Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:58 AM EDT

PDB ID	:	5V2C / pdb_00005v2c
Title	:	RE-REFINEMENT OF CRYSTAL STRUCTURE OF PHOTOSYSTEM II COMPLEX
Authors	:	Wang, J.; Wiwczar, J.M.; Brudvig, G.W.
Deposited on	:	2017-03-03
Resolution	:	1.90 Å(reported)

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

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

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

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

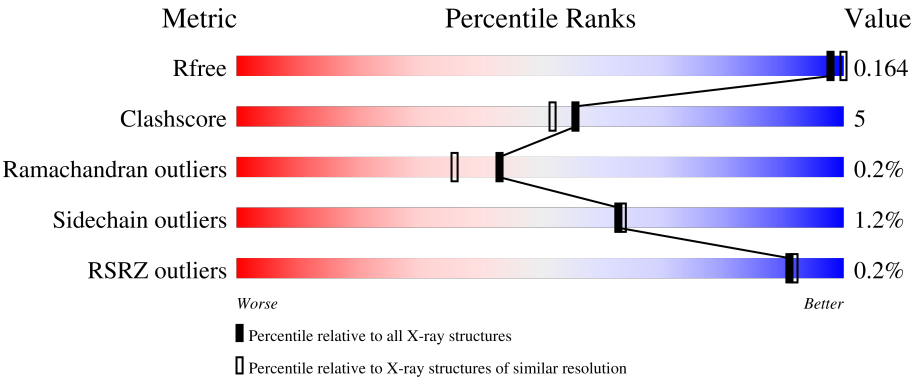
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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.



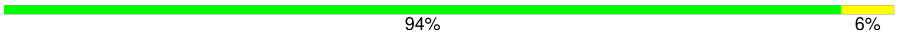
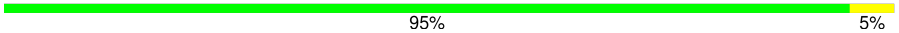
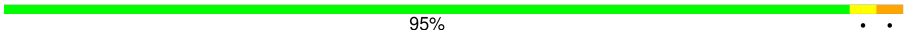
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	344	91% 6% ·
1	a	344	90% 7% ·
2	B	506	93% 7%
2	b	506	92% 7%
3	C	458	91% 7% ·

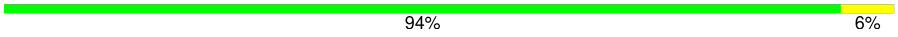
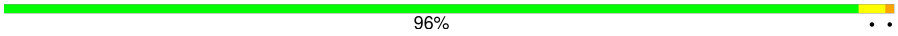
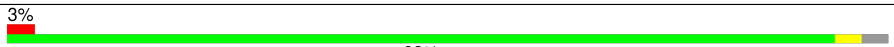
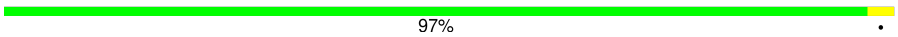
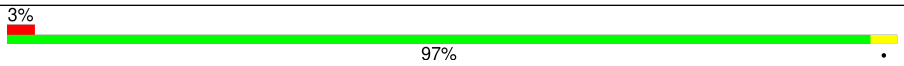
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Mol	Chain	Length	Quality of chain
3	c	458	
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	245	
13	o	245	
14	T	32	
14	t	32	
15	U	104	
15	u	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	41	
18	x	41	
19	Z	62	
19	z	62	

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
22	CL	v	201	-	-	X	-
23	BCT	A	605	-	X	-	-
23	BCT	a	406	-	X	-	-
30	GOL	C	523	-	-	X	-
30	GOL	C	528	-	X	X	-
30	GOL	c	529	-	-	X	-
43	HEC	V	203	X	-	-	-
43	HEC	v	202	X	-	-	-

2 Entry composition (i)

There are 46 unique types of molecules in this entry. The entry contains 57584 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	4	0
			2639	1730	434	460	15			
1	a	334	Total	C	N	O	S	0	4	0
			2639	1730	434	460	15			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	504	Total	C	N	O	S	0	11	0
			4032	2646	671	702	13			
2	b	506	Total	C	N	O	S	0	10	0
			4037	2649	670	705	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	506	SER	-	expression tag	UNP D0VWR1
B	507	ASP	-	expression tag	UNP D0VWR1
b	506	SER	-	expression tag	UNP D0VWR1
b	507	ASP	-	expression tag	UNP D0VWR1

- 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	5	0
			3508	2297	585	613	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	c	458	Total	C	N	O	S	0	4	0
			3553	2324	592	624	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	16	GLU	-	expression tag	UNP D0VWR7
C	17	ALA	-	expression tag	UNP D0VWR7
C	18	ALA	-	expression tag	UNP D0VWR7
C	19	ASN	-	expression tag	UNP D0VWR7
C	20	SER	-	expression tag	UNP D0VWR7
C	21	ILE	-	expression tag	UNP D0VWR7
C	22	PHE	-	expression tag	UNP D0VWR7
c	16	GLU	-	expression tag	UNP D0VWR7
c	17	ALA	-	expression tag	UNP D0VWR7
c	18	ALA	-	expression tag	UNP D0VWR7
c	19	ASN	-	expression tag	UNP D0VWR7
c	20	SER	-	expression tag	UNP D0VWR7
c	21	ILE	-	expression tag	UNP D0VWR7
c	22	PHE	-	expression tag	UNP D0VWR7

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	1	0
			2731	1810	445	464	12			
4	d	342	Total	C	N	O	S	0	2	0
			2741	1815	448	466	12			

- 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	3	0
			676	441	110	125			
5	e	81	Total	C	N	O	0	2	0
			668	436	107	125			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	2	0
			525	351	86	86	2			
7	h	65	Total	C	N	O	S	0	1	0
			519	346	85	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	39	Total	C	N	O	S	0	2	0
			294	197	46	50	1			
9	j	39	Total	C	N	O	S	0	0	0
			281	187	43	50	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	2	GLU	MET	conflict	UNP Q7DGD4
j	2	GLU	MET	conflict	UNP Q7DGD4

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

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

There are 4 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	S	0	1	0
			309	207	48	53	1			
11	l	37	Total	C	N	O	S	0	2	0
			315	211	49	54	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	2	0
			286	190	42	53	1			
12	m	35	Total	C	N	O	S	0	2	0
			289	193	42	52	2			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	245	Total	C	N	O	S	0	6	0
			1904	1192	317	391	4			
13	o	245	Total	C	N	O	S	0	5	0
			1902	1189	320	389	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	2	ALA	-	expression tag	UNP D0VWR2
O	3	ALA	-	expression tag	UNP D0VWR2
o	2	ALA	-	expression tag	UNP D0VWR2
o	3	ALA	-	expression tag	UNP D0VWR2

- 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	2	0
			271	190	36	42	3			
14	t	30	Total	C	N	O	S	0	2	0
			271	190	36	42	3			

- 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	2	0
			786	499	130	157			
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
			1077	683	181	209	4			
16	v	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	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	1	0
			219	145	37	34	3			
17	y	29	Total	C	N	O	S	0	1	0
			220	146	37	33	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	40	Total	C	N	O	S	0	1	0
			300	201	47	51	1			
18	x	40	Total	C	N	O	S	0	0	0
			295	196	47	51	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	initiating methionine	UNP D0VWR4

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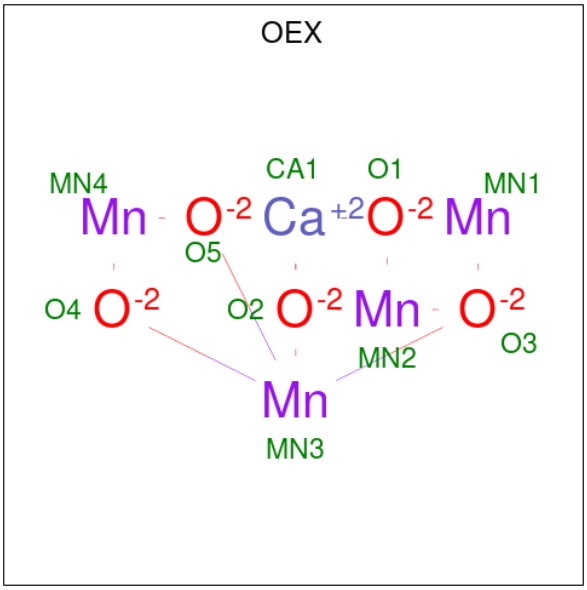
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Chain	Residue	Modelled	Actual	Comment	Reference
x	1	MET	-	initiating methionine	UNP D0VWR4

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



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

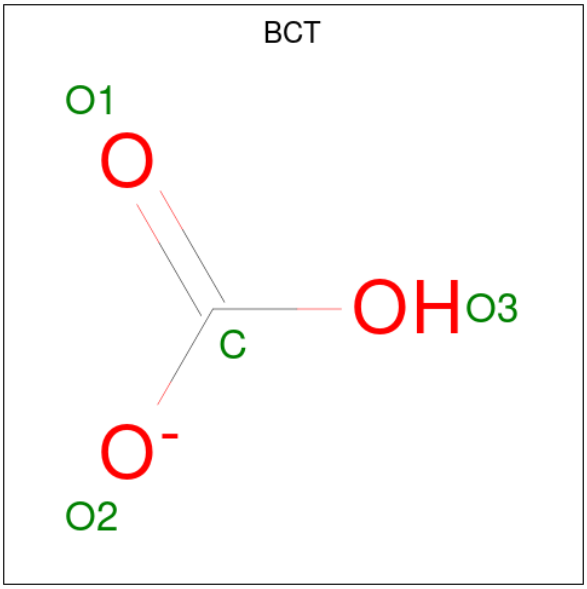
- Molecule 21 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

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

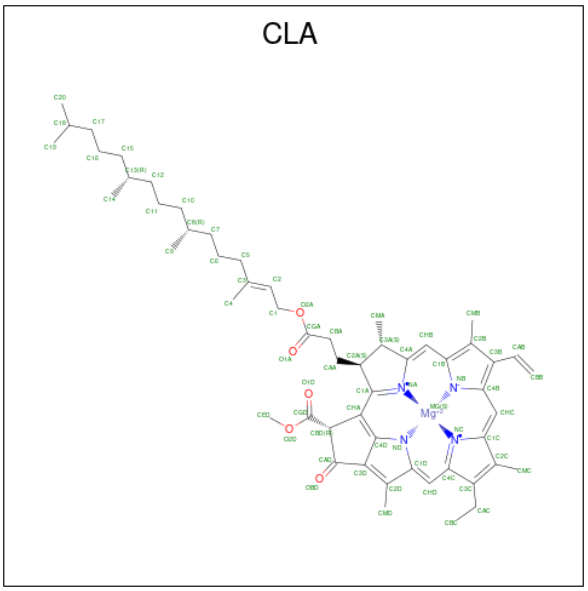
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	A	2	Total Cl 2 2	0	0
22	V	1	Total Cl 1 1	0	0
22	a	2	Total Cl 2 2	0	0
22	v	1	Total Cl 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	1	Total C O 4 1 3	0	0
23	a	1	Total C O 4 1 3	0	0
23	m	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
			60	50	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
			55	45	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
			55	45	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
			60	50	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
			60	50	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
			60	50	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		

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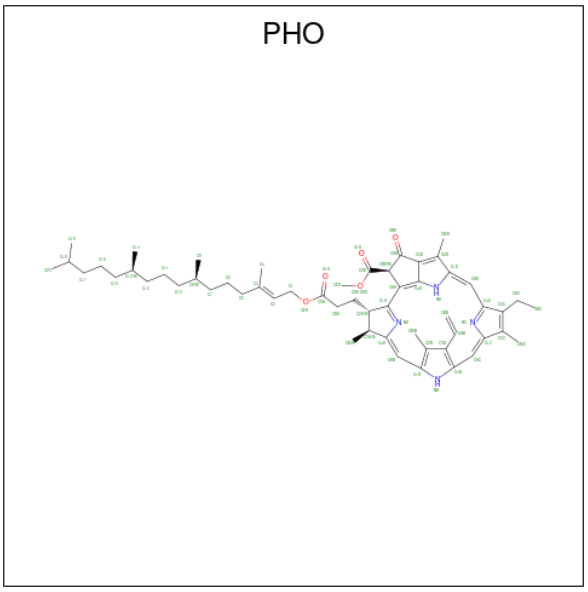
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	a	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	b	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
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
			55	45	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
			60	50	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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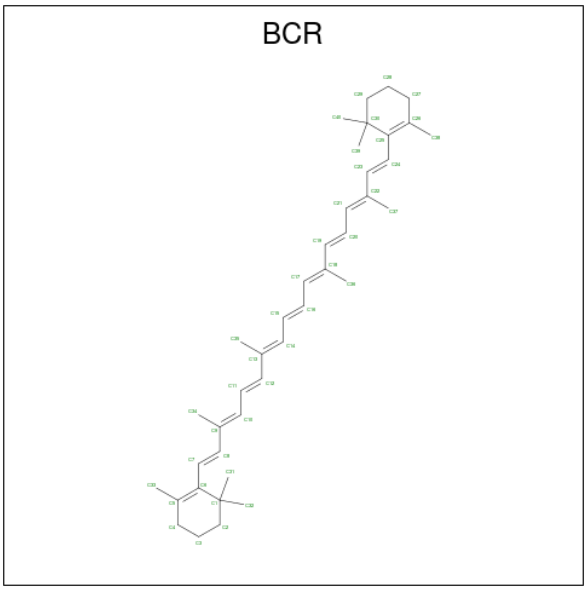
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
24	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
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: $C_{55}H_{74}N_4O_5$).



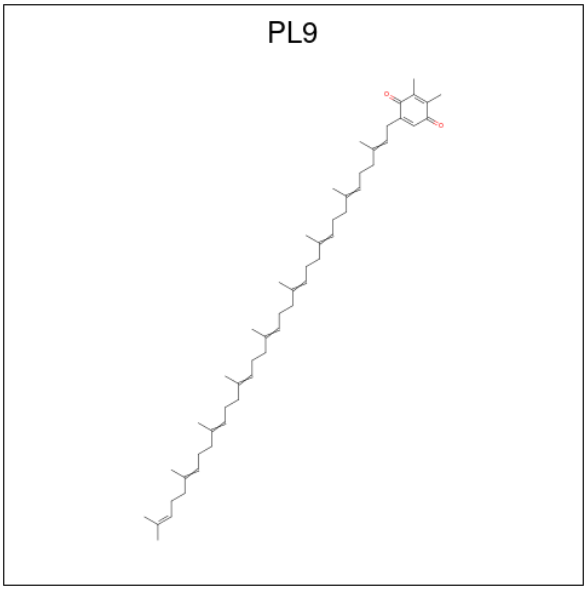
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
25	A	1	Total	C	N	O	0	0
			64	55	4	5		
25	D	1	Total	C	N	O	0	0
			64	55	4	5		
25	a	1	Total	C	N	O	0	0
			64	55	4	5		
25	d	1	Total	C	N	O	0	0
			64	55	4	5		

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



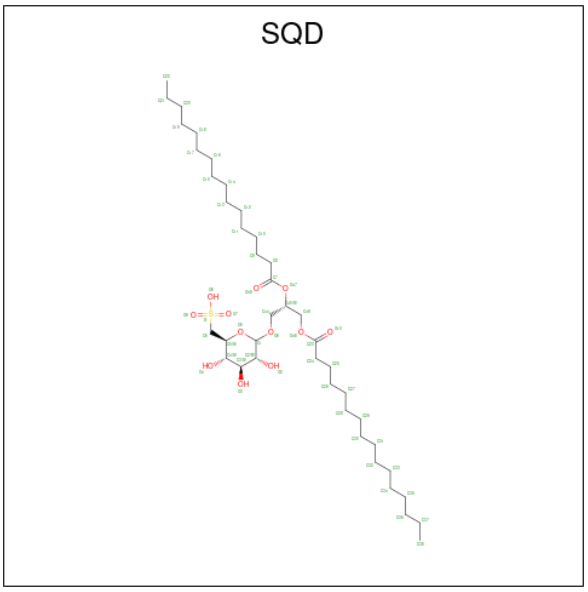
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	B	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	C	1	Total C 40 40	0	0
26	D	1	Total C 40 40	0	0
26	H	1	Total C 40 40	0	0
26	K	1	Total C 40 40	0	0
26	T	1	Total C 40 40	0	0
26	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	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

- Molecule 27 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: $C_{53}H_{80}O_2$).



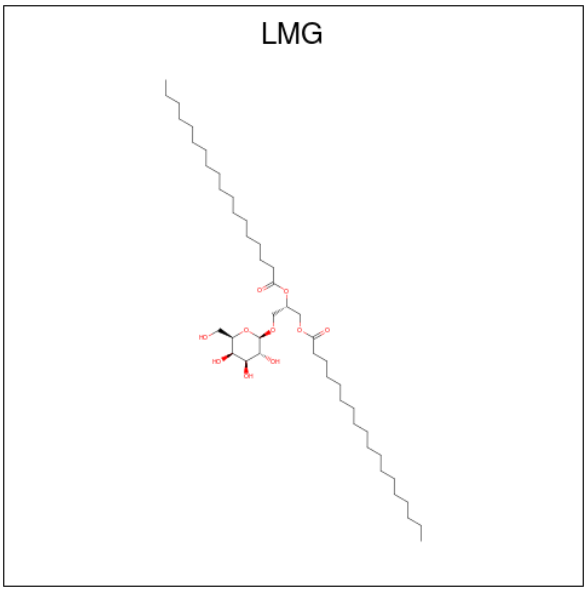
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	1	Total C O 55 53 2	0	0
27	D	1	Total C O 55 53 2	0	0
27	a	1	Total C O 55 53 2	0	0
27	d	1	Total C O 55 53 2	0	0

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



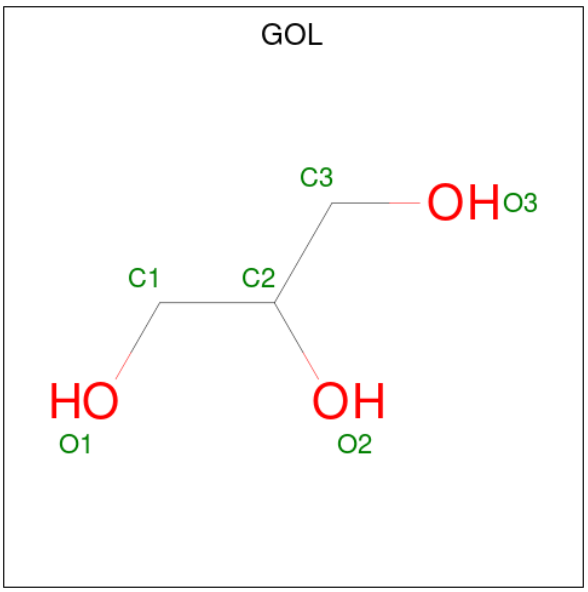
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	A	1	Total	C	O	S	0	0
			54	41	12	1		
28	F	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	a	1	Total	C	O	S	0	0
			54	41	12	1		
28	b	1	Total	C	O	S	0	0
			54	41	12	1		
28	h	1	Total	C	O	S	0	0
			54	41	12	1		
28	l	1	Total	C	O	S	0	0
			54	41	12	1		
28	x	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	1	Total C O 51 41 10	0	0
29	B	1	Total C O 51 41 10	0	0
29	B	1	Total C O 55 45 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 51 41 10	0	0
29	C	1	Total C O 55 45 10	0	0
29	J	1	Total C O 47 37 10	0	0
29	a	1	Total C O 51 41 10	0	0
29	b	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	c	1	Total C O 51 41 10	0	0
29	d	1	Total C O 55 45 10	0	0
29	j	1	Total C O 47 37 10	0	0
29	z	1	Total C O 55 45 10	0	0

- Molecule 30 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			6	3	3		
30	A	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	B	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		
30	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	D	1	Total	C	O	0	0
			6	3	3		
30	D	1	Total	C	O	0	0
			6	3	3		
30	D	1	Total	C	O	0	0
			6	3	3		
30	F	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	O	1	Total	C	O	0	0
			6	3	3		
30	T	1	Total	C	O	0	0
			6	3	3		
30	T	1	Total	C	O	0	0
			6	3	3		
30	U	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	V	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	a	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		

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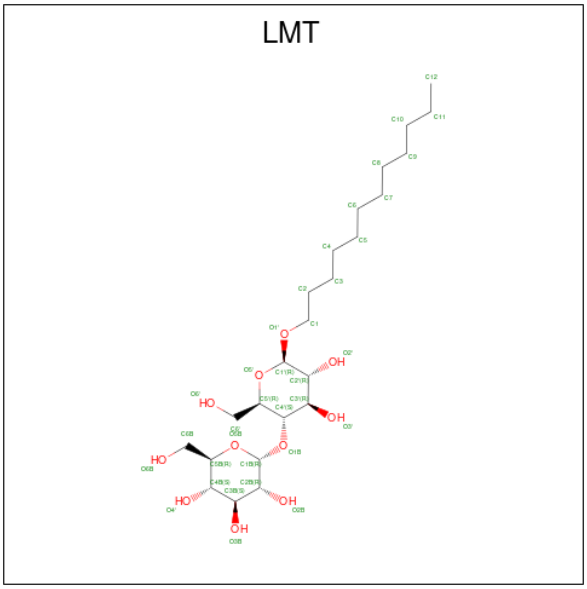
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	b	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	c	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	d	1	Total	C	O	0	0
			6	3	3		
30	e	1	Total	C	O	0	0
			6	3	3		
30	f	1	Total	C	O	0	0
			6	3	3		
30	f	1	Total	C	O	0	0
			6	3	3		
30	m	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	o	1	Total	C	O	0	0
			6	3	3		
30	t	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	u	1	Total	C	O	0	0
			6	3	3		
30	v	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	v	1	Total C O 6 3 3	0	0
30	v	1	Total C O 6 3 3	0	0
30	v	1	Total C O 6 3 3	0	0
30	v	1	Total C O 6 3 3	0	0
30	y	1	Total C O 6 3 3	0	0

- Molecule 31 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



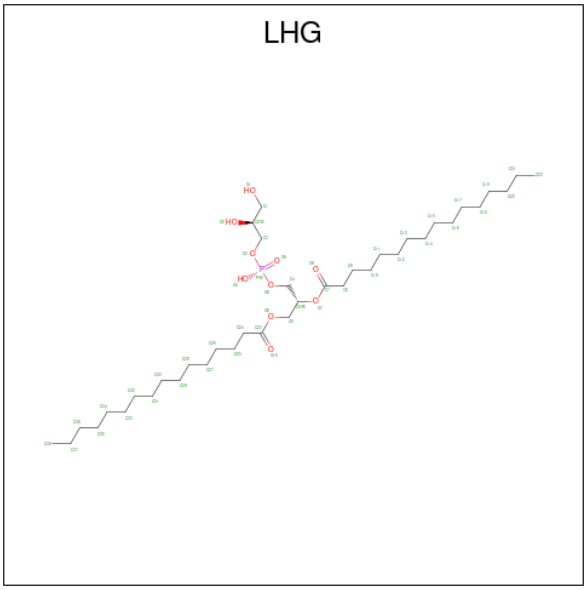
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	A	1	Total C O 35 24 11	0	0
31	B	1	Total C O 35 24 11	0	0
31	C	1	Total C O 35 24 11	0	0
31	F	1	Total C O 35 24 11	0	0
31	I	1	Total C O 35 24 11	0	0
31	J	1	Total C O 35 24 11	0	0

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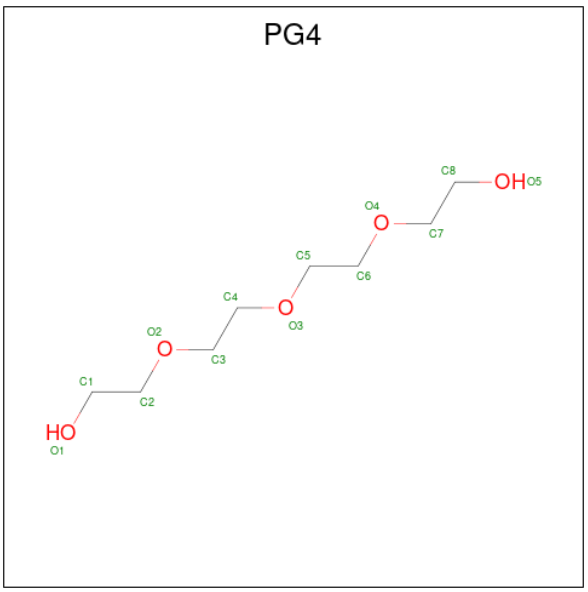
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	M	1	Total C O 35 24 11	0	0
31	M	1	Total C O 35 24 11	0	0
31	Y	1	Total C O 35 24 11	0	0
31	a	1	Total C O 35 24 11	0	0
31	b	1	Total C O 35 24 11	0	0
31	c	1	Total C O 35 24 11	0	0
31	f	1	Total C O 35 24 11	0	0
31	j	1	Total C O 35 24 11	0	0
31	m	1	Total C O 35 24 11	0	0
31	m	1	Total C O 35 24 11	0	0
31	t	1	Total C O 35 24 11	0	0
31	u	1	Total C O 35 24 11	0	0

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	A	1	Total	C	O	P	0	0
			42	31	10	1		
32	B	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	D	1	Total	C	O	P	0	0
			49	38	10	1		
32	E	1	Total	C	O	P	0	0
			42	31	10	1		
32	a	1	Total	C	O	P	0	0
			41	30	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	d	1	Total	C	O	P	0	0
			49	38	10	1		
32	e	1	Total	C	O	P	0	0
			42	31	10	1		
32	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 33 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	B	1	Total C O 13 8 5	0	0
33	C	1	Total C O 13 8 5	0	0
33	C	1	Total C O 13 8 5	0	0
33	C	1	Total C O 13 8 5	0	0
33	C	1	Total C O 13 8 5	0	0
33	C	1	Total C O 13 8 5	0	0
33	D	1	Total C O 13 8 5	0	0
33	E	1	Total C O 13 8 5	0	0
33	E	1	Total C O 13 8 5	0	0
33	H	1	Total C O 13 8 5	0	0
33	H	1	Total C O 13 8 5	0	0
33	H	1	Total C O 13 8 5	0	0
33	H	1	Total C O 13 8 5	0	0
33	I	1	Total C O 13 8 5	0	0

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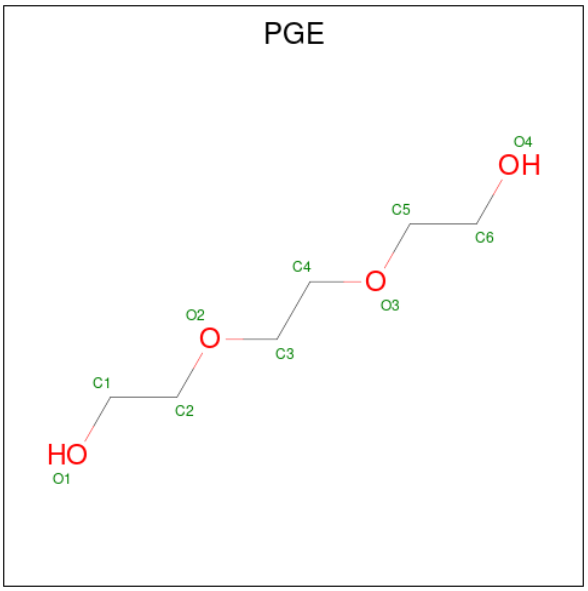
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	I	1	Total C O 13 8 5	0	0
33	I	1	Total C O 13 8 5	0	0
33	J	1	Total C O 13 8 5	0	0
33	J	1	Total C O 13 8 5	0	0
33	K	1	Total C O 13 8 5	0	0
33	U	1	Total C O 13 8 5	0	0
33	V	1	Total C O 13 8 5	0	0
33	V	1	Total C O 13 8 5	0	0
33	V	1	Total C O 13 8 5	0	0
33	V	1	Total C O 13 8 5	0	0
33	V	1	Total C O 13 8 5	0	0
33	X	1	Total C O 13 8 5	0	0
33	X	1	Total C O 13 8 5	0	0
33	X	1	Total C O 13 8 5	0	0
33	a	1	Total C O 13 8 5	0	0
33	a	1	Total C O 13 8 5	0	0
33	b	1	Total C O 13 8 5	0	0
33	b	1	Total C O 13 8 5	0	0
33	b	1	Total C O 13 8 5	0	0
33	b	1	Total C O 13 8 5	0	0
33	c	1	Total C O 13 8 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	c	1	Total C O 13 8 5	0	0
33	c	1	Total C O 13 8 5	0	0
33	c	1	Total C O 13 8 5	0	0
33	d	1	Total C O 13 8 5	0	0
33	e	1	Total C O 13 8 5	0	0
33	e	1	Total C O 13 8 5	0	0
33	h	1	Total C O 13 8 5	0	0
33	i	1	Total C O 13 8 5	0	0
33	i	1	Total C O 13 8 5	0	0
33	i	1	Total C O 13 8 5	0	0
33	i	1	Total C O 13 8 5	0	0
33	j	1	Total C O 13 8 5	0	0
33	l	1	Total C O 13 8 5	0	0
33	x	1	Total C O 13 8 5	0	0

- Molecule 34 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	1	Total C O 7 4 3	0	0
34	A	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	B	1	Total C O 10 6 4	0	0
34	C	1	Total C O 10 6 4	0	0
34	C	1	Total C O 10 6 4	0	0
34	D	1	Total C O 10 6 4	0	0
34	E	1	Total C O 10 6 4	0	0
34	E	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	E	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	H	1	Total	C	O	0	0
			10	6	4		
34	I	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	J	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	O	1	Total	C	O	0	0
			10	6	4		
34	T	1	Total	C	O	0	0
			7	4	3		
34	V	1	Total	C	O	0	0
			10	6	4		
34	V	1	Total	C	O	0	0
			10	6	4		
34	Y	1	Total	C	O	0	0
			10	6	4		
34	a	1	Total	C	O	0	0
			10	6	4		
34	a	1	Total	C	O	0	0
			10	6	4		

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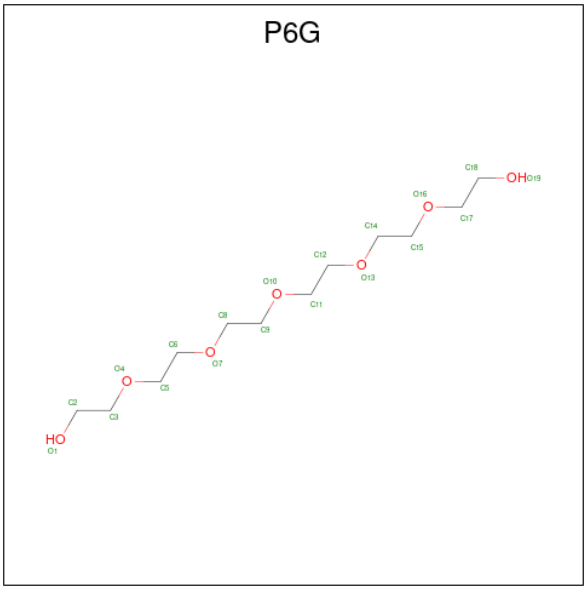
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	b	1	Total C O 10 6 4	0	0
34	c	1	Total C O 10 6 4	0	0
34	c	1	Total C O 10 6 4	0	0
34	c	1	Total C O 10 6 4	0	0
34	c	1	Total C O 10 6 4	0	0
34	c	1	Total C O 10 6 4	0	0
34	f	1	Total C O 10 6 4	0	0
34	h	1	Total C O 10 6 4	0	0
34	h	1	Total C O 10 6 4	0	0
34	h	1	Total C O 10 6 4	0	0
34	h	1	Total C O 10 6 4	0	0
34	i	1	Total C O 10 6 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	i	1	Total C O 10 6 4	0	0
34	j	1	Total C O 10 6 4	0	0
34	o	1	Total C O 10 6 4	0	0
34	o	1	Total C O 10 6 4	0	0
34	o	1	Total C O 10 6 4	0	0
34	o	1	Total C O 10 6 4	0	0
34	t	1	Total C O 10 6 4	0	0
34	t	1	Total C O 7 4 3	0	0
34	x	1	Total C O 10 6 4	0	0

- Molecule 35 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



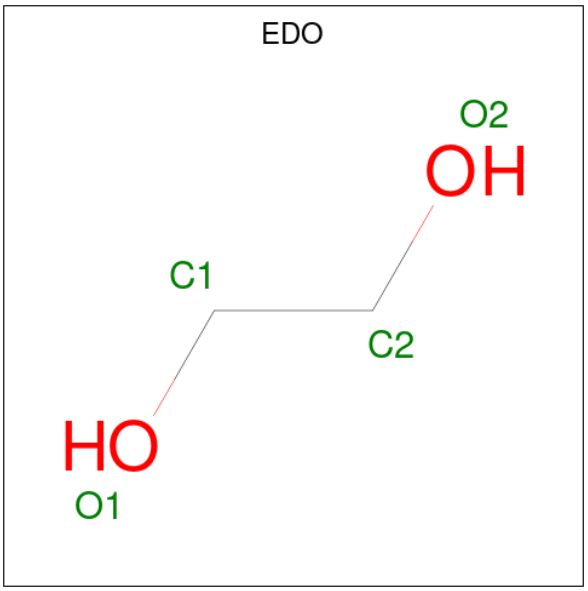
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	1	Total C O 19 12 7	0	0
35	A	1	Total C O 19 12 7	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	B	1	Total C O 19 12 7	0	0
35	B	1	Total C O 19 12 7	0	0
35	C	1	Total C O 19 12 7	0	0
35	D	1	Total C O 19 12 7	0	0
35	D	1	Total C O 19 12 7	0	0
35	D	1	Total C O 19 12 7	0	0
35	E	1	Total C O 19 12 7	0	0
35	I	1	Total C O 19 12 7	0	0
35	T	1	Total C O 19 12 7	0	0
35	b	1	Total C O 19 12 7	0	0
35	b	1	Total C O 19 12 7	0	0
35	c	1	Total C O 19 12 7	0	0
35	d	1	Total C O 19 12 7	0	0
35	d	1	Total C O 19 12 7	0	0
35	j	1	Total C O 19 12 7	0	0

- Molecule 36 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	A	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	B	1	Total	C	O	0	0
			4	2	2		
36	C	1	Total	C	O	0	0
			4	2	2		
36	D	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	E	1	Total	C	O	0	0
			4	2	2		
36	H	1	Total	C	O	0	0
			4	2	2		
36	I	1	Total	C	O	0	0
			4	2	2		
36	J	1	Total	C	O	0	0
			4	2	2		
36	O	1	Total	C	O	0	0
			4	2	2		
36	V	1	Total	C	O	0	0
			4	2	2		

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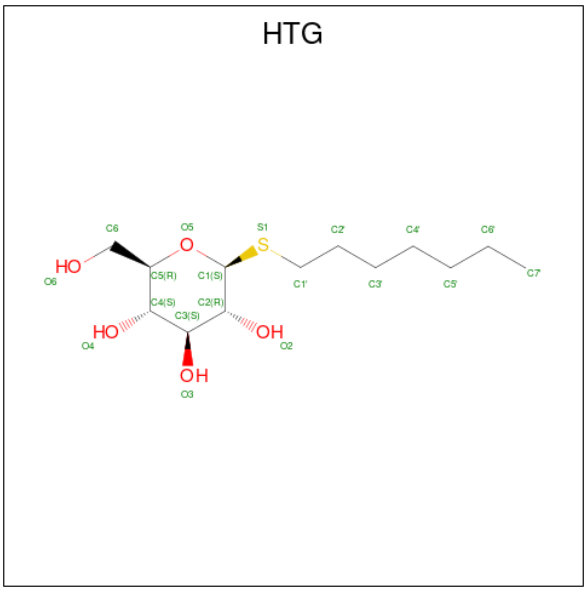
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	X	1	Total C O 4 2 2	0	0
36	a	1	Total C O 4 2 2	0	0
36	c	1	Total C O 4 2 2	0	0
36	d	1	Total C O 4 2 2	0	0
36	e	1	Total C O 4 2 2	0	0
36	i	1	Total C O 4 2 2	0	0
36	o	1	Total C O 4 2 2	0	0
36	o	1	Total C O 4 2 2	0	0

- Molecule 37 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	B	1	Total Ca 1 1	0	0
37	O	1	Total Ca 1 1	0	0
37	b	1	Total Ca 1 1	0	0
37	c	1	Total Ca 1 1	0	0
37	h	1	Total Ca 1 1	0	0
37	o	1	Total Ca 1 1	0	0

- Molecule 38 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: $C_{13}H_{26}O_5S$).



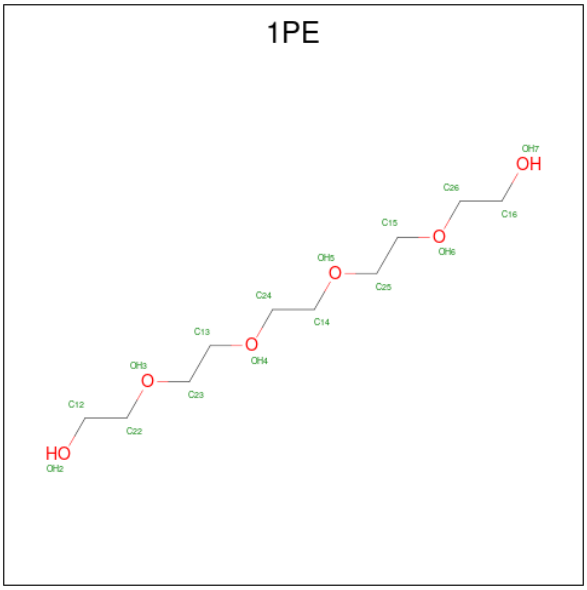
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	B	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	C	1	Total	C	O	S	0	0
			19	13	5	1		
38	H	1	Total	C	O	S	0	0
			19	13	5	1		
38	O	1	Total	C	O	S	0	0
			19	13	5	1		
38	V	1	Total	C	O	S	0	0
			19	13	5	1		
38	a	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	b	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	c	1	Total	C	O	S	0	0
			19	13	5	1		
38	h	1	Total	C	O	S	0	0
			19	13	5	1		
38	o	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 39 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



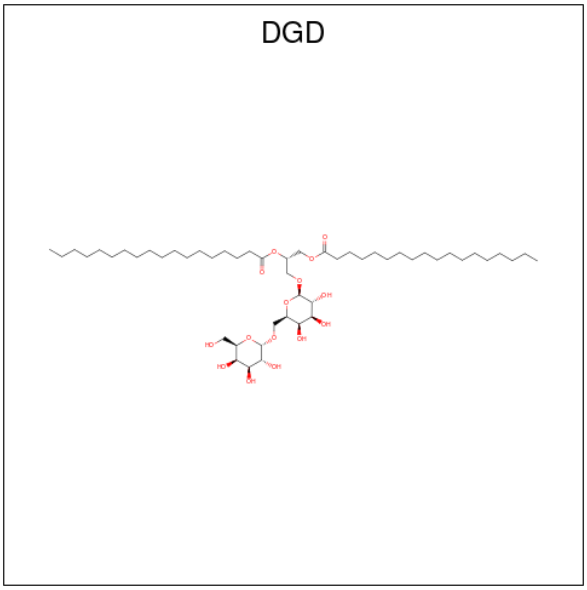
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
39	B	1	Total	C	O	0	0
			16	10	6		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	B	1	Total C O 16 10 6	0	0
39	L	1	Total C O 16 10 6	0	0
39	V	1	Total C O 16 10 6	0	0
39	e	1	Total C O 16 10 6	0	0
39	j	1	Total C O 16 10 6	0	0
39	x	1	Total C O 16 10 6	0	0

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



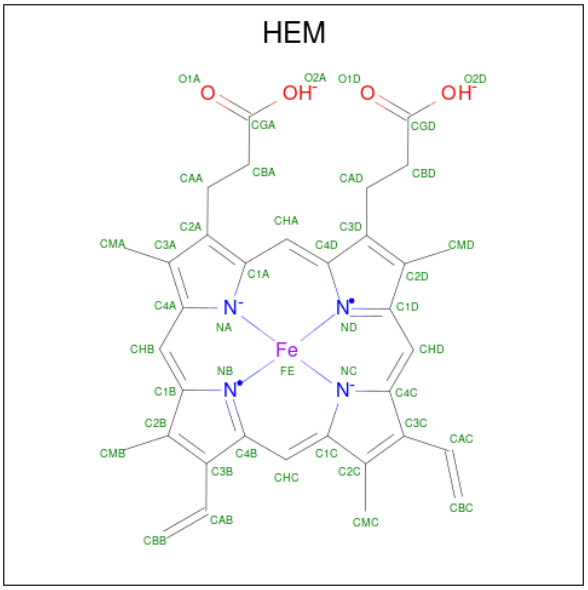
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	C	1	Total C O 62 47 15	0	0
40	C	1	Total C O 56 41 15	0	0
40	C	1	Total C O 62 47 15	0	0
40	D	1	Total C O 66 51 15	0	0
40	H	1	Total C O 62 47 15	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
40	c	1	Total C O 62 47 15	0	0
40	c	1	Total C O 57 42 15	0	0
40	c	1	Total C O 62 47 15	0	0
40	d	1	Total C O 66 51 15	0	0
40	h	1	Total C O 62 47 15	0	0

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 42 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

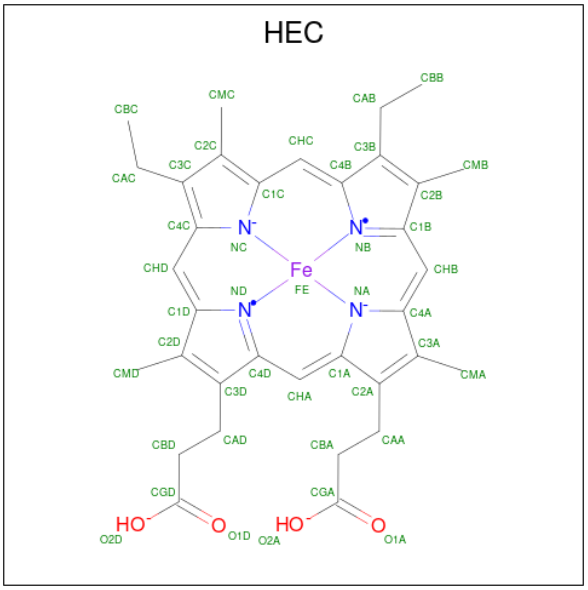
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	F	1	Total Mg 1 1	0	0
42	J	1	Total Mg 1 1	0	0

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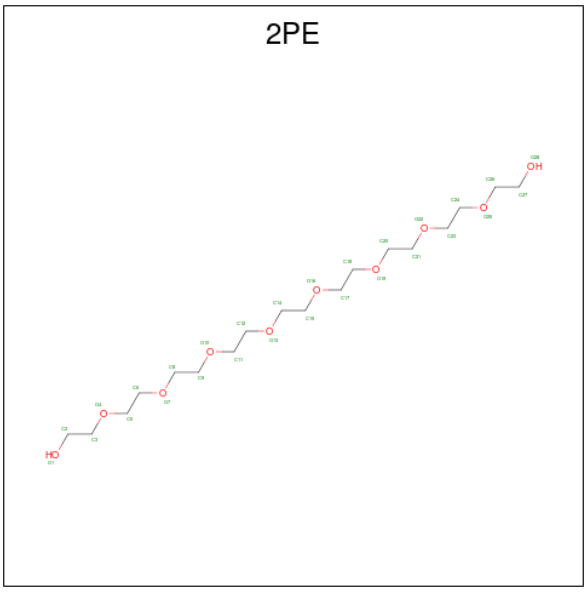
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
42	f	1	Total Mg 1 1	0	0
42	j	1	Total Mg 1 1	0	0

- Molecule 43 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



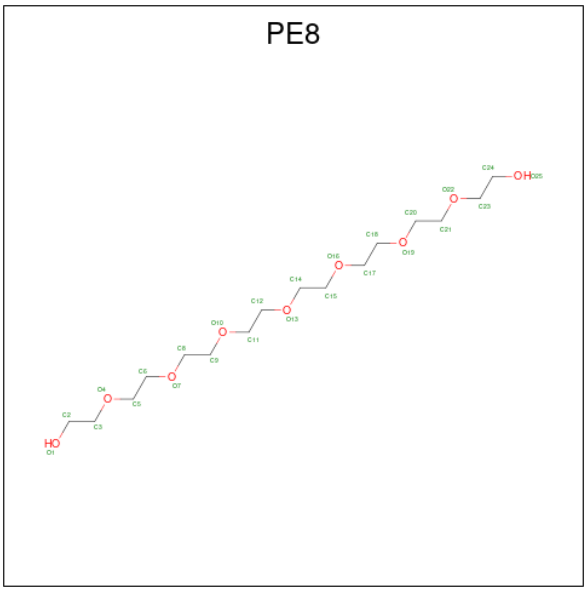
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
43	V	1	Total C Fe N O 43 34 1 4 4	0	0
43	v	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 44 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
44	V	1	Total C O 28 18 10	0	0

- Molecule 45 is 3,6,9,12,15,18,21-HEPTAOXATRICOSANE-1,23-DIOL (CCD ID: PE8) (formula: $C_{16}H_{34}O_9$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
45	i	1	Total C O 25 16 9	0	0

- Molecule 46 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
46	A	191	Total O 191 191	0	0
46	B	413	Total O 413 413	0	0
46	C	320	Total O 320 320	0	0
46	D	169	Total O 170 170	0	1
46	E	57	Total O 57 57	0	0
46	F	17	Total O 17 17	0	0
46	H	63	Total O 63 63	0	0
46	I	16	Total O 16 16	0	0
46	J	17	Total O 17 17	0	0
46	K	15	Total O 15 15	0	0
46	L	23	Total O 23 23	0	0
46	M	33	Total O 33 33	0	0
46	O	254	Total O 254 254	0	0
46	T	27	Total O 27 27	0	0
46	U	112	Total O 112 112	0	0
46	V	149	Total O 149 149	0	0
46	Y	6	Total O 6 6	0	0
46	X	10	Total O 10 10	0	0
46	Z	4	Total O 4 4	0	0
46	a	177	Total O 177 177	0	0
46	b	421	Total O 421 421	0	0
46	c	329	Total O 329 329	0	0

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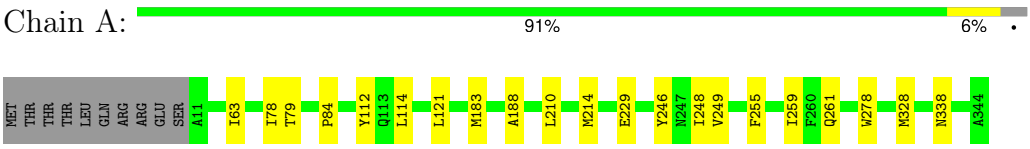
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
46	d	188	Total O 189 189	0	1
46	e	46	Total O 46 46	0	0
46	f	15	Total O 15 15	0	0
46	h	52	Total O 52 52	0	0
46	i	22	Total O 22 22	0	0
46	j	12	Total O 12 12	0	0
46	k	9	Total O 9 9	0	0
46	l	23	Total O 23 23	0	0
46	m	24	Total O 24 24	0	0
46	o	246	Total O 246 246	0	0
46	t	17	Total O 17 17	0	0
46	u	140	Total O 140 140	0	0
46	v	154	Total O 154 154	0	0
46	y	7	Total O 7 7	0	0
46	x	8	Total O 8 8	0	0
46	z	1	Total O 1 1	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.

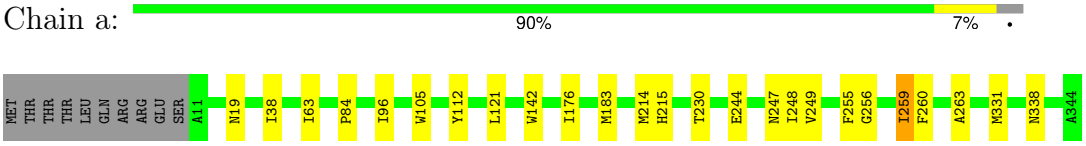
• Molecule 1: Photosystem II protein D1

Chain A:



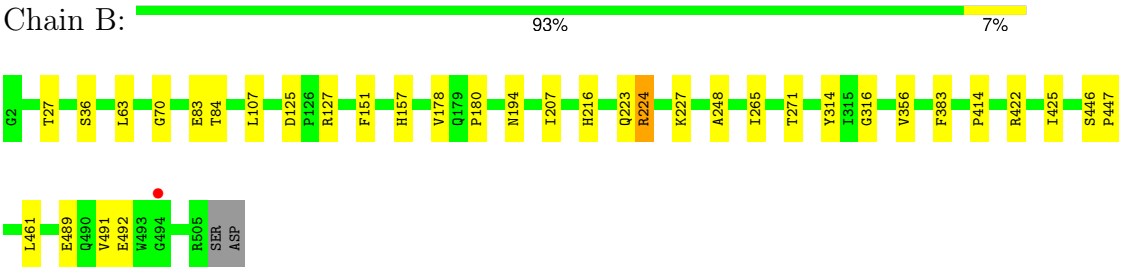
• Molecule 1: Photosystem II protein D1

Chain a:



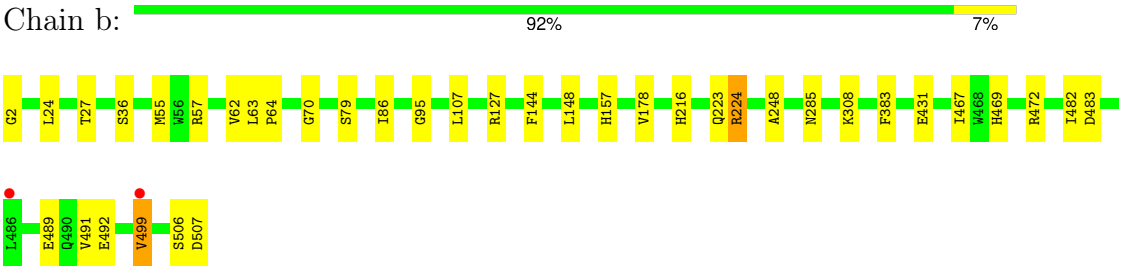
• Molecule 2: Photosystem II CP47 reaction center protein

Chain B:



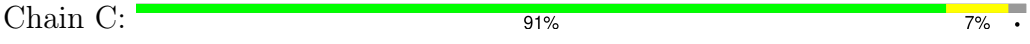
• Molecule 2: Photosystem II CP47 reaction center protein

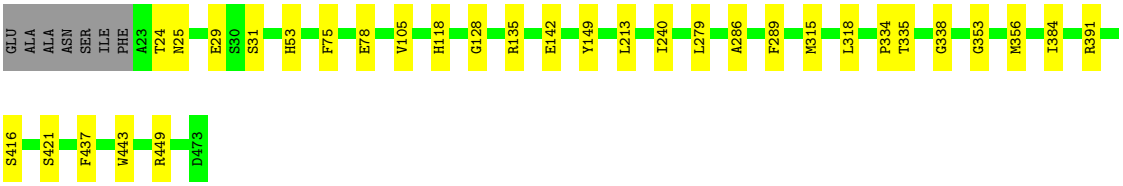
Chain b:



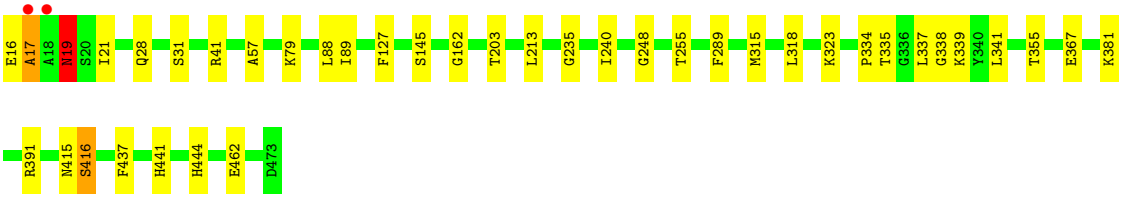
• Molecule 3: Photosystem II CP43 reaction center protein

Chain C:

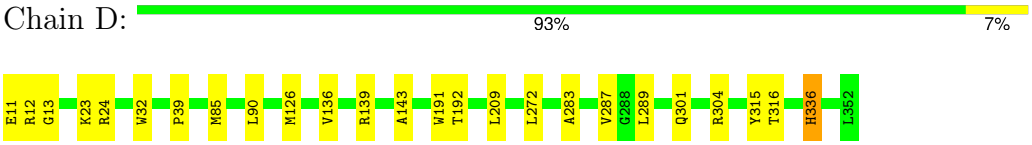




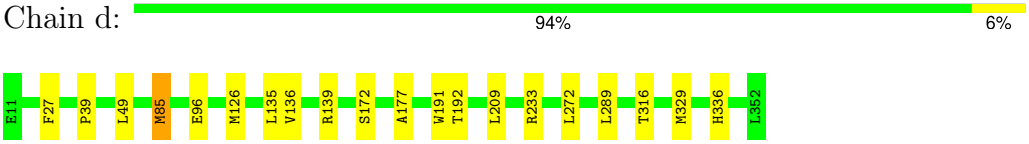
• Molecule 3: Photosystem II CP43 reaction center protein



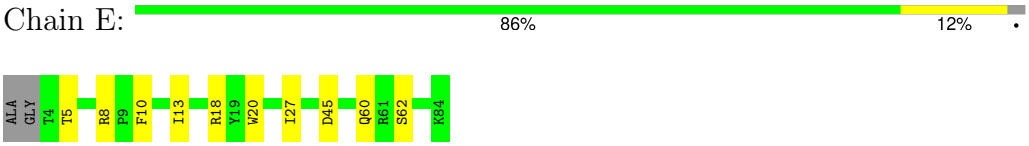
• Molecule 4: Photosystem II D2 protein



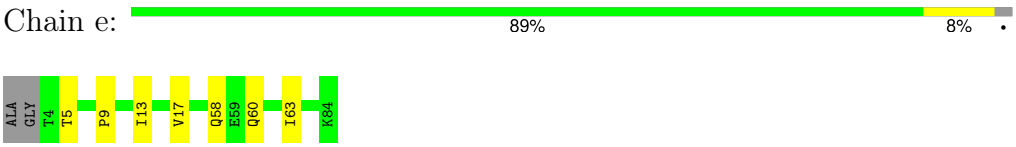
• Molecule 4: Photosystem II D2 protein



• Molecule 5: Cytochrome b559 subunit alpha

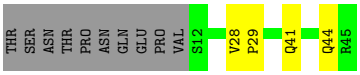


• Molecule 5: Cytochrome b559 subunit alpha



• Molecule 6: Cytochrome b559 subunit beta





• Molecule 6: Cytochrome b559 subunit beta

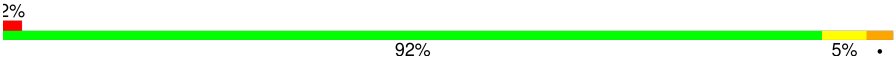
Chain f:

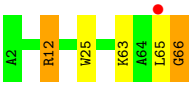




• Molecule 7: Photosystem II reaction center protein H

Chain H:

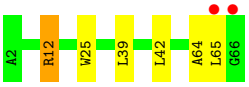




• Molecule 7: Photosystem II reaction center protein H

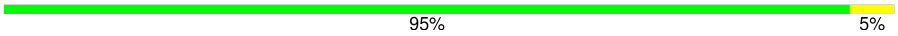
Chain h:





• Molecule 8: Photosystem II reaction center protein I

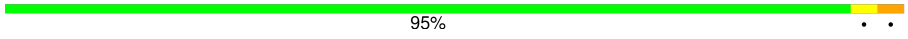
Chain I:





• Molecule 8: Photosystem II reaction center protein I

Chain i:

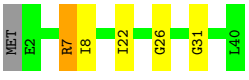




• Molecule 9: Photosystem II reaction center protein J

Chain J:





• Molecule 9: Photosystem II reaction center protein J

Chain j:





• Molecule 10: Photosystem II reaction center protein K

Chain K:

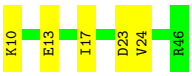




• Molecule 10: Photosystem II reaction center protein K

Chain k:

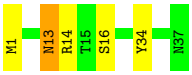




• Molecule 11: Photosystem II reaction center protein L

Chain L:





• Molecule 11: Photosystem II reaction center protein L

Chain l:

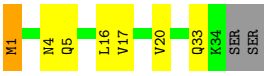




• Molecule 12: Photosystem II reaction center protein M

Chain M:

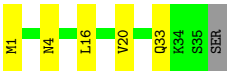




• Molecule 12: Photosystem II reaction center protein M

Chain m:

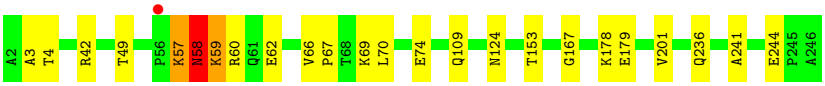




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain O:

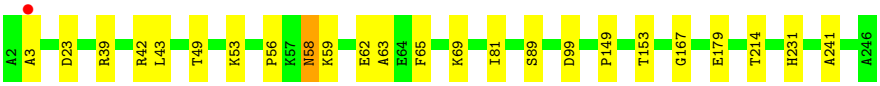




• Molecule 13: Photosystem II manganese-stabilizing polypeptide

Chain o:

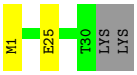




• Molecule 14: Photosystem II reaction center protein T

Chain T:

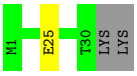




• Molecule 14: Photosystem II reaction center protein T

Chain t:

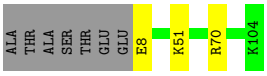




• Molecule 15: Photosystem II 12 kDa extrinsic protein

Chain U:





• Molecule 15: Photosystem II 12 kDa extrinsic protein

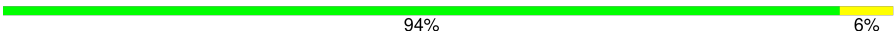
Chain u:

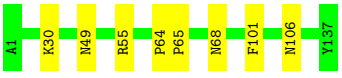




• Molecule 16: Cytochrome c-550

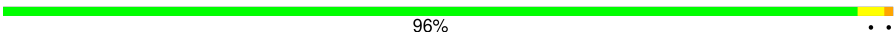
Chain V:

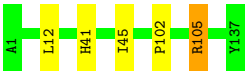




• Molecule 16: Cytochrome c-550

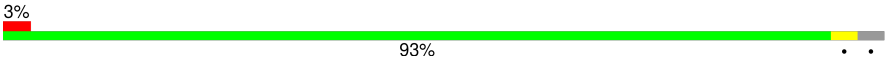
Chain v:

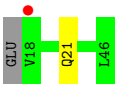




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y:

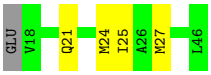




• Molecule 17: Photosystem II reaction center protein Ycf12

Chain y:

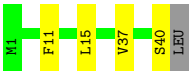




• Molecule 18: Photosystem II reaction center protein X

Chain X:

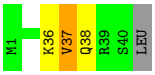




• Molecule 18: Photosystem II reaction center protein X

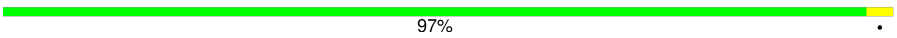
Chain x:





• Molecule 19: Photosystem II reaction center protein Z

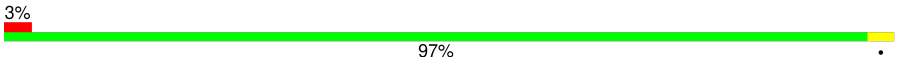
Chain Z:

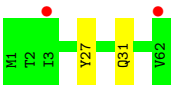




• Molecule 19: Photosystem II reaction center protein Z

Chain z:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	122.19Å 228.51Å 286.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	178.62 – 1.90 178.62 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (178.62-1.90) 99.8 (178.62-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.092 , 0.163 0.093 , 0.164	Depositor DCC
R_{free} test set	31202 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 76.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	57584	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 2PE, DGD, PGE, HEC, HTG, GOL, FME, HEM, PE8, FE2, BCT, 1PE, MG, PL9, CLA, CA, CL, P6G, LMG, SQD, PG4, BCR, MHS, OEX, LMT, EDO, PHO, LHG

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	1.23	1/2736 (0.0%)	1.03	2/3730 (0.1%)
1	a	1.18	3/2736 (0.1%)	1.01	1/3730 (0.0%)
2	B	1.22	6/4205 (0.1%)	1.03	2/5727 (0.0%)
2	b	1.16	4/4207 (0.1%)	1.00	2/5731 (0.0%)
3	C	1.14	3/3636 (0.1%)	0.96	1/4950 (0.0%)
3	c	1.06	3/3679 (0.1%)	0.99	3/5008 (0.1%)
4	D	1.19	1/2816 (0.0%)	1.00	1/3836 (0.0%)
4	d	1.15	1/2829 (0.0%)	0.97	0/3852
5	E	1.19	3/704 (0.4%)	1.00	0/959
5	e	1.05	0/693	0.99	1/944 (0.1%)
6	F	1.02	0/284	0.94	0/387
6	f	1.01	0/265	0.95	0/360
7	H	1.20	2/544 (0.4%)	1.00	0/739
7	h	1.04	1/535 (0.2%)	0.90	0/728
8	I	1.19	0/311	0.92	0/419
8	i	1.07	0/311	0.96	0/419
9	J	1.06	0/306	0.94	0/413
9	j	0.99	0/287	1.04	0/388
10	K	1.08	0/303	1.01	0/416
10	k	1.00	0/303	1.07	0/416
11	L	1.25	1/319 (0.3%)	1.03	0/433
11	l	1.15	0/328	1.01	0/446
12	M	1.32	1/279 (0.4%)	1.13	0/380
12	m	1.16	0/275	1.03	0/375
13	O	1.11	3/1953 (0.2%)	1.01	0/2649
13	o	1.13	1/1948 (0.1%)	1.02	0/2641
14	T	1.24	0/266	1.12	0/362
14	t	1.12	0/266	1.04	0/362
15	U	1.02	0/803	0.94	0/1088
15	u	1.12	0/785	0.95	0/1064
16	V	1.12	1/1104 (0.1%)	0.94	0/1498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	v	1.08	1/1096 (0.1%)	0.96	0/1487
17	Y	1.14	0/223	1.12	0/299
17	y	1.09	0/224	1.19	1/299 (0.3%)
18	X	0.99	0/306	1.05	0/413
18	x	1.10	2/298 (0.7%)	1.11	1/402 (0.2%)
19	Z	0.95	0/490	1.06	0/669
19	z	0.99	1/490 (0.2%)	1.03	0/669
All	All	1.14	39/43143 (0.1%)	1.00	15/58688 (0.0%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	201	VAL	C-O	-7.92	1.15	1.24
7	H	66	GLY	C-OXT	7.35	1.38	1.23
12	M	17	VAL	CA-C	6.96	1.59	1.52
7	H	66	GLY	C-O	6.39	1.36	1.23
2	B	271	THR	N-CA	6.24	1.53	1.45
2	b	62	VAL	C-O	6.16	1.31	1.24
18	x	37	VAL	CA-CB	5.99	1.61	1.54
1	A	278	TRP	N-CA	-5.98	1.42	1.46
2	b	95	GLY	N-CA	-5.78	1.38	1.45
11	L	34	TYR	C-O	5.75	1.31	1.24
3	C	118	HIS	CA-C	5.75	1.60	1.52
3	c	89	ILE	CA-CB	5.75	1.57	1.54
1	a	176	ILE	CA-C	5.74	1.59	1.52
2	b	499	VAL	CA-CB	5.71	1.60	1.54
1	a	38	ILE	C-O	-5.70	1.19	1.24
16	v	105	ARG	N-CA	5.68	1.52	1.46
3	C	384	ILE	C-O	-5.60	1.18	1.24
2	B	151	PHE	N-CA	5.59	1.53	1.46
2	b	2	GLY	N-CA	5.55	1.54	1.45
4	d	85	MET	SD-CE	-5.49	1.65	1.79
3	c	367	GLU	C-O	-5.48	1.19	1.24
7	h	42	LEU	N-CA	5.43	1.52	1.46
5	E	62[A]	SER	C-O	-5.42	1.17	1.24
5	E	62[B]	SER	C-O	-5.42	1.17	1.24
18	x	36	LYS	CA-C	5.41	1.59	1.52
4	D	85	MET	SD-CE	-5.26	1.66	1.79
19	z	27	TYR	C-O	-5.21	1.17	1.24
2	B	356	VAL	C-O	-5.20	1.18	1.24
16	V	101	PHE	CA-C	5.19	1.58	1.52
13	o	214	THR	CA-C	-5.18	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	178	LYS	C-O	-5.16	1.17	1.23
5	E	5	THR	N-CA	5.15	1.52	1.46
3	c	255	THR	CA-C	5.15	1.57	1.52
13	O	244	GLU	CA-C	-5.13	1.47	1.52
3	C	421	SER	N-CA	-5.10	1.39	1.45
2	B	265	ILE	C-O	-5.06	1.17	1.24
2	B	207	ILE	CA-C	5.02	1.59	1.52
2	B	63	LEU	C-O	5.00	1.29	1.24
1	a	259	ILE	CA-C	5.00	1.59	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	142	TRP	N-CA-C	6.49	120.91	112.92
4	D	139	ARG	NE-CZ-NH1	5.93	127.43	121.50
1	A	261	GLN	N-CA-C	5.92	118.22	111.11
3	C	24	THR	CB-CA-C	-5.40	101.75	110.77
2	B	224	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	A	78	ILE	N-CA-C	5.34	116.11	110.72
3	c	79	LYS	CB-CA-C	-5.31	101.15	109.11
18	x	37	VAL	N-CA-CB	5.24	117.16	110.13
3	c	17	ALA	CA-C-N	5.24	131.13	121.70
3	c	17	ALA	C-N-CA	5.24	131.13	121.70
2	b	55	MET	N-CA-C	5.23	117.66	111.33
5	e	58	GLN	N-CA-C	5.20	117.35	111.11
17	y	24	MET	N-CA-C	-5.13	105.58	111.07
2	b	224	ARG	CA-CB-CG	-5.12	103.86	114.10
2	B	414	PRO	N-CA-C	5.12	116.94	110.70

