.39
24	b	625	CLA	CHB-C1B	3.93	1.48	1.39
24	c	508	CLA	C3D-C2D	3.92	1.49	1.39
24	c	511	CLA	C3D-C2D	3.92	1.49	1.39
24	C	506	CLA	CHD-C4C	3.92	1.48	1.39
24	C	505	CLA	O2A-CGA	3.92	1.44	1.33
24	C	512	CLA	CHD-C4C	3.92	1.48	1.39
33	D	415	LMG	O8-C28	3.91	1.44	1.33
24	b	617	CLA	CHD-C4C	3.91	1.48	1.39
24	C	509	CLA	CHB-C1B	3.91	1.48	1.39
24	c	512	CLA	CHD-C1D	3.91	1.46	1.38
33	a	415	LMG	O7-C10	3.91	1.45	1.34
36	C	516	DGD	O1G-C1A	3.90	1.44	1.33
24	b	619	CLA	OBD-CAD	3.90	1.29	1.22
24	B	611	CLA	O2A-CGA	3.90	1.44	1.33
24	B	613	CLA	C3D-C2D	3.90	1.49	1.39
24	b	612	CLA	CHD-C1D	3.89	1.46	1.38
24	B	606	CLA	CHB-C1B	3.89	1.48	1.39
24	C	510	CLA	CHB-C1B	3.89	1.48	1.39
24	c	517	CLA	C3D-C2D	3.89	1.49	1.39
24	b	614	CLA	C3D-C2D	3.88	1.49	1.39
24	B	613	CLA	OBD-CAD	3.88	1.29	1.22
24	c	509	CLA	CHC-C4B	3.88	1.48	1.39
33	C	519	LMG	O7-C10	3.88	1.45	1.34
24	b	620	CLA	CHB-C1B	3.88	1.48	1.39
24	b	618	CLA	C3D-C2D	3.88	1.49	1.39
24	b	612	CLA	C3D-C2D	3.88	1.49	1.39
24	C	509	CLA	C3D-C2D	3.88	1.49	1.39
24	c	512	CLA	CHB-C1B	3.87	1.48	1.39
36	C	517	DGD	O2G-C1B	3.87	1.45	1.34
24	b	623	CLA	C3D-C2D	3.87	1.49	1.39
24	B	615	CLA	CHD-C1D	3.87	1.46	1.38
24	c	516	CLA	OBD-CAD	3.87	1.29	1.22
25	A	408	PHO	O2A-CGA	3.87	1.44	1.33
24	c	513	CLA	C3D-C2D	3.87	1.49	1.39
24	D	404	CLA	CHC-C1C	3.87	1.46	1.38
24	B	607	CLA	CHC-C4B	3.87	1.48	1.39
36	c	521	DGD	O2G-C1B	3.86	1.45	1.34
24	D	404	CLA	CHD-C1D	3.86	1.45	1.38
24	d	404	CLA	C1B-NB	-3.86	1.32	1.37
24	c	509	CLA	CHD-C4C	3.86	1.48	1.39
24	C	502	CLA	CHB-C1B	3.86	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	610	CLA	CHD-C4C	3.86	1.48	1.39
24	B	602	CLA	CHB-C1B	3.86	1.48	1.39
24	d	403	CLA	C3D-C2D	3.86	1.49	1.39
24	b	614	CLA	CHD-C1D	3.86	1.45	1.38
24	B	610	CLA	CHB-C1B	3.86	1.48	1.39
24	c	513	CLA	OBD-CAD	3.86	1.29	1.22
33	b	629	LMG	O8-C28	3.86	1.44	1.33
24	C	507	CLA	C3D-C2D	3.85	1.49	1.39
24	a	412	CLA	CHD-C1D	3.85	1.45	1.38
24	D	405	CLA	CHD-C4C	3.85	1.48	1.39
36	c	520	DGD	O2G-C1B	3.85	1.45	1.34
25	a	411	PHO	O2A-CGA	3.85	1.44	1.33
24	C	505	CLA	CHD-C4C	3.85	1.48	1.39
24	C	501	CLA	CHD-C4C	3.85	1.48	1.39
24	b	615	CLA	C3D-C2D	3.85	1.49	1.39
24	c	511	CLA	CHD-C4C	3.85	1.48	1.39
24	A	406	CLA	CHD-C4C	3.85	1.48	1.39
24	b	614	CLA	O2A-CGA	3.85	1.44	1.33
24	C	508	CLA	C3D-C2D	3.85	1.49	1.39
24	B	608	CLA	CHC-C4B	3.84	1.48	1.39
36	c	519	DGD	O1G-C1A	3.84	1.44	1.33
24	B	612	CLA	CHD-C4C	3.84	1.47	1.39
24	C	513	CLA	C3D-C2D	3.84	1.49	1.39
24	B	605	CLA	O2A-CGA	3.84	1.44	1.33
24	D	405	CLA	C3D-C2D	3.84	1.49	1.39
24	c	505	CLA	CHB-C1B	3.84	1.48	1.39
24	c	511	CLA	CHC-C4B	3.84	1.48	1.39
24	c	507	CLA	C3D-C2D	3.84	1.49	1.39
24	A	405	CLA	OBD-CAD	3.83	1.29	1.22
24	b	617	CLA	OBD-CAD	3.83	1.29	1.22
24	B	603	CLA	CHC-C4B	3.83	1.48	1.39
24	d	404	CLA	CHD-C4C	3.83	1.47	1.39
24	B	606	CLA	CHC-C4B	3.83	1.48	1.39
24	C	513	CLA	CHC-C4B	3.83	1.48	1.39
24	c	514	CLA	CHC-C4B	3.82	1.48	1.39
24	B	602	CLA	C3D-C2D	3.82	1.49	1.39
24	b	617	CLA	CHB-C1B	3.82	1.48	1.39
24	B	603	CLA	C3D-C2D	3.82	1.49	1.39
24	b	621	CLA	C3D-C2D	3.82	1.49	1.39
24	C	502	CLA	CHD-C4C	3.82	1.47	1.39
24	B	609	CLA	C3D-C2D	3.82	1.49	1.39
24	B	613	CLA	CHB-C1B	3.82	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	616	CLA	C3D-C2D	3.82	1.49	1.39
24	b	623	CLA	CHB-C1B	3.82	1.48	1.39
24	b	613	CLA	CHB-C1B	3.81	1.48	1.39
24	A	406	CLA	OBD-CAD	3.81	1.29	1.22
24	A	409	CLA	C3D-C2D	3.81	1.49	1.39
24	B	604	CLA	CHC-C4B	3.81	1.48	1.39
24	b	622	CLA	O2A-CGA	3.81	1.44	1.33
24	A	407	CLA	C3D-C2D	3.81	1.49	1.39
24	D	404	CLA	CHD-C4C	3.81	1.47	1.39
24	c	513	CLA	CHB-C1B	3.80	1.47	1.39
24	C	512	CLA	CHC-C4B	3.80	1.47	1.39
37	L	101	LHG	O7-C7	3.79	1.45	1.34
24	a	412	CLA	C3D-C2D	3.79	1.49	1.39
33	k	101	LMG	O7-C10	3.79	1.45	1.34
24	b	614	CLA	CHD-C4C	3.79	1.47	1.39
24	C	510	CLA	CHC-C4B	3.79	1.47	1.39
24	c	509	CLA	OBD-CAD	3.79	1.29	1.22
24	B	611	CLA	CHB-C1B	3.79	1.47	1.39
24	B	617	CLA	C3D-C2D	3.79	1.49	1.39
24	B	613	CLA	CHD-C1D	3.79	1.45	1.38
37	d	408	LHG	O8-C23	3.79	1.44	1.33
24	c	505	CLA	C3D-C2D	3.79	1.49	1.39
27	a	414	SQD	O47-C7	3.78	1.45	1.34
24	a	410	CLA	CHD-C4C	3.78	1.47	1.39
24	c	515	CLA	C3D-C2D	3.78	1.49	1.39
35	b	632	HTG	C1'-S1	-3.78	1.76	1.81
24	B	603	CLA	CHD-C4C	3.77	1.47	1.39
24	b	625	CLA	CHC-C4B	3.77	1.47	1.39
24	B	611	CLA	C3D-C2D	3.77	1.49	1.39
24	D	405	CLA	CHB-C1B	3.76	1.47	1.39
24	b	619	CLA	O2A-CGA	3.76	1.44	1.33
24	C	505	CLA	CHB-C1B	3.76	1.47	1.39
24	C	501	CLA	OBD-CAD	3.76	1.28	1.22
24	a	409	CLA	O2A-CGA	3.75	1.44	1.33
24	A	407	CLA	CHC-C4B	3.75	1.47	1.39
24	C	509	CLA	CHC-C4B	3.75	1.47	1.39
24	A	407	CLA	O2A-CGA	3.75	1.44	1.33
24	c	514	CLA	OBD-CAD	3.75	1.28	1.22
24	c	517	CLA	CHC-C4B	3.75	1.47	1.39
24	b	622	CLA	C3D-C2D	3.74	1.49	1.39
24	A	409	CLA	CHC-C4B	3.74	1.47	1.39
24	B	614	CLA	CHB-C1B	3.74	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	620	CLA	C3D-C2D	3.74	1.49	1.39
24	B	615	CLA	OBD-CAD	3.74	1.28	1.22
24	C	511	CLA	OBD-CAD	3.74	1.28	1.22
24	d	404	CLA	CHC-C4B	3.74	1.47	1.39
24	b	619	CLA	CHC-C4B	3.73	1.47	1.39
24	b	619	CLA	C1B-NB	-3.73	1.33	1.37
24	b	615	CLA	OBD-CAD	3.73	1.28	1.22
24	a	410	CLA	CHB-C1B	3.73	1.47	1.39
24	B	616	CLA	CHD-C1D	3.73	1.45	1.38
24	B	602	CLA	CHC-C4B	3.73	1.47	1.39
24	B	605	CLA	CHD-C4C	3.72	1.47	1.39
24	B	616	CLA	CHB-C1B	3.72	1.47	1.39
24	C	505	CLA	CHC-C4B	3.72	1.47	1.39
24	C	501	CLA	CHB-C1B	3.72	1.47	1.39
24	D	404	CLA	C3D-C2D	3.72	1.49	1.39
24	d	405	CLA	CHC-C4B	3.72	1.47	1.39
24	c	516	CLA	CHC-C4B	3.71	1.47	1.39
24	B	602	CLA	OBD-CAD	3.71	1.28	1.22
24	C	503	CLA	OBD-CAD	3.71	1.28	1.22
24	b	615	CLA	CHB-C1B	3.71	1.47	1.39
24	b	615	CLA	CHD-C4C	3.71	1.47	1.39
24	b	610	CLA	CHC-C4B	3.71	1.47	1.39
24	b	624	CLA	CHB-C1B	3.70	1.47	1.39
24	c	514	CLA	C3D-C2D	3.70	1.49	1.39
24	B	608	CLA	CHB-C1B	3.70	1.47	1.39
24	b	612	CLA	CHB-C1B	3.69	1.47	1.39
24	c	506	CLA	CHB-C1B	3.69	1.47	1.39
24	d	405	CLA	CHD-C4C	3.69	1.47	1.39
24	C	510	CLA	OBD-CAD	3.69	1.28	1.22
24	b	616	CLA	OBD-CAD	3.69	1.28	1.22
24	b	613	CLA	CHD-C4C	3.68	1.47	1.39
24	c	510	CLA	CHB-C1B	3.68	1.47	1.39
24	b	610	CLA	OBD-CAD	3.68	1.28	1.22
24	b	614	CLA	CHB-C1B	3.68	1.47	1.39
24	b	621	CLA	CHC-C4B	3.68	1.47	1.39
24	d	404	CLA	C1D-ND	3.68	1.42	1.37
24	c	512	CLA	CHD-C4C	3.68	1.47	1.39
24	b	611	CLA	C3D-C2D	3.68	1.49	1.39
24	b	616	CLA	CHB-C1B	3.68	1.47	1.39
24	C	513	CLA	OBD-CAD	3.68	1.28	1.22
24	c	512	CLA	OBD-CAD	3.68	1.28	1.22
24	B	604	CLA	C1B-NB	-3.67	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	515	CLA	CHB-C1B	3.67	1.47	1.39
24	B	609	CLA	OBD-CAD	3.67	1.28	1.22
24	c	511	CLA	OBD-CAD	3.67	1.28	1.22
24	C	507	CLA	OBD-CAD	3.67	1.28	1.22
24	b	616	CLA	CHC-C4B	3.67	1.47	1.39
24	b	620	CLA	C1D-ND	3.66	1.42	1.37
24	c	507	CLA	CHC-C4B	3.66	1.47	1.39
24	C	509	CLA	OBD-CAD	3.66	1.28	1.22
24	c	517	CLA	OBD-CAD	3.66	1.28	1.22
24	A	406	CLA	CHD-C1D	3.65	1.45	1.38
24	D	405	CLA	OBD-CAD	3.65	1.28	1.22
24	C	505	CLA	C3D-C2D	3.65	1.48	1.39
24	B	615	CLA	CHB-C1B	3.65	1.47	1.39
24	a	409	CLA	CHC-C4B	3.65	1.47	1.39
24	a	410	CLA	C3D-C2D	3.65	1.48	1.39
24	b	620	CLA	CHD-C4C	3.64	1.47	1.39
24	B	608	CLA	C3D-C2D	3.64	1.48	1.39
24	B	613	CLA	C1D-ND	3.64	1.42	1.37
24	C	502	CLA	CHC-C4B	3.63	1.47	1.39
24	A	406	CLA	C4B-NB	-3.63	1.33	1.37
24	c	511	CLA	CHB-C1B	3.63	1.47	1.39
24	d	405	CLA	OBD-CAD	3.62	1.28	1.22
24	A	409	CLA	CHB-C1B	3.62	1.47	1.39
24	C	503	CLA	CHB-C1B	3.62	1.47	1.39
24	b	619	CLA	C3D-C2D	3.62	1.48	1.39
24	b	611	CLA	CHB-C1B	3.62	1.47	1.39
24	c	507	CLA	CHD-C4C	3.62	1.47	1.39
24	B	607	CLA	OBD-CAD	3.61	1.28	1.22
24	c	517	CLA	CHB-C1B	3.61	1.47	1.39
35	d	413	HTG	C1'-S1	-3.61	1.76	1.81
24	a	412	CLA	CHB-C1B	3.61	1.47	1.39
24	b	612	CLA	CHC-C4B	3.61	1.47	1.39
24	b	614	CLA	OBD-CAD	3.61	1.28	1.22
24	B	617	CLA	CHB-C1B	3.60	1.47	1.39
24	c	510	CLA	CHC-C4B	3.60	1.47	1.39
24	B	612	CLA	CHC-C4B	3.60	1.47	1.39
24	c	510	CLA	C3D-C2D	3.60	1.48	1.39
24	B	607	CLA	CHD-C4C	3.60	1.47	1.39
24	C	506	CLA	C1B-NB	-3.60	1.33	1.37
24	C	502	CLA	OBD-CAD	3.60	1.28	1.22
24	b	624	CLA	OBD-CAD	3.60	1.28	1.22
24	B	610	CLA	OBD-CAD	3.60	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	611	CLA	CHC-C4B	3.59	1.47	1.39
24	B	606	CLA	OBD-CAD	3.59	1.28	1.22
24	C	513	CLA	CHB-C1B	3.59	1.47	1.39
24	b	612	CLA	CHD-C4C	3.59	1.47	1.39
24	B	604	CLA	C3D-C2D	3.59	1.48	1.39
24	c	508	CLA	CHC-C4B	3.58	1.47	1.39
24	A	407	CLA	OBD-CAD	3.58	1.28	1.22
24	c	513	CLA	CHC-C4B	3.58	1.47	1.39
24	b	615	CLA	C1B-NB	-3.58	1.33	1.37
24	b	616	CLA	CHD-C4C	3.58	1.47	1.39
24	C	508	CLA	OBD-CAD	3.57	1.28	1.22
24	C	512	CLA	OBD-CAD	3.57	1.28	1.22
24	B	617	CLA	OBD-CAD	3.57	1.28	1.22
24	B	606	CLA	C3D-C2D	3.56	1.48	1.39
24	B	616	CLA	CHD-C4C	3.56	1.47	1.39
24	a	409	CLA	OBD-CAD	3.56	1.28	1.22
24	c	505	CLA	C1B-NB	-3.56	1.33	1.37
24	C	504	CLA	CHC-C4B	3.54	1.47	1.39
24	c	512	CLA	CHC-C4B	3.54	1.47	1.39
24	B	607	CLA	CHB-C1B	3.54	1.47	1.39
24	B	614	CLA	CHC-C4B	3.54	1.47	1.39
24	C	505	CLA	OBD-CAD	3.54	1.28	1.22
24	C	506	CLA	CHB-C1B	3.54	1.47	1.39
24	C	512	CLA	CHB-C1B	3.54	1.47	1.39
24	c	515	CLA	OBD-CAD	3.54	1.28	1.22
24	c	508	CLA	CHB-C1B	3.53	1.47	1.39
24	c	507	CLA	OBD-CAD	3.53	1.28	1.22
24	b	620	CLA	CHC-C4B	3.53	1.47	1.39
24	B	617	CLA	CHC-C4B	3.53	1.47	1.39
24	b	625	CLA	OBD-CAD	3.53	1.28	1.22
24	B	615	CLA	CHD-C4C	3.53	1.47	1.39
24	B	616	CLA	OBD-CAD	3.53	1.28	1.22
24	d	405	CLA	CHB-C1B	3.52	1.47	1.39
24	C	504	CLA	CHB-C1B	3.52	1.47	1.39
24	B	613	CLA	CHD-C4C	3.52	1.47	1.39
24	c	509	CLA	C3D-C2D	3.51	1.48	1.39
24	c	507	CLA	CHB-C1B	3.51	1.47	1.39
24	B	605	CLA	CHB-C1B	3.51	1.47	1.39
37	d	408	LHG	O7-C7	3.51	1.44	1.34
24	B	615	CLA	CHC-C4B	3.51	1.47	1.39
24	b	621	CLA	CHD-C4C	3.51	1.47	1.39
24	B	612	CLA	CHB-C1B	3.51	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	405	CLA	C1B-NB	-3.51	1.33	1.37
24	b	618	CLA	CHC-C4B	3.51	1.47	1.39
24	B	613	CLA	CHC-C4B	3.50	1.47	1.39
24	a	409	CLA	CHB-C1B	3.50	1.47	1.39
24	b	613	CLA	CHC-C4B	3.50	1.47	1.39
24	B	605	CLA	C3D-C2D	3.50	1.48	1.39
24	d	403	CLA	CHB-C1B	3.49	1.47	1.39
24	B	609	CLA	CHB-C1B	3.48	1.47	1.39
24	D	404	CLA	CHC-C4B	3.48	1.47	1.39
24	b	616	CLA	C1B-NB	-3.48	1.33	1.37
24	C	508	CLA	CHC-C4B	3.48	1.47	1.39
24	B	608	CLA	OBD-CAD	3.48	1.28	1.22
24	C	505	CLA	C1B-NB	-3.48	1.33	1.37
24	a	412	CLA	OBD-CAD	3.46	1.28	1.22
24	D	405	CLA	CHC-C4B	3.46	1.47	1.39
24	C	504	CLA	OBD-CAD	3.46	1.28	1.22
24	c	508	CLA	C4B-NB	-3.45	1.33	1.37
24	B	607	CLA	C3D-C2D	3.45	1.48	1.39
24	d	403	CLA	OBD-CAD	3.45	1.28	1.22
24	D	404	CLA	CHB-C1B	3.45	1.47	1.39
37	d	409	LHG	O8-C23	3.44	1.43	1.33
24	c	506	CLA	OBD-CAD	3.44	1.28	1.22
24	B	608	CLA	C1B-NB	-3.44	1.33	1.37
24	a	410	CLA	CHC-C4B	3.44	1.47	1.39
24	D	404	CLA	OBD-CAD	3.43	1.28	1.22
38	f	101	HEM	C1B-NB	-3.43	1.34	1.40
24	b	623	CLA	C1B-NB	-3.43	1.33	1.37
24	c	510	CLA	OBD-CAD	3.43	1.28	1.22
24	b	624	CLA	CHC-C4B	3.43	1.47	1.39
24	C	508	CLA	CHB-C1B	3.43	1.47	1.39
24	B	604	CLA	CHB-C1B	3.43	1.47	1.39
24	c	510	CLA	C1B-NB	-3.43	1.33	1.37
24	b	614	CLA	CHC-C4B	3.42	1.47	1.39
24	c	505	CLA	CHC-C4B	3.42	1.47	1.39
24	c	508	CLA	OBD-CAD	3.42	1.28	1.22
35	b	607	HTG	C1'-S1	-3.41	1.76	1.81
24	c	506	CLA	CHC-C4B	3.40	1.47	1.39
24	a	412	CLA	CHC-C4B	3.40	1.47	1.39
24	C	506	CLA	CHC-C4B	3.40	1.47	1.39
24	A	409	CLA	OBD-CAD	3.39	1.28	1.22
24	b	619	CLA	CHB-C1B	3.39	1.47	1.39
24	a	412	CLA	C1B-NB	-3.39	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	603	CLA	C1B-NB	-3.38	1.33	1.37
24	C	511	CLA	CHC-C4B	3.38	1.47	1.39
24	B	612	CLA	OBD-CAD	3.38	1.28	1.22
24	b	622	CLA	C1B-C2B	3.37	1.51	1.43
24	b	623	CLA	CHC-C4B	3.37	1.47	1.39
24	B	609	CLA	C4B-NB	-3.36	1.33	1.37
24	C	507	CLA	CHB-C1B	3.36	1.47	1.39
24	A	406	CLA	C1B-NB	-3.36	1.33	1.37
24	C	506	CLA	OBD-CAD	3.36	1.28	1.22
24	c	515	CLA	CHC-C4B	3.35	1.46	1.39
35	B	631	HTG	C1'-S1	-3.35	1.76	1.81
24	c	516	CLA	CHB-C1B	3.35	1.46	1.39
24	B	610	CLA	CHC-C4B	3.33	1.46	1.39
24	A	405	CLA	CHC-C4B	3.33	1.46	1.39
38	E	103	HEM	C4D-ND	-3.32	1.34	1.40
35	B	632	HTG	C1'-S1	-3.32	1.76	1.81
24	c	508	CLA	C1B-NB	-3.32	1.33	1.37
24	b	622	CLA	C4C-C3C	3.32	1.50	1.45
24	B	603	CLA	CHB-C1B	3.31	1.46	1.39
35	V	206	HTG	C1'-S1	-3.30	1.76	1.81
24	A	406	CLA	CHB-C1B	3.29	1.46	1.39
24	A	406	CLA	CHC-C4B	3.29	1.46	1.39
24	B	605	CLA	CHC-C4B	3.28	1.46	1.39
24	d	403	CLA	C1B-C2B	3.28	1.50	1.43
24	d	404	CLA	CHB-C1B	3.28	1.46	1.39
24	B	613	CLA	C1B-NB	-3.26	1.33	1.37
24	c	509	CLA	C1B-NB	-3.26	1.33	1.37
24	B	612	CLA	C4B-NB	-3.25	1.33	1.37
35	c	524	HTG	C1'-S1	-3.25	1.76	1.81
37	D	409	LHG	O7-C7	3.25	1.43	1.34
24	b	610	CLA	CHB-C1B	3.25	1.46	1.39
35	B	624	HTG	C1'-S1	-3.23	1.76	1.81
24	A	407	CLA	CHB-C1B	3.23	1.46	1.39
24	A	407	CLA	C1B-NB	-3.22	1.33	1.37
24	b	615	CLA	CHC-C4B	3.22	1.46	1.39
24	b	623	CLA	OBD-CAD	3.22	1.28	1.22
24	B	607	CLA	C1B-NB	-3.22	1.33	1.37
24	B	605	CLA	C1B-C2B	3.21	1.50	1.43
24	c	505	CLA	OBD-CAD	3.20	1.28	1.22
35	b	608	HTG	C1'-S1	-3.20	1.76	1.81
24	D	405	CLA	C1B-NB	-3.19	1.33	1.37
24	a	409	CLA	C4B-NB	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	404	CLA	OBD-CAD	3.18	1.28	1.22
24	a	412	CLA	C4B-NB	-3.18	1.33	1.37
24	B	611	CLA	C1B-NB	-3.17	1.33	1.37
24	B	615	CLA	C1B-NB	-3.17	1.33	1.37
24	A	405	CLA	C4C-C3C	3.17	1.50	1.45
24	d	403	CLA	CHC-C4B	3.16	1.46	1.39
24	c	513	CLA	C4B-NB	-3.16	1.33	1.37
24	D	404	CLA	C1B-NB	-3.16	1.33	1.37
24	c	512	CLA	C1B-NB	-3.16	1.33	1.37
24	b	613	CLA	OBD-CAD	3.15	1.27	1.22
24	d	405	CLA	C1B-NB	-3.15	1.33	1.37
24	B	616	CLA	C1B-NB	-3.14	1.33	1.37
38	E	103	HEM	C1B-NB	-3.13	1.34	1.40
38	f	101	HEM	C4D-ND	-3.13	1.34	1.40
24	d	404	CLA	C4B-NB	-3.12	1.33	1.37
24	c	510	CLA	C4B-NB	-3.11	1.33	1.37
24	b	622	CLA	OBD-CAD	3.11	1.27	1.22
35	C	522	HTG	C1'-S1	-3.11	1.77	1.81
24	c	516	CLA	C4B-NB	-3.11	1.33	1.37
24	B	614	CLA	C1B-NB	-3.10	1.33	1.37
24	b	625	CLA	C1B-NB	-3.10	1.33	1.37
40	V	205	HEC	C4D-ND	-3.09	1.33	1.39
24	B	605	CLA	OBD-CAD	3.09	1.27	1.22
24	D	405	CLA	C4B-NB	-3.08	1.33	1.37
24	C	504	CLA	C1B-NB	-3.08	1.33	1.37
24	B	610	CLA	C1B-NB	-3.07	1.33	1.37
24	C	507	CLA	C1B-NB	-3.07	1.33	1.37
24	c	513	CLA	C1B-NB	-3.07	1.33	1.37
24	B	607	CLA	C4B-NB	-3.06	1.33	1.37
24	b	612	CLA	C4B-NB	-3.06	1.33	1.37
24	B	609	CLA	C1B-NB	-3.06	1.33	1.37
35	b	602	HTG	C1'-S1	-3.05	1.77	1.81
35	c	523	HTG	C1'-S1	-3.05	1.77	1.81
24	c	516	CLA	C1B-NB	-3.05	1.33	1.37
24	A	405	CLA	CHB-C1B	3.04	1.46	1.39
24	B	604	CLA	OBD-CAD	3.04	1.27	1.22
24	C	511	CLA	C1B-C2B	3.03	1.50	1.43
35	D	414	HTG	C1'-S1	-3.03	1.77	1.81
24	B	612	CLA	C1B-NB	-3.03	1.33	1.37
24	c	506	CLA	C4D-CHA	3.03	1.48	1.38
24	b	612	CLA	OBD-CAD	3.03	1.27	1.22
24	A	409	CLA	C1B-NB	-3.02	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	610	CLA	C1B-NB	-3.02	1.33	1.37
24	d	403	CLA	C1B-NB	-3.01	1.33	1.37
35	C	523	HTG	C1'-S1	-3.00	1.77	1.81
24	C	510	CLA	C1B-NB	-3.00	1.33	1.37
24	C	503	CLA	C1B-NB	-3.00	1.33	1.37
24	B	610	CLA	C1B-C2B	2.99	1.50	1.43
24	b	620	CLA	C1B-NB	-2.99	1.33	1.37
24	A	409	CLA	C4B-NB	-2.99	1.33	1.37
24	c	506	CLA	C4B-NB	-2.99	1.33	1.37
24	B	606	CLA	C1B-C2B	2.99	1.50	1.43
24	b	621	CLA	C4B-NB	-2.98	1.33	1.37
24	C	508	CLA	C1B-NB	-2.98	1.33	1.37
24	b	612	CLA	C1B-NB	-2.98	1.33	1.37
24	a	412	CLA	C1B-C2B	2.97	1.50	1.43
24	d	403	CLA	C4B-NB	-2.97	1.34	1.37
24	c	505	CLA	C4B-NB	-2.97	1.34	1.37
24	b	611	CLA	C1B-NB	-2.96	1.34	1.37
40	v	206	HEC	C1D-ND	-2.96	1.34	1.39
24	C	506	CLA	C4B-NB	-2.96	1.34	1.37
24	C	510	CLA	C4C-C3C	2.96	1.50	1.45
24	C	505	CLA	C1B-C2B	2.95	1.50	1.43
24	c	515	CLA	C4B-NB	-2.95	1.34	1.37
24	C	501	CLA	C1B-NB	-2.94	1.34	1.37
24	b	620	CLA	OBD-CAD	2.94	1.27	1.22
25	D	401[A]	PHO	CHA-CBD	-2.93	1.48	1.51
24	a	410	CLA	C1B-NB	-2.93	1.34	1.37
24	C	511	CLA	C4B-NB	-2.93	1.34	1.37
40	V	205	HEC	C1B-NB	-2.93	1.34	1.39
24	B	605	CLA	C4D-CHA	2.93	1.48	1.38
24	C	502	CLA	C4B-NB	-2.92	1.34	1.37
24	B	604	CLA	C4B-NB	-2.92	1.34	1.37
24	a	409	CLA	C4C-C3C	2.92	1.50	1.45
24	b	625	CLA	C1B-C2B	2.92	1.50	1.43
24	C	512	CLA	C1B-NB	-2.92	1.34	1.37
24	c	511	CLA	C4D-CHA	2.91	1.48	1.38
24	B	617	CLA	C1B-NB	-2.91	1.34	1.37
24	C	504	CLA	C4B-NB	-2.91	1.34	1.37
24	b	611	CLA	C4B-NB	-2.91	1.34	1.37
24	c	517	CLA	C1B-NB	-2.91	1.34	1.37
24	b	622	CLA	CHC-C4B	2.91	1.45	1.39
24	C	507	CLA	C4D-CHA	2.91	1.48	1.38
24	C	511	CLA	C4D-CHA	2.90	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	501	CLA	C1C-C2C	2.90	1.50	1.44
24	B	617	CLA	C1B-C2B	2.89	1.49	1.43
24	c	517	CLA	C4B-NB	-2.89	1.34	1.37
25	d	402[A]	PHO	C3A-C2A	-2.89	1.52	1.54
24	B	614	CLA	C4C-C3C	2.89	1.49	1.45
24	B	617	CLA	C4D-CHA	2.88	1.48	1.38
24	C	510	CLA	C4B-NB	-2.88	1.34	1.37
24	B	606	CLA	C1C-C2C	2.88	1.50	1.44
24	b	613	CLA	C1B-NB	-2.88	1.34	1.37
24	b	622	CLA	C4D-CHA	2.87	1.48	1.38
24	B	611	CLA	C4D-CHA	2.87	1.48	1.38
24	b	613	CLA	C4D-CHA	2.87	1.48	1.38
24	c	509	CLA	C1B-C2B	2.87	1.49	1.43
24	B	605	CLA	C1B-NB	-2.87	1.34	1.37
24	B	602	CLA	C1B-C2B	2.87	1.49	1.43
24	C	509	CLA	C4B-NB	-2.87	1.34	1.37
24	b	614	CLA	C1B-C2B	2.87	1.49	1.43
24	B	617	CLA	C4B-NB	-2.87	1.34	1.37
24	C	509	CLA	C1B-NB	-2.87	1.34	1.37
24	c	507	CLA	C1B-NB	-2.86	1.34	1.37
24	c	514	CLA	C1B-C2B	2.86	1.49	1.43
24	C	507	CLA	C4B-NB	-2.85	1.34	1.37
24	b	625	CLA	C4D-CHA	2.85	1.48	1.38
24	b	625	CLA	C4B-NB	-2.84	1.34	1.37
35	B	623	HTG	C1'-S1	-2.84	1.77	1.81
24	b	623	CLA	C1B-C2B	2.84	1.49	1.43
24	C	503	CLA	C1C-C2C	2.84	1.50	1.44
24	A	405	CLA	C4B-NB	-2.83	1.34	1.37
24	c	512	CLA	C1B-C2B	2.83	1.49	1.43
24	C	509	CLA	C1B-C2B	2.83	1.49	1.43
40	V	205	HEC	C4B-NB	-2.83	1.34	1.39
24	b	622	CLA	C1B-NB	-2.83	1.34	1.37
24	D	405	CLA	C1B-C2B	2.82	1.49	1.43
24	b	615	CLA	C4B-NB	-2.82	1.34	1.37
24	b	621	CLA	C1B-C2B	2.81	1.49	1.43
24	C	510	CLA	C4D-CHA	2.81	1.48	1.38
24	C	502	CLA	C1B-C2B	2.81	1.49	1.43
24	c	511	CLA	C4B-NB	-2.81	1.34	1.37
24	b	613	CLA	C1B-C2B	2.81	1.49	1.43
24	D	404	CLA	C4B-NB	-2.81	1.34	1.37
24	b	624	CLA	C1B-C2B	2.80	1.49	1.43
24	b	616	CLA	C4D-CHA	2.80	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	404	CLA	C1B-C2B	2.80	1.49	1.43
24	b	616	CLA	C1B-C2B	2.80	1.49	1.43
24	B	606	CLA	C4B-NB	-2.79	1.34	1.37
24	c	513	CLA	C4D-CHA	2.79	1.48	1.38
24	c	505	CLA	C4D-CHA	2.79	1.48	1.38
24	C	509	CLA	C4D-CHA	2.79	1.48	1.38
24	A	409	CLA	C4C-C3C	2.78	1.49	1.45
24	c	511	CLA	C1C-C2C	2.78	1.50	1.44
24	B	609	CLA	CHC-C4B	2.78	1.45	1.39
24	C	505	CLA	C4B-NB	-2.78	1.34	1.37
24	b	620	CLA	C4B-NB	-2.78	1.34	1.37
24	B	609	CLA	C4C-C3C	2.78	1.49	1.45
31	a	416[B]	PL9	C6-C5	2.78	1.48	1.35
31	A	417[B]	PL9	C6-C5	2.77	1.48	1.35
24	C	502	CLA	C1B-NB	-2.77	1.34	1.37
31	d	407[B]	PL9	C6-C5	2.77	1.48	1.35
24	B	606	CLA	C4C-C3C	2.77	1.49	1.45
24	B	608	CLA	C4D-CHA	2.77	1.47	1.38
24	A	409	CLA	C4D-CHA	2.77	1.47	1.38
24	c	506	CLA	C1B-C2B	2.77	1.49	1.43
24	b	614	CLA	C4D-CHA	2.76	1.47	1.38
24	C	512	CLA	C4D-CHA	2.76	1.47	1.38
33	Z	101	LMG	O8-C28	2.76	1.46	1.33
24	A	407	CLA	C1B-C2B	2.75	1.49	1.43
24	c	514	CLA	C4B-NB	-2.75	1.34	1.37
31	a	416[A]	PL9	C6-C5	2.75	1.48	1.35
24	B	602	CLA	C1B-NB	-2.75	1.34	1.37
40	v	206	HEC	C1B-NB	-2.74	1.34	1.39
24	C	506	CLA	C4D-CHA	2.74	1.47	1.38
24	C	501	CLA	C4D-CHA	2.74	1.47	1.38
24	b	624	CLA	C4D-CHA	2.74	1.47	1.38
24	b	620	CLA	C1B-C2B	2.74	1.49	1.43
24	c	515	CLA	C1B-C2B	2.74	1.49	1.43
24	C	513	CLA	C4B-NB	-2.74	1.34	1.37
24	b	621	CLA	C4D-CHA	2.74	1.47	1.38
24	b	617	CLA	C4D-CHA	2.74	1.47	1.38
24	b	614	CLA	C1C-C2C	2.74	1.50	1.44
24	c	507	CLA	C4D-CHA	2.74	1.47	1.38
24	b	610	CLA	C4B-NB	-2.73	1.34	1.37
24	b	616	CLA	C4B-NB	-2.73	1.34	1.37
24	b	618	CLA	C1B-NB	-2.73	1.34	1.37
24	B	615	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	622	CLA	C4B-NB	-2.73	1.34	1.37
24	B	612	CLA	C4C-C3C	2.73	1.49	1.45
31	D	407[B]	PL9	C6-C5	2.72	1.48	1.35
24	c	515	CLA	C1B-NB	-2.72	1.34	1.37
24	C	508	CLA	C4D-CHA	2.72	1.47	1.38
24	b	615	CLA	C4D-CHA	2.72	1.47	1.38
24	B	613	CLA	C4B-NB	-2.72	1.34	1.37
24	B	610	CLA	C4D-CHA	2.72	1.47	1.38
24	c	509	CLA	C4C-C3C	2.72	1.49	1.45
31	A	417[A]	PL9	C6-C5	2.71	1.48	1.35
24	b	621	CLA	C1B-NB	-2.71	1.34	1.37
24	c	507	CLA	C1B-C2B	2.71	1.49	1.43
24	B	609	CLA	C1B-C2B	2.71	1.49	1.43
24	b	620	CLA	C4D-CHA	2.71	1.47	1.38
24	c	514	CLA	C4D-CHA	2.71	1.47	1.38
31	d	407[A]	PL9	C6-C5	2.70	1.48	1.35
24	B	614	CLA	C4D-CHA	2.70	1.47	1.38
24	B	611	CLA	C1B-C2B	2.70	1.49	1.43
38	E	103	HEM	C1C-C2C	-2.70	1.40	1.45
24	C	513	CLA	C1B-NB	-2.70	1.34	1.37
24	B	607	CLA	C1C-C2C	2.70	1.50	1.44
24	c	516	CLA	C4D-CHA	2.70	1.47	1.38
24	b	619	CLA	C4C-C3C	2.70	1.49	1.45
24	b	621	CLA	C1C-C2C	2.70	1.50	1.44
24	A	409	CLA	C1B-C2B	2.69	1.49	1.43
24	c	511	CLA	C1B-C2B	2.69	1.49	1.43
25	A	408	PHO	C3A-C2A	-2.69	1.52	1.54
24	C	502	CLA	C4D-CHA	2.69	1.47	1.38
38	f	101	HEM	C1C-C2C	-2.69	1.40	1.45
24	a	409	CLA	C4D-CHA	2.69	1.47	1.38
24	a	410	CLA	C1B-C2B	2.69	1.49	1.43
24	C	512	CLA	C1C-C2C	2.69	1.50	1.44
24	C	508	CLA	C4B-NB	-2.68	1.34	1.37
40	V	205	HEC	C1D-ND	-2.68	1.34	1.39
24	B	607	CLA	C4D-CHA	2.68	1.47	1.38
24	B	615	CLA	C4D-CHA	2.68	1.47	1.38
24	c	514	CLA	C1B-NB	-2.68	1.34	1.37
24	B	613	CLA	C1C-C2C	2.67	1.49	1.44
25	d	402[A]	PHO	C4B-NB	-2.67	1.33	1.38
24	B	605	CLA	C4B-NB	-2.67	1.34	1.37
24	b	617	CLA	C1B-NB	-2.66	1.34	1.37
24	c	513	CLA	C1B-C2B	2.66	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	511	CLA	C4C-C3C	2.66	1.49	1.45
24	B	602	CLA	C4D-CHA	2.66	1.47	1.38
24	b	611	CLA	C1B-C2B	2.66	1.49	1.43
24	c	507	CLA	C4B-NB	-2.66	1.34	1.37
24	B	608	CLA	C1C-C2C	2.66	1.49	1.44
24	b	615	CLA	C1B-C2B	2.65	1.49	1.43
24	B	602	CLA	C4B-NB	-2.65	1.34	1.37
35	b	631	HTG	C1'-S1	-2.65	1.77	1.81
24	b	612	CLA	C4D-CHA	2.65	1.47	1.38
24	D	404	CLA	C4C-C3C	2.64	1.49	1.45
24	B	612	CLA	C4D-CHA	2.64	1.47	1.38
24	A	406	CLA	C4D-CHA	2.64	1.47	1.38
24	B	608	CLA	C1B-C2B	2.64	1.49	1.43
24	c	512	CLA	C1C-C2C	2.64	1.49	1.44
24	c	508	CLA	C4D-CHA	2.63	1.47	1.38
24	d	404	CLA	C4D-CHA	2.63	1.47	1.38
24	C	512	CLA	C1B-C2B	2.63	1.49	1.43
40	v	206	HEC	C4D-ND	-2.63	1.34	1.39
24	b	610	CLA	C4D-CHA	2.63	1.47	1.38
24	C	504	CLA	C4D-CHA	2.62	1.47	1.38
24	C	511	CLA	C1B-NB	-2.62	1.34	1.37
24	c	517	CLA	C1C-C2C	2.62	1.49	1.44
24	b	618	CLA	C1B-C2B	2.62	1.49	1.43
24	B	610	CLA	C4B-NB	-2.62	1.34	1.37
24	b	613	CLA	C4B-NB	-2.62	1.34	1.37
24	B	603	CLA	C3D-C4D	-2.62	1.38	1.44
24	B	611	CLA	C4B-NB	-2.62	1.34	1.37
24	c	514	CLA	C4C-C3C	2.61	1.49	1.45
24	c	512	CLA	C4D-CHA	2.61	1.47	1.38
24	A	405	CLA	C1C-C2C	2.61	1.49	1.44
24	b	618	CLA	C4D-CHA	2.61	1.47	1.38
24	a	409	CLA	C1B-C2B	2.61	1.49	1.43
24	C	510	CLA	C1B-C2B	2.60	1.49	1.43
24	d	405	CLA	C4D-CHA	2.60	1.47	1.38
24	a	410	CLA	C1C-C2C	2.60	1.49	1.44
24	B	603	CLA	C1B-C2B	2.60	1.49	1.43
24	b	619	CLA	C4D-CHA	2.59	1.47	1.38
24	b	614	CLA	C1B-NB	-2.59	1.34	1.37
24	c	505	CLA	C1B-C2B	2.59	1.49	1.43
24	C	503	CLA	C1B-C2B	2.58	1.49	1.43
31	D	407[A]	PL9	C6-C5	2.58	1.48	1.35
25	a	411	PHO	C3A-C2A	-2.58	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	C4D-CHA	2.58	1.47	1.38
24	C	513	CLA	C3B-C4B	2.57	1.50	1.42
24	a	412	CLA	C4D-CHA	2.57	1.47	1.38
24	B	603	CLA	C4D-CHA	2.57	1.47	1.38
24	b	616	CLA	C3D-C4D	-2.56	1.38	1.44
24	b	622	CLA	C3D-C4D	-2.56	1.38	1.44
25	D	401[B]	PHO	C4B-NB	-2.56	1.34	1.38
24	B	610	CLA	C4C-C3C	2.56	1.49	1.45
24	B	609	CLA	C4D-CHA	2.56	1.47	1.38
24	a	410	CLA	C4B-NB	-2.56	1.34	1.37
24	c	505	CLA	C4C-C3C	2.56	1.49	1.45
24	C	513	CLA	C4D-CHA	2.56	1.47	1.38
24	C	502	CLA	C1C-C2C	2.55	1.49	1.44
24	d	405	CLA	C4B-NB	-2.55	1.34	1.37
24	B	613	CLA	C1B-C2B	2.55	1.49	1.43
24	B	616	CLA	C1C-C2C	2.55	1.49	1.44
24	B	616	CLA	C4D-CHA	2.55	1.47	1.38
24	B	616	CLA	C1B-C2B	2.55	1.49	1.43
24	B	614	CLA	C4B-NB	-2.55	1.34	1.37
24	A	407	CLA	C3D-C4D	-2.54	1.38	1.44
24	B	617	CLA	C3D-C4D	-2.54	1.38	1.44
24	d	405	CLA	C1B-C2B	2.54	1.49	1.43
24	C	501	CLA	C3B-C4B	2.54	1.50	1.42
24	C	505	CLA	C4D-CHA	2.54	1.47	1.38
24	D	405	CLA	C4D-CHA	2.54	1.47	1.38
24	C	509	CLA	C4C-C3C	2.54	1.49	1.45
24	B	614	CLA	C1C-C2C	2.54	1.49	1.44
24	c	515	CLA	C4D-CHA	2.53	1.47	1.38
24	b	610	CLA	C3B-C4B	2.53	1.50	1.42
24	b	615	CLA	C1C-C2C	2.53	1.49	1.44
24	B	611	CLA	C3D-C4D	-2.53	1.38	1.44
24	C	513	CLA	C4C-C3C	2.53	1.49	1.45
24	B	615	CLA	C1C-C2C	2.53	1.49	1.44
25	A	408	PHO	CHA-CBD	-2.53	1.48	1.51
24	c	509	CLA	C4D-CHA	2.53	1.47	1.38
24	B	606	CLA	C3B-C4B	2.53	1.50	1.42
24	B	605	CLA	C4C-C3C	2.53	1.49	1.45
25	D	401[B]	PHO	C1B-NB	-2.52	1.34	1.38
24	c	517	CLA	C1B-C2B	2.52	1.49	1.43
24	B	603	CLA	C1C-C2C	2.52	1.49	1.44
25	a	411	PHO	CHA-CBD	-2.52	1.48	1.51
24	c	517	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	409	CLA	C1B-NB	-2.52	1.34	1.37
24	b	624	CLA	C1B-NB	-2.52	1.34	1.37
24	C	503	CLA	C3B-C4B	2.52	1.50	1.42
24	b	617	CLA	C1B-C2B	2.51	1.49	1.43
24	A	407	CLA	C1C-C2C	2.51	1.49	1.44
24	A	407	CLA	C4B-NB	-2.51	1.34	1.37
24	B	608	CLA	C4C-C3C	2.51	1.49	1.45
24	b	614	CLA	C4B-NB	-2.51	1.34	1.37
24	B	611	CLA	C3B-C4B	2.51	1.50	1.42
24	A	405	CLA	C4D-CHA	2.51	1.47	1.38
24	a	410	CLA	C3D-C4D	-2.51	1.38	1.44
36	D	408	DGD	O3G-C1D	2.50	1.44	1.40
24	C	513	CLA	C1B-C2B	2.50	1.49	1.43
24	c	513	CLA	C1C-C2C	2.50	1.49	1.44
24	b	617	CLA	C3B-C4B	2.50	1.50	1.42
24	B	612	CLA	C1B-C2B	2.50	1.49	1.43
24	B	616	CLA	C4B-NB	-2.50	1.34	1.37
24	D	404	CLA	C4D-CHA	2.50	1.47	1.38
24	b	613	CLA	C1C-C2C	2.50	1.49	1.44
35	b	632	HTG	C1-S1	-2.49	1.76	1.80
24	c	507	CLA	C1C-C2C	2.49	1.49	1.44
24	C	506	CLA	C3D-C4D	-2.49	1.38	1.44
24	b	611	CLA	C4D-CHA	2.49	1.46	1.38
24	b	612	CLA	C1B-C2B	2.49	1.49	1.43
24	B	610	CLA	C3D-C4D	-2.49	1.38	1.44
24	C	506	CLA	C4C-C3C	2.49	1.49	1.45
24	C	512	CLA	C3B-C4B	2.48	1.50	1.42
24	c	516	CLA	C1C-C2C	2.48	1.49	1.44
24	B	602	CLA	C3B-C4B	2.48	1.50	1.42
24	b	612	CLA	C4C-C3C	2.48	1.49	1.45
24	B	604	CLA	C1C-C2C	2.48	1.49	1.44
24	c	506	CLA	C1B-NB	-2.48	1.34	1.37
24	C	507	CLA	C1B-C2B	2.47	1.48	1.43
24	B	612	CLA	C1C-C2C	2.47	1.49	1.44
24	A	409	CLA	C3D-C4D	-2.47	1.38	1.44
24	A	407	CLA	C4D-CHA	2.47	1.46	1.38
24	C	505	CLA	C4C-C3C	2.47	1.49	1.45
24	C	508	CLA	C1B-C2B	2.47	1.48	1.43
24	A	406	CLA	C1B-C2B	2.46	1.48	1.43
24	A	407	CLA	C3B-C4B	2.46	1.49	1.42
24	d	404	CLA	C4C-C3C	2.46	1.49	1.45
24	B	614	CLA	C3B-C2B	2.46	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	d	403	CLA	C4D-CHA	2.46	1.46	1.38
24	B	615	CLA	C4B-NB	-2.46	1.34	1.37
24	B	613	CLA	C3B-C2B	2.46	1.49	1.41
24	c	510	CLA	C3D-C4D	-2.46	1.38	1.44
24	C	501	CLA	C1B-C2B	2.46	1.48	1.43
24	B	616	CLA	C3B-C4B	2.45	1.49	1.42
24	c	511	CLA	C1B-NB	-2.45	1.34	1.37
24	b	612	CLA	C1C-C2C	2.45	1.49	1.44
24	C	508	CLA	C4C-C3C	2.45	1.49	1.45
24	B	608	CLA	C3D-C4D	-2.45	1.38	1.44
24	B	606	CLA	C4D-CHA	2.45	1.46	1.38
24	b	613	CLA	C4C-C3C	2.45	1.49	1.45
24	C	503	CLA	C4D-CHA	2.45	1.46	1.38
24	B	604	CLA	C4D-CHA	2.44	1.46	1.38
29	A	414	LMT	O1'-C1'	2.44	1.44	1.40
24	b	619	CLA	C1B-C2B	2.44	1.48	1.43
24	c	513	CLA	C4C-C3C	2.44	1.49	1.45
24	a	410	CLA	C4D-CHA	2.44	1.46	1.38
24	b	617	CLA	C1C-C2C	2.44	1.49	1.44
24	c	508	CLA	C1C-C2C	2.44	1.49	1.44
24	C	503	CLA	C4C-C3C	2.44	1.49	1.45
24	B	604	CLA	C3D-C4D	-2.43	1.38	1.44
24	c	513	CLA	C3B-C2B	2.43	1.49	1.41
24	b	617	CLA	C4B-NB	-2.43	1.34	1.37
24	C	511	CLA	C3B-C2B	2.43	1.49	1.41
24	C	507	CLA	C1C-C2C	2.43	1.49	1.44
24	c	513	CLA	C3D-C4D	-2.43	1.38	1.44
24	D	404	CLA	C3B-C2B	2.43	1.49	1.41
24	b	611	CLA	C1C-C2C	2.43	1.49	1.44
24	C	509	CLA	C3B-C2B	2.42	1.49	1.41
24	C	504	CLA	C1B-C2B	2.42	1.48	1.43
24	c	517	CLA	C3B-C4B	2.42	1.49	1.42
24	b	620	CLA	C4C-C3C	2.42	1.49	1.45
25	a	411	PHO	C1B-NB	-2.42	1.34	1.38
24	c	505	CLA	C1C-C2C	2.41	1.49	1.44
24	B	609	CLA	C1C-NC	-2.41	1.34	1.37
25	D	401[B]	PHO	CHA-CBD	-2.41	1.48	1.51
24	d	404	CLA	C3D-C4D	-2.41	1.38	1.44
24	b	619	CLA	C4B-NB	-2.41	1.34	1.37
24	B	608	CLA	C4B-NB	-2.41	1.34	1.37
25	d	402[B]	PHO	C3A-C2A	-2.40	1.52	1.54
24	b	618	CLA	C1C-C2C	2.40	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	614	CLA	C3B-C4B	2.40	1.49	1.42
24	C	502	CLA	C3B-C4B	2.40	1.49	1.42
25	D	401[A]	PHO	C1B-NB	-2.40	1.34	1.38
24	c	509	CLA	C3B-C4B	2.39	1.49	1.42
24	a	409	CLA	C1C-C2C	2.39	1.49	1.44
24	B	607	CLA	C3D-C4D	-2.39	1.38	1.44
24	C	505	CLA	C1C-C2C	2.39	1.49	1.44
24	c	516	CLA	C3B-C4B	2.39	1.49	1.42
24	C	507	CLA	C4C-C3C	2.39	1.49	1.45
24	b	610	CLA	C1B-C2B	2.38	1.48	1.43
24	D	404	CLA	C3D-C4D	-2.38	1.38	1.44
24	b	620	CLA	C3D-C4D	-2.38	1.38	1.44
24	b	623	CLA	C4D-CHA	2.37	1.46	1.38
25	D	401[B]	PHO	C3A-C2A	-2.37	1.52	1.54
37	d	408	LHG	O7-C5	-2.37	1.41	1.46
24	B	612	CLA	C3D-C4D	-2.37	1.38	1.44
24	B	605	CLA	C3B-C2B	2.37	1.49	1.41
24	B	606	CLA	C1B-NB	-2.37	1.34	1.37
24	C	505	CLA	C3D-C4D	-2.37	1.38	1.44
24	c	510	CLA	C1B-C2B	2.36	1.48	1.43
24	C	512	CLA	C4C-C3C	2.36	1.49	1.45
35	C	522	HTG	C1-S1	-2.36	1.76	1.80
24	B	603	CLA	C3B-C2B	2.36	1.49	1.41
24	B	614	CLA	C1B-C2B	2.36	1.48	1.43
24	b	625	CLA	C3B-C4B	2.36	1.49	1.42
24	C	501	CLA	C4B-NB	-2.36	1.34	1.37
24	A	406	CLA	C3B-C2B	2.36	1.49	1.41
24	b	624	CLA	C3B-C4B	2.36	1.49	1.42
24	b	621	CLA	C3B-C2B	2.35	1.49	1.41
24	b	612	CLA	C3D-C4D	-2.35	1.38	1.44
24	C	504	CLA	C1C-C2C	2.35	1.49	1.44
24	C	512	CLA	C4B-NB	-2.35	1.34	1.37
24	B	616	CLA	C3D-C4D	-2.34	1.38	1.44
24	B	610	CLA	C3B-C4B	2.34	1.49	1.42
25	D	401[A]	PHO	C3A-C2A	-2.34	1.52	1.54
25	a	411	PHO	C4B-NB	-2.34	1.34	1.38
24	b	610	CLA	C1C-C2C	2.34	1.49	1.44
24	D	405	CLA	C4C-C3C	2.34	1.49	1.45
24	C	504	CLA	C4C-C3C	2.34	1.49	1.45
24	d	403	CLA	C1C-NC	-2.34	1.34	1.37
24	b	613	CLA	C3B-C2B	2.33	1.49	1.41
24	D	405	CLA	C3D-C4D	-2.33	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	CLA	C1C-C2C	2.33	1.49	1.44
24	b	619	CLA	C3B-C2B	2.33	1.49	1.41
24	B	609	CLA	C3D-C4D	-2.32	1.39	1.44
24	c	514	CLA	C3B-C2B	2.32	1.49	1.41
24	c	509	CLA	C1C-C2C	2.32	1.49	1.44
24	c	506	CLA	C3D-C4D	-2.32	1.39	1.44
24	c	506	CLA	C3B-C4B	2.32	1.49	1.42
24	C	504	CLA	C3B-C2B	2.32	1.49	1.41
24	b	614	CLA	C3D-C4D	-2.32	1.39	1.44
24	b	623	CLA	C3D-C4D	-2.32	1.39	1.44
24	B	615	CLA	C3B-C2B	2.32	1.49	1.41
24	b	611	CLA	C3B-C2B	2.32	1.49	1.41
24	C	508	CLA	C3D-C4D	-2.32	1.39	1.44
24	b	616	CLA	C3B-C4B	2.31	1.49	1.42
24	b	610	CLA	C3B-C2B	2.31	1.49	1.41
24	C	508	CLA	C3B-C4B	2.31	1.49	1.42
24	B	604	CLA	C1B-C2B	2.31	1.48	1.43
24	b	618	CLA	C3D-C4D	-2.31	1.39	1.44
24	b	619	CLA	C3D-C4D	-2.31	1.39	1.44
24	c	517	CLA	C3D-C4D	-2.31	1.39	1.44
25	d	402[A]	PHO	CHA-CBD	-2.30	1.49	1.51
24	C	505	CLA	C3B-C4B	2.30	1.49	1.42
25	D	401[A]	PHO	C4B-NB	-2.30	1.34	1.38
24	a	410	CLA	C3B-C4B	2.30	1.49	1.42
24	c	511	CLA	C3B-C2B	2.30	1.48	1.41
24	b	616	CLA	C1C-C2C	2.30	1.49	1.44
24	c	511	CLA	C4C-C3C	2.30	1.48	1.45
24	A	405	CLA	C3B-C2B	2.30	1.48	1.41
24	C	509	CLA	C1C-C2C	2.29	1.49	1.44
24	C	510	CLA	C3B-C2B	2.29	1.48	1.41
24	B	607	CLA	C4C-C3C	2.29	1.48	1.45
24	b	617	CLA	C3D-C4D	-2.29	1.39	1.44
24	a	409	CLA	C3B-C2B	2.29	1.48	1.41
24	C	510	CLA	C3D-C4D	-2.29	1.39	1.44
24	b	623	CLA	C4C-C3C	2.29	1.48	1.45
24	c	508	CLA	C3B-C2B	2.29	1.48	1.41
35	d	413	HTG	C1-S1	-2.28	1.76	1.80
24	b	620	CLA	C3B-C2B	2.28	1.48	1.41
25	d	402[B]	PHO	C1B-NB	-2.28	1.34	1.38
24	d	403	CLA	C3D-C4D	-2.28	1.39	1.44
24	d	405	CLA	C3D-C4D	-2.28	1.39	1.44
24	d	404	CLA	C1C-C2C	2.28	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	618	CLA	C3B-C4B	2.28	1.49	1.42
24	d	404	CLA	C1B-C2B	2.28	1.48	1.43
24	b	623	CLA	C3B-C2B	2.28	1.48	1.41
24	B	602	CLA	C1C-C2C	2.28	1.49	1.44
24	b	622	CLA	C3B-C2B	2.27	1.48	1.41
24	C	508	CLA	C3B-C2B	2.27	1.48	1.41
24	b	625	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	503	CLA	C4B-NB	-2.27	1.34	1.37
24	A	406	CLA	C3D-C4D	-2.27	1.39	1.44
24	C	510	CLA	C1C-C2C	2.27	1.49	1.44
24	A	405	CLA	C3D-C4D	-2.27	1.39	1.44
24	c	517	CLA	C4C-C3C	2.27	1.48	1.45
24	c	512	CLA	C3B-C2B	2.26	1.48	1.41
24	b	611	CLA	C3B-C4B	2.26	1.49	1.42
24	d	405	CLA	C3B-C4B	2.26	1.49	1.42
25	d	402[B]	PHO	CHA-CBD	-2.26	1.49	1.51
24	B	609	CLA	C3B-C2B	2.26	1.48	1.41
24	c	508	CLA	C3D-C4D	-2.26	1.39	1.44
24	c	509	CLA	C3D-C4D	-2.26	1.39	1.44
40	v	206	HEC	C4A-C3A	-2.26	1.40	1.45
24	C	511	CLA	C1C-C2C	2.26	1.49	1.44
24	b	612	CLA	C3B-C2B	2.26	1.48	1.41
24	c	507	CLA	C3D-C4D	-2.25	1.39	1.44
25	d	402[B]	PHO	C4B-NB	-2.25	1.34	1.38
24	c	508	CLA	C1B-C2B	2.25	1.48	1.43
24	B	613	CLA	C4D-CHA	2.25	1.46	1.38
24	B	617	CLA	C3B-C2B	2.25	1.48	1.41
24	a	412	CLA	C3D-C4D	-2.25	1.39	1.44
24	c	515	CLA	C3B-C4B	2.25	1.49	1.42
24	C	502	CLA	C4C-C3C	2.25	1.48	1.45
24	c	506	CLA	C4C-C3C	2.25	1.48	1.45
24	c	510	CLA	C4C-C3C	2.25	1.48	1.45
24	a	410	CLA	C4C-C3C	2.25	1.48	1.45
24	b	618	CLA	C4B-NB	-2.24	1.34	1.37
24	d	405	CLA	C1C-C2C	2.24	1.49	1.44
24	C	509	CLA	C3D-C4D	-2.24	1.39	1.44
24	c	507	CLA	C4C-C3C	2.24	1.48	1.45
24	c	508	CLA	C4C-C3C	2.24	1.48	1.45
24	C	502	CLA	C3B-C2B	2.24	1.48	1.41
24	B	617	CLA	C4C-C3C	2.23	1.48	1.45
36	h	102	DGD	O5D-C1E	2.23	1.43	1.40
24	B	612	CLA	C3B-C2B	2.23	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	617	CLA	C4C-C3C	2.23	1.48	1.45
24	B	611	CLA	C3B-C2B	2.23	1.48	1.41
24	c	506	CLA	C3B-C2B	2.23	1.48	1.41
25	D	401[A]	PHO	C1D-ND	-2.22	1.34	1.38
24	a	412	CLA	C4C-C3C	2.22	1.48	1.45
24	B	604	CLA	C3B-C4B	2.22	1.49	1.42
24	b	615	CLA	C3B-C2B	2.22	1.48	1.41
24	b	611	CLA	C3D-C4D	-2.22	1.39	1.44
24	d	403	CLA	C3B-C2B	2.22	1.48	1.41
24	C	503	CLA	C3D-C4D	-2.22	1.39	1.44
25	a	411	PHO	CBD-CGD	-2.21	1.49	1.52
24	A	405	CLA	C1B-C2B	2.21	1.48	1.43
24	A	407	CLA	C4C-C3C	2.21	1.48	1.45
24	B	611	CLA	C4C-C3C	2.21	1.48	1.45
31	d	407[A]	PL9	C2-C3	2.21	1.40	1.34
24	b	623	CLA	C4B-NB	-2.21	1.35	1.37
24	c	515	CLA	C3B-C2B	2.21	1.48	1.41
24	b	621	CLA	C3B-C4B	2.21	1.49	1.42
24	B	603	CLA	C3B-C4B	2.21	1.49	1.42
24	c	505	CLA	C3B-C2B	2.21	1.48	1.41
24	c	510	CLA	C3B-C2B	2.20	1.48	1.41
24	c	509	CLA	C4B-NB	-2.20	1.35	1.37
24	B	603	CLA	C4C-C3C	2.20	1.48	1.45
24	C	513	CLA	C3D-C4D	-2.20	1.39	1.44
24	B	607	CLA	C1B-C2B	2.20	1.48	1.43
24	c	512	CLA	C4C-C3C	2.20	1.48	1.45
24	c	507	CLA	C3B-C4B	2.20	1.49	1.42
40	v	206	HEC	C4B-NB	-2.19	1.35	1.39
31	a	416[B]	PL9	C2-C3	2.19	1.40	1.34
24	D	404	CLA	C1C-C2C	2.19	1.49	1.44
24	C	513	CLA	C3B-C2B	2.19	1.48	1.41
24	a	412	CLA	C3B-C4B	2.19	1.49	1.42
24	B	615	CLA	C3D-C4D	-2.19	1.39	1.44
24	b	619	CLA	C3B-C4B	2.19	1.49	1.42
24	c	512	CLA	C3D-C4D	-2.19	1.39	1.44
31	a	416[A]	PL9	C2-C3	2.19	1.40	1.34
25	A	408	PHO	C4B-NB	-2.19	1.34	1.38
24	B	606	CLA	C3D-C4D	-2.19	1.39	1.44
24	B	604	CLA	C4C-C3C	2.19	1.48	1.45
24	C	501	CLA	C4C-C3C	2.18	1.48	1.45
24	b	611	CLA	C4C-C3C	2.18	1.48	1.45
24	b	625	CLA	C3B-C2B	2.18	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C3D-C4D	-2.18	1.39	1.44
24	c	512	CLA	C4B-NB	-2.18	1.35	1.37
25	D	401[B]	PHO	C1D-ND	-2.18	1.34	1.38
24	b	623	CLA	C1C-C2C	2.17	1.48	1.44
24	c	514	CLA	C1C-C2C	2.17	1.48	1.44
24	A	409	CLA	C3B-C4B	2.17	1.49	1.42
38	f	101	HEM	C1D-ND	-2.17	1.34	1.38
24	a	410	CLA	C3B-C2B	2.17	1.48	1.41
24	B	602	CLA	C3B-C2B	2.17	1.48	1.41
24	C	511	CLA	C3D-C4D	-2.17	1.39	1.44
24	A	406	CLA	C1C-NC	-2.16	1.34	1.37
24	b	618	CLA	C4C-C3C	2.16	1.48	1.45
24	B	605	CLA	C3D-C4D	-2.16	1.39	1.44
24	C	513	CLA	C1C-C2C	2.15	1.48	1.44
40	V	205	HEC	C1A-C2A	-2.15	1.41	1.45
24	b	617	CLA	C3B-C2B	2.15	1.48	1.41
24	C	506	CLA	C1B-C2B	2.15	1.48	1.43
24	b	614	CLA	C3B-C2B	2.15	1.48	1.41
24	c	510	CLA	C3B-C4B	2.15	1.49	1.42
24	b	624	CLA	C3B-C2B	2.15	1.48	1.41
33	b	629	LMG	O1-C1	2.15	1.43	1.40
24	C	506	CLA	C1C-C2C	2.15	1.48	1.44
24	c	514	CLA	C3D-C4D	-2.15	1.39	1.44
35	D	414	HTG	C1-S1	-2.15	1.77	1.80
24	B	617	CLA	C3B-C4B	2.14	1.49	1.42
31	A	417[B]	PL9	C2-C3	2.14	1.40	1.34
31	A	417[A]	PL9	C2-C3	2.14	1.40	1.34
24	b	615	CLA	C3B-C4B	2.14	1.49	1.42
24	B	602	CLA	C3D-C4D	-2.14	1.39	1.44
24	c	516	CLA	C4C-C3C	2.14	1.48	1.45
24	b	610	CLA	C3D-C4D	-2.14	1.39	1.44
24	b	614	CLA	C4C-C3C	2.14	1.48	1.45
24	C	512	CLA	C3B-C2B	2.13	1.48	1.41
24	B	607	CLA	C3B-C2B	2.13	1.48	1.41
24	B	608	CLA	C3B-C2B	2.13	1.48	1.41
24	d	403	CLA	C4C-C3C	2.13	1.48	1.45
24	b	612	CLA	C3B-C4B	2.13	1.48	1.42
25	d	402[A]	PHO	C1B-NB	-2.13	1.34	1.38
24	A	406	CLA	C4C-C3C	2.13	1.48	1.45
24	c	516	CLA	C3D-C4D	-2.12	1.39	1.44
24	c	511	CLA	C3D-C4D	-2.12	1.39	1.44
35	b	608	HTG	C1-S1	-2.12	1.77	1.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	509	CLA	C3B-C4B	2.11	1.48	1.42
24	b	621	CLA	C4C-C3C	2.11	1.48	1.45
24	A	405	CLA	C3B-C4B	2.11	1.48	1.42
24	c	515	CLA	C4C-C3C	2.11	1.48	1.45
24	b	624	CLA	C4C-C3C	2.11	1.48	1.45
24	b	625	CLA	C4C-C3C	2.11	1.48	1.45
24	B	606	CLA	C1D-C2D	2.10	1.49	1.45
24	b	611	CLA	C1D-C2D	2.10	1.49	1.45
24	c	516	CLA	C1B-C2B	2.10	1.48	1.43
24	C	501	CLA	C3D-C4D	-2.10	1.39	1.44
24	C	504	CLA	C3D-C4D	-2.10	1.39	1.44
24	D	405	CLA	C3B-C4B	2.10	1.48	1.42
35	c	523	HTG	C1-S1	-2.10	1.77	1.80
24	B	605	CLA	C1C-C2C	2.10	1.48	1.44
24	a	409	CLA	C3D-C4D	-2.09	1.39	1.44
24	c	507	CLA	C3B-C2B	2.09	1.48	1.41
24	C	501	CLA	C3B-C2B	2.09	1.48	1.41
29	a	404	LMT	O1'-C1'	2.09	1.43	1.40
24	C	508	CLA	C1C-C2C	2.09	1.48	1.44
24	c	515	CLA	C1D-C2D	2.09	1.49	1.45
24	B	607	CLA	C3B-C4B	2.09	1.48	1.42
24	b	613	CLA	MG-ND	-2.09	2.01	2.05
31	d	407[B]	PL9	C2-C3	2.09	1.39	1.34
24	c	515	CLA	C1C-C2C	2.09	1.48	1.44
24	c	514	CLA	C3B-C4B	2.09	1.48	1.42
25	D	401[B]	PHO	C3D-C4D	-2.09	1.38	1.41
24	B	604	CLA	C3B-C2B	2.09	1.48	1.41
24	B	609	CLA	C3B-C4B	2.09	1.48	1.42
24	B	605	CLA	C3B-C4B	2.08	1.48	1.42
24	b	615	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	602	CLA	C4C-C3C	2.08	1.48	1.45
24	C	507	CLA	C3B-C4B	2.08	1.48	1.42
24	c	516	CLA	C3B-C2B	2.08	1.48	1.41
24	c	505	CLA	C3D-C4D	-2.07	1.39	1.44
36	c	520	DGD	O5D-C1E	2.07	1.43	1.40
24	C	511	CLA	C3B-C4B	2.07	1.48	1.42
24	C	504	CLA	C3B-C4B	2.07	1.48	1.42
24	c	512	CLA	C3B-C4B	2.07	1.48	1.42
29	T	104	LMT	O1'-C1'	2.07	1.43	1.40
33	Z	101	LMG	O1-C1	2.07	1.43	1.40
36	e	101	DGD	O5D-C1E	2.07	1.43	1.40
24	D	405	CLA	C1C-NC	-2.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	D	407[B]	PL9	C2-C3	2.07	1.39	1.34
24	B	611	CLA	C1D-C2D	2.07	1.49	1.45
24	b	622	CLA	C1C-C2C	2.06	1.48	1.44
24	C	512	CLA	C3D-C4D	-2.05	1.39	1.44
24	b	619	CLA	C1D-C2D	2.05	1.49	1.45
24	B	608	CLA	C3B-C4B	2.05	1.48	1.42
24	D	405	CLA	C1C-C2C	2.05	1.48	1.44
24	C	505	CLA	C3B-C2B	2.05	1.48	1.41
24	C	507	CLA	C3B-C2B	2.05	1.48	1.41
29	M	104	LMT	O1'-C1'	2.05	1.43	1.40
24	B	602	CLA	C1D-C2D	2.05	1.49	1.45
24	B	602	CLA	C1C-NC	-2.04	1.34	1.37
31	D	407[A]	PL9	C2-C3	2.04	1.39	1.34
24	C	503	CLA	C3B-C2B	2.04	1.48	1.41
24	a	412	CLA	C1C-C2C	2.04	1.48	1.44
24	d	404	CLA	C3B-C2B	2.04	1.48	1.41
25	d	402[B]	PHO	CBD-CGD	-2.04	1.49	1.52
35	V	206	HTG	C1-S1	-2.03	1.77	1.80
35	c	524	HTG	C1-S1	-2.03	1.77	1.80
24	b	621	CLA	C3D-C4D	-2.03	1.39	1.44
24	b	619	CLA	C1C-C2C	2.03	1.48	1.44
24	c	517	CLA	C3B-C2B	2.03	1.48	1.41
24	b	615	CLA	C4C-C3C	2.03	1.48	1.45
38	f	101	HEM	C3B-C4B	2.03	1.48	1.44
24	c	509	CLA	C3B-C2B	2.03	1.48	1.41
24	c	506	CLA	C1C-NC	-2.03	1.34	1.37
24	A	407	CLA	C3B-C2B	2.02	1.48	1.41
24	A	409	CLA	C1D-C2D	2.02	1.49	1.45
24	b	624	CLA	C1D-C2D	2.02	1.49	1.45
24	d	405	CLA	C3B-C2B	2.02	1.48	1.41
24	B	615	CLA	C4C-C3C	2.02	1.48	1.45
29	e	102	LMT	O1'-C1'	2.02	1.43	1.40
26	b	628	BCR	C30-C25	-2.02	1.51	1.53
24	A	406	CLA	C3B-C4B	2.02	1.48	1.42
24	B	603	CLA	C4B-NB	-2.01	1.35	1.37
26	H	101	BCR	C30-C25	-2.01	1.51	1.53
24	B	615	CLA	C3B-C4B	2.01	1.48	1.42
40	V	205	HEC	C4A-C3A	-2.01	1.41	1.45
24	b	622	CLA	C3B-C4B	2.01	1.48	1.42
24	C	507	CLA	C3D-C4D	-2.01	1.39	1.44
40	V	205	HEC	C1D-C2D	2.00	1.47	1.43
24	C	506	CLA	C3B-C2B	2.00	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	412	CLA	C3B-C2B	2.00	1.47	1.41
40	V	205	HEC	C3B-C4B	2.00	1.49	1.46