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	2639	0	2551	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	2639	0	2551	21	0
2	B	4032	0	3914	30	0
2	b	4037	0	3915	31	0
3	C	3508	0	3440	25	0
3	c	3553	0	3474	25	0
4	D	2731	0	2637	21	0
4	d	2741	0	2647	17	0
5	E	676	0	671	9	0
5	e	668	0	658	7	0
6	F	275	0	282	2	0
6	f	257	0	269	4	0
7	H	525	0	558	5	0
7	h	519	0	545	6	0
8	I	314	0	328	2	0
8	i	314	0	328	2	0
9	J	294	0	309	7	0
9	j	281	0	285	4	0
10	K	293	0	305	4	0
10	k	293	0	305	2	0
11	L	309	0	327	3	0
11	l	315	0	335	4	0
12	M	286	0	303	32	0
12	m	289	0	310	30	0
13	O	1904	0	1887	16	0
13	o	1902	0	1885	14	0
14	T	271	0	277	1	0
14	t	271	0	277	1	0
15	U	786	0	787	1	0
15	u	774	0	773	5	0
16	V	1077	0	1092	8	0
16	v	1072	0	1086	3	0
17	Y	219	0	253	1	0
17	y	220	0	255	3	0
18	X	300	0	340	5	0
18	x	295	0	329	1	0
19	Z	479	0	516	0	0
19	z	479	0	516	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	1	0	0	1	0
22	a	2	0	0	0	0
22	v	1	0	0	2	0
23	A	4	0	0	0	0
23	a	4	0	0	0	0
23	m	8	0	2	0	0
24	A	190	0	203	6	0
24	B	1015	0	1093	27	0
24	C	835	0	910	26	0
24	D	195	0	216	10	0
24	a	190	0	203	6	0
24	b	1025	0	1116	23	0
24	c	835	0	910	22	0
24	d	195	0	216	5	0
25	A	64	0	74	1	0
25	D	64	0	74	1	0
25	a	64	0	74	0	0
25	d	64	0	74	3	0
26	A	40	0	56	3	0
26	B	120	0	168	12	0
26	C	120	0	168	5	0
26	D	40	0	56	2	0
26	H	40	0	56	3	0
26	K	40	0	56	2	0
26	T	40	0	56	8	0
26	a	40	0	56	3	0
26	b	120	0	168	10	0
26	c	120	0	168	7	0
26	d	40	0	56	3	0
26	h	40	0	56	3	0
26	k	40	0	56	6	0
26	t	40	0	56	5	0
27	A	55	0	80	7	0
27	D	55	0	80	0	0
27	a	55	0	80	11	0
27	d	55	0	80	0	0
28	A	162	0	234	5	0
28	F	54	0	78	0	0
28	a	162	0	234	1	0
28	b	54	0	78	2	0
28	h	54	0	78	0	0
28	l	54	0	78	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	x	54	0	78	2	0
29	A	51	0	72	3	0
29	B	106	0	158	7	0
29	C	157	0	230	3	0
29	J	47	0	64	0	0
29	a	51	0	72	1	0
29	b	51	0	72	2	0
29	c	102	0	144	1	0
29	d	55	0	86	2	0
29	j	47	0	64	0	0
29	z	55	0	86	1	0
30	A	12	0	16	4	0
30	B	42	0	56	0	0
30	C	24	0	31	14	0
30	D	18	0	24	2	0
30	F	6	0	8	0	0
30	O	30	0	40	1	0
30	T	12	0	16	1	0
30	U	6	0	8	2	0
30	V	30	0	40	0	0
30	a	12	0	16	2	0
30	b	36	0	48	1	0
30	c	24	0	32	9	0
30	d	12	0	16	1	0
30	e	6	0	8	0	0
30	f	12	0	16	0	0
30	m	6	0	8	0	0
30	o	18	0	24	1	0
30	t	6	0	8	1	0
30	u	12	0	16	0	0
30	v	30	0	40	0	0
30	y	6	0	8	0	0
31	A	35	0	46	0	0
31	B	35	0	46	2	0
31	C	35	0	46	0	0
31	F	35	0	46	0	0
31	I	35	0	46	1	0
31	J	35	0	46	1	0
31	M	70	0	92	5	0
31	Y	35	0	46	1	0
31	a	35	0	46	0	0
31	b	35	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	35	0	46	0	0
31	f	35	0	46	0	0
31	j	35	0	46	0	0
31	m	70	0	92	0	0
31	t	35	0	46	0	0
31	u	35	0	46	3	0
32	A	42	0	54	0	0
32	B	49	0	74	0	0
32	D	147	0	222	2	0
32	E	42	0	57	0	0
32	a	41	0	52	0	0
32	d	147	0	222	3	0
32	e	42	0	57	2	0
32	l	49	0	74	1	0
33	A	13	0	18	0	0
33	B	104	0	144	0	0
33	C	65	0	90	0	0
33	D	13	0	18	0	0
33	E	26	0	36	0	0
33	H	52	0	72	2	0
33	I	39	0	54	2	0
33	J	26	0	36	0	0
33	K	13	0	18	0	0
33	U	13	0	18	0	0
33	V	65	0	90	0	0
33	X	39	0	54	0	0
33	a	26	0	36	0	0
33	b	52	0	72	0	0
33	c	52	0	72	1	0
33	d	13	0	18	0	0
33	e	26	0	36	0	0
33	h	13	0	18	0	0
33	i	52	0	72	0	0
33	j	13	0	18	0	0
33	l	13	0	18	0	0
33	x	13	0	18	0	0
34	A	17	0	23	0	0
34	B	70	0	98	2	0
34	C	20	0	28	0	0
34	D	10	0	14	0	0
34	E	60	0	84	0	0
34	H	40	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	I	10	0	14	0	0
34	J	30	0	42	0	0
34	O	30	0	42	3	0
34	T	7	0	9	0	0
34	V	20	0	28	0	0
34	Y	10	0	14	0	0
34	a	20	0	28	0	0
34	b	100	0	140	0	0
34	c	50	0	70	0	0
34	f	10	0	14	0	0
34	h	40	0	56	0	0
34	i	20	0	28	0	0
34	j	10	0	14	0	0
34	o	40	0	56	2	0
34	t	17	0	23	0	0
34	x	10	0	14	0	0
35	A	38	0	52	0	0
35	B	38	0	52	1	0
35	C	19	0	26	0	0
35	D	57	0	78	0	0
35	E	19	0	26	0	0
35	I	19	0	26	0	0
35	T	19	0	26	2	0
35	b	38	0	52	0	0
35	c	19	0	26	0	0
35	d	38	0	52	0	0
35	j	19	0	26	0	0
36	A	4	0	6	0	0
36	B	16	0	24	0	0
36	C	4	0	6	0	0
36	D	4	0	6	3	0
36	E	8	0	12	0	0
36	H	4	0	6	0	0
36	I	4	0	6	0	0
36	J	4	0	6	0	0
36	O	4	0	6	0	0
36	V	4	0	6	0	0
36	X	4	0	6	0	0
36	a	4	0	6	0	0
36	c	4	0	6	0	0
36	d	4	0	6	0	0
36	e	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	i	4	0	6	0	0
36	o	8	0	12	0	0
37	B	1	0	0	0	0
37	O	1	0	0	0	0
37	b	1	0	0	0	0
37	c	1	0	0	0	0
37	h	1	0	0	0	0
37	o	1	0	0	0	0
38	B	76	0	104	3	0
38	C	114	0	156	4	0
38	H	19	0	26	0	0
38	O	19	0	26	0	0
38	V	19	0	26	0	0
38	a	19	0	26	0	0
38	b	76	0	104	0	0
38	c	76	0	104	0	0
38	h	19	0	26	1	0
38	o	19	0	26	1	0
39	B	32	0	44	0	0
39	L	16	0	22	0	0
39	V	16	0	22	0	0
39	e	16	0	22	0	0
39	j	16	0	22	0	0
39	x	16	0	22	1	0
40	C	180	0	234	0	0
40	D	66	0	96	2	0
40	H	62	0	82	0	0
40	c	181	0	236	0	0
40	d	66	0	96	0	1
40	h	62	0	82	0	0
41	E	43	0	30	5	0
41	e	43	0	30	4	0
42	F	1	0	0	0	0
42	J	1	0	0	0	0
42	f	1	0	0	0	0
42	j	1	0	0	0	0
43	V	43	0	30	1	0
43	v	43	0	30	0	0
44	V	28	0	38	3	0
45	i	25	0	34	1	0
46	A	191	0	0	7	0
46	B	413	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	C	320	0	0	5	0
46	D	170	0	0	5	0
46	E	57	0	0	3	0
46	F	17	0	0	0	0
46	H	63	0	0	2	0
46	I	16	0	0	2	0
46	J	17	0	0	2	0
46	K	15	0	0	0	0
46	L	23	0	0	0	0
46	M	33	0	0	2	0
46	O	254	0	0	8	0
46	T	27	0	0	1	0
46	U	112	0	0	3	0
46	V	149	0	0	6	0
46	X	10	0	0	0	0
46	Y	6	0	0	0	0
46	Z	4	0	0	0	0
46	a	177	0	0	5	0
46	b	421	0	0	12	0
46	c	329	0	0	5	0
46	d	189	0	0	2	0
46	e	46	0	0	0	0
46	f	15	0	0	0	0
46	h	52	0	0	1	0
46	i	22	0	0	1	0
46	j	12	0	0	0	0
46	k	9	0	0	0	0
46	l	23	0	0	1	0
46	m	24	0	0	1	0
46	o	246	0	0	9	0
46	t	17	0	0	0	0
46	u	140	0	0	2	0
46	v	154	0	0	3	1
46	x	8	0	0	0	0
46	y	7	0	0	0	0
46	z	1	0	0	0	0
All	All	57584	0	56553	522	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (522) 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)
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:CD2	1.49	1.41
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD11	1.65	1.26
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD22	1.69	1.22
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:HD13	1.14	1.10
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:CD1	1.85	1.07
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:HD21	1.06	1.05
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CD2	2.32	1.05
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:HD21	1.86	1.04
4:D:301:GLN:OE1	46:D:501:HOH:O	1.76	1.03
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CD2	1.88	1.02
2:B:127[B]:ARG:HH21	2:B:127[B]:ARG:CG	1.73	1.01
38:B:623:HTG:H61	46:O:427:HOH:O	1.64	0.97
1:A:214:MET:HG2	27:A:611:PL9:H102	1.45	0.97
3:C:338:GLY:O	30:C:528:GOL:H32	1.63	0.97
2:B:127[B]:ARG:HH21	2:B:127[B]:ARG:HG3	0.82	0.96
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD13	1.95	0.96
12:M:16[B]:LEU:HD13	12:m:16[B]:LEU:CD1	1.95	0.96
2:B:127[B]:ARG:HG3	2:B:127[B]:ARG:NH2	1.64	0.96
30:A:614:GOL:O2	46:A:701:HOH:O	1.85	0.93
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD1	2.45	0.92
1:a:338:ASN:HD21	30:c:529:GOL:H12	1.36	0.90
12:M:16[B]:LEU:HD22	12:m:16[B]:LEU:HD11	0.90	0.89
30:c:529:GOL:O1	46:c:601:HOH:O	1.91	0.89
22:V:202:CL:CL	46:V:390:HOH:O	2.27	0.88
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CD1	2.53	0.86
3:c:338:GLY:O	30:c:529:GOL:H11	1.75	0.85
26:T:102:BCR:H382	26:T:102:BCR:H23C	1.62	0.81
30:C:528:GOL:O3	46:C:601:HOH:O	1.96	0.81
26:t:102:BCR:H382	26:t:102:BCR:H23C	1.62	0.81
30:A:615:GOL:C3	46:E:201:HOH:O	2.30	0.79
24:D:405:CLA:H192	18:X:15[A]:LEU:HD11	1.65	0.79
10:K:17:ILE:HD12	10:K:17:ILE:H	1.48	0.78
31:M:101:LMT:H121	28:b:633:SQD:H381	1.66	0.77
1:A:338:ASN:HD21	30:C:528:GOL:H31	1.50	0.77
8:I:33:LYS:HG2	46:I:213:HOH:O	1.85	0.77
4:D:11:GLU:N	36:D:419:EDO:HO2	1.83	0.77
30:A:615:GOL:H31	46:E:201:HOH:O	1.83	0.76
12:M:33:GLN:HB2	12:m:33:GLN:HG2	1.65	0.76
4:D:316:THR:HG21	46:D:561:HOH:O	1.85	0.76
38:C:531:HTG:O6	46:C:602:HOH:O	2.03	0.76
11:l:8[B]:GLN:NE2	46:l:201:HOH:O	2.18	0.76
1:a:338:ASN:ND2	30:c:529:GOL:H12	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:m:4:ASN:ND2	46:m:201:HOH:O	2.21	0.73
31:M:102:LMT:H111	24:b:615:CLA:H191	1.69	0.73
2:B:83:GLU:O	46:B:701:HOH:O	2.06	0.73
46:a:527:HOH:O	4:d:139:ARG:HD2	1.88	0.72
1:a:19:ASN:HD22	28:a:424:SQD:H62	1.55	0.72
1:a:338:ASN:HD21	30:c:529:GOL:C1	2.03	0.71
46:A:756:HOH:O	30:C:528:GOL:H11	1.90	0.70
12:M:4:ASN:ND2	46:M:201:HOH:O	2.25	0.69
26:T:102:BCR:HC8	26:T:102:BCR:H311	1.72	0.69
24:b:609:CLA:HMB1	24:b:609:CLA:HBB1	1.76	0.68
16:V:68:ASN:HD21	44:V:216:2PE:H261	1.57	0.68
34:o:308:PGE:H22	46:o:482:HOH:O	1.93	0.68
12:M:16[B]:LEU:HD11	12:m:16[B]:LEU:HD22	0.73	0.68
12:M:33:GLN:HB2	12:m:33:GLN:CG	2.24	0.66
46:b:753:HOH:O	22:v:201:CL:CL	2.50	0.66
31:M:101:LMT:H121	28:b:633:SQD:C38	2.23	0.66
38:C:529:HTG:H7'2	31:I:101:LMT:H123	1.78	0.66
30:a:415:GOL:O2	46:o:401:HOH:O	2.14	0.66
1:A:248:ILE:HD11	46:A:848:HOH:O	1.95	0.65
1:A:249:VAL:HG12	2:B:491:VAL:HG21	1.79	0.65
2:B:491:VAL:HG12	4:D:136[A]:VAL:HG13	1.79	0.65
26:D:406:BCR:H331	26:D:406:BCR:C8	2.26	0.65
38:o:301:HTG:O6	46:o:401:HOH:O	2.13	0.65
46:A:701:HOH:O	13:O:109:GLN:NE2	2.30	0.65
1:A:338:ASN:ND2	30:C:528:GOL:H31	2.12	0.65
16:V:64:PRO:HB2	44:V:216:2PE:H241	1.80	0.64
24:B:611:CLA:HHC	24:B:611:CLA:HBB1	1.79	0.64
16:v:12:LEU:HD22	46:v:305:HOH:O	1.97	0.63
24:C:506:CLA:HBB1	24:C:506:CLA:HMB1	1.79	0.63
1:a:214:MET:HG2	27:a:412:PL9:H102	1.80	0.63
2:b:491:VAL:HG12	4:d:136:VAL:HG13	1.81	0.63
29:b:621:LMG:H291	46:b:903:HOH:O	1.97	0.63
8:i:34:ARG:NH2	46:i:201:HOH:O	2.32	0.63
1:a:183:MET:HA	24:a:407:CLA:HMD2	1.82	0.62
7:h:12[B]:ARG:NH2	46:h:201:HOH:O	2.32	0.62
30:A:615:GOL:H32	46:E:201:HOH:O	1.97	0.62
26:h:103:BCR:HC8	26:h:103:BCR:H331	1.82	0.62
24:a:407:CLA:HMB3	24:a:407:CLA:HBB1	1.80	0.62
40:D:408:DGD:HBG1	30:D:412:GOL:O3	1.99	0.61
24:B:604:CLA:C4D	24:B:606:CLA:H43	2.30	0.61
1:A:183:MET:HA	24:A:606:CLA:HMD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:70:LEU:HD22	34:O:308:PGE:H62	1.82	0.61
24:A:609:CLA:H203	24:C:506:CLA:H142	1.83	0.61
13:o:231:HIS:ND1	46:o:405:HOH:O	2.31	0.60
26:B:620:BCR:H331	26:B:620:BCR:HC8	1.83	0.60
24:B:602:CLA:HHC	24:B:602:CLA:HBB1	1.84	0.60
26:B:619:BCR:H331	26:B:619:BCR:C8	2.32	0.60
24:B:602:CLA:H92	26:H:102:BCR:H403	1.84	0.59
10:k:24:VAL:HG13	17:y:25:ILE:HD13	1.83	0.59
12:M:16[B]:LEU:CG	12:m:16[B]:LEU:HD21	2.31	0.59
24:a:410:CLA:H202	24:c:505:CLA:H13	1.84	0.59
26:h:103:BCR:H331	26:h:103:BCR:C8	2.32	0.59
2:B:224:ARG:HD3	7:H:25:TRP:CE2	2.38	0.59
9:J:7[B]:ARG:NH2	46:J:201:HOH:O	2.35	0.59
2:b:57:ARG:NH1	46:b:701:HOH:O	2.31	0.59
2:B:224:ARG:HD3	7:H:25:TRP:CD2	2.38	0.59
27:a:412:PL9:H512	28:x:101:SQD:H152	1.85	0.59
26:t:102:BCR:HC8	26:t:102:BCR:H311	1.84	0.59
26:A:610:BCR:H331	26:A:610:BCR:C8	2.32	0.59
24:C:504:CLA:C15	32:D:411:LHG:C38	2.81	0.59
26:H:102:BCR:H331	26:H:102:BCR:C8	2.32	0.59
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CD2	2.60	0.59
24:b:612:CLA:HBB1	24:b:612:CLA:HMB1	1.86	0.58
24:B:602:CLA:C7	24:B:602:CLA:H11	2.33	0.58
24:B:602:CLA:H141	34:B:646:PGE:C6	2.33	0.58
31:B:622:LMT:H122	29:B:634:LMG:H453	1.85	0.58
24:b:611:CLA:H192	24:b:611:CLA:H152	1.83	0.58
40:D:408:DGD:HD61	5:E:45:ASP:HB3	1.85	0.58
6:f:41:GLN:OE1	9:j:31:GLY:HA3	2.04	0.58
30:C:523:GOL:C3	46:V:308:HOH:O	2.52	0.57
27:A:611:PL9:H502	4:D:39:PRO:HG3	1.86	0.57
7:H:65:LEU:HB2	7:H:66:GLY:HA2	1.84	0.57
1:A:338:ASN:HD21	30:C:528:GOL:C3	2.17	0.57
13:O:57:LYS:O	13:O:59:LYS:N	2.37	0.57
2:b:216:HIS:CE1	24:b:610:CLA:NA	2.73	0.57
2:B:180:PRO:HB2	35:B:652:P6G:H32	1.86	0.56
26:t:102:BCR:H382	26:t:102:BCR:C23	2.34	0.56
2:B:216:HIS:CE1	24:B:610:CLA:NA	2.73	0.56
2:B:223[A]:GLN:NE2	46:B:706:HOH:O	2.38	0.56
13:O:70:LEU:CD2	34:O:308:PGE:H62	2.35	0.56
3:c:339:LYS:O	46:c:602:HOH:O	2.17	0.56
13:O:69:LYS:NZ	46:O:405:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:16[B]:LEU:HD21	12:m:16[B]:LEU:CG	2.36	0.56
3:C:142:GLU:HG2	46:C:635:HOH:O	2.04	0.56
24:B:602:CLA:H141	34:B:646:PGE:H62	1.87	0.56
8:I:33:LYS:HE2	46:I:213:HOH:O	2.05	0.56
27:a:412:PL9:H353	27:a:412:PL9:H311	1.88	0.55
24:B:602:CLA:H93	33:H:106:PG4:H11	1.88	0.55
2:B:127[A]:ARG:NH1	46:B:707:HOH:O	2.38	0.55
26:B:618:BCR:H382	26:B:618:BCR:H23C	1.87	0.55
24:D:405:CLA:HBB1	24:D:405:CLA:HMB3	1.88	0.55
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.41	0.55
26:B:620:BCR:H331	26:B:620:BCR:C8	2.36	0.55
30:C:523:GOL:H31	46:V:308:HOH:O	2.06	0.55
24:b:608:CLA:H42	29:b:621:LMG:H302	1.88	0.55
24:c:505:CLA:HBB1	24:c:505:CLA:HMB3	1.89	0.55
7:H:12[A]:ARG:HG2	46:H:251:HOH:O	2.06	0.55
5:e:17:VAL:HG23	9:j:7:ARG:HG2	1.89	0.55
1:A:214:MET:HE2	1:A:255:PHE:CE1	2.43	0.54
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.70	0.54
1:a:121[A]:LEU:HD23	29:a:414:LMG:H202	1.90	0.54
8:i:1:FME:H	45:i:107:PE8:H212	1.71	0.54
24:D:405:CLA:H192	18:X:15[A]:LEU:CD1	2.34	0.54
1:a:230:THR:C	46:b:710:HOH:O	2.51	0.54
10:K:17:ILE:H	10:K:17:ILE:CD1	2.18	0.54
3:c:337:LEU:HB2	30:c:529:GOL:H2	1.88	0.54
26:H:102:BCR:H331	26:H:102:BCR:HC8	1.87	0.54
41:e:107:HEM:HMC2	41:e:107:HEM:HBC2	1.89	0.54
2:B:127[B]:ARG:CG	2:B:127[B]:ARG:NH2	2.46	0.54
1:a:249:VAL:HG12	2:b:491:VAL:CG2	2.38	0.54
2:b:127:ARG:NH2	46:b:706:HOH:O	2.39	0.54
2:b:248:ALA:HA	24:b:604:CLA:H42	1.90	0.54
3:c:415:ASN:O	3:c:416[B]:SER:HB2	2.08	0.54
12:M:16[B]:LEU:C	12:M:16[B]:LEU:HD23	2.31	0.54
26:b:620:BCR:H331	26:b:620:BCR:HC8	1.90	0.54
26:b:618:BCR:H382	26:b:618:BCR:H23C	1.90	0.53
29:d:412:LMG:H112	46:d:647:HOH:O	2.08	0.53
5:e:17:VAL:CG2	9:j:7:ARG:HG2	2.37	0.53
24:c:501:CLA:H192	24:c:506:CLA:C1B	2.38	0.53
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.91	0.53
15:u:19:THR:HA	31:u:203:LMT:H3B	1.89	0.53
1:A:246:TYR:OH	46:A:702:HOH:O	2.18	0.53
30:D:402:GOL:H11	12:M:1:FME:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:216:HIS:HE1	24:b:610:CLA:C1A	2.22	0.53
24:c:502:CLA:H61	24:c:512:CLA:H42	1.90	0.53
13:o:56:PRO:HG3	13:o:63:ALA:HB2	1.91	0.53
4:D:336:MHS:HM2	46:D:611:HOH:O	2.09	0.52
3:C:78:GLU:OE2	16:V:106[A]:ASN:ND2	2.42	0.52
13:O:59:LYS:NZ	46:O:407:HOH:O	2.40	0.52
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.38	0.52
29:A:613:LMG:C43	29:A:613:LMG:H242	2.39	0.52
2:B:216:HIS:HE1	24:B:610:CLA:C1A	2.22	0.52
24:C:509:CLA:HBB1	24:C:509:CLA:HMB1	1.91	0.52
27:a:412:PL9:H502	4:d:39:PRO:HG3	1.91	0.52
2:b:224:ARG:HD3	7:h:25:TRP:CD2	2.45	0.52
1:a:214:MET:HE2	1:a:255:PHE:CE1	2.44	0.52
2:b:36[A]:SER:OG	26:b:619:BCR:H362	2.10	0.52
7:h:25:TRP:CD1	38:h:101:HTG:H1	2.45	0.52
24:b:602:CLA:H41	46:b:1040:HOH:O	2.10	0.52
24:c:505:CLA:HBD	24:c:505:CLA:HAA1	1.91	0.52
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.90	0.52
30:T:103:GOL:H32	35:T:105:P6G:H151	1.90	0.52
24:B:602:CLA:H11	24:B:602:CLA:H71	1.92	0.52
24:b:602:CLA:HHC	24:b:602:CLA:HBB1	1.92	0.52
12:M:33:GLN:CD	12:m:33:GLN:HG3	2.34	0.52
27:a:412:PL9:H513	30:d:413:GOL:O2	2.10	0.52
2:b:499:VAL:HG12	4:d:135:LEU:HB3	1.92	0.52
15:u:85:THR:HA	31:u:203:LMT:H1'	1.91	0.52
24:b:616:CLA:HBB1	24:b:616:CLA:HMB3	1.91	0.51
12:M:20:VAL:HG11	12:m:20:VAL:HG22	1.91	0.51
12:M:16[B]:LEU:CG	12:m:16[B]:LEU:CD2	2.86	0.51
24:C:504:CLA:HBB1	24:C:504:CLA:HMB1	1.92	0.51
24:d:405:CLA:HMB1	24:d:405:CLA:HBB1	1.92	0.51
26:d:406:BCR:H331	26:d:406:BCR:C8	2.39	0.51
9:j:11:TRP:CZ2	9:j:12:ILE:HD11	2.45	0.51
10:K:17:ILE:HD12	10:K:17:ILE:N	2.21	0.51
3:C:338:GLY:O	30:C:528:GOL:C3	2.49	0.51
26:k:101:BCR:C23	26:k:101:BCR:H382	2.41	0.51
24:d:404:CLA:HBC3	24:d:404:CLA:HHD	1.93	0.51
29:B:634:LMG:H201	4:D:32:TRP:CE3	2.46	0.51
24:C:506:CLA:HMC2	24:C:507:CLA:H102	1.92	0.51
13:O:124:ASN:O	30:O:305:GOL:H12	2.10	0.51
4:d:191:TRP:CE3	4:d:289:LEU:HD11	2.45	0.51
24:b:611:CLA:HHC	24:b:611:CLA:HBB1	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:ARG:NE	29:C:526:LMG:O5	2.37	0.51
26:C:525:BCR:H331	26:C:525:BCR:C8	2.40	0.51
24:b:604:CLA:C4D	24:b:606:CLA:H43	2.41	0.51
46:b:754:HOH:O	7:h:64:ALA:HB1	2.10	0.50
24:B:610:CLA:HBB1	24:B:610:CLA:HMB1	1.92	0.50
24:C:502:CLA:H193	38:C:521:HTG:H3'1	1.94	0.50
24:C:512:CLA:HMB3	24:C:512:CLA:HBB1	1.94	0.50
13:O:179:GLU:HG2	46:O:620:HOH:O	2.11	0.50
25:d:401:PHO:HBB1	25:d:401:PHO:CMB	2.42	0.50
12:m:16[B]:LEU:C	12:m:16[B]:LEU:HD23	2.37	0.50
38:B:623:HTG:C6	46:O:427:HOH:O	2.38	0.50
27:a:412:PL9:H522	46:a:501:HOH:O	2.12	0.50
2:b:144:PHE:CE2	2:b:148[A]:LEU:HD11	2.47	0.50
4:d:85:MET:CE	4:d:96:GLU:HG2	2.42	0.50
1:A:214:MET:CG	27:A:611:PL9:H102	2.29	0.50
22:v:201:CL:CL	46:v:450:HOH:O	2.56	0.50
24:c:503:CLA:HBB1	24:c:503:CLA:HMB1	1.92	0.50
24:c:510:CLA:HMB1	24:c:510:CLA:HBB1	1.92	0.50
26:c:515:BCR:H382	26:c:515:BCR:H23C	1.93	0.50
46:a:527:HOH:O	4:d:139:ARG:CD	2.52	0.50
24:b:610:CLA:HBB1	24:b:610:CLA:HMB1	1.94	0.50
5:e:13:ILE:HG21	41:e:107:HEM:CAD	2.42	0.49
31:B:622:LMT:C12	29:B:634:LMG:H453	2.42	0.49
3:c:318:LEU:C	3:c:318:LEU:HD23	2.36	0.49
4:D:11:GLU:N	36:D:419:EDO:O2	2.44	0.49
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.12	0.49
12:M:20:VAL:HG11	12:m:20:VAL:CG2	2.42	0.49
24:c:504:CLA:C15	32:d:411:LHG:C38	2.90	0.49
2:b:86:ILE:CG1	46:b:909:HOH:O	2.59	0.49
3:c:88:LEU:HD13	24:c:503:CLA:HED3	1.94	0.49
24:c:506:CLA:HMB3	24:c:506:CLA:HBB1	1.93	0.49
3:C:279:LEU:HD22	24:C:509:CLA:HED2	1.94	0.49
26:b:620:BCR:H331	26:b:620:BCR:C8	2.42	0.49
16:v:102:PRO:O	16:v:105:ARG:HG3	2.12	0.49
46:A:756:HOH:O	30:C:528:GOL:C1	2.54	0.49
24:B:602:CLA:H93	33:H:106:PG4:C1	2.43	0.49
4:d:272:LEU:C	4:d:272:LEU:HD23	2.36	0.49
14:t:25[A]:GLU:HB2	30:t:101:GOL:H2	1.93	0.49
2:b:506:SER:HA	2:b:507:ASP:HB2	1.95	0.49
24:b:608:CLA:HMB1	24:b:608:CLA:HBB1	1.93	0.49
26:b:620:BCR:H383	26:b:620:BCR:H23C	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:42:ARG:O	13:o:241:ALA:HA	2.12	0.49
3:C:75:PHE:CZ	3:C:105:VAL:HG21	2.47	0.48
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.45	0.48
1:a:263:ALA:O	27:a:412:PL9:H152	2.13	0.48
24:c:506:CLA:HMC2	24:c:507:CLA:H102	1.95	0.48
13:o:58:ASN:HA	13:o:59:LYS:HB2	1.94	0.48
27:A:611:PL9:HC2	27:A:611:PL9:H103	1.95	0.48
2:B:125:ASP:OD1	2:B:127[B]:ARG:NH2	2.45	0.48
26:h:103:BCR:H383	26:h:103:BCR:H23C	1.94	0.48
6:f:28:VAL:HB	6:f:29:PRO:HD3	1.94	0.48
24:C:503:CLA:HBB1	24:C:503:CLA:HMB1	1.95	0.48
13:O:74[A]:GLU:OE2	46:O:401:HOH:O	2.20	0.48
26:B:619:BCR:H331	26:B:619:BCR:HC8	1.95	0.48
12:M:16[B]:LEU:CD2	12:m:16[B]:LEU:CG	2.91	0.48
24:B:606:CLA:HHC	24:B:606:CLA:HBB1	1.94	0.48
1:a:247:ASN:HB3	2:b:482:ILE:HD11	1.95	0.48
1:a:331:MET:HE2	46:o:522:HOH:O	2.12	0.48
5:E:10:PHE:HE1	41:E:113:HEM:HBD2	1.79	0.48
26:b:619:BCR:H331	26:b:619:BCR:C8	2.44	0.48
3:C:334:PRO:HA	13:O:153:THR:OG1	2.14	0.48
24:C:510:CLA:HMB3	24:C:510:CLA:HBB1	1.95	0.48
24:B:607:CLA:HMB1	24:B:607:CLA:HBB1	1.96	0.48
4:D:209:LEU:HD23	4:D:209:LEU:C	2.38	0.48
3:c:213:LEU:HD11	26:c:515:BCR:C20	2.44	0.47
24:d:403:CLA:HMB1	24:d:403:CLA:HBB1	1.95	0.47
10:k:23:ASP:OD2	17:y:21:GLN:NE2	2.46	0.47
1:A:63:ILE:HB	3:C:335:THR:HG21	1.95	0.47
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:HD21	2.35	0.47
2:b:86:ILE:HG13	46:b:909:HOH:O	2.13	0.47
2:b:383:PHE:CZ	13:o:167:GLY:HA2	2.50	0.47
11:l:13:ASN:C	11:l:13:ASN:HD22	2.22	0.47
26:t:102:BCR:C23	26:t:102:BCR:C38	2.91	0.47
12:M:16[B]:LEU:CD1	12:m:16[B]:LEU:CG	2.92	0.47
35:T:105:P6G:O19	46:T:201:HOH:O	2.20	0.47
24:b:611:CLA:H192	24:b:611:CLA:C15	2.44	0.47
30:c:525:GOL:H31	46:v:301:HOH:O	2.14	0.47
30:C:523:GOL:O1	43:V:203:HEC:O2D	2.29	0.47
29:A:613:LMG:C43	29:A:613:LMG:C24	2.93	0.47
24:D:403:CLA:HMB1	24:D:403:CLA:HBB1	1.97	0.47
46:a:670:HOH:O	32:d:410:LHG:H381	2.14	0.47
2:b:224:ARG:HD3	7:h:25:TRP:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:c:512:CLA:HMB3	24:c:512:CLA:HBB1	1.96	0.47
4:D:13:GLY:HA3	36:D:419:EDO:H21	1.97	0.47
26:T:102:BCR:H23C	26:T:102:BCR:C38	2.37	0.47
5:e:13:ILE:HG21	41:e:107:HEM:HAD1	1.96	0.47
12:M:5:GLN:C	46:M:203:HOH:O	2.57	0.47
4:d:49:LEU:HD13	26:d:406:BCR:C15	2.45	0.47
2:b:285:ASN:HB3	46:b:977:HOH:O	2.14	0.46
3:c:337:LEU:CB	30:c:529:GOL:H2	2.45	0.46
2:B:223[A]:GLN:OE1	2:B:227:LYS:HD2	2.15	0.46
26:K:101:BCR:H321	26:K:101:BCR:HC8	1.97	0.46
1:a:249:VAL:HG12	2:b:491:VAL:HG23	1.96	0.46
2:B:36[A]:SER:OG	26:B:619:BCR:H362	2.15	0.46
24:B:608:CLA:HMB1	24:B:608:CLA:HBB1	1.98	0.46
24:B:616:CLA:HBB1	24:B:616:CLA:HMB3	1.98	0.46
1:a:215:HIS:HA	27:a:412:PL9:O1	2.16	0.46
15:u:58:VAL:HG12	15:u:79:LEU:HD22	1.96	0.46
24:B:602:CLA:H143	24:B:602:CLA:C1B	2.44	0.46
31:Y:101:LMT:O2B	31:Y:101:LMT:H4'	2.16	0.46
24:a:407:CLA:HBC3	24:a:407:CLA:HMC1	1.97	0.46
26:A:610:BCR:C23	26:A:610:BCR:H382	2.46	0.46
24:B:607:CLA:HBB1	24:B:607:CLA:CMB	2.46	0.46
16:V:30:LYS:NZ	46:V:305:HOH:O	2.49	0.46
2:b:70:GLY:HA2	2:b:178:VAL:HG21	1.97	0.46
2:b:24:LEU:HD21	24:b:617:CLA:CAB	2.46	0.46
24:B:614:CLA:HBB1	24:B:614:CLA:HMB1	1.97	0.46
27:a:412:PL9:H512	28:x:101:SQD:C15	2.45	0.46
2:b:223[B]:GLN:NE2	46:b:714:HOH:O	2.49	0.46
24:c:504:CLA:HBB1	24:c:504:CLA:HMB1	1.98	0.46
1:a:248:ILE:HD11	46:a:596:HOH:O	2.16	0.45
13:o:179:GLU:HG2	34:o:308:PGE:O1	2.16	0.45
26:K:101:BCR:C8	26:K:101:BCR:H311	2.46	0.45
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.52	0.45
17:y:27[B]:MET:HE3	17:y:27[B]:MET:HB3	1.88	0.45
28:A:622:SQD:H382	33:I:104:PG4:H12	1.97	0.45
5:e:9:PRO:HA	32:e:101:LHG:HC2	1.99	0.45
28:A:612:SQD:C38	9:J:22:ILE:HD11	2.46	0.45
24:c:501:CLA:H42	24:c:502:CLA:HMD3	1.99	0.45
29:B:634:LMG:H292	29:B:634:LMG:H122	1.98	0.45
26:k:101:BCR:H321	26:k:101:BCR:HC8	1.97	0.45
4:D:272:LEU:C	4:D:272:LEU:HD23	2.42	0.45
4:D:304:ARG:NH1	46:D:505:HOH:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:O:308:PGE:H5	46:O:548:HOH:O	2.16	0.45
26:T:102:BCR:C38	26:T:102:BCR:C23	2.95	0.45
24:D:404:CLA:HBC3	24:D:404:CLA:HHD	1.99	0.45
26:T:102:BCR:H382	26:T:102:BCR:C23	2.39	0.45
27:A:611:PL9:H103	27:A:611:PL9:C2	2.47	0.45
24:C:511:CLA:HAA1	24:C:511:CLA:HBD	1.98	0.45
31:M:101:LMT:H6D	11:l:9:PRO:HA	1.99	0.45
30:a:416:GOL:H32	5:e:63:ILE:HD11	1.99	0.45
26:b:619:BCR:H331	26:b:619:BCR:HC8	1.99	0.45
3:c:203:THR:O	3:c:235:GLY:HA3	2.17	0.45
2:B:157:HIS:CE1	24:B:607:CLA:NA	2.85	0.45
2:B:461:LEU:HD22	32:D:409:LHG:H301	1.99	0.44
5:E:10:PHE:CE1	41:E:113:HEM:HBD2	2.51	0.44
5:E:8[B]:ARG:HB3	5:E:13:ILE:HD11	1.99	0.44
1:A:114:LEU:C	1:A:114:LEU:HD23	2.42	0.44
24:A:606:CLA:CBD	24:D:403:CLA:HAC2	2.47	0.44
2:B:422:ARG:O	2:B:425:ILE:HG12	2.18	0.44
24:D:405:CLA:H171	18:X:15[A]:LEU:HG	1.99	0.44
11:L:13:ASN:C	11:L:13:ASN:HD22	2.25	0.44
26:b:620:BCR:H383	26:b:620:BCR:C23	2.48	0.44
24:c:505:CLA:HBB1	24:c:505:CLA:CMB	2.47	0.44
41:e:107:HEM:HMC2	6:f:31:ILE:HG13	1.99	0.44
38:B:623:HTG:H4	46:O:427:HOH:O	2.16	0.44
26:T:102:BCR:H311	26:T:102:BCR:C8	2.44	0.44
13:O:58:ASN:ND2	2:b:431:GLU:OE1	2.51	0.44
1:A:84:PRO:HA	1:A:112:TYR:CG	2.52	0.44
2:B:84:THR:HG21	46:o:631:HOH:O	2.18	0.44
3:C:391:ARG:NH1	46:C:612:HOH:O	2.50	0.44
26:C:514:BCR:H353	29:C:526:LMG:H262	1.99	0.44
24:C:505:CLA:HBC2	26:C:515:BCR:H341	2.00	0.44
26:C:515:BCR:H382	26:C:515:BCR:H23C	1.98	0.44
16:V:65:PRO:O	44:V:216:2PE:H242	2.17	0.44
2:b:216:HIS:CE1	24:b:610:CLA:C1A	3.00	0.44
16:v:41:HIS:HA	16:v:45:ILE:O	2.18	0.44
24:B:602:CLA:HHC	24:B:602:CLA:CBB	2.47	0.44
3:c:323:LYS:HD2	30:c:525:GOL:O2	2.17	0.44
3:C:437:PHE:CZ	24:C:510:CLA:HMB2	2.53	0.43
26:a:411:BCR:H24C	26:a:411:BCR:H371	1.89	0.43
46:b:926:HOH:O	30:o:305:GOL:C3	2.66	0.43
46:c:672:HOH:O	13:o:149:PRO:HB2	2.18	0.43
3:C:149:TYR:CZ	24:C:509:CLA:H201	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:58:ASN:O	13:O:60:ARG:N	2.51	0.43
26:d:406:BCR:H11C	26:d:406:BCR:H341	1.93	0.43
29:d:412:LMG:H292	29:d:412:LMG:H122	1.99	0.43
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.53	0.43
16:V:55[B]:ARG:NH1	46:V:306:HOH:O	2.50	0.43
3:c:162:GLY:HA2	3:c:248:GLY:HA2	2.00	0.43
24:c:505:CLA:HBC2	26:c:515:BCR:H341	2.00	0.43
4:d:85:MET:HE1	4:d:96:GLU:HG2	2.00	0.43
15:U:51:LYS:HB2	46:U:348:HOH:O	2.17	0.43
26:c:527:BCR:C12	26:k:101:BCR:H333	2.49	0.43
4:d:209:LEU:HD23	4:d:209:LEU:C	2.43	0.43
3:C:286:ALA:HB2	24:C:502:CLA:HMD2	2.00	0.43
24:C:502:CLA:H61	24:C:512:CLA:H42	1.99	0.43
13:O:66:VAL:HB	13:O:67:PRO:HD2	2.00	0.43
3:c:57:ALA:HA	46:c:846:HOH:O	2.17	0.43
3:c:338:GLY:HA3	3:c:341:LEU:O	2.18	0.43
24:c:504:CLA:H142	29:c:519:LMG:C43	2.48	0.43
3:C:318:LEU:C	3:C:318:LEU:HD23	2.44	0.43
26:k:101:BCR:HC7	26:k:101:BCR:H331	1.89	0.43
26:B:619:BCR:H20C	26:B:619:BCR:H361	1.87	0.43
24:C:507:CLA:H61	24:C:507:CLA:H41	1.83	0.43
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.43
25:A:608:PHO:NC	25:A:608:PHO:ND	2.67	0.43
3:C:353:GLY:H	30:C:528:GOL:C2	2.31	0.43
24:C:505:CLA:HBB1	24:C:505:CLA:HMB3	2.01	0.43
11:L:14:ARG:HB3	14:T:25[A]:GLU:HG2	2.01	0.43
4:d:192:THR:HG23	24:d:404:CLA:HBC2	2.01	0.43
26:B:618:BCR:H24C	26:B:618:BCR:H371	1.88	0.43
26:a:411:BCR:C23	26:a:411:BCR:H382	2.49	0.43
2:B:70:GLY:HA2	2:B:178:VAL:HG21	2.01	0.43
3:C:128:GLY:HA3	24:C:513:CLA:C3C	2.49	0.43
24:D:403:CLA:H203	24:D:403:CLA:H162	1.65	0.43
26:T:102:BCR:HC7	26:T:102:BCR:H331	1.80	0.43
30:U:201:GOL:H12	46:U:366:HOH:O	2.19	0.43
13:o:69:LYS:NZ	46:o:424:HOH:O	2.52	0.43
24:A:607:CLA:HMB1	24:A:607:CLA:HBB1	2.01	0.42
26:A:610:BCR:H382	26:A:610:BCR:H23C	2.01	0.42
28:A:612:SQD:H381	9:J:22:ILE:HD11	2.01	0.42
24:B:615:CLA:H72	26:B:618:BCR:H362	2.01	0.42
5:E:27:ILE:HG12	41:E:113:HEM:HMC3	2.01	0.42
24:c:509:CLA:HMB1	24:c:509:CLA:HBB1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:437:PHE:CE2	24:C:510:CLA:HMB2	2.54	0.42
4:D:192:THR:HG23	24:D:404:CLA:HBC2	2.01	0.42
2:b:63:LEU:N	2:b:64:PRO:HD2	2.34	0.42
1:A:121[A]:LEU:HD23	29:A:613:LMG:H202	2.01	0.42
3:c:17:ALA:HB1	3:c:19:ASN:HD22	1.83	0.42
3:C:356:MET:CE	30:C:528:GOL:H12	2.50	0.42
26:c:514:BCR:H331	26:c:514:BCR:C8	2.49	0.42
4:d:27:PHE:CD1	32:e:101:LHG:HC12	2.55	0.42
3:C:443:TRP:CE2	24:C:508:CLA:HMD2	2.55	0.42
24:C:509:CLA:HBB1	24:C:509:CLA:CMB	2.49	0.42
24:a:408:CLA:HMB1	24:a:408:CLA:HBB1	2.01	0.42
3:c:381:LYS:NZ	13:o:99:ASP:OD2	2.40	0.42
13:o:39[B]:ARG:NE	46:o:413:HOH:O	2.42	0.42
16:V:55[B]:ARG:CZ	46:V:306:HOH:O	2.68	0.42
2:b:467:ILE:HG13	4:d:126:MET:HE1	2.02	0.42
2:b:482:ILE:O	2:b:483:ASP:C	2.63	0.42
3:c:127:PHE:CE1	29:z:101:LMG:H351	2.55	0.42
11:l:13:ASN:ND2	11:l:16:SER:H	2.17	0.42
15:u:70:ARG:HD2	46:u:414:HOH:O	2.19	0.42
24:c:510:CLA:HBC3	24:c:510:CLA:H192	2.01	0.42
24:A:606:CLA:HMB1	24:A:606:CLA:HBB1	2.02	0.42
29:B:634:LMG:H301	29:B:634:LMG:HC91	2.01	0.42
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.02	0.42
7:h:39:LEU:C	7:h:39:LEU:HD23	2.44	0.42
3:C:53:HIS:CB	24:C:512:CLA:HMD1	2.50	0.42
15:u:45:LEU:HD21	15:u:71:GLN:HB3	2.01	0.42
27:A:611:PL9:H532	46:A:848:HOH:O	2.18	0.42
28:A:616:SQD:H222	26:T:102:BCR:C32	2.50	0.42
1:a:96:ILE:HG12	1:a:105:TRP:CE2	2.55	0.42
26:k:101:BCR:H382	26:k:101:BCR:H23C	2.02	0.42
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.02	0.41
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.92	0.41
29:C:526:LMG:H202	38:C:532:HTG:H7'1	2.02	0.41
24:D:405:CLA:H193	18:X:11:PHE:HB3	2.02	0.41
5:E:13:ILE:HG21	41:E:113:HEM:CAD	2.50	0.41
2:b:308:LYS:NZ	30:b:629:GOL:H11	2.35	0.41
25:d:401:PHO:HBC2	25:d:401:PHO:HHD	2.02	0.41
2:B:216:HIS:CE1	24:B:610:CLA:C1A	3.03	0.41
3:C:25:ASN:HD21	3:C:31:SER:HA	1.84	0.41
3:C:449:ARG:NH1	46:C:610:HOH:O	2.50	0.41
1:a:84:PRO:HA	1:a:112:TYR:CG	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:515:BCR:H20C	26:c:515:BCR:H361	1.88	0.41
18:x:38:GLN:HE22	39:x:104:1PE:C22	2.33	0.41
2:B:194:ASN:C	2:B:194:ASN:OD1	2.62	0.41
29:B:634:LMG:H121	4:D:23:LYS:NZ	2.35	0.41
4:D:283:ALA:O	4:D:287:VAL:HG23	2.21	0.41
2:b:157:HIS:CE1	24:b:607:CLA:NA	2.88	0.41
3:c:21:ILE:HD12	33:c:533:PG4:H82	2.02	0.41
3:c:391:ARG:NH2	46:c:607:HOH:O	2.41	0.41
13:o:49[A]:THR:CG2	46:o:610:HOH:O	2.67	0.41
13:o:53:LYS:HE3	13:o:65:PHE:CE1	2.55	0.41
7:H:63[B]:LYS:NZ	46:H:201:HOH:O	2.42	0.41
27:a:412:PL9:H403	6:f:22:ALA:HB2	2.03	0.41
24:B:615:CLA:C10	29:B:621:LMG:C43	2.99	0.41
26:B:618:BCR:H20C	26:B:618:BCR:H361	1.97	0.41
24:C:501:CLA:H192	24:C:506:CLA:C1B	2.50	0.41
1:a:214:MET:HG2	27:a:412:PL9:C10	2.47	0.41
26:b:620:BCR:C23	26:b:620:BCR:C38	2.98	0.41
3:c:437:PHE:CE2	24:c:510:CLA:HMB3	2.55	0.41
4:d:316:THR:HG21	46:d:617:HOH:O	2.19	0.41
26:B:620:BCR:C23	26:B:620:BCR:H383	2.51	0.41
26:D:406:BCR:H383	26:D:406:BCR:H23C	2.01	0.41
5:E:20:TRP:CD1	9:J:8:ILE:HD12	2.56	0.41
1:a:256:GLY:O	1:a:260:PHE:C	2.63	0.41
26:k:101:BCR:HC8	26:k:101:BCR:H311	2.01	0.41
27:A:611:PL9:H251	27:A:611:PL9:H271	1.79	0.41
5:E:18:ARG:NH1	41:E:113:HEM:O2A	2.52	0.41
12:M:20:VAL:HG22	12:m:20:VAL:HG11	2.02	0.41
3:c:334:PRO:HA	13:o:153:THR:OG1	2.20	0.41
31:u:203:LMT:H6D	46:u:408:HOH:O	2.20	0.41
26:B:620:BCR:HC8	26:B:620:BCR:C33	2.47	0.41
9:J:7[A]:ARG:NH2	46:J:202:HOH:O	2.54	0.41
11:L:13:ASN:ND2	11:L:16:SER:H	2.18	0.41
26:c:527:BCR:H23C	26:c:527:BCR:H383	2.03	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.03	0.41
24:A:606:CLA:H203	24:A:606:CLA:H161	1.78	0.41
2:B:248:ALA:HA	24:B:604:CLA:H42	2.02	0.41
24:B:602:CLA:H112	24:B:602:CLA:H142	1.89	0.41
4:D:336:MHS:N	4:D:336:MHS:HM1	2.36	0.41
25:D:401:PHO:HBB1	25:D:401:PHO:HMB1	2.03	0.41
26:a:411:BCR:C8	26:a:411:BCR:H331	2.50	0.41
2:b:27:THR:HG22	2:b:107:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:d:401:PHO:HBB1	25:d:401:PHO:HMB1	2.03	0.41
24:d:403:CLA:H203	24:d:403:CLA:H162	1.74	0.41
30:C:523:GOL:C1	16:V:49:ASN:HD22	2.33	0.41
1:a:63:ILE:HB	3:c:335:THR:HG21	2.02	0.41
24:C:506:CLA:HBB1	24:C:506:CLA:CMB	2.51	0.40
4:D:126:MET:HE3	4:D:143:ALA:O	2.21	0.40
30:U:201:GOL:C1	46:U:366:HOH:O	2.69	0.40
3:c:441:HIS:CE1	24:c:505:CLA:ND	2.90	0.40
4:d:172:SER:HB2	4:d:177:ALA:HB1	2.03	0.40
13:o:43:LEU:HB3	13:o:81:ILE:HB	2.03	0.40
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.02	0.40
3:C:213[B]:LEU:HD21	26:C:515:BCR:C20	2.51	0.40
9:J:26:GLY:HA2	31:J:103:LMT:H81	2.03	0.40
3:c:31:SER:HB2	3:c:41:ARG:HG2	2.02	0.40
31:M:102:LMT:H91	24:b:615:CLA:H201	2.02	0.40
13:O:49[A]:THR:OG1	13:O:236:GLN:HB2	2.21	0.40
3:c:28:GLN:NE2	4:d:233[B]:ARG:HE	2.20	0.40
32:d:409:LHG:O9	32:l:101:LHG:HC81	2.21	0.40
28:A:622:SQD:H382	33:I:104:PG4:C1	2.51	0.40
4:D:316:THR:HG23	46:D:501:HOH:O	2.22	0.40
24:a:407:CLA:HBB1	24:a:407:CLA:CMB	2.50	0.40
2:b:469:HIS:CE1	24:b:612:CLA:NA	2.89	0.40
24:b:615:CLA:H193	24:b:615:CLA:H162	1.92	0.40
26:b:619:BCR:H20C	26:b:619:BCR:H361	1.92	0.40
3:c:444:HIS:CE1	24:c:508:CLA:NA	2.89	0.40
24:b:614:CLA:HBB1	24:b:614:CLA:HMB1	2.03	0.40
26:t:102:BCR:H11C	26:t:102:BCR:H341	1.98	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:d:408:DGD:O5E	46:v:404:HOH:O[4_456]	2.18	0.02

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	336/344 (98%)	332 (99%)	3 (1%)	1 (0%)	36	29
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	36	29
2	B	513/506 (101%)	508 (99%)	5 (1%)	0	100	100
2	b	514/506 (102%)	505 (98%)	9 (2%)	0	100	100
3	C	454/458 (99%)	444 (98%)	9 (2%)	1 (0%)	43	36
3	c	460/458 (100%)	446 (97%)	11 (2%)	3 (1%)	18	10
4	D	340/342 (99%)	331 (97%)	9 (3%)	0	100	100
4	d	341/342 (100%)	334 (98%)	7 (2%)	0	100	100
5	E	82/83 (99%)	82 (100%)	0	0	100	100
5	e	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
6	F	32/44 (73%)	32 (100%)	0	0	100	100
6	f	30/44 (68%)	29 (97%)	0	1 (3%)	3	0
7	H	65/65 (100%)	58 (89%)	7 (11%)	0	100	100
7	h	64/65 (98%)	59 (92%)	4 (6%)	1 (2%)	7	2
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
9	J	39/40 (98%)	39 (100%)	0	0	100	100
9	j	37/40 (92%)	37 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	37/37 (100%)	37 (100%)	0	0	100	100
12	M	34/36 (94%)	34 (100%)	0	0	100	100
12	m	34/36 (94%)	34 (100%)	0	0	100	100
13	O	249/245 (102%)	242 (97%)	3 (1%)	4 (2%)	7	2
13	o	248/245 (101%)	239 (96%)	8 (3%)	1 (0%)	30	22
14	T	29/32 (91%)	29 (100%)	0	0	100	100
14	t	29/32 (91%)	29 (100%)	0	0	100	100
15	U	97/104 (93%)	95 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	u	95/104 (91%)	93 (98%)	2 (2%)	0	100	100
16	V	137/137 (100%)	132 (96%)	5 (4%)	0	100	100
16	v	136/137 (99%)	133 (98%)	3 (2%)	0	100	100
17	Y	28/30 (93%)	28 (100%)	0	0	100	100
17	y	28/30 (93%)	28 (100%)	0	0	100	100
18	X	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
18	x	38/41 (93%)	37 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	57 (95%)	3 (5%)	0	100	100
19	z	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
All	All	5280/5362 (98%)	5161 (98%)	106 (2%)	13 (0%)	43	36

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	O	58	ASN
13	O	59	LYS
3	C	416	SER
3	c	416[A]	SER
3	c	416[B]	SER
13	o	3	ALA
13	O	3	ALA
13	O	4	THR
3	c	19	ASN
7	h	65	LEU
1	A	259	ILE
6	f	15	ILE
1	a	259	ILE

5.3.2 Protein sidechains (i)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	273/279 (98%)	271 (99%)	2 (1%)	76 78
1	a	273/279 (98%)	272 (100%)	1 (0%)	84 87
2	B	413/404 (102%)	411 (100%)	2 (0%)	81 84
2	b	414/404 (102%)	410 (99%)	4 (1%)	68 70
3	C	357/357 (100%)	354 (99%)	3 (1%)	73 75
3	c	361/357 (101%)	351 (97%)	10 (3%)	38 32
4	D	277/276 (100%)	275 (99%)	2 (1%)	76 78
4	d	278/276 (101%)	277 (100%)	1 (0%)	84 87
5	E	75/72 (104%)	75 (100%)	0	100 100
5	e	74/72 (103%)	73 (99%)	1 (1%)	59 59
6	F	28/38 (74%)	27 (96%)	1 (4%)	31 23
6	f	26/38 (68%)	25 (96%)	1 (4%)	29 21
7	H	56/54 (104%)	54 (96%)	2 (4%)	31 23
7	h	55/54 (102%)	53 (96%)	2 (4%)	31 23
8	I	34/34 (100%)	34 (100%)	0	100 100
8	i	34/34 (100%)	34 (100%)	0	100 100
9	J	29/28 (104%)	27 (93%)	2 (7%)	14 7
9	j	27/28 (96%)	26 (96%)	1 (4%)	30 22
10	K	30/30 (100%)	29 (97%)	1 (3%)	33 26
10	k	30/30 (100%)	27 (90%)	3 (10%)	7 3
11	L	36/35 (103%)	34 (94%)	2 (6%)	19 11
11	l	37/35 (106%)	36 (97%)	1 (3%)	39 34
12	M	32/32 (100%)	32 (100%)	0	100 100
12	m	31/32 (97%)	31 (100%)	0	100 100
13	O	212/206 (103%)	209 (99%)	3 (1%)	59 59
13	o	211/206 (102%)	207 (98%)	4 (2%)	50 47
14	T	27/28 (96%)	27 (100%)	0	100 100
14	t	27/28 (96%)	27 (100%)	0	100 100
15	U	86/89 (97%)	84 (98%)	2 (2%)	44 40
15	u	84/89 (94%)	83 (99%)	1 (1%)	63 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	119/117 (102%)	119 (100%)	0	100	100
16	v	118/117 (101%)	118 (100%)	0	100	100
17	Y	23/23 (100%)	23 (100%)	0	100	100
17	y	23/23 (100%)	23 (100%)	0	100	100
18	X	34/34 (100%)	33 (97%)	1 (3%)	37	31
18	x	33/34 (97%)	32 (97%)	1 (3%)	36	30
19	Z	52/52 (100%)	50 (96%)	2 (4%)	29	21
19	z	52/52 (100%)	51 (98%)	1 (2%)	50	47
All	All	4381/4376 (100%)	4324 (99%)	57 (1%)	63	61

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	LEU
1	A	229	GLU
2	B	489	GLU
2	B	492	GLU
3	C	29	GLU
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	90	LEU
6	F	44	GLN
7	H	12[A]	ARG
7	H	12[B]	ARG
9	J	7[A]	ARG
9	J	7[B]	ARG
10	K	10	LYS
11	L	1	MET
11	L	13	ASN
13	O	57	LYS
13	O	58	ASN
13	O	62	GLU
15	U	8	GLU
15	U	70	ARG
18	X	40	SER
19	Z	6	GLN
19	Z	42	LEU
1	a	244	GLU

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Mol	Chain	Res	Type
2	b	79	SER
2	b	472	ARG
2	b	489	GLU
2	b	492	GLU
3	c	16	GLU
3	c	19	ASN
3	c	145[A]	SER
3	c	145[B]	SER
3	c	240	ILE
3	c	289	PHE
3	c	315	MET
3	c	355	THR
3	c	462[A]	GLU
3	c	462[B]	GLU
4	d	329	MET
5	e	5	THR
6	f	44	GLN
7	h	12[A]	ARG
7	h	12[B]	ARG
9	j	7	ARG
10	k	10	LYS
10	k	13	GLU
10	k	17	ILE
11	l	13	ASN
13	o	23	ASP
13	o	58	ASN
13	o	62	GLU
13	o	89	SER
15	u	70	ARG
18	x	37	VAL
19	z	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	165	GLN
1	A	261	GLN
1	A	315	ASN
1	A	338	ASN
2	B	53	ASN
2	B	281	GLN

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Mol	Chain	Res	Type
2	B	282	GLN
2	B	409	GLN
3	C	25	ASN
3	C	201	ASN
3	C	373	ASN
4	D	83	ASN
4	D	98	GLN
4	D	186	GLN
4	D	255	GLN
4	D	301	GLN
4	D	332	GLN
5	E	74	GLN
11	L	13	ASN
13	O	88	ASN
13	O	124	ASN
13	O	147	ASN
13	O	155	ASN
16	V	34	GLN
16	V	118	HIS
19	Z	58	ASN
1	a	165	GLN
1	a	338	ASN
2	b	14	ASN
2	b	53	ASN
2	b	281	GLN
2	b	497	GLN
3	c	19	ASN
3	c	28	GLN
3	c	201	ASN
4	d	83	ASN
4	d	186	GLN
4	d	255	GLN
11	l	13	ASN
12	m	33	GLN
13	o	155	ASN
18	x	38	GLN
19	z	31	GLN
19	z	58	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	I	1	8	8,9,10	0.74	0	8,9,11	1.17	1 (12%)
4	MHS	D	336	4	10,11,12	1.75	2 (20%)	5,14,16	3.92	4 (80%)
14	FME	T	1[A]	-	8,9,10	0.58	0	8,9,11	1.22	2 (25%)
8	FME	i	1	8	8,9,10	0.46	0	8,9,11	1.53	2 (25%)
14	FME	T	1[B]	-	8,9,10	0.48	0	8,9,11	1.10	1 (12%)
12	FME	m	1[B]	-	8,9,10	0.86	0	8,9,11	1.62	2 (25%)
12	FME	m	1[A]	-	8,9,10	0.55	0	8,9,11	1.35	1 (12%)
4	MHS	d	336	4	10,11,12	2.17	3 (30%)	5,14,16	2.86	2 (40%)
12	FME	M	1	12	8,9,10	1.50	1 (12%)	8,9,11	1.32	1 (12%)
14	FME	t	1[A]	-	8,9,10	0.93	0	8,9,11	0.98	0
14	FME	t	1[B]	-	8,9,10	0.70	0	8,9,11	0.98	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
8	FME	I	1	8	-	0/7/9/11	-
4	MHS	D	336	4	-	0/5/6/8	0/1/1/1
14	FME	T	1[A]	-	-	0/7/9/11	-
8	FME	i	1	8	-	0/7/9/11	-
14	FME	T	1[B]	-	-	2/7/9/11	-
12	FME	m	1[B]	-	-	3/7/9/11	-
12	FME	m	1[A]	-	-	1/7/9/11	-
4	MHS	d	336	4	-	0/5/6/8	0/1/1/1
12	FME	M	1	12	-	1/7/9/11	-
14	FME	t	1[A]	-	-	0/7/9/11	-
14	FME	t	1[B]	-	-	2/7/9/11	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	336	MHS	CD2-NE2	-4.37	1.30	1.37
4	d	336	MHS	CG-ND1	-3.96	1.31	1.38
4	D	336	MHS	CD2-NE2	-3.91	1.30	1.37
12	M	1	FME	CA-N	-3.09	1.42	1.46
4	d	336	MHS	CM-ND1	2.55	1.51	1.46
4	D	336	MHS	CG-ND1	-2.45	1.34	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	336	MHS	ND1-CE1-NE2	-6.40	109.13	112.94
4	d	336	MHS	ND1-CE1-NE2	-4.93	110.01	112.94
4	D	336	MHS	CM-ND1-CG	4.20	131.17	126.69
4	d	336	MHS	CM-ND1-CG	3.38	130.28	126.69
4	D	336	MHS	CD2-NE2-CE1	2.92	109.06	105.24
8	i	1	FME	O-C-CA	-2.78	117.61	124.77
4	D	336	MHS	CM-ND1-CE1	-2.69	121.25	126.28
12	M	1	FME	CG-CB-CA	2.67	121.03	112.87
12	m	1[A]	FME	O-C-CA	-2.44	118.48	124.77
12	m	1[B]	FME	CB-CG-SD	-2.41	97.90	113.82
14	T	1[B]	FME	O-C-CA	-2.30	118.85	124.77
14	T	1[A]	FME	O-C-CA	-2.29	118.89	124.77
8	I	1	FME	O-C-CA	-2.16	119.21	124.77
14	T	1[A]	FME	CG-CB-CA	2.16	119.47	112.87
12	m	1[B]	FME	O1-CN-N	-2.09	119.93	125.32
8	i	1	FME	CB-CA-N	2.05	114.24	110.52

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	M	1	FME	O-C-CA-CB
14	T	1[B]	FME	CB-CG-SD-CE
14	t	1[B]	FME	CB-CG-SD-CE
14	T	1[B]	FME	C-CA-CB-CG
14	t	1[B]	FME	C-CA-CB-CG
12	m	1[B]	FME	CB-CG-SD-CE
12	m	1[A]	FME	CA-CB-CG-SD
12	m	1[B]	FME	C-CA-CB-CG
12	m	1[B]	FME	CB-CA-N-CN

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	336	MHS	2	0
8	i	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 447 ligands modelled in this entry, 18 are monoatomic - leaving 429 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	$\#\|Z\| > 2$
40	DGD	C	518	-	63,63,67	0.80	2 (3%)	77,77,81	1.10	6 (7%)
26	BCR	k	101	-	41,41,41	1.01	1 (2%)	56,56,56	1.68	12 (21%)
33	PG4	J	104	-	12,12,12	0.60	0	11,11,11	0.31	0
36	EDO	E	112	-	3,3,3	0.57	0	2,2,2	0.12	0
30	GOL	F	101	42	5,5,5	0.53	0	5,5,5	0.77	0
38	HTG	C	529	-	19,19,19	1.18	2 (10%)	23,24,24	2.05	4 (17%)
24	CLA	c	512	3	69,73,73	1.87	16 (23%)	82,113,113	2.39	27 (32%)
36	EDO	B	655	-	3,3,3	0.41	0	2,2,2	0.46	0
23	BCT	m	104[B]	-	3,3,3	1.08	0	2,3,3	1.84	1 (50%)
33	PG4	A	619	-	12,12,12	0.71	0	11,11,11	0.60	0
34	PGE	c	536	-	9,9,9	0.62	0	8,8,8	0.27	0
28	SQD	l	102	-	52,54,54	1.27	4 (7%)	62,65,65	1.82	13 (20%)
28	SQD	A	616	-	52,54,54	1.12	3 (5%)	62,65,65	1.55	9 (14%)
36	EDO	B	656	-	3,3,3	1.04	0	2,2,2	0.25	0
33	PG4	x	102	-	12,12,12	0.65	0	11,11,11	0.37	0
26	BCR	c	515	-	41,41,41	1.28	3 (7%)	56,56,56	1.68	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	c	506	3	69,73,73	1.94	16 (23%)	82,113,113	2.28	28 (34%)
34	PGE	c	540	-	9,9,9	0.67	0	8,8,8	0.46	0
24	CLA	B	614	2	69,73,73	1.58	12 (17%)	82,113,113	2.02	19 (23%)
31	LMT	A	617	-	36,36,36	1.09	2 (5%)	47,47,47	1.60	9 (19%)
30	GOL	u	202	-	5,5,5	0.84	0	5,5,5	0.39	0
33	PG4	I	102	-	12,12,12	0.61	0	11,11,11	0.41	0
38	HTG	o	301	-	19,19,19	1.88	2 (10%)	23,24,24	1.02	1 (4%)
30	GOL	C	524	-	5,5,5	0.81	0	5,5,5	1.09	0
33	PG4	I	104	-	12,12,12	0.50	0	11,11,11	0.48	0
34	PGE	b	641	-	9,9,9	0.39	0	8,8,8	0.73	0
24	CLA	C	508	3	64,68,73	1.70	16 (25%)	76,107,113	2.27	21 (27%)
33	PG4	C	535	-	12,12,12	0.96	0	11,11,11	0.82	0
33	PG4	C	536	-	12,12,12	0.69	0	11,11,11	0.65	0
30	GOL	c	529	-	5,5,5	1.03	0	5,5,5	1.45	1 (20%)
30	GOL	b	626	-	5,5,5	0.80	0	5,5,5	0.83	0
33	PG4	j	104	-	12,12,12	0.70	0	11,11,11	0.72	0
24	CLA	B	616	2	69,73,73	1.74	18 (26%)	82,113,113	2.27	21 (25%)
36	EDO	X	104	-	3,3,3	0.91	0	2,2,2	0.40	0
30	GOL	B	626	-	5,5,5	0.85	0	5,5,5	0.76	0
38	HTG	b	623	-	19,19,19	1.19	1 (5%)	23,24,24	1.54	5 (21%)
43	HEC	V	203	16	50,50,50	1.59	8 (16%)	68,82,82	1.55	10 (14%)
33	PG4	i	103	-	12,12,12	0.64	0	11,11,11	0.47	0
33	PG4	B	639	-	12,12,12	0.90	0	11,11,11	0.73	0
31	LMT	b	622	-	36,36,36	0.82	1 (2%)	47,47,47	1.44	5 (10%)
24	CLA	B	606	2	69,73,73	1.76	17 (24%)	82,113,113	2.46	30 (36%)
38	HTG	c	523	-	19,19,19	0.87	1 (5%)	23,24,24	1.38	4 (17%)
30	GOL	O	304	-	5,5,5	0.44	0	5,5,5	0.54	0
26	BCR	d	406	-	41,41,41	1.55	4 (9%)	56,56,56	2.25	17 (30%)
33	PG4	a	420	-	12,12,12	0.58	0	11,11,11	0.37	0
24	CLA	B	607	2	59,63,73	1.74	18 (30%)	70,101,113	2.64	26 (37%)
30	GOL	y	101	-	5,5,5	0.69	0	5,5,5	0.72	0
38	HTG	H	101	-	19,19,19	1.04	1 (5%)	23,24,24	1.56	5 (21%)
39	1PE	B	653	-	15,15,15	0.61	0	14,14,14	0.41	0
29	LMG	d	412	-	55,55,55	1.06	3 (5%)	63,63,63	1.18	5 (7%)
29	LMG	j	101	42	47,47,55	1.02	3 (6%)	55,55,63	1.05	3 (5%)
35	P6G	b	648	-	18,18,18	0.62	0	17,17,17	0.74	0
33	PG4	I	103	-	12,12,12	0.74	0	11,11,11	0.57	0
24	CLA	C	501	3	69,73,73	1.73	17 (24%)	82,113,113	2.59	26 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	B	604	2	69,73,73	1.72	16 (23%)	82,113,113	2.23	22 (26%)
38	HTG	c	530	-	19,19,19	1.61	3 (15%)	23,24,24	1.18	3 (13%)
34	PGE	i	105	-	9,9,9	0.66	0	8,8,8	0.68	0
30	GOL	b	629	-	5,5,5	0.71	0	5,5,5	1.16	0
25	PHO	A	608	-	58,69,69	1.96	14 (24%)	55,99,99	2.40	14 (25%)
36	EDO	c	542	-	3,3,3	0.60	0	2,2,2	0.43	0
31	LMT	f	101	-	36,36,36	0.95	1 (2%)	47,47,47	1.34	5 (10%)
30	GOL	v	207	-	5,5,5	0.51	0	5,5,5	0.35	0
24	CLA	b	603	2	69,73,73	1.71	15 (21%)	82,113,113	2.13	24 (29%)
30	GOL	B	629	-	5,5,5	0.94	0	5,5,5	0.39	0
30	GOL	v	205	-	5,5,5	0.45	0	5,5,5	0.62	0
34	PGE	V	215	-	9,9,9	0.87	0	8,8,8	0.62	0
28	SQD	A	622	-	52,54,54	1.32	3 (5%)	62,65,65	1.46	9 (14%)
24	CLA	A	606	1	69,73,73	1.58	15 (21%)	82,113,113	1.99	22 (26%)
26	BCR	B	620	-	41,41,41	1.15	3 (7%)	56,56,56	1.39	7 (12%)
24	CLA	c	510	3	69,73,73	1.87	17 (24%)	82,113,113	2.03	22 (26%)
36	EDO	D	419	-	3,3,3	0.66	0	2,2,2	0.09	0
26	BCR	C	525	-	41,41,41	1.15	4 (9%)	56,56,56	1.69	10 (17%)
24	CLA	b	607	2	59,63,73	1.76	14 (23%)	70,101,113	2.26	27 (38%)
29	LMG	B	634	-	55,55,55	1.26	4 (7%)	63,63,63	1.41	12 (19%)
32	LHG	d	411	-	48,48,48	1.02	3 (6%)	51,54,54	0.85	2 (3%)
35	P6G	D	418	-	18,18,18	0.75	0	17,17,17	0.60	0
33	PG4	V	209	-	12,12,12	0.85	0	11,11,11	1.00	1 (9%)
31	LMT	F	102	-	36,36,36	1.08	3 (8%)	47,47,47	1.26	5 (10%)
33	PG4	V	213	-	12,12,12	0.71	0	11,11,11	0.63	0
24	CLA	b	610	2	69,73,73	1.79	17 (24%)	82,113,113	2.23	22 (26%)
36	EDO	o	311	-	3,3,3	0.45	0	2,2,2	0.32	0
24	CLA	B	613	2	69,73,73	1.55	14 (20%)	82,113,113	1.74	21 (25%)
32	LHG	D	411	-	48,48,48	0.88	2 (4%)	51,54,54	0.86	3 (5%)
26	BCR	D	406	-	41,41,41	1.45	4 (9%)	56,56,56	2.01	14 (25%)
24	CLA	B	610	2	69,73,73	1.55	13 (18%)	82,113,113	2.20	25 (30%)
27	PL9	a	412	-	55,55,55	1.21	2 (3%)	68,69,69	1.82	14 (20%)
40	DGD	c	516	-	63,63,67	0.92	3 (4%)	77,77,81	1.09	4 (5%)
34	PGE	b	644	-	9,9,9	0.63	0	8,8,8	0.37	0
40	DGD	c	517	-	58,58,67	1.01	4 (6%)	72,72,81	1.12	3 (4%)
28	SQD	A	612	-	52,54,54	1.04	3 (5%)	62,65,65	2.08	14 (22%)
38	HTG	B	624	-	19,19,19	0.96	1 (5%)	23,24,24	1.76	5 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	PG4	c	535	-	12,12,12	0.86	0	11,11,11	0.68	0
24	CLA	C	511	3	69,73,73	1.63	11 (15%)	82,113,113	2.14	24 (29%)
26	BCR	T	102	-	41,41,41	1.00	2 (4%)	56,56,56	1.66	12 (21%)
32	LHG	D	409	-	48,48,48	0.86	2 (4%)	51,54,54	1.50	5 (9%)
34	PGE	V	214	-	9,9,9	0.63	0	8,8,8	0.30	0
30	GOL	V	207	-	5,5,5	0.78	0	5,5,5	0.85	0
33	PG4	i	102	-	12,12,12	0.57	0	11,11,11	0.53	0
24	CLA	D	403	46	69,73,73	1.87	17 (24%)	82,113,113	2.18	19 (23%)
29	LMG	b	621	-	51,51,55	1.05	3 (5%)	59,59,63	1.68	6 (10%)
34	PGE	B	649	-	9,9,9	0.90	0	8,8,8	0.55	0
38	HTG	C	531	-	19,19,19	1.24	2 (10%)	23,24,24	0.95	2 (8%)
20	OEX	A	601	3,46,1	0,14,14	-	-	-		
30	GOL	v	203	-	5,5,5	0.78	0	5,5,5	0.68	0
23	BCT	m	104[A]	-	3,3,3	1.60	1 (33%)	2,3,3	0.79	0
30	GOL	B	635	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
34	PGE	B	650	-	9,9,9	0.63	0	8,8,8	0.37	0
34	PGE	h	110	-	9,9,9	0.80	0	8,8,8	0.67	0
27	PL9	A	611	-	55,55,55	1.27	7 (12%)	68,69,69	2.20	18 (26%)
33	PG4	H	104	-	12,12,12	0.62	0	11,11,11	0.34	0
24	CLA	b	615	2	69,73,73	1.68	15 (21%)	82,113,113	2.17	24 (29%)
36	EDO	A	625	-	3,3,3	0.58	0	2,2,2	0.37	0
34	PGE	b	639	-	9,9,9	0.62	0	8,8,8	0.43	0
29	LMG	c	520	-	51,51,55	1.19	3 (5%)	59,59,63	1.21	5 (8%)
28	SQD	a	413	-	52,54,54	1.07	4 (7%)	62,65,65	2.09	12 (19%)
34	PGE	t	104	-	9,9,9	0.83	0	8,8,8	0.69	0
29	LMG	A	613	-	51,51,55	0.98	3 (5%)	59,59,63	1.01	3 (5%)
34	PGE	t	105	-	6,6,9	0.68	0	5,5,8	0.50	0
30	GOL	f	104	-	5,5,5	0.79	0	5,5,5	1.28	1 (20%)
30	GOL	A	614	-	5,5,5	1.20	0	5,5,5	0.92	0
34	PGE	E	106	-	9,9,9	0.69	0	8,8,8	0.60	0
40	DGD	c	518	-	63,63,67	0.92	3 (4%)	77,77,81	0.98	7 (9%)
35	P6G	B	651	-	18,18,18	0.52	0	17,17,17	0.66	0
33	PG4	E	103	-	12,12,12	0.64	0	11,11,11	0.52	0
29	LMG	C	526	-	55,55,55	1.06	2 (3%)	63,63,63	1.51	9 (14%)
33	PG4	B	636	-	12,12,12	0.57	0	11,11,11	0.59	0
34	PGE	h	107	-	9,9,9	0.78	0	8,8,8	0.68	0
34	PGE	H	111	-	9,9,9	0.67	0	8,8,8	0.39	0
26	BCR	K	101	-	41,41,41	0.98	1 (2%)	56,56,56	1.49	9 (16%)
26	BCR	h	103	-	41,41,41	1.12	4 (9%)	56,56,56	1.78	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	PG4	b	636	-	12,12,12	0.78	0	11,11,11	0.68	0
30	GOL	V	205	-	5,5,5	0.95	0	5,5,5	1.14	0
35	P6G	D	417	-	18,18,18	0.64	0	17,17,17	0.88	0
34	PGE	H	108	-	9,9,9	0.60	0	8,8,8	0.59	0
33	PG4	X	101	-	12,12,12	0.66	0	11,11,11	0.51	0
34	PGE	o	308	-	9,9,9	0.70	0	8,8,8	0.55	0
32	LHG	d	410	-	48,48,48	0.82	2 (4%)	51,54,54	1.13	3 (5%)
30	GOL	V	201	-	5,5,5	1.05	0	5,5,5	0.51	0
34	PGE	E	107	-	9,9,9	0.77	0	8,8,8	0.76	0
38	HTG	O	303	-	19,19,19	1.48	2 (10%)	23,24,24	1.02	1 (4%)
30	GOL	c	528	-	5,5,5	0.57	0	5,5,5	0.66	0
33	PG4	C	534	-	12,12,12	0.73	0	11,11,11	0.41	0
30	GOL	T	101	-	5,5,5	0.96	0	5,5,5	0.91	0
35	P6G	E	110	-	18,18,18	0.77	0	17,17,17	0.53	0
31	LMT	m	102	-	36,36,36	0.96	1 (2%)	47,47,47	1.69	7 (14%)
35	P6G	I	106	-	18,18,18	0.64	0	17,17,17	0.78	1 (5%)
24	CLA	D	404	4	69,73,73	1.80	19 (27%)	82,113,113	2.20	27 (32%)
25	PHO	a	409	-	58,69,69	1.97	13 (22%)	55,99,99	2.26	15 (27%)
33	PG4	i	104	-	12,12,12	0.51	0	11,11,11	0.41	0
34	PGE	E	105	-	9,9,9	0.73	0	8,8,8	0.47	0
36	EDO	e	106	-	3,3,3	0.38	0	2,2,2	0.53	0
32	LHG	a	419	-	40,40,48	1.22	3 (7%)	43,46,54	1.39	6 (13%)
33	PG4	J	105	-	12,12,12	0.69	0	11,11,11	0.37	0
35	P6G	j	106	-	18,18,18	0.80	0	17,17,17	0.75	0
38	HTG	C	532	-	19,19,19	1.09	2 (10%)	23,24,24	1.78	5 (21%)
24	CLA	b	602	46	69,73,73	1.87	14 (20%)	82,113,113	2.37	26 (31%)
24	CLA	b	614	2	69,73,73	1.77	17 (24%)	82,113,113	2.16	22 (26%)
26	BCR	A	610	-	41,41,41	1.20	4 (9%)	56,56,56	1.53	12 (21%)
30	GOL	v	206	-	5,5,5	0.31	0	5,5,5	0.55	0
34	PGE	b	638	-	9,9,9	1.00	0	8,8,8	0.70	0
38	HTG	C	522	-	19,19,19	1.04	1 (5%)	23,24,24	1.76	3 (13%)
24	CLA	B	603	2	69,73,73	1.78	15 (21%)	82,113,113	2.23	24 (29%)
38	HTG	b	624	-	19,19,19	1.42	2 (10%)	23,24,24	1.27	2 (8%)
31	LMT	t	103	-	36,36,36	0.84	0	47,47,47	1.41	9 (19%)
34	PGE	b	646	-	9,9,9	0.67	0	8,8,8	0.51	0
30	GOL	A	615	-	5,5,5	0.54	0	5,5,5	1.11	0
30	GOL	O	307	-	5,5,5	0.51	0	5,5,5	0.21	0
24	CLA	d	405	4	69,73,73	1.80	18 (26%)	82,113,113	2.30	25 (30%)
34	PGE	B	646	-	9,9,9	0.54	0	8,8,8	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
26	BCR	C	514	-	41,41,41	1.23	4 (9%)	56,56,56	1.89	13 (23%)
34	PGE	f	105	-	9,9,9	0.59	0	8,8,8	0.26	0
26	BCR	t	102	-	41,41,41	1.11	3 (7%)	56,56,56	2.02	18 (32%)
31	LMT	c	521	-	36,36,36	0.83	0	47,47,47	1.67	12 (25%)
30	GOL	B	628	-	5,5,5	0.77	0	5,5,5	1.75	1 (20%)
30	GOL	B	633	-	5,5,5	1.28	1 (20%)	5,5,5	1.31	0
24	CLA	B	612	2	69,73,73	1.52	15 (21%)	82,113,113	2.31	22 (26%)
35	P6G	d	416	-	18,18,18	0.63	0	17,17,17	0.59	0
31	LMT	M	102	-	36,36,36	0.90	0	47,47,47	1.57	2 (4%)
24	CLA	b	617	2	64,68,73	1.71	15 (23%)	76,107,113	2.47	28 (36%)
34	PGE	J	106	-	9,9,9	0.63	0	8,8,8	0.33	0
24	CLA	B	602	46	69,73,73	1.77	17 (24%)	82,113,113	2.61	32 (39%)
30	GOL	C	527	-	5,5,5	0.49	0	5,5,5	0.29	0
30	GOL	e	102	-	5,5,5	0.71	0	5,5,5	0.85	0
33	PG4	b	635	-	12,12,12	0.84	0	11,11,11	0.78	0
39	1PE	B	654	-	15,15,15	0.77	0	14,14,14	0.89	0
36	EDO	H	112	-	3,3,3	0.47	0	2,2,2	0.37	0
33	PG4	C	537	-	12,12,12	0.66	0	11,11,11	0.57	0
24	CLA	A	609	1	69,73,73	1.82	17 (24%)	82,113,113	2.21	27 (32%)
35	P6G	D	416	-	18,18,18	0.72	0	17,17,17	0.59	0
30	GOL	t	101	-	5,5,5	1.27	0	5,5,5	1.16	1 (20%)
38	HTG	h	101	-	19,19,19	1.10	2 (10%)	23,24,24	1.65	5 (21%)
30	GOL	d	413	-	5,5,5	0.81	0	5,5,5	0.96	0
33	PG4	c	532	-	12,12,12	0.90	0	11,11,11	0.81	0
29	LMG	C	520	-	51,51,55	1.27	3 (5%)	59,59,63	1.28	9 (15%)
32	LHG	E	101	-	41,41,48	1.12	2 (4%)	44,47,54	1.15	3 (6%)
32	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.18	4 (7%)
40	DGD	C	516	-	63,63,67	0.91	5 (7%)	77,77,81	1.29	10 (12%)
33	PG4	B	638	-	12,12,12	0.82	0	11,11,11	0.76	0
24	CLA	d	404	4	69,73,73	1.52	15 (21%)	82,113,113	2.24	24 (29%)
39	1PE	V	217	-	15,15,15	0.95	0	14,14,14	1.01	1 (7%)
38	HTG	c	531	-	19,19,19	1.11	2 (10%)	23,24,24	1.74	6 (26%)
38	HTG	a	418	-	19,19,19	1.30	3 (15%)	23,24,24	1.82	8 (34%)
34	PGE	C	539	-	9,9,9	0.93	0	8,8,8	0.86	0
34	PGE	A	621	-	9,9,9	0.73	0	8,8,8	0.48	0
30	GOL	D	413	-	5,5,5	0.58	0	5,5,5	0.90	0
30	GOL	u	201	-	5,5,5	0.74	0	5,5,5	1.18	0
33	PG4	E	102	-	12,12,12	0.61	0	11,11,11	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	505	3	69,73,73	1.94	17 (24%)	82,113,113	2.15	21 (25%)
24	CLA	b	609	2	69,73,73	1.65	15 (21%)	82,113,113	2.09	23 (28%)
24	CLA	c	511	3	69,73,73	1.73	17 (24%)	82,113,113	2.12	24 (29%)
29	LMG	J	101	42	47,47,55	0.76	2 (4%)	55,55,63	0.91	2 (3%)
33	PG4	U	202	-	12,12,12	0.69	0	11,11,11	0.47	0
43	HEC	v	202	16	50,50,50	1.37	8 (16%)	68,82,82	1.69	16 (23%)
24	CLA	c	502	3	69,73,73	1.75	17 (24%)	82,113,113	2.09	22 (26%)
31	LMT	J	103	-	36,36,36	0.92	1 (2%)	47,47,47	1.57	9 (19%)
34	PGE	J	107	-	9,9,9	0.68	0	8,8,8	0.53	0
33	PG4	X	103	-	12,12,12	0.76	0	11,11,11	0.54	0
24	CLA	B	609	2	69,73,73	1.54	15 (21%)	82,113,113	2.08	20 (24%)
30	GOL	f	103	42	5,5,5	0.69	0	5,5,5	0.93	0
38	HTG	C	530	-	19,19,19	0.99	1 (5%)	23,24,24	1.13	2 (8%)
23	BCT	a	406	21	3,3,3	1.49	1 (33%)	2,3,3	2.80	2 (100%)
30	GOL	D	402	-	5,5,5	0.78	0	5,5,5	1.36	1 (20%)
28	SQD	b	633	-	52,54,54	1.39	4 (7%)	62,65,65	1.96	16 (25%)
30	GOL	V	206	-	5,5,5	0.57	0	5,5,5	0.20	0
33	PG4	H	106	-	12,12,12	0.74	0	11,11,11	0.63	0
34	PGE	i	106	-	9,9,9	0.83	0	8,8,8	0.64	0
34	PGE	Y	102	-	9,9,9	0.79	0	8,8,8	0.61	0
34	PGE	I	105	-	9,9,9	0.96	0	8,8,8	0.74	0
36	EDO	d	417	-	3,3,3	0.67	0	2,2,2	0.31	0
24	CLA	B	611	46	69,73,73	1.82	16 (23%)	82,113,113	2.34	30 (36%)
30	GOL	b	627	-	5,5,5	1.26	1 (20%)	5,5,5	1.42	1 (20%)
26	BCR	b	618	-	41,41,41	1.13	3 (7%)	56,56,56	1.51	7 (12%)
34	PGE	E	109	-	9,9,9	0.85	0	8,8,8	0.57	0
34	PGE	o	306	-	9,9,9	0.61	0	8,8,8	0.24	0
36	EDO	E	111	-	3,3,3	0.64	0	2,2,2	0.35	0
33	PG4	X	102	-	12,12,12	0.85	0	11,11,11	0.79	0
32	LHG	d	409	-	48,48,48	0.87	3 (6%)	51,54,54	1.39	6 (11%)
30	GOL	B	627	-	5,5,5	0.70	0	5,5,5	0.94	0
28	SQD	x	101	-	52,54,54	1.22	3 (5%)	62,65,65	1.74	12 (19%)
33	PG4	C	538	-	12,12,12	0.77	0	11,11,11	0.55	0
34	PGE	B	648	-	9,9,9	0.87	0	8,8,8	0.72	0
35	P6G	B	652	-	18,18,18	0.83	0	17,17,17	1.10	1 (5%)
31	LMT	m	101	-	36,36,36	1.03	1 (2%)	47,47,47	1.10	5 (10%)
34	PGE	C	540	-	9,9,9	0.60	0	8,8,8	0.32	0
30	GOL	C	528	-	5,5,5	0.68	0	5,5,5	3.18	4 (80%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	LMG	z	101	-	55,55,55	1.03	2 (3%)	63,63,63	1.18	6 (9%)
33	PG4	B	643	-	12,12,12	0.55	0	11,11,11	0.55	0
24	CLA	C	503	3	69,73,73	1.86	18 (26%)	82,113,113	2.35	23 (28%)
33	PG4	l	103	-	12,12,12	0.66	0	11,11,11	0.50	0
28	SQD	h	105	-	52,54,54	1.39	5 (9%)	62,65,65	1.47	10 (16%)
34	PGE	c	538	-	9,9,9	0.92	0	8,8,8	0.88	0
38	HTG	C	521	-	19,19,19	0.89	1 (5%)	23,24,24	1.00	1 (4%)
36	EDO	I	107	-	3,3,3	0.71	0	2,2,2	0.12	0
33	PG4	b	637	-	12,12,12	0.78	0	11,11,11	0.56	0
30	GOL	o	304	-	5,5,5	0.50	0	5,5,5	0.93	0
28	SQD	F	104	-	52,54,54	1.42	5 (9%)	62,65,65	2.03	15 (24%)
24	CLA	c	513	3	69,73,73	1.76	17 (24%)	82,113,113	2.28	21 (25%)
24	CLA	c	503	3	69,73,73	1.64	15 (21%)	82,113,113	1.99	25 (30%)
24	CLA	B	615	2	59,63,73	2.00	15 (25%)	70,101,113	2.48	27 (38%)
26	BCR	B	619	-	41,41,41	1.14	4 (9%)	56,56,56	1.48	8 (14%)
30	GOL	c	525	-	5,5,5	0.48	0	5,5,5	1.50	1 (20%)
24	CLA	C	512	3	69,73,73	1.81	15 (21%)	82,113,113	2.08	24 (29%)
34	PGE	b	640	-	9,9,9	0.64	0	8,8,8	0.31	0
33	PG4	h	106	-	12,12,12	0.58	0	11,11,11	0.48	0
33	PG4	K	102	-	12,12,12	0.62	0	11,11,11	0.50	0
33	PG4	d	414	-	12,12,12	0.73	0	11,11,11	0.45	0
29	LMG	B	621	-	51,51,55	1.11	4 (7%)	59,59,63	1.70	8 (13%)
34	PGE	O	308	-	9,9,9	0.99	0	8,8,8	1.27	1 (12%)
30	GOL	b	628	-	5,5,5	0.84	0	5,5,5	0.44	0
33	PG4	B	642	-	12,12,12	0.82	0	11,11,11	0.63	0
34	PGE	c	537	-	9,9,9	0.54	0	8,8,8	0.35	0
20	OEX	a	402	3,46,1	0,14,14	-	-	-		
23	BCT	A	605	21	3,3,3	1.53	1 (33%)	2,3,3	2.54	2 (100%)
34	PGE	b	642	-	9,9,9	0.67	0	8,8,8	0.20	0
34	PGE	b	647	-	9,9,9	0.60	0	8,8,8	0.42	0
36	EDO	a	425	-	3,3,3	0.59	0	2,2,2	0.12	0
26	BCR	c	514	-	41,41,41	1.24	5 (12%)	56,56,56	1.72	14 (25%)
30	GOL	V	208	-	5,5,5	0.48	0	5,5,5	0.47	0
33	PG4	B	637	-	12,12,12	0.81	0	11,11,11	0.55	0
34	PGE	B	645	-	9,9,9	0.73	0	8,8,8	0.67	0
30	GOL	O	305	-	5,5,5	0.46	0	5,5,5	0.35	0
32	LHG	B	632	-	48,48,48	0.81	2 (4%)	51,54,54	1.32	7 (13%)
33	PG4	i	101	-	12,12,12	0.59	0	11,11,11	0.41	0
24	CLA	a	408	46	64,68,73	1.80	17 (26%)	76,107,113	2.36	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	DGD	d	408	-	67,67,67	1.33	4 (5%)	81,81,81	1.77	10 (12%)
41	HEM	e	107	5,6	50,50,50	1.83	13 (26%)	67,82,82	1.66	13 (19%)
30	GOL	b	630	-	5,5,5	0.47	0	5,5,5	0.33	0
27	PL9	D	407	-	55,55,55	1.47	9 (16%)	68,69,69	1.32	6 (8%)
34	PGE	O	309	-	9,9,9	0.81	0	8,8,8	0.98	1 (12%)
36	EDO	V	218	-	3,3,3	0.87	0	2,2,2	0.13	0
25	PHO	D	401	-	58,69,69	2.48	16 (27%)	55,99,99	2.25	12 (21%)
35	P6G	T	105	-	18,18,18	0.68	0	17,17,17	0.95	0
31	LMT	C	533	-	36,36,36	0.69	1 (2%)	47,47,47	1.11	1 (2%)
33	PG4	e	104	-	12,12,12	0.61	0	11,11,11	0.56	0
24	CLA	c	505	3	69,73,73	1.70	16 (23%)	82,113,113	2.39	22 (26%)
30	GOL	C	523	-	5,5,5	0.70	0	5,5,5	2.31	2 (40%)
29	LMG	C	519	-	51,51,55	1.13	3 (5%)	59,59,63	1.54	7 (11%)
24	CLA	c	509	3	69,73,73	1.71	16 (23%)	82,113,113	2.22	25 (30%)
40	DGD	D	408	-	67,67,67	1.22	4 (5%)	81,81,81	1.61	11 (13%)
34	PGE	x	103	-	9,9,9	0.61	0	8,8,8	0.57	0
30	GOL	D	412	-	5,5,5	0.64	0	5,5,5	0.68	0
30	GOL	T	103	-	5,5,5	0.74	0	5,5,5	0.72	0
34	PGE	o	309	-	9,9,9	0.84	0	8,8,8	0.71	0
24	CLA	D	405	4	69,73,73	1.74	13 (18%)	82,113,113	2.12	24 (29%)
24	CLA	a	407	1	69,73,73	1.69	19 (27%)	82,113,113	2.09	25 (30%)
24	CLA	d	403	46	69,73,73	1.70	14 (20%)	82,113,113	2.01	23 (28%)
29	LMG	c	519	-	51,51,55	1.02	3 (5%)	59,59,63	1.39	8 (13%)
34	PGE	b	643	-	9,9,9	0.86	0	8,8,8	0.61	0
35	P6G	b	649	-	18,18,18	0.55	0	17,17,17	0.52	0
24	CLA	C	502	3	69,73,73	1.64	16 (23%)	82,113,113	2.12	20 (24%)
32	LHG	e	101	-	41,41,48	1.13	2 (4%)	44,47,54	1.19	4 (9%)
39	1PE	j	107	-	15,15,15	0.63	0	14,14,14	0.62	0
36	EDO	o	310	-	3,3,3	0.59	0	2,2,2	0.06	0
30	GOL	O	306	-	5,5,5	1.29	1 (20%)	5,5,5	1.20	1 (20%)
24	CLA	c	507	46	69,73,73	1.86	17 (24%)	82,113,113	2.19	24 (29%)
31	LMT	j	103	-	36,36,36	0.75	1 (2%)	47,47,47	1.45	6 (12%)
31	LMT	u	203	-	36,36,36	1.27	2 (5%)	47,47,47	1.70	9 (19%)
24	CLA	B	608	46	69,73,73	1.58	14 (20%)	82,113,113	2.16	22 (26%)
29	LMG	a	414	-	51,51,55	0.86	2 (3%)	59,59,63	1.25	5 (8%)
30	GOL	o	305	-	5,5,5	0.69	0	5,5,5	1.03	0
24	CLA	b	605	2	69,73,73	1.81	17 (24%)	82,113,113	2.61	25 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
24	CLA	C	509	3	69,73,73	1.61	16 (23%)	82,113,113	2.28	25 (30%)
24	CLA	b	611	46	69,73,73	1.66	16 (23%)	82,113,113	2.30	30 (36%)
24	CLA	A	607	46	64,68,73	1.84	16 (25%)	76,107,113	2.34	24 (31%)
36	EDO	J	109	-	3,3,3	0.40	0	2,2,2	0.39	0
45	PE8	i	107	-	24,24,24	0.69	0	23,23,23	0.69	0
34	PGE	B	644	-	9,9,9	0.57	0	8,8,8	0.45	0
33	PG4	e	103	-	12,12,12	0.58	0	11,11,11	0.50	0
40	DGD	H	103	-	63,63,67	1.08	7 (11%)	77,77,81	1.21	12 (15%)
30	GOL	B	625	-	5,5,5	0.69	0	5,5,5	1.99	2 (40%)
28	SQD	a	417	-	52,54,54	1.17	3 (5%)	62,65,65	1.26	5 (8%)
26	BCR	B	618	-	41,41,41	0.95	0	56,56,56	1.55	9 (16%)
33	PG4	V	212	-	12,12,12	0.72	0	11,11,11	0.56	0
24	CLA	c	504	46	64,68,73	1.99	19 (29%)	76,107,113	2.47	25 (32%)
26	BCR	c	527	-	41,41,41	1.02	2 (4%)	56,56,56	1.40	9 (16%)
24	CLA	C	507	46	69,73,73	1.83	17 (24%)	82,113,113	2.34	25 (30%)
33	PG4	H	107	-	12,12,12	0.70	0	11,11,11	0.50	0
34	PGE	J	108	-	9,9,9	0.58	0	8,8,8	0.51	0
24	CLA	C	510	3	69,73,73	1.72	16 (23%)	82,113,113	2.12	25 (30%)
24	CLA	b	606	2	69,73,73	1.89	19 (27%)	82,113,113	2.47	30 (36%)
34	PGE	b	645	-	9,9,9	0.54	0	8,8,8	0.41	0
26	BCR	H	102	-	41,41,41	1.07	4 (9%)	56,56,56	1.78	18 (32%)
33	PG4	c	533	-	12,12,12	0.59	0	11,11,11	0.47	0
30	GOL	a	416	-	5,5,5	0.64	0	5,5,5	0.84	0
38	HTG	c	522	-	19,19,19	0.69	0	23,24,24	1.35	4 (17%)
31	LMT	B	622	-	36,36,36	0.80	1 (2%)	47,47,47	1.46	7 (14%)
26	BCR	a	411	-	41,41,41	1.21	5 (12%)	56,56,56	1.33	7 (12%)
27	PL9	d	407	-	55,55,55	1.31	9 (16%)	68,69,69	1.28	9 (13%)
36	EDO	C	542	-	3,3,3	0.48	0	2,2,2	0.39	0
24	CLA	C	504	46	64,68,73	1.70	14 (21%)	76,107,113	2.15	25 (32%)
30	GOL	a	415	-	5,5,5	1.10	0	5,5,5	1.18	1 (20%)
33	PG4	B	641	-	12,12,12	0.72	0	11,11,11	0.61	0
26	BCR	C	515	-	41,41,41	0.98	2 (4%)	56,56,56	1.65	12 (21%)
44	2PE	V	216	-	27,27,27	0.92	0	26,26,26	0.68	0
34	PGE	a	422	-	9,9,9	0.67	0	8,8,8	0.72	0
30	GOL	m	103	-	5,5,5	0.28	0	5,5,5	0.60	0
34	PGE	H	109	-	9,9,9	0.53	0	8,8,8	0.48	0
24	CLA	b	612	2	69,73,73	1.60	15 (21%)	82,113,113	2.27	25 (30%)
32	LHG	A	618	-	41,41,48	1.22	2 (4%)	44,47,54	1.23	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	GOL	U	201	-	5,5,5	0.54	0	5,5,5	1.15	0
30	GOL	d	402	-	5,5,5	0.64	0	5,5,5	1.04	1 (20%)
33	PG4	b	634	-	12,12,12	0.82	0	11,11,11	0.67	0
26	BCR	b	620	-	41,41,41	0.98	2 (4%)	56,56,56	1.41	5 (8%)
30	GOL	v	204	-	5,5,5	1.18	0	5,5,5	0.91	0
35	P6G	C	541	-	18,18,18	0.66	0	17,17,17	0.43	0
41	HEM	E	113	5,6	50,50,50	1.90	13 (26%)	67,82,82	2.17	20 (29%)
38	HTG	B	623	-	19,19,19	1.00	1 (5%)	23,24,24	1.34	3 (13%)
24	CLA	b	604	2	69,73,73	1.66	17 (24%)	82,113,113	2.25	27 (32%)
30	GOL	O	302	-	5,5,5	1.52	1 (20%)	5,5,5	0.99	0
24	CLA	a	410	1	69,73,73	1.74	13 (18%)	82,113,113	2.15	26 (31%)
26	BCR	b	619	-	41,41,41	1.26	5 (12%)	56,56,56	1.78	14 (25%)
38	HTG	V	204	-	19,19,19	0.94	1 (5%)	23,24,24	2.59	7 (30%)
38	HTG	b	632	-	19,19,19	0.94	1 (5%)	23,24,24	1.61	7 (30%)
35	P6G	A	623	-	18,18,18	0.69	0	17,17,17	0.56	0
38	HTG	B	631	-	19,19,19	1.05	2 (10%)	23,24,24	1.09	2 (8%)
33	PG4	B	640	-	12,12,12	0.67	0	11,11,11	0.43	0
33	PG4	H	105	-	12,12,12	0.74	0	11,11,11	0.48	0
24	CLA	B	605	2	69,73,73	1.76	18 (26%)	82,113,113	2.51	32 (39%)
34	PGE	H	110	-	9,9,9	0.56	0	8,8,8	0.33	0
34	PGE	A	620	-	6,6,9	0.65	0	5,5,8	0.90	0
31	LMT	M	101	-	36,36,36	0.94	2 (5%)	47,47,47	1.82	15 (31%)
24	CLA	b	613	2	69,73,73	1.77	19 (27%)	82,113,113	2.07	22 (26%)
24	CLA	C	513	3	69,73,73	1.62	14 (20%)	82,113,113	2.16	24 (29%)
31	LMT	I	101	-	36,36,36	0.89	1 (2%)	47,47,47	1.54	9 (19%)
34	PGE	h	109	-	9,9,9	0.71	0	8,8,8	0.45	0
34	PGE	E	108	-	9,9,9	0.56	0	8,8,8	0.39	0
34	PGE	a	423	-	9,9,9	0.60	0	8,8,8	0.44	0
31	LMT	Y	101	-	36,36,36	0.58	0	47,47,47	1.26	5 (10%)
34	PGE	c	539	-	9,9,9	0.65	0	8,8,8	0.38	0
24	CLA	B	617	2	64,68,73	1.80	18 (28%)	76,107,113	2.34	26 (34%)
35	P6G	c	541	-	18,18,18	0.51	0	17,17,17	0.41	0
39	1PE	L	101	-	15,15,15	0.68	0	14,14,14	0.66	0
34	PGE	O	310	-	9,9,9	0.61	0	8,8,8	0.36	0
34	PGE	o	307	-	9,9,9	0.78	0	8,8,8	0.55	0
33	PG4	V	210	-	12,12,12	0.91	0	11,11,11	0.78	0
36	EDO	B	658	-	3,3,3	0.45	0	2,2,2	0.47	0
33	PG4	D	414	-	12,12,12	0.67	0	11,11,11	0.51	0
39	1PE	x	104	-	15,15,15	0.62	0	14,14,14	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PGE	h	108	-	9,9,9	0.60	0	8,8,8	0.42	0
34	PGE	D	415	-	9,9,9	0.60	0	8,8,8	0.41	0
33	PG4	a	421	-	12,12,12	0.63	0	11,11,11	0.61	0
24	CLA	c	508	3	64,68,73	1.72	15 (23%)	76,107,113	2.19	21 (27%)
33	PG4	V	211	-	12,12,12	1.03	0	11,11,11	0.80	0
30	GOL	b	625	-	5,5,5	0.53	0	5,5,5	1.63	2 (40%)
25	PHO	d	401	-	58,69,69	2.47	14 (24%)	55,99,99	2.60	17 (30%)
28	SQD	a	424	-	52,54,54	1.28	3 (5%)	62,65,65	1.91	14 (22%)
34	PGE	E	104	-	9,9,9	0.57	0	8,8,8	0.45	0
24	CLA	b	616	2	69,73,73	1.65	11 (15%)	82,113,113	2.29	23 (28%)
35	P6G	d	415	-	18,18,18	0.70	0	17,17,17	0.96	1 (5%)
38	HTG	B	630	-	19,19,19	1.03	2 (10%)	23,24,24	1.52	7 (30%)
34	PGE	B	647	-	9,9,9	0.71	0	8,8,8	0.67	0
24	CLA	c	501	3	69,73,73	1.56	12 (17%)	82,113,113	2.45	24 (29%)
31	LMT	a	401	-	36,36,36	0.84	1 (2%)	47,47,47	1.44	4 (8%)
34	PGE	j	105	-	9,9,9	0.65	0	8,8,8	0.59	0
30	GOL	c	526	-	5,5,5	0.41	0	5,5,5	0.89	0
33	PG4	c	534	-	12,12,12	0.54	0	11,11,11	0.43	0
40	DGD	C	517	-	57,57,67	0.89	3 (5%)	71,71,81	1.10	2 (2%)
24	CLA	C	506	3	69,73,73	1.73	15 (21%)	82,113,113	2.14	22 (26%)
30	GOL	o	303	-	5,5,5	0.79	0	5,5,5	0.67	0
34	PGE	T	104	-	6,6,9	1.04	0	5,5,8	0.53	0
24	CLA	b	608	46	69,73,73	1.54	14 (20%)	82,113,113	1.81	20 (24%)
36	EDO	i	108	-	3,3,3	0.40	0	2,2,2	0.45	0
32	LHG	D	410	-	48,48,48	0.90	3 (6%)	51,54,54	0.99	1 (1%)
36	EDO	O	311	-	3,3,3	0.63	0	2,2,2	0.28	0
35	P6G	A	624	-	18,18,18	0.59	0	17,17,17	0.55	0
39	1PE	e	105	-	15,15,15	0.64	0	14,14,14	0.53	0
36	EDO	B	657	-	3,3,3	0.61	0	2,2,2	0.03	0
38	HTG	b	631	-	19,19,19	1.26	2 (10%)	23,24,24	1.64	6 (26%)
40	DGD	h	104	-	63,63,67	1.13	4 (6%)	77,77,81	1.25	8 (10%)

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
40	DGD	C	518	-	-	10/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	k	101	-	-	0/29/63/63	0/2/2/2
33	PG4	J	104	-	-	3/10/10/10	-
36	EDO	E	112	-	-	0/1/1/1	-
30	GOL	F	101	42	-	2/4/4/4	-
38	HTG	C	529	-	-	3/10/30/30	0/1/1/1
24	CLA	c	512	3	-	7/39/115/115	-
36	EDO	B	655	-	-	0/1/1/1	-
33	PG4	A	619	-	-	3/10/10/10	-
34	PGE	c	536	-	-	3/7/7/7	-
28	SQD	l	102	-	-	19/49/69/69	0/1/1/1
28	SQD	A	616	-	-	17/49/69/69	0/1/1/1
36	EDO	B	656	-	-	1/1/1/1	-
33	PG4	x	102	-	-	3/10/10/10	-
26	BCR	c	515	-	-	0/29/63/63	0/2/2/2
24	CLA	c	506	3	-	7/39/115/115	-
34	PGE	c	540	-	-	4/7/7/7	-
24	CLA	B	614	2	-	2/39/115/115	-
31	LMT	A	617	-	-	8/21/61/61	0/2/2/2
30	GOL	u	202	-	-	0/4/4/4	-
33	PG4	I	102	-	-	6/10/10/10	-
38	HTG	o	301	-	-	0/10/30/30	0/1/1/1
30	GOL	C	524	-	-	0/4/4/4	-
33	PG4	I	104	-	-	4/10/10/10	-
34	PGE	b	641	-	-	3/7/7/7	-
24	CLA	C	508	3	-	2/33/109/115	-
33	PG4	C	535	-	-	3/10/10/10	-
33	PG4	C	536	-	-	5/10/10/10	-
30	GOL	c	529	-	-	2/4/4/4	-
30	GOL	b	626	-	-	0/4/4/4	-
33	PG4	j	104	-	-	8/10/10/10	-
24	CLA	B	616	2	-	6/39/115/115	-
36	EDO	X	104	-	-	0/1/1/1	-
30	GOL	B	626	-	-	0/4/4/4	-
38	HTG	b	623	-	-	2/10/30/30	0/1/1/1
43	HEC	V	203	16	1/1/3/7	6/14/54/54	-
33	PG4	i	103	-	-	6/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PG4	B	639	-	-	4/10/10/10	-
31	LMT	b	622	-	-	9/21/61/61	0/2/2/2
24	CLA	B	606	2	-	5/39/115/115	-
38	HTG	c	523	-	-	1/10/30/30	0/1/1/1
30	GOL	O	304	-	-	0/4/4/4	-
26	BCR	d	406	-	-	2/29/63/63	0/2/2/2
33	PG4	a	420	-	-	3/10/10/10	-
24	CLA	B	607	2	-	2/27/103/115	-
30	GOL	y	101	-	-	2/4/4/4	-
38	HTG	H	101	-	-	3/10/30/30	0/1/1/1
39	1PE	B	653	-	-	4/13/13/13	-
29	LMG	d	412	-	-	24/50/70/70	0/1/1/1
29	LMG	j	101	42	-	9/42/62/70	0/1/1/1
35	P6G	b	648	-	-	6/16/16/16	-
33	PG4	I	103	-	-	5/10/10/10	-
24	CLA	C	501	3	-	4/39/115/115	-
24	CLA	B	604	2	-	1/39/115/115	-
38	HTG	c	530	-	-	3/10/30/30	0/1/1/1
34	PGE	i	105	-	-	4/7/7/7	-
30	GOL	b	629	-	-	2/4/4/4	-
25	PHO	A	608	-	-	2/37/103/103	0/5/6/6
36	EDO	c	542	-	-	1/1/1/1	-
31	LMT	f	101	-	-	2/21/61/61	0/2/2/2
30	GOL	v	207	-	-	2/4/4/4	-
24	CLA	b	603	2	-	2/39/115/115	-
30	GOL	B	629	-	-	0/4/4/4	-
30	GOL	v	205	-	-	2/4/4/4	-
34	PGE	V	215	-	-	4/7/7/7	-
28	SQD	A	622	-	-	24/49/69/69	0/1/1/1
24	CLA	A	606	1	-	5/39/115/115	-
26	BCR	B	620	-	-	1/29/63/63	0/2/2/2
24	CLA	c	510	3	-	4/39/115/115	-
36	EDO	D	419	-	-	0/1/1/1	-
26	BCR	C	525	-	-	2/29/63/63	0/2/2/2
24	CLA	b	607	2	-	1/27/103/115	-
29	LMG	B	634	-	-	18/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LHG	d	411	-	-	10/53/53/53	-
35	P6G	D	418	-	-	7/16/16/16	-
33	PG4	V	209	-	-	5/10/10/10	-
31	LMT	F	102	-	-	6/21/61/61	0/2/2/2
33	PG4	V	213	-	-	4/10/10/10	-
24	CLA	b	610	2	-	0/39/115/115	-
36	EDO	o	311	-	-	1/1/1/1	-
24	CLA	B	613	2	-	2/39/115/115	-
32	LHG	D	411	-	-	8/53/53/53	-
26	BCR	D	406	-	-	0/29/63/63	0/2/2/2
24	CLA	B	610	2	-	1/39/115/115	-
27	PL9	a	412	-	-	10/53/73/73	0/1/1/1
40	DGD	c	516	-	-	16/51/91/95	0/2/2/2
34	PGE	b	644	-	-	3/7/7/7	-
40	DGD	c	517	-	-	15/46/86/95	0/2/2/2
28	SQD	A	612	-	-	11/49/69/69	0/1/1/1
38	HTG	B	624	-	-	3/10/30/30	0/1/1/1
33	PG4	c	535	-	-	3/10/10/10	-
24	CLA	C	511	3	-	0/39/115/115	-
26	BCR	T	102	-	-	1/29/63/63	0/2/2/2
32	LHG	D	409	-	-	7/53/53/53	-
34	PGE	V	214	-	-	4/7/7/7	-
30	GOL	V	207	-	-	0/4/4/4	-
33	PG4	i	102	-	-	4/10/10/10	-
24	CLA	D	403	46	-	3/39/115/115	-
29	LMG	b	621	-	-	13/46/66/70	0/1/1/1
34	PGE	B	649	-	-	3/7/7/7	-
38	HTG	C	531	-	-	7/10/30/30	0/1/1/1
30	GOL	v	203	-	-	0/4/4/4	-
30	GOL	B	635	-	-	0/4/4/4	-
34	PGE	B	650	-	-	2/7/7/7	-
34	PGE	h	110	-	-	3/7/7/7	-
27	PL9	A	611	-	-	10/53/73/73	0/1/1/1
33	PG4	H	104	-	-	3/10/10/10	-
24	CLA	b	615	2	-	9/39/115/115	-
36	EDO	A	625	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	b	639	-	-	3/7/7/7	-
29	LMG	c	520	-	-	17/46/66/70	0/1/1/1
28	SQD	a	413	-	-	19/49/69/69	0/1/1/1
34	PGE	t	104	-	-	2/7/7/7	-
29	LMG	A	613	-	-	19/46/66/70	0/1/1/1
34	PGE	t	105	-	-	1/4/4/7	-
30	GOL	f	104	-	-	4/4/4/4	-
30	GOL	A	614	-	-	0/4/4/4	-
34	PGE	E	106	-	-	3/7/7/7	-
40	DGD	c	518	-	-	15/51/91/95	0/2/2/2
35	P6G	B	651	-	-	5/16/16/16	-
33	PG4	E	103	-	-	4/10/10/10	-
29	LMG	C	526	-	-	27/50/70/70	0/1/1/1
33	PG4	B	636	-	-	3/10/10/10	-
34	PGE	h	107	-	-	4/7/7/7	-
34	PGE	H	111	-	-	3/7/7/7	-
26	BCR	K	101	-	-	2/29/63/63	0/2/2/2
26	BCR	h	103	-	-	0/29/63/63	0/2/2/2
33	PG4	b	636	-	-	6/10/10/10	-
30	GOL	V	205	-	-	0/4/4/4	-
35	P6G	D	417	-	-	8/16/16/16	-
34	PGE	H	108	-	-	5/7/7/7	-
33	PG4	X	101	-	-	3/10/10/10	-
34	PGE	o	308	-	-	5/7/7/7	-
32	LHG	d	410	-	-	8/53/53/53	-
30	GOL	V	201	-	-	0/4/4/4	-
34	PGE	E	107	-	-	5/7/7/7	-
38	HTG	O	303	-	-	1/10/30/30	0/1/1/1
30	GOL	c	528	-	-	3/4/4/4	-
33	PG4	C	534	-	-	5/10/10/10	-
30	GOL	T	101	-	-	0/4/4/4	-
35	P6G	E	110	-	-	11/16/16/16	-
31	LMT	m	102	-	-	3/21/61/61	0/2/2/2
35	P6G	I	106	-	-	10/16/16/16	-
24	CLA	D	404	4	-	3/39/115/115	-
25	PHO	a	409	-	-	1/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PG4	i	104	-	-	5/10/10/10	-
34	PGE	E	105	-	-	4/7/7/7	-
36	EDO	e	106	-	-	1/1/1/1	-
32	LHG	a	419	-	-	21/45/45/53	-
33	PG4	J	105	-	-	6/10/10/10	-
35	P6G	j	106	-	-	7/16/16/16	-
38	HTG	C	532	-	-	2/10/30/30	0/1/1/1
24	CLA	b	602	46	-	14/39/115/115	-
24	CLA	b	614	2	-	0/39/115/115	-
26	BCR	A	610	-	-	2/29/63/63	0/2/2/2
30	GOL	v	206	-	-	2/4/4/4	-
34	PGE	b	638	-	-	3/7/7/7	-
38	HTG	C	522	-	-	3/10/30/30	0/1/1/1
24	CLA	B	603	2	-	2/39/115/115	-
38	HTG	b	624	-	-	4/10/30/30	0/1/1/1
31	LMT	t	103	-	-	7/21/61/61	0/2/2/2
34	PGE	b	646	-	-	4/7/7/7	-
30	GOL	A	615	-	-	1/4/4/4	-
30	GOL	O	307	-	-	2/4/4/4	-
24	CLA	d	405	4	-	4/39/115/115	-
34	PGE	B	646	-	-	4/7/7/7	-
26	BCR	C	514	-	-	0/29/63/63	0/2/2/2
34	PGE	f	105	-	-	2/7/7/7	-
26	BCR	t	102	-	-	1/29/63/63	0/2/2/2
31	LMT	c	521	-	-	9/21/61/61	0/2/2/2
30	GOL	B	628	-	-	0/4/4/4	-
30	GOL	B	633	-	-	4/4/4/4	-
24	CLA	B	612	2	-	3/39/115/115	-
35	P6G	d	416	-	-	8/16/16/16	-
31	LMT	M	102	-	-	7/21/61/61	0/2/2/2
24	CLA	b	617	2	-	5/33/109/115	-
34	PGE	J	106	-	-	3/7/7/7	-
24	CLA	B	602	46	-	12/39/115/115	-
30	GOL	C	527	-	-	2/4/4/4	-
30	GOL	e	102	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PG4	b	635	-	-	5/10/10/10	-
39	1PE	B	654	-	-	4/13/13/13	-
36	EDO	H	112	-	-	1/1/1/1	-
33	PG4	C	537	-	-	6/10/10/10	-
24	CLA	A	609	1	-	10/39/115/115	-
35	P6G	D	416	-	-	9/16/16/16	-
30	GOL	t	101	-	-	0/4/4/4	-
38	HTG	h	101	-	-	4/10/30/30	0/1/1/1
30	GOL	d	413	-	-	4/4/4/4	-
33	PG4	c	532	-	-	6/10/10/10	-
29	LMG	C	520	-	-	17/46/66/70	0/1/1/1
32	LHG	E	101	-	-	16/46/46/53	-
32	LHG	l	101	-	-	12/53/53/53	-
40	DGD	C	516	-	-	17/51/91/95	0/2/2/2
33	PG4	B	638	-	-	6/10/10/10	-
24	CLA	d	404	4	-	1/39/115/115	-
39	1PE	V	217	-	-	4/13/13/13	-
38	HTG	c	531	-	-	8/10/30/30	0/1/1/1
38	HTG	a	418	-	-	7/10/30/30	0/1/1/1
34	PGE	C	539	-	-	3/7/7/7	-
34	PGE	A	621	-	-	3/7/7/7	-
30	GOL	D	413	-	-	2/4/4/4	-
30	GOL	u	201	-	-	0/4/4/4	-
33	PG4	E	102	-	-	8/10/10/10	-
24	CLA	C	505	3	-	2/39/115/115	-
24	CLA	b	609	2	-	1/39/115/115	-
24	CLA	c	511	3	-	2/39/115/115	-
29	LMG	J	101	42	-	6/42/62/70	0/1/1/1
33	PG4	U	202	-	-	3/10/10/10	-
43	HEC	v	202	16	1/1/3/7	4/14/54/54	-
24	CLA	c	502	3	-	2/39/115/115	-
31	LMT	J	103	-	-	10/21/61/61	0/2/2/2
34	PGE	J	107	-	-	3/7/7/7	-
33	PG4	X	103	-	-	4/10/10/10	-
24	CLA	B	609	2	-	1/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	f	103	42	-	1/4/4/4	-
38	HTG	C	530	-	-	3/10/30/30	0/1/1/1
30	GOL	D	402	-	-	2/4/4/4	-
28	SQD	b	633	-	-	18/49/69/69	0/1/1/1
30	GOL	V	206	-	-	0/4/4/4	-
33	PG4	H	106	-	-	4/10/10/10	-
34	PGE	i	106	-	-	4/7/7/7	-
34	PGE	Y	102	-	-	4/7/7/7	-
34	PGE	I	105	-	-	2/7/7/7	-
36	EDO	d	417	-	-	1/1/1/1	-
24	CLA	B	611	46	-	3/39/115/115	-
30	GOL	b	627	-	-	0/4/4/4	-
26	BCR	b	618	-	-	1/29/63/63	0/2/2/2
34	PGE	E	109	-	-	4/7/7/7	-
34	PGE	o	306	-	-	3/7/7/7	-
36	EDO	E	111	-	-	1/1/1/1	-
33	PG4	X	102	-	-	4/10/10/10	-
32	LHG	d	409	-	-	7/53/53/53	-
30	GOL	B	627	-	-	2/4/4/4	-
28	SQD	x	101	-	-	23/49/69/69	0/1/1/1
33	PG4	C	538	-	-	2/10/10/10	-
34	PGE	B	648	-	-	3/7/7/7	-
35	P6G	B	652	-	-	7/16/16/16	-
31	LMT	m	101	-	-	5/21/61/61	0/2/2/2
34	PGE	C	540	-	-	4/7/7/7	-
30	GOL	C	528	-	-	4/4/4/4	-
29	LMG	z	101	-	-	31/50/70/70	0/1/1/1
33	PG4	B	643	-	-	5/10/10/10	-
24	CLA	C	503	3	-	4/39/115/115	-
33	PG4	l	103	-	-	2/10/10/10	-
28	SQD	h	105	-	-	26/49/69/69	0/1/1/1
34	PGE	c	538	-	-	2/7/7/7	-
38	HTG	C	521	-	-	4/10/30/30	0/1/1/1
36	EDO	I	107	-	-	0/1/1/1	-
33	PG4	b	637	-	-	5/10/10/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	o	304	-	-	4/4/4/4	-
28	SQD	F	104	-	-	18/49/69/69	0/1/1/1
24	CLA	c	513	3	-	1/39/115/115	-
24	CLA	c	503	3	-	1/39/115/115	-
24	CLA	B	615	2	-	2/27/103/115	-
26	BCR	B	619	-	-	0/29/63/63	0/2/2/2
30	GOL	c	525	-	-	2/4/4/4	-
24	CLA	C	512	3	-	2/39/115/115	-
34	PGE	b	640	-	-	3/7/7/7	-
33	PG4	h	106	-	-	3/10/10/10	-
33	PG4	K	102	-	-	4/10/10/10	-
33	PG4	d	414	-	-	2/10/10/10	-
29	LMG	B	621	-	-	11/46/66/70	0/1/1/1
34	PGE	O	308	-	-	5/7/7/7	-
30	GOL	b	628	-	-	0/4/4/4	-
33	PG4	B	642	-	-	5/10/10/10	-
34	PGE	c	537	-	-	4/7/7/7	-
34	PGE	b	642	-	-	3/7/7/7	-
34	PGE	b	647	-	-	3/7/7/7	-
36	EDO	a	425	-	-	1/1/1/1	-
26	BCR	c	514	-	-	0/29/63/63	0/2/2/2
30	GOL	V	208	-	-	3/4/4/4	-
33	PG4	B	637	-	-	4/10/10/10	-
34	PGE	B	645	-	-	5/7/7/7	-
30	GOL	O	305	-	-	2/4/4/4	-
32	LHG	B	632	-	-	12/53/53/53	-
33	PG4	i	101	-	-	7/10/10/10	-
24	CLA	a	408	46	-	4/33/109/115	-
40	DGD	d	408	-	-	32/55/95/95	0/2/2/2
41	HEM	e	107	5,6	-	5/14/54/54	-
30	GOL	b	630	-	-	0/4/4/4	-
27	PL9	D	407	-	-	1/53/73/73	0/1/1/1
34	PGE	O	309	-	-	5/7/7/7	-
36	EDO	V	218	-	-	1/1/1/1	-
25	PHO	D	401	-	-	1/37/103/103	0/5/6/6
35	P6G	T	105	-	-	12/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	LMT	C	533	-	-	12/21/61/61	0/2/2/2
33	PG4	e	104	-	-	4/10/10/10	-
24	CLA	c	505	3	-	0/39/115/115	-
30	GOL	C	523	-	-	1/4/4/4	-
29	LMG	C	519	-	-	15/46/66/70	0/1/1/1
24	CLA	c	509	3	-	9/39/115/115	-
40	DGD	D	408	-	-	30/55/95/95	0/2/2/2
34	PGE	x	103	-	-	2/7/7/7	-
30	GOL	D	412	-	-	3/4/4/4	-
30	GOL	T	103	-	-	2/4/4/4	-
34	PGE	o	309	-	-	5/7/7/7	-
24	CLA	D	405	4	-	7/39/115/115	-
24	CLA	a	407	1	-	2/39/115/115	-
24	CLA	d	403	46	-	4/39/115/115	-
29	LMG	c	519	-	-	19/46/66/70	0/1/1/1
34	PGE	b	643	-	-	3/7/7/7	-
35	P6G	b	649	-	-	10/16/16/16	-
24	CLA	C	502	3	-	4/39/115/115	-
32	LHG	e	101	-	-	24/46/46/53	-
39	1PE	j	107	-	-	5/13/13/13	-
36	EDO	o	310	-	-	0/1/1/1	-
30	GOL	O	306	-	-	0/4/4/4	-
24	CLA	c	507	46	-	2/39/115/115	-
31	LMT	j	103	-	-	10/21/61/61	0/2/2/2
31	LMT	u	203	-	-	12/21/61/61	0/2/2/2
24	CLA	B	608	46	-	0/39/115/115	-
29	LMG	a	414	-	-	24/46/66/70	0/1/1/1
30	GOL	o	305	-	-	2/4/4/4	-
24	CLA	b	605	2	-	6/39/115/115	-
24	CLA	C	509	3	-	7/39/115/115	-
24	CLA	b	611	46	-	6/39/115/115	-
24	CLA	A	607	46	-	2/33/109/115	-
36	EDO	J	109	-	-	0/1/1/1	-
45	PE8	i	107	-	-	13/22/22/22	-
34	PGE	B	644	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PG4	e	103	-	-	4/10/10/10	-
40	DGD	H	103	-	-	10/51/91/95	0/2/2/2
30	GOL	B	625	-	-	2/4/4/4	-
28	SQD	a	417	-	-	16/49/69/69	0/1/1/1
26	BCR	B	618	-	-	2/29/63/63	0/2/2/2
33	PG4	V	212	-	-	5/10/10/10	-
24	CLA	c	504	46	-	3/33/109/115	-
26	BCR	c	527	-	-	1/29/63/63	0/2/2/2
24	CLA	C	507	46	-	7/39/115/115	-
33	PG4	H	107	-	-	4/10/10/10	-
34	PGE	J	108	-	-	4/7/7/7	-
24	CLA	C	510	3	-	1/39/115/115	-
24	CLA	b	606	2	-	3/39/115/115	-
34	PGE	b	645	-	-	4/7/7/7	-
26	BCR	H	102	-	-	0/29/63/63	0/2/2/2
33	PG4	c	533	-	-	5/10/10/10	-
30	GOL	a	416	-	-	2/4/4/4	-
38	HTG	c	522	-	-	4/10/30/30	0/1/1/1
31	LMT	B	622	-	-	6/21/61/61	0/2/2/2
26	BCR	a	411	-	-	0/29/63/63	0/2/2/2
27	PL9	d	407	-	-	1/53/73/73	0/1/1/1
36	EDO	C	542	-	-	1/1/1/1	-
24	CLA	C	504	46	-	3/33/109/115	-
30	GOL	a	415	-	-	0/4/4/4	-
33	PG4	B	641	-	-	4/10/10/10	-
26	BCR	C	515	-	-	2/29/63/63	0/2/2/2
44	2PE	V	216	-	-	14/25/25/25	-
34	PGE	a	422	-	-	5/7/7/7	-
30	GOL	m	103	-	-	0/4/4/4	-
34	PGE	H	109	-	-	6/7/7/7	-
24	CLA	b	612	2	-	3/39/115/115	-
32	LHG	A	618	-	-	23/46/46/53	-
30	GOL	U	201	-	-	1/4/4/4	-
30	GOL	d	402	-	-	2/4/4/4	-
33	PG4	b	634	-	-	3/10/10/10	-
26	BCR	b	620	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GOL	v	204	-	-	2/4/4/4	-
35	P6G	C	541	-	-	8/16/16/16	-
41	HEM	E	113	5,6	-	2/14/54/54	-
38	HTG	B	623	-	-	3/10/30/30	0/1/1/1
24	CLA	b	604	2	-	3/39/115/115	-
30	GOL	O	302	-	-	2/4/4/4	-
24	CLA	a	410	1	-	11/39/115/115	-
26	BCR	b	619	-	-	0/29/63/63	0/2/2/2
38	HTG	V	204	-	-	2/10/30/30	0/1/1/1
38	HTG	b	632	-	-	2/10/30/30	0/1/1/1
35	P6G	A	623	-	-	9/16/16/16	-
38	HTG	B	631	-	-	3/10/30/30	0/1/1/1
33	PG4	B	640	-	-	5/10/10/10	-
33	PG4	H	105	-	-	4/10/10/10	-
24	CLA	B	605	2	-	4/39/115/115	-
34	PGE	H	110	-	-	4/7/7/7	-
34	PGE	A	620	-	-	2/4/4/7	-
31	LMT	M	101	-	-	2/21/61/61	0/2/2/2
24	CLA	b	613	2	-	3/39/115/115	-
24	CLA	C	513	3	-	7/39/115/115	-
31	LMT	I	101	-	-	7/21/61/61	0/2/2/2
34	PGE	h	109	-	-	4/7/7/7	-
34	PGE	E	108	-	-	2/7/7/7	-
34	PGE	a	423	-	-	3/7/7/7	-
31	LMT	Y	101	-	-	12/21/61/61	0/2/2/2
34	PGE	c	539	-	-	1/7/7/7	-
24	CLA	B	617	2	-	8/33/109/115	-
35	P6G	c	541	-	-	5/16/16/16	-
39	1PE	L	101	-	-	5/13/13/13	-
34	PGE	O	310	-	-	5/7/7/7	-
34	PGE	o	307	-	-	5/7/7/7	-
33	PG4	V	210	-	-	8/10/10/10	-
36	EDO	B	658	-	-	1/1/1/1	-
33	PG4	D	414	-	-	5/10/10/10	-
39	1PE	x	104	-	-	9/13/13/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	PGE	h	108	-	-	4/7/7/7	-
34	PGE	D	415	-	-	6/7/7/7	-
33	PG4	a	421	-	-	3/10/10/10	-
24	CLA	c	508	3	-	0/33/109/115	-
33	PG4	V	211	-	-	3/10/10/10	-
30	GOL	b	625	-	-	3/4/4/4	-
25	PHO	d	401	-	-	2/37/103/103	0/5/6/6
28	SQD	a	424	-	-	22/49/69/69	0/1/1/1
34	PGE	E	104	-	-	1/7/7/7	-
24	CLA	b	616	2	-	4/39/115/115	-
35	P6G	d	415	-	-	8/16/16/16	-
38	HTG	B	630	-	-	4/10/30/30	0/1/1/1
34	PGE	B	647	-	-	3/7/7/7	-
24	CLA	c	501	3	-	2/39/115/115	-
31	LMT	a	401	-	-	9/21/61/61	0/2/2/2
34	PGE	j	105	-	-	4/7/7/7	-
30	GOL	c	526	-	-	0/4/4/4	-
33	PG4	c	534	-	-	6/10/10/10	-
40	DGD	C	517	-	-	14/45/85/95	0/2/2/2
24	CLA	C	506	3	-	10/39/115/115	-
30	GOL	o	303	-	-	2/4/4/4	-
34	PGE	T	104	-	-	1/4/4/7	-
24	CLA	b	608	46	-	1/39/115/115	-
36	EDO	i	108	-	-	0/1/1/1	-
32	LHG	D	410	-	-	8/53/53/53	-
36	EDO	O	311	-	-	1/1/1/1	-
35	P6G	A	624	-	-	9/16/16/16	-
39	1PE	e	105	-	-	7/13/13/13	-
36	EDO	B	657	-	-	0/1/1/1	-
38	HTG	b	631	-	-	2/10/30/30	0/1/1/1
40	DGD	h	104	-	-	10/51/91/95	0/2/2/2