All (2967) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	402[B]	PHO	C2D-C1D-ND	11.68	117.87	109.43
25	D	401[B]	PHO	C2D-C1D-ND	11.34	117.63	109.43
25	D	401[A]	PHO	C2D-C1D-ND	11.13	117.47	109.43
25	d	402[A]	PHO	C2D-C1D-ND	10.96	117.36	109.43
25	A	408	PHO	C2D-C1D-ND	10.95	117.35	109.43
25	a	411	PHO	C2D-C1D-ND	10.89	117.30	109.43
24	B	613	CLA	C1D-ND-C4D	-10.27	99.11	106.31
24	b	621	CLA	C1D-ND-C4D	-10.20	99.16	106.31
24	B	606	CLA	C1D-ND-C4D	-10.08	99.24	106.31
24	A	407	CLA	C1D-ND-C4D	-10.02	99.28	106.31
24	a	412	CLA	C1D-ND-C4D	-9.95	99.33	106.31
24	c	515	CLA	C1D-ND-C4D	-9.90	99.36	106.31
24	B	615	CLA	C1D-ND-C4D	-9.90	99.37	106.31
24	C	503	CLA	C1D-ND-C4D	-9.89	99.37	106.31
24	b	614	CLA	C1D-ND-C4D	-9.88	99.38	106.31
24	a	410	CLA	C1D-ND-C4D	-9.86	99.40	106.31
24	C	501	CLA	C1D-ND-C4D	-9.77	99.46	106.31
24	c	517	CLA	C1D-ND-C4D	-9.68	99.52	106.31
24	B	611	CLA	C1D-ND-C4D	-9.67	99.52	106.31
24	B	602	CLA	C1D-ND-C4D	-9.67	99.53	106.31
24	b	611	CLA	C1D-ND-C4D	-9.67	99.53	106.31
24	c	509	CLA	C1D-ND-C4D	-9.60	99.58	106.31
24	B	607	CLA	C1D-ND-C4D	-9.43	99.69	106.31
24	b	618	CLA	C1D-ND-C4D	-9.43	99.70	106.31
24	D	404	CLA	C1D-ND-C4D	-9.41	99.71	106.31
24	c	508	CLA	C1D-ND-C4D	-9.38	99.73	106.31
24	C	513	CLA	C1D-ND-C4D	-9.29	99.79	106.31
24	A	406	CLA	C1D-ND-C4D	-9.27	99.81	106.31
24	b	612	CLA	C1D-ND-C4D	-9.26	99.81	106.31
24	C	511	CLA	C1D-ND-C4D	-9.26	99.82	106.31
24	B	603	CLA	C1D-ND-C4D	-9.24	99.83	106.31
24	c	514	CLA	C1D-ND-C4D	-9.19	99.86	106.31
24	D	405	CLA	C1D-ND-C4D	-9.16	99.88	106.31
24	c	505	CLA	C1D-ND-C4D	-9.15	99.89	106.31
24	d	403	CLA	C1D-ND-C4D	-9.14	99.90	106.31
24	B	610	CLA	C1D-ND-C4D	-9.11	99.92	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C1D-ND-C4D	-9.07	99.95	106.31
24	a	409	CLA	C1D-ND-C4D	-9.06	99.96	106.31
24	B	609	CLA	C1D-ND-C4D	-9.05	99.96	106.31
24	c	507	CLA	C1D-ND-C4D	-9.05	99.96	106.31
24	C	509	CLA	C1D-ND-C4D	-9.04	99.97	106.31
24	b	617	CLA	C1D-ND-C4D	-9.03	99.97	106.31
24	b	624	CLA	C1D-ND-C4D	-9.03	99.98	106.31
24	C	512	CLA	C1D-ND-C4D	-9.01	99.99	106.31
24	C	502	CLA	C1D-ND-C4D	-9.00	100.00	106.31
24	b	623	CLA	C1D-ND-C4D	-8.99	100.00	106.31
24	d	405	CLA	C1D-ND-C4D	-8.99	100.01	106.31
24	B	616	CLA	C1D-ND-C4D	-8.97	100.02	106.31
24	B	612	CLA	C1D-ND-C4D	-8.95	100.03	106.31
24	b	625	CLA	C1D-ND-C4D	-8.93	100.04	106.31
25	d	402[A]	PHO	O2D-CGD-CBD	8.93	120.76	110.95
24	b	610	CLA	C1D-ND-C4D	-8.91	100.06	106.31
24	c	511	CLA	C1D-ND-C4D	-8.90	100.07	106.31
24	B	604	CLA	C1D-ND-C4D	-8.89	100.08	106.31
24	c	516	CLA	C1D-ND-C4D	-8.88	100.08	106.31
24	b	619	CLA	C1D-ND-C4D	-8.84	100.11	106.31
24	b	615	CLA	C1D-ND-C4D	-8.84	100.11	106.31
24	C	505	CLA	C1D-ND-C4D	-8.80	100.14	106.31
24	c	512	CLA	C1D-ND-C4D	-8.77	100.16	106.31
24	c	513	CLA	C1D-ND-C4D	-8.77	100.16	106.31
24	C	507	CLA	C1D-ND-C4D	-8.76	100.17	106.31
24	d	404	CLA	C1D-ND-C4D	-8.74	100.18	106.31
25	A	408	PHO	O2D-CGD-CBD	8.70	120.51	110.95
24	c	510	CLA	C1D-ND-C4D	-8.69	100.22	106.31
24	b	620	CLA	C1D-ND-C4D	-8.68	100.22	106.31
24	A	409	CLA	C1D-ND-C4D	-8.66	100.24	106.31
24	C	504	CLA	C1D-ND-C4D	-8.55	100.31	106.31
24	B	608	CLA	C1D-ND-C4D	-8.55	100.31	106.31
24	B	617	CLA	C1D-ND-C4D	-8.55	100.31	106.31
24	c	506	CLA	C1D-ND-C4D	-8.54	100.32	106.31
24	C	510	CLA	C1D-ND-C4D	-8.48	100.36	106.31
25	d	402[B]	PHO	O2D-CGD-CBD	8.47	120.25	110.95
24	b	616	CLA	C1D-ND-C4D	-8.42	100.40	106.31
24	B	614	CLA	C1D-ND-C4D	-8.38	100.43	106.31
24	C	506	CLA	C1D-ND-C4D	-8.02	100.68	106.31
24	B	605	CLA	C1D-ND-C4D	-8.01	100.69	106.31
25	A	408	PHO	C3B-C4B-NB	8.00	112.67	107.46
24	b	613	CLA	C1D-ND-C4D	-7.99	100.70	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	402[A]	PHO	C3B-C4B-NB	7.98	112.66	107.46
25	d	402[B]	PHO	C3B-C4B-NB	7.95	112.64	107.46
25	a	411	PHO	O2D-CGD-CBD	7.92	119.65	110.95
25	a	411	PHO	C3B-C4B-NB	7.88	112.60	107.46
24	b	622	CLA	C1D-ND-C4D	-7.82	100.82	106.31
24	A	405	CLA	C1D-ND-C4D	-7.76	100.86	106.31
25	D	401[A]	PHO	O2D-CGD-CBD	7.45	119.14	110.95
24	d	404	CLA	C4A-NA-C1A	-7.38	103.31	106.68
24	B	611	CLA	CMD-C2D-C1D	7.34	137.66	124.73
25	D	401[B]	PHO	C3B-C4B-NB	7.30	112.22	107.46
24	b	622	CLA	CMD-C2D-C1D	7.29	137.57	124.73
24	b	611	CLA	CMD-C2D-C1D	7.26	137.52	124.73
24	c	516	CLA	C4A-NA-C1A	-7.26	103.37	106.68
24	B	608	CLA	CMD-C2D-C1D	7.17	137.36	124.73
24	b	619	CLA	CMD-C2D-C1D	7.12	137.27	124.73
25	D	401[A]	PHO	C3B-C4B-NB	7.09	112.09	107.46
24	B	607	CLA	CMD-C2D-C1D	7.07	137.17	124.73
24	b	616	CLA	CMD-C2D-C1D	7.03	137.11	124.73
24	A	405	CLA	C4A-NA-C1A	-7.02	103.48	106.68
24	C	503	CLA	C4A-NA-C1A	-7.01	103.48	106.68
24	B	613	CLA	C2D-C1D-ND	6.96	117.01	110.13
24	c	510	CLA	CMD-C2D-C1D	6.87	136.82	124.73
24	c	511	CLA	O2D-CGD-CBD	6.87	123.23	111.23
24	b	621	CLA	C2D-C1D-ND	6.85	116.91	110.13
25	d	402[A]	PHO	C2B-C1B-NB	6.85	114.38	109.43
24	b	621	CLA	CHD-C4C-C3C	-6.85	114.79	124.77
24	c	507	CLA	CMD-C2D-C1D	6.83	136.75	124.73
24	B	605	CLA	CMD-C2D-C1D	6.82	136.74	124.73
24	c	516	CLA	O2D-CGD-CBD	6.79	123.09	111.23
24	B	606	CLA	CMD-C2D-C1D	6.77	136.66	124.73
24	b	623	CLA	O2D-CGD-CBD	6.75	123.04	111.23
24	B	615	CLA	C2D-C1D-ND	6.74	116.80	110.13
24	A	406	CLA	CMD-C2D-C1D	6.69	136.51	124.73
24	B	616	CLA	CHD-C4C-C3C	-6.66	115.06	124.77
24	B	614	CLA	CMD-C2D-C1D	6.66	136.45	124.73
25	D	401[A]	PHO	C2B-C1B-NB	6.64	114.23	109.43
24	a	410	CLA	CMD-C2D-C1D	6.62	136.39	124.73
24	A	405	CLA	CMD-C2D-C1D	6.62	136.38	124.73
24	B	615	CLA	CHD-C4C-C3C	-6.62	115.13	124.77
24	b	614	CLA	CHD-C4C-C3C	-6.61	115.14	124.77
24	a	409	CLA	C4A-NA-C1A	-6.60	103.67	106.68
24	C	509	CLA	CMD-C2D-C1D	6.57	136.29	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	C4A-NA-C1A	-6.54	103.70	106.68
24	b	623	CLA	CMD-C2D-C1D	6.54	136.24	124.73
24	C	504	CLA	CMD-C2D-C1D	6.53	136.22	124.73
24	B	602	CLA	CMD-C2D-C1D	6.51	136.20	124.73
24	C	510	CLA	CMD-C2D-C1D	6.51	136.19	124.73
24	B	603	CLA	CMD-C2D-C1D	6.50	136.17	124.73
24	D	405	CLA	CMD-C2D-C1D	6.49	136.16	124.73
24	B	603	CLA	C4A-NA-C1A	-6.49	103.72	106.68
24	b	624	CLA	CMD-C2D-C1D	6.48	136.14	124.73
24	B	604	CLA	CMD-C2D-C1D	6.48	136.14	124.73
24	b	618	CLA	CMD-C2D-C1D	6.46	136.11	124.73
24	A	407	CLA	CMD-C2D-C1D	6.45	136.09	124.73
24	c	517	CLA	CMD-C2D-C1D	6.44	136.07	124.73
24	c	511	CLA	CHD-C4C-C3C	-6.44	115.38	124.77
24	A	409	CLA	CMD-C2D-C1D	6.44	136.06	124.73
24	B	613	CLA	CHD-C4C-C3C	-6.43	115.39	124.77
25	d	402[B]	PHO	C2B-C1B-NB	6.43	114.08	109.43
24	b	619	CLA	C4A-NA-C1A	-6.43	103.75	106.68
24	b	614	CLA	CMD-C2D-C1D	6.41	136.03	124.73
24	d	403	CLA	CMD-C2D-C1D	6.40	136.01	124.73
25	A	408	PHO	C2B-C1B-NB	6.38	114.04	109.43
24	B	617	CLA	CMD-C2D-C1D	6.38	135.96	124.73
24	C	504	CLA	O2D-CGD-CBD	6.36	122.35	111.23
25	d	402[B]	PHO	C4D-ND-C1D	-6.36	101.25	108.87
24	b	614	CLA	C2D-C1D-ND	6.36	116.42	110.13
24	c	513	CLA	CMD-C2D-C1D	6.35	135.90	124.73
24	b	625	CLA	O2D-CGD-CBD	6.34	122.31	111.23
24	C	513	CLA	CMD-C2D-C1D	6.34	135.89	124.73
24	a	409	CLA	CMD-C2D-C1D	6.33	135.88	124.73
24	c	515	CLA	CMD-C2D-C1D	6.33	135.87	124.73
24	c	507	CLA	CHD-C4C-C3C	-6.33	115.55	124.77
24	C	507	CLA	CMD-C2D-C1D	6.32	135.85	124.73
24	c	508	CLA	C2D-C1D-ND	6.31	116.38	110.13
24	b	610	CLA	O2D-CGD-CBD	6.29	122.22	111.23
24	c	512	CLA	C2D-C1D-ND	6.28	116.34	110.13
24	a	412	CLA	C2D-C1D-ND	6.26	116.33	110.13
24	A	406	CLA	C2D-C1D-ND	6.26	116.32	110.13
24	B	607	CLA	CHD-C4C-C3C	-6.24	115.67	124.77
24	c	511	CLA	CMD-C2D-C1D	6.24	135.72	124.73
24	c	512	CLA	CHD-C4C-C3C	-6.24	115.67	124.77
24	c	514	CLA	CMD-C2D-C1D	6.23	135.70	124.73
24	C	503	CLA	CHD-C4C-C3C	-6.21	115.72	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
24	C	512	CLA	CHD-C4C-C3C	-6.21	115.72	124.77
24	b	615	CLA	CMD-C2D-C1D	6.20	135.65	124.73
24	B	603	CLA	CHD-C4C-C3C	-6.19	115.74	124.77
24	b	615	CLA	CHD-C4C-C3C	-6.18	115.77	124.77
24	a	410	CLA	CHD-C4C-C3C	-6.16	115.79	124.77
24	C	501	CLA	C2D-C1D-ND	6.15	116.22	110.13
24	D	404	CLA	C2D-C1D-ND	6.15	116.21	110.13
24	C	506	CLA	CMD-C2D-C1D	6.14	135.54	124.73
24	d	405	CLA	CHD-C4C-C3C	-6.14	115.82	124.77
24	C	501	CLA	O2D-CGD-CBD	6.13	121.95	111.23
24	C	512	CLA	C2D-C1D-ND	6.13	116.19	110.13
24	B	609	CLA	CMD-C2D-C1D	6.12	135.51	124.73
24	c	511	CLA	C2D-C1D-ND	6.12	116.18	110.13
24	C	503	CLA	CMD-C2D-C1D	6.12	135.50	124.73
24	C	503	CLA	C2D-C1D-ND	6.11	116.17	110.13
24	b	624	CLA	CHD-C4C-C3C	-6.11	115.87	124.77
24	c	508	CLA	CMD-C2D-C1D	6.10	135.47	124.73
24	C	502	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
24	c	515	CLA	C2D-C1D-ND	6.09	116.15	110.13
24	c	509	CLA	CMD-C2D-C1D	6.09	135.44	124.73
24	b	615	CLA	C2D-C1D-ND	6.08	116.15	110.13
24	c	505	CLA	C2D-C1D-ND	6.08	116.14	110.13
24	B	607	CLA	C2D-C1D-ND	6.07	116.14	110.13
24	b	618	CLA	C2D-C1D-ND	6.07	116.13	110.13
24	b	610	CLA	CMD-C2D-C1D	6.06	135.41	124.73
24	b	613	CLA	C4A-NA-C1A	-6.06	103.91	106.68
24	b	625	CLA	C4A-NA-C1A	-6.05	103.92	106.68
24	B	613	CLA	O2D-CGD-CBD	6.05	121.80	111.23
24	B	607	CLA	C4A-NA-C1A	-6.05	103.92	106.68
24	b	618	CLA	CHD-C4C-C3C	-6.05	115.96	124.77
24	c	507	CLA	C2D-C1D-ND	6.02	116.09	110.13
24	d	405	CLA	CMD-C2D-C1D	6.02	135.34	124.73
24	C	508	CLA	CMD-C2D-C1D	6.02	135.33	124.73
24	B	610	CLA	CMD-C2D-C1D	6.02	135.33	124.73
24	b	611	CLA	C4A-NA-C1A	-6.02	103.93	106.68
24	B	616	CLA	C2D-C1D-ND	6.02	116.08	110.13
24	C	501	CLA	CHD-C4C-C3C	-6.01	116.00	124.77
24	b	612	CLA	CHD-C4C-C3C	-6.01	116.00	124.77
24	a	410	CLA	C2D-C1D-ND	6.00	116.07	110.13
24	B	602	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
24	b	616	CLA	CHD-C4C-C3C	-5.99	116.04	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	625	CLA	CHD-C4C-C3C	-5.99	116.04	124.77
24	C	512	CLA	O2D-CGD-CBD	5.98	121.69	111.23
24	C	502	CLA	C2D-C1D-ND	5.98	116.04	110.13
25	d	402[A]	PHO	C4D-ND-C1D	-5.98	101.71	108.87
24	d	403	CLA	C2C-C1C-NC	5.98	116.26	109.98
24	B	602	CLA	O2D-CGD-CBD	5.97	121.67	111.23
24	b	617	CLA	C4A-NA-C1A	-5.97	103.96	106.68
24	C	511	CLA	C2D-C1D-ND	5.97	116.03	110.13
24	B	612	CLA	C4A-NA-C1A	-5.96	103.96	106.68
24	C	507	CLA	CHD-C4C-C3C	-5.95	116.10	124.77
24	c	505	CLA	CMD-C2D-C1D	5.94	135.19	124.73
24	b	613	CLA	O2D-CGD-CBD	5.94	121.61	111.23
24	C	507	CLA	C2D-C1D-ND	5.93	116.00	110.13
24	D	404	CLA	CMD-C2D-C1D	5.93	135.17	124.73
24	b	612	CLA	C2D-C1D-ND	5.92	115.99	110.13
24	B	611	CLA	CHD-C4C-C3C	-5.92	116.14	124.77
24	b	611	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
24	b	622	CLA	C2C-C1C-NC	5.90	116.18	109.98
24	b	610	CLA	CHD-C4C-C3C	-5.89	116.18	124.77
24	B	614	CLA	C2D-C1D-ND	5.89	115.96	110.13
24	b	624	CLA	C2D-C1D-ND	5.89	115.96	110.13
24	B	617	CLA	O2D-CGD-CBD	5.89	121.53	111.23
25	D	401[B]	PHO	O2D-CGD-CBD	5.89	117.42	110.95
24	b	613	CLA	CMD-C2D-C1D	5.87	135.07	124.73
24	D	404	CLA	C2C-C1C-NC	5.87	116.15	109.98
35	C	522	HTG	C1'-S1-C1	5.87	113.13	100.45
24	d	403	CLA	C2D-C1D-ND	5.87	115.94	110.13
24	A	407	CLA	C2D-C1D-ND	5.87	115.93	110.13
24	C	511	CLA	CMD-C2D-C1D	5.86	135.05	124.73
24	B	604	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
24	C	501	CLA	CMD-C2D-C1D	5.86	135.05	124.73
24	c	509	CLA	C4A-NA-C1A	-5.86	104.01	106.68
25	D	401[B]	PHO	C2B-C1B-NB	5.86	113.66	109.43
24	B	617	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
24	c	517	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
24	C	505	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
24	b	613	CLA	C2D-C1D-ND	5.84	115.91	110.13
24	C	508	CLA	O2D-CGD-CBD	5.84	121.44	111.23
24	B	612	CLA	C2D-C1D-ND	5.84	115.90	110.13
24	B	615	CLA	O2D-CGD-CBD	5.84	121.43	111.23
27	L	102	SQD	O6-C1-C2	5.83	117.13	108.27
24	B	611	CLA	C2D-C1D-ND	5.83	115.90	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	614	CLA	C4A-NA-C1A	-5.83	104.02	106.68
24	b	622	CLA	C3B-C4B-NB	5.83	115.73	110.53
24	b	623	CLA	C2D-C1D-ND	5.82	115.89	110.13
24	A	407	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
24	B	615	CLA	CMD-C2D-C1D	5.82	134.97	124.73
24	A	405	CLA	C2B-C1B-NB	5.81	116.35	110.33
24	B	616	CLA	CMD-C2D-C1D	5.80	134.95	124.73
24	b	612	CLA	C4A-NA-C1A	-5.80	104.03	106.68
24	D	404	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
24	C	505	CLA	C4A-NA-C1A	-5.79	104.04	106.68
24	b	617	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
24	B	610	CLA	C2D-C1D-ND	5.78	115.85	110.13
24	B	606	CLA	C2D-C1D-ND	5.78	115.85	110.13
25	A	408	PHO	C4D-ND-C1D	-5.78	101.95	108.87
24	c	517	CLA	C2D-C1D-ND	5.76	115.83	110.13
24	B	609	CLA	C2C-C1C-NC	5.76	116.03	109.98
24	b	612	CLA	CMD-C2D-C1D	5.75	134.86	124.73
24	c	515	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
24	C	504	CLA	C2D-C1D-ND	5.75	115.81	110.13
24	B	602	CLA	C2D-C1D-ND	5.74	115.81	110.13
24	A	406	CLA	CHD-C4C-C3C	-5.74	116.41	124.77
25	D	401[B]	PHO	C4D-ND-C1D	-5.74	102.00	108.87
35	d	413	HTG	C1'-S1-C1	5.73	112.83	100.45
24	b	621	CLA	O2D-CGD-CBD	5.73	121.25	111.23
24	c	509	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
24	B	605	CLA	C2D-C1D-ND	5.73	115.79	110.13
24	C	504	CLA	C4A-NA-C1A	-5.71	104.07	106.68
24	b	625	CLA	C2D-C1D-ND	5.71	115.78	110.13
24	D	405	CLA	C2D-C1D-ND	5.71	115.77	110.13
24	b	617	CLA	C2D-C1D-ND	5.68	115.75	110.13
24	a	412	CLA	O2D-CGD-CBD	5.68	121.16	111.23
24	d	404	CLA	CMD-C2D-C1D	5.68	134.73	124.73
24	b	616	CLA	C2D-C1D-ND	5.67	115.74	110.13
24	d	405	CLA	C2D-C1D-ND	5.66	115.73	110.13
24	b	611	CLA	C2D-C1D-ND	5.66	115.72	110.13
24	C	505	CLA	CMD-C2D-C1D	5.66	134.69	124.73
24	c	508	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
24	C	505	CLA	O2D-CGD-CBD	5.64	121.10	111.23
24	C	509	CLA	C2D-C1D-ND	5.63	115.70	110.13
24	c	506	CLA	CHD-C4C-C3C	-5.63	116.56	124.77
24	b	620	CLA	C2C-C1C-NC	5.63	115.89	109.98
24	c	505	CLA	CHD-C4C-C3C	-5.63	116.57	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Y	101	BCR	C33-C5-C6	-5.63	118.34	124.48
24	c	505	CLA	O2D-CGD-CBD	5.61	121.04	111.23
24	b	620	CLA	C2D-C1D-ND	5.61	115.68	110.13
24	c	513	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
24	b	618	CLA	O2D-CGD-CBD	5.61	121.03	111.23
24	C	502	CLA	CMD-C2D-C1D	5.60	134.60	124.73
24	B	604	CLA	O2D-CGD-CBD	5.59	121.01	111.23
24	b	613	CLA	C2C-C1C-NC	5.59	115.86	109.98
24	b	613	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
24	B	605	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
24	b	623	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
24	c	516	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
24	B	612	CLA	CHD-C4C-C3C	-5.56	116.67	124.77
24	a	412	CLA	CHD-C4C-C3C	-5.55	116.68	124.77
24	c	516	CLA	C2B-C1B-NB	5.55	116.08	110.33
24	D	404	CLA	C4A-NA-C1A	-5.55	104.15	106.68
24	b	625	CLA	CMD-C2D-C1D	5.54	134.49	124.73
24	c	509	CLA	O2D-CGD-CBD	5.54	120.91	111.23
24	b	612	CLA	O2D-CGD-CBD	5.53	120.90	111.23
24	B	605	CLA	C2C-C1C-NC	5.52	115.78	109.98
24	b	614	CLA	O2D-CGD-CBD	5.52	120.89	111.23
25	a	411	PHO	C2B-C1B-NB	5.52	113.42	109.43
24	B	608	CLA	C2D-C1D-ND	5.52	115.59	110.13
24	B	617	CLA	C4A-NA-C1A	-5.51	104.17	106.68
24	c	514	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
24	d	405	CLA	C4A-NA-C1A	-5.50	104.17	106.68
24	C	508	CLA	C2D-C1D-ND	5.48	115.55	110.13
24	d	404	CLA	C2D-C1D-ND	5.48	115.55	110.13
24	B	609	CLA	C2D-C1D-ND	5.47	115.54	110.13
24	B	617	CLA	C2D-C1D-ND	5.46	115.53	110.13
25	d	402[A]	PHO	C1-C2-C3	-5.46	117.25	126.20
25	d	402[B]	PHO	C3D-C4D-ND	5.45	114.69	107.71
24	c	508	CLA	O2D-CGD-CBD	5.45	120.75	111.23
24	b	610	CLA	C2D-C1D-ND	5.45	115.52	110.13
24	B	604	CLA	C2D-C1D-ND	5.45	115.52	110.13
24	C	513	CLA	C2D-C1D-ND	5.44	115.51	110.13
25	D	401[A]	PHO	C4D-ND-C1D	-5.43	102.37	108.87
35	B	624	HTG	O5-C1-C2	5.42	117.80	110.32
24	C	509	CLA	CHD-C4C-C3C	-5.42	116.86	124.77
26	C	515	BCR	C7-C8-C9	-5.42	118.22	126.23
24	B	605	CLA	O2D-CGD-CBD	5.41	120.69	111.23
24	B	614	CLA	CHD-C4C-C3C	-5.41	116.88	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	610	CLA	CHD-C4C-C3C	-5.41	116.89	124.77
38	E	103	HEM	CHC-C4B-NB	5.40	130.24	124.42
24	c	516	CLA	CMD-C2D-C1D	5.40	134.24	124.73
24	c	516	CLA	C3B-C2B-C1B	-5.40	100.81	107.17
25	D	401[A]	PHO	C1-C2-C3	-5.40	117.35	126.20
27	f	102	SQD	O47-C7-C8	5.38	123.12	111.48
24	B	612	CLA	C2C-C1C-NC	5.37	115.63	109.98
25	a	411	PHO	C4D-ND-C1D	-5.37	102.44	108.87
24	B	603	CLA	C2D-C1D-ND	5.37	115.44	110.13
24	c	506	CLA	C2D-C1D-ND	5.37	115.44	110.13
24	A	407	CLA	O2D-CGD-CBD	5.36	120.60	111.23
24	c	516	CLA	C2D-C1D-ND	5.36	115.43	110.13
24	c	506	CLA	CMD-C2D-C1D	5.36	134.16	124.73
24	B	614	CLA	C2C-C1C-NC	5.36	115.61	109.98
24	a	412	CLA	CMD-C2D-C1D	5.36	134.16	124.73
25	d	402[A]	PHO	C3D-C4D-ND	5.35	114.57	107.71
24	c	513	CLA	C2D-C1D-ND	5.35	115.42	110.13
24	B	612	CLA	CMD-C2D-C1D	5.35	134.15	124.73
24	C	506	CLA	C2D-C1D-ND	5.34	115.42	110.13
24	c	509	CLA	C2D-C1D-ND	5.34	115.41	110.13
24	c	514	CLA	C2D-C1D-ND	5.34	115.41	110.13
24	d	403	CLA	C3B-C4B-NB	5.34	115.30	110.53
24	C	508	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
24	C	511	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
24	a	409	CLA	C2C-C1C-NC	5.33	115.58	109.98
24	A	406	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
24	C	510	CLA	O2D-CGD-CBD	5.32	120.54	111.23
24	b	624	CLA	C4A-NA-C1A	-5.32	104.25	106.68
25	d	402[B]	PHO	C1-C2-C3	-5.32	117.48	126.20
24	b	619	CLA	CHD-C4C-C3C	-5.30	117.04	124.77
24	b	617	CLA	CMD-C2D-C1D	5.30	134.06	124.73
24	C	504	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
24	d	403	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
24	c	517	CLA	C4A-NA-C1A	-5.30	104.26	106.68
24	d	404	CLA	CHD-C4C-C3C	-5.28	117.07	124.77
24	b	619	CLA	C2D-C1D-ND	5.28	115.35	110.13
24	B	610	CLA	C2C-C1C-NC	5.27	115.52	109.98
24	b	616	CLA	O2D-CGD-CBD	5.26	120.43	111.23
24	c	514	CLA	O2D-CGD-CBD	5.26	120.43	111.23
24	C	507	CLA	C3B-C2B-C1B	-5.26	100.97	107.17
24	b	610	CLA	C4A-NA-C1A	-5.26	104.28	106.68
24	d	404	CLA	C2C-C1C-NC	5.26	115.50	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	503	CLA	O2D-CGD-CBD	5.25	120.42	111.23
24	C	512	CLA	C4A-NA-C1A	-5.25	104.28	106.68
24	a	409	CLA	C2D-C1D-ND	5.25	115.32	110.13
24	d	405	CLA	O2D-CGD-CBD	5.25	120.40	111.23
24	b	611	CLA	C3B-C2B-C1B	-5.25	100.99	107.17
25	D	401[B]	PHO	C3D-C4D-ND	5.24	114.43	107.71
25	A	408	PHO	C3D-C4D-ND	5.24	114.42	107.71
24	B	608	CLA	C4A-NA-C1A	-5.22	104.30	106.68
24	D	405	CLA	CHD-C4C-C3C	-5.21	117.18	124.77
24	b	620	CLA	CMD-C2D-C1D	5.20	133.88	124.73
24	c	514	CLA	C2C-C1C-NC	5.20	115.44	109.98
24	B	606	CLA	O2D-CGD-CBD	5.19	120.31	111.23
24	b	620	CLA	CHD-C4C-C3C	-5.19	117.20	124.77
24	A	406	CLA	C2C-C1C-NC	5.19	115.44	109.98
24	B	611	CLA	C4A-NA-C1A	-5.19	104.31	106.68
24	c	513	CLA	O2D-CGD-CBD	5.19	120.30	111.23
24	c	510	CLA	C2D-C1D-ND	5.19	115.26	110.13
24	B	604	CLA	C4A-NA-C1A	-5.18	104.31	106.68
24	b	617	CLA	O2D-CGD-CBD	5.18	120.29	111.23
24	C	506	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
24	c	512	CLA	O2D-CGD-CBD	5.17	120.27	111.23
24	c	506	CLA	C3B-C2B-C1B	-5.17	101.07	107.17
24	C	508	CLA	C4A-NA-C1A	-5.17	104.32	106.68
24	C	510	CLA	CHD-C4C-C3C	-5.17	117.24	124.77
24	c	510	CLA	CHD-C4C-C3C	-5.17	117.24	124.77
24	C	510	CLA	C2C-C1C-NC	5.16	115.41	109.98
24	A	405	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
24	B	603	CLA	O2D-CGD-CBD	5.16	120.25	111.23
24	c	506	CLA	C4A-NA-C1A	-5.16	104.33	106.68
24	a	409	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
24	C	504	CLA	C2B-C1B-NB	5.15	115.67	110.33
24	B	612	CLA	O2D-CGD-CBD	5.15	120.23	111.23
24	C	513	CLA	CHD-C4C-C3C	-5.15	117.27	124.77
24	C	512	CLA	CMD-C2D-C1D	5.14	133.78	124.73
24	c	510	CLA	C2C-C1C-NC	5.14	115.38	109.98
24	A	406	CLA	C2B-C1B-NB	5.14	115.65	110.33
24	B	608	CLA	CHD-C4C-C3C	-5.13	117.29	124.77
24	C	508	CLA	C2B-C1B-NB	5.13	115.64	110.33
24	b	610	CLA	C2B-C1B-NB	5.13	115.64	110.33
24	A	409	CLA	C2C-C1C-NC	5.12	115.36	109.98
24	b	614	CLA	C4A-NA-C1A	-5.12	104.34	106.68
24	A	409	CLA	C3B-C2B-C1B	-5.12	101.13	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	CLA	C3D-C4D-ND	5.12	118.30	109.99
24	C	509	CLA	O2D-CGD-CBD	5.11	120.17	111.23
24	C	506	CLA	C2C-C1C-NC	5.11	115.35	109.98
40	v	206	HEC	CBB-CAB-C3B	-5.11	117.22	127.43
24	C	504	CLA	C3B-C2B-C1B	-5.11	101.15	107.17
24	c	510	CLA	C4A-NA-C1A	-5.10	104.35	106.68
24	c	508	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
24	C	513	CLA	C2B-C1B-NB	5.09	115.61	110.33
26	D	406	BCR	C7-C8-C9	-5.09	118.71	126.23
24	C	513	CLA	C4A-NA-C1A	-5.08	104.36	106.68
24	b	620	CLA	O2D-CGD-CBD	5.08	120.11	111.23
26	H	101	BCR	C7-C8-C9	-5.07	118.73	126.23
24	A	406	CLA	C3D-C2D-C1D	-5.07	98.91	105.83
24	C	510	CLA	C2D-C1D-ND	5.07	115.14	110.13
24	B	608	CLA	O2D-CGD-CBD	5.07	120.09	111.23
25	D	401[A]	PHO	C3D-C4D-ND	5.06	114.20	107.71
24	c	515	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
24	b	619	CLA	C2B-C1B-NB	5.05	115.56	110.33
24	b	622	CLA	C2D-C1D-ND	5.05	115.12	110.13
24	A	407	CLA	C2B-C1B-NB	5.04	115.55	110.33
24	D	405	CLA	O2D-CGD-CBD	5.04	120.04	111.23
24	A	409	CLA	C2D-C1D-ND	5.03	115.10	110.13
24	c	512	CLA	C2C-C1C-NC	5.02	115.25	109.98
24	b	615	CLA	O2D-CGD-CBD	5.01	120.00	111.23
24	c	507	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
26	T	103	BCR	C33-C5-C6	-5.00	119.03	124.48
24	c	509	CLA	C2C-C1C-NC	4.99	115.22	109.98
24	A	406	CLA	O2D-CGD-CBD	4.99	119.95	111.23
24	C	513	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
24	C	505	CLA	C2D-C1D-ND	4.99	115.06	110.13
24	C	501	CLA	C4A-NA-C1A	-4.98	104.41	106.68
27	F	101	SQD	O47-C7-C8	4.98	122.25	111.48
24	A	409	CLA	CHD-C4C-C3C	-4.97	117.52	124.77
24	b	618	CLA	C4A-NA-C1A	-4.97	104.41	106.68
24	B	606	CLA	C3D-C4D-ND	4.97	118.06	109.99
24	a	410	CLA	C4A-NA-C1A	-4.97	104.41	106.68
24	b	612	CLA	C2C-C1C-NC	4.97	115.20	109.98
24	C	509	CLA	C1-C2-C3	-4.97	118.06	126.20
24	b	611	CLA	C2B-C1B-NB	4.96	115.47	110.33
24	c	513	CLA	C2C-C1C-NC	4.96	115.19	109.98
24	b	623	CLA	C3B-C2B-C1B	-4.96	101.33	107.17
24	c	511	CLA	C3B-C2B-C1B	-4.95	101.33	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
24	B	609	CLA	CHD-C4C-C3C	-4.95	117.55	124.77
25	a	411	PHO	C3D-C4D-ND	4.95	114.05	107.71
24	b	621	CLA	CMD-C2D-C1D	4.95	133.44	124.73
24	c	513	CLA	C4A-NA-C1A	-4.94	104.42	106.68
24	D	405	CLA	C2C-C1C-NC	4.94	115.17	109.98
24	b	611	CLA	O2D-CGD-CBD	4.94	119.86	111.23
24	a	412	CLA	C2C-C1C-NC	4.94	115.17	109.98
24	b	615	CLA	C2C-C1C-NC	4.94	115.17	109.98
24	C	511	CLA	C3B-C2B-C1B	-4.93	101.36	107.17
24	b	615	CLA	C4A-NA-C1A	-4.93	104.43	106.68
24	a	410	CLA	O2D-CGD-CBD	4.92	119.84	111.23
24	b	618	CLA	C3D-C2D-C1D	-4.92	99.11	105.83
24	B	613	CLA	C3D-C4D-ND	4.92	117.99	109.99
25	D	401[B]	PHO	C1-C2-C3	-4.92	118.14	126.20
24	b	623	CLA	C3D-C2D-C1D	-4.91	99.13	105.83
24	C	505	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
24	c	505	CLA	C3B-C2B-C1B	-4.91	101.39	107.17
24	d	403	CLA	C1C-C2C-C3C	-4.90	101.82	106.98
24	C	507	CLA	O2D-CGD-CBD	4.90	119.80	111.23
24	b	623	CLA	C2C-C1C-NC	4.90	115.13	109.98
24	C	507	CLA	C4A-NA-C1A	-4.90	104.44	106.68
24	d	403	CLA	C3D-C2D-C1D	-4.90	99.15	105.83
24	B	612	CLA	C3B-C2B-C1B	-4.90	101.40	107.17
24	b	624	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
24	b	616	CLA	C3D-C2D-C1D	-4.89	99.16	105.83
27	B	621	SQD	O47-C7-C8	4.88	122.04	111.48
24	c	513	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
24	C	504	CLA	C3D-C2D-C1D	-4.88	99.17	105.83
24	B	611	CLA	C3D-C2D-C1D	-4.87	99.18	105.83
24	B	617	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
24	c	512	CLA	C4A-NA-C1A	-4.87	104.46	106.68
35	B	624	HTG	C1'-S1-C1	4.87	110.96	100.45
24	b	614	CLA	C3D-C2D-C1D	-4.87	99.19	105.83
24	A	407	CLA	C3B-C2B-C1B	-4.87	101.43	107.17
24	B	615	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
24	B	608	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
24	b	618	CLA	C2C-C1C-NC	4.85	115.08	109.98
27	A	411	SQD	O6-C1-C2	4.85	115.64	108.27
26	k	102	BCR	C20-C21-C22	-4.85	120.47	127.28
24	A	406	CLA	C4A-NA-C1A	-4.85	104.47	106.68
24	C	506	CLA	C4A-NA-C1A	-4.85	104.47	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	613	CLA	C3D-C2D-C1D	-4.84	99.22	105.83
24	b	610	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
24	b	615	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
24	C	502	CLA	C1-C2-C3	-4.84	118.27	126.20
24	A	405	CLA	CHD-C4C-C3C	-4.84	117.72	124.77
24	A	409	CLA	C2B-C1B-NB	4.84	115.34	110.33
24	B	607	CLA	O2D-CGD-CBD	4.84	119.69	111.23
24	b	615	CLA	C3D-C2D-C1D	-4.83	99.23	105.83
24	C	511	CLA	C2C-C1C-NC	4.83	115.06	109.98
24	d	405	CLA	C2B-C1B-NB	4.83	115.34	110.33
24	B	605	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
24	b	619	CLA	C3B-C2B-C1B	-4.82	101.48	107.17
24	a	409	CLA	CHD-C4C-C3C	-4.82	117.74	124.77
24	b	615	CLA	C2B-C1B-NB	4.82	115.33	110.33
24	C	513	CLA	C2C-C1C-NC	4.82	115.04	109.98
24	c	512	CLA	CMD-C2D-C1D	4.81	133.19	124.73
24	b	621	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
24	B	610	CLA	CMB-C2B-C1B	4.81	132.74	125.42
24	B	611	CLA	C2B-C1B-NB	4.80	115.31	110.33
24	C	509	CLA	C2C-C1C-NC	4.80	115.02	109.98
24	c	512	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
27	a	414	SQD	O6-C1-C2	4.80	115.56	108.27
24	c	508	CLA	C3D-C2D-C1D	-4.80	99.29	105.83
24	a	409	CLA	C2B-C1B-NB	4.80	115.30	110.33
24	B	608	CLA	C2C-C1C-NC	4.79	115.02	109.98
24	B	604	CLA	C2B-C1B-NB	4.79	115.29	110.33
24	c	506	CLA	C2B-C1B-NB	4.79	115.29	110.33
24	B	611	CLA	C3B-C2B-C1B	-4.79	101.53	107.17
24	B	605	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
24	B	606	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
24	c	517	CLA	C3D-C4D-ND	4.78	117.76	109.99
24	b	612	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
24	D	404	CLA	C1-C2-C3	-4.78	118.37	126.20
24	c	517	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
24	B	607	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
24	C	506	CLA	O2D-CGD-CBD	4.77	119.57	111.23
24	c	507	CLA	C2C-C1C-NC	4.77	114.99	109.98
24	c	507	CLA	C3B-C2B-C1B	-4.77	101.55	107.17
36	e	101	DGD	O2G-C1B-C2B	4.77	121.79	111.48
24	B	607	CLA	CHD-C1D-ND	-4.77	118.10	124.80
24	b	624	CLA	C2C-C1C-NC	4.76	114.99	109.98
24	D	404	CLA	C3B-C2B-C1B	-4.76	101.56	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
35	C	523	HTG	C1-O5-C5	4.76	121.10	112.56
36	e	101	DGD	O6E-C5E-C4E	4.76	118.27	109.70
24	D	404	CLA	C1C-C2C-C3C	-4.76	101.98	106.98
26	y	101	BCR	C33-C5-C6	-4.75	119.30	124.48
24	c	509	CLA	C3D-C4D-ND	4.75	117.72	109.99
35	B	623	HTG	C1'-S1-C1	4.75	110.71	100.45
24	c	515	CLA	C2B-C1B-NB	4.74	115.24	110.33
24	B	605	CLA	C4A-NA-C1A	-4.74	104.52	106.68
24	C	504	CLA	C2C-C1C-NC	4.74	114.96	109.98
24	b	613	CLA	C1C-C2C-C3C	-4.73	102.00	106.98
24	B	614	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
24	C	508	CLA	C3B-C2B-C1B	-4.73	101.59	107.17
24	b	611	CLA	C3D-C4D-ND	4.73	117.68	109.99
27	A	411	SQD	O47-C7-C8	4.73	121.72	111.48
24	c	515	CLA	C4A-NA-C1A	-4.73	104.52	106.68
24	C	502	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
24	B	604	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	C	510	CLA	C4A-NA-C1A	-4.73	104.52	106.68
24	C	502	CLA	C3B-C2B-C1B	-4.73	101.60	107.17
24	C	512	CLA	C2B-C1B-NB	4.73	115.23	110.33
24	a	412	CLA	C3D-C4D-ND	4.72	117.67	109.99
24	B	615	CLA	C4A-NA-C1A	-4.72	104.53	106.68
24	d	405	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
24	c	505	CLA	C2C-C1C-NC	4.71	114.93	109.98
24	B	617	CLA	C2C-C1C-NC	4.71	114.93	109.98
24	c	505	CLA	C3D-C2D-C1D	-4.71	99.41	105.83
24	C	513	CLA	C3D-C4D-ND	4.71	117.64	109.99
27	a	414	SQD	O47-C7-C8	4.70	121.65	111.48
24	C	503	CLA	C3D-C4D-ND	4.70	117.63	109.99
24	b	619	CLA	C2C-C1C-NC	4.69	114.91	109.98
24	A	405	CLA	C2D-C1D-ND	4.69	114.77	110.13
24	B	615	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
24	C	511	CLA	C1-C2-C3	-4.69	118.52	126.20
24	a	409	CLA	C3D-C4D-ND	4.68	117.60	109.99
24	C	507	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
24	c	511	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
24	b	622	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
24	B	603	CLA	C3D-C4D-ND	4.68	117.59	109.99
24	C	511	CLA	C4A-NA-C1A	-4.68	104.55	106.68
24	C	505	CLA	C2C-C1C-NC	4.67	114.89	109.98
24	C	501	CLA	C3D-C4D-ND	4.67	117.58	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	516	CLA	C3D-C4D-ND	4.67	117.57	109.99
24	c	515	CLA	C3D-C4D-ND	4.66	117.57	109.99
24	b	625	CLA	C3B-C2B-C1B	-4.66	101.67	107.17
24	B	602	CLA	C3D-C4D-ND	4.66	117.56	109.99
24	c	506	CLA	C2C-C1C-NC	4.65	114.87	109.98
24	C	512	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
24	b	622	CLA	CHD-C4C-C3C	-4.65	118.00	124.77
24	A	405	CLA	C2C-C1C-NC	4.65	114.86	109.98
24	B	613	CLA	C3B-C2B-C1B	-4.65	101.69	107.17
24	a	410	CLA	C3D-C4D-ND	4.64	117.54	109.99
24	C	512	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
24	B	607	CLA	C2B-C1B-NB	4.64	115.14	110.33
24	B	609	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
24	D	405	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	a	412	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
24	D	405	CLA	C4A-NA-C1A	-4.64	104.56	106.68
24	C	506	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
24	a	410	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	B	607	CLA	C2C-C1C-NC	4.63	114.85	109.98
24	B	616	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
24	B	610	CLA	C3D-C2D-C1D	-4.63	99.52	105.83
24	b	610	CLA	C3D-C4D-ND	4.62	117.50	109.99
24	C	503	CLA	C3B-C2B-C1B	-4.62	101.72	107.17
24	b	612	CLA	C1D-CHD-C4C	-4.62	116.20	126.02
24	a	410	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
24	B	611	CLA	C3D-C4D-ND	4.61	117.49	109.99
27	F	101	SQD	O5-C5-C4	4.61	118.00	109.70
35	c	523	HTG	C1'-S1-C1	4.61	110.40	100.45
24	D	405	CLA	C3B-C2B-C1B	-4.60	101.74	107.17
24	b	614	CLA	C3D-C4D-ND	4.60	117.47	109.99
26	K	101	BCR	C7-C8-C9	-4.60	119.42	126.23
24	A	409	CLA	C4A-NA-C1A	-4.60	104.58	106.68
24	a	412	CLA	C2B-C1B-NB	4.60	115.09	110.33
24	c	514	CLA	C1-C2-C3	-4.60	118.66	126.20
24	D	404	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
24	B	611	CLA	CHD-C1D-ND	-4.60	118.33	124.80
24	b	612	CLA	C2B-C1B-NB	4.59	115.09	110.33
24	B	610	CLA	C4A-NA-C1A	-4.59	104.58	106.68
24	C	503	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
24	B	606	CLA	C4A-NA-C1A	-4.58	104.59	106.68
24	d	404	CLA	C3D-C4D-ND	4.58	117.43	109.99
24	b	614	CLA	C3B-C2B-C1B	-4.57	101.78	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
24	c	511	CLA	C2C-C1C-NC	4.57	114.78	109.98
24	C	503	CLA	C2B-C1B-NB	4.57	115.06	110.33
24	c	506	CLA	O2D-CGD-CBD	4.57	119.21	111.23
24	b	622	CLA	C4A-NA-C1A	-4.57	104.60	106.68
24	B	603	CLA	C3B-C2B-C1B	-4.56	101.79	107.17
24	b	621	CLA	C3D-C4D-ND	4.56	117.40	109.99
24	C	505	CLA	C3D-C4D-ND	4.56	117.40	109.99
24	b	623	CLA	C4A-NA-C1A	-4.56	104.60	106.68
26	B	618	BCR	C33-C5-C6	-4.56	119.51	124.48
24	B	613	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
24	C	508	CLA	C3D-C4D-ND	4.56	117.39	109.99
24	A	409	CLA	C3D-C4D-ND	4.55	117.38	109.99
24	c	514	CLA	C3D-C4D-ND	4.55	117.38	109.99
24	d	404	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	d	403	CLA	C3B-C2B-C1B	-4.55	101.81	107.17
24	d	403	CLA	O2D-CGD-CBD	4.55	119.18	111.23
24	B	617	CLA	C2B-C1B-NB	4.54	115.04	110.33
24	b	621	CLA	C2C-C1C-NC	4.54	114.75	109.98
24	A	407	CLA	CHD-C1D-ND	-4.54	118.41	124.80
24	C	511	CLA	C2B-C1B-NB	4.53	115.03	110.33
24	c	514	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
24	a	410	CLA	C2C-C1C-NC	4.53	114.74	109.98
24	b	616	CLA	C2C-C1C-NC	4.53	114.74	109.98
24	c	508	CLA	C2B-C1B-NB	4.53	115.02	110.33
24	B	602	CLA	C2B-C1B-NB	4.53	115.02	110.33
24	C	502	CLA	O2D-CGD-CBD	4.52	119.13	111.23
24	B	602	CLA	C3B-C2B-C1B	-4.52	101.84	107.17
24	C	510	CLA	C1-C2-C3	-4.52	118.80	126.20
24	b	617	CLA	C3D-C4D-ND	4.51	117.32	109.99
24	C	509	CLA	C4A-NA-C1A	-4.51	104.62	106.68
24	A	409	CLA	O2D-CGD-CBD	4.51	119.11	111.23
24	c	517	CLA	C2B-C1B-NB	4.51	115.00	110.33
24	A	406	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
24	B	617	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	B	606	CLA	C2C-C1C-NC	4.50	114.71	109.98
24	C	509	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
24	d	403	CLA	C3D-C4D-ND	4.50	117.30	109.99
33	a	415	LMG	O7-C10-C11	4.50	121.21	111.48
24	B	609	CLA	C3D-C4D-ND	4.50	117.30	109.99
24	d	405	CLA	C3D-C2D-C1D	-4.50	99.70	105.83
24	c	515	CLA	CHD-C1D-ND	-4.49	118.48	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	625	CLA	C3D-C2D-C1D	-4.49	99.70	105.83
31	D	407[B]	PL9	C7-C8-C9	-4.49	119.09	126.83
24	c	517	CLA	C2C-C1C-NC	4.49	114.70	109.98
24	b	614	CLA	C2C-C1C-NC	4.49	114.69	109.98
24	C	504	CLA	CHD-C1D-ND	-4.48	118.49	124.80
24	B	603	CLA	C2C-C1C-NC	4.48	114.69	109.98
24	D	405	CLA	C3D-C4D-ND	4.48	117.27	109.99
24	B	603	CLA	C2B-C1B-NB	4.48	114.97	110.33
24	B	610	CLA	C3D-C4D-ND	4.48	117.27	109.99
24	b	618	CLA	C3D-C4D-ND	4.48	117.27	109.99
24	C	502	CLA	C4A-NA-C1A	-4.47	104.64	106.68
24	b	617	CLA	C2B-C1B-NB	4.47	114.96	110.33
24	c	507	CLA	C4A-NA-C1A	-4.47	104.64	106.68
24	C	507	CLA	C2C-C1C-NC	4.47	114.68	109.98
24	d	405	CLA	C3D-C4D-ND	4.47	117.25	109.99
24	C	502	CLA	C2C-C1C-NC	4.47	114.68	109.98
24	b	611	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	C	510	CLA	C3B-C2B-C1B	-4.47	101.90	107.17
24	C	511	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
24	B	610	CLA	O2D-CGD-CBD	4.47	119.04	111.23
24	c	512	CLA	C3C-C4C-NC	4.46	116.15	110.43
25	a	411	PHO	O1D-CGD-CBD	-4.46	117.95	124.72
24	C	507	CLA	C2B-C1B-NB	4.46	114.95	110.33
37	D	411	LHG	O7-C7-C8	4.46	121.14	111.48
24	b	621	CLA	C3C-C4C-NC	4.46	116.14	110.43
24	B	615	CLA	C2C-C1C-NC	4.46	114.67	109.98
24	c	508	CLA	C2C-C1C-NC	4.46	114.67	109.98
24	b	612	CLA	C3D-C4D-ND	4.46	117.23	109.99
24	c	507	CLA	C1D-CHD-C4C	-4.46	116.54	126.02
35	B	632	HTG	C1'-S1-C1	4.46	110.07	100.45
24	b	611	CLA	CHD-C1D-ND	-4.46	118.53	124.80
24	B	616	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
24	c	510	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	C	505	CLA	C2B-C1B-NB	4.45	114.94	110.33
24	B	609	CLA	C2B-C1B-NB	4.45	114.94	110.33
24	B	606	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
24	A	406	CLA	CHD-C1D-ND	-4.44	118.55	124.80
24	C	501	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
24	d	404	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
31	D	407[B]	PL9	C42-C43-C44	-4.44	117.47	127.62
26	D	406	BCR	C24-C23-C22	-4.43	119.67	126.23
24	c	513	CLA	C2B-C1B-NB	4.43	114.92	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	407	CLA	C4A-NA-C1A	-4.43	104.66	106.68
24	B	602	CLA	C2C-C1C-NC	4.43	114.63	109.98
24	D	404	CLA	C3D-C4D-ND	4.42	117.18	109.99
24	a	412	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
24	c	510	CLA	CHD-C1D-ND	-4.42	118.58	124.80
24	b	613	CLA	C3B-C2B-C1B	-4.42	101.97	107.17
24	c	515	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
24	B	616	CLA	C2B-C1B-NB	4.41	114.90	110.33
24	b	614	CLA	CHD-C1D-ND	-4.41	118.59	124.80
24	a	412	CLA	C3B-C4B-NB	4.41	114.46	110.53
29	D	403	LMT	O1B-C4'-C3'	4.41	118.43	107.23
24	C	512	CLA	C2C-C1C-NC	4.40	114.61	109.98
24	C	511	CLA	C3D-C4D-ND	4.40	117.14	109.99
24	b	623	CLA	C3D-C4D-ND	4.40	117.14	109.99
24	C	511	CLA	O2D-CGD-CBD	4.40	118.92	111.23
24	b	625	CLA	C3D-C4D-ND	4.40	117.14	109.99
24	b	620	CLA	C3B-C2B-C1B	-4.40	101.99	107.17
24	b	619	CLA	C3D-C4D-ND	4.40	117.13	109.99
24	B	606	CLA	C2B-C1B-NB	4.40	114.88	110.33
24	B	612	CLA	C3D-C4D-ND	4.39	117.13	109.99
24	d	404	CLA	CHD-C1D-ND	-4.39	118.62	124.80
24	C	502	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	B	604	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	A	407	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	b	612	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	b	619	CLA	O2D-CGD-CBD	4.39	118.90	111.23
24	b	619	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
24	c	507	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	C	503	CLA	CHD-C1D-ND	-4.39	118.63	124.80
24	b	625	CLA	C2B-C1B-NB	4.39	114.88	110.33
24	b	623	CLA	C2B-C1B-NB	4.39	114.87	110.33
24	C	503	CLA	C2C-C1C-NC	4.38	114.59	109.98
24	B	615	CLA	C3D-C4D-ND	4.38	117.11	109.99
27	B	621	SQD	O6-C1-C2	4.38	114.93	108.27
24	C	510	CLA	C3D-C4D-ND	4.38	117.11	109.99
24	C	501	CLA	C2C-C1C-NC	4.38	114.58	109.98
24	B	612	CLA	C2B-C1B-NB	4.38	114.87	110.33
24	B	612	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
24	c	505	CLA	C2B-C1B-NB	4.37	114.86	110.33
33	C	520	LMG	O7-C10-C11	4.37	120.94	111.48
24	b	624	CLA	C2B-C1B-NB	4.37	114.86	110.33
33	c	522	LMG	O7-C10-C11	4.37	120.93	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	O2D-CGD-CBD	4.37	118.86	111.23
35	b	632	HTG	C1'-S1-C1	4.36	109.88	100.45
40	v	206	HEC	CHC-C4B-NB	4.36	129.20	124.45
24	B	615	CLA	C2B-C1B-NB	4.36	114.85	110.33
24	b	616	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
24	B	609	CLA	O2D-CGD-CBD	4.36	118.85	111.23
24	C	508	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
24	b	621	CLA	C3B-C2B-C1B	-4.35	102.05	107.17
24	C	509	CLA	C2B-C1B-NB	4.34	114.83	110.33
24	c	514	CLA	C4A-NA-C1A	-4.34	104.70	106.68
24	B	614	CLA	C3B-C2B-C1B	-4.34	102.05	107.17
35	c	524	HTG	C1'-S1-C1	4.34	109.82	100.45
24	c	510	CLA	C2B-C1B-NB	4.34	114.82	110.33
24	a	410	CLA	C2B-C1B-NB	4.34	114.82	110.33
24	b	624	CLA	C3D-C4D-ND	4.33	117.03	109.99
24	A	406	CLA	C3D-C4D-ND	4.33	117.03	109.99
24	B	609	CLA	C1C-C2C-C3C	-4.33	102.42	106.98
24	B	604	CLA	C2C-C1C-NC	4.33	114.53	109.98
24	a	409	CLA	CHD-C1D-ND	-4.33	118.71	124.80
24	B	613	CLA	C2C-C1C-NC	4.33	114.53	109.98
24	D	405	CLA	C2B-C1B-NB	4.33	114.81	110.33
24	b	610	CLA	C2C-C1C-NC	4.33	114.53	109.98
24	d	403	CLA	CHD-C1D-ND	-4.32	118.72	124.80
24	c	507	CLA	C3C-C4C-NC	4.32	115.97	110.43
24	C	511	CLA	C3B-C4B-NB	4.32	114.39	110.53
24	B	608	CLA	C3B-C2B-C1B	-4.32	102.08	107.17
24	B	616	CLA	C3D-C4D-ND	4.32	117.00	109.99
24	b	620	CLA	C3D-C4D-ND	4.32	117.00	109.99
24	b	624	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
24	c	517	CLA	C3D-C2D-C1D	-4.31	99.96	105.83
24	B	602	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
24	C	502	CLA	C3D-C4D-ND	4.30	116.98	109.99
38	f	101	HEM	CHC-C4B-NB	4.30	129.06	124.42
24	B	609	CLA	C3B-C4B-NB	4.30	114.37	110.53
24	b	619	CLA	C1-C2-C3	-4.30	119.15	126.20
24	B	602	CLA	CHD-C1D-ND	-4.30	118.75	124.80
24	c	513	CLA	C3D-C2D-C1D	-4.30	99.96	105.83
24	C	509	CLA	C3D-C4D-ND	4.30	116.98	109.99
33	A	419	LMG	O7-C10-C11	4.30	120.78	111.48
24	C	508	CLA	CHD-C1D-ND	-4.30	118.76	124.80
24	C	501	CLA	C2B-C1B-NB	4.30	114.78	110.33
24	B	615	CLA	C3C-C4C-NC	4.30	115.93	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C3D-C4D-ND	4.30	116.97	109.99
24	c	517	CLA	O2D-CGD-CBD	4.29	118.74	111.23
24	c	508	CLA	C3D-C4D-ND	4.29	116.96	109.99
24	c	510	CLA	C1C-C2C-C3C	-4.29	102.47	106.98
24	B	602	CLA	C4A-NA-C1A	-4.29	104.72	106.68
24	C	512	CLA	C3D-C4D-ND	4.29	116.96	109.99
24	c	511	CLA	C3C-C4C-NC	4.29	115.92	110.43
24	c	517	CLA	CHD-C1D-ND	-4.29	118.77	124.80
24	b	610	CLA	C3D-C2D-C1D	-4.29	99.98	105.83
24	d	405	CLA	C2C-C1C-NC	4.28	114.48	109.98
24	B	603	CLA	CHD-C1D-ND	-4.28	118.77	124.80
26	T	103	BCR	C11-C10-C9	-4.28	121.28	127.28
24	C	513	CLA	CHD-C1D-ND	-4.28	118.78	124.80
24	B	609	CLA	C4A-NA-C1A	-4.28	104.73	106.68
24	D	404	CLA	CHD-C1D-ND	-4.27	118.79	124.80
24	B	609	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
24	b	616	CLA	C4A-NA-C1A	-4.27	104.73	106.68
24	a	412	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
24	a	409	CLA	C1C-C2C-C3C	-4.26	102.50	106.98
24	b	619	CLA	CHD-C1D-ND	-4.26	118.81	124.80
24	C	505	CLA	C3C-C4C-NC	4.26	115.88	110.43
27	L	102	SQD	O47-C7-C8	4.26	120.69	111.48
24	c	513	CLA	C3D-C4D-ND	4.25	116.90	109.99
24	c	510	CLA	C3D-C4D-ND	4.25	116.90	109.99
36	C	516	DGD	O2G-C1B-C2B	4.25	120.68	111.48
24	B	607	CLA	C3D-C4D-ND	4.25	116.89	109.99
35	C	523	HTG	C1'-S1-C1	4.25	109.62	100.45
24	C	513	CLA	C3D-C2D-C1D	-4.24	100.04	105.83
24	B	613	CLA	C3C-C4C-NC	4.24	115.86	110.43
24	C	501	CLA	C3B-C2B-C1B	-4.24	102.17	107.17
24	B	616	CLA	C3C-C4C-NC	4.24	115.86	110.43
29	A	414	LMT	C1'-O5'-C5'	4.24	122.00	113.72
26	b	626	BCR	C15-C14-C13	-4.24	121.34	127.28
24	b	624	CLA	CHD-C1D-ND	-4.24	118.84	124.80
24	c	506	CLA	C3D-C4D-ND	4.24	116.87	109.99
24	B	611	CLA	C2C-C1C-NC	4.23	114.43	109.98
25	d	402[A]	PHO	O2D-CGD-O1D	-4.23	115.62	123.85
24	B	605	CLA	C3C-C4C-NC	4.23	115.84	110.43
24	b	614	CLA	C3C-C4C-NC	4.22	115.84	110.43
24	c	508	CLA	C4A-NA-C1A	-4.22	104.75	106.68
26	H	101	BCR	C38-C26-C25	-4.22	119.88	124.48
24	b	622	CLA	C3B-C2B-C1B	-4.22	102.20	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t	102	BCR	C33-C5-C6	-4.22	119.88	124.48
24	b	620	CLA	C1-C2-C3	-4.22	119.29	126.20
24	A	405	CLA	C3D-C4D-ND	4.22	116.84	109.99
24	B	610	CLA	C3B-C2B-C1B	-4.21	102.20	107.17
24	B	610	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	d	404	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	c	505	CLA	C3D-C4D-ND	4.21	116.83	109.99
24	c	510	CLA	C3B-C2B-C1B	-4.21	102.21	107.17
24	B	606	CLA	CHD-C1D-ND	-4.21	118.88	124.80
24	A	407	CLA	C2C-C1C-NC	4.21	114.40	109.98
24	b	618	CLA	CHD-C1D-ND	-4.21	118.88	124.80
27	a	405	SQD	O47-C7-C8	4.21	120.58	111.48
24	b	615	CLA	C1D-CHD-C4C	-4.20	117.08	126.02
24	B	605	CLA	C2B-C1B-NB	4.20	114.68	110.33
24	c	512	CLA	C3B-C2B-C1B	-4.20	102.22	107.17
24	b	617	CLA	C3D-C2D-C1D	-4.20	100.10	105.83
24	b	610	CLA	CHD-C1D-ND	-4.20	118.90	124.80
24	C	508	CLA	C2C-C1C-NC	4.19	114.39	109.98
24	b	625	CLA	C1D-CHD-C4C	-4.19	117.11	126.02
24	d	404	CLA	C1C-C2C-C3C	-4.19	102.57	106.98
35	b	631	HTG	C1'-S1-C1	4.19	109.50	100.45
24	C	506	CLA	C3B-C2B-C1B	-4.19	102.23	107.17
24	A	409	CLA	CAC-C3C-C4C	4.19	130.24	124.79
24	b	622	CLA	C2B-C1B-NB	4.18	114.66	110.33
24	A	409	CLA	C3D-C2D-C1D	-4.18	100.12	105.83
24	c	516	CLA	CHD-C1D-ND	-4.18	118.92	124.80
24	c	508	CLA	CHD-C1D-ND	-4.18	118.92	124.80
24	B	616	CLA	C2C-C1C-NC	4.18	114.37	109.98
24	B	613	CLA	CMC-C2C-C1C	4.18	131.56	125.03
24	b	617	CLA	C1-C2-C3	-4.18	119.35	126.20
29	A	414	LMT	O5'-C5'-C4'	4.18	118.36	109.72
24	b	617	CLA	C2C-C1C-NC	4.18	114.37	109.98
24	b	620	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
24	B	614	CLA	C2B-C1B-NB	4.17	114.65	110.33
24	B	603	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
24	B	613	CLA	CMD-C2D-C1D	4.16	132.06	124.73
24	D	404	CLA	O2D-CGD-CBD	4.16	118.50	111.23
24	c	507	CLA	O2D-CGD-CBD	4.16	118.50	111.23
24	C	509	CLA	CHD-C1D-ND	-4.16	118.95	124.80
24	B	616	CLA	C1D-CHD-C4C	-4.16	117.19	126.02
31	d	407[B]	PL9	C42-C43-C44	-4.16	118.11	127.62
24	c	506	CLA	C3D-C2D-C1D	-4.15	100.17	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	C1-C2-C3	-4.15	119.40	126.20
26	C	515	BCR	C33-C5-C6	-4.15	119.96	124.48
24	C	504	CLA	C3D-C4D-ND	4.14	116.72	109.99
24	b	614	CLA	C2B-C1B-NB	4.14	114.61	110.33
24	B	617	CLA	C3D-C4D-ND	4.14	116.71	109.99
24	C	510	CLA	C3D-C2D-C1D	-4.13	100.19	105.83
24	b	623	CLA	O2D-CGD-O1D	-4.13	115.81	123.85
24	A	405	CLA	C1D-CHD-C4C	-4.13	117.24	126.02
24	B	608	CLA	C2B-C1B-NB	4.13	114.61	110.33
24	b	620	CLA	C1C-C2C-C3C	-4.13	102.64	106.98
31	a	416[A]	PL9	C22-C23-C24	-4.13	118.18	127.62
24	C	503	CLA	C3C-C4C-NC	4.12	115.71	110.43
24	A	406	CLA	CBC-CAC-C3C	-4.12	101.25	112.42
35	D	414	HTG	C1'-S1-C1	4.12	109.34	100.45
24	c	515	CLA	C2C-C1C-NC	4.12	114.31	109.98
27	L	102	SQD	C3-C4-C5	4.11	117.69	110.23
24	D	405	CLA	CHD-C1D-ND	-4.11	119.01	124.80
36	D	408	DGD	O2G-C1B-C2B	4.11	120.38	111.48
24	B	607	CLA	C3C-C4C-NC	4.11	115.70	110.43
24	c	505	CLA	CHD-C1D-ND	-4.11	119.02	124.80
24	B	606	CLA	C1D-CHD-C4C	-4.11	117.28	126.02
24	C	510	CLA	C2B-C1B-NB	4.11	114.59	110.33
24	c	511	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
24	C	502	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
38	E	103	HEM	CAD-CBD-CGD	4.09	124.53	113.67
24	C	503	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
24	B	617	CLA	C1D-CHD-C4C	-4.09	117.33	126.02
40	V	205	HEC	CBB-CAB-C3B	-4.09	119.26	127.43
24	B	608	CLA	CHD-C1D-ND	-4.09	119.05	124.80
24	b	615	CLA	CHD-C1D-ND	-4.09	119.05	124.80
24	b	618	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
24	c	507	CLA	C3D-C4D-ND	4.08	116.62	109.99
24	b	615	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	A	405	CLA	CAC-C3C-C4C	4.08	130.09	124.79
24	B	612	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
24	c	514	CLA	C3D-C2D-C1D	-4.07	100.27	105.83
24	b	621	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
24	B	612	CLA	CHD-C1D-ND	-4.07	119.07	124.80
24	b	620	CLA	C4A-NA-C1A	-4.07	104.82	106.68
31	a	416[A]	PL9	C32-C33-C34	-4.07	118.32	127.62
24	B	614	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
26	y	101	BCR	C15-C14-C13	-4.06	121.58	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	506	CLA	C3D-C4D-ND	4.06	116.59	109.99
24	A	405	CLA	C3B-C4B-NB	4.06	114.16	110.53
24	b	616	CLA	CHD-C1D-ND	-4.06	119.09	124.80
24	A	405	CLA	CAA-C2A-C3A	-4.06	102.03	113.00
24	d	404	CLA	C3D-C2D-C1D	-4.06	100.30	105.83
37	E	101	LHG	O7-C7-C8	4.05	120.25	111.48
24	c	512	CLA	C3D-C4D-ND	4.05	116.58	109.99
26	B	620	BCR	C15-C14-C13	-4.05	121.60	127.28
24	A	405	CLA	C3D-C2D-C1D	-4.05	100.31	105.83
24	b	610	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
24	B	610	CLA	CHD-C1D-ND	-4.05	119.11	124.80
24	c	514	CLA	C2B-C1B-NB	4.05	114.52	110.33
24	C	507	CLA	C3D-C4D-ND	4.04	116.56	109.99
24	C	513	CLA	O2D-CGD-CBD	4.04	118.30	111.23
24	B	614	CLA	CHD-C1D-ND	-4.04	119.12	124.80
24	d	405	CLA	C1D-CHD-C4C	-4.04	117.43	126.02
24	C	506	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
24	b	616	CLA	C2B-C1B-NB	4.03	114.51	110.33
36	c	519	DGD	O2G-C1B-C2B	4.03	120.20	111.48
26	c	526	BCR	C15-C14-C13	-4.03	121.62	127.28
35	B	622	HTG	C1'-S1-C1	4.03	109.16	100.45
24	C	511	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
29	a	404	LMT	C1'-O5'-C5'	4.03	121.59	113.72
24	a	409	CLA	C3D-C2D-C1D	-4.03	100.33	105.83
26	b	628	BCR	C24-C23-C22	-4.03	120.28	126.23
24	c	505	CLA	C4A-NA-C1A	-4.03	104.84	106.68
24	B	604	CLA	CHD-C1D-ND	-4.02	119.14	124.80
24	A	409	CLA	CMB-C2B-C1B	4.02	131.53	125.42
24	c	515	CLA	O2D-CGD-CBD	4.01	118.25	111.23
24	B	609	CLA	CHD-C1D-ND	-4.01	119.15	124.80
27	F	101	SQD	O6-C1-C2	4.01	114.36	108.27
35	B	631	HTG	C1'-S1-C1	4.01	109.10	100.45
36	e	101	DGD	C3E-C4E-C5E	4.01	117.50	110.23
24	C	504	CLA	C1D-CHD-C4C	-4.01	117.51	126.02
24	C	511	CLA	CAC-C3C-C4C	4.00	130.00	124.79
24	c	511	CLA	C3D-C4D-ND	4.00	116.49	109.99
24	b	618	CLA	C2B-C1B-NB	4.00	114.47	110.33
24	C	512	CLA	C3C-C4C-NC	4.00	115.56	110.43
24	C	504	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
24	B	605	CLA	C3B-C4B-NB	4.00	114.10	110.53
24	D	404	CLA	C2B-C1B-NB	4.00	114.47	110.33
24	b	611	CLA	C2C-C1C-NC	4.00	114.18	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	513	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
36	c	521	DGD	O2G-C1B-C2B	4.00	120.13	111.48
24	C	507	CLA	CHD-C1D-ND	-3.99	119.18	124.80
36	D	408	DGD	C1D-C2D-C3D	3.99	118.41	110.01
26	Y	101	BCR	C15-C14-C13	-3.99	121.68	127.28
24	b	614	CLA	O2D-CGD-O1D	-3.99	116.08	123.85
24	b	622	CLA	CAC-C3C-C4C	3.99	129.98	124.79
24	b	616	CLA	C3D-C4D-ND	3.99	116.47	109.99
24	B	602	CLA	C1D-CHD-C4C	-3.99	117.55	126.02
24	c	509	CLA	C3C-C4C-NC	3.98	115.53	110.43
26	b	627	BCR	C15-C14-C13	-3.98	121.70	127.28
24	b	623	CLA	CHD-C1D-ND	-3.98	119.20	124.80
24	c	511	CLA	C4A-NA-C1A	-3.98	104.86	106.68
24	c	509	CLA	C3B-C2B-C1B	-3.98	102.48	107.17
24	a	410	CLA	CHD-C1D-ND	-3.98	119.20	124.80
24	c	511	CLA	CHD-C1D-ND	-3.97	119.22	124.80
24	d	403	CLA	C2B-C1B-NB	3.96	114.44	110.33
25	A	408	PHO	CBC-CAC-C3C	-3.96	107.20	112.87
24	B	606	CLA	CMB-C2B-C1B	3.96	131.45	125.42
24	B	610	CLA	C1C-C2C-C3C	-3.96	102.81	106.98
29	a	404	LMT	O5'-C5'-C4'	3.96	117.92	109.72
24	c	517	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
24	b	624	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
24	C	506	CLA	C2B-C1B-NB	3.96	114.43	110.33
24	c	512	CLA	C2B-C1B-NB	3.96	114.43	110.33
24	B	612	CLA	C3C-C4C-NC	3.96	115.50	110.43
38	f	101	HEM	CHD-C1D-ND	3.96	128.68	124.42
40	V	205	HEC	CHC-C4B-NB	3.96	128.76	124.45
24	d	403	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
24	C	506	CLA	CHD-C1D-ND	-3.96	119.24	124.80
24	c	514	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
24	a	410	CLA	C1D-CHD-C4C	-3.95	117.63	126.02
24	C	510	CLA	CHD-C1D-ND	-3.94	119.25	124.80
24	c	510	CLA	C3B-C4B-NB	3.94	114.05	110.53
24	b	622	CLA	C1C-C2C-C3C	-3.94	102.83	106.98
24	C	501	CLA	CHD-C1D-ND	-3.94	119.26	124.80
24	B	603	CLA	O2D-CGD-O1D	-3.93	116.19	123.85
24	B	604	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
24	B	605	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
24	c	516	CLA	C2C-C1C-NC	3.93	114.11	109.98
24	b	623	CLA	C1-C2-C3	-3.93	119.76	126.20
24	d	405	CLA	CHD-C1D-ND	-3.92	119.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C3C-C4C-NC	3.92	115.45	110.43
24	C	501	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
24	B	607	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
25	D	401[B]	PHO	C1A-C2A-C3A	-3.92	99.11	102.84
24	b	615	CLA	C3D-C4D-ND	3.92	116.36	109.99
24	c	508	CLA	C1D-CHD-C4C	-3.92	117.69	126.02
24	b	611	CLA	O2D-CGD-O1D	-3.92	116.22	123.85
24	b	625	CLA	C2C-C1C-NC	3.91	114.09	109.98
24	B	615	CLA	C1D-CHD-C4C	-3.91	117.70	126.02
24	b	615	CLA	C3C-C4C-NC	3.91	115.44	110.43
24	a	412	CLA	CHD-C1D-ND	-3.91	119.30	124.80
24	B	615	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
24	c	505	CLA	O2D-CGD-O1D	-3.90	116.25	123.85
27	A	413	SQD	O47-C7-C8	3.90	119.92	111.48
24	C	511	CLA	CHD-C1D-ND	-3.90	119.31	124.80
24	b	622	CLA	C4B-C3B-C2B	-3.90	102.46	107.30
31	A	417[B]	PL9	C37-C38-C39	-3.90	118.70	127.62
24	C	501	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
24	B	608	CLA	C3D-C4D-ND	3.89	116.31	109.99
24	C	512	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
24	c	514	CLA	CHD-C1D-ND	-3.88	119.34	124.80
24	c	513	CLA	C1C-C2C-C3C	-3.88	102.90	106.98
26	D	406	BCR	C38-C26-C25	-3.88	120.25	124.48
27	B	621	SQD	O7-S-C6	3.88	112.55	106.76
24	A	406	CLA	C3B-C4B-NB	3.88	113.99	110.53
24	C	505	CLA	C1D-CHD-C4C	-3.88	117.78	126.02
24	C	513	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
26	c	518	BCR	C15-C14-C13	-3.87	121.85	127.28
37	d	410	LHG	O7-C7-C8	3.87	119.85	111.48
24	c	506	CLA	C1-C2-C3	-3.87	119.86	126.20
24	A	409	CLA	CHD-C1D-ND	-3.86	119.36	124.80
38	E	103	HEM	CHD-C1D-ND	3.86	128.58	124.42
24	c	514	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
24	C	508	CLA	C3B-C4B-NB	3.86	113.98	110.53
24	b	616	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
24	b	613	CLA	CMC-C2C-C1C	3.86	131.06	125.03
24	c	512	CLA	C1D-CHD-C4C	-3.85	117.83	126.02
24	B	603	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
24	b	620	CLA	C2B-C1B-NB	3.85	114.32	110.33
24	B	614	CLA	C3D-C4D-ND	3.85	116.24	109.99
24	b	610	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
24	b	612	CLA	C3C-C4C-NC	3.85	115.36	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	C3C-C4C-NC	3.84	115.35	110.43
24	c	515	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
31	d	407[A]	PL9	C42-C43-C44	-3.84	118.84	127.62
27	A	413	SQD	O48-C23-C24	3.84	123.53	111.83
24	B	613	CLA	CHD-C1D-ND	-3.83	119.41	124.80
24	C	507	CLA	C1D-CHD-C4C	-3.83	117.88	126.02
26	b	626	BCR	C7-C8-C9	-3.83	120.57	126.23
24	C	503	CLA	O2D-CGD-O1D	-3.83	116.40	123.85
31	a	416[A]	PL9	C15-C14-C16	3.83	121.87	115.23
24	b	623	CLA	C1D-CHD-C4C	-3.83	117.89	126.02
24	c	506	CLA	C1D-CHD-C4C	-3.83	117.89	126.02
24	b	613	CLA	C2B-C1B-NB	3.82	114.29	110.33
24	A	405	CLA	CHD-C1D-ND	-3.82	119.42	124.80
24	c	509	CLA	CHD-C1D-ND	-3.82	119.42	124.80
24	C	502	CLA	C3C-C4C-NC	3.82	115.33	110.43
24	b	617	CLA	CHD-C1D-ND	-3.82	119.42	124.80
24	c	513	CLA	C3B-C4B-NB	3.82	113.94	110.53
24	D	405	CLA	C3B-C4B-NB	3.81	113.94	110.53
24	c	516	CLA	C3D-C2D-C1D	-3.81	100.63	105.83
24	B	611	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
24	b	616	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
33	C	519	LMG	O7-C10-C11	3.81	119.72	111.48
24	C	513	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
24	B	603	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
24	c	511	CLA	C2B-C1B-NB	3.81	114.27	110.33
24	B	608	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
24	C	513	CLA	C1-C2-C3	-3.80	119.97	126.20
24	a	409	CLA	C3B-C4B-NB	3.80	113.92	110.53
24	c	507	CLA	C1-C2-C3	-3.80	119.97	126.20
24	b	623	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
24	b	614	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
24	C	501	CLA	O2D-CGD-O1D	-3.79	116.46	123.85
24	b	613	CLA	C3C-C4C-NC	3.79	115.29	110.43
26	t	102	BCR	C3-C4-C5	-3.79	107.30	114.06
24	B	615	CLA	CHD-C1D-ND	-3.79	119.47	124.80
24	A	406	CLA	C1D-CHD-C4C	-3.79	117.96	126.02
24	c	510	CLA	O2D-CGD-CBD	3.79	117.85	111.23
24	b	620	CLA	C3B-C4B-NB	3.79	113.91	110.53
33	a	415	LMG	C8-O7-C10	-3.79	108.74	117.80
24	b	616	CLA	C3C-C4C-NC	3.78	115.28	110.43
24	c	512	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
24	A	407	CLA	O2D-CGD-O1D	-3.78	116.48	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
24	b	621	CLA	C2B-C1B-NB	3.78	114.25	110.33
24	b	622	CLA	C3D-C4D-ND	3.78	116.14	109.99
24	B	617	CLA	C3B-C4B-NB	3.78	113.91	110.53
24	b	622	CLA	CHD-C1D-ND	-3.78	119.48	124.80
24	C	506	CLA	CBC-CAC-C3C	-3.78	102.17	112.42
24	C	510	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
24	b	612	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
24	a	409	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
24	B	603	CLA	C3C-C4C-NC	3.77	115.26	110.43
24	a	412	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
24	c	512	CLA	C1-C2-C3	-3.77	120.02	126.20
24	B	604	CLA	CAA-C2A-C3A	-3.77	102.81	113.00
24	B	617	CLA	CHD-C1D-ND	-3.77	119.50	124.80
24	C	510	CLA	C3B-C4B-NB	3.77	113.89	110.53
24	B	614	CLA	C3C-C4C-NC	3.77	115.26	110.43
24	D	405	CLA	CMB-C2B-C1B	3.77	131.15	125.42
24	B	610	CLA	C3B-C4B-NB	3.76	113.89	110.53
31	A	417[B]	PL9	C7-C3-C4	3.76	120.01	116.91
24	B	614	CLA	C1-C2-C3	-3.76	120.04	126.20
31	a	416[B]	PL9	C32-C33-C34	-3.75	119.04	127.62
24	b	622	CLA	C1-C2-C3	-3.75	120.06	126.20
24	b	621	CLA	C4A-NA-C1A	-3.75	104.97	106.68
24	C	509	CLA	C3B-C4B-NB	3.74	113.87	110.53
24	c	514	CLA	C3B-C4B-NB	3.74	113.87	110.53
24	B	616	CLA	CHD-C1D-ND	-3.74	119.54	124.80
24	c	517	CLA	C3C-C4C-NC	3.74	115.22	110.43
24	a	412	CLA	CMB-C2B-C1B	3.74	131.11	125.42
24	b	612	CLA	CHD-C1D-ND	-3.73	119.55	124.80
24	b	620	CLA	CHD-C1D-ND	-3.73	119.55	124.80
24	c	513	CLA	CHD-C1D-ND	-3.73	119.55	124.80
24	C	508	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
24	c	509	CLA	C2B-C1B-NB	3.73	114.19	110.33
26	b	627	BCR	C29-C30-C25	3.73	115.85	110.44
24	C	506	CLA	CAC-C3C-C4C	3.72	129.63	124.79
31	d	407[B]	PL9	C7-C8-C9	-3.72	120.42	126.83
24	d	403	CLA	CBC-CAC-C3C	-3.72	102.33	112.42
24	B	608	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
24	a	410	CLA	C3C-C4C-NC	3.72	115.19	110.43
24	b	619	CLA	CAC-C3C-C4C	3.72	129.62	124.79
33	Z	101	LMG	O7-C10-C11	3.71	119.52	111.48
26	b	626	BCR	C33-C5-C6	-3.71	120.43	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	406	BCR	C28-C27-C26	-3.71	107.44	114.06
24	B	609	CLA	C1D-CHD-C4C	-3.70	118.14	126.02
24	B	607	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
31	D	407[A]	PL9	C42-C43-C44	-3.70	119.15	127.62
24	C	505	CLA	CMB-C2B-C1B	3.70	131.06	125.42
24	a	410	CLA	C1C-C2C-C3C	-3.70	103.09	106.98
24	b	613	CLA	C1D-CHD-C4C	-3.70	118.15	126.02
31	a	416[A]	PL9	C7-C3-C4	3.70	119.96	116.91
24	B	610	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
24	a	409	CLA	CAA-C2A-C3A	-3.70	103.01	113.00
24	c	506	CLA	CHD-C1D-ND	-3.69	119.60	124.80
36	c	520	DGD	O2G-C1B-C2B	3.69	119.46	111.48
24	c	506	CLA	C3C-C4C-NC	3.69	115.16	110.43
26	C	514	BCR	C7-C8-C9	-3.69	120.78	126.23
24	B	613	CLA	C4A-NA-C1A	-3.68	105.00	106.68
35	b	632	HTG	O5-C1-C2	3.68	115.40	110.32
24	D	404	CLA	C3B-C4B-NB	3.68	113.82	110.53
24	B	614	CLA	C3B-C4B-NB	3.68	113.81	110.53
24	c	516	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
24	C	507	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
24	C	509	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
24	b	620	CLA	C3C-C4C-NC	3.68	115.14	110.43
24	c	508	CLA	C1C-C2C-C3C	-3.67	103.11	106.98
24	C	501	CLA	CMC-C2C-C1C	3.67	130.77	125.03
24	b	617	CLA	O2D-CGD-O1D	-3.67	116.71	123.85
24	b	611	CLA	C3C-C4C-NC	3.66	115.12	110.43
24	B	605	CLA	CHD-C1D-ND	-3.66	119.65	124.80
24	b	622	CLA	C1D-CHD-C4C	-3.66	118.24	126.02
24	b	625	CLA	C3C-C4C-NC	3.66	115.12	110.43
31	A	417[B]	PL9	C7-C3-C2	-3.66	119.08	123.39
24	C	502	CLA	CHD-C1D-ND	-3.65	119.66	124.80
26	c	518	BCR	C16-C17-C18	-3.65	122.16	127.28
24	A	409	CLA	C1C-C2C-C3C	-3.65	103.14	106.98
24	b	622	CLA	CHC-C1C-C2C	-3.65	116.58	126.95
24	D	405	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
29	T	104	LMT	C1'-O5'-C5'	3.65	120.84	113.72
24	c	509	CLA	C1D-CHD-C4C	-3.65	118.27	126.02
24	C	512	CLA	CHD-C1D-ND	-3.64	119.68	124.80
24	d	404	CLA	C3C-C4C-NC	3.64	115.10	110.43
24	c	510	CLA	C1D-CHD-C4C	-3.64	118.28	126.02
24	c	514	CLA	C4-C3-C5	3.64	121.55	115.23
24	b	613	CLA	C3D-C4D-ND	3.64	115.90	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	604	CLA	C3C-C4C-NC	3.64	115.09	110.43
26	H	101	BCR	C24-C23-C22	-3.64	120.85	126.23
24	c	505	CLA	C3C-C4C-NC	3.64	115.09	110.43
24	b	621	CLA	CHD-C1D-ND	-3.64	119.68	124.80
24	B	602	CLA	C3B-C4B-NB	3.64	113.78	110.53
24	c	507	CLA	CHD-C1D-ND	-3.64	119.69	124.80
24	b	618	CLA	C1D-CHD-C4C	-3.64	118.29	126.02
24	b	624	CLA	O2D-CGD-CBD	3.63	117.58	111.23
24	B	613	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	D	405	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	A	407	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
24	C	507	CLA	C3C-C4C-NC	3.63	115.08	110.43
24	B	604	CLA	C1C-C2C-C3C	-3.63	103.17	106.98
27	A	411	SQD	C45-O47-C7	-3.63	109.12	117.80
26	d	406	BCR	C38-C26-C25	-3.62	120.53	124.48
24	A	406	CLA	CAA-C2A-C3A	-3.62	103.21	113.00
26	d	406	BCR	C24-C23-C22	-3.62	120.88	126.23
24	b	615	CLA	C3B-C4B-NB	3.62	113.76	110.53
24	c	505	CLA	C1C-C2C-C3C	-3.62	103.17	106.98
24	c	509	CLA	C3D-C2D-C1D	-3.61	100.90	105.83
26	Y	101	BCR	C10-C11-C12	-3.61	112.73	123.20
24	c	512	CLA	C3B-C4B-NB	3.61	113.75	110.53
24	d	403	CLA	CHC-C1C-C2C	-3.61	116.68	126.95
24	B	611	CLA	CAA-C2A-C3A	-3.61	103.25	113.00
24	C	501	CLA	C3C-C4C-NC	3.61	115.05	110.43
24	b	619	CLA	C3C-C4C-NC	3.61	115.05	110.43
24	b	624	CLA	C3C-C4C-NC	3.61	115.05	110.43
27	a	405	SQD	O48-C23-C24	3.60	122.83	111.83
24	B	616	CLA	CMB-C2B-C1B	3.60	130.90	125.42
24	C	504	CLA	C3B-C4B-NB	3.60	113.74	110.53
24	C	509	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	b	617	CLA	C1D-CHD-C4C	-3.60	118.37	126.02
24	C	505	CLA	CAC-C3C-C4C	3.60	129.47	124.79
24	c	509	CLA	C1C-C2C-C3C	-3.59	103.20	106.98
24	A	409	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
35	b	607	HTG	C1'-S1-C1	3.59	108.21	100.45
24	b	610	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
24	b	611	CLA	C1D-CHD-C4C	-3.59	118.39	126.02
26	c	526	BCR	C33-C5-C6	-3.59	120.57	124.48
24	D	405	CLA	C3C-C4C-NC	3.59	115.03	110.43
33	D	415	LMG	O7-C10-C11	3.59	119.24	111.48
24	D	404	CLA	C3C-C4C-NC	3.58	115.02	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	412	CLA	C1-C2-C3	-3.58	120.33	126.20
24	b	621	CLA	O2A-CGA-CBA	3.58	122.74	111.83
24	d	405	CLA	C3C-C4C-NC	3.57	115.01	110.43
24	B	613	CLA	C1D-CHD-C4C	-3.57	118.42	126.02
24	d	405	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
31	A	417[A]	PL9	C37-C38-C39	-3.57	119.45	127.62
24	B	617	CLA	C3C-C4C-NC	3.57	115.00	110.43
24	b	617	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
24	c	508	CLA	C3C-C4C-NC	3.57	115.00	110.43
31	a	416[B]	PL9	C22-C23-C24	-3.56	119.47	127.62
24	d	404	CLA	O2A-CGA-CBA	3.56	122.70	111.83
24	b	614	CLA	CMB-C2B-C1B	3.56	130.84	125.42
24	c	513	CLA	C3C-C4C-NC	3.56	114.99	110.43
24	c	515	CLA	C1-C2-C3	-3.56	120.37	126.20
24	b	616	CLA	CAA-C2A-C3A	-3.56	103.39	113.00
24	b	617	CLA	C3C-C4C-NC	3.56	114.98	110.43
31	a	416[B]	PL9	C7-C3-C4	3.55	119.84	116.91
24	b	613	CLA	C3B-C4B-NB	3.55	113.70	110.53
24	B	608	CLA	CAA-C2A-C3A	-3.55	103.40	113.00
24	b	614	CLA	C1C-C2C-C3C	-3.55	103.24	106.98
24	B	605	CLA	C1D-CHD-C4C	-3.55	118.47	126.02
24	C	506	CLA	C1D-CHD-C4C	-3.55	118.48	126.02
24	c	510	CLA	C4B-C3B-C2B	-3.55	102.89	107.30
24	d	404	CLA	C1-C2-C3	-3.55	120.39	126.20
24	b	621	CLA	C3B-C4B-NB	3.55	113.69	110.53
24	d	404	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
24	b	613	CLA	CHD-C1D-ND	-3.54	119.82	124.80
24	c	505	CLA	C1D-CHD-C4C	-3.54	118.50	126.02
26	h	101	BCR	C38-C26-C25	-3.54	120.62	124.48
24	c	505	CLA	CAC-C3C-C4C	3.54	129.39	124.79
24	c	517	CLA	C1C-C2C-C3C	-3.53	103.26	106.98
33	d	415	LMG	O7-C10-C11	3.53	119.13	111.48
24	B	602	CLA	C3C-C4C-NC	3.53	114.96	110.43
26	H	101	BCR	C16-C17-C18	-3.53	122.32	127.28
24	C	505	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
24	b	625	CLA	CHD-C1D-ND	-3.53	119.83	124.80
24	C	505	CLA	C3D-C2D-C1D	-3.53	101.02	105.83
24	b	612	CLA	C3B-C4B-NB	3.52	113.68	110.53
24	D	404	CLA	CBC-CAC-C3C	-3.52	102.87	112.42
24	D	405	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
24	B	602	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
38	E	103	HEM	C1B-NB-C4B	3.51	109.37	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	407[B]	PL9	C10-C9-C11	3.51	121.33	115.23
24	a	410	CLA	O2D-CGD-O1D	-3.51	117.02	123.85
26	T	103	BCR	C12-C13-C14	-3.51	113.50	119.01
24	c	516	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
24	d	403	CLA	C4A-NA-C1A	-3.50	105.08	106.68
24	B	613	CLA	C2B-C1B-NB	3.50	113.96	110.33
29	C	521	LMT	O1B-C4'-C3'	3.50	116.13	107.23
24	A	405	CLA	C3C-C4C-NC	3.50	114.91	110.43
24	b	625	CLA	C4C-C3C-C2C	-3.49	101.81	106.89
24	c	509	CLA	CMB-C2B-C1B	3.49	130.74	125.42
24	C	510	CLA	C1D-CHD-C4C	-3.49	118.60	126.02
25	d	402[B]	PHO	C1A-C2A-C3A	-3.49	99.52	102.84
24	b	622	CLA	O2D-CGD-CBD	3.49	117.33	111.23
24	b	621	CLA	C4C-C3C-C2C	-3.49	101.82	106.89
24	C	511	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
24	D	404	CLA	C1D-CHD-C4C	-3.48	118.61	126.02
24	A	407	CLA	CMB-C2B-C1B	3.48	130.72	125.42
24	c	511	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
24	A	409	CLA	C3C-C4C-NC	3.48	114.89	110.43
24	B	611	CLA	O2A-CGA-CBA	3.48	122.44	111.83
24	B	616	CLA	CMC-C2C-C1C	3.48	130.47	125.03
24	b	624	CLA	C3B-C4B-NB	3.47	113.63	110.53
36	C	517	DGD	O2G-C1B-C2B	3.47	119.00	111.48
31	a	416[B]	PL9	C27-C28-C29	-3.47	119.68	127.62
27	f	102	SQD	C1-O5-C5	3.47	120.50	113.72
24	b	623	CLA	C3C-C4C-NC	3.47	114.88	110.43
24	c	513	CLA	C1-C2-C3	-3.46	120.52	126.20
26	d	406	BCR	C29-C30-C25	3.46	115.47	110.44
24	b	616	CLA	CBC-CAC-C3C	-3.46	103.03	112.42
24	b	619	CLA	C1D-CHD-C4C	-3.46	118.67	126.02
25	d	402[A]	PHO	C1A-C2A-C3A	-3.46	99.55	102.84
33	z	101	LMG	O7-C10-C11	3.45	118.95	111.48
31	D	407[A]	PL9	C40-C39-C41	3.45	121.22	115.23
37	L	101	LHG	O7-C7-C8	3.45	118.95	111.48
24	B	612	CLA	C1D-CHD-C4C	-3.45	118.68	126.02
24	B	614	CLA	CAC-C3C-C4C	3.45	129.28	124.79
24	B	609	CLA	CHC-C1C-C2C	-3.45	117.15	126.95
31	a	416[B]	PL9	C7-C8-C9	-3.45	120.89	126.83
24	b	623	CLA	C3B-C4B-NB	3.45	113.61	110.53
24	c	510	CLA	CBC-CAC-C3C	-3.45	103.08	112.42
24	b	620	CLA	C1D-CHD-C4C	-3.45	118.70	126.02
31	a	416[B]	PL9	C7-C3-C2	-3.44	119.33	123.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	417[B]	PL9	C22-C23-C24	-3.44	119.75	127.62
24	C	510	CLA	C3C-C4C-NC	3.44	114.83	110.43
24	b	611	CLA	CAA-C2A-C3A	-3.44	103.71	113.00
31	a	416[B]	PL9	C15-C14-C16	3.43	121.19	115.23
26	b	626	BCR	C16-C17-C18	-3.43	122.46	127.28
31	A	417[A]	PL9	C32-C33-C34	-3.43	119.77	127.62
38	f	101	HEM	CHD-C4C-NC	3.43	128.19	124.45
26	B	620	BCR	C28-C27-C26	-3.43	107.94	114.06
24	b	612	CLA	CAA-C2A-C3A	-3.43	103.72	113.00
26	Y	101	BCR	C24-C23-C22	-3.43	121.16	126.23
24	d	403	CLA	CAA-C2A-C3A	-3.43	103.74	113.00
24	B	615	CLA	C3B-C4B-NB	3.43	113.59	110.53
24	B	610	CLA	C3C-C4C-NC	3.43	114.82	110.43
24	b	625	CLA	C3B-C4B-NB	3.42	113.59	110.53
31	a	416[A]	PL9	C17-C18-C19	-3.42	119.79	127.62
24	B	608	CLA	C3C-C4C-NC	3.42	114.81	110.43
24	C	509	CLA	C3C-C4C-NC	3.42	114.81	110.43
24	d	403	CLA	C4B-C3B-C2B	-3.42	103.05	107.30
24	B	613	CLA	C4-C3-C5	3.42	121.16	115.23
24	B	614	CLA	C1D-CHD-C4C	-3.42	118.76	126.02
26	a	413	BCR	C20-C21-C22	-3.42	122.49	127.28
24	D	404	CLA	O2A-CGA-CBA	3.42	122.25	111.83
24	b	620	CLA	CAC-C3C-C4C	3.41	129.22	124.79
24	A	405	CLA	O2A-CGA-CBA	3.41	122.22	111.83
24	C	502	CLA	CAC-C3C-C4C	3.40	129.22	124.79
24	b	621	CLA	C1C-C2C-C3C	-3.40	103.40	106.98
25	A	408	PHO	C1A-C2A-C3A	-3.40	99.60	102.84
24	c	510	CLA	C1-C2-C3	-3.40	120.62	126.20
24	c	507	CLA	C4C-C3C-C2C	-3.40	101.94	106.89
31	a	416[A]	PL9	C7-C8-C9	-3.40	120.97	126.83
25	d	402[A]	PHO	C4-C3-C5	3.40	121.12	115.23
31	a	416[B]	PL9	C17-C18-C19	-3.40	119.85	127.62
24	B	615	CLA	C4C-C3C-C2C	-3.39	101.95	106.89
25	d	402[A]	PHO	C4D-CHA-CBD	3.39	110.08	108.45
33	k	101	LMG	O7-C10-C11	3.39	118.82	111.48
24	b	614	CLA	O2A-CGA-O1A	-3.39	115.15	123.63
24	c	507	CLA	CMB-C2B-C1B	3.39	130.58	125.42
26	T	103	BCR	C21-C20-C19	-3.39	113.39	123.20
24	c	509	CLA	C1-C2-C3	-3.39	120.65	126.20
24	C	509	CLA	CAC-C3C-C4C	3.39	129.19	124.79
24	c	511	CLA	CMC-C2C-C1C	3.38	130.32	125.03
31	A	417[B]	PL9	C32-C33-C34	-3.38	119.88	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	625	CLA	CAC-C3C-C4C	3.38	129.19	124.79
35	V	206	HTG	C1'-S1-C1	3.38	107.75	100.45
24	C	505	CLA	CHD-C1D-ND	-3.38	120.05	124.80
24	B	612	CLA	C1-C2-C3	-3.38	120.67	126.20
40	V	205	HEC	CHD-C4C-NC	3.37	128.12	124.45
31	A	417[A]	PL9	C7-C3-C4	3.37	119.69	116.91
24	b	625	CLA	O2D-CGD-O1D	-3.37	117.29	123.85
24	b	613	CLA	C1-C2-C3	-3.36	120.68	126.20
24	c	516	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
24	b	620	CLA	CHC-C1C-C2C	-3.36	117.39	126.95
31	a	416[A]	PL9	C42-C43-C44	-3.36	119.94	127.62
24	b	622	CLA	C3C-C4C-NC	3.36	114.73	110.43
24	c	505	CLA	C3B-C4B-NB	3.35	113.52	110.53
24	D	405	CLA	CAC-C3C-C4C	3.35	129.15	124.79
24	C	508	CLA	C3C-C4C-NC	3.35	114.72	110.43
24	c	514	CLA	C3C-C4C-NC	3.35	114.72	110.43
24	D	405	CLA	C4-C3-C5	3.35	121.04	115.23
24	B	610	CLA	CHC-C1C-C2C	-3.35	117.44	126.95
24	A	407	CLA	C1D-CHD-C4C	-3.35	118.91	126.02
24	B	612	CLA	C3B-C4B-NB	3.34	113.51	110.53
24	C	512	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
27	F	101	SQD	C3-C4-C5	3.34	116.29	110.23
24	b	624	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
24	C	501	CLA	CBC-CAC-C3C	-3.34	103.37	112.42
24	b	616	CLA	CMB-C2B-C1B	3.34	130.50	125.42
24	c	515	CLA	CAC-C3C-C4C	3.34	129.13	124.79
40	V	205	HEC	CBC-CAC-C3C	-3.34	120.77	127.43
29	C	521	LMT	C1'-O5'-C5'	3.34	120.23	113.72
26	K	101	BCR	C24-C23-C22	-3.33	121.30	126.23
24	C	510	CLA	CAC-C3C-C4C	3.33	129.12	124.79
24	c	516	CLA	CBC-CAC-C3C	-3.33	103.39	112.42
24	b	613	CLA	CAC-C3C-C4C	3.33	129.12	124.79
26	B	619	BCR	C28-C27-C26	-3.33	108.12	114.06
24	a	412	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	A	407	CLA	C3C-C4C-NC	3.33	114.69	110.43
24	b	619	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
24	B	604	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	C	506	CLA	C3C-C4C-NC	3.32	114.69	110.43
24	B	605	CLA	C3D-C4D-ND	3.32	115.39	109.99
24	B	611	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
36	h	102	DGD	O2G-C1B-C2B	3.32	118.66	111.48
24	c	506	CLA	C4C-C3C-C2C	-3.32	102.06	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t	102	BCR	C15-C16-C17	-3.32	116.73	123.52
26	B	619	BCR	C33-C5-C6	-3.32	120.87	124.48
24	c	516	CLA	C1-C2-C3	-3.31	120.77	126.20
24	c	511	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
24	B	608	CLA	C3B-C4B-NB	3.31	113.48	110.53
24	B	605	CLA	CAC-C3C-C4C	3.31	129.09	124.79
31	A	417[A]	PL9	C20-C19-C21	3.31	120.97	115.23
24	B	617	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
38	E	103	HEM	CHD-C4C-NC	3.31	128.05	124.45
24	B	616	CLA	O2D-CGD-CBD	3.30	117.01	111.23
26	D	406	BCR	C28-C27-C26	-3.30	108.17	114.06
24	B	604	CLA	O2A-CGA-CBA	3.30	121.90	111.83
24	B	611	CLA	CHD-C4C-NC	3.30	129.35	124.23
24	B	604	CLA	O2A-CGA-O1A	-3.30	115.38	123.63
24	c	512	CLA	C4-C3-C5	3.30	120.95	115.23
24	B	609	CLA	C4B-C3B-C2B	-3.30	103.20	107.30
24	C	506	CLA	C4-C3-C5	3.29	120.94	115.23
24	C	512	CLA	C1-C2-C3	-3.29	120.80	126.20
24	a	410	CLA	CAA-C2A-C3A	-3.29	104.10	113.00
35	c	524	HTG	C1-O5-C5	3.29	118.47	112.56
24	b	610	CLA	CHD-C4C-NC	3.29	129.34	124.23
24	A	409	CLA	C4-C3-C5	3.29	120.94	115.23
24	b	614	CLA	C4C-C3C-C2C	-3.29	102.10	106.89
26	c	518	BCR	C38-C26-C25	-3.29	120.89	124.48
24	B	608	CLA	CAC-C3C-C4C	3.29	129.07	124.79
24	C	502	CLA	C1C-C2C-C3C	-3.29	103.52	106.98
36	H	102	DGD	O2G-C1B-C2B	3.29	118.59	111.48
26	t	102	BCR	C20-C21-C22	-3.28	122.67	127.28
37	D	411	LHG	O8-C23-C24	3.28	121.85	111.83
24	A	406	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
24	B	606	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
27	a	414	SQD	C1-C2-C3	-3.28	103.11	110.01
24	c	506	CLA	CAC-C3C-C4C	3.28	129.06	124.79
24	C	511	CLA	C3C-C4C-NC	3.28	114.63	110.43
24	c	515	CLA	C3B-C4B-NB	3.28	113.45	110.53
24	B	615	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
24	a	412	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
24	C	508	CLA	C4C-C3C-C2C	-3.27	102.13	106.89
31	D	407[B]	PL9	C27-C28-C29	-3.27	120.14	127.62
24	b	621	CLA	C1-C2-C3	-3.27	120.84	126.20
27	a	405	SQD	O8-S-C6	3.26	112.27	105.97
24	c	515	CLA	C3C-C4C-NC	3.26	114.61	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
26	A	410	BCR	C33-C5-C6	-3.26	120.93	124.48
31	D	407[A]	PL9	C7-C8-C9	-3.26	121.22	126.83
24	B	614	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
31	D	407[B]	PL9	C22-C23-C24	-3.25	120.19	127.62
31	A	417[B]	PL9	C20-C19-C21	3.25	120.87	115.23
24	C	506	CLA	CAA-C2A-C3A	-3.25	104.22	113.00
26	B	620	BCR	C36-C18-C19	3.25	123.05	118.09
24	a	410	CLA	CMB-C2B-C1B	3.24	130.36	125.42
24	A	405	CLA	C4C-C3C-C2C	-3.24	102.17	106.89
24	C	504	CLA	C3C-C4C-NC	3.24	114.58	110.43
24	c	506	CLA	CMB-C2B-C1B	3.24	130.36	125.42
24	C	503	CLA	C4C-C3C-C2C	-3.24	102.18	106.89
24	c	516	CLA	C3C-C4C-NC	3.24	114.58	110.43
24	b	621	CLA	C4-C3-C5	3.24	120.84	115.23
24	C	502	CLA	C3B-C4B-NB	3.23	113.42	110.53
24	D	404	CLA	CHC-C1C-C2C	-3.23	117.77	126.95
24	C	509	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
26	D	406	BCR	C33-C5-C6	-3.23	120.97	124.48
37	E	101	LHG	O8-C23-C24	3.22	121.67	111.83
26	B	618	BCR	C7-C8-C9	-3.22	121.47	126.23
26	Y	101	BCR	C40-C30-C25	-3.22	105.19	110.24
24	a	409	CLA	C3C-C4C-NC	3.22	114.56	110.43
24	B	612	CLA	CAC-C3C-C4C	3.22	128.98	124.79
24	A	409	CLA	CAA-C2A-C3A	-3.22	104.30	113.00
33	C	519	LMG	O8-C28-C29	3.22	121.64	111.83
24	c	511	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
24	b	619	CLA	C3B-C4B-NB	3.22	113.40	110.53
24	B	613	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
24	B	612	CLA	CMA-C3A-C4A	-3.21	103.14	111.77
24	b	618	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
37	b	634	LHG	O7-C7-C8	3.21	118.43	111.48
24	C	503	CLA	CMB-C2B-C1B	3.21	130.31	125.42
24	b	625	CLA	C1-C2-C3	-3.21	120.94	126.20
24	b	614	CLA	C2A-C1A-CHA	-3.20	118.31	123.87
24	B	603	CLA	CAA-C2A-C3A	-3.20	104.34	113.00
24	c	510	CLA	CHC-C1C-C2C	-3.20	117.85	126.95
27	F	101	SQD	C1-C2-C3	-3.20	103.27	110.01
24	c	515	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
26	t	102	BCR	C7-C8-C9	-3.20	121.50	126.23
24	C	503	CLA	C1C-C2C-C3C	-3.20	103.61	106.98
24	d	405	CLA	CMB-C2B-C1B	3.20	130.29	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	405	CLA	C3B-C4B-NB	3.20	113.38	110.53
26	T	103	BCR	C15-C16-C17	-3.20	116.98	123.52
38	E	103	HEM	CHB-C1B-NB	3.19	128.32	124.37
24	C	512	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
24	c	512	CLA	C4C-C3C-C2C	-3.19	102.24	106.89
40	V	205	HEC	CHA-C1A-NA	3.19	127.93	124.45
24	d	403	CLA	C1-C2-C3	-3.19	120.97	126.20
31	a	416[A]	PL9	C27-C28-C29	-3.19	120.32	127.62
31	A	417[A]	PL9	C8-C7-C3	3.19	120.27	112.03
31	A	417[A]	PL9	C22-C23-C24	-3.19	120.32	127.62
24	d	404	CLA	C1D-CHD-C4C	-3.19	119.25	126.02
24	C	501	CLA	CMB-C2B-C1B	3.19	130.27	125.42
24	B	611	CLA	C3C-C4C-NC	3.19	114.51	110.43
25	D	401[A]	PHO	C4-C3-C5	3.19	120.76	115.23
24	d	405	CLA	CHD-C4C-NC	3.18	129.17	124.23
24	a	412	CLA	CBC-CAC-C3C	-3.18	103.79	112.42
24	A	405	CLA	O2D-CGD-CBD	3.18	116.80	111.23
24	A	407	CLA	C3B-C4B-NB	3.18	113.37	110.53
26	D	406	BCR	C29-C30-C25	3.18	115.06	110.44
26	C	514	BCR	C15-C14-C13	-3.18	122.82	127.28
24	C	507	CLA	CMB-C2B-C1B	3.18	130.26	125.42
31	D	407[A]	PL9	C10-C9-C11	3.18	120.75	115.23
24	B	616	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
24	c	512	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
24	B	609	CLA	C3C-C4C-NC	3.18	114.50	110.43
24	c	510	CLA	CAA-C2A-C3A	-3.18	104.42	113.00
24	C	505	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
24	a	412	CLA	CHC-C1C-C2C	-3.17	117.93	126.95
24	A	406	CLA	CHD-C4C-NC	3.17	129.15	124.23
24	b	618	CLA	CMB-C2B-C1B	3.17	130.25	125.42
33	k	101	LMG	O8-C28-C29	3.17	121.50	111.83
24	B	616	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
24	B	615	CLA	O2A-CGA-CBA	3.17	121.50	111.83
25	d	402[B]	PHO	C4-C3-C5	3.17	120.73	115.23
24	c	511	CLA	CMB-C2B-C1B	3.17	130.24	125.42
24	c	513	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
24	B	617	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
24	C	513	CLA	C3C-C4C-NC	3.17	114.49	110.43
24	b	610	CLA	C3C-C4C-NC	3.17	114.49	110.43
24	C	504	CLA	CBC-CAC-C3C	-3.17	103.84	112.42
24	B	605	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
24	B	605	CLA	O2A-CGA-CBA	3.17	121.49	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	405	CLA	C1C-C2C-C3C	-3.16	103.65	106.98
24	B	602	CLA	O2A-CGA-CBA	3.16	121.48	111.83
24	b	611	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
31	a	416[B]	PL9	C42-C43-C44	-3.16	120.39	127.62
26	a	413	BCR	C15-C14-C13	-3.16	122.84	127.28
24	c	506	CLA	CHC-C1C-C2C	-3.16	117.97	126.95
36	e	101	DGD	O5D-C1E-C2E	3.16	113.07	108.27
26	K	101	BCR	C33-C5-C6	-3.16	121.04	124.48
24	a	412	CLA	C3C-C4C-NC	3.16	114.47	110.43
31	a	416[A]	PL9	C20-C19-C21	3.16	120.71	115.23
31	A	417[B]	PL9	C7-C8-C9	-3.16	121.39	126.83
26	Y	101	BCR	C16-C17-C18	-3.16	122.85	127.28
24	B	612	CLA	CMC-C2C-C1C	3.16	129.97	125.03
36	D	408	DGD	O1G-C1A-C2A	3.15	121.45	111.83
24	c	506	CLA	C1C-C2C-C3C	-3.15	103.67	106.98
24	C	508	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
24	B	606	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
35	B	624	HTG	C1-O5-C5	3.15	118.21	112.56
24	b	621	CLA	O2A-CGA-O1A	-3.15	115.75	123.63
24	B	616	CLA	CAC-C3C-C4C	3.15	128.89	124.79
24	c	515	CLA	O2A-CGA-CBA	3.15	121.43	111.83
24	c	506	CLA	C3B-C4B-NB	3.15	113.34	110.53
24	b	624	CLA	C4-C3-C5	3.14	120.68	115.23
24	A	405	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
31	D	407[B]	PL9	C40-C39-C41	3.14	120.68	115.23
24	A	405	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
31	A	417[B]	PL9	C27-C28-C29	-3.14	120.44	127.62
24	C	504	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
24	B	609	CLA	CAC-C3C-C4C	3.14	128.87	124.79
24	c	517	CLA	CMB-C2B-C1B	3.14	130.19	125.42
33	b	629	LMG	O7-C10-C11	3.14	118.26	111.48
24	b	619	CLA	C1C-C2C-C3C	-3.13	103.68	106.98
24	c	505	CLA	CBC-CAC-C3C	-3.13	103.93	112.42
24	A	406	CLA	C3C-C4C-NC	3.13	114.44	110.43
24	c	513	CLA	CAC-C3C-C4C	3.13	128.86	124.79
24	c	509	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
24	b	624	CLA	CHD-C4C-NC	3.13	129.08	124.23
24	b	611	CLA	C1-C2-C3	-3.13	121.07	126.20
24	b	611	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
24	B	616	CLA	CHD-C4C-NC	3.12	129.08	124.23
26	b	628	BCR	C15-C14-C13	-3.12	122.90	127.28
24	B	606	CLA	C2A-C1A-CHA	-3.12	118.45	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	d	403	CLA	C2A-C1A-CHA	-3.12	118.45	123.87
24	C	513	CLA	CAC-C3C-C4C	3.12	128.85	124.79
24	b	621	CLA	C4B-C3B-C2B	-3.12	103.42	107.30
31	a	416[A]	PL9	C10-C9-C11	3.12	120.64	115.23
24	c	508	CLA	CMC-C2C-C1C	3.12	129.91	125.03
36	H	102	DGD	O1G-C1A-C2A	3.12	121.34	111.83
24	b	624	CLA	C4C-C3C-C2C	-3.12	102.35	106.89
24	B	605	CLA	CHC-C1C-C2C	-3.12	118.09	126.95
36	C	518	DGD	O1G-C1A-C2A	3.12	121.34	111.83
24	b	621	CLA	CHD-C4C-NC	3.12	129.06	124.23
24	D	404	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
31	d	407[B]	PL9	C40-C39-C41	3.11	120.63	115.23
24	C	505	CLA	C1C-C2C-C3C	-3.11	103.71	106.98
24	C	504	CLA	C4-C3-C5	3.11	120.62	115.23
24	C	502	CLA	C4C-C3C-C2C	-3.11	102.37	106.89
37	d	409	LHG	O7-C7-C8	3.10	118.19	111.48
24	C	510	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
24	C	506	CLA	C3B-C4B-NB	3.10	113.30	110.53
24	b	622	CLA	CMB-C2B-C1B	3.10	130.14	125.42
24	C	508	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
24	a	409	CLA	O2D-CGD-CBD	3.10	116.64	111.23
26	T	103	BCR	C35-C13-C12	3.10	122.82	118.09
26	C	514	BCR	C33-C5-C6	-3.09	121.11	124.48
24	D	405	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
26	H	101	BCR	C31-C1-C6	-3.09	105.39	110.24
24	b	614	CLA	CHD-C4C-NC	3.09	129.03	124.23
24	C	506	CLA	CHC-C1C-C2C	-3.09	118.16	126.95
38	f	101	HEM	CHA-C4D-ND	3.09	128.19	124.37
24	A	407	CLA	CHD-C4C-NC	3.09	129.02	124.23
24	c	512	CLA	CHD-C1D-ND	-3.09	120.46	124.80
24	a	410	CLA	CHD-C4C-NC	3.09	129.02	124.23
24	B	602	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
24	b	618	CLA	C3B-C4B-NB	3.09	113.28	110.53
29	M	104	LMT	O5'-C5'-C4'	3.09	116.10	109.72
24	B	614	CLA	C4-C3-C5	3.09	120.58	115.23
24	c	517	CLA	C4C-C3C-C2C	-3.08	102.40	106.89
24	b	624	CLA	CMB-C2B-C1B	3.08	130.11	125.42
24	b	613	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
24	B	602	CLA	CHD-C4C-NC	3.08	129.01	124.23
24	c	515	CLA	CHD-C4C-NC	3.08	129.00	124.23
24	a	409	CLA	CHC-C1C-C2C	-3.08	118.20	126.95
33	b	629	LMG	O8-C28-C29	3.08	121.22	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	m	103	LMT	C1B-O5B-C5B	3.08	119.73	113.72
24	c	517	CLA	CMC-C2C-C1C	3.07	129.84	125.03
24	c	517	CLA	CAC-C3C-C4C	3.07	128.79	124.79
24	B	603	CLA	CHD-C4C-NC	3.07	128.99	124.23
24	A	407	CLA	CBC-CAC-C3C	-3.07	104.09	112.42
24	a	409	CLA	O2A-CGA-CBA	3.07	121.20	111.83
24	B	606	CLA	CAC-C3C-C4C	3.07	128.78	124.79
24	a	409	CLA	C2A-C1A-CHA	-3.07	118.54	123.87
24	b	620	CLA	C4B-C3B-C2B	-3.07	103.49	107.30
24	B	607	CLA	CMC-C2C-C1C	3.07	129.83	125.03
24	a	409	CLA	CAA-C2A-C1A	-3.07	101.92	111.97
26	d	406	BCR	C16-C15-C14	-3.07	117.25	123.52
24	B	608	CLA	CMC-C2C-C1C	3.07	129.82	125.03
24	b	612	CLA	CBC-CAC-C3C	-3.06	104.11	112.42
24	b	612	CLA	CAC-C3C-C4C	3.06	128.78	124.79
26	k	102	BCR	C24-C23-C22	-3.06	121.70	126.23
37	d	408	LHG	O8-C23-O10	-3.06	115.97	123.63
31	d	407[A]	PL9	C37-C38-C39	-3.06	120.62	127.62
27	L	102	SQD	O48-C23-C24	3.06	121.17	111.83
26	y	101	BCR	C10-C11-C12	-3.06	114.34	123.20
31	a	416[B]	PL9	C37-C38-C39	-3.06	120.63	127.62
24	b	618	CLA	C1-C2-C3	-3.06	121.19	126.20
24	B	611	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
27	A	411	SQD	O48-C23-C24	3.06	121.15	111.83
27	a	414	SQD	C1-O5-C5	-3.05	107.75	113.72
24	B	602	CLA	C4B-C3B-C2B	-3.05	103.50	107.30
24	B	605	CLA	CMB-C2B-C1B	3.05	130.07	125.42
24	c	514	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
24	b	610	CLA	C3B-C4B-NB	3.05	113.25	110.53
24	B	613	CLA	C1-C2-C3	-3.05	121.20	126.20
24	c	509	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
24	a	409	CLA	O2A-CGA-O1A	-3.04	116.02	123.63
24	C	506	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
24	B	608	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
24	C	512	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
33	M	101	LMG	O8-C28-C29	3.04	121.11	111.83
24	C	501	CLA	CHD-C4C-NC	3.04	128.94	124.23
37	L	101	LHG	C5-O7-C7	-3.04	110.52	117.80
26	c	518	BCR	C21-C20-C19	-3.04	114.40	123.20
24	B	611	CLA	C4C-C3C-C2C	-3.03	102.47	106.89
24	B	607	CLA	C4-C3-C5	3.03	120.50	115.23
24	b	625	CLA	CHC-C1C-C2C	-3.03	118.33	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	409	CLA	C3B-C4B-NB	3.03	113.24	110.53
24	b	611	CLA	C3B-C4B-NB	3.03	113.24	110.53
24	b	613	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
31	d	407[A]	PL9	C40-C39-C41	3.03	120.49	115.23
26	Y	101	BCR	C38-C26-C25	-3.03	121.18	124.48
24	B	615	CLA	CHD-C4C-NC	3.03	128.93	124.23
26	C	515	BCR	C24-C23-C22	-3.03	121.75	126.23
24	d	405	CLA	CAC-C3C-C4C	3.03	128.73	124.79
24	b	612	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
24	b	623	CLA	CBC-CAC-C3C	-3.03	104.22	112.42
24	B	610	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
24	b	615	CLA	C4B-C3B-C2B	-3.02	103.54	107.30
24	B	606	CLA	C3B-C4B-NB	3.02	113.23	110.53
24	b	616	CLA	C3B-C4B-NB	3.02	113.23	110.53
24	d	405	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
24	A	406	CLA	O2A-CGA-O1A	-3.02	116.07	123.63
24	b	623	CLA	O2A-CGA-CBA	3.02	121.04	111.83
24	b	619	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
24	C	506	CLA	C1-C2-C3	-3.02	121.25	126.20
31	a	416[A]	PL9	C37-C38-C39	-3.02	120.72	127.62
24	B	613	CLA	C4C-C3C-C2C	-3.01	102.50	106.89
24	C	511	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
24	c	515	CLA	C4-C3-C5	3.01	120.46	115.23
37	a	420	LHG	O7-C7-C8	3.01	118.00	111.48
24	B	611	CLA	C3B-C4B-NB	3.01	113.22	110.53
36	C	518	DGD	O2G-C1B-C2B	3.01	117.99	111.48
24	c	508	CLA	C4-C3-C5	3.01	120.45	115.23
24	c	513	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
24	d	404	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
33	c	522	LMG	C3-C4-C5	3.00	115.68	110.23
24	B	606	CLA	CHD-C4C-NC	3.00	128.89	124.23
24	d	404	CLA	C3B-C4B-NB	3.00	113.21	110.53
24	b	623	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
24	b	625	CLA	O2A-CGA-CBA	3.00	120.98	111.83
24	B	614	CLA	CMC-C2C-C1C	3.00	129.72	125.03
24	B	608	CLA	CBC-CAC-C3C	-3.00	104.29	112.42
24	B	610	CLA	C1-O2A-CGA	3.00	123.91	116.65
24	C	509	CLA	C4B-C3B-C2B	-3.00	103.58	107.30
35	C	523	HTG	O5-C5-C4	3.00	115.10	109.70
24	b	619	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
24	C	510	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
24	C	511	CLA	CHC-C1C-C2C	-2.99	118.44	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	514	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
31	A	417[A]	PL9	C12-C13-C14	-2.99	120.77	127.62
27	a	414	SQD	C45-O47-C7	-2.99	110.63	117.80
24	b	613	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
33	Z	101	LMG	C1-O6-C5	2.99	119.56	113.72
24	b	622	CLA	C4C-C3C-C2C	-2.99	102.54	106.89
24	a	412	CLA	CMA-C3A-C4A	-2.99	103.74	111.77
24	b	615	CLA	C4-C3-C5	2.99	120.42	115.23
24	A	409	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
24	d	403	CLA	C3C-C4C-NC	2.99	114.26	110.43
24	b	624	CLA	CHC-C1C-C2C	-2.99	118.45	126.95
26	c	518	BCR	C33-C5-C6	-2.99	121.22	124.48
24	D	405	CLA	CAA-C2A-C3A	-2.99	104.93	113.00
24	d	405	CLA	CMC-C2C-C1C	2.99	129.70	125.03
24	b	622	CLA	O2A-CGA-CBA	2.99	120.94	111.83
24	C	504	CLA	CAC-C3C-C4C	2.99	128.67	124.79
31	d	407[B]	PL9	C12-C13-C14	-2.98	120.79	127.62
24	B	612	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
25	d	402[B]	PHO	CMA-C3A-C4A	-2.98	108.19	114.61
26	K	101	BCR	C10-C11-C12	-2.98	114.56	123.20
24	C	503	CLA	C4-C3-C5	2.98	120.40	115.23
26	t	102	BCR	C21-C20-C19	-2.98	114.56	123.20
24	a	412	CLA	CHD-C4C-NC	2.98	128.85	124.23
31	A	417[A]	PL9	C45-C44-C46	2.98	120.40	115.23
24	c	516	CLA	C4-C3-C5	2.98	120.39	115.23
37	D	409	LHG	O8-C23-C24	2.98	120.91	111.83
24	C	502	CLA	CMC-C2C-C1C	2.98	129.68	125.03
26	h	101	BCR	C7-C8-C9	-2.98	121.83	126.23
24	B	604	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
33	c	522	LMG	O6-C5-C4	2.97	115.06	109.70
24	a	409	CLA	C4-C3-C5	2.97	120.38	115.23
24	C	504	CLA	CMC-C2C-C1C	2.97	129.67	125.03
24	b	625	CLA	CHD-C4C-NC	2.97	128.83	124.23
24	b	614	CLA	C4-C3-C5	2.97	120.38	115.23
31	A	417[A]	PL9	C53-C6-C1	2.97	121.36	115.28
26	h	101	BCR	C16-C17-C18	-2.97	123.12	127.28
24	c	505	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
24	D	404	CLA	CMB-C2B-C1B	2.97	129.94	125.42
31	D	407[A]	PL9	C15-C14-C16	2.97	120.38	115.23
37	D	409	LHG	O7-C7-C8	2.97	117.90	111.48
24	c	509	CLA	CAC-C3C-C4C	2.97	128.65	124.79
31	A	417[A]	PL9	C27-C28-C29	-2.97	120.84	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	C1-C2-C3	-2.97	121.34	126.20
24	B	617	CLA	CHC-C1C-C2C	-2.96	118.52	126.95
24	c	511	CLA	C1-C2-C3	-2.96	121.34	126.20
31	a	416[B]	PL9	C20-C19-C21	2.96	120.37	115.23
37	d	408	LHG	O7-C7-C8	2.96	117.89	111.48
24	b	610	CLA	C4-C3-C5	2.96	120.37	115.23
36	c	519	DGD	C2G-O2G-C1B	-2.96	110.71	117.80
24	B	604	CLA	C3B-C4B-NB	2.96	113.17	110.53
24	A	409	CLA	CHC-C1C-C2C	-2.96	118.54	126.95
24	C	507	CLA	CHD-C4C-NC	2.96	128.82	124.23
24	D	405	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
24	B	614	CLA	CHC-C1C-C2C	-2.96	118.55	126.95
24	c	507	CLA	C3B-C4B-NB	2.96	113.17	110.53
24	B	602	CLA	CMB-C2B-C1B	2.95	129.92	125.42
24	B	606	CLA	O2A-CGA-O1A	-2.95	116.24	123.63
31	a	416[B]	PL9	C10-C9-C11	2.95	120.36	115.23
24	C	508	CLA	C1C-C2C-C3C	-2.95	103.87	106.98
36	h	102	DGD	O1G-C1A-C2A	2.95	120.84	111.83
24	C	503	CLA	CMC-C2C-C1C	2.95	129.65	125.03
24	D	405	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
24	b	617	CLA	O2A-CGA-CBA	2.95	120.83	111.83
24	b	616	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
26	B	620	BCR	C38-C26-C25	-2.95	121.27	124.48
24	D	405	CLA	C1-C2-C3	-2.95	121.37	126.20
24	b	624	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
24	B	605	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
24	C	508	CLA	CAC-C3C-C4C	2.94	128.62	124.79
24	c	512	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
24	b	613	CLA	O2A-CGA-CBA	2.94	120.81	111.83
24	B	610	CLA	CAC-C3C-C4C	2.94	128.62	124.79
27	F	101	SQD	O48-C23-C24	2.94	120.81	111.83
24	B	603	CLA	C1-C2-C3	-2.94	121.38	126.20
24	b	615	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
24	C	502	CLA	CHD-C4C-NC	2.94	128.79	124.23
24	b	615	CLA	CHD-C4C-NC	2.94	128.79	124.23
24	B	612	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
24	C	510	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
24	C	507	CLA	CMC-C2C-C1C	2.94	129.63	125.03
24	d	405	CLA	CBC-CAC-C3C	-2.94	104.46	112.42
24	C	502	CLA	CMB-C2B-C1B	2.94	129.89	125.42
24	c	509	CLA	CHC-C1C-C2C	-2.94	118.61	126.95
27	A	411	SQD	O8-S-C6	2.93	111.64	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	508	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
24	b	625	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
24	d	403	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
33	C	519	LMG	C8-O7-C10	-2.93	110.78	117.80
24	d	403	CLA	CMA-C3A-C2A	-2.93	102.66	113.98
24	C	507	CLA	C1-C2-C3	-2.93	121.40	126.20
31	a	416[A]	PL9	C35-C34-C36	2.93	120.31	115.23
24	C	501	CLA	CAC-C3C-C4C	2.93	128.60	124.79
24	b	612	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
24	c	516	CLA	CHD-C4C-NC	2.92	128.77	124.23
31	D	407[B]	PL9	C7-C3-C2	-2.92	119.94	123.39
24	c	510	CLA	C3C-C4C-NC	2.92	114.17	110.43
31	d	407[A]	PL9	C10-C9-C11	2.92	120.30	115.23
24	a	410	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
24	A	406	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
24	B	617	CLA	CHD-C4C-NC	2.92	128.76	124.23
24	b	612	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
24	b	610	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
24	B	605	CLA	O2A-CGA-O1A	-2.91	116.34	123.63
35	B	624	HTG	C1-C2-C3	2.91	116.24	110.55
37	d	408	LHG	O8-C23-C24	2.91	120.71	111.83
26	D	406	BCR	C15-C14-C13	-2.91	123.19	127.28
24	d	404	CLA	CBC-CAC-C3C	-2.91	104.53	112.42
24	A	407	CLA	C4-C3-C5	2.91	120.28	115.23
24	B	613	CLA	CHD-C4C-NC	2.91	128.74	124.23
26	d	406	BCR	C15-C14-C13	-2.91	123.20	127.28
26	b	626	BCR	C29-C30-C25	2.91	114.66	110.44
24	B	603	CLA	C4C-C3C-C2C	-2.91	102.66	106.89
36	C	516	DGD	C3G-C2G-C1G	-2.91	105.01	111.78
24	c	513	CLA	CMC-C2C-C1C	2.91	129.57	125.03
24	c	509	CLA	C3B-C4B-NB	2.91	113.12	110.53
26	c	518	BCR	C11-C10-C9	-2.91	123.20	127.28
24	c	505	CLA	C4C-C3C-C2C	-2.90	102.66	106.89
24	c	505	CLA	CMC-C2C-C1C	2.90	129.57	125.03
24	c	515	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
25	D	401[A]	PHO	CMB-C2B-C3B	2.90	130.49	124.68
24	C	508	CLA	C1-C2-C3	-2.90	121.44	126.20
24	c	508	CLA	CAC-C3C-C4C	2.90	128.57	124.79
24	C	513	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
24	B	617	CLA	CMB-C2B-C1B	2.90	129.84	125.42
33	z	101	LMG	O8-C28-C29	2.90	120.68	111.83
24	D	405	CLA	CBC-CAC-C3C	-2.90	104.56	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	404	CLA	O2A-CGA-O1A	-2.90	116.38	123.63
27	f	102	SQD	O5-C5-C4	2.90	114.92	109.70
36	c	521	DGD	O1G-C1A-C2A	2.90	120.66	111.83
24	b	611	CLA	CHD-C4C-NC	2.89	128.72	124.23
24	C	512	CLA	CHD-C4C-NC	2.89	128.72	124.23
24	B	602	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
24	c	508	CLA	C3B-C4B-NB	2.89	113.11	110.53
24	B	606	CLA	CMC-C2C-C1C	2.89	129.55	125.03
24	B	604	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
24	B	607	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
27	a	414	SQD	O8-S-C6	2.89	111.55	105.97
24	A	407	CLA	C1-C2-C3	-2.89	121.46	126.20
24	b	623	CLA	CAC-C3C-C4C	2.89	128.55	124.79
26	t	102	BCR	C1-C6-C7	2.89	123.48	115.65
24	c	512	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
24	D	404	CLA	CAA-C2A-C3A	-2.89	105.20	113.00
24	b	620	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
24	d	403	CLA	CMB-C2B-C1B	2.89	129.81	125.42
24	b	618	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
24	a	410	CLA	C3B-C4B-NB	2.89	113.11	110.53
24	b	614	CLA	O2A-CGA-CBA	2.88	120.63	111.83
26	B	619	BCR	C29-C30-C25	2.88	114.63	110.44
31	A	417[A]	PL9	C7-C8-C9	-2.88	121.87	126.83
24	c	516	CLA	O2A-CGA-CBA	2.88	120.62	111.83
24	C	512	CLA	C3B-C4B-NB	2.88	113.10	110.53
24	b	623	CLA	CMC-C2C-C1C	2.88	129.53	125.03
24	b	618	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
26	C	514	BCR	C38-C26-C25	-2.88	121.34	124.48
24	d	403	CLA	CHD-C4C-NC	2.88	128.69	124.23
24	C	508	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
24	a	412	CLA	CHB-C4A-NA	2.87	128.55	124.40
24	b	619	CLA	O2A-CGA-CBA	2.87	120.60	111.83
24	d	404	CLA	C2A-C1A-CHA	-2.87	118.88	123.87
24	B	614	CLA	O2D-CGD-CBD	2.87	116.25	111.23
24	B	615	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
24	C	509	CLA	C1-O2A-CGA	2.87	123.60	116.65
24	C	503	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
24	b	615	CLA	CAA-C2A-C3A	-2.87	105.24	113.00
24	B	604	CLA	CHD-C4C-NC	2.87	128.68	124.23
24	b	617	CLA	CHD-C4C-NC	2.87	128.68	124.23
24	C	501	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
24	b	616	CLA	CHD-C4C-NC	2.87	128.68	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	c	518	BCR	C3-C4-C5	-2.87	108.94	114.06
24	A	409	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
24	D	404	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
24	c	511	CLA	CHD-C4C-NC	2.87	128.68	124.23
26	b	627	BCR	C38-C26-C25	-2.86	121.36	124.48
24	c	517	CLA	C2A-C1A-CHA	-2.86	118.90	123.87
24	b	614	CLA	C3B-C4B-NB	2.86	113.09	110.53
24	B	617	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
24	B	603	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
24	a	412	CLA	C4-C3-C5	2.86	120.20	115.23
31	d	407[B]	PL9	C27-C28-C29	-2.86	121.07	127.62
36	H	102	DGD	O1G-C1A-O1A	-2.86	116.47	123.63
33	z	101	LMG	C8-O7-C10	-2.86	110.95	117.80
24	b	618	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
31	d	407[A]	PL9	C27-C28-C29	-2.86	121.08	127.62
26	h	101	BCR	C10-C11-C12	-2.86	114.92	123.20
24	C	509	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
24	b	612	CLA	CHC-C1C-C2C	-2.85	118.84	126.95
24	D	404	CLA	CHD-C4C-NC	2.85	128.66	124.23
24	B	614	CLA	O2A-CGA-CBA	2.85	120.53	111.83
31	D	407[B]	PL9	C37-C38-C39	-2.85	121.09	127.62
24	b	617	CLA	CBC-CAC-C3C	-2.85	104.69	112.42
24	c	513	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
24	B	603	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
29	M	104	LMT	O1B-C1B-C2B	2.85	115.10	108.09
24	b	620	CLA	CMB-C2B-C1B	2.85	129.75	125.42
24	c	507	CLA	C4-C3-C5	2.85	120.17	115.23
24	C	506	CLA	CMC-C2C-C1C	2.85	129.48	125.03
24	B	603	CLA	C3B-C4B-NB	2.85	113.07	110.53
26	k	102	BCR	C3-C4-C5	-2.85	108.98	114.06
24	C	511	CLA	C4C-C3C-C2C	-2.84	102.75	106.89
24	B	605	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
24	C	505	CLA	C3B-C4B-NB	2.84	113.07	110.53
24	c	511	CLA	C4-C3-C5	2.84	120.16	115.23
24	c	515	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
24	B	602	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
24	b	612	CLA	CHD-C4C-NC	2.84	128.63	124.23
26	k	102	BCR	C15-C14-C13	-2.84	123.30	127.28
31	A	417[B]	PL9	C42-C43-C44	-2.84	121.13	127.62
24	c	508	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
24	B	607	CLA	CHD-C4C-NC	2.84	128.63	124.23
24	b	616	CLA	CHC-C1C-C2C	-2.84	118.89	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	C4B-C3B-C2B	-2.84	103.78	107.30
24	b	620	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
24	b	617	CLA	C2A-C1A-CHA	-2.84	118.94	123.87
31	a	416[A]	PL9	C40-C39-C41	2.84	120.15	115.23
24	a	410	CLA	O2A-CGA-CBA	2.84	120.48	111.83
37	d	408	LHG	O7-C7-O9	-2.83	117.08	123.70
24	B	615	CLA	C2A-C1A-CHA	-2.83	118.95	123.87
24	b	617	CLA	CMC-C2C-C1C	2.83	129.46	125.03
24	b	617	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
24	c	506	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
24	B	608	CLA	CHC-C1C-C2C	-2.83	118.91	126.95
24	d	404	CLA	CMC-C2C-C1C	2.83	129.45	125.03
24	C	509	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
24	d	404	CLA	C4-C3-C5	2.82	120.13	115.23
24	b	615	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
24	a	410	CLA	C4-C3-C5	2.82	120.12	115.23
37	L	101	LHG	O8-C23-C24	2.82	120.43	111.83
26	t	102	BCR	C37-C22-C23	2.82	122.39	118.09
31	d	407[B]	PL9	C10-C9-C11	2.82	120.12	115.23
24	b	616	CLA	CMC-C2C-C1C	2.82	129.44	125.03
24	b	611	CLA	C2A-C1A-CHA	-2.82	118.98	123.87
25	D	401[B]	PHO	C4-C3-C5	2.82	120.12	115.23
24	C	508	CLA	O2A-CGA-CBA	2.82	120.42	111.83
24	B	615	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
31	a	416[A]	PL9	C7-C3-C2	-2.82	120.07	123.39
24	C	504	CLA	CHC-C1C-C2C	-2.82	118.95	126.95
31	a	416[B]	PL9	C35-C34-C36	2.81	120.11	115.23
24	a	412	CLA	CMA-C3A-C2A	-2.81	103.11	113.98
24	B	613	CLA	C2A-C1A-CHA	-2.81	118.99	123.87
38	f	101	HEM	C4D-ND-C1D	2.81	108.54	105.21
24	C	502	CLA	O2A-CGA-CBA	2.81	120.41	111.83
33	Z	101	LMG	C8-O7-C10	-2.81	111.07	117.80
24	C	513	CLA	C3B-C4B-NB	2.81	113.04	110.53
24	b	612	CLA	O2A-CGA-CBA	2.81	120.40	111.83
24	C	502	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
24	b	618	CLA	CHD-C4C-NC	2.81	128.58	124.23
38	f	101	HEM	C1B-NB-C4B	2.81	108.53	105.21
31	a	416[A]	PL9	C53-C6-C1	2.81	121.03	115.28
24	c	510	CLA	CHD-C4C-NC	2.81	128.58	124.23
24	b	610	CLA	CHC-C1C-C2C	-2.81	118.97	126.95
27	F	101	SQD	C44-O6-C1	-2.81	107.78	113.80
24	C	507	CLA	C4C-C3C-C2C	-2.80	102.81	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	628	BCR	C38-C26-C25	-2.80	121.42	124.48
26	b	628	BCR	C8-C7-C6	-2.80	119.51	127.00
26	K	101	BCR	C3-C4-C5	-2.80	109.06	114.06
27	a	414	SQD	O48-C23-C24	2.80	120.38	111.83
26	Y	101	BCR	C15-C16-C17	-2.80	117.79	123.52
38	f	101	HEM	CBD-CAD-C3D	-2.80	104.79	112.53
24	B	612	CLA	CHC-C1C-C2C	-2.80	118.99	126.95
24	C	504	CLA	C4B-C3B-C2B	-2.80	103.82	107.30
26	b	628	BCR	C3-C4-C5	-2.80	109.07	114.06
24	B	610	CLA	C1-C2-C3	-2.80	121.61	126.20
24	C	505	CLA	CHC-C1C-C2C	-2.80	119.00	126.95
24	c	510	CLA	CAC-C3C-C4C	2.80	128.43	124.79
31	d	407[B]	PL9	C37-C38-C39	-2.80	121.22	127.62
24	b	611	CLA	C4-C3-C5	2.79	120.07	115.23
24	B	617	CLA	O2A-CGA-CBA	2.79	120.34	111.83
33	b	629	LMG	O8-C28-O10	-2.79	116.65	123.63
24	c	505	CLA	O2A-CGA-CBA	2.79	120.33	111.83
24	C	511	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
24	b	619	CLA	CMA-C3A-C4A	-2.79	104.28	111.77
26	c	526	BCR	C20-C21-C22	-2.79	123.37	127.28
24	c	514	CLA	O2A-CGA-CBA	2.79	120.33	111.83
24	C	503	CLA	CHD-C4C-NC	2.78	128.55	124.23
24	B	606	CLA	O2A-CGA-CBA	2.78	120.33	111.83
24	C	509	CLA	CMC-C2C-C1C	2.78	129.38	125.03
24	B	609	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
24	B	614	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
37	d	409	LHG	O8-C23-O10	-2.78	116.67	123.63
24	c	517	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
24	b	620	CLA	O2A-CGA-CBA	2.78	120.30	111.83
24	c	517	CLA	CHD-C4C-NC	2.78	128.54	124.23
24	c	517	CLA	O2A-CGA-CBA	2.78	120.30	111.83
26	B	618	BCR	C16-C17-C18	-2.78	123.39	127.28
31	D	407[B]	PL9	C53-C6-C1	2.77	120.96	115.28
24	d	405	CLA	CHC-C1C-C2C	-2.77	119.06	126.95
24	a	410	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
24	A	405	CLA	CAA-C2A-C1A	-2.77	102.89	111.97
24	c	514	CLA	CHD-C4C-NC	2.77	128.53	124.23
37	d	410	LHG	O8-C23-C24	2.77	120.29	111.83
24	B	608	CLA	C1-O2A-CGA	2.77	123.36	116.65
26	K	101	BCR	C20-C21-C22	-2.77	123.39	127.28
24	B	607	CLA	CAA-C2A-C3A	-2.77	105.52	113.00
31	A	417[B]	PL9	C12-C13-C14	-2.77	121.29	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	K	101	BCR	C2-C1-C6	2.77	114.46	110.44
24	c	513	CLA	C4C-C3C-C2C	-2.77	102.87	106.89
29	m	103	LMT	O5'-C5'-C4'	2.76	115.43	109.72
24	C	510	CLA	O2A-CGA-CBA	2.76	120.26	111.83
40	v	206	HEC	CBC-CAC-C3C	-2.76	121.92	127.43
24	B	611	CLA	C1-C2-C3	-2.76	121.68	126.20
40	v	206	HEC	CHA-C1A-NA	2.76	127.46	124.45
24	A	407	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
27	a	414	SQD	O47-C7-O49	-2.76	117.26	123.70
24	B	603	CLA	C4-C3-C5	2.76	120.01	115.23
24	B	610	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
24	d	405	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
24	b	620	CLA	CBC-CAC-C3C	-2.76	104.95	112.42
33	M	101	LMG	O7-C10-C11	2.75	117.44	111.48
24	c	514	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
24	d	404	CLA	CAC-C3C-C4C	2.75	128.37	124.79
24	b	616	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
24	c	516	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
26	c	526	BCR	C28-C27-C26	-2.75	109.16	114.06
24	d	405	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
24	C	507	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
24	b	612	CLA	CMC-C2C-C1C	2.74	129.32	125.03
24	c	507	CLA	CHD-C4C-NC	2.74	128.48	124.23
24	C	512	CLA	CMB-C2B-C1B	2.74	129.59	125.42
24	C	507	CLA	O2A-CGA-CBA	2.74	120.19	111.83
25	a	411	PHO	CBA-CAA-C2A	-2.74	105.70	113.78
24	b	622	CLA	O2A-CGA-O1A	-2.74	116.78	123.63
24	c	508	CLA	CHD-C4C-NC	2.74	128.47	124.23
24	d	404	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
24	c	507	CLA	CAC-C3C-C4C	2.74	128.35	124.79
31	A	417[B]	PL9	C53-C6-C1	2.73	120.88	115.28
24	B	613	CLA	C3B-C4B-NB	2.73	112.97	110.53
31	a	416[A]	PL9	C25-C24-C26	2.73	119.97	115.23
26	T	103	BCR	C2-C1-C6	2.73	114.41	110.44
24	d	403	CLA	C1-O2A-CGA	2.73	123.27	116.65
24	b	623	CLA	CHD-C4C-NC	2.73	128.47	124.23
24	a	412	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
24	C	510	CLA	C4-C3-C5	2.73	119.97	115.23
26	K	101	BCR	C29-C30-C25	2.73	114.40	110.44
24	A	407	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
24	C	512	CLA	C4B-C3B-C2B	-2.73	103.91	107.30
24	b	618	CLA	C4-C3-C5	2.73	119.96	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	621	CLA	CMC-C2C-C1C	2.73	129.29	125.03
24	c	513	CLA	O2A-CGA-CBA	2.73	120.14	111.83
31	D	407[A]	PL9	C22-C23-C24	-2.72	121.39	127.62
24	C	512	CLA	O2A-CGA-CBA	2.72	120.14	111.83
31	A	417[B]	PL9	C8-C7-C3	2.72	119.06	112.03
25	D	401[A]	PHO	O2D-CGD-O1D	-2.72	118.55	123.85
26	h	101	BCR	C24-C23-C22	-2.72	122.21	126.23
24	B	607	CLA	O2A-CGA-O1A	-2.72	116.83	123.63
24	d	404	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
24	B	605	CLA	CMC-C2C-C1C	2.72	129.28	125.03
26	c	518	BCR	C37-C22-C23	2.72	122.24	118.09
31	D	407[A]	PL9	C37-C38-C39	-2.72	121.41	127.62
24	B	606	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
26	y	101	BCR	C21-C20-C19	-2.72	115.33	123.20
31	D	407[A]	PL9	C53-C6-C1	2.71	120.84	115.28
31	D	407[A]	PL9	C2-C1-C6	2.71	122.22	119.00
24	A	405	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
31	D	407[B]	PL9	C12-C13-C14	-2.71	121.42	127.62
24	c	505	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
26	k	102	BCR	C36-C18-C19	2.71	122.23	118.09
27	f	102	SQD	O47-C7-O49	-2.71	117.37	123.70
25	a	411	PHO	CED-O2D-CGD	2.71	122.06	115.92
35	b	608	HTG	C1'-S1-C1	2.71	106.30	100.45
25	d	402[B]	PHO	CMB-C2B-C3B	2.71	130.09	124.68
25	D	401[A]	PHO	C1A-C2A-C3A	-2.71	100.26	102.84
38	f	101	HEM	CAD-CBD-CGD	2.71	120.84	113.67
25	D	401[A]	PHO	C4A-C3A-C2A	-2.71	100.27	102.84
24	b	618	CLA	CBC-CAC-C3C	-2.70	105.09	112.42
24	C	505	CLA	C1-O2A-CGA	2.70	123.20	116.65
25	A	408	PHO	CMA-C3A-C4A	-2.70	108.78	114.61
24	B	617	CLA	O2D-CGD-O1D	-2.70	118.58	123.85
40	V	205	HEC	CMD-C2D-C1D	2.70	129.54	125.42
24	C	502	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
26	a	413	BCR	C38-C26-C25	-2.70	121.54	124.48
24	C	511	CLA	CMC-C2C-C1C	2.70	129.25	125.03
27	A	413	SQD	O48-C23-O10	-2.70	116.88	123.63
26	c	518	BCR	C7-C8-C9	-2.70	122.24	126.23
24	c	513	CLA	CHD-C4C-NC	2.70	128.41	124.23
24	C	509	CLA	O2A-CGA-CBA	2.70	120.06	111.83
25	A	408	PHO	O2D-CGD-O1D	-2.70	118.60	123.85
24	B	612	CLA	C4B-C3B-C2B	-2.70	103.95	107.30
24	B	607	CLA	CHC-C1C-C2C	-2.70	119.28	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	512	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
24	B	604	CLA	C4-C3-C5	2.70	119.91	115.23
24	C	511	CLA	O2A-CGA-CBA	2.69	120.05	111.83
24	c	506	CLA	O2A-CGA-CBA	2.69	120.05	111.83
24	B	604	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
24	A	406	CLA	C1-C2-C3	-2.69	121.79	126.20
24	b	619	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
24	c	508	CLA	CHC-C1C-C2C	-2.69	119.30	126.95
26	T	103	BCR	C1-C6-C7	2.69	122.95	115.65
24	A	407	CLA	CHC-C1C-C2C	-2.69	119.31	126.95
24	d	404	CLA	CMB-C2B-C1B	2.69	129.51	125.42
24	C	503	CLA	CAC-C3C-C4C	2.69	128.29	124.79
26	a	413	BCR	C33-C5-C6	-2.69	121.55	124.48
26	c	526	BCR	C29-C30-C25	2.69	114.34	110.44
24	d	404	CLA	O2A-CGA-O1A	-2.68	116.91	123.63
25	d	402[B]	PHO	O2D-CGD-O1D	-2.68	118.62	123.85
24	b	621	CLA	CMB-C2B-C1B	2.68	129.50	125.42
24	C	505	CLA	C4-C3-C5	2.68	119.88	115.23
24	b	611	CLA	C1-O2A-CGA	2.68	123.14	116.65
36	C	517	DGD	O1G-C1A-C2A	2.68	120.00	111.83
35	b	602	HTG	C1-O5-C5	2.68	117.36	112.56
25	A	408	PHO	C1-C2-C3	-2.68	121.81	126.20
24	a	410	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
24	C	513	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
24	B	603	CLA	CMA-C3A-C2A	-2.67	103.65	113.98
24	b	615	CLA	CMC-C2C-C1C	2.67	129.21	125.03
24	b	623	CLA	C4C-C3C-C2C	-2.67	103.00	106.89
24	C	511	CLA	CHD-C4C-NC	2.67	128.37	124.23
31	A	417[B]	PL9	C45-C44-C46	2.67	119.86	115.23
31	D	407[B]	PL9	C25-C24-C26	2.67	119.86	115.23
24	B	616	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
24	C	501	CLA	C1-C2-C3	-2.67	121.83	126.20
26	y	101	BCR	C40-C30-C25	-2.67	106.06	110.24
24	B	609	CLA	CBC-CAC-C3C	-2.67	105.19	112.42
40	v	206	HEC	C2A-C1A-NA	-2.67	107.75	110.32
24	A	407	CLA	C2A-C1A-CHA	-2.67	119.24	123.87
24	C	504	CLA	CHD-C4C-NC	2.67	128.37	124.23
37	b	634	LHG	O8-C23-C24	2.67	119.96	111.83
31	d	407[A]	PL9	C20-C19-C21	2.67	119.85	115.23
24	c	507	CLA	CHC-C1C-C2C	-2.67	119.37	126.95
24	a	409	CLA	CAC-C3C-C4C	2.66	128.26	124.79
31	A	417[B]	PL9	C15-C14-C16	2.66	119.85	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	618	CLA	O2A-CGA-CBA	2.66	119.96	111.83
24	a	410	CLA	C2A-C1A-CHA	-2.66	119.25	123.87
24	c	508	CLA	O2A-CGA-CBA	2.66	119.95	111.83
31	a	416[B]	PL9	C25-C24-C26	2.66	119.85	115.23
26	t	102	BCR	C11-C10-C9	-2.66	123.55	127.28
24	c	509	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
24	c	515	CLA	CMC-C2C-C1C	2.66	129.19	125.03
24	b	613	CLA	C6-C5-C3	-2.66	107.00	113.47
24	C	506	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
24	B	614	CLA	CED-O2D-CGD	2.66	121.94	115.92
31	D	407[A]	PL9	C27-C28-C29	-2.66	121.54	127.62
24	B	603	CLA	C2A-C1A-CHA	-2.66	119.26	123.87
24	c	508	CLA	CAA-C2A-C3A	-2.65	105.83	113.00
40	v	206	HEC	CHA-C4D-ND	2.65	128.67	123.86
24	B	607	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
24	a	412	CLA	O2A-CGA-CBA	2.65	119.91	111.83
24	c	505	CLA	CHD-C4C-NC	2.65	128.34	124.23
26	k	102	BCR	C10-C11-C12	-2.65	115.53	123.20
24	b	623	CLA	C2A-C1A-CHA	-2.65	119.27	123.87
24	a	409	CLA	C4B-C3B-C2B	-2.65	104.01	107.30
24	B	615	CLA	CAC-C3C-C4C	2.65	128.24	124.79
26	b	628	BCR	C21-C20-C19	-2.65	115.53	123.20
24	c	505	CLA	O2A-CGA-O1A	-2.65	117.01	123.63
24	B	615	CLA	C4-C3-C5	2.64	119.82	115.23
26	d	406	BCR	C33-C5-C6	-2.64	121.60	124.48
31	D	407[A]	PL9	C7-C3-C4	2.64	119.09	116.91
24	B	607	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	b	621	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
26	c	526	BCR	C16-C17-C18	-2.64	123.57	127.28
26	A	410	BCR	C2-C1-C6	2.64	114.28	110.44
27	f	102	SQD	O48-C23-C24	2.64	119.88	111.83
26	B	620	BCR	C10-C11-C12	-2.64	115.55	123.20
24	C	509	CLA	CHD-C4C-NC	2.64	128.32	124.23
24	b	615	CLA	CBC-CAC-C3C	-2.64	105.27	112.42
24	a	410	CLA	CMC-C2C-C1C	2.64	129.15	125.03
24	a	410	CLA	C1-C2-C3	-2.64	121.88	126.20
24	b	621	CLA	CHC-C1C-C2C	-2.63	119.46	126.95
27	A	411	SQD	O48-C23-O10	-2.63	117.04	123.63
24	B	611	CLA	CMB-C2B-C1B	2.63	129.43	125.42
24	B	616	CLA	C2A-C1A-CHA	-2.63	119.30	123.87
24	c	511	CLA	CAC-C3C-C4C	2.63	128.21	124.79
24	C	509	CLA	C4-C3-C5	2.63	119.79	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	C	515	BCR	C15-C16-C17	-2.63	118.14	123.52
26	T	103	BCR	C15-C14-C13	2.62	130.96	127.28
33	Z	101	LMG	O6-C5-C4	2.62	114.43	109.70
24	c	505	CLA	CMB-C2B-C1B	2.62	129.41	125.42
24	c	511	CLA	O1D-CGD-CBD	-2.62	119.35	124.52
24	b	624	CLA	CAC-C3C-C4C	2.62	128.20	124.79
31	a	416[B]	PL9	C53-C6-C1	2.62	120.64	115.28
24	B	606	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
24	c	512	CLA	CAA-C2A-C3A	-2.62	105.92	113.00
24	c	514	CLA	C2A-C1A-CHA	-2.62	119.32	123.87
24	B	610	CLA	CHD-C4C-NC	2.62	128.29	124.23
33	a	415	LMG	O8-C28-C29	2.62	119.82	111.83
37	a	420	LHG	O8-C23-C24	2.62	119.82	111.83
31	A	417[B]	PL9	C17-C18-C19	-2.62	121.63	127.62
24	B	613	CLA	CBC-CAC-C3C	-2.62	105.33	112.42
26	y	101	BCR	C16-C17-C18	-2.62	123.61	127.28
31	D	407[A]	PL9	C25-C24-C26	2.61	119.77	115.23
24	C	508	CLA	CHD-C4C-NC	2.61	128.28	124.23
38	E	103	HEM	CBD-CAD-C3D	-2.61	105.31	112.53
24	B	612	CLA	C2A-C1A-CHA	-2.61	119.33	123.87
24	c	506	CLA	CHD-C4C-NC	2.61	128.28	124.23
24	b	610	CLA	C4C-C3C-C2C	-2.61	103.09	106.89
36	c	520	DGD	C2G-O2G-C1B	-2.61	111.54	117.80
38	E	103	HEM	CHA-C1A-NA	2.61	128.60	123.86
31	A	417[A]	PL9	C25-C24-C26	2.61	119.76	115.23
24	b	614	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
24	a	410	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
24	C	502	CLA	O2A-CGA-O1A	-2.61	117.10	123.63
27	A	411	SQD	O47-C7-O49	-2.61	117.60	123.70
26	B	618	BCR	C21-C20-C19	-2.61	115.64	123.20
24	b	611	CLA	CMB-C2B-C1B	2.61	129.39	125.42
31	A	417[A]	PL9	C30-C29-C31	2.61	119.75	115.23
24	b	617	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
31	A	417[A]	PL9	C7-C3-C2	-2.61	120.32	123.39
24	B	610	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
31	A	417[A]	PL9	C42-C43-C44	-2.60	121.66	127.62
24	D	405	CLA	O2A-CGA-CBA	2.60	119.78	111.83
24	C	501	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
24	b	617	CLA	C4B-C3B-C2B	-2.60	104.07	107.30
24	B	610	CLA	CBC-CAC-C3C	-2.60	105.37	112.42
24	C	513	CLA	CBC-CAC-C3C	-2.60	105.37	112.42
24	B	613	CLA	O2A-CGA-CBA	2.60	119.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	a	411	PHO	C4-C3-C5	2.60	119.74	115.23
24	b	611	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
24	c	516	CLA	CHC-C1C-C2C	-2.60	119.57	126.95
24	B	608	CLA	C4C-C3C-C2C	-2.60	103.11	106.89
31	d	407[B]	PL9	C17-C18-C19	-2.60	121.68	127.62
26	b	628	BCR	C2-C1-C6	2.59	114.21	110.44
26	B	620	BCR	C24-C23-C22	-2.59	122.40	126.23
24	b	623	CLA	CAA-C2A-C3A	-2.59	106.00	113.00
24	B	611	CLA	C4-C3-C5	2.59	119.72	115.23
24	A	409	CLA	C2A-C1A-CHA	-2.59	119.38	123.87
40	v	206	HEC	CHB-C1B-NB	2.59	128.55	123.86
24	b	623	CLA	O2A-CGA-O1A	-2.58	117.16	123.63
24	C	513	CLA	CHD-C4C-NC	2.58	128.24	124.23
35	b	607	HTG	C1-O5-C5	2.58	117.20	112.56
24	C	510	CLA	C6-C7-C8	-2.58	107.38	115.97
36	C	516	DGD	O1G-C1A-O1A	-2.58	117.18	123.63
24	C	506	CLA	C4C-C3C-C2C	-2.58	103.14	106.89
24	B	613	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
24	c	513	CLA	C1-O2A-CGA	2.57	122.88	116.65
24	A	406	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
24	C	513	CLA	CMC-C2C-C1C	2.57	129.05	125.03
26	H	101	BCR	C16-C15-C14	-2.57	118.26	123.52
24	D	404	CLA	C4-C3-C5	2.57	119.69	115.23
26	D	406	BCR	C10-C11-C12	-2.57	115.75	123.20
26	T	103	BCR	C7-C6-C5	-2.57	115.64	121.56
24	b	614	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
24	c	517	CLA	C1-C2-C3	-2.57	121.99	126.20
24	C	513	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
24	a	412	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
24	d	405	CLA	C4-C3-C5	2.57	119.68	115.23
24	b	623	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
24	b	616	CLA	CAC-C3C-C4C	2.56	128.13	124.79
24	C	513	CLA	O2A-CGA-CBA	2.56	119.65	111.83
37	d	408	LHG	C5-O7-C7	-2.56	111.66	117.80
33	Z	101	LMG	C9-O8-C28	2.56	123.41	117.08
24	c	508	CLA	O2A-CGA-O1A	-2.56	117.22	123.63
24	b	615	CLA	O2A-CGA-CBA	2.56	119.65	111.83
24	C	513	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
24	c	514	CLA	CBC-CAC-C3C	-2.56	105.48	112.42
26	k	102	BCR	C11-C10-C9	-2.56	123.69	127.28
26	D	406	BCR	C21-C20-C19	-2.56	115.78	123.20
24	b	617	CLA	O2A-CGA-O1A	-2.56	117.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	510	CLA	O2A-CGA-O1A	-2.56	117.23	123.63
26	t	102	BCR	C7-C6-C5	-2.56	115.66	121.56
31	D	407[B]	PL9	C51-C49-C50	2.56	120.47	114.59
33	a	415	LMG	C7-O1-C1	-2.56	108.31	113.80
24	B	616	CLA	C3B-C4B-NB	2.56	112.81	110.53
24	C	501	CLA	C3B-C4B-NB	2.56	112.81	110.53
24	b	622	CLA	C4-C3-C5	2.56	119.67	115.23
24	c	515	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
31	d	407[B]	PL9	C20-C19-C21	2.56	119.66	115.23
24	c	516	CLA	CMC-C2C-C1C	2.55	129.02	125.03
24	C	503	CLA	O2A-CGA-CBA	2.55	119.62	111.83
24	B	612	CLA	CBC-CAC-C3C	-2.55	105.50	112.42
27	F	101	SQD	O47-C7-O49	-2.55	117.74	123.70
24	c	509	CLA	C4-C3-C5	2.55	119.66	115.23
25	a	411	PHO	CMA-C3A-C4A	-2.55	109.12	114.61
24	b	619	CLA	C4-C3-C5	2.55	119.65	115.23
24	A	407	CLA	CAA-C2A-C3A	-2.55	106.11	113.00
24	b	615	CLA	C1-O2A-CGA	2.55	122.82	116.65
26	C	514	BCR	C20-C21-C22	-2.55	123.70	127.28
24	b	625	CLA	CMB-C2B-C1B	2.55	129.30	125.42
24	B	615	CLA	C1-O2A-CGA	2.55	122.82	116.65
26	C	515	BCR	C21-C20-C19	-2.55	115.82	123.20
33	c	522	LMG	O8-C28-C29	2.55	119.60	111.83
24	C	505	CLA	C4B-C3B-C2B	-2.55	104.14	107.30
24	c	512	CLA	CHD-C4C-NC	2.55	128.18	124.23
24	c	508	CLA	C4B-C3B-C2B	-2.55	104.14	107.30
24	C	512	CLA	CMC-C2C-C1C	2.54	129.01	125.03
24	a	410	CLA	CMA-C3A-C2A	-2.54	104.16	113.98
24	B	602	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	C	512	CLA	C4-C3-C5	2.54	119.64	115.23
31	D	407[A]	PL9	C12-C13-C14	-2.54	121.81	127.62
24	B	604	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	b	610	CLA	C2A-C1A-CHA	-2.54	119.46	123.87
24	C	512	CLA	CAC-C3C-C4C	2.54	128.09	124.79
24	B	608	CLA	C1-C2-C3	-2.54	122.04	126.20
26	C	514	BCR	C23-C24-C25	-2.53	120.23	127.00
24	c	516	CLA	CBA-CAA-C2A	-2.53	106.25	113.79
24	c	515	CLA	CMB-C2B-C1B	2.53	129.28	125.42
26	y	101	BCR	C37-C22-C23	2.53	121.95	118.09
33	k	101	LMG	C8-O7-C10	-2.53	111.74	117.80
24	d	405	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
31	a	416[A]	PL9	C30-C29-C31	2.53	119.61	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	409	CLA	C4C-C3C-C2C	-2.53	103.21	106.89
25	d	402[A]	PHO	CMB-C2B-C3B	2.53	129.73	124.68
31	d	407[B]	PL9	C25-C24-C26	2.53	119.61	115.23
24	b	611	CLA	CAC-C3C-C4C	2.52	128.07	124.79
24	B	614	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
31	d	407[B]	PL9	C22-C23-C24	-2.52	121.85	127.62
31	A	417[A]	PL9	C15-C14-C16	2.52	119.61	115.23
24	c	512	CLA	O2A-CGA-CBA	2.52	119.53	111.83
25	A	408	PHO	O1D-CGD-CBD	-2.52	120.90	124.72
26	B	619	BCR	C30-C25-C26	-2.52	119.19	122.64
31	a	416[B]	PL9	C40-C39-C41	2.52	119.60	115.23
24	c	507	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
24	B	611	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
24	b	617	CLA	C3B-C4B-NB	2.52	112.78	110.53
40	V	205	HEC	CHB-C1B-NB	2.52	128.43	123.86
33	A	419	LMG	C8-O7-C10	-2.52	111.77	117.80
24	D	404	CLA	C4C-C3C-C2C	-2.51	103.23	106.89
31	A	417[B]	PL9	C25-C24-C26	2.51	119.59	115.23
26	h	101	BCR	C11-C10-C9	-2.51	123.76	127.28
24	A	409	CLA	CHB-C4A-NA	2.51	128.02	124.40
31	D	407[A]	PL9	C42-C41-C39	-2.51	104.88	113.19
24	b	616	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
24	B	612	CLA	CMB-C2B-C1B	2.51	129.23	125.42
24	c	517	CLA	CHC-C1C-C2C	-2.50	119.83	126.95
24	A	405	CLA	CMA-C3A-C4A	-2.50	105.05	111.77
24	A	409	CLA	CMC-C2C-C1C	2.50	128.94	125.03
24	d	403	CLA	CHB-C1B-NB	-2.50	120.30	124.05
24	B	607	CLA	C3B-C4B-NB	2.50	112.76	110.53
37	d	409	LHG	C6-C5-C4	-2.50	105.96	111.78
24	c	517	CLA	C3B-C4B-NB	2.50	112.76	110.53
24	d	405	CLA	C2A-C1A-CHA	-2.50	119.53	123.87
33	Z	101	LMG	C1-C2-C3	2.50	115.26	110.01
24	B	608	CLA	C4-C3-C5	2.49	119.56	115.23
26	K	101	BCR	C31-C1-C6	-2.49	106.33	110.24
31	D	407[B]	PL9	C7-C3-C4	2.49	118.96	116.91
24	B	605	CLA	C4-C3-C5	2.49	119.55	115.23
24	B	609	CLA	O2A-CGA-CBA	2.49	119.43	111.83
26	C	514	BCR	C16-C17-C18	-2.49	123.78	127.28
24	b	611	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
24	c	516	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
24	C	508	CLA	C2A-C1A-CHA	-2.49	119.55	123.87
24	C	506	CLA	CHD-C4C-NC	2.49	128.09	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	620	BCR	C29-C30-C25	2.49	114.05	110.44
24	C	504	CLA	C4C-C3C-C2C	-2.49	103.27	106.89
27	a	414	SQD	C44-O6-C1	-2.49	108.47	113.80
26	t	102	BCR	C2-C1-C6	2.49	114.05	110.44
26	y	101	BCR	C32-C1-C6	-2.49	106.34	110.24
24	C	503	CLA	C4B-C3B-C2B	-2.48	104.21	107.30
31	a	416[B]	PL9	C45-C44-C46	2.48	119.54	115.23
24	c	509	CLA	C2A-C1A-CHA	-2.48	119.56	123.87
24	a	409	CLA	C1-C2-C3	-2.48	122.13	126.20
36	C	517	DGD	C1E-O6E-C5E	-2.48	108.87	113.72
24	d	405	CLA	O2A-CGA-CBA	2.48	119.40	111.83
25	a	411	PHO	C1A-C2A-C3A	-2.48	100.48	102.84
27	B	621	SQD	O48-C23-C24	2.48	119.40	111.83
24	b	624	CLA	C11-C10-C8	-2.48	107.72	115.97
24	b	614	CLA	CMA-C3A-C2A	-2.48	104.40	113.98
27	L	102	SQD	O8-S-C6	2.48	110.76	105.97
31	d	407[A]	PL9	C53-C6-C1	2.48	120.35	115.28
24	b	613	CLA	CHD-C4C-NC	2.48	128.07	124.23
33	d	415	LMG	O8-C28-C29	2.48	119.39	111.83
24	a	412	CLA	C2A-C1A-CHA	-2.48	119.57	123.87
24	B	611	CLA	CAA-CBA-CGA	-2.48	106.18	113.21
24	B	615	CLA	O2A-CGA-O1A	-2.47	117.44	123.63
36	C	517	DGD	O6E-C5E-C6E	2.47	112.56	106.44
24	c	517	CLA	C4B-C3B-C2B	-2.47	104.23	107.30
36	e	101	DGD	O1G-C1A-C2A	2.47	119.36	111.83
25	D	401[B]	PHO	O2A-CGA-CBA	2.47	119.36	111.83
24	C	508	CLA	C4-C3-C5	2.47	119.51	115.23
24	c	511	CLA	CHC-C1C-C2C	-2.46	119.95	126.95
24	b	616	CLA	CGD-CBD-CAD	-2.46	102.88	110.85
27	L	102	SQD	O47-C7-O49	-2.46	117.95	123.70
24	c	514	CLA	CMB-C2B-C1B	2.46	129.16	125.42
24	C	501	CLA	CHC-C1C-C2C	-2.46	119.96	126.95
35	V	206	HTG	C1-C2-C3	-2.46	105.74	110.55
24	c	510	CLA	C4-C3-C5	2.46	119.50	115.23
24	B	608	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
24	c	509	CLA	CHD-C4C-NC	2.46	128.04	124.23
29	M	104	LMT	C1B-O5B-C5B	2.46	118.52	113.72
35	b	632	HTG	C1-O5-C5	2.46	116.97	112.56
24	B	615	CLA	CMB-C2B-C1B	2.46	129.16	125.42
24	b	619	CLA	CAA-CBA-CGA	-2.46	106.23	113.21
24	B	615	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
24	B	609	CLA	O2D-CGD-O1D	-2.45	119.07	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	416[A]	PL9	C51-C49-C50	2.45	120.23	114.59
26	Y	101	BCR	C21-C20-C19	-2.45	116.09	123.20
31	d	407[A]	PL9	C12-C13-C14	-2.45	122.01	127.62
24	c	515	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
24	B	606	CLA	C4B-C3B-C2B	-2.45	104.25	107.30
37	D	411	LHG	O8-C23-O10	-2.45	117.50	123.63
24	B	616	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
26	c	526	BCR	C11-C10-C9	-2.45	123.84	127.28
24	c	507	CLA	O2A-CGA-CBA	2.45	119.31	111.83
31	D	407[A]	PL9	C32-C33-C34	-2.45	122.02	127.62
33	C	520	LMG	O8-C28-C29	2.45	119.30	111.83
24	C	511	CLA	C4-C3-C5	2.45	119.48	115.23
24	C	501	CLA	O2A-CGA-CBA	2.45	119.30	111.83
37	d	409	LHG	O8-C23-C24	2.45	119.30	111.83
24	D	404	CLA	C2A-C1A-CHA	-2.45	119.62	123.87
24	a	410	CLA	CAC-C3C-C4C	2.45	127.97	124.79
24	B	616	CLA	C4-C3-C5	2.45	119.47	115.23
24	b	618	CLA	CMC-C2C-C1C	2.44	128.85	125.03
24	c	514	CLA	CAC-C3C-C4C	2.44	127.97	124.79
25	d	402[B]	PHO	O2A-CGA-CBA	2.44	119.28	111.83
24	C	513	CLA	CMB-C2B-C1B	2.44	129.13	125.42
36	h	102	DGD	O1G-C1A-O1A	-2.44	117.52	123.63
27	A	411	SQD	C1-C2-C3	-2.44	104.88	110.01
24	a	410	CLA	OBD-CAD-C3D	-2.44	122.72	128.42
24	B	607	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
36	D	408	DGD	O6D-C5D-C6D	2.44	111.53	106.69
24	B	617	CLA	C1-O2A-CGA	2.44	122.55	116.65
24	C	507	CLA	CAC-C3C-C4C	2.44	127.96	124.79
38	E	103	HEM	CHD-C1D-C2D	-2.43	121.18	125.03
26	H	101	BCR	C10-C11-C12	-2.43	116.15	123.20
26	b	626	BCR	C37-C22-C23	2.43	121.81	118.09
24	D	405	CLA	C2A-C1A-CHA	-2.43	119.65	123.87
24	D	404	CLA	CMC-C2C-C1C	2.43	128.83	125.03
24	c	510	CLA	O2A-CGA-CBA	2.43	119.25	111.83
24	B	613	CLA	CAC-C3C-C4C	2.43	127.95	124.79
26	d	406	BCR	C21-C20-C19	-2.43	116.17	123.20
24	c	514	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
29	M	102	LMT	O5'-C1'-O1'	-2.42	104.32	110.04
24	b	612	CLA	C2A-C1A-CHA	-2.42	119.66	123.87
25	A	408	PHO	C4-C3-C5	2.42	119.43	115.23
24	A	405	CLA	CAA-CBA-CGA	-2.42	106.33	113.21
24	c	516	CLA	CMB-C2B-C1B	2.42	129.10	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	B	619	BCR	C24-C23-C22	-2.42	122.66	126.23
26	B	620	BCR	C16-C17-C18	-2.41	123.89	127.28
24	c	506	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
27	a	414	SQD	O9-S-C6	2.41	110.36	106.76
31	A	417[A]	PL9	C17-C18-C19	-2.41	122.10	127.62
27	B	621	SQD	O47-C7-O49	-2.41	118.07	123.70
31	A	417[B]	PL9	C10-C9-C11	2.41	119.41	115.23
33	C	520	LMG	C3-C4-C5	2.41	114.60	110.23
40	v	206	HEC	CHD-C4C-NC	2.41	127.08	124.45
27	a	405	SQD	O48-C23-O10	-2.41	117.60	123.63
24	B	609	CLA	CMB-C2B-C1B	2.41	129.09	125.42
24	b	617	CLA	CAC-C3C-C4C	2.41	127.92	124.79
31	A	417[A]	PL9	C10-C9-C11	2.41	119.40	115.23
24	A	405	CLA	CMB-C2B-C3B	2.40	132.21	126.55
25	A	408	PHO	CBA-CAA-C2A	-2.40	106.70	113.78
25	D	401[B]	PHO	CMA-C3A-C4A	-2.40	109.43	114.61
35	B	632	HTG	C1-O5-C5	2.40	116.87	112.56
24	A	409	CLA	O2A-CGA-CBA	2.40	119.16	111.83
24	C	503	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
24	b	616	CLA	C2A-C1A-CHA	-2.40	119.70	123.87
24	b	618	CLA	C1-O2A-CGA	2.40	122.46	116.65
24	c	510	CLA	CMC-C2C-C1C	2.40	128.78	125.03
40	v	206	HEC	O2D-CGD-CBD	2.40	121.58	114.00
24	B	602	CLA	C1-O2A-CGA	2.40	122.46	116.65
24	C	504	CLA	CAA-C2A-C3A	-2.40	106.52	113.00
24	b	625	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
24	B	610	CLA	C4-C3-C5	2.40	119.39	115.23
24	b	612	CLA	C4-C3-C5	2.40	119.39	115.23
24	A	409	CLA	C1-C2-C3	-2.40	122.27	126.20
24	C	513	CLA	C4-C3-C5	2.39	119.39	115.23
24	c	515	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
26	T	103	BCR	C16-C17-C18	-2.39	123.92	127.28
24	B	609	CLA	CHD-C4C-NC	2.39	127.94	124.23
35	C	523	HTG	O5-C1-C2	2.39	113.61	110.32
26	b	627	BCR	C20-C21-C22	-2.39	123.93	127.28
24	A	409	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
33	A	419	LMG	O8-C28-C29	2.39	119.12	111.83
26	K	101	BCR	C15-C16-C17	-2.39	118.63	123.52
24	d	403	CLA	C4C-C3C-C2C	-2.39	103.42	106.89
26	B	619	BCR	C37-C22-C21	-2.39	118.95	122.82
25	a	411	PHO	O2A-CGA-CBA	2.38	119.11	111.83
27	A	411	SQD	O9-S-C6	2.38	110.31	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	510	CLA	CHD-C4C-NC	2.38	127.92	124.23
24	C	502	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
33	c	522	LMG	C8-O7-C10	-2.38	112.10	117.80
24	B	610	CLA	CMA-C3A-C4A	-2.38	105.37	111.77
24	c	516	CLA	C3B-C4B-NB	2.38	112.66	110.53
24	b	611	CLA	O2A-CGA-CBA	2.38	119.09	111.83
24	B	611	CLA	O2A-CGA-O1A	-2.38	117.67	123.63
24	c	511	CLA	O2A-CGA-CBA	2.38	119.09	111.83
31	A	417[B]	PL9	C30-C29-C31	2.38	119.36	115.23
26	t	102	BCR	C33-C5-C4	2.38	118.67	113.60
24	b	612	CLA	CMA-C3A-C2A	-2.38	104.79	113.98
31	D	407[B]	PL9	C17-C18-C19	-2.38	122.18	127.62
24	B	608	CLA	CMB-C2B-C1B	2.38	129.04	125.42
25	d	402[B]	PHO	O1D-CGD-CBD	-2.38	121.12	124.72
24	C	505	CLA	CMC-C2C-C1C	2.37	128.74	125.03
24	A	406	CLA	O2A-CGA-CBA	2.37	119.07	111.83
24	b	617	CLA	C11-C12-C13	-2.37	108.09	115.97
24	C	511	CLA	CBC-CAC-C3C	-2.37	106.00	112.42
36	c	519	DGD	O2G-C1B-O1B	-2.37	118.17	123.70
24	b	619	CLA	CHD-C4C-NC	2.37	127.90	124.23
31	D	407[B]	PL9	C45-C44-C46	2.37	119.33	115.23
24	c	508	CLA	CBC-CAC-C3C	-2.36	106.01	112.42
24	a	409	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
24	b	623	CLA	CMB-C2B-C1B	2.36	129.02	125.42
24	B	608	CLA	CHD-C4C-NC	2.36	127.90	124.23
24	b	613	CLA	CMB-C2B-C1B	2.36	129.02	125.42
26	d	406	BCR	C10-C11-C12	-2.36	116.35	123.20
24	C	508	CLA	CBC-CAC-C3C	-2.36	106.02	112.42
24	b	614	CLA	CMC-C2C-C1C	2.36	128.72	125.03
24	B	612	CLA	C1-O2A-CGA	2.36	122.36	116.65
24	B	611	CLA	CMA-C3A-C2A	-2.36	104.87	113.98
26	T	103	BCR	C37-C22-C23	2.36	121.69	118.09
24	c	511	CLA	C3B-C4B-NB	2.36	112.63	110.53
24	c	516	CLA	CHB-C1B-C2B	-2.36	120.59	127.43
24	C	510	CLA	O1D-CGD-CBD	-2.35	119.87	124.52
24	b	612	CLA	O2A-CGA-O1A	-2.35	117.74	123.63
31	a	416[B]	PL9	C30-C29-C31	2.35	119.31	115.23
24	b	613	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
38	f	101	HEM	CHB-C1B-NB	2.35	127.28	124.37
31	D	407[A]	PL9	C51-C49-C50	2.35	120.00	114.59
26	c	526	BCR	C38-C26-C25	-2.35	121.92	124.48
24	B	617	CLA	O1D-CGD-CBD	-2.35	119.89	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	616	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
24	b	614	CLA	CBC-CAC-C3C	-2.35	106.06	112.42
24	C	501	CLA	C2A-C1A-CHA	-2.35	119.79	123.87
24	C	505	CLA	CHD-C4C-NC	2.35	127.87	124.23
24	C	513	CLA	CAA-C2A-C3A	-2.35	106.66	113.00
37	D	409	LHG	O8-C23-O10	-2.35	117.76	123.63
27	A	413	SQD	O8-S-C6	2.35	110.50	105.97
25	d	402[A]	PHO	C4A-C3A-C2A	-2.34	100.61	102.84
40	V	205	HEC	C4B-NB-C1B	2.34	109.64	105.82
24	B	617	CLA	CAC-C3C-C4C	2.34	127.83	124.79
31	D	407[B]	PL9	C32-C33-C34	-2.34	122.27	127.62
24	B	614	CLA	CHD-C4C-NC	2.34	127.86	124.23
33	a	415	LMG	O7-C10-O9	-2.34	118.23	123.70
25	A	408	PHO	C4A-C3A-C2A	-2.34	100.61	102.84
24	a	409	CLA	CMB-C2B-C1B	2.34	128.98	125.42
26	y	101	BCR	C29-C30-C25	2.34	113.83	110.44
24	C	504	CLA	O1D-CGD-CBD	-2.34	119.91	124.52
24	C	509	CLA	C11-C12-C13	-2.34	108.20	115.97
24	c	514	CLA	C4-C3-C2	-2.34	117.63	123.63
24	c	516	CLA	C11-C12-C13	-2.34	108.20	115.97
38	E	103	HEM	CBA-CAA-C2A	-2.34	106.07	112.53
27	L	102	SQD	C1-C2-C3	-2.33	105.10	110.01
24	C	505	CLA	C2A-C1A-CHA	-2.33	119.81	123.87
36	c	520	DGD	O1G-C1A-C2A	2.33	118.95	111.83
24	C	507	CLA	O2A-CGA-O1A	-2.33	117.80	123.63
31	D	407[A]	PL9	C40-C39-C38	-2.33	117.64	123.63
24	C	509	CLA	C2A-C1A-CHA	-2.33	119.83	123.87
27	L	102	SQD	C44-O6-C1	-2.33	108.80	113.80
24	d	403	CLA	O2A-CGA-CBA	2.33	118.93	111.83
27	F	101	SQD	C1-O5-C5	2.33	118.26	113.72
24	A	405	CLA	CHB-C1B-C2B	-2.33	120.68	127.43
24	c	513	CLA	C2A-C1A-CHA	-2.32	119.83	123.87
24	c	512	CLA	O2A-CGA-O1A	-2.32	117.81	123.63
24	d	404	CLA	CHD-C4C-NC	2.32	127.83	124.23
33	M	101	LMG	O1-C7-C8	-2.32	105.17	110.82
26	b	628	BCR	C16-C15-C14	-2.32	118.77	123.52
36	e	101	DGD	C1E-O6E-C5E	2.32	118.25	113.72
24	C	513	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
24	B	609	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
24	A	406	CLA	CMB-C2B-C3B	2.32	132.00	126.55
24	A	407	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
29	E	102	LMT	O5'-C5'-C4'	2.32	114.51	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d	407[B]	PL9	C7-C3-C4	2.32	118.82	116.91
24	B	612	CLA	CHD-C4C-NC	2.32	127.82	124.23
24	c	514	CLA	O2A-CGA-O1A	-2.31	117.84	123.63
24	B	604	CLA	C1-O2A-CGA	2.31	122.25	116.65
26	B	620	BCR	C37-C22-C23	2.31	121.62	118.09
24	C	501	CLA	C4-C3-C5	2.31	119.24	115.23
31	a	416[A]	PL9	C8-C7-C3	2.31	118.00	112.03
24	B	611	CLA	C11-C12-C13	-2.31	108.28	115.97
24	B	613	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
40	V	205	HEC	O2D-CGD-CBD	2.31	121.30	114.00
24	c	507	CLA	C1-O2A-CGA	2.31	122.24	116.65
24	C	503	CLA	C1-C2-C3	-2.31	122.42	126.20
24	C	503	CLA	C3B-C4B-NB	2.31	112.59	110.53
38	E	103	HEM	C4C-CHD-C1D	-2.31	121.11	126.02
26	D	406	BCR	C16-C17-C18	-2.31	124.04	127.28
24	c	514	CLA	C6-C7-C8	-2.31	108.30	115.97
24	b	618	CLA	CAC-C3C-C4C	2.31	127.79	124.79
24	c	513	CLA	C4-C3-C5	2.30	119.23	115.23
35	V	206	HTG	O5-C1-C2	-2.30	107.14	110.32
40	v	206	HEC	CAA-C2A-C3A	-2.30	123.55	127.87
25	D	401[B]	PHO	OBD-CAD-C3D	-2.30	124.30	127.89
24	A	406	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
24	c	515	CLA	C2A-C1A-CHA	-2.30	119.87	123.87
24	c	508	CLA	C2A-C1A-CHA	-2.30	119.88	123.87
24	D	405	CLA	CHD-C4C-NC	2.30	127.80	124.23
36	C	516	DGD	C4E-C3E-C2E	-2.30	106.79	110.83
24	C	506	CLA	O2A-CGA-CBA	2.30	118.84	111.83
31	A	417[B]	PL9	C40-C39-C41	2.30	119.22	115.23
24	c	513	CLA	CBC-CAC-C3C	-2.30	106.20	112.42
24	B	617	CLA	CED-O2D-CGD	2.30	121.12	115.92
24	A	409	CLA	C4B-C3B-C2B	-2.29	104.45	107.30
31	D	407[B]	PL9	C2-C1-C6	2.29	121.72	119.00
24	B	603	CLA	O2A-CGA-CBA	2.29	118.82	111.83
24	B	607	CLA	C1-C2-C3	-2.29	122.44	126.20
35	b	607	HTG	O5-C5-C4	2.29	113.82	109.70
24	B	614	CLA	C7-C6-C5	-2.29	107.17	113.26
26	a	413	BCR	C37-C22-C21	-2.29	119.11	122.82
26	t	102	BCR	C12-C13-C14	-2.29	115.41	119.01
24	B	604	CLA	CMC-C2C-C1C	2.28	128.60	125.03
26	t	102	BCR	C35-C13-C12	2.28	121.58	118.09
24	c	510	CLA	C4C-C3C-C2C	-2.28	103.57	106.89
36	c	519	DGD	O1G-C1A-C2A	2.28	118.79	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	615	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
24	b	622	CLA	CED-O2D-CGD	2.28	121.08	115.92
24	c	508	CLA	CMB-C2B-C1B	2.28	128.89	125.42
24	b	621	CLA	O1D-CGD-CBD	-2.28	120.03	124.52
24	B	603	CLA	C1-O2A-CGA	2.28	122.16	116.65
24	A	406	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
40	v	206	HEC	O2A-CGA-CBA	2.27	121.19	114.00
24	B	615	CLA	CMC-C2C-C1C	2.27	128.59	125.03
24	c	507	CLA	CMC-C2C-C1C	2.27	128.59	125.03
24	B	614	CLA	CAA-C2A-C3A	-2.27	106.86	113.00
36	H	102	DGD	C3G-O3G-C1D	-2.27	108.92	113.80
24	d	403	CLA	C4-C3-C5	2.27	119.17	115.23
31	d	407[A]	PL9	C25-C24-C26	2.27	119.17	115.23
36	C	517	DGD	O1G-C1A-O1A	-2.27	117.95	123.63
40	V	205	HEC	CHA-C4D-ND	2.27	127.98	123.86
24	C	508	CLA	CHB-C4A-NA	2.27	127.67	124.40
24	A	406	CLA	CMA-C3A-C2A	-2.27	105.21	113.98
24	b	622	CLA	OBD-CAD-C3D	-2.27	123.11	128.42
38	f	101	HEM	C2A-C1A-NA	-2.27	107.64	110.15
24	b	610	CLA	CMC-C2C-C1C	2.27	128.58	125.03
24	b	619	CLA	O2A-CGA-O1A	-2.27	117.96	123.63
24	C	502	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
33	d	415	LMG	O6-C5-C4	2.27	113.78	109.70
36	e	101	DGD	O2G-C1B-O1B	-2.26	118.41	123.70
24	C	510	CLA	CMC-C2C-C1C	2.26	128.57	125.03
24	B	612	CLA	C4-C3-C5	2.26	119.16	115.23
25	D	401[B]	PHO	CED-O2D-CGD	2.26	121.05	115.92
31	d	407[A]	PL9	C15-C14-C16	2.26	119.16	115.23
24	b	619	CLA	CBC-CAC-C3C	-2.26	106.29	112.42
26	b	628	BCR	C10-C11-C12	-2.26	116.65	123.20
24	B	606	CLA	C4-C3-C5	2.26	119.15	115.23
24	C	510	CLA	C2A-C1A-CHA	-2.26	119.94	123.87
24	C	507	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
24	b	613	CLA	CHA-C1A-NA	-2.26	121.27	126.39
26	B	619	BCR	C2-C1-C6	2.26	113.72	110.44
24	b	611	CLA	CMC-C2C-C1C	2.26	128.56	125.03
26	a	413	BCR	C36-C18-C19	2.26	121.53	118.09
24	B	608	CLA	C2A-C1A-CHA	-2.25	119.96	123.87
33	d	415	LMG	C1-O6-C5	2.25	118.12	113.72
36	C	517	DGD	O3G-C1D-C2D	2.25	111.69	108.27
35	b	608	HTG	C1-O5-C5	2.25	116.60	112.56
24	c	507	CLA	C2A-C1A-CHA	-2.25	119.96	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	b	626	BCR	C36-C18-C19	2.25	121.53	118.09
24	b	621	CLA	CAC-C3C-C4C	2.25	127.72	124.79
37	E	101	LHG	O8-C23-O10	-2.25	118.00	123.63
24	b	620	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
31	d	407[B]	PL9	C45-C44-C46	2.25	119.12	115.23
24	b	616	CLA	O2A-CGA-CBA	2.24	118.68	111.83
37	E	101	LHG	C5-O7-C7	-2.24	112.42	117.80
33	D	415	LMG	O8-C28-O10	-2.24	118.02	123.63
24	C	502	CLA	CED-O2D-CGD	2.24	121.00	115.92
33	b	629	LMG	O6-C5-C6	2.24	112.00	106.44
31	d	407[B]	PL9	C30-C29-C31	2.24	119.12	115.23
24	b	621	CLA	C2A-C1A-CHA	-2.24	119.98	123.87
24	a	409	CLA	CMC-C2C-C1C	2.24	128.53	125.03
24	C	509	CLA	CMB-C2B-C1B	2.24	128.83	125.42
24	b	610	CLA	CBC-CAC-C3C	-2.24	106.35	112.42
24	B	602	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
26	b	627	BCR	C37-C22-C21	-2.24	119.19	122.82
24	b	620	CLA	C2A-C1A-CHA	-2.24	119.99	123.87
26	C	515	BCR	C11-C10-C9	-2.24	124.14	127.28
26	k	102	BCR	C2-C1-C6	2.23	113.69	110.44
24	B	609	CLA	C1-C2-C3	-2.23	122.54	126.20
26	a	413	BCR	C37-C22-C23	2.23	121.50	118.09
24	B	610	CLA	O2A-CGA-CBA	2.23	118.64	111.83
29	M	104	LMT	O5B-C5B-C4B	2.23	113.72	109.70
24	b	624	CLA	O2A-CGA-CBA	2.23	118.64	111.83
33	C	519	LMG	O8-C28-O10	-2.23	118.05	123.63
24	a	409	CLA	CHD-C4C-NC	2.23	127.69	124.23
24	C	502	CLA	C4-C3-C5	2.23	119.09	115.23
40	v	206	HEC	CHD-C1D-ND	2.23	127.90	123.86
31	A	417[B]	PL9	C35-C34-C36	2.22	119.09	115.23
24	B	605	CLA	CHA-C1A-NA	-2.22	121.36	126.39
24	C	507	CLA	C4-C3-C5	2.22	119.09	115.23
24	c	507	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
24	B	602	CLA	CAC-C3C-C4C	2.22	127.68	124.79
31	d	407[B]	PL9	C7-C3-C2	-2.22	120.77	123.39
27	a	414	SQD	O48-C23-O10	-2.22	118.08	123.63
35	b	608	HTG	O5-C1-C2	2.22	113.38	110.32
31	a	416[B]	PL9	C51-C49-C50	2.22	119.69	114.59
33	z	101	LMG	C7-O1-C1	-2.22	109.04	113.80
24	c	516	CLA	C4B-C3B-C2B	-2.22	104.55	107.30
24	C	505	CLA	C1-C2-C3	-2.22	122.57	126.20
36	c	519	DGD	O3G-C3G-C2G	-2.21	105.43	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
36	c	520	DGD	C3B-C2B-C1B	-2.21	105.59	113.69
26	C	514	BCR	C11-C10-C9	-2.21	124.18	127.28
24	B	603	CLA	CMB-C2B-C1B	2.21	128.79	125.42
24	b	620	CLA	CHD-C4C-NC	2.21	127.66	124.23
24	b	614	CLA	OBD-CAD-C3D	-2.21	123.25	128.42
24	B	604	CLA	CHB-C1B-C2B	-2.21	121.01	127.43
38	E	103	HEM	C3B-C4B-NB	-2.21	107.88	109.47
24	C	512	CLA	CHB-C4A-NA	2.21	127.59	124.40
31	D	407[B]	PL9	C15-C14-C16	2.21	119.06	115.23
37	d	410	LHG	O8-C23-O10	-2.21	118.10	123.63
26	B	620	BCR	C8-C7-C6	-2.21	121.10	127.00
25	D	401[B]	PHO	CMB-C2B-C3B	2.21	129.09	124.68
24	b	617	CLA	C11-C10-C8	-2.21	108.63	115.97
24	C	512	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
36	C	518	DGD	O3G-C3G-C2G	-2.21	105.45	110.82
24	B	615	CLA	CED-O2D-CGD	2.20	120.92	115.92
24	c	509	CLA	CMC-C2C-C1C	2.20	128.47	125.03
24	b	616	CLA	CMA-C3A-C2A	-2.20	105.48	113.98
24	b	618	CLA	C2A-C1A-CHA	-2.20	120.05	123.87
24	A	407	CLA	CMC-C2C-C1C	2.20	128.47	125.03
27	f	102	SQD	O7-S-C6	2.20	110.04	106.76
24	B	612	CLA	O2A-CGA-CBA	2.20	118.53	111.83
25	D	401[A]	PHO	O2A-CGA-CBA	2.20	118.53	111.83
24	c	505	CLA	C4-C3-C5	2.20	119.04	115.23
29	A	414	LMT	C6'-C5'-C4'	-2.19	107.21	113.38
24	c	509	CLA	O2A-CGA-CBA	2.19	118.53	111.83
24	B	603	CLA	C11-C12-C13	-2.19	108.67	115.97
24	c	505	CLA	OBD-CAD-C3D	-2.19	123.29	128.42
24	B	603	CLA	CMC-C2C-C1C	2.19	128.46	125.03
33	d	415	LMG	C6-C5-C4	-2.19	107.63	113.02
24	c	517	CLA	O2A-CGA-O1A	-2.19	118.14	123.63
36	c	519	DGD	O1G-C1A-O1A	-2.19	118.14	123.63
24	B	616	CLA	O2A-CGA-CBA	2.19	118.52	111.83
24	d	404	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
26	A	410	BCR	C38-C26-C25	-2.19	122.09	124.48
33	D	415	LMG	O8-C28-C29	2.19	118.51	111.83
24	C	510	CLA	O2D-CGD-O1D	-2.19	119.59	123.85
26	b	626	BCR	C10-C11-C12	-2.19	116.86	123.20
24	A	407	CLA	CMA-C3A-C4A	-2.19	105.90	111.77
26	d	406	BCR	C38-C26-C27	2.19	118.26	113.60
27	L	102	SQD	C1-O5-C5	-2.19	109.45	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	D	406	BCR	C1-C6-C7	2.19	121.58	115.65
26	Y	101	BCR	C35-C13-C12	2.19	121.43	118.09
40	V	205	HEC	C2A-C1A-NA	-2.18	108.22	110.32
29	T	104	LMT	C6'-C5'-C4'	-2.18	107.24	113.38
26	B	618	BCR	C15-C14-C13	-2.18	124.22	127.28
29	a	404	LMT	C1B-O1B-C4'	-2.18	112.81	117.98
27	A	411	SQD	C44-O6-C1	-2.18	109.12	113.80
37	L	101	LHG	O4-P-O5	2.18	122.58	112.44
29	m	103	LMT	C1'-O5'-C5'	2.18	117.97	113.72
24	b	610	CLA	C1-O2A-CGA	2.18	121.92	116.65
27	F	101	SQD	O48-C23-O10	-2.18	118.19	123.63
26	k	102	BCR	C34-C9-C8	2.17	121.41	118.09
24	c	517	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
24	A	405	CLA	CHB-C4A-NA	2.17	127.54	124.40
24	c	516	CLA	CAC-C3C-C4C	2.17	127.62	124.79
27	A	413	SQD	O6-C44-C45	-2.17	105.54	110.82
26	B	618	BCR	C38-C26-C25	-2.17	122.11	124.48
25	A	408	PHO	C4D-CHA-CBD	2.17	109.50	108.45
24	B	616	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
24	c	517	CLA	C4-C3-C5	2.17	118.99	115.23
24	b	625	CLA	CHC-C1C-NC	2.17	127.58	124.31
24	A	405	CLA	C2A-C1A-CHA	-2.17	120.10	123.87
38	f	101	HEM	C4C-NC-C1C	2.17	109.35	105.82
29	C	521	LMT	O5'-C5'-C4'	2.17	114.20	109.72
26	k	102	BCR	C7-C8-C9	-2.17	123.03	126.23
24	b	620	CLA	CHB-C4A-NA	2.17	127.53	124.40
24	C	510	CLA	CBC-CAC-C3C	-2.17	106.55	112.42
36	C	517	DGD	O6D-C5D-C6D	2.17	110.99	106.69
24	A	409	CLA	CHD-C4C-NC	2.16	127.59	124.23
35	d	413	HTG	C1-O5-C5	2.16	116.44	112.56
26	d	406	BCR	C40-C30-C25	-2.16	106.85	110.24
31	D	407[B]	PL9	C30-C29-C31	2.16	118.98	115.23
24	B	604	CLA	CAC-C3C-C4C	2.16	127.60	124.79
24	A	407	CLA	CHB-C4A-NA	2.16	127.52	124.40
40	V	205	HEC	CBA-CAA-C2A	-2.16	106.56	112.53
25	A	408	PHO	C16-C15-C13	-2.16	108.79	115.97
24	b	619	CLA	O1D-CGD-CBD	-2.16	120.26	124.52
40	v	206	HEC	CHB-C1B-C2B	-2.16	121.16	127.43
24	C	504	CLA	C1-C2-C3	-2.16	122.67	126.20
24	c	517	CLA	O2D-CGD-O1D	-2.16	119.65	123.85
24	A	406	CLA	C6-C7-C8	-2.16	108.80	115.97
24	b	611	CLA	CMD-C2D-C3D	-2.15	122.75	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	C6-C7-C8	-2.15	108.81	115.97
24	B	617	CLA	C4-C3-C5	2.15	118.96	115.23
38	E	103	HEM	CHA-C4D-ND	2.15	127.03	124.37
24	c	510	CLA	CED-O2D-CGD	2.15	120.80	115.92
24	B	605	CLA	OBD-CAD-C3D	-2.15	123.39	128.42
31	d	407[B]	PL9	C15-C14-C16	2.15	118.96	115.23
33	k	101	LMG	O8-C28-O10	-2.15	118.25	123.63
24	C	501	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
33	C	519	LMG	O7-C10-O9	-2.15	118.68	123.70
40	v	206	HEC	CBA-CAA-C2A	-2.15	106.59	112.53
31	d	407[A]	PL9	C22-C23-C24	-2.15	122.70	127.62
36	D	408	DGD	O6D-C1D-C2D	2.15	114.79	110.37
24	c	513	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
31	A	417[A]	PL9	C47-C46-C44	-2.15	106.06	113.19
36	c	521	DGD	O1G-C1A-O1A	-2.15	118.25	123.63
27	A	411	SQD	C1-O5-C5	-2.15	109.53	113.72
24	b	625	CLA	C4-C3-C5	2.15	118.95	115.23
36	C	516	DGD	O1G-C1A-C2A	2.15	118.38	111.83
26	B	620	BCR	C36-C18-C17	-2.15	119.34	122.82
24	B	607	CLA	CAC-C3C-C4C	2.14	127.58	124.79
24	b	625	CLA	CBC-CAC-C3C	-2.14	106.61	112.42
24	c	512	CLA	CAC-C3C-C4C	2.14	127.58	124.79
31	D	407[B]	PL9	C20-C19-C21	2.14	118.94	115.23
31	d	407[A]	PL9	O1-C4-C3	-2.14	118.47	120.73
24	b	610	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
24	b	623	CLA	C4-C3-C5	2.14	118.94	115.23
35	c	523	HTG	C1-O5-C5	2.14	116.40	112.56
26	A	410	BCR	C21-C20-C19	-2.14	117.00	123.20
26	d	406	BCR	C7-C8-C9	-2.14	123.07	126.23
40	v	206	HEC	C4D-ND-C1D	2.14	109.30	105.82
29	a	419	LMT	C1B-O1B-C4'	-2.14	112.92	117.98
26	c	518	BCR	C34-C9-C8	2.13	121.35	118.09
24	C	508	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
26	a	413	BCR	C40-C30-C25	-2.13	106.90	110.24
38	f	101	HEM	CHA-C1A-NA	2.13	127.72	123.86
24	A	406	CLA	CAA-CBA-CGA	2.13	119.26	113.21
24	b	611	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
24	B	611	CLA	CAC-C3C-C4C	2.13	127.56	124.79
24	C	508	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
25	a	411	PHO	CAC-C3C-C4C	2.13	129.50	124.03
24	c	515	CLA	CBC-CAC-C3C	-2.13	106.65	112.42
37	L	101	LHG	O8-C23-O10	-2.13	118.31	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	409	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
26	b	628	BCR	C11-C10-C9	-2.13	124.30	127.28
31	d	407[B]	PL9	C32-C33-C34	-2.13	122.76	127.62
24	B	607	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
31	D	407[A]	PL9	C47-C48-C49	-2.12	120.56	127.64
24	c	507	CLA	CBC-CAC-C3C	-2.12	106.66	112.42
24	c	511	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
36	c	520	DGD	O5D-C1E-C2E	2.12	111.50	108.27
24	d	405	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
24	C	508	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
24	b	622	CLA	CHB-C1B-NB	-2.12	120.87	124.05
31	A	417[B]	PL9	C47-C48-C49	-2.12	120.58	127.64
26	K	101	BCR	C15-C14-C13	-2.12	124.31	127.28
31	D	407[B]	PL9	C47-C48-C49	-2.12	120.59	127.64
24	B	605	CLA	CHD-C4C-NC	2.12	127.51	124.23
24	b	615	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
24	B	611	CLA	CBC-CAC-C3C	-2.11	106.69	112.42
24	b	625	CLA	C2A-C1A-CHA	-2.11	120.20	123.87
26	d	406	BCR	C37-C22-C23	2.11	121.31	118.09
24	B	603	CLA	CMA-C3A-C4A	-2.11	106.10	111.77
24	c	512	CLA	CMB-C2B-C1B	2.11	128.63	125.42
35	V	206	HTG	C3-C4-C5	2.11	114.06	110.23
31	D	407[B]	PL9	C36-C37-C38	-2.11	101.58	112.02
26	K	101	BCR	C36-C18-C19	2.11	121.31	118.09
26	B	618	BCR	C24-C23-C22	-2.11	123.11	126.23
24	B	602	CLA	CHB-C4A-NA	2.11	127.44	124.40
31	D	407[A]	PL9	C20-C19-C21	2.11	118.89	115.23
37	D	410	LHG	O7-C7-C8	2.11	116.04	111.48
31	d	407[A]	PL9	C40-C39-C38	-2.11	118.22	123.63
26	b	626	BCR	C20-C21-C22	-2.10	124.33	127.28
31	D	407[A]	PL9	C7-C3-C2	-2.10	120.91	123.39
33	c	522	LMG	O7-C10-O9	-2.10	118.79	123.70
26	b	626	BCR	C37-C22-C21	-2.10	119.41	122.82
24	B	607	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
25	a	411	PHO	C1-C2-C3	-2.10	122.75	126.20
33	k	101	LMG	O6-C5-C6	2.10	111.65	106.44
24	C	508	CLA	CHB-C1B-C2B	-2.10	121.33	127.43
26	H	101	BCR	C21-C20-C19	-2.10	117.11	123.20
24	A	409	CLA	CMA-C3A-C2A	-2.10	105.86	113.98
29	A	414	LMT	C4B-C3B-C2B	-2.10	107.14	110.83
24	c	509	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
24	D	405	CLA	O2A-CGA-O1A	-2.10	118.38	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	619	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
24	b	622	CLA	O2D-CGD-O1D	-2.10	119.77	123.85
31	a	416[A]	PL9	C45-C44-C46	2.10	118.87	115.23
24	B	607	CLA	CMB-C2B-C1B	2.10	128.61	125.42
24	B	611	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
27	L	102	SQD	C4-C3-C2	2.10	114.51	110.83
24	C	508	CLA	CHC-C1C-NC	2.10	127.47	124.31
24	C	512	CLA	O1D-CGD-CBD	-2.10	120.39	124.52
31	D	407[A]	PL9	C35-C34-C36	2.09	118.86	115.23
24	c	511	CLA	C4B-C3B-C2B	-2.09	104.70	107.30
24	b	624	CLA	O2D-CGD-O1D	-2.09	119.77	123.85
25	d	402[A]	PHO	CMA-C3A-C4A	-2.09	110.10	114.61
36	C	517	DGD	C3G-O3G-C1D	-2.09	109.31	113.80
24	B	614	CLA	CHB-C4A-NA	2.09	127.42	124.40
24	C	504	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
33	Z	101	LMG	O6-C1-C2	2.09	114.67	110.37
31	A	417[A]	PL9	C2-C1-C6	2.09	121.48	119.00
24	b	625	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
36	C	518	DGD	O1G-C1A-O1A	-2.09	118.40	123.63
24	C	503	CLA	C1-O2A-CGA	2.09	121.71	116.65
26	C	515	BCR	C37-C22-C23	2.09	121.28	118.09
29	e	102	LMT	O5'-C5'-C4'	2.09	114.04	109.72
24	c	512	CLA	C2A-C1A-CHA	-2.09	120.24	123.87
37	D	410	LHG	O8-C23-C24	2.09	118.20	111.83
31	A	417[B]	PL9	C51-C49-C50	2.09	119.39	114.59
37	d	409	LHG	O7-C7-O9	-2.09	118.83	123.70
24	C	511	CLA	C2A-C1A-CHA	-2.09	120.25	123.87
36	H	102	DGD	C3E-C4E-C5E	-2.08	106.45	110.23
24	A	407	CLA	O2A-CGA-CBA	2.08	118.19	111.83
24	b	614	CLA	C1-C2-C3	-2.08	122.78	126.20
35	B	631	HTG	C6-C5-C4	-2.08	107.91	113.02
33	d	415	LMG	C4-C3-C2	-2.08	107.17	110.83
26	y	101	BCR	C8-C7-C6	-2.08	121.44	127.00
27	L	102	SQD	O48-C23-O10	-2.08	118.42	123.63
25	a	411	PHO	C4A-C3A-C2A	-2.08	100.86	102.84
24	C	509	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
24	B	613	CLA	CMB-C2B-C1B	2.08	128.58	125.42
24	c	512	CLA	CMC-C2C-C1C	2.08	128.28	125.03
36	C	517	DGD	C2G-O2G-C1B	-2.08	112.83	117.80
24	B	609	CLA	CHB-C4A-NA	2.08	127.40	124.40
24	B	609	CLA	C2A-C1A-CHA	-2.08	120.26	123.87
29	t	101	LMT	C1'-O5'-C5'	2.08	117.77	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	V	205	HEC	CHB-C1B-C2B	-2.08	121.40	127.43
31	d	407[A]	PL9	C8-C7-C3	2.08	117.39	112.03
36	C	516	DGD	C2G-O2G-C1B	-2.07	112.83	117.80
24	C	510	CLA	C4-C3-C2	-2.07	118.30	123.63
24	b	613	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
26	B	619	BCR	C37-C22-C23	2.07	121.25	118.09
26	B	618	BCR	C16-C15-C14	-2.07	119.28	123.52
26	Y	101	BCR	C37-C22-C23	2.07	121.25	118.09
25	A	408	PHO	CMB-C2B-C3B	2.07	128.82	124.68
24	B	615	CLA	CHB-C4A-NA	2.07	127.39	124.40
24	B	609	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
24	C	512	CLA	C1-O2A-CGA	2.07	121.66	116.65
36	c	520	DGD	O2G-C1B-O1B	-2.07	118.87	123.70
24	c	514	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	D	407[A]	PL9	C36-C37-C38	-2.07	101.80	112.02
26	T	103	BCR	C29-C30-C25	2.06	113.44	110.44
24	b	619	CLA	CMB-C2B-C1B	2.06	128.56	125.42
31	D	407[B]	PL9	C10-C9-C8	-2.06	118.33	123.63
26	t	102	BCR	C29-C28-C27	-2.06	106.74	111.28
33	c	522	LMG	O8-C28-O10	-2.06	118.47	123.63
31	a	416[B]	PL9	C8-C7-C3	2.06	117.36	112.03
24	b	625	CLA	CHA-C1A-NA	-2.06	121.73	126.39
24	d	403	CLA	CHB-C4A-NA	2.06	127.37	124.40
36	c	521	DGD	O2G-C1B-O1B	-2.06	118.89	123.70
33	b	629	LMG	C9-C8-C7	-2.06	106.98	111.78
24	B	615	CLA	C4D-CHA-C1A	-2.06	118.79	121.24
24	b	625	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
24	c	505	CLA	CAA-C2A-C3A	-2.06	107.44	113.00
26	C	515	BCR	C28-C27-C26	-2.06	110.39	114.06
24	B	610	CLA	CED-O2D-CGD	2.05	120.58	115.92
33	C	520	LMG	C8-O7-C10	-2.05	112.88	117.80
24	a	409	CLA	CHB-C4A-NA	2.05	127.36	124.40
26	a	413	BCR	C8-C7-C6	-2.05	121.51	127.00
24	b	622	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
29	m	103	LMT	O5B-C5B-C4B	2.05	113.40	109.70
26	K	101	BCR	C16-C17-C18	-2.05	124.40	127.28
25	a	411	PHO	C16-C15-C13	-2.05	109.15	115.97
26	B	619	BCR	C31-C1-C6	-2.05	107.03	110.24
26	a	413	BCR	C29-C30-C25	2.05	113.42	110.44
38	E	103	HEM	C2A-C1A-NA	-2.05	107.88	110.15
24	b	618	CLA	CED-O2D-CGD	2.05	120.56	115.92
24	b	617	CLA	CMB-C2B-C1B	2.05	128.53	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	617	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
24	A	405	CLA	C1-C2-C3	-2.04	122.85	126.20
24	b	620	CLA	C7-C6-C5	-2.04	107.81	113.26
24	C	506	CLA	OBD-CAD-C3D	-2.04	123.64	128.42
24	b	610	CLA	CHB-C1B-C2B	-2.04	121.49	127.43
24	b	615	CLA	CAC-C3C-C4C	2.04	127.45	124.79
24	b	616	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
24	b	615	CLA	CHA-C1A-NA	-2.04	121.77	126.39
25	d	402[A]	PHO	O2A-CGA-CBA	2.04	118.06	111.83
24	b	610	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
24	b	619	CLA	CHA-C1A-NA	-2.04	121.77	126.39
36	H	102	DGD	C2G-O2G-C1B	-2.04	112.92	117.80
33	d	415	LMG	O8-C28-O10	-2.04	118.53	123.63
24	C	510	CLA	CMB-C2B-C1B	2.04	128.52	125.42
24	A	405	CLA	CED-O2D-CGD	2.04	120.54	115.92
24	B	612	CLA	CHB-C4A-NA	2.04	127.34	124.40
26	H	101	BCR	C7-C6-C5	2.04	126.25	121.56
24	c	505	CLA	C2A-C1A-CHA	-2.04	120.33	123.87
24	A	406	CLA	C6-C5-C3	-2.04	108.51	113.47
24	b	618	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
24	c	508	CLA	CHB-C4A-NA	2.03	127.34	124.40
26	C	515	BCR	C15-C14-C13	-2.03	124.42	127.28
26	C	515	BCR	C10-C11-C12	-2.03	117.31	123.20
24	A	407	CLA	CAA-C2A-C1A	-2.03	105.31	111.97
35	B	623	HTG	C1-O5-C5	2.03	116.21	112.56
25	d	402[B]	PHO	C4-C3-C2	-2.03	118.41	123.63
26	Y	101	BCR	C34-C9-C8	2.03	121.19	118.09
26	b	627	BCR	C37-C22-C23	2.03	121.19	118.09
24	C	507	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
24	C	506	CLA	C2A-C1A-CHA	-2.03	120.34	123.87
26	b	627	BCR	C33-C5-C6	-2.03	122.27	124.48
26	h	101	BCR	C16-C15-C14	-2.03	119.37	123.52
24	b	614	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
26	D	406	BCR	C38-C26-C27	2.03	117.92	113.60
24	C	510	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
24	B	606	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
24	b	617	CLA	C4-C3-C5	2.03	118.75	115.23
24	C	511	CLA	CMB-C2B-C1B	2.03	128.50	125.42
26	D	406	BCR	C30-C25-C24	2.03	121.14	115.65
31	d	407[A]	PL9	C35-C34-C36	2.03	118.74	115.23
24	C	510	CLA	CHB-C4A-NA	2.02	127.32	124.40
26	B	619	BCR	C21-C20-C19	-2.02	117.34	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	624	CLA	C1-C2-C3	-2.02	122.89	126.20
26	D	406	BCR	C3-C4-C5	-2.02	110.45	114.06
31	A	417[A]	PL9	C40-C39-C41	2.02	118.74	115.23
24	a	412	CLA	C4A-NA-C1A	-2.02	105.76	106.68
38	E	103	HEM	O2A-CGA-CBA	2.02	120.39	114.00
24	b	611	CLA	CMA-C3A-C2A	-2.02	106.17	113.98
24	b	621	CLA	CMA-C3A-C2A	-2.02	106.18	113.98
24	C	511	CLA	CED-O2D-CGD	2.02	120.49	115.92
25	d	402[B]	PHO	OBD-CAD-C3D	-2.02	124.75	127.89
24	b	611	CLA	CHB-C4A-NA	2.02	127.31	124.40
24	B	617	CLA	C2A-C1A-CHA	-2.02	120.37	123.87
29	M	104	LMT	O1'-C1'-C2'	2.01	111.33	108.27
27	F	101	SQD	O7-S-C6	2.01	109.76	106.76
33	C	520	LMG	O7-C10-O9	-2.01	119.00	123.70
31	A	417[A]	PL9	C51-C49-C50	2.01	119.22	114.59
24	b	620	CLA	CMC-C2C-C1C	2.01	128.18	125.03
40	v	206	HEC	C4C-NC-C1C	2.01	109.10	105.82
24	c	507	CLA	O2D-CGD-O1D	-2.01	119.93	123.85
37	b	634	LHG	O4-P-O5	2.01	121.80	112.44
37	D	409	LHG	O7-C7-O9	-2.01	119.00	123.70
35	V	206	HTG	O5-C5-C4	2.01	113.32	109.70
40	V	205	HEC	CHD-C1D-ND	2.01	127.50	123.86
24	b	610	CLA	C11-C12-C13	-2.01	109.29	115.97
24	b	610	CLA	CMB-C2B-C1B	2.01	128.48	125.42
24	c	511	CLA	CHB-C4A-NA	2.01	127.30	124.40
24	d	405	CLA	C1-O2A-CGA	2.01	121.51	116.65
24	C	505	CLA	CHA-C1A-NA	-2.01	121.85	126.39
24	C	506	CLA	CMB-C2B-C1B	2.01	128.47	125.42
29	M	104	LMT	C1'-O5'-C5'	2.01	117.64	113.72
24	c	516	CLA	CHA-C1A-NA	-2.01	121.85	126.39
24	c	513	CLA	OBD-CAD-C3D	-2.00	123.73	128.42
24	a	412	CLA	CAC-C3C-C4C	2.00	127.39	124.79
24	b	621	CLA	CAA-C2A-C3A	-2.00	107.59	113.00