All (1512) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	d	401	PHO	C1B-C2B	9.15	1.49	1.39
25	d	401	PHO	C1D-C2D	8.98	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	C1D-C2D	8.83	1.49	1.39
38	o	301	HTG	C1'-S1	-7.16	1.71	1.81
25	D	401	PHO	C3B-C2B	7.09	1.50	1.40
24	D	404	CLA	C1D-ND	6.75	1.46	1.37
24	b	607	CLA	C1D-ND	6.52	1.46	1.37
24	D	403	CLA	OBD-CAD	6.50	1.33	1.22
24	B	606	CLA	C2-C3	6.41	1.47	1.33
24	c	506	CLA	C1D-ND	6.38	1.46	1.37
24	B	615	CLA	C1B-NB	-6.12	1.29	1.37
26	d	406	BCR	C30-C25	-6.09	1.46	1.53
25	D	401	PHO	C1B-C2B	6.09	1.46	1.39
40	D	408	DGD	O2G-C1B	6.06	1.51	1.34
24	B	602	CLA	O2A-CGA	5.93	1.50	1.33
24	b	606	CLA	C2-C3	5.91	1.46	1.33
27	a	412	PL9	C7-C3	5.86	1.59	1.51
41	e	107	HEM	FE-NB	5.85	2.12	1.94
24	c	510	CLA	C1D-ND	5.84	1.45	1.37
25	d	401	PHO	C3B-C4B	5.81	1.47	1.41
25	a	409	PHO	C1D-C2D	5.79	1.45	1.39
24	C	505	CLA	C1D-ND	5.79	1.45	1.37
24	B	615	CLA	CHC-C1C	5.74	1.50	1.38
24	b	602	CLA	O2D-CGD	5.73	1.47	1.33
24	b	606	CLA	O2D-CGD	5.72	1.47	1.33
24	D	405	CLA	C1D-ND	5.72	1.45	1.37
24	C	504	CLA	C4B-NB	-5.72	1.30	1.37
24	C	506	CLA	C1D-ND	5.64	1.45	1.37
24	b	614	CLA	OBD-CAD	5.64	1.32	1.22
40	d	408	DGD	O2G-C1B	5.64	1.50	1.34
25	a	409	PHO	C1B-C2B	5.63	1.45	1.39
28	F	104	SQD	O48-C23	5.63	1.49	1.33
24	B	605	CLA	C2-C3	5.59	1.45	1.33
24	a	410	CLA	CHC-C1C	5.59	1.49	1.38
24	B	611	CLA	CHD-C1D	5.58	1.49	1.38
24	a	407	CLA	C1D-ND	5.50	1.45	1.37
24	C	505	CLA	OBD-CAD	5.47	1.31	1.22
25	A	608	PHO	C1B-C2B	5.45	1.45	1.39
24	b	605	CLA	C2-C3	5.45	1.45	1.33
24	b	602	CLA	O2A-CGA	5.35	1.48	1.33
24	b	606	CLA	C3C-C2C	5.35	1.48	1.36
24	B	604	CLA	C3C-C2C	5.33	1.48	1.36
29	C	526	LMG	O7-C10	5.31	1.49	1.34
24	b	614	CLA	C3C-C2C	5.24	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	508	CLA	C3C-C2C	5.22	1.48	1.36
24	a	410	CLA	C1D-ND	5.19	1.44	1.37
25	A	608	PHO	C1D-C2D	5.18	1.45	1.39
25	a	409	PHO	C3B-C2B	5.15	1.47	1.40
25	A	608	PHO	C3B-C2B	5.13	1.47	1.40
24	A	607	CLA	C1D-ND	5.12	1.44	1.37
28	x	101	SQD	O48-C23	5.12	1.48	1.33
29	C	520	LMG	O8-C28	5.10	1.48	1.33
25	D	401	PHO	C3D-C2D	5.09	1.48	1.39
24	B	615	CLA	C1D-ND	5.07	1.44	1.37
41	E	113	HEM	C1B-NB	-5.06	1.31	1.40
25	d	401	PHO	OBD-CAD	5.06	1.28	1.22
24	C	510	CLA	C1D-ND	5.05	1.44	1.37
28	l	102	SQD	O8-S	5.02	1.66	1.47
28	b	633	SQD	O47-C7	5.01	1.48	1.34
40	d	408	DGD	O1G-C1A	4.98	1.47	1.33
25	A	608	PHO	C4D-CHA	4.96	1.47	1.39
24	C	511	CLA	CHB-C1B	4.96	1.50	1.39
24	B	617	CLA	C1D-ND	4.96	1.44	1.37
38	O	303	HTG	C1'-S1	-4.96	1.74	1.81
26	D	406	BCR	C30-C25	-4.95	1.47	1.53
29	C	520	LMG	O7-C10	4.95	1.48	1.34
24	d	404	CLA	CHC-C1C	4.93	1.48	1.38
25	D	401	PHO	OBD-CAD	4.91	1.28	1.22
28	h	105	SQD	O48-C23	4.91	1.47	1.33
24	B	603	CLA	CHC-C1C	4.90	1.48	1.38
24	C	507	CLA	C1D-ND	4.90	1.44	1.37
24	c	503	CLA	C1D-ND	4.90	1.44	1.37
24	c	505	CLA	C1D-ND	4.89	1.44	1.37
24	A	609	CLA	C1D-ND	4.88	1.44	1.37
32	a	419	LHG	O8-C23	4.88	1.47	1.33
24	b	610	CLA	O2D-CGD	4.88	1.45	1.33
28	A	622	SQD	O47-C7	4.88	1.48	1.34
24	b	605	CLA	MG-ND	-4.87	1.96	2.05
32	A	618	LHG	O7-C7	4.87	1.48	1.34
24	C	505	CLA	C1B-NB	-4.86	1.31	1.37
29	C	519	LMG	O8-C28	4.85	1.47	1.33
26	c	515	BCR	C1-C6	-4.85	1.47	1.53
28	h	105	SQD	O47-C7	4.84	1.47	1.34
24	B	613	CLA	CHC-C1C	4.83	1.48	1.38
24	c	504	CLA	C4B-NB	-4.83	1.31	1.37
24	A	607	CLA	CHD-C1D	4.83	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	506	CLA	O2D-CGD	4.82	1.45	1.33
24	B	611	CLA	C1D-ND	4.82	1.44	1.37
24	C	501	CLA	C1D-ND	4.82	1.44	1.37
24	d	403	CLA	CHC-C1C	4.82	1.48	1.38
43	V	203	HEC	FE-NB	4.80	2.09	1.94
29	c	520	LMG	O8-C28	4.80	1.47	1.33
24	b	616	CLA	OBD-CAD	4.79	1.30	1.22
38	c	530	HTG	O2-C2	4.79	1.54	1.43
28	A	622	SQD	O48-C23	4.79	1.47	1.33
24	B	603	CLA	OBD-CAD	4.79	1.30	1.22
24	b	603	CLA	CHC-C1C	4.78	1.48	1.38
29	B	621	LMG	O8-C28	4.78	1.47	1.33
28	F	104	SQD	O47-C7	4.78	1.47	1.34
24	C	512	CLA	C1D-ND	4.77	1.44	1.37
29	B	634	LMG	O8-C28	4.76	1.47	1.33
24	b	605	CLA	CHC-C1C	4.76	1.48	1.38
24	d	403	CLA	C1C-NC	-4.76	1.30	1.37
24	b	615	CLA	O2A-CGA	4.76	1.47	1.33
24	c	511	CLA	C1D-ND	4.75	1.44	1.37
24	A	606	CLA	OBD-CAD	4.74	1.30	1.22
24	A	606	CLA	C3C-C2C	4.74	1.47	1.36
28	b	633	SQD	O48-C23	4.73	1.47	1.33
24	D	403	CLA	C1D-ND	4.72	1.44	1.37
28	a	417	SQD	O48-C23	4.72	1.47	1.33
24	C	512	CLA	CHC-C1C	4.70	1.47	1.38
24	B	616	CLA	C1D-ND	4.68	1.44	1.37
28	a	424	SQD	O47-C7	4.68	1.47	1.34
28	b	633	SQD	O8-S	4.67	1.64	1.47
40	D	408	DGD	O1G-C1A	4.66	1.46	1.33
24	b	616	CLA	C1D-ND	4.65	1.44	1.37
32	A	618	LHG	O8-C23	4.65	1.46	1.33
25	a	409	PHO	C4D-CHA	4.65	1.46	1.39
28	h	105	SQD	O8-S	4.64	1.64	1.47
32	e	101	LHG	O8-C23	4.64	1.46	1.33
24	b	616	CLA	C3C-C2C	4.64	1.46	1.36
24	C	503	CLA	CHC-C1C	4.64	1.47	1.38
24	c	512	CLA	C1D-ND	4.63	1.43	1.37
24	b	610	CLA	CHD-C1D	4.63	1.47	1.38
24	C	507	CLA	O2D-CGD	4.63	1.44	1.33
27	A	611	PL9	C7-C3	4.63	1.57	1.51
24	b	615	CLA	C4B-NB	-4.63	1.31	1.37
41	e	107	HEM	FE-NC	4.62	2.10	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	e	107	HEM	C1B-NB	-4.61	1.32	1.40
41	E	113	HEM	FE-NB	4.59	2.09	1.94
25	d	401	PHO	C4D-CHA	4.59	1.46	1.39
29	d	412	LMG	O8-C28	4.59	1.46	1.33
24	c	509	CLA	OBD-CAD	4.59	1.30	1.22
24	C	513	CLA	CHC-C1C	4.57	1.47	1.38
24	a	408	CLA	C1D-ND	4.57	1.43	1.37
24	b	617	CLA	CHB-C1B	4.56	1.49	1.39
24	c	507	CLA	OBD-CAD	4.55	1.30	1.22
24	A	609	CLA	CHB-C1B	4.54	1.49	1.39
25	D	401	PHO	C3B-C4B	4.54	1.46	1.41
29	B	634	LMG	O7-C10	4.54	1.47	1.34
24	b	608	CLA	C3C-C2C	4.54	1.46	1.36
24	c	508	CLA	C1D-ND	4.54	1.43	1.37
28	A	622	SQD	O8-S	4.53	1.64	1.47
28	a	424	SQD	O48-C23	4.53	1.46	1.33
32	e	101	LHG	O7-C7	4.53	1.47	1.34
29	c	520	LMG	O7-C10	4.52	1.47	1.34
24	C	505	CLA	C3C-C2C	4.49	1.46	1.36
28	a	424	SQD	O8-S	4.48	1.64	1.47
24	C	512	CLA	CHD-C1D	4.47	1.47	1.38
24	c	504	CLA	MG-ND	-4.46	1.96	2.05
24	c	507	CLA	C3C-C2C	4.46	1.46	1.36
24	c	507	CLA	CHC-C1C	4.45	1.47	1.38
24	C	503	CLA	C1D-ND	4.45	1.43	1.37
24	b	611	CLA	C3C-C2C	4.43	1.46	1.36
24	B	604	CLA	C1B-C2B	4.43	1.53	1.43
24	c	507	CLA	C1D-ND	4.42	1.43	1.37
24	C	503	CLA	O2D-CGD	4.42	1.44	1.33
28	x	101	SQD	O8-S	4.42	1.63	1.47
25	D	401	PHO	C4D-CHA	4.41	1.46	1.39
25	d	401	PHO	C3A-C2A	-4.40	1.50	1.54
24	c	502	CLA	O2D-CGD	4.39	1.44	1.33
24	b	613	CLA	OBD-CAD	4.38	1.30	1.22
24	b	614	CLA	O2D-CGD	4.38	1.44	1.33
24	c	513	CLA	C3D-C4D	-4.37	1.34	1.44
24	c	503	CLA	O2D-CGD	4.35	1.43	1.33
27	D	407	PL9	C36-C37	-4.34	1.39	1.53
32	E	101	LHG	O8-C23	4.33	1.46	1.33
24	D	403	CLA	CHC-C4B	4.32	1.49	1.39
24	B	607	CLA	CHC-C1C	4.32	1.47	1.38
24	C	511	CLA	C3C-C2C	4.32	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	OBD-CAD	4.32	1.29	1.22
24	c	512	CLA	C3C-C2C	4.32	1.46	1.36
24	b	602	CLA	C1D-ND	4.31	1.43	1.37
24	c	503	CLA	CHC-C1C	4.30	1.47	1.38
32	a	419	LHG	O7-C7	4.30	1.46	1.34
24	B	603	CLA	CHB-C1B	4.30	1.49	1.39
24	D	403	CLA	MG-ND	-4.30	1.97	2.05
24	C	510	CLA	O2D-CGD	4.30	1.43	1.33
24	b	610	CLA	OBD-CAD	4.30	1.29	1.22
24	c	504	CLA	C1D-ND	4.29	1.43	1.37
24	c	506	CLA	MG-ND	-4.29	1.97	2.05
43	v	202	HEC	FE-NB	4.29	2.08	1.94
24	c	504	CLA	CHD-C4C	4.28	1.48	1.39
24	C	501	CLA	C3C-C2C	4.27	1.46	1.36
24	b	604	CLA	C3C-C2C	4.27	1.46	1.36
28	a	417	SQD	O47-C7	4.26	1.46	1.34
29	A	613	LMG	O7-C10	4.26	1.46	1.34
24	C	508	CLA	CHC-C1C	4.25	1.47	1.38
28	F	104	SQD	O8-S	4.25	1.63	1.47
29	z	101	LMG	O8-C28	4.25	1.45	1.33
24	B	614	CLA	C1D-ND	4.24	1.43	1.37
24	d	405	CLA	C1B-NB	-4.24	1.32	1.37
38	b	624	HTG	C1'-S1	-4.24	1.75	1.81
24	b	602	CLA	CHC-C4B	4.23	1.48	1.39
24	B	614	CLA	CHC-C1C	4.22	1.46	1.38
24	b	616	CLA	C3D-C2D	4.21	1.50	1.39
24	c	512	CLA	MG-ND	-4.21	1.97	2.05
24	c	502	CLA	C1D-ND	4.20	1.43	1.37
24	B	612	CLA	CHC-C1C	4.20	1.46	1.38
24	b	615	CLA	CHB-C1B	4.19	1.48	1.39
24	c	507	CLA	O2D-CGD	4.18	1.43	1.33
24	b	610	CLA	CHC-C1C	4.18	1.46	1.38
28	A	616	SQD	O48-C23	4.18	1.45	1.33
24	D	405	CLA	CHC-C1C	4.18	1.46	1.38
24	B	605	CLA	C1D-ND	4.18	1.43	1.37
24	c	502	CLA	CHB-C1B	4.18	1.48	1.39
24	C	503	CLA	C3C-C2C	4.17	1.45	1.36
24	C	511	CLA	C3D-C2D	4.17	1.50	1.39
24	c	508	CLA	C3C-C2C	4.17	1.45	1.36
24	c	505	CLA	C3C-C2C	4.17	1.45	1.36
24	B	617	CLA	CHB-C1B	4.16	1.48	1.39
24	c	504	CLA	C1B-NB	-4.16	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	z	101	LMG	O7-C10	4.15	1.46	1.34
32	E	101	LHG	O7-C7	4.15	1.46	1.34
24	c	502	CLA	C3D-C4D	-4.15	1.34	1.44
24	D	405	CLA	CHB-C1B	4.14	1.48	1.39
24	B	606	CLA	O2D-CGD	4.14	1.43	1.33
24	C	502	CLA	CHC-C1C	4.14	1.46	1.38
24	B	608	CLA	CHB-C1B	4.13	1.48	1.39
29	c	519	LMG	O8-C28	4.13	1.45	1.33
24	B	602	CLA	C3D-C4D	-4.12	1.34	1.44
24	B	611	CLA	C3C-C2C	4.11	1.45	1.36
28	A	616	SQD	O47-C7	4.11	1.45	1.34
25	a	409	PHO	C3D-C2D	4.11	1.46	1.39
40	h	104	DGD	O5D-C1E	4.11	1.47	1.40
24	b	602	CLA	C3D-C4D	-4.10	1.35	1.44
28	a	417	SQD	O8-S	4.10	1.62	1.47
24	C	512	CLA	O2A-CGA	4.09	1.45	1.33
24	c	507	CLA	CHB-C1B	4.08	1.48	1.39
24	D	405	CLA	C3C-C2C	4.07	1.45	1.36
28	A	612	SQD	O8-S	4.07	1.62	1.47
24	c	513	CLA	C1D-ND	4.07	1.43	1.37
24	b	614	CLA	C1D-ND	4.06	1.43	1.37
24	C	507	CLA	CHB-C1B	4.06	1.48	1.39
24	C	501	CLA	C4B-NB	-4.06	1.32	1.37
24	A	607	CLA	CHC-C1C	4.06	1.46	1.38
41	E	113	HEM	FE-NC	4.04	2.08	1.95
28	a	413	SQD	O8-S	4.03	1.62	1.47
24	C	509	CLA	C3D-C4D	-4.02	1.35	1.44
24	c	511	CLA	CHD-C4C	4.02	1.48	1.39
28	l	102	SQD	O48-C23	4.02	1.45	1.33
24	C	502	CLA	C4B-NB	-4.02	1.32	1.37
24	C	509	CLA	OBD-CAD	4.02	1.29	1.22
24	b	613	CLA	CHC-C4B	4.00	1.48	1.39
24	C	502	CLA	C3C-C2C	4.00	1.45	1.36
28	x	101	SQD	O47-C7	3.99	1.45	1.34
24	c	512	CLA	CHC-C1C	3.99	1.46	1.38
24	A	607	CLA	C4B-NB	-3.99	1.32	1.37
43	V	203	HEC	C4B-NB	-3.98	1.33	1.40
29	j	101	LMG	O7-C10	3.97	1.45	1.34
24	c	513	CLA	OBD-CAD	3.97	1.29	1.22
24	B	615	CLA	CHB-C1B	3.97	1.48	1.39
24	B	609	CLA	C1D-ND	3.97	1.43	1.37
24	a	410	CLA	CHB-C1B	3.97	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	604	CLA	CHC-C1C	3.95	1.46	1.38
24	B	603	CLA	C3C-C2C	3.95	1.45	1.36
24	C	510	CLA	C3C-C2C	3.95	1.45	1.36
24	c	513	CLA	O2D-CGD	3.94	1.42	1.33
24	c	505	CLA	CHD-C1D	3.94	1.46	1.38
24	A	607	CLA	MG-NB	-3.94	1.98	2.05
24	C	501	CLA	OBD-CAD	3.94	1.29	1.22
24	c	511	CLA	C3D-C4D	-3.94	1.35	1.44
24	c	513	CLA	C3C-C2C	3.93	1.45	1.36
29	B	634	LMG	O1-C1	3.93	1.46	1.40
24	B	614	CLA	C3C-C2C	3.92	1.45	1.36
24	b	609	CLA	C3C-C2C	3.92	1.45	1.36
24	D	403	CLA	C3C-C2C	3.91	1.45	1.36
24	a	408	CLA	CHB-C1B	3.91	1.48	1.39
24	c	512	CLA	O2D-CGD	3.91	1.42	1.33
24	d	403	CLA	OBD-CAD	3.90	1.29	1.22
24	c	501	CLA	C4B-NB	-3.90	1.32	1.37
24	b	605	CLA	O2D-CGD	3.90	1.42	1.33
24	b	607	CLA	CHC-C4B	3.89	1.48	1.39
24	c	506	CLA	C3D-C4D	-3.89	1.35	1.44
24	B	611	CLA	C3D-C2D	3.89	1.49	1.39
24	c	506	CLA	CHB-C1B	3.88	1.48	1.39
28	A	612	SQD	O47-C7	3.88	1.45	1.34
24	C	502	CLA	C1D-ND	3.87	1.42	1.37
24	b	611	CLA	CHC-C1C	3.87	1.46	1.38
24	B	613	CLA	CHD-C4C	3.87	1.48	1.39
24	B	614	CLA	OBD-CAD	3.86	1.29	1.22
24	b	609	CLA	CHD-C1D	3.86	1.45	1.38
24	c	504	CLA	C3D-C2D	3.86	1.49	1.39
24	a	407	CLA	C3C-C2C	3.86	1.45	1.36
24	C	511	CLA	C3D-C4D	-3.85	1.35	1.44
24	b	604	CLA	C1D-ND	3.85	1.42	1.37
24	d	405	CLA	C4B-NB	-3.85	1.32	1.37
24	B	609	CLA	C3C-C2C	3.85	1.45	1.36
24	d	405	CLA	C3C-C2C	3.85	1.45	1.36
24	B	602	CLA	C1D-ND	3.85	1.42	1.37
24	c	513	CLA	CHC-C4B	3.85	1.48	1.39
24	A	609	CLA	CHC-C4B	3.85	1.48	1.39
24	c	504	CLA	C3C-C2C	3.85	1.45	1.36
24	c	510	CLA	CHC-C4B	3.84	1.48	1.39
24	C	512	CLA	C3D-C2D	3.84	1.49	1.39
43	V	203	HEC	C1D-ND	-3.84	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	519	LMG	O7-C10	3.84	1.45	1.34
24	b	603	CLA	OBD-CAD	3.84	1.29	1.22
24	C	512	CLA	C3D-C4D	-3.84	1.35	1.44
32	d	411	LHG	O7-C7	3.84	1.45	1.34
24	b	613	CLA	O2D-CGD	3.84	1.42	1.33
24	B	615	CLA	O2A-CGA	3.83	1.44	1.33
24	c	512	CLA	C3D-C2D	3.83	1.49	1.39
29	C	526	LMG	O8-C28	3.82	1.44	1.33
24	b	603	CLA	CHB-C1B	3.80	1.47	1.39
24	c	506	CLA	CHD-C4C	3.80	1.47	1.39
41	E	113	HEM	C4D-ND	-3.79	1.33	1.40
24	b	611	CLA	C1D-ND	3.79	1.42	1.37
24	B	604	CLA	O2A-CGA	3.79	1.44	1.33
24	B	607	CLA	CHB-C1B	3.79	1.47	1.39
27	D	407	PL9	C41-C39	3.79	1.59	1.51
24	c	510	CLA	CHD-C4C	3.79	1.47	1.39
24	C	507	CLA	C3C-C2C	3.78	1.44	1.36
24	c	501	CLA	C1D-ND	3.78	1.42	1.37
24	c	509	CLA	C3D-C4D	-3.78	1.35	1.44
24	B	613	CLA	OBD-CAD	3.77	1.29	1.22
24	B	607	CLA	C3C-C2C	3.77	1.44	1.36
24	c	509	CLA	O2D-CGD	3.77	1.42	1.33
27	A	611	PL9	O1-C4	-3.77	1.14	1.23
26	D	406	BCR	C1-C6	-3.76	1.49	1.53
25	D	401	PHO	C3D-C4D	-3.75	1.36	1.41
24	b	613	CLA	C1B-C2B	3.75	1.51	1.43
24	b	614	CLA	O2A-CGA	3.75	1.44	1.33
24	c	510	CLA	C3D-C2D	3.75	1.49	1.39
40	d	408	DGD	O3G-C1D	3.74	1.46	1.40
24	c	507	CLA	CHD-C1D	3.74	1.45	1.38
24	d	403	CLA	CHB-C1B	3.74	1.47	1.39
24	c	509	CLA	C3C-C2C	3.74	1.44	1.36
24	d	403	CLA	C1D-ND	3.73	1.42	1.37
24	c	511	CLA	OBD-CAD	3.73	1.28	1.22
24	C	503	CLA	C3D-C4D	-3.73	1.35	1.44
24	B	616	CLA	C1B-C2B	3.72	1.51	1.43
24	C	507	CLA	C3D-C2D	3.72	1.49	1.39
24	C	511	CLA	O2D-CGD	3.72	1.42	1.33
28	l	102	SQD	O47-C7	3.71	1.44	1.34
28	A	616	SQD	O8-S	3.71	1.61	1.47
24	b	608	CLA	CHC-C1C	3.71	1.45	1.38
24	c	508	CLA	O2A-CGA	3.71	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	609	CLA	CHD-C1D	3.70	1.45	1.38
24	c	501	CLA	CHB-C1B	3.70	1.47	1.39
24	c	512	CLA	C3D-C4D	-3.70	1.35	1.44
24	C	501	CLA	CHC-C1C	3.70	1.45	1.38
24	b	606	CLA	O2A-CGA	3.69	1.44	1.33
24	c	506	CLA	C3C-C2C	3.69	1.44	1.36
24	b	612	CLA	C1D-ND	3.69	1.42	1.37
24	C	512	CLA	CHB-C1B	3.69	1.47	1.39
24	B	608	CLA	CHC-C1C	3.69	1.45	1.38
24	d	405	CLA	OBD-CAD	3.68	1.28	1.22
24	b	602	CLA	C3C-C2C	3.68	1.44	1.36
24	c	501	CLA	C3C-C2C	3.67	1.44	1.36
24	B	616	CLA	C1B-NB	-3.67	1.33	1.37
24	b	605	CLA	CHB-C1B	3.66	1.47	1.39
24	C	513	CLA	C3C-C2C	3.66	1.44	1.36
40	h	104	DGD	O1G-C1A	3.66	1.44	1.33
24	b	612	CLA	CHB-C1B	3.66	1.47	1.39
24	c	507	CLA	C3D-C2D	3.66	1.49	1.39
24	B	610	CLA	C1B-C2B	3.66	1.51	1.43
24	C	506	CLA	C3D-C4D	-3.66	1.36	1.44
31	u	203	LMT	O1'-C1'	3.66	1.46	1.40
24	A	606	CLA	O2D-CGD	3.65	1.42	1.33
24	B	610	CLA	C3C-C2C	3.65	1.44	1.36
24	b	610	CLA	C1D-ND	3.65	1.42	1.37
24	C	501	CLA	C3D-C2D	3.65	1.48	1.39
24	D	405	CLA	O2D-CGD	3.65	1.42	1.33
24	c	510	CLA	O2D-CGD	3.65	1.42	1.33
24	B	607	CLA	C1B-NB	-3.64	1.33	1.37
24	a	408	CLA	OBD-CAD	3.64	1.28	1.22
24	C	507	CLA	CHD-C1D	3.63	1.45	1.38
24	B	608	CLA	C3C-C2C	3.63	1.44	1.36
24	C	505	CLA	CHD-C1D	3.63	1.45	1.38
24	B	602	CLA	O2D-CGD	3.62	1.42	1.33
24	B	606	CLA	CHC-C4B	3.62	1.47	1.39
24	B	610	CLA	O2D-CGD	3.61	1.42	1.33
24	c	513	CLA	C3D-C2D	3.61	1.48	1.39
32	l	101	LHG	O8-C23	3.61	1.43	1.33
24	a	410	CLA	C3D-C4D	-3.61	1.36	1.44
24	b	603	CLA	C3C-C2C	3.61	1.44	1.36
24	C	505	CLA	C1B-C2B	3.61	1.51	1.43
24	B	608	CLA	C1B-C2B	3.60	1.51	1.43
29	c	519	LMG	O7-C10	3.60	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	513	CLA	O2D-CGD	3.60	1.42	1.33
24	A	609	CLA	C3C-C2C	3.60	1.44	1.36
24	b	617	CLA	CHC-C1C	3.60	1.45	1.38
24	B	604	CLA	CHC-C1C	3.59	1.45	1.38
29	a	414	LMG	O7-C10	3.59	1.44	1.34
24	c	512	CLA	CHB-C1B	3.59	1.47	1.39
24	C	501	CLA	CHC-C4B	3.58	1.47	1.39
24	c	512	CLA	OBD-CAD	3.57	1.28	1.22
24	C	513	CLA	C3D-C4D	-3.57	1.36	1.44
24	a	407	CLA	OBD-CAD	3.57	1.28	1.22
24	B	608	CLA	O2D-CGD	3.57	1.42	1.33
24	d	405	CLA	C1D-ND	3.56	1.42	1.37
24	C	506	CLA	CHB-C1B	3.56	1.47	1.39
24	b	615	CLA	OBD-CAD	3.56	1.28	1.22
38	C	531	HTG	C1'-S1	-3.56	1.76	1.81
24	B	606	CLA	CHD-C1D	3.55	1.45	1.38
40	c	517	DGD	O1G-C1A	3.55	1.43	1.33
24	B	602	CLA	CHC-C1C	3.55	1.45	1.38
24	C	509	CLA	C1B-C2B	3.55	1.51	1.43
24	D	405	CLA	C3D-C2D	3.55	1.48	1.39
24	B	611	CLA	O2D-CGD	3.54	1.41	1.33
27	D	407	PL9	C38-C39	-3.53	1.24	1.33
24	b	605	CLA	C4B-NB	-3.53	1.33	1.37
27	d	407	PL9	C36-C37	-3.53	1.42	1.53
24	d	405	CLA	C3D-C2D	3.53	1.48	1.39
24	C	504	CLA	OBD-CAD	3.53	1.28	1.22
24	a	410	CLA	C3C-C2C	3.53	1.44	1.36
24	D	403	CLA	CHC-C1C	3.53	1.45	1.38
25	D	401	PHO	C3A-C2A	-3.53	1.51	1.54
24	A	609	CLA	CHC-C1C	3.53	1.45	1.38
24	d	405	CLA	C1C-NC	-3.52	1.32	1.37
24	b	608	CLA	C3D-C2D	3.52	1.48	1.39
24	A	607	CLA	CHC-C4B	3.52	1.47	1.39
24	b	608	CLA	C1B-C2B	3.52	1.51	1.43
24	B	610	CLA	CHC-C1C	3.52	1.45	1.38
24	b	609	CLA	CHB-C1B	3.52	1.47	1.39
24	C	507	CLA	C4B-NB	-3.51	1.33	1.37
24	c	506	CLA	C1B-NB	-3.51	1.33	1.37
24	c	508	CLA	CHD-C1D	3.51	1.45	1.38
24	C	513	CLA	CHB-C1B	3.51	1.47	1.39
24	C	508	CLA	C1D-ND	3.51	1.42	1.37
24	B	617	CLA	C1C-NC	-3.51	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	OBD-CAD	3.50	1.28	1.22
24	B	611	CLA	C3D-C4D	-3.50	1.36	1.44
24	c	509	CLA	O2A-CGA	3.50	1.43	1.33
24	b	616	CLA	O2A-CGA	3.49	1.43	1.33
24	a	408	CLA	CHC-C1C	3.49	1.45	1.38
24	b	608	CLA	CHB-C1B	3.49	1.47	1.39
24	C	512	CLA	O2D-CGD	3.49	1.41	1.33
24	B	605	CLA	O2A-CGA	3.49	1.43	1.33
24	b	611	CLA	MG-ND	-3.48	1.98	2.05
24	C	512	CLA	CHD-C4C	3.48	1.47	1.39
24	c	512	CLA	CHD-C4C	3.48	1.47	1.39
24	b	613	CLA	C3C-C2C	3.48	1.44	1.36
24	c	512	CLA	O2A-CGA	3.48	1.43	1.33
24	A	607	CLA	C3D-C4D	-3.47	1.36	1.44
24	c	513	CLA	O2A-CGA	3.47	1.43	1.33
26	d	406	BCR	C1-C6	-3.47	1.49	1.53
24	B	613	CLA	C1D-ND	3.47	1.42	1.37
24	c	503	CLA	CHB-C1B	3.47	1.47	1.39
24	A	606	CLA	CHC-C1C	3.47	1.45	1.38
24	c	511	CLA	CHB-C1B	3.47	1.47	1.39
24	B	609	CLA	CHD-C1D	3.47	1.45	1.38
24	A	607	CLA	O2D-CGD	3.47	1.41	1.33
25	d	401	PHO	C3D-C2D	3.46	1.45	1.39
24	B	604	CLA	C3D-C2D	3.46	1.48	1.39
24	c	509	CLA	CHB-C1B	3.46	1.47	1.39
24	b	602	CLA	CHC-C1C	3.46	1.45	1.38
24	B	611	CLA	CHC-C1C	3.46	1.45	1.38
24	B	616	CLA	CHD-C4C	3.46	1.47	1.39
24	C	509	CLA	CHD-C1D	3.45	1.45	1.38
24	c	506	CLA	CHC-C1C	3.44	1.45	1.38
40	c	518	DGD	O1G-C1A	3.44	1.43	1.33
24	C	507	CLA	CHC-C1C	3.44	1.45	1.38
24	B	609	CLA	O2A-CGA	3.44	1.43	1.33
25	a	409	PHO	OBD-CAD	3.43	1.26	1.22
24	B	602	CLA	C3D-C2D	3.43	1.48	1.39
24	B	616	CLA	MG-NB	-3.43	1.99	2.05
24	c	504	CLA	O2D-CGD	3.43	1.41	1.33
43	v	202	HEC	FE-NC	3.43	2.06	1.95
24	c	510	CLA	CHB-C1B	3.43	1.47	1.39
24	b	615	CLA	CHD-C4C	3.43	1.47	1.39
24	a	408	CLA	MG-ND	-3.42	1.99	2.05
38	b	631	HTG	C1'-S1	-3.42	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	608	PHO	C3D-C2D	3.41	1.45	1.39
24	c	506	CLA	O2D-CGD	3.41	1.41	1.33
24	B	616	CLA	MG-ND	-3.41	1.99	2.05
24	C	502	CLA	O2D-CGD	3.40	1.41	1.33
32	d	411	LHG	O8-C23	3.40	1.43	1.33
24	c	508	CLA	MG-ND	-3.40	1.99	2.05
24	B	603	CLA	O2D-CGD	3.40	1.41	1.33
24	C	508	CLA	CHB-C1B	3.40	1.47	1.39
24	c	508	CLA	CHC-C1C	3.39	1.45	1.38
24	c	506	CLA	C1C-NC	-3.39	1.32	1.37
24	B	614	CLA	MG-NB	-3.39	1.99	2.05
24	c	510	CLA	C3C-C2C	3.39	1.44	1.36
24	B	610	CLA	MG-NB	-3.39	1.99	2.05
24	C	513	CLA	C1D-ND	3.38	1.42	1.37
24	C	503	CLA	OBD-CAD	3.38	1.28	1.22
24	c	511	CLA	O2D-CGD	3.38	1.41	1.33
24	C	504	CLA	C1D-ND	3.38	1.42	1.37
24	C	505	CLA	CHC-C4B	3.38	1.47	1.39
24	C	504	CLA	CHD-C4C	3.38	1.46	1.39
24	D	404	CLA	CHB-C1B	3.37	1.47	1.39
24	B	616	CLA	O2D-CGD	3.37	1.41	1.33
24	c	513	CLA	CHB-C1B	3.37	1.47	1.39
24	b	616	CLA	C3D-C4D	-3.37	1.36	1.44
24	c	504	CLA	C3D-C4D	-3.37	1.36	1.44
24	C	502	CLA	CHB-C1B	3.36	1.47	1.39
24	C	506	CLA	C3C-C2C	3.36	1.44	1.36
24	c	506	CLA	CHD-C1D	3.36	1.45	1.38
25	A	608	PHO	O2D-CGD	3.36	1.41	1.33
25	A	608	PHO	OBD-CAD	3.36	1.26	1.22
24	B	606	CLA	O2A-CGA	3.36	1.43	1.33
29	A	613	LMG	O8-C28	3.36	1.43	1.33
24	A	609	CLA	C3D-C4D	-3.35	1.36	1.44
24	D	405	CLA	C3D-C4D	-3.35	1.36	1.44
29	b	621	LMG	O7-C8	-3.35	1.38	1.46
24	b	613	CLA	C3D-C2D	3.35	1.48	1.39
24	D	404	CLA	CHC-C4B	3.35	1.46	1.39
24	b	617	CLA	O2D-CGD	3.35	1.41	1.33
28	a	413	SQD	O47-C7	3.35	1.43	1.34
24	C	503	CLA	O2A-CGA	3.34	1.43	1.33
24	b	612	CLA	CHD-C4C	3.34	1.46	1.39
24	c	508	CLA	C1B-NB	-3.34	1.33	1.37
24	b	612	CLA	C4B-NB	-3.34	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	CHB-C1B	3.34	1.46	1.39
29	B	621	LMG	O7-C10	3.34	1.43	1.34
31	F	102	LMT	O1'-C1'	3.34	1.45	1.40
24	a	410	CLA	C3D-C2D	3.33	1.48	1.39
40	h	104	DGD	O2G-C1B	3.33	1.43	1.34
41	E	113	HEM	C4B-NB	-3.32	1.32	1.38
24	d	404	CLA	CHC-C4B	3.31	1.46	1.39
24	b	617	CLA	C3C-C2C	3.31	1.43	1.36
40	c	516	DGD	O1G-C1A	3.31	1.43	1.33
24	C	504	CLA	O2D-CGD	3.31	1.41	1.33
24	b	603	CLA	C3D-C4D	-3.30	1.36	1.44
29	b	621	LMG	O7-C10	3.30	1.43	1.34
24	B	609	CLA	C3D-C2D	3.30	1.48	1.39
24	c	508	CLA	C3D-C2D	3.30	1.48	1.39
25	A	608	PHO	C3B-C4B	3.30	1.44	1.41
24	b	611	CLA	CHC-C4B	3.30	1.46	1.39
24	b	603	CLA	MG-ND	-3.30	1.99	2.05
24	C	507	CLA	C3D-C4D	-3.30	1.36	1.44
24	B	613	CLA	C3C-C2C	3.29	1.43	1.36
24	C	511	CLA	O2A-CGA	3.28	1.42	1.33
24	B	602	CLA	CHD-C1D	3.28	1.44	1.38
24	c	502	CLA	CHC-C4B	3.28	1.46	1.39
24	b	612	CLA	C3C-C2C	3.28	1.43	1.36
24	a	408	CLA	C3C-C2C	3.28	1.43	1.36
24	D	403	CLA	C1B-NB	-3.28	1.33	1.37
24	D	403	CLA	MG-NB	-3.28	1.99	2.05
24	b	612	CLA	MG-ND	-3.28	1.99	2.05
24	B	615	CLA	MG-ND	-3.28	1.99	2.05
24	C	510	CLA	CHC-C1C	3.28	1.45	1.38
24	c	501	CLA	C3D-C4D	-3.28	1.36	1.44
24	B	614	CLA	CHB-C1B	3.28	1.46	1.39
24	b	612	CLA	CHD-C1D	3.27	1.44	1.38
29	d	412	LMG	O7-C10	3.27	1.43	1.34
24	b	617	CLA	OBD-CAD	3.27	1.28	1.22
24	B	617	CLA	C3D-C2D	3.27	1.47	1.39
24	d	405	CLA	CHC-C1C	3.27	1.45	1.38
24	C	503	CLA	CHC-C4B	3.27	1.46	1.39
24	b	602	CLA	CHD-C1D	3.27	1.44	1.38
24	C	504	CLA	C3C-C2C	3.26	1.43	1.36
24	B	617	CLA	OBD-CAD	3.26	1.28	1.22
24	c	505	CLA	CHC-C1C	3.26	1.45	1.38
24	b	604	CLA	C3D-C4D	-3.25	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	608	CLA	MG-ND	-3.25	1.99	2.05
31	f	101	LMT	O1'-C1'	3.25	1.45	1.40
24	c	508	CLA	CHB-C1B	3.25	1.46	1.39
24	B	603	CLA	CHC-C4B	3.24	1.46	1.39
24	b	612	CLA	O2D-CGD	3.24	1.41	1.33
24	B	610	CLA	C1D-ND	3.23	1.42	1.37
24	C	503	CLA	C1B-NB	-3.23	1.33	1.37
24	b	613	CLA	CHB-C1B	3.23	1.46	1.39
24	b	617	CLA	CHC-C4B	3.23	1.46	1.39
24	d	403	CLA	O2D-CGD	3.23	1.41	1.33
24	d	405	CLA	CAA-C2A	-3.23	1.48	1.54
24	C	506	CLA	C3D-C2D	3.23	1.47	1.39
24	C	502	CLA	C3D-C2D	3.22	1.47	1.39
24	D	405	CLA	CHD-C1D	3.22	1.44	1.38
24	a	408	CLA	C3D-C2D	3.22	1.47	1.39
24	c	502	CLA	CHC-C1C	3.22	1.44	1.38
24	c	507	CLA	C1B-C2B	3.22	1.50	1.43
24	C	504	CLA	C1C-NC	-3.22	1.32	1.37
25	D	401	PHO	C4B-NB	-3.22	1.32	1.38
24	b	606	CLA	C3D-C4D	-3.21	1.37	1.44
24	d	403	CLA	C3C-C2C	3.21	1.43	1.36
24	C	505	CLA	O2A-CGA	3.21	1.42	1.33
24	A	609	CLA	C1B-C2B	3.21	1.50	1.43
24	c	501	CLA	O2A-CGA	3.21	1.42	1.33
24	C	501	CLA	C3D-C4D	-3.20	1.37	1.44
24	B	617	CLA	CHC-C1C	3.20	1.44	1.38
43	V	203	HEC	C1B-NB	-3.20	1.32	1.38
29	C	520	LMG	O1-C1	3.20	1.45	1.40
32	D	411	LHG	O8-C23	3.20	1.42	1.33
40	C	517	DGD	O1G-C1A	3.19	1.42	1.33
24	B	608	CLA	C3D-C2D	3.19	1.47	1.39
24	C	513	CLA	C4B-NB	-3.19	1.33	1.37
24	B	616	CLA	OBD-CAD	3.19	1.28	1.22
24	B	611	CLA	C1B-C2B	3.19	1.50	1.43
24	B	604	CLA	OBD-CAD	3.19	1.28	1.22
24	b	607	CLA	O2D-CGD	3.19	1.41	1.33
24	C	510	CLA	C3D-C2D	3.19	1.47	1.39
24	c	511	CLA	C3D-C2D	3.19	1.47	1.39
24	B	603	CLA	C3D-C4D	-3.19	1.37	1.44
24	d	403	CLA	CHD-C4C	3.19	1.46	1.39
24	b	617	CLA	O2A-CGA	3.19	1.42	1.33
24	C	513	CLA	C3D-C2D	3.19	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	407	CLA	O2D-CGD	3.18	1.41	1.33
25	A	608	PHO	O2A-CGA	3.18	1.42	1.33
24	b	605	CLA	C1D-C2D	3.18	1.51	1.45
24	B	603	CLA	C1B-C2B	3.18	1.50	1.43
24	c	501	CLA	CHD-C1D	3.17	1.44	1.38
38	C	530	HTG	C1'-S1	-3.17	1.77	1.81
24	c	513	CLA	CHC-C1C	3.17	1.44	1.38
24	b	609	CLA	C1D-ND	3.17	1.42	1.37
24	c	503	CLA	C3D-C4D	-3.17	1.37	1.44
24	B	612	CLA	C1D-ND	3.17	1.42	1.37
41	e	107	HEM	C4D-ND	-3.16	1.34	1.40
24	c	506	CLA	O2A-CGA	3.16	1.42	1.33
24	B	617	CLA	O2D-CGD	3.16	1.41	1.33
25	D	401	PHO	CBD-CGD	-3.16	1.48	1.52
24	B	612	CLA	CHB-C1B	3.16	1.46	1.39
24	B	606	CLA	CHB-C1B	3.16	1.46	1.39
24	a	407	CLA	CHC-C4B	3.16	1.46	1.39
24	c	513	CLA	CHD-C4C	3.16	1.46	1.39
24	B	606	CLA	C1C-NC	-3.16	1.32	1.37
24	b	604	CLA	C3D-C2D	3.15	1.47	1.39
25	D	401	PHO	O2D-CGD	3.15	1.41	1.33
24	C	513	CLA	O2A-CGA	3.15	1.42	1.33
24	b	611	CLA	C3D-C2D	3.15	1.47	1.39
24	a	407	CLA	CHB-C1B	3.14	1.46	1.39
24	D	405	CLA	O2A-CGA	3.14	1.42	1.33
25	A	608	PHO	CBD-CGD	-3.14	1.48	1.52
24	b	602	CLA	CHB-C1B	3.14	1.46	1.39
24	d	404	CLA	C3D-C2D	3.14	1.47	1.39
24	C	507	CLA	CHD-C4C	3.13	1.46	1.39
24	b	603	CLA	C1D-ND	3.13	1.42	1.37
24	C	509	CLA	C3C-C2C	3.13	1.43	1.36
24	C	509	CLA	O2A-CGA	3.12	1.42	1.33
24	C	505	CLA	MG-ND	-3.12	1.99	2.05
24	c	513	CLA	CHD-C1D	3.12	1.44	1.38
40	c	516	DGD	O5D-C1E	3.12	1.45	1.40
24	B	617	CLA	C4B-NB	-3.12	1.33	1.37
24	c	510	CLA	C3D-C4D	-3.12	1.37	1.44
24	b	604	CLA	OBD-CAD	3.12	1.27	1.22
24	c	504	CLA	CHD-C1D	3.11	1.44	1.38
24	B	609	CLA	CHC-C4B	3.11	1.46	1.39
24	c	511	CLA	O2A-CGA	3.11	1.42	1.33
32	D	410	LHG	O8-C23	3.11	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	O2D-CGD	3.10	1.40	1.33
41	E	113	HEM	C4D-C3D	3.10	1.50	1.45
24	B	612	CLA	C3C-C2C	3.10	1.43	1.36
24	B	611	CLA	C1B-NB	-3.10	1.33	1.37
24	c	509	CLA	C1B-C2B	3.10	1.50	1.43
24	b	610	CLA	CHB-C1B	3.10	1.46	1.39
24	a	408	CLA	CHD-C4C	3.10	1.46	1.39
24	a	407	CLA	MG-ND	-3.10	1.99	2.05
24	b	610	CLA	C3C-C2C	3.10	1.43	1.36
24	C	509	CLA	CHC-C1C	3.09	1.44	1.38
24	b	603	CLA	C1B-C2B	3.09	1.50	1.43
27	a	412	PL9	C6-C5	3.09	1.50	1.35
24	c	504	CLA	C1B-C2B	3.09	1.50	1.43
24	c	505	CLA	C1C-C2C	3.09	1.50	1.44
24	c	508	CLA	O2D-CGD	3.08	1.40	1.33
24	C	512	CLA	C3C-C2C	3.08	1.43	1.36
24	D	405	CLA	CHC-C4B	3.08	1.46	1.39
24	b	603	CLA	C3D-C2D	3.08	1.47	1.39
38	b	623	HTG	C1-C2	3.08	1.58	1.53
24	b	614	CLA	CHC-C1C	3.08	1.44	1.38
24	B	602	CLA	C1B-C2B	3.07	1.50	1.43
24	A	609	CLA	C3D-C2D	3.07	1.47	1.39
24	B	603	CLA	C1B-NB	-3.07	1.33	1.37
24	b	603	CLA	O2A-CGA	3.07	1.42	1.33
24	d	404	CLA	O2A-CGA	3.06	1.42	1.33
24	b	607	CLA	CHB-C1B	3.06	1.46	1.39
27	d	407	PL9	C41-C39	3.06	1.57	1.51
24	D	404	CLA	C4B-NB	-3.06	1.33	1.37
24	b	604	CLA	CHD-C1D	3.06	1.44	1.38
24	b	603	CLA	CHB-C4A	-3.06	1.30	1.37
24	c	512	CLA	CHC-C4B	3.06	1.46	1.39
24	C	510	CLA	C3D-C4D	-3.06	1.37	1.44
24	b	604	CLA	O2D-CGD	3.06	1.40	1.33
24	B	616	CLA	CHC-C1C	3.05	1.44	1.38
24	C	503	CLA	C1B-C2B	3.05	1.50	1.43
27	d	407	PL9	C38-C39	-3.05	1.26	1.33
24	b	613	CLA	CHC-C1C	3.05	1.44	1.38
24	c	507	CLA	C4B-NB	-3.05	1.33	1.37
24	c	502	CLA	CHD-C1D	3.05	1.44	1.38
24	c	505	CLA	C1C-NC	-3.05	1.33	1.37
24	c	503	CLA	C3D-C2D	3.05	1.47	1.39
24	C	505	CLA	O2D-CGD	3.05	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	605	CLA	CHC-C1C	3.04	1.44	1.38
24	C	511	CLA	C1B-C2B	3.04	1.50	1.43
24	d	403	CLA	MG-ND	-3.04	1.99	2.05
24	C	511	CLA	OBD-CAD	3.03	1.27	1.22
24	c	505	CLA	CHB-C1B	3.03	1.46	1.39
38	C	532	HTG	C1'-S1	-3.03	1.77	1.81
40	C	516	DGD	O2G-C1B	3.03	1.42	1.34
24	a	410	CLA	C1B-C2B	3.03	1.50	1.43
29	c	520	LMG	O1-C1	3.03	1.45	1.40
24	C	504	CLA	C3D-C2D	3.02	1.47	1.39
24	d	405	CLA	O2A-CGA	3.02	1.42	1.33
24	c	502	CLA	O2A-CGA	3.02	1.42	1.33
32	B	632	LHG	O8-C23	3.02	1.42	1.33
24	C	506	CLA	O2A-CGA	3.02	1.42	1.33
24	C	512	CLA	C4C-C3C	3.02	1.50	1.45
24	b	617	CLA	C3D-C2D	3.02	1.47	1.39
24	A	607	CLA	C3D-C2D	3.02	1.47	1.39
24	C	509	CLA	CHB-C1B	3.01	1.46	1.39
24	d	405	CLA	C3D-C4D	-3.01	1.37	1.44
24	A	606	CLA	C3D-C2D	3.01	1.47	1.39
24	c	504	CLA	O2A-CGA	3.00	1.42	1.33
26	c	514	BCR	C30-C25	-3.00	1.49	1.53
38	c	530	HTG	C1'-S1	-3.00	1.77	1.81
24	b	602	CLA	C3D-C2D	3.00	1.47	1.39
32	l	101	LHG	O7-C7	3.00	1.42	1.34
24	a	408	CLA	C3D-C4D	-3.00	1.37	1.44
24	C	507	CLA	CHC-C4B	2.99	1.46	1.39
24	B	610	CLA	CHD-C1D	2.99	1.44	1.38
24	a	408	CLA	C1C-NC	-2.99	1.33	1.37
38	C	521	HTG	C1-S1	-2.99	1.75	1.80
24	C	507	CLA	OBD-CAD	2.99	1.27	1.22
24	b	616	CLA	MG-NB	-2.98	1.99	2.05
40	D	408	DGD	O5D-C1E	2.98	1.45	1.40
32	D	410	LHG	O7-C7	2.98	1.42	1.34
24	B	602	CLA	CHC-C4B	2.98	1.46	1.39
24	A	607	CLA	OBD-CAD	2.98	1.27	1.22
24	b	609	CLA	C3D-C2D	2.98	1.47	1.39
38	H	101	HTG	C1'-S1	-2.98	1.77	1.81
40	H	103	DGD	O5D-C1E	2.97	1.45	1.40
24	b	610	CLA	O2A-CGA	2.97	1.42	1.33
24	C	504	CLA	CHB-C1B	2.97	1.46	1.39
24	c	511	CLA	CHD-C1D	2.97	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	609	CLA	C1C-NC	-2.96	1.33	1.37
24	b	605	CLA	C3D-C4D	-2.96	1.37	1.44
24	A	606	CLA	C1D-ND	2.96	1.41	1.37
24	b	607	CLA	CHC-C1C	2.96	1.44	1.38
24	D	404	CLA	OBD-CAD	2.96	1.27	1.22
24	c	501	CLA	CHC-C1C	2.96	1.44	1.38
24	A	609	CLA	OBD-CAD	2.96	1.27	1.22
25	d	401	PHO	C4B-NB	-2.96	1.33	1.38
24	c	504	CLA	C1D-C2D	2.96	1.51	1.45
24	A	607	CLA	C1C-NC	-2.95	1.33	1.37
24	C	512	CLA	C1B-C2B	2.95	1.50	1.43
24	c	503	CLA	C1B-NB	-2.95	1.34	1.37
26	a	411	BCR	C36-C18	2.95	1.56	1.50
24	b	611	CLA	C4B-NB	-2.95	1.34	1.37
24	c	509	CLA	CHC-C4B	2.95	1.46	1.39
27	A	611	PL9	C6-C5	2.95	1.49	1.35
24	b	609	CLA	CHC-C1C	2.95	1.44	1.38
24	b	609	CLA	OBD-CAD	2.94	1.27	1.22
29	d	412	LMG	O1-C1	2.94	1.45	1.40
24	B	605	CLA	OBD-CAD	2.94	1.27	1.22
24	c	511	CLA	CHC-C4B	2.94	1.46	1.39
24	A	609	CLA	C4B-NB	-2.94	1.34	1.37
40	c	518	DGD	O2G-C1B	2.94	1.42	1.34
24	b	617	CLA	C3D-C4D	-2.93	1.37	1.44
24	C	501	CLA	CHD-C4C	2.93	1.45	1.39
24	D	403	CLA	O2D-CGD	2.93	1.40	1.33
24	A	606	CLA	CHB-C1B	2.93	1.46	1.39
24	B	606	CLA	CHC-C1C	2.93	1.44	1.38
24	b	606	CLA	MG-ND	-2.93	2.00	2.05
24	c	502	CLA	C3D-C2D	2.93	1.47	1.39
24	b	615	CLA	C3D-C4D	-2.93	1.37	1.44
24	c	509	CLA	C3D-C2D	2.92	1.47	1.39
41	e	107	HEM	C4C-NC	-2.92	1.34	1.39
28	a	413	SQD	O48-C23	2.92	1.41	1.33
24	C	511	CLA	CHC-C1C	2.92	1.44	1.38
24	d	403	CLA	O2A-CGA	2.92	1.41	1.33
24	b	607	CLA	CHD-C1D	2.92	1.44	1.38
38	C	529	HTG	O5-C1	2.92	1.47	1.42
24	c	504	CLA	OBD-CAD	2.92	1.27	1.22
24	B	613	CLA	CHC-C4B	2.92	1.46	1.39
24	b	607	CLA	CHD-C4C	2.91	1.45	1.39
24	c	510	CLA	CHC-C1C	2.91	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	511	CLA	C3C-C2C	2.91	1.43	1.36
24	B	612	CLA	OBD-CAD	2.91	1.27	1.22
24	B	615	CLA	CHB-C4A	-2.91	1.30	1.37
24	C	506	CLA	CHC-C4B	2.91	1.45	1.39
24	C	503	CLA	CHD-C4C	2.91	1.45	1.39
40	c	517	DGD	O2G-C1B	2.91	1.42	1.34
24	b	612	CLA	CHC-C1C	2.91	1.44	1.38
27	D	407	PL9	C18-C19	2.91	1.39	1.33
24	b	605	CLA	C3C-C2C	2.91	1.43	1.36
26	c	514	BCR	C1-C6	-2.91	1.50	1.53
24	c	509	CLA	C1D-ND	2.91	1.41	1.37
24	B	607	CLA	C3D-C4D	-2.90	1.37	1.44
24	D	404	CLA	MG-ND	-2.90	2.00	2.05
24	b	613	CLA	MG-ND	-2.90	2.00	2.05
29	j	101	LMG	O8-C28	2.90	1.41	1.33
24	D	404	CLA	C3C-C2C	2.90	1.43	1.36
25	d	401	PHO	O2D-CGD	2.90	1.40	1.33
24	b	616	CLA	CHD-C4C	2.90	1.45	1.39
24	a	408	CLA	CHD-C1D	2.90	1.44	1.38
24	B	611	CLA	CHC-C4B	2.89	1.45	1.39
31	A	617	LMT	O1'-C1'	2.89	1.45	1.40
24	C	504	CLA	O2A-CGA	2.89	1.41	1.33
24	b	614	CLA	C3D-C2D	2.89	1.46	1.39
24	B	602	CLA	C3C-C2C	2.89	1.43	1.36
24	C	506	CLA	CHC-C1C	2.88	1.44	1.38
24	A	609	CLA	CHD-C4C	2.88	1.45	1.39
40	c	517	DGD	O5D-C1E	2.88	1.45	1.40
24	b	606	CLA	MG-NB	-2.87	2.00	2.05
26	C	514	BCR	C30-C25	-2.87	1.50	1.53
24	b	609	CLA	C1B-C2B	2.87	1.49	1.43
24	b	609	CLA	O2A-CGA	2.86	1.41	1.33
24	B	612	CLA	C3D-C2D	2.86	1.46	1.39
24	b	608	CLA	CHC-C4B	2.86	1.45	1.39
24	c	511	CLA	C4B-NB	-2.86	1.34	1.37
24	B	611	CLA	C1C-NC	-2.86	1.33	1.37
24	b	611	CLA	C3D-C4D	-2.86	1.37	1.44
24	b	613	CLA	O2A-CGA	2.86	1.41	1.33
24	b	603	CLA	CHC-C4B	2.86	1.45	1.39
25	d	401	PHO	C1D-ND	-2.85	1.33	1.38
24	b	615	CLA	CHC-C4B	2.85	1.45	1.39
24	d	405	CLA	C1B-C2B	2.85	1.49	1.43
24	c	504	CLA	CHC-C1C	2.85	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	CLA	C4B-NB	-2.85	1.34	1.37
24	c	503	CLA	OBD-CAD	2.84	1.27	1.22
24	C	505	CLA	C3D-C2D	2.84	1.46	1.39
24	b	613	CLA	CMB-C2B	-2.84	1.44	1.50
24	a	408	CLA	O2D-CGD	2.84	1.40	1.33
40	d	408	DGD	O5D-C1E	2.84	1.44	1.40
24	B	610	CLA	C3D-C2D	2.84	1.46	1.39
24	B	610	CLA	CHD-C4C	2.84	1.45	1.39
25	a	409	PHO	C3A-C2A	-2.84	1.52	1.54
24	B	614	CLA	C3D-C2D	2.84	1.46	1.39
24	C	503	CLA	C1C-NC	-2.83	1.33	1.37
24	c	505	CLA	C1B-C2B	2.83	1.49	1.43
24	B	604	CLA	CHD-C4C	2.83	1.45	1.39
24	b	614	CLA	CHC-C4B	2.83	1.45	1.39
24	B	610	CLA	O2A-CGA	2.83	1.41	1.33
38	h	101	HTG	C1-S1	-2.83	1.76	1.80
24	B	605	CLA	CHC-C4B	2.83	1.45	1.39
24	b	604	CLA	CHD-C4C	2.83	1.45	1.39
24	B	603	CLA	CHD-C1D	2.83	1.43	1.38
40	C	517	DGD	O2G-C1B	2.82	1.42	1.34
24	C	502	CLA	C1B-C2B	2.82	1.49	1.43
24	c	509	CLA	CHD-C1D	2.82	1.43	1.38
31	I	101	LMT	O1'-C1'	2.82	1.44	1.40
24	B	605	CLA	O2D-CGD	2.82	1.40	1.33
43	v	202	HEC	C1B-NB	-2.81	1.33	1.38
24	c	505	CLA	O2D-CGD	2.81	1.40	1.33
24	B	616	CLA	C4C-C3C	2.81	1.49	1.45
29	b	621	LMG	O8-C28	2.80	1.41	1.33
24	B	611	CLA	CHB-C1B	2.80	1.45	1.39
24	c	501	CLA	C3D-C2D	2.80	1.46	1.39
24	C	508	CLA	O2A-CGA	2.80	1.41	1.33
24	c	503	CLA	C1B-C2B	2.80	1.49	1.43
24	b	615	CLA	O2D-CGD	2.80	1.40	1.33
24	b	612	CLA	C1B-C2B	2.80	1.49	1.43
24	c	508	CLA	C1B-C2B	2.79	1.49	1.43
24	c	506	CLA	C1C-C2C	2.79	1.50	1.44
41	E	113	HEM	C1C-C2C	-2.79	1.39	1.45
24	B	606	CLA	C3D-C2D	2.79	1.46	1.39
24	d	404	CLA	CHD-C1D	2.79	1.43	1.38
38	B	624	HTG	C1'-S1	-2.79	1.77	1.81
24	D	403	CLA	C1C-NC	-2.79	1.33	1.37
24	B	613	CLA	CHD-C1D	2.78	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	O2D-CGD	2.78	1.40	1.33
24	b	608	CLA	O2D-CGD	2.78	1.40	1.33
24	b	615	CLA	C3C-C2C	2.78	1.42	1.36
24	C	513	CLA	CHD-C1D	2.78	1.43	1.38
24	D	404	CLA	C1C-C2C	2.78	1.50	1.44
24	c	506	CLA	C1B-C2B	2.78	1.49	1.43
26	c	514	BCR	C8-C9	2.77	1.51	1.46
24	D	404	CLA	O2D-CGD	2.77	1.40	1.33
24	c	501	CLA	C1B-C2B	2.77	1.49	1.43
24	B	617	CLA	CHD-C4C	2.77	1.45	1.39
24	c	502	CLA	C1C-NC	-2.77	1.33	1.37
24	b	616	CLA	C4B-NB	-2.77	1.34	1.37
24	b	617	CLA	C1C-NC	-2.77	1.33	1.37
24	B	607	CLA	CHD-C4C	2.77	1.45	1.39
24	a	407	CLA	CHC-C1C	2.76	1.44	1.38
24	B	612	CLA	C4C-C3C	2.76	1.49	1.45
24	b	609	CLA	CHC-C4B	2.76	1.45	1.39
27	A	611	PL9	C2-C3	2.76	1.41	1.34
40	C	516	DGD	O1G-C1A	2.76	1.41	1.33
24	C	508	CLA	C3D-C2D	2.76	1.46	1.39
31	a	401	LMT	O1'-C1'	2.76	1.44	1.40
24	B	605	CLA	MG-NB	-2.75	2.00	2.05
24	b	613	CLA	MG-NB	-2.75	2.00	2.05
24	c	512	CLA	CHD-C1D	2.75	1.43	1.38
24	B	617	CLA	C1B-C2B	2.75	1.49	1.43
24	b	605	CLA	O2A-CGA	2.75	1.41	1.33
24	b	617	CLA	C1B-C2B	2.75	1.49	1.43
32	D	409	LHG	O8-C23	2.74	1.41	1.33
31	b	622	LMT	O3B-C3B	2.74	1.49	1.43
24	b	607	CLA	C3C-C2C	2.74	1.42	1.36
24	c	505	CLA	OBD-CAD	2.74	1.27	1.22
24	C	502	CLA	CHD-C4C	2.74	1.45	1.39
24	B	608	CLA	CHD-C1D	2.74	1.43	1.38
24	b	614	CLA	CHD-C4C	2.74	1.45	1.39
27	D	407	PL9	C6-C5	2.74	1.48	1.35
24	b	610	CLA	MG-ND	-2.73	2.00	2.05
24	B	616	CLA	O2A-CGA	2.73	1.41	1.33
24	b	611	CLA	OBD-CAD	2.73	1.27	1.22
24	c	510	CLA	CMC-C2C	-2.73	1.45	1.50
24	b	602	CLA	CHD-C4C	2.73	1.45	1.39
26	B	619	BCR	C24-C25	2.73	1.54	1.45
26	t	102	BCR	C29-C30	-2.73	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	510	CLA	MG-ND	-2.73	2.00	2.05
24	c	502	CLA	C1B-C2B	2.72	1.49	1.43
24	C	503	CLA	CHD-C1D	2.72	1.43	1.38
40	c	516	DGD	O2G-C1B	2.72	1.42	1.34
24	C	509	CLA	MG-NB	-2.72	2.00	2.05
24	b	614	CLA	C3D-C4D	-2.72	1.38	1.44
24	B	616	CLA	C3C-C2C	2.71	1.42	1.36
24	c	503	CLA	CHD-C1D	2.71	1.43	1.38
24	C	508	CLA	C1C-C2C	2.71	1.50	1.44
24	B	605	CLA	C1C-C2C	2.71	1.50	1.44
24	c	503	CLA	CHC-C4B	2.71	1.45	1.39
24	D	405	CLA	CHD-C4C	2.71	1.45	1.39
24	b	606	CLA	CHC-C1C	2.71	1.43	1.38
24	B	614	CLA	O2A-CGA	2.70	1.41	1.33
24	B	614	CLA	O2D-CGD	2.70	1.39	1.33
24	B	617	CLA	O2A-CGA	2.70	1.41	1.33
24	c	507	CLA	CHC-C4B	2.70	1.45	1.39
25	D	401	PHO	O2A-C1	-2.70	1.38	1.46
24	c	510	CLA	C1B-C2B	2.70	1.49	1.43
24	B	605	CLA	CHD-C4C	2.70	1.45	1.39
40	H	103	DGD	O5D-C6D	2.70	1.48	1.43
24	b	610	CLA	CMC-C2C	-2.70	1.45	1.50
38	c	530	HTG	C1-C2	2.70	1.58	1.53
24	c	507	CLA	CHD-C4C	2.70	1.45	1.39
24	c	510	CLA	CHD-C1D	2.70	1.43	1.38
24	c	502	CLA	OBD-CAD	2.69	1.27	1.22
24	b	617	CLA	C4B-NB	-2.69	1.34	1.37
24	B	612	CLA	CHC-C4B	2.69	1.45	1.39
24	C	512	CLA	CHC-C4B	2.68	1.45	1.39
24	d	403	CLA	CHC-C4B	2.68	1.45	1.39
24	C	504	CLA	C3D-C4D	-2.68	1.38	1.44
24	b	606	CLA	CHB-C1B	2.68	1.45	1.39
24	C	507	CLA	CBD-CGD	-2.67	1.44	1.52
24	B	615	CLA	C1B-C2B	2.67	1.49	1.43
24	B	612	CLA	C3D-C4D	-2.67	1.38	1.44
30	O	302	GOL	O1-C1	2.67	1.53	1.42
24	B	604	CLA	CHD-C1D	2.67	1.43	1.38
24	B	610	CLA	OBD-CAD	2.66	1.27	1.22
24	B	607	CLA	OBD-CAD	2.66	1.27	1.22
26	b	619	BCR	C24-C25	2.66	1.54	1.45
24	D	404	CLA	O1D-CGD	2.66	1.28	1.21
38	o	301	HTG	C1-C2	2.66	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	510	CLA	C4B-NB	-2.66	1.34	1.37
43	V	203	HEC	FE-NA	2.66	2.03	1.95
24	B	617	CLA	C3C-C2C	2.66	1.42	1.36
26	a	411	BCR	C8-C9	2.66	1.51	1.46
24	b	606	CLA	C1D-ND	2.66	1.41	1.37
24	D	404	CLA	C1B-C2B	2.66	1.49	1.43
24	C	501	CLA	CHD-C1D	2.65	1.43	1.38
24	B	614	CLA	CHD-C4C	2.65	1.45	1.39
24	c	509	CLA	CHC-C1C	2.65	1.43	1.38
24	b	609	CLA	C3D-C4D	-2.65	1.38	1.44
24	b	613	CLA	C3D-C4D	-2.65	1.38	1.44
28	h	105	SQD	O6-C1	2.65	1.44	1.40
24	C	509	CLA	C4B-NB	-2.64	1.34	1.37
24	b	605	CLA	CHC-C4B	2.64	1.45	1.39
24	d	405	CLA	CHD-C1D	2.64	1.43	1.38
24	B	603	CLA	C3D-C2D	2.64	1.46	1.39
26	d	406	BCR	C32-C1	-2.64	1.48	1.53
24	D	403	CLA	C3D-C2D	2.64	1.46	1.39
24	C	508	CLA	O2D-CED	-2.64	1.39	1.45
24	b	604	CLA	C1B-C2B	2.64	1.49	1.43
24	B	616	CLA	CHC-C4B	2.63	1.45	1.39
24	b	606	CLA	C3D-C2D	2.63	1.46	1.39
38	a	418	HTG	C1'-S1	-2.63	1.77	1.81
24	B	613	CLA	CHB-C1B	2.63	1.45	1.39
26	K	101	BCR	C30-C25	-2.63	1.50	1.53
25	a	409	PHO	O2D-CGD	2.63	1.39	1.33
24	b	607	CLA	C1B-C2B	2.63	1.49	1.43
24	b	608	CLA	C1D-C2D	2.63	1.50	1.45
24	D	404	CLA	C3D-C4D	-2.62	1.38	1.44
24	B	607	CLA	MG-NB	-2.62	2.00	2.05
26	H	102	BCR	C8-C9	2.62	1.51	1.46
41	E	113	HEM	C3C-C4C	-2.62	1.41	1.46
24	D	404	CLA	CHC-C1C	2.62	1.43	1.38
24	C	505	CLA	C3D-C4D	-2.62	1.38	1.44
24	C	510	CLA	C1B-NB	-2.62	1.34	1.37
24	b	607	CLA	C3D-C4D	-2.62	1.38	1.44
26	b	618	BCR	C8-C9	2.62	1.51	1.46
24	B	608	CLA	OBD-CAD	2.62	1.27	1.22
24	c	511	CLA	CMB-C2B	-2.62	1.45	1.50
24	c	507	CLA	C1D-C2D	2.62	1.50	1.45
24	c	511	CLA	CHC-C1C	2.62	1.43	1.38
24	C	505	CLA	C4C-C3C	2.62	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	J	101	LMG	O7-C10	2.62	1.41	1.34
24	C	503	CLA	MG-NB	-2.61	2.00	2.05
40	c	518	DGD	O2G-C2G	-2.61	1.40	1.46
26	A	610	BCR	C40-C30	-2.61	1.48	1.53
24	D	405	CLA	C1B-C2B	2.61	1.49	1.43
24	c	505	CLA	O2A-CGA	2.61	1.41	1.33
26	h	103	BCR	C27-C26	2.61	1.55	1.51
24	A	606	CLA	CHC-C4B	2.61	1.45	1.39
24	C	507	CLA	C1B-C2B	2.61	1.49	1.43
43	V	203	HEC	FE-NC	2.61	2.03	1.95
24	b	602	CLA	OBD-CAD	2.61	1.27	1.22
25	A	608	PHO	CHA-CBD	-2.61	1.48	1.51
38	h	101	HTG	C1'-S1	-2.61	1.77	1.81
26	B	620	BCR	C23-C22	2.61	1.51	1.46
24	b	610	CLA	C3D-C2D	2.60	1.46	1.39
24	d	405	CLA	O2D-CGD	2.60	1.39	1.33
24	b	603	CLA	CHD-C4C	2.60	1.45	1.39
25	a	409	PHO	C4B-NB	-2.60	1.33	1.38
28	A	612	SQD	O48-C23	2.60	1.40	1.33
24	D	404	CLA	MG-NB	-2.59	2.00	2.05
24	B	606	CLA	C1B-C2B	2.59	1.49	1.43
40	H	103	DGD	O1G-C1A	2.59	1.40	1.33
24	B	605	CLA	C3C-C2C	2.59	1.42	1.36
25	d	401	PHO	C3D-C4D	-2.58	1.37	1.41
40	H	103	DGD	O2G-C1B	2.58	1.41	1.34
24	B	604	CLA	C3D-C4D	-2.58	1.38	1.44
24	C	509	CLA	CHC-C4B	2.58	1.45	1.39
24	C	503	CLA	C1C-C2C	2.58	1.49	1.44
24	C	508	CLA	CHD-C1D	2.58	1.43	1.38
41	e	107	HEM	C3B-C4B	2.58	1.49	1.44
24	B	606	CLA	MG-ND	-2.58	2.00	2.05
24	a	410	CLA	O2A-CGA	2.58	1.40	1.33
32	D	411	LHG	O7-C7	2.58	1.41	1.34
24	C	502	CLA	C3D-C4D	-2.57	1.38	1.44
24	C	505	CLA	CHB-C1B	2.57	1.45	1.39
24	D	403	CLA	O2A-CGA	2.57	1.40	1.33
31	B	622	LMT	O1'-C1'	2.57	1.44	1.40
24	B	606	CLA	C4B-NB	-2.57	1.34	1.37
24	a	407	CLA	C4B-NB	-2.57	1.34	1.37
32	d	411	LHG	O8-C6	-2.57	1.39	1.45
24	b	605	CLA	O2A-C1	-2.57	1.39	1.46
24	B	609	CLA	O2D-CGD	2.57	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	604	CLA	CHB-C1B	2.57	1.45	1.39
24	B	608	CLA	CHD-C4C	2.57	1.45	1.39
24	C	503	CLA	O2D-CED	-2.57	1.39	1.45
23	A	605	BCT	O1-C	2.57	1.34	1.25
24	C	505	CLA	CHC-C1C	2.57	1.43	1.38
24	b	613	CLA	CMC-C2C	-2.56	1.45	1.50
24	C	509	CLA	C3D-C2D	2.56	1.46	1.39
27	d	407	PL9	C15-C14	-2.56	1.44	1.50
24	B	617	CLA	C3D-C4D	-2.56	1.38	1.44
38	c	531	HTG	O5-C1	2.56	1.46	1.42
24	b	615	CLA	C1D-ND	2.55	1.41	1.37
31	m	102	LMT	O4'-C4B	2.55	1.49	1.43
24	b	603	CLA	C1D-C2D	2.55	1.50	1.45
24	b	611	CLA	O2D-CGD	2.55	1.39	1.33
24	a	410	CLA	CHC-C4B	2.55	1.45	1.39
25	a	409	PHO	C3D-C4D	-2.55	1.37	1.41
24	a	407	CLA	C3D-C2D	2.55	1.45	1.39
24	C	501	CLA	C1C-C2C	2.55	1.49	1.44
24	B	609	CLA	CHB-C1B	2.55	1.45	1.39
24	B	614	CLA	C3D-C4D	-2.55	1.38	1.44
24	C	510	CLA	CHD-C4C	2.55	1.45	1.39
24	c	502	CLA	O2A-C1	-2.55	1.39	1.46
24	C	506	CLA	CHD-C4C	2.54	1.45	1.39
26	C	514	BCR	C8-C9	2.54	1.51	1.46
24	b	615	CLA	CHC-C1C	2.54	1.43	1.38
32	d	409	LHG	O8-C23	2.54	1.40	1.33
41	e	107	HEM	C1D-ND	-2.54	1.33	1.38
40	C	518	DGD	O1G-C1A	2.54	1.40	1.33
24	a	407	CLA	CHD-C4C	2.54	1.45	1.39
24	b	616	CLA	C1B-C2B	2.54	1.49	1.43
41	E	113	HEM	FE-NA	2.54	2.03	1.95
24	D	403	CLA	C1B-C2B	2.54	1.49	1.43
38	c	531	HTG	C1'-S1	-2.53	1.77	1.81
24	B	617	CLA	C2-C3	2.53	1.38	1.33
25	D	401	PHO	C1D-ND	-2.53	1.34	1.38
24	c	505	CLA	CHD-C4C	2.53	1.45	1.39
24	A	606	CLA	MG-ND	-2.53	2.00	2.05
24	B	605	CLA	C3D-C2D	2.53	1.45	1.39
24	d	404	CLA	C3C-C2C	2.53	1.42	1.36
24	c	512	CLA	C1B-NB	-2.53	1.34	1.37
24	B	615	CLA	CHD-C1D	2.52	1.43	1.38
24	c	505	CLA	C4B-NB	-2.52	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	613	CLA	C1B-C2B	2.52	1.49	1.43
24	c	509	CLA	C4B-NB	-2.52	1.34	1.37
24	A	609	CLA	C3B-C4B	2.52	1.50	1.42
24	b	605	CLA	C1D-ND	2.52	1.41	1.37
24	c	502	CLA	CHD-C4C	2.52	1.44	1.39
24	b	614	CLA	C1B-C2B	2.51	1.49	1.43
24	B	610	CLA	CHB-C1B	2.51	1.45	1.39
24	a	408	CLA	C1B-C2B	2.51	1.49	1.43
26	T	102	BCR	C38-C26	-2.51	1.46	1.50
26	c	514	BCR	C23-C22	2.51	1.51	1.46
24	D	404	CLA	C3B-C4B	2.51	1.50	1.42
24	a	407	CLA	CMD-C2D	-2.51	1.45	1.50
24	a	407	CLA	C1D-C2D	2.51	1.50	1.45
24	b	606	CLA	C1B-NB	-2.51	1.34	1.37
24	B	615	CLA	C3C-C2C	2.50	1.42	1.36
24	b	604	CLA	O2A-CGA	2.50	1.40	1.33
24	b	607	CLA	C3D-C2D	2.50	1.45	1.39
24	a	407	CLA	C3D-C4D	-2.50	1.38	1.44
29	a	414	LMG	O8-C28	2.50	1.40	1.33
24	c	513	CLA	C1B-C2B	2.50	1.49	1.43
25	a	409	PHO	C3B-C4B	2.50	1.44	1.41
24	B	616	CLA	CHB-C1B	2.49	1.45	1.39
24	C	507	CLA	MG-ND	-2.49	2.00	2.05
24	c	503	CLA	CHD-C4C	2.49	1.44	1.39
24	B	608	CLA	C1B-NB	-2.49	1.34	1.37
24	B	611	CLA	OBD-CAD	2.49	1.26	1.22
40	C	516	DGD	O5D-C1E	2.49	1.44	1.40
32	d	409	LHG	O7-C5	-2.49	1.40	1.46
31	m	101	LMT	O1'-C1'	2.49	1.44	1.40
24	d	405	CLA	C1D-C2D	2.49	1.50	1.45
24	b	617	CLA	CHD-C1D	2.48	1.43	1.38
29	C	519	LMG	O7-C8	-2.48	1.40	1.46
24	A	607	CLA	C1B-C2B	2.48	1.49	1.43
24	B	604	CLA	C1D-ND	2.48	1.41	1.37
26	A	610	BCR	C23-C22	2.48	1.51	1.46
25	a	409	PHO	O2A-CGA	2.48	1.40	1.33
43	v	202	HEC	FE-NA	2.48	2.03	1.95
40	D	408	DGD	O3G-C1D	2.48	1.44	1.40
24	d	403	CLA	C3D-C4D	-2.48	1.38	1.44
38	B	631	HTG	O5-C1	2.47	1.46	1.42
38	c	523	HTG	C1'-S1	-2.47	1.78	1.81
26	C	525	BCR	C1-C6	-2.47	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	516	DGD	O5D-C6D	-2.47	1.39	1.43
26	c	515	BCR	C8-C9	2.47	1.51	1.46
26	B	619	BCR	C35-C13	2.47	1.55	1.50
24	C	504	CLA	MG-ND	-2.46	2.00	2.05
24	B	606	CLA	C1D-C2D	2.46	1.50	1.45
23	m	104[A]	BCT	O1-C	2.46	1.34	1.25
24	B	604	CLA	C4-C3	-2.46	1.44	1.50
24	B	605	CLA	C1B-C2B	2.46	1.48	1.43
24	d	405	CLA	CHC-C4B	2.46	1.44	1.39
32	d	410	LHG	O7-C7	2.46	1.41	1.34
24	b	613	CLA	C4B-NB	-2.45	1.34	1.37
25	D	401	PHO	O2A-CGA	2.45	1.40	1.33
38	C	532	HTG	C1-S1	-2.45	1.76	1.80
24	c	505	CLA	C3D-C4D	-2.45	1.38	1.44
26	C	525	BCR	C30-C25	-2.45	1.50	1.53
24	b	612	CLA	O2A-CGA	2.45	1.40	1.33
24	C	503	CLA	C4B-NB	-2.45	1.34	1.37
24	d	403	CLA	C3D-C2D	2.45	1.45	1.39
24	b	611	CLA	O2D-CED	-2.44	1.39	1.45
24	C	507	CLA	O2A-CGA	2.44	1.40	1.33
24	B	609	CLA	MG-ND	-2.44	2.00	2.05
24	A	607	CLA	C3C-C2C	2.44	1.42	1.36
23	a	406	BCT	O1-C	2.44	1.34	1.25
24	c	504	CLA	CHB-C1B	2.44	1.44	1.39
24	B	606	CLA	C1D-ND	2.44	1.41	1.37
24	c	508	CLA	OBD-CAD	2.44	1.26	1.22
24	d	403	CLA	C4B-NB	-2.43	1.34	1.37
24	B	602	CLA	MG-NC	-2.43	2.00	2.06
24	C	503	CLA	C3D-C2D	2.43	1.45	1.39
41	E	113	HEM	C4C-NC	-2.43	1.35	1.39
43	v	202	HEC	C4B-NB	-2.43	1.36	1.40
24	B	612	CLA	C1B-C2B	2.43	1.48	1.43
24	B	608	CLA	C4B-NB	-2.43	1.34	1.37
24	B	603	CLA	C1D-ND	2.43	1.41	1.37
24	C	501	CLA	C1C-NC	-2.43	1.34	1.37
24	C	509	CLA	C1D-ND	2.43	1.41	1.37
24	C	506	CLA	C1B-NB	-2.42	1.34	1.37
24	C	510	CLA	MG-ND	-2.42	2.01	2.05
24	a	408	CLA	C3B-C4B	2.42	1.49	1.42
24	B	617	CLA	MG-ND	-2.42	2.01	2.05
24	b	609	CLA	C4D-CHA	2.42	1.46	1.38
24	b	616	CLA	O2D-CGD	2.42	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	D	401	PHO	CMC-C2C	-2.41	1.46	1.50
24	B	607	CLA	C1C-C2C	2.41	1.49	1.44
38	V	204	HTG	O5-C1	2.41	1.46	1.42
24	B	608	CLA	C3D-C4D	-2.41	1.38	1.44
24	b	611	CLA	CHD-C4C	2.41	1.44	1.39
24	b	603	CLA	O2D-CGD	2.41	1.39	1.33
27	D	407	PL9	C51-C49	-2.40	1.44	1.50
26	b	618	BCR	C40-C30	-2.40	1.49	1.53
24	B	616	CLA	C3D-C4D	-2.40	1.38	1.44
24	C	508	CLA	C4B-NB	-2.40	1.34	1.37
24	d	405	CLA	CHD-C4C	2.40	1.44	1.39
24	c	504	CLA	CHC-C4B	2.40	1.44	1.39
24	B	607	CLA	C3D-C2D	2.40	1.45	1.39
24	A	609	CLA	CHB-C4A	-2.40	1.31	1.37
24	c	502	CLA	C3C-C2C	2.40	1.41	1.36
30	B	633	GOL	O2-C2	2.40	1.50	1.43
24	c	512	CLA	C4C-C3C	2.39	1.49	1.45
24	c	505	CLA	MG-ND	-2.39	2.01	2.05
24	B	605	CLA	MG-ND	-2.39	2.01	2.05
24	D	403	CLA	CHB-C1B	2.39	1.44	1.39
24	b	605	CLA	C3D-C2D	2.38	1.45	1.39
24	B	612	CLA	O2D-CGD	2.38	1.39	1.33
31	M	101	LMT	O4'-C4B	2.38	1.48	1.43
26	H	102	BCR	C12-C13	2.38	1.51	1.46
24	b	610	CLA	CHC-C4B	2.38	1.44	1.39
27	A	611	PL9	C11-C9	-2.38	1.46	1.51
24	c	512	CLA	C1B-C2B	2.38	1.48	1.43
27	d	407	PL9	C2-C1	-2.38	1.38	1.44
26	D	406	BCR	C2-C3	-2.38	1.47	1.52
24	b	610	CLA	C1B-C2B	2.38	1.48	1.43
24	b	617	CLA	C2-C3	2.38	1.38	1.33
24	B	616	CLA	C3D-C2D	2.38	1.45	1.39
24	C	508	CLA	OBD-CAD	2.38	1.26	1.22
40	c	517	DGD	O5D-C6D	-2.38	1.39	1.43
25	A	608	PHO	C4D-ND	-2.38	1.35	1.38
24	b	604	CLA	C3A-C2A	-2.37	1.48	1.54
24	b	611	CLA	CHB-C1B	2.37	1.44	1.39
41	E	113	HEM	C1C-NC	-2.37	1.35	1.39
24	C	506	CLA	OBD-CAD	2.37	1.26	1.22
27	D	407	PL9	O1-C4	2.37	1.28	1.23
24	b	609	CLA	CHD-C4C	2.36	1.44	1.39
24	D	404	CLA	CMB-C2B	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	J	103	LMT	O1'-C1'	2.36	1.44	1.40
24	D	404	CLA	CHD-C1D	2.36	1.43	1.38
24	B	612	CLA	CHD-C4C	2.35	1.44	1.39
24	c	509	CLA	C1C-NC	-2.35	1.34	1.37
27	d	407	PL9	C6-C5	2.35	1.46	1.35
30	O	306	GOL	O2-C2	2.34	1.50	1.43
24	B	606	CLA	O1D-CGD	2.34	1.27	1.21
26	b	619	BCR	C5-C6	2.34	1.38	1.34
24	C	505	CLA	CMD-C2D	-2.34	1.46	1.50
24	c	501	CLA	CHD-C4C	2.34	1.44	1.39
24	c	503	CLA	O2D-CED	-2.34	1.40	1.45
24	d	405	CLA	CHB-C1B	2.34	1.44	1.39
24	B	603	CLA	CHD-C4C	2.33	1.44	1.39
24	d	404	CLA	C1C-NC	-2.33	1.34	1.37
28	l	102	SQD	O5-C1	2.33	1.47	1.41
24	b	614	CLA	CHD-C1D	2.33	1.42	1.38
32	D	409	LHG	C24-C23	2.33	1.57	1.50
24	c	505	CLA	CHC-C4B	2.33	1.44	1.39
31	A	617	LMT	O3B-C3B	2.33	1.48	1.43
24	A	606	CLA	CHD-C4C	2.33	1.44	1.39
24	A	606	CLA	C3D-C4D	-2.33	1.39	1.44
29	c	519	LMG	O7-C8	-2.32	1.41	1.46
24	B	605	CLA	CHB-C4A	-2.32	1.31	1.37
26	k	101	BCR	C30-C25	-2.32	1.50	1.53
28	b	633	SQD	O6-C1	2.32	1.44	1.40
24	b	610	CLA	C1D-C2D	2.31	1.49	1.45
24	B	616	CLA	CHD-C1D	2.31	1.42	1.38
24	b	612	CLA	C3D-C4D	-2.31	1.39	1.44
24	B	604	CLA	C4C-C3C	2.31	1.49	1.45
24	b	613	CLA	C1D-ND	2.31	1.40	1.37
29	B	621	LMG	O10-C28	-2.31	1.15	1.22
24	b	612	CLA	C1C-C2C	2.31	1.49	1.44
25	d	401	PHO	CMA-C3A	-2.30	1.49	1.53
24	D	403	CLA	CHD-C4C	2.30	1.44	1.39
26	b	620	BCR	C12-C13	2.30	1.50	1.46
24	A	609	CLA	C1B-NB	-2.30	1.34	1.37
29	A	613	LMG	O1-C1	2.29	1.44	1.40
27	A	611	PL9	C6-C1	2.29	1.52	1.48
24	B	615	CLA	CHD-C4C	2.29	1.44	1.39
24	b	614	CLA	C1B-NB	-2.29	1.34	1.37
24	B	603	CLA	C1C-NC	-2.29	1.34	1.37
24	B	607	CLA	C1B-C2B	2.29	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	406	BCR	C8-C9	2.29	1.50	1.46
24	a	410	CLA	O2A-C1	-2.29	1.40	1.46
24	B	612	CLA	CMD-C2D	-2.29	1.46	1.50
24	C	508	CLA	C3D-C4D	-2.28	1.39	1.44
24	C	501	CLA	CHB-C1B	2.28	1.44	1.39
24	b	607	CLA	OBD-CAD	2.28	1.26	1.22
26	C	514	BCR	C15-C14	2.28	1.50	1.43
24	a	408	CLA	C1B-NB	-2.28	1.34	1.37
24	D	404	CLA	CHD-C4C	2.28	1.44	1.39
31	F	102	LMT	C4B-C5B	2.28	1.57	1.53
24	c	511	CLA	CMD-C2D	-2.28	1.46	1.50
24	C	502	CLA	CHD-C1D	2.27	1.42	1.38
24	b	610	CLA	C4B-NB	-2.27	1.34	1.37
24	c	513	CLA	MG-NA	-2.27	2.00	2.06
24	A	609	CLA	O2A-CGA	2.27	1.40	1.33
24	C	513	CLA	CHC-C4B	2.27	1.44	1.39
40	C	518	DGD	O2G-C2G	-2.26	1.41	1.46
24	D	403	CLA	C4D-CHA	2.26	1.46	1.38
38	B	630	HTG	C1'-S1	-2.26	1.78	1.81
41	e	107	HEM	C1D-C2D	2.26	1.49	1.44
24	c	506	CLA	C3D-C2D	2.26	1.45	1.39
26	a	411	BCR	C20-C21	2.26	1.50	1.43
26	C	515	BCR	C12-C13	2.26	1.50	1.46
24	a	408	CLA	CHC-C4B	2.26	1.44	1.39
24	B	612	CLA	O2A-CGA	2.26	1.39	1.33
27	d	407	PL9	C45-C44	2.26	1.56	1.50
29	j	101	LMG	O7-C8	-2.26	1.41	1.46
24	b	608	CLA	O2A-CGA	2.25	1.39	1.33
24	B	604	CLA	MG-NB	-2.25	2.01	2.05
24	B	602	CLA	CBD-CGD	-2.25	1.45	1.52
24	B	609	CLA	OBD-CAD	2.25	1.26	1.22
38	a	418	HTG	O2-C2	2.25	1.48	1.43
24	B	604	CLA	C1C-NC	-2.25	1.34	1.37
40	C	517	DGD	O5D-C1E	2.25	1.43	1.40
43	v	202	HEC	C4A-NA	-2.24	1.35	1.39
24	C	510	CLA	C4C-C3C	2.24	1.48	1.45
26	T	102	BCR	C15-C14	2.24	1.50	1.43
24	d	404	CLA	MG-NB	-2.24	2.01	2.05
26	b	619	BCR	C34-C9	2.24	1.55	1.50
24	B	602	CLA	C2-C3	2.24	1.38	1.33
38	b	632	HTG	O5-C1	2.23	1.46	1.42
32	d	409	LHG	P-O4	-2.23	1.45	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	617	CLA	CHD-C1D	2.23	1.42	1.38
24	B	609	CLA	CHC-C1C	2.23	1.43	1.38
41	e	107	HEM	CHD-C4C	-2.23	1.34	1.38
32	B	632	LHG	O7-C7	2.23	1.40	1.34
24	b	606	CLA	C1B-C2B	2.23	1.48	1.43
24	b	604	CLA	C1C-C2C	2.23	1.49	1.44
24	B	606	CLA	OBD-CAD	2.23	1.26	1.22
24	d	404	CLA	C3D-C4D	-2.23	1.39	1.44
24	C	506	CLA	C1C-C2C	2.23	1.49	1.44
25	d	401	PHO	CBD-CGD	-2.22	1.49	1.52
41	e	107	HEM	C3C-C4C	-2.22	1.42	1.46
24	C	509	CLA	C1B-NB	-2.22	1.34	1.37
38	C	522	HTG	C1'-S1	-2.22	1.78	1.81
24	c	502	CLA	MG-ND	-2.22	2.01	2.05
24	d	404	CLA	CMB-C2B	-2.22	1.46	1.50
24	B	602	CLA	C4D-CHA	2.22	1.46	1.38
24	C	508	CLA	MG-ND	-2.22	2.01	2.05
24	c	503	CLA	C3C-C2C	2.21	1.41	1.36
31	u	203	LMT	C1B-C2B	2.21	1.59	1.52
24	B	611	CLA	CHD-C4C	2.21	1.44	1.39
24	C	512	CLA	C1C-C2C	2.21	1.49	1.44
24	b	602	CLA	C3B-C4B	2.21	1.49	1.42
38	a	418	HTG	C1-S1	-2.21	1.77	1.80
24	C	508	CLA	O2D-CGD	2.21	1.38	1.33
24	C	513	CLA	C1D-C2D	2.21	1.49	1.45
31	C	533	LMT	O1'-C1'	2.21	1.43	1.40
24	c	510	CLA	CAA-C2A	-2.21	1.50	1.54
26	b	619	BCR	C30-C25	-2.20	1.51	1.53
26	B	620	BCR	C29-C28	-2.20	1.47	1.52
38	O	303	HTG	C1-C2	2.20	1.57	1.53
26	a	411	BCR	C27-C26	2.20	1.55	1.51
24	B	608	CLA	CHC-C4B	2.20	1.44	1.39
24	a	407	CLA	C4D-CHA	2.20	1.46	1.38
24	b	614	CLA	CHB-C1B	2.20	1.44	1.39
24	B	614	CLA	C4D-CHA	2.20	1.45	1.38
29	B	621	LMG	O7-C8	-2.20	1.41	1.46
24	C	510	CLA	C1C-C2C	2.20	1.49	1.44
25	d	401	PHO	CMC-C2C	-2.20	1.47	1.50
24	B	615	CLA	CBA-CGA	2.19	1.57	1.50
24	c	508	CLA	CMD-C2D	-2.19	1.46	1.50
24	c	509	CLA	C1C-C2C	2.19	1.49	1.44
24	b	612	CLA	C1B-NB	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	504	CLA	C1C-NC	-2.19	1.34	1.37
26	c	527	BCR	C8-C9	2.19	1.50	1.46
24	c	506	CLA	OBD-CAD	2.18	1.26	1.22
24	C	508	CLA	CMD-C2D	-2.18	1.46	1.50
24	b	615	CLA	CHD-C1D	2.18	1.42	1.38
24	C	507	CLA	C1C-C2C	2.18	1.48	1.44
26	b	620	BCR	C1-C6	-2.18	1.51	1.53
41	E	113	HEM	C1A-NA	-2.18	1.35	1.39
26	D	406	BCR	C26-C25	2.17	1.38	1.34
26	h	103	BCR	C24-C25	2.17	1.52	1.45
26	A	610	BCR	C31-C1	-2.17	1.49	1.53
24	D	405	CLA	C1C-NC	-2.17	1.34	1.37
24	B	609	CLA	CHD-C4C	2.17	1.44	1.39
24	b	607	CLA	O2A-CGA	2.17	1.39	1.33
25	A	608	PHO	C1B-NB	-2.17	1.34	1.38
24	C	504	CLA	CHC-C4B	2.17	1.44	1.39
43	v	202	HEC	CHC-C4B	2.17	1.42	1.38
24	c	513	CLA	C1B-NB	-2.17	1.35	1.37
26	h	103	BCR	C19-C18	2.16	1.50	1.46
26	A	610	BCR	C20-C21	2.16	1.49	1.43
24	B	609	CLA	C3D-C4D	-2.16	1.39	1.44
29	J	101	LMG	O8-C28	2.16	1.39	1.33
38	B	623	HTG	C1-C2	2.16	1.57	1.53
27	A	611	PL9	C48-C49	2.16	1.38	1.32
41	e	107	HEM	O2D-CGD	-2.16	1.23	1.30
24	B	612	CLA	C4D-CHA	2.16	1.45	1.38
24	B	607	CLA	C1D-ND	2.16	1.40	1.37
24	b	608	CLA	CHD-C1D	2.16	1.42	1.38
24	B	607	CLA	O2A-CGA	2.15	1.39	1.33
43	V	203	HEC	CMC-C2C	2.15	1.55	1.50
24	B	617	CLA	CHC-C4B	2.15	1.44	1.39
24	A	606	CLA	CHD-C1D	2.15	1.42	1.38
24	B	615	CLA	C1C-NC	-2.15	1.34	1.37
24	c	509	CLA	C4C-C3C	2.15	1.48	1.45
26	B	620	BCR	C15-C14	2.15	1.49	1.43
24	b	606	CLA	CHB-C4A	-2.15	1.32	1.37
31	F	102	LMT	O4'-C4B	2.15	1.48	1.43
24	b	611	CLA	C1C-NC	-2.15	1.34	1.37
24	c	501	CLA	OBD-CAD	2.15	1.26	1.22
24	b	613	CLA	C3B-C4B	2.15	1.49	1.42
24	B	611	CLA	MG-ND	-2.14	2.01	2.05
24	B	602	CLA	C1C-NC	-2.14	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	602	CLA	CHB-C1B	2.14	1.44	1.39
24	b	612	CLA	C1C-NC	-2.14	1.34	1.37
24	B	605	CLA	C4B-NB	-2.14	1.35	1.37
24	C	511	CLA	CHD-C4C	2.14	1.44	1.39
24	C	501	CLA	O2A-CGA	2.14	1.39	1.33
24	b	602	CLA	C1C-C2C	2.13	1.48	1.44
27	d	407	PL9	C50-C49	-2.13	1.44	1.50
24	c	507	CLA	C1C-C2C	2.13	1.48	1.44
24	b	605	CLA	C1C-NC	-2.13	1.34	1.37
24	d	404	CLA	C1B-NB	-2.13	1.35	1.37
24	d	404	CLA	MG-ND	-2.13	2.01	2.05
24	b	615	CLA	C3D-C2D	2.13	1.44	1.39
24	b	606	CLA	CHC-C4B	2.13	1.44	1.39
24	C	502	CLA	O2A-CGA	2.13	1.39	1.33
24	C	506	CLA	CHD-C1D	2.13	1.42	1.38
24	B	615	CLA	C3D-C4D	-2.13	1.39	1.44
24	B	603	CLA	MG-ND	-2.13	2.01	2.05
24	b	615	CLA	C1B-NB	-2.12	1.35	1.37
24	B	615	CLA	C3B-C4B	2.12	1.48	1.42
24	c	507	CLA	C3D-C4D	-2.12	1.39	1.44
24	b	604	CLA	CHB-C1B	2.12	1.44	1.39
32	D	410	LHG	O7-C5	-2.12	1.41	1.46
40	C	516	DGD	O1G-C1G	-2.12	1.40	1.45
24	C	510	CLA	CMC-C2C	-2.12	1.46	1.50
24	b	608	CLA	CMB-C2B	-2.12	1.46	1.50
24	B	607	CLA	C4D-CHA	2.12	1.45	1.38
38	C	529	HTG	C1-C2	2.12	1.57	1.53
24	C	509	CLA	CHD-C4C	2.12	1.44	1.39
24	b	614	CLA	C3B-C4B	2.12	1.48	1.42
26	t	102	BCR	C16-C17	2.11	1.49	1.43
24	b	611	CLA	C1B-C2B	2.11	1.48	1.43
24	a	410	CLA	C1C-NC	-2.11	1.34	1.37
24	A	609	CLA	MG-NA	-2.11	2.01	2.06
24	c	502	CLA	C4B-NB	-2.11	1.35	1.37
24	D	403	CLA	C3D-C4D	-2.11	1.39	1.44
24	B	605	CLA	CBD-CGD	-2.11	1.46	1.52
24	b	614	CLA	C1C-NC	-2.11	1.34	1.37
24	C	502	CLA	CHC-C4B	2.11	1.44	1.39
26	c	514	BCR	C12-C13	2.11	1.50	1.46
25	a	409	PHO	CMD-C2D	-2.11	1.47	1.51
24	C	506	CLA	MG-ND	-2.11	2.01	2.05
28	a	413	SQD	O47-C45	-2.11	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	b	613	CLA	C1B-NB	-2.10	1.35	1.37
24	b	606	CLA	CHD-C1D	2.10	1.42	1.38
24	c	510	CLA	O2A-CGA	2.10	1.39	1.33
32	d	410	LHG	O8-C23	2.10	1.39	1.33
24	C	504	CLA	CAC-C3C	-2.10	1.45	1.51
24	A	606	CLA	C2-C3	2.10	1.37	1.33
28	F	104	SQD	C3-C2	2.10	1.57	1.52
31	j	103	LMT	O1'-C1'	2.10	1.43	1.40
24	c	503	CLA	O2A-CGA	2.10	1.39	1.33
24	C	511	CLA	C4B-NB	-2.10	1.35	1.37
24	d	404	CLA	O2D-CGD	2.10	1.38	1.33
38	b	631	HTG	O4-C4	2.09	1.48	1.43
26	b	619	BCR	C19-C18	2.09	1.50	1.46
24	B	606	CLA	C3B-C4B	2.09	1.48	1.42
24	c	507	CLA	C1C-NC	-2.09	1.34	1.37
27	D	407	PL9	C31-C29	2.09	1.55	1.51
24	C	513	CLA	C1B-C2B	2.09	1.48	1.43
26	C	515	BCR	C1-C6	-2.09	1.51	1.53
24	b	605	CLA	OBD-CAD	2.09	1.26	1.22
24	c	511	CLA	CMC-C2C	-2.09	1.46	1.50
24	B	613	CLA	O2A-CGA	2.09	1.39	1.33
24	C	501	CLA	C1B-C2B	2.09	1.48	1.43
24	B	604	CLA	C1B-NB	-2.09	1.35	1.37
24	C	508	CLA	C4D-CHA	2.09	1.45	1.38
24	B	607	CLA	CMA-C3A	-2.09	1.48	1.53
24	A	607	CLA	CBB-CAB	-2.09	1.20	1.30
24	b	604	CLA	C4C-C3C	2.08	1.48	1.45
24	b	610	CLA	C1C-C2C	2.08	1.48	1.44
24	c	508	CLA	C3D-C4D	-2.08	1.39	1.44
24	B	613	CLA	C1B-NB	-2.08	1.35	1.37
24	b	617	CLA	MG-ND	-2.08	2.01	2.05
41	e	107	HEM	C1C-C2C	-2.08	1.41	1.45
30	b	627	GOL	O3-C3	2.08	1.51	1.42
38	B	630	HTG	O2-C2	2.08	1.48	1.43
24	b	608	CLA	CBD-CGD	-2.08	1.46	1.52
24	C	509	CLA	O2D-CGD	2.08	1.38	1.33
26	C	525	BCR	C8-C9	2.08	1.50	1.46
24	B	602	CLA	MG-ND	-2.08	2.01	2.05
24	a	407	CLA	MG-NB	-2.08	2.01	2.05
24	B	607	CLA	C4B-NB	-2.08	1.35	1.37
24	C	510	CLA	CHC-C4B	2.07	1.44	1.39
43	V	203	HEC	CHA-C4D	-2.07	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	502	CLA	C4D-CHA	2.07	1.45	1.38
24	C	513	CLA	C1C-NC	-2.07	1.34	1.37
24	b	605	CLA	C1C-C2C	2.07	1.48	1.44
24	B	608	CLA	C1D-C2D	2.07	1.49	1.45
26	b	618	BCR	C12-C13	2.07	1.50	1.46
26	c	515	BCR	C15-C14	2.07	1.49	1.43
24	C	512	CLA	MG-ND	-2.07	2.01	2.05
25	A	608	PHO	C4B-NB	-2.07	1.34	1.38
24	C	505	CLA	C1C-NC	-2.06	1.34	1.37
24	A	607	CLA	O2A-CGA	2.06	1.39	1.33
24	b	614	CLA	CMB-C2B	-2.06	1.46	1.50
24	B	607	CLA	MG-ND	-2.06	2.01	2.05
24	C	502	CLA	OBD-CAD	2.06	1.26	1.22
24	C	501	CLA	C4D-CHA	2.06	1.45	1.38
24	B	613	CLA	C3D-C2D	2.06	1.44	1.39
24	b	606	CLA	C1C-C2C	2.06	1.48	1.44
24	b	610	CLA	C1C-NC	-2.06	1.34	1.37
24	C	502	CLA	MG-ND	-2.06	2.01	2.05
24	b	608	CLA	C3D-C4D	-2.06	1.39	1.44
26	C	514	BCR	C10-C9	-2.06	1.31	1.35
40	H	103	DGD	O6E-C1E	2.06	1.47	1.41
26	B	619	BCR	C19-C18	2.05	1.50	1.46
24	b	611	CLA	CHD-C1D	2.05	1.42	1.38
24	a	410	CLA	C4C-C3C	2.05	1.48	1.45
40	h	104	DGD	O4E-C4E	2.05	1.48	1.43
24	c	510	CLA	CMD-C2D	-2.05	1.46	1.50
24	a	410	CLA	C3A-C2A	-2.05	1.48	1.54
24	b	606	CLA	C5-C3	2.05	1.55	1.51
24	A	606	CLA	C1B-C2B	2.05	1.47	1.43
24	B	605	CLA	C3A-C2A	-2.05	1.48	1.54
24	d	404	CLA	C1B-C2B	2.05	1.47	1.43
24	d	404	CLA	C4D-CHA	2.04	1.45	1.38
43	v	202	HEC	C1D-ND	-2.04	1.36	1.40
24	b	607	CLA	MG-NB	-2.04	2.01	2.05
24	B	613	CLA	C4-C3	-2.04	1.45	1.50
26	H	102	BCR	C23-C22	2.04	1.50	1.46
41	e	107	HEM	C4B-NB	-2.04	1.34	1.38
26	h	103	BCR	C1-C6	-2.04	1.51	1.53
24	c	513	CLA	C1C-C2C	2.04	1.48	1.44
24	b	604	CLA	C1B-NB	-2.04	1.35	1.37
27	d	407	PL9	C2-C3	2.04	1.39	1.34
24	a	407	CLA	C3A-C2A	-2.03	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	609	CLA	C3B-C4B	2.03	1.48	1.42
26	c	527	BCR	C5-C6	2.03	1.37	1.34
27	D	407	PL9	C13-C14	2.03	1.37	1.33
24	a	407	CLA	C1B-C2B	2.03	1.47	1.43
24	A	606	CLA	C1D-C2D	2.03	1.49	1.45
28	F	104	SQD	C4-C5	2.03	1.57	1.53
28	h	105	SQD	C46-C45	2.03	1.57	1.50
40	H	103	DGD	O4E-C4E	2.03	1.48	1.43
24	b	604	CLA	MG-NB	-2.03	2.01	2.05
31	M	101	LMT	C3B-C2B	2.03	1.57	1.52
24	A	607	CLA	C4D-CHA	2.03	1.45	1.38
24	a	407	CLA	CHD-C1D	2.03	1.42	1.38
24	b	615	CLA	C1B-C2B	2.03	1.47	1.43
24	b	606	CLA	CHD-C4C	2.02	1.43	1.39
24	c	504	CLA	C1C-C2C	2.02	1.48	1.44
24	B	617	CLA	CMC-C2C	-2.02	1.46	1.50
24	c	511	CLA	C1B-C2B	2.02	1.47	1.43
26	t	102	BCR	C23-C22	2.02	1.50	1.46
41	E	113	HEM	C1D-C2D	2.02	1.48	1.44
24	B	607	CLA	O2D-CGD	2.02	1.38	1.33
38	B	631	HTG	C1'-S1	-2.02	1.78	1.81
24	B	610	CLA	CHC-C4B	2.02	1.43	1.39
24	b	613	CLA	C1C-NC	-2.02	1.34	1.37
24	C	501	CLA	C1B-NB	-2.01	1.35	1.37
26	C	525	BCR	C31-C1	-2.01	1.49	1.53
24	c	513	CLA	CHB-C4A	-2.01	1.32	1.37
32	a	419	LHG	C4-C5	2.01	1.57	1.50
29	B	634	LMG	C30-C29	2.01	1.59	1.52
26	B	619	BCR	C12-C13	2.01	1.50	1.46
38	b	624	HTG	O5-C1	2.01	1.45	1.42
40	H	103	DGD	O6D-C1D	2.01	1.47	1.41
24	B	616	CLA	C1C-C2C	2.01	1.48	1.44
26	a	411	BCR	C30-C25	-2.01	1.51	1.53
24	c	508	CLA	C3B-C4B	2.01	1.48	1.42
24	B	611	CLA	O2A-CGA	2.00	1.39	1.33
24	B	609	CLA	C4B-NB	-2.00	1.35	1.37
38	C	531	HTG	O5-C1	2.00	1.45	1.42
24	c	507	CLA	O2A-CGA	2.00	1.39	1.33
26	H	102	BCR	C33-C5	2.00	1.54	1.50
24	D	404	CLA	CMC-C2C	-2.00	1.46	1.50

All (2716) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	d	401	PHO	C3B-C4B-NB	10.42	114.26	107.46
28	a	413	SQD	O6-C1-C2	9.34	122.46	108.27
40	d	408	DGD	O3G-C1D-C2D	9.10	122.09	108.27
25	A	608	PHO	C3B-C4B-NB	8.95	113.30	107.46
28	F	104	SQD	O6-C1-C2	8.89	121.78	108.27
25	D	401	PHO	C2B-C1B-NB	8.87	115.84	109.43
25	a	409	PHO	C3B-C4B-NB	8.80	113.20	107.46
24	C	501	CLA	O2D-CGD-CBD	8.45	126.00	111.23
31	M	102	LMT	C1-O1'-C1'	8.42	128.06	113.68
26	d	406	BCR	C40-C30-C25	-8.30	97.22	110.24
24	B	605	CLA	C1-C2-C3	-8.19	112.78	126.20
38	V	204	HTG	O5-C1-C2	-8.11	99.14	110.32
24	B	610	CLA	C2C-C1C-NC	8.04	118.43	109.98
24	C	501	CLA	O2D-CGD-O1D	-7.95	108.37	123.85
24	d	404	CLA	C2C-C1C-NC	7.90	118.28	109.98
24	C	501	CLA	C2C-C1C-NC	7.79	118.16	109.98
24	c	504	CLA	C3B-C4B-NB	7.70	117.40	110.53
24	B	612	CLA	C2C-C1C-NC	7.61	117.98	109.98
26	D	406	BCR	C40-C30-C25	-7.52	98.45	110.24
24	c	501	CLA	C2C-C1C-NC	7.46	117.82	109.98
40	D	408	DGD	O2G-C1B-C2B	7.44	127.58	111.48
27	A	611	PL9	C3-C4-C5	7.43	127.83	118.57
24	b	605	CLA	C2C-C1C-NC	7.39	117.75	109.98
24	d	404	CLA	C3B-C4B-NB	7.35	117.09	110.53
25	A	608	PHO	C2D-C1D-ND	7.34	114.73	109.43
24	C	505	CLA	C2C-C1C-NC	7.32	117.67	109.98
27	A	611	PL9	C7-C3-C2	7.32	132.01	123.39
24	B	605	CLA	C5-C3-C2	-7.32	104.74	121.17
24	C	504	CLA	C2C-C1C-NC	7.29	117.64	109.98
38	C	529	HTG	C1'-S1-C1	7.23	116.06	100.45
24	b	609	CLA	C2C-C1C-NC	7.22	117.56	109.98
25	D	401	PHO	C3B-C4B-NB	7.17	112.14	107.46
24	B	608	CLA	C2C-C1C-NC	7.14	117.48	109.98
24	c	501	CLA	C3B-C4B-NB	7.12	116.88	110.53
24	c	504	CLA	C2C-C1C-NC	7.11	117.44	109.98
24	c	508	CLA	C2C-C1C-NC	7.05	117.39	109.98
25	d	401	PHO	O2D-CGD-CBD	7.02	118.66	110.95
24	c	505	CLA	C3C-C4C-NC	7.00	119.40	110.43
24	B	616	CLA	C2C-C1C-NC	7.00	117.33	109.98
24	D	403	CLA	C2C-C1C-NC	7.00	117.33	109.98
24	C	506	CLA	C2C-C1C-NC	6.96	117.30	109.98
24	B	615	CLA	C2B-C1B-NB	6.95	117.53	110.33
24	b	611	CLA	C2C-C1C-NC	6.93	117.26	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	A	612	SQD	C1-O5-C5	-6.90	100.24	113.72
24	B	614	CLA	CMD-C2D-C1D	6.89	136.87	124.73
24	b	616	CLA	C2C-C1C-NC	6.88	117.21	109.98
24	c	512	CLA	C2C-C1C-NC	6.87	117.20	109.98
24	B	604	CLA	C2C-C1C-NC	6.86	117.18	109.98
41	E	113	HEM	CAD-CBD-CGD	6.85	131.84	113.67
24	B	616	CLA	C3B-C4B-NB	6.83	116.63	110.53
24	b	616	CLA	C3B-C2B-C1B	-6.81	99.14	107.17
29	C	519	LMG	O8-C28-C29	6.78	132.50	111.83
24	C	509	CLA	C2C-C1C-NC	6.76	117.08	109.98
24	C	502	CLA	C3B-C4B-NB	6.73	116.54	110.53
24	c	506	CLA	C3B-C4B-NB	6.71	116.52	110.53
24	b	605	CLA	C1-C2-C3	-6.69	115.23	126.20
24	b	606	CLA	CMD-C2D-C1D	6.69	136.51	124.73
24	B	607	CLA	C2C-C1C-NC	6.67	116.99	109.98
24	a	410	CLA	C2C-C1C-NC	6.67	116.99	109.98
24	d	404	CLA	C1C-C2C-C3C	-6.66	99.97	106.98
24	D	403	CLA	C3B-C4B-NB	6.66	116.47	110.53
24	b	610	CLA	C3C-C4C-NC	6.66	118.96	110.43
24	C	507	CLA	C2C-C1C-NC	6.65	116.97	109.98
24	c	504	CLA	C2B-C1B-NB	6.65	117.22	110.33
24	D	404	CLA	C2C-C1C-NC	6.61	116.92	109.98
24	B	607	CLA	C3B-C4B-NB	6.60	116.43	110.53
24	b	612	CLA	C2C-C1C-NC	6.60	116.91	109.98
24	c	513	CLA	CMD-C2D-C1D	6.60	136.34	124.73
24	b	617	CLA	C2C-C1C-NC	6.57	116.89	109.98
27	a	412	PL9	C7-C3-C4	6.56	122.31	116.91
28	l	102	SQD	O6-C1-C2	6.56	118.23	108.27
24	b	613	CLA	C3C-C4C-NC	6.56	118.83	110.43
24	B	606	CLA	C3C-C4C-NC	6.55	118.82	110.43
24	A	609	CLA	C2C-C1C-NC	6.55	116.86	109.98
24	B	609	CLA	C2C-C1C-NC	6.53	116.84	109.98
25	d	401	PHO	C2B-C1B-NB	6.53	114.15	109.43
24	a	408	CLA	C3B-C4B-NB	6.52	116.35	110.53
24	C	512	CLA	C3B-C4B-NB	6.47	116.31	110.53
24	b	617	CLA	C3C-C4C-NC	6.47	118.72	110.43
24	C	503	CLA	C2B-C1B-NB	6.46	117.02	110.33
24	c	511	CLA	C2C-C1C-NC	6.45	116.75	109.98
25	a	409	PHO	O2D-CGD-CBD	6.42	118.01	110.95
25	A	608	PHO	C2B-C1B-NB	6.42	114.07	109.43
24	b	602	CLA	O2D-CGD-CBD	6.40	122.42	111.23
26	C	525	BCR	C7-C8-C9	-6.39	116.79	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	621	LMG	O7-C10-C11	6.38	125.29	111.48
24	B	602	CLA	C2C-C1C-NC	6.36	116.66	109.98
31	c	521	LMT	O1B-C4'-C3'	6.35	123.37	107.23
24	a	408	CLA	C2C-C1C-NC	6.33	116.63	109.98
24	c	502	CLA	C2C-C1C-NC	6.32	116.62	109.98
24	B	605	CLA	C2C-C1C-NC	6.32	116.61	109.98
24	B	617	CLA	C2C-C1C-NC	6.31	116.61	109.98
24	B	602	CLA	O2D-CGD-CBD	6.31	122.25	111.23
24	C	509	CLA	CMD-C2D-C1D	6.28	135.79	124.73
24	c	513	CLA	C2C-C1C-NC	6.27	116.57	109.98
24	C	508	CLA	C2C-C1C-NC	6.27	116.57	109.98
24	a	410	CLA	C3B-C4B-NB	6.26	116.12	110.53
24	b	604	CLA	C2C-C1C-NC	6.26	116.56	109.98
24	b	605	CLA	C3C-C4C-NC	6.23	118.41	110.43
24	A	607	CLA	C2C-C1C-NC	6.21	116.50	109.98
24	a	408	CLA	C3C-C4C-NC	6.20	118.37	110.43
24	c	505	CLA	CAC-C3C-C4C	6.19	132.85	124.79
24	c	512	CLA	C2B-C1B-NB	6.19	116.75	110.33
40	d	408	DGD	O2G-C1B-C2B	6.15	124.78	111.48
24	c	501	CLA	O2D-CGD-O1D	-6.15	111.89	123.85
24	c	507	CLA	C2C-C1C-NC	6.14	116.43	109.98
24	b	604	CLA	C3B-C4B-NB	6.11	115.99	110.53
24	D	405	CLA	C2C-C1C-NC	6.11	116.40	109.98
24	b	614	CLA	C2C-C1C-NC	6.09	116.38	109.98
24	B	606	CLA	C2C-C1C-NC	6.09	116.38	109.98
28	A	612	SQD	C1-C2-C3	-6.09	97.20	110.01
24	C	503	CLA	C3C-C4C-NC	6.08	118.21	110.43
24	c	513	CLA	CHD-C4C-C3C	-6.07	115.93	124.77
24	C	503	CLA	C3B-C4B-NB	6.06	115.94	110.53
24	b	603	CLA	C3C-C4C-NC	6.05	118.19	110.43
24	a	407	CLA	C2C-C1C-NC	6.04	116.33	109.98
24	c	504	CLA	C1C-C2C-C3C	-6.02	100.65	106.98
24	b	610	CLA	C2C-C1C-NC	6.01	116.29	109.98
24	C	503	CLA	C3B-C2B-C1B	-6.01	100.09	107.17
24	b	616	CLA	C1C-C2C-C3C	-6.00	100.67	106.98
28	b	633	SQD	O6-C1-C2	6.00	117.39	108.27
24	D	404	CLA	C3B-C4B-NB	6.00	115.89	110.53
24	B	607	CLA	C1C-C2C-C3C	-5.98	100.69	106.98
24	c	508	CLA	C3B-C4B-NB	5.96	115.85	110.53
31	m	102	LMT	O1'-C1'-C2'	5.96	117.32	108.27
24	c	512	CLA	C3B-C4B-NB	5.94	115.83	110.53
24	A	607	CLA	CAC-C3C-C4C	5.94	132.51	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	506	CLA	C2B-C1B-NB	5.94	116.48	110.33
26	t	102	BCR	C31-C1-C6	5.93	119.54	110.24
24	c	509	CLA	C2C-C1C-NC	5.91	116.19	109.98
24	B	611	CLA	C3C-C4C-NC	5.91	118.00	110.43
24	B	602	CLA	C3B-C2B-C1B	-5.89	100.22	107.17
24	b	602	CLA	C2C-C1C-NC	5.88	116.16	109.98
28	a	424	SQD	O47-C7-C8	5.88	124.20	111.48
24	b	605	CLA	C5-C3-C2	-5.86	108.02	121.17
24	C	507	CLA	C3C-C4C-NC	5.85	117.92	110.43
24	c	505	CLA	C1D-ND-C4D	-5.84	102.21	106.31
24	D	404	CLA	CMD-C2D-C1D	5.84	135.01	124.73
32	D	409	LHG	O8-C23-O10	-5.82	109.06	123.63
24	C	508	CLA	C2B-C1B-NB	5.82	116.36	110.33
24	b	617	CLA	O2D-CGD-CBD	5.81	121.38	111.23
24	C	507	CLA	C3B-C2B-C1B	-5.80	100.33	107.17
24	B	602	CLA	CMC-C2C-C1C	5.80	134.10	125.03
24	C	501	CLA	C3B-C4B-NB	5.79	115.70	110.53
24	C	503	CLA	CHD-C4C-C3C	-5.79	116.33	124.77
24	d	405	CLA	C2C-C1C-NC	5.78	116.05	109.98
24	A	607	CLA	C3B-C2B-C1B	-5.77	100.37	107.17
24	C	504	CLA	C1C-C2C-C3C	-5.77	100.92	106.98
40	D	408	DGD	O3G-C1D-C2D	5.76	117.02	108.27
24	B	616	CLA	C2B-C1B-NB	5.75	116.29	110.33
24	d	405	CLA	C2B-C1B-NB	5.74	116.28	110.33
24	B	608	CLA	C3B-C4B-NB	5.73	115.64	110.53
43	v	202	HEC	C4B-NB-C1B	5.73	111.99	105.21
26	k	101	BCR	C39-C30-C25	-5.72	101.28	110.24
24	b	606	CLA	C3C-C4C-NC	5.71	117.75	110.43
24	C	513	CLA	C3B-C2B-C1B	-5.71	100.44	107.17
24	C	509	CLA	C3B-C4B-NB	5.71	115.62	110.53
24	B	612	CLA	C2B-C1B-NB	5.71	116.24	110.33
24	B	610	CLA	C3B-C4B-NB	5.70	115.62	110.53
24	c	503	CLA	CMD-C2D-C1D	5.70	134.76	124.73
24	c	513	CLA	CMC-C2C-C1C	5.70	133.93	125.03
38	V	204	HTG	C1-O5-C5	-5.69	102.35	112.56
24	B	612	CLA	C3B-C2B-C1B	-5.69	100.46	107.17
24	C	508	CLA	C3B-C4B-NB	5.69	115.61	110.53
24	c	505	CLA	C2C-C1C-NC	5.68	115.95	109.98
24	D	403	CLA	C1C-C2C-C3C	-5.68	101.01	106.98
24	D	403	CLA	C2B-C1B-NB	5.65	116.19	110.33
24	C	509	CLA	C3B-C2B-C1B	-5.65	100.51	107.17
24	B	611	CLA	C2C-C1C-NC	5.65	115.91	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	424	SQD	O9-S-C6	5.64	115.18	106.76
24	C	513	CLA	C3C-C4C-NC	5.64	117.66	110.43
24	C	507	CLA	C2B-C1B-NB	5.64	116.17	110.33
29	B	621	LMG	O7-C10-O9	-5.64	110.53	123.70
24	B	604	CLA	O2D-CGD-CBD	5.62	121.05	111.23
24	b	612	CLA	C3B-C4B-NB	5.60	115.53	110.53
24	d	405	CLA	C3B-C4B-NB	5.60	115.53	110.53
24	C	511	CLA	O2D-CGD-CBD	5.59	121.00	111.23
24	b	604	CLA	C1D-ND-C4D	-5.59	102.39	106.31
29	C	526	LMG	O7-C10-C11	5.58	123.56	111.48
24	c	504	CLA	C3B-C2B-C1B	-5.58	100.59	107.17
24	b	616	CLA	C2B-C1B-NB	5.57	116.11	110.33
24	C	508	CLA	C3C-C4C-NC	5.57	117.57	110.43
24	A	607	CLA	C2B-C1B-NB	5.57	116.10	110.33
32	a	419	LHG	O7-C7-C8	5.56	123.52	111.48
24	B	611	CLA	C2B-C1B-NB	5.56	116.09	110.33
24	c	510	CLA	C3C-C4C-NC	5.55	117.55	110.43
24	B	609	CLA	C2B-C1B-NB	5.55	116.09	110.33
24	a	407	CLA	C2B-C1B-NB	5.55	116.09	110.33
24	B	612	CLA	C1C-C2C-C3C	-5.55	101.14	106.98
24	B	612	CLA	C3C-C4C-NC	5.55	117.54	110.43
24	B	603	CLA	C3B-C4B-NB	5.54	115.48	110.53
24	C	506	CLA	C1C-C2C-C3C	-5.54	101.15	106.98
24	C	501	CLA	C1C-C2C-C3C	-5.54	101.16	106.98
24	B	606	CLA	C2B-C1B-NB	5.53	116.06	110.33
24	B	614	CLA	C2C-C1C-NC	5.52	115.78	109.98
29	B	621	LMG	O8-C28-C29	5.52	128.68	111.83
24	B	605	CLA	C3B-C4B-NB	5.52	115.46	110.53
24	B	602	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
24	b	613	CLA	CHD-C4C-C3C	-5.52	116.73	124.77
24	B	607	CLA	O2D-CGD-CBD	5.51	120.87	111.23
24	C	510	CLA	C2C-C1C-NC	5.51	115.77	109.98
24	B	604	CLA	O2D-CGD-O1D	-5.51	113.13	123.85
24	C	508	CLA	C1C-C2C-C3C	-5.51	101.19	106.98
24	c	509	CLA	C3C-C4C-NC	5.50	117.48	110.43
29	b	621	LMG	O8-C28-C29	5.50	128.62	111.83
24	b	605	CLA	C2B-C1B-NB	5.50	116.03	110.33
24	C	511	CLA	C2B-C1B-NB	5.50	116.03	110.33
24	b	609	CLA	C3B-C4B-NB	5.49	115.43	110.53
24	c	513	CLA	C3B-C2B-C1B	-5.48	100.70	107.17
24	D	403	CLA	CMD-C2D-C1D	5.48	134.38	124.73
24	C	511	CLA	C3B-C4B-NB	5.48	115.42	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	505	CLA	C2B-C1B-NB	5.47	116.00	110.33
24	A	606	CLA	C4A-NA-C1A	-5.47	104.18	106.68
24	b	613	CLA	C3B-C4B-NB	5.47	115.41	110.53
24	A	607	CLA	CMD-C2D-C1D	5.46	134.35	124.73
24	c	503	CLA	C2C-C1C-NC	5.46	115.71	109.98
30	C	528	GOL	C3-C2-C1	5.46	131.81	111.80
31	I	101	LMT	O1B-C4'-C3'	5.45	121.08	107.23
24	c	505	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
24	c	507	CLA	C3B-C4B-NB	5.45	115.39	110.53
24	b	614	CLA	CMD-C2D-C1D	5.44	134.31	124.73
24	c	509	CLA	C3B-C2B-C1B	-5.43	100.76	107.17
24	B	609	CLA	C3C-C4C-NC	5.43	117.38	110.43
28	a	413	SQD	C1-O5-C5	-5.42	103.13	113.72
25	D	401	PHO	C3D-C4D-ND	5.42	114.66	107.71
24	C	513	CLA	C2C-C1C-NC	5.42	115.67	109.98
24	a	408	CLA	C2B-C1B-NB	5.42	115.94	110.33
24	c	506	CLA	CMD-C2D-C1D	5.42	134.27	124.73
24	c	511	CLA	C1C-C2C-C3C	-5.42	101.28	106.98
24	B	615	CLA	C2C-C1C-NC	5.40	115.66	109.98
24	c	511	CLA	CMC-C2C-C1C	5.40	133.47	125.03
24	c	508	CLA	C4D-C3D-CAD	-5.40	102.24	108.11
24	B	605	CLA	CMD-C2D-C1D	5.40	134.23	124.73
38	C	522	HTG	C1'-S1-C1	5.39	112.10	100.45
24	b	605	CLA	C4-C3-C5	-5.38	105.88	115.23
24	B	604	CLA	CMC-C2C-C1C	5.38	133.44	125.03
24	b	613	CLA	C2C-C1C-NC	5.38	115.63	109.98
24	B	611	CLA	C3B-C2B-C1B	-5.38	100.83	107.17
24	c	506	CLA	C3C-C4C-NC	5.37	117.31	110.43
24	d	403	CLA	CMD-C2D-C1D	5.37	134.18	124.73
24	B	617	CLA	O2D-CGD-CBD	5.36	120.61	111.23
24	A	606	CLA	C2C-C1C-NC	5.35	115.60	109.98
24	C	503	CLA	C2C-C1C-NC	5.35	115.60	109.98
24	c	509	CLA	C2B-C1B-NB	5.34	115.87	110.33
24	B	615	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
41	E	113	HEM	C1B-NB-C4B	5.33	111.52	105.21
24	B	616	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
24	b	611	CLA	C3C-C4C-NC	5.32	117.25	110.43
24	C	507	CLA	CMD-C2D-C1D	5.32	134.10	124.73
24	b	614	CLA	C3B-C4B-NB	5.31	115.27	110.53
24	B	611	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
24	B	602	CLA	CMD-C2D-C1D	5.30	134.07	124.73
27	a	412	PL9	C3-C4-C5	5.30	125.18	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C3C-C4C-NC	5.29	117.21	110.43
29	b	621	LMG	O7-C10-O9	-5.29	111.33	123.70
24	b	610	CLA	C2B-C1B-NB	5.29	115.81	110.33
24	b	614	CLA	CAC-C3C-C4C	5.28	131.67	124.79
28	A	612	SQD	O47-C7-C8	5.28	122.91	111.48
24	B	603	CLA	CMD-C2D-C1D	5.28	134.03	124.73
24	b	617	CLA	C3B-C2B-C1B	-5.28	100.95	107.17
24	b	606	CLA	C5-C3-C2	-5.27	109.34	121.17
24	c	502	CLA	C4D-C3D-CAD	-5.27	102.38	108.11
24	C	501	CLA	CMD-C2D-C1D	5.27	134.00	124.73
26	b	618	BCR	C7-C8-C9	-5.26	118.45	126.23
24	b	609	CLA	C3C-C4C-NC	5.25	117.16	110.43
24	c	509	CLA	CAC-C3C-C4C	5.25	131.62	124.79
24	B	604	CLA	C3B-C4B-NB	5.25	115.22	110.53
24	B	616	CLA	C3C-C4C-NC	5.24	117.14	110.43
24	C	509	CLA	CAC-C3C-C4C	5.24	131.61	124.79
24	b	612	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
24	d	405	CLA	C3B-C2B-C1B	-5.23	101.00	107.17
24	B	607	CLA	C4A-NA-C1A	-5.23	104.29	106.68
24	c	501	CLA	C2B-C1B-NB	5.23	115.75	110.33
24	c	501	CLA	C1C-C2C-C3C	-5.23	101.48	106.98
24	B	610	CLA	C3C-C4C-NC	5.23	117.13	110.43
24	b	610	CLA	C3B-C4B-NB	5.22	115.19	110.53
29	b	621	LMG	O7-C10-C11	5.22	122.78	111.48
24	B	616	CLA	CMD-C2D-C1D	5.22	133.92	124.73
24	C	502	CLA	C2C-C1C-NC	5.22	115.47	109.98
24	b	603	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
24	D	405	CLA	C3B-C4B-NB	5.22	115.19	110.53
24	b	607	CLA	C1D-ND-C4D	-5.22	102.65	106.31
24	C	511	CLA	CMD-C2D-C1D	5.22	133.91	124.73
24	B	615	CLA	C1D-ND-C4D	-5.21	102.65	106.31
24	B	603	CLA	C1D-ND-C4D	-5.21	102.65	106.31
24	a	407	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
24	B	602	CLA	C2B-C1B-NB	5.20	115.72	110.33
24	b	602	CLA	CHD-C4C-C3C	-5.20	117.19	124.77
24	c	512	CLA	CMD-C2D-C1D	5.20	133.88	124.73
24	B	602	CLA	C3C-C4C-NC	5.20	117.09	110.43
24	B	606	CLA	CHD-C4C-C3C	-5.19	117.20	124.77
24	c	513	CLA	C3C-C4C-NC	5.19	117.08	110.43
24	c	511	CLA	C3B-C2B-C1B	-5.19	101.06	107.17
24	B	603	CLA	C3C-C4C-NC	5.18	117.07	110.43
24	b	612	CLA	C1C-C2C-C3C	-5.18	101.53	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	602	CLA	C3C-C4C-NC	5.18	117.07	110.43
24	B	609	CLA	C3B-C4B-NB	5.18	115.15	110.53
24	c	510	CLA	C2C-C1C-NC	5.17	115.42	109.98
24	b	602	CLA	CMD-C2D-C1D	5.17	133.83	124.73
25	d	401	PHO	C3D-C4D-ND	5.17	114.33	107.71
24	B	606	CLA	C1-C2-C3	-5.16	117.74	126.20
24	b	608	CLA	C3B-C4B-NB	5.16	115.13	110.53
24	c	512	CLA	O2D-CGD-CBD	5.15	120.24	111.23
24	c	510	CLA	C3B-C2B-C1B	-5.15	101.10	107.17
28	x	101	SQD	O8-S-C6	5.15	115.92	105.97
24	D	405	CLA	C3C-C4C-NC	5.15	117.02	110.43
24	C	510	CLA	CMD-C2D-C1D	5.14	133.78	124.73
24	b	605	CLA	CAC-C3C-C4C	5.14	131.48	124.79
24	B	612	CLA	CMC-C2C-C1C	5.14	133.06	125.03
24	b	607	CLA	C2C-C1C-NC	5.14	115.38	109.98
38	B	624	HTG	C1'-S1-C1	5.13	111.54	100.45
24	b	615	CLA	O2D-CGD-CBD	5.13	120.20	111.23
38	C	532	HTG	C1-O5-C5	5.13	121.76	112.56
24	C	512	CLA	C2C-C1C-NC	5.13	115.37	109.98
24	B	605	CLA	C3C-C4C-NC	5.12	116.99	110.43
29	c	519	LMG	O8-C28-C29	5.12	127.44	111.83
24	B	612	CLA	C3B-C4B-NB	5.12	115.10	110.53
28	A	612	SQD	O6-C1-C2	5.11	116.04	108.27
24	b	617	CLA	CAC-C3C-C4C	5.11	131.44	124.79
24	c	501	CLA	C3B-C2B-C1B	-5.11	101.14	107.17
24	c	501	CLA	CMD-C2D-C1D	5.11	133.72	124.73
24	c	513	CLA	C1C-C2C-C3C	-5.10	101.61	106.98
24	b	617	CLA	O2A-CGA-CBA	5.09	127.36	111.83
24	c	507	CLA	C3C-C4C-NC	5.09	116.95	110.43
24	c	510	CLA	C2B-C1B-NB	5.07	115.58	110.33
24	C	503	CLA	CMD-C2D-C1D	5.06	133.64	124.73
25	a	409	PHO	C2D-C1D-ND	5.05	113.08	109.43
24	b	613	CLA	CAC-C3C-C4C	5.05	131.36	124.79
24	C	505	CLA	C3C-C4C-NC	5.05	116.89	110.43
24	B	606	CLA	C3B-C2B-C1B	-5.04	101.23	107.17
28	b	633	SQD	O5-C1-C2	-5.04	100.02	110.37
24	A	607	CLA	C3C-C4C-NC	5.04	116.88	110.43
24	b	612	CLA	CMC-C2C-C1C	5.03	132.90	125.03
24	b	602	CLA	C2B-C1B-NB	5.03	115.55	110.33
24	b	611	CLA	CAC-C3C-C4C	5.03	131.34	124.79
24	B	614	CLA	C3C-C4C-NC	5.03	116.88	110.43
24	c	510	CLA	O2D-CGD-CBD	5.03	120.02	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	610	CLA	O2D-CGD-O1D	-5.02	114.08	123.85
24	b	615	CLA	C2C-C1C-NC	5.01	115.25	109.98
38	C	522	HTG	C1-O5-C5	5.01	121.56	112.56
24	c	509	CLA	CMD-C2D-C1D	5.01	133.56	124.73
24	b	605	CLA	CMD-C2D-C1D	5.01	133.54	124.73
24	C	503	CLA	CMC-C2C-C1C	5.00	132.85	125.03
24	C	506	CLA	C3C-C4C-NC	5.00	116.83	110.43
24	c	502	CLA	C1C-C2C-C3C	-4.99	101.73	106.98
24	C	504	CLA	C3B-C4B-NB	4.98	114.98	110.53
24	b	606	CLA	C1D-ND-C4D	-4.98	102.82	106.31
24	d	405	CLA	CMD-C2D-C1D	4.98	133.50	124.73
24	b	612	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
38	c	531	HTG	C1'-S1-C1	4.98	111.20	100.45
24	B	608	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
24	C	501	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
24	b	610	CLA	O2D-CGD-CBD	4.97	119.92	111.23
32	e	101	LHG	O7-C7-C8	4.96	122.22	111.48
40	c	517	DGD	O2G-C1B-C2B	4.96	122.21	111.48
24	c	508	CLA	C3C-C4C-NC	4.96	116.78	110.43
24	c	511	CLA	C2B-C1B-NB	4.96	115.47	110.33
24	B	615	CLA	C3B-C2B-C1B	-4.95	101.33	107.17
24	b	616	CLA	CMD-C2D-C1D	4.94	133.43	124.73
24	C	511	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
24	B	607	CLA	C1D-ND-C4D	-4.94	102.84	106.31
24	C	508	CLA	C4D-C3D-CAD	-4.94	102.74	108.11
24	A	609	CLA	C2B-C1B-NB	4.94	115.45	110.33
24	a	410	CLA	C3C-C4C-NC	4.94	116.75	110.43
24	c	506	CLA	C2C-C1C-NC	4.93	115.17	109.98
24	c	502	CLA	C3B-C4B-NB	4.93	114.94	110.53
24	D	405	CLA	C2B-C1B-NB	4.93	115.44	110.33
24	B	603	CLA	C2C-C1C-NC	4.93	115.16	109.98
31	a	401	LMT	C1'-O5'-C5'	4.93	123.34	113.72
24	b	606	CLA	C2C-C1C-NC	4.93	115.16	109.98
24	b	615	CLA	C1D-ND-C4D	-4.93	102.86	106.31
24	b	615	CLA	CMD-C2D-C1D	4.92	133.40	124.73
24	C	510	CLA	C3C-C4C-NC	4.91	116.73	110.43
28	A	612	SQD	O9-S-C6	4.91	114.08	106.76
24	B	603	CLA	CHD-C4C-C3C	-4.90	117.62	124.77
26	B	619	BCR	C40-C30-C25	-4.90	102.55	110.24
24	b	617	CLA	C2B-C1B-NB	4.90	115.41	110.33
24	C	510	CLA	C2B-C1B-NB	4.89	115.40	110.33
24	b	616	CLA	CMC-C2C-C1C	4.89	132.68	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	605	CLA	C3B-C4B-NB	4.89	114.89	110.53
24	c	506	CLA	CHD-C4C-C3C	-4.89	117.65	124.77
24	C	509	CLA	C2B-C1B-NB	4.88	115.39	110.33
24	d	405	CLA	CAC-C3C-C4C	4.87	131.13	124.79
24	C	504	CLA	CMD-C2D-C1D	4.87	133.31	124.73
24	c	508	CLA	C1C-C2C-C3C	-4.87	101.86	106.98
28	a	413	SQD	O9-S-C6	4.86	114.02	106.76
24	C	507	CLA	CHD-C4C-C3C	-4.86	117.69	124.77
32	d	409	LHG	O8-C23-O10	-4.85	111.50	123.63
29	b	621	LMG	O8-C28-O10	-4.85	111.50	123.63
25	a	409	PHO	C2B-C1B-NB	4.85	112.93	109.43
24	c	512	CLA	C1C-C2C-C3C	-4.85	101.88	106.98
24	B	607	CLA	C2B-C1B-NB	4.83	115.34	110.33
24	b	613	CLA	C4C-C3C-C2C	-4.83	99.86	106.89
24	B	617	CLA	C3C-C4C-NC	4.83	116.61	110.43
24	B	604	CLA	C1C-C2C-C3C	-4.82	101.91	106.98
24	B	611	CLA	C4C-C3C-C2C	-4.82	99.87	106.89
24	a	407	CLA	CAC-C3C-C4C	4.82	131.06	124.79
41	E	113	HEM	CHC-C4B-NB	4.82	129.61	124.42
26	C	514	BCR	C23-C24-C25	-4.82	114.12	127.00
24	b	606	CLA	CHD-C4C-C3C	-4.82	117.75	124.77
24	B	617	CLA	CMD-C2D-C1D	4.82	133.21	124.73
29	C	526	LMG	C1-C2-C3	-4.81	99.90	110.01
24	c	503	CLA	C3B-C4B-NB	4.80	114.82	110.53
24	A	606	CLA	C3B-C4B-NB	4.80	114.81	110.53
28	a	424	SQD	C44-O6-C1	4.80	124.08	113.80
27	A	611	PL9	C2-C1-C6	4.79	124.69	119.00
24	C	512	CLA	CAC-C3C-C4C	4.79	131.02	124.79
24	c	501	CLA	O2D-CGD-CBD	4.79	119.60	111.23
24	C	511	CLA	C2C-C1C-NC	4.79	115.01	109.98
24	B	602	CLA	O2A-C1-C2	4.78	126.51	108.11
43	V	203	HEC	CHA-C4D-ND	4.78	129.57	124.42
24	B	606	CLA	C4-C3-C2	-4.78	111.36	123.63
24	c	507	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
28	F	104	SQD	O3-C3-C2	4.77	121.62	110.38
38	H	101	HTG	C1-O5-C5	4.77	121.11	112.56
24	c	502	CLA	C2B-C1B-NB	4.76	115.26	110.33
24	c	505	CLA	C4C-C3C-C2C	-4.76	99.97	106.89
24	C	508	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
29	a	414	LMG	O7-C10-C11	4.75	121.76	111.48
24	c	503	CLA	CHD-C4C-C3C	-4.75	117.85	124.77
24	B	609	CLA	CHD-C4C-C3C	-4.74	117.86	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	C2B-C1B-NB	4.74	115.24	110.33
24	b	617	CLA	CHD-C4C-C3C	-4.74	117.87	124.77
24	D	404	CLA	C3C-C4C-NC	4.74	116.50	110.43
24	d	405	CLA	O2D-CGD-CBD	4.73	119.49	111.23
24	b	602	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
24	d	405	CLA	CHD-C4C-C3C	-4.72	117.89	124.77
40	C	517	DGD	O2G-C1B-O1B	-4.72	112.68	123.70
28	A	616	SQD	O47-C7-C8	4.71	121.66	111.48
24	B	611	CLA	CMD-C2D-C1D	4.70	133.01	124.73
27	D	407	PL9	C40-C39-C41	4.70	123.39	115.23
24	b	615	CLA	C3B-C4B-NB	4.70	114.72	110.53
31	B	622	LMT	O1'-C1'-C2'	4.70	115.41	108.27
24	c	505	CLA	CHD-C4C-C3C	-4.69	117.93	124.77
24	b	605	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
24	C	505	CLA	CMD-C2D-C1D	4.69	132.99	124.73
24	B	607	CLA	CMC-C2C-C1C	4.69	132.36	125.03
25	A	608	PHO	C3D-C4D-ND	4.68	113.71	107.71
24	B	611	CLA	CAC-C3C-C4C	4.68	130.88	124.79
24	C	505	CLA	CAC-C3C-C4C	4.67	130.87	124.79
24	C	502	CLA	C2B-C1B-NB	4.67	115.16	110.33
31	j	103	LMT	C1-O1'-C1'	4.66	121.64	113.68
24	c	501	CLA	CMC-C2C-C1C	4.66	132.31	125.03
26	C	514	BCR	C24-C23-C22	-4.66	119.35	126.23
24	C	505	CLA	C3B-C4B-NB	4.66	114.69	110.53
24	b	603	CLA	O2D-CGD-O1D	-4.65	114.79	123.85
24	C	504	CLA	C3B-C2B-C1B	-4.65	101.68	107.17
24	b	605	CLA	C4-C3-C2	-4.65	111.69	123.63
24	A	606	CLA	CAC-C3C-C4C	4.64	130.83	124.79
24	A	606	CLA	C3C-C4C-NC	4.64	116.38	110.43
24	c	502	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
32	E	101	LHG	O7-C7-C8	4.64	121.53	111.48
24	c	503	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
26	T	102	BCR	C20-C21-C22	-4.64	120.77	127.28
24	C	512	CLA	C3C-C4C-NC	4.64	116.37	110.43
24	B	607	CLA	CHD-C4C-C3C	-4.64	118.01	124.77
24	d	405	CLA	C3C-C4C-NC	4.63	116.36	110.43
24	B	617	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
24	b	603	CLA	C3B-C4B-NB	4.62	114.66	110.53
24	d	404	CLA	C4B-C3B-C2B	-4.62	101.55	107.30
24	B	610	CLA	C1C-C2C-C3C	-4.62	102.12	106.98
24	B	610	CLA	C2B-C1B-NB	4.62	115.12	110.33
24	C	512	CLA	C2B-C1B-NB	4.61	115.11	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	d	406	BCR	C40-C30-C39	4.61	121.82	108.63
28	b	633	SQD	C4-C3-C2	4.60	118.91	110.83
24	D	405	CLA	CMD-C2D-C1D	4.60	132.83	124.73
24	c	507	CLA	CHD-C4C-C3C	-4.60	118.07	124.77
24	C	513	CLA	O2D-CGD-CBD	4.59	119.25	111.23
24	b	612	CLA	C2B-C1B-NB	4.59	115.08	110.33
24	A	609	CLA	C4D-C3D-CAD	-4.59	103.12	108.11
28	A	616	SQD	O6-C1-C2	4.58	115.23	108.27
24	d	403	CLA	C3B-C4B-NB	4.58	114.62	110.53
24	b	608	CLA	C3C-C4C-NC	4.58	116.30	110.43
24	C	504	CLA	C2B-C1B-NB	4.58	115.08	110.33
24	a	408	CLA	CMD-C2D-C1D	4.58	132.79	124.73
27	A	611	PL9	C7-C8-C9	-4.58	118.95	126.83
24	c	511	CLA	CHD-C4C-C3C	-4.57	118.10	124.77
26	C	514	BCR	C7-C8-C9	-4.57	119.47	126.23
24	C	507	CLA	C1C-C2C-C3C	-4.57	102.17	106.98
24	B	606	CLA	C4C-C3C-C2C	-4.57	100.24	106.89
24	C	502	CLA	CMC-C2C-C1C	4.57	132.17	125.03
24	a	407	CLA	C3B-C4B-NB	4.56	114.61	110.53
24	b	611	CLA	CMD-C2D-C1D	4.56	132.76	124.73
24	c	505	CLA	C3B-C4B-NB	4.56	114.60	110.53
24	b	606	CLA	CMC-C2C-C1C	4.56	132.16	125.03
24	c	512	CLA	C1-C2-C3	-4.56	118.73	126.20
24	A	609	CLA	C3B-C4B-NB	4.55	114.60	110.53
24	B	617	CLA	C3B-C4B-NB	4.55	114.59	110.53
24	d	403	CLA	C2C-C1C-NC	4.55	114.76	109.98
24	c	508	CLA	CMD-C2D-C1D	4.54	132.73	124.73
24	C	506	CLA	CHD-C4C-C3C	-4.54	118.15	124.77
24	B	605	CLA	C2B-C1B-NB	4.54	115.03	110.33
24	B	617	CLA	CAC-C3C-C4C	4.54	130.70	124.79
26	b	619	BCR	C37-C22-C23	4.54	125.02	118.09
24	d	403	CLA	C2B-C1B-NB	4.54	115.03	110.33
24	C	510	CLA	C3B-C2B-C1B	-4.53	101.82	107.17
24	d	404	CLA	C3C-C4C-NC	4.53	116.24	110.43
24	b	604	CLA	C4B-C3B-C2B	-4.53	101.67	107.30
24	b	615	CLA	O2D-CGD-O1D	-4.53	115.03	123.85
24	c	502	CLA	CHD-C4C-C3C	-4.53	118.17	124.77
24	C	510	CLA	CAC-C3C-C4C	4.52	130.67	124.79
26	t	102	BCR	C39-C30-C25	-4.52	103.15	110.24
24	c	509	CLA	C3B-C4B-NB	4.52	114.57	110.53
24	B	606	CLA	C1D-ND-C4D	-4.52	103.14	106.31
26	d	406	BCR	C30-C25-C26	-4.51	116.47	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	501	CLA	C2B-C1B-NB	4.50	115.00	110.33
24	C	510	CLA	CHD-C4C-C3C	-4.50	118.21	124.77
24	c	512	CLA	C3B-C2B-C1B	-4.50	101.86	107.17
24	D	404	CLA	C1C-C2C-C3C	-4.50	102.25	106.98
24	B	610	CLA	C3B-C2B-C1B	-4.50	101.87	107.17
24	A	606	CLA	C2B-C1B-NB	4.49	114.98	110.33
24	C	513	CLA	C2B-C1B-NB	4.48	114.97	110.33
24	C	511	CLA	CHD-C4C-C3C	-4.47	118.25	124.77
24	c	512	CLA	C3C-C4C-NC	4.47	116.16	110.43
24	d	403	CLA	CHD-C4C-C3C	-4.47	118.26	124.77
24	B	607	CLA	CMD-C2D-C1D	4.47	132.59	124.73
28	A	622	SQD	C44-O6-C1	4.47	123.37	113.80
24	B	604	CLA	CHD-C4C-C3C	-4.47	118.26	124.77
24	c	508	CLA	C2B-C1B-NB	4.47	114.96	110.33
24	b	617	CLA	C4C-C3C-C2C	-4.46	100.40	106.89
26	T	102	BCR	C7-C8-C9	-4.46	119.64	126.23
31	b	622	LMT	O1'-C1'-C2'	4.45	115.03	108.27
24	C	513	CLA	CAC-C3C-C4C	4.45	130.58	124.79
24	B	612	CLA	CHD-C4C-C3C	-4.44	118.30	124.77
24	D	403	CLA	C3C-C4C-NC	4.44	116.12	110.43
24	b	612	CLA	C1D-ND-C4D	-4.44	103.20	106.31
24	c	505	CLA	CMD-C2D-C1D	4.43	132.53	124.73
24	c	504	CLA	CMD-C2D-C1D	4.43	132.53	124.73
24	C	506	CLA	CMC-C2C-C1C	4.43	131.95	125.03
24	C	506	CLA	O2D-CGD-CBD	4.42	118.96	111.23
24	B	607	CLA	C3C-C4C-NC	4.42	116.09	110.43
25	A	608	PHO	O2D-CGD-CBD	4.42	115.80	110.95
24	b	612	CLA	C3C-C4C-NC	4.41	116.08	110.43
24	C	510	CLA	CMC-C2C-C1C	4.41	131.93	125.03
27	A	611	PL9	C53-C6-C1	4.41	124.31	115.28
28	b	633	SQD	O9-S-C6	4.41	113.34	106.76
24	c	508	CLA	C4B-C3B-C2B	-4.41	101.82	107.30
41	E	113	HEM	CMD-C2D-C1D	4.41	131.93	125.03
28	a	417	SQD	O48-C23-C24	4.41	125.28	111.83
24	C	508	CLA	CMD-C2D-C1D	4.41	132.49	124.73
24	C	502	CLA	CMD-C2D-C1D	4.41	132.49	124.73
24	c	507	CLA	CMD-C2D-C1D	4.41	132.49	124.73
40	C	517	DGD	O2G-C1B-C2B	4.40	121.01	111.48
24	c	504	CLA	CMC-C2C-C1C	4.40	131.91	125.03
24	d	403	CLA	C3C-C4C-NC	4.40	116.06	110.43
24	b	614	CLA	C2B-C1B-NB	4.40	114.89	110.33
24	B	605	CLA	C1C-C2C-C3C	-4.40	102.36	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	606	CLA	C3B-C4B-NB	4.39	114.45	110.53
24	B	606	CLA	C5-C3-C2	-4.39	111.30	121.17
24	C	509	CLA	C3C-C4C-NC	4.39	116.06	110.43
24	b	611	CLA	C3B-C2B-C1B	-4.39	101.99	107.17
24	B	608	CLA	C1C-C2C-C3C	-4.39	102.36	106.98
24	a	408	CLA	CHD-C4C-C3C	-4.39	118.38	124.77
24	c	509	CLA	CHD-C4C-C3C	-4.39	118.38	124.77
40	C	516	DGD	O2G-C1B-C2B	4.39	120.97	111.48
24	b	610	CLA	C4C-C3C-C2C	-4.38	100.51	106.89
24	b	606	CLA	CMB-C2B-C1B	4.38	132.09	125.42
24	C	509	CLA	C1C-C2C-C3C	-4.38	102.37	106.98
28	a	424	SQD	O6-C1-C2	4.38	114.93	108.27
28	x	101	SQD	O47-C7-C8	4.38	120.95	111.48
29	C	519	LMG	O7-C10-C11	4.38	120.95	111.48
24	C	513	CLA	CHD-C4C-C3C	-4.38	118.39	124.77
28	a	413	SQD	C1-C2-C3	-4.37	100.81	110.01
24	C	506	CLA	C3B-C2B-C1B	-4.37	102.02	107.17
24	b	604	CLA	C3C-C4C-NC	4.37	116.03	110.43
24	b	604	CLA	CMD-C2D-C1D	4.37	132.42	124.73
24	C	505	CLA	C2B-C1B-NB	4.37	114.86	110.33
24	b	610	CLA	C3B-C2B-C1B	-4.36	102.03	107.17
24	b	603	CLA	CMD-C2D-C1D	4.36	132.41	124.73
24	b	608	CLA	C2C-C1C-NC	4.36	114.56	109.98
24	C	502	CLA	C1C-C2C-C3C	-4.36	102.40	106.98
26	h	103	BCR	C38-C26-C25	-4.35	119.74	124.48
24	B	603	CLA	O2D-CGD-O1D	-4.35	115.39	123.85
24	B	602	CLA	C4D-C3D-CAD	-4.34	103.39	108.11
26	c	515	BCR	C32-C1-C6	-4.34	103.44	110.24
24	c	507	CLA	C2B-C1B-NB	4.34	114.82	110.33
28	h	105	SQD	O7-S-C6	4.33	113.22	106.76
24	B	609	CLA	C1C-C2C-C3C	-4.33	102.43	106.98
24	b	609	CLA	C2B-C1B-NB	4.33	114.81	110.33
26	c	514	BCR	C7-C8-C9	-4.32	119.84	126.23
24	b	617	CLA	C3B-C4B-NB	4.32	114.39	110.53
26	C	515	BCR	C3-C4-C5	-4.32	106.36	114.06
24	B	602	CLA	C3B-C4B-NB	4.32	114.38	110.53
24	c	502	CLA	CMC-C2C-C1C	4.31	131.78	125.03
24	c	506	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
24	B	608	CLA	CMD-C2D-C1D	4.31	132.31	124.73
24	B	604	CLA	C3B-C2B-C1B	-4.31	102.09	107.17
24	A	609	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
25	a	409	PHO	C3D-C4D-ND	4.30	113.22	107.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	609	CLA	CED-O2D-CGD	4.30	125.66	115.92
31	A	617	LMT	O2'-C2'-C1'	4.29	120.30	110.08
24	B	608	CLA	C4A-NA-C1A	-4.29	104.72	106.68
24	b	607	CLA	C3B-C2B-C1B	-4.29	102.11	107.17
24	B	603	CLA	C3D-C4D-ND	4.29	116.96	109.99
24	B	603	CLA	O2D-CGD-CBD	4.29	118.72	111.23
24	c	503	CLA	C2B-C1B-NB	4.28	114.76	110.33
24	B	616	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
41	E	113	HEM	C1D-C2D-C3D	-4.27	102.49	106.98
24	C	506	CLA	CMD-C2D-C1D	4.27	132.24	124.73
24	B	608	CLA	C3C-C4C-NC	4.27	115.90	110.43
26	t	102	BCR	C38-C26-C25	-4.26	119.83	124.48
31	A	617	LMT	C1-O1'-C1'	4.26	120.96	113.68
26	K	101	BCR	C37-C22-C23	4.26	124.59	118.09
32	d	409	LHG	O8-C23-C24	4.26	124.82	111.83
24	b	617	CLA	CMD-C2D-C1D	4.26	132.22	124.73
24	a	407	CLA	C1C-C2C-C3C	-4.25	102.51	106.98
24	b	606	CLA	C4-C3-C2	-4.25	112.70	123.63
29	B	634	LMG	O7-C10-C11	4.25	120.68	111.48
32	D	409	LHG	O8-C23-C24	4.25	124.80	111.83
24	c	510	CLA	CHD-C4C-C3C	-4.25	118.58	124.77
24	d	404	CLA	C2B-C1B-NB	4.25	114.73	110.33
24	B	605	CLA	C6-C5-C3	-4.25	103.12	113.47
28	x	101	SQD	C1-O5-C5	4.25	122.01	113.72
24	B	615	CLA	O2A-CGA-O1A	-4.25	113.01	123.63
24	a	408	CLA	C4C-C3C-C2C	-4.24	100.71	106.89
24	b	605	CLA	C1C-C2C-C3C	-4.24	102.52	106.98
24	A	607	CLA	CHD-C4C-C3C	-4.24	118.59	124.77
27	a	412	PL9	O1-C4-C3	-4.24	116.26	120.73
28	l	102	SQD	O47-C7-C8	4.23	120.64	111.48
24	B	616	CLA	CMC-C2C-C1C	4.23	131.65	125.03
24	C	506	CLA	C2B-C1B-NB	4.23	114.71	110.33
24	C	511	CLA	C3C-C4C-NC	4.23	115.85	110.43
40	d	408	DGD	C3G-O3G-C1D	4.23	122.86	113.80
24	b	615	CLA	C3B-C2B-C1B	-4.23	102.19	107.17
24	b	602	CLA	C2A-C1A-CHA	-4.23	116.53	123.87
24	b	603	CLA	C2C-C1C-NC	4.22	114.42	109.98
28	x	101	SQD	O9-S-C6	4.22	113.06	106.76
24	b	602	CLA	C1C-C2C-C3C	-4.21	102.55	106.98
24	B	604	CLA	C3C-C4C-NC	4.21	115.83	110.43
24	D	404	CLA	C2B-C1B-NB	4.21	114.69	110.33
24	B	602	CLA	C1C-C2C-C3C	-4.21	102.56	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	u	203	LMT	O1'-C1'-C2'	4.20	114.65	108.27
24	b	612	CLA	O2D-CGD-CBD	4.20	118.56	111.23
24	c	511	CLA	C3C-C4C-NC	4.19	115.80	110.43
24	c	507	CLA	CAC-C3C-C4C	4.19	130.24	124.79
24	B	617	CLA	C1D-ND-C4D	-4.18	103.38	106.31
24	b	617	CLA	O2A-CGA-O1A	-4.18	113.17	123.63
24	B	603	CLA	C4C-C3C-C2C	-4.18	100.80	106.89
24	C	505	CLA	O2D-CGD-O1D	-4.18	115.71	123.85
24	c	501	CLA	C4D-C3D-CAD	-4.18	103.56	108.11
38	h	101	HTG	O5-C1-C2	4.18	116.08	110.32
24	b	611	CLA	C1C-C2C-C3C	-4.17	102.59	106.98
24	B	613	CLA	O2D-CGD-CBD	4.17	118.53	111.23
24	c	512	CLA	CHD-C4C-C3C	-4.17	118.69	124.77
24	B	611	CLA	C3D-C2D-C1D	-4.17	100.15	105.83
24	b	604	CLA	C1C-C2C-C3C	-4.16	102.60	106.98
24	b	610	CLA	CMD-C2D-C1D	4.16	132.06	124.73
24	C	512	CLA	CMD-C2D-C1D	4.16	132.05	124.73
24	C	505	CLA	CHD-C4C-C3C	-4.16	118.71	124.77
24	c	507	CLA	O2D-CGD-CBD	4.16	118.49	111.23
24	b	606	CLA	C1-C2-C3	-4.15	119.39	126.20
24	b	607	CLA	C3C-C4C-NC	4.15	115.75	110.43
28	A	622	SQD	C45-O47-C7	4.15	127.74	117.80
28	l	102	SQD	O7-S-C6	4.15	112.96	106.76
26	C	514	BCR	C28-C27-C26	-4.15	106.65	114.06
38	V	204	HTG	C1-C2-C3	-4.15	102.43	110.55
43	V	203	HEC	C4B-NB-C1B	4.15	110.12	105.21
24	B	612	CLA	CAC-C3C-C4C	4.15	130.19	124.79
24	b	605	CLA	C6-C5-C3	-4.14	103.38	113.47
26	b	620	BCR	C40-C30-C25	-4.14	103.75	110.24
24	A	609	CLA	C1C-C2C-C3C	-4.14	102.62	106.98
28	a	413	SQD	O5-C1-C2	-4.14	101.87	110.37
26	b	619	BCR	C28-C27-C26	-4.14	106.68	114.06
24	B	616	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
24	b	605	CLA	CHD-C4C-C3C	-4.13	118.75	124.77
24	b	616	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
25	A	608	PHO	C4D-ND-C1D	-4.12	103.94	108.87
24	A	609	CLA	C4A-NA-C1A	-4.12	104.80	106.68
24	c	513	CLA	C2B-C1B-NB	4.12	114.60	110.33
24	C	507	CLA	C3B-C4B-NB	4.12	114.20	110.53
28	x	101	SQD	O48-C23-C24	4.11	124.38	111.83
28	A	622	SQD	O9-S-C6	4.11	112.89	106.76
24	B	613	CLA	C2C-C1C-NC	4.11	114.30	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	C3B-C4B-NB	4.11	114.20	110.53
24	B	613	CLA	C3C-C4C-NC	4.11	115.69	110.43
28	b	633	SQD	O47-C7-C8	4.10	120.36	111.48
24	C	503	CLA	C4C-C3C-C2C	-4.10	100.92	106.89
24	b	611	CLA	CHD-C4C-C3C	-4.10	118.79	124.77
24	b	611	CLA	CED-O2D-CGD	4.09	125.20	115.92
24	b	609	CLA	CHD-C4C-C3C	-4.09	118.81	124.77
24	B	615	CLA	C3C-C4C-NC	4.09	115.67	110.43
26	c	527	BCR	C7-C8-C9	-4.09	120.18	126.23
28	F	104	SQD	O9-S-C6	4.09	112.86	106.76
24	b	603	CLA	O2D-CGD-CBD	4.08	118.37	111.23
28	b	633	SQD	O48-C23-C24	4.08	124.27	111.83
24	C	505	CLA	C4C-C3C-C2C	-4.08	100.96	106.89
24	b	605	CLA	CMC-C2C-C1C	4.08	131.40	125.03
28	l	102	SQD	O48-C46-C45	4.08	120.14	108.40
24	C	512	CLA	C3B-C2B-C1B	-4.07	102.37	107.17
24	C	513	CLA	C4C-C3C-C2C	-4.07	100.96	106.89
24	C	513	CLA	C2A-C1A-CHA	-4.07	116.80	123.87
24	b	609	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
24	B	609	CLA	CMD-C2D-C1D	4.07	131.90	124.73
24	b	608	CLA	CMD-C2D-C1D	4.07	131.89	124.73
26	b	619	BCR	C40-C30-C25	-4.06	103.87	110.24
24	B	605	CLA	C4-C3-C2	-4.06	113.19	123.63
24	b	611	CLA	C2B-C1B-NB	4.06	114.54	110.33
24	b	602	CLA	CMB-C2B-C1B	4.06	131.60	125.42
27	a	412	PL9	C53-C6-C1	4.06	123.59	115.28
24	C	501	CLA	C3C-C4C-NC	4.06	115.63	110.43
30	C	523	GOL	O2-C2-C1	4.06	125.99	109.18
24	c	511	CLA	C3B-C4B-NB	4.06	114.15	110.53
24	b	615	CLA	C3C-C4C-NC	4.05	115.62	110.43
24	B	610	CLA	CMC-C2C-C1C	4.05	131.36	125.03
24	b	603	CLA	C3D-C4D-ND	4.05	116.57	109.99
26	B	618	BCR	C7-C8-C9	-4.04	120.25	126.23
24	b	603	CLA	C4C-C3C-C2C	-4.04	101.01	106.89
31	m	102	LMT	O5'-C1'-O1'	-4.03	100.52	110.04
27	d	407	PL9	C40-C39-C41	4.03	122.22	115.23
31	u	203	LMT	O5B-C1B-C2B	4.03	118.65	110.37
26	C	514	BCR	C20-C21-C22	-4.02	121.63	127.28
24	c	502	CLA	C3C-C4C-NC	4.02	115.58	110.43
24	C	501	CLA	CMC-C2C-C1C	4.02	131.31	125.03
24	c	501	CLA	C3C-C4C-NC	4.02	115.58	110.43
29	c	519	LMG	O7-C10-C11	4.02	120.17	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	505	CLA	C3B-C2B-C1B	-4.01	102.44	107.17
24	C	502	CLA	C4D-C3D-CAD	-4.01	103.75	108.11
24	c	504	CLA	C7-C6-C5	-4.01	102.57	113.26
24	a	410	CLA	CAC-C3C-C4C	4.01	130.01	124.79
24	B	617	CLA	CHD-C4C-C3C	-4.01	118.93	124.77
26	d	406	BCR	C38-C26-C25	-4.01	120.11	124.48
41	e	107	HEM	O2D-CGD-CBD	4.01	126.66	114.00
24	A	609	CLA	C3C-C4C-NC	4.00	115.56	110.43
24	b	616	CLA	CHD-C4C-C3C	-4.00	118.94	124.77
24	c	505	CLA	C3D-C4D-ND	4.00	116.48	109.99
24	B	608	CLA	CMC-C2C-C1C	4.00	131.28	125.03
24	A	607	CLA	C4-C3-C5	3.99	122.16	115.23
24	c	503	CLA	C3C-C4C-NC	3.99	115.54	110.43
28	a	413	SQD	O8-S-C6	3.99	113.68	105.97
26	D	406	BCR	C7-C8-C9	-3.99	120.33	126.23
26	D	406	BCR	C37-C22-C23	3.99	124.18	118.09
24	A	607	CLA	C3B-C4B-NB	3.99	114.09	110.53
24	C	502	CLA	C3B-C2B-C1B	-3.99	102.47	107.17
41	E	113	HEM	CHD-C1D-C2D	-3.98	118.74	125.03
24	b	606	CLA	O2D-CGD-CBD	3.98	118.19	111.23
24	a	408	CLA	CAC-C3C-C4C	3.98	129.97	124.79
26	d	406	BCR	C31-C1-C6	-3.98	104.01	110.24
26	D	406	BCR	C32-C1-C6	3.97	116.48	110.24
24	a	410	CLA	CHD-C4C-C3C	-3.97	118.98	124.77
24	D	405	CLA	CHD-C4C-C3C	-3.97	118.99	124.77
24	B	617	CLA	C1C-C2C-C3C	-3.97	102.81	106.98
26	b	620	BCR	C7-C8-C9	-3.97	120.37	126.23
24	a	408	CLA	C4B-C3B-C2B	-3.96	102.37	107.30
24	B	615	CLA	CMD-C2D-C1D	3.96	131.70	124.73
24	B	615	CLA	C3B-C4B-NB	3.96	114.06	110.53
24	c	509	CLA	C4C-C3C-C2C	-3.96	101.13	106.89
41	E	113	HEM	O2D-CGD-CBD	3.96	126.50	114.00
24	B	607	CLA	C4B-C3B-C2B	-3.96	102.38	107.30
24	B	613	CLA	CAC-C3C-C4C	3.95	129.94	124.79
24	D	403	CLA	CAC-C3C-C4C	3.95	129.94	124.79
24	d	404	CLA	CMD-C2D-C1D	3.95	131.69	124.73
24	b	611	CLA	CMC-C2C-C1C	3.95	131.21	125.03
24	C	501	CLA	CHD-C4C-C3C	-3.95	119.01	124.77
24	D	403	CLA	CHD-C4C-C3C	-3.95	119.02	124.77
24	B	613	CLA	C3B-C4B-NB	3.95	114.05	110.53
24	b	606	CLA	O2D-CGD-O1D	-3.95	116.17	123.85
24	B	612	CLA	CMD-C2D-C1D	3.94	131.67	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	l	102	SQD	O2-C2-C1	3.94	119.47	110.08
24	A	607	CLA	C3D-C4D-ND	3.94	116.39	109.99
24	b	603	CLA	C3B-C2B-C1B	-3.94	102.53	107.17
24	b	610	CLA	CHD-C4C-C3C	-3.94	119.03	124.77
24	d	403	CLA	C4C-C3C-C2C	-3.94	101.16	106.89
24	B	603	CLA	C4B-C3B-C2B	-3.94	102.41	107.30
24	b	615	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
24	a	410	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
31	C	533	LMT	O1B-C4'-C3'	3.93	117.22	107.23
25	d	401	PHO	C4-C3-C5	3.93	122.05	115.23
40	D	408	DGD	C2G-O2G-C1B	3.93	127.19	117.80
24	B	602	CLA	CMB-C2B-C1B	3.92	131.39	125.42
27	A	611	PL9	C37-C36-C34	-3.92	100.19	113.19
24	b	607	CLA	C2A-C1A-CHA	-3.92	117.06	123.87
31	f	101	LMT	O5'-C5'-C6'	3.92	116.15	106.44
24	a	410	CLA	C2B-C1B-NB	3.92	114.39	110.33
26	c	514	BCR	C24-C23-C22	-3.92	120.44	126.23
24	c	504	CLA	C3C-C4C-NC	3.92	115.45	110.43
24	C	503	CLA	C4D-C3D-CAD	-3.92	103.85	108.11
24	b	604	CLA	O2D-CGD-CBD	3.91	118.07	111.23
24	b	614	CLA	CHD-C4C-C3C	-3.91	119.07	124.77
24	B	607	CLA	O2D-CGD-O1D	-3.91	116.24	123.85
31	m	102	LMT	C1'-O5'-C5'	-3.91	106.09	113.72
31	u	203	LMT	O5B-C5B-C6B	3.91	116.12	106.44
24	B	617	CLA	O2A-CGA-O1A	-3.90	113.86	123.63
26	D	406	BCR	C40-C30-C39	3.90	119.81	108.63
24	b	607	CLA	CMD-C2D-C1D	3.90	131.60	124.73
27	A	611	PL9	O1-C4-C3	-3.90	116.61	120.73
31	j	103	LMT	C3B-C4B-C5B	3.90	117.30	110.23
24	b	602	CLA	CAC-C3C-C4C	3.89	129.86	124.79
24	b	602	CLA	C4D-CHA-C1A	-3.89	116.60	121.24
24	D	405	CLA	O2D-CGD-CBD	3.89	118.03	111.23
24	C	509	CLA	CMC-C2C-C1C	3.89	131.11	125.03
26	b	618	BCR	C8-C7-C6	-3.89	116.61	127.00
41	E	113	HEM	CHA-C4D-ND	3.89	129.18	124.37
31	A	617	LMT	O5'-C1'-C2'	-3.89	102.38	110.37
24	A	609	CLA	CMD-C2D-C1D	3.89	131.57	124.73
24	D	404	CLA	C3A-C2A-C1A	-3.89	95.52	101.34
24	b	604	CLA	CMC-C2C-C1C	3.89	131.11	125.03
31	M	101	LMT	O1'-C1'-C2'	3.88	114.17	108.27
24	b	608	CLA	C2B-C1B-NB	3.88	114.35	110.33
24	b	606	CLA	C4C-C3C-C2C	-3.88	101.24	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	608	CLA	CHD-C4C-C3C	-3.88	119.12	124.77
24	b	615	CLA	CMC-C2C-C1C	3.88	131.10	125.03
24	C	510	CLA	C3B-C4B-NB	3.87	113.99	110.53
24	B	606	CLA	CAC-C3C-C4C	3.87	129.83	124.79
24	B	616	CLA	CMB-C2B-C1B	3.87	131.31	125.42
24	b	607	CLA	C1C-C2C-C3C	-3.87	102.91	106.98
24	C	506	CLA	O2D-CGD-O1D	-3.86	116.33	123.85
24	d	405	CLA	C4C-C3C-C2C	-3.86	101.27	106.89
24	C	502	CLA	CAC-C3C-C4C	3.86	129.81	124.79
24	b	607	CLA	C2B-C1B-NB	3.85	114.32	110.33
24	B	617	CLA	C2B-C1B-NB	3.85	114.32	110.33
31	J	103	LMT	C1B-O5B-C5B	3.85	121.24	113.72
24	C	512	CLA	O2D-CGD-CBD	3.85	117.95	111.23
40	c	516	DGD	O2G-C1B-C2B	3.85	119.80	111.48
24	C	505	CLA	CMC-C2C-C1C	3.85	131.04	125.03
24	B	610	CLA	C4D-C3D-CAD	-3.84	103.93	108.11
24	a	408	CLA	C3D-C4D-ND	3.84	116.24	109.99
24	B	610	CLA	CHD-C4C-C3C	-3.84	119.17	124.77
24	D	405	CLA	C1C-C2C-C3C	-3.84	102.94	106.98
24	D	404	CLA	C2A-C1A-CHA	-3.84	117.21	123.87
24	c	504	CLA	O2D-CGD-CBD	3.84	117.94	111.23
40	c	517	DGD	O2G-C1B-O1B	-3.84	114.73	123.70
24	c	510	CLA	CAC-C3C-C4C	3.84	129.78	124.79
24	B	611	CLA	C4D-C3D-CAD	-3.84	103.94	108.11
24	c	510	CLA	C3B-C4B-NB	3.84	113.95	110.53
24	B	609	CLA	C3B-C2B-C1B	-3.83	102.65	107.17
32	B	632	LHG	O7-C7-O9	-3.83	114.75	123.70
24	b	602	CLA	CMC-C2C-C1C	3.83	131.01	125.03
24	b	613	CLA	CMD-C2D-C1D	3.82	131.46	124.73
24	b	610	CLA	CAC-C3C-C4C	3.82	129.76	124.79
28	a	413	SQD	O47-C7-C8	3.82	119.74	111.48
31	M	101	LMT	O2B-C2B-C1B	-3.81	100.99	110.08
24	C	507	CLA	CMC-C2C-C1C	3.81	130.99	125.03
26	a	411	BCR	C7-C8-C9	-3.81	120.60	126.23
24	B	614	CLA	C4D-C3D-CAD	-3.81	103.97	108.11
24	B	612	CLA	C2A-C1A-CHA	-3.81	117.26	123.87
24	b	614	CLA	C1-C2-C3	-3.81	119.96	126.20
24	C	501	CLA	C2A-C1A-CHA	-3.80	117.26	123.87
24	b	607	CLA	CHD-C4C-C3C	-3.80	119.23	124.77
24	c	506	CLA	C4C-C3C-C2C	-3.80	101.36	106.89
25	d	401	PHO	O2D-CGD-O1D	-3.80	116.45	123.85
24	C	509	CLA	CHD-C4C-C3C	-3.80	119.23	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	CLA	CMB-C2B-C1B	3.80	131.20	125.42
26	C	525	BCR	C24-C23-C22	-3.80	120.62	126.23
26	c	527	BCR	C24-C23-C22	-3.79	120.62	126.23
41	e	107	HEM	C1B-NB-C4B	3.79	109.70	105.21
28	a	424	SQD	O48-C23-C24	3.79	123.39	111.83
24	b	616	CLA	C3C-C4C-NC	3.79	115.28	110.43
24	c	503	CLA	CMC-C2C-C1C	3.78	130.95	125.03
27	a	412	PL9	C2-C3-C4	-3.78	113.69	118.78
31	F	102	LMT	O4'-C4B-C5B	3.78	118.63	109.32
31	u	203	LMT	C1B-O5B-C5B	3.78	121.10	113.72
24	B	602	CLA	OBD-CAD-C3D	-3.78	119.59	128.42
24	B	606	CLA	C2A-C1A-CHA	-3.78	117.31	123.87
24	b	613	CLA	C3B-C2B-C1B	-3.78	102.72	107.17
24	b	605	CLA	O2D-CGD-CBD	3.77	117.83	111.23
29	c	520	LMG	C4-C3-C2	3.77	117.45	110.83
24	D	405	CLA	C4D-C3D-CAD	-3.77	104.01	108.11
28	A	622	SQD	O48-C23-C24	3.77	123.33	111.83
24	c	510	CLA	C4C-C3C-C2C	-3.77	101.40	106.89
24	C	507	CLA	C4A-NA-C1A	-3.77	104.96	106.68
24	D	403	CLA	C3B-C2B-C1B	-3.77	102.73	107.17
24	B	615	CLA	O2D-CGD-CBD	3.76	117.81	111.23
24	a	407	CLA	CMC-C2C-C1C	3.76	130.91	125.03
32	d	410	LHG	O8-C23-O10	-3.76	114.22	123.63
43	V	203	HEC	CHA-C4D-C3D	-3.76	119.29	124.77
24	c	501	CLA	CHD-C4C-C3C	-3.76	119.29	124.77
24	A	609	CLA	CHD-C4C-C3C	-3.75	119.30	124.77
24	b	609	CLA	C3B-C2B-C1B	-3.75	102.74	107.17
41	e	107	HEM	CHD-C1D-ND	3.75	128.46	124.42
24	A	607	CLA	C3D-C2D-C1D	-3.75	100.71	105.83
24	C	507	CLA	O2D-CGD-CBD	3.75	117.78	111.23
24	B	614	CLA	C2B-C1B-NB	3.75	114.21	110.33
24	a	410	CLA	CMD-C2D-C1D	3.75	131.33	124.73
24	B	602	CLA	O2A-CGA-CBA	3.75	123.26	111.83
24	D	404	CLA	C1D-ND-C4D	-3.74	103.69	106.31
24	B	615	CLA	C1C-C2C-C3C	-3.74	103.05	106.98
29	C	519	LMG	O7-C10-O9	-3.73	114.97	123.70
29	z	101	LMG	O7-C10-C11	3.73	119.56	111.48
24	b	616	CLA	C3B-C4B-NB	3.73	113.86	110.53
24	c	502	CLA	CMD-C2D-C1D	3.72	131.28	124.73
24	B	615	CLA	CED-O2D-CGD	3.71	124.34	115.92
24	B	608	CLA	C3D-C2D-C1D	-3.71	100.77	105.83
24	a	407	CLA	C3C-C4C-NC	3.71	115.19	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	614	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
24	C	502	CLA	C4B-C3B-C2B	-3.71	102.69	107.30
24	c	505	CLA	C2A-C1A-CHA	-3.71	117.44	123.87
24	c	513	CLA	C3D-C4D-ND	3.71	116.01	109.99
24	B	615	CLA	CMB-C2B-C1B	3.70	131.06	125.42
27	A	611	PL9	C7-C3-C4	-3.70	113.86	116.91
26	c	515	BCR	C24-C23-C22	-3.70	120.76	126.23
26	c	515	BCR	C7-C8-C9	-3.70	120.76	126.23
24	b	608	CLA	C3B-C2B-C1B	-3.69	102.81	107.17
24	B	602	CLA	O2D-CGD-O1D	-3.69	116.66	123.85
24	d	403	CLA	CBC-CAC-C3C	-3.69	102.41	112.42
24	C	507	CLA	O1D-CGD-CBD	-3.69	117.24	124.52
26	h	103	BCR	C40-C30-C25	-3.69	104.45	110.24
29	d	412	LMG	O7-C10-O9	-3.69	115.08	123.70
40	C	516	DGD	O2G-C1B-O1B	-3.69	115.08	123.70
24	b	602	CLA	CED-O2D-CGD	3.69	124.28	115.92
24	b	607	CLA	CAC-C3C-C4C	3.68	129.58	124.79
24	D	405	CLA	C3B-C2B-C1B	-3.68	102.83	107.17
28	F	104	SQD	C3-C4-C5	3.68	116.91	110.23
24	b	615	CLA	O2A-CGA-O1A	-3.68	114.42	123.63
24	C	501	CLA	CAC-C3C-C4C	3.68	129.58	124.79
26	H	102	BCR	C7-C8-C9	-3.68	120.79	126.23
24	d	403	CLA	C3B-C2B-C1B	-3.68	102.83	107.17
26	h	103	BCR	C37-C22-C23	3.68	123.71	118.09
38	c	531	HTG	C1-O5-C5	3.68	119.16	112.56
24	C	504	CLA	O2D-CGD-CBD	3.68	117.66	111.23
24	B	615	CLA	O2D-CGD-O1D	-3.68	116.69	123.85
24	c	508	CLA	C3D-C2D-C1D	-3.67	100.82	105.83
24	C	507	CLA	C2A-C1A-CHA	-3.67	117.50	123.87
41	e	107	HEM	CMD-C2D-C1D	3.67	130.77	125.03
40	H	103	DGD	O3G-C1D-C2D	-3.67	102.70	108.27
24	C	513	CLA	C4-C3-C5	3.67	121.59	115.23
24	a	408	CLA	O2D-CGD-CBD	3.67	117.64	111.23
24	b	613	CLA	C2B-C1B-NB	3.67	114.13	110.33
24	d	404	CLA	C4-C3-C5	3.66	121.59	115.23