All (63) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
24	A	405	CLA	ND
24	A	406	CLA	ND
24	B	602	CLA	ND
24	B	603	CLA	ND
24	B	604	CLA	ND

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Mol	Chain	Res	Type	Atom
24	B	605	CLA	ND
24	B	606	CLA	ND
24	B	607	CLA	ND
24	B	608	CLA	ND
24	B	610	CLA	ND
24	B	611	CLA	ND
24	B	612	CLA	ND
24	B	613	CLA	ND
24	B	614	CLA	ND
24	B	615	CLA	ND
24	B	616	CLA	ND
24	B	617	CLA	ND
24	C	501	CLA	ND
24	C	502	CLA	ND
24	C	503	CLA	ND
24	C	504	CLA	ND
24	C	505	CLA	ND
24	C	506	CLA	ND
24	C	507	CLA	ND
24	C	508	CLA	ND
24	C	509	CLA	ND
24	C	510	CLA	ND
24	C	512	CLA	ND
24	C	513	CLA	ND
24	D	404	CLA	ND
24	D	405	CLA	ND
24	a	409	CLA	ND
24	a	412	CLA	ND
24	b	610	CLA	ND
24	b	611	CLA	ND
24	b	612	CLA	ND
24	b	613	CLA	ND
24	b	614	CLA	ND
24	b	615	CLA	ND
24	b	616	CLA	ND
24	b	618	CLA	ND
24	b	619	CLA	ND
24	b	620	CLA	ND
24	b	621	CLA	ND
24	b	622	CLA	ND
24	b	623	CLA	ND
24	b	624	CLA	ND

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Mol	Chain	Res	Type	Atom
24	b	625	CLA	ND
24	c	505	CLA	ND
24	c	506	CLA	ND
24	c	507	CLA	ND
24	c	508	CLA	ND
24	c	509	CLA	ND
24	c	510	CLA	ND
24	c	511	CLA	ND
24	c	512	CLA	ND
24	c	513	CLA	ND
24	c	514	CLA	ND
24	c	515	CLA	ND
24	c	516	CLA	ND
24	d	403	CLA	ND
24	d	404	CLA	ND
24	d	405	CLA	ND

All (1384) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	607	CLA	C2B-C3B-CAB-CBB
24	B	607	CLA	C4B-C3B-CAB-CBB
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	B	615	CLA	C2-C3-C5-C6
24	C	502	CLA	C4B-C3B-CAB-CBB
24	C	505	CLA	C2B-C3B-CAB-CBB
24	C	505	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	C4B-C3B-CAB-CBB
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D
24	C	509	CLA	C2-C1-O2A-CGA
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	616	CLA	C4B-C3B-CAB-CBB
24	b	623	CLA	CAD-CBD-CGD-O1D
24	b	623	CLA	CAD-CBD-CGD-O2D
24	b	623	CLA	C2-C3-C5-C6
24	c	508	CLA	C2-C3-C5-C6
24	c	508	CLA	C4-C3-C5-C6
24	c	511	CLA	CHA-CBD-CGD-O1D
24	c	511	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	c	516	CLA	C2B-C3B-CAB-CBB
24	c	516	CLA	C4B-C3B-CAB-CBB
26	C	515	BCR	C7-C8-C9-C10
26	D	406	BCR	C7-C8-C9-C10
26	D	406	BCR	C21-C22-C23-C24
26	Y	101	BCR	C1-C6-C7-C8
26	Y	101	BCR	C5-C6-C7-C8
26	Y	101	BCR	C21-C22-C23-C24
26	d	406	BCR	C21-C22-C23-C24
26	d	406	BCR	C37-C22-C23-C24
26	t	102	BCR	C7-C8-C9-C10
26	y	101	BCR	C1-C6-C7-C8
26	y	101	BCR	C5-C6-C7-C8
27	A	413	SQD	O6-C44-C45-O47
27	B	621	SQD	O5-C1-O6-C44
27	B	621	SQD	O49-C7-O47-C45
27	F	101	SQD	O49-C7-O47-C45
27	F	101	SQD	C5-C6-S-O7
27	F	101	SQD	C5-C6-S-O9
27	L	102	SQD	O5-C1-O6-C44
27	L	102	SQD	O49-C7-O47-C45
27	a	405	SQD	O6-C44-C45-O47
27	a	405	SQD	O5-C5-C6-S
27	f	102	SQD	O49-C7-O47-C45
27	f	102	SQD	C8-C7-O47-C45
27	f	102	SQD	C5-C6-S-O7
27	f	102	SQD	C5-C6-S-O8
27	f	102	SQD	C5-C6-S-O9
28	B	626	GOL	O1-C1-C2-O2
28	B	626	GOL	O1-C1-C2-C3
28	B	627	GOL	O1-C1-C2-O2
28	B	629	GOL	O1-C1-C2-C3
28	D	402	GOL	C1-C2-C3-O3
28	T	102	GOL	O1-C1-C2-O2
28	T	102	GOL	O1-C1-C2-C3
28	V	201	GOL	C1-C2-C3-O3
28	a	401	GOL	C1-C2-C3-O3
28	a	402	GOL	O1-C1-C2-C3
28	a	421	GOL	O1-C1-C2-C3
28	b	604	GOL	C1-C2-C3-O3
28	b	605	GOL	O1-C1-C2-C3
28	b	606	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	b	606	GOL	O1-C1-C2-C3
28	c	502	GOL	O1-C1-C2-C3
28	v	202	GOL	O1-C1-C2-C3
29	A	414	LMT	O5'-C1'-O1'-C1
29	E	102	LMT	O5'-C1'-O1'-C1
29	M	104	LMT	O5'-C1'-O1'-C1
29	a	404	LMT	C2'-C1'-O1'-C1
29	a	404	LMT	O5'-C1'-O1'-C1
29	b	630	LMT	C2'-C1'-O1'-C1
29	b	630	LMT	O5'-C1'-O1'-C1
33	A	419	LMG	C11-C10-O7-C8
33	C	520	LMG	C11-C10-O7-C8
33	Z	101	LMG	O6-C1-O1-C7
33	Z	101	LMG	O9-C10-O7-C8
33	Z	101	LMG	C11-C10-O7-C8
33	z	101	LMG	O6-C1-O1-C7
33	z	101	LMG	O9-C10-O7-C8
35	B	623	HTG	C2'-C1'-S1-C1
35	B	624	HTG	O5-C1-S1-C1'
35	V	206	HTG	C2-C1-S1-C1'
36	D	408	DGD	C2B-C1B-O2G-C2G
36	D	408	DGD	O1B-C1B-O2G-C2G
36	e	101	DGD	C2B-C1B-O2G-C2G
36	e	101	DGD	O1B-C1B-O2G-C2G
36	e	101	DGD	C2D-C1D-O3G-C3G
36	e	101	DGD	O6E-C1E-O5D-C6D
37	D	409	LHG	C4-O6-P-O5
37	D	410	LHG	C4-O6-P-O3
37	D	410	LHG	C4-O6-P-O4
37	E	101	LHG	C3-O3-P-O6
37	E	101	LHG	C4-O6-P-O3
37	E	101	LHG	C4-O6-P-O5
37	L	101	LHG	C4-O6-P-O3
37	L	101	LHG	C4-O6-P-O4
37	a	420	LHG	C3-O3-P-O5
37	a	420	LHG	C3-O3-P-O6
37	a	420	LHG	C4-O6-P-O5
37	a	420	LHG	C24-C23-O8-C6
37	b	634	LHG	O1-C1-C2-C3
37	b	634	LHG	C4-O6-P-O3
37	b	634	LHG	C4-O6-P-O4
37	d	408	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
37	d	408	LHG	C4-O6-P-O5
37	d	409	LHG	C3-O3-P-O4
37	d	409	LHG	C3-O3-P-O6
38	E	103	HEM	C2B-C3B-CAB-CBB
38	E	103	HEM	C2C-C3C-CAC-CBC
38	E	103	HEM	C4C-C3C-CAC-CBC
40	V	205	HEC	C2B-C3B-CAB-CBB
40	V	205	HEC	C4B-C3B-CAB-CBB
40	V	205	HEC	C2C-C3C-CAC-CBC
40	V	205	HEC	C4C-C3C-CAC-CBC
40	v	206	HEC	C2B-C3B-CAB-CBB
40	v	206	HEC	C4B-C3B-CAB-CBB
29	C	521	LMT	C3'-C4'-O1B-C1B
29	D	403	LMT	C3'-C4'-O1B-C1B
37	E	101	LHG	O10-C23-O8-C6
37	a	420	LHG	O10-C23-O8-C6
37	E	101	LHG	C24-C23-O8-C6
33	A	419	LMG	O9-C10-O7-C8
33	C	520	LMG	O9-C10-O7-C8
24	A	409	CLA	C3-C5-C6-C7
24	B	617	CLA	C3-C5-C6-C7
24	a	412	CLA	C3-C5-C6-C7
24	b	623	CLA	C3-C5-C6-C7
24	c	510	CLA	C3-C5-C6-C7
33	z	101	LMG	O6-C5-C6-O5
27	B	621	SQD	C8-C7-O47-C45
27	F	101	SQD	C8-C7-O47-C45
27	L	102	SQD	C8-C7-O47-C45
33	z	101	LMG	C11-C10-O7-C8
24	B	615	CLA	C4-C3-C5-C6
24	b	614	CLA	C4-C3-C5-C6
24	b	623	CLA	C4-C3-C5-C6
31	a	416[A]	PL9	C12-C11-C9-C10
31	a	416[B]	PL9	C12-C11-C9-C10
24	B	615	CLA	C3-C5-C6-C7
35	c	523	HTG	S1-C1'-C2'-C3'
24	B	602	CLA	C3-C5-C6-C7
24	c	515	CLA	CBD-CGD-O2D-CED
29	M	104	LMT	O5'-C5'-C6'-O6'
35	B	624	HTG	O5-C5-C6-O6
24	C	509	CLA	CBD-CGD-O2D-CED
33	C	520	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
36	e	101	DGD	C4E-C5E-C6E-O5E
31	A	417[A]	PL9	C25-C24-C26-C27
31	A	417[B]	PL9	C25-C24-C26-C27
31	a	416[A]	PL9	C15-C14-C16-C17
31	a	416[A]	PL9	C20-C19-C21-C22
31	a	416[B]	PL9	C20-C19-C21-C22
24	b	614	CLA	C2-C3-C5-C6
31	A	417[A]	PL9	C23-C24-C26-C27
31	a	416[A]	PL9	C13-C14-C16-C17
31	a	416[A]	PL9	C23-C24-C26-C27
31	a	416[B]	PL9	C13-C14-C16-C17
31	a	416[B]	PL9	C18-C19-C21-C22
31	a	416[B]	PL9	C23-C24-C26-C27
29	M	102	LMT	O5B-C5B-C6B-O6B
29	m	103	LMT	O5'-C5'-C6'-O6'
35	C	523	HTG	O5-C5-C6-O6
31	D	407[A]	PL9	C39-C41-C42-C43
31	D	407[B]	PL9	C39-C41-C42-C43
31	a	416[B]	PL9	C9-C11-C12-C13
31	d	407[A]	PL9	C39-C41-C42-C43
31	d	407[B]	PL9	C39-C41-C42-C43
33	z	101	LMG	C4-C5-C6-O5
24	d	405	CLA	CBD-CGD-O2D-CED
24	C	509	CLA	O1A-CGA-O2A-C1
29	C	521	LMT	O5'-C1'-O1'-C1
29	T	104	LMT	O5'-C1'-O1'-C1
29	a	419	LMT	O5'-C1'-O1'-C1
29	e	102	LMT	O5'-C1'-O1'-C1
29	t	101	LMT	O5'-C1'-O1'-C1
36	D	408	DGD	O6D-C1D-O3G-C3G
36	e	101	DGD	O6D-C1D-O3G-C3G
29	M	104	LMT	C4'-C5'-C6'-O6'
24	C	509	CLA	CBA-CGA-O2A-C1
37	D	411	LHG	C24-C23-O8-C6
24	C	501	CLA	CBD-CGD-O2D-CED
24	b	613	CLA	CBD-CGD-O2D-CED
24	c	507	CLA	CBD-CGD-O2D-CED
37	D	411	LHG	O10-C23-O8-C6
29	e	102	LMT	C4'-C5'-C6'-O6'
24	a	410	CLA	CBD-CGD-O2D-CED
33	a	415	LMG	C17-C18-C19-C20
24	a	412	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	a	412	CLA	CBA-CGA-O2A-C1
29	m	102	LMT	O5'-C5'-C6'-O6'
24	B	606	CLA	C4-C3-C5-C6
31	a	416[A]	PL9	C25-C24-C26-C27
31	a	416[B]	PL9	C15-C14-C16-C17
31	a	416[B]	PL9	C25-C24-C26-C27
24	B	606	CLA	C2-C3-C5-C6
31	A	417[B]	PL9	C23-C24-C26-C27
31	a	416[A]	PL9	C12-C11-C9-C8
24	B	602	CLA	C11-C10-C8-C9
24	B	617	CLA	C6-C7-C8-C9
24	C	501	CLA	C11-C12-C13-C14
24	b	620	CLA	C11-C12-C13-C14
24	c	510	CLA	C6-C7-C8-C9
24	c	513	CLA	C11-C10-C8-C9
29	A	414	LMT	C2'-C1'-O1'-C1
29	C	521	LMT	C2'-C1'-O1'-C1
29	E	102	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	C2'-C1'-O1'-C1
29	a	419	LMT	C2'-C1'-O1'-C1
29	e	102	LMT	C2'-C1'-O1'-C1
29	t	101	LMT	C2'-C1'-O1'-C1
36	D	408	DGD	C2D-C1D-O3G-C3G
37	E	101	LHG	O2-C2-C3-O3
26	C	515	BCR	C7-C8-C9-C34
26	C	515	BCR	C37-C22-C23-C24
26	D	406	BCR	C7-C8-C9-C34
26	D	406	BCR	C37-C22-C23-C24
26	Y	101	BCR	C37-C22-C23-C24
26	t	102	BCR	C7-C8-C9-C34
36	c	521	DGD	C1A-C2A-C3A-C4A
27	A	413	SQD	C18-C19-C20-C21
24	B	615	CLA	C8-C10-C11-C12
24	C	508	CLA	C10-C11-C12-C13
36	H	102	DGD	O6E-C5E-C6E-O5E
28	B	629	GOL	O2-C2-C3-O3
28	a	402	GOL	O1-C1-C2-O2
24	b	623	CLA	CBD-CGD-O2D-CED
29	C	521	LMT	O5B-C5B-C6B-O6B
24	B	616	CLA	C11-C12-C13-C15
24	b	615	CLA	C12-C13-C15-C16
37	d	410	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	M	102	LMT	O5'-C5'-C6'-O6'
33	Z	101	LMG	C10-C11-C12-C13
29	T	104	LMT	O1'-C1-C2-C3
29	M	102	LMT	C4B-C5B-C6B-O6B
35	B	624	HTG	C4-C5-C6-O6
36	H	102	DGD	C4E-C5E-C6E-O5E
27	A	413	SQD	C23-C24-C25-C26
27	B	621	SQD	C7-C8-C9-C10
33	c	522	LMG	C10-C11-C12-C13
24	B	615	CLA	C10-C11-C12-C13
24	C	506	CLA	C5-C6-C7-C8
24	b	615	CLA	C13-C15-C16-C17
36	C	516	DGD	O6D-C5D-C6D-O5D
24	B	607	CLA	C2A-CAA-CBA-CGA
24	A	409	CLA	C13-C15-C16-C17
24	B	616	CLA	C8-C10-C11-C12
24	b	624	CLA	C10-C11-C12-C13
24	c	513	CLA	C13-C15-C16-C17
29	e	102	LMT	O5'-C5'-C6'-O6'
33	k	101	LMG	C10-C11-C12-C13
36	C	517	DGD	C1B-C2B-C3B-C4B
37	D	409	LHG	C23-C24-C25-C26
24	B	605	CLA	C3-C5-C6-C7
33	d	415	LMG	C19-C20-C21-C22
24	A	409	CLA	C10-C11-C12-C13
24	B	615	CLA	C5-C6-C7-C8
24	b	615	CLA	C10-C11-C12-C13
24	c	512	CLA	C15-C16-C17-C18
24	c	505	CLA	CBD-CGD-O2D-CED
33	C	520	LMG	C4-C5-C6-O5
33	a	415	LMG	C10-C11-C12-C13
24	b	623	CLA	C5-C6-C7-C8
24	d	405	CLA	C4-C3-C5-C6
37	d	410	LHG	O10-C23-O8-C6
37	d	410	LHG	C25-C26-C27-C28
24	a	410	CLA	C10-C11-C12-C13
24	b	623	CLA	C13-C15-C16-C17
24	c	517	CLA	C10-C11-C12-C13
27	B	621	SQD	C24-C23-O48-C46
27	L	102	SQD	C24-C23-O48-C46
29	m	102	LMT	C4'-C5'-C6'-O6'
35	b	632	HTG	S1-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
36	C	517	DGD	CBB-CCB-CDB-CEB
24	c	515	CLA	O1D-CGD-O2D-CED
37	b	634	LHG	C7-C8-C9-C10
37	E	101	LHG	C1-C2-C3-O3
24	B	602	CLA	C10-C11-C12-C13
24	C	509	CLA	C13-C15-C16-C17
24	b	620	CLA	C8-C10-C11-C12
36	C	516	DGD	C2A-C3A-C4A-C5A
37	E	101	LHG	C23-C24-C25-C26
24	B	617	CLA	C10-C11-C12-C13
24	b	610	CLA	C8-C10-C11-C12
31	a	416[A]	PL9	C30-C29-C31-C32
31	a	416[A]	PL9	C18-C19-C21-C22
36	C	516	DGD	C4D-C5D-C6D-O5D
24	a	412	CLA	C15-C16-C17-C18
33	k	101	LMG	C11-C10-O7-C8
37	D	410	LHG	C32-C33-C34-C35
33	k	101	LMG	O9-C10-O7-C8
29	M	104	LMT	C2'-C1'-O1'-C1
36	C	517	DGD	C2E-C1E-O5D-C6D
36	c	520	DGD	C2E-C1E-O5D-C6D
36	e	101	DGD	C2E-C1E-O5D-C6D
31	a	416[A]	PL9	C9-C11-C12-C13
36	e	101	DGD	O6D-C5D-C6D-O5D
36	e	101	DGD	O6E-C5E-C6E-O5E
24	b	622	CLA	C16-C17-C18-C19
26	b	628	BCR	C11-C12-C13-C35
27	B	621	SQD	O10-C23-O48-C46
24	b	615	CLA	C2A-CAA-CBA-CGA
28	B	627	GOL	O1-C1-C2-C3
28	B	628	GOL	O1-C1-C2-C3
28	B	629	GOL	C1-C2-C3-O3
28	O	301	GOL	C1-C2-C3-O3
28	V	202	GOL	O1-C1-C2-C3
28	V	204	GOL	C1-C2-C3-O3
28	o	301	GOL	O1-C1-C2-C3
28	v	204	GOL	O1-C1-C2-C3
37	D	409	LHG	O1-C1-C2-C3
37	E	101	LHG	C7-C8-C9-C10
24	b	610	CLA	C16-C17-C18-C20
37	a	420	LHG	C11-C12-C13-C14
36	C	517	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
36	c	520	DGD	O6E-C1E-O5D-C6D
24	C	506	CLA	C13-C15-C16-C17
36	C	518	DGD	O6E-C5E-C6E-O5E
36	C	518	DGD	C6B-C7B-C8B-C9B
24	B	617	CLA	C2-C1-O2A-CGA
24	b	610	CLA	C2-C1-O2A-CGA
24	c	513	CLA	C2-C1-O2A-CGA
24	a	412	CLA	C16-C17-C18-C19
24	b	610	CLA	C16-C17-C18-C19
24	b	620	CLA	C16-C17-C18-C19
27	L	102	SQD	O10-C23-O48-C46
27	A	411	SQD	C9-C10-C11-C12
33	C	519	LMG	C11-C12-C13-C14
27	F	101	SQD	C26-C27-C28-C29
33	M	101	LMG	C29-C30-C31-C32
36	C	516	DGD	C4B-C5B-C6B-C7B
36	C	517	DGD	C9A-CAA-CBA-CCA
36	c	519	DGD	C8B-C9B-CAB-CBB
36	e	101	DGD	C5A-C6A-C7A-C8A
24	C	501	CLA	C15-C16-C17-C18
29	M	104	LMT	C2-C3-C4-C5
36	D	408	DGD	C7A-C8A-C9A-CAA
36	e	101	DGD	C2A-C3A-C4A-C5A
37	d	410	LHG	C29-C30-C31-C32
27	a	414	SQD	C11-C12-C13-C14
33	C	519	LMG	C12-C13-C14-C15
36	C	518	DGD	CAA-CBA-CCA-CDA
28	B	629	GOL	O1-C1-C2-O2
28	D	402	GOL	O2-C2-C3-O3
28	V	201	GOL	O2-C2-C3-O3
28	V	204	GOL	O2-C2-C3-O3
28	a	401	GOL	O2-C2-C3-O3
28	a	421	GOL	O1-C1-C2-O2
28	b	605	GOL	O1-C1-C2-O2
28	v	202	GOL	O1-C1-C2-O2
28	v	204	GOL	O1-C1-C2-O2
24	C	509	CLA	O1D-CGD-O2D-CED
24	c	507	CLA	O1D-CGD-O2D-CED
24	A	407	CLA	C4B-C3B-CAB-CBB
24	A	409	CLA	C4B-C3B-CAB-CBB
24	B	615	CLA	C4B-C3B-CAB-CBB
24	C	504	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
24	d	405	CLA	C4B-C3B-CAB-CBB
35	b	632	HTG	C1'-C2'-C3'-C4'
24	d	405	CLA	O1D-CGD-O2D-CED
33	A	419	LMG	C30-C31-C32-C33
36	c	520	DGD	C9A-CAA-CBA-CCA
37	D	409	LHG	C11-C12-C13-C14
24	b	612	CLA	C6-C7-C8-C10
36	c	519	DGD	O6D-C5D-C6D-O5D
27	a	405	SQD	C23-C24-C25-C26
36	e	101	DGD	C2A-C1A-O1G-C1G
33	k	101	LMG	C32-C33-C34-C35
35	B	623	HTG	C2'-C3'-C4'-C5'
37	b	634	LHG	C33-C34-C35-C36
27	L	102	SQD	C29-C30-C31-C32
24	c	516	CLA	CBA-CGA-O2A-C1
35	B	623	HTG	C4-C5-C6-O6
29	t	101	LMT	C3-C4-C5-C6
33	Z	101	LMG	C19-C20-C21-C22
33	d	415	LMG	C38-C39-C40-C41
36	c	519	DGD	CAB-CBB-CCB-CDB
36	e	101	DGD	C8B-C9B-CAB-CBB
36	h	102	DGD	CAA-CBA-CCA-CDA
27	L	102	SQD	C32-C33-C34-C35
27	a	414	SQD	C9-C10-C11-C12
36	c	519	DGD	C5A-C6A-C7A-C8A
37	L	101	LHG	C14-C15-C16-C17
33	d	415	LMG	C16-C17-C18-C19
29	t	101	LMT	C11-C10-C9-C8
33	a	415	LMG	C14-C15-C16-C17
36	C	516	DGD	C1B-C2B-C3B-C4B
24	A	407	CLA	C2B-C3B-CAB-CBB
24	C	502	CLA	C2B-C3B-CAB-CBB
24	C	507	CLA	C2B-C3B-CAB-CBB
24	b	616	CLA	C2B-C3B-CAB-CBB
26	B	618	BCR	C1-C6-C7-C8
26	B	618	BCR	C5-C6-C7-C8
36	c	521	DGD	C7A-C8A-C9A-CAA
37	b	634	LHG	C11-C10-C9-C8
24	B	605	CLA	CBD-CGD-O2D-CED
24	a	409	CLA	CBD-CGD-O2D-CED
33	z	101	LMG	C13-C14-C15-C16
36	e	101	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
27	F	101	SQD	C34-C35-C36-C37
36	H	102	DGD	C7A-C8A-C9A-CAA
36	c	521	DGD	C6A-C7A-C8A-C9A
24	d	405	CLA	C2-C3-C5-C6
27	L	102	SQD	C14-C15-C16-C17
29	T	104	LMT	C11-C10-C9-C8
33	d	415	LMG	C35-C36-C37-C38
37	E	101	LHG	C24-C25-C26-C27
37	b	634	LHG	C27-C28-C29-C30
33	C	520	LMG	C28-C29-C30-C31
24	A	409	CLA	CBA-CGA-O2A-C1
37	d	409	LHG	C24-C23-O8-C6
24	b	623	CLA	C11-C10-C8-C9
27	a	414	SQD	C15-C16-C17-C18
29	e	102	LMT	C4-C5-C6-C7
35	b	602	HTG	C3'-C4'-C5'-C6'
33	Z	101	LMG	C2-C1-O1-C7
33	C	520	LMG	C14-C15-C16-C17
33	z	101	LMG	C12-C13-C14-C15
29	T	104	LMT	C1-C2-C3-C4
29	m	103	LMT	C2-C3-C4-C5
36	D	408	DGD	C2A-C3A-C4A-C5A
24	c	515	CLA	CBA-CGA-O2A-C1
24	B	611	CLA	C16-C17-C18-C19
24	B	616	CLA	C16-C17-C18-C19
33	A	419	LMG	C14-C15-C16-C17
29	C	521	LMT	O5B-C1B-O1B-C4'
24	A	407	CLA	C13-C15-C16-C17
24	b	610	CLA	C10-C11-C12-C13
24	c	513	CLA	C15-C16-C17-C18
27	A	411	SQD	C13-C14-C15-C16
33	b	629	LMG	C30-C31-C32-C33
36	c	519	DGD	C9A-CAA-CBA-CCA
36	C	517	DGD	CAB-CBB-CCB-CDB
37	a	420	LHG	C24-C25-C26-C27
35	c	523	HTG	C1'-C2'-C3'-C4'
24	b	613	CLA	C13-C15-C16-C17
24	b	615	CLA	C15-C16-C17-C18
26	t	102	BCR	C11-C12-C13-C35
27	A	411	SQD	C15-C16-C17-C18
27	f	102	SQD	C24-C25-C26-C27
36	e	101	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
33	d	415	LMG	C14-C15-C16-C17
24	B	611	CLA	C16-C17-C18-C20
24	B	616	CLA	C16-C17-C18-C20
24	a	412	CLA	C16-C17-C18-C20
24	b	622	CLA	C16-C17-C18-C20
24	b	624	CLA	C16-C17-C18-C20
29	T	104	LMT	C4-C5-C6-C7
37	D	409	LHG	C24-C25-C26-C27
31	D	407[B]	PL9	C45-C44-C46-C47
31	d	407[B]	PL9	C45-C44-C46-C47
35	b	631	HTG	C2'-C3'-C4'-C5'
29	A	414	LMT	O1'-C1-C2-C3
29	M	102	LMT	C1-C2-C3-C4
27	L	102	SQD	C35-C36-C37-C38
33	d	415	LMG	C15-C16-C17-C18
36	c	521	DGD	CBB-CCB-CDB-CEB
24	A	409	CLA	O1A-CGA-O2A-C1
37	d	409	LHG	O10-C23-O8-C6
24	a	412	CLA	C10-C11-C12-C13
36	C	517	DGD	C4B-C5B-C6B-C7B
29	C	521	LMT	O5'-C5'-C6'-O6'
24	B	614	CLA	C13-C15-C16-C17
38	E	103	HEM	C4B-C3B-CAB-CBB
27	a	414	SQD	C29-C30-C31-C32
35	b	631	HTG	C3'-C4'-C5'-C6'
24	c	516	CLA	O1A-CGA-O2A-C1
35	C	523	HTG	S1-C1'-C2'-C3'
36	C	517	DGD	C1A-C2A-C3A-C4A
24	C	501	CLA	O1D-CGD-O2D-CED
36	C	516	DGD	C3B-C4B-C5B-C6B
29	b	630	LMT	C3'-C4'-O1B-C1B
24	A	406	CLA	C2C-C3C-CAC-CBC
24	C	511	CLA	CBA-CGA-O2A-C1
35	b	607	HTG	C2'-C3'-C4'-C5'
24	b	623	CLA	C10-C11-C12-C13
29	A	414	LMT	C6-C7-C8-C9
33	b	629	LMG	C38-C39-C40-C41
37	L	101	LHG	C12-C13-C14-C15
24	b	612	CLA	C5-C6-C7-C8
27	L	102	SQD	C28-C29-C30-C31
33	D	415	LMG	C19-C20-C21-C22
36	D	408	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	C7B-C8B-C9B-CAB
37	d	408	LHG	C25-C26-C27-C28
27	B	621	SQD	C11-C10-C9-C8
24	b	612	CLA	CBD-CGD-O2D-CED
36	c	519	DGD	O6E-C5E-C6E-O5E
24	a	410	CLA	O1D-CGD-O2D-CED
33	b	629	LMG	C37-C38-C39-C40
36	D	408	DGD	C8B-C9B-CAB-CBB
24	B	602	CLA	C8-C10-C11-C12
24	C	504	CLA	C15-C16-C17-C18
27	L	102	SQD	C10-C11-C12-C13
33	A	419	LMG	C13-C14-C15-C16
28	V	202	GOL	O1-C1-C2-O2
28	b	604	GOL	O2-C2-C3-O3
28	c	502	GOL	O1-C1-C2-O2
24	c	515	CLA	O1A-CGA-O2A-C1
24	C	509	CLA	C3-C5-C6-C7
24	c	513	CLA	C3-C5-C6-C7
36	H	102	DGD	C7B-C8B-C9B-CAB
29	m	103	LMT	C1-C2-C3-C4
36	e	101	DGD	C4D-C5D-C6D-O5D
29	a	404	LMT	C7-C8-C9-C10
27	L	102	SQD	C13-C14-C15-C16
29	a	404	LMT	C2-C3-C4-C5
37	L	101	LHG	C13-C14-C15-C16
33	A	419	LMG	C10-C11-C12-C13
24	A	409	CLA	C6-C7-C8-C10
24	B	615	CLA	C12-C13-C15-C16
24	C	501	CLA	C12-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C7
24	D	404	CLA	C12-C13-C15-C16
24	b	623	CLA	C11-C12-C13-C15
24	b	624	CLA	C16-C17-C18-C19
24	C	511	CLA	O1A-CGA-O2A-C1
24	B	610	CLA	C4-C3-C5-C6
31	D	407[A]	PL9	C15-C14-C16-C17
24	B	610	CLA	C2-C3-C5-C6
31	D	407[B]	PL9	C43-C44-C46-C47
31	d	407[B]	PL9	C13-C14-C16-C17
33	C	519	LMG	C31-C32-C33-C34
36	C	516	DGD	C6A-C7A-C8A-C9A
24	B	611	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
24	C	501	CLA	C14-C13-C15-C16
24	b	610	CLA	C11-C10-C8-C9
24	b	612	CLA	C6-C7-C8-C9
24	b	623	CLA	C11-C12-C13-C14
33	k	101	LMG	C36-C37-C38-C39
33	A	419	LMG	O6-C5-C6-O5
37	d	408	LHG	C32-C33-C34-C35
36	C	516	DGD	O6E-C5E-C6E-O5E
35	c	524	HTG	C4-C5-C6-O6
36	C	516	DGD	C2E-C1E-O5D-C6D
27	B	621	SQD	C44-C45-C46-O48
27	F	101	SQD	C44-C45-C46-O48
27	a	405	SQD	O6-C44-C45-C46
27	a	414	SQD	O6-C44-C45-C46
33	Z	101	LMG	C7-C8-C9-O8
36	e	101	DGD	O1G-C1G-C2G-C3G
37	a	420	LHG	C4-C5-C6-O8
29	D	403	LMT	O1'-C1-C2-C3
35	b	632	HTG	O5-C5-C6-O6
27	a	414	SQD	C30-C31-C32-C33
24	C	509	CLA	C5-C6-C7-C8
29	m	103	LMT	C4'-C5'-C6'-O6'
33	A	419	LMG	C39-C40-C41-C42
36	c	520	DGD	C3B-C4B-C5B-C6B
29	D	403	LMT	O5B-C5B-C6B-O6B
24	c	513	CLA	C16-C17-C18-C19
33	A	419	LMG	C36-C37-C38-C39
33	C	520	LMG	C39-C40-C41-C42
36	c	521	DGD	CBA-CCA-CDA-CEA
36	c	521	DGD	C7B-C8B-C9B-CAB
29	A	414	LMT	O5B-C5B-C6B-O6B
27	A	413	SQD	C24-C25-C26-C27
24	b	613	CLA	O1D-CGD-O2D-CED
24	A	409	CLA	C8-C10-C11-C12
24	c	507	CLA	C8-C10-C11-C12
33	Z	101	LMG	O6-C5-C6-O5
25	d	402[B]	PHO	C2C-C3C-CAC-CBC
24	a	409	CLA	C2C-C3C-CAC-CBC
31	D	407[A]	PL9	C13-C14-C16-C17
31	D	407[B]	PL9	C28-C29-C31-C32
31	d	407[B]	PL9	C43-C44-C46-C47
24	b	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
29	M	104	LMT	O5B-C5B-C6B-O6B
33	D	415	LMG	O6-C5-C6-O5
33	d	415	LMG	O6-C5-C6-O5
24	b	617	CLA	C13-C15-C16-C17
24	c	510	CLA	C15-C16-C17-C18
36	c	519	DGD	C4D-C5D-C6D-O5D
24	C	503	CLA	C8-C10-C11-C12
29	e	102	LMT	C9-C10-C11-C12
33	C	520	LMG	C10-C11-C12-C13
36	D	408	DGD	C3B-C4B-C5B-C6B
36	h	102	DGD	C6A-C7A-C8A-C9A
37	D	409	LHG	C34-C35-C36-C37
36	D	408	DGD	C1B-C2B-C3B-C4B
24	D	405	CLA	C3-C5-C6-C7
27	F	101	SQD	C30-C31-C32-C33
24	b	623	CLA	C15-C16-C17-C18
27	a	405	SQD	C25-C26-C27-C28
24	B	615	CLA	CBA-CGA-O2A-C1
31	a	416[A]	PL9	C28-C29-C31-C32
24	c	510	CLA	C16-C17-C18-C19
35	b	602	HTG	C2'-C3'-C4'-C5'
29	m	102	LMT	C9-C10-C11-C12
36	c	520	DGD	C2A-C3A-C4A-C5A
27	f	102	SQD	O6-C44-C45-O47
33	Z	101	LMG	O1-C7-C8-O7
33	a	415	LMG	O7-C8-C9-O8
37	D	411	LHG	O7-C5-C6-O8
37	E	101	LHG	O7-C5-C6-O8
33	b	629	LMG	C40-C41-C42-C43
35	b	607	HTG	C4'-C5'-C6'-C7'
27	F	101	SQD	C7-C8-C9-C10
24	B	602	CLA	C2A-CAA-CBA-CGA
33	A	419	LMG	C12-C13-C14-C15
27	a	414	SQD	C19-C20-C21-C22
36	C	518	DGD	C2A-C1A-O1G-C1G
36	c	521	DGD	C2A-C1A-O1G-C1G
33	a	415	LMG	C12-C13-C14-C15
24	b	623	CLA	C16-C17-C18-C19
24	C	510	CLA	C4-C3-C5-C6
24	b	625	CLA	C4-C3-C5-C6
24	C	512	CLA	CBA-CGA-O2A-C1
24	b	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	C	519	LMG	C29-C28-O8-C9
24	c	516	CLA	C15-C16-C17-C18
27	F	101	SQD	C31-C32-C33-C34
27	A	411	SQD	C12-C13-C14-C15
36	c	520	DGD	C4A-C5A-C6A-C7A
36	c	520	DGD	C7A-C8A-C9A-CAA
28	B	628	GOL	O1-C1-C2-O2
37	D	409	LHG	O1-C1-C2-O2
37	b	634	LHG	O1-C1-C2-O2
24	A	409	CLA	C6-C7-C8-C9
24	B	616	CLA	C14-C13-C15-C16
24	C	512	CLA	C11-C10-C8-C9
24	a	410	CLA	C11-C10-C8-C9
24	b	612	CLA	C11-C10-C8-C9
24	c	513	CLA	C6-C7-C8-C9
24	A	409	CLA	C15-C16-C17-C18
37	L	101	LHG	C35-C36-C37-C38
24	B	608	CLA	C4B-C3B-CAB-CBB
24	B	617	CLA	C4B-C3B-CAB-CBB
24	C	506	CLA	C4B-C3B-CAB-CBB
24	D	405	CLA	C4B-C3B-CAB-CBB
24	b	625	CLA	C4B-C3B-CAB-CBB
24	c	505	CLA	C4B-C3B-CAB-CBB
24	c	506	CLA	C4B-C3B-CAB-CBB
24	c	508	CLA	C4B-C3B-CAB-CBB
24	d	404	CLA	C4B-C3B-CAB-CBB
24	A	405	CLA	C13-C15-C16-C17
36	C	517	DGD	C4A-C5A-C6A-C7A
29	M	102	LMT	C4'-C5'-C6'-O6'
36	c	521	DGD	C6B-C7B-C8B-C9B
37	D	411	LHG	C29-C30-C31-C32
36	h	102	DGD	CDA-CEA-CFA-CGA
24	a	410	CLA	C11-C10-C8-C7
24	b	610	CLA	C6-C7-C8-C10
24	b	612	CLA	C11-C10-C8-C7
24	c	510	CLA	C6-C7-C8-C10
24	c	513	CLA	C6-C7-C8-C10
24	B	615	CLA	O1A-CGA-O2A-C1
35	B	623	HTG	O5-C5-C6-O6
24	c	513	CLA	C16-C17-C18-C20
24	B	608	CLA	C3A-C2A-CAA-CBA
24	B	610	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C4-C3-C5-C6
24	C	513	CLA	C3A-C2A-CAA-CBA
24	a	412	CLA	C3A-C2A-CAA-CBA
24	c	514	CLA	C4-C3-C5-C6
31	D	407[B]	PL9	C15-C14-C16-C17
31	a	416[A]	PL9	C45-C44-C46-C47
36	h	102	DGD	O2G-C1B-C2B-C3B
24	B	616	CLA	C2-C3-C5-C6
36	h	102	DGD	C5B-C6B-C7B-C8B
26	h	101	BCR	C9-C10-C11-C12
24	b	614	CLA	C8-C10-C11-C12
29	t	101	LMT	C2-C3-C4-C5
33	k	101	LMG	C21-C22-C23-C24
24	c	514	CLA	C8-C10-C11-C12
27	L	102	SQD	C44-C45-C46-O48
33	a	415	LMG	C7-C8-C9-O8
33	k	101	LMG	C7-C8-C9-O8
36	D	408	DGD	O1G-C1G-C2G-C3G
37	D	411	LHG	C4-C5-C6-O8
37	E	101	LHG	C4-C5-C6-O8
29	m	102	LMT	C11-C10-C9-C8
24	b	623	CLA	C16-C17-C18-C20
24	C	501	CLA	C13-C15-C16-C17
24	C	507	CLA	C15-C16-C17-C18
27	A	413	SQD	C30-C31-C32-C33
27	B	621	SQD	C17-C18-C19-C20
33	A	419	LMG	C29-C30-C31-C32
33	a	415	LMG	C33-C34-C35-C36
37	d	410	LHG	C33-C34-C35-C36
33	b	629	LMG	C33-C34-C35-C36
31	d	407[B]	PL9	C15-C14-C16-C17
24	C	510	CLA	C2-C3-C5-C6
24	c	505	CLA	O1D-CGD-O2D-CED
29	E	102	LMT	C2-C3-C4-C5
33	k	101	LMG	C39-C40-C41-C42
35	B	631	HTG	C4'-C5'-C6'-C7'
24	C	512	CLA	C2B-C3B-CAB-CBB
26	C	515	BCR	C1-C6-C7-C8
26	D	406	BCR	C23-C24-C25-C30
29	b	630	LMT	C6-C7-C8-C9
33	M	101	LMG	C31-C32-C33-C34
36	e	101	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
24	C	504	CLA	C13-C15-C16-C17
35	B	624	HTG	C3'-C4'-C5'-C6'
36	c	521	DGD	C2A-C3A-C4A-C5A
27	f	102	SQD	C31-C32-C33-C34
36	c	519	DGD	C3A-C4A-C5A-C6A
24	A	405	CLA	C15-C16-C17-C18
24	B	607	CLA	C10-C11-C12-C13
27	B	621	SQD	O47-C45-C46-O48
27	F	101	SQD	O47-C45-C46-O48
27	L	102	SQD	O47-C45-C46-O48
27	a	414	SQD	O6-C44-C45-O47
36	D	408	DGD	O2G-C2G-C3G-O3G
31	A	417[A]	PL9	C4-C3-C7-C8
31	A	417[B]	PL9	C4-C3-C7-C8
31	a	416[A]	PL9	C4-C3-C7-C8
31	a	416[B]	PL9	C4-C3-C7-C8
35	V	206	HTG	O5-C1-S1-C1'
27	a	405	SQD	C29-C30-C31-C32
33	a	415	LMG	C35-C36-C37-C38
37	L	101	LHG	C26-C27-C28-C29
31	d	407[A]	PL9	C45-C44-C46-C47
24	D	405	CLA	C8-C10-C11-C12
24	c	514	CLA	C2-C3-C5-C6
31	A	417[A]	PL9	C2-C3-C7-C8
36	c	520	DGD	C6A-C7A-C8A-C9A
37	D	411	LHG	C12-C13-C14-C15
24	A	407	CLA	C11-C10-C8-C9
24	B	615	CLA	C14-C13-C15-C16
24	b	610	CLA	C6-C7-C8-C9
36	C	518	DGD	C9A-CAA-CBA-CCA
24	B	614	CLA	C10-C11-C12-C13
29	M	102	LMT	O5'-C1'-O1'-C1
36	C	516	DGD	O6E-C1E-O5D-C6D
33	z	101	LMG	C15-C16-C17-C18
27	a	405	SQD	C28-C29-C30-C31
31	D	407[B]	PL9	C9-C11-C12-C13
29	m	102	LMT	C5-C6-C7-C8
28	C	524	GOL	O1-C1-C2-O2
28	V	204	GOL	O1-C1-C2-O2
28	v	203	GOL	O1-C1-C2-O2
24	A	406	CLA	C3-C5-C6-C7
31	A	417[A]	PL9	C15-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
36	c	519	DGD	CCA-CDA-CEA-CFA
26	T	103	BCR	C13-C14-C15-C16
26	t	102	BCR	C13-C14-C15-C16
24	b	625	CLA	C2-C3-C5-C6
31	d	407[A]	PL9	C43-C44-C46-C47
24	b	620	CLA	C16-C17-C18-C20
24	b	625	CLA	C16-C17-C18-C19
37	E	101	LHG	C8-C7-O7-C5
24	b	610	CLA	O1A-CGA-O2A-C1
36	c	521	DGD	C5B-C6B-C7B-C8B
27	A	413	SQD	C7-C8-C9-C10
27	f	102	SQD	C25-C26-C27-C28
33	b	629	LMG	C17-C18-C19-C20
24	C	510	CLA	CBA-CGA-O2A-C1
24	b	623	CLA	O1D-CGD-O2D-CED
24	c	510	CLA	C16-C17-C18-C20
27	A	411	SQD	C18-C19-C20-C21
26	K	101	BCR	C36-C18-C19-C20
26	b	626	BCR	C36-C18-C19-C20
24	A	407	CLA	C11-C10-C8-C7
24	B	616	CLA	C12-C13-C15-C16
24	B	617	CLA	C6-C7-C8-C10
24	C	501	CLA	C11-C12-C13-C15
24	C	505	CLA	C11-C12-C13-C15
24	c	510	CLA	C11-C10-C8-C7
24	d	404	CLA	C11-C12-C13-C15
29	a	404	LMT	C3-C4-C5-C6
33	C	520	LMG	C29-C30-C31-C32
24	c	513	CLA	C10-C11-C12-C13
27	B	621	SQD	C19-C20-C21-C22
37	d	410	LHG	C35-C36-C37-C38
26	C	515	BCR	C21-C22-C23-C24
26	K	101	BCR	C17-C18-C19-C20
33	k	101	LMG	C20-C21-C22-C23
33	C	519	LMG	O10-C28-O8-C9
27	F	101	SQD	C5-C6-S-O8
37	E	101	LHG	C25-C26-C27-C28
27	A	413	SQD	C11-C12-C13-C14
33	a	415	LMG	C29-C30-C31-C32
27	A	411	SQD	C8-C7-O47-C45
36	C	517	DGD	C8A-C9A-CAA-CBA
24	C	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	a	411	PHO	C2-C3-C5-C6
31	a	416[A]	PL9	C43-C44-C46-C47
38	f	101	HEM	C2B-C3B-CAB-CBB
38	f	101	HEM	C2C-C3C-CAC-CBC
37	d	408	LHG	C33-C34-C35-C36
28	v	201	GOL	O1-C1-C2-C3
28	v	203	GOL	O1-C1-C2-C3
37	d	410	LHG	C11-C10-C9-C8
27	L	102	SQD	C46-C45-O47-C7
36	C	518	DGD	O1A-C1A-O1G-C1G
33	b	629	LMG	C39-C40-C41-C42
27	L	102	SQD	C33-C34-C35-C36
36	C	517	DGD	C3B-C4B-C5B-C6B
24	B	602	CLA	C16-C17-C18-C20
24	b	619	CLA	C16-C17-C18-C20
35	B	623	HTG	C4'-C5'-C6'-C7'
36	C	518	DGD	CDA-CEA-CFA-CGA
33	A	419	LMG	C11-C12-C13-C14
36	c	521	DGD	O1A-C1A-O1G-C1G
33	b	629	LMG	C35-C36-C37-C38
37	L	101	LHG	C17-C18-C19-C20
24	b	615	CLA	C8-C10-C11-C12
24	d	405	CLA	C15-C16-C17-C18
29	D	403	LMT	O5'-C1'-O1'-C1
33	A	419	LMG	O6-C1-O1-C7
27	A	413	SQD	O6-C44-C45-C46
31	a	416[A]	PL9	C39-C41-C42-C43
33	z	101	LMG	O1-C7-C8-C9
37	E	101	LHG	C19-C20-C21-C22
24	C	509	CLA	C10-C11-C12-C13
24	b	625	CLA	C10-C11-C12-C13
37	D	411	LHG	C28-C29-C30-C31
24	C	510	CLA	O1A-CGA-O2A-C1
25	a	411	PHO	C4-C3-C5-C6
31	D	407[A]	PL9	C45-C44-C46-C47
31	D	407[B]	PL9	C13-C14-C16-C17
33	A	419	LMG	O1-C7-C8-O7
33	Z	101	LMG	O7-C8-C9-O8
24	C	505	CLA	C11-C12-C13-C14
24	b	618	CLA	C6-C7-C8-C9
24	c	510	CLA	C11-C10-C8-C9
24	b	619	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
33	A	419	LMG	C32-C33-C34-C35
27	f	102	SQD	C26-C27-C28-C29
36	H	102	DGD	C5A-C6A-C7A-C8A
24	c	514	CLA	O1A-CGA-O2A-C1
33	M	101	LMG	C16-C17-C18-C19
36	C	517	DGD	C8B-C9B-CAB-CBB
33	a	415	LMG	C31-C32-C33-C34
37	d	408	LHG	C29-C30-C31-C32
27	a	414	SQD	C33-C34-C35-C36
29	a	419	LMT	C6-C7-C8-C9
36	h	102	DGD	CCA-CDA-CEA-CFA
29	D	403	LMT	C2'-C1'-O1'-C1
24	B	604	CLA	C5-C6-C7-C8
29	m	103	LMT	O1'-C1-C2-C3
33	D	415	LMG	C13-C14-C15-C16
31	A	417[A]	PL9	C13-C14-C16-C17
37	D	410	LHG	C13-C14-C15-C16
27	a	405	SQD	C31-C32-C33-C34
37	D	409	LHG	C25-C26-C27-C28
29	M	104	LMT	C2B-C1B-O1B-C4'
24	B	614	CLA	C15-C16-C17-C18
24	a	409	CLA	O1D-CGD-O2D-CED
35	V	206	HTG	C4-C5-C6-O6
33	C	520	LMG	C13-C14-C15-C16
37	E	101	LHG	O9-C7-O7-C5
29	M	104	LMT	C2-C1-O1'-C1'
31	D	407[A]	PL9	C9-C11-C12-C13
27	A	411	SQD	C14-C15-C16-C17
24	C	501	CLA	C1A-C2A-CAA-CBA
24	C	506	CLA	C1A-C2A-CAA-CBA
24	C	512	CLA	C4B-C3B-CAB-CBB
24	c	510	CLA	C1A-C2A-CAA-CBA
24	c	512	CLA	C1A-C2A-CAA-CBA
24	c	515	CLA	C1A-C2A-CAA-CBA
31	A	417[B]	PL9	C15-C14-C16-C17
29	M	102	LMT	C11-C10-C9-C8
26	H	101	BCR	C7-C8-C9-C10
27	B	621	SQD	C14-C15-C16-C17
36	e	101	DGD	C3A-C4A-C5A-C6A
27	a	405	SQD	C24-C25-C26-C27
24	C	509	CLA	C8-C10-C11-C12
27	a	414	SQD	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
36	D	408	DGD	C4B-C5B-C6B-C7B
27	B	621	SQD	C5-C6-S-O7
27	a	414	SQD	C17-C18-C19-C20
24	C	505	CLA	C12-C13-C15-C16
24	C	506	CLA	C12-C13-C15-C16
24	b	625	CLA	C12-C13-C15-C16
33	Z	101	LMG	C13-C14-C15-C16
24	c	514	CLA	CBA-CGA-O2A-C1
36	D	408	DGD	C2B-C3B-C4B-C5B
33	D	415	LMG	C34-C35-C36-C37
40	v	206	HEC	C4C-C3C-CAC-CBC
27	a	414	SQD	C35-C36-C37-C38
27	A	411	SQD	O49-C7-O47-C45
38	f	101	HEM	C3D-CAD-CBD-CGD
24	a	409	CLA	C4C-C3C-CAC-CBC
24	B	610	CLA	C6-C7-C8-C9
24	B	616	CLA	C11-C12-C13-C14
37	D	411	LHG	C10-C11-C12-C13
36	e	101	DGD	CAB-CBB-CCB-CDB
37	d	410	LHG	C24-C25-C26-C27
24	b	614	CLA	O1A-CGA-O2A-C1
33	k	101	LMG	O1-C7-C8-O7
33	k	101	LMG	O7-C8-C9-O8
36	e	101	DGD	O1G-C1G-C2G-O2G
37	a	420	LHG	O7-C5-C6-O8
37	D	409	LHG	C33-C34-C35-C36
36	C	517	DGD	CCA-CDA-CEA-CFA
33	A	419	LMG	O1-C7-C8-C9
33	Z	101	LMG	O1-C7-C8-C9
36	D	408	DGD	C1G-C2G-C3G-O3G
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	606	CLA	CAD-CBD-CGD-O2D
24	B	608	CLA	CAD-CBD-CGD-O2D
24	B	610	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	b	614	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
24	c	508	CLA	CAD-CBD-CGD-O2D
24	c	510	CLA	CAD-CBD-CGD-O2D
36	h	102	DGD	C9B-CAB-CBB-CCB
29	m	103	LMT	C3-C4-C5-C6
27	L	102	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
33	D	415	LMG	C30-C31-C32-C33
33	D	415	LMG	C20-C21-C22-C23
33	M	101	LMG	C33-C34-C35-C36
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	608	CLA	CAD-CBD-CGD-O1D
24	B	610	CLA	CAD-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	b	610	CLA	CAD-CBD-CGD-O1D
24	b	614	CLA	CAD-CBD-CGD-O1D
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	508	CLA	CAD-CBD-CGD-O1D
24	c	510	CLA	CAD-CBD-CGD-O1D
24	c	513	CLA	CHA-CBD-CGD-O1D
24	c	513	CLA	CHA-CBD-CGD-O2D
37	D	409	LHG	C4-O6-P-O3
37	D	410	LHG	C4-O6-P-O5
37	E	101	LHG	C3-O3-P-O5
37	L	101	LHG	C4-O6-P-O5
37	b	634	LHG	C4-O6-P-O5
37	d	408	LHG	C4-O6-P-O4
40	v	206	HEC	C2C-C3C-CAC-CBC
24	B	615	CLA	C2B-C3B-CAB-CBB
24	C	504	CLA	C2B-C3B-CAB-CBB
24	d	405	CLA	C2B-C3B-CAB-CBB
26	H	101	BCR	C5-C6-C7-C8
27	a	414	SQD	C27-C28-C29-C30
36	e	101	DGD	CAA-CBA-CCA-CDA
25	A	408	PHO	C2-C3-C5-C6
37	L	101	LHG	C23-C24-C25-C26
35	c	524	HTG	O5-C5-C6-O6
26	H	101	BCR	C7-C8-C9-C34
26	c	518	BCR	C7-C8-C9-C34
37	D	411	LHG	C2-C3-O3-P
37	d	410	LHG	C2-C3-O3-P
29	T	104	LMT	C7-C8-C9-C10
24	B	602	CLA	CAA-CBA-CGA-O2A
27	a	405	SQD	C27-C28-C29-C30
37	a	420	LHG	C23-C24-C25-C26
33	a	415	LMG	C21-C22-C23-C24
37	d	408	LHG	C11-C10-C9-C8
36	c	520	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
24	B	613	CLA	C8-C10-C11-C12
24	C	503	CLA	C5-C6-C7-C8
33	D	415	LMG	C16-C17-C18-C19
27	B	621	SQD	C46-C45-O47-C7
33	M	101	LMG	C9-C8-O7-C10
25	A	408	PHO	C4-C3-C5-C6
37	d	408	LHG	C26-C27-C28-C29
31	a	416[A]	PL9	C14-C16-C17-C18
24	c	508	CLA	C15-C16-C17-C18
31	A	417[B]	PL9	C43-C44-C46-C47
31	d	407[B]	PL9	C18-C19-C21-C22
37	d	410	LHG	C30-C31-C32-C33
29	e	102	LMT	C2B-C1B-O1B-C4'
24	b	611	CLA	C16-C17-C18-C19
37	L	101	LHG	O6-C4-C5-C6
37	b	634	LHG	O6-C4-C5-C6
24	C	508	CLA	C3-C5-C6-C7
24	B	615	CLA	C6-C7-C8-C9
24	a	410	CLA	C14-C13-C15-C16
24	b	625	CLA	C14-C13-C15-C16
24	d	404	CLA	C11-C12-C13-C14
24	B	602	CLA	C16-C17-C18-C19
27	B	621	SQD	C31-C32-C33-C34
36	c	520	DGD	C5B-C6B-C7B-C8B
27	A	413	SQD	C24-C23-O48-C46
33	a	415	LMG	C30-C31-C32-C33
33	A	419	LMG	C2-C1-O1-C7
31	a	416[B]	PL9	C12-C11-C9-C8
24	B	613	CLA	CBD-CGD-O2D-CED
33	d	415	LMG	C29-C30-C31-C32
27	A	413	SQD	O10-C23-O48-C46
33	c	522	LMG	O9-C10-O7-C8
33	c	522	LMG	O7-C8-C9-O8
33	z	101	LMG	O1-C7-C8-O7
27	A	413	SQD	C15-C16-C17-C18
27	f	102	SQD	C30-C31-C32-C33
33	c	522	LMG	C11-C10-O7-C8
24	C	510	CLA	C8-C10-C11-C12
24	A	405	CLA	CBD-CGD-O2D-CED
36	e	101	DGD	C4A-C5A-C6A-C7A
24	d	403	CLA	C2C-C3C-CAC-CBC
24	b	610	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
36	C	517	DGD	C5A-C6A-C7A-C8A
27	f	102	SQD	O6-C44-C45-C46
33	k	101	LMG	O1-C7-C8-C9
24	b	614	CLA	CBA-CGA-O2A-C1
24	c	507	CLA	C5-C6-C7-C8
36	c	519	DGD	C5D-C6D-O5D-C1E
36	c	520	DGD	C2G-C3G-O3G-C1D
36	c	520	DGD	C5D-C6D-O5D-C1E
24	b	622	CLA	O1D-CGD-O2D-CED
24	c	510	CLA	C13-C15-C16-C17
24	B	603	CLA	C2A-CAA-CBA-CGA
24	b	625	CLA	C16-C17-C18-C20
36	H	102	DGD	C6B-C7B-C8B-C9B
31	A	417[A]	PL9	C45-C44-C46-C47
31	A	417[B]	PL9	C45-C44-C46-C47
29	m	102	LMT	C1-C2-C3-C4
35	B	622	HTG	C4'-C5'-C6'-C7'
24	C	505	CLA	C14-C13-C15-C16
24	a	410	CLA	C6-C7-C8-C9
37	a	420	LHG	C14-C15-C16-C17
24	a	412	CLA	C4B-C3B-CAB-CBB
27	A	413	SQD	C26-C27-C28-C29
36	C	517	DGD	C3A-C4A-C5A-C6A
24	C	502	CLA	C16-C17-C18-C20
24	B	606	CLA	C10-C11-C12-C13
24	a	412	CLA	C4-C3-C5-C6
24	c	517	CLA	C4-C3-C5-C6
31	D	407[B]	PL9	C35-C34-C36-C37
29	C	521	LMT	C5'-C4'-O1B-C1B
27	B	621	SQD	C15-C16-C17-C18
29	e	102	LMT	C5-C6-C7-C8
31	A	417[A]	PL9	C43-C44-C46-C47
36	C	518	DGD	C8A-C9A-CAA-CBA
31	A	417[B]	PL9	C19-C21-C22-C23
31	a	416[B]	PL9	C14-C16-C17-C18
38	f	101	HEM	C4B-C3B-CAB-CBB
38	f	101	HEM	C4C-C3C-CAC-CBC
33	C	519	LMG	C29-C30-C31-C32
29	D	403	LMT	C5-C6-C7-C8
24	a	410	CLA	C6-C7-C8-C10
37	d	409	LHG	O2-C2-C3-O3
33	C	519	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
27	B	621	SQD	C9-C10-C11-C12
35	d	413	HTG	C1'-C2'-C3'-C4'
25	a	411	PHO	C2C-C3C-CAC-CBC
27	L	102	SQD	O6-C44-C45-O47
37	d	410	LHG	O7-C5-C6-O8
36	e	101	DGD	CCA-CDA-CEA-CFA
24	c	511	CLA	C2A-CAA-CBA-CGA
36	c	520	DGD	C3A-C4A-C5A-C6A
29	m	102	LMT	O5'-C1'-O1'-C1
29	m	103	LMT	O5'-C1'-O1'-C1
36	c	519	DGD	O6E-C1E-O5D-C6D
36	C	518	DGD	C3B-C4B-C5B-C6B
24	C	510	CLA	C2-C1-O2A-CGA
40	V	205	HEC	CAD-CBD-CGD-O2D
33	z	101	LMG	C16-C17-C18-C19
40	V	205	HEC	CAD-CBD-CGD-O1D
31	a	416[B]	PL9	C45-C44-C46-C47
38	f	101	HEM	C2A-CAA-CBA-CGA
24	a	412	CLA	C2-C3-C5-C6
24	c	517	CLA	C2-C3-C5-C6
31	A	417[B]	PL9	C13-C14-C16-C17
33	b	629	LMG	C16-C17-C18-C19
33	d	415	LMG	C36-C37-C38-C39
31	A	417[A]	PL9	C19-C21-C22-C23
24	B	602	CLA	C14-C13-C15-C16
24	B	604	CLA	C6-C7-C8-C9
24	C	504	CLA	C11-C12-C13-C14
24	C	506	CLA	C14-C13-C15-C16
24	b	619	CLA	C11-C12-C13-C14
24	c	513	CLA	C14-C13-C15-C16
27	F	101	SQD	C32-C33-C34-C35
36	C	516	DGD	C7B-C8B-C9B-CAB
28	V	204	GOL	O1-C1-C2-C3
35	B	623	HTG	C1'-C2'-C3'-C4'
24	C	501	CLA	C16-C17-C18-C19
27	a	414	SQD	C16-C17-C18-C19
33	C	520	LMG	C15-C16-C17-C18
33	M	101	LMG	C7-C8-O7-C10
24	A	406	CLA	C4C-C3C-CAC-CBC
33	M	101	LMG	C20-C21-C22-C23
24	c	506	CLA	C16-C17-C18-C19
36	H	102	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
33	C	520	LMG	C37-C38-C39-C40
28	C	525	GOL	O1-C1-C2-O2
28	O	301	GOL	O2-C2-C3-O3
29	M	102	LMT	C2'-C1'-O1'-C1
29	T	104	LMT	C4'-C5'-C6'-O6'
24	c	505	CLA	C2A-CAA-CBA-CGA
36	D	408	DGD	C4A-C5A-C6A-C7A
37	D	409	LHG	C28-C29-C30-C31
29	C	521	LMT	C4B-C5B-C6B-O6B
37	b	634	LHG	O6-C4-C5-O7
33	D	415	LMG	C14-C15-C16-C17
29	m	102	LMT	O1'-C1-C2-C3
24	A	409	CLA	C2B-C3B-CAB-CBB
24	B	608	CLA	C2B-C3B-CAB-CBB
24	D	405	CLA	C2B-C3B-CAB-CBB
24	a	412	CLA	C2B-C3B-CAB-CBB
24	b	611	CLA	C2B-C3B-CAB-CBB
24	c	505	CLA	C2B-C3B-CAB-CBB
24	c	506	CLA	C2B-C3B-CAB-CBB
24	c	508	CLA	C2B-C3B-CAB-CBB
24	d	404	CLA	C2B-C3B-CAB-CBB
26	C	515	BCR	C5-C6-C7-C8
26	D	406	BCR	C23-C24-C25-C26
26	c	518	BCR	C1-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C30
36	c	519	DGD	C2A-C3A-C4A-C5A
24	c	511	CLA	C5-C6-C7-C8
24	b	610	CLA	C4-C3-C5-C6
31	D	407[A]	PL9	C43-C44-C46-C47
31	a	416[B]	PL9	C43-C44-C46-C47
27	A	411	SQD	C16-C17-C18-C19
35	b	607	HTG	C3'-C4'-C5'-C6'
37	D	409	LHG	C27-C28-C29-C30
37	d	410	LHG	C9-C10-C11-C12
29	D	403	LMT	C4-C5-C6-C7
24	B	602	CLA	C11-C10-C8-C7
24	B	614	CLA	C12-C13-C15-C16
24	C	504	CLA	C12-C13-C15-C16
29	D	403	LMT	C2-C3-C4-C5
27	F	101	SQD	O6-C44-C45-O47
38	E	103	HEM	CAD-CBD-CGD-O1D
37	E	101	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
29	T	104	LMT	O5'-C5'-C6'-O6'
27	B	621	SQD	C35-C36-C37-C38
24	C	513	CLA	C4-C3-C5-C6
31	A	417[A]	PL9	C20-C19-C21-C22
31	A	417[A]	PL9	C40-C39-C41-C42
31	A	417[B]	PL9	C30-C29-C31-C32
24	B	612	CLA	C10-C11-C12-C13
24	C	508	CLA	C5-C6-C7-C8
33	c	522	LMG	C31-C32-C33-C34
27	A	413	SQD	C25-C26-C27-C28
24	C	506	CLA	C6-C7-C8-C9
24	b	625	CLA	C11-C12-C13-C14
29	M	102	LMT	C7-C8-C9-C10
36	C	517	DGD	C7B-C8B-C9B-CAB
37	d	408	LHG	C34-C35-C36-C37
24	a	409	CLA	C13-C15-C16-C17
31	A	417[A]	PL9	C30-C29-C31-C32
31	d	407[B]	PL9	C35-C34-C36-C37
36	C	516	DGD	O2G-C1B-C2B-C3B
24	B	606	CLA	O1A-CGA-O2A-C1
24	b	619	CLA	C2A-CAA-CBA-CGA
24	b	623	CLA	C2A-CAA-CBA-CGA
35	C	522	HTG	C1'-C2'-C3'-C4'
38	E	103	HEM	CAD-CBD-CGD-O2D
33	a	415	LMG	C19-C20-C21-C22
28	D	402	GOL	O1-C1-C2-O2
31	D	407[A]	PL9	C35-C34-C36-C37
27	B	621	SQD	C32-C33-C34-C35
37	E	101	LHG	C10-C11-C12-C13
40	v	206	HEC	CAD-CBD-CGD-O2D
33	a	415	LMG	O8-C28-C29-C30
24	C	508	CLA	C13-C15-C16-C17
29	a	404	LMT	C6-C7-C8-C9
24	B	604	CLA	C4B-C3B-CAB-CBB
24	b	611	CLA	C4B-C3B-CAB-CBB
24	b	615	CLA	C4B-C3B-CAB-CBB
24	c	511	CLA	C4B-C3B-CAB-CBB
33	M	101	LMG	C36-C37-C38-C39
35	C	523	HTG	C4-C5-C6-O6
29	a	404	LMT	C9-C10-C11-C12
24	C	507	CLA	C2A-CAA-CBA-CGA
29	M	104	LMT	O5B-C1B-O1B-C4'

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Mol	Chain	Res	Type	Atoms
29	e	102	LMT	O5B-C1B-O1B-C4'
36	C	516	DGD	C5B-C6B-C7B-C8B
24	A	405	CLA	C16-C17-C18-C19
36	D	408	DGD	O1G-C1G-C2G-O2G
37	d	409	LHG	O7-C5-C6-O8
33	a	415	LMG	C22-C23-C24-C25
24	A	407	CLA	C10-C11-C12-C13
37	d	410	LHG	C31-C32-C33-C34
24	b	615	CLA	C11-C10-C8-C7
29	t	101	LMT	C4-C5-C6-C7
37	E	101	LHG	C16-C17-C18-C19
24	C	501	CLA	C16-C17-C18-C20
40	v	206	HEC	CAD-CBD-CGD-O1D
26	c	518	BCR	C7-C8-C9-C10
24	C	510	CLA	C6-C7-C8-C9
24	b	615	CLA	C11-C10-C8-C9
24	b	624	CLA	C13-C15-C16-C17
29	e	102	LMT	C1-C2-C3-C4
36	H	102	DGD	C8A-C9A-CAA-CBA
27	B	621	SQD	C5-C6-S-O8
33	z	101	LMG	C8-C7-O1-C1
36	C	516	DGD	C5D-C6D-O5D-C1E
36	D	408	DGD	C2G-C3G-O3G-C1D
29	M	102	LMT	C5-C6-C7-C8
24	b	611	CLA	C16-C17-C18-C20
36	C	518	DGD	CBA-CCA-CDA-CEA
24	A	407	CLA	C3A-C2A-CAA-CBA
24	b	618	CLA	C3A-C2A-CAA-CBA
31	A	417[A]	PL9	C28-C29-C31-C32
36	c	520	DGD	C8A-C9A-CAA-CBA
24	C	513	CLA	C3-C5-C6-C7
25	d	402[B]	PHO	C8-C10-C11-C12
36	h	102	DGD	O1B-C1B-C2B-C3B
27	a	405	SQD	C24-C23-O48-C46
27	A	411	SQD	C7-C8-C9-C10
37	d	409	LHG	C35-C36-C37-C38
24	C	506	CLA	C3-C5-C6-C7
31	D	407[B]	PL9	C30-C29-C31-C32
36	h	102	DGD	C9A-CAA-CBA-CCA
24	b	622	CLA	CBD-CGD-O2D-CED
27	A	413	SQD	O5-C1-O6-C44
33	a	415	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
36	C	516	DGD	C1G-C2G-C3G-O3G
27	a	405	SQD	O10-C23-O48-C46
28	o	301	GOL	O1-C1-C2-O2
37	a	420	LHG	O1-C1-C2-O2
33	c	522	LMG	C37-C38-C39-C40
24	C	509	CLA	C15-C16-C17-C18
33	c	522	LMG	C34-C35-C36-C37
36	D	408	DGD	C9B-CAB-CBB-CCB
29	A	414	LMT	C11-C10-C9-C8
24	B	607	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
33	d	415	LMG	C17-C18-C19-C20
24	d	403	CLA	C13-C15-C16-C17
27	A	411	SQD	C11-C10-C9-C8
24	C	512	CLA	CAA-CBA-CGA-O2A
37	a	420	LHG	C13-C14-C15-C16
35	b	602	HTG	C1'-C2'-C3'-C4'
24	b	615	CLA	C14-C13-C15-C16
24	C	506	CLA	C16-C17-C18-C20
36	c	520	DGD	O2G-C1B-C2B-C3B
24	C	513	CLA	O1A-CGA-O2A-C1
24	C	510	CLA	CAA-CBA-CGA-O2A
24	A	409	CLA	C12-C13-C15-C16
24	B	604	CLA	C6-C7-C8-C10
24	C	506	CLA	C6-C7-C8-C10
24	b	620	CLA	C11-C12-C13-C15
24	b	625	CLA	C11-C12-C13-C15
24	c	513	CLA	C11-C10-C8-C7
24	c	513	CLA	C12-C13-C15-C16
24	c	514	CLA	C12-C13-C15-C16
36	C	517	DGD	C6B-C7B-C8B-C9B
37	b	634	LHG	C23-C24-C25-C26
24	B	604	CLA	C2B-C3B-CAB-CBB
24	B	617	CLA	C2B-C3B-CAB-CBB
24	C	506	CLA	C2B-C3B-CAB-CBB
24	b	625	CLA	C2B-C3B-CAB-CBB
26	c	518	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	t	102	BCR	C1-C6-C7-C8
26	t	102	BCR	C5-C6-C7-C8
33	A	419	LMG	O8-C28-C29-C30
37	D	411	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
24	b	622	CLA	C2-C1-O2A-CGA
33	a	415	LMG	C18-C19-C20-C21
36	c	519	DGD	C2E-C1E-O5D-C6D
31	A	417[A]	PL9	C9-C11-C12-C13
37	d	409	LHG	C11-C10-C9-C8
36	c	520	DGD	C4B-C5B-C6B-C7B
31	d	407[A]	PL9	C30-C29-C31-C32
27	f	102	SQD	O47-C7-C8-C9
37	a	420	LHG	O8-C23-C24-C25
31	d	407[A]	PL9	C28-C29-C31-C32
35	b	632	HTG	C2'-C1'-S1-C1
35	c	523	HTG	C2'-C1'-S1-C1
24	B	608	CLA	C2A-CAA-CBA-CGA
36	D	408	DGD	CBA-CCA-CDA-CEA
24	C	502	CLA	C3-C5-C6-C7
27	L	102	SQD	C27-C28-C29-C30
24	C	513	CLA	CBA-CGA-O2A-C1
26	H	101	BCR	C9-C10-C11-C12
29	E	102	LMT	C1-C2-C3-C4
37	E	101	LHG	O8-C23-C24-C25
29	a	419	LMT	C7-C8-C9-C10
24	D	404	CLA	C14-C13-C15-C16
24	b	625	CLA	C6-C7-C8-C9
27	f	102	SQD	C35-C36-C37-C38
27	L	102	SQD	O6-C44-C45-C46
24	B	610	CLA	C1A-C2A-CAA-CBA
24	C	503	CLA	C4B-C3B-CAB-CBB
24	c	517	CLA	C1A-C2A-CAA-CBA
24	B	614	CLA	CAA-CBA-CGA-O2A
33	Z	101	LMG	O7-C10-C11-C12
36	e	101	DGD	O2G-C1B-C2B-C3B
26	b	626	BCR	C17-C18-C19-C20
26	k	102	BCR	C17-C18-C19-C20
26	t	102	BCR	C11-C12-C13-C14
33	k	101	LMG	C35-C36-C37-C38
36	C	517	DGD	O2G-C1B-C2B-C3B
37	L	101	LHG	O7-C7-C8-C9
24	B	615	CLA	C2A-CAA-CBA-CGA
36	h	102	DGD	C7B-C8B-C9B-CAB
24	B	602	CLA	O1D-CGD-O2D-CED
37	d	409	LHG	C26-C27-C28-C29
24	a	409	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
24	b	614	CLA	C16-C17-C18-C19
24	c	516	CLA	CAA-CBA-CGA-O2A
36	c	521	DGD	O1G-C1A-C2A-C3A
24	B	613	CLA	O1D-CGD-O2D-CED
24	d	403	CLA	C15-C16-C17-C18
27	B	621	SQD	C5-C6-S-O9
24	C	513	CLA	C8-C10-C11-C12
24	b	612	CLA	C4-C3-C5-C6
24	B	614	CLA	C2-C1-O2A-CGA
24	b	623	CLA	C2-C1-O2A-CGA
24	c	516	CLA	C2-C1-O2A-CGA
24	c	517	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
24	b	622	CLA	CAA-CBA-CGA-O2A
36	D	408	DGD	O1G-C1A-C2A-C3A
24	B	604	CLA	C11-C10-C8-C7
24	C	509	CLA	C11-C12-C13-C15
24	b	623	CLA	C12-C13-C15-C16
24	b	624	CLA	C11-C12-C13-C15
24	c	508	CLA	C12-C13-C15-C16
24	d	403	CLA	C11-C10-C8-C7
24	C	513	CLA	C2-C3-C5-C6
24	d	403	CLA	C16-C17-C18-C20
29	C	521	LMT	C3-C4-C5-C6
27	A	413	SQD	C13-C14-C15-C16
36	H	102	DGD	CCA-CDA-CEA-CFA
38	f	101	HEM	CAD-CBD-CGD-O1D
37	D	409	LHG	C17-C18-C19-C20
24	b	622	CLA	C13-C15-C16-C17
37	b	634	LHG	C31-C32-C33-C34
33	M	101	LMG	C15-C16-C17-C18
38	f	101	HEM	CAA-CBA-CGA-O1A
31	a	416[B]	PL9	C26-C27-C28-C29
24	b	624	CLA	C5-C6-C7-C8
35	B	622	HTG	S1-C1'-C2'-C3'
24	b	620	CLA	O1A-CGA-O2A-C1
36	c	520	DGD	O1B-C1B-C2B-C3B
33	b	629	LMG	O8-C28-C29-C30
38	f	101	HEM	CAD-CBD-CGD-O2D
31	a	416[A]	PL9	C2-C3-C7-C8
33	A	419	LMG	C16-C17-C18-C19
24	B	606	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C6-C7-C8-C9
24	c	514	CLA	C6-C7-C8-C9
36	C	518	DGD	C2B-C3B-C4B-C5B
29	D	403	LMT	O5B-C1B-O1B-C4'
36	C	518	DGD	C8B-C9B-CAB-CBB
29	M	104	LMT	O1'-C1-C2-C3
24	C	512	CLA	CAA-CBA-CGA-O1A
27	f	102	SQD	O49-C7-C8-C9
27	A	411	SQD	O5-C5-C6-S
27	A	413	SQD	O5-C5-C6-S
24	d	403	CLA	C4C-C3C-CAC-CBC
33	Z	101	LMG	O9-C10-C11-C12
24	b	619	CLA	C15-C16-C17-C18
24	b	622	CLA	O1A-CGA-O2A-C1
26	b	628	BCR	C11-C12-C13-C14
24	c	516	CLA	CAA-CBA-CGA-O1A
36	D	408	DGD	O1A-C1A-C2A-C3A
37	a	420	LHG	C15-C16-C17-C18
24	b	623	CLA	C8-C10-C11-C12
27	A	411	SQD	C45-C44-O6-C1
27	B	621	SQD	C45-C44-O6-C1
33	M	101	LMG	C8-C7-O1-C1
36	C	517	DGD	C5D-C6D-O5D-C1E
36	h	102	DGD	C2G-C3G-O3G-C1D
29	t	101	LMT	C7-C8-C9-C10
36	c	521	DGD	C8A-C9A-CAA-CBA
27	A	413	SQD	C2-C1-O6-C44
24	C	510	CLA	CAA-CBA-CGA-O1A
24	b	619	CLA	C5-C6-C7-C8
29	C	521	LMT	C2B-C1B-O1B-C4'
24	c	506	CLA	C16-C17-C18-C20
33	C	519	LMG	O1-C7-C8-C9
38	f	101	HEM	CAA-CBA-CGA-O2A
37	d	410	LHG	C14-C15-C16-C17
36	C	517	DGD	O1B-C1B-C2B-C3B
36	c	521	DGD	O1A-C1A-C2A-C3A
37	a	420	LHG	O10-C23-C24-C25
31	A	417[B]	PL9	C26-C27-C28-C29
31	a	416[B]	PL9	C21-C22-C23-C24
24	c	507	CLA	C15-C16-C17-C18
36	e	101	DGD	O1B-C1B-C2B-C3B
24	b	610	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	b	622	CLA	CAD-CBD-CGD-O2D
24	b	612	CLA	O1D-CGD-O2D-CED
24	c	515	CLA	C2-C1-O2A-CGA
37	L	101	LHG	O9-C7-C8-C9
33	M	101	LMG	O8-C28-C29-C30
37	d	408	LHG	O8-C23-C24-C25
36	c	519	DGD	CBA-CCA-CDA-CEA
33	b	629	LMG	O10-C28-C29-C30
33	M	101	LMG	C28-C29-C30-C31
36	c	520	DGD	C1A-C2A-C3A-C4A
33	C	519	LMG	O7-C10-C11-C12
33	k	101	LMG	O7-C10-C11-C12
37	b	634	LHG	O7-C7-C8-C9
24	d	404	CLA	C15-C16-C17-C18
37	d	408	LHG	O10-C23-C24-C25
37	d	410	LHG	C7-C8-C9-C10
33	z	101	LMG	O8-C28-C29-C30
37	E	101	LHG	O10-C23-C24-C25

There are no ring outliers.

174 monomers are involved in 417 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	615	CLA	8	0
25	a	411	PHO	2	0
26	K	101	BCR	3	0
28	T	102	GOL	3	0
24	b	610	CLA	2	0
37	E	101	LHG	2	0
37	d	408	LHG	5	0
33	a	415	LMG	5	0
37	d	409	LHG	1	0
29	m	102	LMT	1	0
24	D	404	CLA	3	0
31	a	416[B]	PL9	11	0
24	c	507	CLA	4	0
24	B	605	CLA	3	0
24	b	625	CLA	4	0
31	D	407[B]	PL9	3	0
24	a	412	CLA	2	0
35	c	523	HTG	1	0
36	H	102	DGD	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	D	403	LMT	1	0
24	c	512	CLA	10	0
25	D	401[A]	PHO	2	0
35	b	631	HTG	1	0
37	D	410	LHG	2	0
26	C	514	BCR	1	0
24	d	403	CLA	4	0
36	C	517	DGD	3	0
28	B	629	GOL	2	0
35	b	602	HTG	2	0
26	c	526	BCR	4	0
38	f	101	HEM	4	0
24	B	611	CLA	3	0
24	c	515	CLA	2	0
26	y	101	BCR	2	0
36	h	102	DGD	1	0
24	b	619	CLA	1	0
26	b	628	BCR	3	0
28	a	421	GOL	1	0
31	a	416[A]	PL9	8	0
37	L	101	LHG	2	0
28	D	402	GOL	2	0
28	b	603	GOL	1	0
24	B	606	CLA	6	0
24	B	616	CLA	4	0
24	d	405	CLA	4	0
24	B	607	CLA	7	0
33	d	415	LMG	4	0
24	a	409	CLA	6	0
24	A	409	CLA	2	0
24	c	513	CLA	1	0
29	E	102	LMT	1	0
24	A	407	CLA	5	0
24	A	405	CLA	4	0
26	B	619	BCR	5	0
27	f	102	SQD	3	0
27	a	414	SQD	2	0
24	B	602	CLA	2	0
28	a	402	GOL	1	0
26	d	406	BCR	1	0
26	A	410	BCR	1	0
24	C	509	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	e	101	DGD	7	0
27	L	102	SQD	2	0
24	C	501	CLA	3	0
26	T	103	BCR	6	0
24	C	505	CLA	5	0
26	b	626	BCR	2	0
26	t	102	BCR	6	0
27	B	621	SQD	1	0
26	D	406	BCR	2	0
37	D	411	LHG	7	0
38	E	103	HEM	2	0
33	A	419	LMG	3	0
30	a	418[B]	OEX	1	0
25	A	408	PHO	1	0
31	A	417[B]	PL9	3	0
29	M	102	LMT	3	0
28	T	101	GOL	1	0
29	a	404	LMT	1	0
24	c	510	CLA	2	0
24	B	609	CLA	1	0
24	b	611	CLA	1	0
24	c	505	CLA	5	0
36	c	520	DGD	3	0
28	v	202	GOL	1	0
24	C	508	CLA	4	0
24	C	511	CLA	2	0
27	A	411	SQD	3	0
33	c	522	LMG	5	0
36	D	408	DGD	2	0
24	b	612	CLA	3	0
24	b	618	CLA	4	0
37	b	634	LHG	4	0
27	A	413	SQD	1	0
27	a	405	SQD	2	0
26	B	618	BCR	2	0
26	a	413	BCR	1	0
24	b	614	CLA	5	0
33	z	101	LMG	6	0
24	d	404	CLA	4	0
24	B	617	CLA	6	0
26	h	101	BCR	5	0
24	B	604	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Y	101	BCR	6	0
26	c	518	BCR	2	0
31	A	417[A]	PL9	5	0
24	c	506	CLA	3	0
33	C	519	LMG	2	0
24	C	506	CLA	6	0
37	d	410	LHG	8	0
24	B	614	CLA	4	0
28	c	502	GOL	1	0
24	b	624	CLA	6	0
35	B	624	HTG	1	0
24	B	610	CLA	4	0
33	D	415	LMG	1	0
35	b	607	HTG	1	0
36	C	518	DGD	1	0
24	C	512	CLA	4	0
29	A	414	LMT	3	0
24	B	608	CLA	3	0
24	a	410	CLA	4	0
37	a	420	LHG	4	0
24	c	511	CLA	3	0
24	b	617	CLA	1	0
24	A	406	CLA	1	0
24	C	503	CLA	4	0
24	c	509	CLA	5	0
24	C	502	CLA	3	0
29	e	102	LMT	1	0
33	b	629	LMG	3	0
24	B	603	CLA	2	0
26	B	620	BCR	4	0
24	b	613	CLA	5	0
25	d	402[B]	PHO	3	0
37	D	409	LHG	3	0
33	k	101	LMG	2	0
33	Z	101	LMG	2	0
24	D	405	CLA	1	0
24	c	514	CLA	4	0
36	C	516	DGD	2	0
24	b	621	CLA	1	0
36	c	521	DGD	3	0
24	b	623	CLA	3	0
33	M	101	LMG	3	0

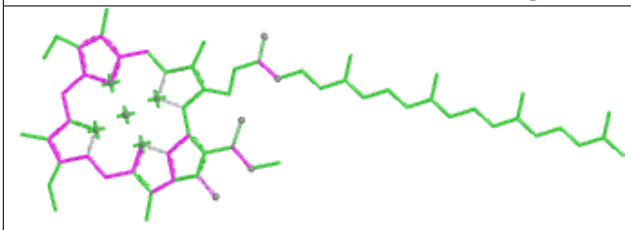
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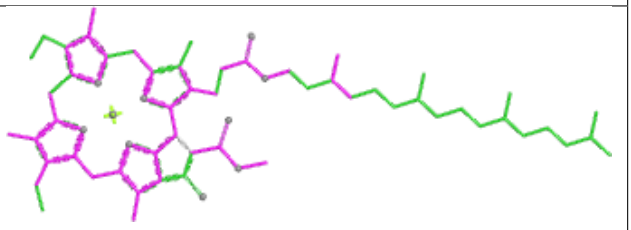
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	613	CLA	4	0
35	b	608	HTG	1	0
24	b	622	CLA	7	0
26	H	101	BCR	5	0
24	C	507	CLA	4	0
26	k	102	BCR	1	0
33	C	520	LMG	2	0
29	T	104	LMT	1	0
35	C	522	HTG	1	0
36	c	519	DGD	3	0
29	C	521	LMT	2	0
35	d	413	HTG	3	0
35	D	414	HTG	2	0
24	C	513	CLA	5	0
24	c	517	CLA	6	0
25	d	402[A]	PHO	2	0
24	b	620	CLA	2	0
26	b	627	BCR	1	0
28	C	524	GOL	2	0
24	c	508	CLA	1	0
28	v	201	GOL	1	0
29	m	103	LMT	2	0
25	D	401[B]	PHO	1	0
35	V	206	HTG	1	0
35	b	632	HTG	1	0
24	C	510	CLA	6	0
24	c	516	CLA	4	0
26	C	515	BCR	2	0
28	a	401	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

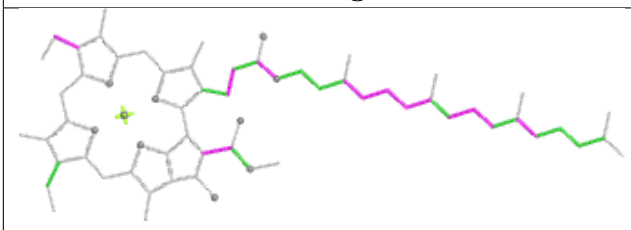
Ligand CLA B 615



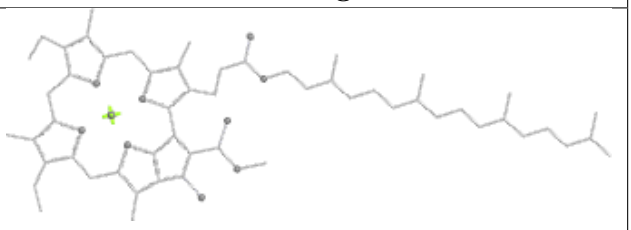
Bond lengths



Bond angles



Torsions

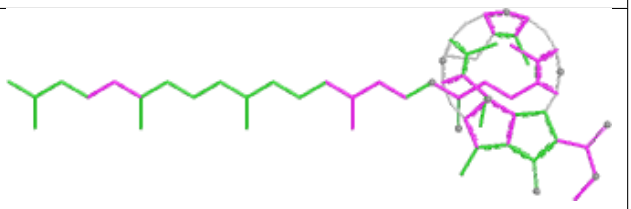


Rings

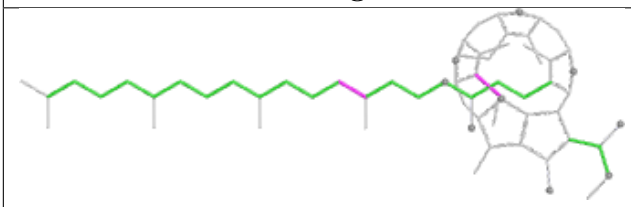
Ligand PHO a 411



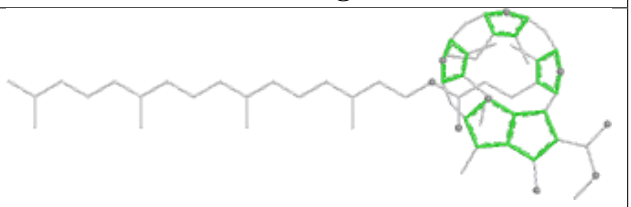
Bond lengths



Bond angles

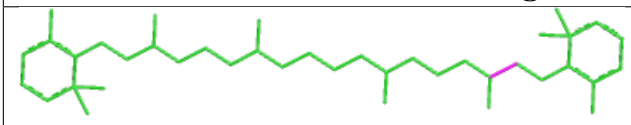


Torsions

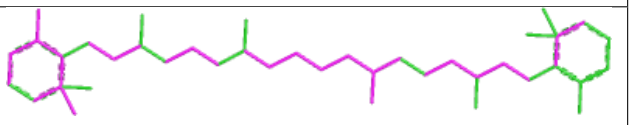


Rings

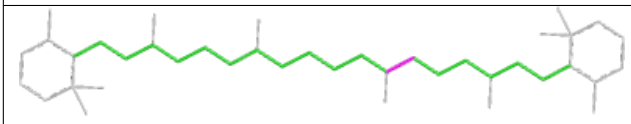
Ligand BCR K 101



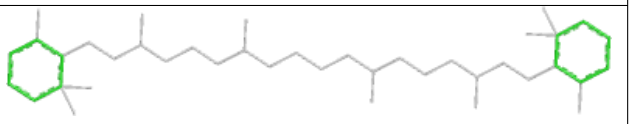
Bond lengths



Bond angles

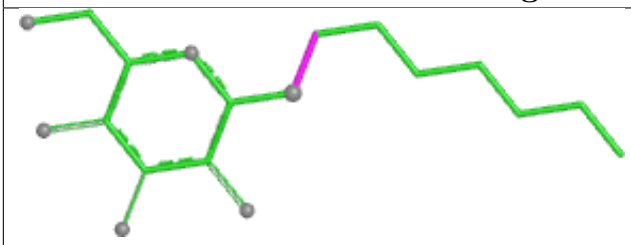


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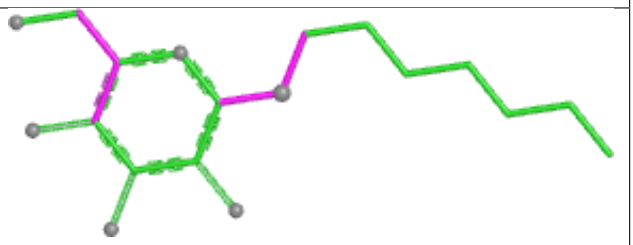


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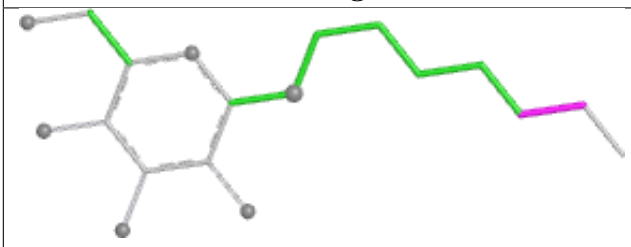
Ligand HTG B 631



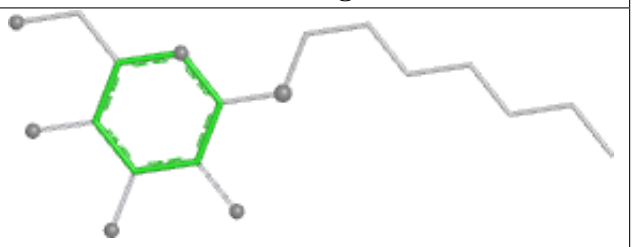
Bond lengths



Bond angles

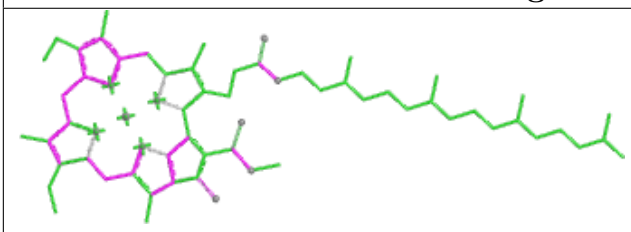


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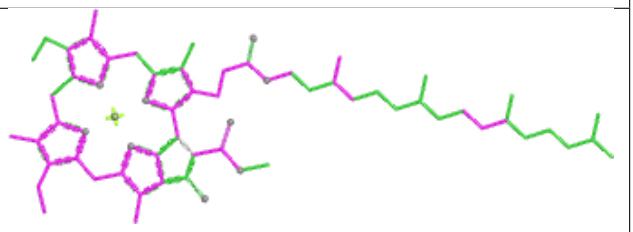


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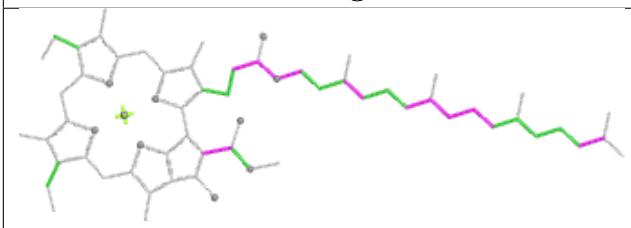
Ligand CLA b 610



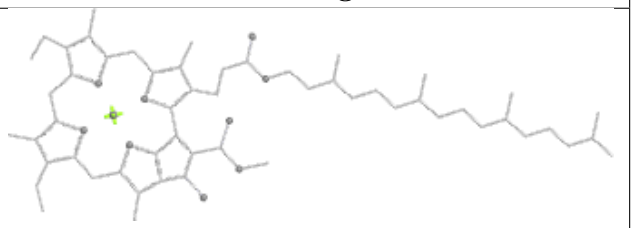
Bond lengths



Bond angles

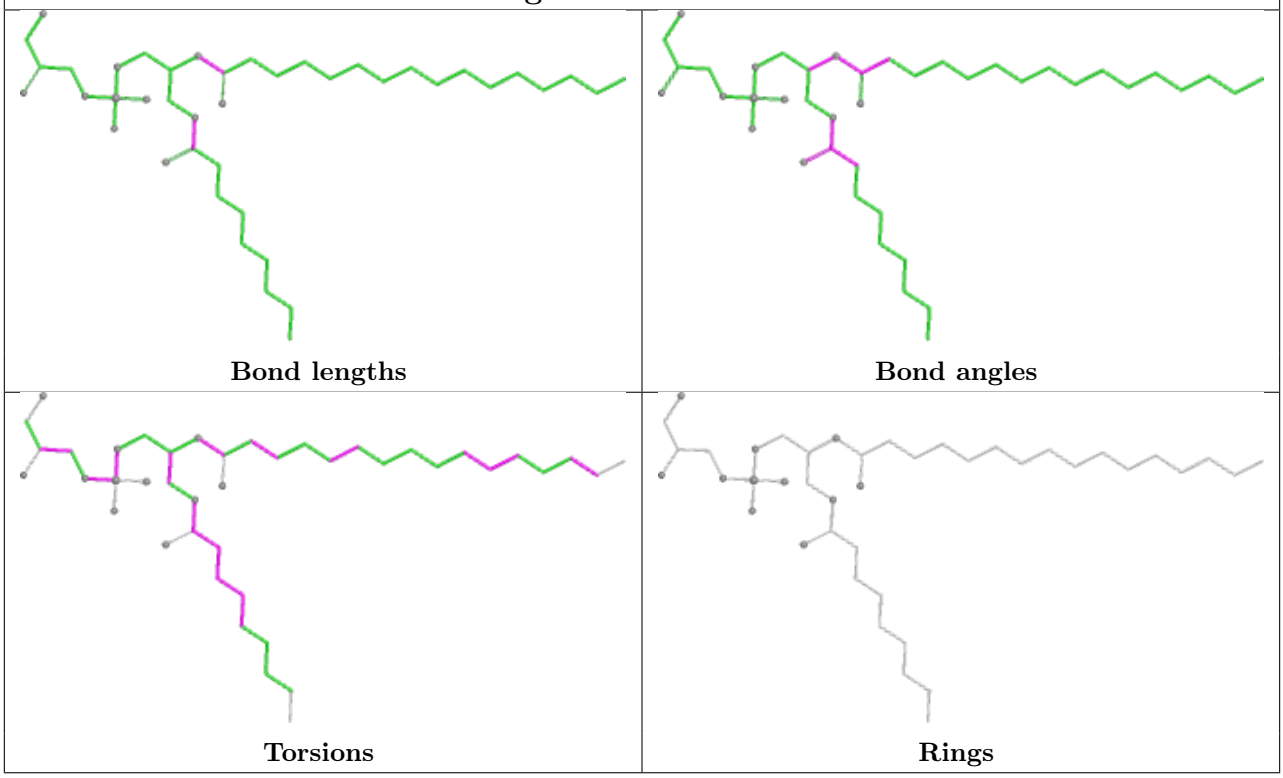


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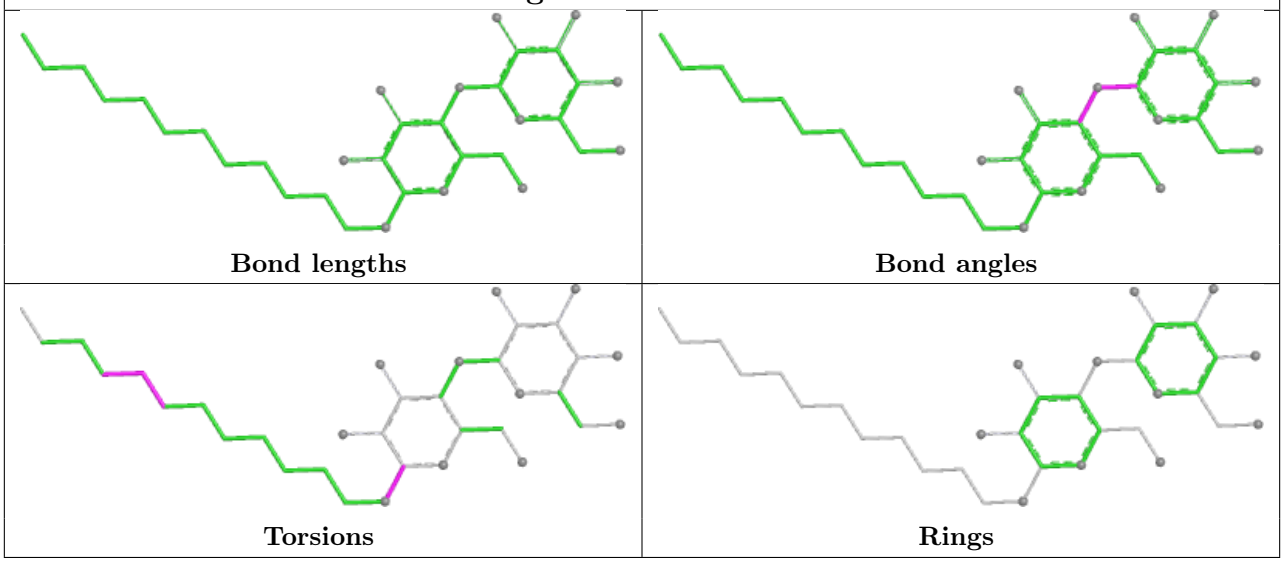


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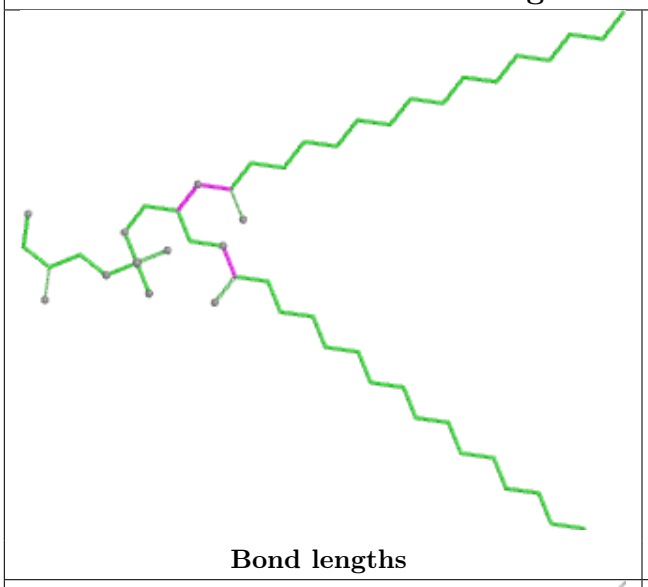
Ligand LHG E 101



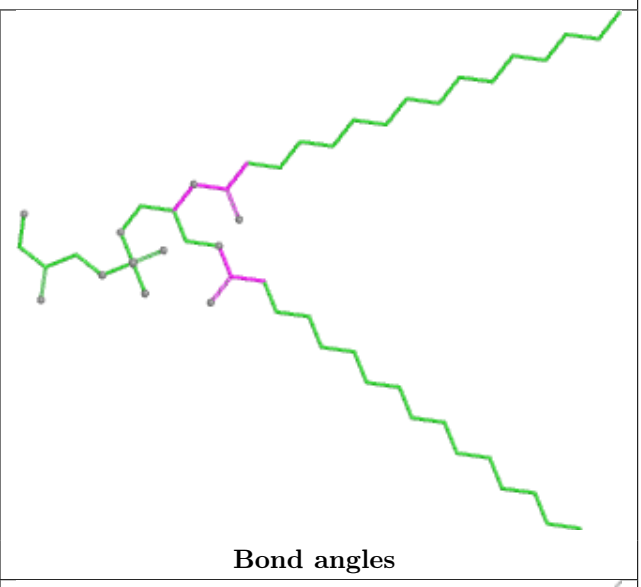
Ligand LMT a 419



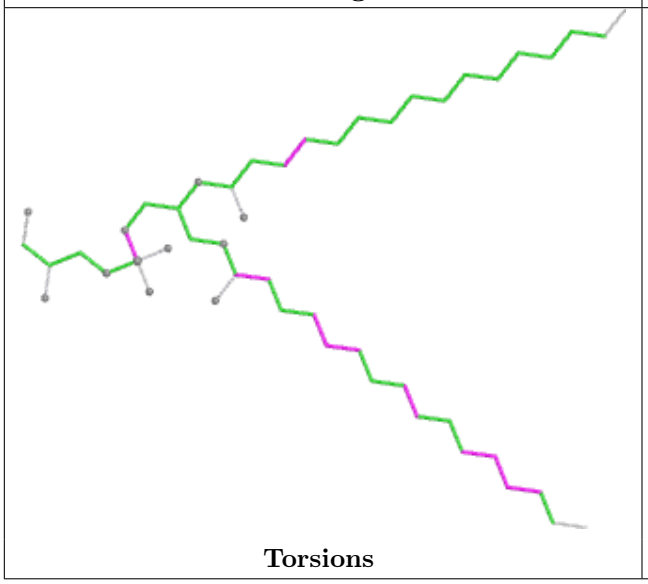
Ligand LHG d 408



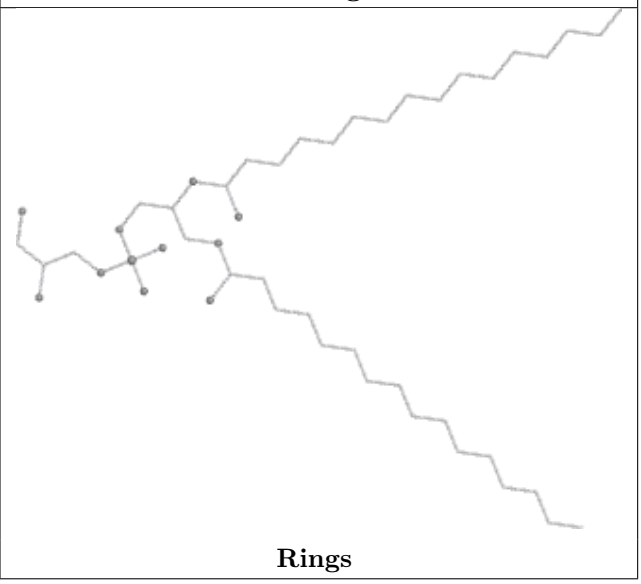
Bond lengths



Bond angles

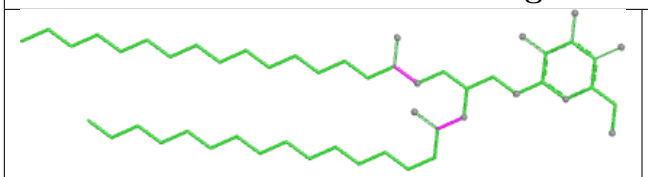


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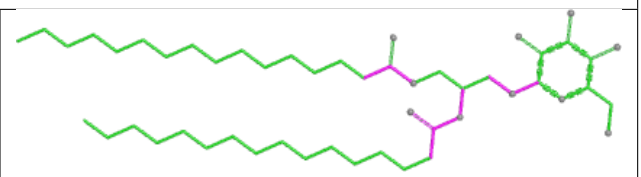


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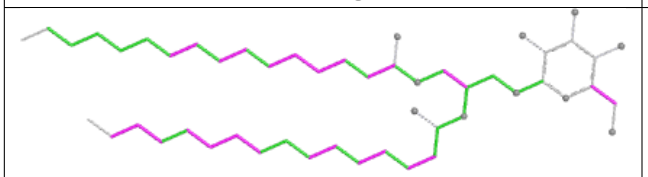
Ligand LMG a 415



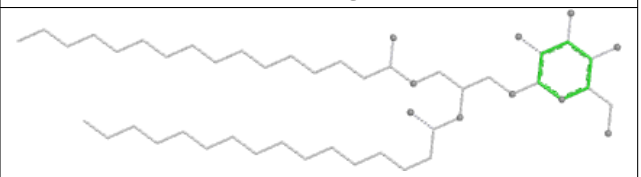
Bond lengths



Bond angles

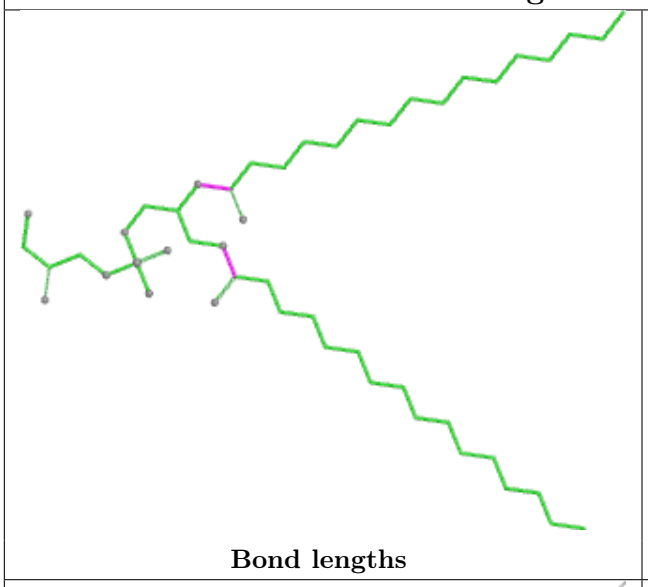


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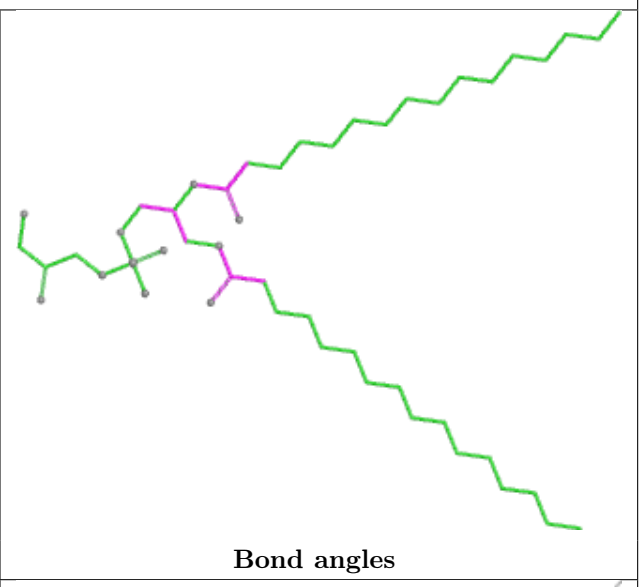


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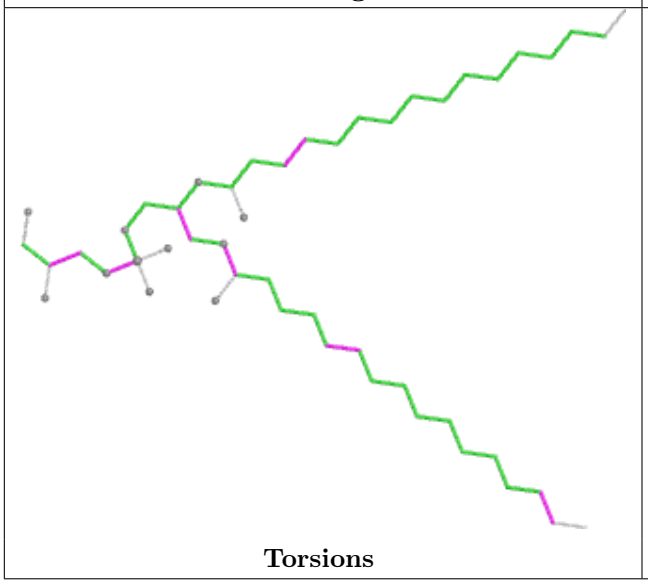
Ligand LHG d 409



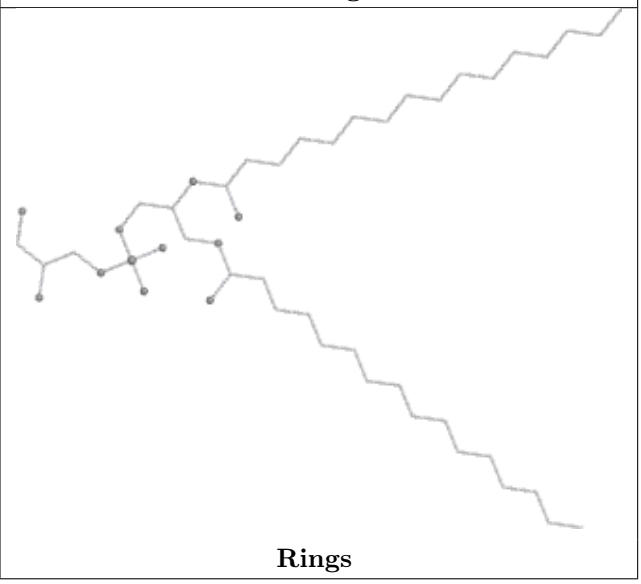
Bond lengths



Bond angles

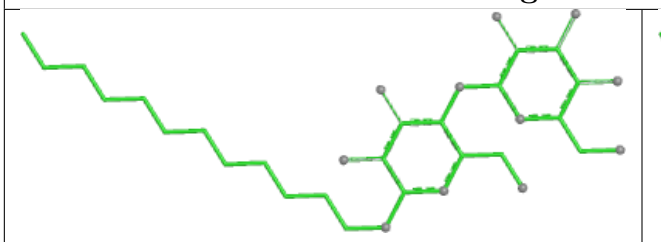


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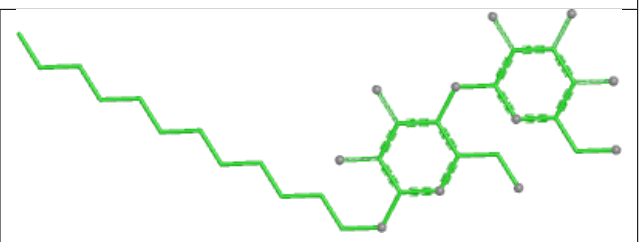


Rings

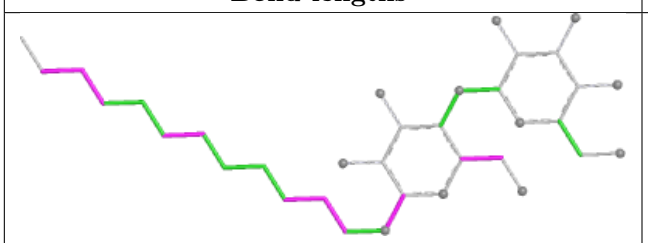
Ligand LMT m 102



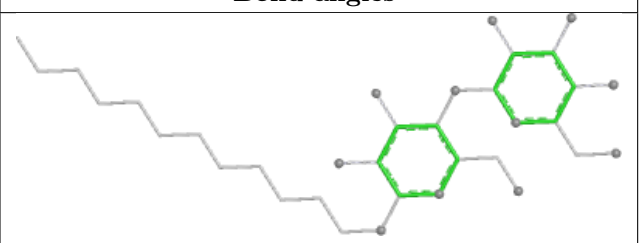
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Bond angles

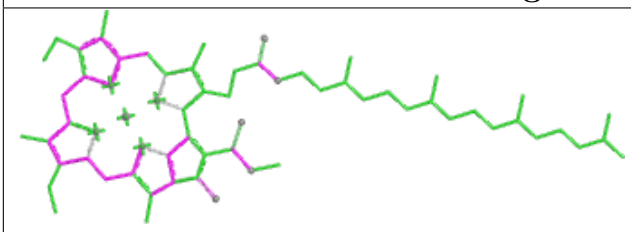


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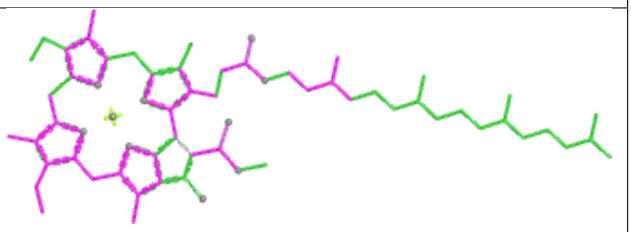