24	B	615	CLA	CMC-C2C-C1C	3.66	130.76	125.03
28	b	633	SQD	O3-C3-C4	-3.66	101.75	110.38
25	D	401	PHO	CED-O2D-CGD	3.66	124.21	115.92
24	B	607	CLA	C3B-C2B-C1B	-3.65	102.86	107.17
24	A	609	CLA	C1D-ND-C4D	-3.65	103.75	106.31
24	b	603	CLA	C2B-C1B-NB	3.65	114.11	110.33
24	b	608	CLA	C4C-C3C-C2C	-3.65	101.58	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	405	CLA	CAC-C3C-C4C	3.64	129.53	124.79
24	c	501	CLA	C2A-C1A-CHA	-3.64	117.55	123.87
24	B	614	CLA	C3B-C2B-C1B	-3.64	102.88	107.17
24	B	603	CLA	C4A-NA-C1A	-3.64	105.02	106.68
24	C	502	CLA	CHD-C4C-C3C	-3.64	119.47	124.77
24	b	602	CLA	C1-O2A-CGA	3.64	125.45	116.65
24	D	403	CLA	C4B-C3B-C2B	-3.63	102.79	107.30
24	C	513	CLA	CMD-C2D-C1D	3.63	131.12	124.73
24	C	513	CLA	O2D-CGD-O1D	-3.63	116.79	123.85
24	B	611	CLA	C3B-C4B-NB	3.63	113.77	110.53
24	C	505	CLA	O2D-CGD-CBD	3.63	117.57	111.23
24	b	609	CLA	C4C-C3C-C2C	-3.62	101.62	106.89
24	B	602	CLA	CAC-C3C-C4C	3.62	129.50	124.79
38	b	631	HTG	C4-C3-C2	3.62	117.18	110.83
24	a	410	CLA	C3D-C4D-ND	3.61	115.86	109.99
24	B	602	CLA	CHB-C4A-NA	3.61	129.61	124.40
24	B	606	CLA	C3D-C4D-ND	3.61	115.85	109.99
26	A	610	BCR	C7-C8-C9	-3.61	120.90	126.23
24	b	615	CLA	C3D-C4D-ND	3.60	115.85	109.99
35	B	652	P6G	O4-C3-C2	3.60	126.00	110.11
24	b	611	CLA	O2D-CGD-CBD	3.60	117.53	111.23
24	c	511	CLA	C3D-C4D-ND	3.60	115.83	109.99
24	b	602	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
24	c	502	CLA	CAC-C3C-C4C	3.60	129.47	124.79
40	d	408	DGD	C2G-O2G-C1B	3.60	126.40	117.80
24	b	614	CLA	C4B-C3B-C2B	-3.59	102.83	107.30
24	a	410	CLA	C3B-C2B-C1B	-3.59	102.93	107.17
24	b	610	CLA	C3D-C4D-ND	3.59	115.83	109.99
24	C	508	CLA	CHD-C4C-C3C	-3.59	119.54	124.77
26	c	515	BCR	C19-C18-C17	-3.59	113.36	119.01
31	a	401	LMT	O1'-C1'-C2'	3.59	113.72	108.27
24	D	405	CLA	C4C-C3C-C2C	-3.59	101.67	106.89
24	b	612	CLA	C3D-C4D-ND	3.59	115.82	109.99
29	c	520	LMG	O1-C1-C2	3.59	113.72	108.27
24	C	512	CLA	CHD-C4C-C3C	-3.59	119.54	124.77
24	C	504	CLA	CMC-C2C-C1C	3.58	130.63	125.03
24	B	606	CLA	CMD-C2D-C1D	3.58	131.04	124.73
24	c	507	CLA	C3D-C2D-C1D	-3.58	100.94	105.83
26	c	514	BCR	C23-C24-C25	-3.58	117.43	127.00
41	e	107	HEM	C4B-C3B-C2B	-3.58	103.99	107.28
31	b	622	LMT	O1B-C4'-C5'	-3.58	100.08	109.48
24	c	513	CLA	C6-C5-C3	-3.58	104.75	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	102	BCR	C24-C23-C22	-3.58	120.94	126.23
24	c	506	CLA	CMC-C2C-C1C	3.58	130.62	125.03
24	c	507	CLA	CMC-C2C-C1C	3.58	130.62	125.03
24	a	407	CLA	CHD-C4C-C3C	-3.57	119.56	124.77
24	b	604	CLA	CHD-C4C-C3C	-3.57	119.56	124.77
26	d	406	BCR	C33-C5-C6	-3.57	120.58	124.48
24	b	606	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
28	l	102	SQD	O48-C23-C24	3.57	122.72	111.83
24	B	603	CLA	CMC-C2C-C1C	3.56	130.60	125.03
24	c	503	CLA	C1C-C2C-C3C	-3.56	103.23	106.98
31	f	101	LMT	O4'-C4B-C5B	3.56	118.09	109.32
24	c	511	CLA	CMD-C2D-C1D	3.56	130.99	124.73
24	c	507	CLA	C4C-C3C-C2C	-3.55	101.72	106.89
24	b	604	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
24	B	617	CLA	CED-O2D-CGD	3.55	123.96	115.92
24	d	405	CLA	C4-C3-C5	3.55	121.38	115.23
26	C	515	BCR	C7-C8-C9	-3.54	120.99	126.23
24	c	503	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
24	A	609	CLA	O2D-CGD-CBD	3.54	117.42	111.23
31	Y	101	LMT	O1B-C4'-C3'	3.54	116.24	107.23
24	C	510	CLA	CED-O2D-CGD	3.54	123.95	115.92
24	B	604	CLA	C2B-C1B-NB	3.54	114.00	110.33
24	C	511	CLA	C3D-C2D-C1D	-3.54	101.00	105.83
31	B	622	LMT	O1B-C4'-C5'	-3.54	100.19	109.48
24	B	604	CLA	C2A-C1A-CHA	-3.54	117.73	123.87
24	b	604	CLA	C3D-C4D-ND	3.54	115.74	109.99
31	u	203	LMT	C3B-C4B-C5B	3.54	116.64	110.23
31	M	102	LMT	O1'-C1'-C2'	3.53	113.64	108.27
26	C	525	BCR	C32-C1-C6	-3.53	104.70	110.24
40	C	518	DGD	O3G-C3G-C2G	-3.53	102.22	110.82
24	b	611	CLA	C4C-C3C-C2C	-3.53	101.75	106.89
28	A	616	SQD	O48-C23-C24	3.53	122.59	111.83
24	c	506	CLA	C4B-C3B-C2B	-3.53	102.92	107.30
28	F	104	SQD	O8-S-C6	3.53	112.78	105.97
24	c	504	CLA	C4B-C3B-C2B	-3.53	102.92	107.30
26	B	619	BCR	C29-C28-C27	-3.53	103.52	111.28
24	c	507	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
41	E	113	HEM	C4B-C3B-C2B	-3.52	104.05	107.28
24	b	611	CLA	C3B-C4B-NB	3.52	113.67	110.53
24	b	611	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
24	b	606	CLA	C3D-C2D-C1D	-3.51	101.04	105.83
25	D	401	PHO	C2D-C1D-ND	3.51	111.97	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	C4D-C3D-CAD	-3.51	104.29	108.11
24	b	605	CLA	C4C-C3C-C2C	-3.51	101.78	106.89
24	b	615	CLA	C2B-C1B-NB	3.51	113.96	110.33
24	c	503	CLA	C2A-C1A-CHA	-3.50	117.79	123.87
24	B	617	CLA	C3D-C2D-C1D	-3.50	101.05	105.83
24	b	617	CLA	C3D-C2D-C1D	-3.50	101.06	105.83
24	B	610	CLA	CMD-C2D-C1D	3.50	130.89	124.73
24	b	603	CLA	CAC-C3C-C4C	3.49	129.34	124.79
31	J	103	LMT	O5B-C5B-C4B	3.49	115.99	109.70
24	B	609	CLA	O2D-CGD-CBD	3.49	117.33	111.23
24	B	610	CLA	CAC-C3C-C4C	3.48	129.32	124.79
32	B	632	LHG	O4-P-O5	3.48	128.63	112.44
24	b	606	CLA	C2B-C1B-NB	3.48	113.93	110.33
24	c	506	CLA	CED-O2D-CGD	3.47	123.80	115.92
24	c	504	CLA	C3D-C4D-ND	3.47	115.63	109.99
26	b	619	BCR	C38-C26-C25	-3.47	120.70	124.48
24	b	611	CLA	O2A-CGA-O1A	-3.47	114.95	123.63
28	h	105	SQD	O47-C7-C8	3.47	118.98	111.48
24	b	606	CLA	C6-C5-C3	-3.47	105.02	113.47
24	d	405	CLA	CMB-C2B-C1B	3.47	130.70	125.42
24	B	605	CLA	C3B-C2B-C1B	-3.46	103.08	107.17
24	B	609	CLA	C4B-C3B-C2B	-3.46	103.00	107.30
41	e	107	HEM	O1D-CGD-CBD	-3.46	112.11	123.09
24	B	614	CLA	C4C-C3C-C2C	-3.46	101.85	106.89
24	c	512	CLA	O2A-CGA-CBA	3.46	122.39	111.83
27	A	611	PL9	C2-C3-C4	-3.46	114.12	118.78
24	d	404	CLA	CMC-C2C-C1C	3.46	130.44	125.03
32	A	618	LHG	O8-C23-C24	3.45	122.37	111.83
24	A	607	CLA	C1D-ND-C4D	-3.45	103.89	106.31
24	C	510	CLA	C4C-C3C-C2C	-3.45	101.87	106.89
24	C	503	CLA	C1D-ND-C4D	-3.45	103.89	106.31
29	J	101	LMG	O8-C28-O10	-3.45	115.01	123.63
24	d	405	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
24	a	407	CLA	CMD-C2D-C1D	3.44	130.79	124.73
24	C	511	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
24	C	505	CLA	C4B-C3B-C2B	-3.44	103.02	107.30
31	f	101	LMT	C1B-O5B-C5B	3.44	120.44	113.72
29	A	613	LMG	O1-C1-C2	3.44	113.50	108.27
31	t	103	LMT	C4B-C3B-C2B	3.44	116.87	110.83
24	C	501	CLA	C1D-ND-C4D	-3.44	103.90	106.31
24	a	408	CLA	CMC-C2C-C1C	3.43	130.40	125.03
26	C	515	BCR	C15-C16-C17	-3.43	116.50	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	v	202	HEC	CHB-C1B-NB	3.43	128.11	124.42
24	B	613	CLA	C2B-C1B-NB	3.43	113.88	110.33
24	C	502	CLA	O2D-CGD-O1D	-3.43	117.18	123.85
24	C	503	CLA	CAC-C3C-C4C	3.42	129.25	124.79
26	C	515	BCR	C2-C3-C4	3.42	118.79	111.28
24	b	608	CLA	CAC-C3C-C4C	3.42	129.23	124.79
27	a	412	PL9	C37-C38-C39	-3.41	119.81	127.62
24	D	404	CLA	CHD-C4C-C3C	-3.41	119.80	124.77
24	B	613	CLA	CHD-C4C-C3C	-3.41	119.80	124.77
24	b	614	CLA	C4C-C3C-C2C	-3.41	101.93	106.89
31	I	101	LMT	C2'-C3'-C4'	-3.41	101.94	109.68
24	d	403	CLA	C4-C3-C5	3.40	121.14	115.23
24	b	616	CLA	O2D-CGD-CBD	3.40	117.18	111.23
27	a	412	PL9	C2-C1-C6	3.40	123.04	119.00
31	b	622	LMT	O5'-C5'-C4'	3.40	116.76	109.72
24	C	506	CLA	CAC-C3C-C4C	3.40	129.22	124.79
24	b	615	CLA	CAC-C3C-C4C	3.40	129.22	124.79
26	b	619	BCR	C29-C28-C27	-3.40	103.80	111.28
24	a	408	CLA	C1C-C2C-C3C	-3.40	103.41	106.98
38	b	631	HTG	O5-C1-C2	-3.39	105.64	110.32
28	a	424	SQD	O5-C5-C4	3.39	115.81	109.70
25	d	401	PHO	C4B-NB-C1B	-3.39	103.87	108.82
24	C	512	CLA	C4C-C3C-C2C	-3.39	101.96	106.89
26	t	102	BCR	C36-C18-C19	3.39	123.26	118.09
28	h	105	SQD	O48-C46-C45	3.39	118.16	108.40
26	B	618	BCR	C8-C7-C6	-3.39	117.95	127.00
26	B	618	BCR	C16-C15-C14	-3.39	116.59	123.52
40	c	516	DGD	C3B-C2B-C1B	-3.38	101.31	113.69
28	b	633	SQD	O47-C45-C46	3.38	120.47	108.34
24	B	606	CLA	CMC-C2C-C1C	3.38	130.31	125.03
24	C	501	CLA	C3D-C4D-ND	3.38	115.48	109.99
24	D	403	CLA	CBC-CAC-C3C	-3.38	103.26	112.42
26	k	101	BCR	C38-C26-C25	-3.38	120.80	124.48
40	d	408	DGD	C1E-O6E-C5E	3.38	120.31	113.72
24	D	405	CLA	C2A-C1A-CHA	-3.37	118.02	123.87
26	D	406	BCR	C29-C30-C25	3.37	115.33	110.44
24	B	604	CLA	C3D-C4D-ND	3.36	115.45	109.99
24	d	405	CLA	CMC-C2C-C1C	3.36	130.29	125.03
24	D	404	CLA	C3B-C2B-C1B	-3.36	103.21	107.17
24	d	405	CLA	C2A-C1A-CHA	-3.36	118.04	123.87
38	a	418	HTG	C1-O5-C5	3.36	118.59	112.56
24	c	501	CLA	C4B-C3B-C2B	-3.36	103.13	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	a	417	SQD	O47-C7-C8	3.35	118.74	111.48
24	c	507	CLA	C2A-C1A-CHA	-3.35	118.06	123.87
28	A	616	SQD	C1-O5-C5	-3.35	107.18	113.72
28	A	612	SQD	O8-S-C6	3.35	112.44	105.97
26	C	525	BCR	C20-C21-C22	-3.35	122.58	127.28
24	B	617	CLA	O2A-CGA-CBA	3.35	122.03	111.83
24	b	614	CLA	C3D-C2D-C1D	-3.34	101.27	105.83
24	c	506	CLA	CHB-C1B-NB	-3.34	119.04	124.05
24	B	605	CLA	C1D-ND-C4D	-3.34	103.97	106.31
24	b	602	CLA	C3D-C4D-ND	3.34	115.41	109.99
24	C	510	CLA	C4D-C3D-CAD	-3.34	104.48	108.11
24	B	613	CLA	O2D-CGD-O1D	-3.34	117.36	123.85
24	c	509	CLA	C3D-C4D-ND	3.33	115.41	109.99
31	b	622	LMT	O5'-C1'-O1'	-3.33	102.17	110.04
24	a	408	CLA	C3B-C2B-C1B	-3.33	103.25	107.17
24	B	611	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
24	C	511	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
38	c	523	HTG	C1'-S1-C1	3.32	107.62	100.45
29	C	520	LMG	O8-C28-C29	3.32	121.95	111.83
40	D	408	DGD	O2G-C1B-O1B	-3.31	115.96	123.70
26	d	406	BCR	C32-C1-C6	3.31	115.44	110.24
38	c	522	HTG	O5-C1-C2	-3.31	105.75	110.32
24	C	507	CLA	O2A-CGA-O1A	-3.31	115.35	123.63
24	c	512	CLA	CHC-C1C-C2C	-3.31	117.55	126.95
28	F	104	SQD	O5-C1-C2	-3.31	103.58	110.37
24	b	609	CLA	C4B-C3B-C2B	-3.30	103.19	107.30
24	a	410	CLA	C4D-C3D-CAD	-3.30	104.52	108.11
24	a	408	CLA	C1D-ND-C4D	-3.30	104.00	106.31
24	a	410	CLA	C4C-C3C-C2C	-3.30	102.09	106.89
24	B	614	CLA	O2A-CGA-CBA	3.30	121.90	111.83
24	b	608	CLA	C3D-C2D-C1D	-3.30	101.33	105.83
24	b	609	CLA	CMD-C2D-C1D	3.30	130.54	124.73
38	h	101	HTG	O5-C1-S1	-3.29	100.89	109.94
28	F	104	SQD	O48-C23-C24	3.29	121.88	111.83
24	b	604	CLA	C4-C3-C5	3.29	120.94	115.23
38	B	623	HTG	C1-C2-C3	3.29	116.98	110.55
43	V	203	HEC	CHB-C1B-NB	3.29	127.96	124.42
38	C	532	HTG	C3-C4-C5	3.28	116.19	110.23
32	A	618	LHG	O8-C23-O10	-3.28	115.42	123.63
24	d	405	CLA	C3D-C4D-ND	3.28	115.32	109.99
26	t	102	BCR	C37-C22-C23	3.28	123.10	118.09
26	t	102	BCR	C23-C22-C21	-3.28	113.85	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	H	102	BCR	C37-C22-C23	3.28	123.10	118.09
24	A	606	CLA	C3D-C2D-C1D	-3.28	101.36	105.83
26	C	515	BCR	C24-C23-C22	-3.28	121.39	126.23
28	a	424	SQD	O48-C23-O10	-3.28	115.44	123.63
24	c	502	CLA	C3D-C2D-C1D	-3.27	101.36	105.83
26	h	103	BCR	C30-C25-C26	-3.27	118.16	122.64
29	C	520	LMG	O7-C10-C11	3.27	118.56	111.48
24	b	602	CLA	CHB-C4A-NA	3.26	129.11	124.40
40	d	408	DGD	O2G-C1B-O1B	-3.26	116.07	123.70
40	h	104	DGD	O2G-C1B-C2B	3.26	118.54	111.48
24	c	509	CLA	CMB-C2B-C1B	3.26	130.39	125.42
24	c	509	CLA	C16-C15-C13	-3.26	105.12	115.97
24	C	506	CLA	C3B-C4B-NB	3.26	113.44	110.53
24	A	606	CLA	C1C-C2C-C3C	-3.26	103.55	106.98
24	b	612	CLA	C1-C2-C3	-3.26	120.86	126.20
38	a	418	HTG	O2-C2-C3	3.26	118.05	110.38
29	C	520	LMG	C4-C3-C2	3.25	116.54	110.83
24	d	403	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
38	V	204	HTG	O2-C2-C1	3.25	116.08	110.30
26	K	101	BCR	C39-C30-C25	-3.25	105.14	110.24
24	c	510	CLA	C3D-C4D-ND	3.25	115.27	109.99
26	b	619	BCR	C30-C25-C26	-3.25	118.19	122.64
24	D	403	CLA	C3D-C2D-C1D	-3.25	101.40	105.83
24	C	503	CLA	C2A-C1A-CHA	-3.25	118.23	123.87
32	D	409	LHG	O7-C7-O9	-3.25	116.11	123.70
26	T	102	BCR	C19-C18-C17	-3.25	113.90	119.01
24	c	505	CLA	CMC-C2C-C1C	3.24	130.10	125.03
24	b	607	CLA	CHC-C1C-C2C	-3.24	117.73	126.95
26	C	514	BCR	C8-C7-C6	-3.24	118.35	127.00
24	C	512	CLA	C2A-C1A-CHA	-3.23	118.26	123.87
26	t	102	BCR	C15-C16-C17	-3.23	116.91	123.52
24	b	606	CLA	C2A-C1A-CHA	-3.22	118.27	123.87
24	c	501	CLA	CBC-CAC-C3C	-3.22	103.69	112.42
26	c	515	BCR	C38-C26-C25	-3.22	120.97	124.48
24	B	611	CLA	CED-O2D-CGD	3.22	123.22	115.92
24	b	604	CLA	C2B-C1B-NB	3.22	113.66	110.33
24	B	617	CLA	C4C-C3C-C2C	-3.22	102.21	106.89
31	B	622	LMT	C3B-C4B-C5B	3.22	116.06	110.23
24	C	504	CLA	C4D-C3D-CAD	-3.21	104.62	108.11
24	c	512	CLA	C3D-C2D-C1D	-3.21	101.45	105.83
24	d	404	CLA	O2D-CGD-CBD	3.21	116.84	111.23
26	C	525	BCR	C37-C22-C23	3.21	122.99	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	e	107	HEM	CHA-C4D-ND	3.21	128.34	124.37
24	c	501	CLA	C3D-C2D-C1D	-3.21	101.45	105.83
24	B	614	CLA	C3D-C2D-C1D	-3.21	101.46	105.83
26	h	103	BCR	C7-C8-C9	-3.20	121.50	126.23
29	d	412	LMG	O7-C10-C11	3.20	118.41	111.48
24	c	511	CLA	CAA-C2A-C1A	3.20	122.47	111.97
24	c	509	CLA	CMC-C2C-C1C	3.20	130.04	125.03
24	A	609	CLA	OBD-CAD-C3D	-3.20	120.93	128.42
24	b	604	CLA	C4D-C3D-CAD	-3.20	104.63	108.11
26	B	620	BCR	C38-C26-C25	-3.20	120.99	124.48
24	C	503	CLA	C1C-C2C-C3C	-3.20	103.62	106.98
24	C	508	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
24	a	410	CLA	C2A-C1A-CHA	-3.20	118.32	123.87
24	b	612	CLA	CBC-CAC-C3C	-3.19	103.76	112.42
24	B	613	CLA	C3B-C2B-C1B	-3.19	103.41	107.17
29	c	520	LMG	O7-C10-C11	3.19	118.39	111.48
24	c	508	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
24	a	407	CLA	C3D-C4D-ND	3.19	115.17	109.99
24	A	606	CLA	C4C-C3C-C2C	-3.19	102.25	106.89
28	x	101	SQD	C3-C4-C5	3.19	116.01	110.23
24	C	508	CLA	C2A-C1A-CHA	-3.19	118.33	123.87
24	b	613	CLA	C4D-CHA-C1A	-3.19	117.44	121.24
38	C	529	HTG	C1-O5-C5	3.19	118.28	112.56
28	h	105	SQD	O6-C1-C2	3.19	113.11	108.27
24	C	508	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
24	b	609	CLA	O2D-CGD-CBD	3.19	116.80	111.23
26	H	102	BCR	C29-C28-C27	-3.18	104.28	111.28
24	b	603	CLA	O2A-CGA-O1A	-3.18	115.67	123.63
24	B	614	CLA	CHD-C4C-C3C	-3.18	120.13	124.77
24	B	607	CLA	C3D-C4D-ND	3.18	115.16	109.99
31	Y	101	LMT	O1B-C1B-C2B	3.18	115.92	108.09
24	D	404	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
24	c	507	CLA	C3D-C4D-ND	3.18	115.16	109.99
41	E	113	HEM	CBD-CAD-C3D	-3.18	103.74	112.53
29	a	414	LMG	C7-O1-C1	-3.18	106.98	113.80
25	A	608	PHO	C4D-CHA-CBD	-3.18	106.93	108.45
28	A	612	SQD	O2-C2-C1	3.18	117.65	110.08
24	C	510	CLA	C1C-C2C-C3C	-3.18	103.64	106.98
24	B	603	CLA	C4-C3-C5	3.18	120.75	115.23
31	F	102	LMT	C1B-O5B-C5B	3.18	119.92	113.72
24	B	605	CLA	C7-C6-C5	-3.17	104.80	113.26
24	D	404	CLA	C3D-C2D-C1D	-3.17	101.50	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	c	519	LMG	O8-C28-O10	-3.17	115.69	123.63
24	b	607	CLA	C3B-C4B-NB	3.17	113.36	110.53
31	F	102	LMT	O5'-C5'-C6'	3.17	114.29	106.44
24	A	607	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
28	A	612	SQD	O47-C7-O49	-3.17	116.30	123.70
26	B	619	BCR	C39-C30-C25	3.17	115.21	110.24
29	C	519	LMG	O8-C28-O10	-3.17	115.71	123.63
24	B	604	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
40	h	104	DGD	C3E-C4E-C5E	-3.16	104.50	110.23
24	d	404	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
29	B	634	LMG	O8-C28-C29	3.16	121.47	111.83
24	C	509	CLA	CMD-C2D-C3D	-3.16	120.44	127.69
24	b	607	CLA	O2A-CGA-O1A	-3.16	115.73	123.63
24	c	512	CLA	CMC-C2C-C1C	3.16	129.97	125.03
24	B	609	CLA	CMC-C2C-C1C	3.16	129.97	125.03
26	H	102	BCR	C40-C30-C25	-3.16	105.29	110.24
41	E	113	HEM	O2A-CGA-CBA	3.16	123.97	114.00
24	b	613	CLA	C4B-C3B-C2B	-3.15	103.38	107.30
38	b	632	HTG	C1-O5-C5	3.15	118.22	112.56
29	c	520	LMG	O8-C28-C29	3.15	121.43	111.83
24	b	607	CLA	C4D-CHA-C1A	-3.15	117.49	121.24
24	c	506	CLA	C1D-ND-C4D	-3.15	104.11	106.31
40	c	517	DGD	O1G-C1A-O1A	-3.15	115.76	123.63
41	E	113	HEM	C2D-C1D-ND	3.15	113.54	109.90
28	F	104	SQD	O8-S-O7	-3.15	103.53	111.40
24	b	612	CLA	C2A-C1A-CHA	-3.14	118.41	123.87
24	C	506	CLA	C4D-C3D-CAD	-3.14	104.69	108.11
26	t	102	BCR	C7-C8-C9	-3.14	121.58	126.23
24	C	506	CLA	C3D-C2D-C1D	-3.14	101.54	105.83
31	j	103	LMT	O1B-C1B-C2B	3.14	115.82	108.09
26	C	514	BCR	C30-C25-C26	-3.14	118.34	122.64
28	A	616	SQD	C44-O6-C1	3.14	120.53	113.80
26	H	102	BCR	C32-C1-C6	3.14	115.17	110.24
24	a	410	CLA	C1-C2-C3	-3.14	121.06	126.20
24	b	616	CLA	C2A-C1A-CHA	-3.14	118.42	123.87
24	A	607	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
24	b	613	CLA	C2A-C1A-CHA	-3.14	118.42	123.87
24	b	611	CLA	C1D-ND-C4D	-3.14	104.11	106.31
31	u	203	LMT	O1B-C1B-C2B	3.14	115.80	108.09
24	B	606	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
26	c	515	BCR	C37-C22-C23	3.13	122.87	118.09
41	E	113	HEM	O2D-CGD-O1D	-3.13	115.28	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	609	CLA	C3D-C4D-ND	3.13	115.08	109.99
38	b	624	HTG	O5-C1-C2	3.13	114.63	110.32
24	B	616	CLA	C3D-C2D-C1D	-3.13	101.56	105.83
24	D	404	CLA	CHB-C4A-NA	3.13	128.92	124.40
30	C	528	GOL	O3-C3-C2	3.13	124.46	110.38
40	H	103	DGD	O1G-C1A-O1A	-3.13	115.81	123.63
24	B	605	CLA	C3D-C2D-C1D	-3.13	101.57	105.83
38	B	624	HTG	C1-C2-C3	3.12	116.66	110.55
24	C	502	CLA	OBD-CAD-C3D	-3.12	121.12	128.42
26	H	102	BCR	C36-C18-C19	3.12	122.86	118.09
24	A	607	CLA	O2D-CGD-CBD	3.12	116.69	111.23
24	d	403	CLA	C1D-ND-C4D	-3.12	104.12	106.31
25	D	401	PHO	CMB-C2B-C3B	3.12	130.92	124.68
24	b	609	CLA	C4A-NA-C1A	-3.12	105.26	106.68
40	h	104	DGD	O1G-C1A-O1A	-3.12	115.83	123.63
24	c	511	CLA	O2D-CGD-CBD	3.12	116.68	111.23
26	A	610	BCR	C20-C21-C22	-3.11	122.91	127.28
29	c	519	LMG	O1-C7-C8	-3.11	103.24	110.82
24	C	512	CLA	C3D-C2D-C1D	-3.11	101.58	105.83
26	t	102	BCR	C35-C13-C12	3.11	122.84	118.09
24	B	616	CLA	C11-C10-C8	-3.11	105.62	115.97
24	c	506	CLA	C3D-C4D-ND	3.11	115.05	109.99
26	C	525	BCR	C38-C26-C25	-3.11	121.09	124.48
32	d	409	LHG	O7-C7-O9	-3.11	116.43	123.70
31	A	617	LMT	C1'-O5'-C5'	3.11	119.79	113.72
24	C	505	CLA	C1C-C2C-C3C	-3.11	103.71	106.98
24	c	509	CLA	C1C-C2C-C3C	-3.11	103.71	106.98
24	c	504	CLA	CHB-C1B-NB	-3.11	119.39	124.05
24	b	616	CLA	CHB-C4A-NA	3.10	128.88	124.40
24	b	606	CLA	CAC-C3C-C4C	3.10	128.83	124.79
30	C	523	GOL	C3-C2-C1	-3.10	100.41	111.80
24	B	612	CLA	C4D-C3D-CAD	-3.10	104.74	108.11
32	A	618	LHG	O8-C6-C5	3.10	117.33	108.40
40	d	408	DGD	O1G-C1A-C2A	3.10	121.28	111.83
24	c	508	CLA	CHD-C4C-C3C	-3.10	120.26	124.77
30	B	625	GOL	O2-C2-C3	-3.10	96.36	109.18
26	d	406	BCR	C1-C6-C5	-3.09	118.41	122.64
24	C	503	CLA	C3D-C2D-C1D	-3.09	101.61	105.83
24	b	607	CLA	O2D-CGD-CBD	3.09	116.64	111.23
38	b	632	HTG	C3-C4-C5	3.09	115.84	110.23
38	C	529	HTG	O5-C5-C6	3.09	114.10	106.44
24	B	614	CLA	O2A-CGA-O1A	-3.09	115.90	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	513	CLA	C2A-C1A-CHA	-3.09	118.51	123.87
24	B	609	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
24	C	508	CLA	O2D-CGD-CBD	3.09	116.63	111.23
24	b	617	CLA	C3D-C4D-ND	3.09	115.01	109.99
24	B	611	CLA	O2D-CGD-CBD	3.09	116.63	111.23
24	c	506	CLA	O2D-CGD-O1D	-3.09	117.84	123.85
31	M	101	LMT	C1'-O5'-C5'	-3.09	107.69	113.72
24	B	616	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
31	F	102	LMT	C1'-O5'-C5'	3.08	119.74	113.72
40	C	518	DGD	O1G-C1A-C2A	3.08	121.22	111.83
24	B	606	CLA	CMB-C2B-C1B	3.07	130.10	125.42
26	H	102	BCR	C20-C21-C22	-3.07	122.97	127.28
38	a	418	HTG	O3-C3-C4	-3.07	103.13	110.38
29	C	519	LMG	O10-C28-C29	-3.07	111.77	123.78
28	a	417	SQD	O48-C23-O10	-3.07	115.95	123.63
24	A	609	CLA	O2A-CGA-O1A	-3.07	115.95	123.63
40	D	408	DGD	O1G-C1A-C2A	3.07	121.19	111.83
24	c	501	CLA	C1D-ND-C4D	-3.07	104.16	106.31
28	a	424	SQD	O8-S-C6	3.07	111.89	105.97
38	B	630	HTG	C4-C3-C2	3.07	116.21	110.83
26	k	101	BCR	C23-C24-C25	-3.06	118.82	127.00
26	d	406	BCR	C28-C27-C26	-3.06	108.59	114.06
24	d	404	CLA	C4A-NA-C1A	-3.06	105.28	106.68
28	x	101	SQD	O5-C5-C4	3.06	115.22	109.70
24	a	410	CLA	C1D-ND-C4D	-3.06	104.16	106.31
25	d	401	PHO	C4D-ND-C1D	-3.06	105.20	108.87
24	B	610	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
24	c	508	CLA	C3B-C2B-C1B	-3.06	103.56	107.17
24	b	605	CLA	C4D-C3D-CAD	-3.06	104.78	108.11
24	b	605	CLA	C3D-C2D-C1D	-3.06	101.66	105.83
26	c	514	BCR	C20-C21-C22	-3.06	122.99	127.28
26	h	103	BCR	C29-C28-C27	-3.06	104.56	111.28
26	k	101	BCR	C29-C28-C27	3.06	117.99	111.28
24	A	606	CLA	C3B-C2B-C1B	-3.05	103.57	107.17
31	J	103	LMT	C3B-C4B-C5B	3.05	115.77	110.23
29	j	101	LMG	O7-C10-C11	3.05	118.08	111.48
28	A	612	SQD	O5-C1-C2	-3.05	104.10	110.37
24	c	512	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
24	B	615	CLA	C2A-C1A-CHA	-3.05	118.57	123.87
25	D	401	PHO	C4-C3-C5	3.05	120.52	115.23
25	d	401	PHO	C2D-C1D-ND	3.05	111.63	109.43
31	f	101	LMT	C1-O1'-C1'	3.04	118.88	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	t	102	BCR	C12-C13-C14	-3.04	114.22	119.01
24	C	510	CLA	C3D-C2D-C1D	-3.04	101.68	105.83
24	C	509	CLA	CMB-C2B-C1B	3.04	130.05	125.42
24	a	408	CLA	C2A-C1A-CHA	-3.04	118.59	123.87
38	c	523	HTG	O5-C1-C2	-3.04	106.12	110.32
32	B	632	LHG	O7-C7-C8	3.04	118.06	111.48
24	C	506	CLA	C2A-C1A-CHA	-3.04	118.59	123.87
24	C	513	CLA	C3B-C4B-NB	3.04	113.24	110.53
31	I	101	LMT	O3'-C3'-C4'	3.04	117.73	109.94
43	v	202	HEC	CHD-C1D-ND	3.04	128.13	124.37
24	B	616	CLA	C2A-C1A-CHA	-3.04	118.59	123.87
24	c	504	CLA	CHD-C4C-C3C	-3.04	120.34	124.77
24	B	613	CLA	C3D-C4D-ND	3.04	114.92	109.99
41	E	113	HEM	CHD-C1D-ND	3.04	127.69	124.42
24	c	511	CLA	C2A-C1A-CHA	-3.04	118.60	123.87
24	C	512	CLA	C1-O2A-CGA	3.03	123.99	116.65
24	c	509	CLA	C2A-C1A-CHA	-3.03	118.61	123.87
41	e	107	HEM	CBA-CAA-C2A	-3.03	104.16	112.53
31	M	101	LMT	O5'-C1'-O1'	-3.03	102.89	110.04
26	C	515	BCR	C36-C18-C19	3.03	122.72	118.09
24	d	404	CLA	CHD-C4C-C3C	-3.03	120.36	124.77
38	b	623	HTG	O5-C1-C2	3.02	114.49	110.32
24	C	511	CLA	CMC-C2C-C1C	3.02	129.76	125.03
32	e	101	LHG	O8-C23-C24	3.02	121.06	111.83
41	e	107	HEM	CHD-C1D-C2D	-3.02	120.25	125.03
24	B	605	CLA	O2D-CGD-CBD	3.02	116.52	111.23
24	D	404	CLA	O2D-CGD-CBD	3.02	116.52	111.23
24	b	612	CLA	C4D-C3D-CAD	-3.02	104.82	108.11
31	j	103	LMT	C1B-O1B-C4'	3.02	125.14	117.98
25	d	401	PHO	C1A-C2A-C3A	-3.02	99.97	102.84
24	d	405	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
24	c	504	CLA	C2A-C1A-CHA	-3.02	118.63	123.87
28	a	424	SQD	C46-O48-C23	3.02	128.15	117.12
24	B	615	CLA	C1-O2A-CGA	3.02	123.95	116.65
24	C	502	CLA	C3C-C4C-NC	3.01	114.29	110.43
24	C	507	CLA	CAC-C3C-C4C	3.01	128.71	124.79
24	b	602	CLA	OBD-CAD-C3D	-3.01	121.38	128.42
24	b	609	CLA	C2A-C1A-CHA	-3.01	118.64	123.87
38	B	631	HTG	C1'-S1-C1	3.01	106.95	100.45
26	B	618	BCR	C33-C5-C6	-3.01	121.20	124.48
31	M	101	LMT	O5'-C5'-C6'	3.01	113.89	106.44
24	B	614	CLA	C1-C2-C3	-3.01	121.27	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	CMC-C2C-C1C	3.01	129.73	125.03
28	F	104	SQD	O4-C4-C3	-3.01	103.29	110.38
25	a	409	PHO	C4D-ND-C1D	-3.01	105.27	108.87
41	e	107	HEM	CHA-C4D-C3D	-3.00	119.69	125.23
24	b	611	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
26	T	102	BCR	C16-C17-C18	-3.00	123.07	127.28
24	B	615	CLA	C3D-C4D-ND	3.00	114.86	109.99
24	a	407	CLA	C4D-C3D-CAD	-3.00	104.85	108.11
26	b	620	BCR	C23-C24-C25	-3.00	118.99	127.00
24	b	614	CLA	CMC-C2C-C1C	3.00	129.72	125.03
24	B	603	CLA	C2B-C1B-NB	3.00	113.43	110.33
24	C	509	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
24	D	404	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
24	d	405	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
24	b	610	CLA	C2A-C1A-CHA	-2.99	118.68	123.87
24	C	513	CLA	OBD-CAD-C3D	-2.99	121.43	128.42
24	b	617	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
26	C	514	BCR	C11-C10-C9	-2.99	123.09	127.28
26	c	514	BCR	C39-C30-C25	-2.99	105.56	110.24
24	B	616	CLA	CAC-C3C-C4C	2.99	128.68	124.79
26	D	406	BCR	C30-C25-C26	-2.99	118.55	122.64
28	A	622	SQD	O48-C23-O10	-2.99	116.16	123.63
26	C	514	BCR	C31-C1-C6	-2.99	105.56	110.24
43	v	202	HEC	CHD-C4C-NC	2.98	129.27	123.86
26	h	103	BCR	C31-C1-C6	-2.98	105.56	110.24
43	v	202	HEC	CHC-C4B-NB	2.98	128.06	124.37
24	B	615	CLA	CAC-C3C-C4C	2.98	128.67	124.79
24	b	603	CLA	C1-C2-C3	-2.98	121.31	126.20
26	c	514	BCR	C37-C22-C23	2.98	122.64	118.09
27	A	611	PL9	C37-C38-C39	-2.98	120.80	127.62
28	A	622	SQD	O6-C1-C2	2.98	112.80	108.27
23	A	605	BCT	O2-C-O1	2.98	127.30	119.68
24	A	606	CLA	CMD-C2D-C1D	2.98	129.98	124.73
31	J	103	LMT	O3'-C3'-C4'	2.98	117.58	109.94
24	C	508	CLA	C3D-C2D-C1D	-2.98	101.77	105.83
24	b	603	CLA	C2A-C1A-CHA	-2.98	118.70	123.87
24	b	607	CLA	C4A-NA-C1A	2.97	108.04	106.68
31	J	103	LMT	C1-O1'-C1'	-2.97	108.60	113.68
29	b	621	LMG	C1-O6-C5	-2.97	107.92	113.72
24	C	501	CLA	CBC-CAC-C3C	-2.97	104.37	112.42
24	A	606	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
38	h	101	HTG	C2'-C1'-S1	-2.97	102.37	112.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	604	CLA	C2A-C1A-CHA	-2.97	118.72	123.87
27	A	611	PL9	C35-C34-C36	2.96	120.37	115.23
26	a	411	BCR	C28-C27-C26	-2.96	108.77	114.06
24	b	607	CLA	C4B-CHC-C1C	-2.96	119.28	126.25
24	b	611	CLA	C3D-C4D-ND	2.96	114.80	109.99
24	b	613	CLA	CMC-C2C-C1C	2.96	129.66	125.03
24	C	507	CLA	CBC-CAC-C3C	-2.96	104.39	112.42
24	C	504	CLA	C3C-C4C-NC	2.96	114.22	110.43
24	B	617	CLA	C3D-C4D-ND	2.96	114.80	109.99
24	C	501	CLA	C3D-C2D-C1D	-2.96	101.79	105.83
24	A	607	CLA	CMC-C2C-C1C	2.96	129.66	125.03
29	B	634	LMG	C3-C4-C5	2.96	115.60	110.23
26	A	610	BCR	C2-C1-C6	2.96	114.73	110.44
24	B	611	CLA	C14-C13-C15	-2.96	100.74	111.27
24	b	610	CLA	C4D-C3D-CAD	-2.96	104.90	108.11
31	F	102	LMT	C1-O1'-C1'	2.95	118.73	113.68
24	c	509	CLA	CED-O2D-CGD	2.95	122.61	115.92
26	B	620	BCR	C37-C22-C23	2.95	122.60	118.09
24	c	502	CLA	O2D-CGD-CBD	2.95	116.39	111.23
38	V	204	HTG	O5-C1-S1	2.95	118.04	109.94
24	b	615	CLA	CED-O2D-CGD	2.95	122.60	115.92
29	B	634	LMG	C7-O1-C1	2.95	120.12	113.80
24	B	608	CLA	C1-C2-C3	-2.95	121.37	126.20
31	m	102	LMT	C1B-C2B-C3B	2.95	116.21	110.01
24	b	616	CLA	CAC-C3C-C4C	2.95	128.62	124.79
26	c	515	BCR	C1-C6-C5	-2.95	118.61	122.64
24	B	605	CLA	C4B-C3B-C2B	-2.94	103.64	107.30
40	D	408	DGD	O3G-C3G-C2G	2.94	117.97	110.82
24	c	512	CLA	CHB-C1B-NB	-2.94	119.64	124.05
24	B	614	CLA	CMD-C2D-C3D	-2.94	120.95	127.69
24	a	407	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
24	D	405	CLA	C3D-C2D-C1D	-2.94	101.82	105.83
26	A	610	BCR	C24-C23-C22	-2.93	121.89	126.23
24	C	506	CLA	C3D-C4D-ND	2.93	114.75	109.99
24	c	505	CLA	CHD-C1D-ND	-2.93	120.67	124.80
25	a	409	PHO	C4D-CHA-CBD	-2.93	107.05	108.45
38	a	418	HTG	C3-C4-C5	2.93	115.55	110.23
26	C	515	BCR	C39-C30-C25	-2.93	105.65	110.24
24	c	503	CLA	O2A-CGA-O1A	-2.93	116.30	123.63
24	c	504	CLA	CHB-C4A-NA	2.93	128.63	124.40
24	b	609	CLA	C3D-C4D-ND	2.93	114.75	109.99
24	B	613	CLA	C1D-ND-C4D	-2.93	104.26	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	C	520	LMG	O1-C1-C2	2.93	112.72	108.27
26	k	101	BCR	C32-C1-C6	2.92	114.83	110.24
24	b	611	CLA	CMB-C2B-C1B	2.92	129.86	125.42
24	B	607	CLA	C4-C3-C5	2.92	120.30	115.23
40	D	408	DGD	O6D-C5D-C6D	2.92	112.48	106.69
28	A	616	SQD	O48-C23-O10	-2.92	116.33	123.63
30	c	525	GOL	O1-C1-C2	2.92	123.50	110.38
31	M	101	LMT	O1'-C1-C2	-2.91	99.48	109.37
24	B	617	CLA	C2A-C1A-CHA	-2.91	118.81	123.87
26	d	406	BCR	C38-C26-C27	2.91	119.80	113.60
31	Y	101	LMT	C3B-C4B-C5B	2.91	115.51	110.23
24	b	614	CLA	C3B-C2B-C1B	-2.91	103.74	107.17
24	B	606	CLA	C4D-C3D-CAD	-2.91	104.95	108.11
24	b	614	CLA	C3D-C4D-ND	2.90	114.71	109.99
28	b	633	SQD	O48-C23-O10	-2.90	116.37	123.63
24	a	410	CLA	C5-C3-C2	-2.90	114.65	121.17
31	m	102	LMT	O5B-C5B-C4B	2.90	114.92	109.70
24	C	507	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
24	b	604	CLA	CAC-C3C-C4C	2.90	128.56	124.79
26	c	515	BCR	C8-C7-C6	-2.90	119.26	127.00
28	A	612	SQD	O9-S-O7	-2.90	104.41	113.82
32	D	410	LHG	O8-C23-O10	-2.89	116.39	123.63
32	l	101	LHG	O8-C23-O10	-2.89	116.39	123.63
24	B	611	CLA	CHB-C4A-NA	2.89	128.57	124.40
23	a	406	BCT	O2-C-O1	2.89	127.07	119.68
31	c	521	LMT	C1B-O1B-C4'	2.89	124.83	117.98
31	M	101	LMT	C1B-C2B-C3B	2.89	116.09	110.01
24	A	609	CLA	C2A-C1A-CHA	-2.89	118.85	123.87
29	a	414	LMG	C8-O7-C10	-2.89	110.88	117.80
24	b	615	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
41	E	113	HEM	O2A-CGA-O1A	-2.89	115.91	123.33
26	B	619	BCR	C30-C25-C26	-2.88	118.69	122.64
24	c	510	CLA	C2A-C1A-CHA	-2.88	118.86	123.87
28	a	417	SQD	C1-C2-C3	-2.88	103.94	110.01
24	C	512	CLA	C1-C2-C3	-2.88	121.47	126.20
26	H	102	BCR	C31-C1-C6	-2.88	105.72	110.24
24	b	617	CLA	C2A-C1A-CHA	-2.88	118.86	123.87
24	c	505	CLA	C3D-C2D-C1D	-2.88	101.90	105.83
43	v	202	HEC	CBD-CAD-C3D	-2.88	104.57	112.53
25	a	409	PHO	CMA-C3A-C4A	-2.88	108.41	114.61
24	b	607	CLA	C3D-C2D-C1D	-2.88	101.90	105.83
24	B	610	CLA	C2A-C1A-CHA	-2.88	118.87	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	a	407	CLA	C3D-C2D-C1D	-2.88	101.91	105.83
24	B	611	CLA	O2A-CGA-O1A	-2.88	116.43	123.63
24	c	510	CLA	CMD-C2D-C1D	2.88	129.79	124.73
24	D	404	CLA	C4D-C3D-CAD	-2.88	104.98	108.11
40	C	516	DGD	C3G-C2G-C1G	-2.87	105.08	111.78
43	v	202	HEC	CHA-C4D-ND	2.87	127.51	124.42
24	c	513	CLA	C3B-C4B-NB	2.87	113.09	110.53
24	c	504	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
26	t	102	BCR	C24-C23-C22	-2.87	121.99	126.23
24	B	614	CLA	C2A-C1A-CHA	-2.87	118.89	123.87
38	B	624	HTG	O5-C1-C2	2.87	114.27	110.32
24	b	606	CLA	C3B-C2B-C1B	-2.87	103.79	107.17
24	B	614	CLA	CAC-C3C-C4C	2.86	128.52	124.79
24	B	602	CLA	C1-C2-C3	-2.86	121.51	126.20
26	h	103	BCR	C24-C23-C22	-2.86	122.00	126.23
26	h	103	BCR	C2-C1-C6	2.86	114.59	110.44
24	c	510	CLA	C4D-C3D-CAD	-2.86	105.00	108.11
24	C	507	CLA	CMB-C2B-C1B	2.86	129.77	125.42
24	B	616	CLA	CHB-C1B-NB	-2.86	119.77	124.05
31	M	101	LMT	C1-O1'-C1'	2.86	118.56	113.68
24	d	403	CLA	C3D-C2D-C1D	-2.85	101.94	105.83
24	c	505	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
24	B	613	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
24	C	512	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
28	a	424	SQD	O6-C44-C45	2.85	117.75	110.82
29	c	519	LMG	O7-C10-O9	-2.85	117.05	123.70
24	C	513	CLA	C3D-C4D-ND	2.85	114.61	109.99
26	K	101	BCR	C38-C26-C25	-2.85	121.38	124.48
31	M	101	LMT	O4'-C4B-C3B	2.85	117.08	110.38
24	c	507	CLA	O2A-CGA-O1A	-2.84	116.51	123.63
24	b	606	CLA	CHD-C1D-ND	-2.84	120.81	124.80
31	u	203	LMT	O1B-C1B-O5B	-2.84	103.22	110.69
24	b	608	CLA	CMC-C2C-C1C	2.84	129.47	125.03
24	B	608	CLA	C2A-C1A-CHA	-2.84	118.94	123.87
26	b	618	BCR	C15-C16-C17	-2.84	117.71	123.52
26	A	610	BCR	C37-C22-C23	2.84	122.42	118.09
24	C	511	CLA	C3D-C4D-ND	2.84	114.60	109.99
43	v	202	HEC	C3C-C4C-NC	-2.84	107.00	110.15
29	C	519	LMG	O8-C9-C8	2.84	116.57	108.40
24	C	502	CLA	C1-C2-C3	-2.84	121.55	126.20
26	h	103	BCR	C36-C18-C19	2.83	122.42	118.09
33	V	209	PG4	C7-O4-C6	2.83	125.66	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	403	CLA	CHC-C1C-C2C	-2.83	118.89	126.95
26	b	618	BCR	C16-C17-C18	-2.83	123.31	127.28
24	c	510	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
24	b	615	CLA	C3D-C2D-C1D	-2.82	101.98	105.83
26	k	101	BCR	C37-C22-C23	2.82	122.40	118.09
24	a	407	CLA	C1D-CHD-C4C	-2.82	120.02	126.02
26	b	619	BCR	C37-C22-C21	-2.82	118.25	122.82
31	M	101	LMT	C3'-C4'-C5'	-2.82	104.68	110.93
24	b	607	CLA	C1-C2-C3	-2.82	121.58	126.20
24	B	610	CLA	C3D-C4D-ND	2.82	114.57	109.99
24	c	506	CLA	C2A-C1A-CHA	-2.82	118.98	123.87
24	b	617	CLA	C1D-ND-C4D	-2.82	104.33	106.31
32	l	101	LHG	O7-C7-C8	2.82	117.58	111.48
24	B	611	CLA	OBD-CAD-C3D	-2.82	121.83	128.42
26	k	101	BCR	C20-C21-C22	-2.82	123.33	127.28
24	B	607	CLA	C2A-C1A-CHA	-2.82	118.98	123.87
24	B	606	CLA	C6-C5-C3	-2.82	106.61	113.47
38	C	532	HTG	O5-C5-C4	2.82	114.77	109.70
24	B	602	CLA	C2A-C1A-CHA	-2.82	118.98	123.87
24	b	609	CLA	OBD-CAD-C3D	-2.82	121.83	128.42
26	C	514	BCR	C39-C30-C25	-2.81	105.83	110.24
24	c	503	CLA	C4D-C3D-CAD	-2.81	105.05	108.11
24	c	502	CLA	CMB-C2B-C1B	2.81	129.70	125.42
24	B	604	CLA	C1D-ND-C4D	-2.81	104.34	106.31
24	C	504	CLA	C1D-ND-C4D	-2.81	104.34	106.31
24	A	607	CLA	C4D-C3D-CAD	-2.81	105.05	108.11
24	C	511	CLA	CAC-C3C-C4C	2.81	128.45	124.79
24	B	608	CLA	O1D-CGD-CBD	-2.81	118.97	124.52
40	h	104	DGD	O4E-C4E-C5E	2.81	116.24	109.32
32	d	410	LHG	O8-C23-C24	2.81	120.39	111.83
24	a	408	CLA	C3D-C2D-C1D	-2.81	102.00	105.83
25	D	401	PHO	OBD-CAD-C3D	-2.80	123.52	127.89
24	A	609	CLA	C3D-C2D-C1D	-2.80	102.01	105.83
24	A	606	CLA	C2A-C1A-CHA	-2.80	119.00	123.87
28	F	104	SQD	O7-S-C6	2.80	110.94	106.76
24	b	612	CLA	CMD-C2D-C1D	2.80	129.66	124.73
24	B	613	CLA	C4D-C3D-CAD	-2.80	105.07	108.11
32	d	409	LHG	C6-O8-C23	2.80	127.35	117.12
24	b	611	CLA	C1-C2-C3	-2.80	121.61	126.20
24	B	605	CLA	CAC-C3C-C4C	2.80	128.43	124.79
24	b	612	CLA	CAC-C3C-C4C	2.80	128.43	124.79
24	B	610	CLA	C4B-C3B-C2B	-2.80	103.83	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	513	CLA	O2A-CGA-CBA	2.80	120.36	111.83
24	B	613	CLA	CMD-C2D-C1D	2.79	129.65	124.73
38	c	522	HTG	O2-C2-C1	-2.79	105.33	110.30
24	b	616	CLA	C1D-ND-C4D	-2.79	104.35	106.31
28	a	413	SQD	O47-C7-O49	-2.79	117.17	123.70
26	a	411	BCR	C23-C24-C25	-2.79	119.54	127.00
26	T	102	BCR	C39-C30-C25	-2.79	105.87	110.24
24	b	604	CLA	CHD-C1D-ND	-2.79	120.88	124.80
28	h	105	SQD	O48-C23-C24	2.79	120.33	111.83
28	A	622	SQD	O5-C5-C4	2.79	114.72	109.70
24	c	506	CLA	CHB-C4A-NA	2.79	128.42	124.40
32	D	409	LHG	C6-O8-C23	2.79	127.30	117.12
31	M	101	LMT	C1B-O1B-C4'	2.79	124.58	117.98
24	b	604	CLA	C3D-C2D-C1D	-2.79	102.03	105.83
24	B	612	CLA	CHC-C1C-C2C	-2.78	119.03	126.95
24	a	408	CLA	C4D-C3D-CAD	-2.78	105.08	108.11
41	e	107	HEM	CHC-C4B-NB	2.78	127.42	124.42
28	h	105	SQD	O9-S-C6	2.78	110.91	106.76
24	c	512	CLA	C1-O2A-CGA	2.78	123.38	116.65
38	C	530	HTG	O5-C5-C6	2.78	113.33	106.44
24	c	510	CLA	CMB-C2B-C1B	2.78	129.65	125.42
24	A	607	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
31	c	521	LMT	O3'-C3'-C4'	2.78	117.05	109.94
24	b	616	CLA	CMB-C2B-C3B	2.78	133.08	126.55
24	D	405	CLA	CHB-C1B-NB	-2.77	119.89	124.05
24	C	504	CLA	CMB-C2B-C1B	2.77	129.64	125.42
24	D	404	CLA	CMC-C2C-C1C	2.77	129.36	125.03
38	h	101	HTG	O2-C2-C1	2.77	115.22	110.30
24	b	617	CLA	C4D-C3D-CAD	-2.77	105.10	108.11
24	c	513	CLA	C3D-C2D-C1D	-2.77	102.05	105.83
24	B	602	CLA	C6-C5-C3	2.77	120.21	113.47
24	c	512	CLA	CMB-C2B-C1B	2.77	129.63	125.42
24	C	508	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
24	b	612	CLA	C4B-C3B-C2B	-2.76	103.86	107.30
24	b	615	CLA	O2A-CGA-CBA	2.76	120.26	111.83
24	B	610	CLA	C4C-C3C-C2C	-2.76	102.87	106.89
24	b	616	CLA	C6-C5-C3	-2.76	106.74	113.47
24	C	504	CLA	C7-C6-C5	-2.76	105.90	113.26
26	B	618	BCR	C24-C23-C22	-2.76	122.15	126.23
24	B	605	CLA	CHD-C4C-C3C	-2.76	120.75	124.77
24	D	403	CLA	C3D-C4D-ND	2.76	114.47	109.99
24	c	512	CLA	CHB-C4A-NA	2.76	128.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	503	CLA	C3D-C4D-ND	2.76	114.47	109.99
24	d	403	CLA	C3D-C4D-ND	2.76	114.47	109.99
29	C	526	LMG	O3-C3-C4	2.76	116.88	110.38
24	d	403	CLA	C4A-NA-C1A	2.76	107.94	106.68
24	B	609	CLA	C3D-C4D-ND	2.76	114.47	109.99
24	b	603	CLA	CHB-C4A-NA	2.76	128.38	124.40
24	C	502	CLA	O2D-CGD-CBD	2.76	116.05	111.23
24	c	501	CLA	C3D-C4D-ND	2.76	114.47	109.99
25	A	608	PHO	C1A-C2A-C3A	-2.76	100.22	102.84
24	B	602	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
38	b	631	HTG	O3-C3-C2	-2.75	103.89	110.38
24	b	605	CLA	CAA-C2A-C1A	2.75	121.00	111.97
24	B	612	CLA	C3D-C4D-ND	2.75	114.46	109.99
24	B	606	CLA	CHB-C4A-NA	2.75	128.37	124.40
24	b	604	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
24	c	505	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	I	101	LMT	O1'-C1'-C2'	2.75	112.44	108.27
24	C	506	CLA	C1D-ND-C4D	-2.74	104.39	106.31
26	A	610	BCR	C8-C7-C6	-2.74	119.68	127.00
24	A	609	CLA	CMC-C2C-C1C	2.74	129.32	125.03
24	B	612	CLA	C1-C2-C3	-2.74	121.71	126.20
27	D	407	PL9	C35-C34-C36	2.74	119.98	115.23
24	b	611	CLA	C2A-C1A-CHA	-2.74	119.11	123.87
40	C	516	DGD	C4E-C3E-C2E	-2.74	106.02	110.83
24	C	511	CLA	CMB-C2B-C1B	2.74	129.59	125.42
24	c	512	CLA	C3D-C4D-ND	2.74	114.44	109.99
24	C	509	CLA	C2A-C1A-CHA	-2.74	119.12	123.87
24	b	616	CLA	C3D-C4D-ND	2.74	114.44	109.99
24	C	504	CLA	CHC-C1C-C2C	-2.74	119.17	126.95
24	B	615	CLA	O2A-CGA-CBA	2.74	120.18	111.83
26	H	102	BCR	C38-C26-C25	-2.74	121.50	124.48
24	B	615	CLA	C4B-C3B-C2B	-2.73	103.90	107.30
24	b	603	CLA	CMC-C2C-C1C	2.73	129.31	125.03
24	c	502	CLA	CHC-C1C-C2C	-2.73	119.18	126.95
24	D	405	CLA	CHB-C4A-NA	2.73	128.34	124.40
24	B	606	CLA	CAA-C2A-C1A	2.73	120.92	111.97
25	d	401	PHO	CBC-CAC-C3C	2.73	116.78	112.87
24	C	501	CLA	CMB-C2B-C1B	2.73	129.58	125.42
24	b	602	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
24	B	603	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
24	C	505	CLA	C4D-CHA-C1A	-2.73	117.99	121.24
24	B	605	CLA	C4-C3-C5	-2.73	110.49	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	512	CLA	O1D-CGD-CBD	-2.73	119.14	124.52
24	C	507	CLA	C3D-C2D-C1D	-2.73	102.11	105.83
24	b	617	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
24	b	615	CLA	C2A-C1A-CHA	-2.72	119.14	123.87
24	b	606	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
24	B	609	CLA	CHB-C1B-NB	-2.72	119.97	124.05
31	B	622	LMT	C1-O1'-C1'	-2.72	109.04	113.68
24	c	506	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
29	C	519	LMG	O1-C7-C8	-2.72	104.21	110.82
24	B	606	CLA	C4-C3-C5	-2.71	110.52	115.23
24	b	610	CLA	C4B-C3B-C2B	-2.71	103.93	107.30
24	A	606	CLA	C3D-C4D-ND	2.71	114.40	109.99
40	H	103	DGD	C3E-C4E-C5E	-2.71	105.31	110.23
24	C	509	CLA	O2A-CGA-O1A	-2.71	116.84	123.63
26	A	610	BCR	C39-C30-C25	-2.71	105.99	110.24
40	h	104	DGD	O1G-C1A-C2A	2.71	120.10	111.83
24	B	609	CLA	C4-C3-C5	2.71	119.93	115.23
26	t	102	BCR	C11-C10-C9	-2.71	123.48	127.28
26	K	101	BCR	C37-C22-C21	-2.71	118.43	122.82
43	v	202	HEC	C4C-CHD-C1D	-2.71	119.88	126.25
24	c	508	CLA	O2D-CGD-CBD	2.71	115.97	111.23
41	E	113	HEM	CBA-CAA-C2A	-2.71	105.05	112.53
24	b	613	CLA	C3D-C4D-ND	2.71	114.39	109.99
28	A	612	SQD	O7-S-C6	-2.70	102.72	106.76
24	b	608	CLA	C2A-C1A-CHA	-2.70	119.17	123.87
29	C	526	LMG	O6-C5-C4	2.70	114.57	109.70
24	C	511	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
23	a	406	BCT	O3-C-O1	-2.70	112.76	119.68
26	B	619	BCR	C37-C22-C23	2.70	122.22	118.09
32	A	618	LHG	O7-C7-C8	2.70	117.33	111.48
24	B	608	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
31	c	521	LMT	C2'-C3'-C4'	-2.70	103.55	109.68
38	b	632	HTG	O5-C5-C6	2.70	113.13	106.44
24	A	606	CLA	C4-C3-C5	2.70	119.91	115.23
24	c	512	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
24	B	612	CLA	O2D-CGD-CBD	2.70	115.95	111.23
24	B	615	CLA	C4C-C3C-C2C	-2.70	102.96	106.89
24	b	608	CLA	CHD-C4C-C3C	-2.70	120.84	124.77
24	b	607	CLA	C3D-C4D-ND	2.70	114.37	109.99
24	B	608	CLA	CAC-C3C-C4C	2.70	128.30	124.79
24	b	614	CLA	C7-C6-C5	-2.70	106.08	113.26
24	C	503	CLA	CAA-C2A-C1A	2.69	120.80	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	509	CLA	C3D-C4D-ND	2.69	114.36	109.99
31	I	101	LMT	O3B-C3B-C2B	-2.69	104.04	110.38
25	D	401	PHO	C4D-ND-C1D	-2.69	105.65	108.87
24	c	504	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
29	a	414	LMG	C4-C3-C2	2.68	115.54	110.83
28	l	102	SQD	C1-C2-C3	-2.68	104.36	110.01
24	C	509	CLA	CHC-C1C-C2C	-2.68	119.32	126.95
24	B	602	CLA	C3D-C4D-ND	2.68	114.35	109.99
25	A	608	PHO	C1-C2-C3	-2.68	121.80	126.20
24	d	403	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
24	C	501	CLA	C4D-C3D-CAD	-2.68	105.19	108.11
24	b	607	CLA	C4D-C3D-CAD	-2.68	105.19	108.11
24	b	612	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
24	a	410	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
27	d	407	PL9	C10-C9-C11	2.68	119.88	115.23
43	v	202	HEC	CHA-C4D-C3D	-2.68	120.87	124.77
24	B	617	CLA	C4A-NA-C1A	-2.68	105.46	106.68
43	V	203	HEC	CBD-CAD-C3D	-2.68	105.13	112.53
24	c	501	CLA	CHB-C1B-NB	-2.68	120.03	124.05
24	c	511	CLA	CHB-C4A-NA	2.68	128.26	124.40
24	b	606	CLA	C4A-NA-C1A	-2.68	105.46	106.68
29	z	101	LMG	C1-C2-C3	-2.68	104.38	110.01
24	B	611	CLA	C20-C18-C19	-2.68	98.59	110.53
24	a	408	CLA	C4-C3-C5	2.68	119.87	115.23
26	c	514	BCR	C31-C1-C6	-2.68	106.05	110.24
32	l	101	LHG	O8-C6-C5	2.67	116.11	108.40
25	d	401	PHO	O2A-CGA-O1A	-2.67	116.94	123.63
38	C	529	HTG	O5-C1-C2	-2.67	106.63	110.32
40	H	103	DGD	O5E-C6E-C5E	-2.67	102.23	111.33
40	D	408	DGD	O5D-C6D-C5D	2.67	115.44	109.42
24	a	407	CLA	C4C-C3C-C2C	-2.67	103.01	106.89
24	c	509	CLA	CHB-C4A-NA	2.67	128.25	124.40
28	F	104	SQD	C1-C2-C3	-2.67	104.39	110.01
26	A	610	BCR	C11-C10-C9	-2.67	123.54	127.28
26	H	102	BCR	C16-C17-C18	-2.67	123.54	127.28
31	J	103	LMT	O1'-C1'-C2'	2.67	112.32	108.27
24	D	404	CLA	C3D-C4D-ND	2.67	114.32	109.99
24	b	608	CLA	C3D-C4D-ND	2.67	114.32	109.99
24	C	503	CLA	O2D-CGD-CBD	2.67	115.89	111.23
24	c	513	CLA	CHB-C4A-NA	2.67	128.25	124.40
24	B	614	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
24	b	616	CLA	C1D-CHD-C4C	-2.66	120.36	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	611	CLA	C4D-C3D-CAD	-2.66	105.21	108.11
24	B	612	CLA	C4C-C3C-C2C	-2.66	103.01	106.89
31	t	103	LMT	O5B-C5B-C4B	2.66	114.50	109.70
24	b	609	CLA	CAC-C3C-C4C	2.66	128.25	124.79
38	a	418	HTG	C1-C2-C3	-2.66	105.34	110.55
24	A	607	CLA	C4A-NA-C1A	2.66	107.89	106.68
24	C	512	CLA	CHB-C4A-NA	2.66	128.24	124.40
24	c	513	CLA	CMD-C2D-C3D	-2.66	121.59	127.69
26	H	102	BCR	C16-C15-C14	-2.66	118.08	123.52
24	B	606	CLA	C4A-NA-C1A	2.66	107.89	106.68
24	A	609	CLA	C4D-CHA-C1A	-2.66	118.07	121.24
24	B	615	CLA	C1D-CHD-C4C	-2.66	120.37	126.02
24	b	609	CLA	C4D-C3D-CAD	-2.66	105.22	108.11
24	C	510	CLA	O2A-CGA-O1A	-2.66	116.99	123.63
26	t	102	BCR	C28-C27-C26	-2.65	109.32	114.06
24	C	512	CLA	C4B-C3B-C2B	-2.65	104.00	107.30
24	D	405	CLA	CHC-C1C-C2C	-2.65	119.41	126.95
24	C	510	CLA	C1D-ND-C4D	-2.65	104.45	106.31
26	h	103	BCR	C11-C10-C9	-2.65	123.56	127.28
24	b	610	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
24	c	506	CLA	CAC-C3C-C4C	2.65	128.24	124.79
38	b	623	HTG	C2'-C1'-S1	2.65	121.27	112.36
24	c	507	CLA	CHB-C1B-NB	-2.65	120.08	124.05
27	d	407	PL9	C20-C19-C21	2.65	119.82	115.23
24	b	606	CLA	C4D-C3D-CAD	-2.65	105.23	108.11
24	B	614	CLA	C3B-C4B-NB	2.64	112.89	110.53
26	a	411	BCR	C37-C22-C21	-2.64	118.53	122.82
24	C	509	CLA	OBD-CAD-C3D	-2.64	122.24	128.42
24	C	507	CLA	C3D-C4D-ND	2.64	114.28	109.99
24	B	602	CLA	C3D-C2D-C1D	-2.64	102.22	105.83
31	t	103	LMT	O5'-C1'-O1'	-2.64	103.80	110.04
24	c	512	CLA	CAC-C3C-C4C	2.64	128.23	124.79
27	A	611	PL9	C27-C28-C29	-2.64	121.58	127.62
38	H	101	HTG	C3-C4-C5	2.64	115.02	110.23
24	C	513	CLA	CMB-C2B-C3B	2.64	132.76	126.55
38	a	418	HTG	O2-C2-C1	2.64	114.98	110.30
26	t	102	BCR	C7-C6-C5	-2.64	115.48	121.56
24	c	501	CLA	CHC-C1C-C2C	-2.64	119.45	126.95
29	A	613	LMG	C3-C4-C5	2.64	115.01	110.23
24	B	608	CLA	C3D-C4D-ND	2.64	114.27	109.99
24	d	404	CLA	CHB-C4A-NA	2.63	128.20	124.40
38	c	523	HTG	O5-C5-C4	2.63	114.45	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	C	521	HTG	O5-C5-C6	2.63	112.97	106.44
24	B	614	CLA	C3D-C4D-ND	2.63	114.27	109.99
26	B	620	BCR	C2-C1-C6	2.63	114.26	110.44
24	b	609	CLA	CMB-C2B-C1B	2.63	129.43	125.42
24	a	407	CLA	C1D-ND-C4D	-2.63	104.47	106.31
24	c	506	CLA	C4D-CHA-C1A	-2.63	118.11	121.24
38	B	623	HTG	O4-C4-C5	2.63	115.80	109.32
38	c	530	HTG	C1'-S1-C1	2.63	106.12	100.45
31	M	101	LMT	C3B-C4B-C5B	-2.62	105.47	110.23
29	B	634	LMG	C30-C29-C28	2.62	123.31	113.69
24	C	510	CLA	C3D-C4D-ND	2.62	114.25	109.99
24	b	609	CLA	CMC-C2C-C1C	2.62	129.13	125.03
24	d	405	CLA	CHB-C1B-NB	-2.62	120.12	124.05
28	h	105	SQD	O3-C3-C4	2.62	116.55	110.38
27	D	407	PL9	C40-C39-C38	-2.62	116.91	123.63
24	B	608	CLA	C4B-C3B-C2B	-2.61	104.05	107.30
24	B	603	CLA	C16-C15-C13	-2.61	107.28	115.97
29	B	634	LMG	C4-C3-C2	2.61	115.42	110.83
24	C	513	CLA	C3D-C2D-C1D	-2.61	102.27	105.83
24	B	609	CLA	C4D-C3D-CAD	-2.61	105.27	108.11
24	b	606	CLA	C4-C3-C5	-2.61	110.70	115.23
24	a	408	CLA	C3A-C2A-C1A	-2.61	97.43	101.34
31	J	103	LMT	C1B-O1B-C4'	2.61	124.16	117.98
24	D	404	CLA	C2A-C3A-C4A	2.61	106.08	101.87
24	C	502	CLA	C2A-C1A-CHA	-2.61	119.34	123.87
40	C	518	DGD	C6B-C5B-C4B	-2.61	101.20	114.37
24	D	404	CLA	CHC-C1C-C2C	-2.61	119.54	126.95
40	C	516	DGD	C3D-C4D-C5D	-2.60	105.51	110.23
24	C	507	CLA	C1D-ND-C4D	-2.60	104.49	106.31
24	b	611	CLA	C14-C13-C15	-2.60	102.00	111.27
26	b	619	BCR	C16-C15-C14	-2.60	118.20	123.52
24	b	603	CLA	CED-O2D-CGD	2.60	121.81	115.92
24	B	604	CLA	CHC-C1C-NC	-2.59	120.40	124.31
38	b	623	HTG	C1-C2-C3	2.59	115.62	110.55
27	a	412	PL9	O2-C1-C2	-2.59	115.93	121.83
24	a	408	CLA	CHC-C1C-C2C	-2.59	119.58	126.95
24	b	612	CLA	C1D-CHD-C4C	-2.59	120.51	126.02
29	B	621	LMG	O8-C28-O10	-2.59	117.15	123.63
24	B	616	CLA	C1D-CHD-C4C	-2.59	120.52	126.02
24	C	509	CLA	C4C-C3C-C2C	-2.59	103.12	106.89
29	C	520	LMG	O3-C3-C4	-2.59	104.27	110.38
31	m	101	LMT	O2'-C2'-C1'	2.59	116.24	110.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	605	CLA	CAA-C2A-C1A	2.58	120.44	111.97
24	C	512	CLA	CMC-C2C-C1C	2.58	129.07	125.03
32	a	419	LHG	O7-C5-C4	2.58	117.61	108.34
24	a	410	CLA	CHB-C4A-NA	2.58	128.13	124.40
25	d	401	PHO	CMB-C2B-C3B	2.58	129.84	124.68
30	C	528	GOL	O1-C1-C2	-2.58	98.76	110.38
32	d	411	LHG	O8-C23-O10	-2.58	117.18	123.63
26	B	618	BCR	C20-C21-C22	-2.58	123.66	127.28
26	H	102	BCR	C37-C22-C21	-2.58	118.64	122.82
24	b	604	CLA	C4A-NA-C1A	-2.58	105.50	106.68
24	c	507	CLA	CMB-C2B-C1B	2.58	129.34	125.42
41	e	107	HEM	C4C-NC-C1C	2.58	110.02	105.82
24	d	403	CLA	C4D-C3D-CAD	-2.58	105.31	108.11
28	h	105	SQD	O2-C2-C1	2.57	116.21	110.08
24	C	509	CLA	O2A-CGA-CBA	2.57	119.69	111.83
26	B	618	BCR	C37-C22-C23	2.57	122.02	118.09
32	D	409	LHG	C11-C10-C9	-2.57	101.36	114.37
38	c	530	HTG	O5-C5-C4	2.57	114.34	109.70
38	b	623	HTG	O5-C5-C4	2.57	114.33	109.70
40	d	408	DGD	C3G-C2G-C1G	-2.57	105.80	111.78
28	l	102	SQD	O8-S-C6	2.57	110.93	105.97
24	C	502	CLA	C16-C17-C18	-2.57	104.48	115.94
24	b	606	CLA	C3D-C4D-ND	2.57	114.16	109.99
24	b	613	CLA	CED-O2D-CGD	2.57	121.73	115.92
27	a	412	PL9	C37-C36-C34	-2.57	104.68	113.19
28	a	424	SQD	O47-C45-C46	2.56	117.54	108.34
24	B	602	CLA	C4C-C3C-C2C	-2.56	103.16	106.89
29	B	634	LMG	O8-C28-O10	-2.56	117.22	123.63
24	B	611	CLA	C2A-C1A-CHA	-2.56	119.42	123.87
29	A	613	LMG	C7-O1-C1	-2.56	108.30	113.80
27	d	407	PL9	C50-C49-C48	-2.56	114.97	122.66
24	B	610	CLA	C3D-C2D-C1D	-2.56	102.33	105.83
28	b	633	SQD	C45-O47-C7	2.56	123.93	117.80
24	B	604	CLA	CMD-C2D-C1D	2.56	129.24	124.73
24	b	610	CLA	CED-O2D-CGD	2.56	121.72	115.92
24	d	405	CLA	C6-C7-C8	-2.56	107.46	115.97
40	c	518	DGD	O6E-C5E-C6E	2.56	112.78	106.44
26	H	102	BCR	C30-C25-C26	-2.56	119.14	122.64
24	C	501	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
25	a	409	PHO	C1A-C2A-C3A	-2.55	100.41	102.84
24	b	604	CLA	C7-C6-C5	-2.55	106.46	113.26
24	B	615	CLA	CHB-C1B-C2B	-2.55	120.02	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	H	103	DGD	O4E-C4E-C5E	2.55	115.61	109.32
25	a	409	PHO	CED-O2D-CGD	2.55	121.70	115.92
24	a	407	CLA	CMB-C2B-C1B	2.55	129.30	125.42
24	c	512	CLA	C2A-C1A-CHA	-2.55	119.44	123.87
29	z	101	LMG	O1-C7-C8	2.55	117.02	110.82
26	c	527	BCR	C20-C21-C22	-2.55	123.71	127.28
24	b	610	CLA	C6-C5-C3	2.55	119.67	113.47
40	d	408	DGD	O6D-C1D-C2D	-2.54	105.14	110.37
38	B	624	HTG	O5-C5-C4	-2.54	105.11	109.70
24	b	611	CLA	CAA-CBA-CGA	-2.54	105.98	113.21
24	b	614	CLA	O2A-CGA-CBA	2.54	119.58	111.83
24	d	403	CLA	CHB-C1B-NB	-2.54	120.24	124.05
26	b	618	BCR	C20-C21-C22	-2.54	123.72	127.28
31	J	103	LMT	O2'-C2'-C3'	-2.54	104.39	110.38
24	C	507	CLA	CMA-C3A-C4A	2.54	118.59	111.77
24	B	604	CLA	CAC-C3C-C4C	2.54	128.09	124.79
24	B	605	CLA	C4D-C3D-CAD	-2.54	105.35	108.11
29	z	101	LMG	C3-C4-C5	2.53	114.83	110.23
24	B	605	CLA	CMB-C2B-C1B	2.53	129.28	125.42
24	D	405	CLA	C1D-ND-C4D	-2.53	104.53	106.31
24	c	509	CLA	C1D-ND-C4D	-2.53	104.53	106.31
24	a	410	CLA	C4-C3-C5	2.53	119.62	115.23
40	h	104	DGD	O5D-C6D-C5D	-2.53	103.72	109.42
31	t	103	LMT	C1-O1'-C1'	2.53	118.00	113.68
24	b	608	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
24	B	608	CLA	O2D-CGD-CBD	2.53	115.65	111.23
24	c	513	CLA	O2A-CGA-CBA	2.53	119.55	111.83
24	B	611	CLA	CMB-C2B-C1B	2.53	129.27	125.42
24	d	403	CLA	C2A-C1A-CHA	-2.53	119.48	123.87
24	c	501	CLA	OBD-CAD-C3D	-2.53	122.51	128.42
26	H	102	BCR	C19-C18-C17	-2.53	115.03	119.01
24	B	602	CLA	O1A-CGA-CBA	-2.53	113.90	123.78
24	d	404	CLA	C3D-C4D-ND	2.53	114.09	109.99
26	C	525	BCR	C15-C16-C17	-2.53	118.35	123.52
24	B	608	CLA	CBC-CAC-C3C	-2.52	105.58	112.42
24	b	606	CLA	O2A-CGA-O1A	-2.52	117.31	123.63
29	B	634	LMG	O7-C10-O9	-2.52	117.81	123.70
24	b	615	CLA	C4D-CHA-C1A	-2.52	118.23	121.24
24	c	512	CLA	CBC-CAC-C3C	-2.52	105.59	112.42
28	x	101	SQD	O9-S-O7	-2.52	105.62	113.82
24	c	503	CLA	CED-O2D-CGD	2.52	121.63	115.92
24	B	613	CLA	C2A-C1A-CHA	-2.52	119.50	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	c	516	DGD	C1D-O6D-C5D	-2.52	108.80	113.72
26	T	102	BCR	C11-C12-C13	-2.52	119.46	126.36
24	b	606	CLA	OBD-CAD-C3D	-2.52	122.53	128.42
26	A	610	BCR	C15-C16-C17	-2.52	118.37	123.52
24	B	616	CLA	CHC-C1C-C2C	-2.52	119.80	126.95
28	h	105	SQD	O5-C1-C2	2.52	115.54	110.37
31	B	622	LMT	C6B-C5B-C4B	-2.51	106.84	113.02
24	B	612	CLA	O2D-CGD-O1D	-2.51	118.95	123.85
24	A	609	CLA	C4-C3-C5	2.51	119.59	115.23
31	I	101	LMT	C6B-C5B-C4B	2.51	119.19	113.02
27	A	611	PL9	C22-C21-C19	-2.51	104.86	113.19
24	B	617	CLA	CMC-C2C-C1C	2.51	128.96	125.03
26	c	527	BCR	C8-C7-C6	-2.51	120.29	127.00
31	A	617	LMT	O3B-C3B-C4B	2.51	116.29	110.38
27	a	412	PL9	C16-C14-C13	-2.51	115.53	121.17
40	c	518	DGD	C3A-C2A-C1A	-2.51	104.50	113.69
24	b	603	CLA	C4B-C3B-C2B	-2.51	104.18	107.30
24	C	511	CLA	C2A-C1A-CHA	-2.51	119.52	123.87
24	b	611	CLA	CHB-C4A-NA	2.50	128.01	124.40
26	B	619	BCR	C38-C26-C25	-2.50	121.75	124.48
40	C	516	DGD	C1D-O6D-C5D	-2.50	108.83	113.72
24	c	506	CLA	C1D-CHD-C4C	-2.50	120.70	126.02
35	d	415	P6G	O16-C17-C18	-2.50	99.08	110.11
24	C	508	CLA	C7-C6-C5	-2.50	106.59	113.26
24	B	609	CLA	CAC-C3C-C4C	2.50	128.05	124.79
25	a	409	PHO	CMC-C2C-C1C	2.50	129.24	124.73
24	C	512	CLA	OBD-CAD-C3D	-2.50	122.57	128.42
31	m	102	LMT	O1'-C1-C2	-2.50	100.88	109.37
26	C	515	BCR	C2-C1-C6	2.50	114.07	110.44
25	A	608	PHO	CMB-C2B-C3B	2.50	129.68	124.68
29	j	101	LMG	O8-C28-O10	-2.50	117.38	123.63
24	A	606	CLA	C4D-C3D-CAD	-2.50	105.39	108.11
24	B	604	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
24	d	404	CLA	C3B-C2B-C1B	-2.49	104.23	107.17
24	c	503	CLA	C1D-CHD-C4C	-2.49	120.72	126.02
26	B	620	BCR	C23-C22-C21	-2.49	115.09	119.01
24	c	508	CLA	C4C-C3C-C2C	-2.49	103.26	106.89
28	l	102	SQD	O9-S-O7	-2.49	105.72	113.82
26	c	514	BCR	C33-C5-C6	-2.49	121.77	124.48
29	B	621	LMG	C38-C37-C36	-2.49	101.78	114.37
24	C	511	CLA	C4B-C3B-C2B	-2.49	104.20	107.30
24	a	410	CLA	O2D-CGD-CBD	2.49	115.58	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c	522	HTG	C1'-S1-C1	2.49	105.82	100.45
24	b	617	CLA	CED-O2D-CGD	2.49	121.56	115.92
24	C	509	CLA	C4D-C3D-CAD	-2.49	105.41	108.11
26	T	102	BCR	C36-C18-C19	2.48	121.88	118.09
24	b	603	CLA	C1D-ND-C4D	-2.48	104.57	106.31
24	C	513	CLA	C5-C3-C2	-2.48	115.60	121.17
24	b	614	CLA	C17-C16-C15	-2.48	102.17	113.28
24	b	616	CLA	C11-C10-C8	-2.48	107.72	115.97
28	a	413	SQD	C45-O47-C7	-2.48	111.86	117.80
24	C	505	CLA	C3D-C4D-ND	2.48	114.01	109.99
24	b	616	CLA	C4D-C3D-CAD	-2.48	105.42	108.11
31	t	103	LMT	C1'-C2'-C3'	2.48	115.22	110.01
38	b	624	HTG	O4-C4-C3	2.47	116.21	110.38
24	C	501	CLA	CHC-C1C-C2C	-2.47	119.92	126.95
31	b	622	LMT	C3'-C4'-C5'	2.47	116.41	110.93
26	C	525	BCR	C16-C17-C18	-2.47	123.81	127.28
24	B	610	CLA	CED-O2D-CGD	2.47	121.52	115.92
38	b	632	HTG	C1'-S1-C1	2.47	105.78	100.45
26	C	514	BCR	C29-C30-C25	2.47	114.02	110.44
24	c	502	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
26	b	619	BCR	C8-C9-C10	-2.47	115.13	119.01
24	B	603	CLA	CAC-C3C-C4C	2.47	128.00	124.79
24	C	510	CLA	C2A-C1A-CHA	-2.47	119.59	123.87
28	a	417	SQD	O6-C1-C2	2.46	112.02	108.27
26	K	101	BCR	C8-C9-C10	-2.46	115.14	119.01
24	B	617	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
24	a	407	CLA	O2A-CGA-O1A	-2.46	117.47	123.63
26	K	101	BCR	C21-C20-C19	-2.46	116.07	123.20
24	c	507	CLA	C1D-ND-C4D	-2.46	104.59	106.31
24	C	510	CLA	C6-C5-C3	2.46	119.46	113.47
26	b	620	BCR	C1-C6-C5	-2.46	119.28	122.64
24	C	503	CLA	C3D-C4D-ND	2.46	113.98	109.99
38	o	301	HTG	C1'-S1-C1	2.46	105.76	100.45
24	d	405	CLA	C5-C3-C2	-2.46	115.65	121.17
26	B	619	BCR	C32-C1-C6	-2.46	106.39	110.24
29	B	621	LMG	O10-C28-C29	-2.46	114.17	123.78
31	M	101	LMT	O5B-C1B-C2B	-2.46	105.32	110.37
32	a	419	LHG	C25-C24-C23	-2.45	104.71	113.69
29	C	520	LMG	O4-C4-C5	2.45	115.36	109.32
28	a	413	SQD	O9-S-O7	-2.45	105.85	113.82
38	H	101	HTG	C1-C2-C3	-2.45	105.75	110.55
29	d	412	LMG	O1-C1-C2	2.45	112.00	108.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	c	507	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
28	l	102	SQD	C26-C25-C24	-2.45	104.13	113.13
24	C	506	CLA	C1-O2A-CGA	2.45	122.57	116.65
24	b	608	CLA	CHC-C1C-C2C	-2.45	120.00	126.95
43	v	202	HEC	C2B-C1B-NB	-2.44	107.08	109.90
24	b	615	CLA	C4C-C3C-C2C	-2.44	103.33	106.89
24	C	506	CLA	CHC-C1C-C2C	-2.44	120.00	126.95
24	B	603	CLA	C3B-C2B-C1B	-2.44	104.29	107.17
24	B	616	CLA	C1D-ND-C4D	-2.44	104.60	106.31
24	D	404	CLA	CBC-CAC-C3C	-2.44	105.80	112.42
24	A	609	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
24	d	405	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
41	E	113	HEM	CHB-C1B-NB	2.44	127.39	124.37
28	A	616	SQD	O47-C7-O49	-2.44	118.00	123.70
38	b	631	HTG	C1-O5-C5	2.44	116.94	112.56
40	C	518	DGD	C4D-C3D-C2D	-2.44	106.55	110.83
38	h	101	HTG	C1-O5-C5	2.44	116.93	112.56
26	c	514	BCR	C32-C1-C6	2.44	114.06	110.24
24	b	604	CLA	C3B-C2B-C1B	-2.43	104.30	107.17
27	d	407	PL9	C40-C39-C38	-2.43	117.37	123.63
40	H	103	DGD	O5D-C6D-C5D	-2.43	103.94	109.42
43	V	203	HEC	CBC-CAC-C3C	2.43	119.01	112.42
24	a	410	CLA	CMC-C2C-C1C	2.43	128.83	125.03
26	C	515	BCR	C32-C1-C6	-2.43	106.43	110.24
25	D	401	PHO	O2D-CGD-CBD	2.43	113.62	110.95
40	C	518	DGD	O1G-C1A-O1A	-2.43	117.55	123.63
24	b	604	CLA	C2D-C1D-ND	2.43	112.53	110.13
24	c	506	CLA	CMB-C2B-C1B	2.43	129.12	125.42
24	a	410	CLA	C16-C15-C13	2.43	124.03	115.97
26	T	102	BCR	C31-C1-C6	2.43	114.05	110.24
24	C	510	CLA	CHB-C4A-NA	2.42	127.90	124.40
25	d	401	PHO	CED-O2D-CGD	2.42	121.42	115.92
24	A	609	CLA	CMB-C2B-C1B	2.42	129.11	125.42
24	C	510	CLA	O2D-CGD-CBD	2.42	115.47	111.23
27	A	611	PL9	O2-C1-C2	-2.42	116.32	121.83
26	c	515	BCR	C39-C30-C25	-2.42	106.44	110.24
26	t	102	BCR	C40-C30-C25	2.42	114.04	110.24
30	b	627	GOL	O3-C3-C2	2.42	121.27	110.38
24	C	512	CLA	C3D-C4D-ND	2.42	113.92	109.99
30	D	402	GOL	O2-C2-C1	-2.42	99.17	109.18
25	d	401	PHO	C4D-CHA-CBD	2.42	109.61	108.45
24	B	605	CLA	O1D-CGD-CBD	-2.42	119.75	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	c	516	DGD	CDB-CCB-CBB	-2.42	102.16	114.37
24	B	613	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
26	B	620	BCR	C31-C1-C6	-2.41	106.46	110.24
24	C	508	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
24	B	611	CLA	C3D-C4D-ND	2.41	113.91	109.99
24	c	511	CLA	C2D-C1D-ND	-2.41	107.74	110.13
24	a	410	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
24	b	609	CLA	C11-C12-C13	-2.41	107.97	115.97
24	a	408	CLA	O2A-CGA-O1A	-2.41	117.61	123.63
24	c	505	CLA	C4D-C3D-CAD	-2.40	105.49	108.11
31	A	617	LMT	C1B-O5B-C5B	2.40	118.42	113.72
31	m	101	LMT	C1-O1'-C1'	2.40	117.79	113.68
31	a	401	LMT	O2'-C2'-C1'	2.40	115.80	110.08
24	D	405	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
26	C	515	BCR	C8-C7-C6	-2.40	120.58	127.00
24	b	605	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
23	m	104[B]	BCT	O2-C-O1	-2.40	113.53	119.68
28	b	633	SQD	O6-C44-C45	2.40	116.66	110.82
26	a	411	BCR	C24-C23-C22	-2.40	122.69	126.23
26	h	103	BCR	C33-C5-C4	-2.40	108.49	113.60
24	b	612	CLA	OBD-CAD-C3D	-2.39	122.82	128.42
31	t	103	LMT	C1B-O5B-C5B	2.39	118.39	113.72
24	B	604	CLA	CBC-CAC-C3C	-2.39	105.93	112.42
30	a	415	GOL	O1-C1-C2	2.39	121.15	110.38
24	C	504	CLA	C3D-C4D-ND	2.39	113.88	109.99
31	a	401	LMT	O5'-C1'-O1'	-2.39	104.39	110.04
24	A	609	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
26	K	101	BCR	C15-C16-C17	-2.39	118.63	123.52
28	l	102	SQD	O47-C7-O49	-2.39	118.12	123.70
40	D	408	DGD	C3G-O3G-C1D	2.39	118.92	113.80
26	h	103	BCR	C16-C17-C18	-2.39	123.93	127.28
27	d	407	PL9	C11-C9-C8	-2.39	115.81	121.17
24	c	504	CLA	C1D-CHD-C4C	-2.39	120.95	126.02
24	A	607	CLA	CMB-C2B-C1B	2.39	129.05	125.42
29	B	634	LMG	C9-O8-C28	2.39	125.84	117.12
30	B	625	GOL	O2-C2-C1	2.39	119.05	109.18
24	C	507	CLA	OBD-CAD-C3D	-2.38	122.84	128.42
24	b	617	CLA	C1-O2A-CGA	2.38	122.42	116.65
26	h	103	BCR	C37-C22-C21	-2.38	118.96	122.82
26	c	527	BCR	C29-C30-C25	2.38	113.89	110.44
26	t	102	BCR	C1-C6-C7	2.38	122.10	115.65
28	b	633	SQD	C1-O5-C5	-2.38	109.08	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	508	CLA	C3D-C4D-ND	2.38	113.85	109.99
24	c	508	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
24	c	509	CLA	CHB-C1B-NB	-2.38	120.48	124.05
38	b	631	HTG	O4-C4-C5	2.37	115.17	109.32
26	A	610	BCR	C28-C27-C26	-2.37	109.82	114.06
29	C	526	LMG	O9-C10-C11	-2.37	114.50	123.78
24	B	616	CLA	C4B-C3B-C2B	-2.37	104.35	107.30
26	D	406	BCR	C15-C16-C17	-2.37	118.67	123.52
29	z	101	LMG	O1-C1-C2	2.37	111.87	108.27
31	M	101	LMT	O5B-C5B-C4B	2.37	113.97	109.70
24	B	615	CLA	C4D-C3D-CAD	-2.37	105.53	108.11
29	C	526	LMG	C3-C4-C5	2.37	114.53	110.23
26	d	406	BCR	C10-C11-C12	-2.37	116.33	123.20
24	C	510	CLA	C4B-C3B-C2B	-2.37	104.36	107.30
24	C	505	CLA	C2A-C1A-CHA	-2.37	119.76	123.87
28	a	424	SQD	O47-C7-O49	-2.37	118.17	123.70
27	D	407	PL9	C22-C23-C24	-2.37	122.21	127.62
24	c	513	CLA	O2D-CGD-CBD	2.37	115.37	111.23
24	b	602	CLA	O2A-CGA-CBA	2.36	119.05	111.83
24	B	617	CLA	C4D-C3D-CAD	-2.36	105.54	108.11
38	C	532	HTG	O2-C2-C1	2.36	114.50	110.30
24	A	606	CLA	CHB-C1B-NB	-2.36	120.50	124.05
26	d	406	BCR	C4-C5-C6	2.36	125.90	122.70
26	A	610	BCR	C15-C14-C13	-2.36	123.97	127.28
24	C	507	CLA	O2A-CGA-CBA	2.36	119.03	111.83
29	C	520	LMG	O8-C28-O10	-2.36	117.72	123.63
24	C	513	CLA	CMC-C2C-C1C	2.36	128.72	125.03
28	a	413	SQD	C46-C45-C44	2.36	117.28	111.78
26	C	514	BCR	C37-C22-C23	2.36	121.69	118.09
24	a	407	CLA	C4A-NA-C1A	-2.36	105.60	106.68
24	B	607	CLA	CED-O2D-CGD	2.36	121.26	115.92
24	D	405	CLA	C3D-C4D-ND	2.36	113.82	109.99
28	l	102	SQD	C45-O47-C7	-2.35	112.16	117.80
24	c	506	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
26	b	619	BCR	C24-C25-C26	2.35	126.97	121.56
24	B	607	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
26	H	102	BCR	C28-C27-C26	2.35	118.25	114.06
24	c	503	CLA	C7-C6-C5	-2.35	107.00	113.26
24	c	501	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
38	C	532	HTG	C4-C3-C2	-2.35	106.71	110.83
29	d	412	LMG	O6-C5-C4	2.35	113.93	109.70
24	C	505	CLA	CHC-C1C-NC	-2.35	120.78	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	V	203	HEC	CHD-C1D-ND	2.35	127.27	124.37
38	H	101	HTG	O2-C2-C1	2.35	114.47	110.30
24	b	603	CLA	C1D-CHD-C4C	-2.35	121.03	126.02
24	B	617	CLA	O2A-C1-C2	2.34	117.13	108.11
24	C	511	CLA	C1-O2A-CGA	2.34	122.33	116.65
31	A	617	LMT	O5B-C1B-C2B	2.34	115.19	110.37
24	B	603	CLA	C2A-C1A-CHA	-2.34	119.80	123.87
26	c	515	BCR	C15-C16-C17	-2.34	118.73	123.52
24	d	403	CLA	CAC-C3C-C4C	2.34	127.84	124.79
24	a	410	CLA	OBD-CAD-C3D	-2.34	122.95	128.42
27	a	412	PL9	C15-C14-C16	2.34	119.28	115.23
24	B	606	CLA	O2A-C1-C2	-2.34	99.12	108.11
24	b	608	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
24	B	602	CLA	C11-C10-C8	2.33	123.72	115.97
24	C	507	CLA	C4D-CHA-C1A	-2.33	118.46	121.24
30	B	628	GOL	C3-C2-C1	2.33	120.34	111.80
24	d	404	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
30	b	625	GOL	O2-C2-C1	2.33	118.82	109.18
26	c	527	BCR	C23-C24-C25	-2.33	120.78	127.00
40	d	408	DGD	C4D-C3D-C2D	2.33	114.92	110.83
24	B	609	CLA	C11-C12-C13	-2.33	108.23	115.97
24	B	603	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
31	c	521	LMT	O1B-C1B-C2B	2.33	113.81	108.09
26	B	618	BCR	C15-C14-C13	-2.32	124.02	127.28
24	c	503	CLA	OBD-CAD-C3D	-2.32	122.98	128.42
24	C	504	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
24	b	617	CLA	CMB-C2B-C3B	2.32	132.01	126.55
24	A	607	CLA	C2A-C1A-CHA	-2.32	119.83	123.87
24	B	605	CLA	CED-O2D-CGD	2.32	121.18	115.92
24	C	502	CLA	CHB-C4A-NA	2.32	127.75	124.40
27	A	611	PL9	C8-C7-C3	2.32	118.02	112.03
24	b	608	CLA	CMB-C2B-C1B	2.32	128.95	125.42
24	C	513	CLA	CED-O2D-CGD	2.32	121.17	115.92
24	c	513	CLA	C4C-C3C-C2C	-2.32	103.52	106.89
24	b	607	CLA	C2A-C3A-C4A	2.32	105.61	101.87
24	b	611	CLA	C20-C18-C19	-2.32	100.19	110.53
38	b	632	HTG	C1-C2-C3	2.32	115.08	110.55
28	A	622	SQD	O47-C7-C8	2.32	116.49	111.48
32	a	419	LHG	O7-C7-O9	-2.32	118.29	123.70
38	B	630	HTG	C1-O5-C5	2.32	116.72	112.56
24	c	511	CLA	CHC-C1C-C2C	-2.32	120.37	126.95
24	c	505	CLA	CAA-C2A-C1A	2.31	119.56	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	a	418	HTG	O3-C3-C2	2.31	115.83	110.38
31	I	101	LMT	C1B-O5B-C5B	2.31	118.24	113.72
24	C	512	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
31	B	622	LMT	O1B-C4'-C3'	2.31	113.11	107.23
24	B	604	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
24	b	602	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
32	E	101	LHG	O7-C7-O9	-2.31	118.31	123.70
26	D	406	BCR	C10-C11-C12	-2.31	116.51	123.20
24	c	512	CLA	CBA-CAA-C2A	-2.31	106.93	113.79
24	C	513	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
29	C	526	LMG	O8-C28-C29	2.31	118.87	111.83
24	c	509	CLA	C4D-CHA-C1A	-2.31	118.49	121.24
24	c	511	CLA	C1D-CHD-C4C	-2.31	121.12	126.02
43	V	203	HEC	CMC-C2C-C1C	2.31	128.93	125.42
29	d	412	LMG	O3-C3-C4	2.30	115.81	110.38
26	D	406	BCR	C37-C22-C21	-2.30	119.09	122.82
24	D	404	CLA	CED-O2D-CGD	2.30	121.14	115.92
24	b	611	CLA	OBD-CAD-C3D	-2.30	123.04	128.42
38	C	531	HTG	O2-C2-C1	2.30	114.39	110.30
24	b	603	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
27	a	412	PL9	C22-C21-C19	-2.30	105.56	113.19
38	b	623	HTG	C1-O5-C5	2.30	116.69	112.56
26	d	406	BCR	C23-C24-C25	-2.30	120.86	127.00
24	B	605	CLA	CHB-C4A-NA	2.30	127.71	124.40
24	c	511	CLA	CMB-C2B-C1B	2.29	128.91	125.42
24	b	616	CLA	CHB-C1B-C2B	-2.29	120.77	127.43
30	c	529	GOL	O3-C3-C2	-2.29	100.06	110.38
24	B	615	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
28	A	612	SQD	O4-C4-C3	-2.29	104.98	110.38
26	K	101	BCR	C23-C24-C25	-2.29	120.88	127.00
24	b	603	CLA	CMB-C2B-C3B	2.29	131.94	126.55
24	b	602	CLA	C4-C3-C5	2.29	119.20	115.23
24	D	403	CLA	C4C-C3C-C2C	-2.29	103.56	106.89
24	c	509	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
26	c	515	BCR	C36-C18-C19	2.29	121.58	118.09
24	A	607	CLA	CHB-C1B-C2B	-2.29	120.79	127.43
24	b	606	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
29	C	520	LMG	O6-C5-C6	2.29	112.11	106.44
24	b	613	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
24	C	503	CLA	CMB-C2B-C1B	2.29	128.90	125.42
24	b	604	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
28	F	104	SQD	C46-O48-C23	2.28	125.47	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	CMC-C2C-C1C	2.28	128.60	125.03
24	B	606	CLA	O2D-CGD-CBD	2.28	115.22	111.23
24	C	505	CLA	CMB-C2B-C3B	2.28	131.92	126.55
24	c	504	CLA	CAC-C3C-C4C	2.28	127.76	124.79
24	c	505	CLA	O2A-CGA-O1A	-2.28	117.92	123.63
24	a	410	CLA	CHA-C4D-ND	-2.28	127.84	132.55
24	C	501	CLA	CHD-C1D-ND	-2.28	121.60	124.80
24	B	605	CLA	C4C-C3C-C2C	-2.28	103.58	106.89
24	c	506	CLA	C16-C17-C18	2.28	126.11	115.94
38	b	632	HTG	C6-C5-C4	-2.28	107.43	113.02
24	c	503	CLA	C4B-C3B-C2B	-2.28	104.47	107.30
32	D	411	LHG	O7-C7-O9	-2.28	118.38	123.70
24	C	504	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
24	d	404	CLA	C2A-C1A-CHA	-2.28	119.92	123.87
24	B	612	CLA	C11-C12-C13	-2.28	108.40	115.97
24	D	403	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
28	F	104	SQD	O47-C7-C8	2.27	116.40	111.48
24	d	404	CLA	C4D-CHA-C1A	-2.27	118.53	121.24
26	C	515	BCR	C4-C5-C6	-2.27	119.63	122.70
24	B	605	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
26	B	619	BCR	C15-C16-C17	-2.27	118.87	123.52
31	A	617	LMT	O1B-C1B-O5B	-2.27	104.71	110.69
24	a	407	CLA	C2A-C1A-CHA	-2.27	119.92	123.87
24	c	501	CLA	CAC-C3C-C4C	2.27	127.74	124.79
30	t	101	GOL	C3-C2-C1	2.27	120.12	111.80
24	d	404	CLA	CHC-C1C-C2C	-2.27	120.50	126.95
24	C	511	CLA	CED-O2D-CGD	2.27	121.06	115.92
24	b	617	CLA	O2A-C1-C2	2.27	116.83	108.11
24	C	503	CLA	C4B-C3B-C2B	-2.27	104.48	107.30
28	A	612	SQD	O48-C23-O10	-2.27	117.96	123.63
27	d	407	PL9	C51-C49-C48	2.26	129.45	122.66
24	B	607	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
43	V	203	HEC	CAD-C3D-C4D	2.26	128.64	124.70
24	B	611	CLA	CAA-CBA-CGA	-2.26	106.78	113.21
24	c	513	CLA	CMB-C2B-C3B	2.26	131.87	126.55
24	C	505	CLA	C4D-C3D-CAD	-2.26	105.65	108.11
24	D	405	CLA	CMA-C3A-C4A	-2.26	105.69	111.77
24	B	610	CLA	C3A-C2A-C1A	-2.26	97.95	101.34
24	b	614	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
40	h	104	DGD	O4D-C4D-C3D	-2.26	105.05	110.38
24	b	614	CLA	C4D-C3D-CAD	-2.26	105.65	108.11
24	c	503	CLA	CHB-C1B-NB	-2.26	120.66	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	B	621	LMG	C1-O6-C5	-2.26	109.31	113.72
24	A	606	CLA	CHB-C4A-NA	2.26	127.66	124.40
24	b	605	CLA	C2A-C1A-CHA	-2.26	119.95	123.87
24	A	607	CLA	CHA-C4D-ND	-2.26	127.89	132.55
24	b	612	CLA	CMB-C2B-C1B	2.26	128.86	125.42
26	K	101	BCR	C10-C11-C12	-2.26	116.66	123.20
24	C	510	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
40	C	516	DGD	C1G-O1G-C1A	2.26	125.37	117.12
26	T	102	BCR	C15-C16-C17	-2.26	118.90	123.52
24	b	611	CLA	CHC-C1C-C2C	-2.26	120.54	126.95
38	c	531	HTG	O2-C2-C3	2.25	115.69	110.38
24	d	404	CLA	C4D-C3D-CAD	-2.25	105.66	108.11
26	B	620	BCR	C20-C21-C22	-2.25	124.12	127.28
26	c	514	BCR	C36-C18-C19	2.25	121.53	118.09
24	c	503	CLA	CHC-C1C-C2C	-2.25	120.55	126.95
39	V	217	1PE	OH3-C22-C12	2.25	120.03	110.11
24	d	403	CLA	C1C-C2C-C3C	-2.25	104.61	106.98
24	c	510	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
26	H	102	BCR	C15-C14-C13	2.25	130.43	127.28
24	D	403	CLA	CMC-C2C-C1C	2.25	128.54	125.03
29	c	519	LMG	C3-C4-C5	2.25	114.30	110.23
24	B	617	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
24	b	615	CLA	C1-O2A-CGA	2.24	122.08	116.65
24	c	505	CLA	O2D-CGD-CBD	2.24	115.15	111.23
24	C	512	CLA	O2A-CGA-CBA	2.24	118.67	111.83
24	c	502	CLA	C1-C2-C3	-2.24	122.53	126.20
29	J	101	LMG	O6-C1-C2	2.24	114.97	110.37
24	D	405	CLA	OBD-CAD-C3D	-2.24	123.18	128.42
24	a	407	CLA	CAA-CBA-CGA	-2.24	106.85	113.21
24	C	501	CLA	OBD-CAD-C3D	-2.24	123.18	128.42
24	B	610	CLA	CHC-C1C-C2C	-2.24	120.59	126.95
26	B	620	BCR	C11-C10-C9	-2.24	124.14	127.28
31	J	103	LMT	C1'-C2'-C3'	2.24	114.72	110.01
27	a	412	PL9	C20-C19-C21	2.24	119.11	115.23
32	D	411	LHG	O8-C23-O10	-2.24	118.03	123.63
32	d	410	LHG	O2-C2-C1	-2.24	99.92	109.18
24	B	607	CLA	CHC-C1C-C2C	-2.24	120.60	126.95
28	b	633	SQD	O2-C2-C3	2.23	115.64	110.38
24	c	502	CLA	C2A-C1A-CHA	-2.23	119.99	123.87
27	D	407	PL9	C53-C6-C1	2.23	119.85	115.28
26	b	618	BCR	C35-C13-C12	2.23	121.49	118.09
24	b	604	CLA	C5-C3-C2	-2.23	116.16	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	612	CLA	CHB-C1B-NB	-2.23	120.71	124.05
24	b	614	CLA	CHB-C1B-NB	-2.23	120.71	124.05
28	x	101	SQD	O8-S-O7	-2.23	105.83	111.40
24	C	503	CLA	CHB-C1B-NB	-2.23	120.71	124.05
31	c	521	LMT	C3'-C4'-C5'	-2.22	106.00	110.93
27	a	412	PL9	C7-C8-C9	2.22	130.66	126.83
32	B	632	LHG	O8-C23-O10	-2.22	118.06	123.63
24	c	510	CLA	O2A-C1-C2	-2.22	99.55	108.11
24	c	508	CLA	CHC-C1C-C2C	-2.22	120.63	126.95
24	B	609	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
31	c	521	LMT	O5'-C1'-O1'	-2.22	104.79	110.04
24	c	512	CLA	C4D-C3D-CAD	-2.22	105.69	108.11
29	C	526	LMG	C9-C8-C7	-2.22	106.60	111.78
24	c	510	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	c	507	CLA	C4-C3-C5	2.22	119.08	115.23
24	D	405	CLA	C4B-C3B-C2B	-2.22	104.54	107.30
38	b	632	HTG	O5-C1-C2	2.22	113.38	110.32
27	d	407	PL9	C7-C3-C4	2.22	118.74	116.91
24	b	610	CLA	CMC-C2C-C1C	2.22	128.50	125.03
24	a	407	CLA	C5-C3-C2	-2.22	116.19	121.17
24	B	610	CLA	CBC-CAC-C3C	-2.22	106.41	112.42
38	B	630	HTG	O2-C2-C3	2.22	115.60	110.38
24	C	512	CLA	C17-C16-C15	-2.22	103.34	113.28
24	b	607	CLA	C1D-CHD-C4C	-2.22	121.31	126.02
32	B	632	LHG	O3-P-O5	-2.22	100.16	108.94
24	B	610	CLA	CHC-C1C-NC	-2.21	120.97	124.31
28	b	633	SQD	C1-C2-C3	-2.21	105.35	110.01
24	C	509	CLA	C16-C17-C18	-2.21	106.05	115.94
43	v	202	HEC	C3B-C4B-NB	-2.21	107.74	110.17
24	d	405	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
40	c	518	DGD	O1G-C1A-C2A	2.21	118.58	111.83
40	c	518	DGD	C6B-C5B-C4B	-2.21	103.18	114.37
32	e	101	LHG	O7-C7-O9	-2.21	118.53	123.70
24	C	504	CLA	CBC-CAC-C3C	-2.21	106.42	112.42
24	b	613	CLA	C11-C12-C13	-2.21	108.61	115.97
24	B	602	CLA	C1D-CHD-C4C	-2.21	121.32	126.02
24	D	403	CLA	C4D-C3D-CAD	-2.21	105.70	108.11
28	a	424	SQD	O8-S-O7	-2.21	105.87	111.40
24	C	504	CLA	C2A-C1A-CHA	-2.21	120.03	123.87
38	b	631	HTG	O5-C1-S1	2.21	116.00	109.94
24	b	613	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
24	B	617	CLA	O1D-CGD-CBD	-2.21	120.16	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	611	CLA	O2A-CGA-CBA	2.21	118.56	111.83
24	D	404	CLA	C4C-C3C-C2C	-2.21	103.68	106.89
24	b	607	CLA	C1-O2A-CGA	2.21	121.99	116.65
26	k	101	BCR	C1-C6-C7	2.20	121.63	115.65
38	V	204	HTG	O5-C5-C6	2.20	111.90	106.44
24	b	602	CLA	C4-C3-C2	-2.20	117.97	123.63
38	H	101	HTG	C2'-C1'-S1	-2.20	104.94	112.36
31	c	521	LMT	O5'-C1'-C2'	2.20	114.90	110.37
26	D	406	BCR	C24-C25-C26	2.20	126.63	121.56
24	C	511	CLA	C4D-C3D-CAD	-2.20	105.71	108.11
24	B	605	CLA	C3D-C4D-ND	2.20	113.57	109.99
26	b	619	BCR	C24-C23-C22	-2.20	122.98	126.23
24	C	504	CLA	C4B-C3B-C2B	-2.20	104.56	107.30
24	B	610	CLA	CMB-C2B-C3B	2.20	131.73	126.55
24	a	410	CLA	CHC-C1C-C2C	-2.20	120.69	126.95
26	t	102	BCR	C19-C18-C17	-2.20	115.55	119.01
24	B	605	CLA	OBD-CAD-C3D	-2.20	123.27	128.42
24	c	503	CLA	CAC-C3C-C4C	2.20	127.65	124.79
26	T	102	BCR	C7-C6-C5	-2.20	116.49	121.56
24	b	603	CLA	C16-C17-C18	-2.20	106.12	115.94
26	c	514	BCR	C38-C26-C25	-2.20	122.08	124.48
24	B	608	CLA	CHC-C1C-C2C	-2.20	120.70	126.95
24	b	608	CLA	C4D-C3D-CAD	-2.20	105.72	108.11
24	B	606	CLA	CHC-C1C-NC	-2.20	121.00	124.31
24	B	614	CLA	C7-C6-C5	-2.20	107.41	113.26
24	b	612	CLA	C4C-C3C-C2C	-2.20	103.69	106.89
31	t	103	LMT	O1B-C4'-C3'	2.20	112.81	107.23
32	A	618	LHG	C6-O8-C23	2.20	125.14	117.12
26	d	406	BCR	C15-C16-C17	-2.20	119.03	123.52
24	C	504	CLA	CAC-C3C-C4C	2.20	127.65	124.79
24	d	404	CLA	CED-O2D-CGD	2.19	120.89	115.92
29	j	101	LMG	O2-C2-C1	-2.19	104.85	110.08
24	B	613	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
24	b	617	CLA	C4A-NA-C1A	-2.19	105.68	106.68
24	c	502	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
40	C	516	DGD	O3G-C3G-C2G	-2.18	105.50	110.82
31	m	101	LMT	O1'-C1'-C2'	2.18	111.59	108.27
40	D	408	DGD	C1D-O6D-C5D	-2.18	109.46	113.72
25	D	401	PHO	C1-C2-C3	-2.18	122.62	126.20
26	d	406	BCR	C2-C1-C6	2.18	113.61	110.44
24	C	508	CLA	CMB-C2B-C1B	2.18	128.74	125.42
24	c	511	CLA	C11-C10-C8	-2.18	108.72	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	606	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
24	d	403	CLA	CHD-C1D-ND	-2.18	121.74	124.80
24	B	613	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
25	a	409	PHO	OBD-CAD-C3D	-2.18	124.50	127.89
38	c	530	HTG	C1-O5-C5	2.18	116.47	112.56
24	c	510	CLA	CHB-C1B-NB	-2.18	120.78	124.05
24	b	609	CLA	CHC-C1C-C2C	-2.18	120.77	126.95
26	A	610	BCR	C23-C24-C25	-2.18	121.19	127.00
32	E	101	LHG	O8-C23-O10	-2.17	118.19	123.63
24	c	504	CLA	C5-C3-C2	-2.17	116.29	121.17
24	B	609	CLA	CHC-C1C-C2C	-2.17	120.77	126.95
28	x	101	SQD	O47-C7-O49	-2.17	118.62	123.70
28	A	616	SQD	O9-S-C6	2.17	110.00	106.76
24	C	501	CLA	C4C-C3C-C2C	-2.17	103.73	106.89
24	B	611	CLA	C5-C3-C2	-2.17	116.29	121.17
31	c	521	LMT	O4'-C4B-C3B	2.17	115.50	110.38
31	t	103	LMT	O3B-C3B-C4B	-2.17	105.25	110.38
24	C	512	CLA	C1C-C2C-C3C	-2.17	104.70	106.98
26	k	101	BCR	C21-C20-C19	-2.17	116.91	123.20
40	h	104	DGD	C6D-C5D-C4D	2.17	116.62	112.07
30	O	306	GOL	C3-C2-C1	-2.17	103.84	111.80
24	c	508	CLA	OBD-CAD-C3D	-2.17	123.35	128.42
26	c	527	BCR	C15-C16-C17	-2.17	119.08	123.52
24	B	607	CLA	C1D-CHD-C4C	-2.17	121.41	126.02
26	k	101	BCR	C4-C5-C6	2.17	125.63	122.70
24	D	404	CLA	CAC-C3C-C4C	2.17	127.61	124.79
32	B	632	LHG	C6-C5-C4	-2.17	106.73	111.78
30	d	402	GOL	O2-C2-C1	-2.17	100.20	109.18
24	C	509	CLA	C1-C2-C3	-2.17	122.65	126.20
27	d	407	PL9	C12-C13-C14	-2.17	122.66	127.62
24	b	609	CLA	C5-C3-C2	-2.16	116.31	121.17
43	V	203	HEC	O2A-CGA-O1A	-2.16	117.77	123.33
26	c	514	BCR	C12-C13-C14	-2.16	115.61	119.01
32	a	419	LHG	O8-C23-C24	2.16	118.43	111.83
24	c	507	CLA	CBC-CAC-C3C	-2.16	106.55	112.42
29	B	634	LMG	C1-O6-C5	2.16	117.94	113.72
26	B	618	BCR	C8-C9-C10	2.16	122.41	119.01
24	c	502	CLA	OBD-CAD-C3D	-2.16	123.36	128.42
38	B	630	HTG	O3-C3-C4	-2.16	105.28	110.38
26	c	514	BCR	C15-C14-C13	-2.16	124.25	127.28
24	C	504	CLA	C5-C3-C2	-2.16	116.32	121.17
24	b	612	CLA	C7-C6-C5	-2.16	107.50	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	607	CLA	CHC-C4B-C3B	-2.16	118.00	127.37
24	c	511	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
43	v	202	HEC	C4C-NC-C1C	2.16	109.34	105.82
24	C	506	CLA	C4D-CHA-C1A	-2.16	118.67	121.24
24	b	613	CLA	O2A-CGA-CBA	2.16	118.41	111.83
24	b	614	CLA	C2A-C1A-CHA	-2.16	120.12	123.87
38	C	522	HTG	O5-C5-C4	2.16	113.58	109.70
24	B	615	CLA	C4-C3-C5	2.16	118.97	115.23
24	c	506	CLA	O1D-CGD-CBD	2.15	128.77	124.52
31	u	203	LMT	O2B-C2B-C1B	2.15	115.21	110.08
25	d	401	PHO	C5-C3-C2	-2.15	116.33	121.17
38	B	623	HTG	C1-O5-C5	2.15	116.42	112.56
31	Y	101	LMT	C1B-O1B-C4'	2.15	123.08	117.98
25	A	608	PHO	CAC-C3C-C4C	2.15	129.56	124.03
24	b	611	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
24	C	508	CLA	CMC-C2C-C1C	2.15	128.39	125.03
38	c	531	HTG	C4-C3-C2	-2.15	107.06	110.83
26	b	619	BCR	C7-C8-C9	-2.15	123.06	126.23
24	c	509	CLA	C4D-C3D-CAD	-2.15	105.77	108.11
24	B	602	CLA	C7-C6-C5	2.15	118.98	113.26
40	C	518	DGD	O3E-C3E-C4E	-2.15	105.32	110.38
24	c	508	CLA	CHB-C4A-NA	2.14	127.50	124.40
41	e	107	HEM	CAD-CBD-CGD	2.14	119.35	113.67
24	A	606	CLA	CHD-C4C-C3C	-2.14	121.65	124.77
26	C	514	BCR	C32-C1-C31	2.14	114.76	108.63
24	B	605	CLA	CMC-C2C-C1C	2.14	128.38	125.03
24	B	602	CLA	C1-O2A-CGA	2.14	121.83	116.65
24	b	617	CLA	CMC-C2C-C1C	2.14	128.38	125.03
24	b	612	CLA	CHB-C4A-NA	2.14	127.49	124.40
24	c	506	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	c	510	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
24	b	615	CLA	C20-C18-C19	2.14	120.07	110.53
40	c	518	DGD	O3G-C3G-C2G	-2.14	105.62	110.82
24	B	611	CLA	CHB-C1B-C2B	-2.14	121.22	127.43
24	C	503	CLA	O2A-CGA-O1A	-2.14	118.29	123.63
38	B	630	HTG	C1'-S1-C1	2.13	105.06	100.45
38	c	531	HTG	O5-C5-C6	2.13	111.73	106.44
40	H	103	DGD	C1D-O6D-C5D	-2.13	109.55	113.72
24	b	604	CLA	O2A-CGA-O1A	-2.13	118.29	123.63
24	d	405	CLA	CGD-CBD-CAD	-2.13	103.94	110.85
28	l	102	SQD	O8-S-O9	-2.13	106.06	111.40
38	B	631	HTG	O5-C1-S1	2.13	115.79	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	v	202	HEC	CHA-C1A-NA	2.13	126.78	124.45
32	d	411	LHG	O7-C7-C8	2.13	116.09	111.48
38	C	530	HTG	C1'-S1-C1	2.13	105.06	100.45
24	B	607	CLA	OBD-CAD-C3D	-2.13	123.43	128.42
24	d	405	CLA	OBD-CAD-C3D	-2.13	123.43	128.42
34	O	309	PGE	C5-O3-C4	2.13	122.59	113.26
26	c	527	BCR	C37-C22-C21	-2.13	119.36	122.82
28	x	101	SQD	O48-C23-O10	-2.13	118.30	123.63
24	B	617	CLA	C4B-C3B-C2B	-2.13	104.65	107.30
31	m	101	LMT	O1B-C1B-C2B	2.13	113.32	108.09
25	a	409	PHO	O1D-CGD-CBD	-2.13	121.50	124.72
41	E	113	HEM	CHA-C4D-C3D	-2.13	121.31	125.23
24	b	609	CLA	C6-C7-C8	-2.13	108.90	115.97
24	b	613	CLA	OBD-CAD-C3D	-2.13	123.45	128.42
26	k	101	BCR	C1-C6-C5	-2.13	119.73	122.64
24	A	606	CLA	C7-C6-C5	-2.13	107.59	113.26
24	c	506	CLA	CHC-C1C-C2C	-2.13	120.91	126.95
28	b	633	SQD	O4-C4-C3	2.12	115.38	110.38
24	A	606	CLA	C1D-ND-C4D	-2.12	104.82	106.31
24	c	513	CLA	C1D-ND-C4D	-2.12	104.82	106.31
26	c	514	BCR	C8-C7-C6	-2.12	121.33	127.00
31	u	203	LMT	O2'-C2'-C1'	2.12	115.13	110.08
28	A	612	SQD	O3-C3-C4	2.12	115.38	110.38
31	I	101	LMT	C4B-C3B-C2B	2.12	114.55	110.83
24	B	602	CLA	C4D-CHA-C1A	-2.12	118.71	121.24
24	b	608	CLA	CHB-C1B-NB	-2.12	120.87	124.05
26	D	406	BCR	C8-C7-C6	-2.12	121.33	127.00
24	A	606	CLA	CMC-C2C-C1C	2.12	128.35	125.03
24	c	510	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
24	B	605	CLA	CHD-C1D-ND	-2.12	121.82	124.80
24	b	613	CLA	C4D-C3D-CAD	-2.12	105.81	108.11
28	a	424	SQD	C45-O47-C7	2.12	122.86	117.80
31	f	101	LMT	C6'-C5'-C4'	-2.12	107.43	113.38
25	A	608	PHO	C4B-NB-C1B	-2.11	105.73	108.82
31	M	101	LMT	C2'-C3'-C4'	2.11	114.48	109.68
25	A	608	PHO	CBA-CAA-C2A	-2.11	107.55	113.78
24	B	604	CLA	CED-O2D-CGD	2.11	120.71	115.92
24	a	408	CLA	CED-O2D-CGD	2.11	120.71	115.92
32	d	409	LHG	C11-C10-C9	-2.11	103.69	114.37
40	C	516	DGD	CDB-CCB-CBB	-2.11	103.69	114.37
31	I	101	LMT	O6B-C6B-C5B	2.11	118.52	111.33
24	D	403	CLA	C4A-NA-C1A	-2.11	105.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	B	624	HTG	O2-C2-C3	-2.11	105.40	110.38
26	D	406	BCR	C21-C20-C19	-2.11	117.08	123.20
24	B	603	CLA	CHD-C1D-ND	-2.11	121.83	124.80
26	C	525	BCR	C33-C5-C6	-2.11	122.18	124.48
30	b	625	GOL	O2-C2-C3	-2.11	100.45	109.18
38	C	531	HTG	C1'-S1-C1	2.11	105.00	100.45
24	c	502	CLA	C3D-C4D-ND	2.11	113.41	109.99
38	c	531	HTG	O3-C3-C2	2.11	115.34	110.38
29	B	634	LMG	O2-C2-C3	-2.11	105.41	110.38
29	c	519	LMG	C7-O1-C1	2.10	118.31	113.80
24	c	511	CLA	C1-O2A-CGA	2.10	121.74	116.65
24	c	503	CLA	CBC-CAC-C3C	-2.10	106.72	112.42
28	F	104	SQD	C1-O5-C5	-2.10	109.61	113.72
32	e	101	LHG	O8-C23-O10	-2.10	118.37	123.63
27	D	407	PL9	C20-C19-C21	2.10	118.88	115.23
24	B	611	CLA	C1D-ND-C4D	-2.10	104.84	106.31
24	a	408	CLA	CHB-C1B-NB	-2.10	120.90	124.05
24	A	609	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
24	b	616	CLA	CHC-C1C-C2C	-2.10	120.98	126.95
24	c	508	CLA	C2A-C1A-CHA	-2.10	120.23	123.87
24	C	502	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
24	b	617	CLA	CHB-C4A-NA	2.10	127.43	124.40
32	B	632	LHG	C9-C8-C7	-2.10	106.01	113.69
24	b	610	CLA	CHB-C1B-NB	-2.10	120.90	124.05
24	C	510	CLA	OBD-CAD-C3D	-2.10	123.52	128.42
31	m	102	LMT	O5'-C5'-C6'	2.10	111.64	106.44
24	c	502	CLA	C4C-C3C-C2C	-2.09	103.84	106.89
38	B	630	HTG	O4-C4-C5	2.09	114.48	109.32
43	v	202	HEC	O2A-CGA-O1A	-2.09	117.95	123.33
31	c	521	LMT	O1'-C1'-C2'	2.09	111.45	108.27
24	B	604	CLA	C6-C5-C3	2.09	118.56	113.47
24	A	609	CLA	C4C-C3C-C2C	-2.09	103.85	106.89
24	b	602	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
26	a	411	BCR	C39-C30-C25	-2.09	106.97	110.24
24	C	509	CLA	CHB-C1B-NB	-2.09	120.92	124.05
40	H	103	DGD	O2G-C1B-C2B	2.09	116.00	111.48
24	B	603	CLA	C1-C2-C3	-2.09	122.78	126.20
24	C	506	CLA	CHB-C4A-NA	2.09	127.41	124.40
26	D	406	BCR	C32-C1-C2	-2.09	100.94	108.95
24	C	510	CLA	C6-C7-C8	-2.09	109.03	115.97
24	C	504	CLA	CHD-C1D-ND	-2.09	121.87	124.80
38	B	630	HTG	O5-C1-C2	-2.09	107.44	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	O	303	HTG	O5-C1-C2	-2.09	107.44	110.32
35	I	106	P6G	C17-O16-C15	2.08	122.38	113.26
38	c	523	HTG	C1-O5-C5	2.08	116.30	112.56
26	T	102	BCR	C35-C13-C12	2.08	121.27	118.09
24	c	508	CLA	CMC-C2C-C1C	2.08	128.29	125.03
41	E	113	HEM	C4C-NC-C1C	2.08	109.22	105.82
30	B	635	GOL	O1-C1-C2	2.08	119.75	110.38
24	D	405	CLA	CHA-C4D-ND	-2.08	128.25	132.55
26	c	515	BCR	C20-C19-C18	-2.08	120.66	126.36
26	b	619	BCR	C11-C10-C9	-2.08	124.36	127.28
29	a	414	LMG	O1-C1-C2	2.08	111.43	108.27
24	C	504	CLA	CHD-C4C-C3C	-2.08	121.74	124.77
24	b	607	CLA	CAA-C2A-C1A	2.08	118.79	111.97
24	A	609	CLA	CAC-C3C-C4C	2.08	127.50	124.79
32	l	101	LHG	O4-P-O5	2.08	122.12	112.44
24	C	511	CLA	C3A-C2A-C1A	2.08	104.45	101.34
31	A	617	LMT	O2B-C2B-C3B	-2.08	105.48	110.38
25	a	409	PHO	CAA-CBA-CGA	-2.08	107.31	113.21
40	c	518	DGD	O1G-C1A-O1A	-2.08	118.43	123.63
24	b	602	CLA	C4D-C3D-CAD	-2.08	105.85	108.11
29	c	519	LMG	C6-C5-C4	-2.08	107.92	113.02
24	B	606	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
29	c	520	LMG	O8-C28-O10	-2.08	118.44	123.63
24	c	504	CLA	C4D-CHA-C1A	-2.07	118.77	121.24
24	c	504	CLA	C6-C7-C8	-2.07	109.07	115.97
26	d	406	BCR	C16-C15-C14	-2.07	119.28	123.52
24	c	509	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
43	v	202	HEC	O2A-CGA-CBA	2.07	120.55	114.00
24	B	605	CLA	CHC-C1C-C2C	-2.07	121.07	126.95
24	C	513	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
28	A	622	SQD	O6-C44-C45	-2.07	105.79	110.82
24	c	511	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
24	d	404	CLA	CHC-C1C-NC	-2.07	121.20	124.31
29	C	520	LMG	C9-O8-C28	2.07	124.67	117.12
40	C	516	DGD	O1G-C1A-O1A	-2.07	118.46	123.63
24	C	504	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
40	H	103	DGD	C3D-C4D-C5D	-2.06	106.49	110.23
24	C	508	CLA	C4A-NA-C1A	-2.06	105.74	106.68
24	b	610	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
24	c	508	CLA	CMA-C3A-C4A	-2.06	106.23	111.77
31	j	103	LMT	O1B-C4'-C3'	2.06	112.47	107.23
24	a	408	CLA	O2D-CGD-O1D	-2.06	119.83	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	C	501	CLA	C4D-CHA-C1A	-2.06	118.78	121.24
26	b	619	BCR	C34-C9-C10	2.06	126.16	122.82
31	c	521	LMT	O6B-C6B-C5B	2.06	118.35	111.33
24	C	509	CLA	O2D-CGD-CBD	2.06	114.83	111.23
30	C	528	GOL	O2-C2-C1	2.06	117.71	109.18
27	A	611	PL9	C25-C24-C26	2.06	118.80	115.23
38	V	204	HTG	O4-C4-C3	2.06	115.23	110.38
26	h	103	BCR	C28-C27-C26	2.06	117.73	114.06
26	H	102	BCR	C2-C1-C6	2.06	113.43	110.44
29	B	634	LMG	O7-C8-C9	2.06	115.73	108.34
24	C	501	CLA	CHB-C4A-NA	2.06	127.37	124.40
27	A	611	PL9	C21-C19-C18	-2.06	116.55	121.17
24	B	607	CLA	C4D-C3D-CAD	-2.06	105.87	108.11
24	C	511	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
32	d	409	LHG	C27-C26-C25	-2.05	103.98	114.37
31	c	521	LMT	C1'-O5'-C5'	2.05	117.73	113.72
40	D	408	DGD	O5D-C1E-C2E	2.05	111.39	108.27
28	F	104	SQD	O48-C23-O10	-2.05	118.50	123.63
24	d	404	CLA	C5-C3-C2	-2.05	116.56	121.17
24	A	607	CLA	C1-C2-C3	2.05	129.55	126.20
31	t	103	LMT	O1B-C1B-O5B	2.05	116.08	110.69
24	b	605	CLA	C3D-C4D-ND	2.05	113.31	109.99
24	C	511	CLA	CHC-C1C-C2C	-2.05	121.13	126.95
24	b	611	CLA	O2A-CGA-CBA	2.05	118.07	111.83
24	b	613	CLA	C1C-C2C-C3C	-2.04	104.83	106.98
26	t	102	BCR	C32-C1-C6	-2.04	107.04	110.24
28	a	413	SQD	O2-C2-C1	2.04	114.94	110.08
24	B	610	CLA	O2D-CGD-CBD	2.04	114.80	111.23
40	H	103	DGD	C6E-C5E-C4E	2.04	118.03	113.02
29	b	621	LMG	C4-C3-C2	-2.04	107.24	110.83
24	B	608	CLA	C6-C7-C8	-2.04	109.18	115.97
24	B	610	CLA	CHC-C4B-C3B	-2.04	118.51	127.37
24	a	407	CLA	C7-C6-C5	-2.04	107.82	113.26
28	b	633	SQD	O2-C2-C1	2.04	114.94	110.08
24	c	503	CLA	CMB-C2B-C1B	2.04	128.53	125.42
24	c	511	CLA	C4-C3-C5	2.04	118.77	115.23
24	c	510	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
40	c	518	DGD	O6D-C1D-C2D	2.04	114.56	110.37
29	B	621	LMG	O5-C6-C5	-2.04	104.39	111.33
29	z	101	LMG	O8-C28-C29	2.04	118.05	111.83
41	E	113	HEM	CHD-C4C-NC	2.04	126.67	124.45
24	C	506	CLA	CMB-C2B-C1B	2.04	128.52	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	D	404	CLA	CHB-C1B-C2B	-2.04	121.52	127.43
24	d	403	CLA	CHB-C4A-NA	2.04	127.34	124.40
24	B	611	CLA	CGD-CBD-CAD	-2.04	104.26	110.85
38	a	418	HTG	O5-C5-C4	2.03	113.37	109.70
24	B	612	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
24	c	507	CLA	CHC-C1C-C2C	-2.03	121.17	126.95
24	c	511	CLA	C5-C3-C2	-2.03	116.60	121.17
24	c	505	CLA	C16-C15-C13	-2.03	109.21	115.97
24	B	616	CLA	C9-C8-C7	-2.03	104.03	111.27
32	a	419	LHG	C6-O8-C23	2.03	124.54	117.12
24	C	503	CLA	OBD-CAD-C3D	-2.03	123.67	128.42
24	a	407	CLA	OBD-CAD-C3D	-2.03	123.67	128.42
24	B	606	CLA	C2D-C1D-ND	2.03	112.14	110.13
31	Y	101	LMT	C4B-C3B-C2B	2.03	114.39	110.83
31	B	622	LMT	O5B-C5B-C6B	2.03	111.46	106.44
40	H	103	DGD	C6D-C5D-C4D	2.03	116.32	112.07
24	b	605	CLA	OBD-CAD-C3D	-2.03	123.68	128.42
24	a	408	CLA	CHA-C4D-ND	-2.03	128.37	132.55
34	O	308	PGE	O3-C5-C6	2.02	119.04	110.11
24	B	613	CLA	O2A-CGA-CBA	2.02	118.01	111.83
24	c	513	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
26	b	618	BCR	C21-C20-C19	-2.02	117.34	123.20
30	f	104	GOL	O3-C3-C2	2.02	119.48	110.38
24	b	617	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
24	c	503	CLA	C4C-C3C-C2C	-2.02	103.95	106.89
24	c	504	CLA	C1-O2A-CGA	2.02	121.55	116.65
26	C	525	BCR	C11-C10-C9	-2.02	124.44	127.28
24	b	607	CLA	CHB-C4A-NA	2.02	127.32	124.40
24	D	404	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
26	b	620	BCR	C21-C20-C19	-2.02	117.35	123.20
24	c	504	CLA	CMB-C2B-C3B	2.02	131.30	126.55
24	C	505	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
24	b	608	CLA	O2D-CGD-CBD	2.02	114.76	111.23
27	A	611	PL9	C20-C19-C21	2.02	118.73	115.23
24	b	615	CLA	C4B-C3B-C2B	-2.02	104.79	107.30
31	j	103	LMT	O5'-C5'-C4'	2.02	113.89	109.72
26	k	101	BCR	C34-C9-C10	2.02	126.08	122.82
31	m	101	LMT	C3B-C4B-C5B	2.02	113.89	110.23
24	c	501	CLA	O1D-CGD-CBD	2.01	128.49	124.52
26	d	406	BCR	C36-C18-C19	2.01	121.17	118.09
24	c	506	CLA	CHC-C4B-NB	-2.01	121.03	124.05
23	A	605	BCT	O3-C-O1	-2.01	114.53	119.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	B	613	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
24	B	602	CLA	C1D-ND-C4D	-2.01	104.90	106.31
40	H	103	DGD	O1G-C1A-C2A	2.01	117.97	111.83
29	C	526	LMG	C1-O6-C5	-2.01	109.79	113.72
28	x	101	SQD	C46-O48-C23	2.01	124.47	117.12
26	c	527	BCR	C37-C22-C23	2.01	121.16	118.09
26	C	515	BCR	C29-C30-C25	2.01	113.36	110.44
25	d	401	PHO	C3D-CAD-CBD	2.01	110.25	107.61
24	b	617	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
24	b	610	CLA	CHC-C1C-C2C	-2.01	121.23	126.95
25	a	409	PHO	C7-C6-C5	-2.01	107.90	113.26
24	b	607	CLA	OBD-CAD-C3D	-2.01	123.72	128.42
24	b	605	CLA	CHB-C1B-NB	-2.01	121.03	124.05
26	a	411	BCR	C2-C1-C6	2.01	113.36	110.44
24	c	509	CLA	C15-C13-C12	-2.01	101.89	112.07
24	B	611	CLA	C3A-C2A-C1A	-2.01	98.33	101.34
28	A	616	SQD	C4-C3-C2	-2.01	107.31	110.83
38	c	522	HTG	O5-C5-C4	-2.01	106.08	109.70
25	D	401	PHO	CMC-C2C-C1C	2.01	128.34	124.73
24	c	509	CLA	C1-C2-C3	-2.00	122.91	126.20
24	B	612	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
25	A	608	PHO	OBD-CAD-CBD	-2.00	122.88	125.82
28	h	105	SQD	O5-C1-O6	-2.00	105.31	110.04
24	B	603	CLA	C14-C13-C12	-2.00	104.14	111.27
24	c	507	CLA	C4B-C3B-C2B	-2.00	104.81	107.30
32	D	411	LHG	O7-C7-C8	2.00	115.81	111.48
26	T	102	BCR	C40-C30-C25	2.00	113.38	110.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
43	V	203	HEC	NA
43	v	202	HEC	NA