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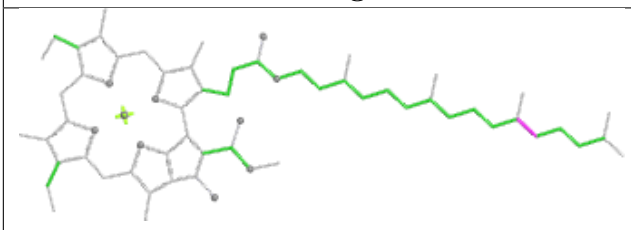
Ligand CLA D 404



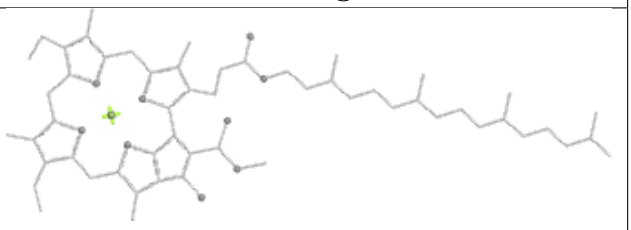
Bond lengths



Bond angles



Torsions

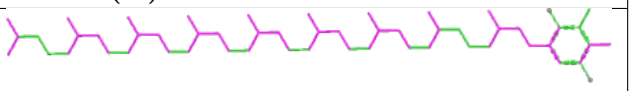


Rings

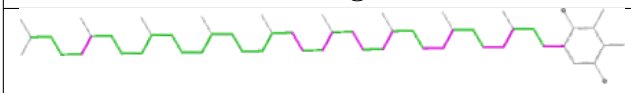
Ligand PL9 a 416 (B)



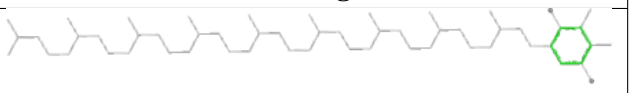
Bond lengths



Bond angles

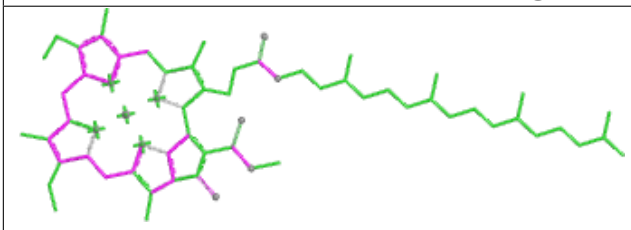


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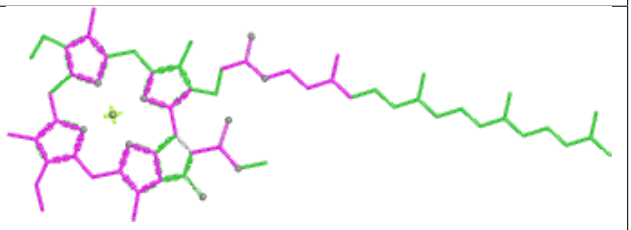


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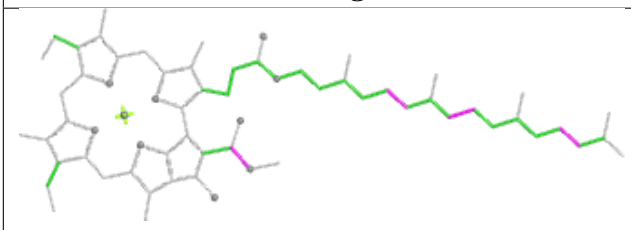
Ligand CLA c 507



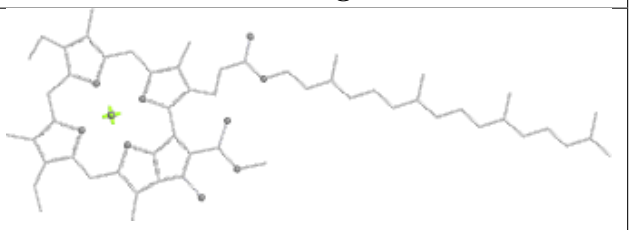
Bond lengths



Bond angles

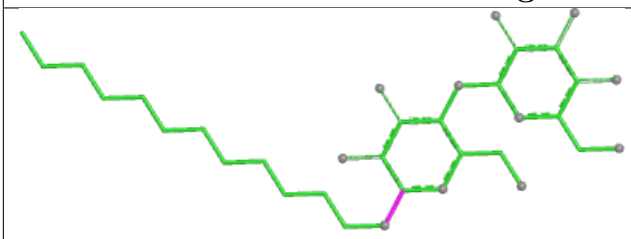


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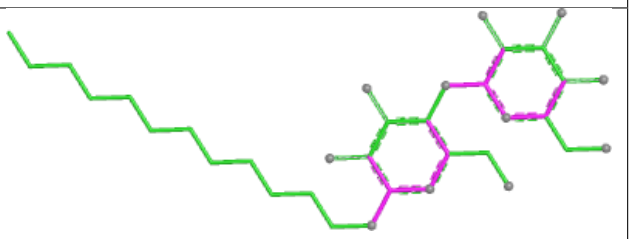


Rings

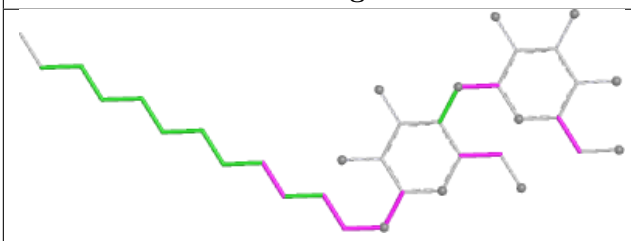
Ligand LMT M 104



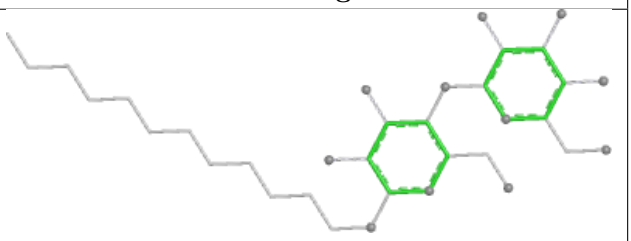
Bond lengths



Bond angles

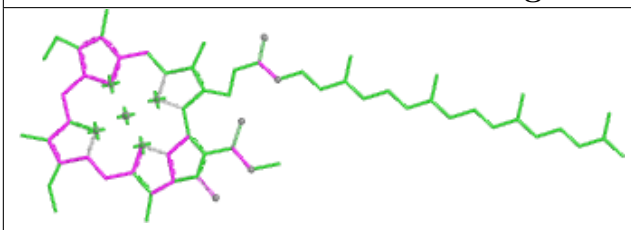


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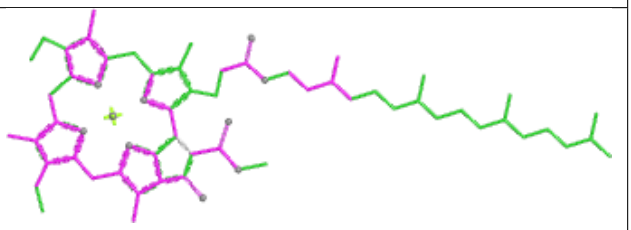


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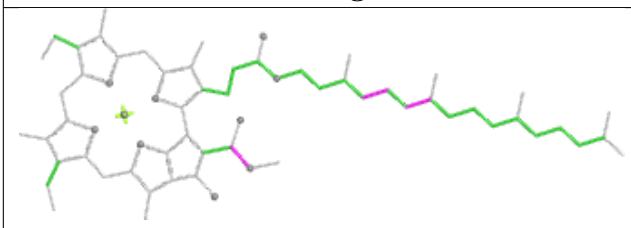
Ligand CLA B 605



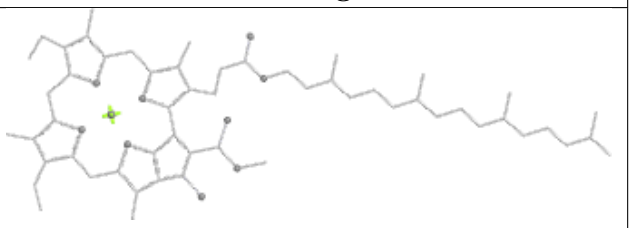
Bond lengths



Bond angles

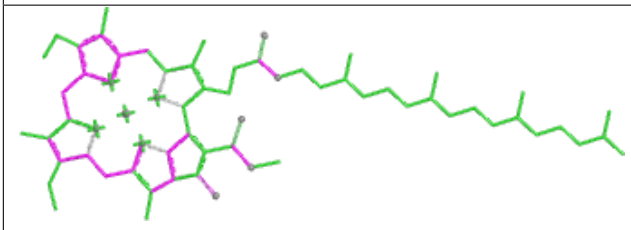


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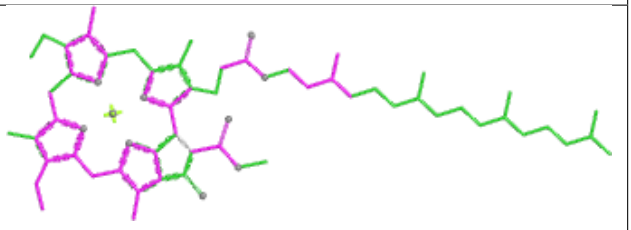


Rings

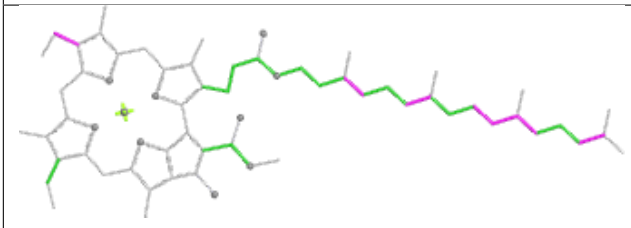
Ligand CLA b 625



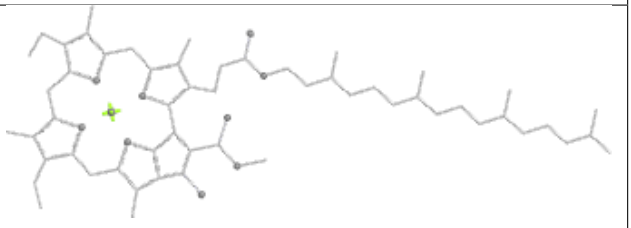
Bond lengths



Bond angles



Torsions

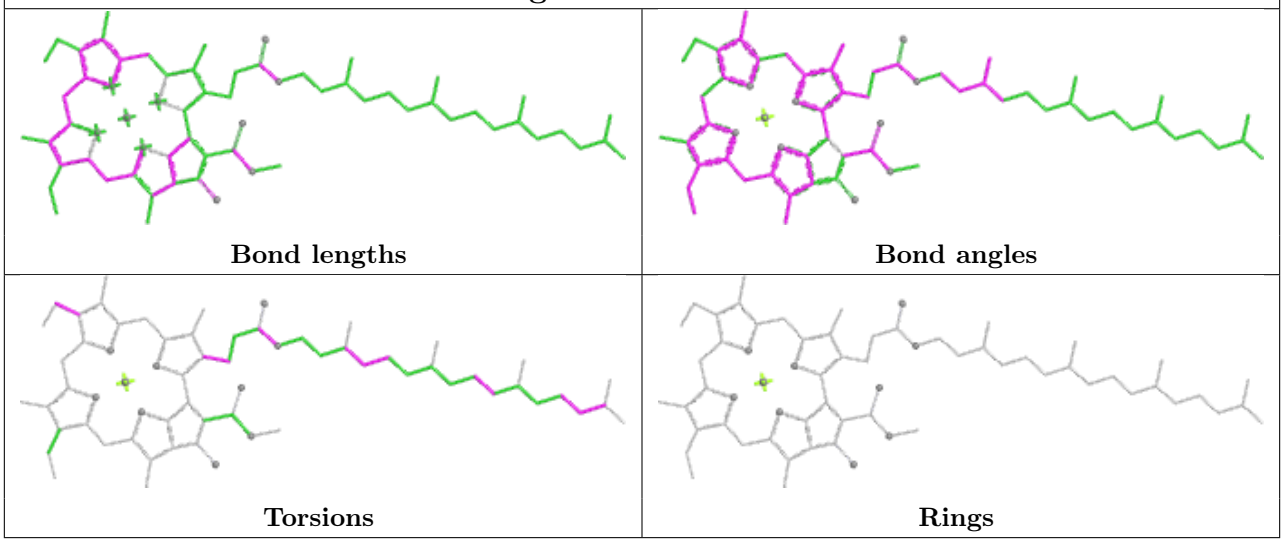


Rings

Ligand PL9 D 407 (B)



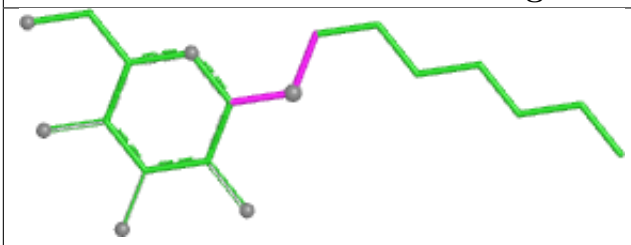
Ligand CLA a 412



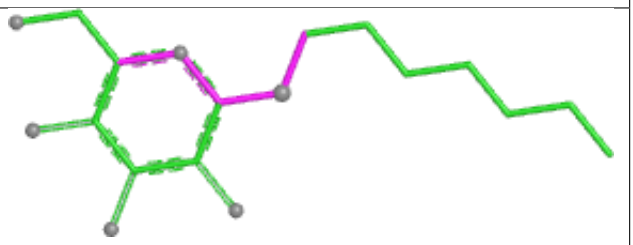
Ligand PL9 d 407 (A)



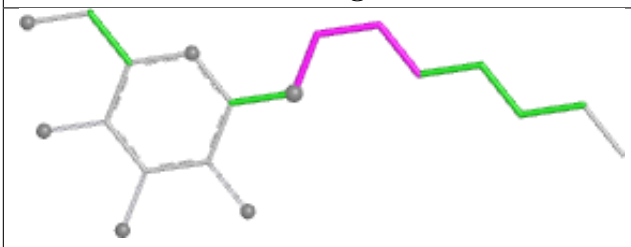
Ligand HTG c 523



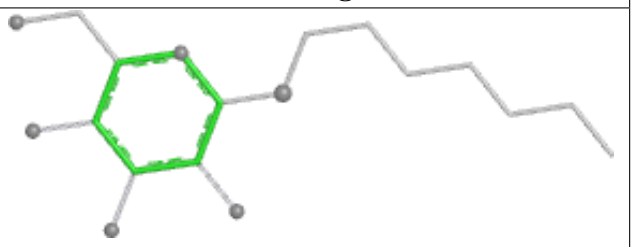
Bond lengths



Bond angles

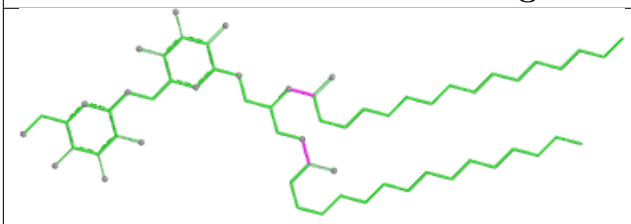


Torsions

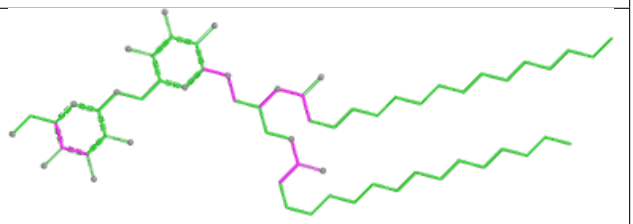


Rings

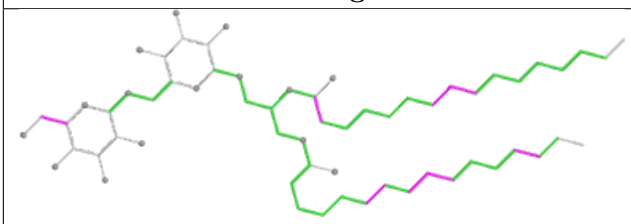
Ligand DGD H 102



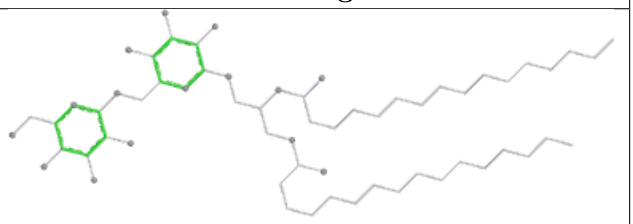
Bond lengths



Bond angles

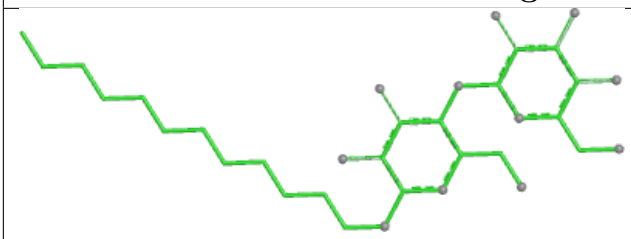


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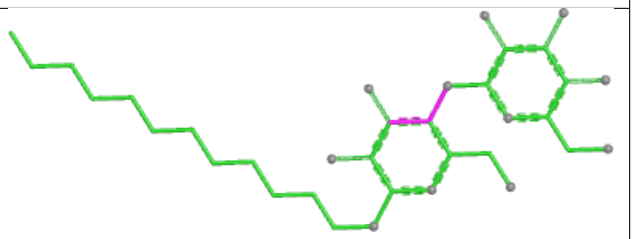


Rings

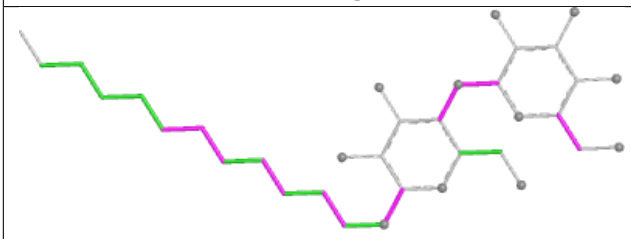
Ligand LMT D 403



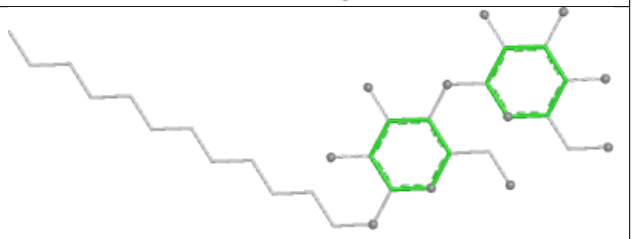
Bond lengths



Bond angles

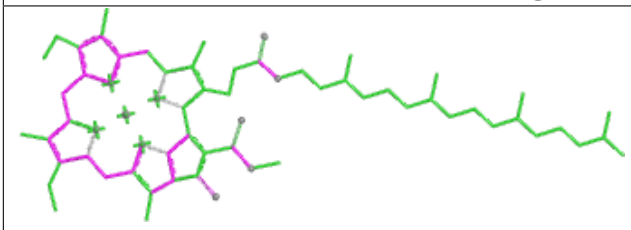


Torsions

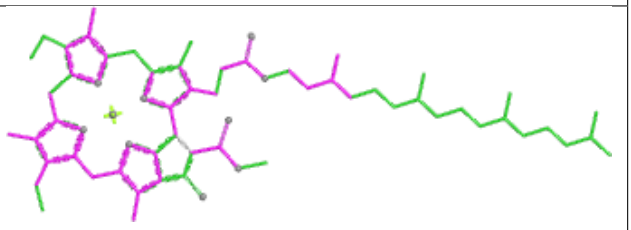


Rings

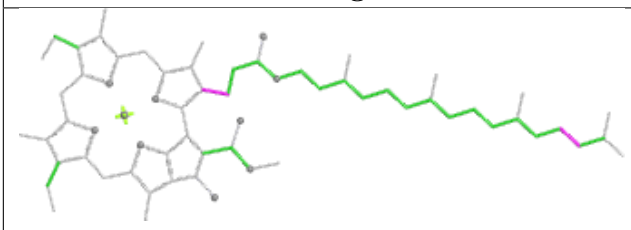
Ligand CLA c 512



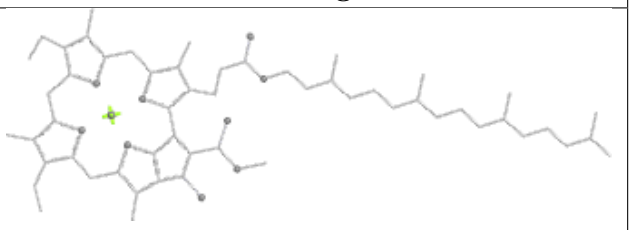
Bond lengths



Bond angles

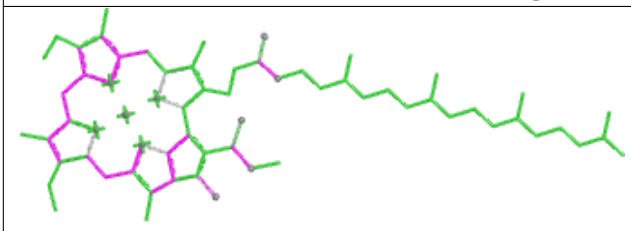


Torsions

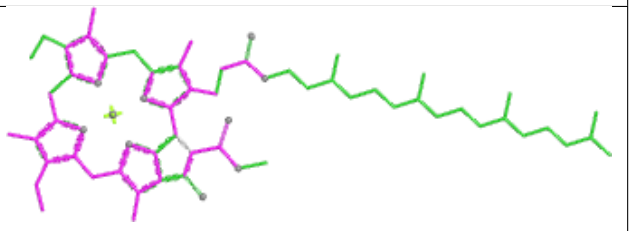


Rings

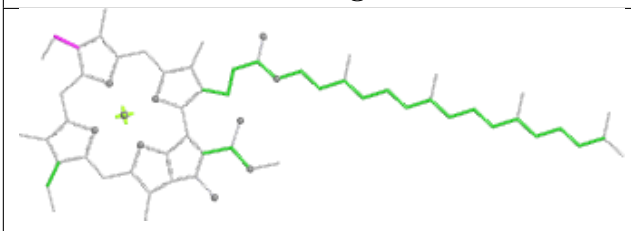
Ligand CLA b 616



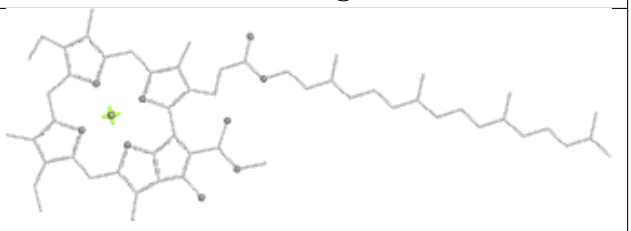
Bond lengths



Bond angles

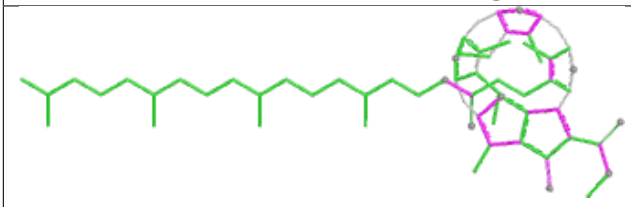


Torsions

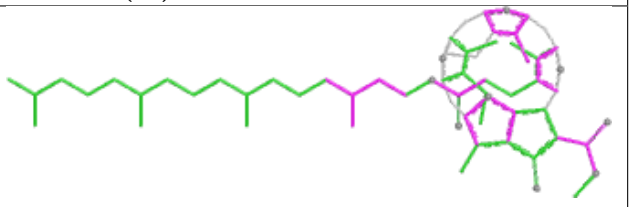


Rings

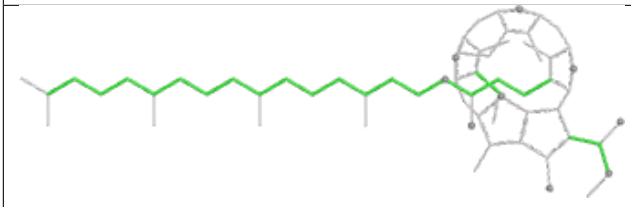
Ligand PHO D 401 (A)



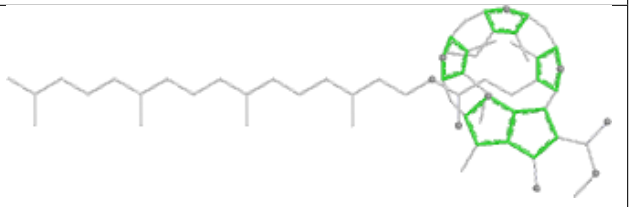
Bond lengths



Bond angles

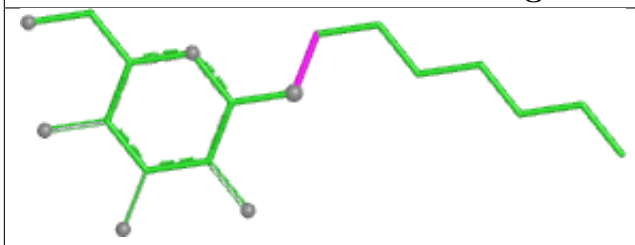


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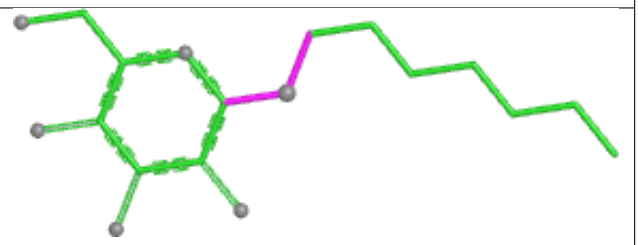


Rings

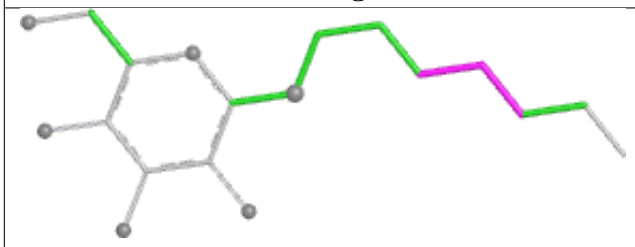
Ligand HTG b 631



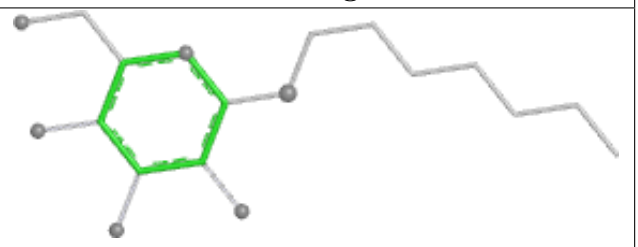
Bond lengths



Bond angles

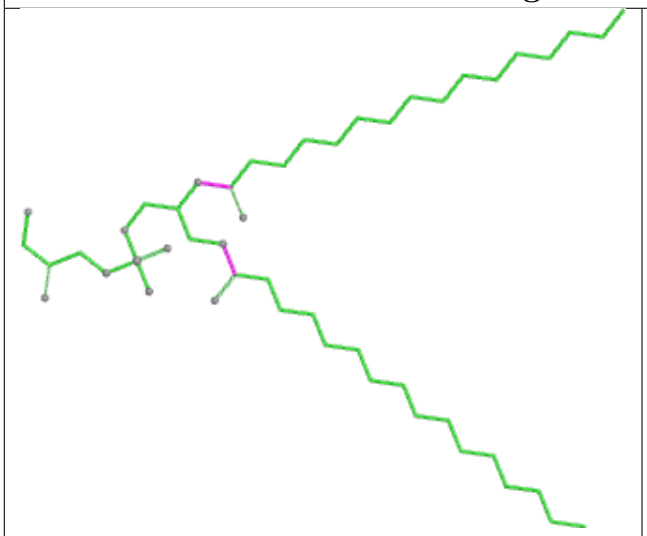


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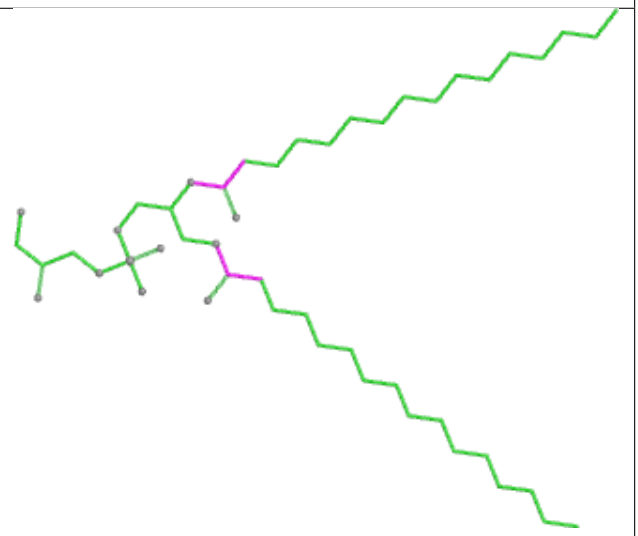


Rings

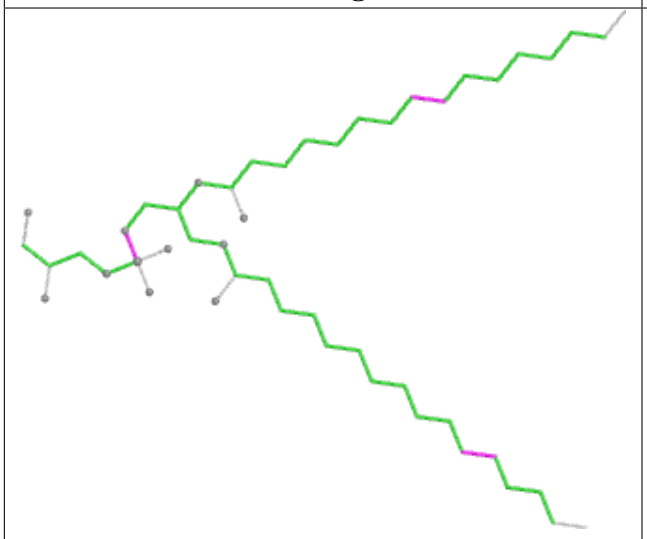
Ligand LHG D 410



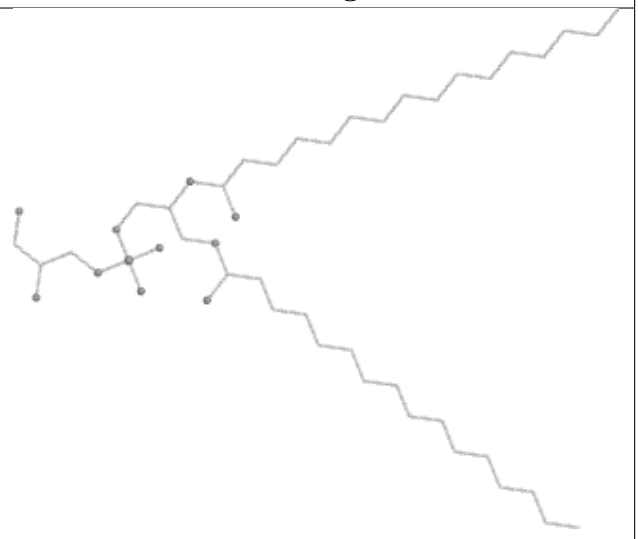
Bond lengths



Bond angles

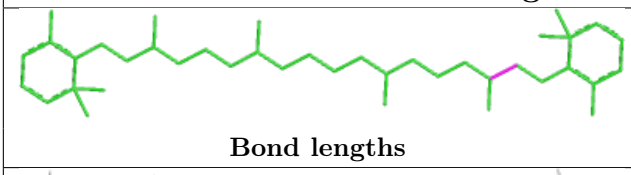


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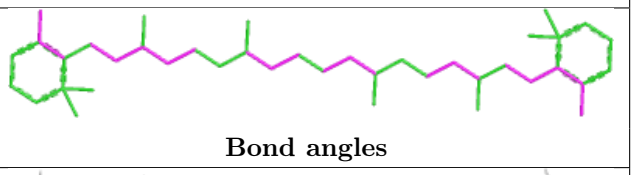


Rings

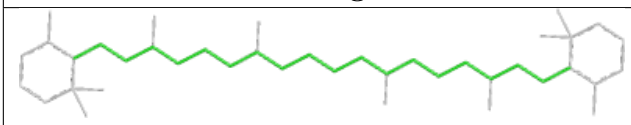
Ligand BCR C 514



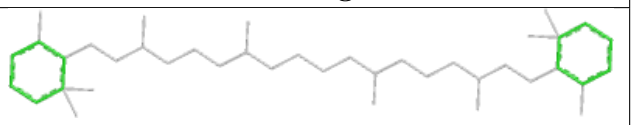
Bond lengths



Bond angles

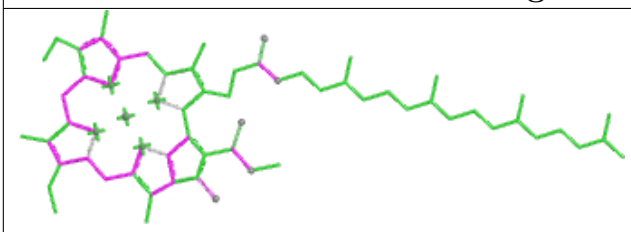


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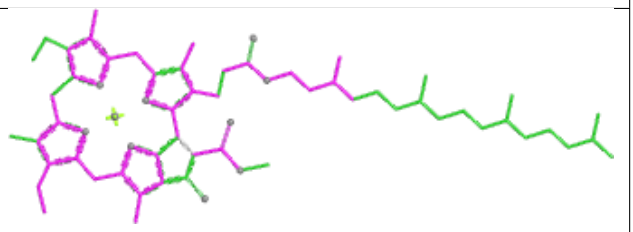


Rings

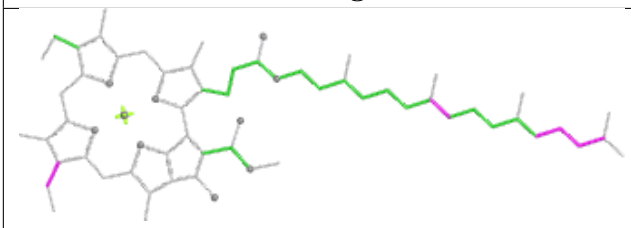
Ligand CLA d 403



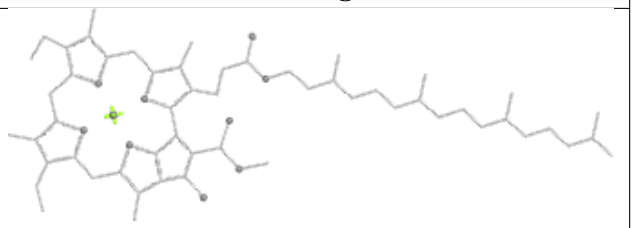
Bond lengths



Bond angles

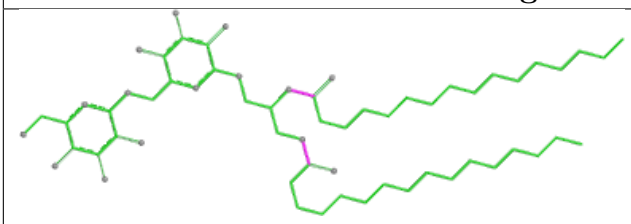


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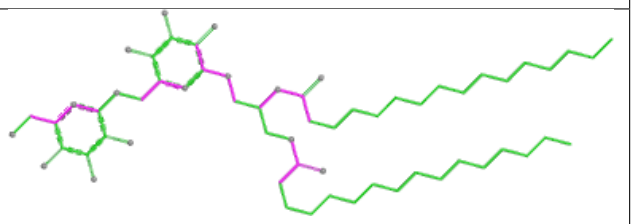


Rings

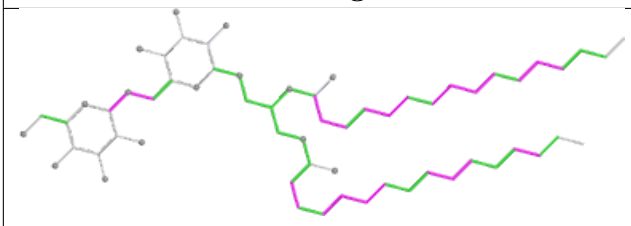
Ligand DGD C 517



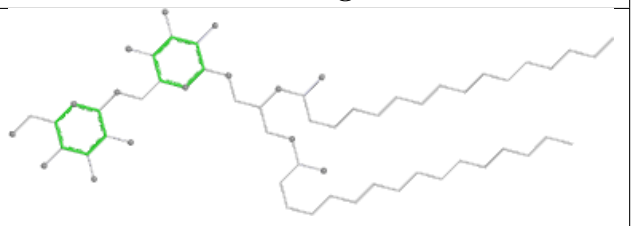
Bond lengths



Bond angles

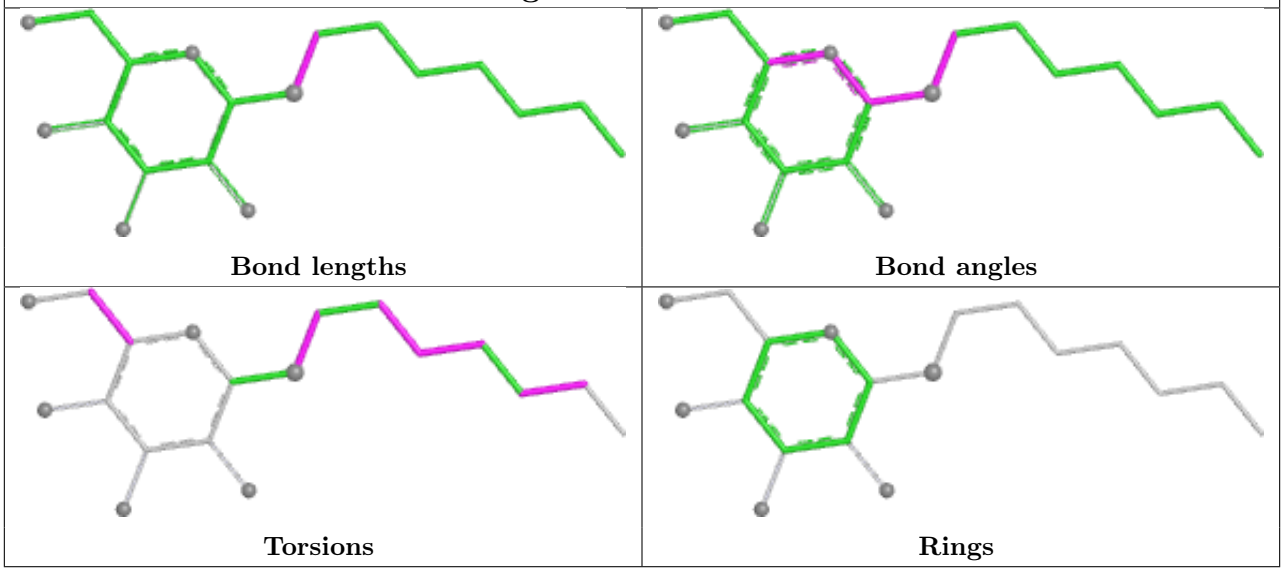


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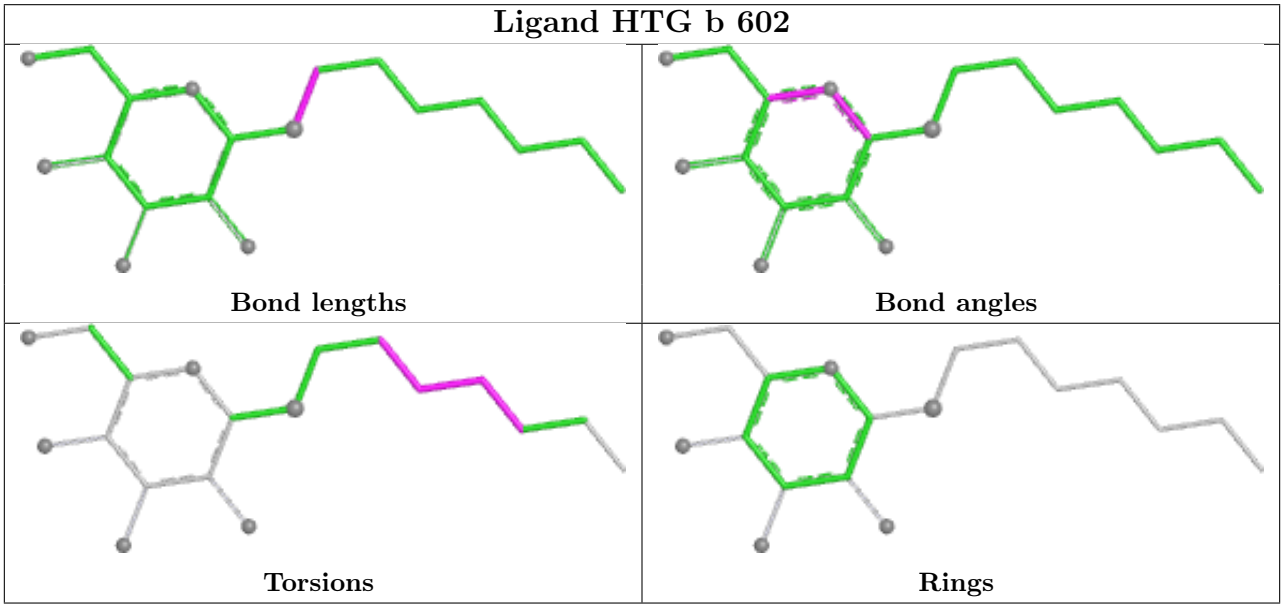


Rings

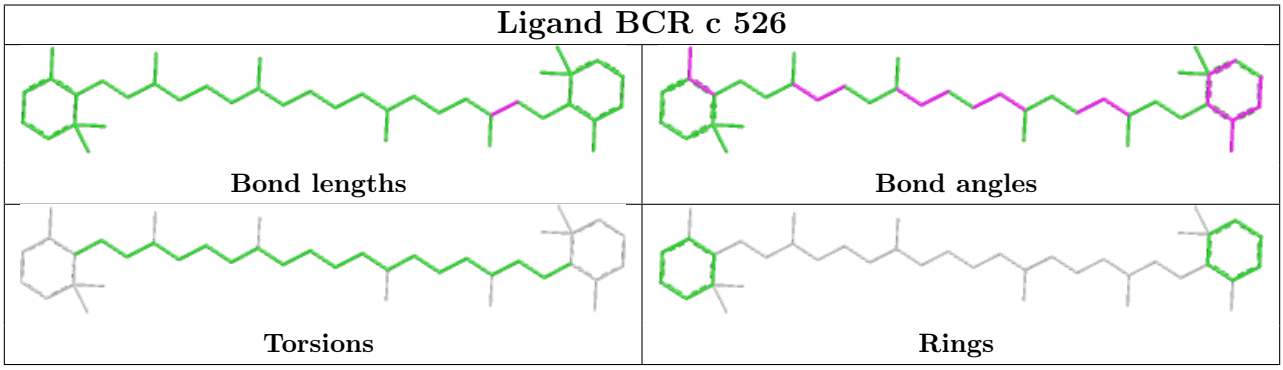
Ligand HTG B 623



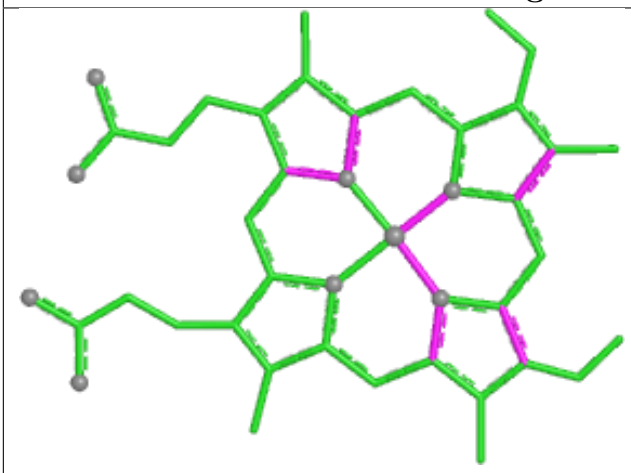
Ligand HTG b 602



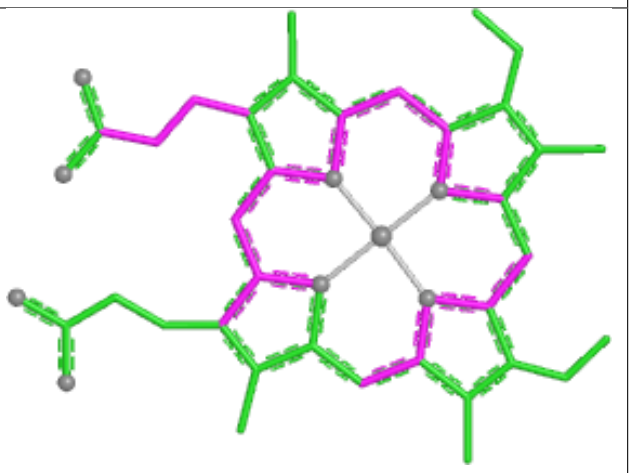
Ligand BCR c 526



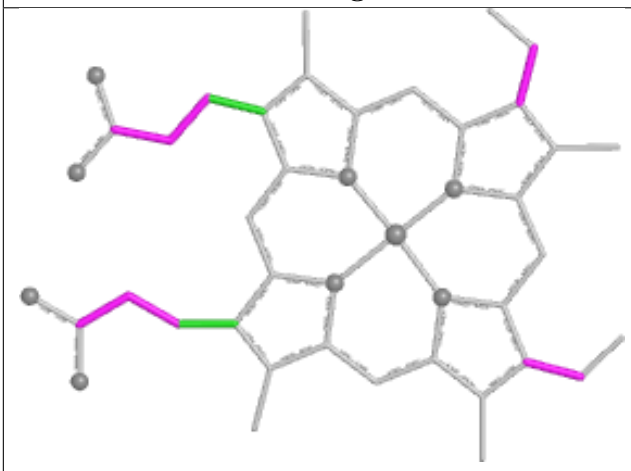
Ligand HEM f 101



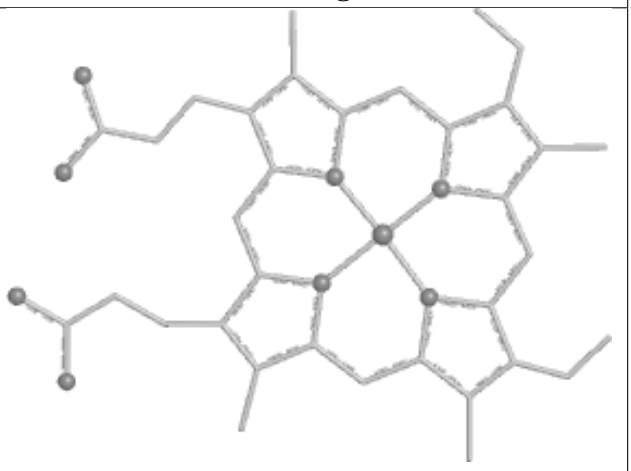
Bond lengths



Bond angles

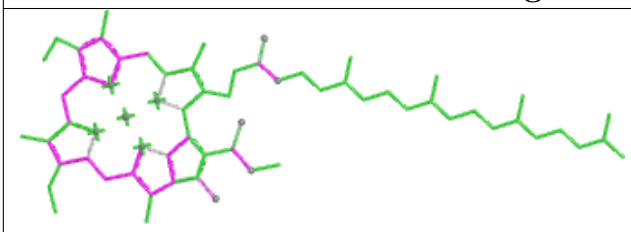


Torsions

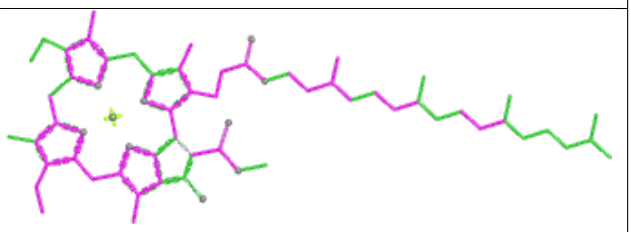


Rings

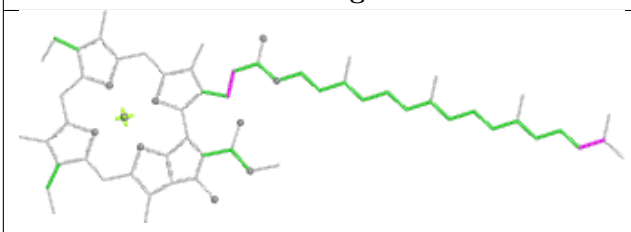
Ligand CLA B 611



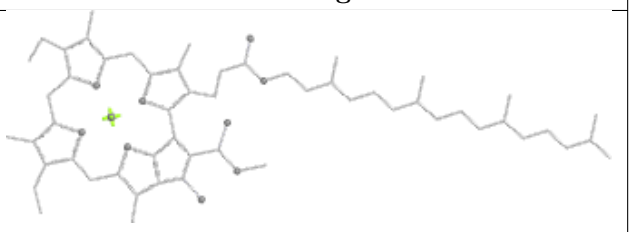
Bond lengths



Bond angles

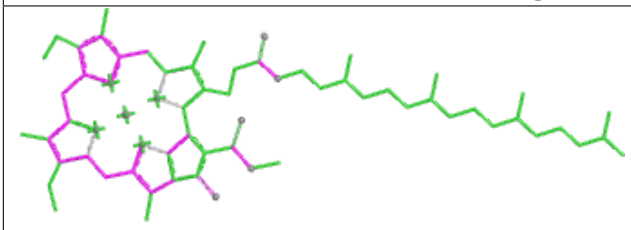


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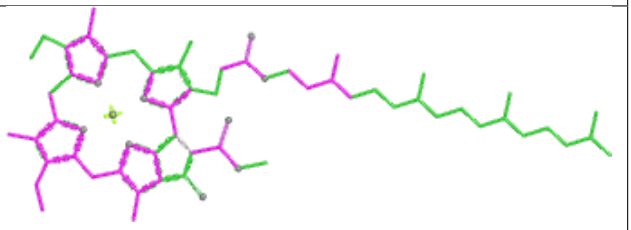


Rings

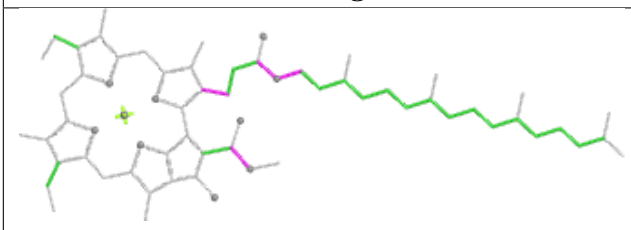
Ligand CLA c 515



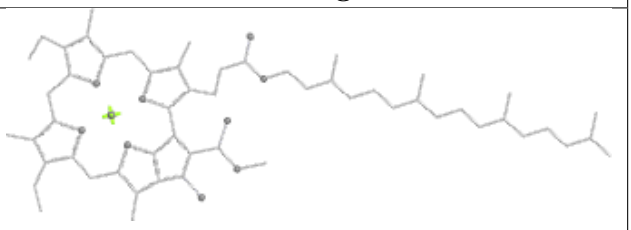
Bond lengths



Bond angles



Torsions

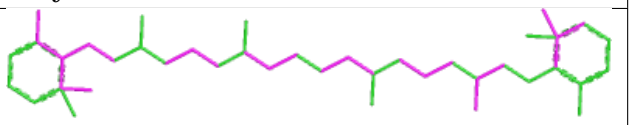


Rings

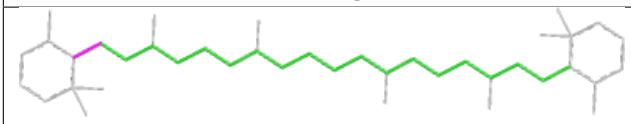
Ligand BCR y 101



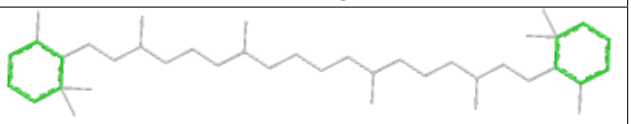
Bond lengths



Bond angles

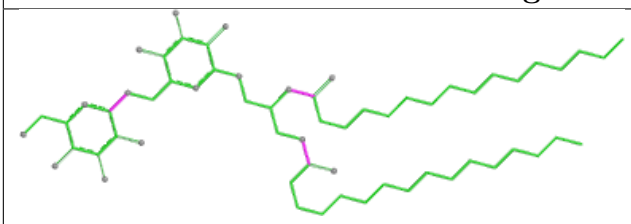


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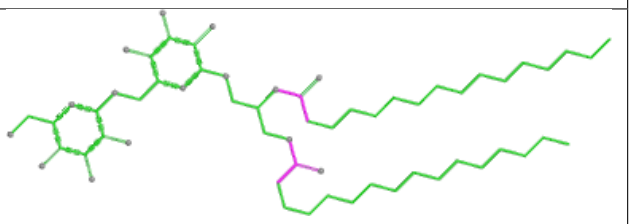


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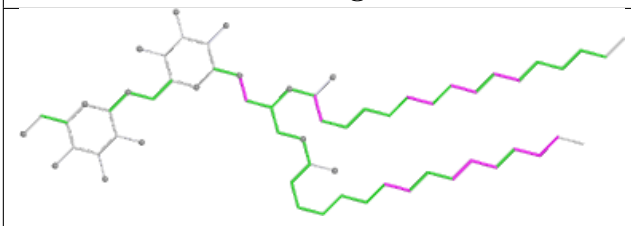
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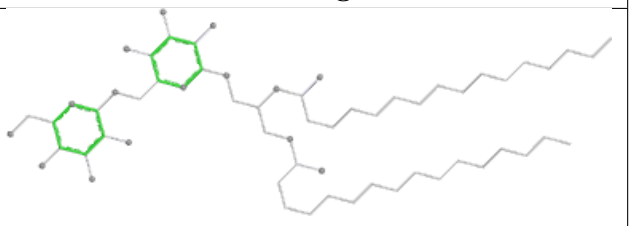
Bond lengths



Bond angles

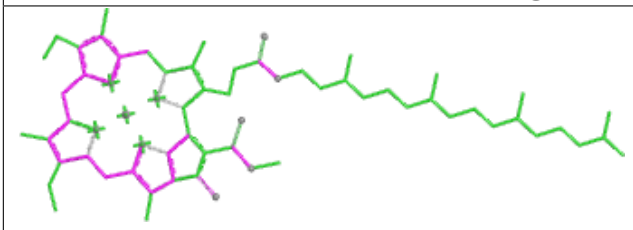


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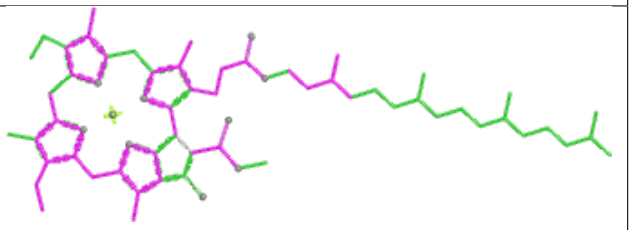


Rings

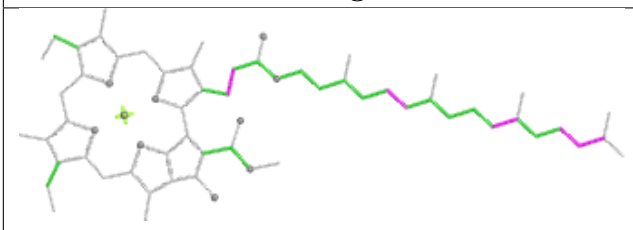
Ligand CLA b 619



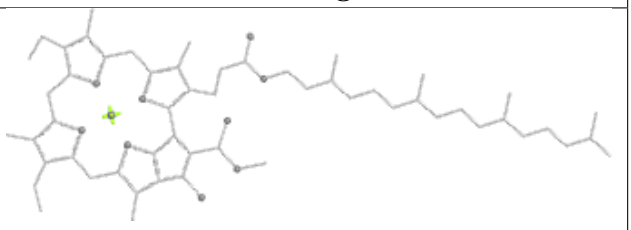
Bond lengths



Bond angles



Torsions

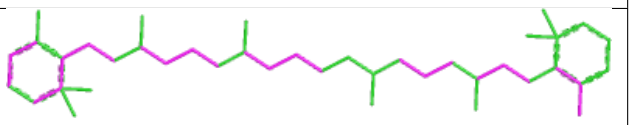


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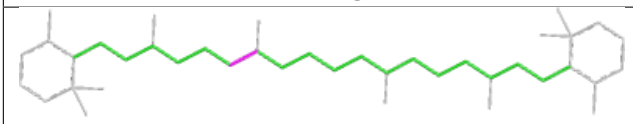
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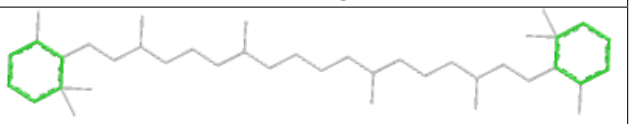
Bond lengths



Bond angles

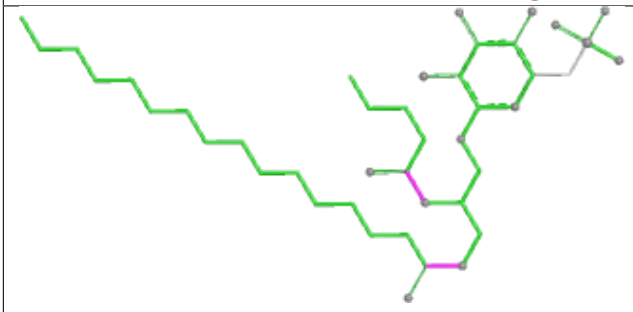


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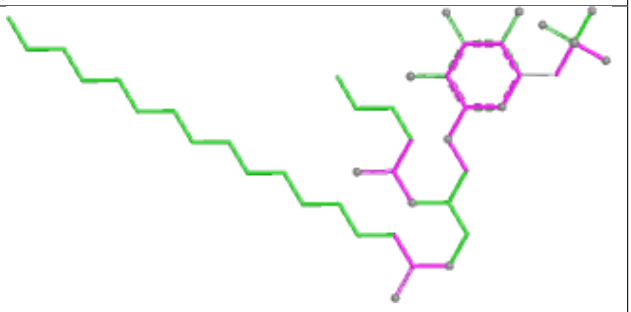


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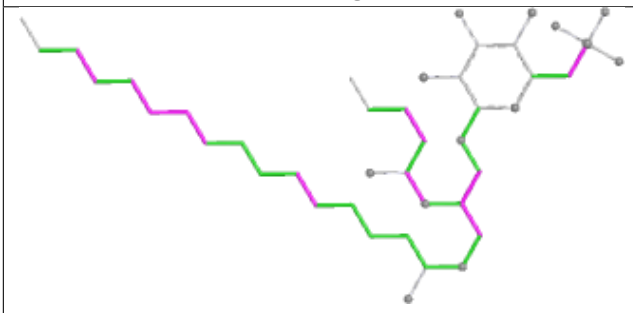
Ligand SQD F 101



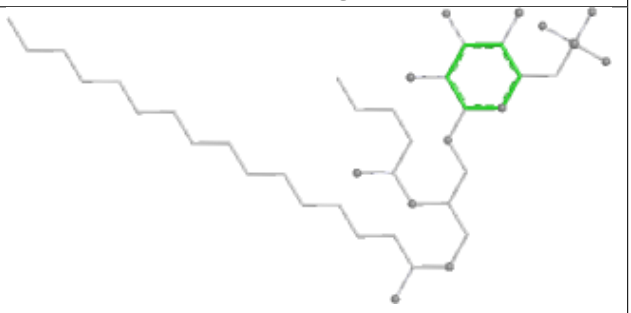
Bond lengths



Bond angles

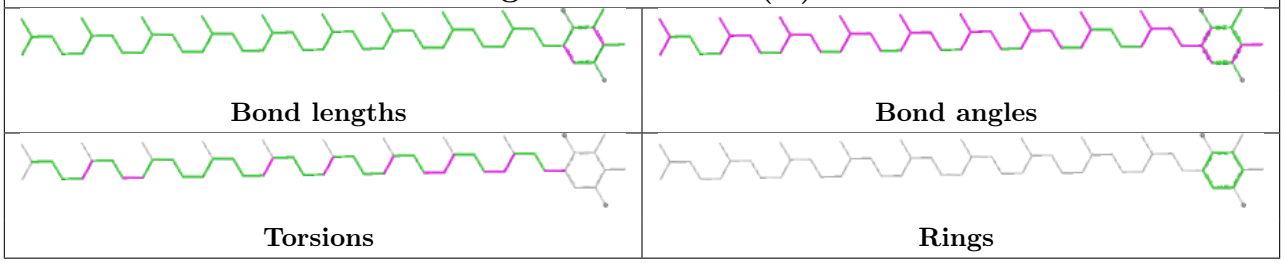


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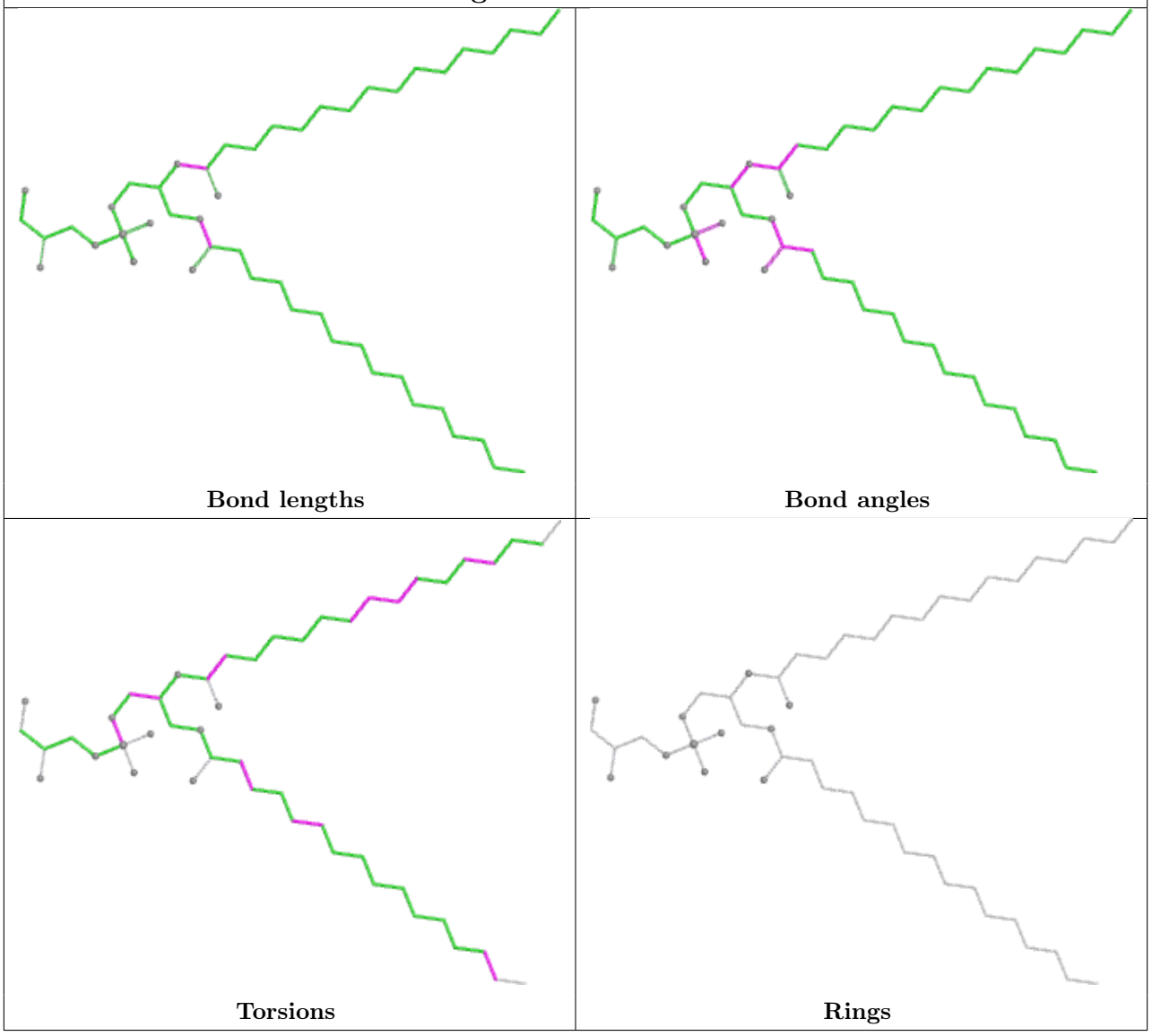


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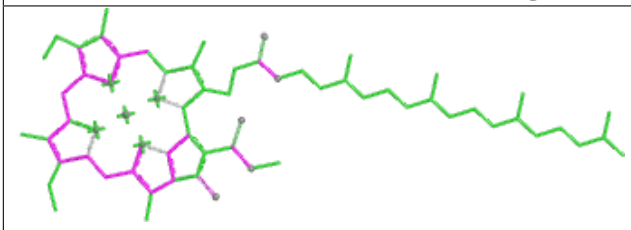
Ligand PL9 a 416 (A)



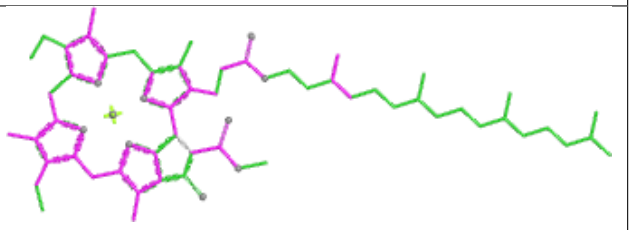
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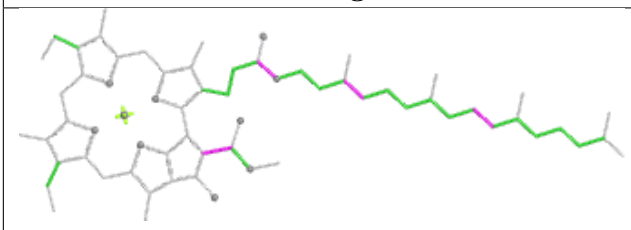
Ligand CLA B 606



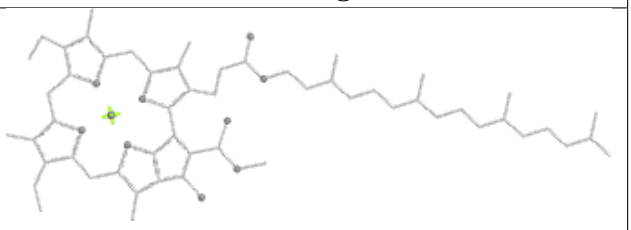
Bond lengths



Bond angles

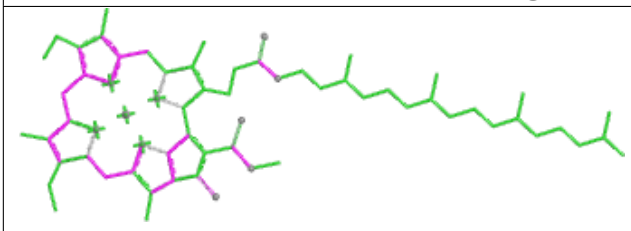


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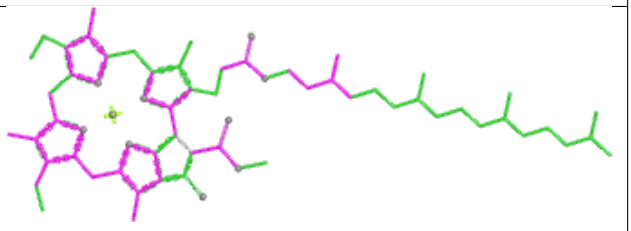


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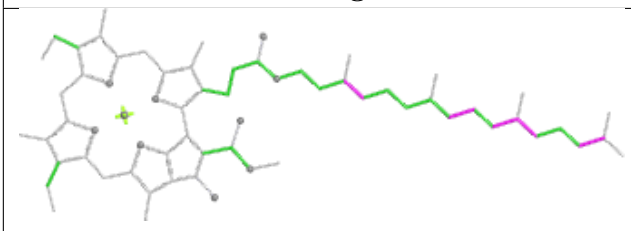
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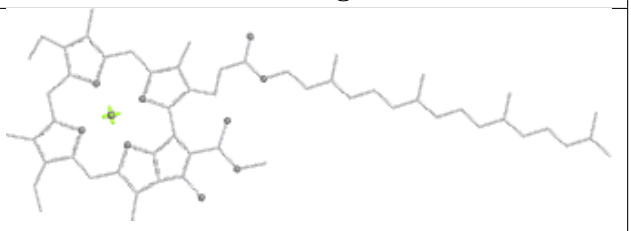
Bond lengths



Bond angles

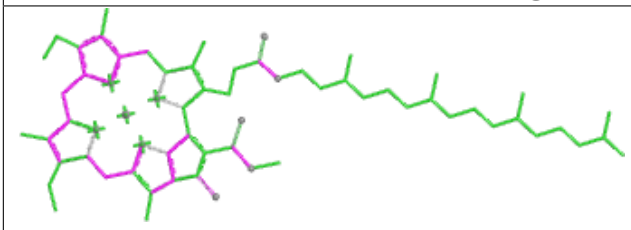


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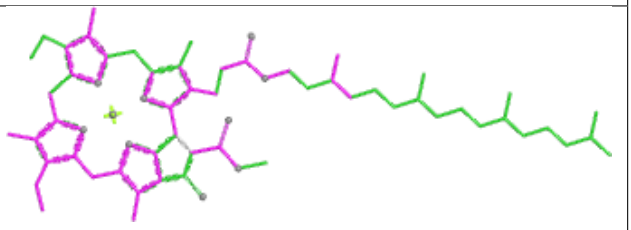


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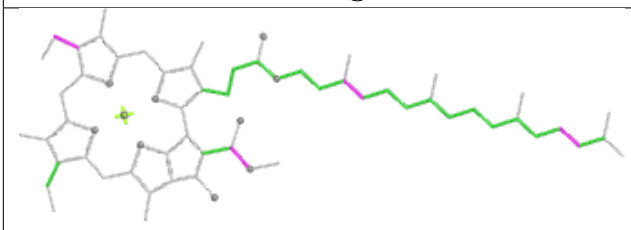
Ligand CLA d 405



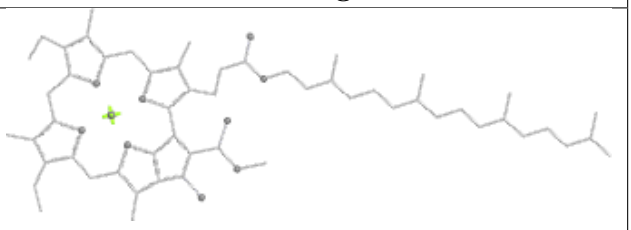
Bond lengths



Bond angles

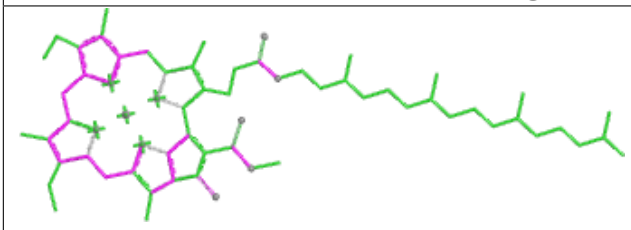


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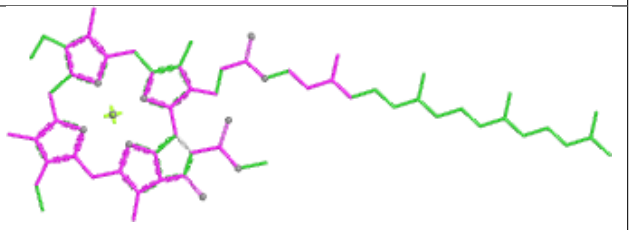


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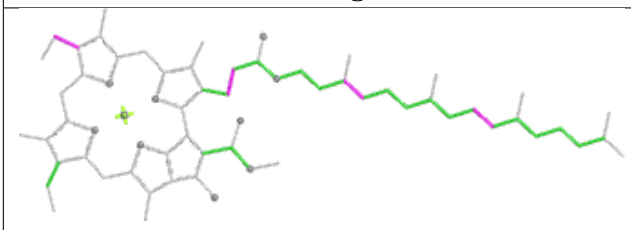
Ligand CLA B 607



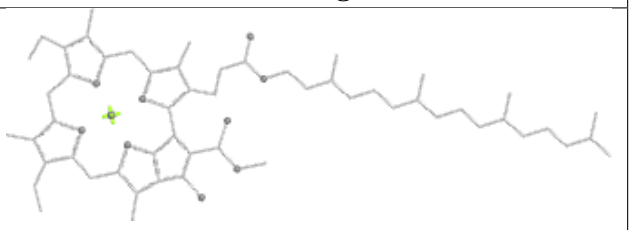
Bond lengths



Bond angles

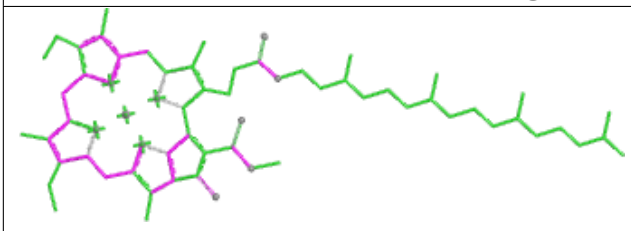


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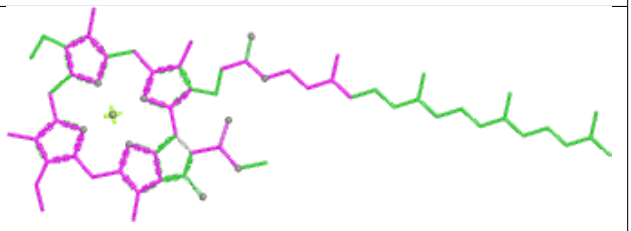


Rings

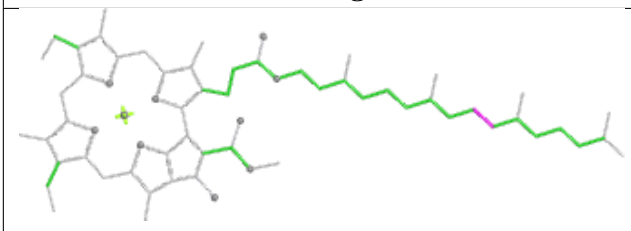
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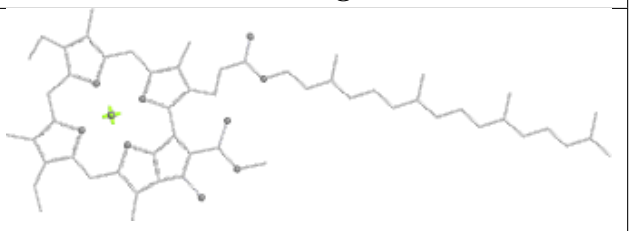
Bond lengths



Bond angles

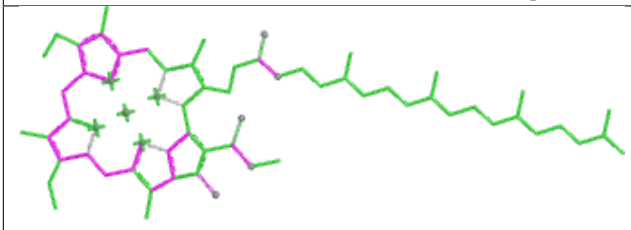


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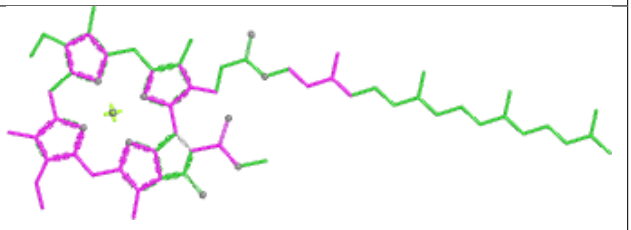


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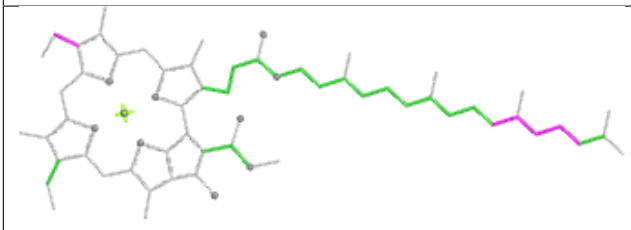
Ligand CLA C 504



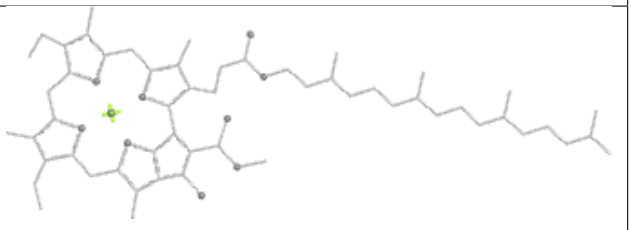
Bond lengths



Bond angles



Torsions

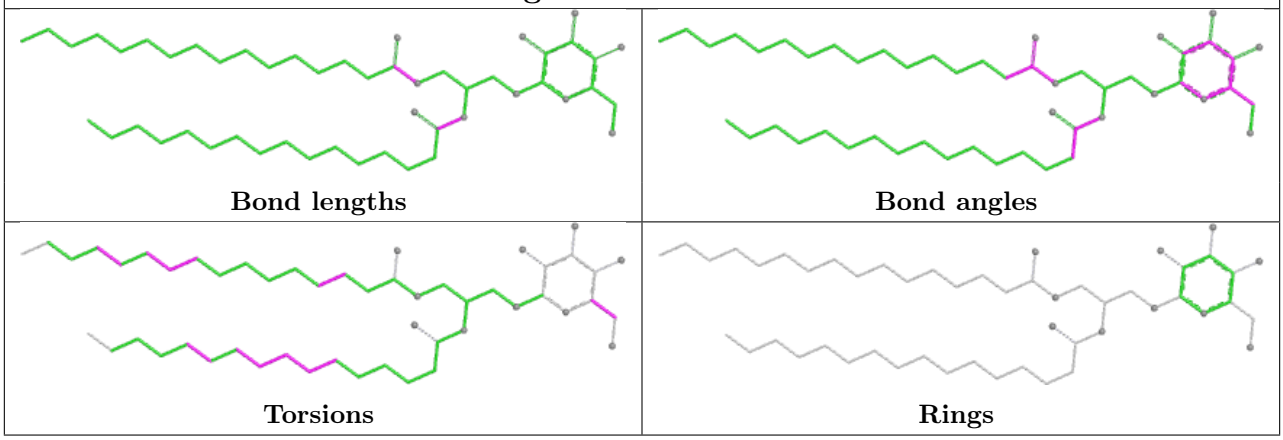


Rings

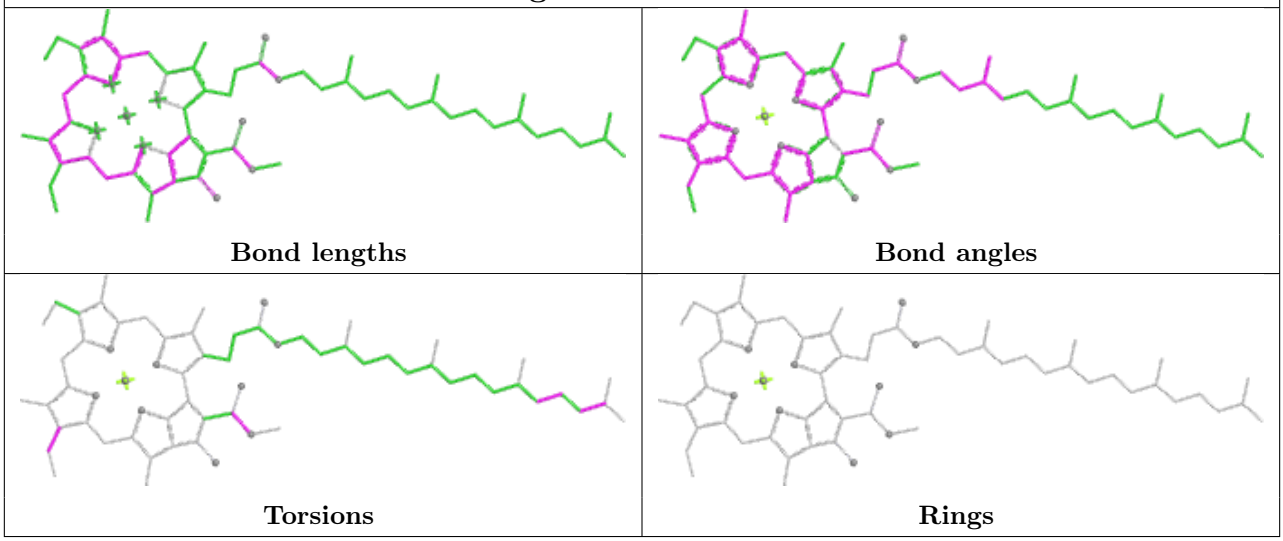
Ligand PL9 D 407 (A)



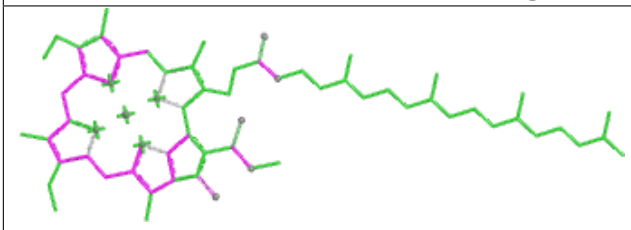
Ligand LMG d 415



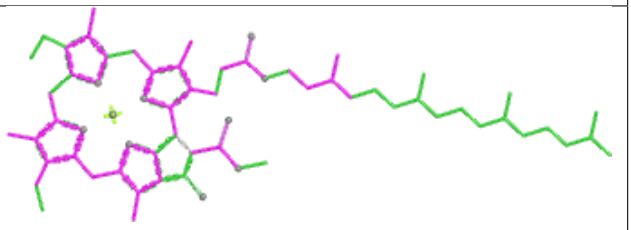
Ligand CLA a 409



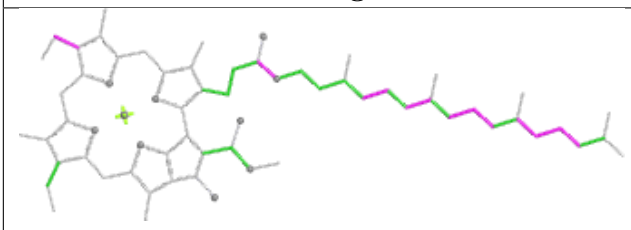
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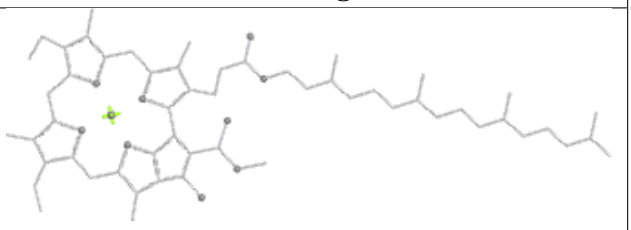
Bond lengths



Bond angles

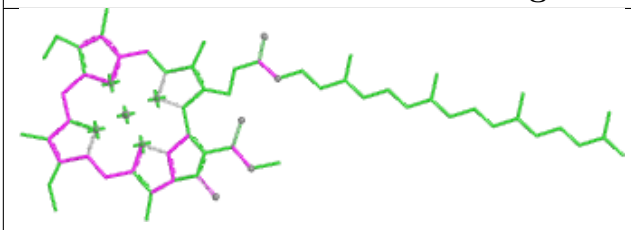


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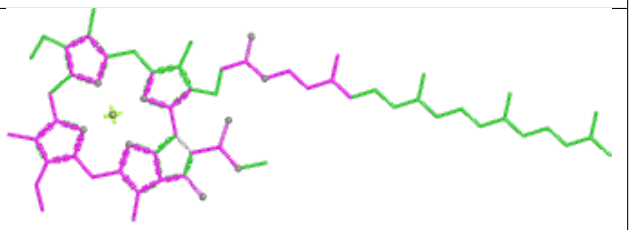


Rings

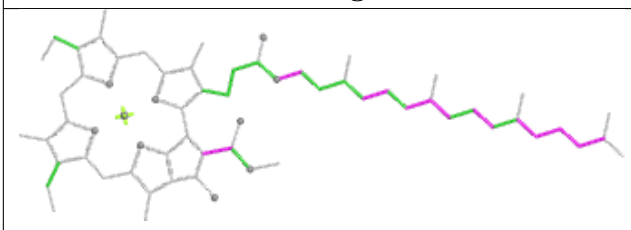
Ligand CLA c 513



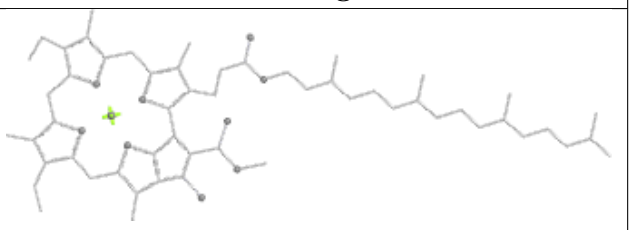
Bond lengths



Bond angles

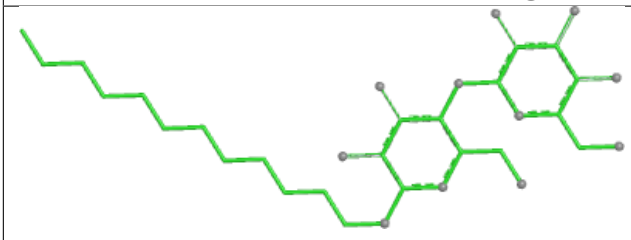


Torsions

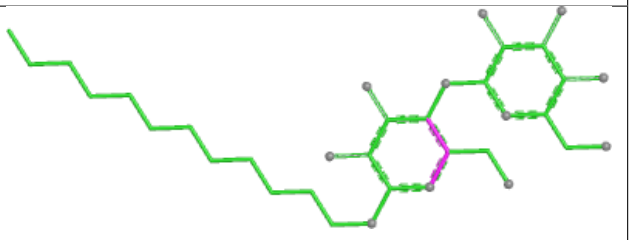


Rings

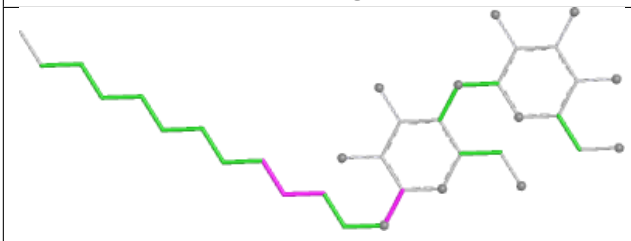
Ligand LMT E 102



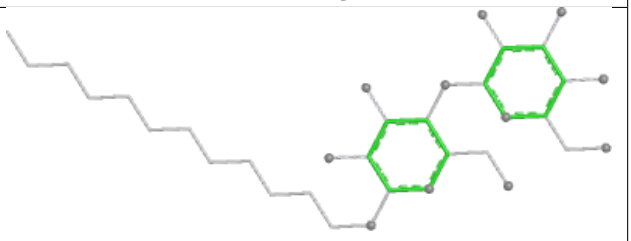
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Bond angles

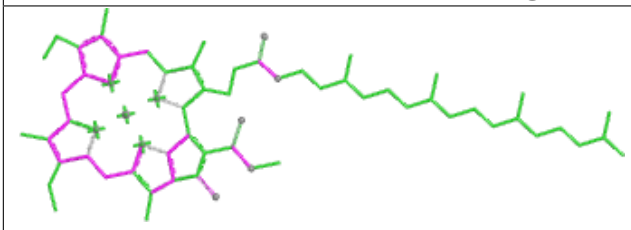


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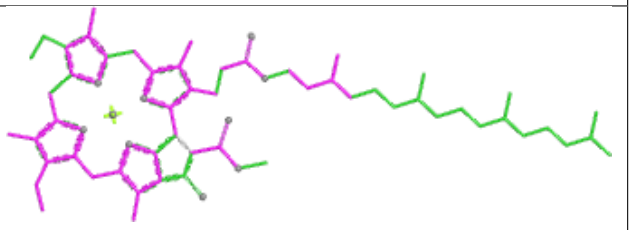


Rings

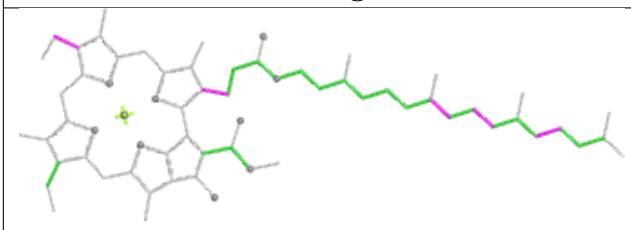
Ligand CLA A 407



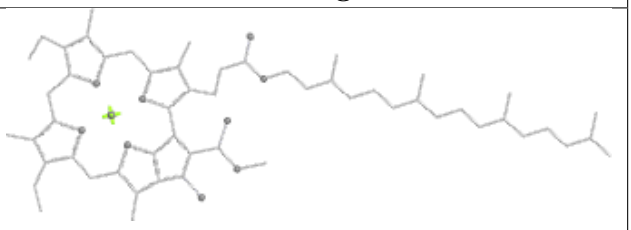
Bond lengths



Bond angles

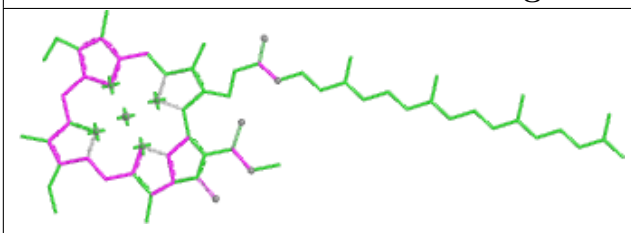


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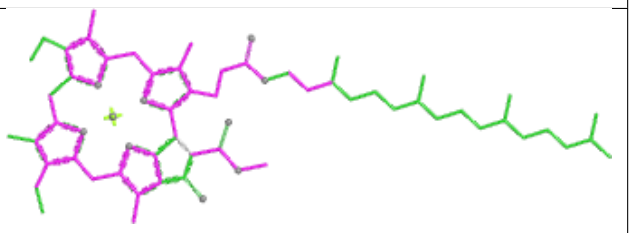


Rings

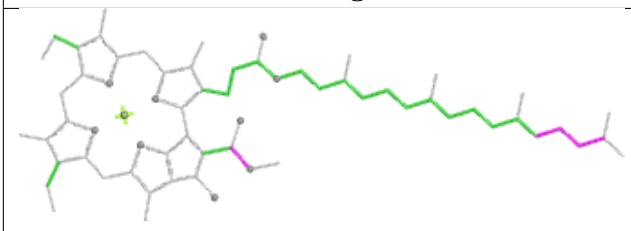
Ligand CLA A 405



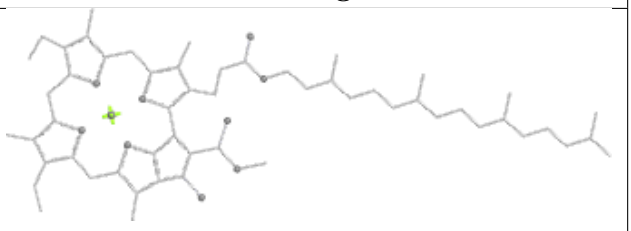
Bond lengths



Bond angles

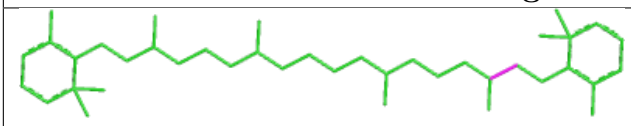


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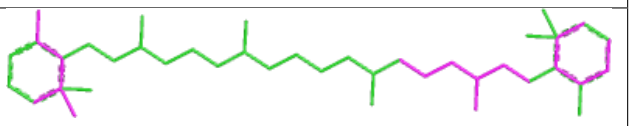


Rings

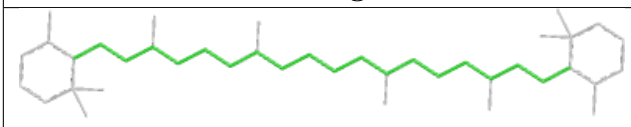
Ligand BCR B 619



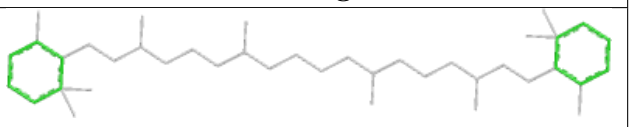
Bond lengths



Bond angles

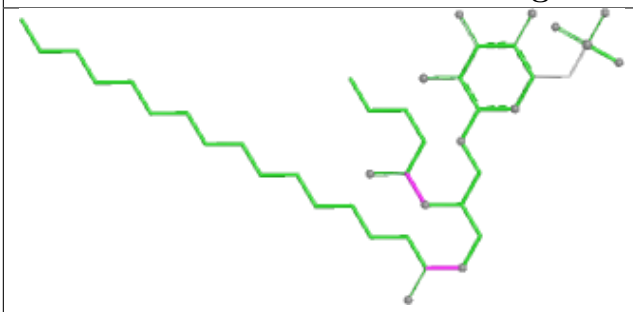


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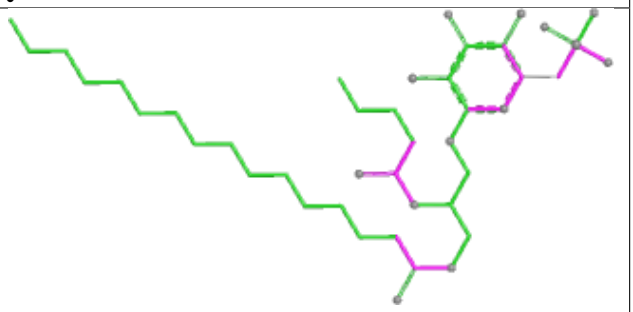


Rings

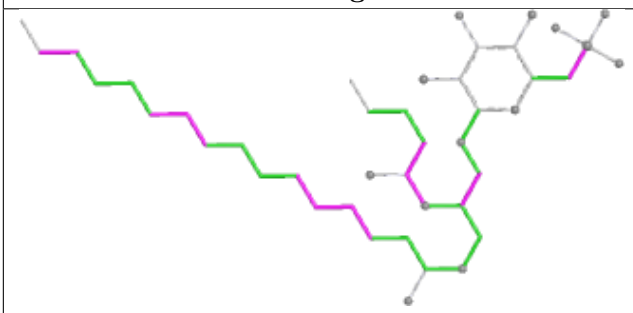
Ligand SQD f 102



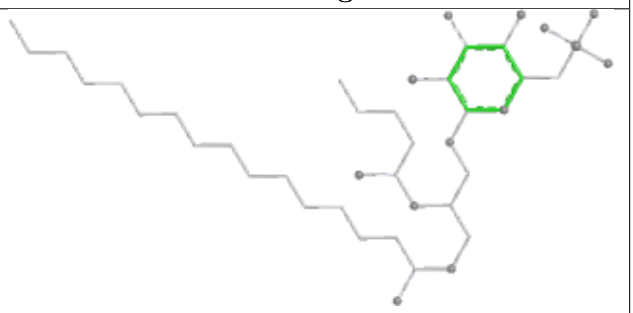
Bond lengths



Bond angles

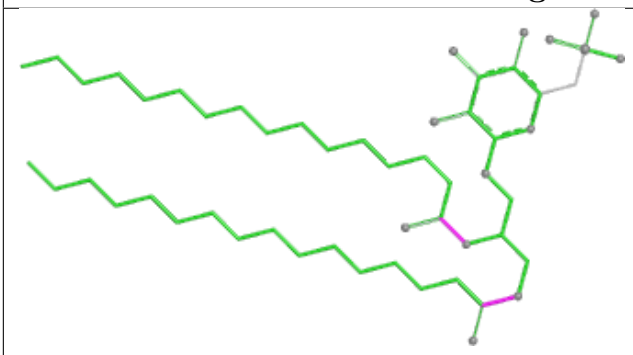


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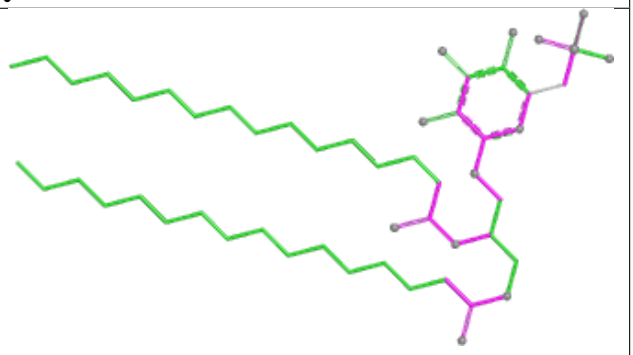


Rings

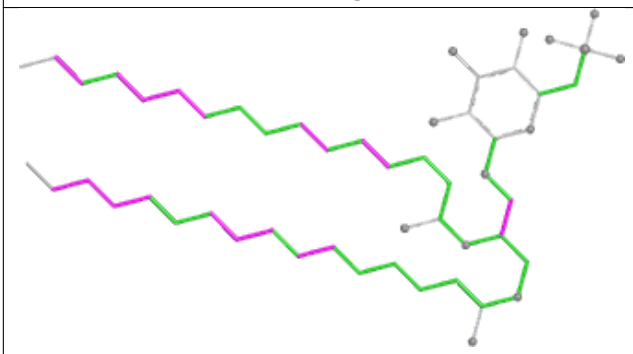
Ligand SQD a 414



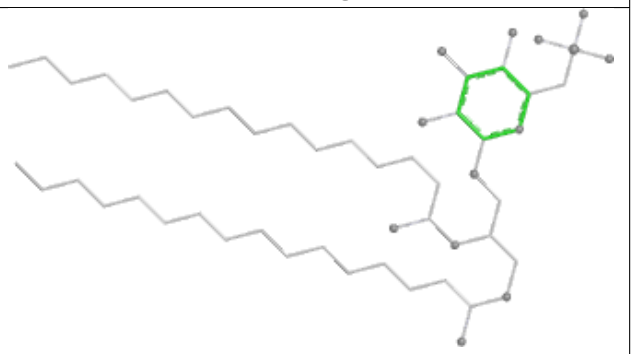
Bond lengths



Bond angles

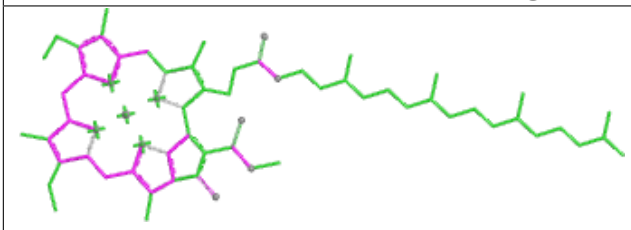


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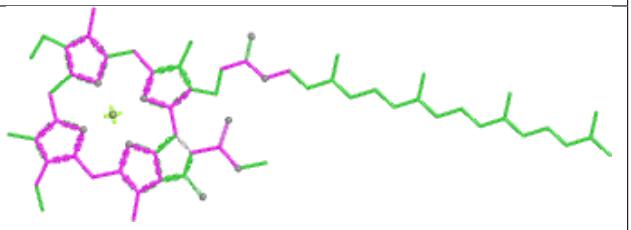


Rings

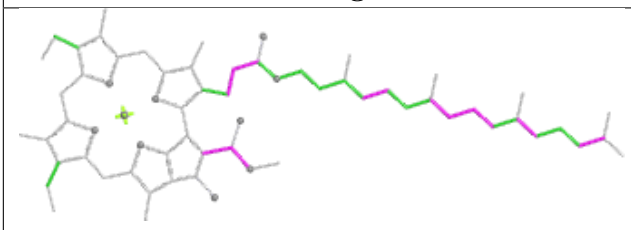
Ligand CLA B 602



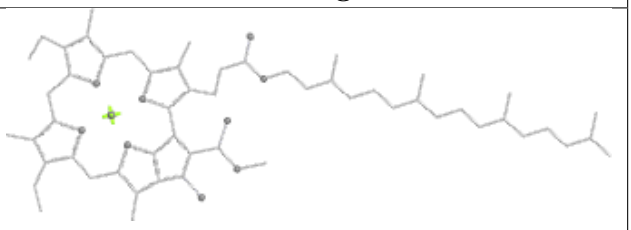
Bond lengths



Bond angles

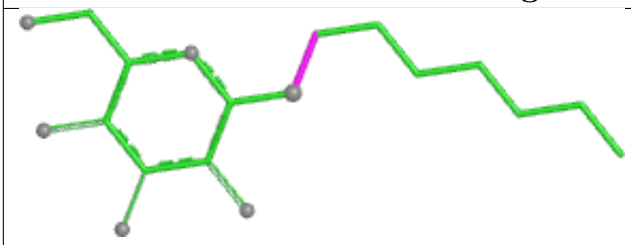


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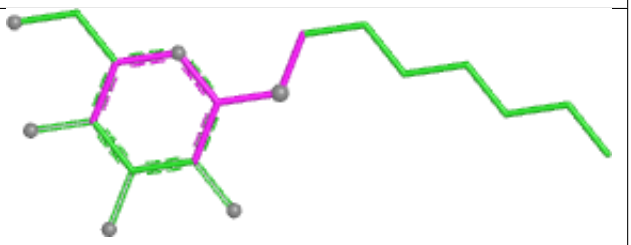


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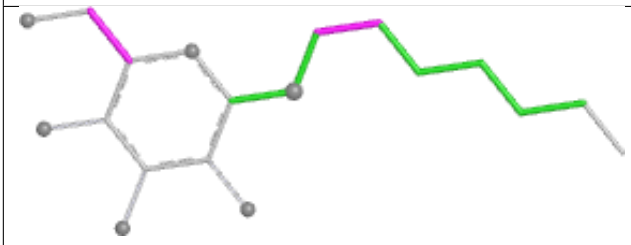
Ligand HTG C 523



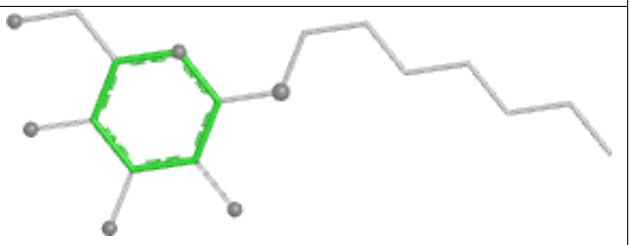
Bond lengths



Bond angles

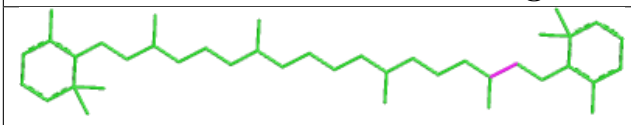


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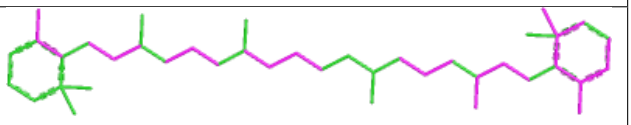


Rings

Ligand BCR d 406



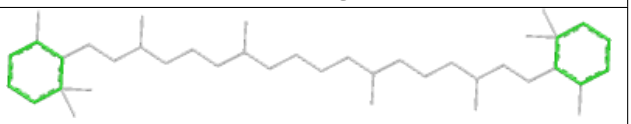
Bond lengths



Bond angles

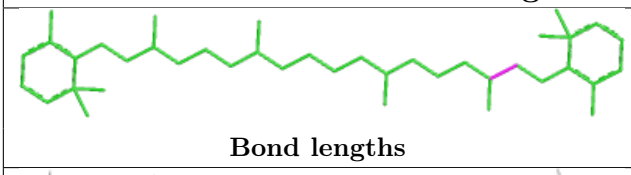


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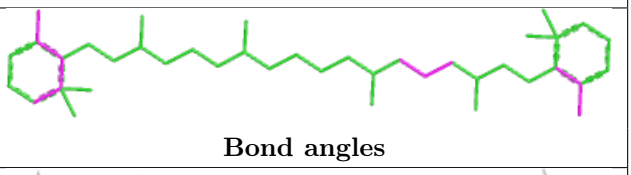


Rings

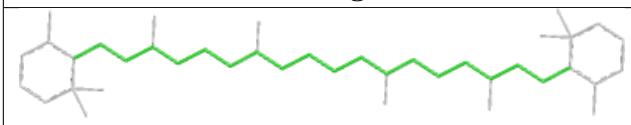
Ligand BCR A 410



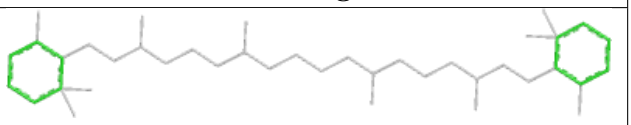
Bond lengths



Bond angles

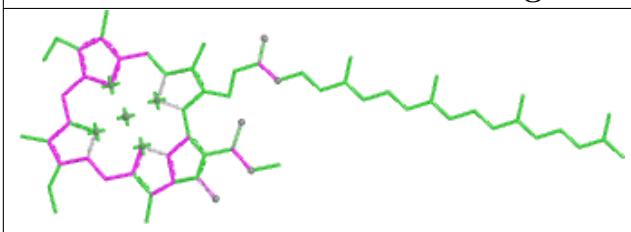


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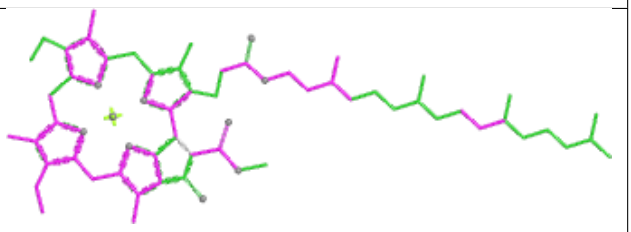


Rings

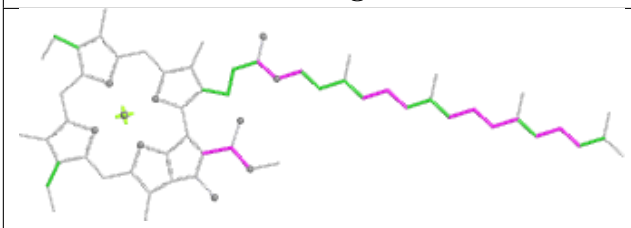
Ligand CLA C 509



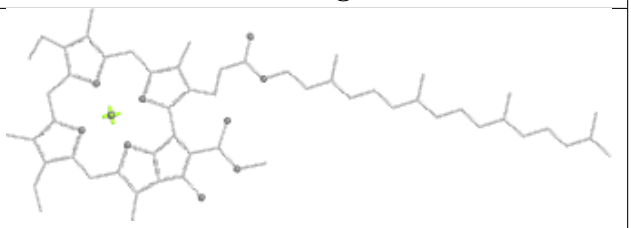
Bond lengths



Bond angles

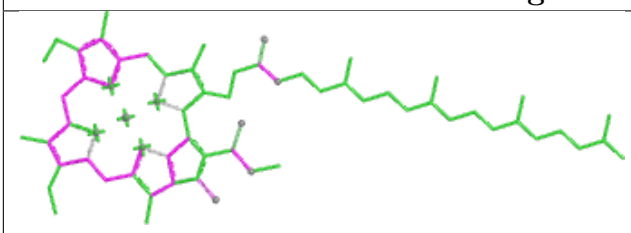


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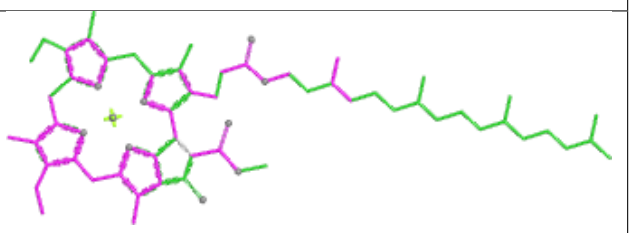


Rings

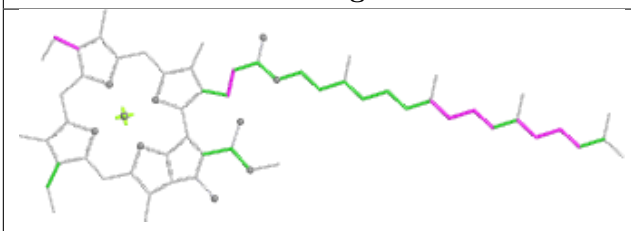
Ligand CLA b 615



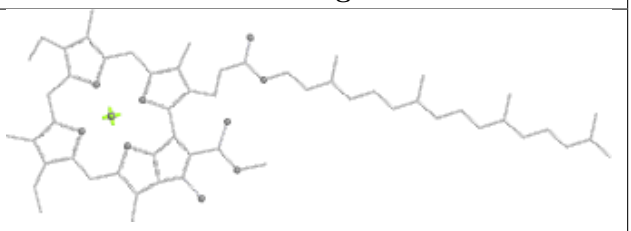
Bond lengths



Bond angles

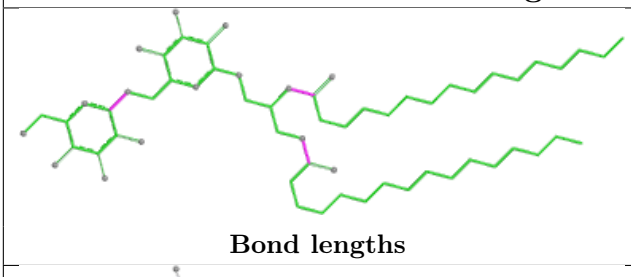


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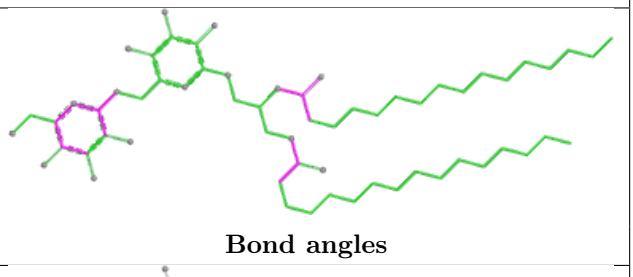


Rings

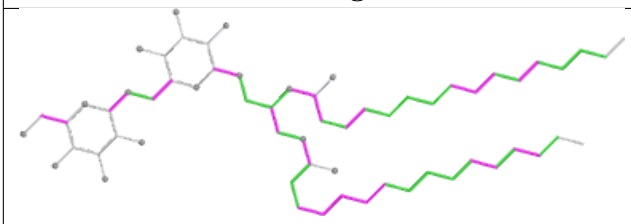
Ligand DGD e 101



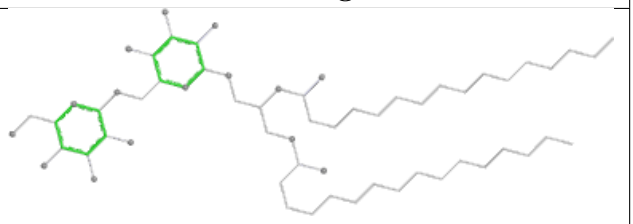
Bond lengths



Bond angles

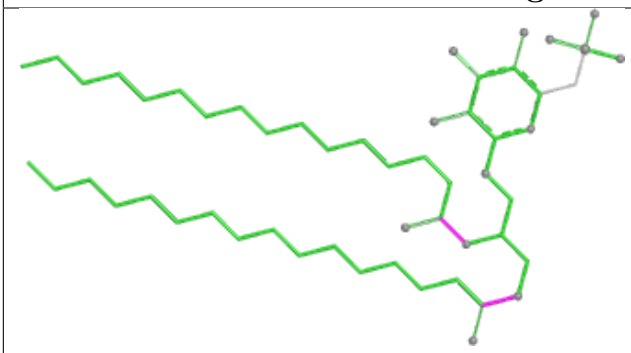


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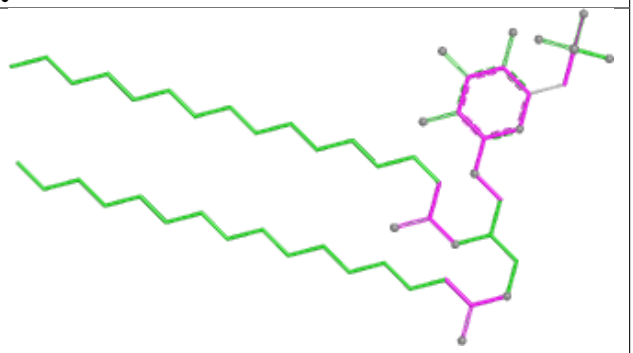


Rings

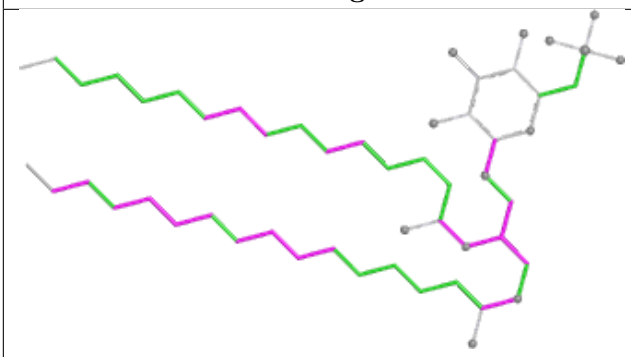
Ligand SQD L 102



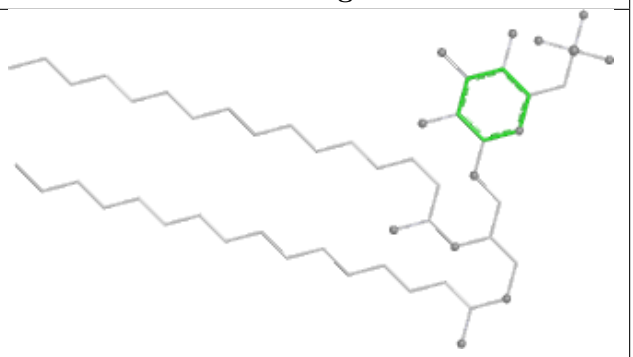
Bond lengths



Bond angles

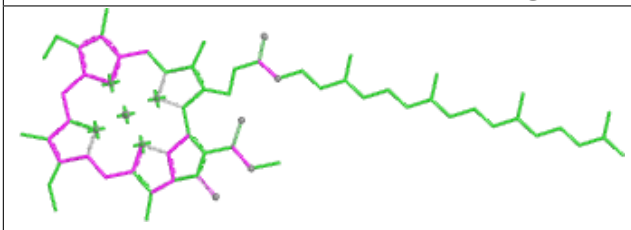


Torsions

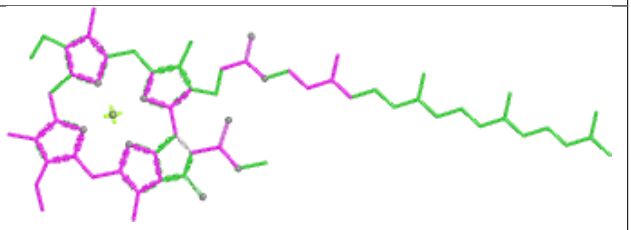


Rings

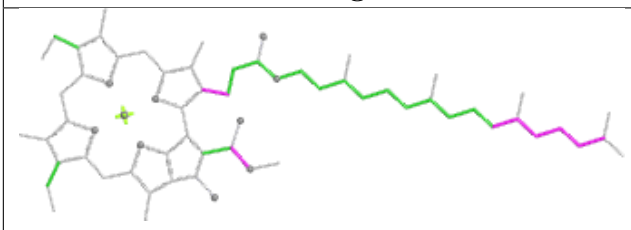
Ligand CLA C 501



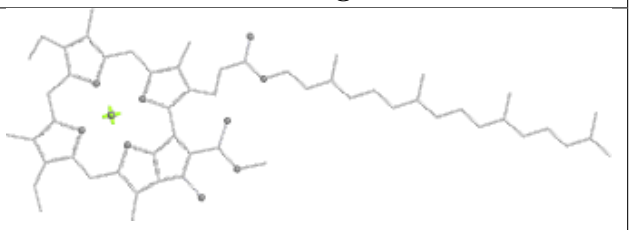
Bond lengths



Bond angles



Torsions

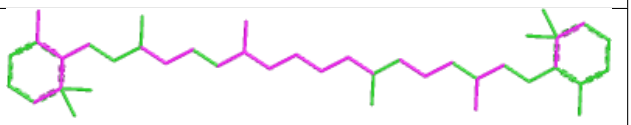


Rings

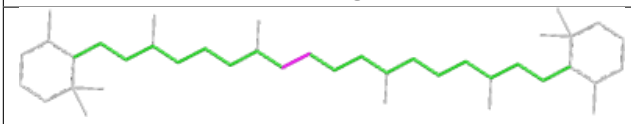
Ligand BCR T 103



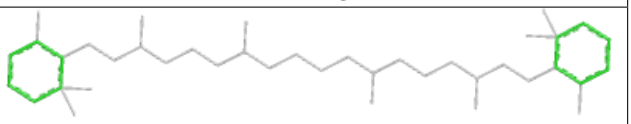
Bond lengths



Bond angles

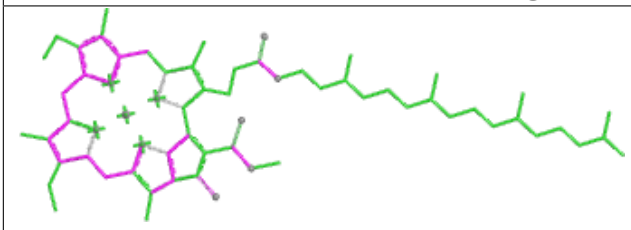


Torsions

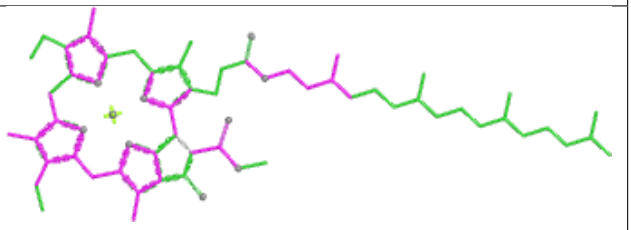


Rings

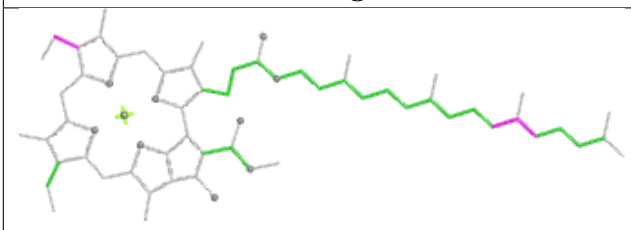
Ligand CLA C 505



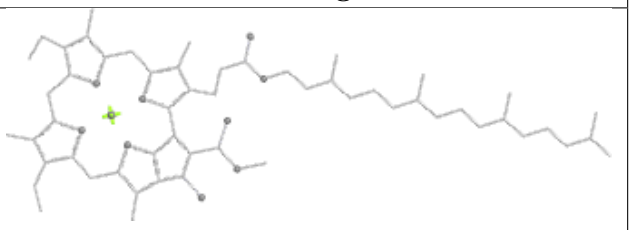
Bond lengths



Bond angles

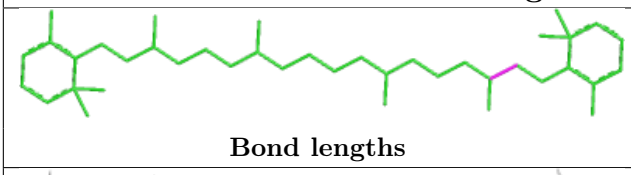


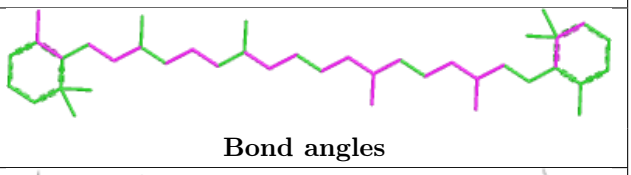
Torsions

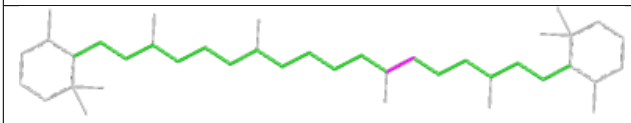


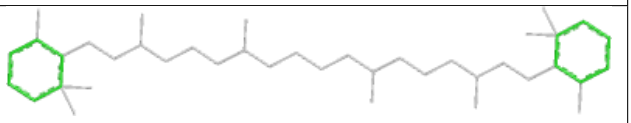
Rings

Ligand BCR b 626


Bond lengths

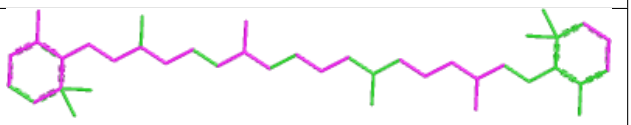

Bond angles

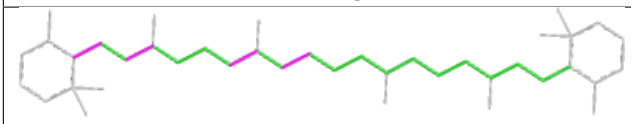

Torsions

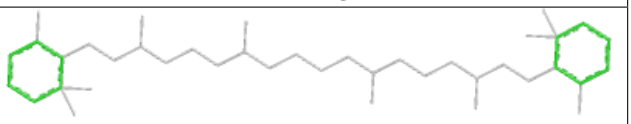

Rings

Ligand BCR t 102

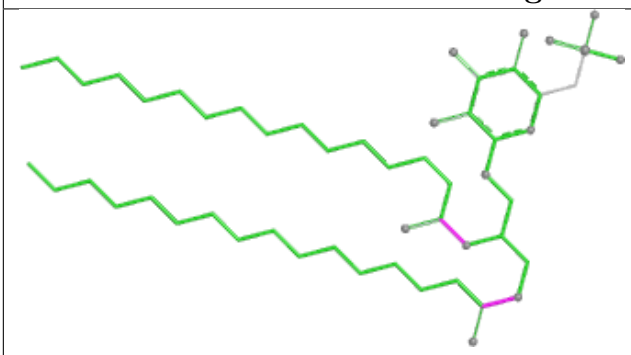

Bond lengths

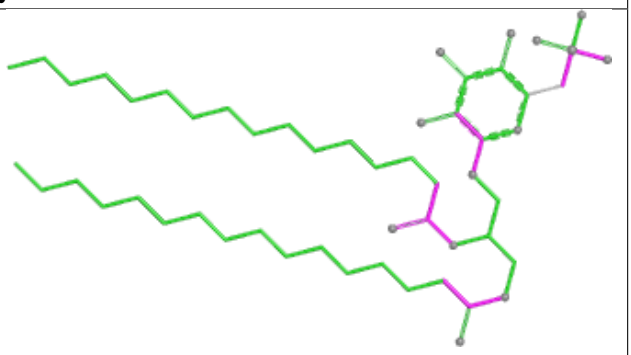

Bond angles

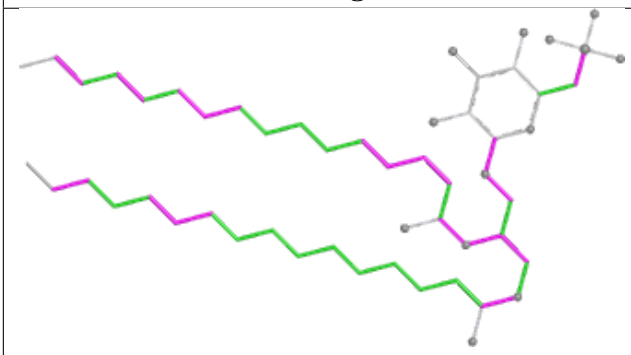

Torsions

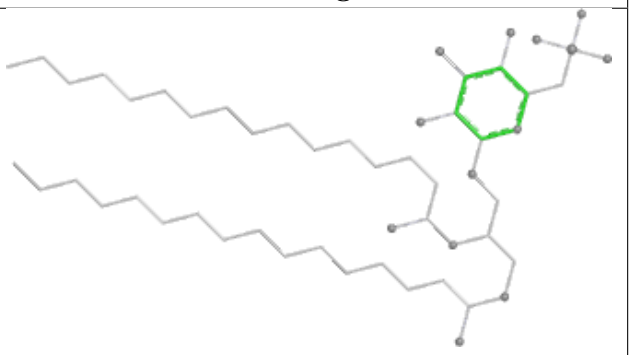

Rings

Ligand SQD B 621

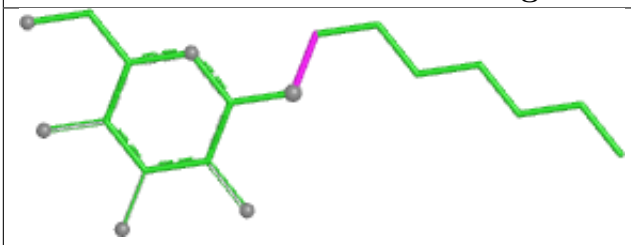

Bond lengths


Bond angles

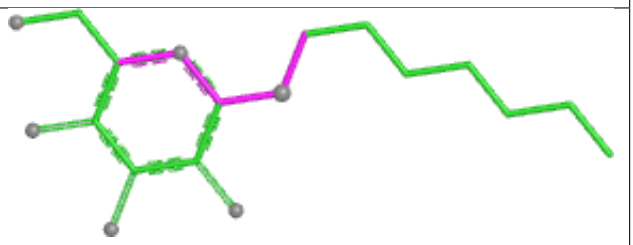

Torsions


Rings

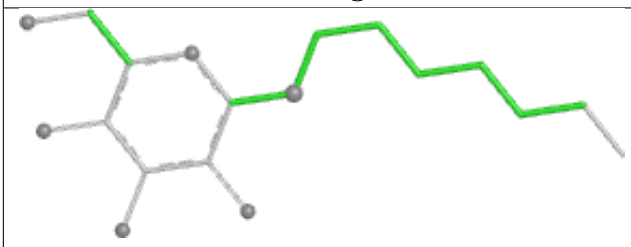
Ligand HTG B 632



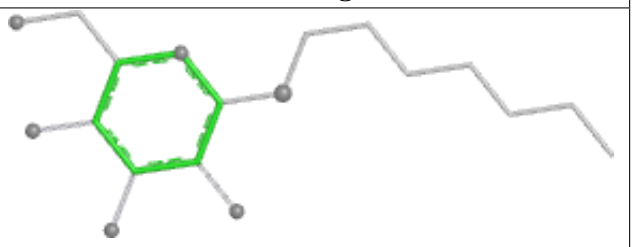
Bond lengths



Bond angles



Torsions

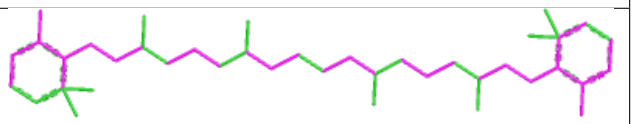


Rings

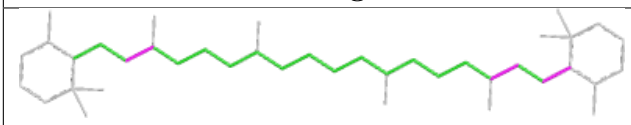
Ligand BCR D 406



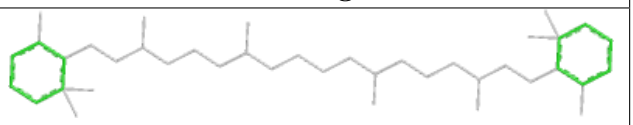
Bond lengths



Bond angles

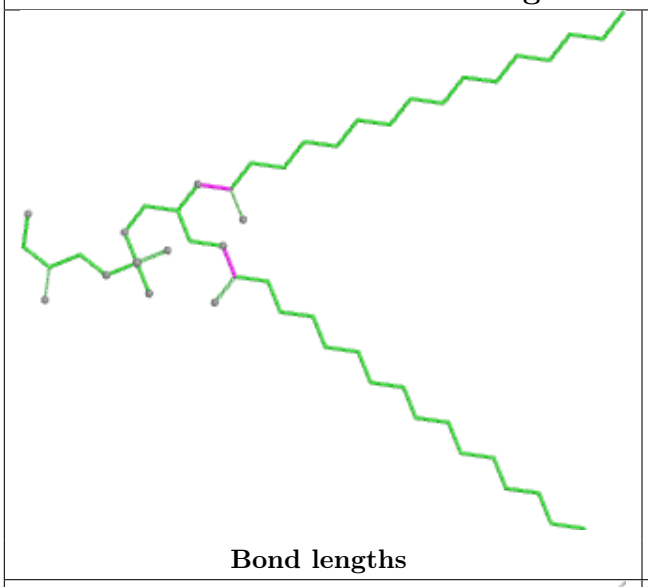


Torsions

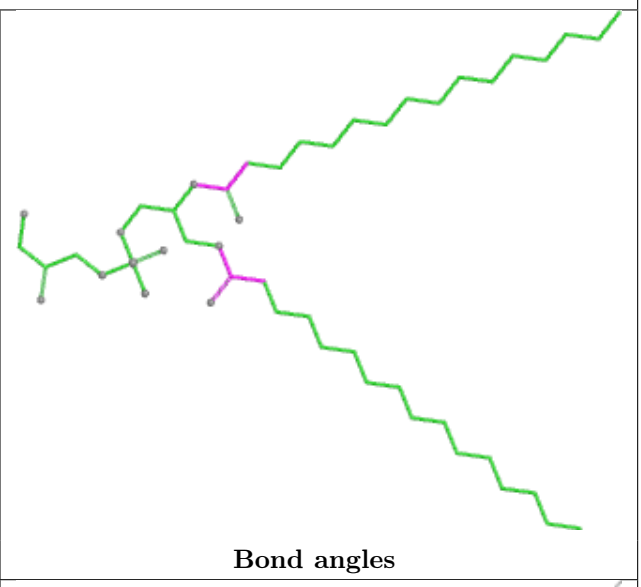


Rings

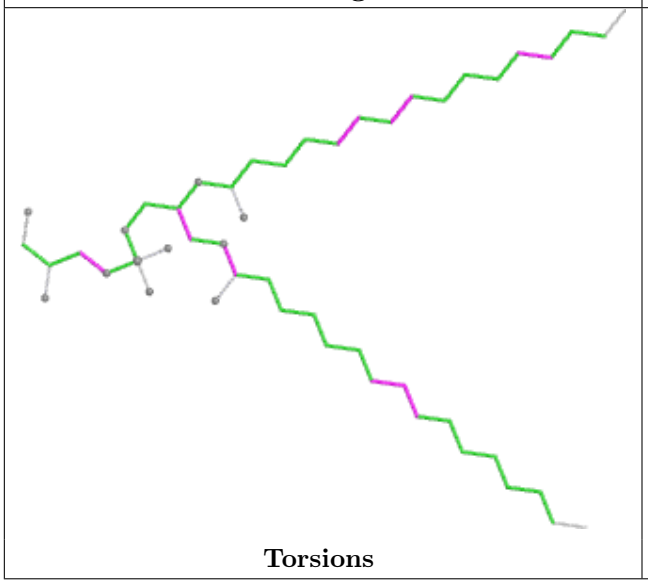
Ligand LHG D 411



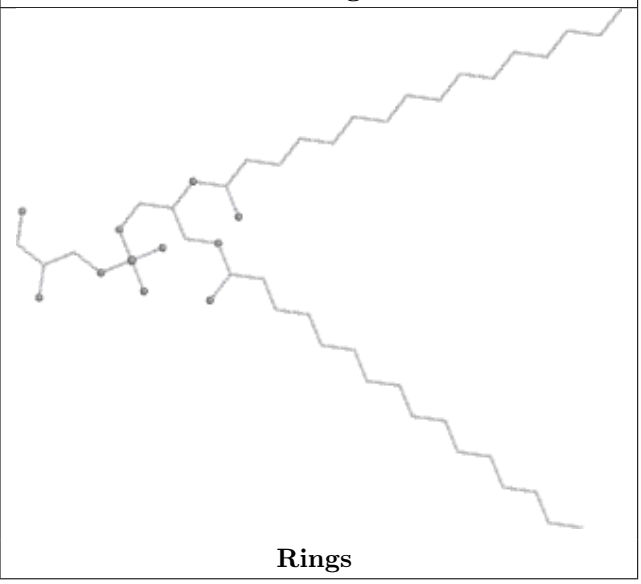
Bond lengths



Bond angles

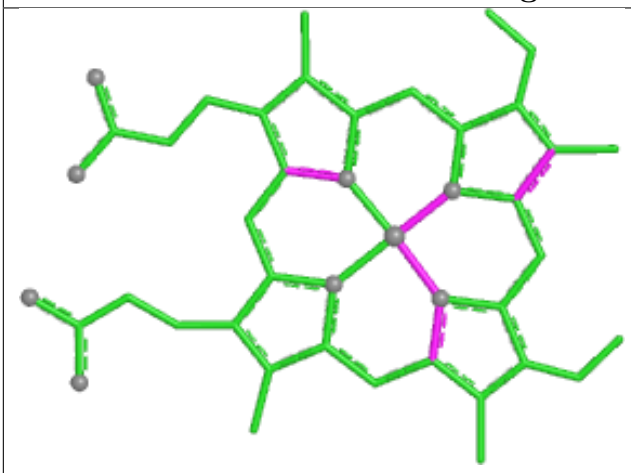


Torsions

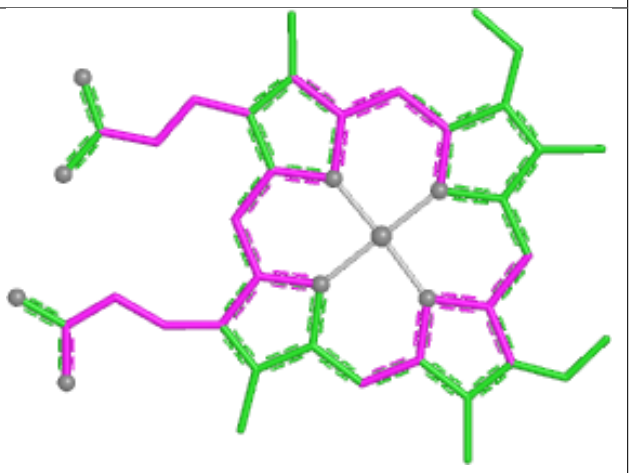


Rings

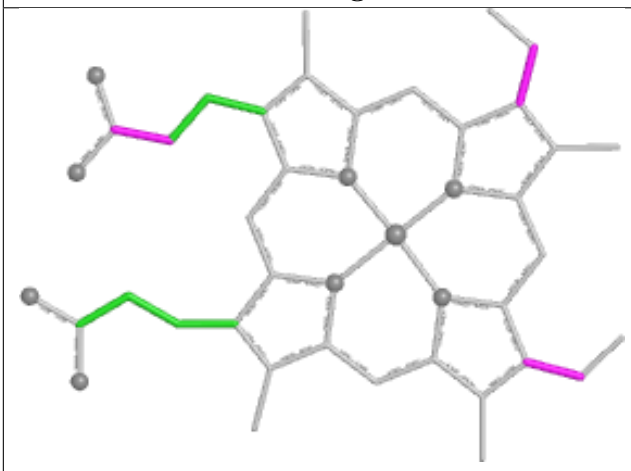
Ligand HEM E 103



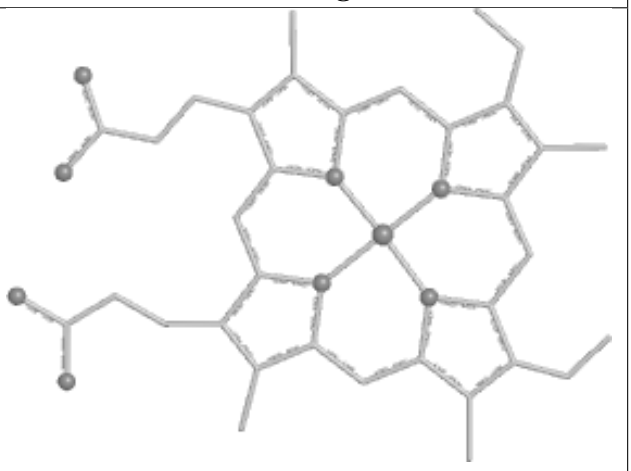
Bond lengths



Bond angles

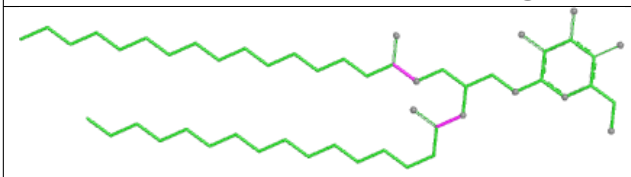


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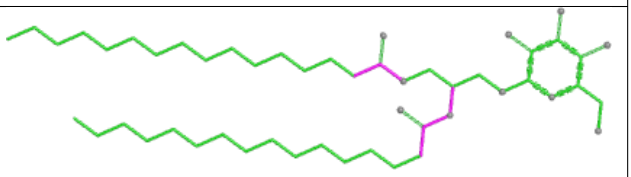


Rings

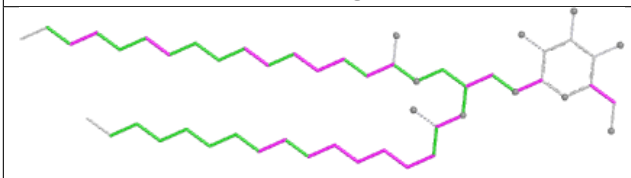
Ligand LMG A 419



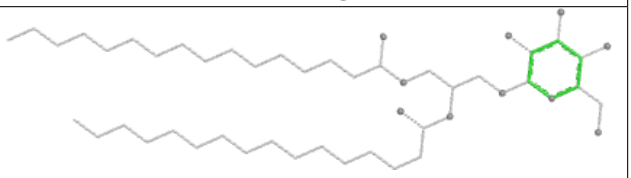
Bond lengths



Bond angles

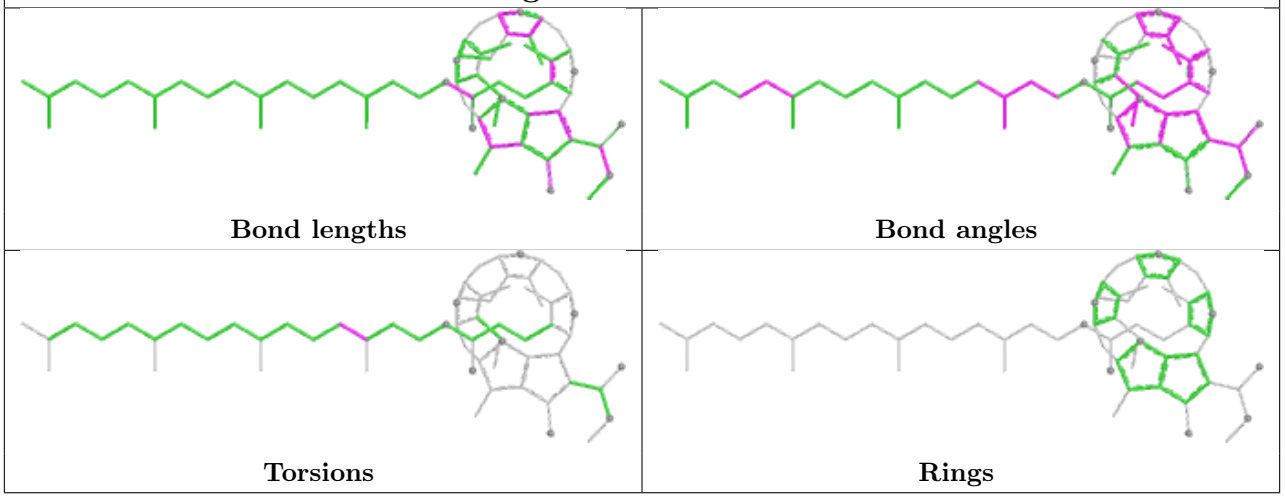


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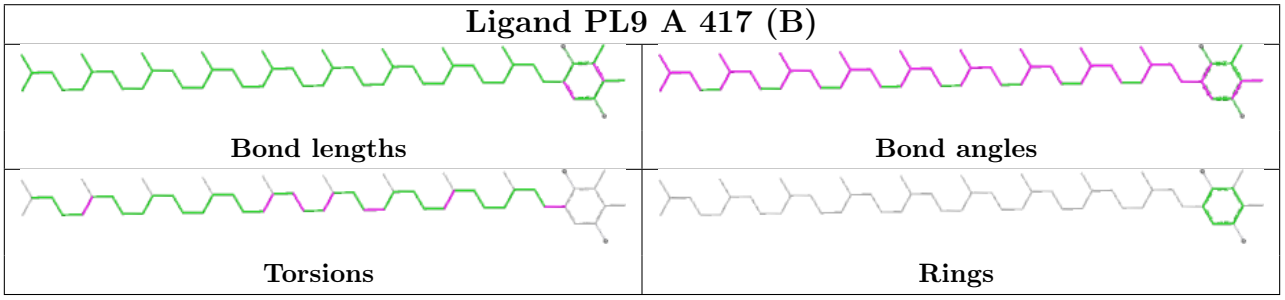


Rings

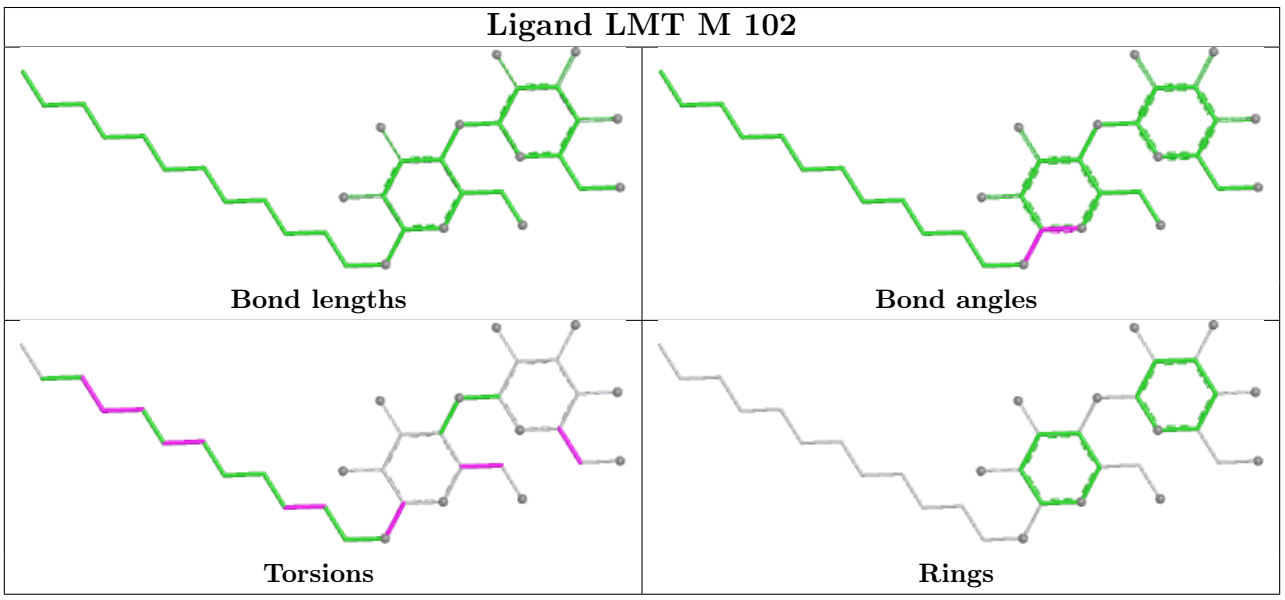
Ligand PHO A 408



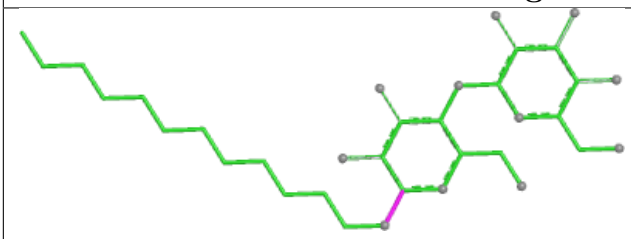
Ligand PL9 A 417 (B)



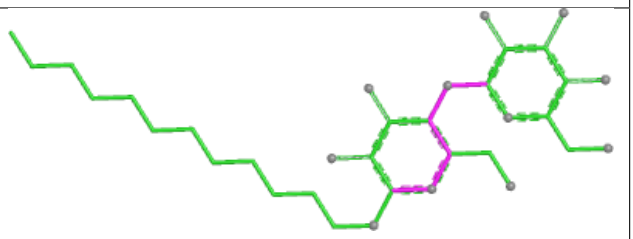
Ligand LMT M 102



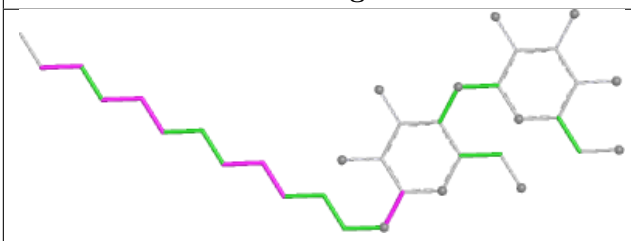
Ligand LMT a 404



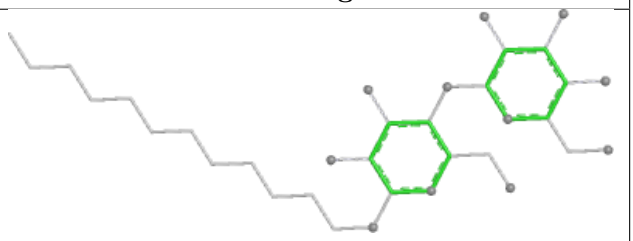
Bond lengths



Bond angles

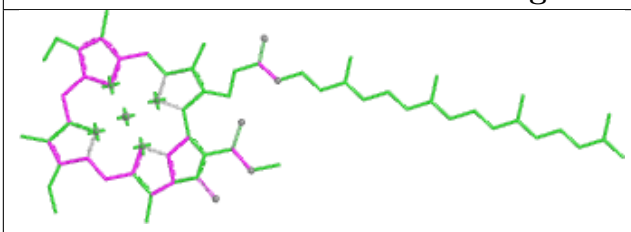


Torsions

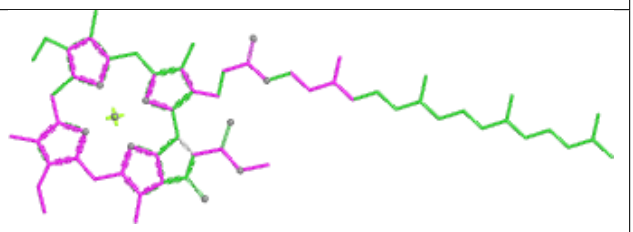


Rings

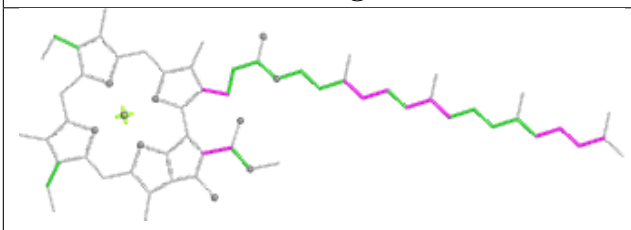
Ligand CLA c 510



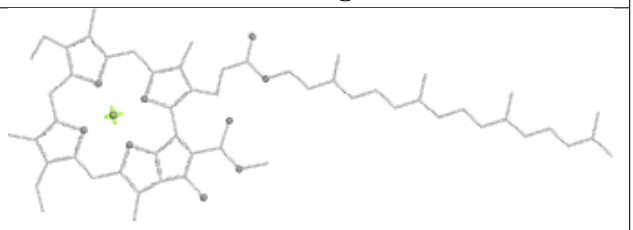
Bond lengths



Bond angles

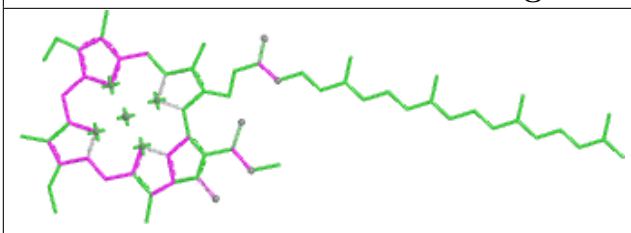


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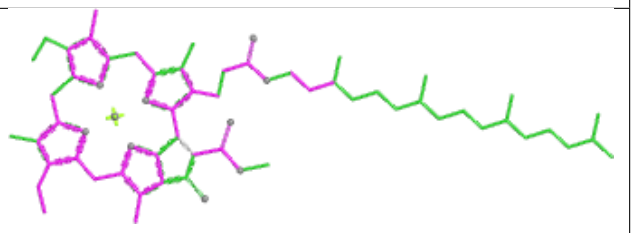


Rings

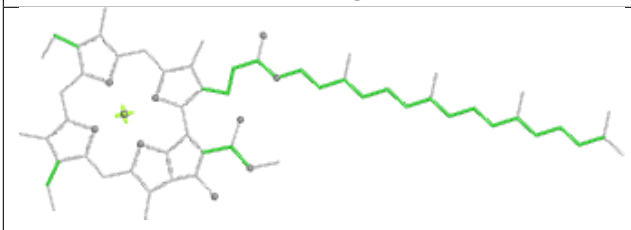
Ligand CLA B 609



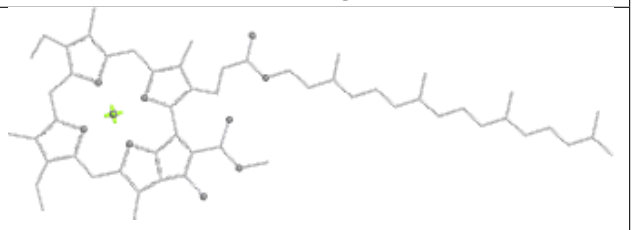
Bond lengths



Bond angles

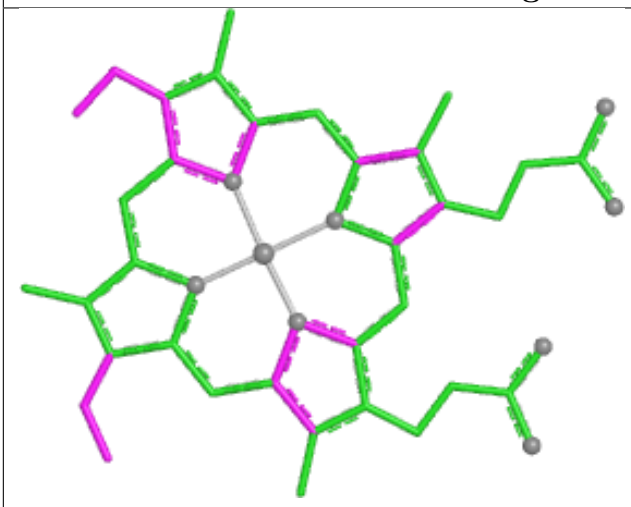


Torsions

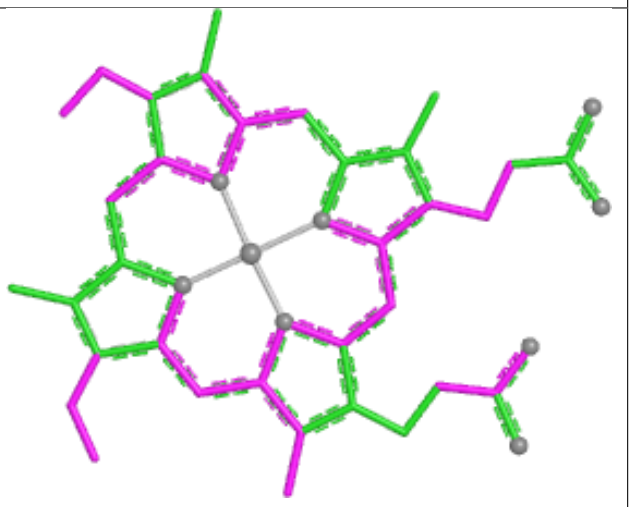


Rings

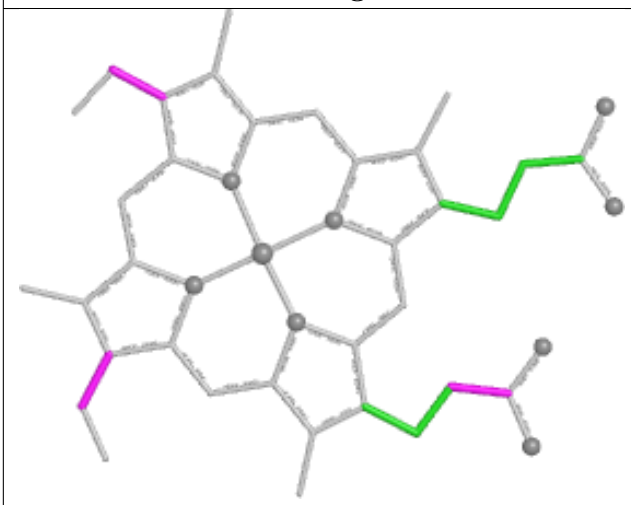
Ligand HEC V 205



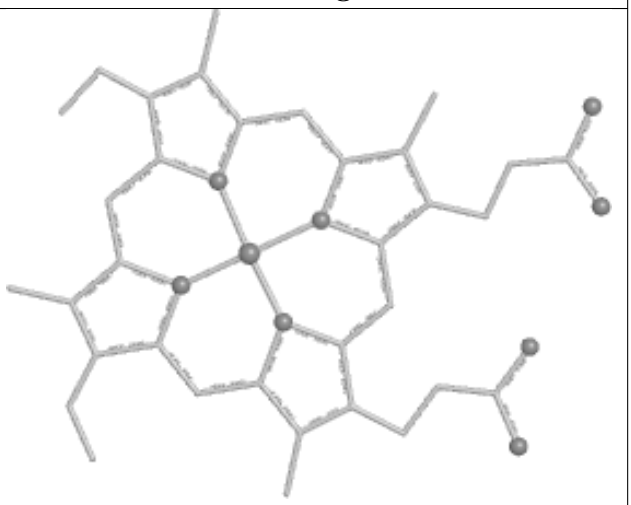
Bond lengths



Bond angles

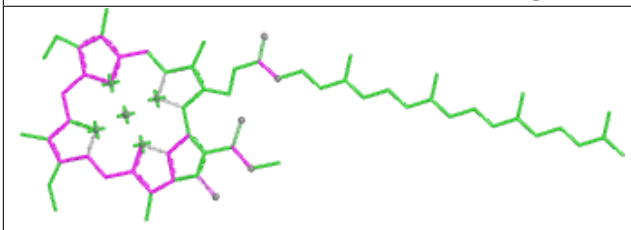


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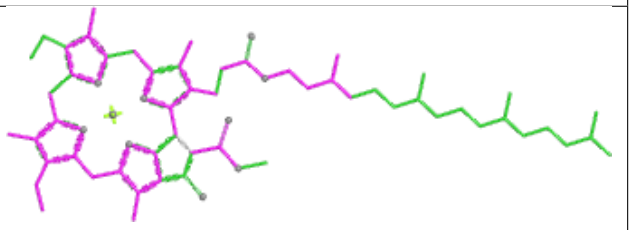


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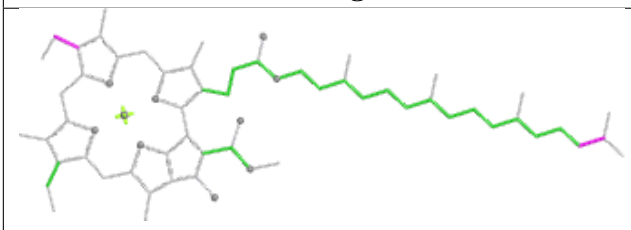
Ligand CLA b 611



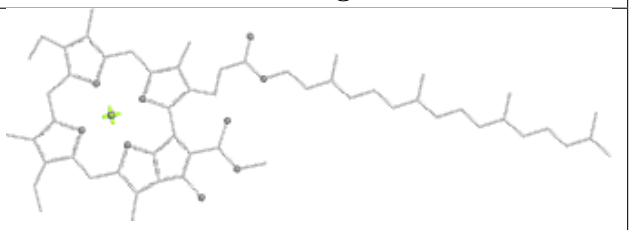
Bond lengths



Bond angles

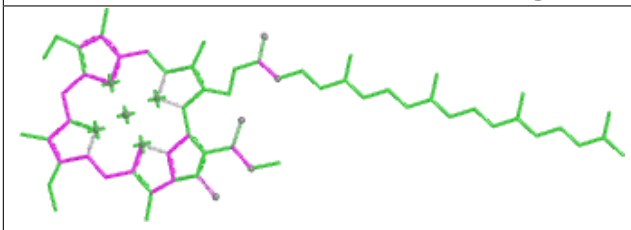


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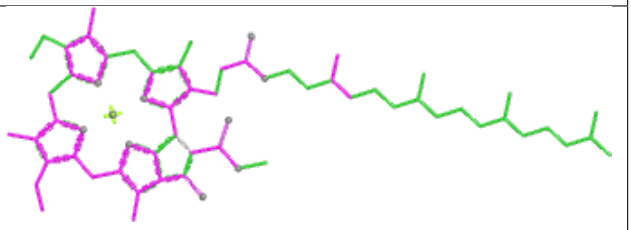


Rings

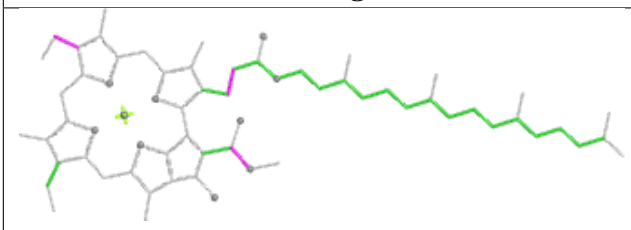
Ligand CLA c 505



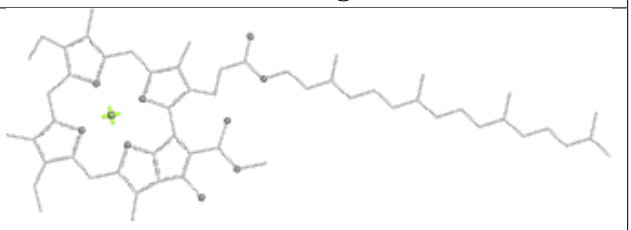
Bond lengths



Bond angles

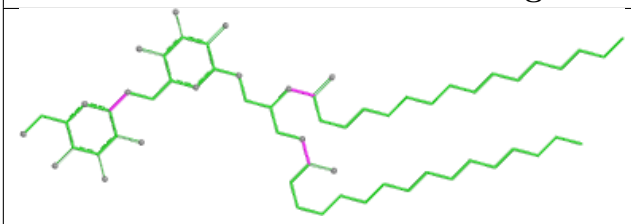


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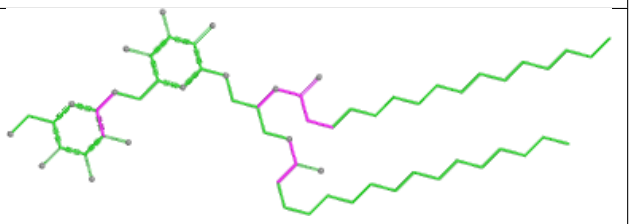


Rings

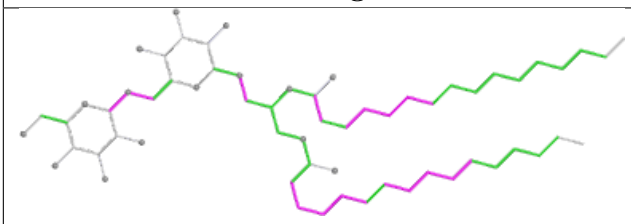
Ligand DGD c 520



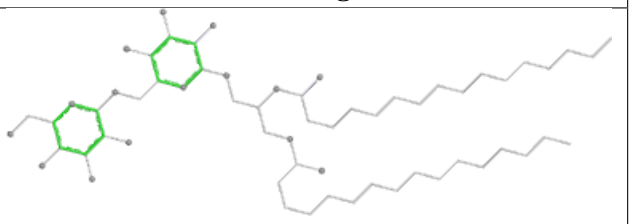
Bond lengths



Bond angles

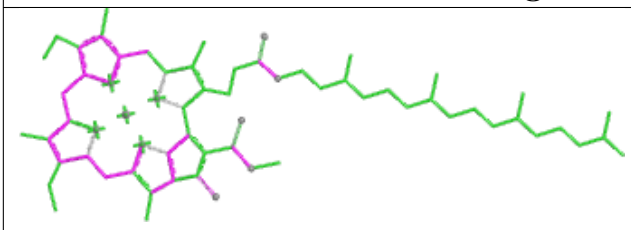


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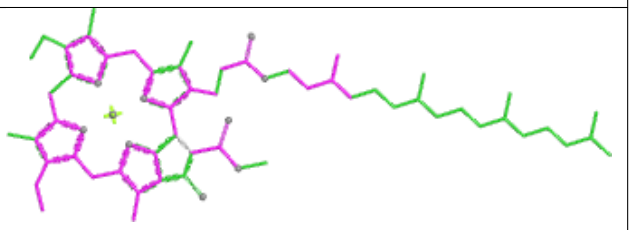


Rings

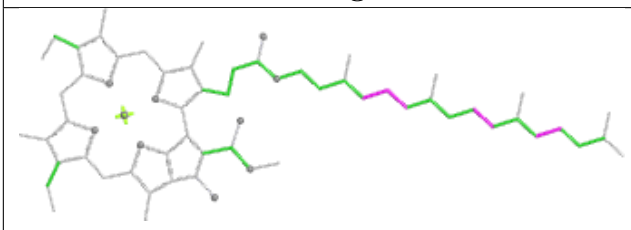
Ligand CLA C 508



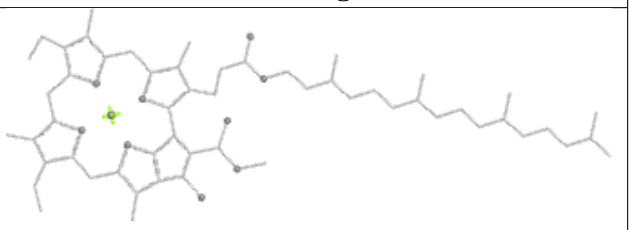
Bond lengths



Bond angles

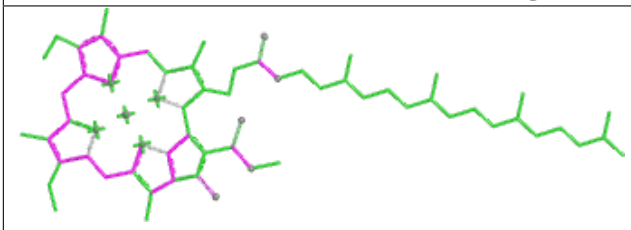


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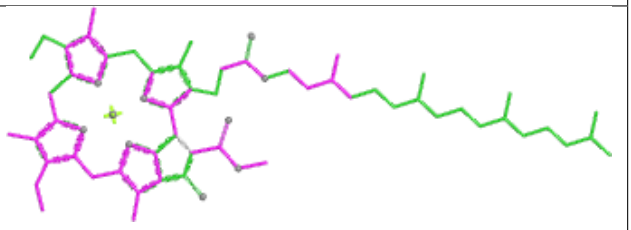


Rings

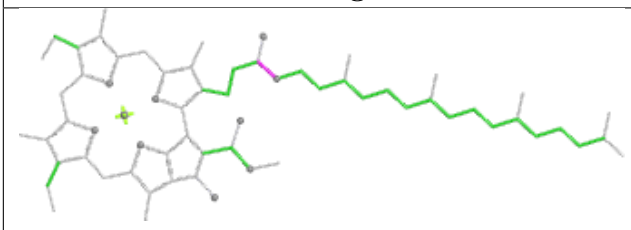
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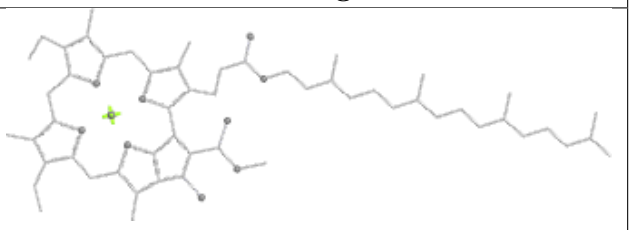
Bond lengths



Bond angles

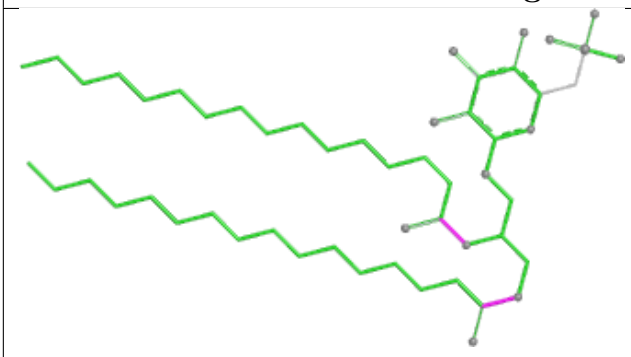


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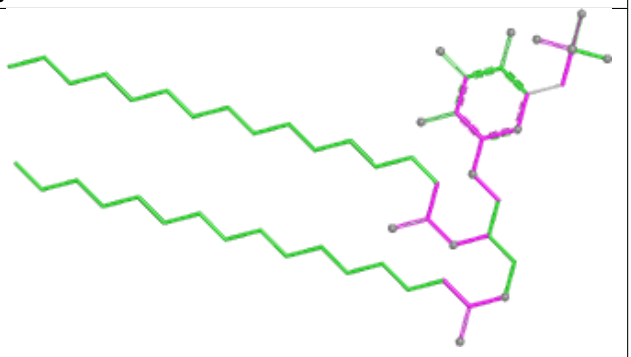


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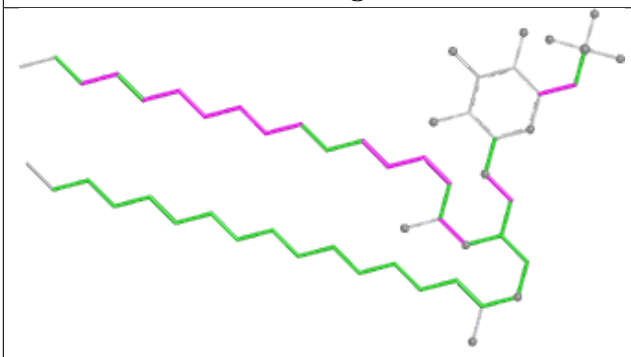
Ligand SQD A 411



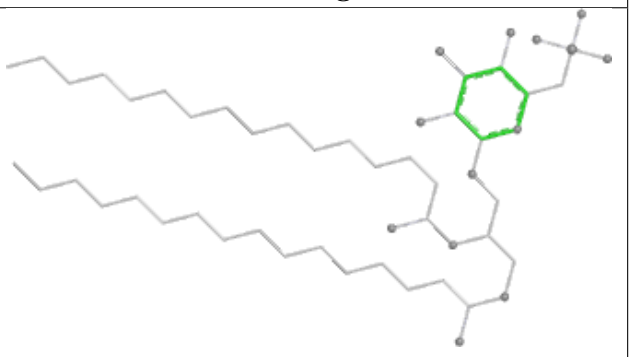
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Bond angles

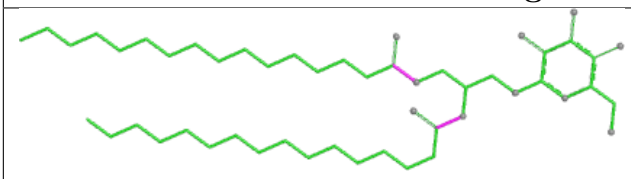


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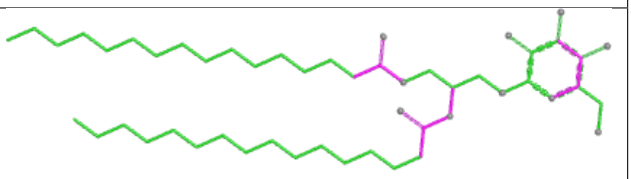


Rings

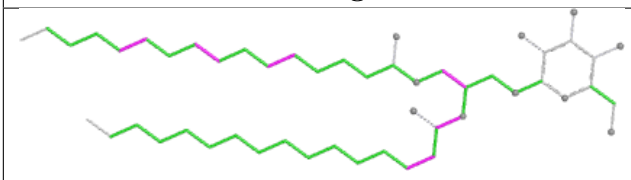
Ligand LMG c 522



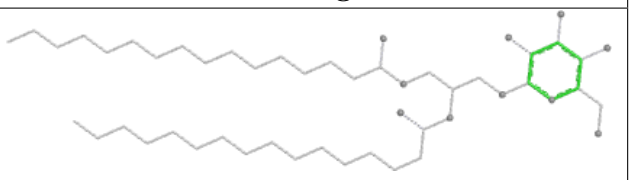
Bond lengths



Bond angles

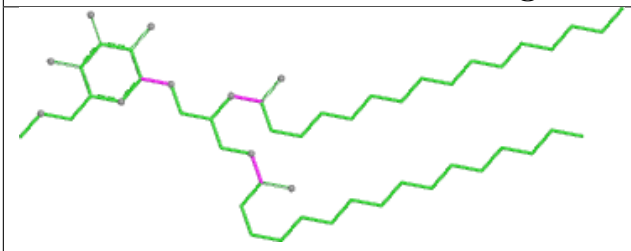


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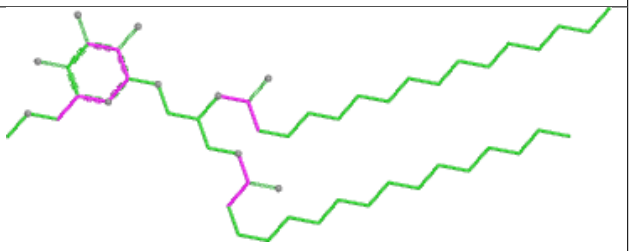


Rings

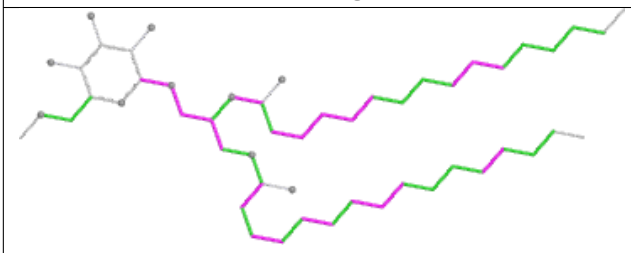
Ligand DGD D 408



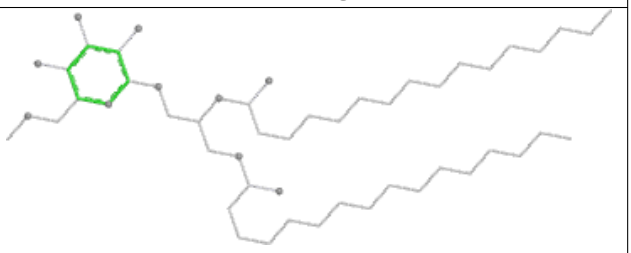
Bond lengths



Bond angles

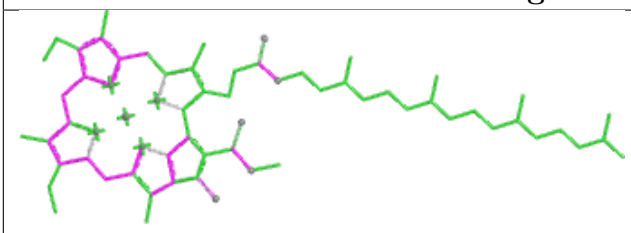


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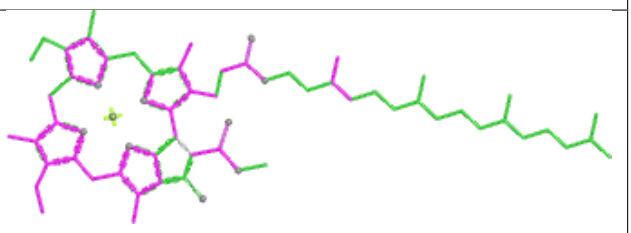


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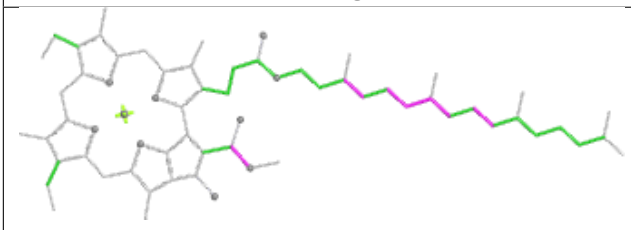
Ligand CLA b 612



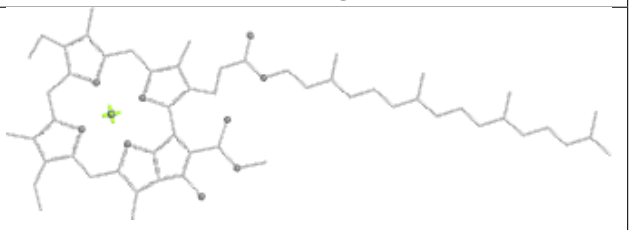
Bond lengths



Bond angles

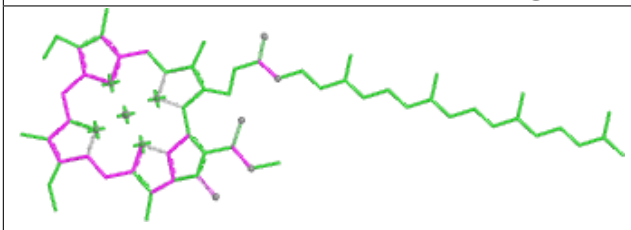


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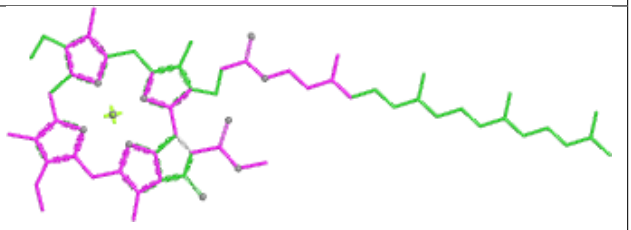


Rings

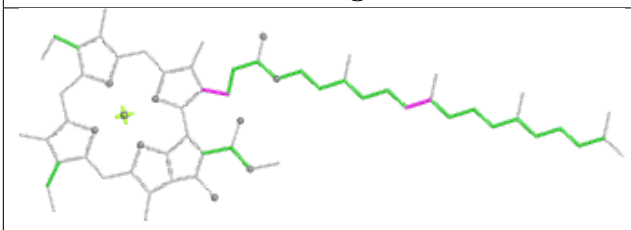
Ligand CLA b 618



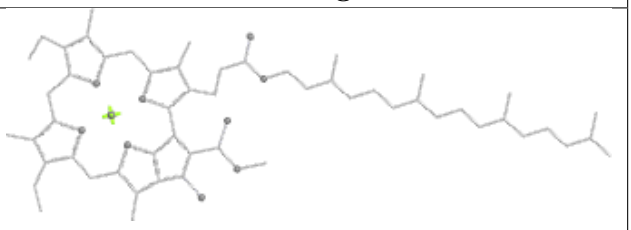
Bond lengths



Bond angles

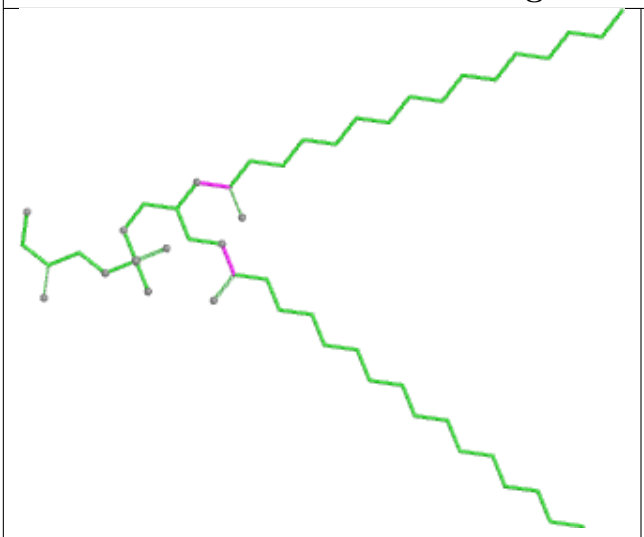


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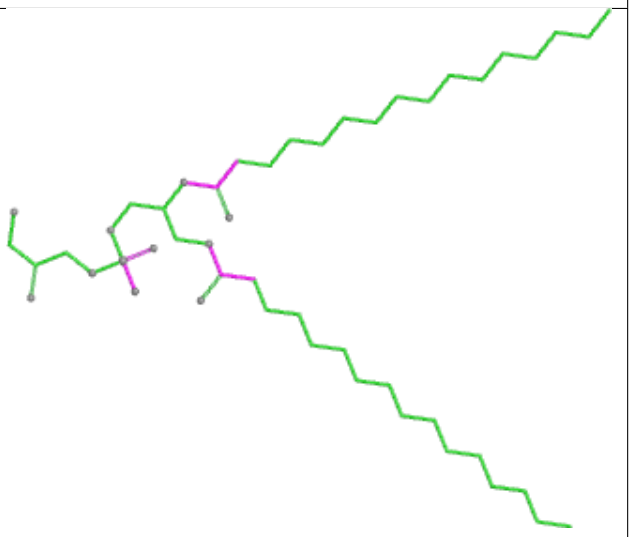


Rings

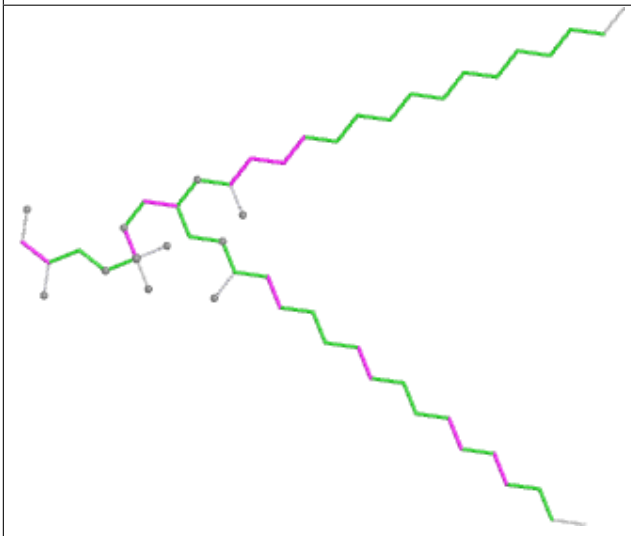
Ligand LHG b 634



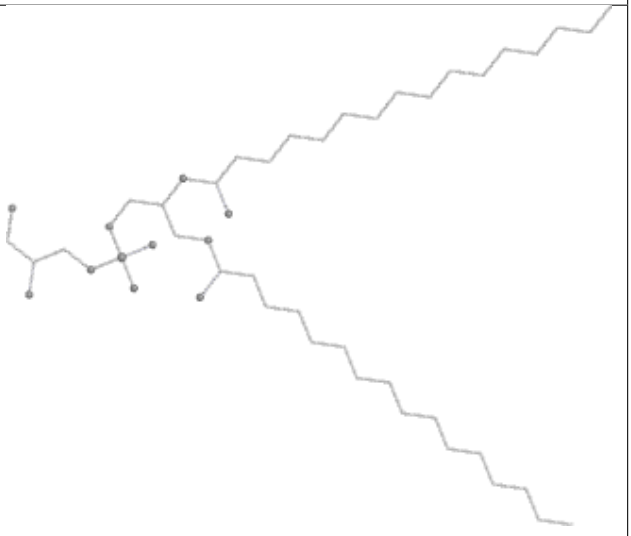
Bond lengths



Bond angles

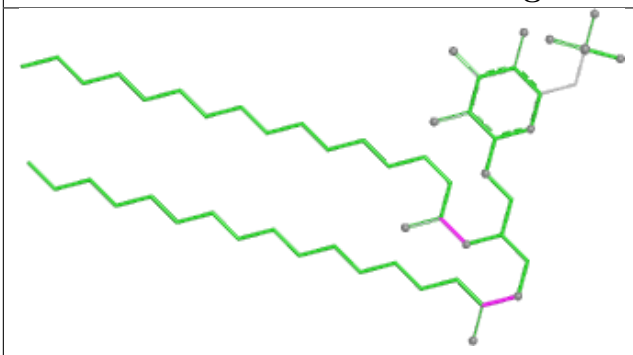


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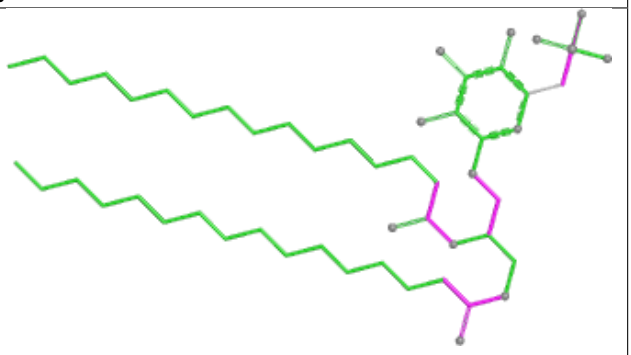


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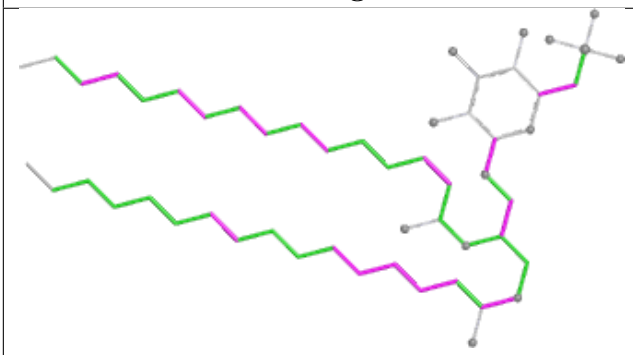
Ligand SQD A 413



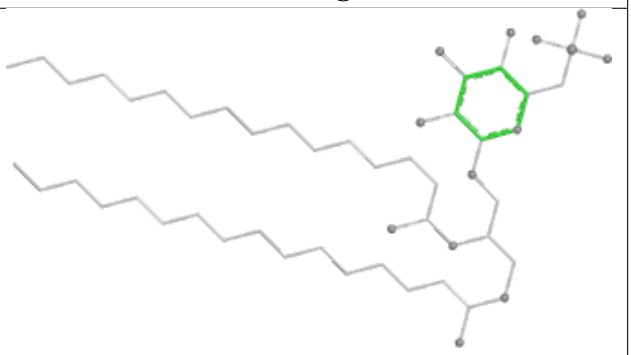
Bond lengths



Bond angles

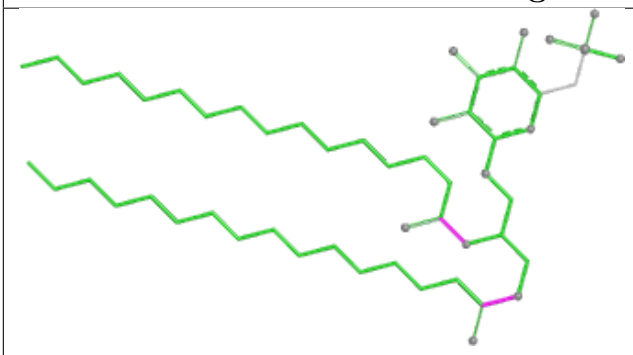


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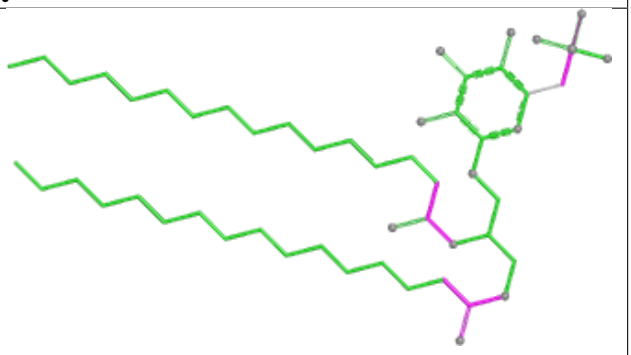


Rings

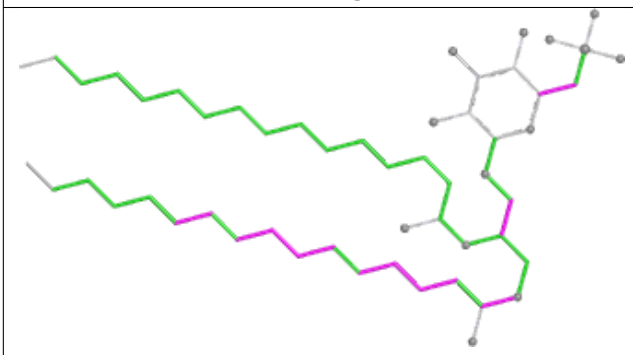
Ligand SQD a 405



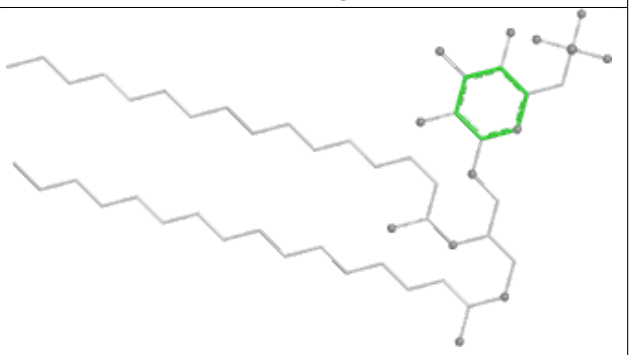
Bond lengths



Bond angles

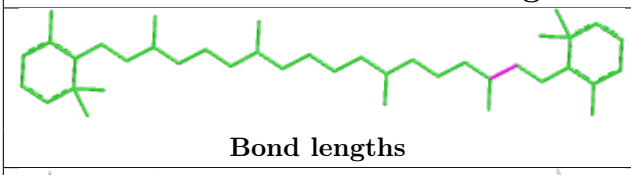


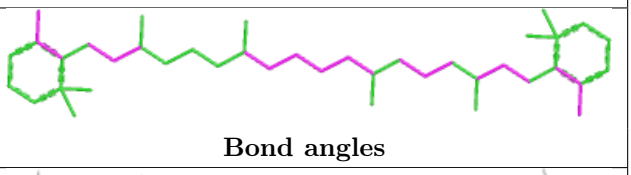
Torsions

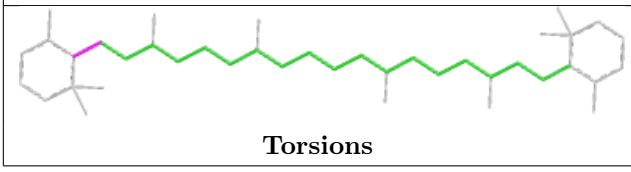


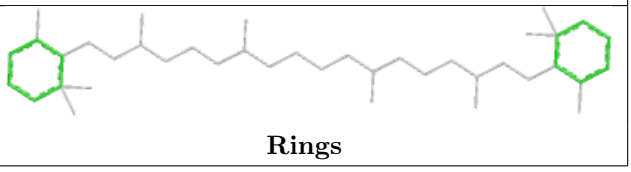
Rings

Ligand BCR B 618

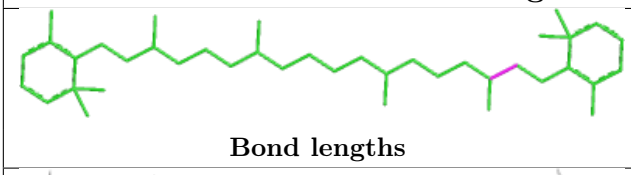

Bond lengths

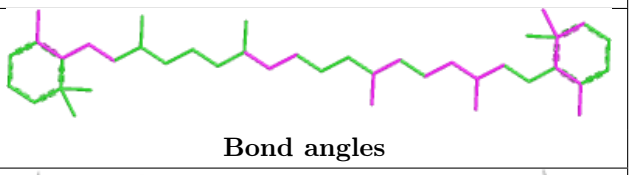

Bond angles

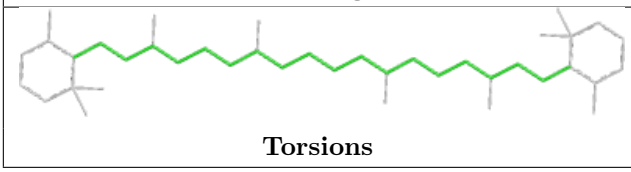

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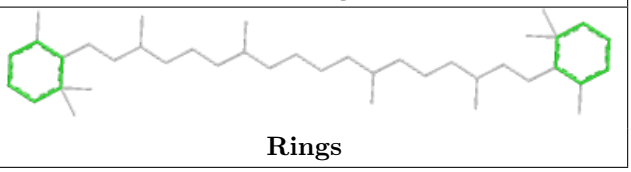

Rings

Ligand BCR a 413

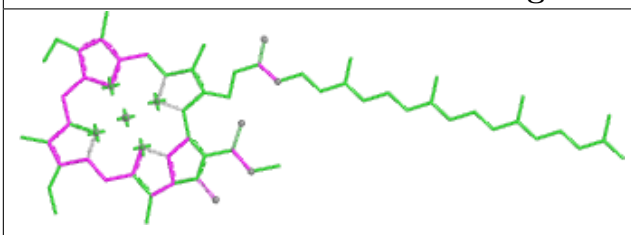

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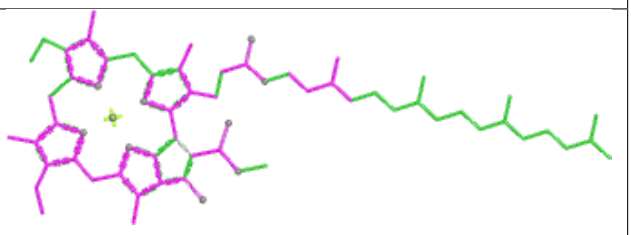

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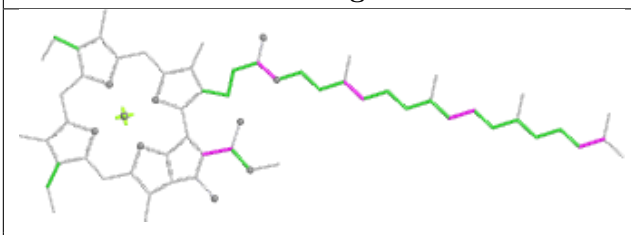

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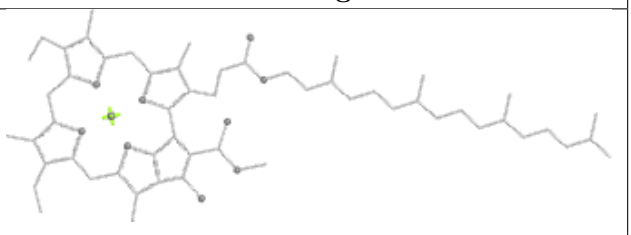

Rings

Ligand CLA b 614

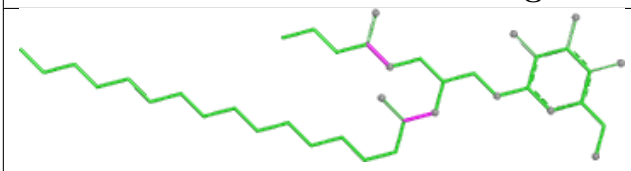

Bond lengths

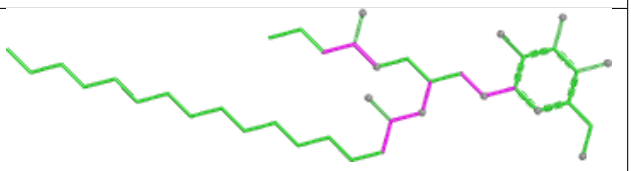

Bond angles

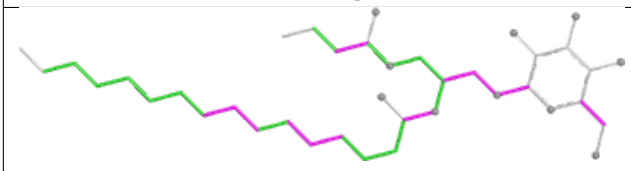

Torsions

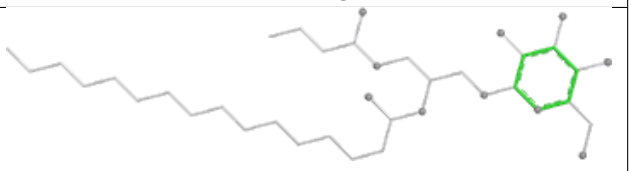

Rings

Ligand LMG z 101

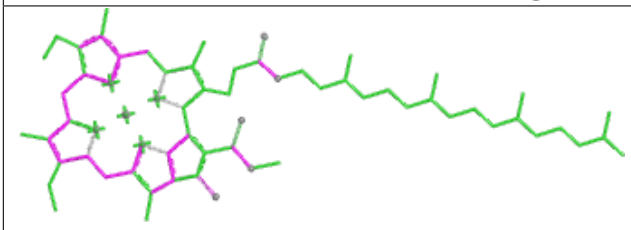

Bond lengths


Bond angles

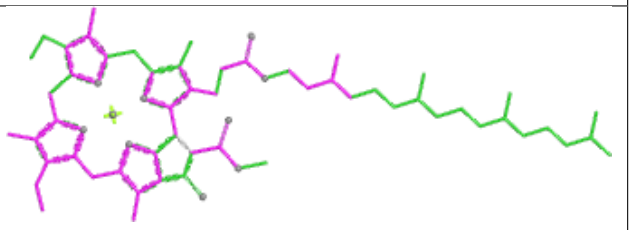

Torsions


Rings

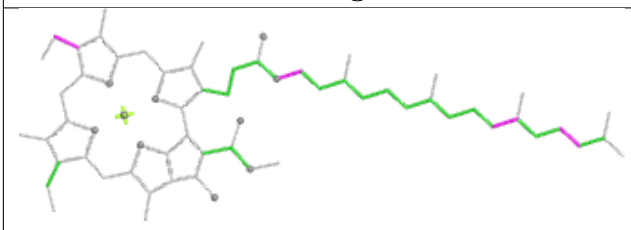
Ligand CLA d 404



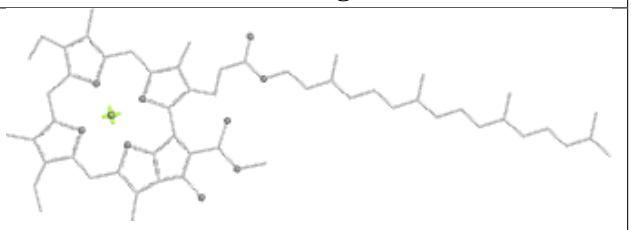
Bond lengths



Bond angles



Torsions



Rings

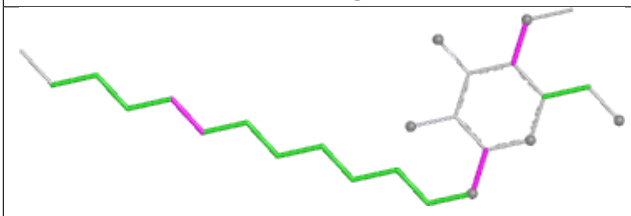
Ligand LMT b 630



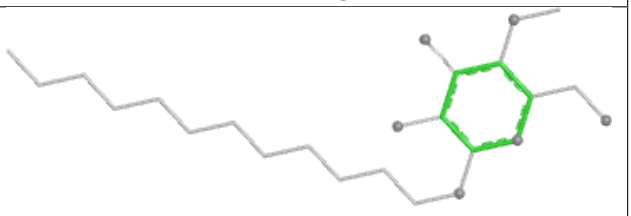
Bond lengths



Bond angles

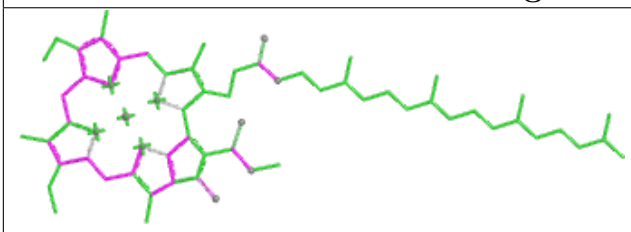


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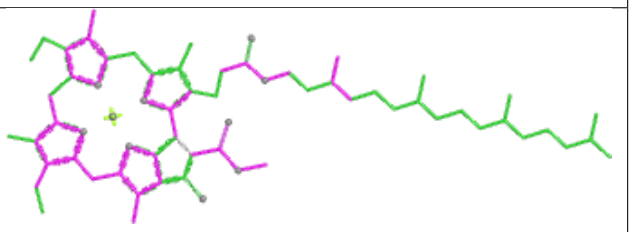


Rings

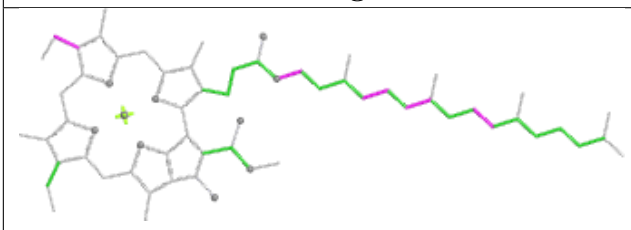
Ligand CLA B 617



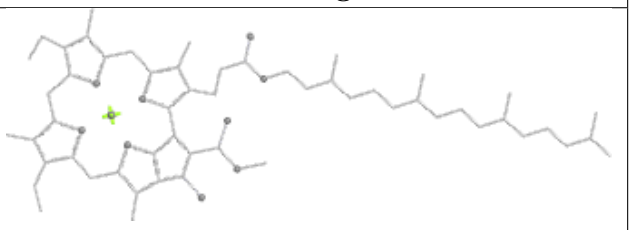
Bond lengths



Bond angles

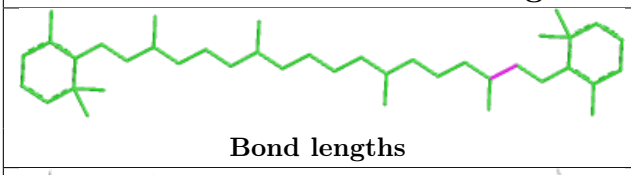


Torsions

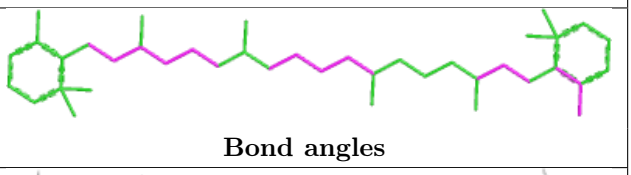


Rings

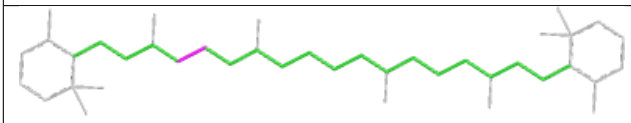
Ligand BCR h 101



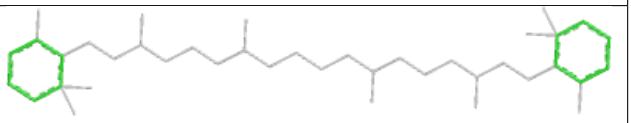
Bond lengths



Bond angles

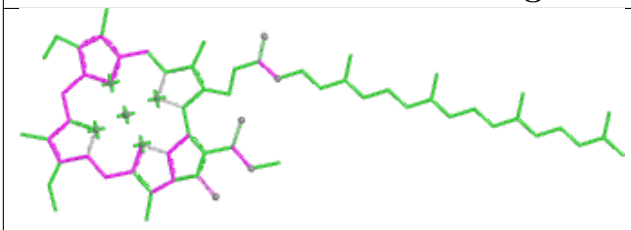


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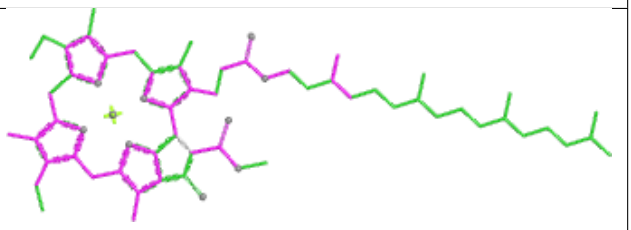


Rings

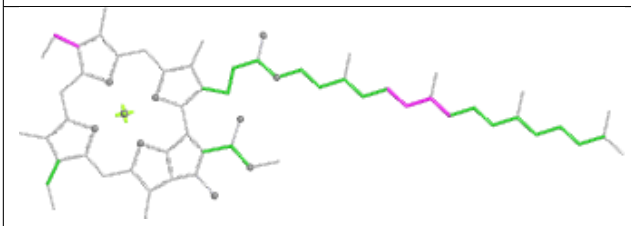
Ligand CLA B 604



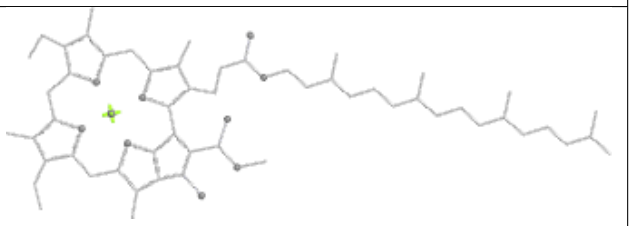
Bond lengths



Bond angles

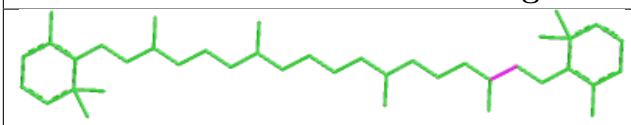


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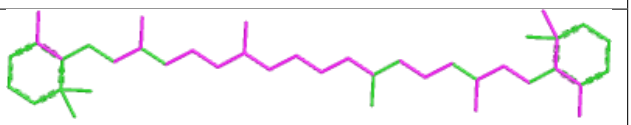


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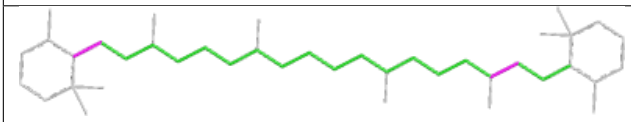
Ligand BCR Y 101



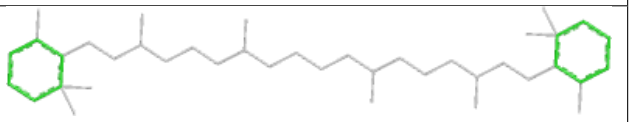
Bond lengths



Bond angles

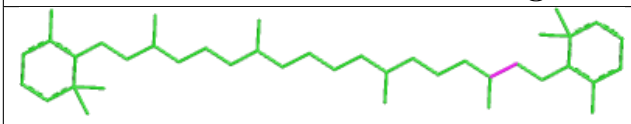


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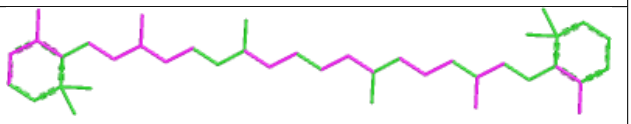


Rings

Ligand BCR c 518



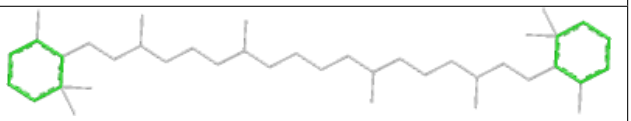
Bond lengths



Bond angles

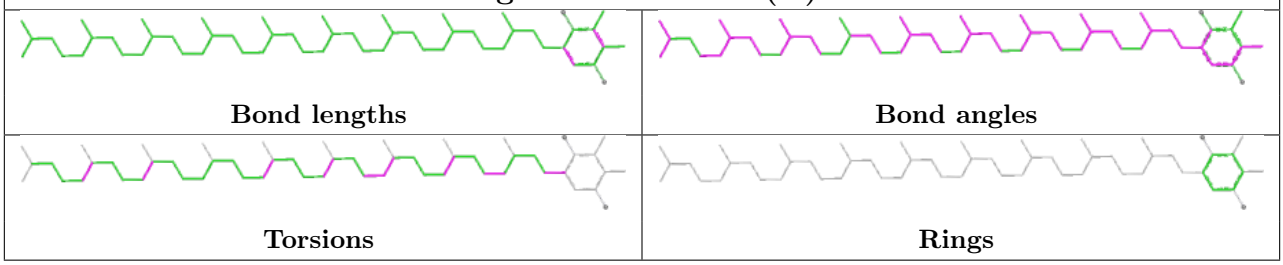


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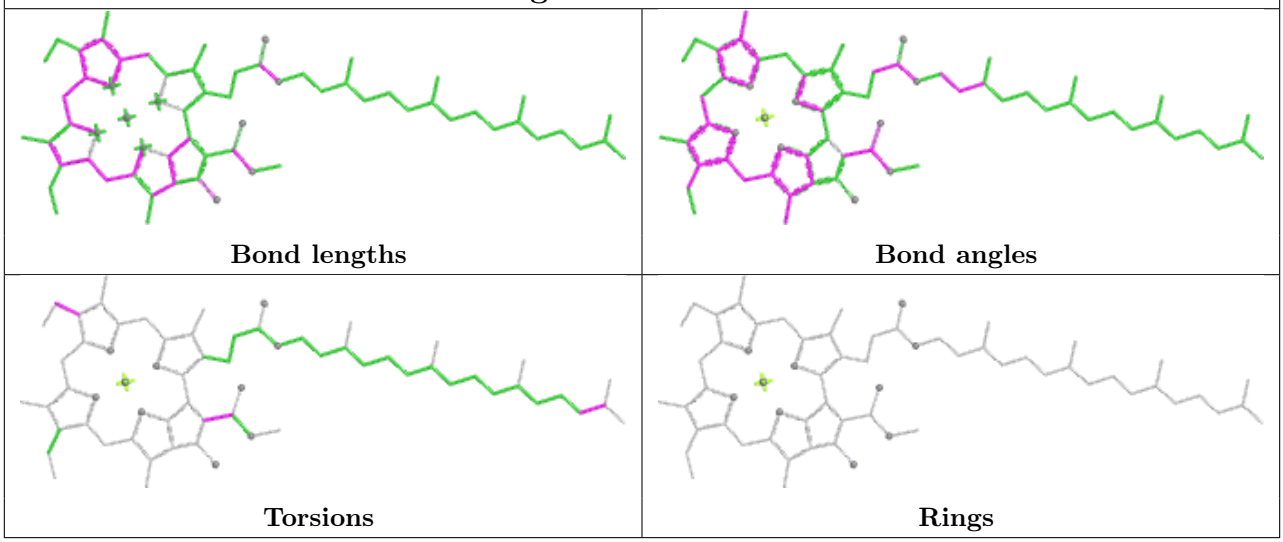


Rings

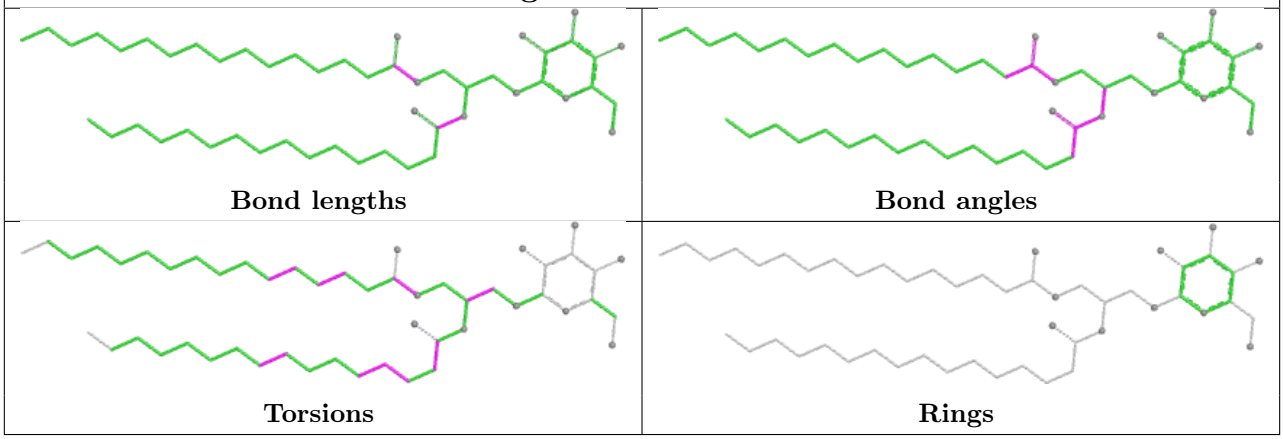
Ligand PL9 A 417 (A)



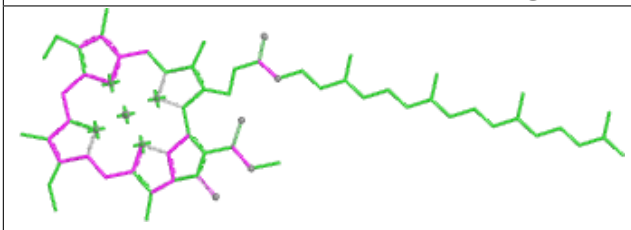
Ligand CLA c 506



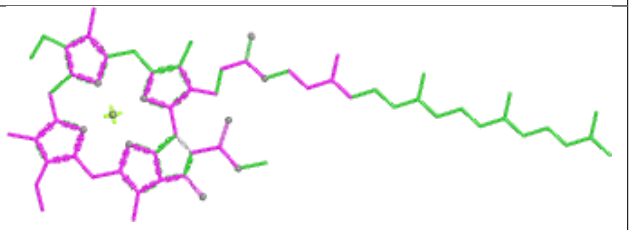
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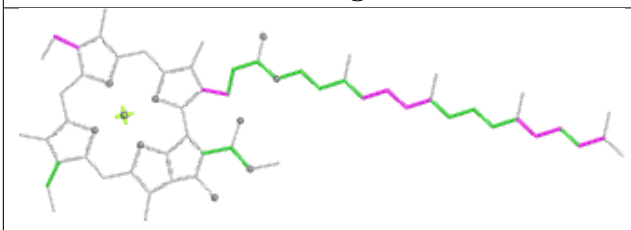
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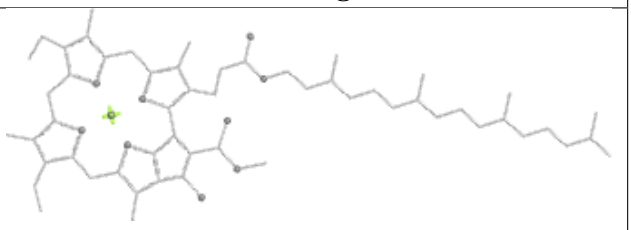
Bond lengths



Bond angles

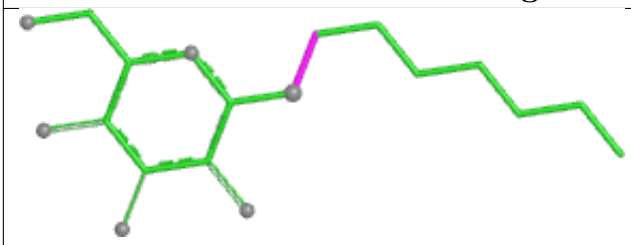


Torsions

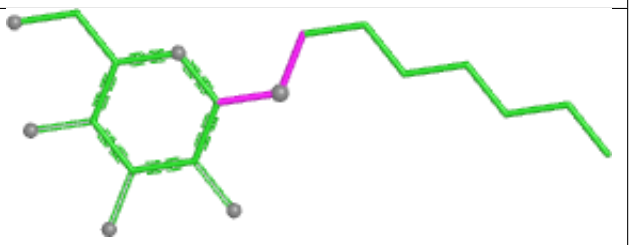


Rings

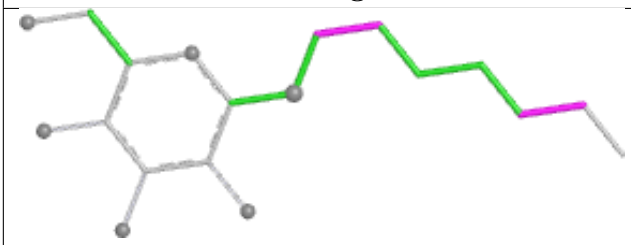
Ligand HTG B 622



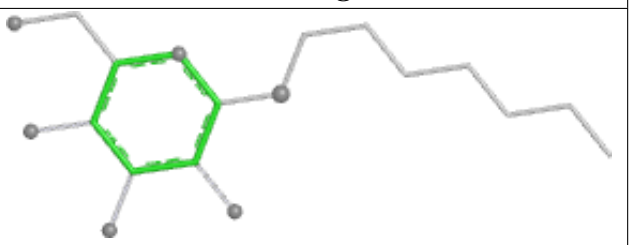
Bond lengths



Bond angles

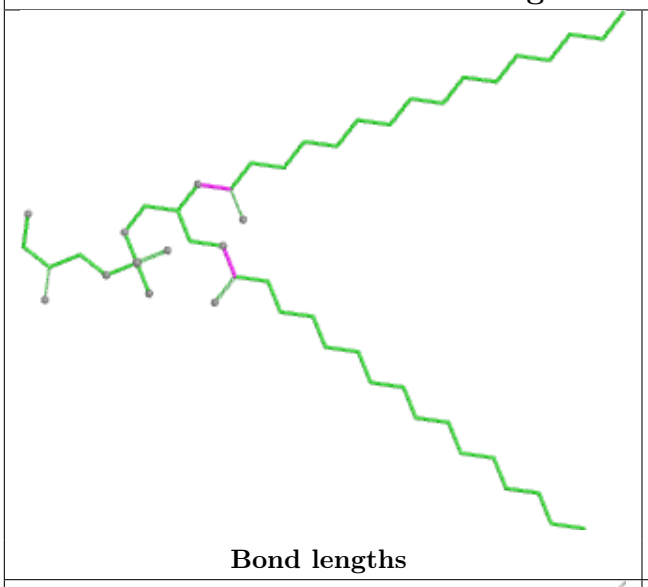


Torsions

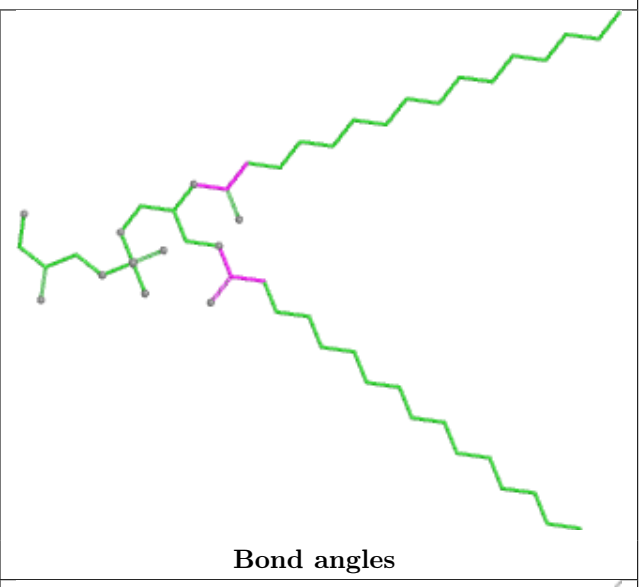


Rings

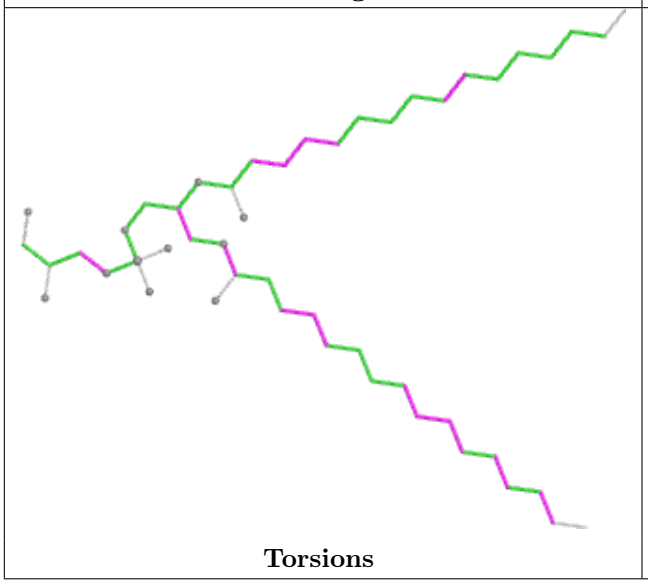
Ligand LHG d 410



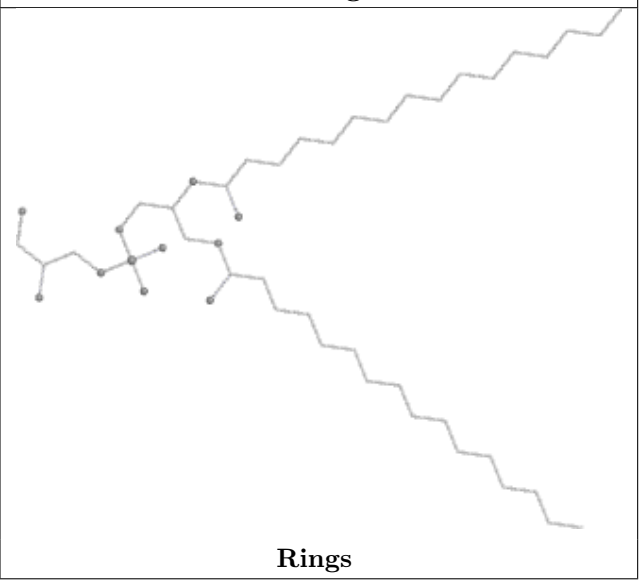
Bond lengths



Bond angles

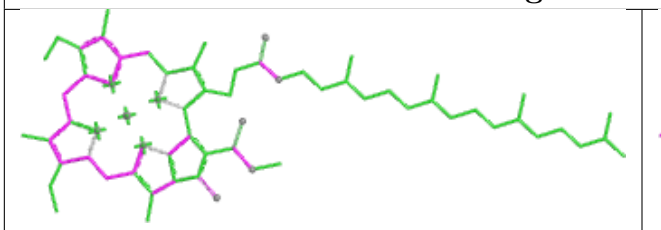


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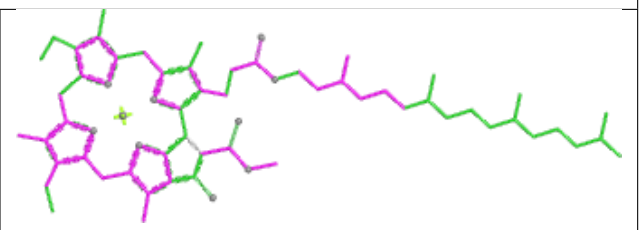


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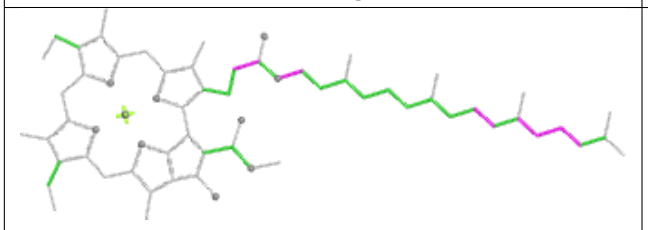
Ligand CLA B 614



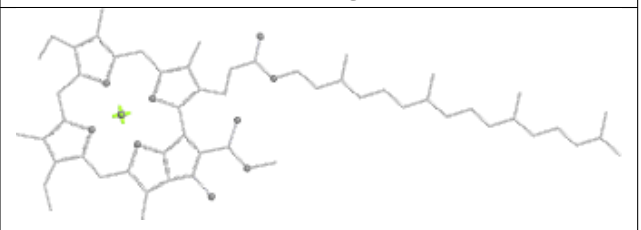
Bond lengths



Bond angles

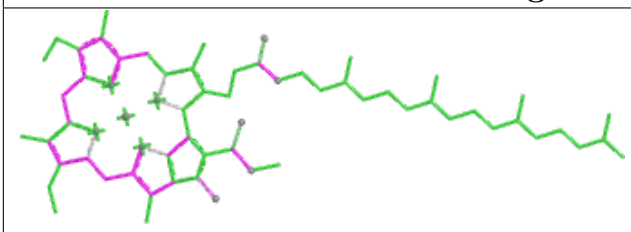


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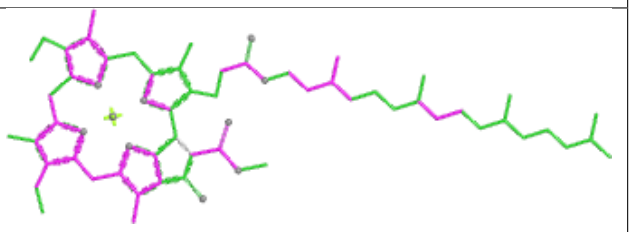


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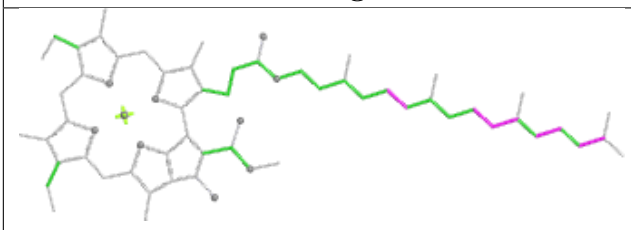
Ligand CLA b 624



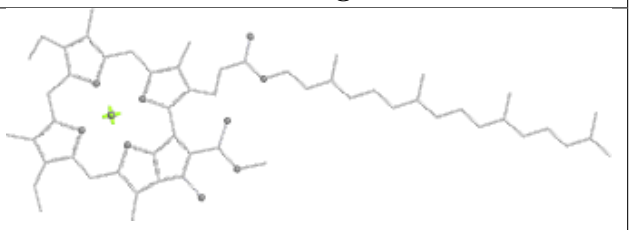
Bond lengths



Bond angles

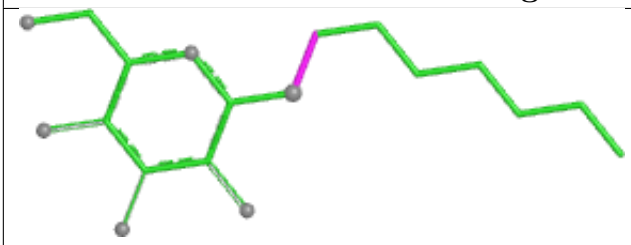


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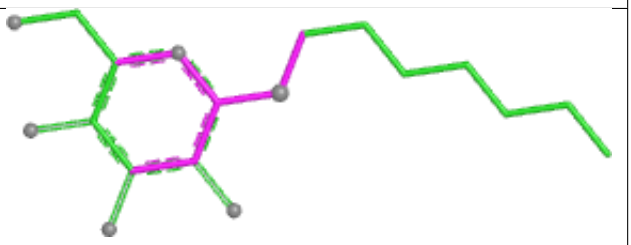


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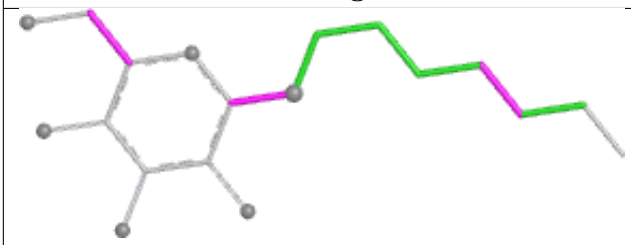
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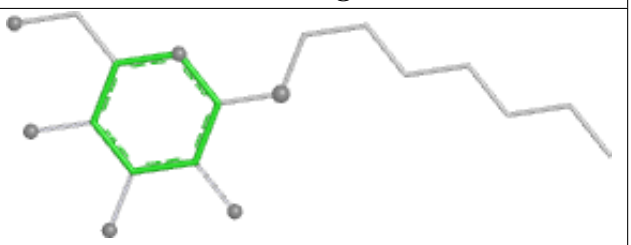
Bond lengths



Bond angles

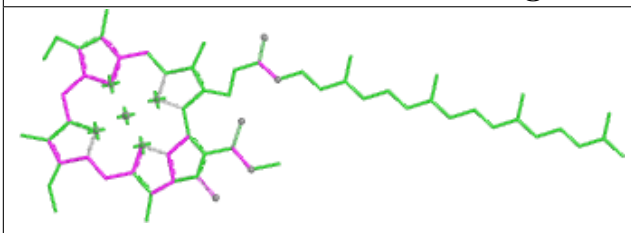


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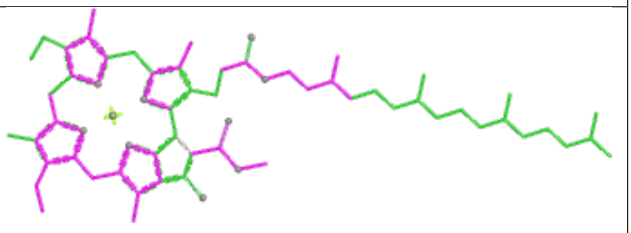


Rings

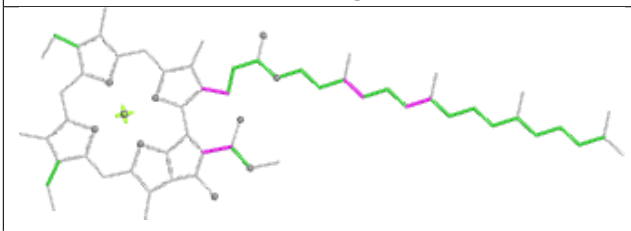
Ligand CLA B 610



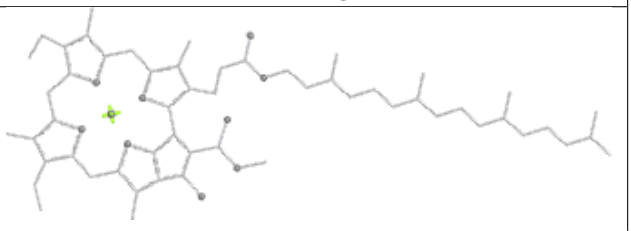
Bond lengths



Bond angles

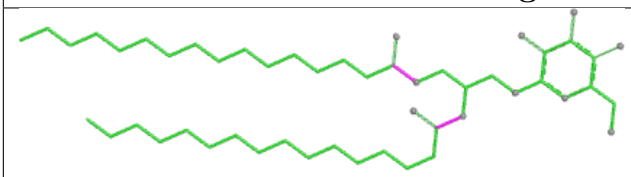


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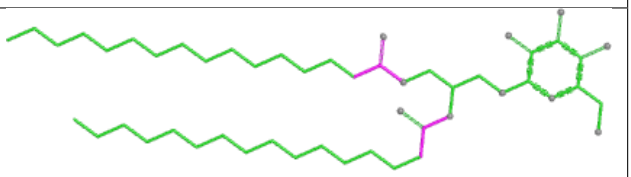


Rings

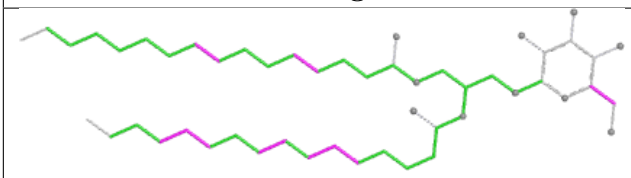
Ligand LMG D 415



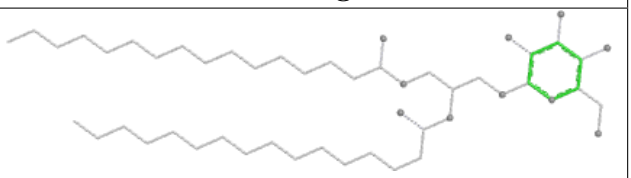
Bond lengths



Bond angles

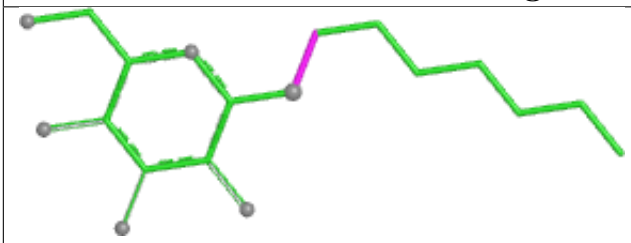


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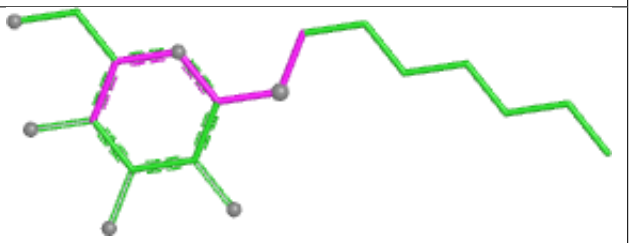


Rings

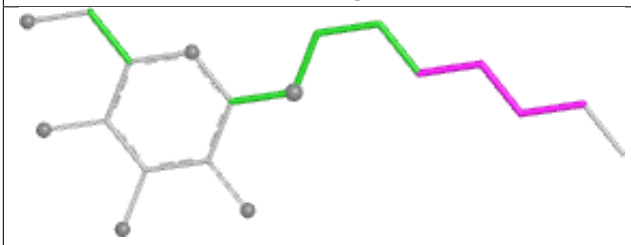
Ligand HTG b 607



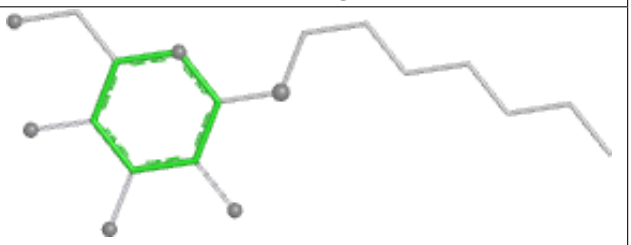
Bond lengths



Bond angles

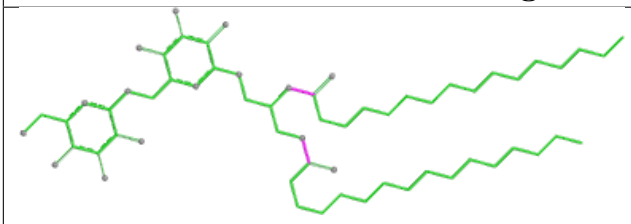


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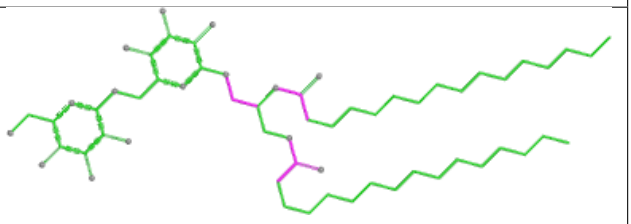


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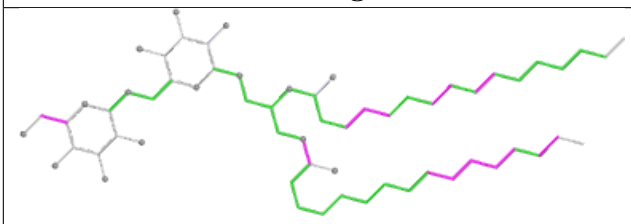
Ligand DGD C 518



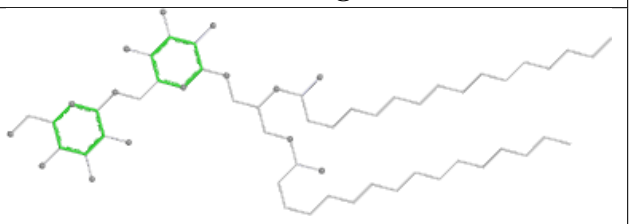
Bond lengths



Bond angles

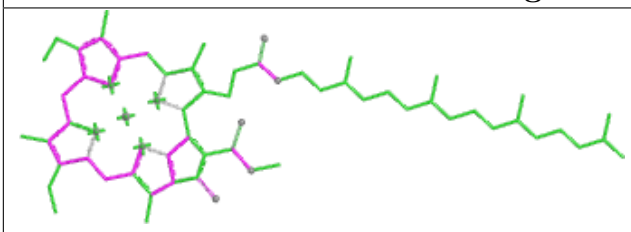


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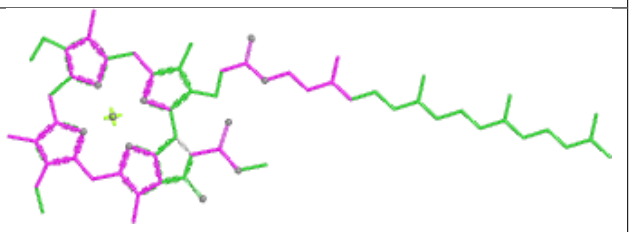


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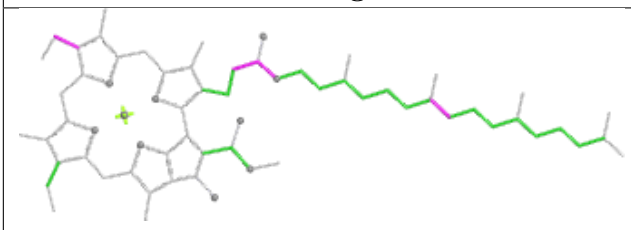
Ligand CLA C 512



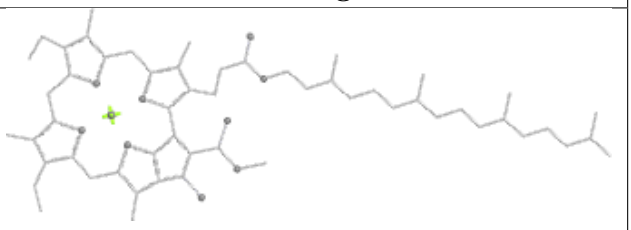
Bond lengths



Bond angles

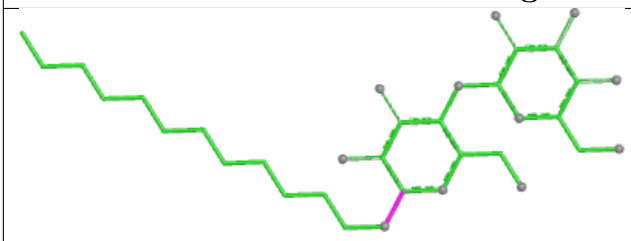


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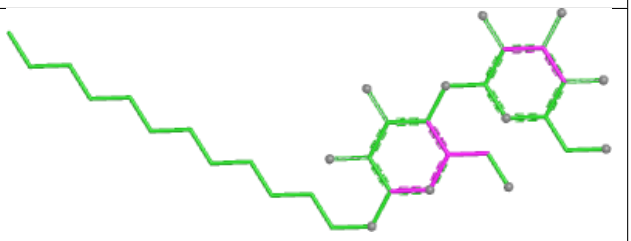


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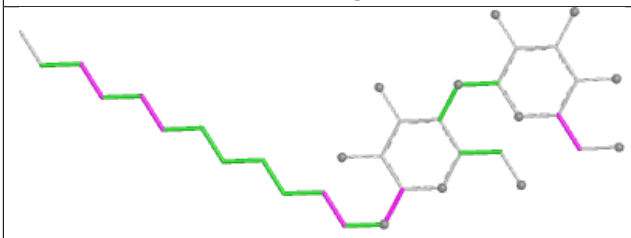
Ligand LMT A 414



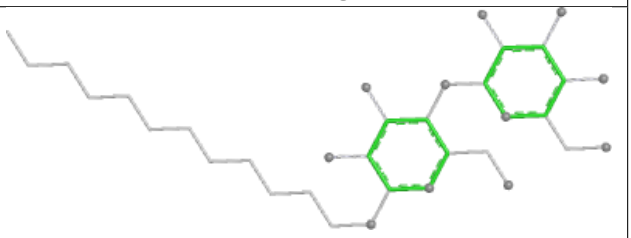
Bond lengths



Bond angles

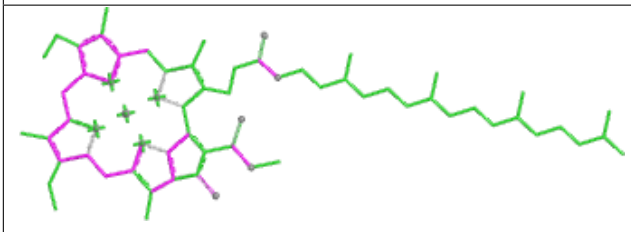


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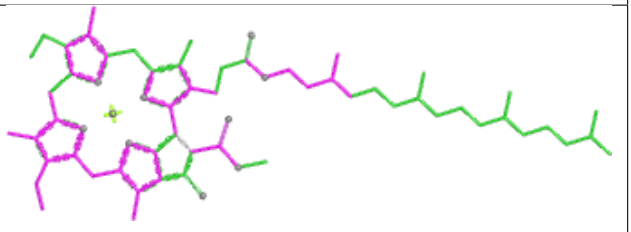


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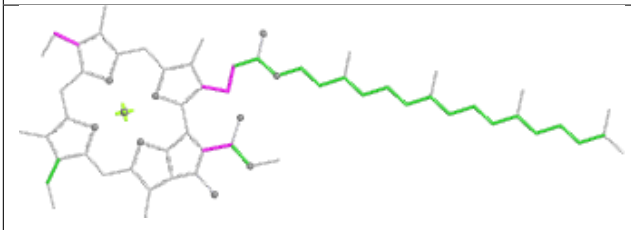
Ligand CLA B 608



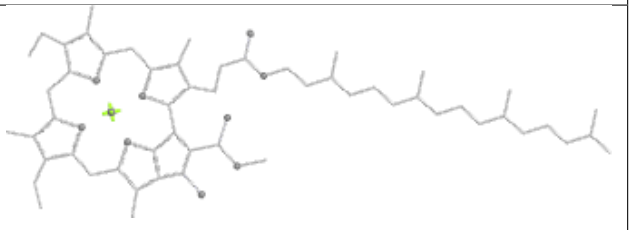
Bond lengths



Bond angles

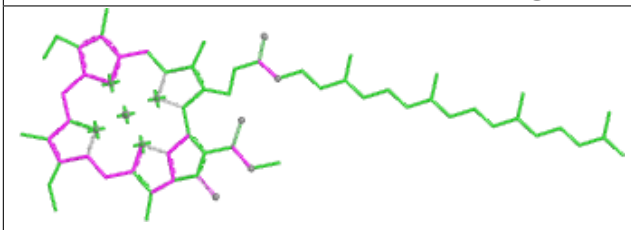


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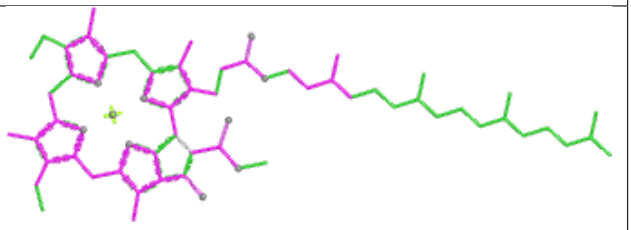


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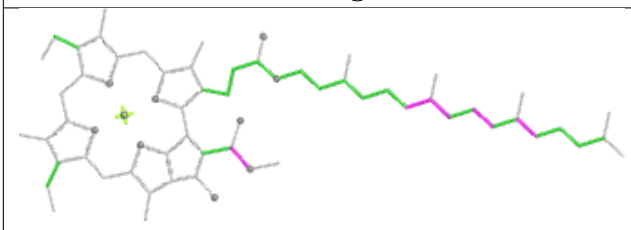
Ligand CLA a 410



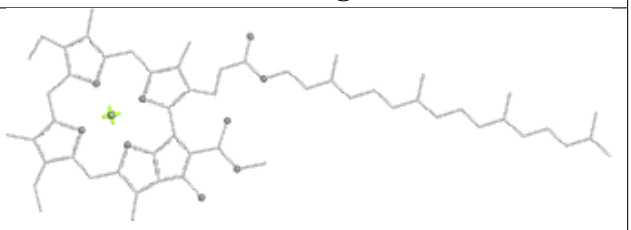
Bond lengths



Bond angles

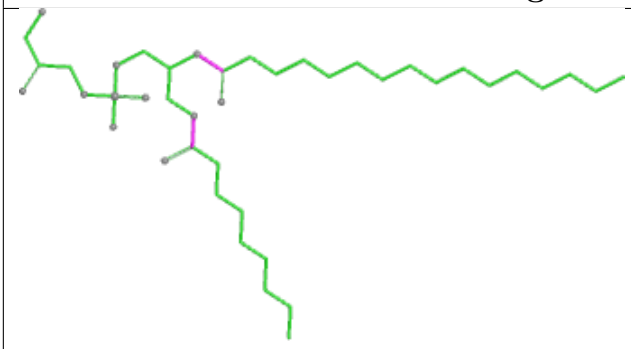


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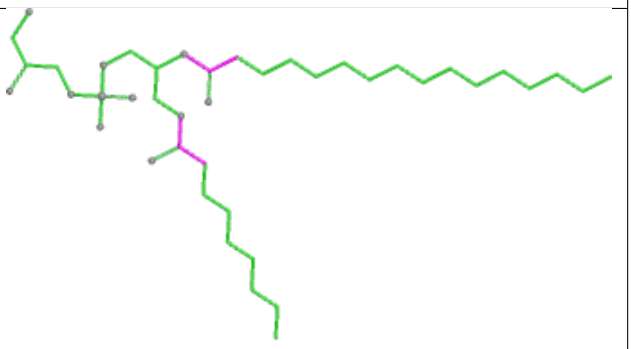


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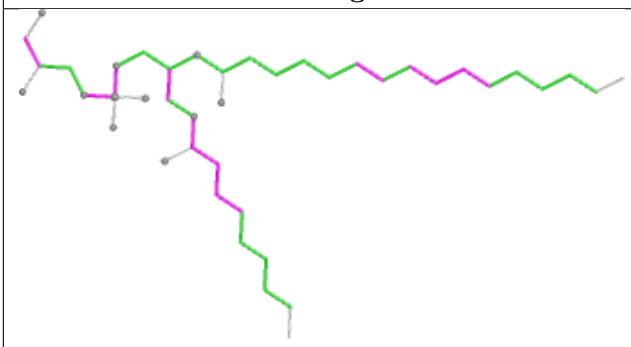
Ligand LHG a 420



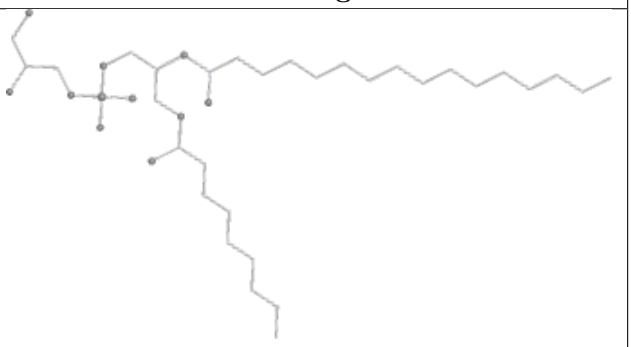
Bond lengths



Bond angles

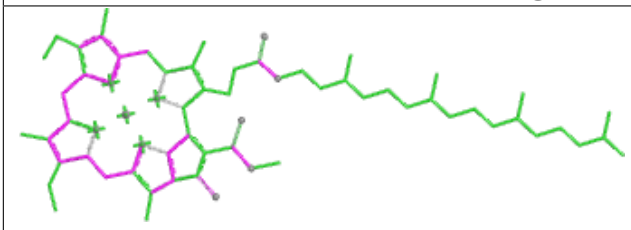


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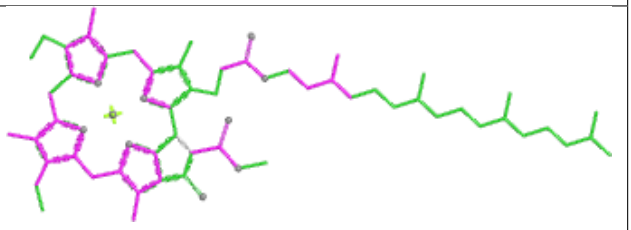


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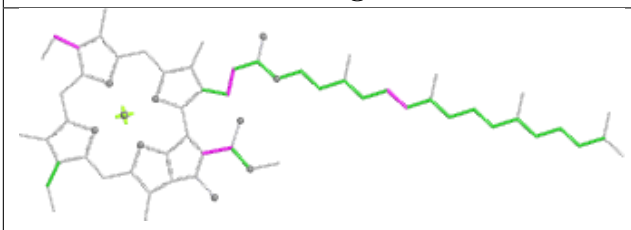
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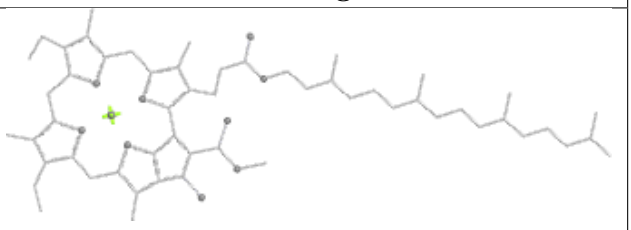
Bond lengths



Bond angles

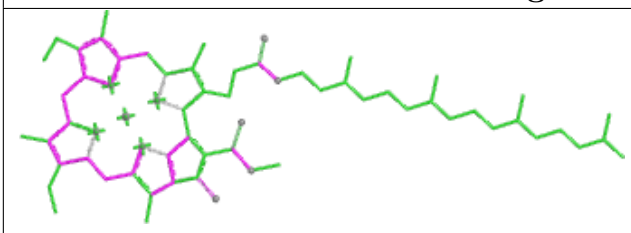


Torsions

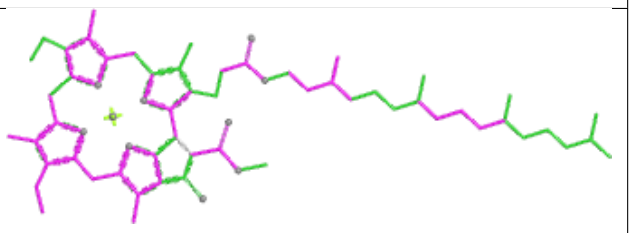


Rings

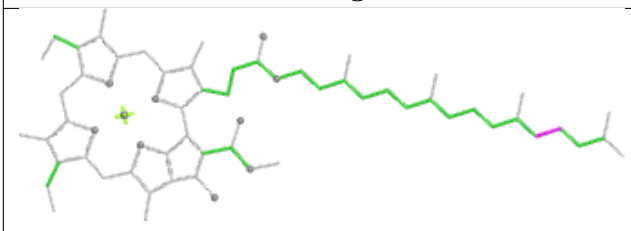
Ligand CLA b 617



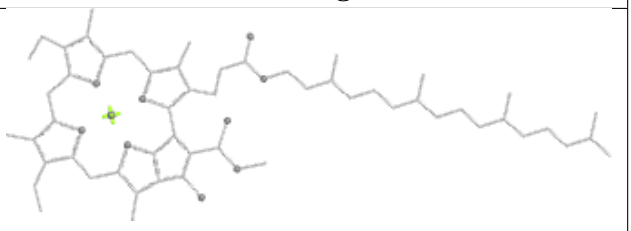
Bond lengths



Bond angles

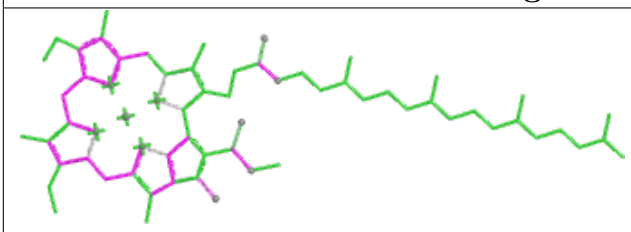


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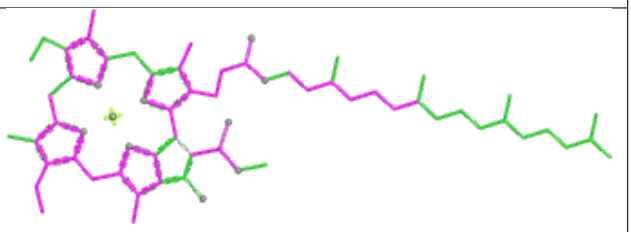


Rings

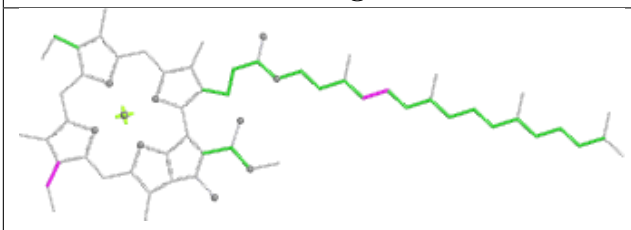
Ligand CLA A 406



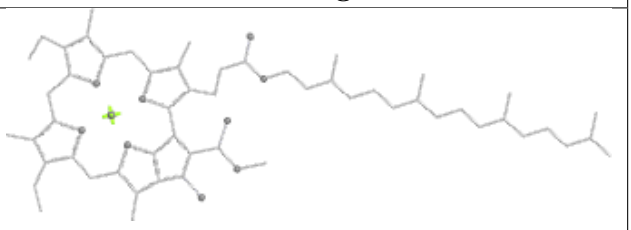
Bond lengths



Bond angles

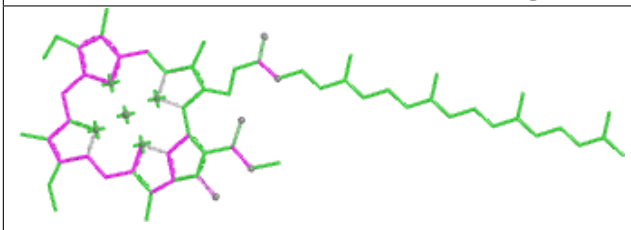


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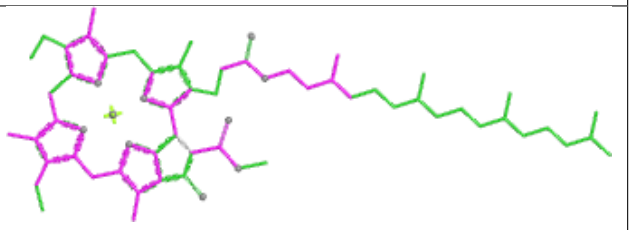


Rings

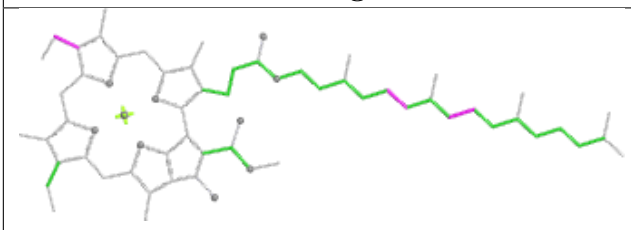
Ligand CLA C 503



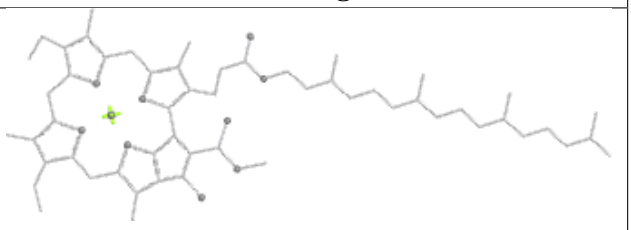
Bond lengths



Bond angles

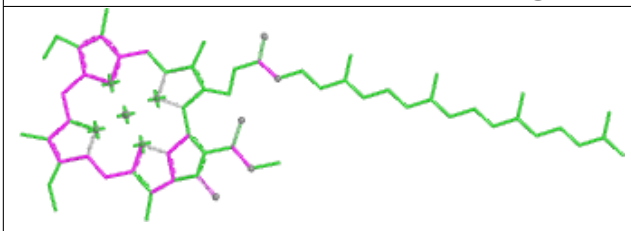


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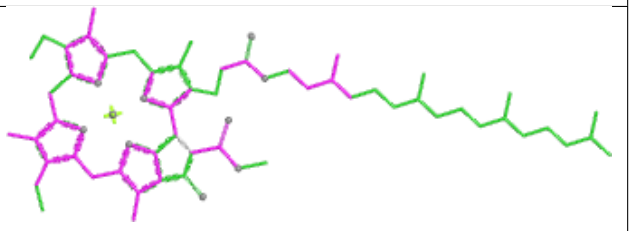


Rings

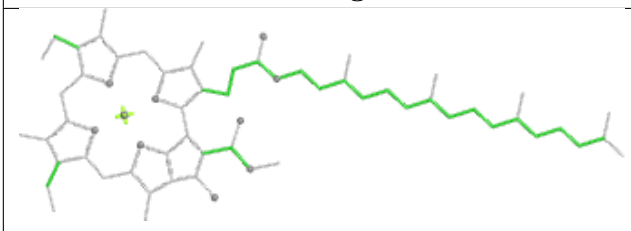
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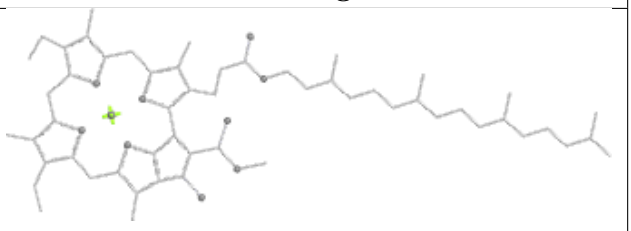
Bond lengths



Bond angles

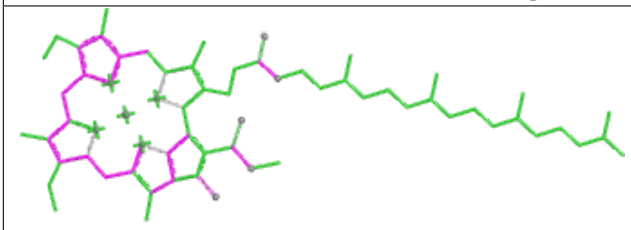


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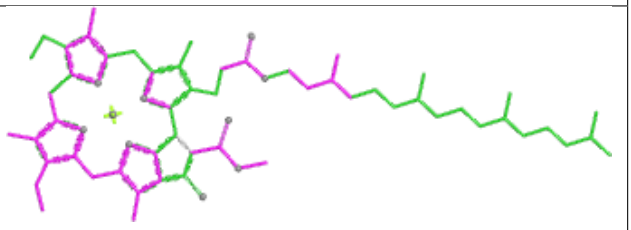


Rings

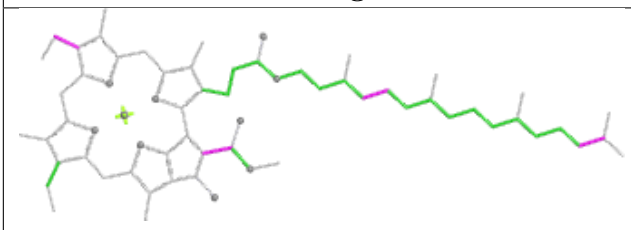
Ligand CLA C 502



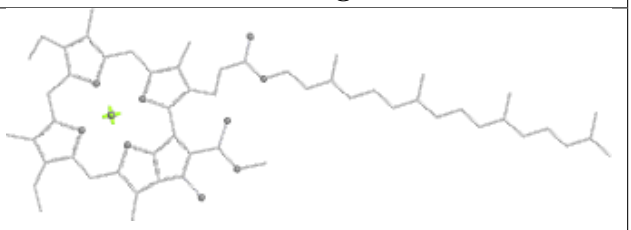
Bond lengths



Bond angles

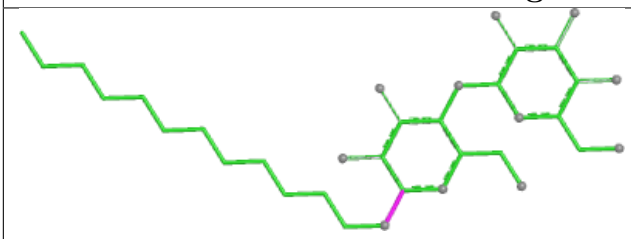


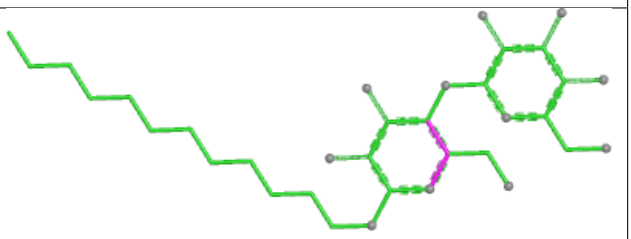
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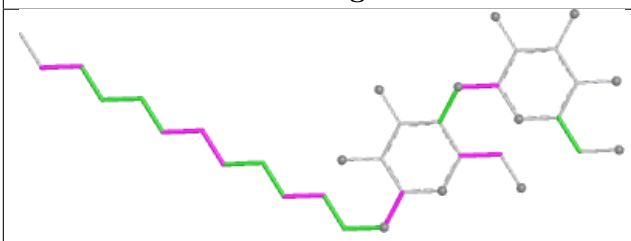


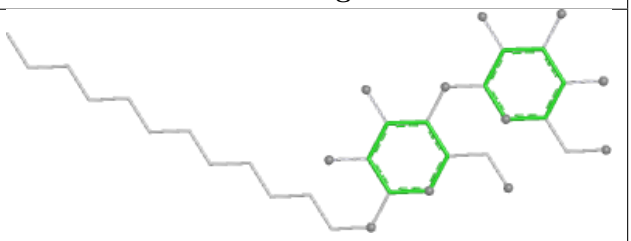
Rings

Ligand LMT e 102

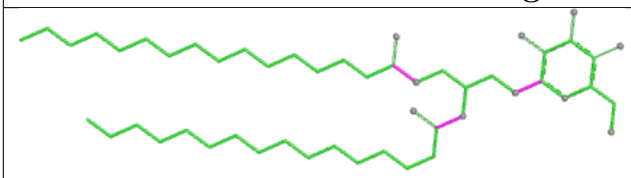

Bond lengths

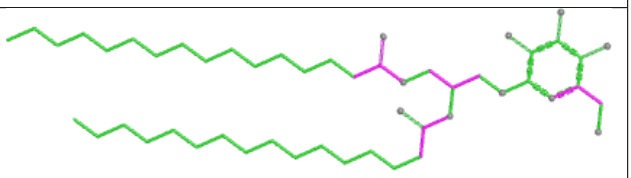

Bond angles

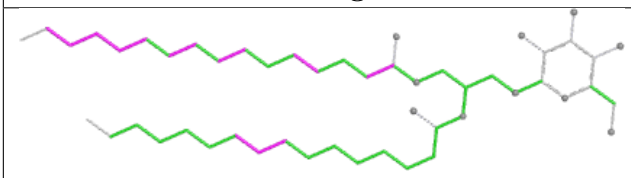

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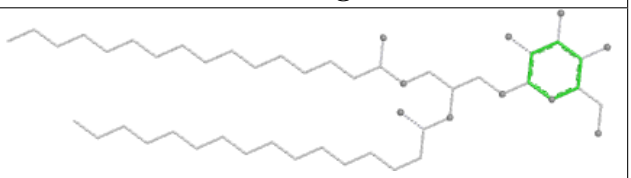

Rings

Ligand LMG b 629

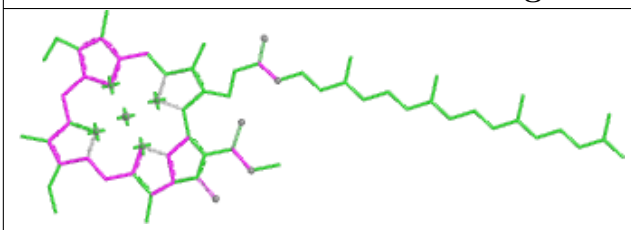

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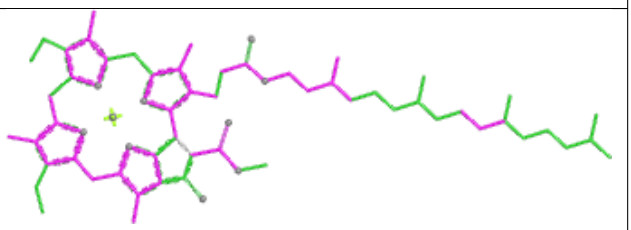

Bond angles

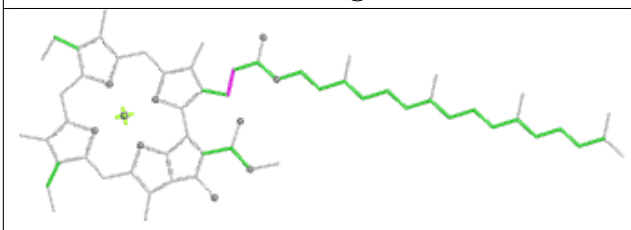

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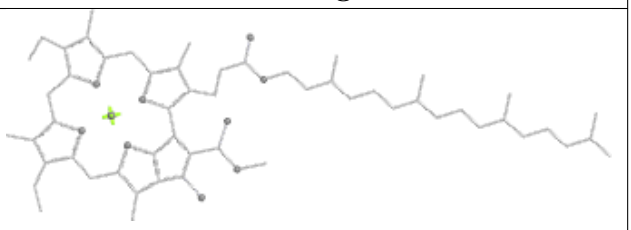

Rings

Ligand CLA B 603

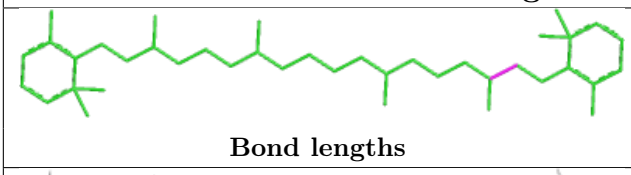

Bond lengths


Bond angles

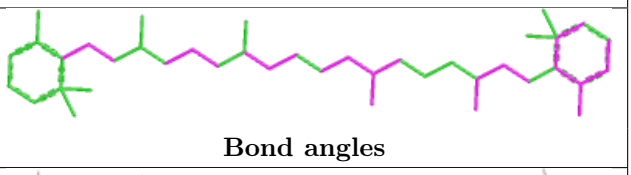

Torsions


Rings

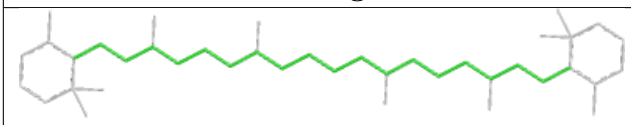
Ligand BCR B 620



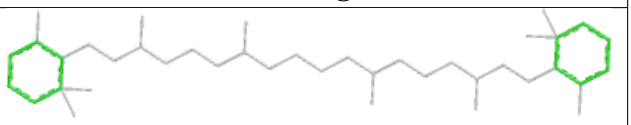
Bond lengths



Bond angles

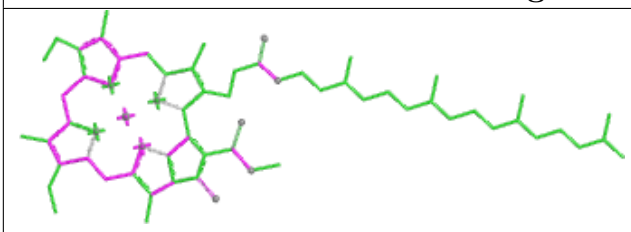


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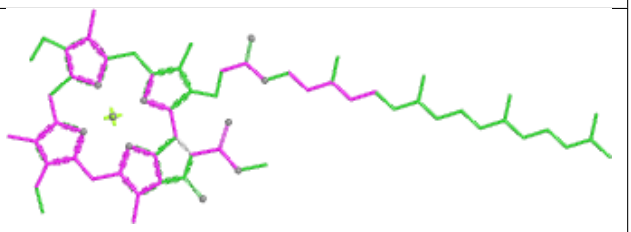


Rings

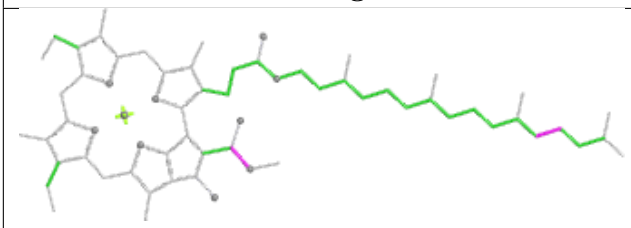
Ligand CLA b 613



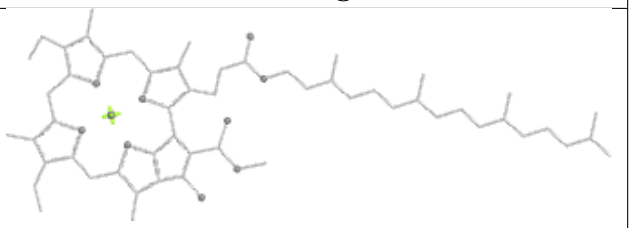
Bond lengths



Bond angles

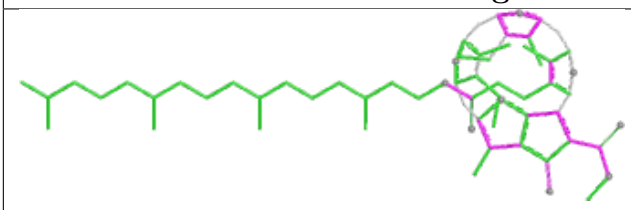


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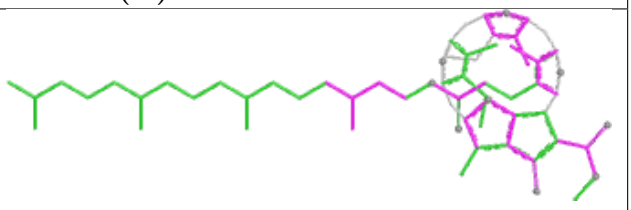


Rings

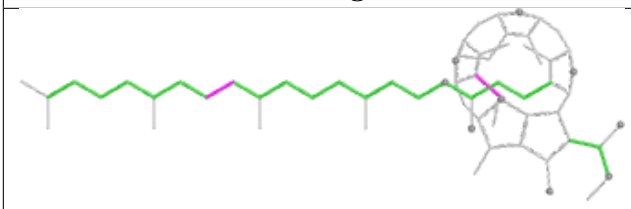
Ligand PHO d 402 (B)



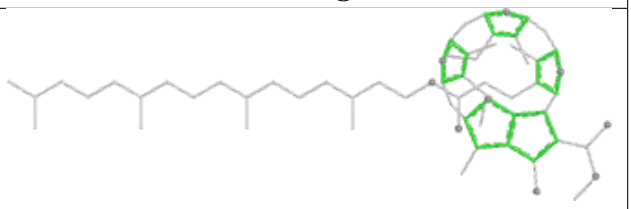
Bond lengths



Bond angles

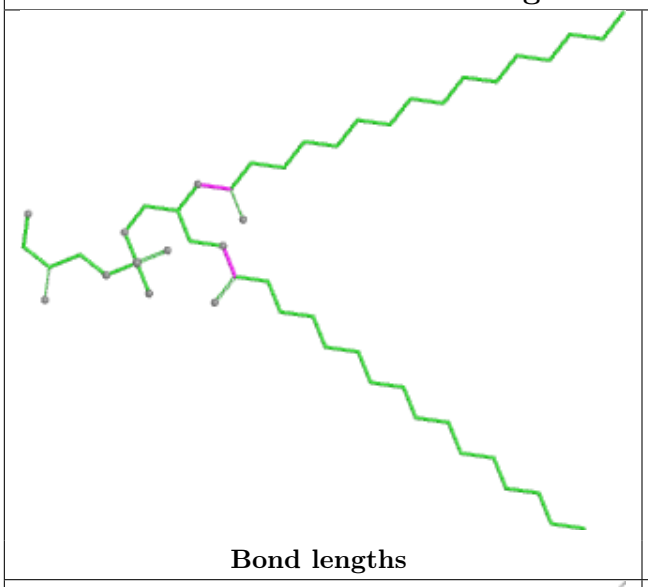


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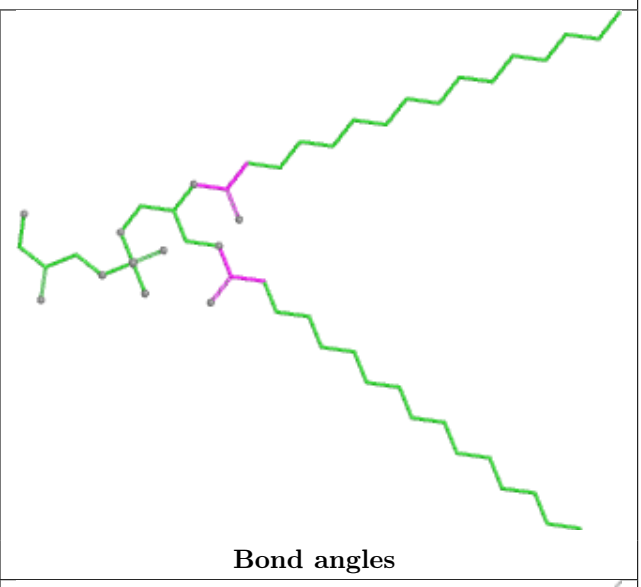


Rings

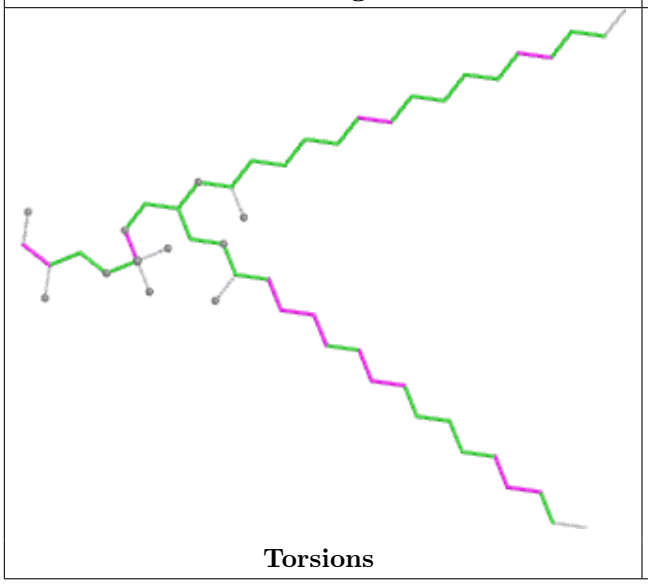
Ligand LHG D 409



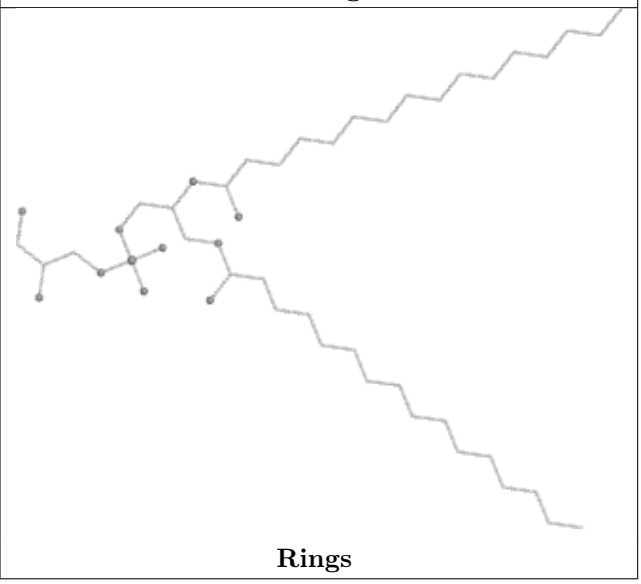
Bond lengths



Bond angles

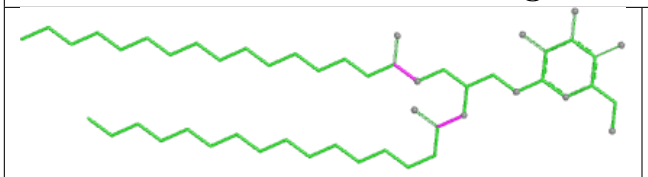


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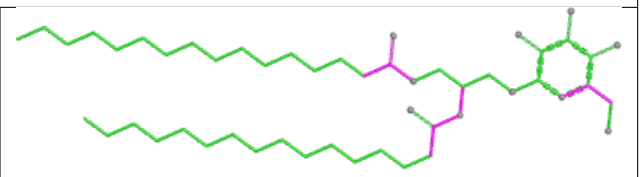


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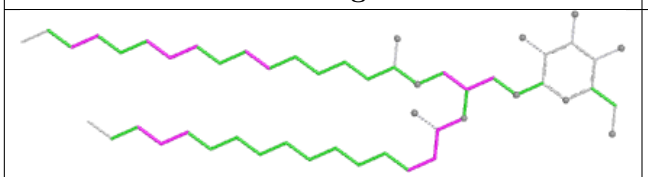
Ligand LMG k 101



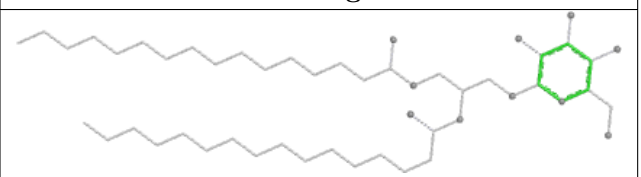
Bond lengths



Bond angles

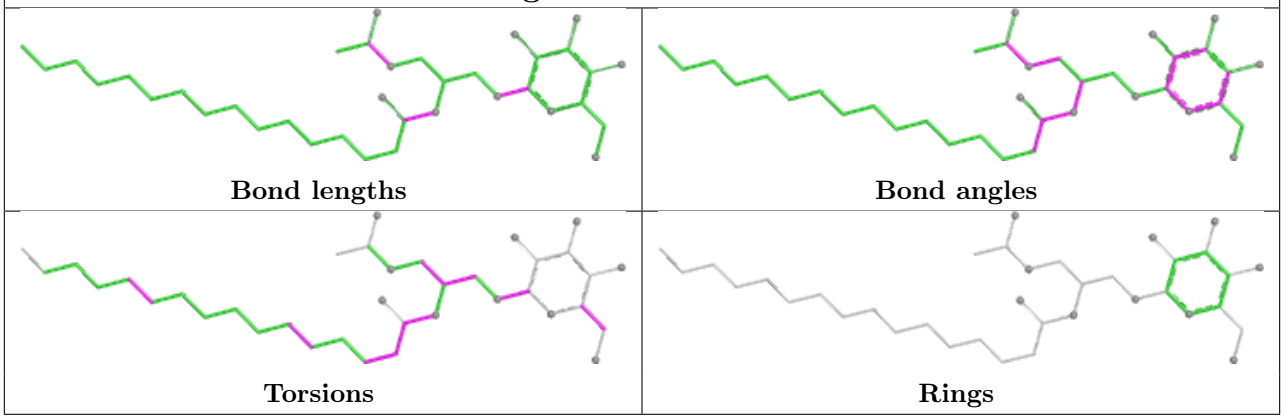


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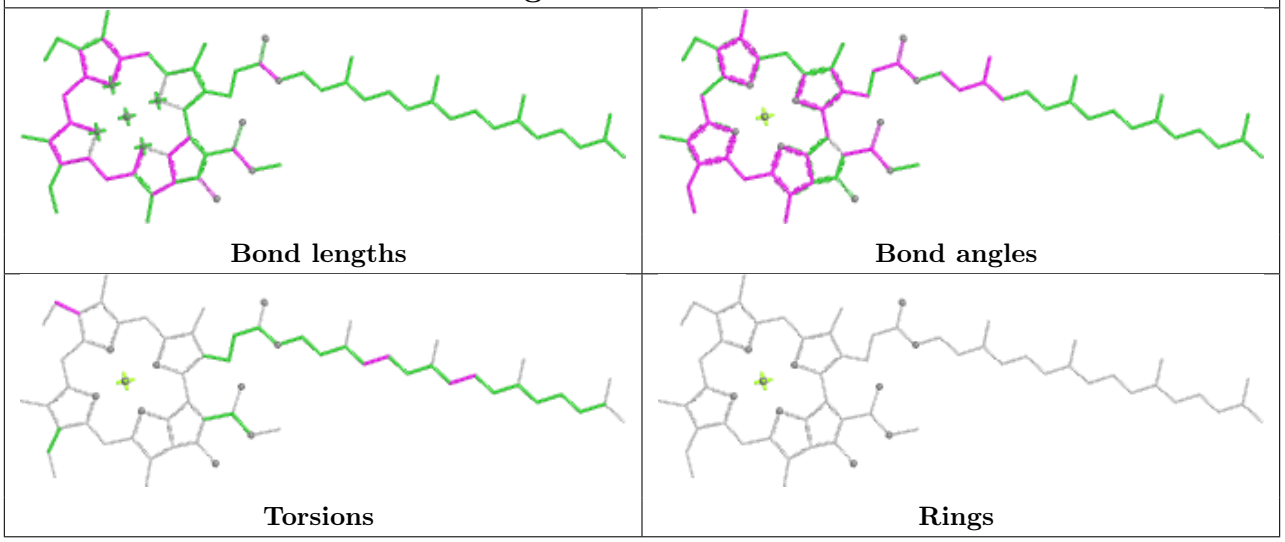


Rings

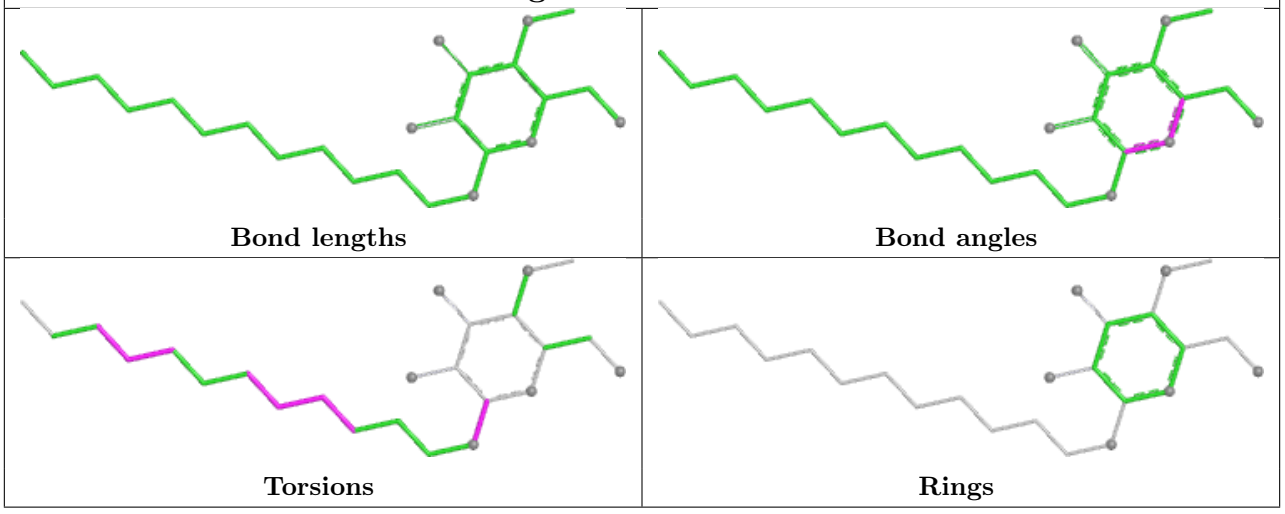
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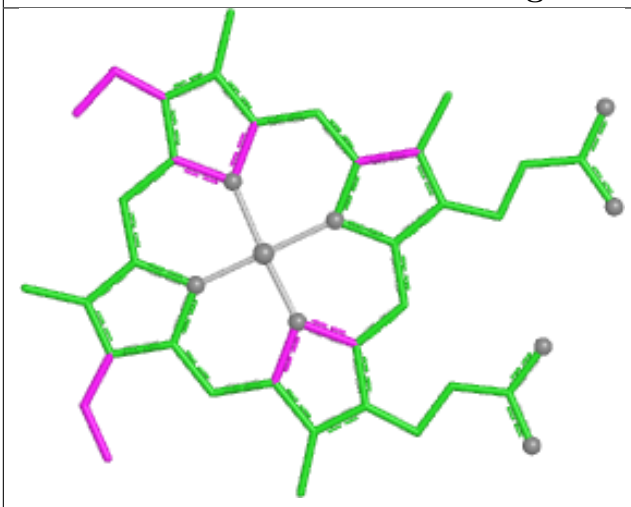
Ligand CLA D 405



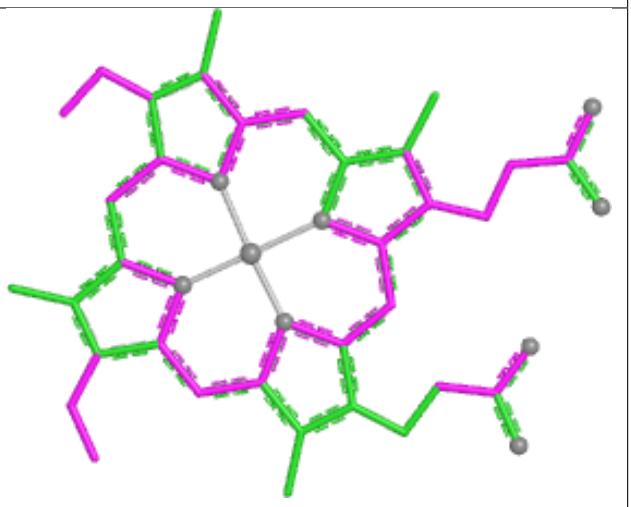
Ligand LMT t 101



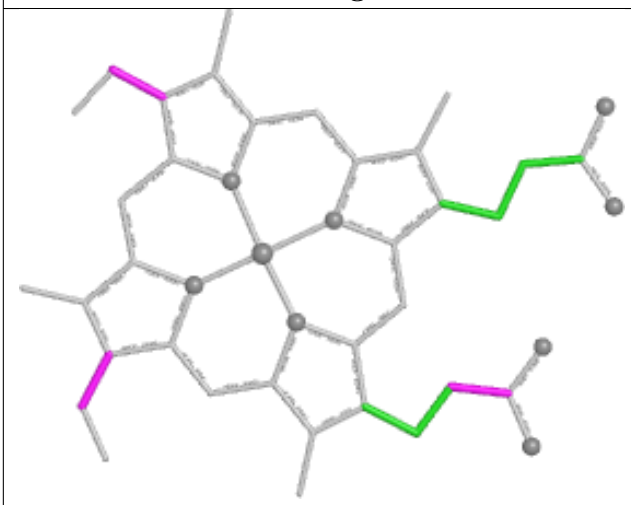
Ligand HEC v 206



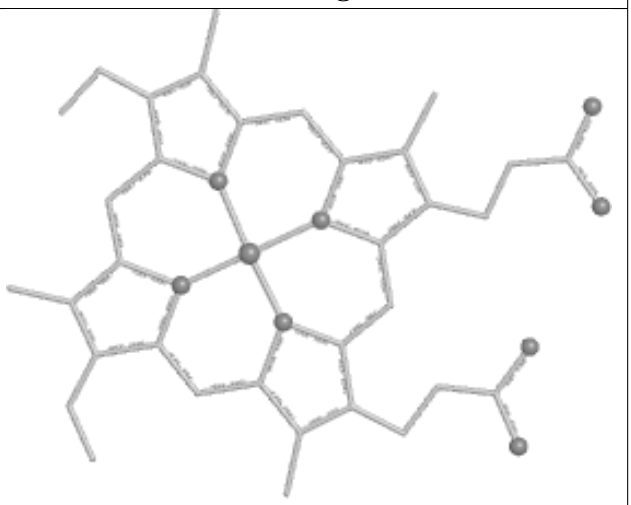
Bond lengths



Bond angles

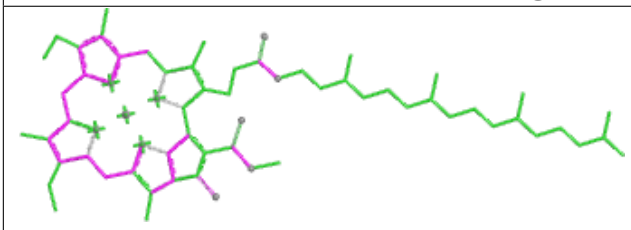


Torsions

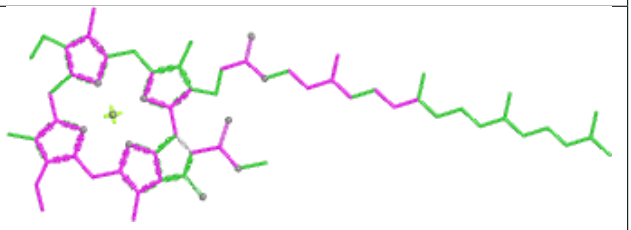


Rings

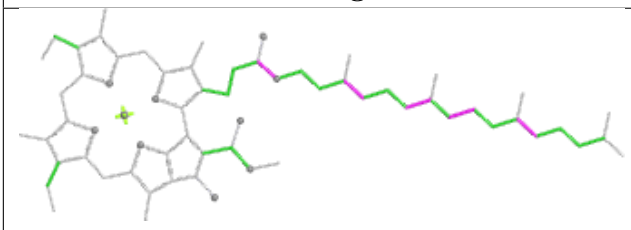
Ligand CLA c 514



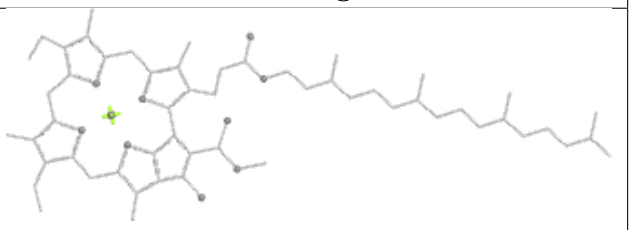
Bond lengths



Bond angles

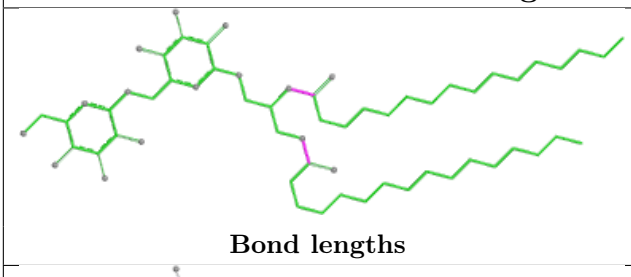


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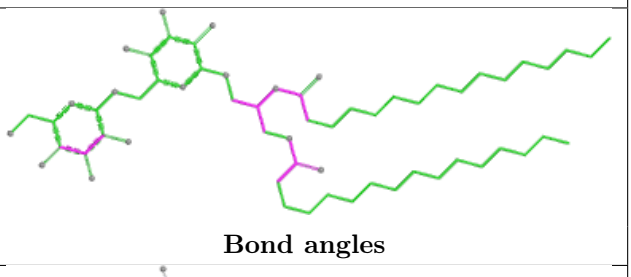


Rings

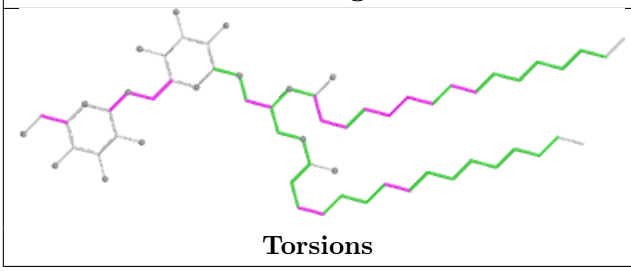
Ligand DGD C 516



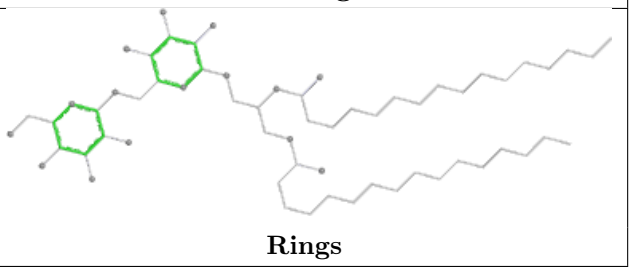
Bond lengths



Bond angles

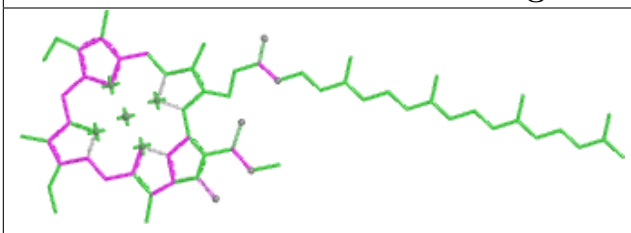


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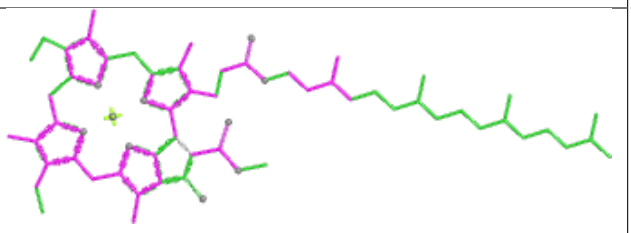


Rings

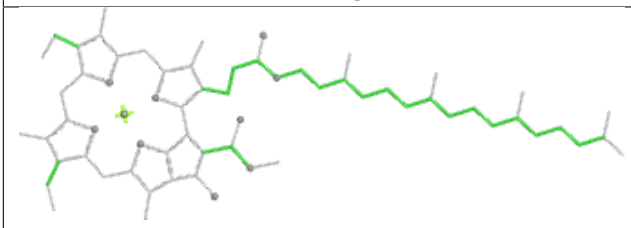
Ligand CLA b 621



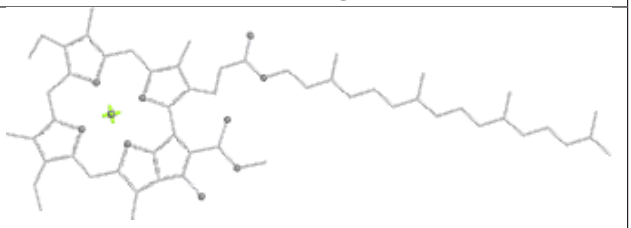
Bond lengths



Bond angles

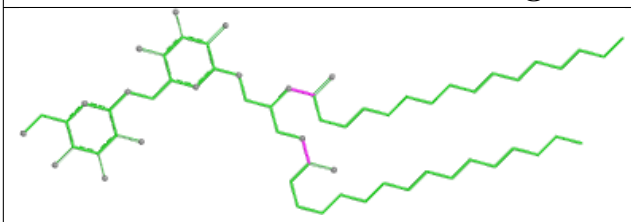


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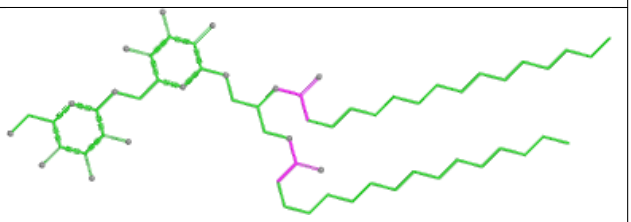


Rings

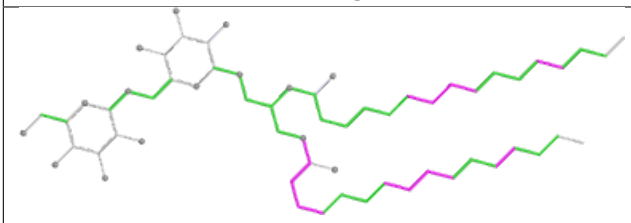
Ligand DGD c 521



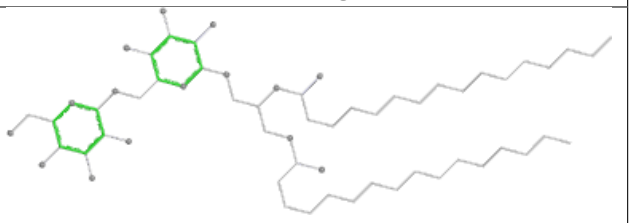
Bond lengths



Bond angles

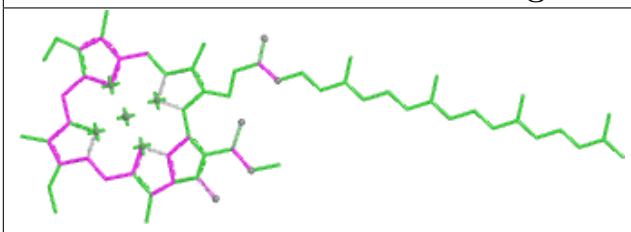


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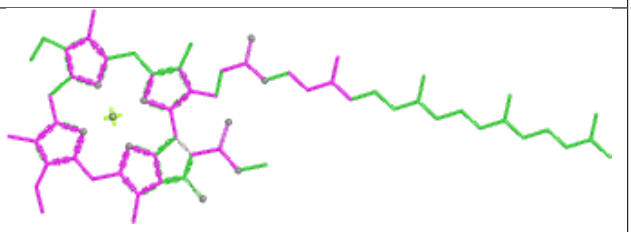


Rings

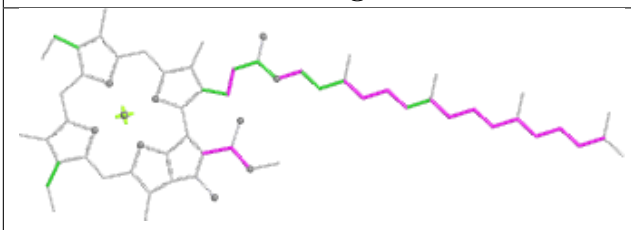
Ligand CLA b 623



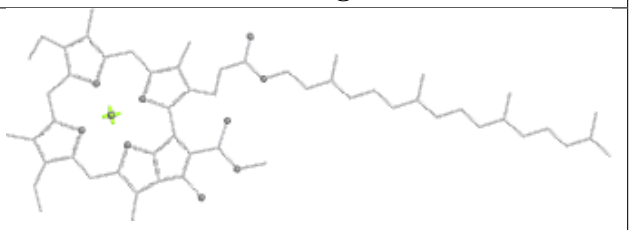
Bond lengths



Bond angles

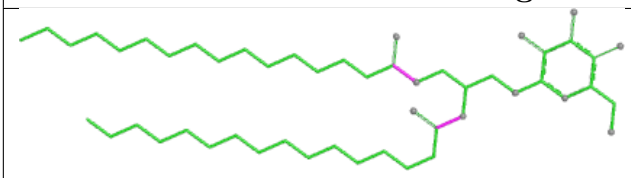


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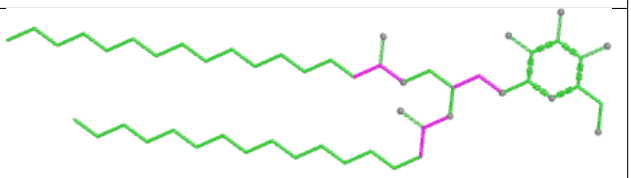


Rings

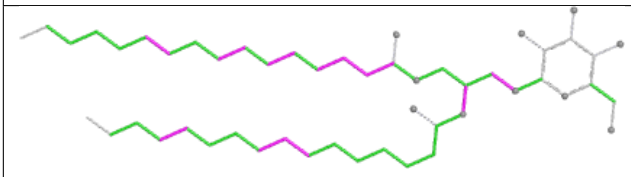
Ligand LMG M 101



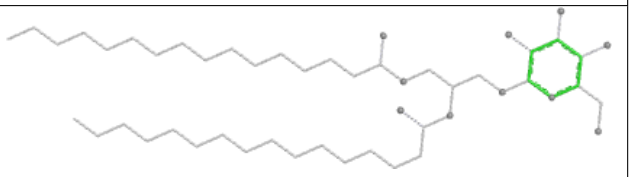
Bond lengths



Bond angles

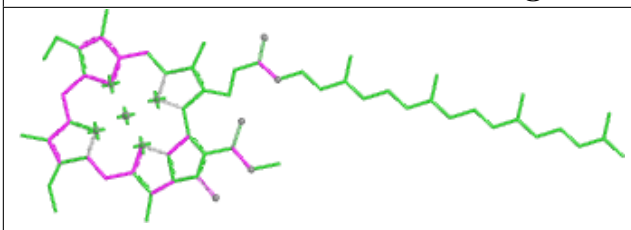


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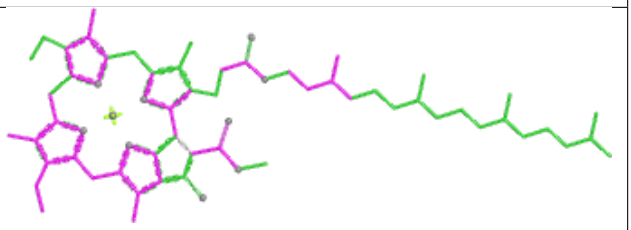


Rings

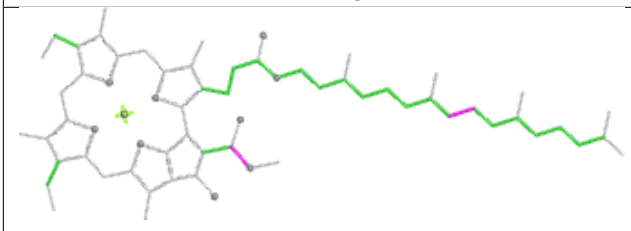
Ligand CLA B 613



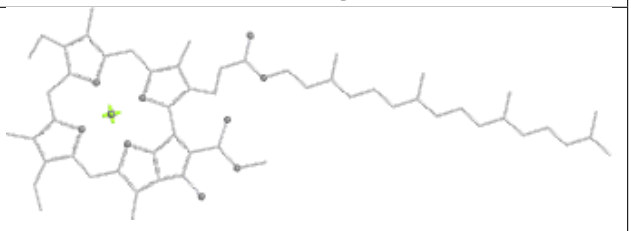
Bond lengths



Bond angles

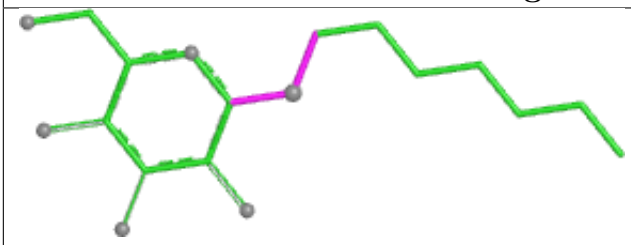


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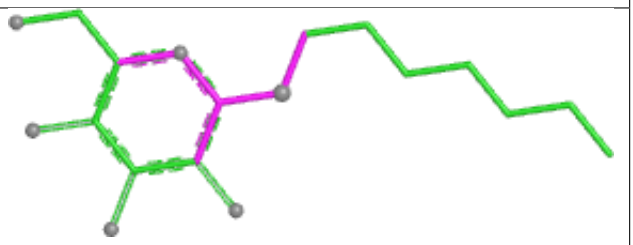


Rings

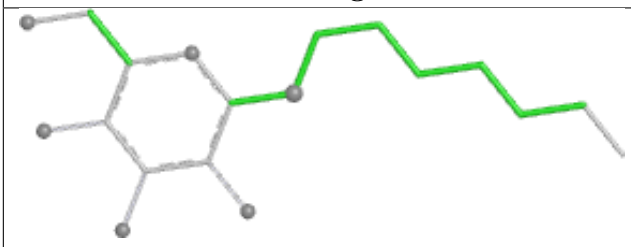
Ligand HTG b 608



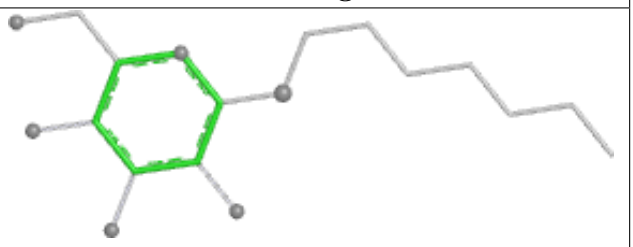
Bond lengths



Bond angles

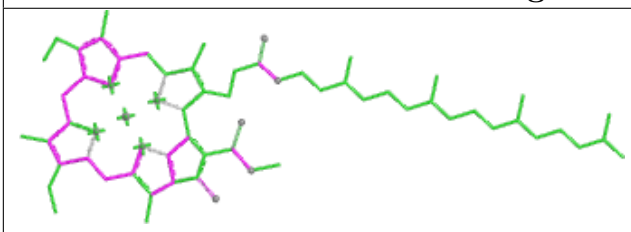


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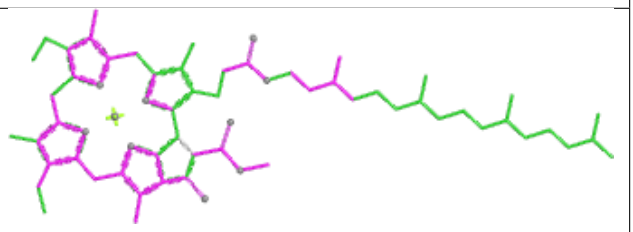


Rings

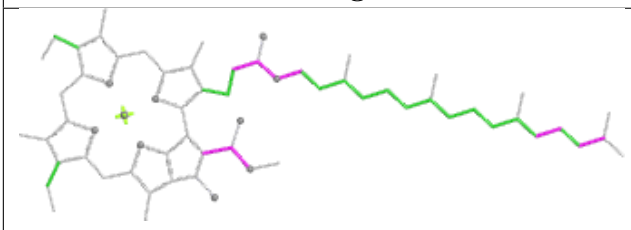
Ligand CLA b 622



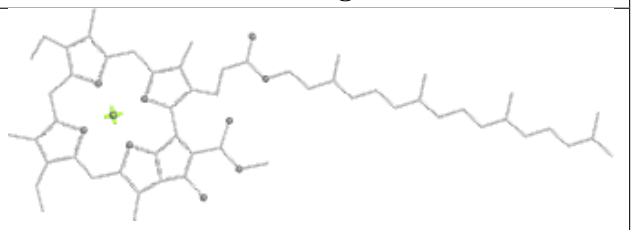
Bond lengths



Bond angles

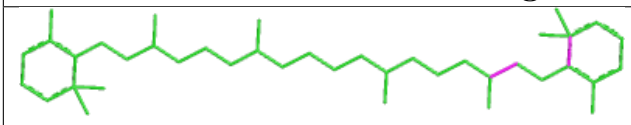


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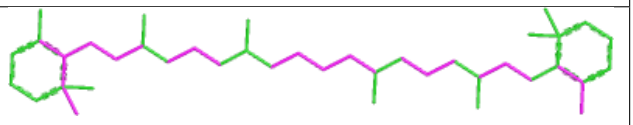


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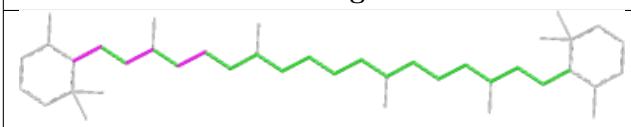
Ligand BCR H 101



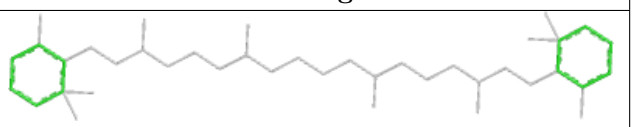
Bond lengths



Bond angles

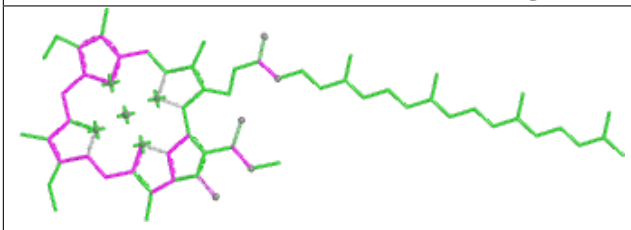


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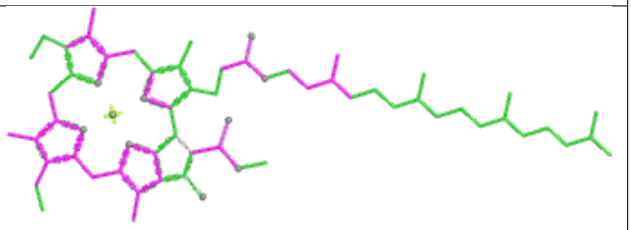


Rings

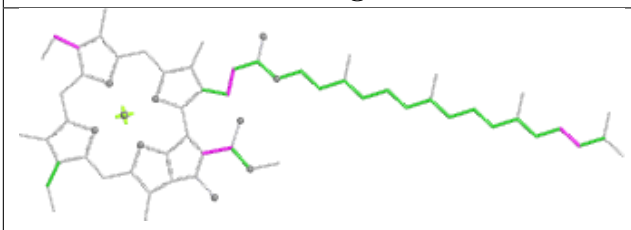
Ligand CLA C 507



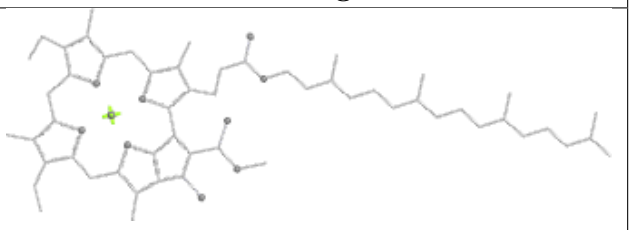
Bond lengths



Bond angles



Torsions



Rings

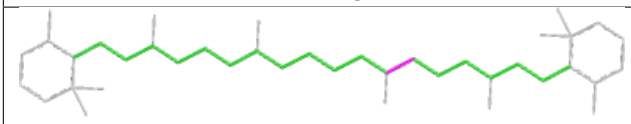
Ligand BCR k 102



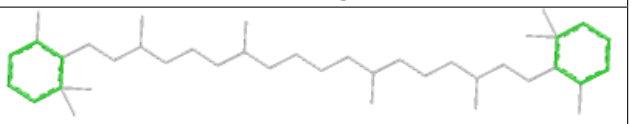
Bond lengths



Bond angles

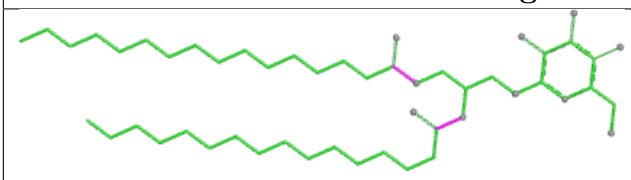


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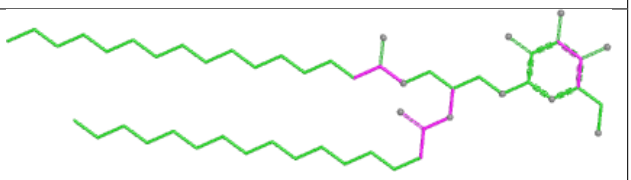


Rings

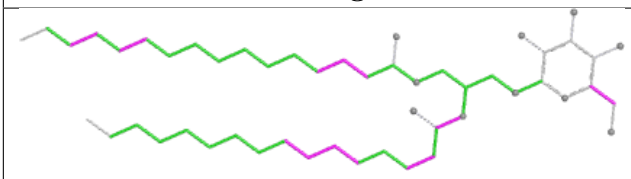
Ligand LMG C 520



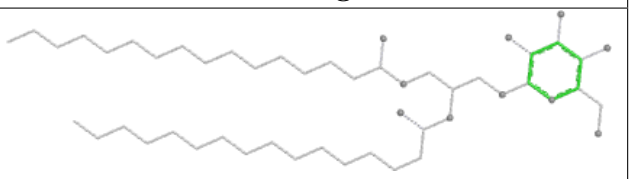
Bond lengths



Bond angles

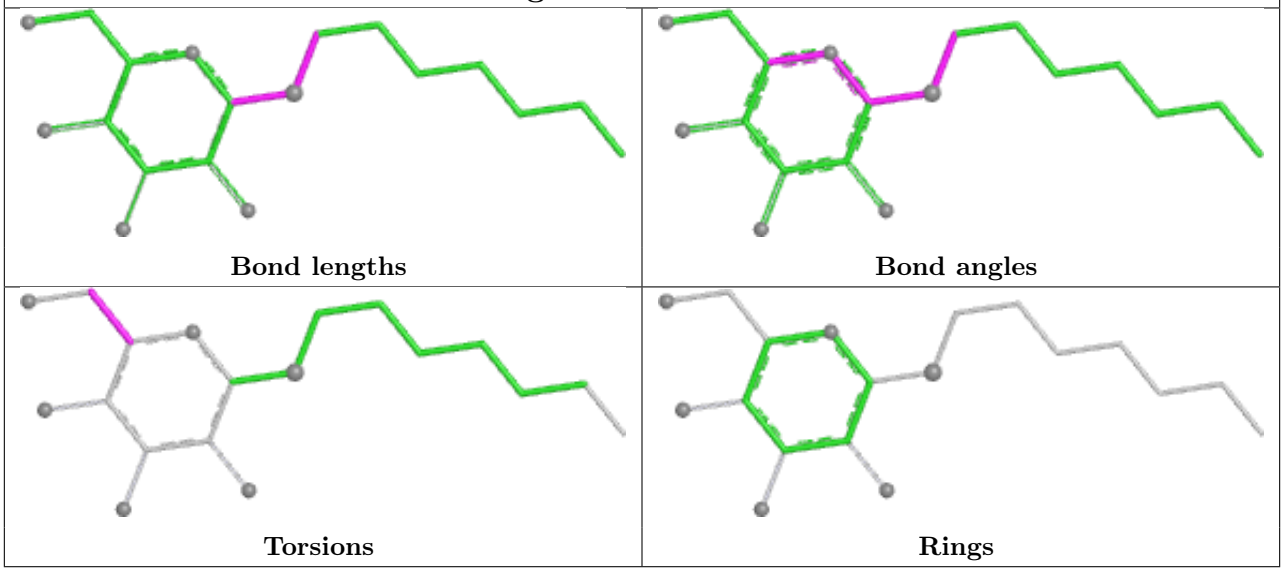


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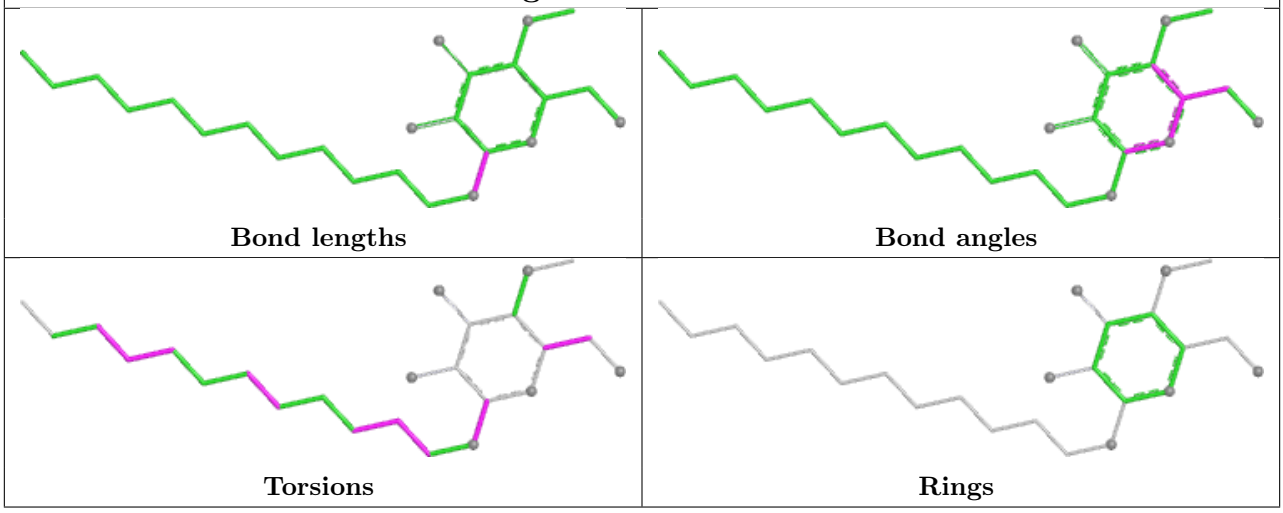


Rings

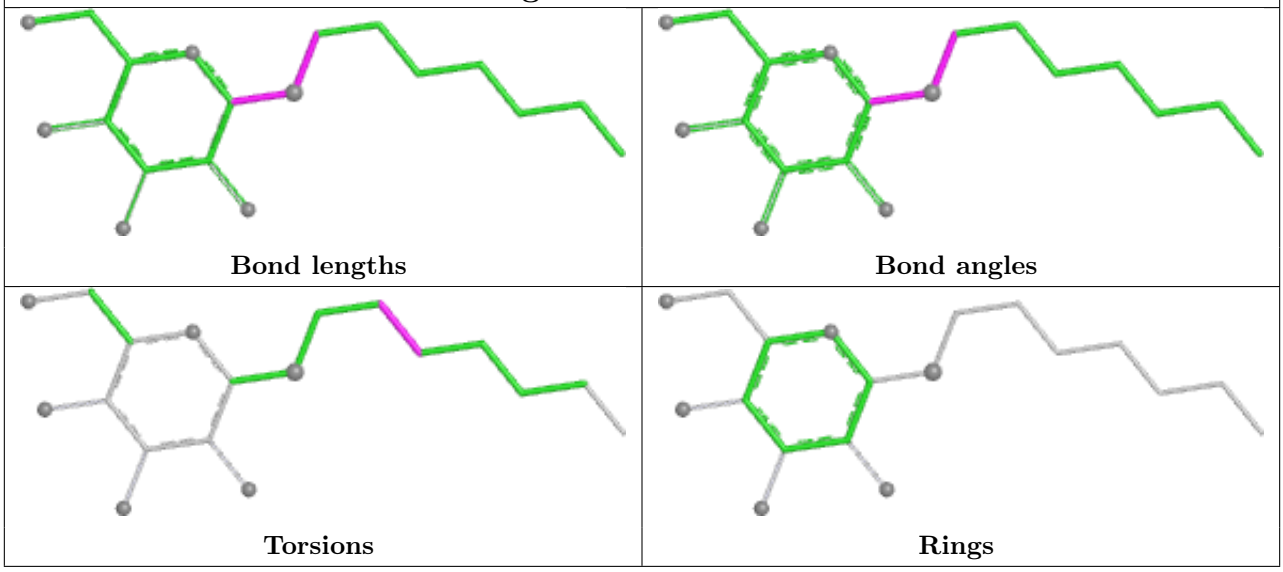
Ligand HTG c 524



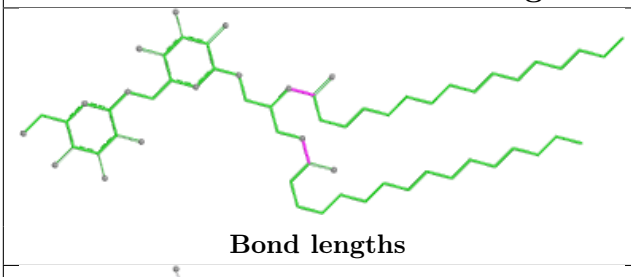
Ligand LMT T 104



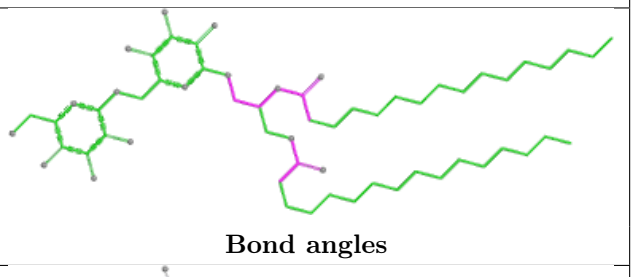
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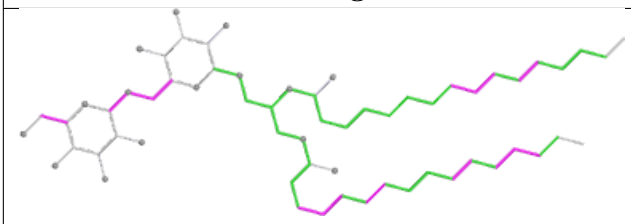
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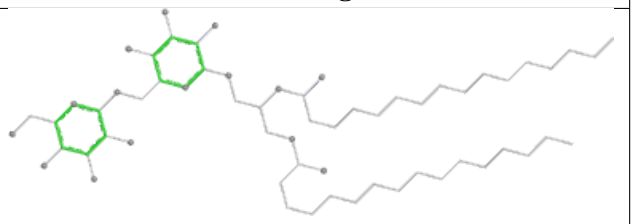
Bond lengths



Bond angles

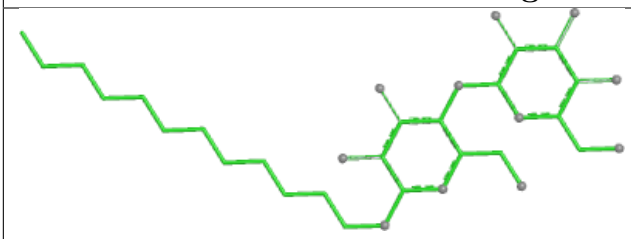


Torsions

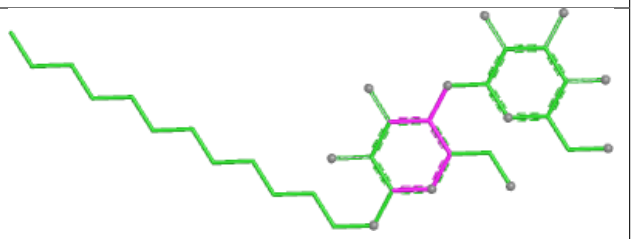


Rings

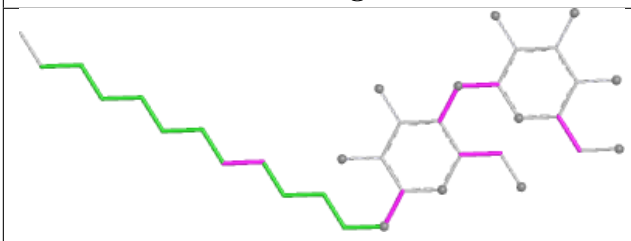
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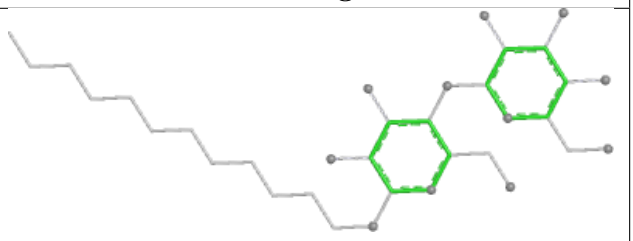
Bond lengths



Bond angles

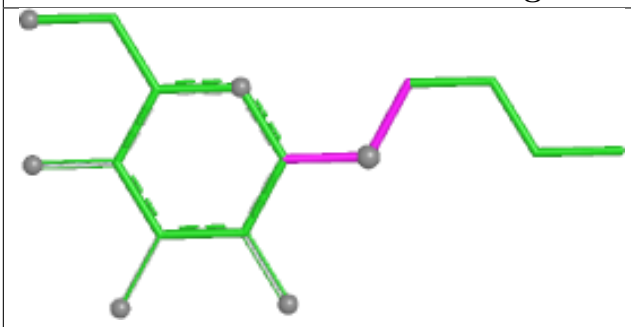


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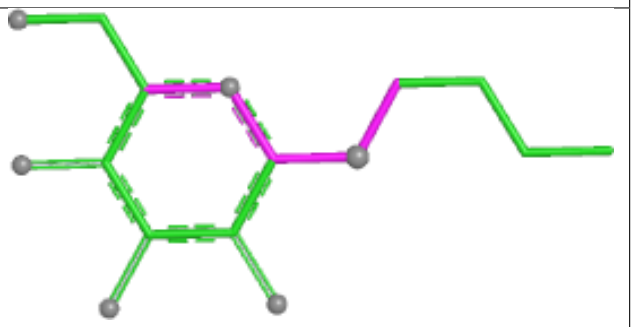


Rings

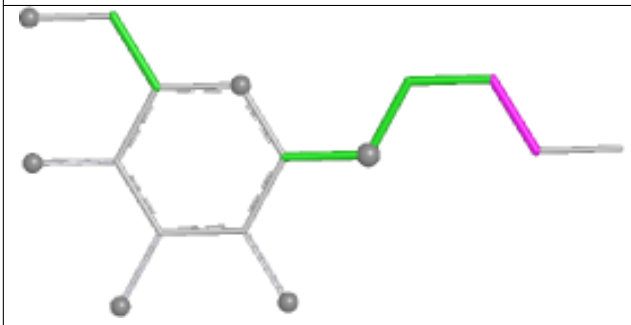
Ligand HTG d 413



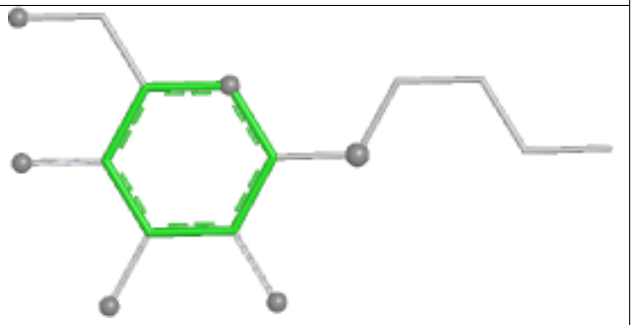
Bond lengths



Bond angles

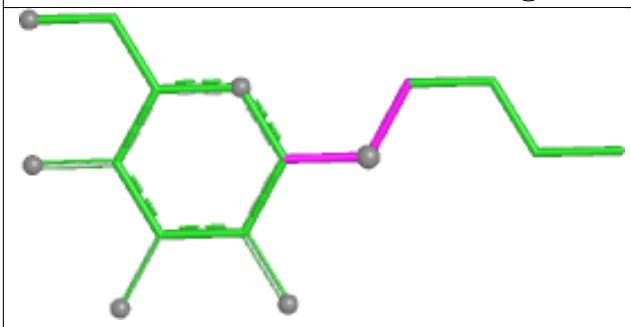


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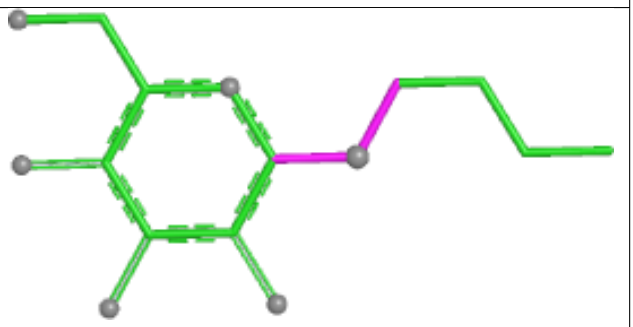


Rings

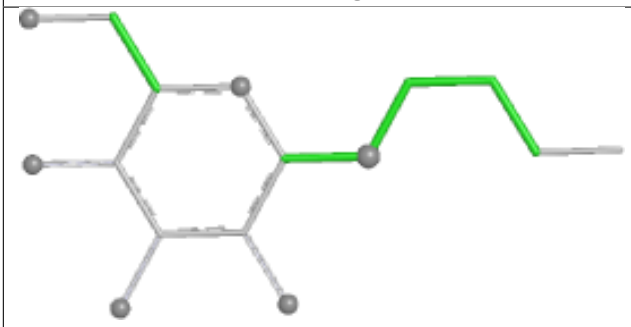
Ligand HTG D 414



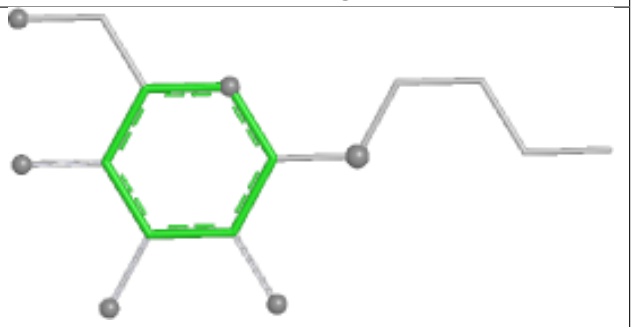
Bond lengths



Bond angles

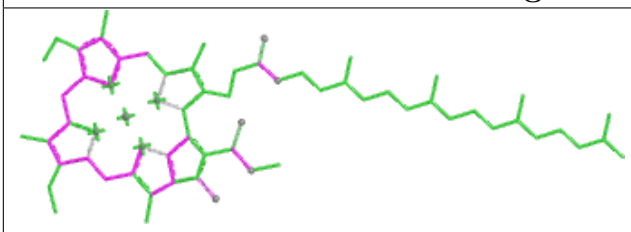


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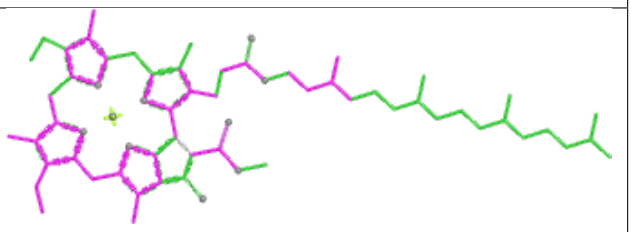


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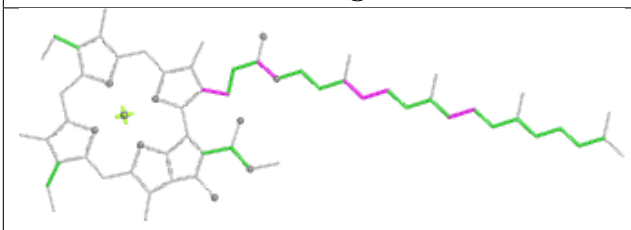
Ligand CLA C 513



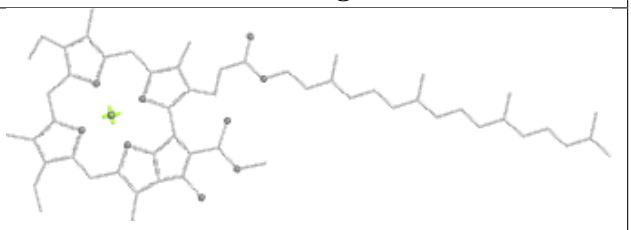
Bond lengths



Bond angles



Torsions

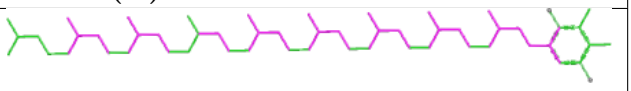


Rings

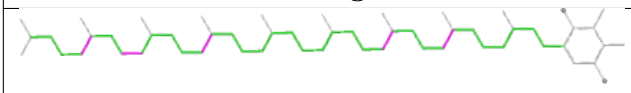
Ligand PL9 d 407 (B)



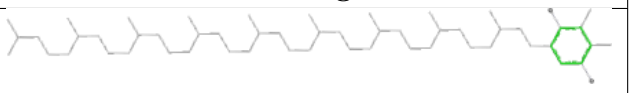
Bond lengths



Bond angles

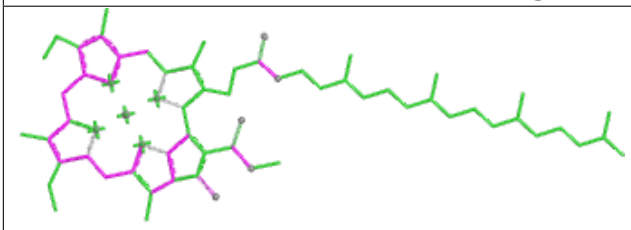


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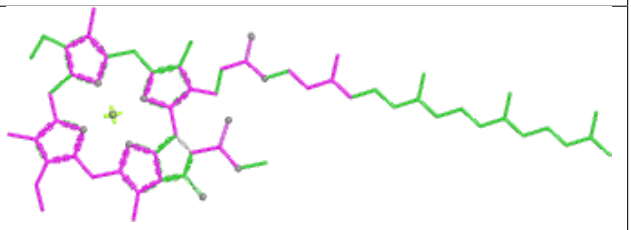


Rings

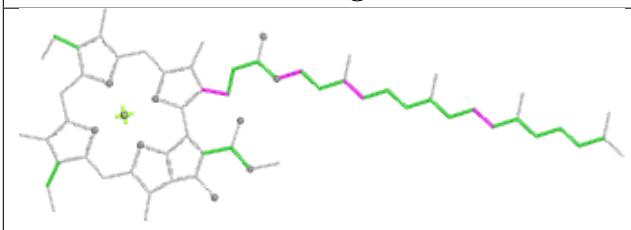
Ligand CLA c 517



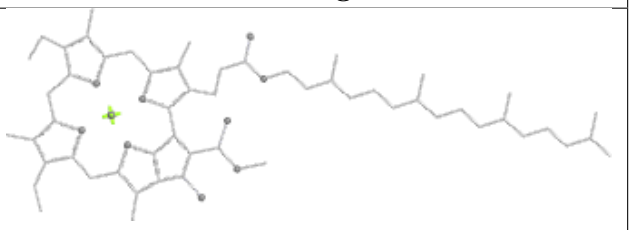
Bond lengths



Bond angles

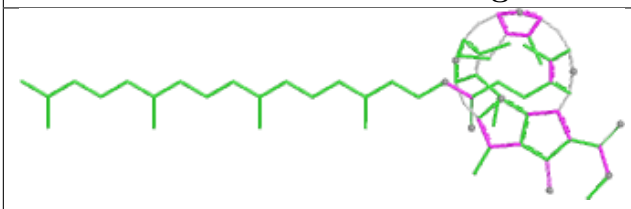


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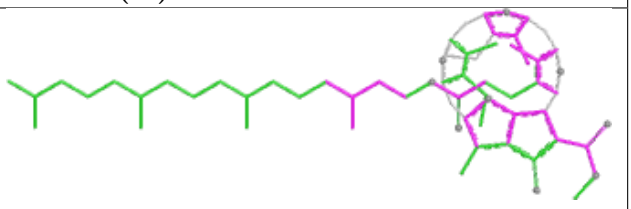


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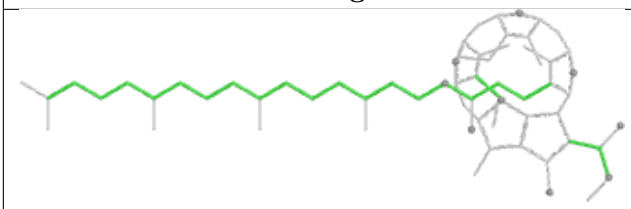
Ligand PHO d 402 (A)



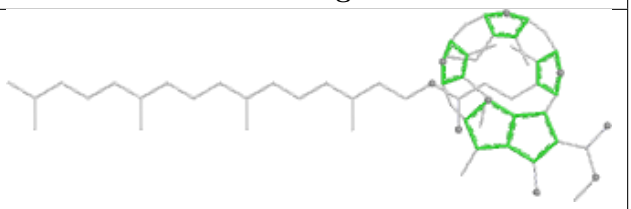
Bond lengths



Bond angles

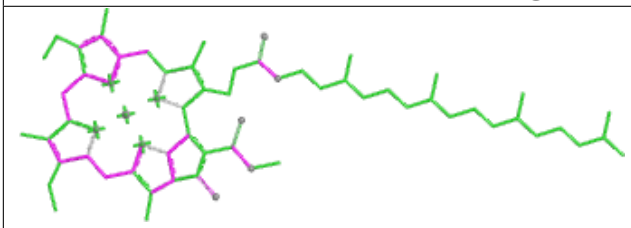


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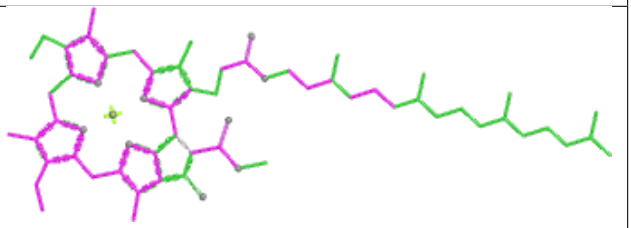


Rings

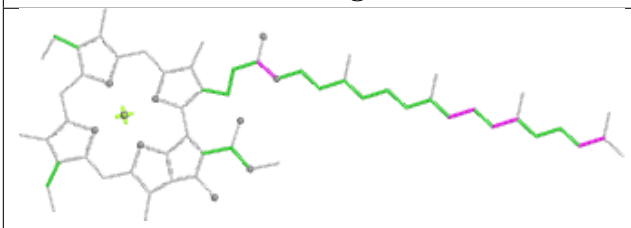
Ligand CLA b 620



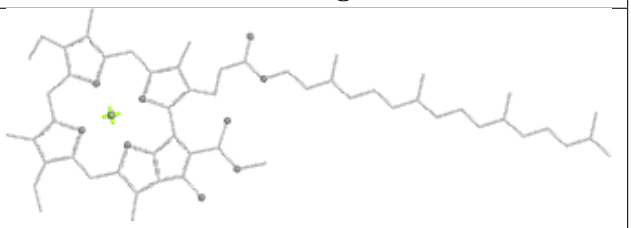
Bond lengths



Bond angles

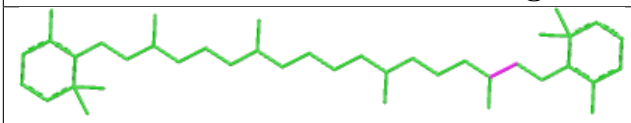


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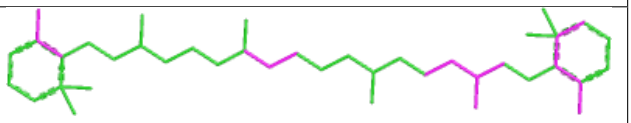


Rings

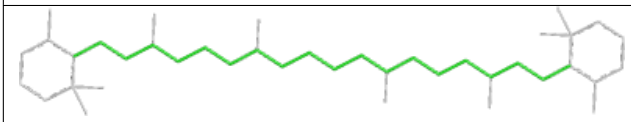
Ligand BCR b 627



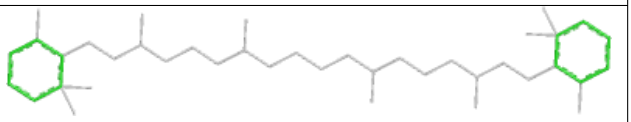
Bond lengths



Bond angles

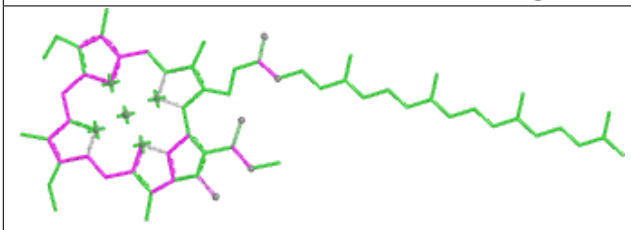


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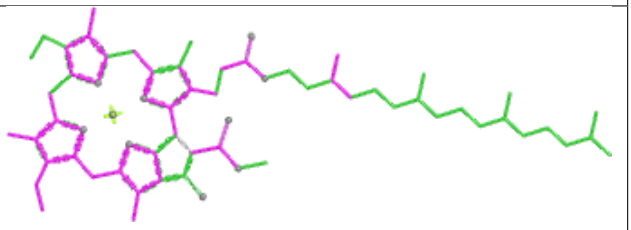


Rings

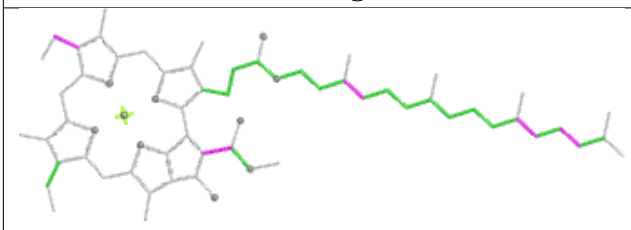
Ligand CLA c 508



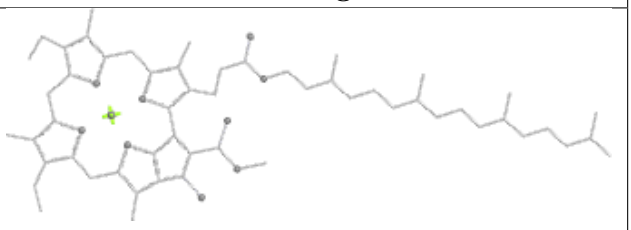
Bond lengths



Bond angles

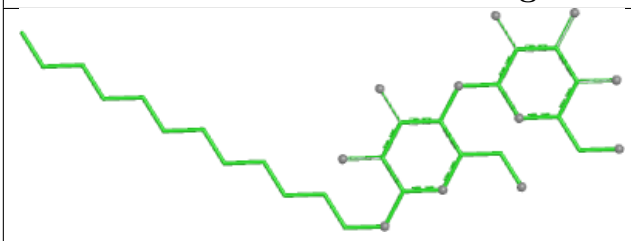


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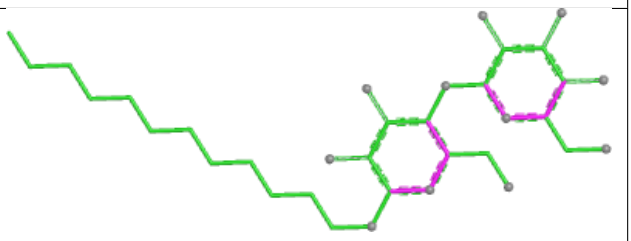


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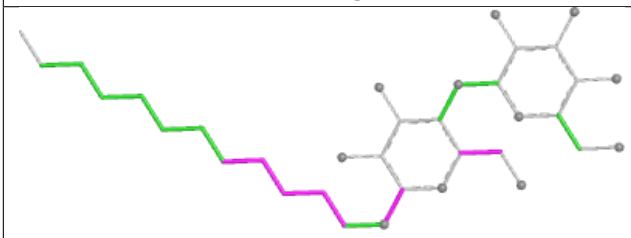
Ligand LMT m 103



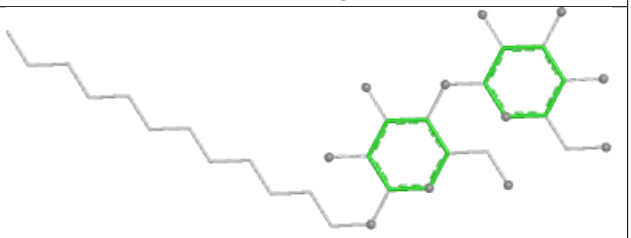
Bond lengths



Bond angles

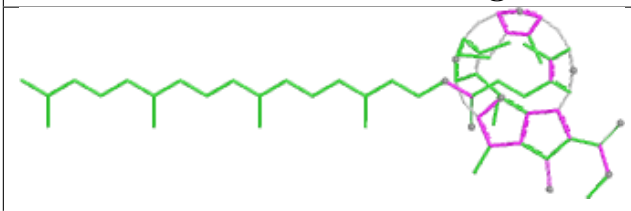


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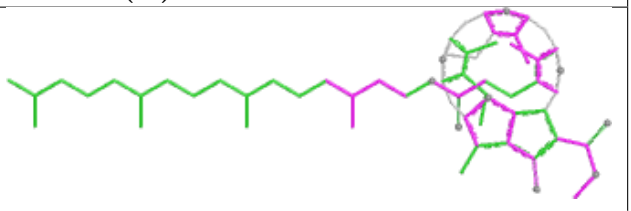


Rings

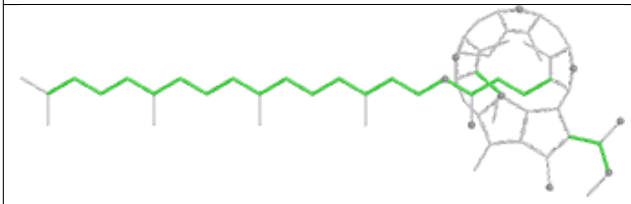
Ligand PHO D 401 (B)



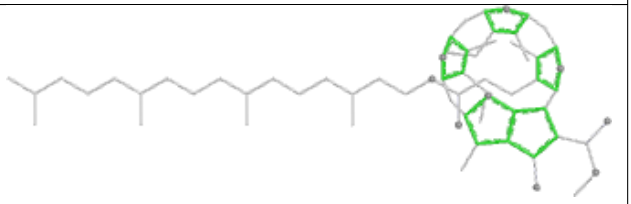
Bond lengths



Bond angles

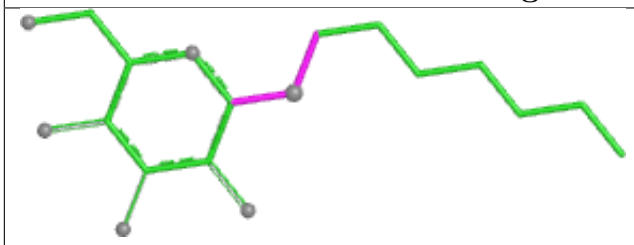


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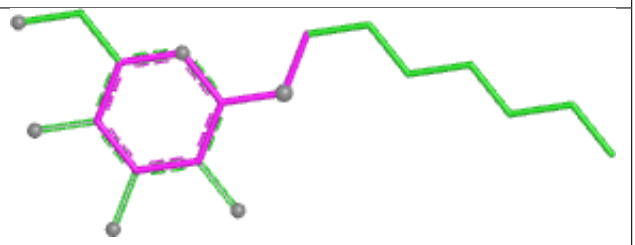


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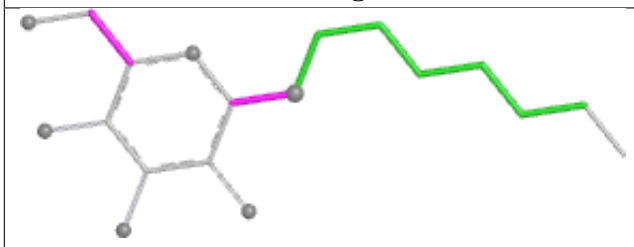
Ligand HTG V 206



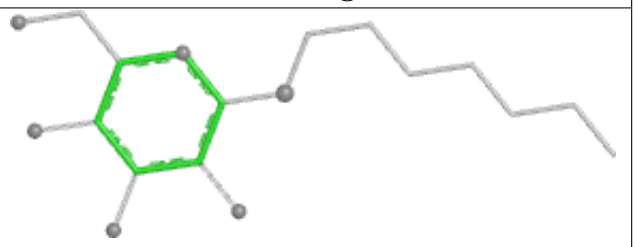
Bond lengths



Bond angles

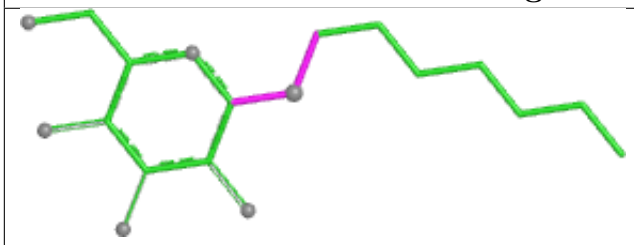


Torsions

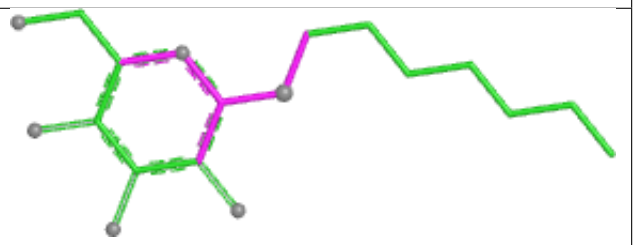


Rings

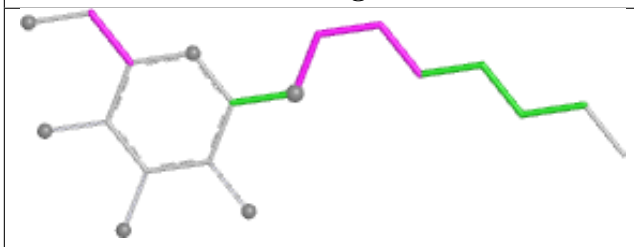
Ligand HTG b 632



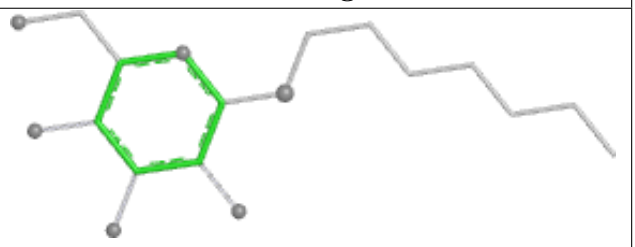
Bond lengths



Bond angles

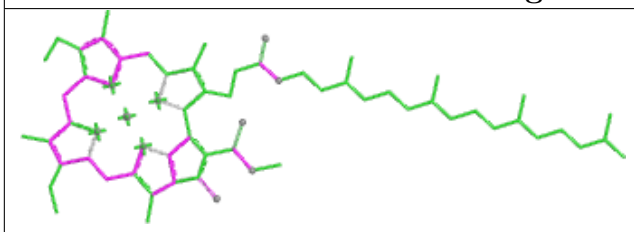


Torsions

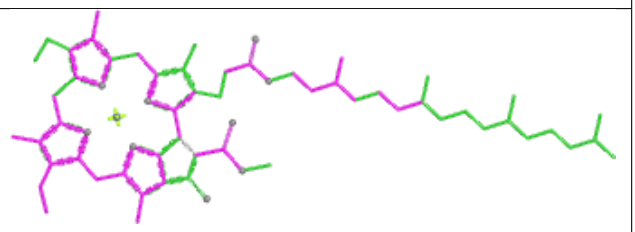


Rings

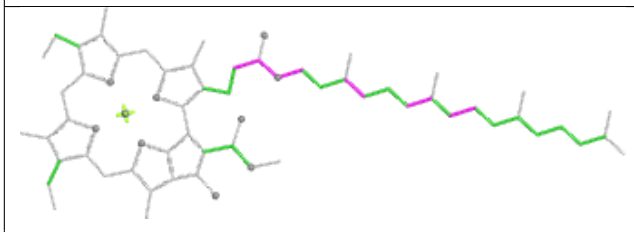
Ligand CLA C 510



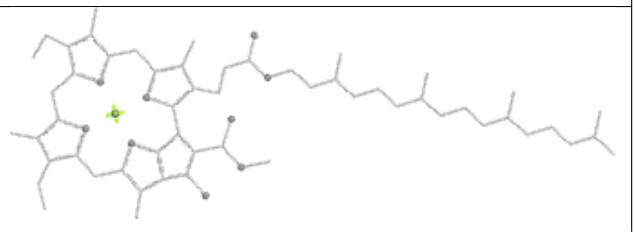
Bond lengths



Bond angles

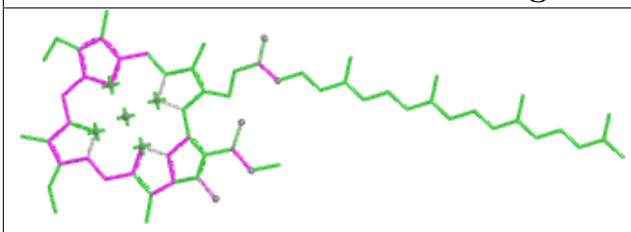


Torsions

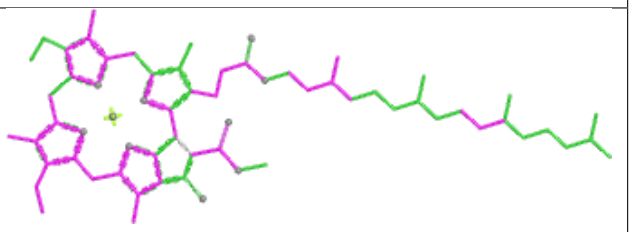


Rings

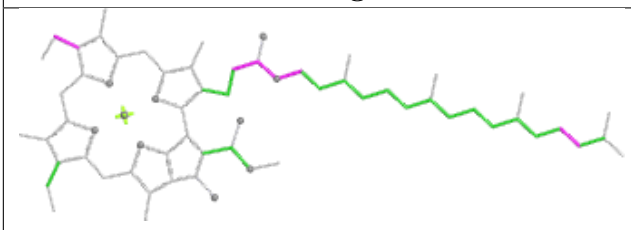
Ligand CLA c 516



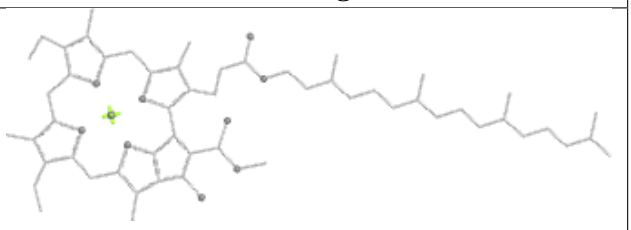
Bond lengths



Bond angles



Torsions

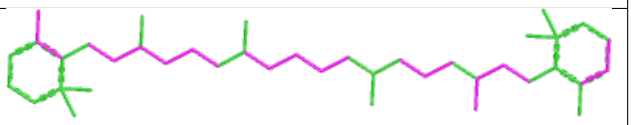


Rings

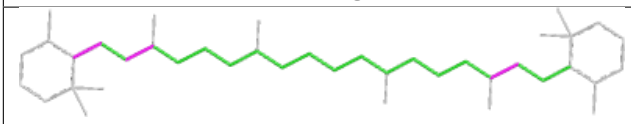
Ligand BCR C 515



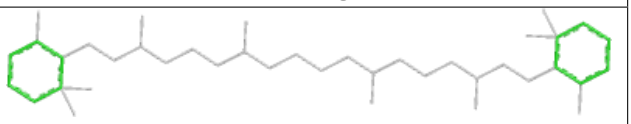
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.53	0 100 100	21, 47, 72, 117	53 (15%)
1	a	334/344 (97%)	-0.52	1 (0%) 90 88	22, 48, 80, 156	55 (16%)
2	B	504/505 (99%)	-0.47	1 (0%) 91 89	31, 54, 93, 141	10 (1%)
2	b	503/505 (99%)	-0.44	3 (0%) 85 83	31, 54, 96, 194	12 (2%)
3	C	451/455 (99%)	-0.45	0 100 100	21, 62, 87, 140	7 (1%)
3	c	455/455 (100%)	-0.43	0 100 100	23, 65, 87, 139	13 (2%)
4	D	341/342 (99%)	-0.60	0 100 100	24, 50, 76, 139	16 (4%)
4	d	341/342 (99%)	-0.55	0 100 100	24, 51, 74, 122	16 (4%)
5	E	81/84 (96%)	-0.10	0 100 100	40, 78, 113, 169	2 (2%)
5	e	81/84 (96%)	-0.06	2 (2%) 58 54	42, 78, 131, 187	2 (2%)
6	F	34/44 (77%)	-0.18	0 100 100	59, 70, 111, 118	0
6	f	32/44 (72%)	-0.22	1 (3%) 51 47	57, 69, 132, 154	0
7	H	65/65 (100%)	-0.30	2 (3%) 51 47	40, 65, 86, 160	1 (1%)
7	h	65/65 (100%)	-0.46	1 (1%) 72 68	54, 67, 85, 172	0
8	I	37/38 (97%)	-0.06	0 100 100	53, 67, 127, 178	0
8	i	37/38 (97%)	-0.23	1 (2%) 56 52	49, 64, 131, 156	0
9	J	38/39 (97%)	-0.04	1 (2%) 57 53	58, 76, 160, 184	0
9	j	39/39 (100%)	-0.11	0 100 100	59, 71, 147, 178	0
10	K	37/37 (100%)	-0.28	0 100 100	65, 77, 94, 113	0
10	k	37/37 (100%)	-0.35	0 100 100	65, 76, 98, 113	0
11	L	37/37 (100%)	-0.60	0 100 100	25, 44, 98, 137	1 (2%)
11	l	37/37 (100%)	-0.48	0 100 100	28, 46, 98, 140	1 (2%)
12	M	33/36 (91%)	-0.53	0 100 100	27, 46, 80, 122	1 (3%)
12	m	33/36 (91%)	-0.61	0 100 100	39, 48, 87, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	243/244 (99%)	-0.52	0 100 100	31, 59, 100, 159	8 (3%)
13	o	243/244 (99%)	-0.44	0 100 100	34, 63, 115, 176	5 (2%)
14	T	29/32 (90%)	-0.67	0 100 100	36, 45, 78, 136	1 (3%)
14	t	29/32 (90%)	-0.54	1 (3%) 48 44	36, 45, 71, 137	1 (3%)
15	U	97/104 (93%)	-0.59	0 100 100	46, 59, 89, 121	0
15	u	97/104 (93%)	-0.57	0 100 100	47, 61, 81, 129	0
16	V	137/137 (100%)	-0.58	0 100 100	25, 59, 83, 119	2 (1%)
16	v	137/137 (100%)	-0.49	0 100 100	26, 69, 98, 139	1 (0%)
17	Y	29/30 (96%)	0.71	3 (10%) 12 9	81, 91, 187, 209	0
17	y	29/30 (96%)	0.27	1 (3%) 48 44	82, 96, 146, 162	0
18	X	39/40 (97%)	-0.04	0 100 100	62, 73, 120, 151	0
18	x	38/40 (95%)	0.17	2 (5%) 32 28	63, 72, 133, 157	0
19	Z	62/62 (100%)	0.05	1 (1%) 70 66	78, 93, 132, 152	0
19	z	62/62 (100%)	0.23	2 (3%) 50 46	83, 97, 151, 188	0
20	R	18/34 (52%)	1.84	8 (44%) 0 0	96, 143, 171, 174	0
All	All	5275/5384 (97%)	-0.42	31 (0%) 85 83	21, 58, 106, 209	208 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
20	R	15	ALA	3.9
17	Y	20	ALA	3.6
7	H	65	LEU	3.4
7	h	65	LEU	3.1
5	e	4	THR	3.0
8	i	37	LEU	3.0
18	x	37	VAL	2.9
1	a	248[A]	ILE	2.8
5	e	5	THR	2.8
2	B	479	PHE	2.7
2	b	486	LEU	2.7
17	y	20	ALA	2.6
19	z	3	ILE	2.5
20	R	3	TRP	2.5
14	t	30	THR	2.4
9	J	2	SER	2.4
20	R	6	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	b	495	PHE	2.4
17	Y	18	VAL	2.4
20	R	14	LEU	2.4
2	b	502	VAL	2.3
17	Y	19	ILE	2.3
20	R	12	VAL	2.3
20	R	9	LEU	2.3
19	z	62	VAL	2.3
20	R	5	VAL	2.3
18	x	2	THR	2.2
7	H	66	GLY	2.2
20	R	13	LEU	2.1
19	Z	62	VAL	2.1
6	f	14	PRO	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	FME	t	1	10/11	0.92	0.08	33,45,52,103	0
14	FME	T	1	10/11	0.93	0.08	40,51,58,129	0
12	FME	m	1	10/11	0.95	0.09	37,59,100,111	0
8	FME	I	1	10/11	0.95	0.07	36,59,66,70	0
12	FME	M	1	10/11	0.97	0.07	38,56,95,98	0
8	FME	i	1	10/11	0.97	0.07	45,62,71,72	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	DGD	e	101	62/66	0.68	0.17	89,127,190,192	0
36	DGD	D	408	52/66	0.70	0.15	75,107,156,165	0
32	UNL	m	101	10/-	0.70	0.18	64,66,90,92	0
29	LMT	E	102	35/35	0.73	0.17	116,153,169,172	0
27	SQD	f	102	43/54	0.73	0.16	109,123,162,167	0
32	UNL	J	101	10/-	0.75	0.17	61,84,93,93	0
29	LMT	C	521	35/35	0.75	0.14	96,134,162,166	0
32	UNL	a	403	30/-	0.76	0.14	77,96,125,131	0
29	LMT	b	630	25/35	0.76	0.16	80,112,160,160	0
37	LHG	a	420	42/49	0.76	0.11	75,138,182,183	0
32	UNL	C	527	34/-	0.77	0.14	92,125,135,139	0
32	UNL	j	101	10/-	0.77	0.15	76,91,98,99	0
32	UNL	A	418	28/-	0.77	0.14	65,94,113,117	0
34	CA	f	103	1/1	0.78	0.07	124,124,124,124	0
37	LHG	E	101	42/49	0.78	0.12	73,119,141,142	0
32	UNL	i	101	40/-	0.78	0.14	54,88,139,142	0
29	LMT	a	419	35/35	0.79	0.13	104,129,159,162	0
29	LMT	e	102	35/35	0.79	0.14	86,143,166,167	0
35	HTG	D	414	16/19	0.79	0.12	81,137,154,157	0
35	HTG	V	206	19/19	0.79	0.14	62,103,129,237	0
29	LMT	A	414	35/35	0.80	0.13	59,96,114,123	0
32	UNL	d	412	36/-	0.80	0.13	69,89,135,139	0
29	LMT	M	104	35/35	0.81	0.13	56,102,155,159	0
35	HTG	d	413	16/19	0.81	0.12	72,110,117,122	0
29	LMT	D	403	35/35	0.81	0.12	75,127,151,153	0
32	UNL	D	413	40/-	0.81	0.12	63,88,132,140	0
35	HTG	B	632	19/19	0.81	0.11	55,118,140,210	0
32	UNL	I	101	40/-	0.81	0.14	60,95,150,153	0
33	LMG	C	520	51/55	0.82	0.12	67,122,137,143	0
32	UNL	B	633	33/-	0.82	0.14	62,87,128,133	0
35	HTG	b	608	19/19	0.82	0.11	55,112,147,160	0
28	GOL	V	201	6/6	0.82	0.16	81,91,96,100	0
35	HTG	c	524	19/19	0.83	0.11	90,122,133,164	0
32	UNL	M	103	10/-	0.83	0.10	48,53,74,76	0
29	LMT	a	404	35/35	0.83	0.12	42,99,122,150	0
32	UNL	c	525	32/-	0.83	0.13	85,102,136,143	0
27	SQD	F	101	43/54	0.83	0.12	80,119,134,139	0
33	LMG	Z	101	37/55	0.83	0.14	72,131,146,147	0
28	GOL	A	412	6/6	0.84	0.12	76,86,88,92	0
33	LMG	z	101	39/55	0.84	0.13	77,125,148,160	0
34	CA	b	609	1/1	0.84	0.09	134,134,134,134	0
32	UNL	b	633	33/-	0.84	0.14	58,97,147,148	0
35	HTG	B	624	19/19	0.84	0.11	78,133,147,176	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	a	402	6/6	0.84	0.13	93,97,103,103	0
35	HTG	C	523	19/19	0.84	0.12	78,117,141,143	0
28	GOL	O	301	6/6	0.84	0.10	74,89,90,93	0
33	LMG	c	522	51/55	0.85	0.12	59,111,124,132	0
27	SQD	L	102	54/54	0.85	0.11	54,82,126,138	0
29	LMT	t	101	25/35	0.85	0.13	52,86,147,149	0
31	PL9	a	416[A]	55/55	0.85	0.16	87,114,123,124	55
31	PL9	a	416[B]	55/55	0.85	0.16	87,114,123,124	55
35	HTG	c	523	19/19	0.85	0.11	91,114,126,129	0
31	PL9	A	417[B]	55/55	0.86	0.15	84,104,120,121	55
35	HTG	b	631	19/19	0.86	0.14	67,83,98,102	0
35	HTG	b	632	19/19	0.86	0.12	77,138,158,165	0
27	SQD	a	405	54/54	0.86	0.10	40,83,122,127	0
35	HTG	B	623	19/19	0.86	0.13	60,79,91,92	0
27	SQD	A	413	54/54	0.86	0.10	56,81,130,137	0
29	LMT	T	104	25/35	0.86	0.14	43,83,140,150	0
29	LMT	m	103	35/35	0.86	0.10	46,103,128,129	0
27	SQD	B	621	54/54	0.86	0.12	56,82,141,145	0
31	PL9	A	417[A]	55/55	0.86	0.15	85,104,120,121	55
28	GOL	T	101	6/6	0.87	0.19	70,88,93,93	0
28	GOL	v	202	6/6	0.87	0.12	83,96,98,100	0
28	GOL	B	627	6/6	0.87	0.12	71,86,88,88	0
29	LMT	m	102	35/35	0.88	0.11	56,93,121,125	0
34	CA	F	102	1/1	0.88	0.10	119,119,119,119	0
22	CL	A	403[A]	1/1	0.88	0.12	47,47,47,47	1
22	CL	A	403[B]	1/1	0.88	0.12	45,45,45,45	1
33	LMG	A	419	51/55	0.88	0.10	57,90,109,115	0
33	LMG	C	519	51/55	0.88	0.10	62,99,117,120	0
28	GOL	C	524	6/6	0.88	0.15	86,89,104,108	0
28	GOL	b	605	6/6	0.88	0.15	66,82,107,110	0
22	CL	v	205	1/1	0.88	0.09	128,128,128,128	0
33	LMG	k	101	51/55	0.88	0.11	62,94,123,126	0
24	CLA	C	513	65/65	0.89	0.10	61,87,117,123	0
28	GOL	T	102	6/6	0.89	0.12	104,114,118,118	0
28	GOL	c	502	6/6	0.89	0.16	85,111,119,127	0
28	GOL	t	103	6/6	0.89	0.17	60,88,99,102	0
35	HTG	C	522	19/19	0.89	0.10	91,102,119,121	0
28	GOL	B	629	6/6	0.89	0.13	55,69,74,78	0
28	GOL	b	606	6/6	0.90	0.10	70,91,98,100	0
24	CLA	C	506	65/65	0.90	0.10	52,75,116,119	0
32	UNL	d	411	17/-	0.90	0.11	57,77,101,101	0
28	GOL	a	421	6/6	0.90	0.10	88,100,106,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
32	UNL	d	414	18/-	0.90	0.13	76,84,116,118	0
24	CLA	B	602	65/65	0.90	0.10	57,74,114,132	0
28	GOL	v	203	6/6	0.90	0.12	96,105,112,124	0
34	CA	B	601	1/1	0.91	0.06	135,135,135,135	0
29	LMT	M	102	35/35	0.91	0.10	46,102,124,132	0
28	GOL	b	601	6/6	0.91	0.10	55,59,64,68	0
22	CL	U	201	1/1	0.91	0.12	117,117,117,117	0
24	CLA	b	610	65/65	0.91	0.10	57,79,127,133	0
24	CLA	c	517	65/65	0.91	0.09	76,94,106,111	0
35	HTG	B	631	19/19	0.91	0.10	52,105,123,128	0
33	LMG	a	415	51/55	0.91	0.09	61,90,100,101	0
28	GOL	o	301	6/6	0.91	0.10	84,90,97,98	0
37	LHG	D	411	49/49	0.91	0.10	51,71,118,127	0
27	SQD	A	411	54/54	0.91	0.10	52,94,103,105	0
32	UNL	X	101	18/-	0.91	0.10	70,77,101,105	0
26	BCR	d	406	40/40	0.92	0.08	48,61,83,91	0
23	BCT	A	404[A]	4/4	0.92	0.11	72,74,78,88	4
36	DGD	C	517	62/66	0.92	0.09	55,71,102,113	0
33	LMG	d	415	51/55	0.92	0.09	53,70,112,122	0
24	CLA	C	504	65/65	0.92	0.09	45,67,93,102	0
23	BCT	A	404[B]	4/4	0.92	0.11	71,72,78,90	4
33	LMG	D	415	51/55	0.92	0.10	51,73,119,129	0
26	BCR	C	514	40/40	0.92	0.09	58,81,93,94	0
32	UNL	D	412	17/-	0.93	0.09	46,71,89,96	0
26	BCR	c	526	40/40	0.93	0.09	72,87,94,96	0
24	CLA	B	615	65/65	0.93	0.09	34,46,97,100	0
28	GOL	B	626	6/6	0.93	0.10	56,67,87,100	0
26	BCR	y	101	40/40	0.93	0.08	58,70,81,83	0
35	HTG	b	602	19/19	0.93	0.08	46,64,75,77	0
33	LMG	b	629	51/55	0.93	0.08	40,57,76,83	0
28	GOL	B	628	6/6	0.93	0.11	56,69,75,78	0
23	BCT	d	401[B]	4/4	0.93	0.12	85,85,88,93	4
28	GOL	B	630	6/6	0.93	0.11	59,95,102,108	0
28	GOL	B	634	6/6	0.93	0.08	56,58,65,66	0
24	CLA	c	510	65/65	0.93	0.08	52,74,96,102	0
23	BCT	d	401[A]	4/4	0.93	0.12	86,88,90,94	4
24	CLA	C	512	65/65	0.93	0.08	62,81,95,102	0
26	BCR	D	406	40/40	0.93	0.09	52,65,99,107	0
26	BCR	K	101	40/40	0.93	0.09	58,71,80,87	0
28	GOL	V	203	6/6	0.93	0.09	68,76,82,85	0
27	SQD	a	414	54/54	0.93	0.09	54,87,114,116	0
24	CLA	B	607	65/65	0.94	0.08	40,54,94,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
31	PL9	d	407[A]	55/55	0.94	0.07	31,46,53,59	55
31	PL9	d	407[B]	55/55	0.94	0.07	31,45,55,63	55
24	CLA	d	405	65/65	0.94	0.08	49,64,115,122	0
25	PHO	d	402[A]	64/64	0.94	0.07	39,50,56,59	64
25	PHO	d	402[B]	64/64	0.94	0.07	40,50,56,60	64
26	BCR	A	410	40/40	0.94	0.07	37,48,57,65	0
26	BCR	B	620	40/40	0.94	0.07	39,53,64,79	0
35	HTG	B	622	19/19	0.94	0.09	53,65,88,92	0
24	CLA	A	409	65/65	0.94	0.09	40,58,123,132	0
24	CLA	a	412	65/65	0.94	0.10	40,59,116,123	0
26	BCR	H	101	40/40	0.94	0.08	45,64,78,85	0
24	CLA	C	508	65/65	0.94	0.08	46,66,133,146	0
26	BCR	Y	101	40/40	0.94	0.08	62,72,92,98	0
26	BCR	b	627	40/40	0.94	0.07	37,52,68,78	0
28	GOL	D	402	6/6	0.94	0.13	55,64,73,77	0
24	CLA	b	615	65/65	0.94	0.08	41,54,100,112	0
24	CLA	b	625	65/65	0.94	0.08	40,61,106,112	0
35	HTG	b	607	19/19	0.94	0.07	52,88,101,103	0
26	BCR	h	101	40/40	0.94	0.07	46,66,76,77	0
24	CLA	c	507	65/65	0.94	0.08	50,62,75,87	0
28	GOL	V	202	6/6	0.94	0.09	54,65,76,78	0
24	CLA	C	510	65/65	0.94	0.07	55,71,84,92	0
28	GOL	V	204	6/6	0.94	0.10	90,103,105,112	0
24	CLA	c	511	65/65	0.94	0.09	53,68,79,83	0
36	DGD	C	516	62/66	0.94	0.08	40,58,89,91	0
24	CLA	c	512	65/65	0.94	0.08	44,59,125,141	0
24	CLA	c	516	65/65	0.94	0.08	63,79,91,99	0
36	DGD	c	519	62/66	0.94	0.08	41,62,97,101	0
36	DGD	c	520	62/66	0.94	0.08	47,65,115,133	0
36	DGD	c	521	62/66	0.94	0.08	51,62,87,100	0
33	LMG	M	101	51/55	0.94	0.08	41,61,83,89	0
36	DGD	h	102	62/66	0.94	0.07	44,60,79,85	0
37	LHG	D	409	49/49	0.94	0.08	39,56,65,72	0
31	PL9	D	407[A]	55/55	0.94	0.08	34,45,52,64	55
31	PL9	D	407[B]	55/55	0.94	0.08	34,45,53,67	55
28	GOL	b	603	6/6	0.94	0.10	60,73,78,87	0
37	LHG	d	410	49/49	0.94	0.10	42,65,113,119	0
26	BCR	T	103	40/40	0.95	0.06	32,51,66,72	0
24	CLA	b	624	65/65	0.95	0.07	42,56,74,78	0
24	CLA	B	609	65/65	0.95	0.07	42,53,62,66	0
26	BCR	b	628	40/40	0.95	0.07	41,59,69,72	0
26	BCR	c	518	40/40	0.95	0.07	49,63,73,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
28	GOL	a	401	6/6	0.95	0.10	55,63,75,82	0
24	CLA	c	505	65/65	0.95	0.08	50,67,75,77	0
24	CLA	c	506	65/65	0.95	0.07	47,61,79,88	0
24	CLA	C	507	65/65	0.95	0.08	51,71,84,91	0
26	BCR	k	102	40/40	0.95	0.08	54,75,85,87	0
28	GOL	b	604	6/6	0.95	0.09	62,73,80,84	0
26	BCR	t	102	40/40	0.95	0.07	36,53,75,77	0
24	CLA	c	508	65/65	0.95	0.07	49,62,85,99	0
24	CLA	c	509	65/65	0.95	0.07	43,56,75,78	0
24	CLA	B	614	65/65	0.95	0.07	31,45,67,82	0
24	CLA	C	509	65/65	0.95	0.09	49,72,86,92	0
24	CLA	A	407	65/65	0.95	0.07	33,47,101,110	0
24	CLA	c	513	65/65	0.95	0.09	53,68,85,94	0
28	GOL	v	204	6/6	0.95	0.10	59,64,71,78	0
24	CLA	c	515	65/65	0.95	0.08	51,73,89,101	0
24	CLA	C	511	65/65	0.95	0.08	56,74,89,101	0
24	CLA	B	617	65/65	0.95	0.11	45,62,136,139	0
24	CLA	C	502	65/65	0.95	0.07	45,66,73,81	0
28	GOL	B	625	6/6	0.95	0.08	55,65,74,83	0
36	DGD	C	518	62/66	0.95	0.07	45,63,82,96	0
24	CLA	D	405	65/65	0.95	0.08	47,62,111,116	0
36	DGD	H	102	62/66	0.95	0.08	41,58,95,103	0
24	CLA	a	410	65/65	0.95	0.07	38,51,113,120	0
24	CLA	C	503	65/65	0.95	0.07	50,62,77,82	0
26	BCR	B	619	40/40	0.95	0.06	37,51,64,71	0
24	CLA	B	608	65/65	0.95	0.07	32,45,58,70	0
24	CLA	C	505	65/65	0.95	0.07	48,60,75,91	0
26	BCR	C	515	40/40	0.95	0.07	47,63,75,80	0
24	CLA	b	618	65/65	0.95	0.07	45,57,67,77	0
28	GOL	F	103	6/6	0.95	0.07	88,95,100,104	0
24	CLA	b	620	65/65	0.95	0.07	35,49,59,65	0
37	LHG	d	408	49/49	0.95	0.07	44,60,70,72	0
24	CLA	b	623	65/65	0.95	0.07	31,47,93,106	0
39	MG	j	102	1/1	0.95	0.06	70,70,70,70	0
25	PHO	A	408	64/64	0.96	0.06	28,44,52,61	0
25	PHO	D	401[A]	64/64	0.96	0.07	41,51,60,63	64
25	PHO	D	401[B]	64/64	0.96	0.07	40,50,59,64	64
24	CLA	b	622	65/65	0.96	0.06	36,49,62,68	0
24	CLA	B	611	65/65	0.96	0.08	42,56,67,71	0
24	CLA	B	612	65/65	0.96	0.06	35,46,54,63	0
26	BCR	B	618	40/40	0.96	0.05	36,49,59,62	0
24	CLA	B	613	65/65	0.96	0.07	32,47,57,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	A	405	65/65	0.96	0.06	32,41,52,62	0
24	CLA	B	603	65/65	0.96	0.06	40,53,62,66	0
24	CLA	B	616	65/65	0.96	0.06	40,56,68,77	0
28	GOL	c	501	6/6	0.96	0.07	47,52,56,58	0
24	CLA	b	611	65/65	0.96	0.07	41,57,65,73	0
24	CLA	b	612	65/65	0.96	0.06	45,55,63,71	0
24	CLA	b	613	65/65	0.96	0.07	32,48,75,84	0
24	CLA	b	614	65/65	0.96	0.07	36,46,60,70	0
24	CLA	B	605	65/65	0.96	0.06	31,45,75,79	0
26	BCR	a	413	40/40	0.96	0.06	34,47,58,61	0
26	BCR	b	626	40/40	0.96	0.05	36,49,59,64	0
24	CLA	b	616	65/65	0.96	0.06	31,42,54,62	0
28	GOL	C	525	6/6	0.96	0.08	52,54,59,60	0
37	LHG	D	410	49/49	0.96	0.07	34,49,75,92	0
24	CLA	c	514	65/65	0.96	0.07	47,64,74,80	0
24	CLA	b	617	65/65	0.96	0.06	43,57,64,73	0
24	CLA	C	501	65/65	0.96	0.07	50,62,87,97	0
37	LHG	b	634	49/49	0.96	0.07	39,54,68,82	0
24	CLA	B	610	65/65	0.96	0.07	38,58,67,75	0
37	LHG	d	409	49/49	0.96	0.07	35,51,69,90	0
24	CLA	d	403	65/65	0.96	0.05	35,44,53,57	0
24	CLA	b	621	65/65	0.96	0.07	35,50,59,63	0
24	CLA	A	406	65/65	0.97	0.05	31,42,51,53	0
24	CLA	b	619	65/65	0.97	0.07	41,58,66,77	0
28	GOL	v	201	6/6	0.97	0.08	74,84,87,96	0
37	LHG	L	101	49/49	0.97	0.06	39,52,64,67	0
25	PHO	a	411	64/64	0.97	0.05	38,45,54,63	0
24	CLA	B	606	65/65	0.97	0.06	36,47,58,61	0
24	CLA	D	404	65/65	0.97	0.06	30,42,61,69	0
24	CLA	d	404	65/65	0.97	0.06	32,45,58,73	0
24	CLA	B	604	65/65	0.97	0.07	43,55,63,68	0
38	HEM	E	103	43/43	0.97	0.08	63,82,103,115	0
38	HEM	f	101	43/43	0.97	0.09	66,90,130,144	0
39	MG	J	102	1/1	0.97	0.05	71,71,71,71	0
24	CLA	a	409	65/65	0.97	0.06	34,44,56,71	0
34	CA	o	302	1/1	0.98	0.03	97,97,97,97	0
22	CL	a	408[B]	1/1	0.98	0.04	49,49,49,49	1
34	CA	O	302	1/1	0.98	0.03	100,100,100,100	0
22	CL	a	408[A]	1/1	0.98	0.04	49,49,49,49	1
34	CA	c	503	1/1	0.98	0.09	77,77,77,77	0
34	CA	C	526	1/1	0.98	0.06	87,87,87,87	0
40	HEC	V	205	43/43	0.98	0.06	44,53,65,67	0

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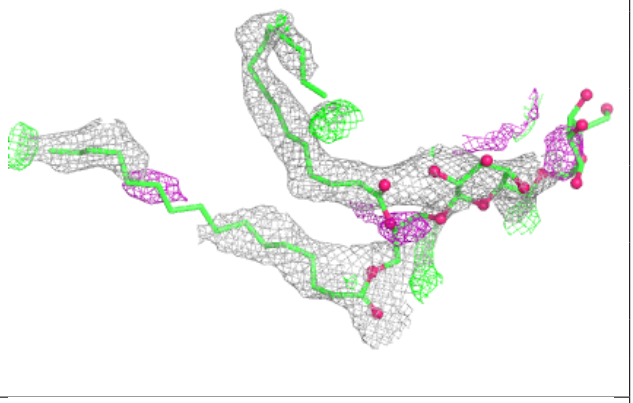
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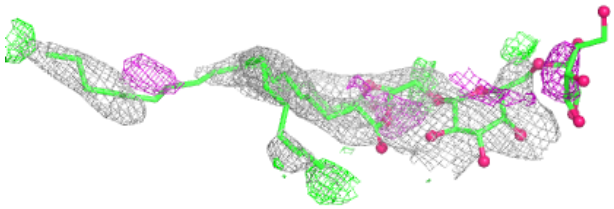
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
40	HEC	v	206	43/43	0.98	0.06	51,65,74,75	0
21	FE2	A	401[B]	1/1	0.99	0.03	65,65,65,65	1
21	FE2	a	406[A]	1/1	0.99	0.02	62,62,62,62	1
22	CL	a	407[A]	1/1	0.99	0.07	43,43,43,43	1
22	CL	a	407[B]	1/1	0.99	0.07	45,45,45,45	1
21	FE2	a	406[B]	1/1	0.99	0.02	62,62,62,62	1
22	CL	A	402[A]	1/1	0.99	0.04	41,41,41,41	1
34	CA	c	504	1/1	0.99	0.03	84,84,84,84	0
30	OEX	A	415[A]	10/10	0.99	0.03	47,57,59,70	10
30	OEX	A	416[B]	10/10	0.99	0.03	43,52,60,68	10
30	OEX	a	417[A]	10/10	0.99	0.04	47,51,57,61	10
30	OEX	a	418[B]	10/10	0.99	0.04	47,51,57,60	10
22	CL	A	402[B]	1/1	0.99	0.04	41,41,41,41	1
21	FE2	A	401[A]	1/1	0.99	0.03	66,66,66,66	1

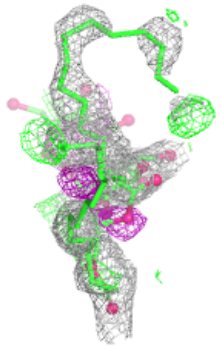
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around DGD e 101:

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

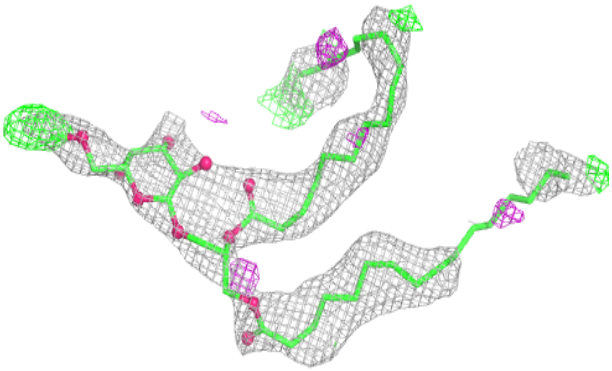


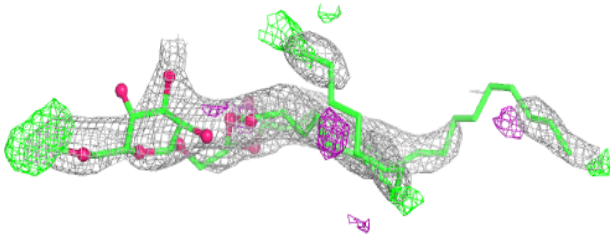


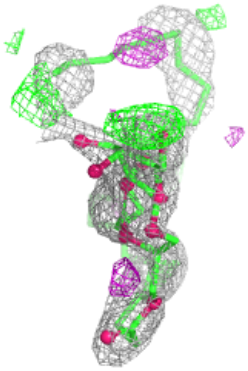


Electron density around DGD D 408:

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

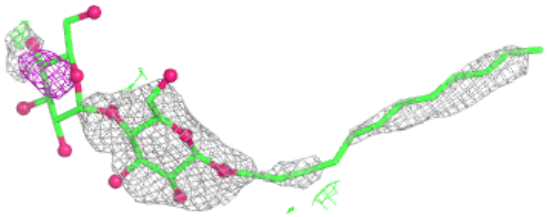


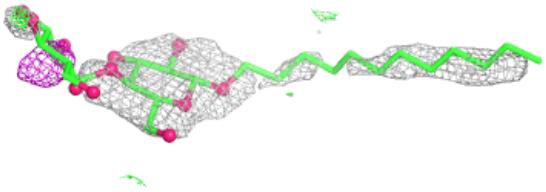


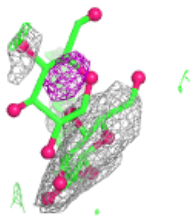


Electron density around LMT E 102:

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

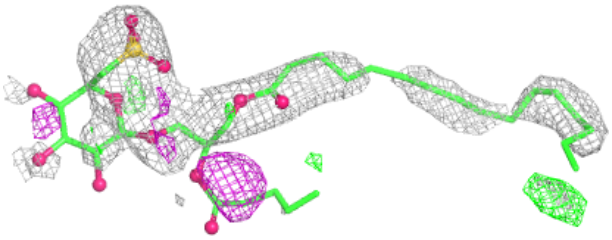


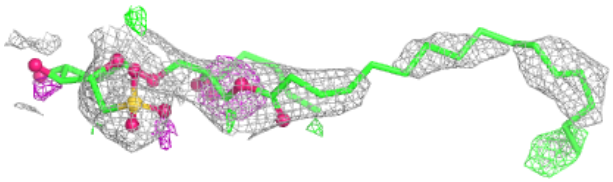


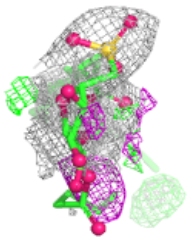


Electron density around SQD f 102:

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

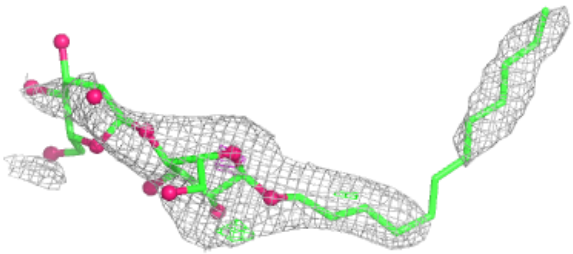


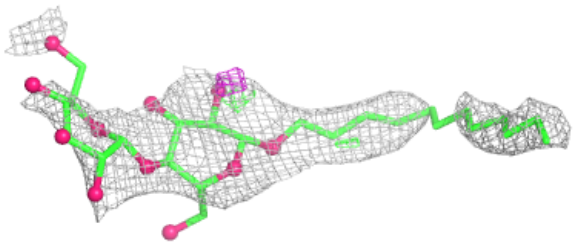


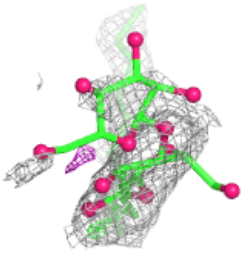


Electron density around LMT C 521:

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

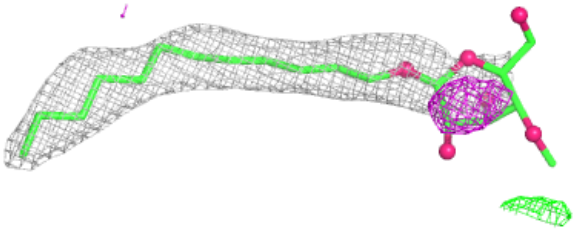


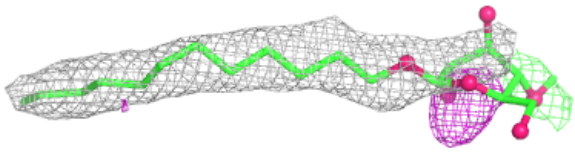


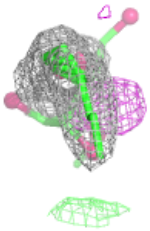


Electron density around LMT b 630:

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

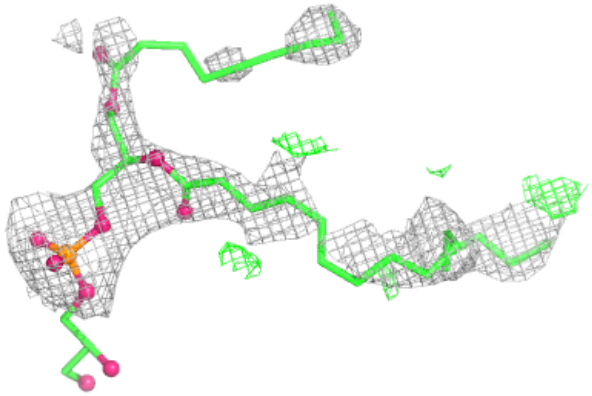


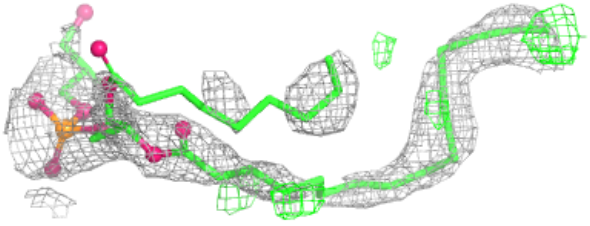


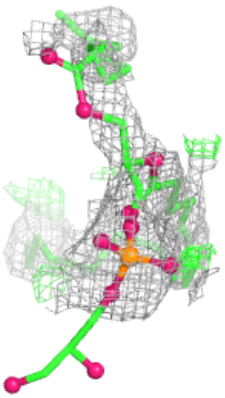


Electron density around LHG a 420:

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

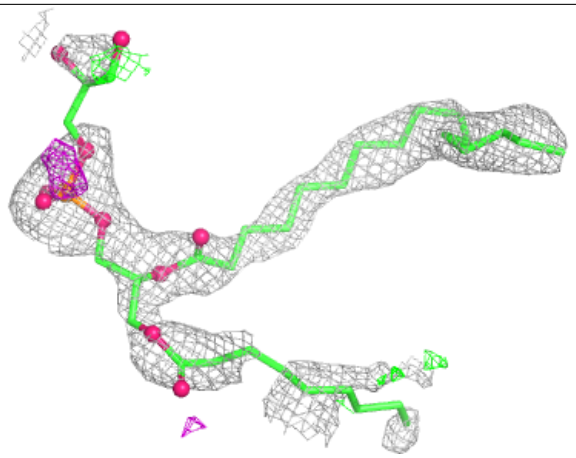


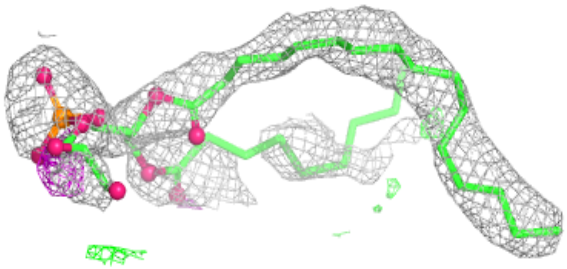




Electron density around LHG E 101:

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



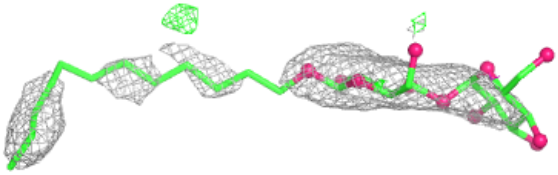


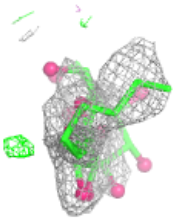


Electron density around LMT a 419:

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

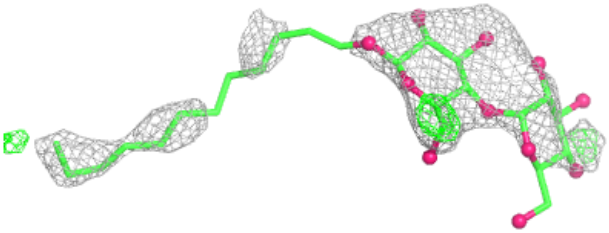


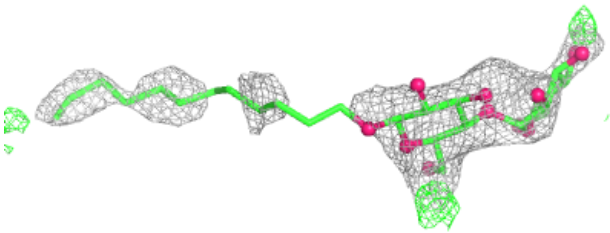


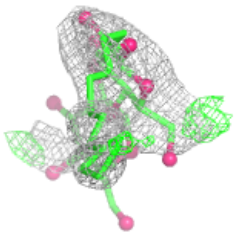


Electron density around LMT e 102:

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

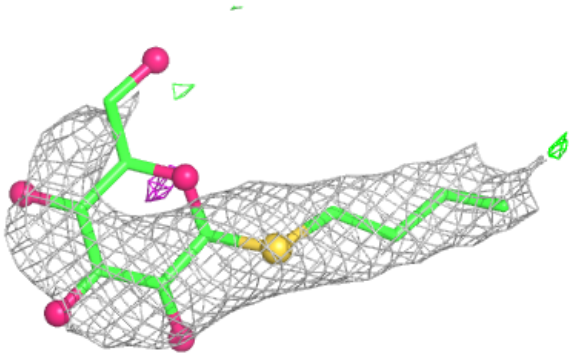


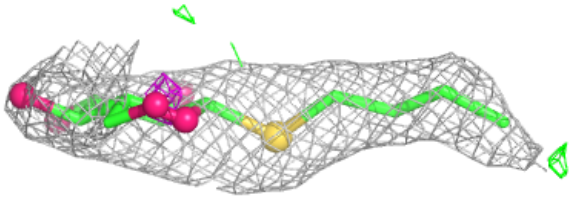


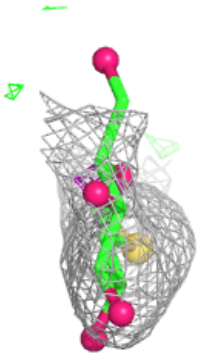


Electron density around HTG D 414:

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

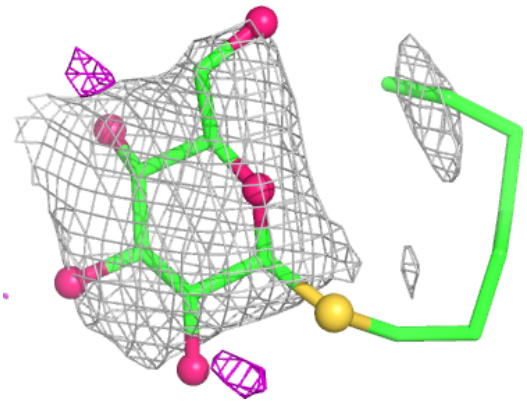


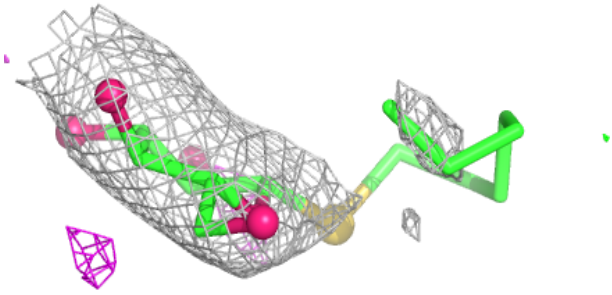


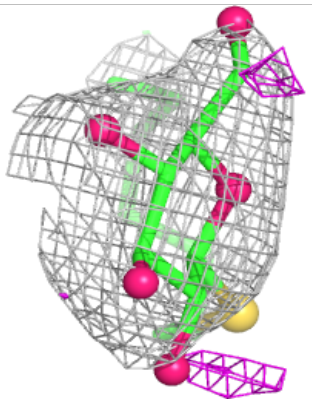


Electron density around HTG V 206:

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

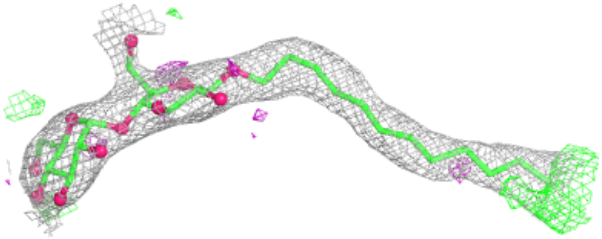


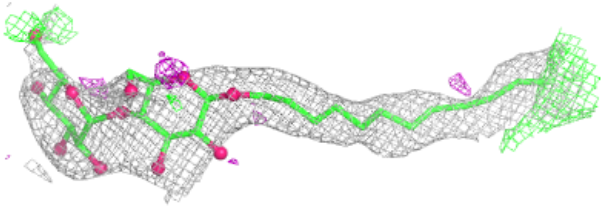


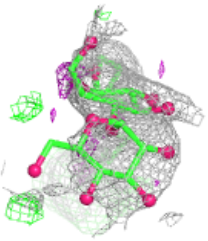


Electron density around LMT A 414:

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

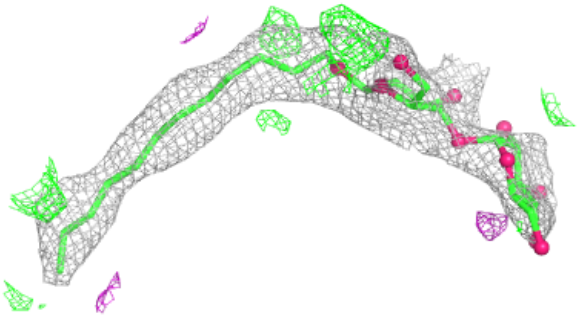


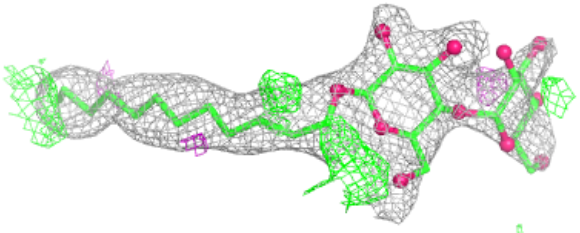


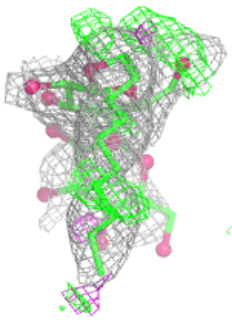


Electron density around LMT M 104:

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



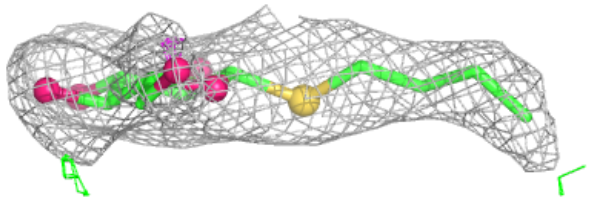


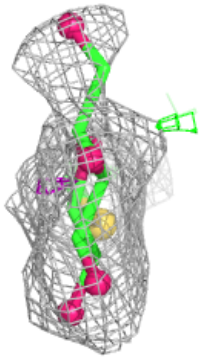


Electron density around HTG d 413:

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

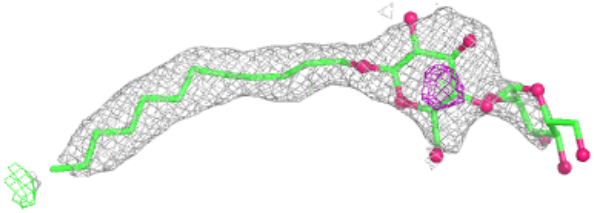


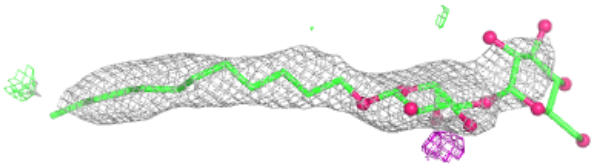


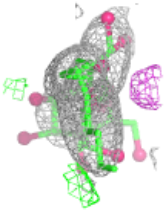


Electron density around LMT D 403:

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

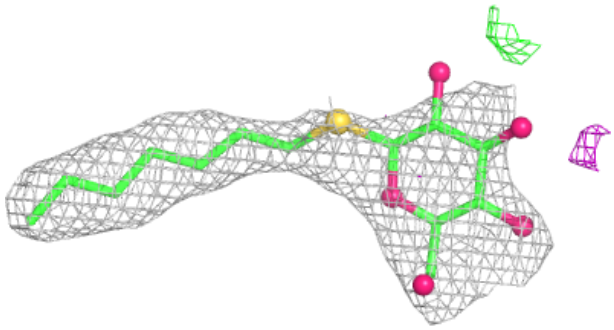


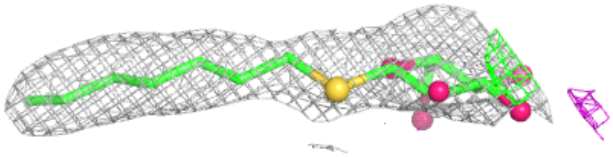


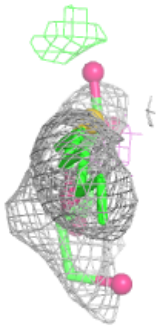


Electron density around HTG B 632:

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

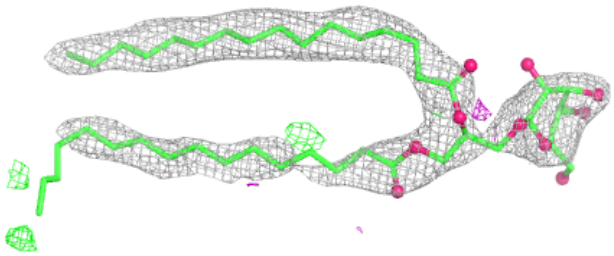


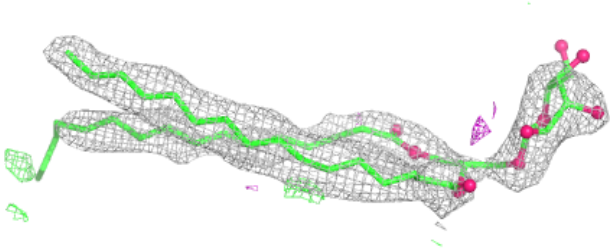


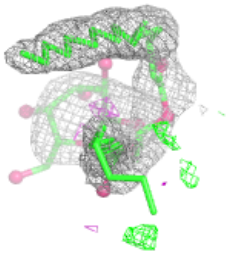


Electron density around LMG C 520:

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

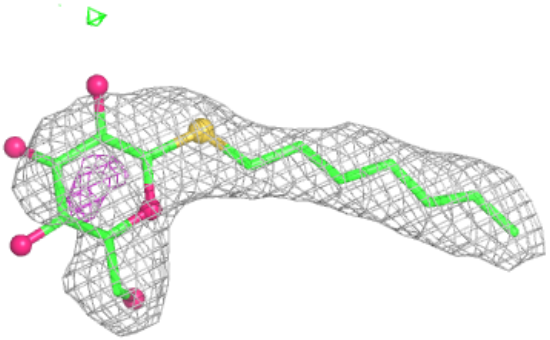


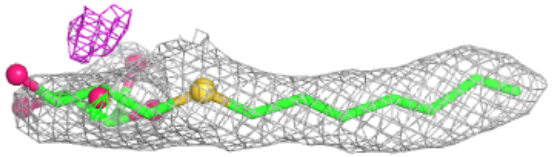


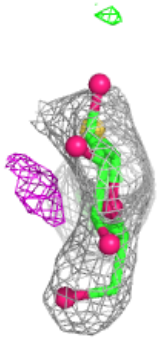


Electron density around HTG b 608:

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

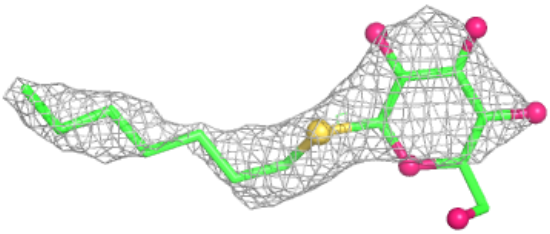


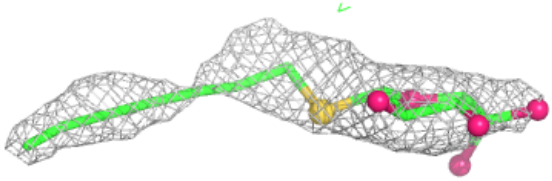


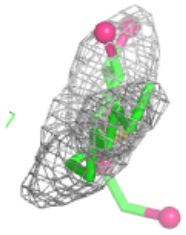


Electron density around HTG c 524:

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

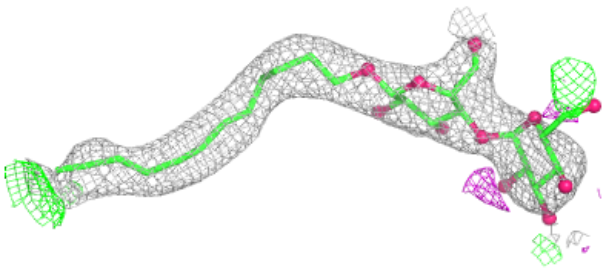


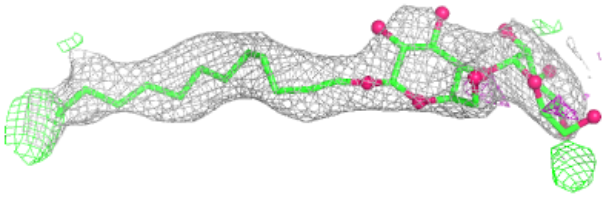


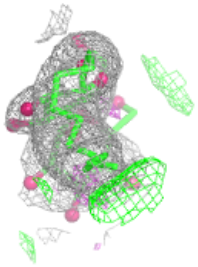


Electron density around LMT a 404:

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

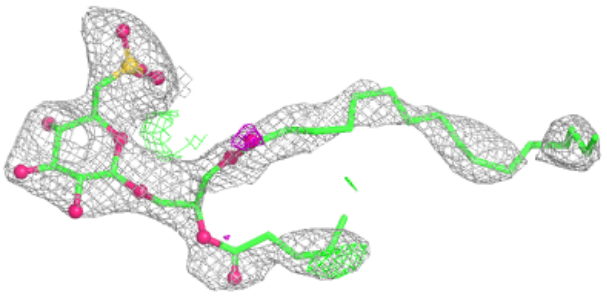


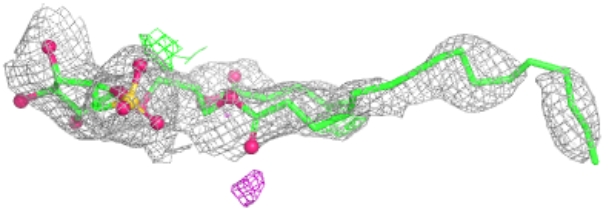


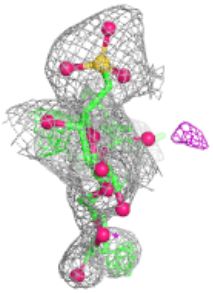


Electron density around SQD F 101:

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

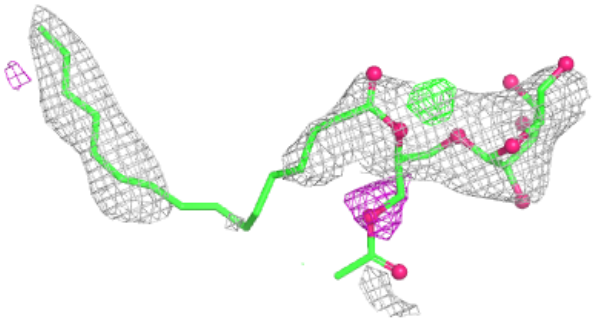


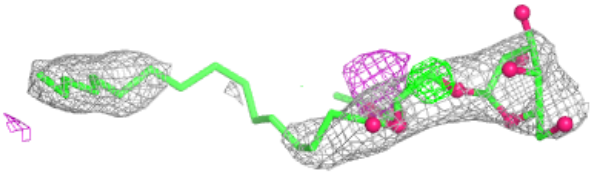


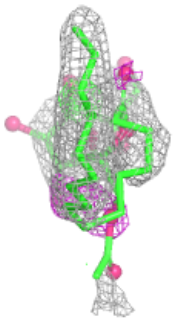


Electron density around LMG Z 101:

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

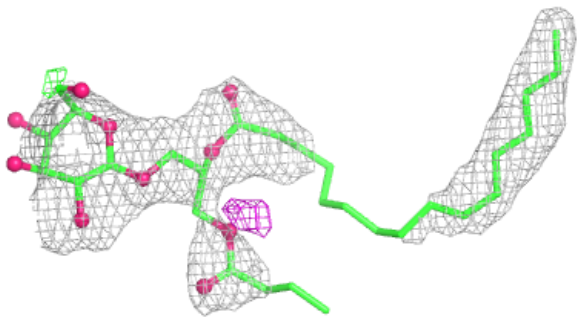


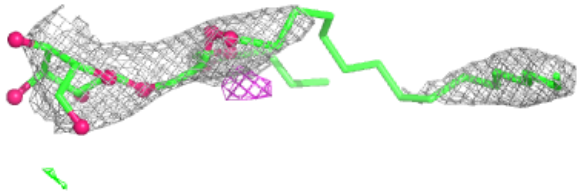


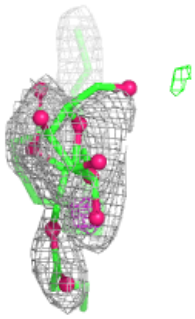


Electron density around LMG z 101:

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

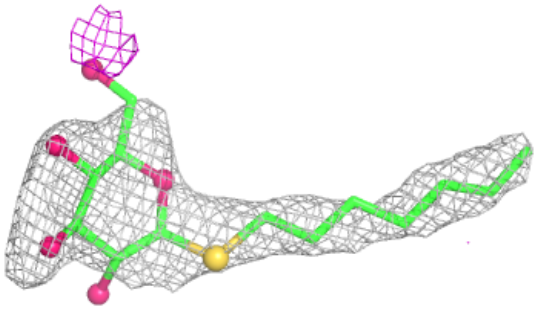


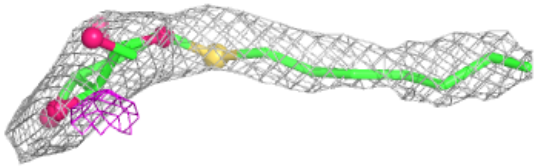


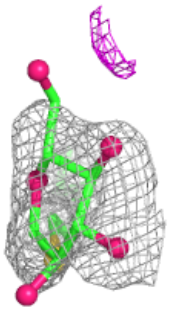


Electron density around HTG B 624:

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

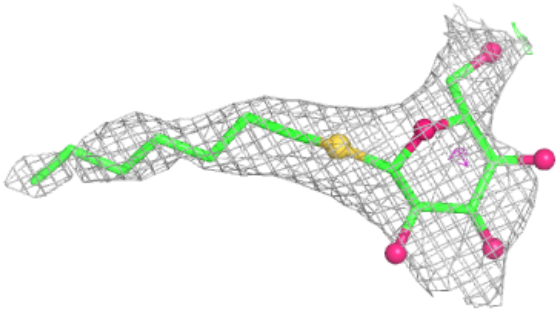


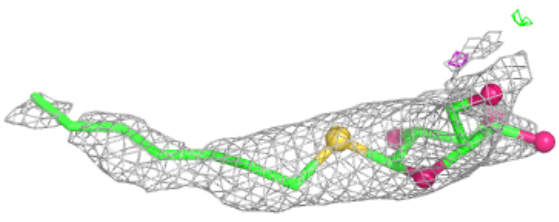


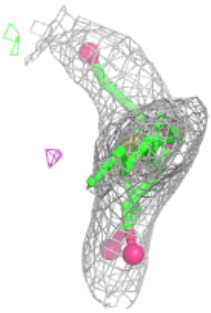


Electron density around HTG C 523:

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

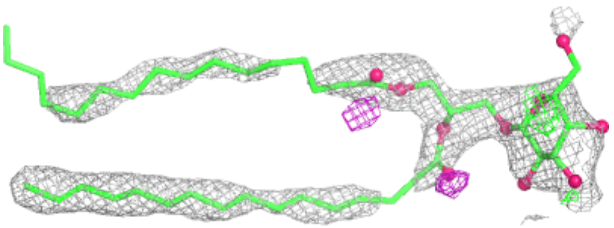


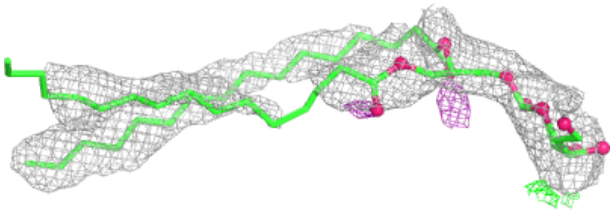


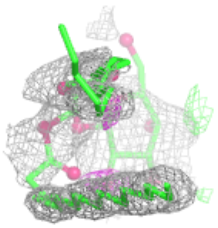


Electron density around LMG c 522:

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

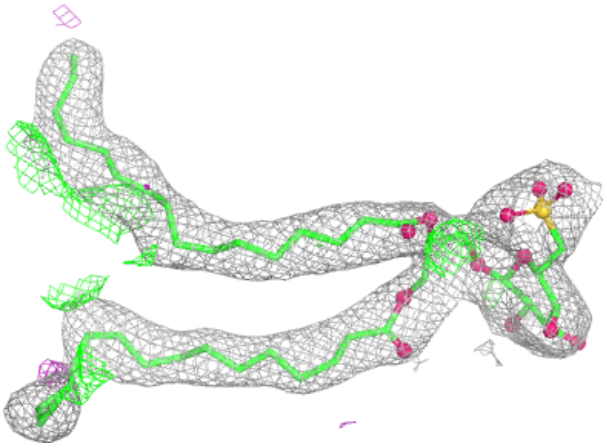


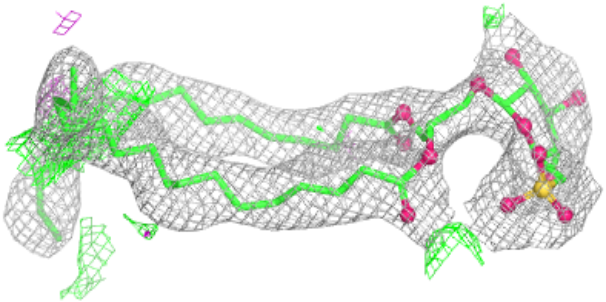


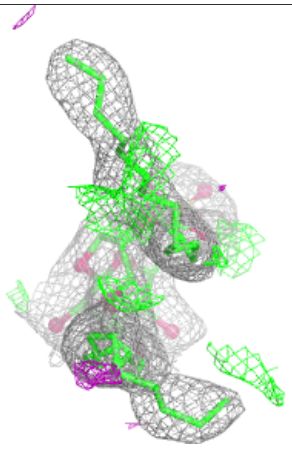


Electron density around SQD L 102:

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

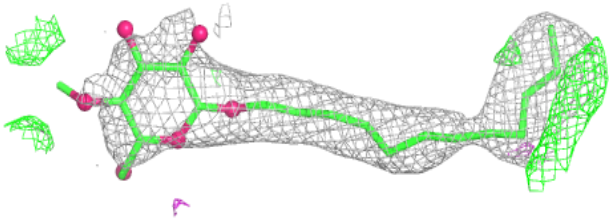


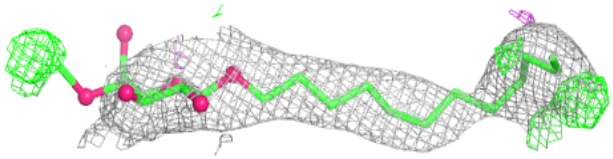


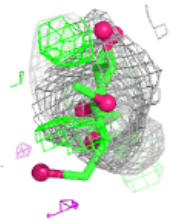


Electron density around LMT t 101:

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

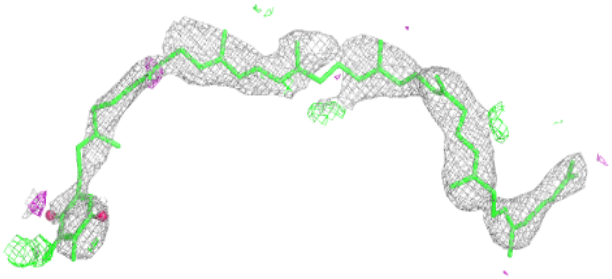


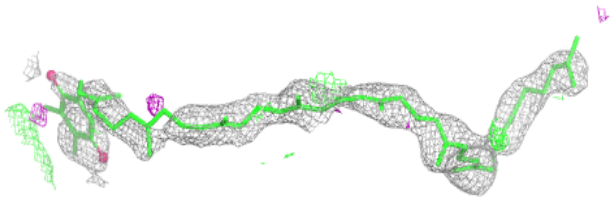


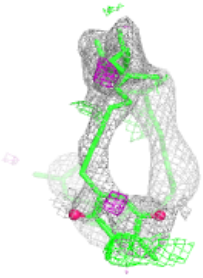


Electron density around PL9 a 416 (A):

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

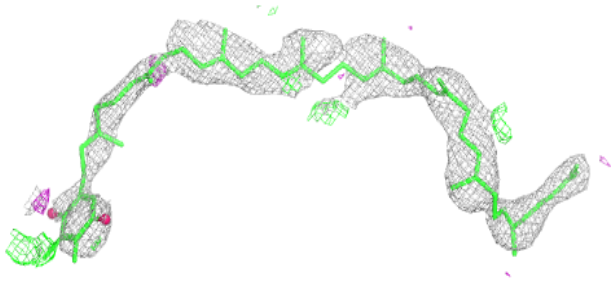


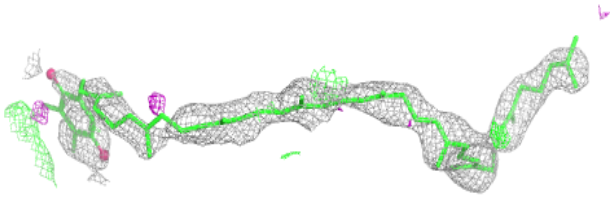


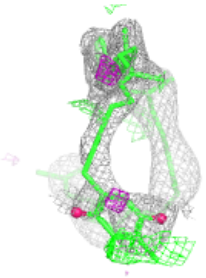


Electron density around PL9 a 416 (B):

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

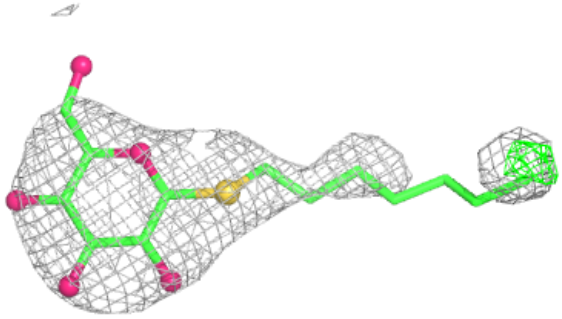


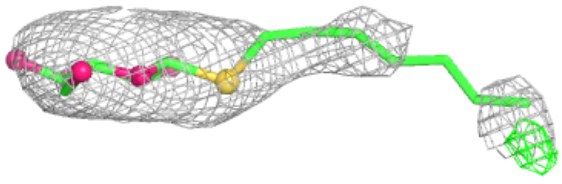


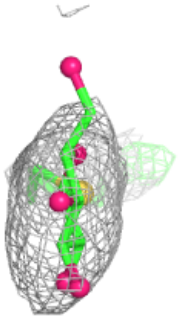


Electron density around HTG c 523:

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

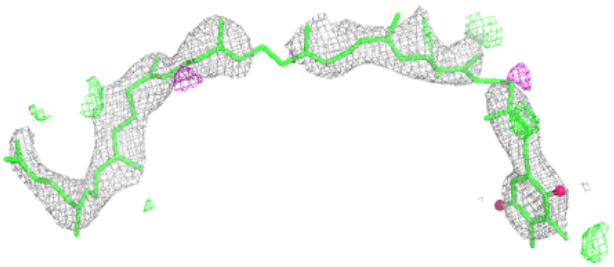


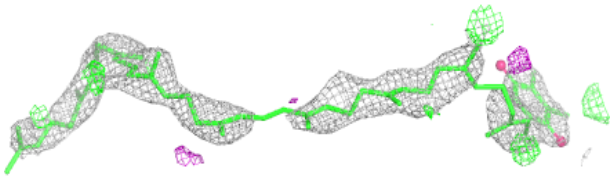


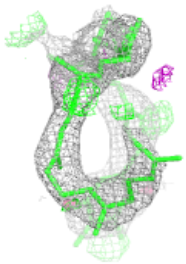


Electron density around PL9 A 417 (B):

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

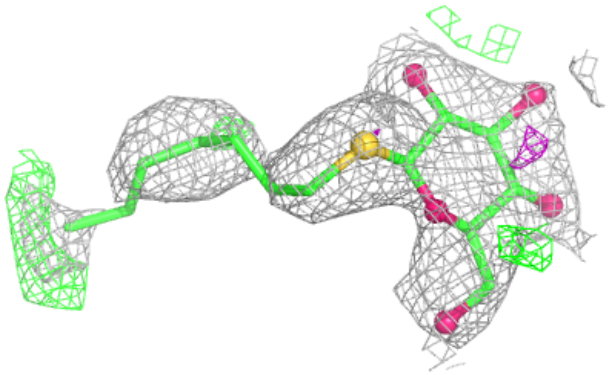


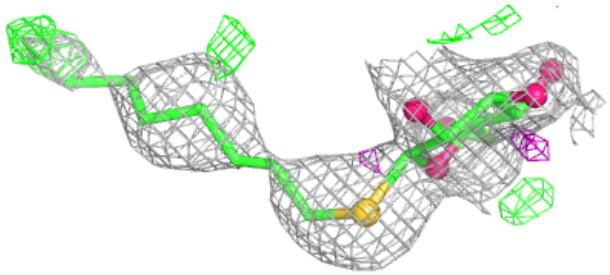


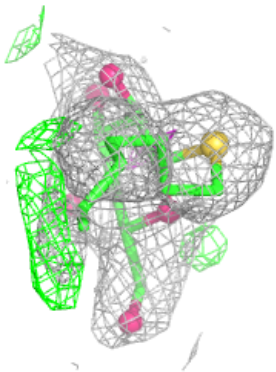


Electron density around HTG b 631:

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

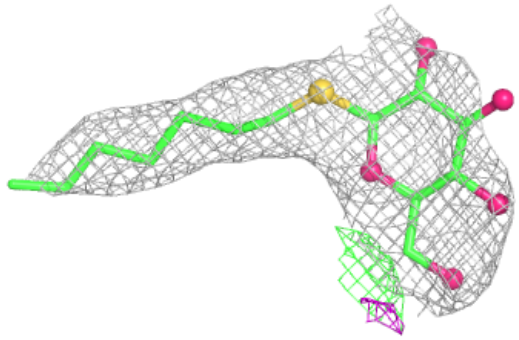


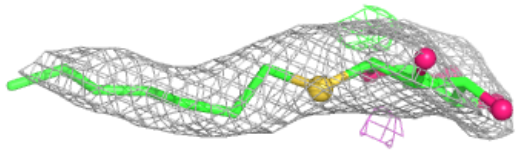


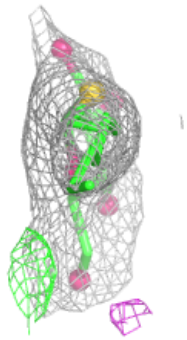


Electron density around HTG b 632:

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

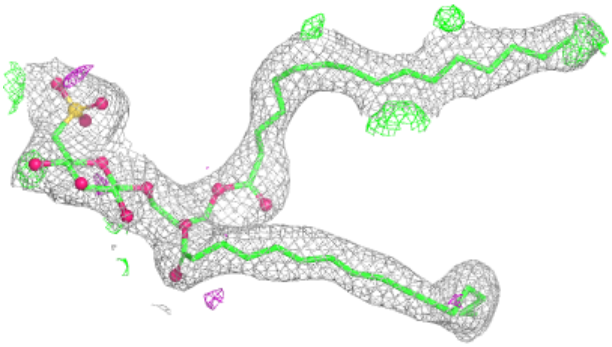


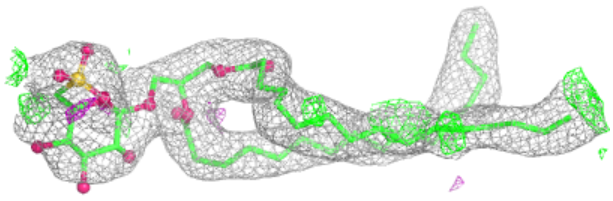


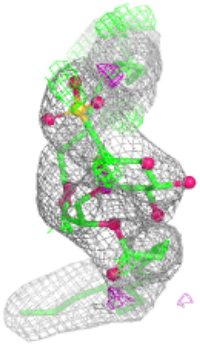


Electron density around SQD a 405:

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

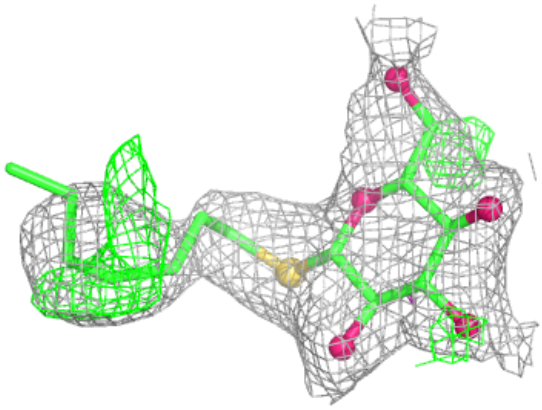


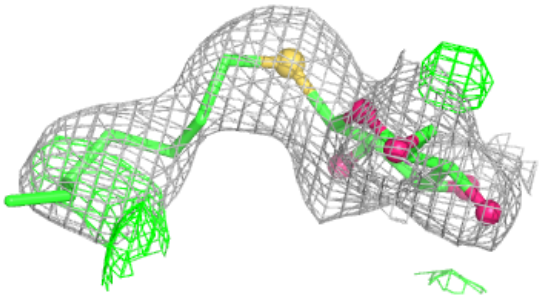


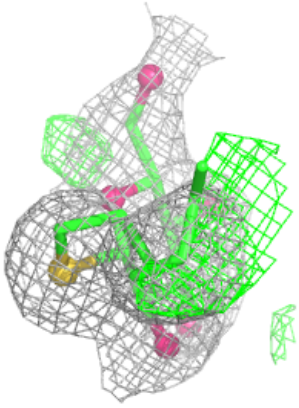


Electron density around HTG B 623:

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

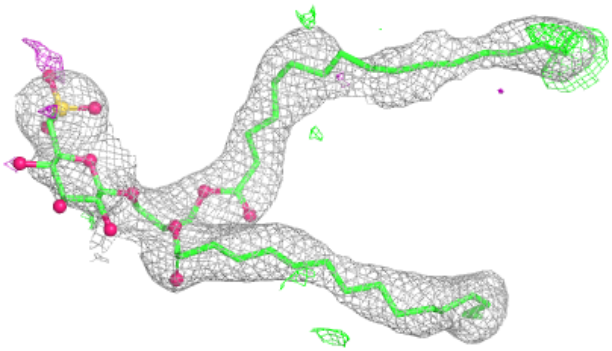


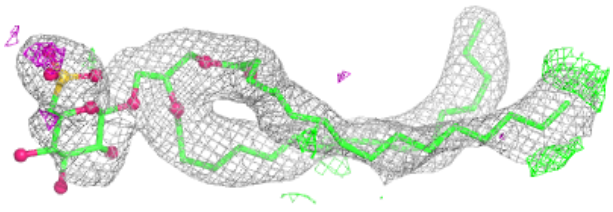


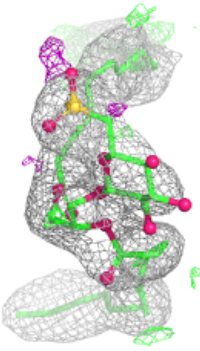


Electron density around SQD A 413:

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

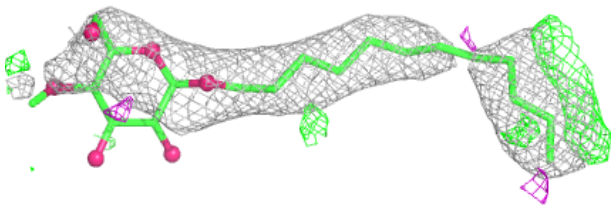


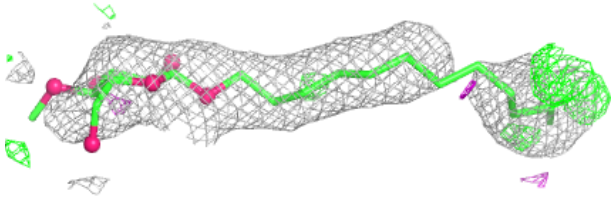


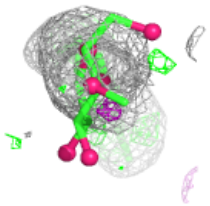


Electron density around LMT T 104:

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

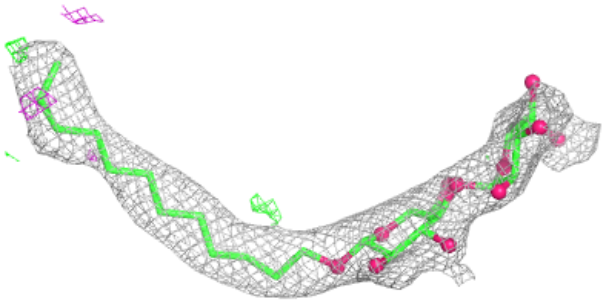


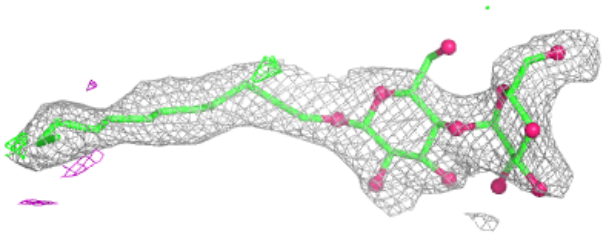


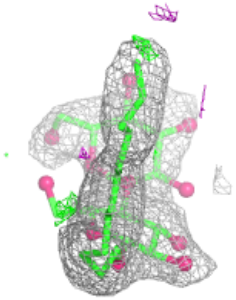


Electron density around LMT m 103:

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

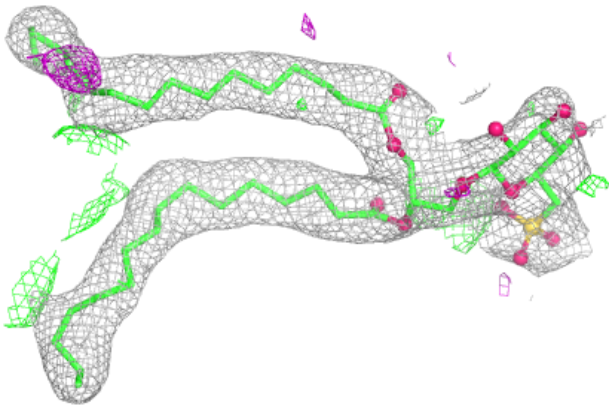


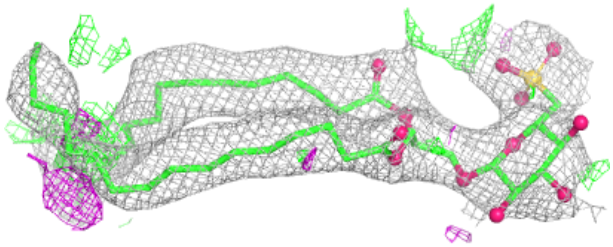


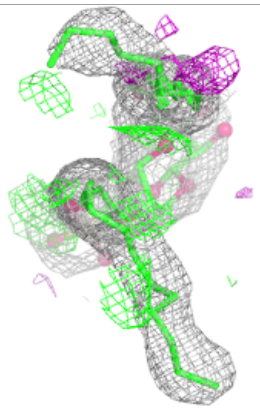


Electron density around SQD B 621:

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

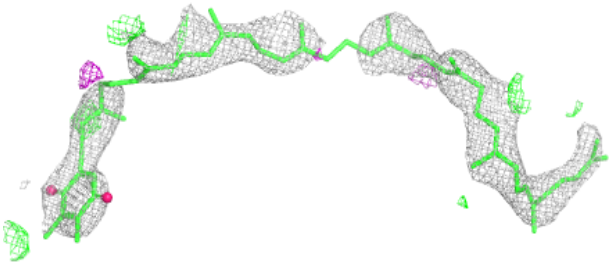


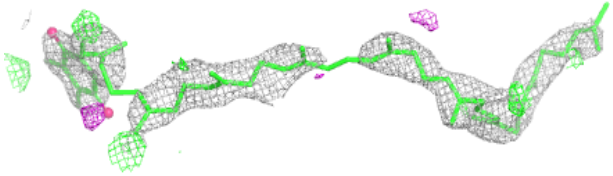


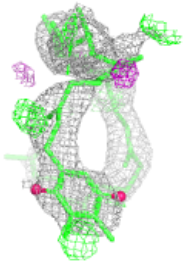


Electron density around PL9 A 417 (A):

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

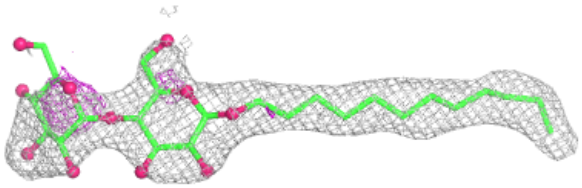


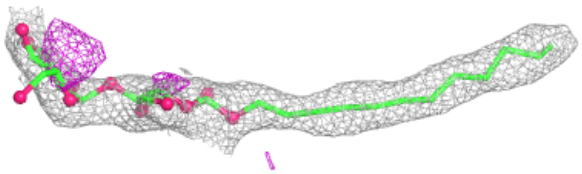


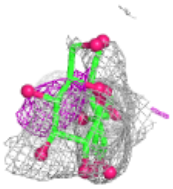


Electron density around LMT m 102:

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

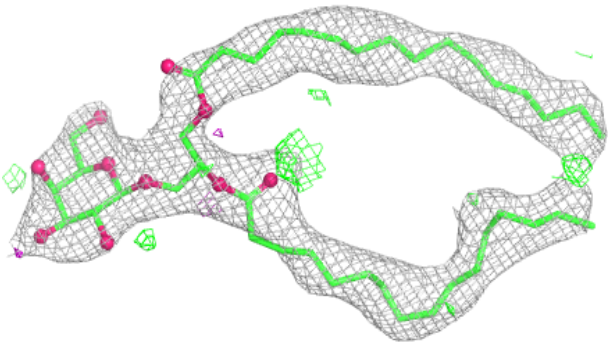


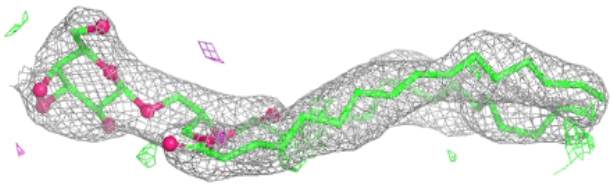


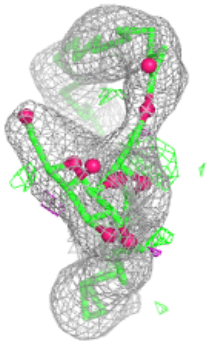


Electron density around LMG A 419:

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

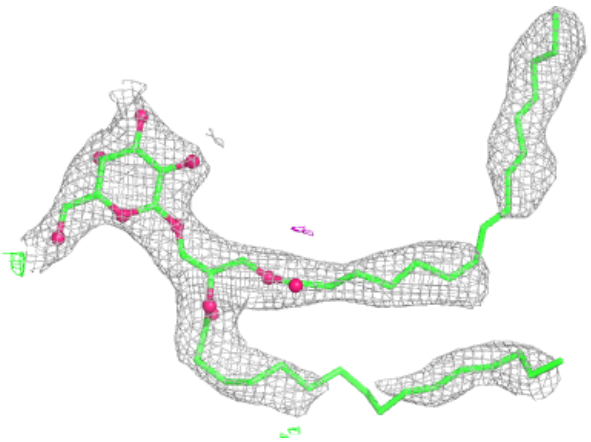


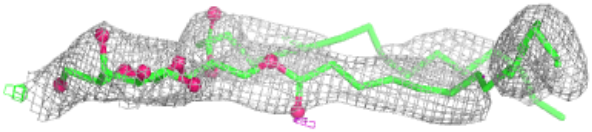


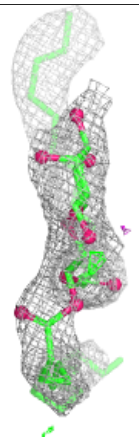


Electron density around LMG C 519:

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

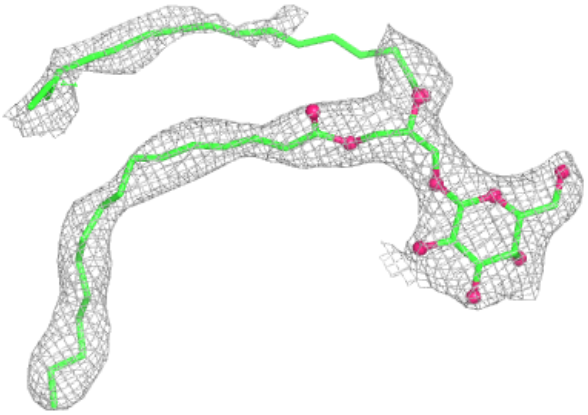


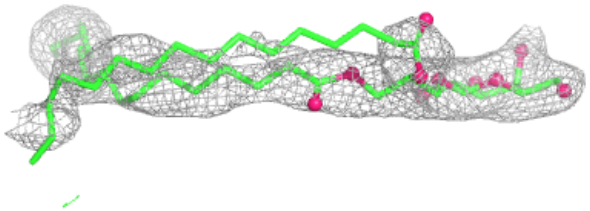


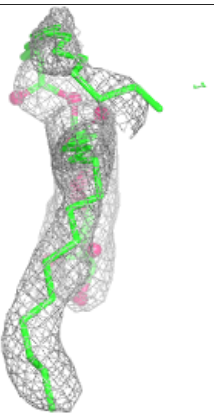


Electron density around LMG k 101:

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

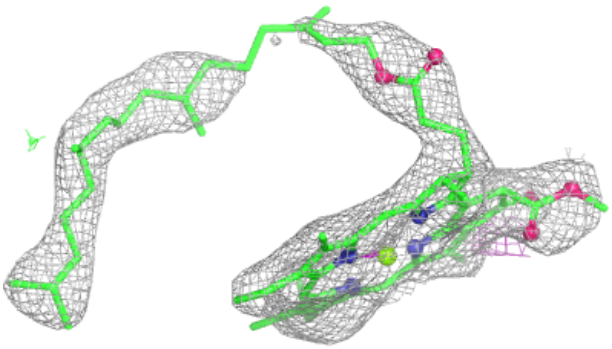


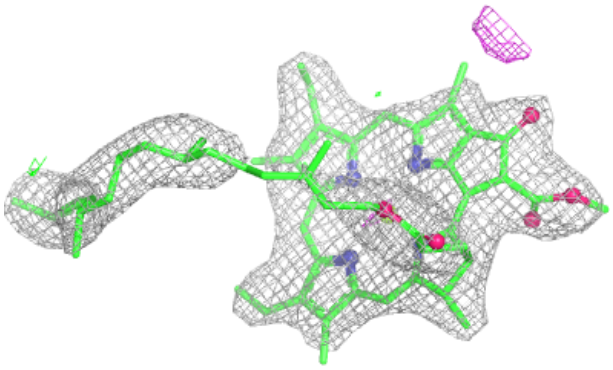


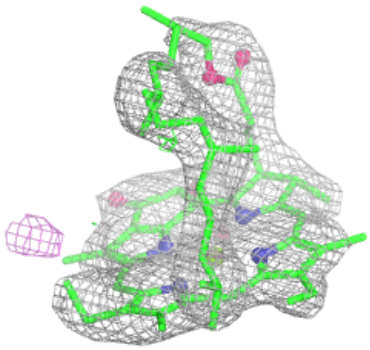


Electron density around CLA C 513:

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

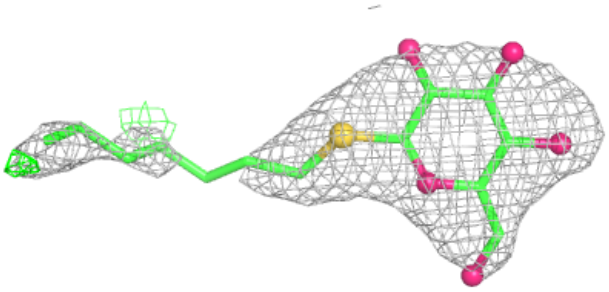


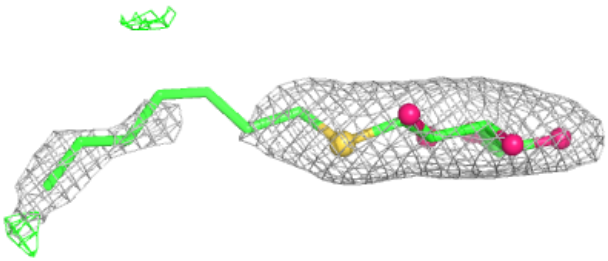


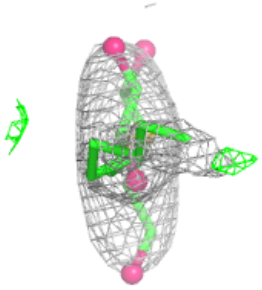


Electron density around HTG C 522:

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

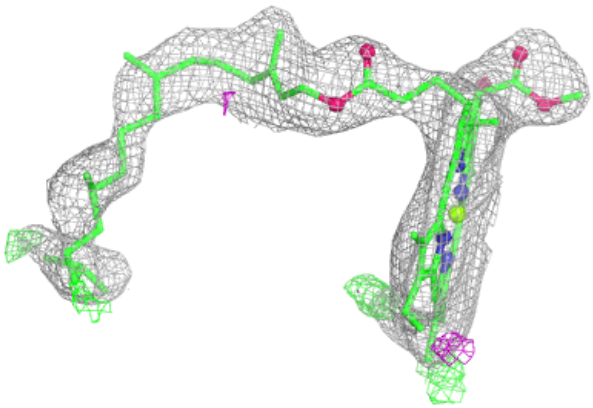


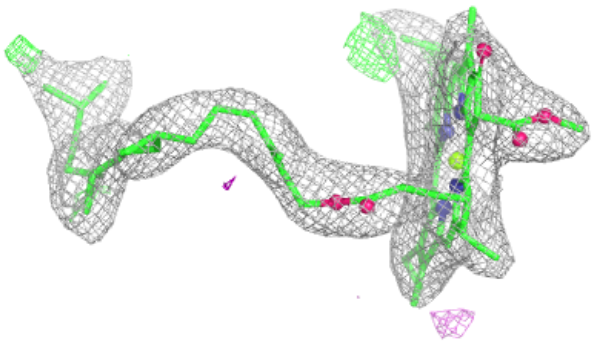


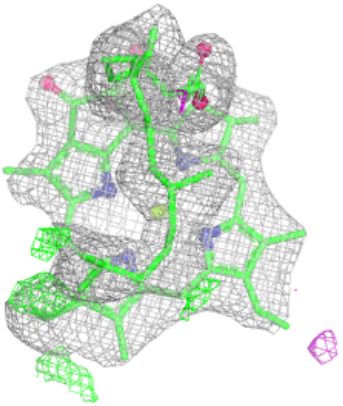


Electron density around CLA C 506:

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

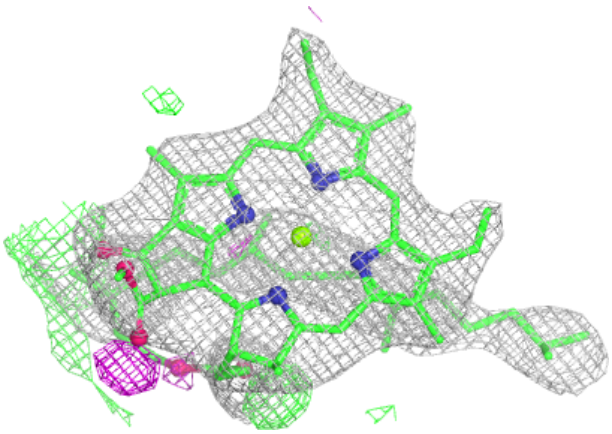


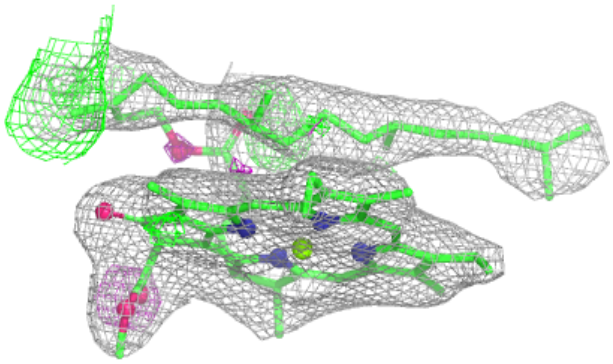


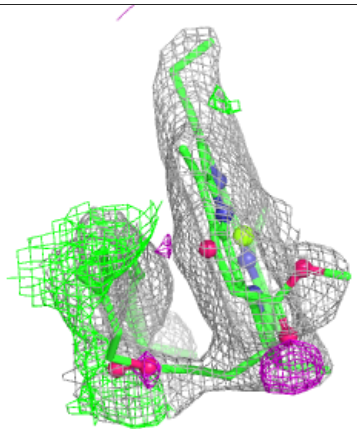


Electron density around CLA B 602:

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

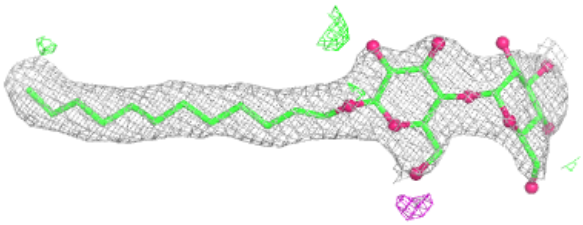


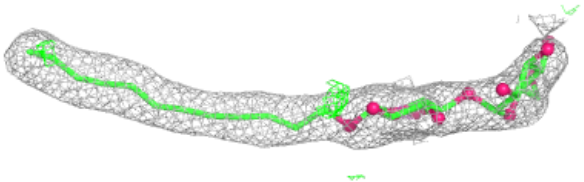


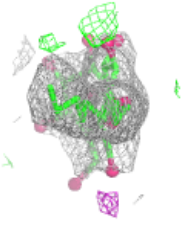


Electron density around LMT M 102:

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

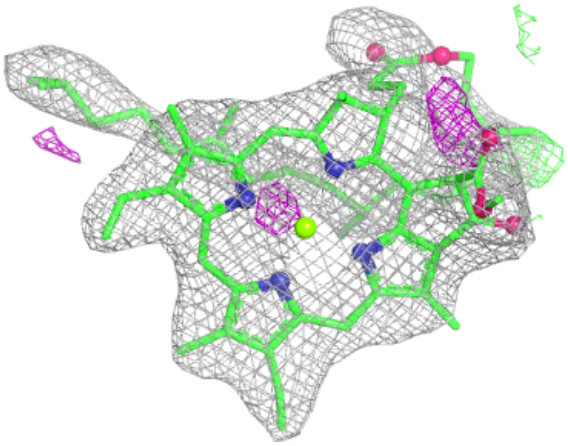


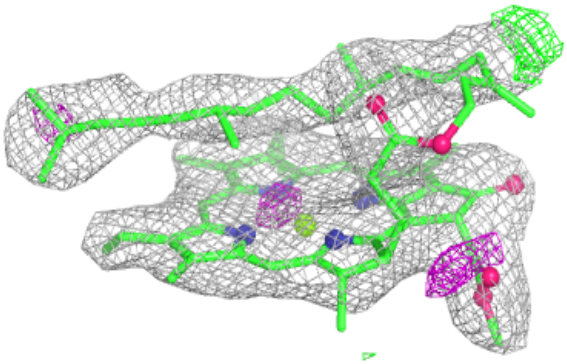


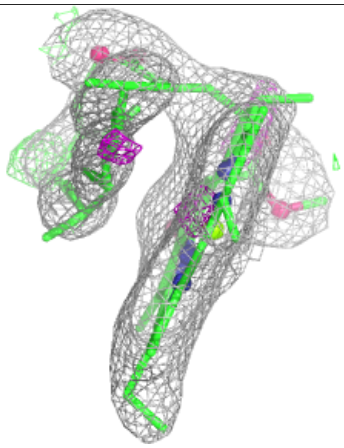


Electron density around CLA b 610:

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

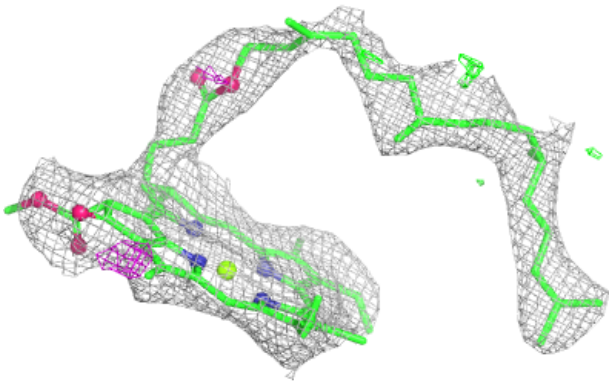


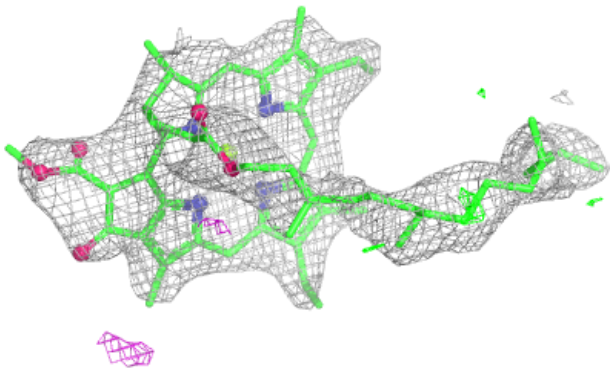




Electron density around CLA c 517:

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

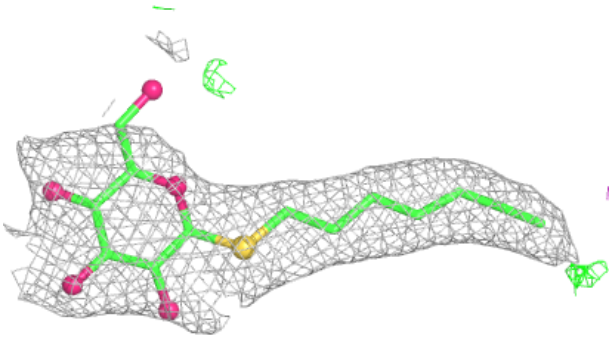


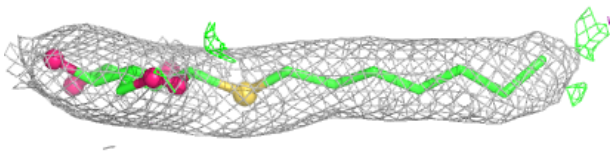


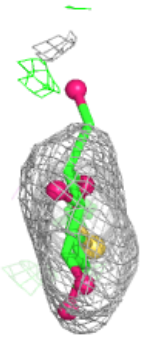


Electron density around HTG B 631:

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

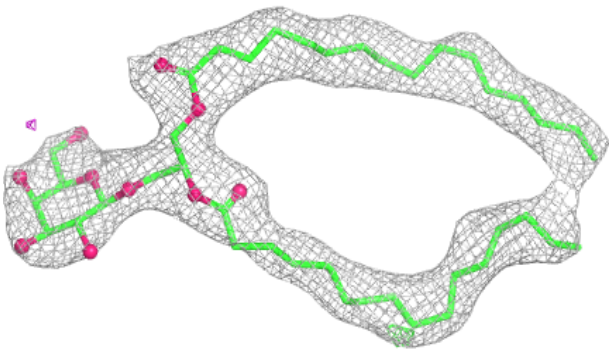


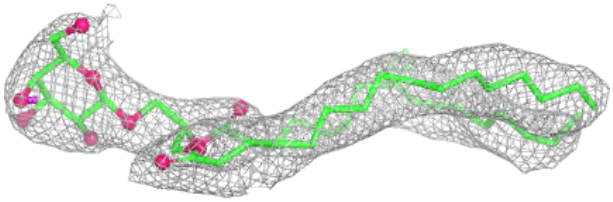


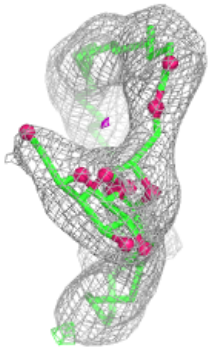


Electron density around LMG a 415:

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

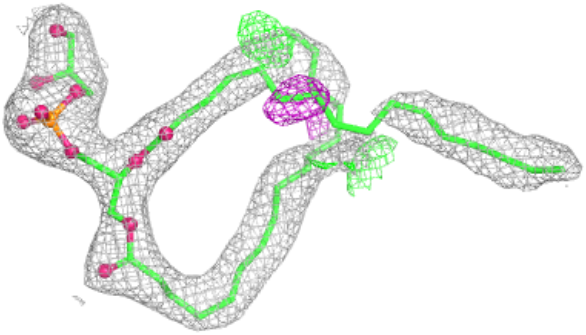


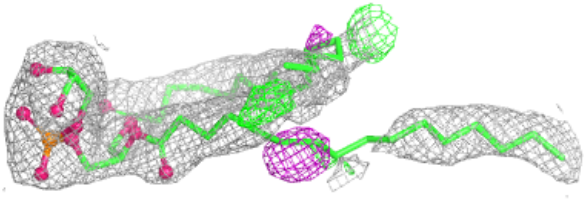


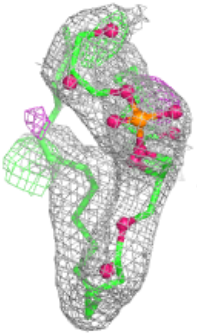


Electron density around LHG D 411:

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

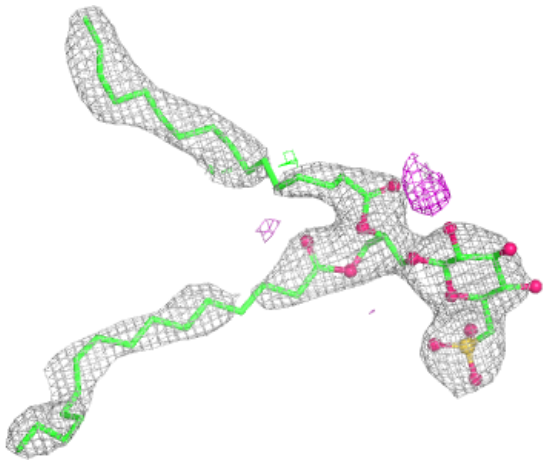


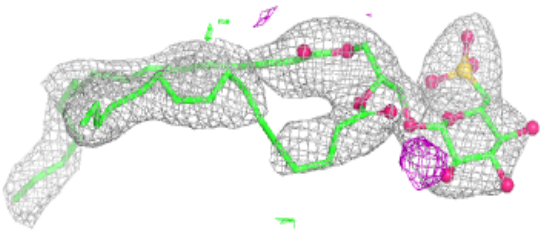


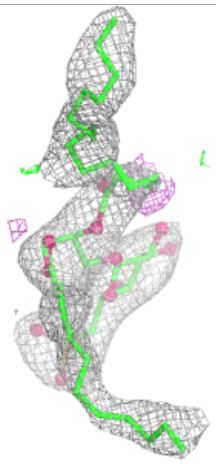


Electron density around SQD A 411:

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

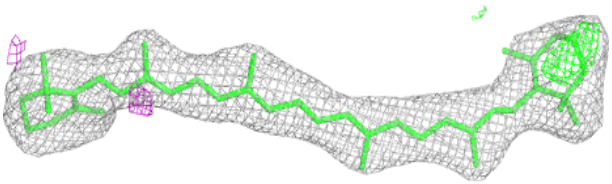


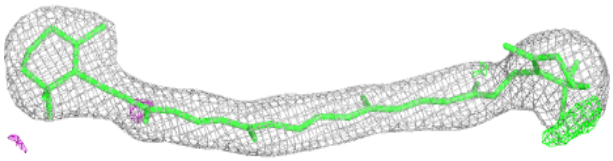


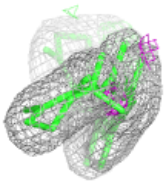


Electron density around BCR d 406:

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

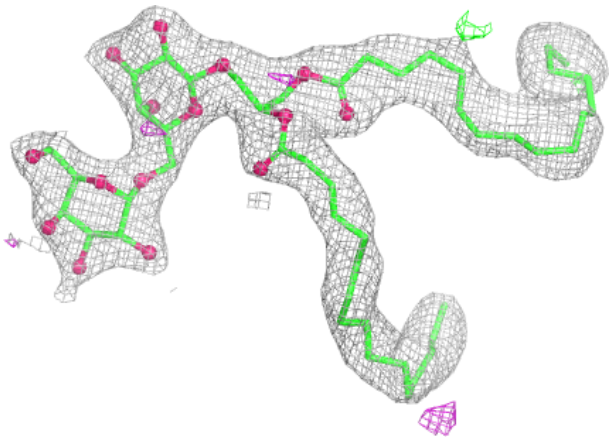


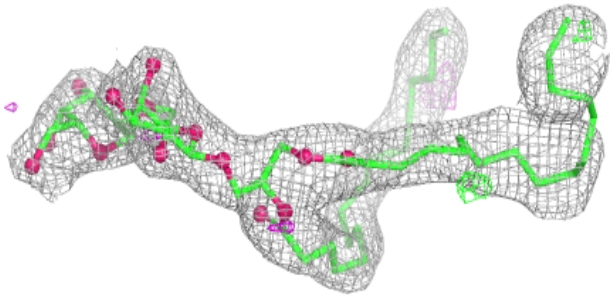


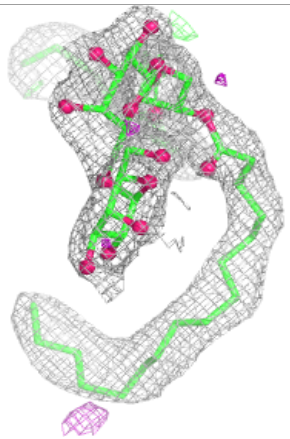


Electron density around DGD C 517:

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

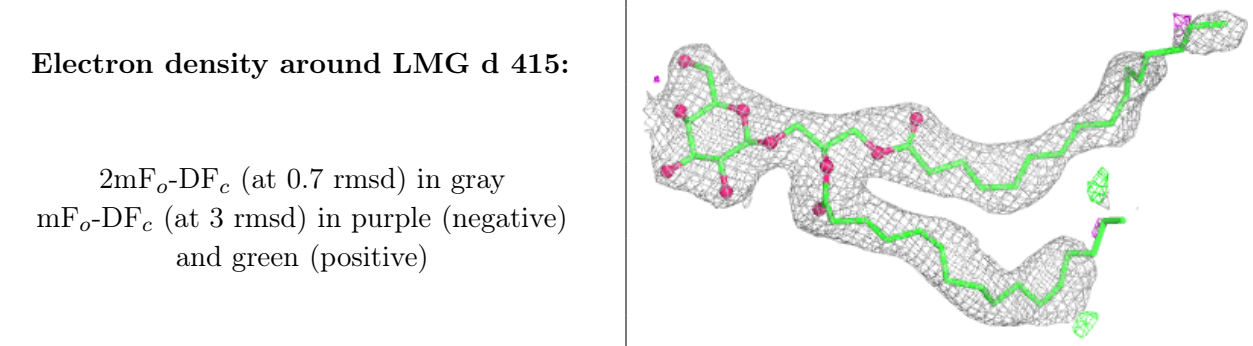


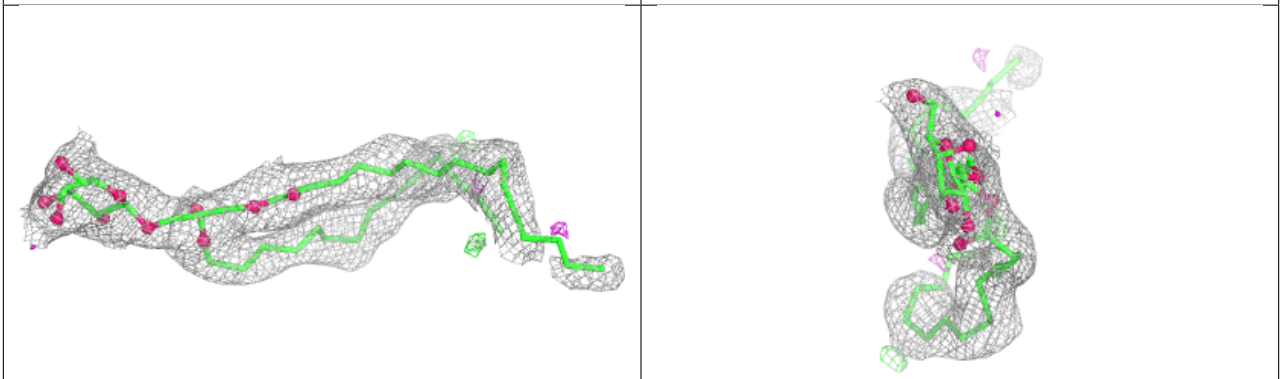




Electron density around LMG d 415:

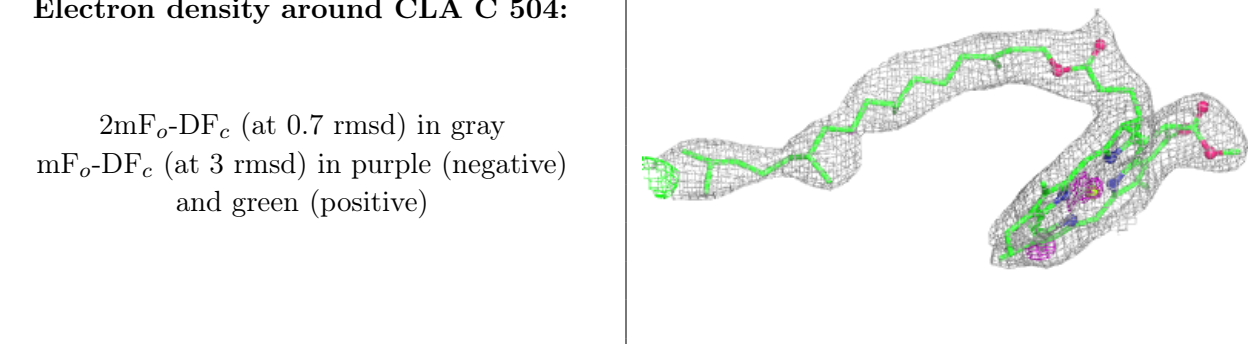
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

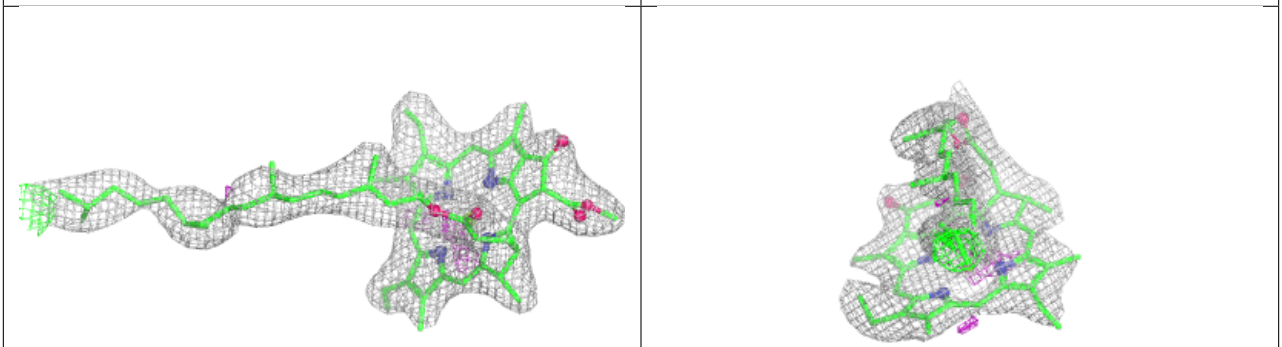




Electron density around CLA C 504:

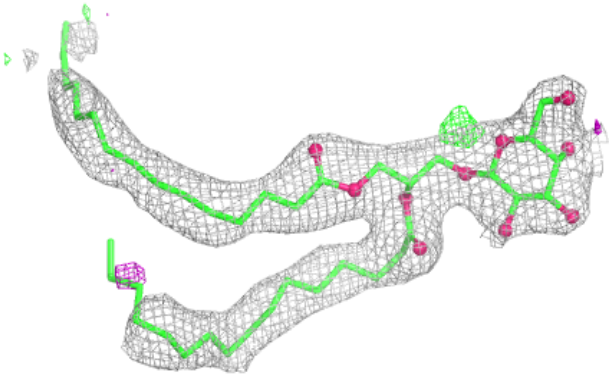
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

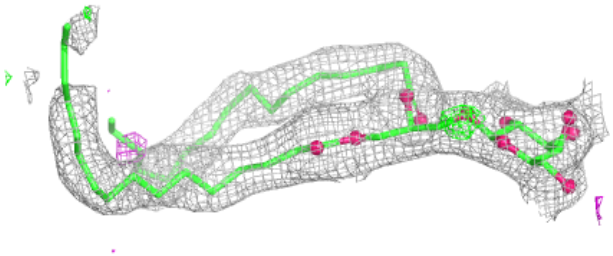


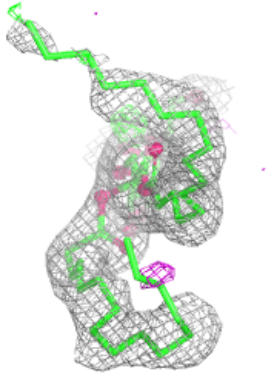


Electron density around LMG D 415:

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

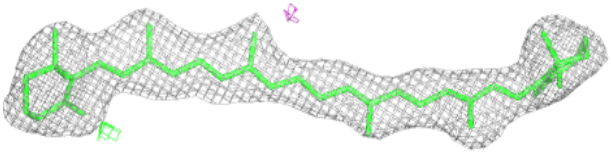


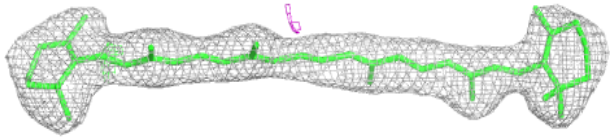


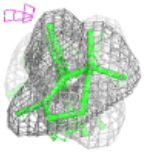


Electron density around BCR C 514:

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

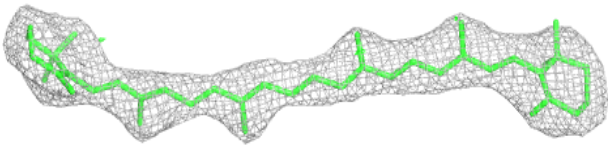


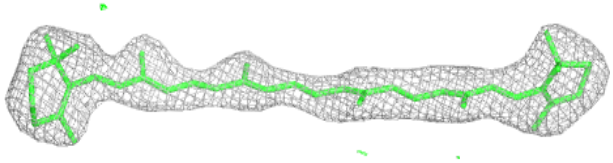


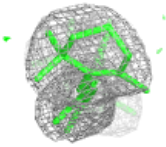


Electron density around BCR c 526:

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

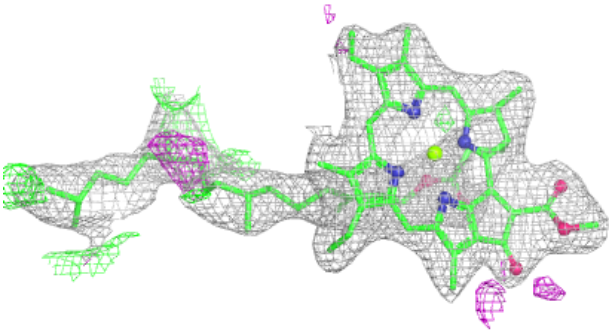


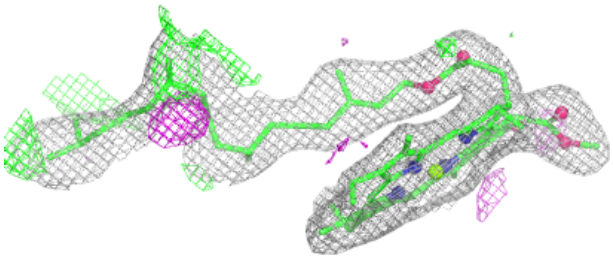


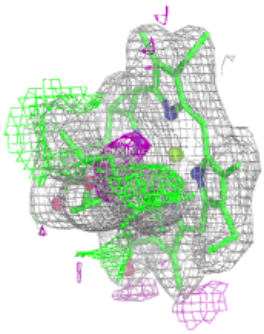


Electron density around CLA B 615:

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

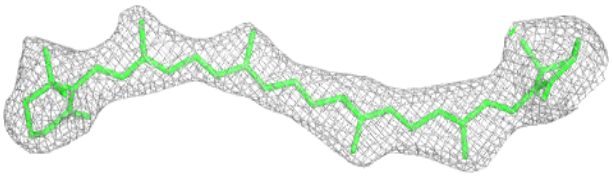


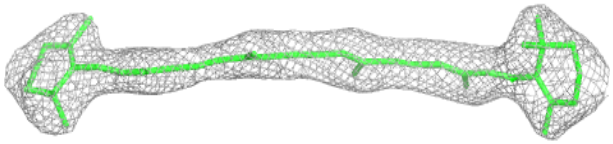


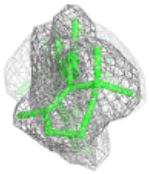


Electron density around BCR y 101:

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

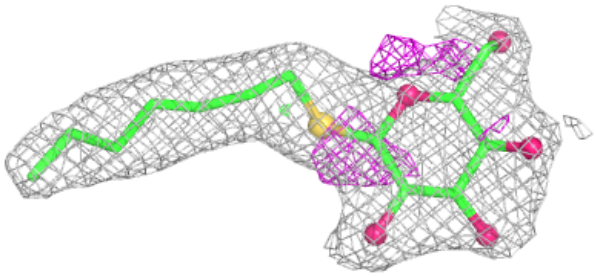


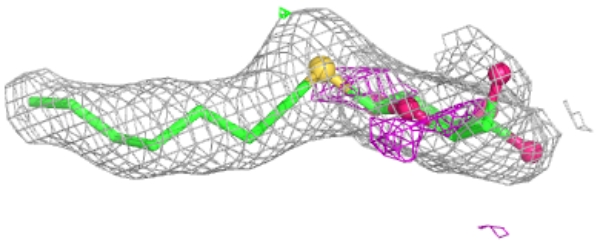


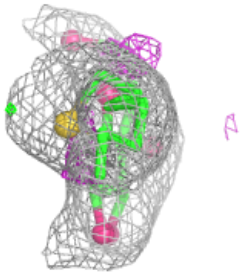


Electron density around HTG b 602:

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

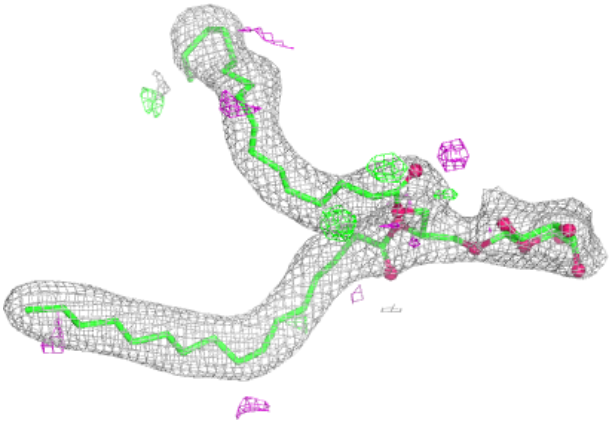


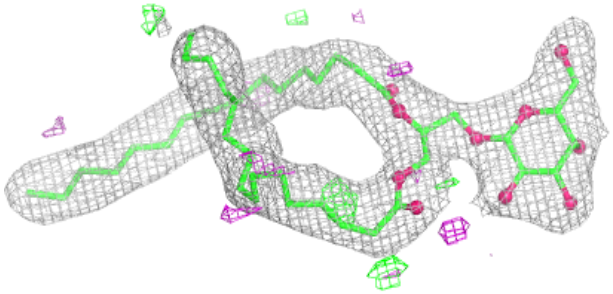


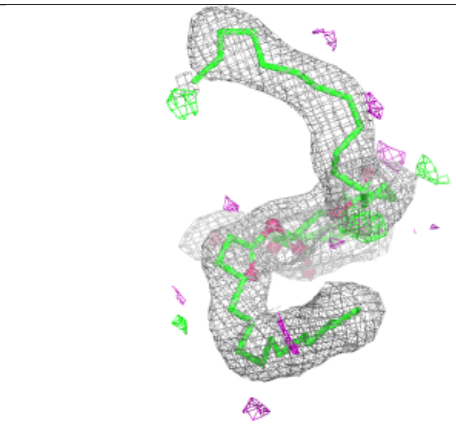


Electron density around LMG b 629:

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

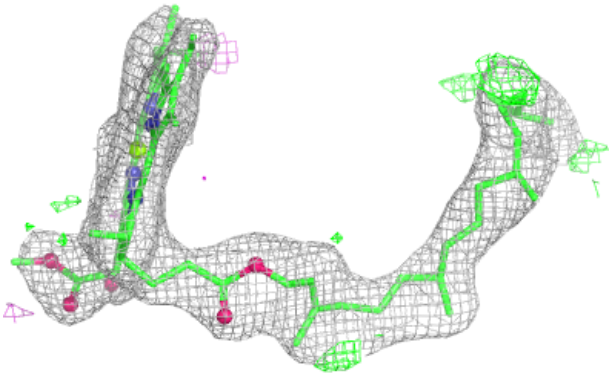


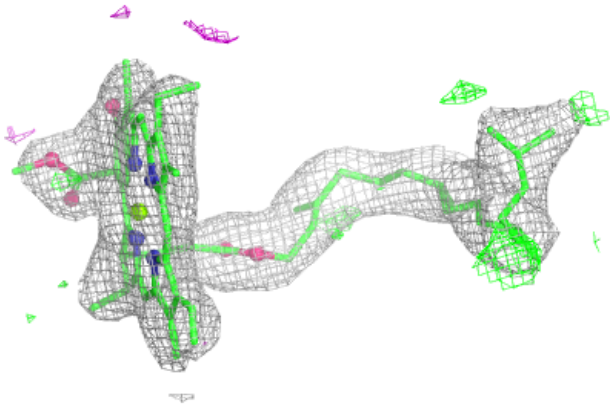


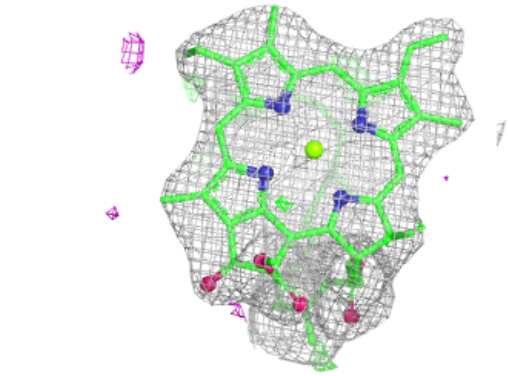


Electron density around CLA c 510:

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

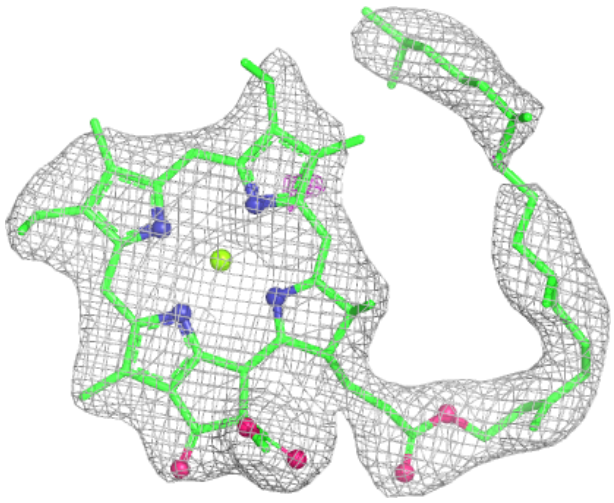


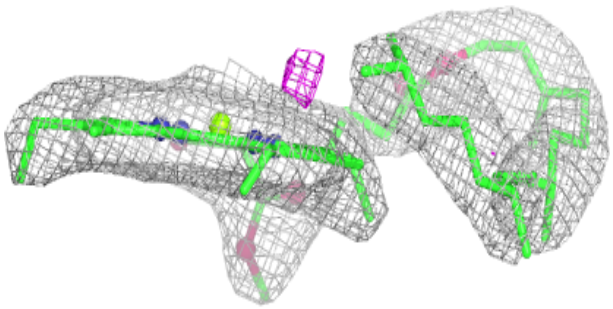


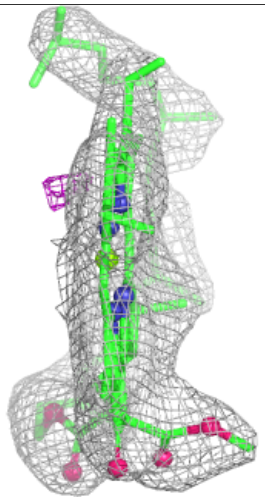


Electron density around CLA C 512:

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

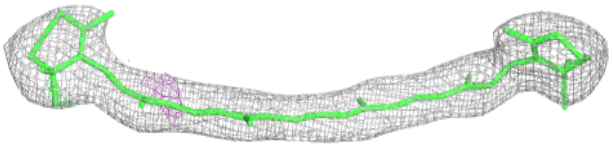


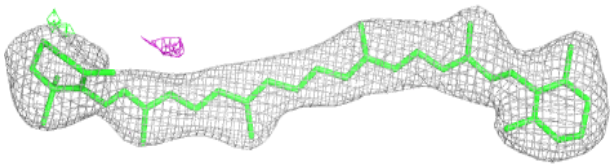


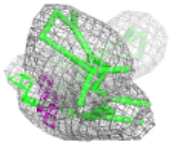


Electron density around BCR D 406:

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

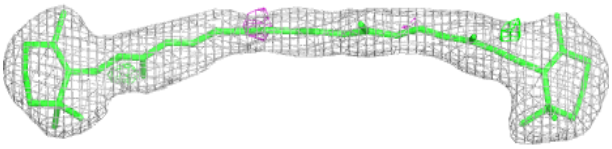


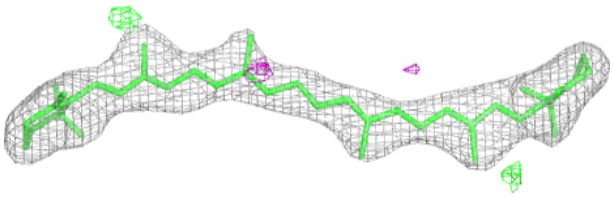


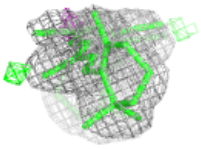


Electron density around BCR K 101:

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

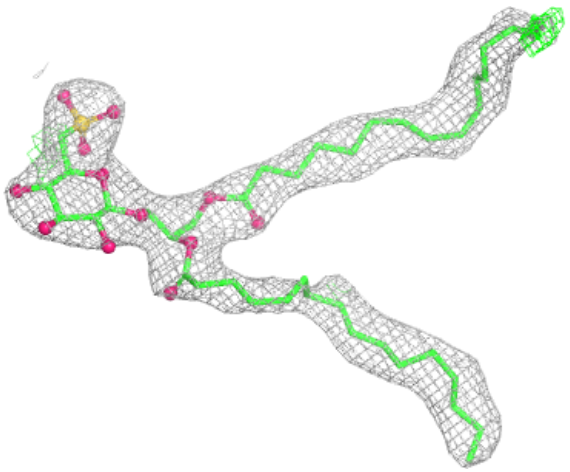


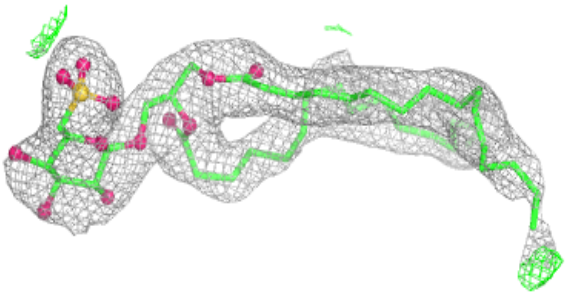


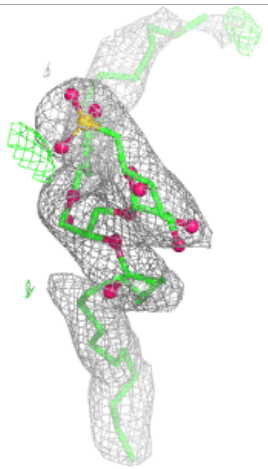


Electron density around SQD a 414:

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

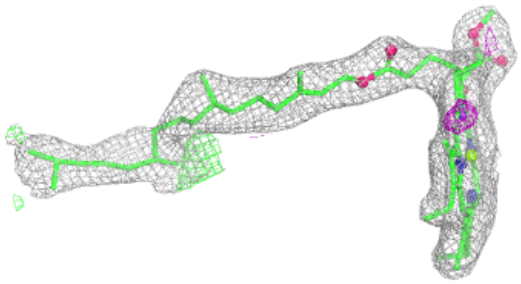


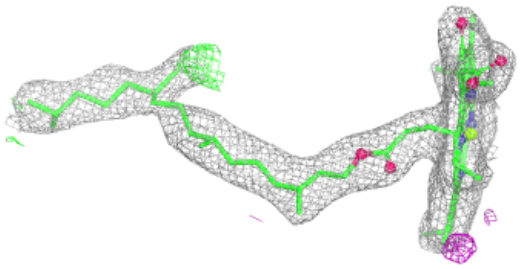


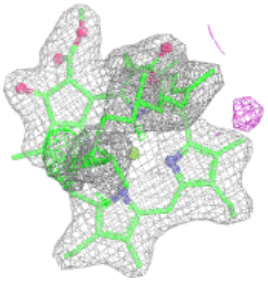


Electron density around CLA B 607:

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

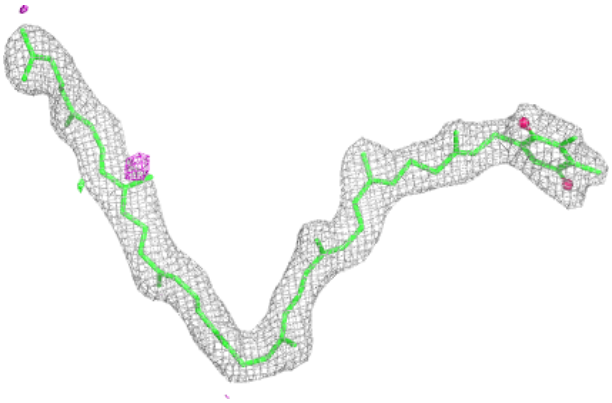


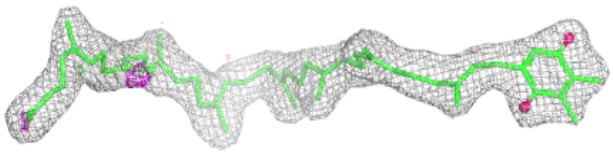


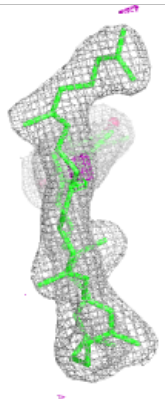


Electron density around PL9 d 407 (A):

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

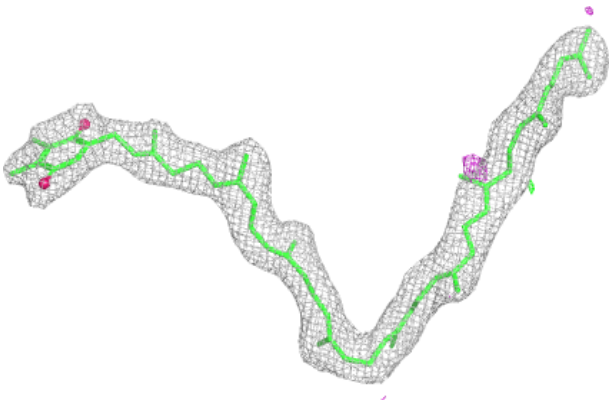


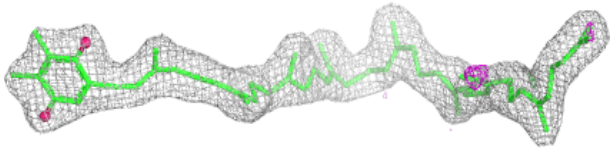




Electron density around PL9 d 407 (B):

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

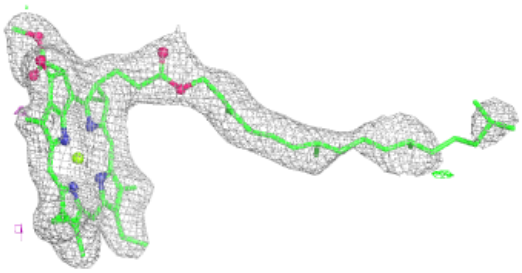


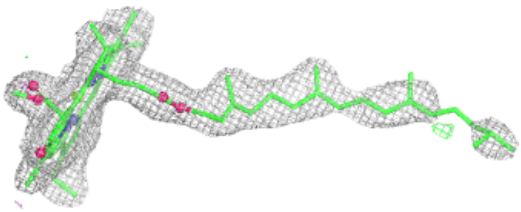


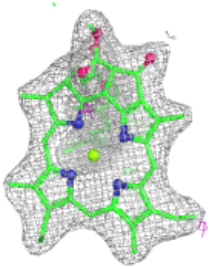


Electron density around CLA d 405:

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

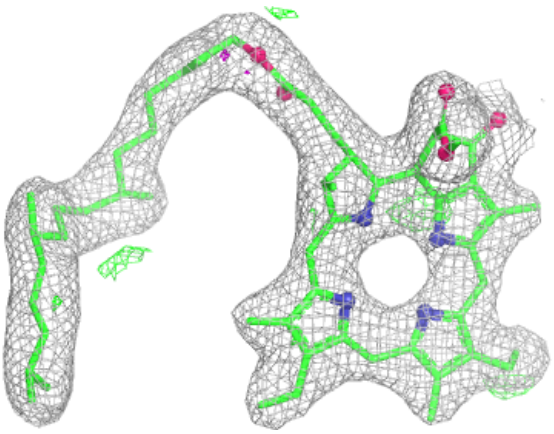


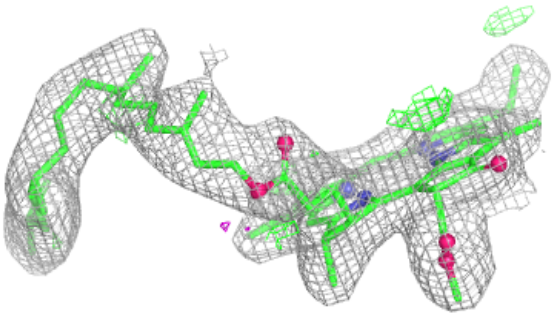


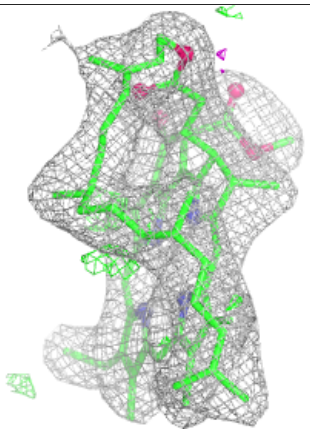


Electron density around PHO d 402 (A):

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

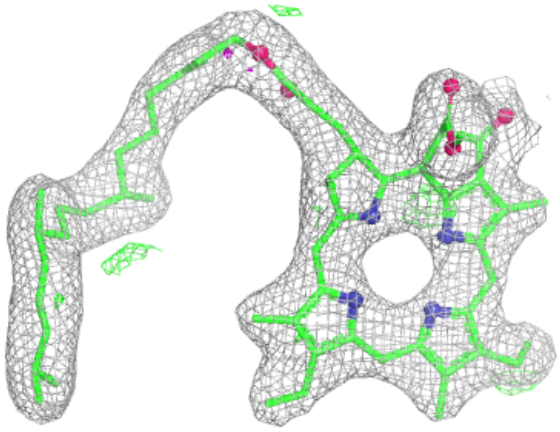


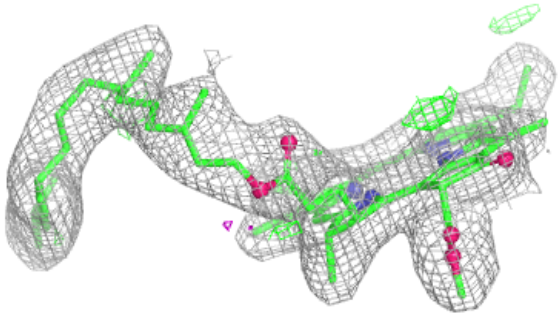


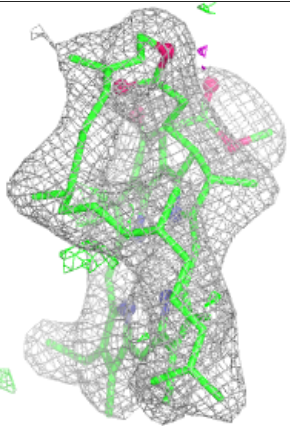


Electron density around PHO d 402 (B):

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

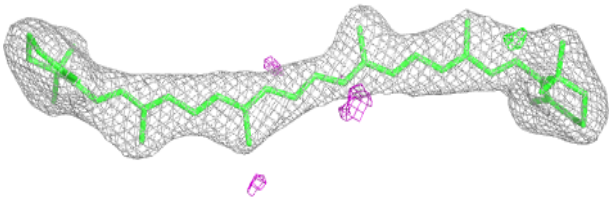


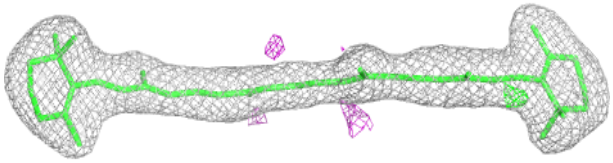


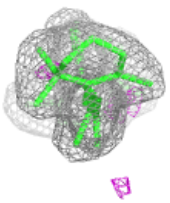


Electron density around BCR A 410:

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

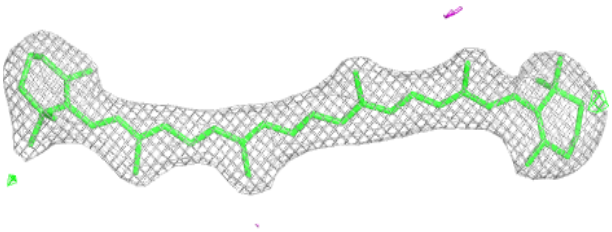


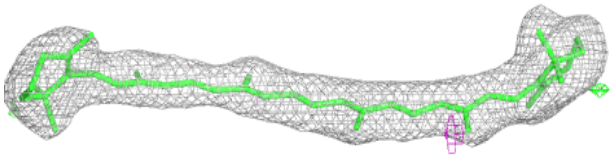


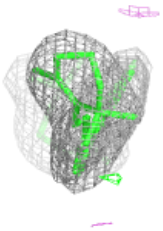


Electron density around BCR B 620:

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

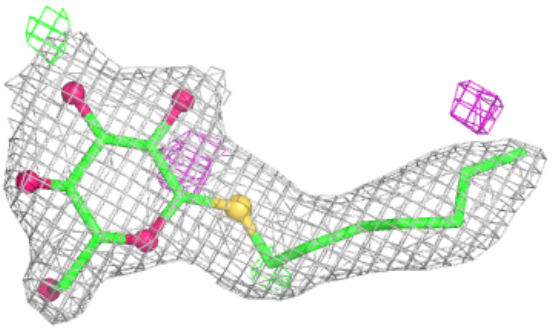


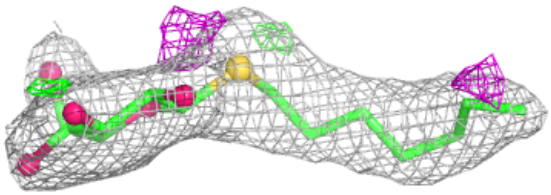


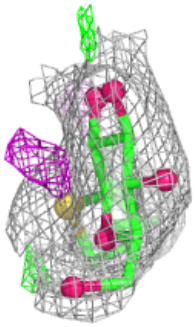


Electron density around HTG B 622:

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

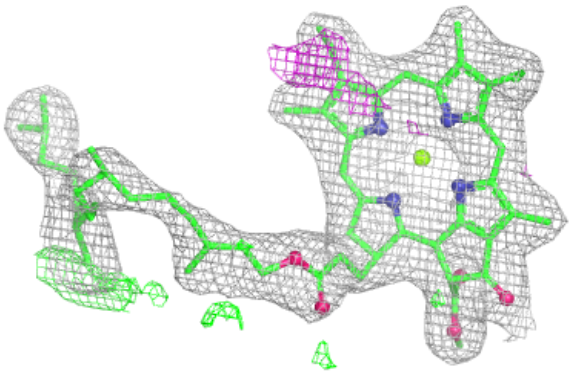


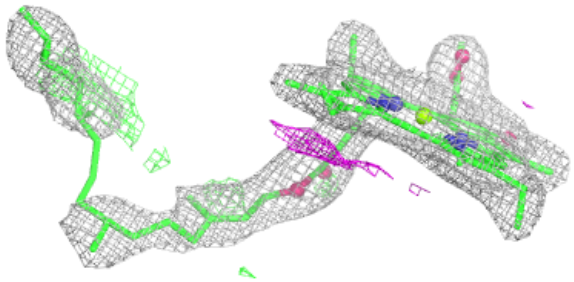


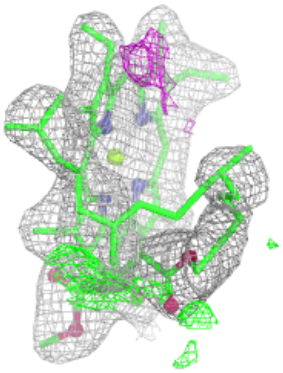


Electron density around CLA A 409:

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

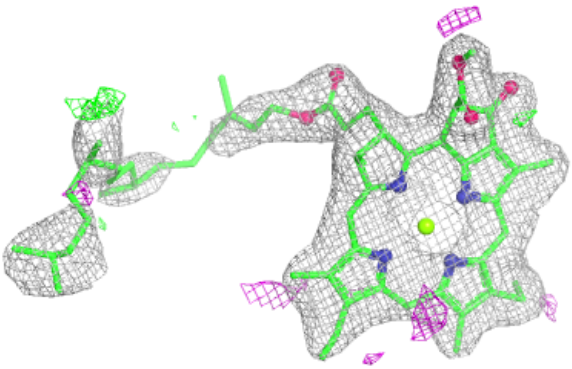


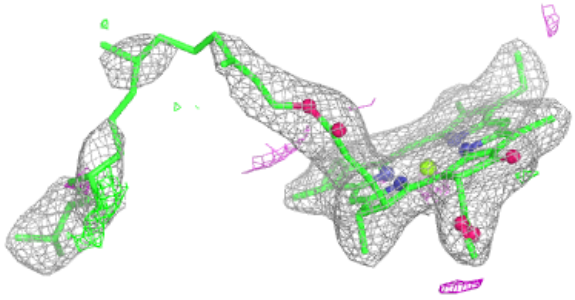


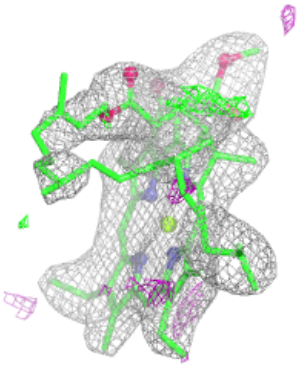


Electron density around CLA a 412:

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

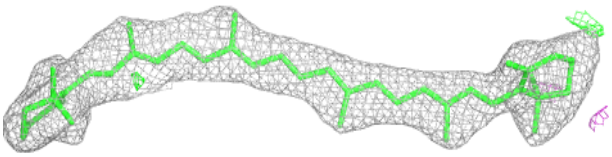


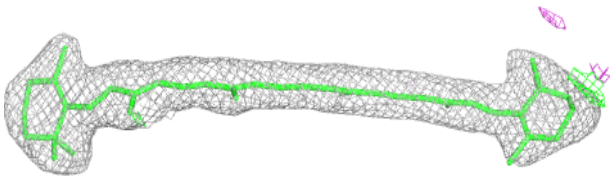


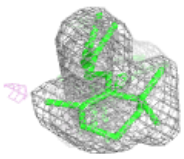


Electron density around BCR H 101:

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

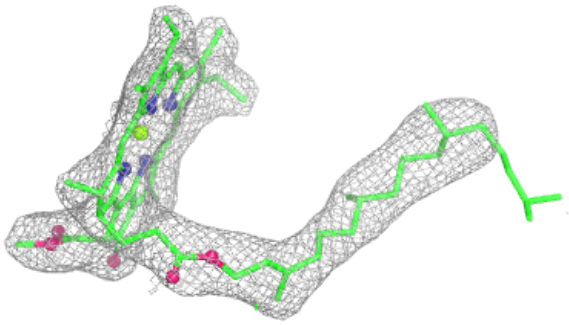


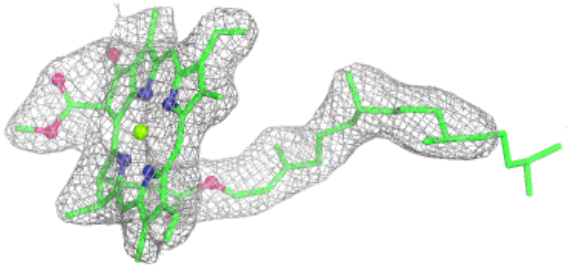


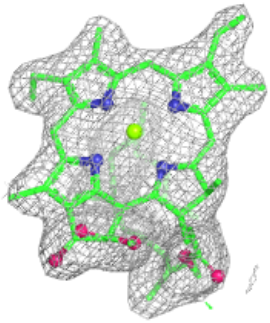


Electron density around CLA C 508:

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

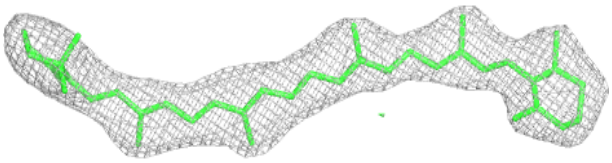


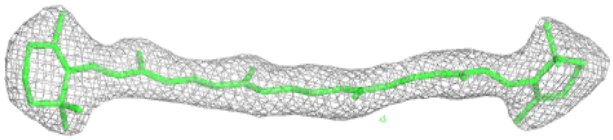


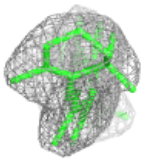


Electron density around BCR Y 101:

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

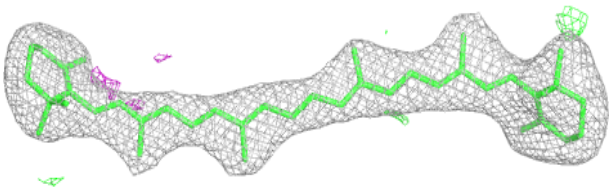


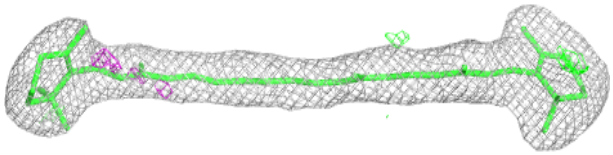


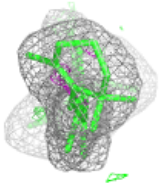


Electron density around BCR b 627:

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

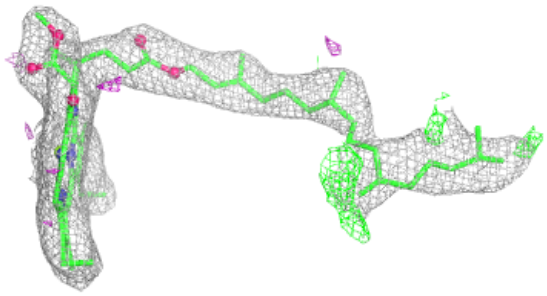


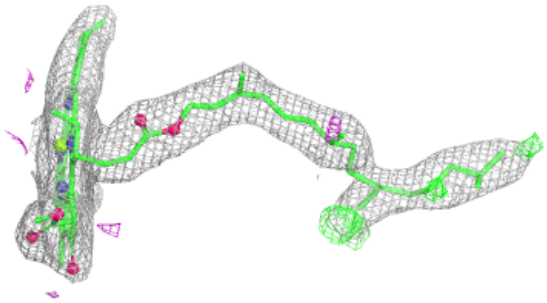


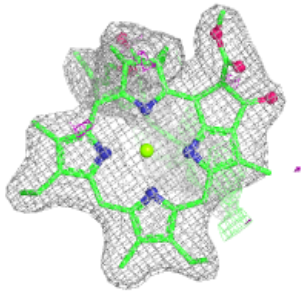


Electron density around CLA b 615:

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

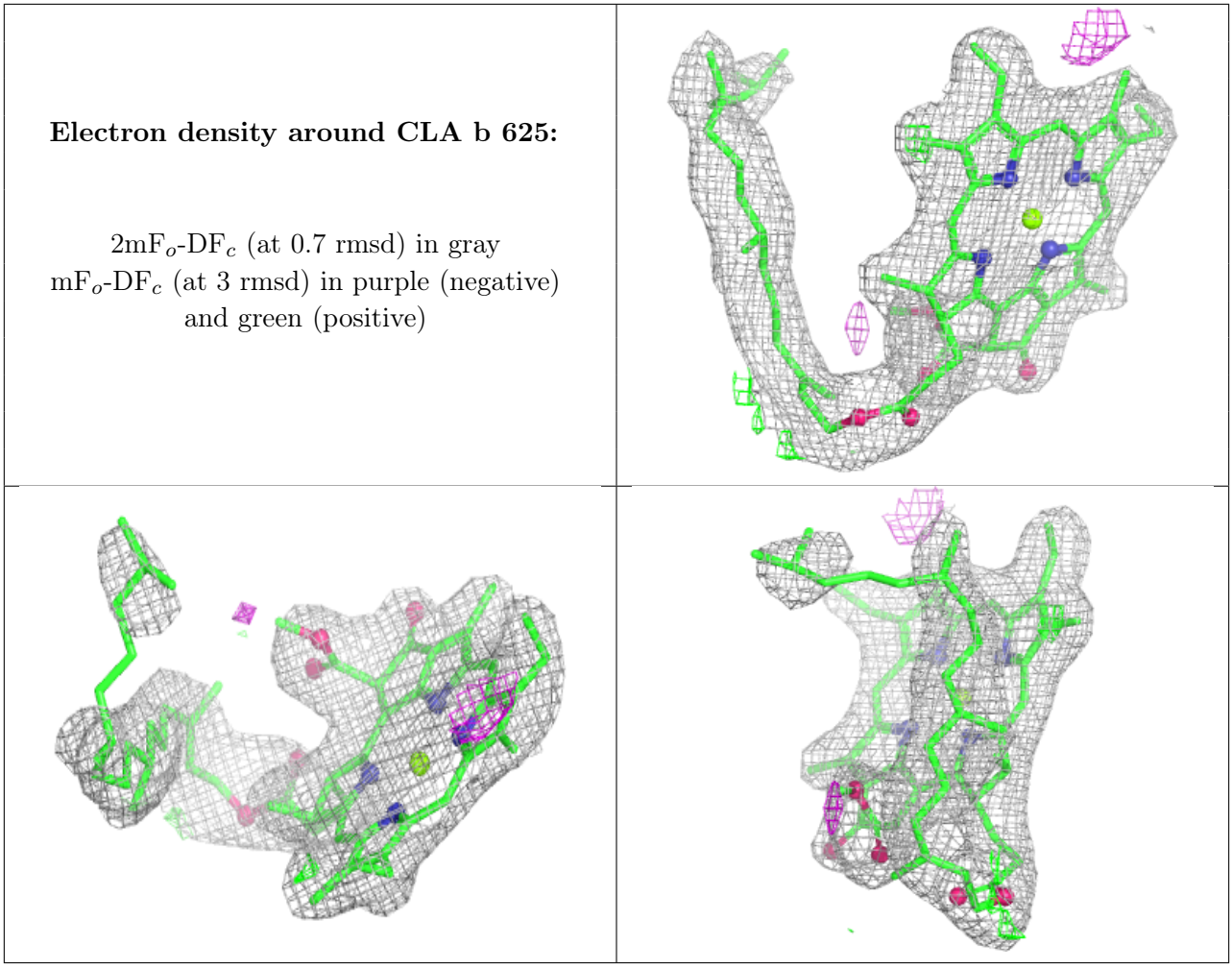






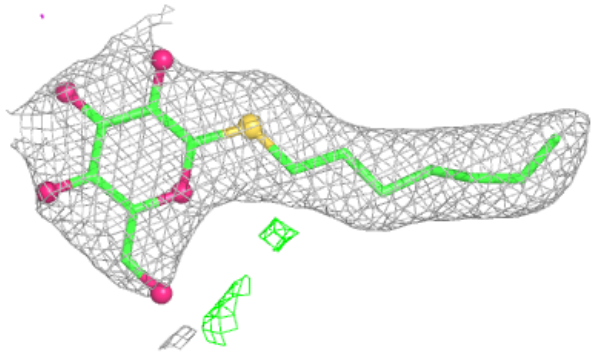
Electron density around CLA b 625:

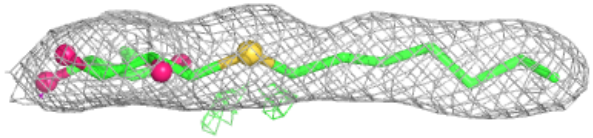
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

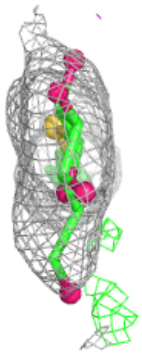


Electron density around HTG b 607:

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

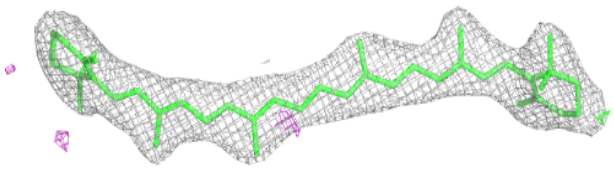


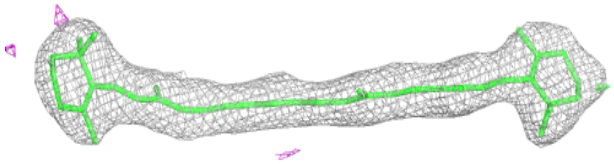


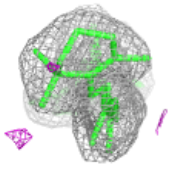


Electron density around BCR h 101:

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

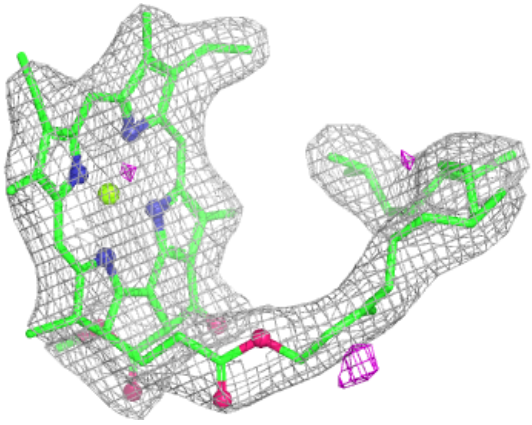


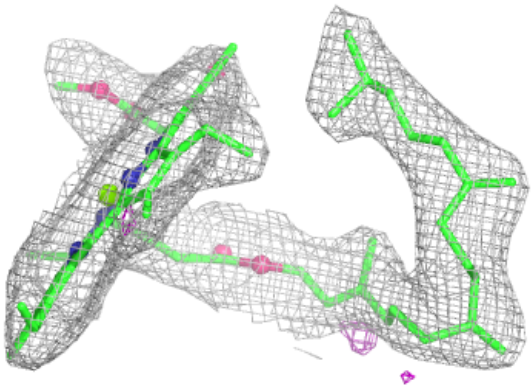


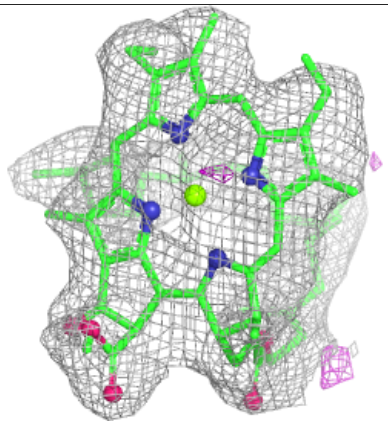


Electron density around CLA c 507:

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

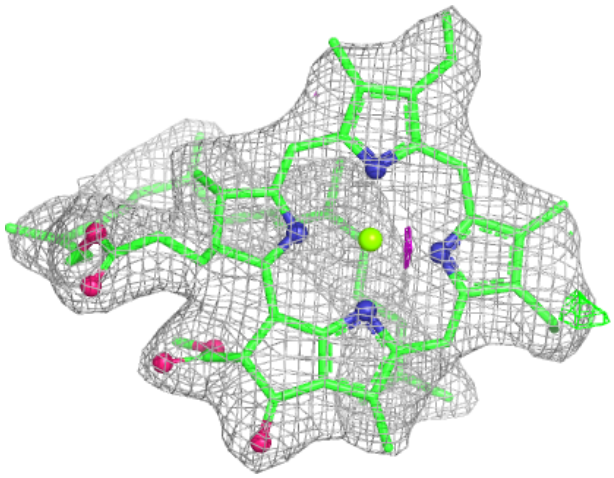


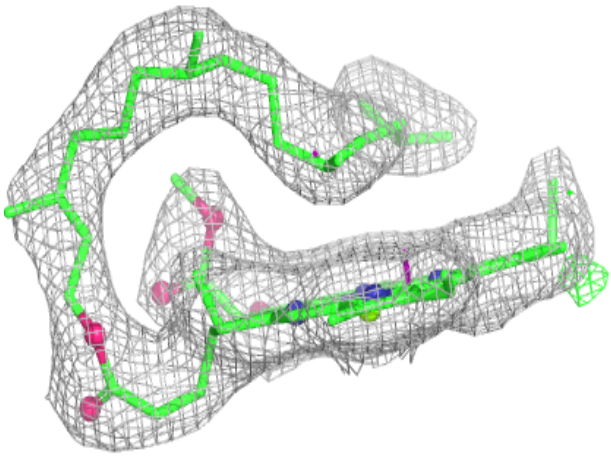


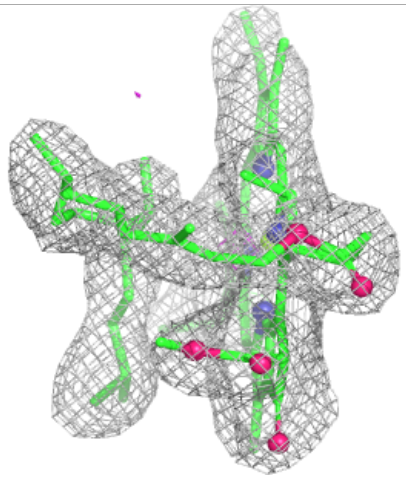


Electron density around CLA C 510:

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

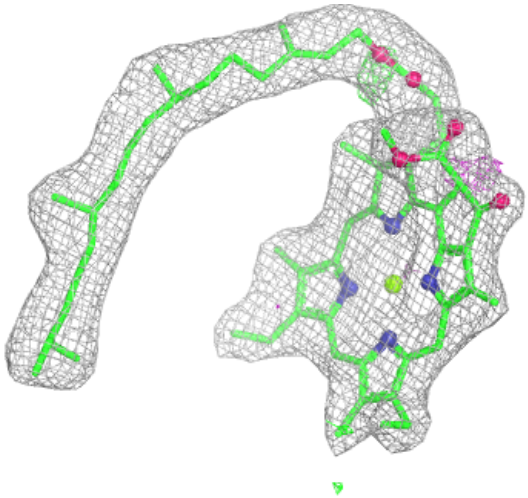


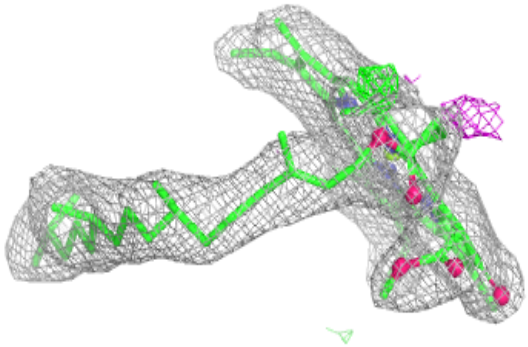


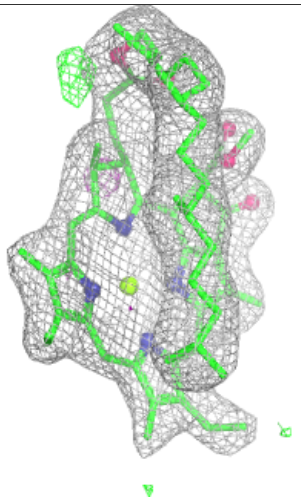


Electron density around CLA c 511:

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

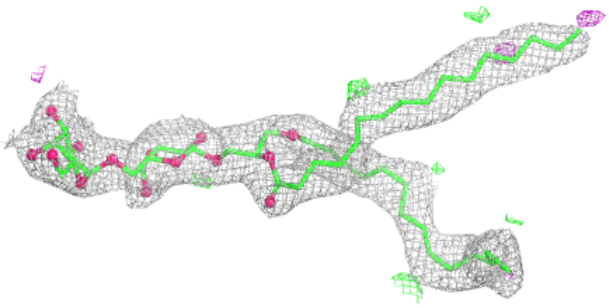


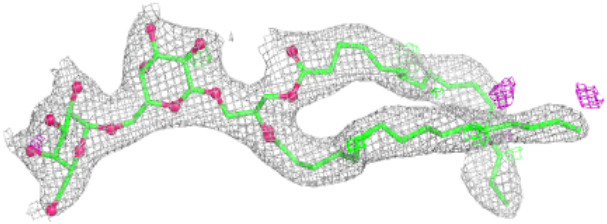


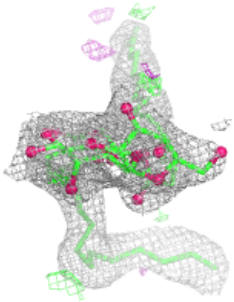


Electron density around DGD C 516:

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

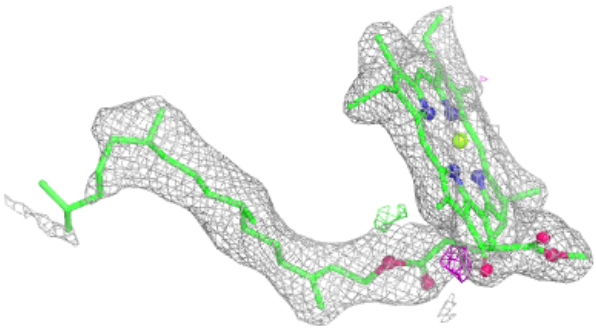


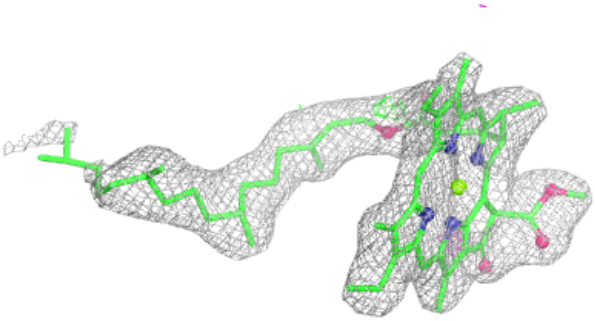


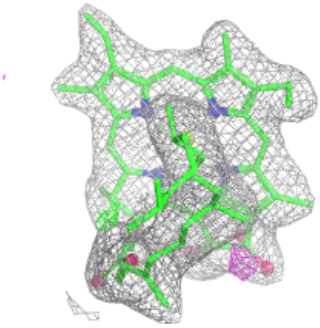


Electron density around CLA c 512:

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

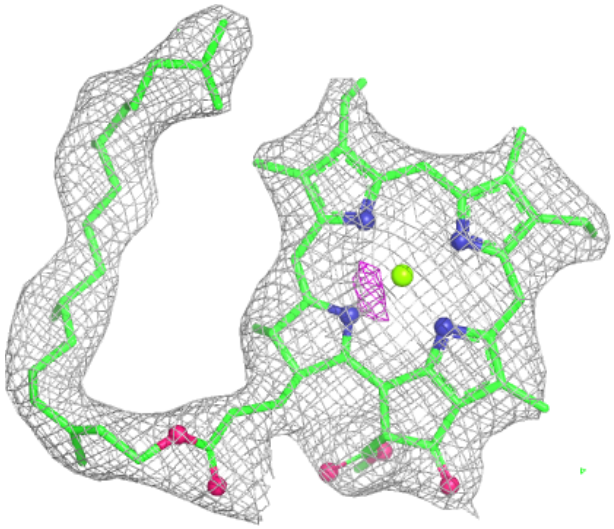


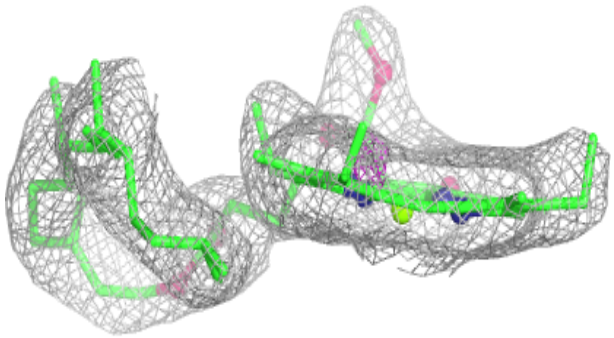


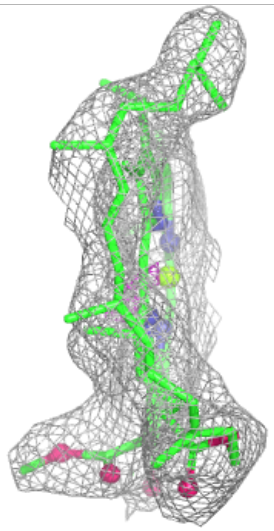


Electron density around CLA c 516:

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

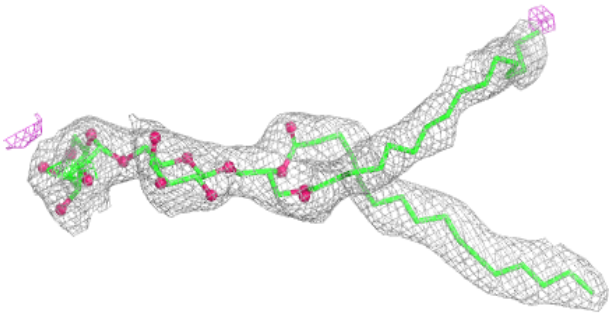


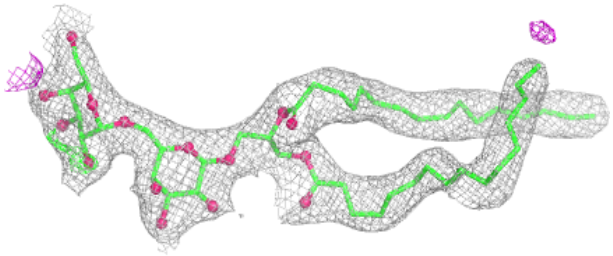


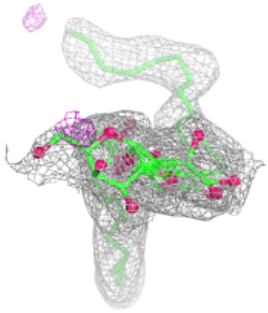


Electron density around DGD c 519:

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

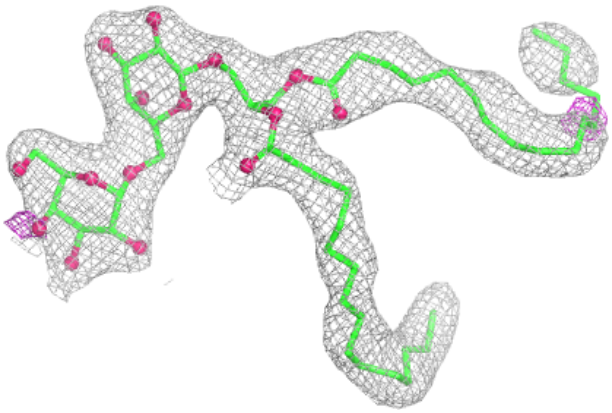


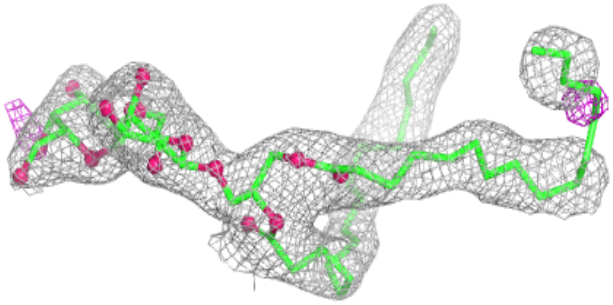




Electron density around DGD c 520:

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

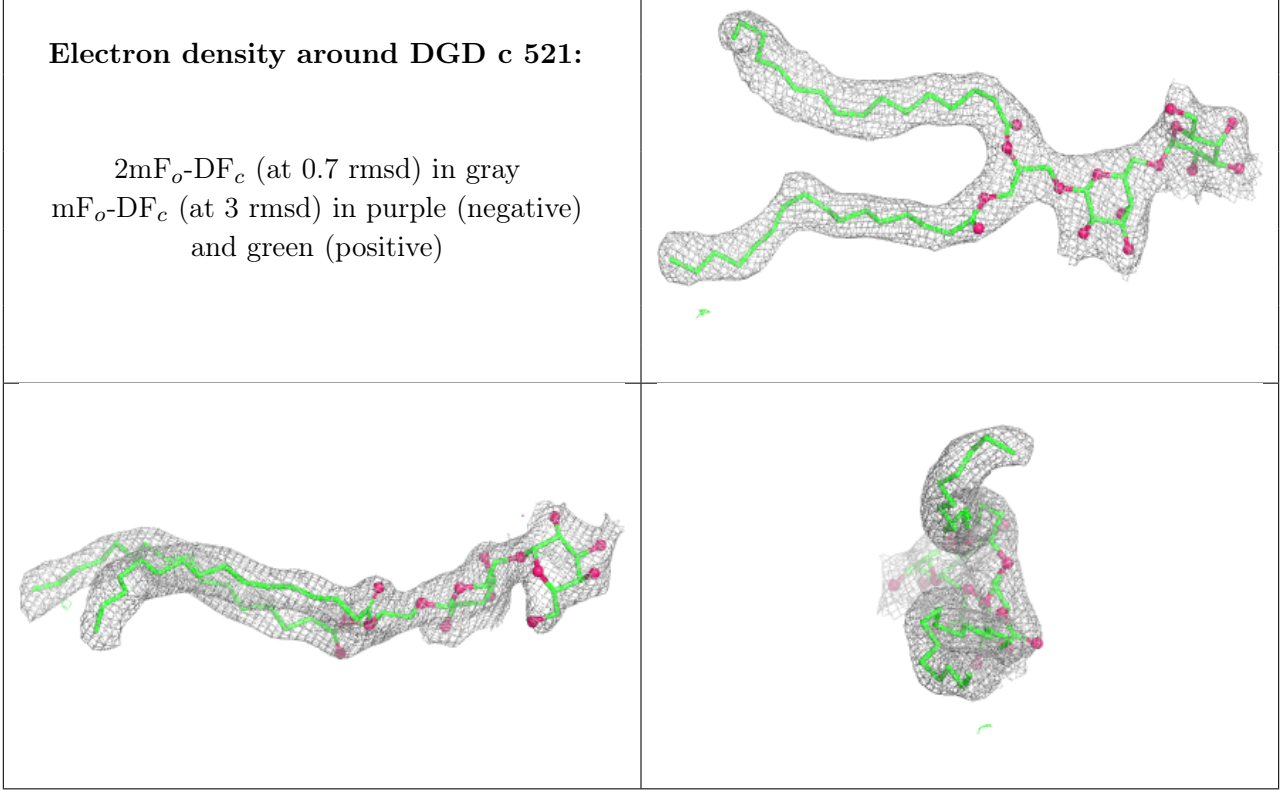






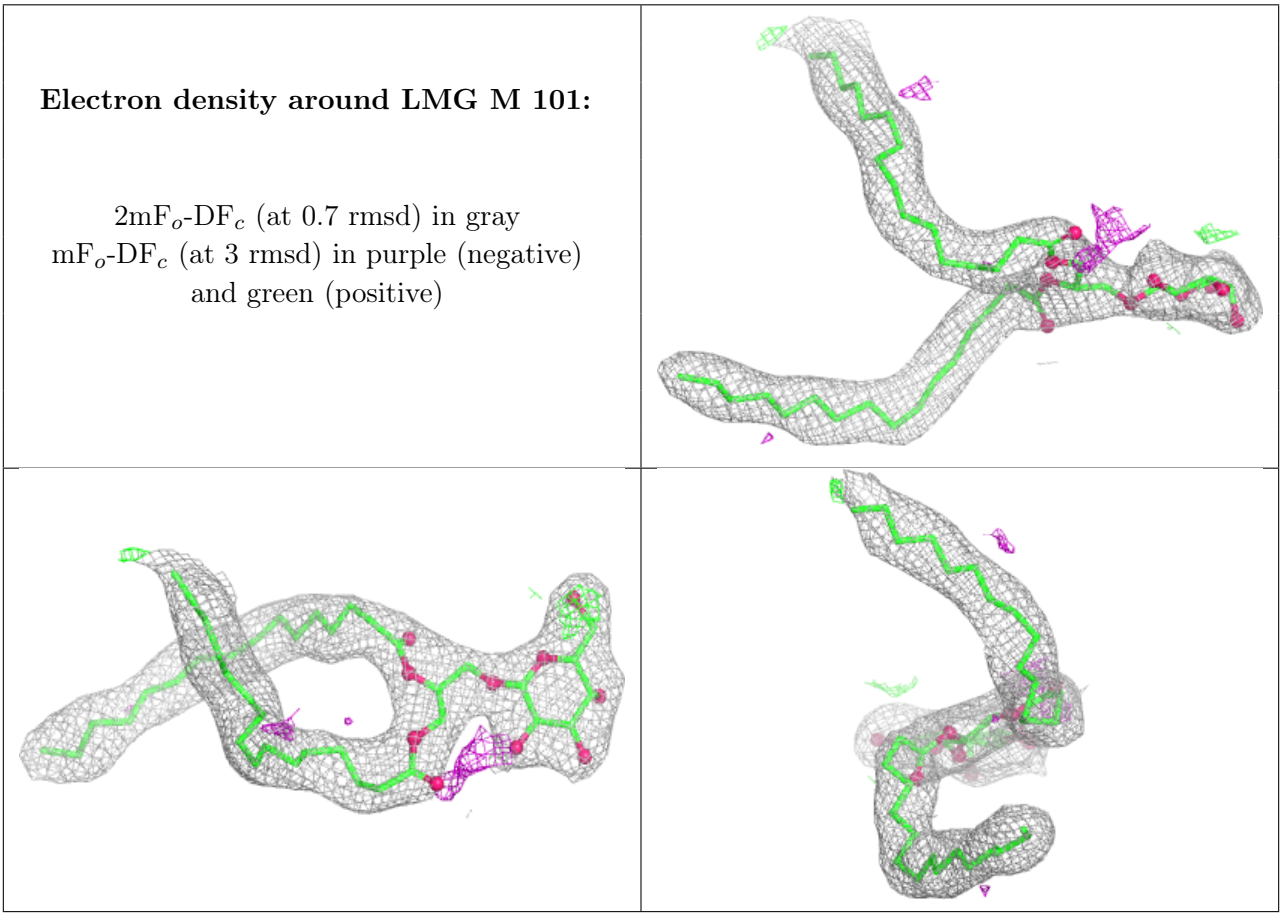
Electron density around DGD c 521:

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



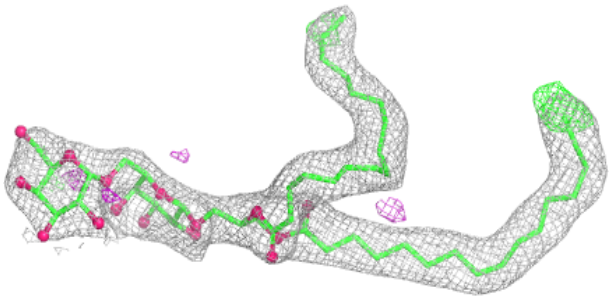
Electron density around LMG M 101:

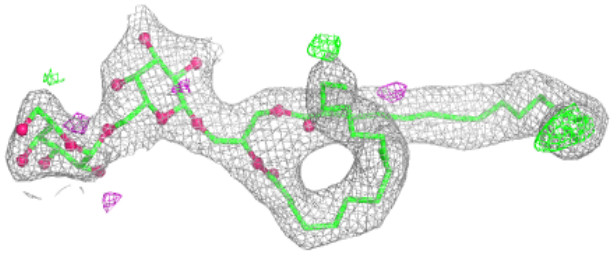
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around DGD h 102:

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

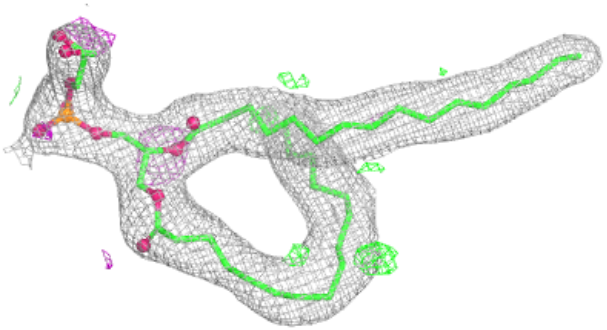


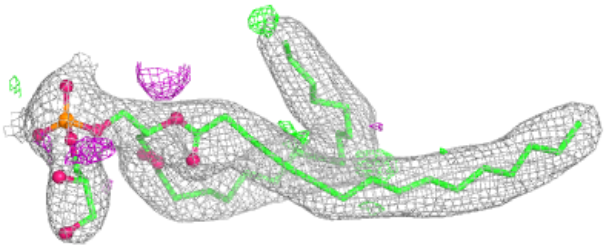


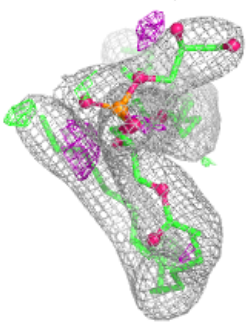


Electron density around LHG D 409:

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

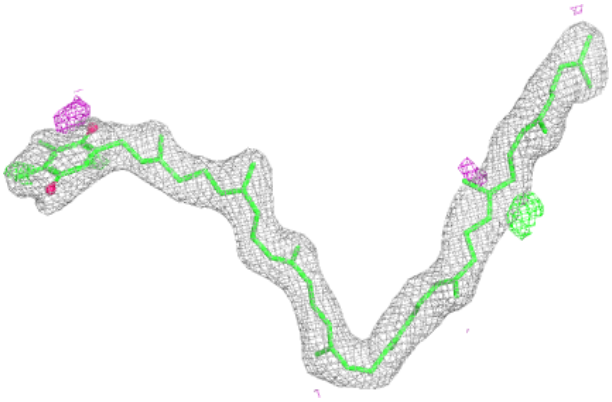


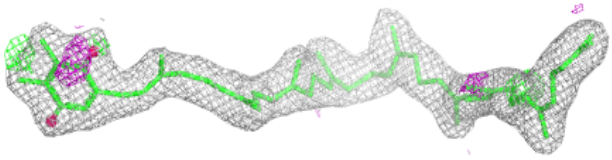


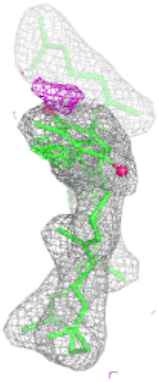


Electron density around PL9 D 407 (A):

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

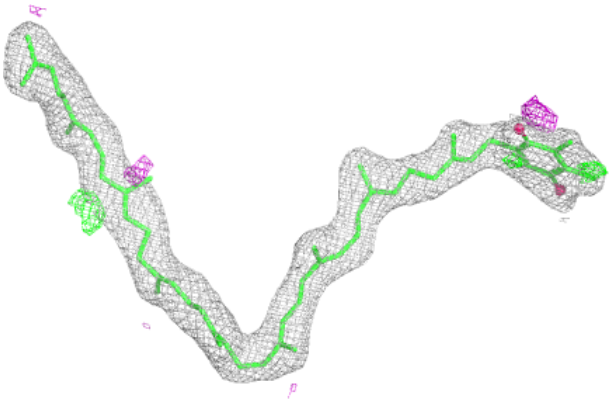


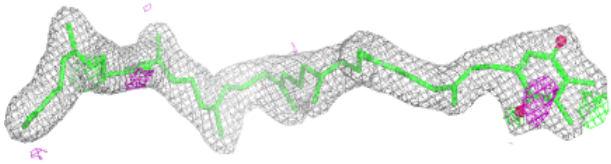


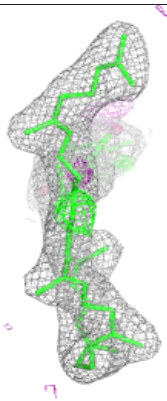


Electron density around PL9 D 407 (B):

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

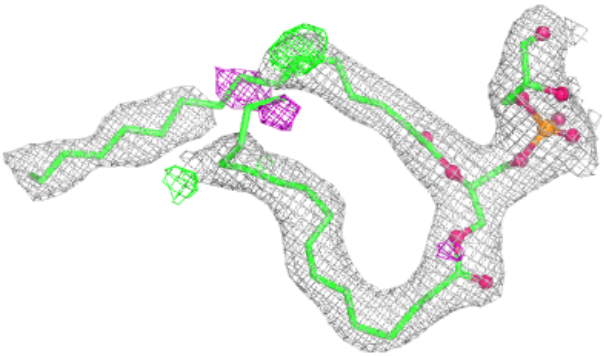


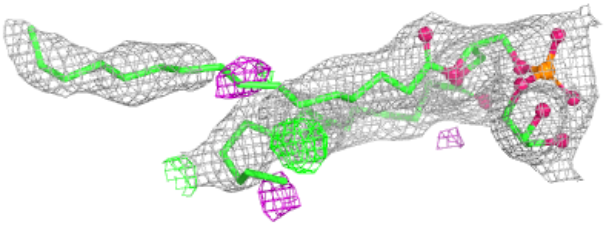


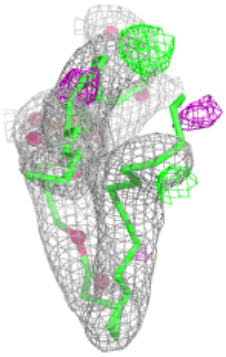


Electron density around LHG d 410:

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

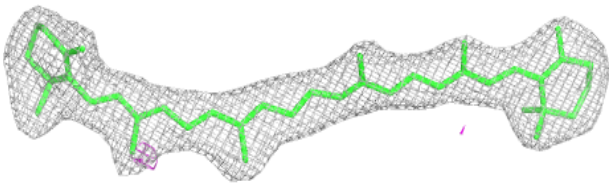


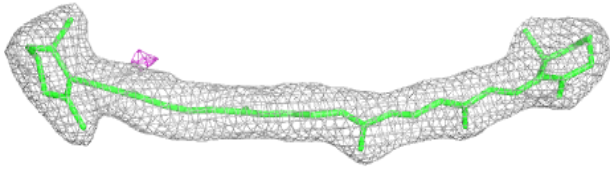


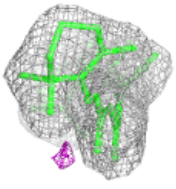


Electron density around BCR T 103:

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

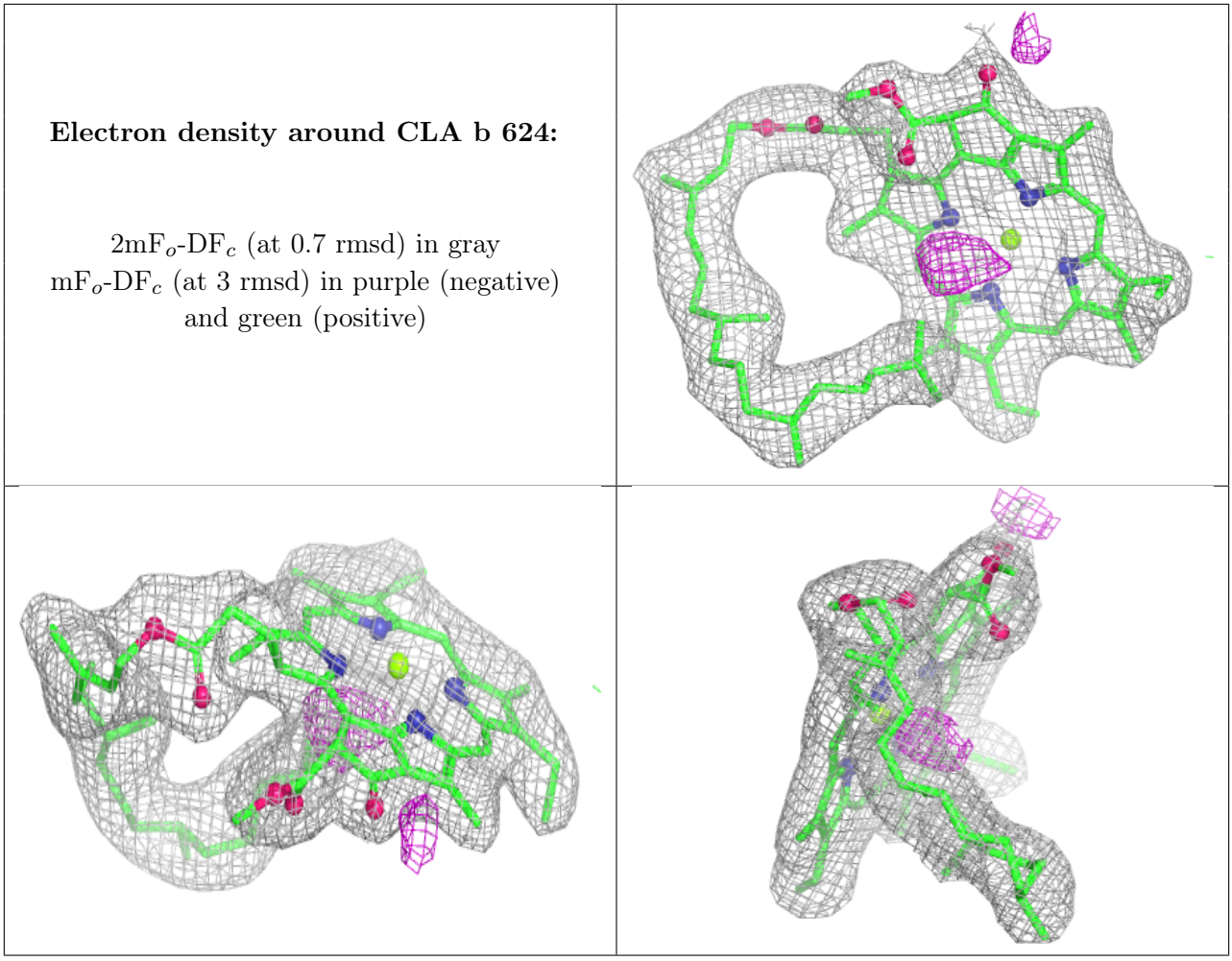






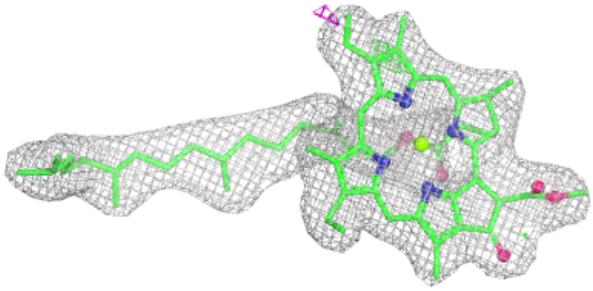
Electron density around CLA b 624:

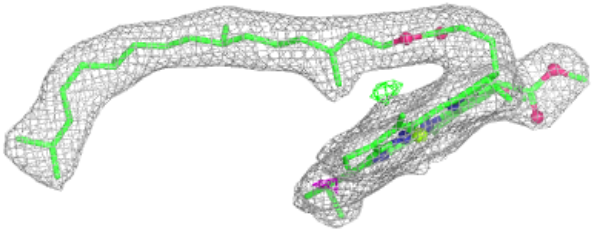
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

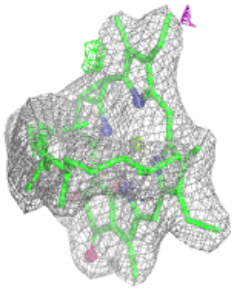


Electron density around CLA B 609:

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

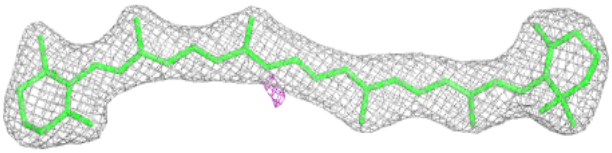


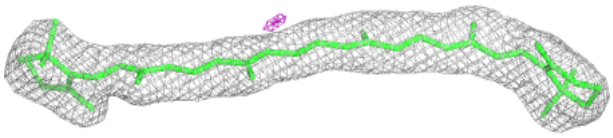


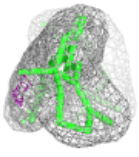


Electron density around BCR b 628:

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

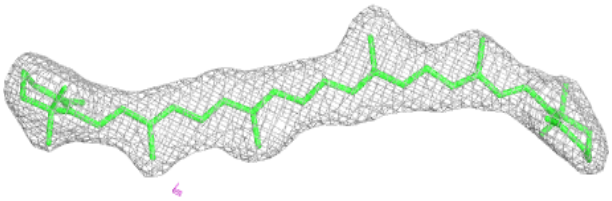


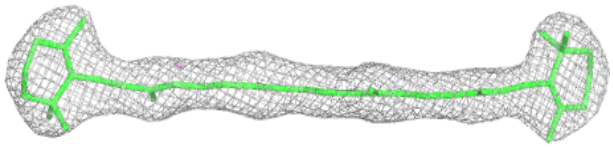


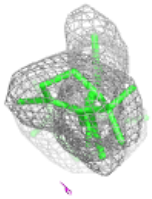


Electron density around BCR c 518:

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

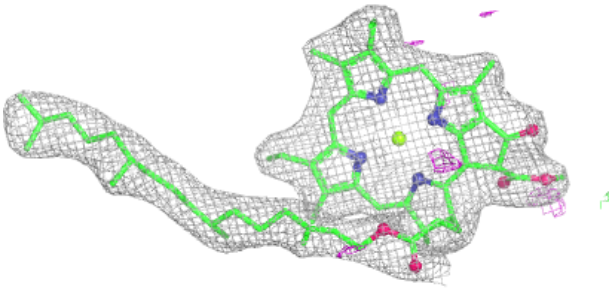


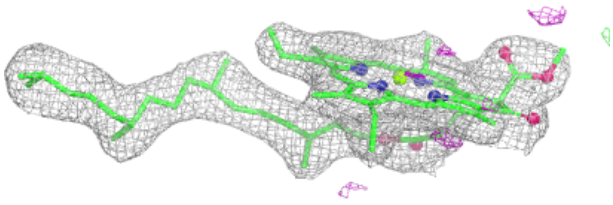


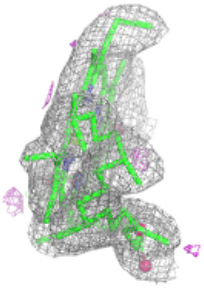


Electron density around CLA c 505:

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

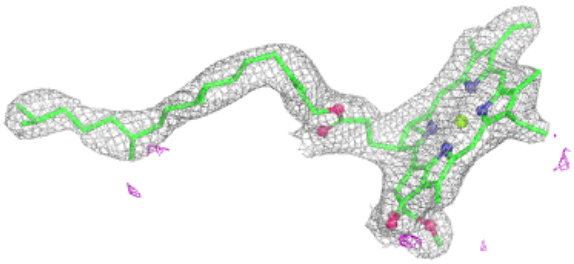


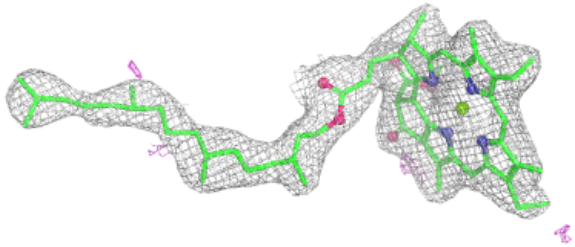


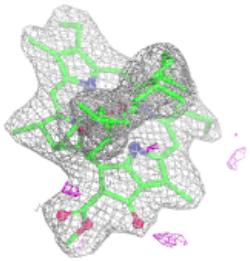


Electron density around CLA c 506:

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

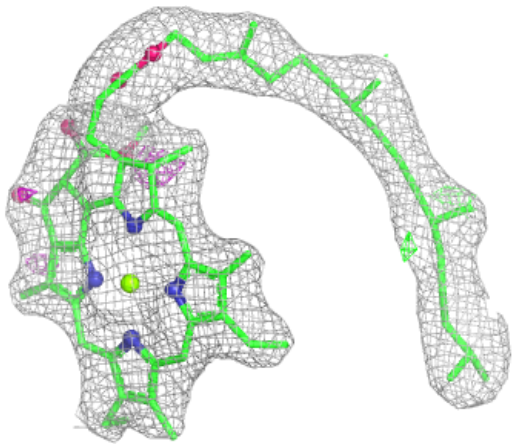


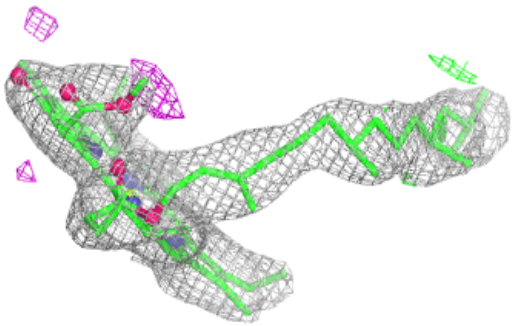


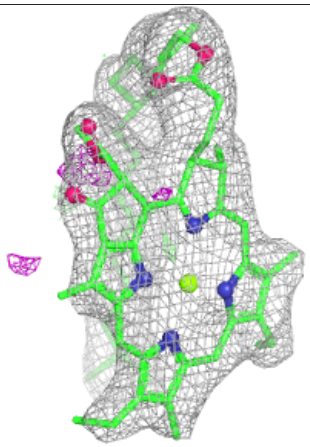


Electron density around CLA C 507:

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

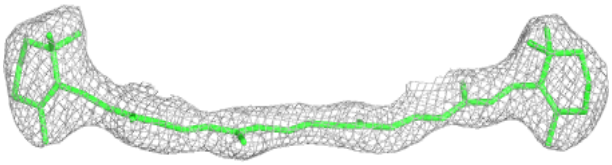


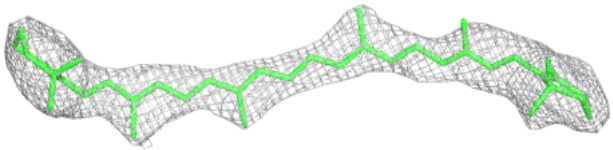


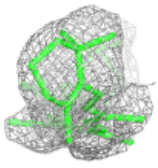


Electron density around BCR k 102:

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

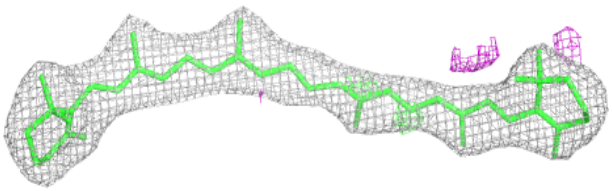


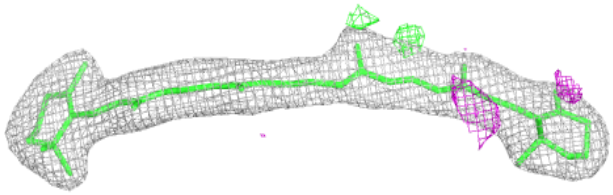


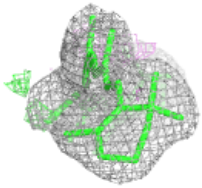


Electron density around BCR t 102:

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

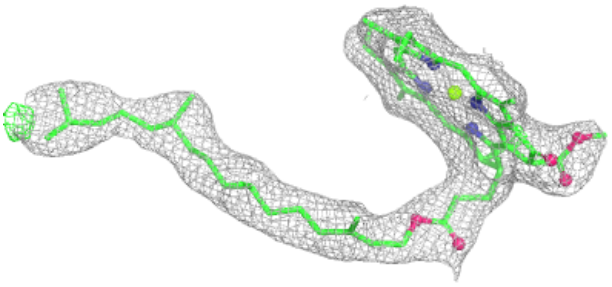


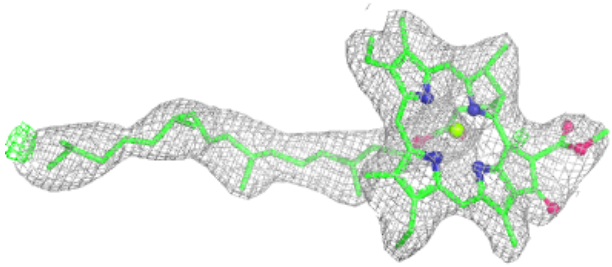


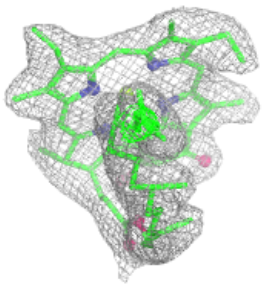


Electron density around CLA c 508:

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

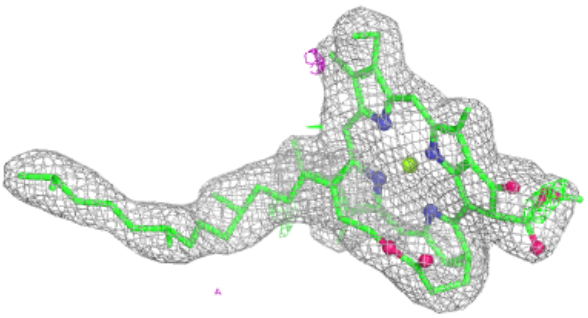


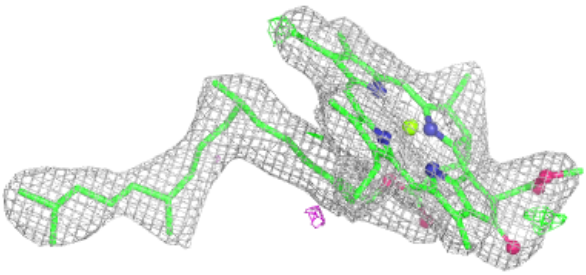


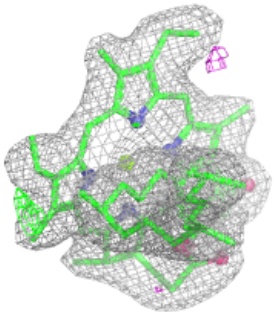


Electron density around CLA c 509:

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

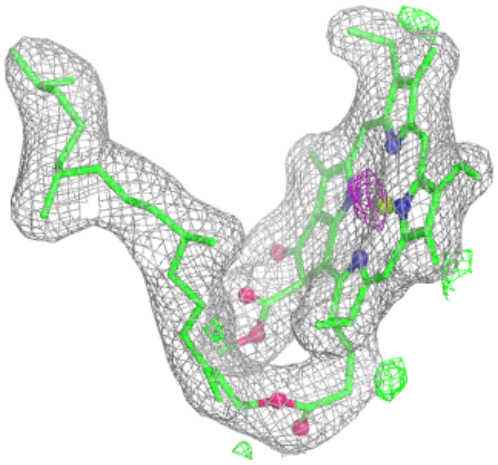


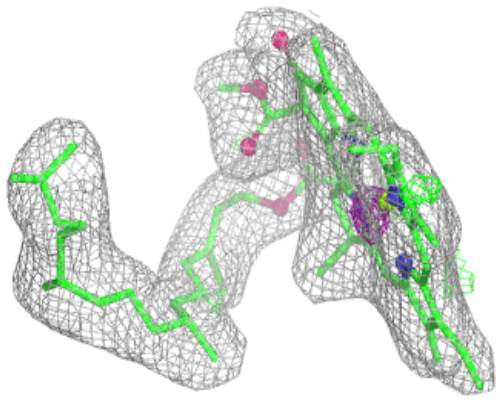


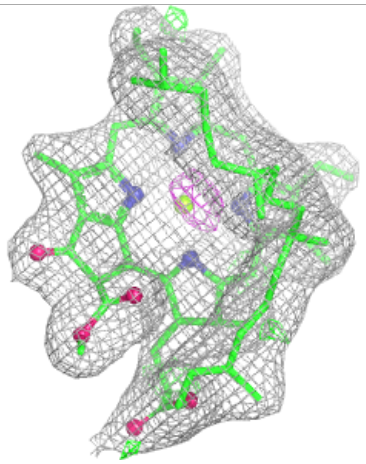


Electron density around CLA B 614:

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

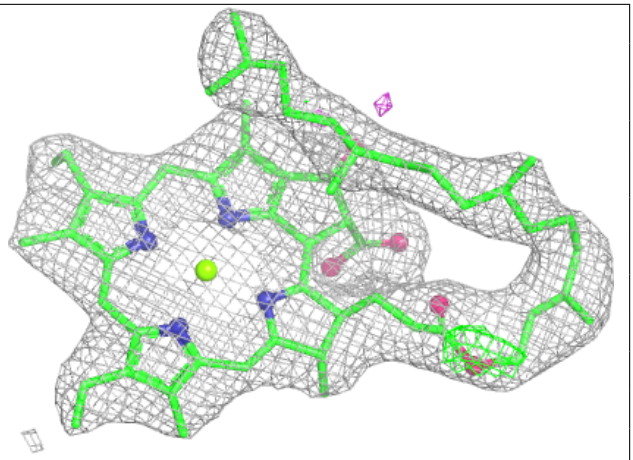


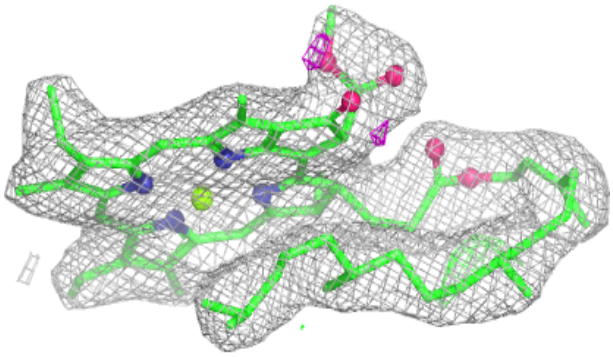


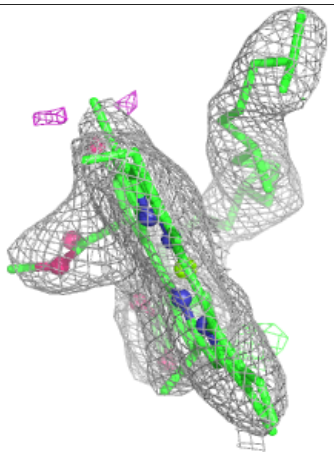


Electron density around CLA C 509:

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

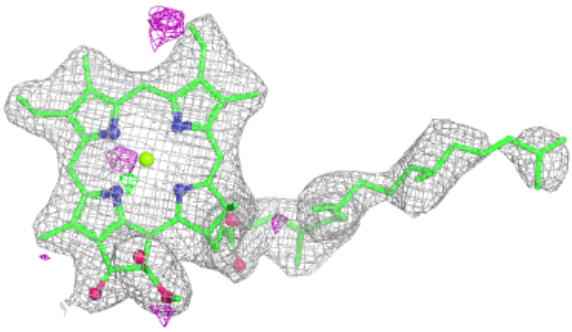


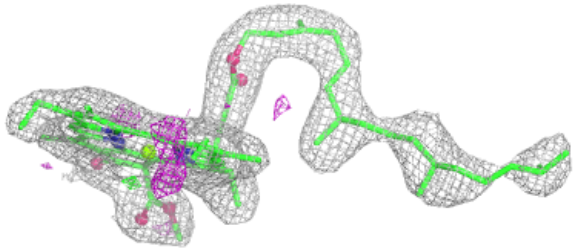


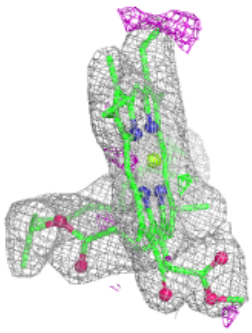


Electron density around CLA A 407:

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

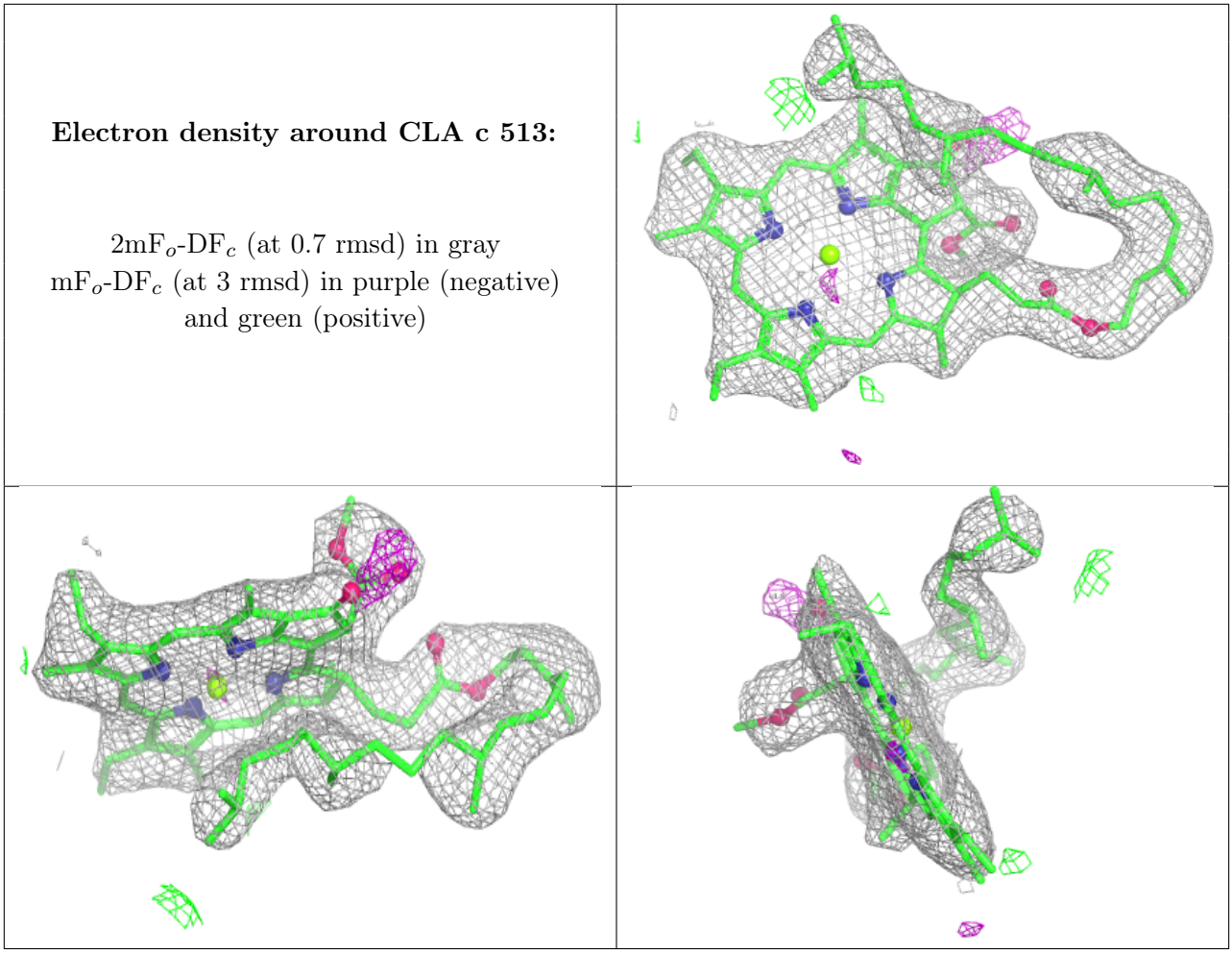






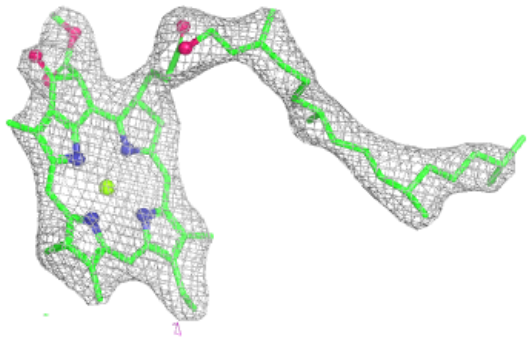
Electron density around CLA c 513:

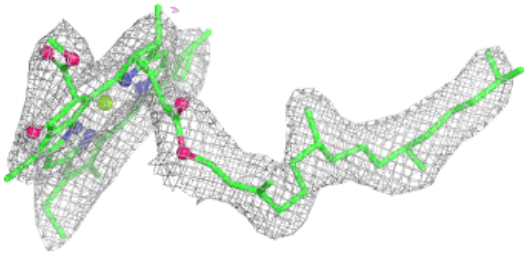
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

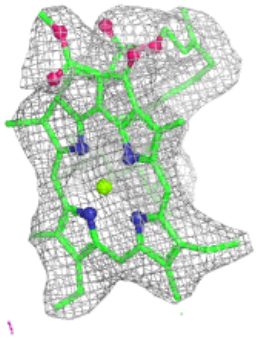


Electron density around CLA c 515:

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

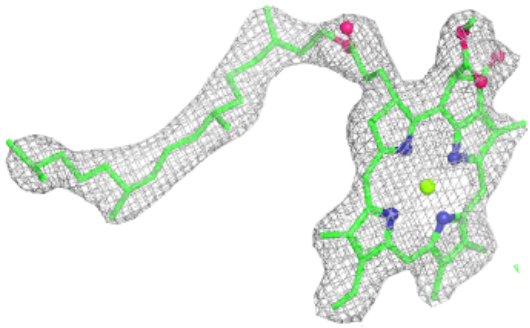


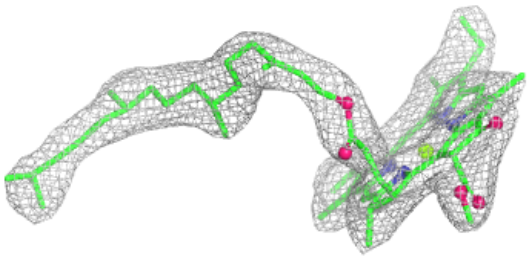


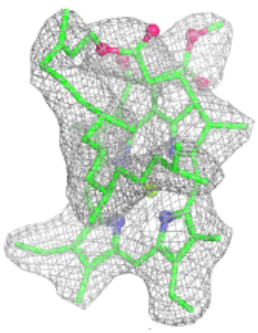


Electron density around CLA C 511:

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

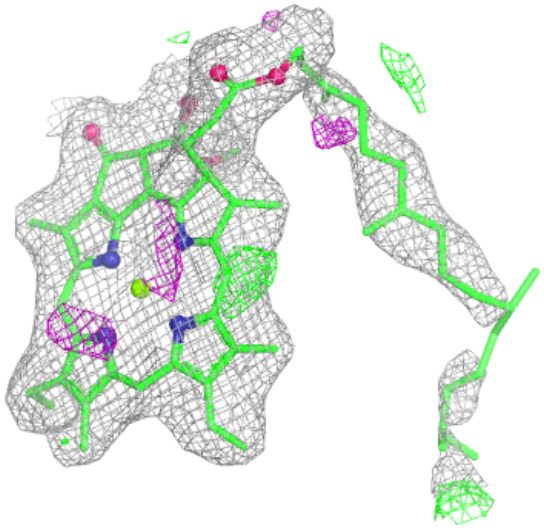


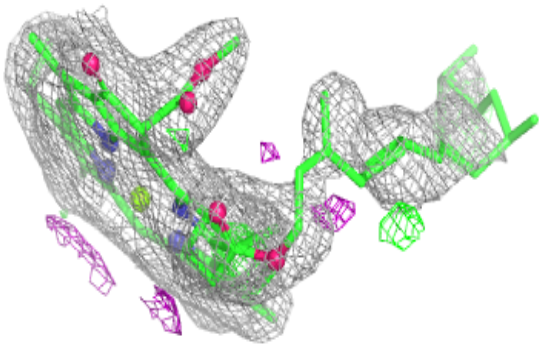


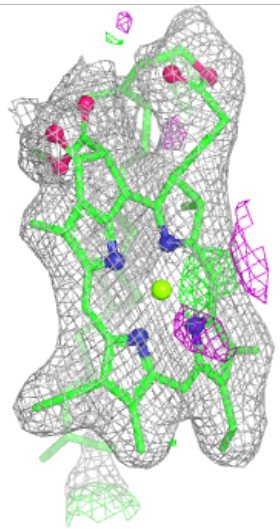


Electron density around CLA B 617:

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

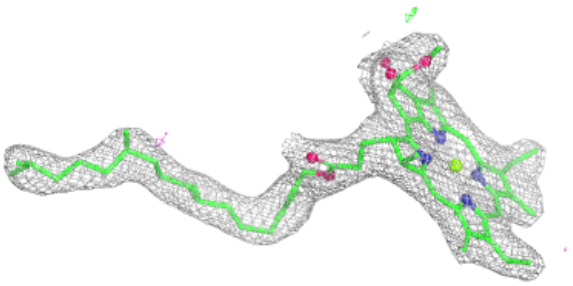


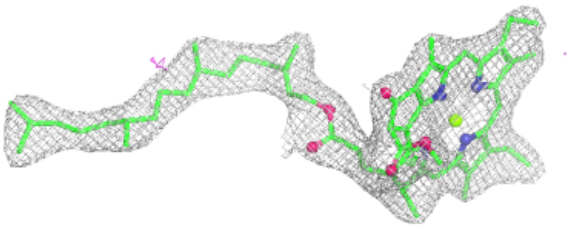


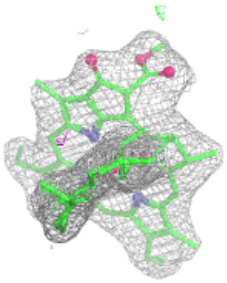


Electron density around CLA C 502:

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

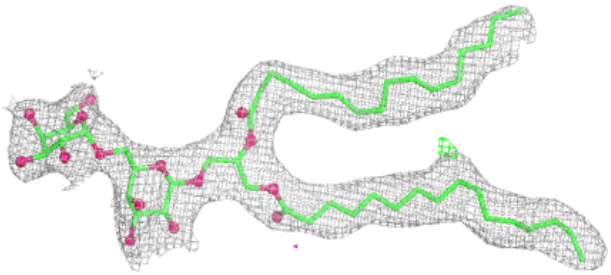


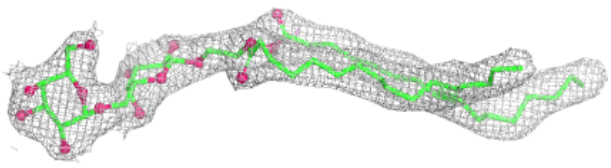


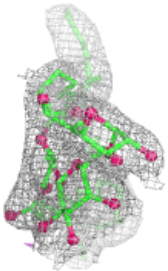


Electron density around DGD C 518:

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

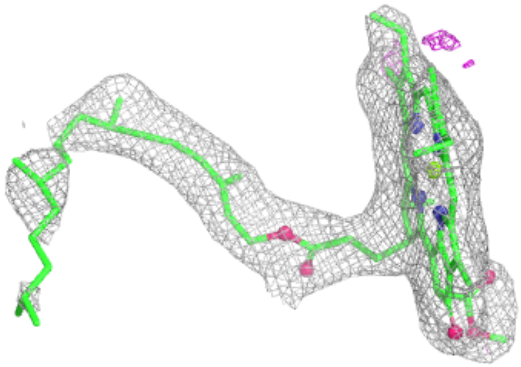


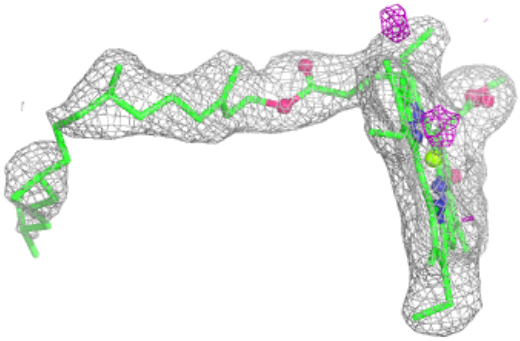


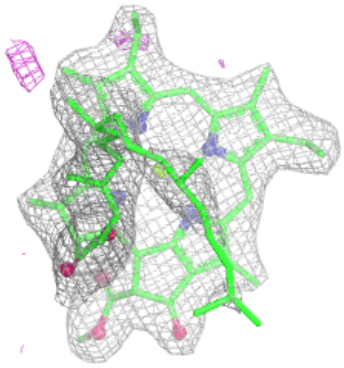


Electron density around CLA D 405:

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

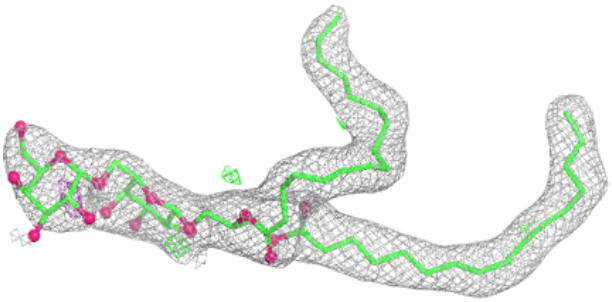


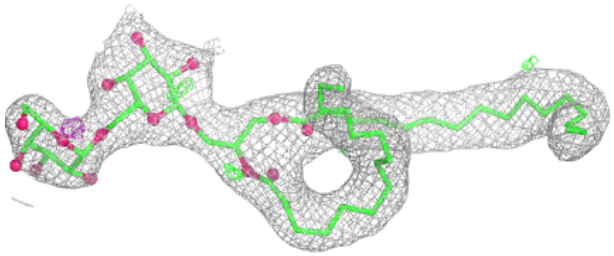




Electron density around DGD H 102:

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

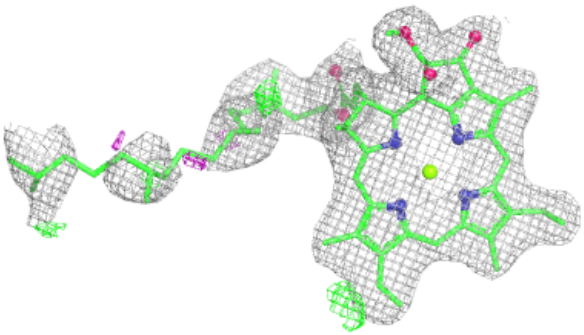


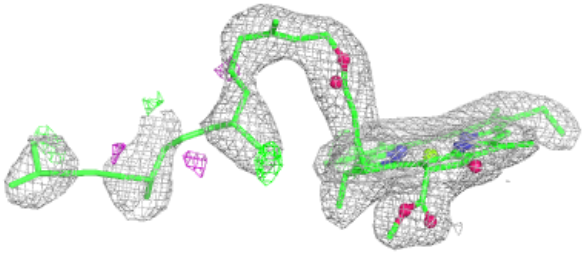


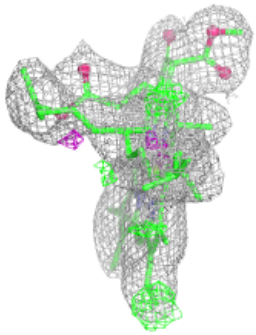


Electron density around CLA a 410:

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

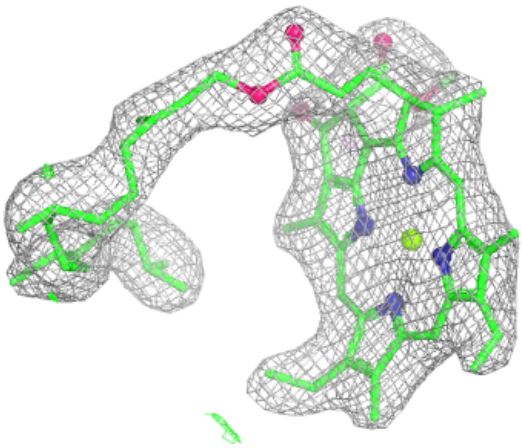


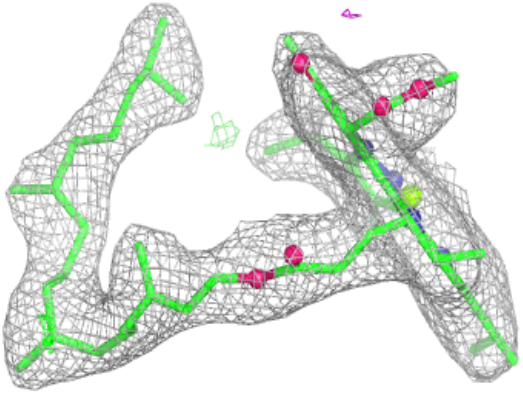


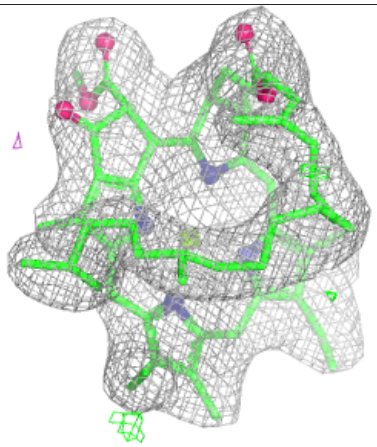


Electron density around CLA C 503:

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

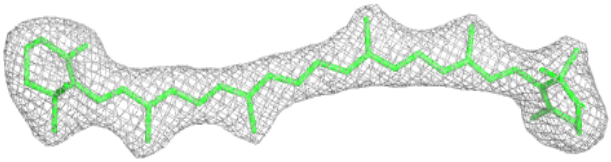


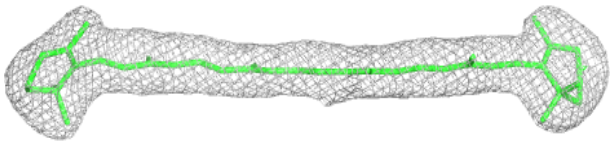


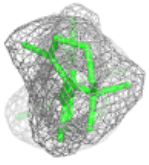


Electron density around BCR B 619:

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

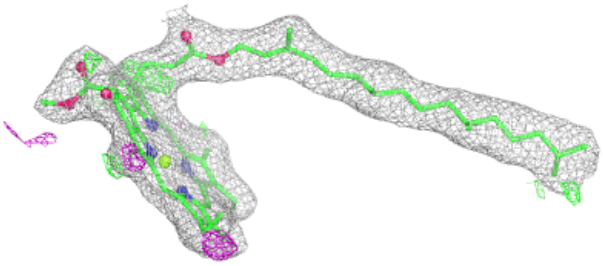


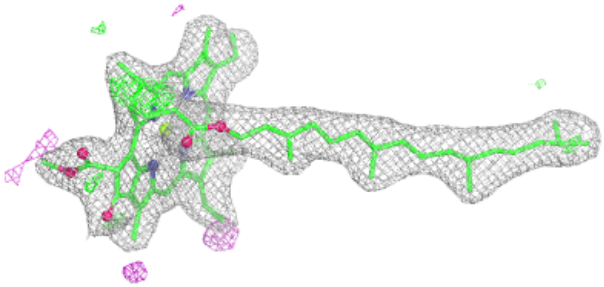


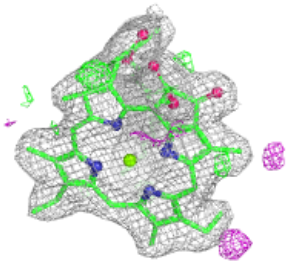


Electron density around CLA B 608:

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

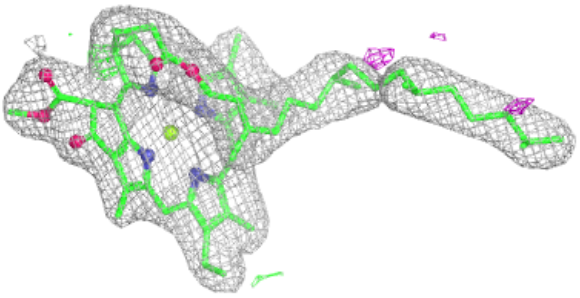


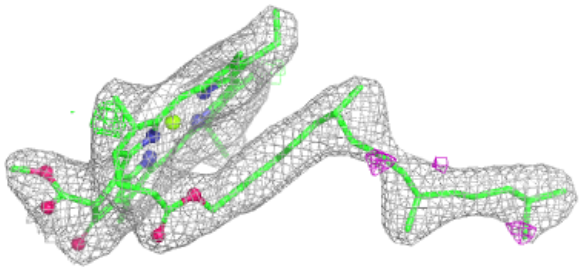


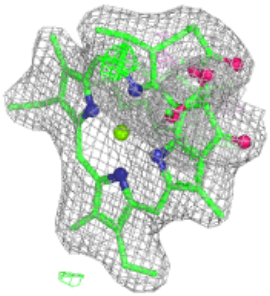


Electron density around CLA C 505:

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

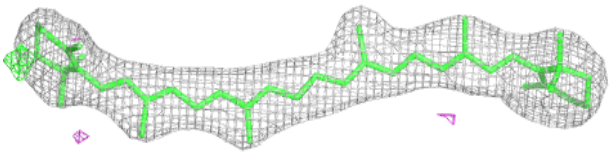


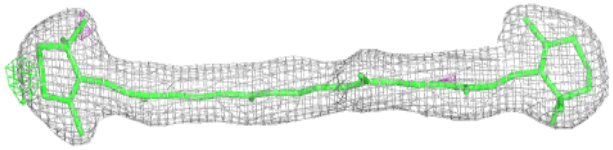


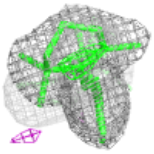


Electron density around BCR C 515:

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

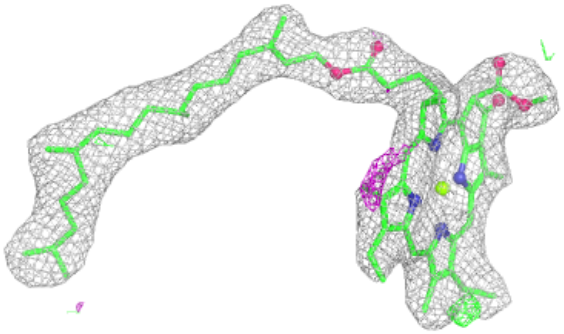


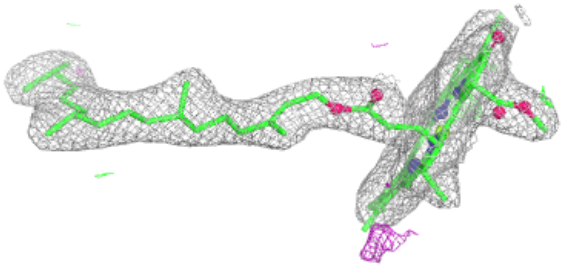


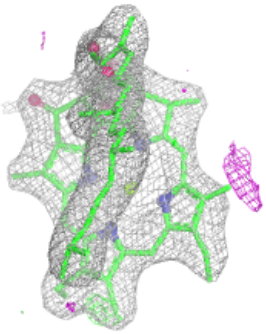


Electron density around CLA b 618:

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

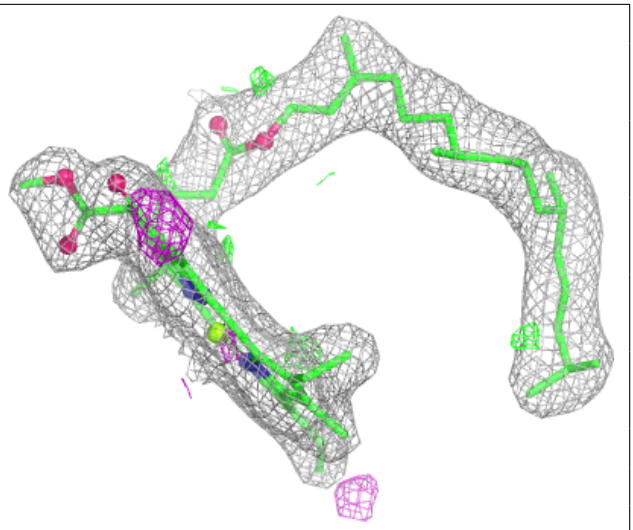


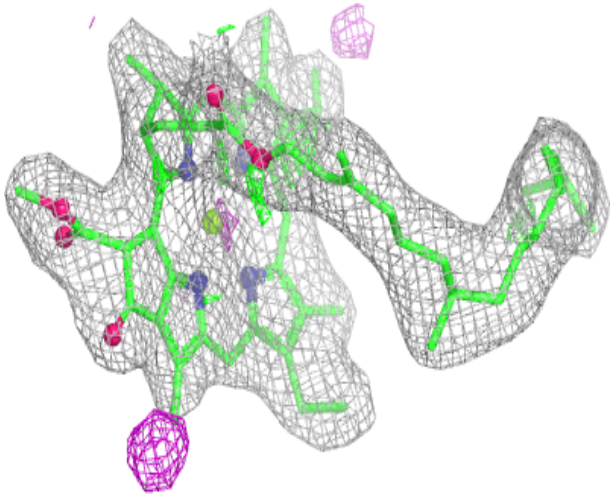


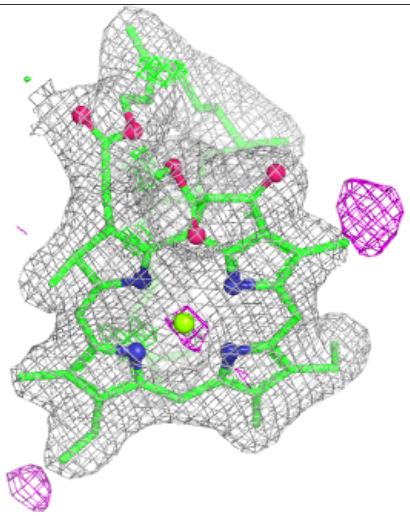


Electron density around CLA b 620:

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

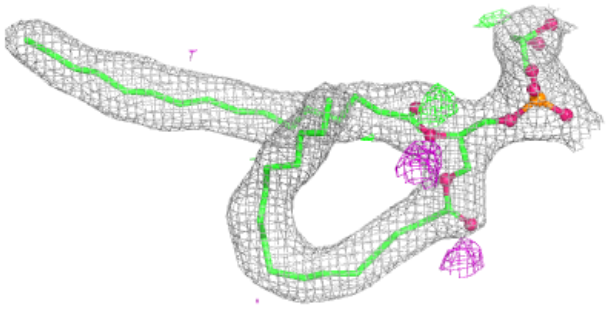


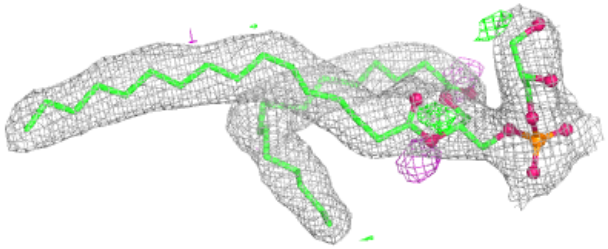


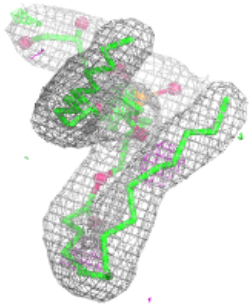


Electron density around LHG d 408:

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

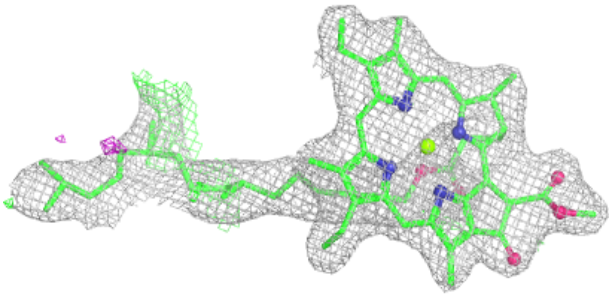


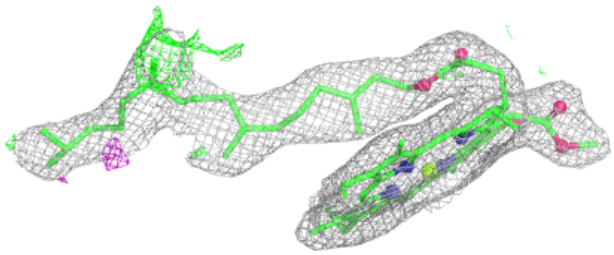


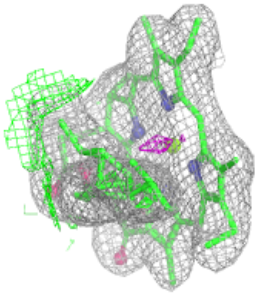


Electron density around CLA b 623:

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

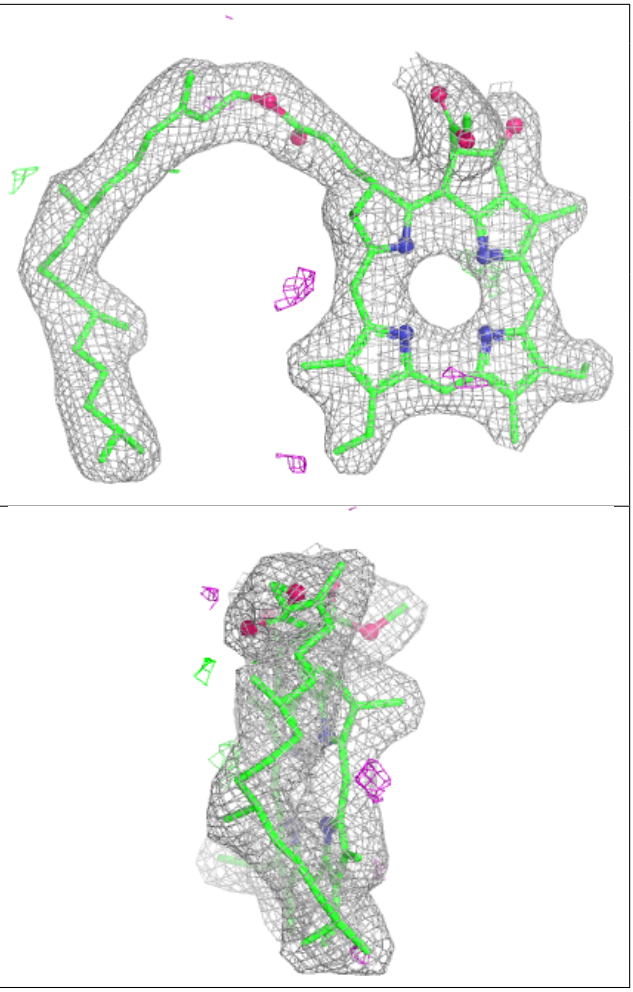






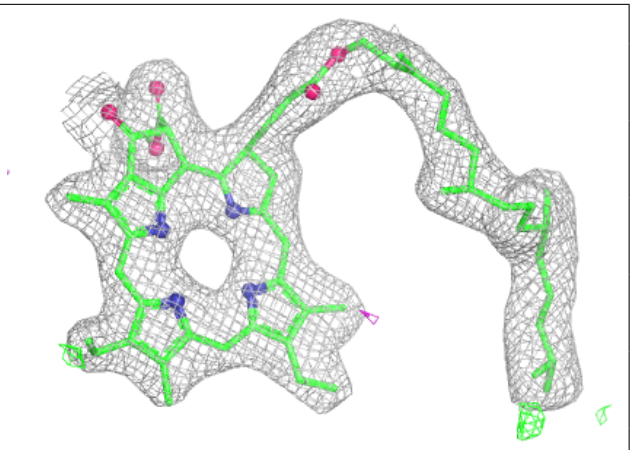
Electron density around PHO A 408:

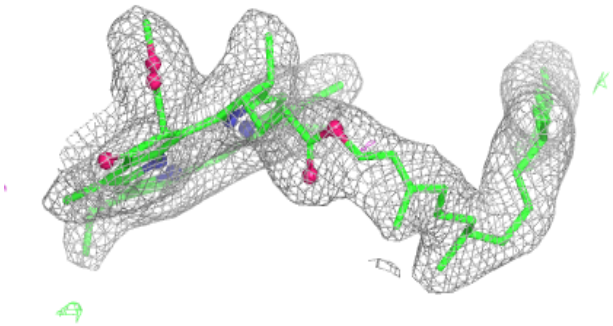
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

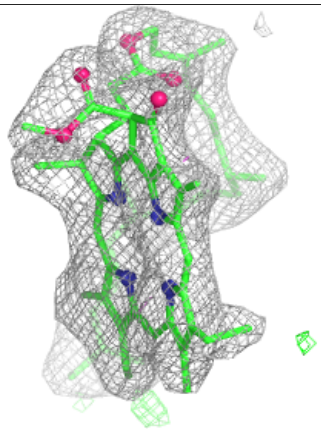


Electron density around PHO D 401 (A):

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

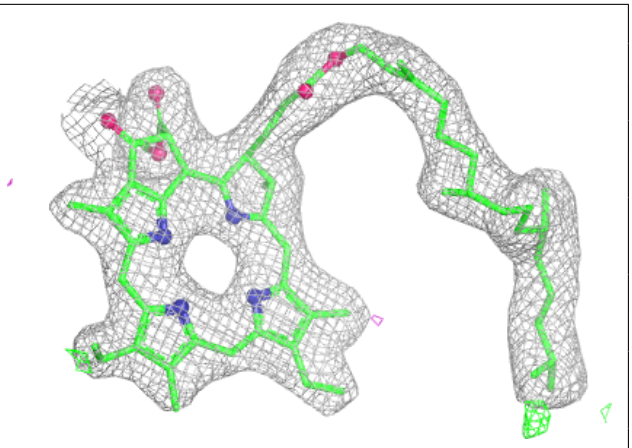


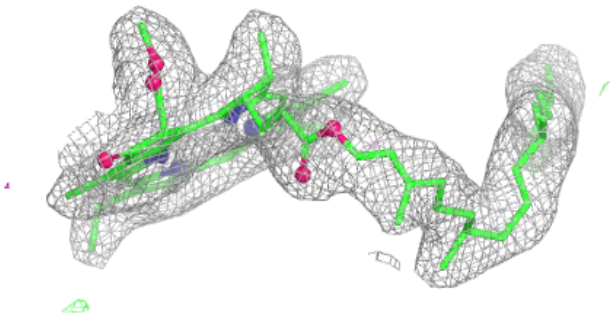


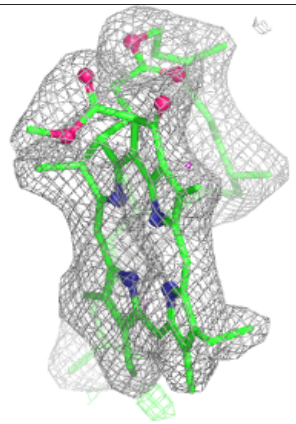


Electron density around PHO D 401 (B):

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

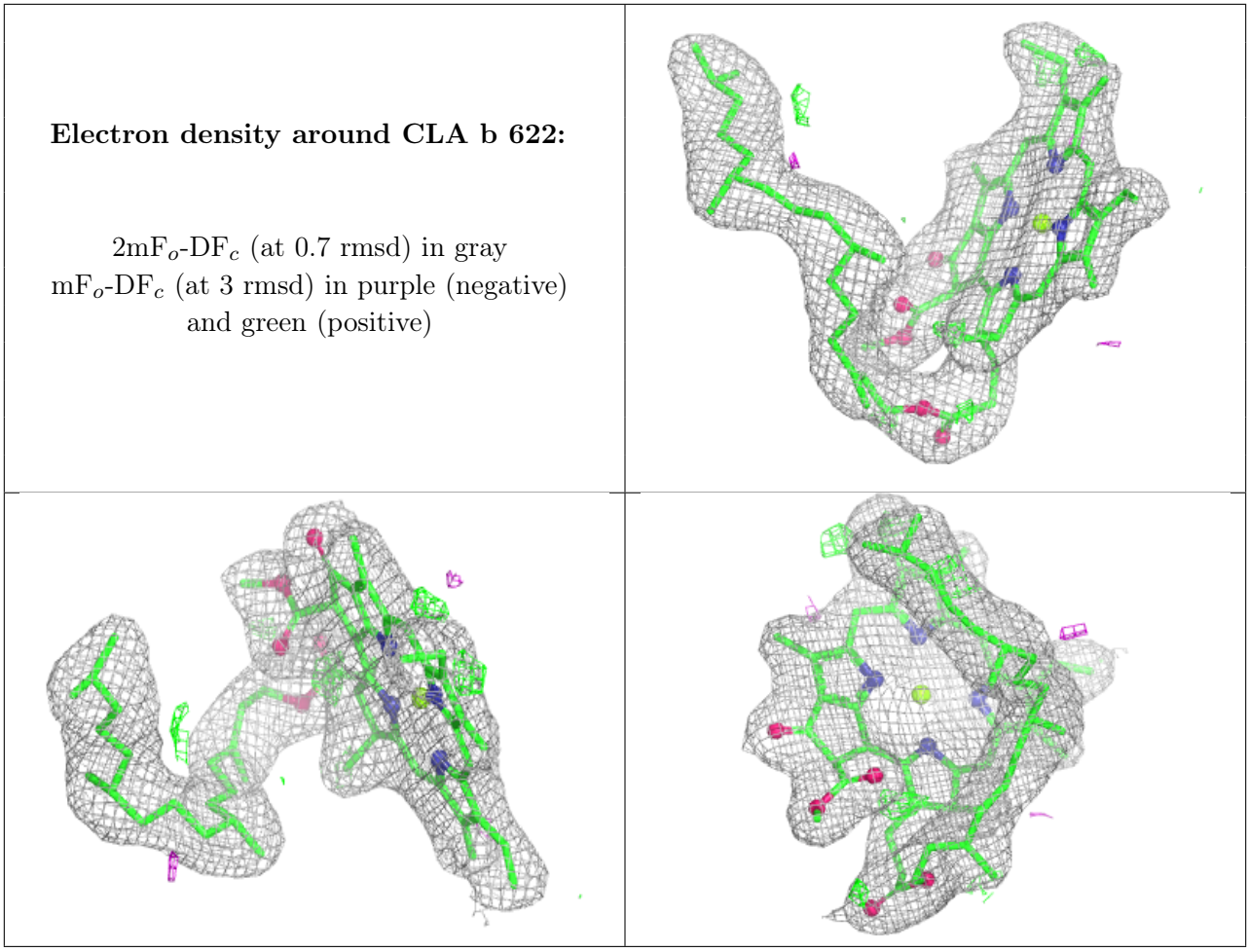






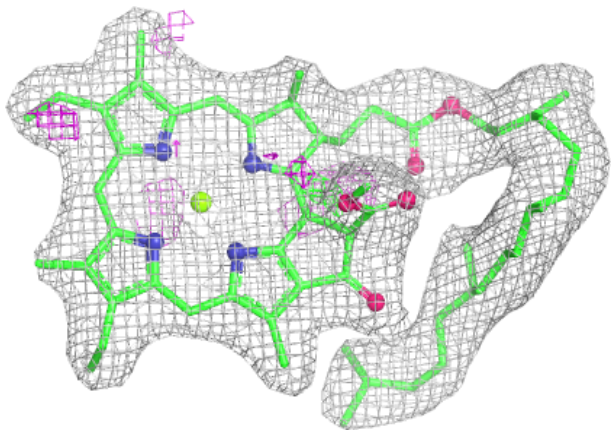
Electron density around CLA b 622:

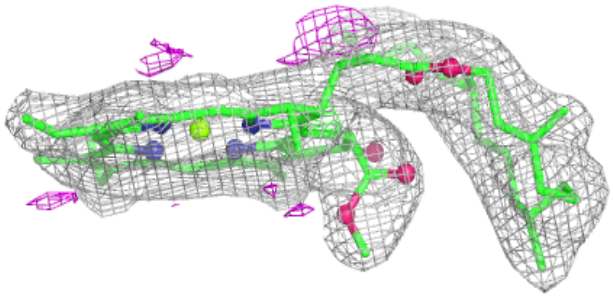
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

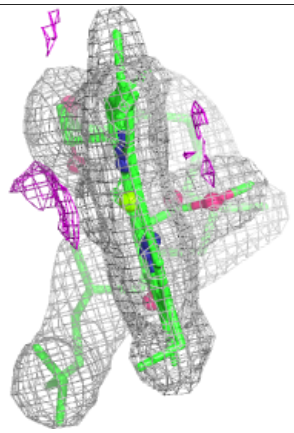


Electron density around CLA B 611:

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

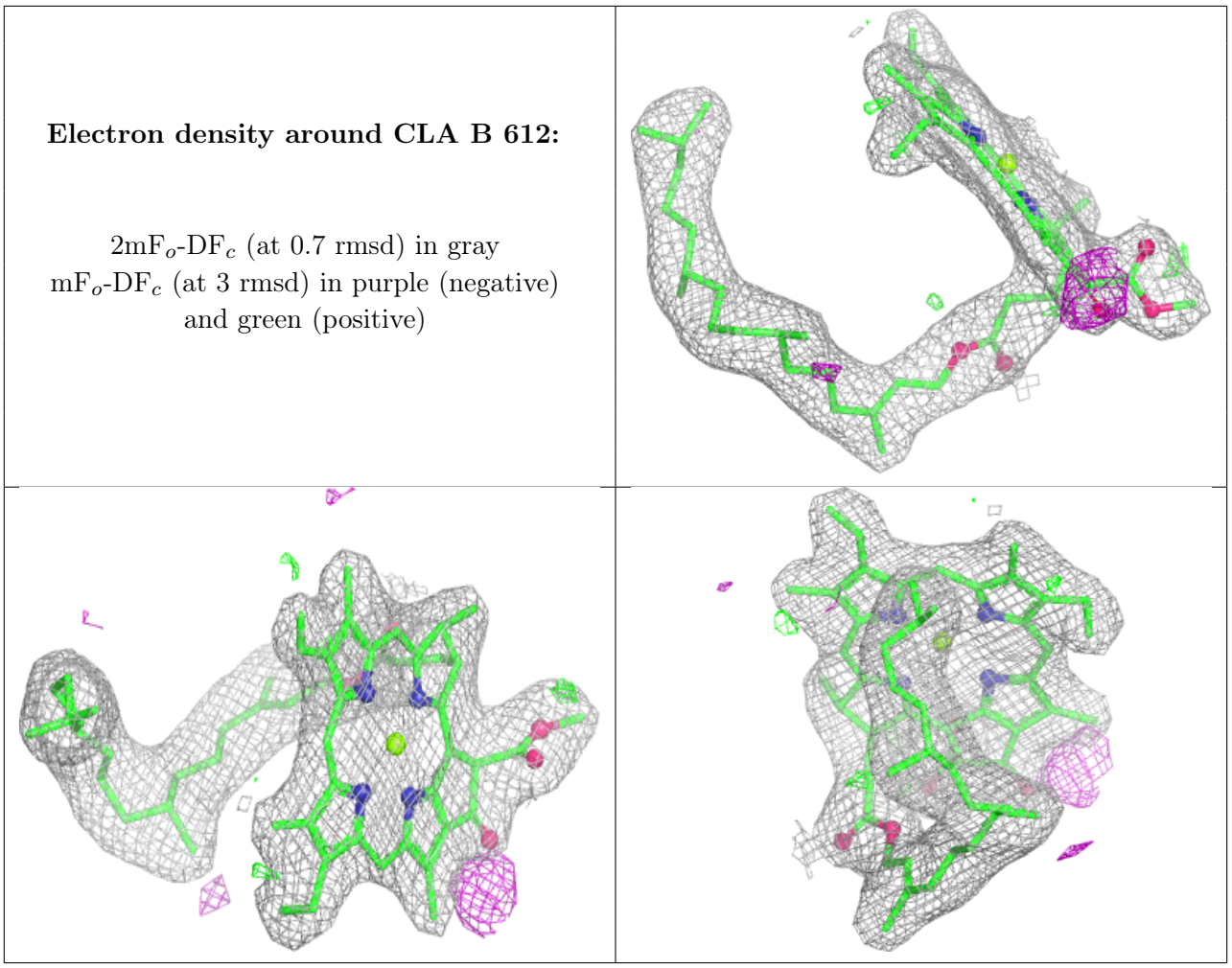






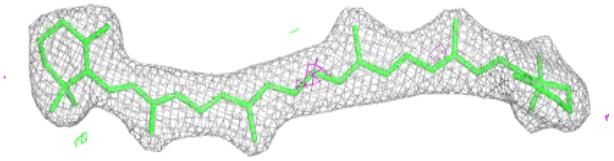
Electron density around CLA B 612:

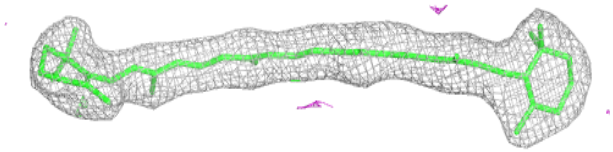
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

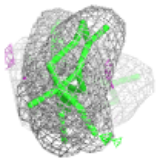


Electron density around BCR B 618:

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

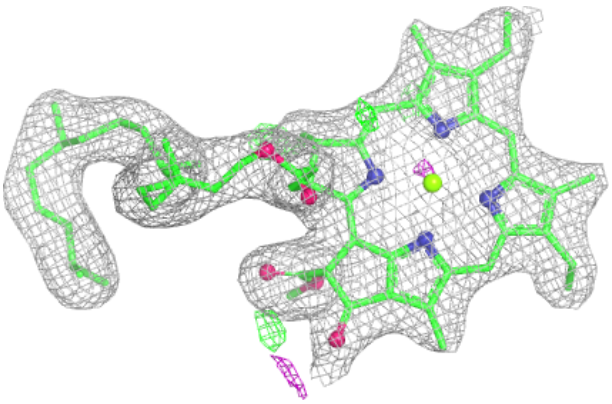


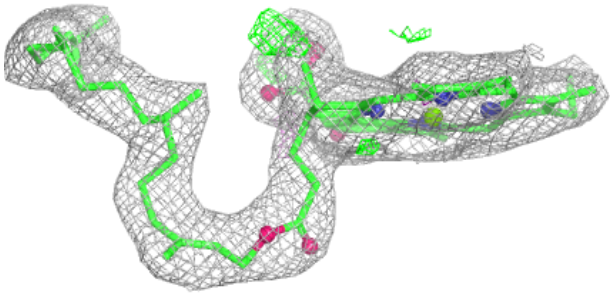


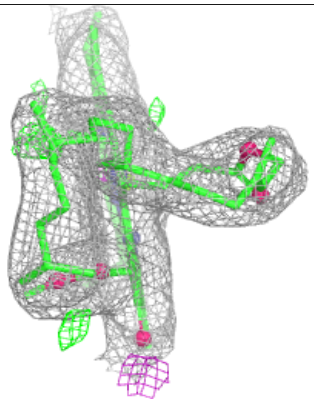


Electron density around CLA B 613:

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

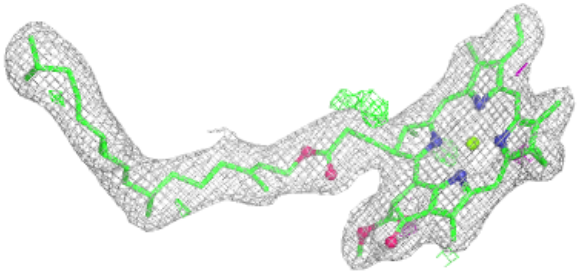


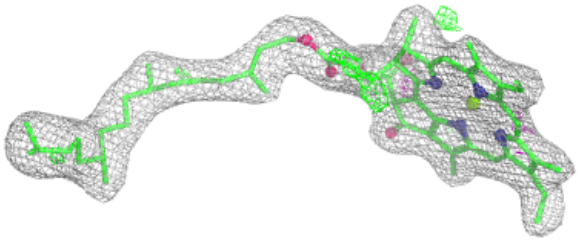


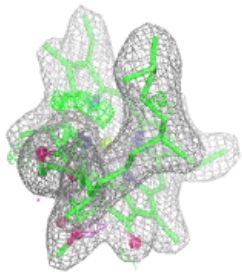


Electron density around CLA A 405:

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

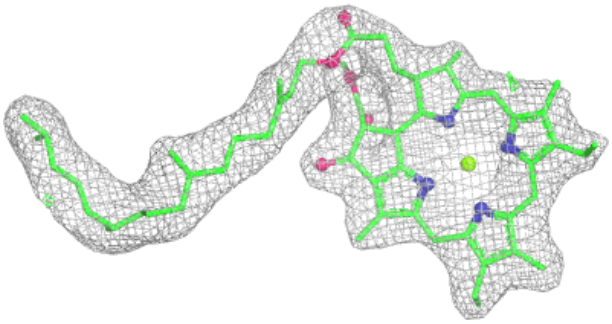


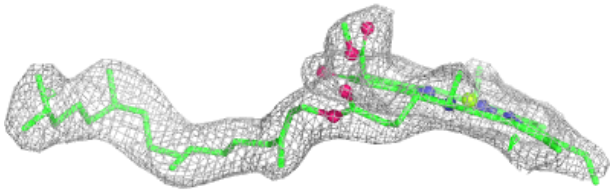




Electron density around CLA B 603:

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

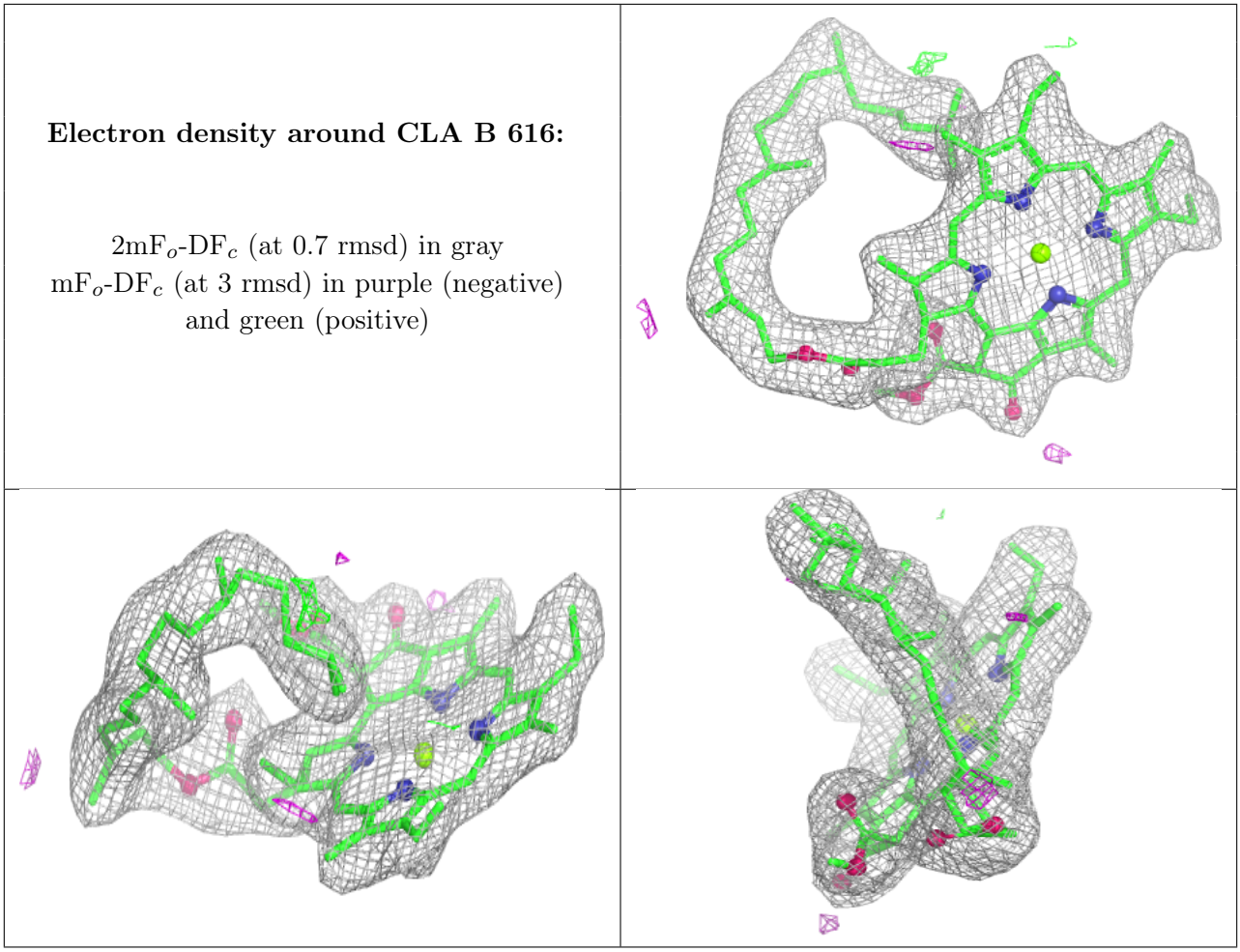






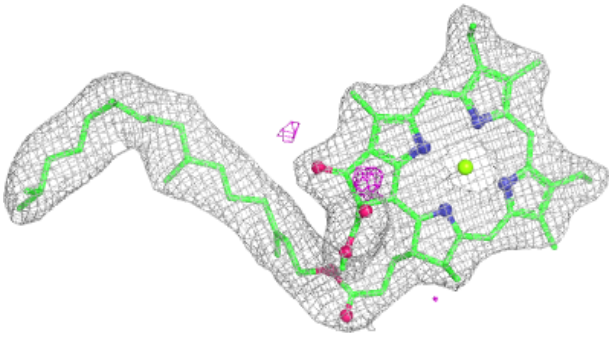
Electron density around CLA B 616:

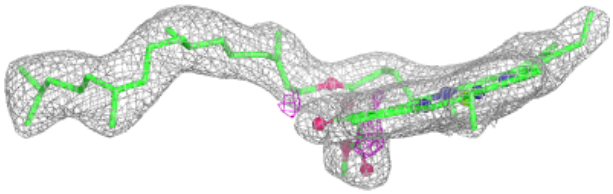
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

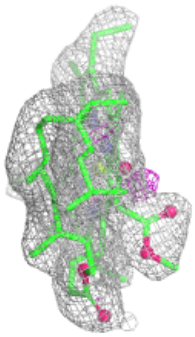


Electron density around CLA b 611:

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

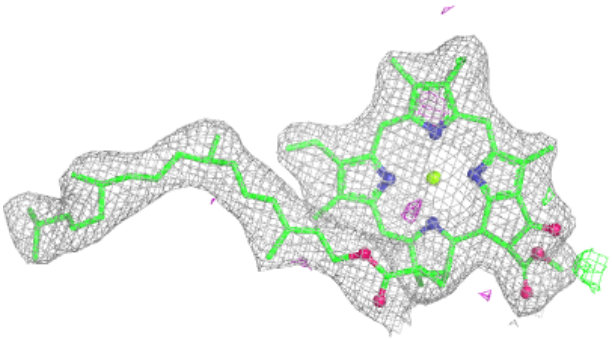


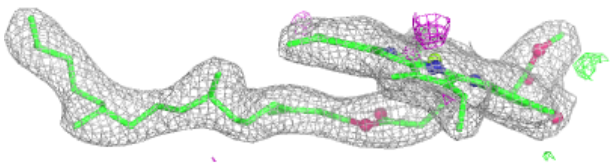


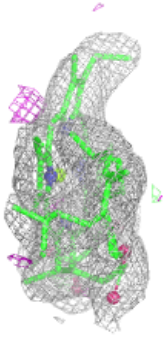


Electron density around CLA b 612:

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

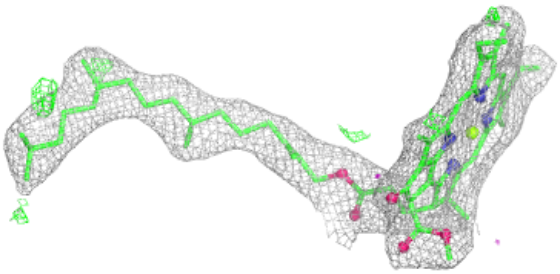


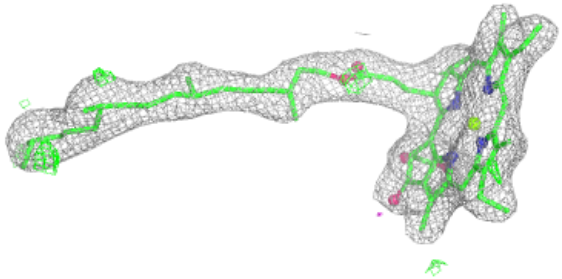


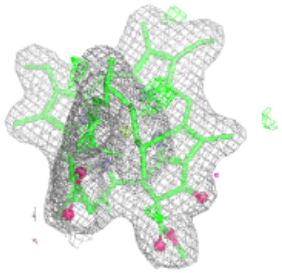


Electron density around CLA b 613:

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

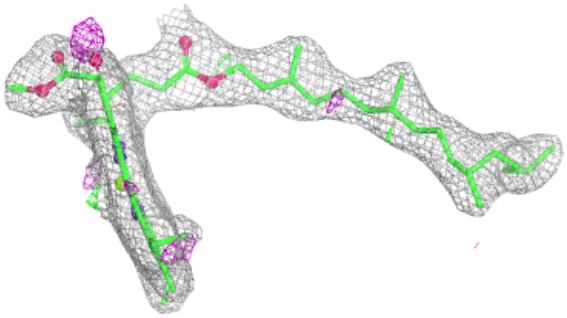


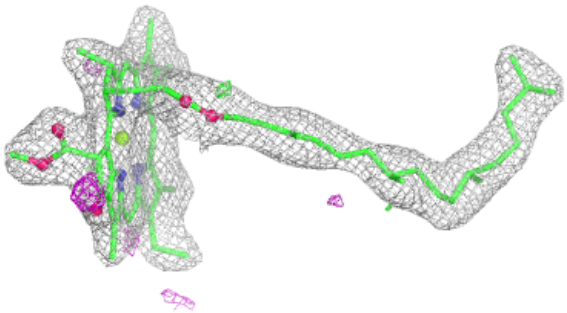


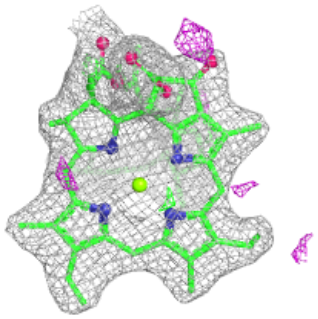


Electron density around CLA b 614:

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

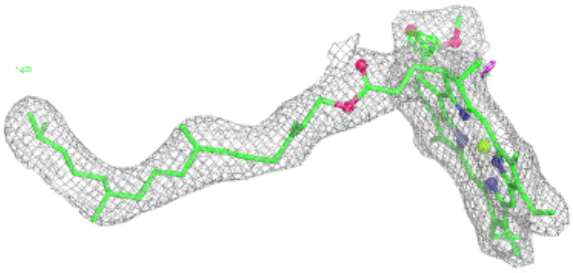


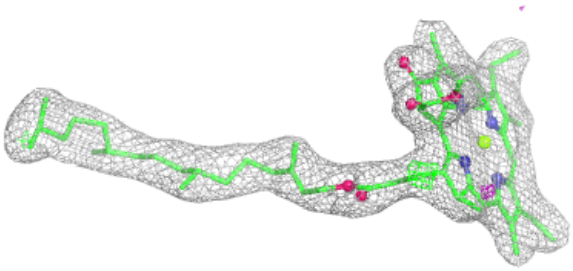


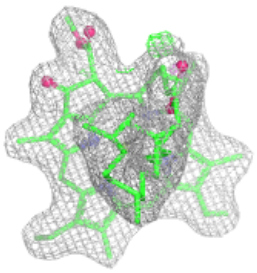


Electron density around CLA B 605:

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

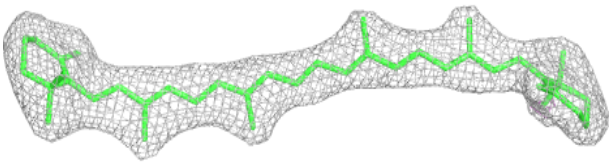


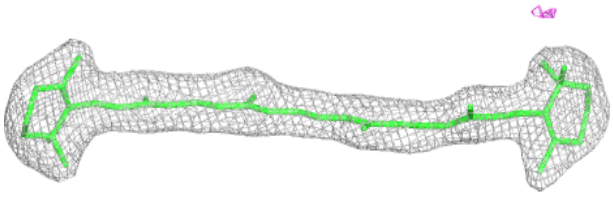


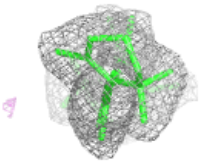


Electron density around BCR a 413:

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

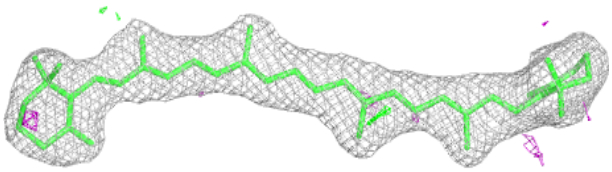


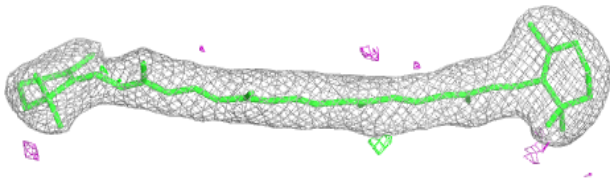


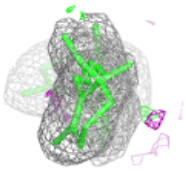


Electron density around BCR b 626:

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

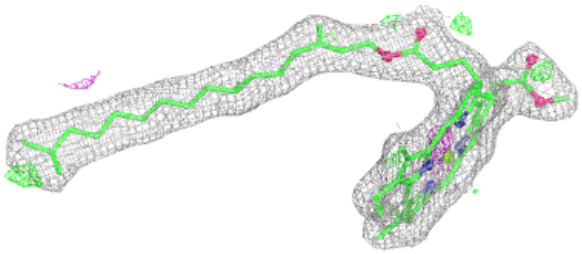


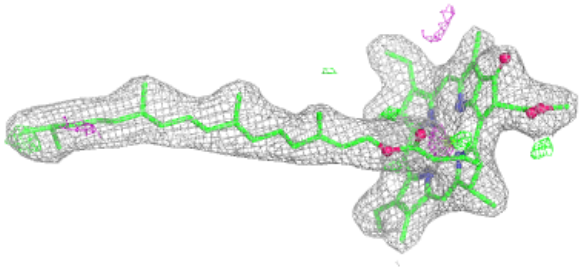


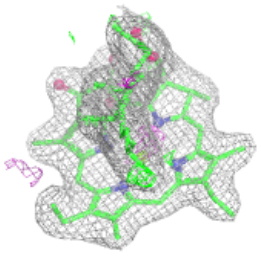


Electron density around CLA b 616:

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

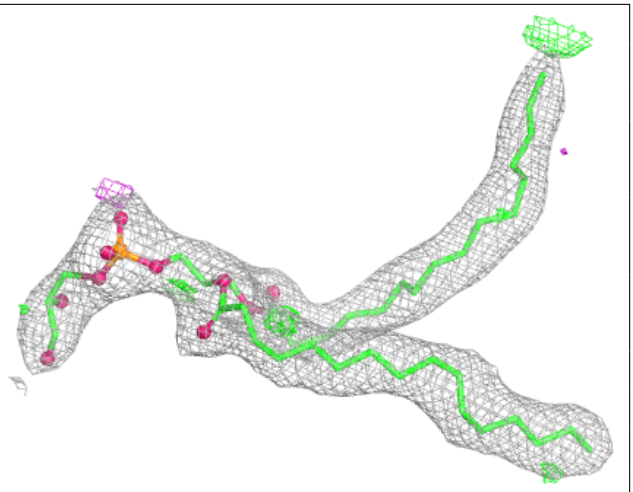


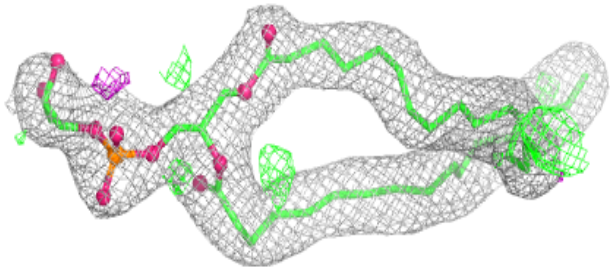


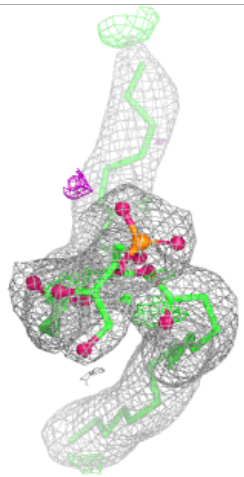


Electron density around LHG D 410:

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

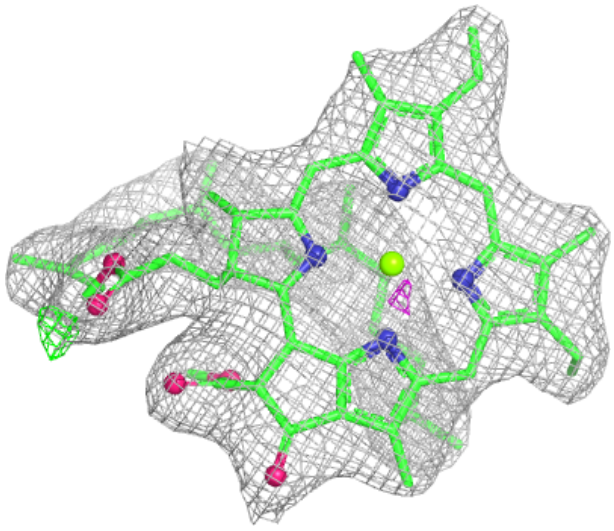


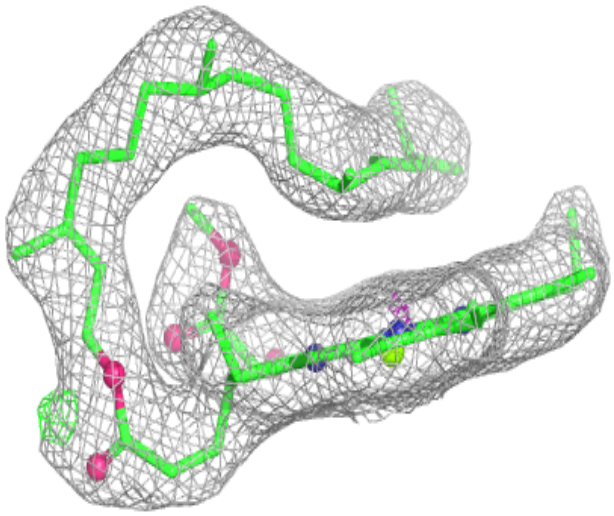


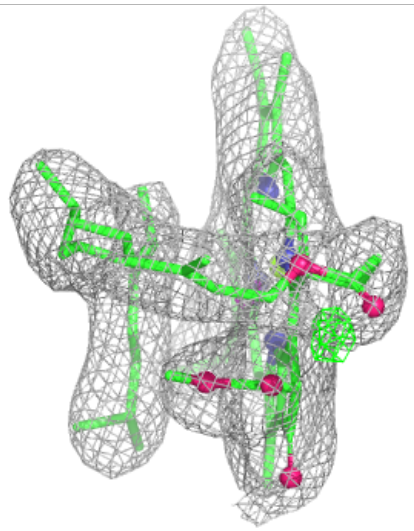


Electron density around CLA c 514:

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

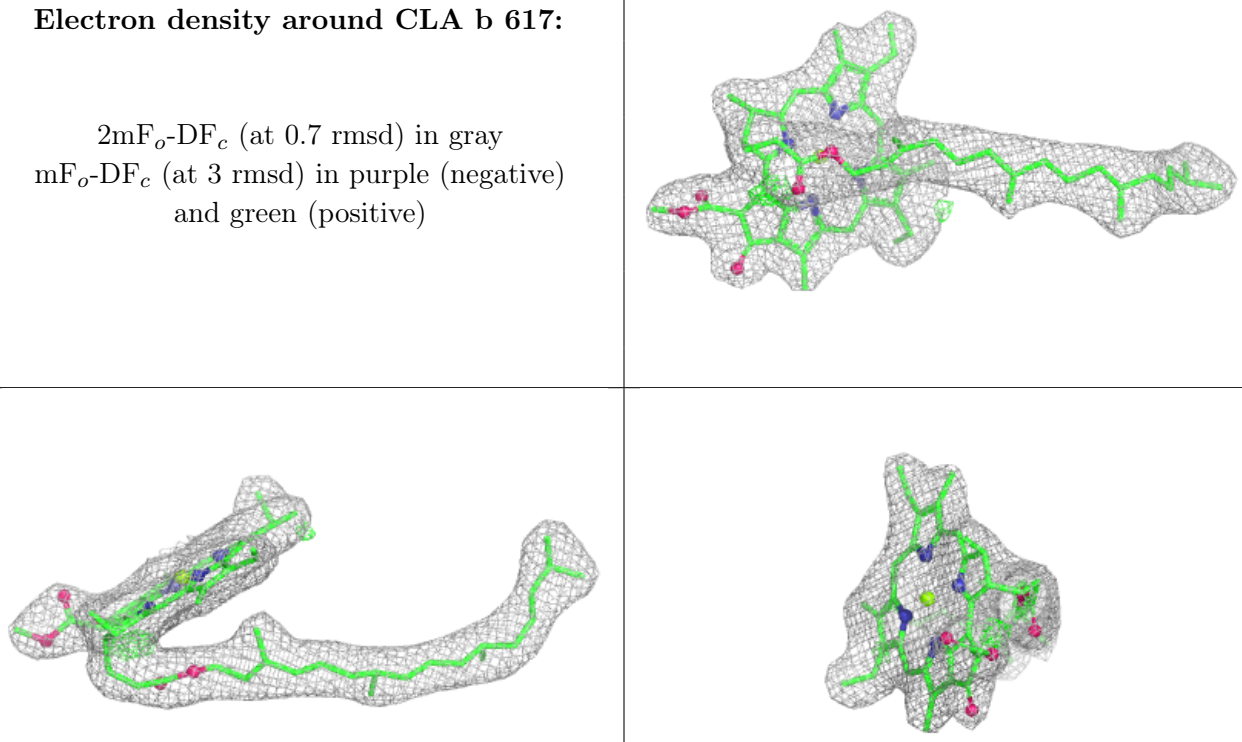






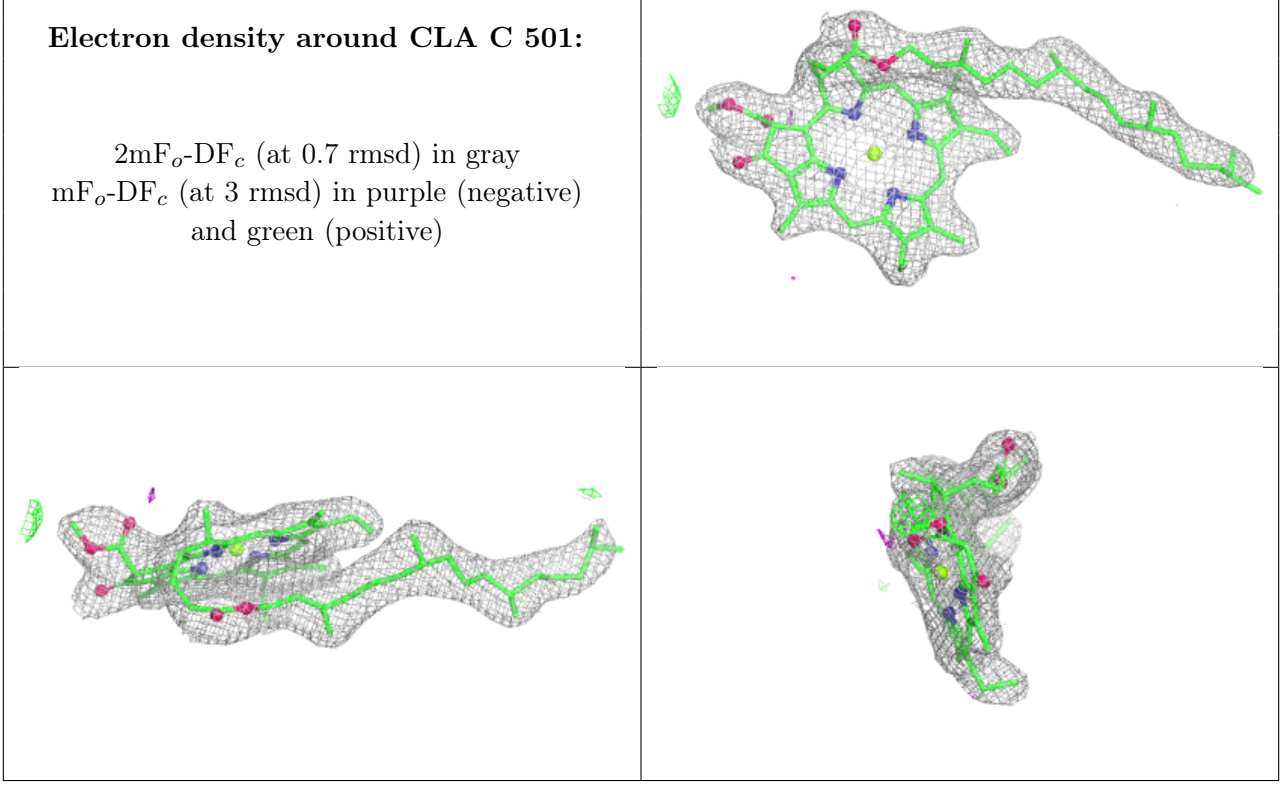
Electron density around CLA b 617:

$2mF_o$-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 C 501:

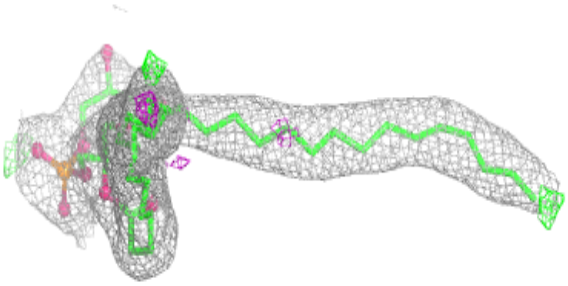
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

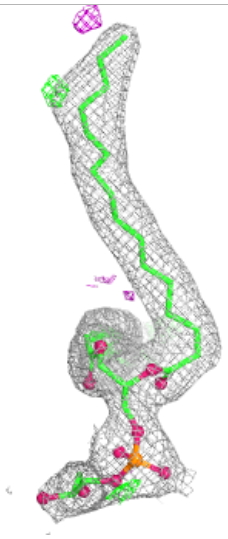


Electron density around LHG b 634:

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

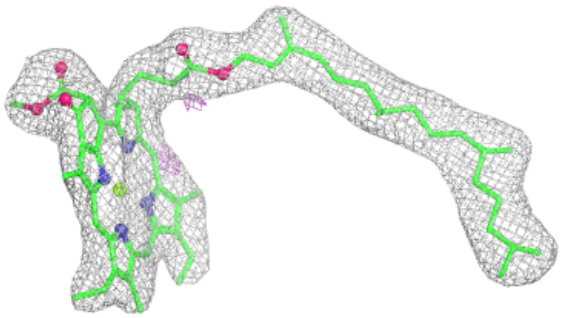


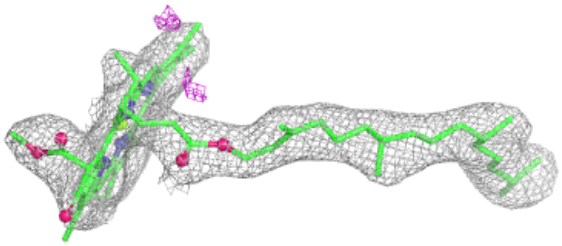


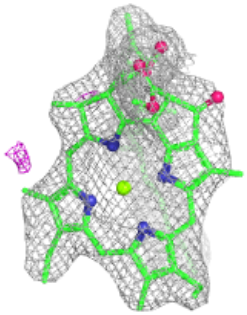


Electron density around CLA B 610:

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

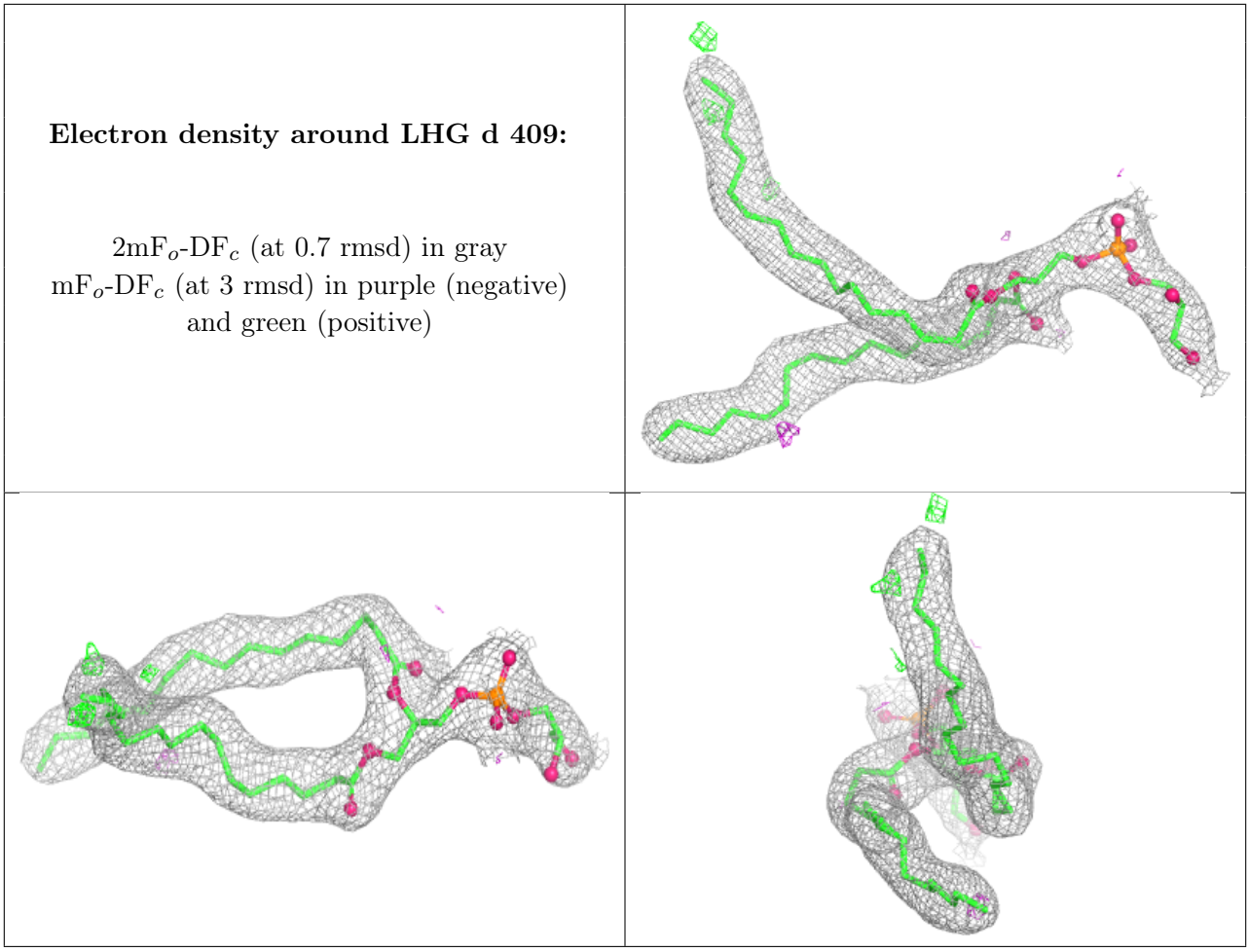






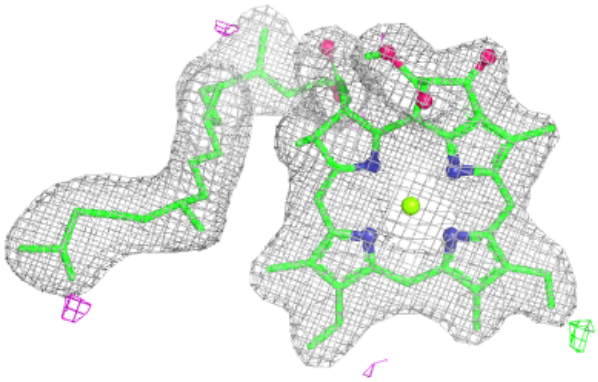
Electron density around LHG d 409:

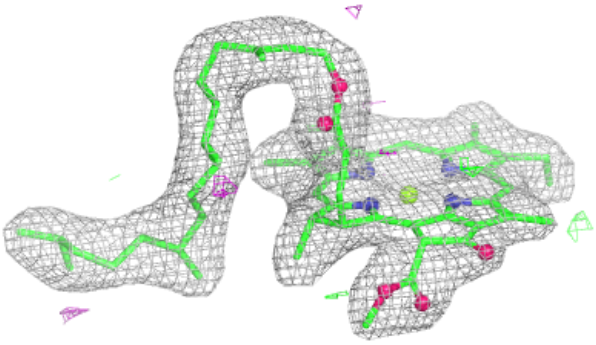
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA d 403:

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

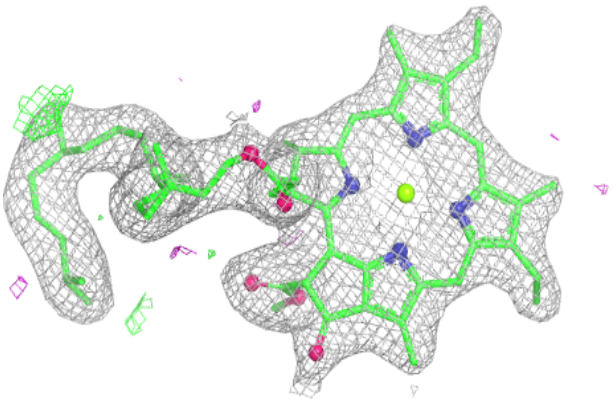


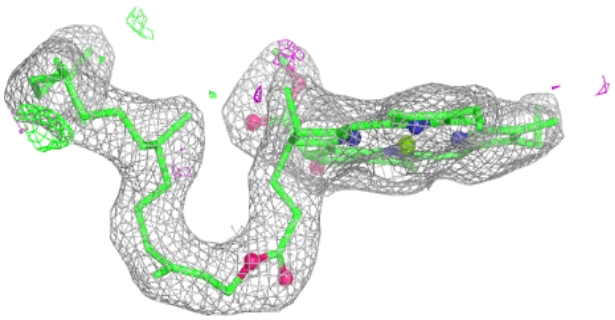


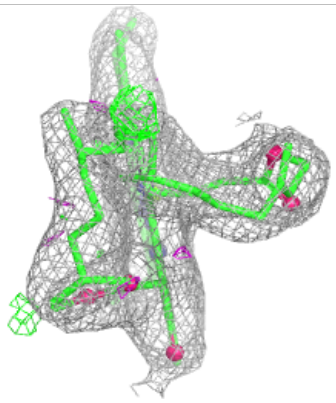


Electron density around CLA b 621:

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

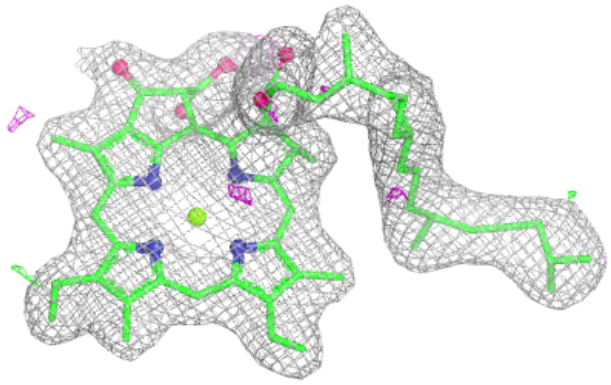


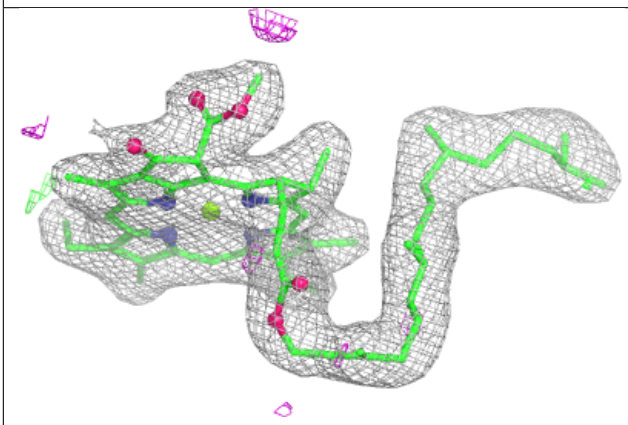


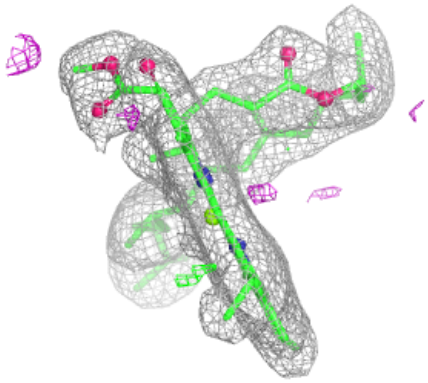


Electron density around CLA A 406:

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

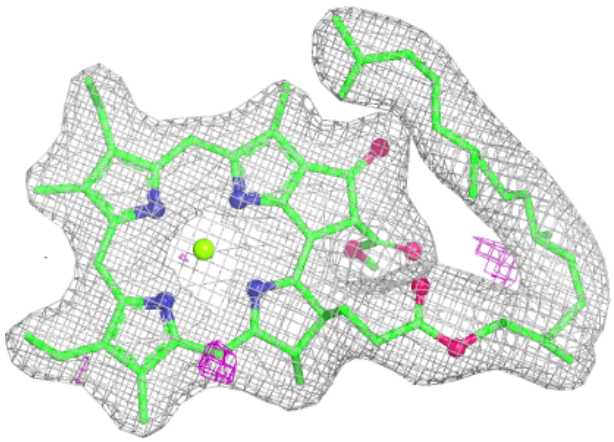


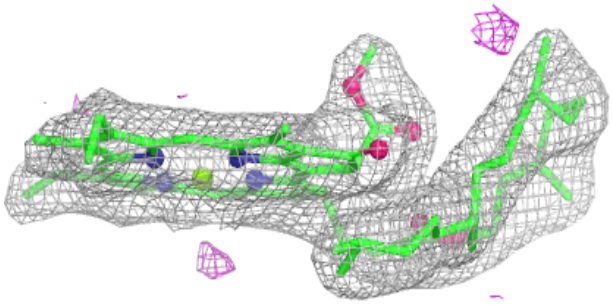


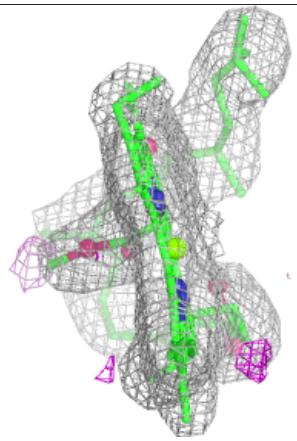


Electron density around CLA b 619:

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



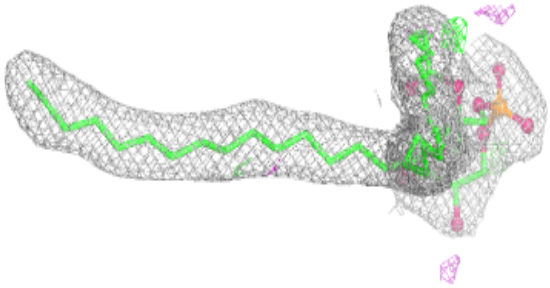


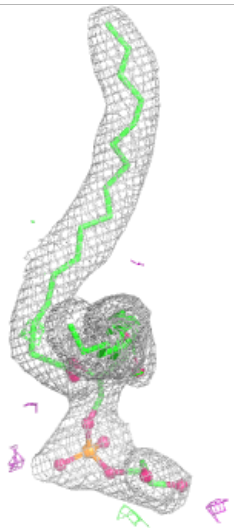


Electron density around LHG L 101:

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

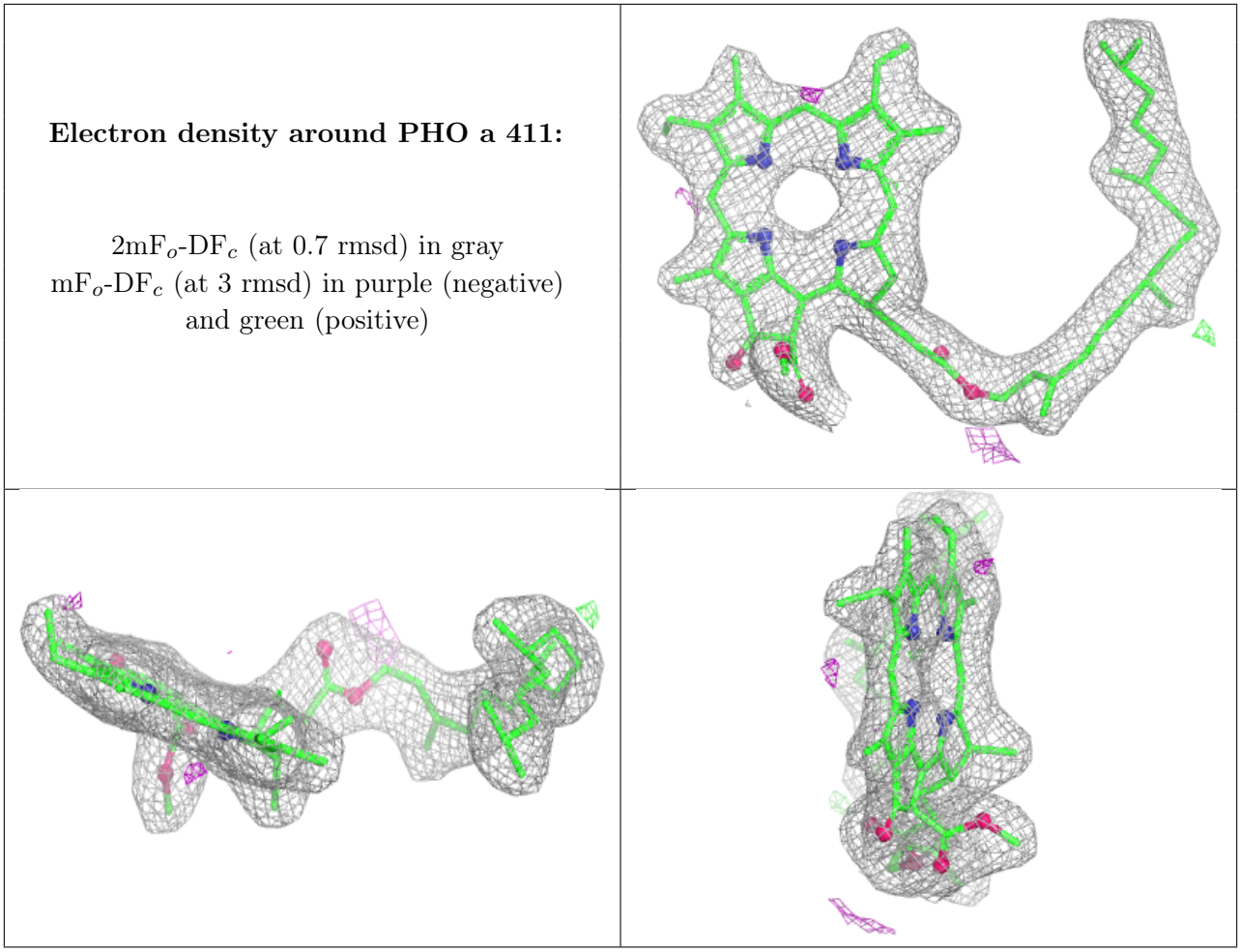






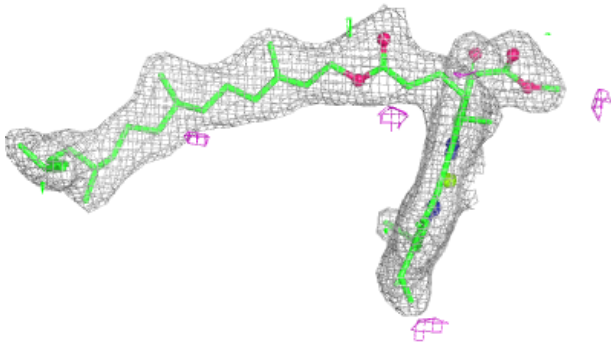
Electron density around PHO a 411:

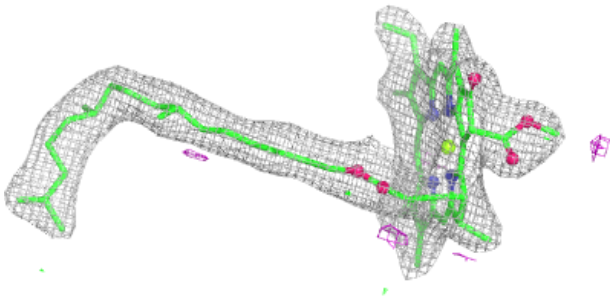
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

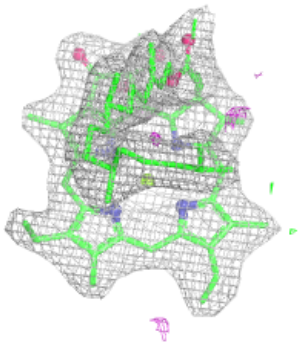


Electron density around CLA B 606:

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

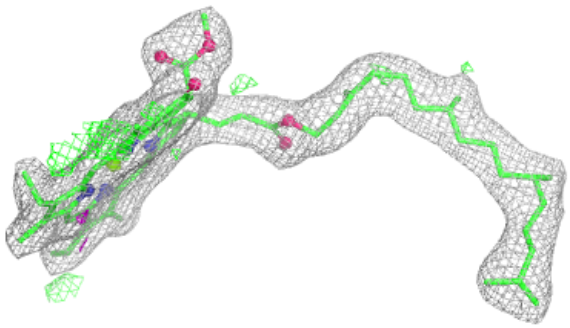


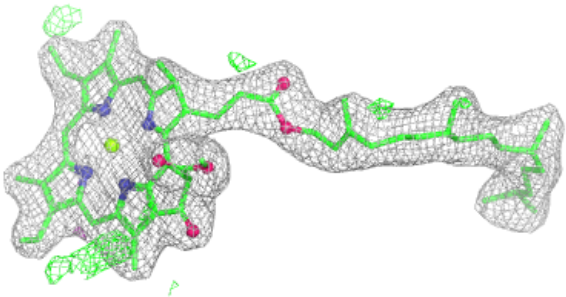


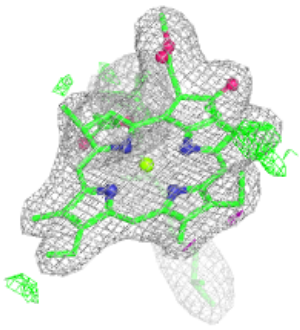


Electron density around CLA D 404:

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

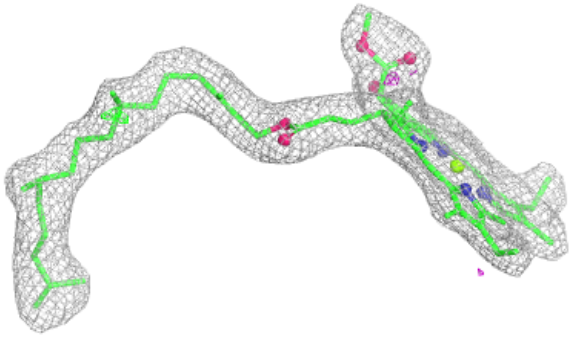


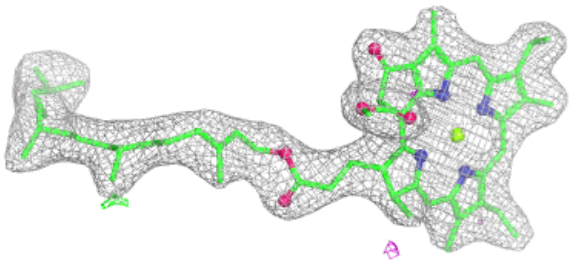


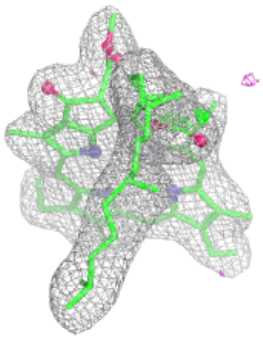


Electron density around CLA d 404:

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

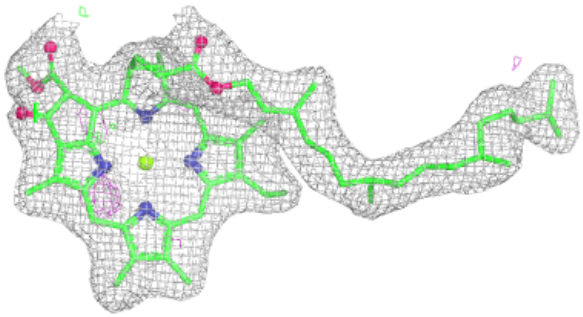


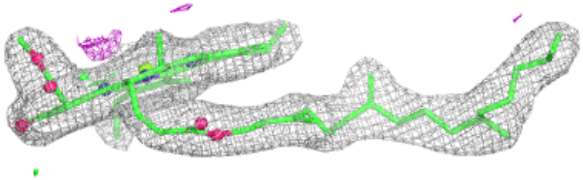


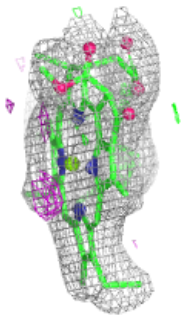


Electron density around CLA B 604:

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

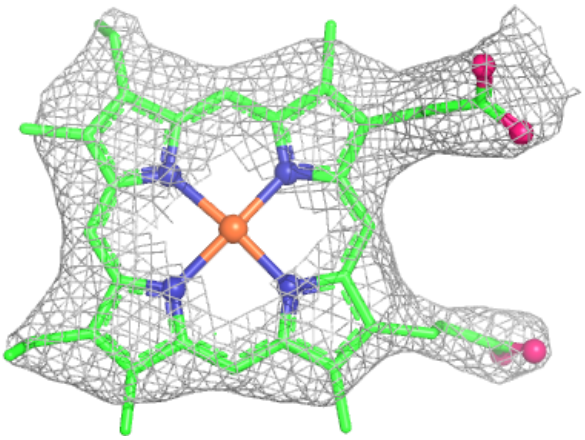


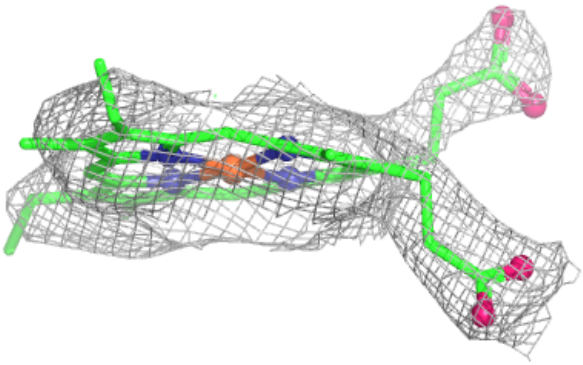


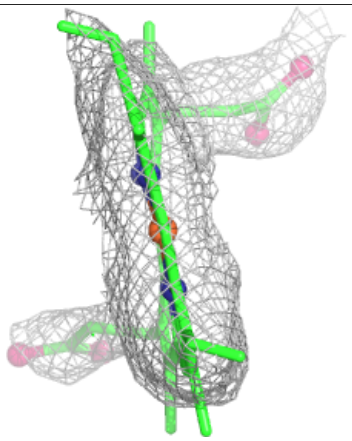


Electron density around HEM E 103:

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

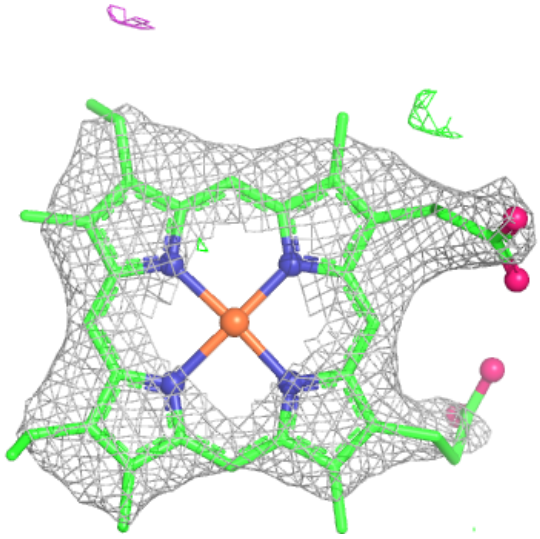


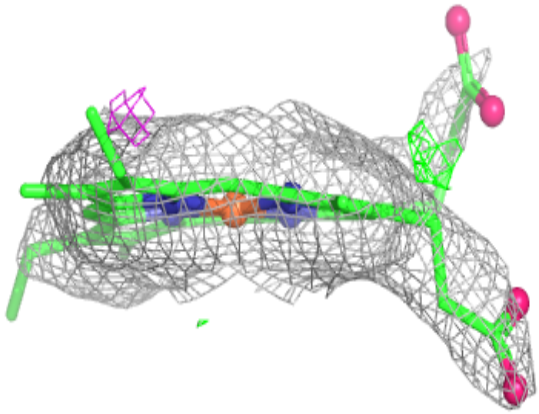


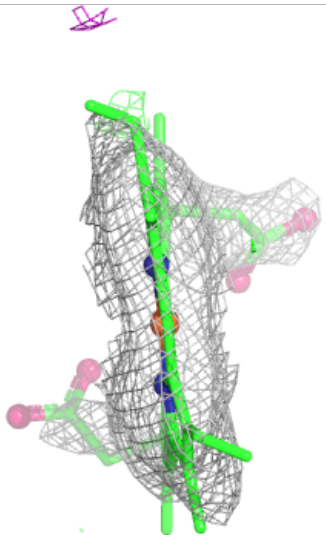


Electron density around HEM f 101:

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

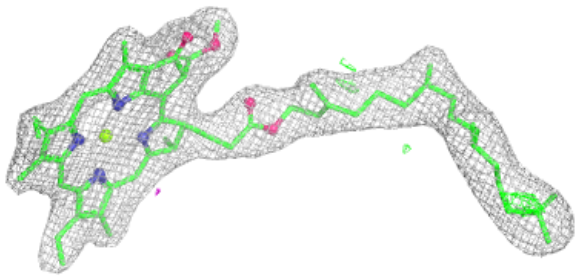


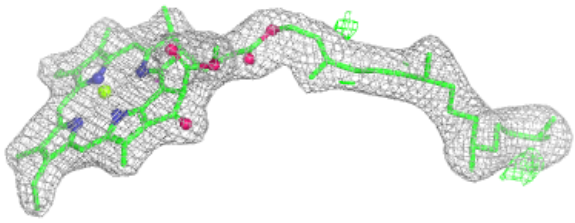


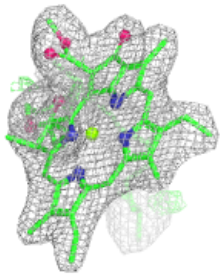


Electron density around CLA a 409:

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

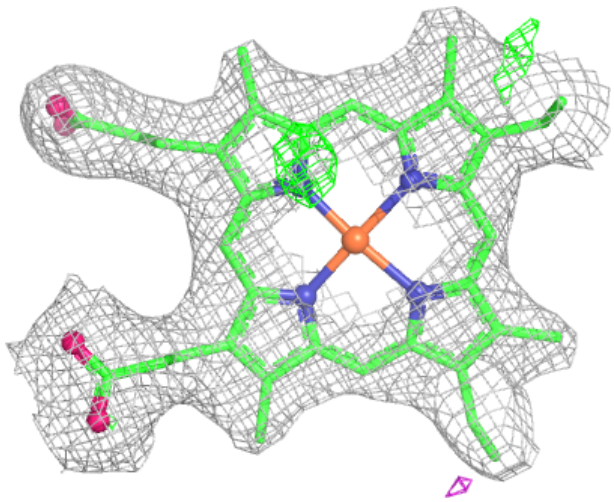


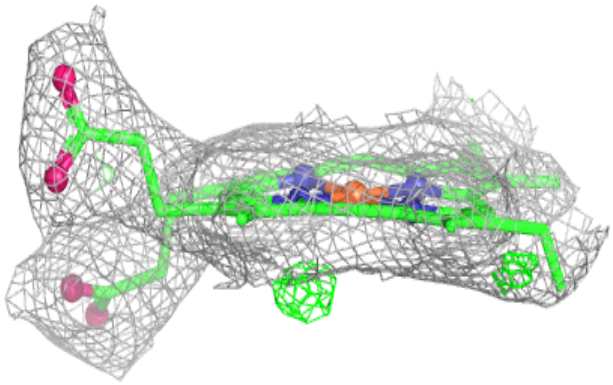




Electron density around HEC V 205:

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

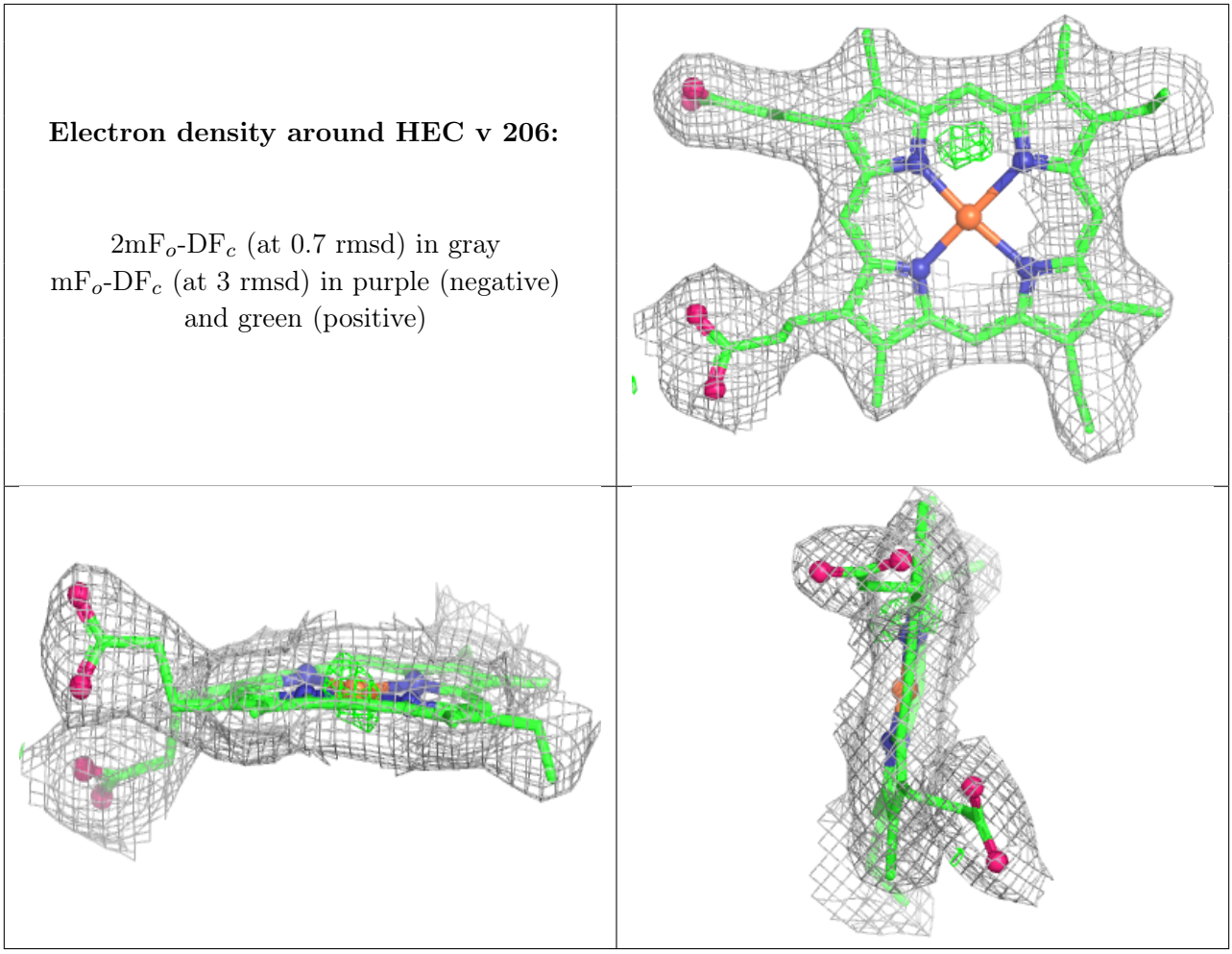






Electron density around HEC v 206:

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



6.5 Other polymers

There are no such residues in this entry.