All (2104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	B	605	CLA	C1-C2-C3-C4
24	B	615	CLA	CAD-CBD-CGD-O1D
24	B	615	CLA	CAD-CBD-CGD-O2D
24	C	507	CLA	CHA-CBD-CGD-O1D
24	C	507	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
24	b	605	CLA	C1-C2-C3-C4
24	b	615	CLA	CAD-CBD-CGD-O1D
24	b	615	CLA	CAD-CBD-CGD-O2D
24	c	507	CLA	CHA-CBD-CGD-O1D
24	c	507	CLA	CHA-CBD-CGD-O2D
26	C	525	BCR	C7-C8-C9-C10
27	A	611	PL9	C23-C24-C26-C27
28	A	616	SQD	O6-C44-C45-O47
28	F	104	SQD	C8-C7-O47-C45
28	a	417	SQD	O6-C44-C45-O47
28	a	424	SQD	C2-C1-O6-C44
28	a	424	SQD	O5-C1-O6-C44
28	b	633	SQD	C8-C7-O47-C45
28	x	101	SQD	C2-C1-O6-C44
28	x	101	SQD	O5-C1-O6-C44
29	B	634	LMG	O9-C10-O7-C8
29	B	634	LMG	O10-C28-O8-C9
29	B	634	LMG	C29-C28-O8-C9
29	C	519	LMG	O7-C8-C9-O8
29	C	526	LMG	C2-C1-O1-C7
29	C	526	LMG	O6-C1-O1-C7
29	d	412	LMG	C2-C1-O1-C7
29	d	412	LMG	O6-C1-O1-C7
29	d	412	LMG	O9-C10-O7-C8
29	d	412	LMG	C11-C10-O7-C8
30	B	633	GOL	C1-C2-C3-O3
30	O	305	GOL	C1-C2-C3-O3
30	a	416	GOL	C1-C2-C3-O3
30	c	525	GOL	O1-C1-C2-O2
30	c	525	GOL	O1-C1-C2-C3
30	d	402	GOL	C1-C2-C3-O3
30	d	413	GOL	O1-C1-C2-C3
30	d	413	GOL	C1-C2-C3-O3
30	d	413	GOL	O2-C2-C3-O3
30	f	104	GOL	O1-C1-C2-C3
30	o	303	GOL	O1-C1-C2-C3
30	o	304	GOL	O1-C1-C2-C3
30	o	305	GOL	O1-C1-C2-C3
30	v	205	GOL	O1-C1-C2-O2
30	v	205	GOL	O1-C1-C2-C3
30	v	206	GOL	C1-C2-C3-O3
30	v	206	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	y	101	GOL	O1-C1-C2-C3
31	F	102	LMT	C2-C1-O1'-C1'
31	M	102	LMT	C2'-C1'-O1'-C1
31	M	102	LMT	O5'-C1'-O1'-C1
31	Y	101	LMT	C2-C1-O1'-C1'
31	j	103	LMT	O5'-C1'-O1'-C1
31	m	101	LMT	O5'-C1'-O1'-C1
32	A	618	LHG	C3-O3-P-O4
32	A	618	LHG	C3-O3-P-O5
32	A	618	LHG	C3-O3-P-O6
32	A	618	LHG	C4-O6-P-O3
32	A	618	LHG	C4-O6-P-O5
32	B	632	LHG	C4-O6-P-O3
32	B	632	LHG	C4-O6-P-O4
32	D	410	LHG	C3-O3-P-O4
32	D	410	LHG	C3-O3-P-O5
32	D	410	LHG	C3-O3-P-O6
32	a	419	LHG	C3-O3-P-O4
32	a	419	LHG	C3-O3-P-O5
32	a	419	LHG	C3-O3-P-O6
32	a	419	LHG	C8-C7-O7-C5
32	d	410	LHG	C3-O3-P-O5
32	d	410	LHG	C3-O3-P-O6
32	e	101	LHG	O1-C1-C2-C3
32	l	101	LHG	C4-O6-P-O3
32	l	101	LHG	C4-O6-P-O4
38	B	624	HTG	O5-C1-S1-C1'
38	C	531	HTG	O5-C1-S1-C1'
38	b	624	HTG	O5-C1-S1-C1'
38	c	522	HTG	O5-C1-S1-C1'
38	c	531	HTG	C2-C1-S1-C1'
40	D	408	DGD	C2B-C1B-O2G-C2G
40	D	408	DGD	O1B-C1B-O2G-C2G
40	D	408	DGD	C2D-C1D-O3G-C3G
40	d	408	DGD	O1B-C1B-O2G-C2G
40	d	408	DGD	C2D-C1D-O3G-C3G
41	E	113	HEM	C3D-CAD-CBD-CGD
31	I	101	LMT	C3'-C4'-O1B-C1B
31	Y	101	LMT	C2B-C1B-O1B-C4'
31	c	521	LMT	C3'-C4'-O1B-C1B
35	c	541	P6G	C14-C15-O16-C17
24	B	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	b	633	SQD	O10-C23-O48-C46
28	h	105	SQD	O10-C23-O48-C46
28	l	102	SQD	O10-C23-O48-C46
28	x	101	SQD	O10-C23-O48-C46
29	C	526	LMG	O10-C28-O8-C9
29	d	412	LMG	O10-C28-O8-C9
29	z	101	LMG	O10-C28-O8-C9
32	A	618	LHG	O10-C23-O8-C6
32	a	419	LHG	O10-C23-O8-C6
40	D	408	DGD	O1A-C1A-O1G-C1G
40	d	408	DGD	O1A-C1A-O1G-C1G
33	H	106	PG4	C3-C4-O3-C5
31	J	103	LMT	O5B-C1B-O1B-C4'
31	C	533	LMT	C3'-C4'-O1B-C1B
28	F	104	SQD	O49-C7-O47-C45
28	b	633	SQD	O49-C7-O47-C45
29	z	101	LMG	O9-C10-O7-C8
32	a	419	LHG	O9-C7-O7-C5
24	C	513	CLA	C3-C5-C6-C7
24	b	605	CLA	C3-C5-C6-C7
24	b	615	CLA	C3-C5-C6-C7
31	j	103	LMT	C2B-C1B-O1B-C4'
24	B	602	CLA	CBA-CGA-O2A-C1
28	A	622	SQD	C24-C23-O48-C46
28	l	102	SQD	C24-C23-O48-C46
29	C	526	LMG	C29-C28-O8-C9
29	d	412	LMG	C29-C28-O8-C9
29	z	101	LMG	C29-C28-O8-C9
32	A	618	LHG	C24-C23-O8-C6
32	a	419	LHG	C24-C23-O8-C6
40	D	408	DGD	C2A-C1A-O1G-C1G
24	C	501	CLA	CBD-CGD-O2D-CED
29	B	634	LMG	C11-C10-O7-C8
29	z	101	LMG	C11-C10-O7-C8
40	d	408	DGD	C2B-C1B-O2G-C2G
24	B	605	CLA	C2-C3-C5-C6
24	b	605	CLA	C2-C3-C5-C6
24	b	606	CLA	C2-C3-C5-C6
24	C	513	CLA	CBD-CGD-O2D-CED
24	B	617	CLA	C3-C5-C6-C7
24	B	617	CLA	CBA-CGA-O2A-C1
24	b	617	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	b	633	SQD	C24-C23-O48-C46
28	h	105	SQD	C24-C23-O48-C46
28	x	101	SQD	C24-C23-O48-C46
40	d	408	DGD	C2A-C1A-O1G-C1G
33	X	102	PG4	C4-C3-O2-C2
29	C	520	LMG	O6-C5-C6-O5
31	j	103	LMT	O5B-C5B-C6B-O6B
31	t	103	LMT	O5'-C5'-C6'-O6'
31	u	203	LMT	C2B-C1B-O1B-C4'
28	A	622	SQD	O10-C23-O48-C46
32	e	101	LHG	O10-C23-O8-C6
29	c	520	LMG	O6-C5-C6-O5
32	D	410	LHG	O2-C2-C3-O3
32	d	410	LHG	O2-C2-C3-O3
32	e	101	LHG	C24-C23-O8-C6
24	b	617	CLA	O1A-CGA-O2A-C1
38	B	631	HTG	C4-C5-C6-O6
38	H	101	HTG	O5-C5-C6-O6
38	b	632	HTG	O5-C5-C6-O6
31	t	103	LMT	C4'-C5'-C6'-O6'
28	l	102	SQD	C8-C7-O47-C45
28	x	101	SQD	C8-C7-O47-C45
38	h	101	HTG	O5-C5-C6-O6
38	B	623	HTG	S1-C1'-C2'-C3'
38	C	522	HTG	S1-C1'-C2'-C3'
27	A	611	PL9	C25-C24-C26-C27
24	B	606	CLA	C2-C3-C5-C6
24	B	617	CLA	O1A-CGA-O2A-C1
31	C	533	LMT	O5B-C5B-C6B-O6B
38	b	624	HTG	O5-C5-C6-O6
27	A	611	PL9	C9-C11-C12-C13
27	a	412	PL9	C19-C21-C22-C23
33	B	637	PG4	O2-C3-C4-O3
34	i	105	PGE	O2-C3-C4-O3
45	i	107	PE8	O7-C8-C9-O10
29	C	520	LMG	C4-C5-C6-O5
29	c	520	LMG	C4-C5-C6-O5
33	E	102	PG4	O3-C5-C6-O4
33	E	103	PG4	O3-C5-C6-O4
33	h	106	PG4	O3-C5-C6-O4
34	J	106	PGE	O2-C3-C4-O3
34	b	638	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
34	o	308	PGE	O2-C3-C4-O3
35	A	623	P6G	O10-C11-C12-O13
35	A	623	P6G	O13-C14-C15-O16
35	B	652	P6G	O10-C11-C12-O13
35	I	106	P6G	O13-C14-C15-O16
35	d	415	P6G	O10-C11-C12-O13
28	F	104	SQD	O5-C1-O6-C44
29	z	101	LMG	O6-C1-O1-C7
40	d	408	DGD	O6E-C1E-O5D-C6D
33	V	210	PG4	O3-C5-C6-O4
35	D	417	P6G	O4-C5-C6-O7
35	c	541	P6G	O10-C11-C12-O13
39	L	101	1PE	OH6-C15-C25-OH5
39	j	107	1PE	OH4-C13-C23-OH3
31	M	102	LMT	O5'-C5'-C6'-O6'
33	a	420	PG4	O3-C5-C6-O4
34	V	214	PGE	O2-C3-C4-O3
34	o	306	PGE	O2-C3-C4-O3
39	B	654	1PE	OH4-C13-C23-OH3
39	B	654	1PE	OH6-C15-C25-OH5
31	Y	101	LMT	O5B-C5B-C6B-O6B
31	u	203	LMT	O5B-C5B-C6B-O6B
31	A	617	LMT	C4B-C5B-C6B-O6B
31	j	103	LMT	C4B-C5B-C6B-O6B
38	B	630	HTG	C4-C5-C6-O6
33	B	637	PG4	O3-C5-C6-O4
33	C	536	PG4	O2-C3-C4-O3
34	x	103	PGE	O2-C3-C4-O3
35	b	649	P6G	O10-C11-C12-O13
31	J	103	LMT	O5'-C5'-C6'-O6'
33	c	534	PG4	O3-C5-C6-O4
33	l	103	PG4	O2-C3-C4-O3
34	a	422	PGE	O2-C3-C4-O3
35	b	648	P6G	O4-C5-C6-O7
34	O	309	PGE	C3-C4-O3-C5
35	D	418	P6G	O7-C8-C9-O10
33	V	213	PG4	O4-C7-C8-O5
28	l	102	SQD	O49-C7-O47-C45
28	x	101	SQD	O49-C7-O47-C45
32	a	419	LHG	C1-C2-C3-O3
32	d	410	LHG	C1-C2-C3-O3
33	D	414	PG4	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
38	B	631	HTG	O5-C5-C6-O6
33	J	105	PG4	O3-C5-C6-O4
33	i	101	PG4	O3-C5-C6-O4
34	i	106	PGE	O2-C3-C4-O3
35	C	541	P6G	O10-C11-C12-O13
35	b	649	P6G	O4-C5-C6-O7
40	c	516	DGD	C2A-C3A-C4A-C5A
34	I	105	PGE	O2-C3-C4-O3
34	J	108	PGE	O2-C3-C4-O3
31	C	533	LMT	C4B-C5B-C6B-O6B
31	M	102	LMT	C4'-C5'-C6'-O6'
31	Y	101	LMT	C4B-C5B-C6B-O6B
33	i	104	PG4	O3-C5-C6-O4
35	B	651	P6G	O7-C8-C9-O10
24	b	602	CLA	C3-C5-C6-C7
31	c	521	LMT	C4'-C5'-C6'-O6'
38	b	632	HTG	C4-C5-C6-O6
28	F	104	SQD	C2-C1-O6-C44
29	z	101	LMG	C2-C1-O1-C7
40	d	408	DGD	C2E-C1E-O5D-C6D
40	C	516	DGD	C1B-C2B-C3B-C4B
33	j	104	PG4	O2-C3-C4-O3
35	T	105	P6G	O13-C14-C15-O16
33	V	209	PG4	C8-C7-O4-C6
31	I	101	LMT	C4'-C5'-C6'-O6'
33	c	532	PG4	O3-C5-C6-O4
33	e	103	PG4	O3-C5-C6-O4
35	B	652	P6G	O4-C5-C6-O7
45	i	107	PE8	O16-C17-C18-O19
31	J	103	LMT	C2B-C1B-O1B-C4'
26	C	525	BCR	C7-C8-C9-C34
38	C	521	HTG	S1-C1'-C2'-C3'
38	C	529	HTG	S1-C1'-C2'-C3'
33	H	104	PG4	O3-C5-C6-O4
33	V	209	PG4	O2-C3-C4-O3
34	C	540	PGE	O2-C3-C4-O3
35	A	624	P6G	O7-C8-C9-O10
28	A	612	SQD	C7-C8-C9-C10
32	E	101	LHG	C7-C8-C9-C10
33	i	101	PG4	O2-C3-C4-O3
31	J	103	LMT	C4'-C5'-C6'-O6'
40	d	408	DGD	O6D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
33	i	103	PG4	O2-C3-C4-O3
34	O	310	PGE	O2-C3-C4-O3
39	e	105	1PE	OH5-C14-C24-OH4
24	A	609	CLA	CBA-CGA-O2A-C1
33	B	640	PG4	O2-C3-C4-O3
24	b	602	CLA	C15-C16-C17-C18
29	C	526	LMG	C10-C11-C12-C13
34	c	538	PGE	O2-C3-C4-O3
35	d	415	P6G	O7-C8-C9-O10
24	C	501	CLA	O1D-CGD-O2D-CED
24	B	616	CLA	C5-C6-C7-C8
33	X	102	PG4	O3-C5-C6-O4
33	b	635	PG4	O2-C3-C4-O3
39	B	653	1PE	OH6-C15-C25-OH5
30	b	629	GOL	O1-C1-C2-O2
30	d	402	GOL	O2-C2-C3-O3
29	c	519	LMG	C10-C11-C12-C13
40	D	408	DGD	C1A-C2A-C3A-C4A
33	C	538	PG4	O3-C5-C6-O4
35	j	106	P6G	O4-C5-C6-O7
24	C	513	CLA	O1D-CGD-O2D-CED
31	c	521	LMT	O1'-C1-C2-C3
24	b	604	CLA	CBD-CGD-O2D-CED
29	B	634	LMG	O6-C5-C6-O5
38	B	630	HTG	O5-C5-C6-O6
24	d	403	CLA	C2C-C3C-CAC-CBC
33	i	102	PG4	O3-C5-C6-O4
34	O	308	PGE	O2-C3-C4-O3
35	D	417	P6G	O10-C11-C12-O13
35	E	110	P6G	O4-C5-C6-O7
35	I	106	P6G	O7-C8-C9-O10
24	A	606	CLA	C15-C16-C17-C18
24	b	602	CLA	C10-C11-C12-C13
31	f	101	LMT	O1'-C1-C2-C3
33	V	213	PG4	O3-C5-C6-O4
33	j	104	PG4	O3-C5-C6-O4
34	h	107	PGE	O2-C3-C4-O3
34	o	307	PGE	O2-C3-C4-O3
33	B	639	PG4	O1-C1-C2-O2
33	C	536	PG4	O1-C1-C2-O2
33	K	102	PG4	O4-C7-C8-O5
33	e	103	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
34	B	649	PGE	O1-C1-C2-O2
34	E	108	PGE	O1-C1-C2-O2
34	H	108	PGE	O1-C1-C2-O2
34	c	536	PGE	O1-C1-C2-O2
34	c	539	PGE	O3-C5-C6-O4
34	c	540	PGE	O3-C5-C6-O4
34	h	107	PGE	O1-C1-C2-O2
34	h	108	PGE	O1-C1-C2-O2
34	o	306	PGE	O3-C5-C6-O4
35	A	624	P6G	O16-C17-C18-O19
39	e	105	1PE	OH7-C16-C26-OH6
39	x	104	1PE	OH7-C16-C26-OH6
27	A	611	PL9	C24-C26-C27-C28
31	u	203	LMT	C4B-C5B-C6B-O6B
31	C	533	LMT	O1'-C1-C2-C3
34	A	621	PGE	O2-C3-C4-O3
34	Y	102	PGE	O2-C3-C4-O3
35	B	651	P6G	O4-C5-C6-O7
29	z	101	LMG	O6-C5-C6-O5
31	a	401	LMT	O5B-C5B-C6B-O6B
28	a	417	SQD	C23-C24-C25-C26
32	D	409	LHG	C23-C24-C25-C26
40	C	517	DGD	C1B-C2B-C3B-C4B
40	c	516	DGD	C1B-C2B-C3B-C4B
24	a	410	CLA	C8-C10-C11-C12
40	D	408	DGD	O6D-C5D-C6D-O5D
38	b	624	HTG	C4-C5-C6-O6
43	V	203	HEC	C4C-C3C-CAC-CBC
33	B	641	PG4	O3-C5-C6-O4
34	f	105	PGE	O2-C3-C4-O3
39	j	107	1PE	OH5-C14-C24-OH4
24	A	609	CLA	C8-C10-C11-C12
24	B	616	CLA	C10-C11-C12-C13
24	C	506	CLA	C5-C6-C7-C8
24	b	602	CLA	C8-C10-C11-C12
24	d	405	CLA	C8-C10-C11-C12
31	A	617	LMT	O5B-C5B-C6B-O6B
33	J	105	PG4	O2-C3-C4-O3
28	A	616	SQD	C23-C24-C25-C26
28	h	105	SQD	C23-C24-C25-C26
29	C	519	LMG	C10-C11-C12-C13
32	d	409	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
40	c	517	DGD	C1A-C2A-C3A-C4A
38	C	531	HTG	S1-C1'-C2'-C3'
28	b	633	SQD	O5-C1-O6-C44
33	V	211	PG4	O3-C5-C6-O4
34	H	109	PGE	O2-C3-C4-O3
31	a	401	LMT	C4B-C5B-C6B-O6B
31	u	203	LMT	O5B-C1B-O1B-C4'
24	C	506	CLA	C10-C11-C12-C13
24	b	615	CLA	C10-C11-C12-C13
24	b	615	CLA	C15-C16-C17-C18
24	c	506	CLA	C10-C11-C12-C13
32	A	618	LHG	O2-C2-C3-O3
32	a	419	LHG	O2-C2-C3-O3
38	C	532	HTG	O5-C5-C6-O6
38	H	101	HTG	C4-C5-C6-O6
38	h	101	HTG	C4-C5-C6-O6
24	C	509	CLA	C8-C10-C11-C12
31	J	103	LMT	O1'-C1-C2-C3
31	M	102	LMT	O1'-C1-C2-C3
44	V	216	2PE	C23-C24-O25-C26
33	B	638	PG4	O3-C5-C6-O4
31	Y	101	LMT	O1'-C1-C2-C3
24	B	602	CLA	C5-C6-C7-C8
35	j	106	P6G	O13-C14-C15-O16
32	A	618	LHG	C23-C24-C25-C26
40	d	408	DGD	C4D-C5D-C6D-O5D
24	b	615	CLA	C5-C6-C7-C8
24	b	615	CLA	C8-C10-C11-C12
24	a	410	CLA	CBA-CGA-O2A-C1
33	I	102	PG4	O2-C3-C4-O3
35	d	416	P6G	O4-C5-C6-O7
24	A	609	CLA	O1A-CGA-O2A-C1
34	b	645	PGE	O2-C3-C4-O3
32	d	411	LHG	C12-C13-C14-C15
27	a	412	PL9	C31-C32-C33-C34
33	A	619	PG4	O1-C1-C2-O2
33	B	637	PG4	O1-C1-C2-O2
33	E	102	PG4	O1-C1-C2-O2
33	I	103	PG4	O4-C7-C8-O5
33	J	105	PG4	O1-C1-C2-O2
33	V	210	PG4	O1-C1-C2-O2
33	V	210	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
33	X	101	PG4	O1-C1-C2-O2
33	b	635	PG4	O4-C7-C8-O5
33	c	532	PG4	O1-C1-C2-O2
33	c	534	PG4	O4-C7-C8-O5
33	j	104	PG4	O1-C1-C2-O2
33	j	104	PG4	O4-C7-C8-O5
34	B	644	PGE	O3-C5-C6-O4
34	B	648	PGE	O3-C5-C6-O4
34	E	108	PGE	O3-C5-C6-O4
34	H	108	PGE	O3-C5-C6-O4
34	O	308	PGE	O3-C5-C6-O4
34	O	309	PGE	O3-C5-C6-O4
34	f	105	PGE	O3-C5-C6-O4
34	h	110	PGE	O3-C5-C6-O4
34	o	308	PGE	O3-C5-C6-O4
34	x	103	PGE	O3-C5-C6-O4
35	B	651	P6G	O16-C17-C18-O19
35	D	416	P6G	O16-C17-C18-O19
35	E	110	P6G	O16-C17-C18-O19
35	I	106	P6G	O16-C17-C18-O19
39	B	654	1PE	OH7-C16-C26-OH6
44	V	216	2PE	O25-C26-C27-O28
31	B	622	LMT	C5'-C4'-O1B-C1B
32	A	618	LHG	C1-C2-C3-O3
32	D	410	LHG	C1-C2-C3-O3
33	A	619	PG4	O2-C3-C4-O3
33	E	102	PG4	O2-C3-C4-O3
33	I	104	PG4	O3-C5-C6-O4
35	E	110	P6G	O7-C8-C9-O10
24	b	602	CLA	CBA-CGA-O2A-C1
28	F	104	SQD	C24-C23-O48-C46
29	A	613	LMG	C29-C28-O8-C9
32	E	101	LHG	C24-C23-O8-C6
24	b	612	CLA	C15-C16-C17-C18
31	j	103	LMT	O5B-C1B-O1B-C4'
31	m	101	LMT	O1'-C1-C2-C3
34	b	646	PGE	O2-C3-C4-O3
35	B	652	P6G	O7-C8-C9-O10
39	e	105	1PE	OH6-C15-C25-OH5
40	D	408	DGD	C4D-C5D-C6D-O5D
28	l	102	SQD	C7-C8-C9-C10
24	B	612	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	D	405	CLA	C8-C10-C11-C12
43	V	203	HEC	C2B-C3B-CAB-CBB
35	d	416	P6G	O10-C11-C12-O13
24	c	509	CLA	C8-C10-C11-C12
34	B	646	PGE	O2-C3-C4-O3
31	t	103	LMT	O5B-C5B-C6B-O6B
33	B	641	PG4	O2-C3-C4-O3
28	h	105	SQD	C8-C7-O47-C45
32	e	101	LHG	C8-C7-O7-C5
35	D	418	P6G	O10-C11-C12-O13
34	j	105	PGE	C4-C3-O2-C2
32	e	101	LHG	O9-C7-O7-C5
29	c	519	LMG	C28-C29-C30-C31
40	c	517	DGD	C1B-C2B-C3B-C4B
27	a	412	PL9	C9-C11-C12-C13
27	a	412	PL9	C14-C16-C17-C18
31	u	203	LMT	O1'-C1-C2-C3
34	c	540	PGE	O2-C3-C4-O3
35	D	417	P6G	O13-C14-C15-O16
34	o	309	PGE	O2-C3-C4-O3
38	c	530	HTG	C4-C5-C6-O6
26	C	515	BCR	C37-C22-C23-C24
38	c	531	HTG	S1-C1'-C2'-C3'
33	J	104	PG4	O3-C5-C6-O4
24	B	607	CLA	C2A-CAA-CBA-CGA
24	b	607	CLA	C2A-CAA-CBA-CGA
24	c	506	CLA	C15-C16-C17-C18
30	B	625	GOL	C1-C2-C3-O3
30	B	627	GOL	O1-C1-C2-C3
30	B	633	GOL	O1-C1-C2-C3
30	C	527	GOL	O1-C1-C2-C3
30	D	402	GOL	C1-C2-C3-O3
30	D	413	GOL	C1-C2-C3-O3
30	F	101	GOL	C1-C2-C3-O3
30	O	302	GOL	C1-C2-C3-O3
30	O	307	GOL	C1-C2-C3-O3
30	T	103	GOL	O1-C1-C2-C3
30	b	629	GOL	O1-C1-C2-C3
30	c	528	GOL	C1-C2-C3-O3
30	c	529	GOL	O1-C1-C2-C3
30	f	103	GOL	C1-C2-C3-O3
30	f	104	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	o	304	GOL	C1-C2-C3-O3
24	b	611	CLA	CBD-CGD-O2D-CED
29	B	634	LMG	C9-C8-O7-C10
24	C	506	CLA	C16-C17-C18-C19
24	b	611	CLA	C16-C17-C18-C20
24	b	602	CLA	O1A-CGA-O2A-C1
33	D	414	PG4	O2-C3-C4-O3
33	B	641	PG4	O4-C7-C8-O5
33	C	538	PG4	O4-C7-C8-O5
33	D	414	PG4	O1-C1-C2-O2
33	D	414	PG4	O4-C7-C8-O5
33	I	102	PG4	O4-C7-C8-O5
33	K	102	PG4	O1-C1-C2-O2
33	a	420	PG4	O1-C1-C2-O2
34	C	540	PGE	O3-C5-C6-O4
34	O	310	PGE	O1-C1-C2-O2
34	b	638	PGE	O1-C1-C2-O2
34	b	640	PGE	O3-C5-C6-O4
34	b	642	PGE	O1-C1-C2-O2
34	b	642	PGE	O3-C5-C6-O4
34	b	644	PGE	O3-C5-C6-O4
34	h	107	PGE	O3-C5-C6-O4
34	j	105	PGE	O1-C1-C2-O2
34	o	308	PGE	O1-C1-C2-O2
35	A	623	P6G	O16-C17-C18-O19
35	C	541	P6G	O1-C2-C3-O4
35	C	541	P6G	O16-C17-C18-O19
35	I	106	P6G	O1-C2-C3-O4
35	T	105	P6G	O1-C2-C3-O4
39	j	107	1PE	OH7-C16-C26-OH6
28	h	105	SQD	O49-C7-O47-C45
39	x	104	1PE	OH6-C15-C25-OH5
38	V	204	HTG	C1'-C2'-C3'-C4'
24	C	503	CLA	CBD-CGD-O2D-CED
35	d	415	P6G	O13-C14-C15-O16
31	B	622	LMT	C3'-C4'-O1B-C1B
24	c	506	CLA	C16-C17-C18-C20
35	E	110	P6G	C14-C15-O16-C17
34	J	107	PGE	O2-C3-C4-O3
32	E	101	LHG	C5-C6-O8-C23
29	J	101	LMG	C39-C40-C41-C42
29	a	414	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	d	412	LMG	C13-C14-C15-C16
32	E	101	LHG	C15-C16-C17-C18
40	c	518	DGD	CBA-CCA-CDA-CEA
28	A	612	SQD	C15-C16-C17-C18
28	A	622	SQD	C28-C29-C30-C31
29	A	613	LMG	C19-C20-C21-C22
29	B	621	LMG	C31-C32-C33-C34
29	C	526	LMG	C38-C39-C40-C41
29	b	621	LMG	C30-C31-C32-C33
29	j	101	LMG	C13-C14-C15-C16
32	l	101	LHG	C14-C15-C16-C17
38	h	101	HTG	C3'-C4'-C5'-C6'
40	D	408	DGD	CDA-CEA-CFA-CGA
28	A	622	SQD	C24-C25-C26-C27
28	l	102	SQD	C18-C19-C20-C21
29	b	621	LMG	C33-C34-C35-C36
29	d	412	LMG	C29-C30-C31-C32
31	J	103	LMT	C11-C10-C9-C8
31	a	401	LMT	C7-C8-C9-C10
32	E	101	LHG	C18-C19-C20-C21
40	C	516	DGD	C4A-C5A-C6A-C7A
40	C	516	DGD	C7A-C8A-C9A-CAA
28	F	104	SQD	O10-C23-O48-C46
28	a	424	SQD	C33-C34-C35-C36
29	C	519	LMG	C16-C17-C18-C19
29	a	414	LMG	C18-C19-C20-C21
29	c	519	LMG	C13-C14-C15-C16
33	a	420	PG4	O2-C3-C4-O3
30	B	625	GOL	O2-C2-C3-O3
30	B	633	GOL	O2-C2-C3-O3
30	D	402	GOL	O2-C2-C3-O3
30	O	302	GOL	O2-C2-C3-O3
30	c	529	GOL	O1-C1-C2-O2
30	d	413	GOL	O1-C1-C2-O2
30	f	104	GOL	O1-C1-C2-O2
30	f	104	GOL	O2-C2-C3-O3
30	o	303	GOL	O1-C1-C2-O2
30	o	304	GOL	O2-C2-C3-O3
30	o	305	GOL	O1-C1-C2-O2
30	y	101	GOL	O1-C1-C2-O2
31	J	103	LMT	C2-C1-O1'-C1'
32	e	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	A	616	SQD	C34-C35-C36-C37
28	F	104	SQD	C26-C27-C28-C29
32	d	409	LHG	C27-C28-C29-C30
40	c	517	DGD	C8B-C9B-CAB-CBB
24	D	405	CLA	C13-C15-C16-C17
38	a	418	HTG	C1'-C2'-C3'-C4'
29	B	634	LMG	C17-C18-C19-C20
29	C	520	LMG	C31-C32-C33-C34
29	j	101	LMG	C15-C16-C17-C18
31	t	103	LMT	C11-C10-C9-C8
24	C	506	CLA	C16-C17-C18-C20
28	l	102	SQD	C26-C27-C28-C29
29	C	519	LMG	C39-C40-C41-C42
29	z	101	LMG	C23-C24-C25-C26
28	A	622	SQD	C8-C7-O47-C45
32	d	411	LHG	C34-C35-C36-C37
33	d	414	PG4	O2-C3-C4-O3
28	a	424	SQD	C18-C19-C20-C21
29	A	613	LMG	C13-C14-C15-C16
40	C	518	DGD	CAA-CBA-CCA-CDA
31	F	102	LMT	C1-C2-C3-C4
31	J	103	LMT	C1-C2-C3-C4
31	a	401	LMT	C1-C2-C3-C4
31	I	101	LMT	O5'-C5'-C6'-O6'
28	A	612	SQD	C32-C33-C34-C35
28	l	102	SQD	C9-C10-C11-C12
29	J	101	LMG	C38-C39-C40-C41
29	z	101	LMG	C34-C35-C36-C37
31	u	203	LMT	C5-C6-C7-C8
31	u	203	LMT	C6-C7-C8-C9
40	H	103	DGD	CBB-CCB-CDB-CEB
43	V	203	HEC	C2C-C3C-CAC-CBC
28	x	101	SQD	C33-C34-C35-C36
40	C	518	DGD	C8A-C9A-CAA-CBA
40	c	517	DGD	C5A-C6A-C7A-C8A
28	b	633	SQD	C26-C27-C28-C29
29	c	520	LMG	C30-C31-C32-C33
29	z	101	LMG	C13-C14-C15-C16
31	B	622	LMT	C7-C8-C9-C10
32	a	419	LHG	C9-C10-C11-C12
38	C	529	HTG	C2'-C3'-C4'-C5'
24	A	609	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
24	C	507	CLA	C5-C6-C7-C8
32	E	101	LHG	C14-C15-C16-C17
32	E	101	LHG	O10-C23-O8-C6
28	A	612	SQD	C11-C12-C13-C14
28	A	612	SQD	C16-C17-C18-C19
32	e	101	LHG	C15-C16-C17-C18
24	a	407	CLA	C2C-C3C-CAC-CBC
33	B	636	PG4	O1-C1-C2-O2
33	B	638	PG4	O4-C7-C8-O5
33	E	103	PG4	O4-C7-C8-O5
33	H	107	PG4	O1-C1-C2-O2
33	c	533	PG4	O4-C7-C8-O5
34	A	620	PGE	O2-C3-C4-O3
34	A	621	PGE	O1-C1-C2-O2
34	H	111	PGE	O3-C5-C6-O4
34	a	422	PGE	O3-C5-C6-O4
34	b	639	PGE	O1-C1-C2-O2
34	b	641	PGE	O3-C5-C6-O4
34	b	645	PGE	O3-C5-C6-O4
34	c	537	PGE	O1-C1-C2-O2
34	h	109	PGE	O1-C1-C2-O2
35	A	623	P6G	O1-C2-C3-O4
35	D	417	P6G	O1-C2-C3-O4
35	D	418	P6G	O16-C17-C18-O19
35	c	541	P6G	O1-C2-C3-O4
39	x	104	1PE	OH2-C12-C22-OH3
44	V	216	2PE	O1-C2-C3-O4
31	I	101	LMT	C5-C6-C7-C8
29	c	520	LMG	C29-C28-O8-C9
29	B	634	LMG	C16-C17-C18-C19
29	a	414	LMG	C13-C14-C15-C16
35	T	105	P6G	O4-C5-C6-O7
28	A	616	SQD	C18-C19-C20-C21
28	x	101	SQD	C18-C19-C20-C21
29	C	519	LMG	C32-C33-C34-C35
29	c	519	LMG	C18-C19-C20-C21
29	c	519	LMG	C37-C38-C39-C40
29	c	520	LMG	C16-C17-C18-C19
31	C	533	LMT	C3-C4-C5-C6
32	D	411	LHG	C29-C30-C31-C32
32	E	101	LHG	C26-C27-C28-C29
32	e	101	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
40	C	517	DGD	CAB-CBB-CCB-CDB
40	D	408	DGD	C4A-C5A-C6A-C7A
40	c	518	DGD	CCB-CDB-CEB-CFB
29	A	613	LMG	O10-C28-O8-C9
33	i	104	PG4	O2-C3-C4-O3
28	a	417	SQD	C18-C19-C20-C21
29	c	520	LMG	C37-C38-C39-C40
31	c	521	LMT	C6-C7-C8-C9
40	H	103	DGD	C7A-C8A-C9A-CAA
36	d	417	EDO	O1-C1-C2-O2
29	c	520	LMG	C15-C16-C17-C18
40	D	408	DGD	CBA-CCA-CDA-CEA
29	C	520	LMG	C38-C39-C40-C41
24	A	609	CLA	C16-C17-C18-C19
24	b	603	CLA	C16-C17-C18-C19
29	C	520	LMG	C10-C11-C12-C13
31	I	101	LMT	O1'-C1-C2-C3
40	d	408	DGD	O6E-C5E-C6E-O5E
26	B	618	BCR	C1-C6-C7-C8
26	K	101	BCR	C5-C6-C7-C8
26	b	620	BCR	C5-C6-C7-C8
26	d	406	BCR	C23-C24-C25-C26
26	d	406	BCR	C23-C24-C25-C30
28	x	101	SQD	C11-C12-C13-C14
28	x	101	SQD	C12-C13-C14-C15
29	a	414	LMG	C20-C21-C22-C23
29	c	519	LMG	C14-C15-C16-C17
32	d	411	LHG	C29-C30-C31-C32
24	B	602	CLA	CBD-CGD-O2D-CED
29	C	519	LMG	C29-C28-O8-C9
35	D	417	P6G	O7-C8-C9-O10
31	F	102	LMT	C5-C6-C7-C8
31	u	203	LMT	C4-C5-C6-C7
28	h	105	SQD	C12-C13-C14-C15
32	D	409	LHG	C29-C30-C31-C32
38	H	101	HTG	C3'-C4'-C5'-C6'
40	D	408	DGD	C2B-C3B-C4B-C5B
40	H	103	DGD	CBA-CCA-CDA-CEA
40	c	516	DGD	C4B-C5B-C6B-C7B
32	a	419	LHG	C10-C11-C12-C13
40	C	516	DGD	C4B-C5B-C6B-C7B
24	a	410	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	a	417	SQD	C27-C28-C29-C30
25	d	401	PHO	C2C-C3C-CAC-CBC
24	a	410	CLA	C10-C11-C12-C13
28	a	424	SQD	C9-C10-C11-C12
29	z	101	LMG	C18-C19-C20-C21
32	D	411	LHG	C13-C14-C15-C16
24	b	602	CLA	C11-C10-C8-C9
29	B	621	LMG	C34-C35-C36-C37
40	C	518	DGD	C2A-C3A-C4A-C5A
40	c	516	DGD	C5B-C6B-C7B-C8B
40	d	408	DGD	CDB-CEB-CFB-CGB
24	C	506	CLA	C13-C15-C16-C17
24	c	512	CLA	C15-C16-C17-C18
35	D	416	P6G	O13-C14-C15-O16
28	a	424	SQD	C26-C27-C28-C29
29	C	526	LMG	C40-C41-C42-C43
29	a	414	LMG	C29-C30-C31-C32
40	C	516	DGD	CAA-CBA-CCA-CDA
40	c	516	DGD	C4D-C5D-C6D-O5D
28	A	616	SQD	C32-C33-C34-C35
28	F	104	SQD	C24-C25-C26-C27
28	a	413	SQD	C29-C30-C31-C32
31	t	103	LMT	C4-C5-C6-C7
40	D	408	DGD	C7A-C8A-C9A-CAA
40	D	408	DGD	C7B-C8B-C9B-CAB
28	h	105	SQD	C2-C1-O6-C44
24	C	509	CLA	C10-C11-C12-C13
24	d	405	CLA	C15-C16-C17-C18
29	d	412	LMG	C31-C32-C33-C34
31	F	102	LMT	C4-C5-C6-C7
28	a	424	SQD	C11-C10-C9-C8
31	B	622	LMT	C6-C7-C8-C9
24	C	502	CLA	C16-C17-C18-C20
29	c	519	LMG	C11-C10-O7-C8
32	E	101	LHG	C8-C7-O7-C5
28	A	622	SQD	C17-C18-C19-C20
24	b	609	CLA	C13-C15-C16-C17
38	C	522	HTG	O5-C5-C6-O6
33	C	537	PG4	O4-C7-C8-O5
33	V	213	PG4	O1-C1-C2-O2
33	i	102	PG4	O4-C7-C8-O5
33	i	103	PG4	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
34	B	645	PGE	O1-C1-C2-O2
34	E	106	PGE	O3-C5-C6-O4
34	V	215	PGE	O1-C1-C2-O2
34	b	643	PGE	O1-C1-C2-O2
34	b	647	PGE	O3-C5-C6-O4
35	D	417	P6G	O16-C17-C18-O19
28	A	622	SQD	O49-C7-O47-C45
29	c	519	LMG	O9-C10-O7-C8
32	D	409	LHG	C30-C31-C32-C33
32	e	101	LHG	C27-C28-C29-C30
40	C	516	DGD	C5B-C6B-C7B-C8B
34	V	215	PGE	O2-C3-C4-O3
31	t	103	LMT	C7-C8-C9-C10
34	c	537	PGE	O2-C3-C4-O3
38	a	418	HTG	C4-C5-C6-O6
29	a	414	LMG	C10-C11-C12-C13
33	C	534	PG4	O2-C3-C4-O3
28	a	424	SQD	C45-C44-O6-C1
29	C	526	LMG	C8-C7-O1-C1
29	z	101	LMG	C8-C7-O1-C1
40	C	517	DGD	C2G-C3G-O3G-C1D
28	b	633	SQD	C9-C10-C11-C12
24	B	611	CLA	C16-C17-C18-C20
24	b	603	CLA	C16-C17-C18-C20
24	c	512	CLA	C16-C17-C18-C19
39	x	104	1PE	OH5-C14-C24-OH4
28	b	633	SQD	C25-C26-C27-C28
29	C	526	LMG	C18-C19-C20-C21
40	c	516	DGD	O6D-C5D-C6D-O5D
29	C	526	LMG	C41-C42-C43-C44
29	z	101	LMG	C32-C33-C34-C35
32	d	409	LHG	C30-C31-C32-C33
34	b	639	PGE	C6-C5-O3-C4
31	j	103	LMT	C1-C2-C3-C4
35	E	110	P6G	O10-C11-C12-O13
35	b	649	P6G	O13-C14-C15-O16
39	B	653	1PE	OH5-C14-C24-OH4
33	B	641	PG4	C4-C3-O2-C2
35	B	652	P6G	C11-C12-O13-C14
29	c	520	LMG	O10-C28-O8-C9
29	J	101	LMG	O6-C5-C6-O5
29	c	520	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	A	622	SQD	C25-C26-C27-C28
29	j	101	LMG	C14-C15-C16-C17
28	h	105	SQD	C24-C25-C26-C27
29	B	634	LMG	C13-C14-C15-C16
40	c	517	DGD	C3A-C4A-C5A-C6A
29	a	414	LMG	C11-C10-O7-C8
33	U	202	PG4	O3-C5-C6-O4
34	D	415	PGE	O2-C3-C4-O3
34	h	109	PGE	O2-C3-C4-O3
29	c	520	LMG	C38-C39-C40-C41
33	c	533	PG4	O3-C5-C6-O4
35	d	416	P6G	O7-C8-C9-O10
35	j	106	P6G	O10-C11-C12-O13
29	A	613	LMG	C12-C13-C14-C15
31	j	103	LMT	C7-C8-C9-C10
38	C	530	HTG	C3'-C4'-C5'-C6'
43	v	202	HEC	C2B-C3B-CAB-CBB
28	l	102	SQD	C15-C16-C17-C18
29	B	634	LMG	C18-C19-C20-C21
29	C	519	LMG	C35-C36-C37-C38
29	J	101	LMG	C12-C13-C14-C15
31	A	617	LMT	O1'-C1-C2-C3
32	a	419	LHG	O7-C5-C6-O8
40	d	408	DGD	C2B-C3B-C4B-C5B
28	F	104	SQD	C31-C32-C33-C34
31	a	401	LMT	C11-C10-C9-C8
32	A	618	LHG	C11-C12-C13-C14
31	I	101	LMT	O5B-C5B-C6B-O6B
38	C	531	HTG	C4-C5-C6-O6
28	l	102	SQD	C28-C29-C30-C31
31	u	203	LMT	C2-C3-C4-C5
38	C	531	HTG	C2'-C3'-C4'-C5'
24	b	617	CLA	C2-C1-O2A-CGA
29	j	101	LMG	O6-C5-C6-O5
24	b	611	CLA	C16-C17-C18-C19
31	Y	101	LMT	C1-C2-C3-C4
28	a	413	SQD	C10-C11-C12-C13
28	a	413	SQD	C33-C34-C35-C36
32	D	411	LHG	C34-C35-C36-C37
33	B	638	PG4	O1-C1-C2-O2
33	B	639	PG4	O4-C7-C8-O5
33	B	642	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
33	B	643	PG4	O4-C7-C8-O5
33	C	535	PG4	O1-C1-C2-O2
33	C	535	PG4	O4-C7-C8-O5
33	I	102	PG4	O1-C1-C2-O2
33	V	209	PG4	O4-C7-C8-O5
33	V	212	PG4	O1-C1-C2-O2
33	X	103	PG4	O1-C1-C2-O2
33	a	421	PG4	O1-C1-C2-O2
33	a	421	PG4	O4-C7-C8-O5
33	b	636	PG4	O1-C1-C2-O2
33	c	532	PG4	O4-C7-C8-O5
33	h	106	PG4	O4-C7-C8-O5
33	i	101	PG4	O4-C7-C8-O5
33	i	104	PG4	O1-C1-C2-O2
33	l	103	PG4	O4-C7-C8-O5
34	B	645	PGE	O3-C5-C6-O4
34	B	647	PGE	O1-C1-C2-O2
34	C	540	PGE	O1-C1-C2-O2
34	H	109	PGE	O1-C1-C2-O2
34	H	109	PGE	O3-C5-C6-O4
34	H	110	PGE	O1-C1-C2-O2
34	H	111	PGE	O1-C1-C2-O2
34	O	310	PGE	O3-C5-C6-O4
34	T	104	PGE	O2-C3-C4-O3
34	V	214	PGE	O3-C5-C6-O4
34	i	105	PGE	O1-C1-C2-O2
34	o	309	PGE	O3-C5-C6-O4
35	A	624	P6G	O1-C2-C3-O4
35	D	418	P6G	O1-C2-C3-O4
35	b	648	P6G	O16-C17-C18-O19
35	b	649	P6G	O1-C2-C3-O4
35	b	649	P6G	O16-C17-C18-O19
35	j	106	P6G	O16-C17-C18-O19
45	i	107	PE8	O1-C2-C3-O4
28	l	102	SQD	C10-C11-C12-C13
40	D	408	DGD	CEB-CFB-CGB-CHB
40	c	518	DGD	C2A-C3A-C4A-C5A
28	b	633	SQD	C34-C35-C36-C37
29	C	520	LMG	C37-C38-C39-C40
31	M	102	LMT	C2-C3-C4-C5
32	l	101	LHG	C5-C6-O8-C23
32	B	632	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	C5-C6-C7-C8
29	A	613	LMG	C10-C11-C12-C13
28	a	413	SQD	C34-C35-C36-C37
29	z	101	LMG	C15-C16-C17-C18
28	h	105	SQD	C15-C16-C17-C18
29	b	621	LMG	C35-C36-C37-C38
30	a	416	GOL	O2-C2-C3-O3
24	b	611	CLA	O1D-CGD-O2D-CED
33	B	636	PG4	O3-C5-C6-O4
35	C	541	P6G	O13-C14-C15-O16
24	B	611	CLA	C13-C15-C16-C17
31	b	622	LMT	C3'-C4'-O1B-C1B
29	c	519	LMG	C32-C33-C34-C35
40	d	408	DGD	C5A-C6A-C7A-C8A
34	b	643	PGE	O2-C3-C4-O3
29	A	613	LMG	C18-C19-C20-C21
32	D	409	LHG	C27-C28-C29-C30
32	d	411	LHG	C15-C16-C17-C18
29	d	412	LMG	O6-C5-C6-O5
29	a	414	LMG	O9-C10-O7-C8
28	A	622	SQD	C26-C27-C28-C29
29	d	412	LMG	C11-C12-C13-C14
33	A	619	PG4	O3-C5-C6-O4
40	C	516	DGD	O6D-C5D-C6D-O5D
24	c	509	CLA	C13-C15-C16-C17
29	c	520	LMG	C10-C11-C12-C13
40	d	408	DGD	C6A-C7A-C8A-C9A
28	l	102	SQD	C27-C28-C29-C30
29	C	519	LMG	O10-C28-O8-C9
24	b	602	CLA	C6-C7-C8-C9
28	h	105	SQD	C31-C32-C33-C34
34	E	105	PGE	O2-C3-C4-O3
40	c	516	DGD	CAA-CBA-CCA-CDA
31	J	103	LMT	O5B-C5B-C6B-O6B
31	I	101	LMT	C4-C5-C6-C7
32	d	409	LHG	C29-C30-C31-C32
33	b	636	PG4	O4-C7-C8-O5
34	D	415	PGE	O1-C1-C2-O2
34	E	109	PGE	O3-C5-C6-O4
34	J	107	PGE	O3-C5-C6-O4
34	O	308	PGE	O1-C1-C2-O2
34	b	640	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
34	h	108	PGE	O3-C5-C6-O4
32	E	101	LHG	O9-C7-O7-C5
28	A	622	SQD	C2-C1-O6-C44
40	C	516	DGD	O6E-C5E-C6E-O5E
28	a	424	SQD	C23-C24-C25-C26
33	X	102	PG4	O2-C3-C4-O3
28	A	622	SQD	C44-C45-C46-O48
28	a	413	SQD	O6-C44-C45-C46
29	A	613	LMG	C7-C8-C9-O8
29	B	634	LMG	C7-C8-C9-O8
29	C	519	LMG	C7-C8-C9-O8
29	a	414	LMG	C7-C8-C9-O8
29	z	101	LMG	C7-C8-C9-O8
32	A	618	LHG	C4-C5-C6-O8
32	a	419	LHG	C4-C5-C6-O8
32	e	101	LHG	C4-C5-C6-O8
40	D	408	DGD	O1G-C1G-C2G-C3G
40	D	408	DGD	C1G-C2G-C3G-O3G
31	u	203	LMT	C11-C10-C9-C8
28	A	622	SQD	C27-C28-C29-C30
38	O	303	HTG	C3'-C4'-C5'-C6'
24	A	606	CLA	C2C-C3C-CAC-CBC
28	a	413	SQD	C9-C10-C11-C12
33	e	104	PG4	O3-C5-C6-O4
40	c	516	DGD	O6E-C5E-C6E-O5E
24	A	607	CLA	C11-C12-C13-C15
24	A	609	CLA	C16-C17-C18-C20
32	D	411	LHG	C17-C18-C19-C20
36	B	656	EDO	O1-C1-C2-O2
36	C	542	EDO	O1-C1-C2-O2
36	o	311	EDO	O1-C1-C2-O2
24	b	616	CLA	C10-C11-C12-C13
40	c	518	DGD	C9B-CAB-CBB-CCB
35	D	418	P6G	O4-C5-C6-O7
31	B	622	LMT	C2-C3-C4-C5
40	d	408	DGD	C4A-C5A-C6A-C7A
31	c	521	LMT	O5'-C5'-C6'-O6'
33	B	643	PG4	O2-C3-C4-O3
29	B	634	LMG	C29-C30-C31-C32
33	C	537	PG4	O3-C5-C6-O4
28	a	424	SQD	C28-C29-C30-C31
32	E	101	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
31	b	622	LMT	C5'-C4'-O1B-C1B
26	C	515	BCR	C21-C22-C23-C24
24	b	604	CLA	C5-C6-C7-C8
33	H	105	PG4	O3-C5-C6-O4
34	E	109	PGE	O2-C3-C4-O3
33	B	642	PG4	O2-C3-C4-O3
30	C	528	GOL	O1-C1-C2-C3
30	b	625	GOL	O1-C1-C2-C3
28	a	424	SQD	C46-C45-O47-C7
28	b	633	SQD	C46-C45-O47-C7
31	Y	101	LMT	C11-C10-C9-C8
39	L	101	1PE	OH5-C14-C24-OH4
28	F	104	SQD	C9-C10-C11-C12
32	e	101	LHG	C11-C12-C13-C14
28	h	105	SQD	C27-C28-C29-C30
29	a	414	LMG	C33-C34-C35-C36
40	d	408	DGD	CDA-CEA-CFA-CGA
33	B	637	PG4	O4-C7-C8-O5
33	B	640	PG4	O4-C7-C8-O5
33	C	534	PG4	O1-C1-C2-O2
33	H	106	PG4	O4-C7-C8-O5
33	V	211	PG4	O1-C1-C2-O2
33	i	101	PG4	O1-C1-C2-O2
34	o	307	PGE	O3-C5-C6-O4
34	o	309	PGE	O1-C1-C2-O2
32	a	419	LHG	C31-C32-C33-C34
40	d	408	DGD	C7A-C8A-C9A-CAA
29	d	412	LMG	C24-C25-C26-C27
29	a	414	LMG	C35-C36-C37-C38
24	C	507	CLA	C2-C3-C5-C6
28	b	633	SQD	C33-C34-C35-C36
29	A	613	LMG	C34-C35-C36-C37
29	c	519	LMG	C16-C17-C18-C19
29	c	519	LMG	C21-C22-C23-C24
40	c	516	DGD	C4A-C5A-C6A-C7A
24	b	615	CLA	C16-C17-C18-C20
29	A	613	LMG	C17-C18-C19-C20
29	C	526	LMG	C42-C43-C44-C45
38	B	630	HTG	C4'-C5'-C6'-C7'
25	D	401	PHO	C2C-C3C-CAC-CBC
32	B	632	LHG	C13-C14-C15-C16
28	a	413	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
39	L	101	1PE	C12-C22-OH3-C23
29	A	613	LMG	C30-C31-C32-C33
29	C	526	LMG	C29-C30-C31-C32
29	b	621	LMG	C39-C40-C41-C42
29	z	101	LMG	C12-C13-C14-C15
32	B	632	LHG	C28-C29-C30-C31
32	l	101	LHG	C13-C14-C15-C16
33	H	105	PG4	O2-C3-C4-O3
28	h	105	SQD	C19-C20-C21-C22
28	a	413	SQD	C15-C16-C17-C18
32	E	101	LHG	C10-C11-C12-C13
40	C	517	DGD	C4A-C5A-C6A-C7A
28	x	101	SQD	C35-C36-C37-C38
28	A	616	SQD	C30-C31-C32-C33
32	B	632	LHG	C14-C15-C16-C17
40	d	408	DGD	C1A-C2A-C3A-C4A
28	a	413	SQD	C31-C32-C33-C34
40	h	104	DGD	CCA-CDA-CEA-CFA
24	C	509	CLA	C13-C15-C16-C17
24	c	513	CLA	C10-C11-C12-C13
24	C	503	CLA	O1D-CGD-O2D-CED
27	A	611	PL9	C30-C29-C31-C32
29	B	621	LMG	C30-C31-C32-C33
33	i	102	PG4	O2-C3-C4-O3
38	b	623	HTG	C4'-C5'-C6'-C7'
28	h	105	SQD	C32-C33-C34-C35
29	C	526	LMG	C11-C12-C13-C14
29	C	526	LMG	C33-C34-C35-C36
35	A	624	P6G	O4-C5-C6-O7
33	X	102	PG4	O4-C7-C8-O5
34	j	105	PGE	O3-C5-C6-O4
29	d	412	LMG	C14-C15-C16-C17
30	B	633	GOL	O1-C1-C2-O2
30	C	527	GOL	O1-C1-C2-O2
30	D	412	GOL	O1-C1-C2-O2
30	F	101	GOL	O2-C2-C3-O3
30	O	307	GOL	O2-C2-C3-O3
24	c	509	CLA	C3-C5-C6-C7
24	A	609	CLA	C11-C10-C8-C9
31	C	533	LMT	C7-C8-C9-C10
38	V	204	HTG	C2'-C3'-C4'-C5'
28	a	417	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
29	j	101	LMG	C16-C17-C18-C19
40	C	517	DGD	CBB-CCB-CDB-CEB
40	c	517	DGD	C7B-C8B-C9B-CAB
33	H	107	PG4	O2-C3-C4-O3
40	d	408	DGD	CFB-CGB-CHB-CIB
31	c	521	LMT	C7-C8-C9-C10
28	A	612	SQD	C28-C29-C30-C31
29	a	414	LMG	C39-C40-C41-C42
29	z	101	LMG	C21-C22-C23-C24
32	A	618	LHG	C14-C15-C16-C17
32	e	101	LHG	C23-C24-C25-C26
31	a	401	LMT	C9-C10-C11-C12
32	a	419	LHG	O6-C4-C5-C6
28	a	424	SQD	C16-C17-C18-C19
28	b	633	SQD	C30-C31-C32-C33
29	B	621	LMG	C29-C30-C31-C32
40	c	516	DGD	C9A-CAA-CBA-CCA
24	A	609	CLA	C11-C10-C8-C7
24	b	602	CLA	C6-C7-C8-C10
28	A	616	SQD	C19-C20-C21-C22
29	c	520	LMG	C40-C41-C42-C43
32	A	618	LHG	C15-C16-C17-C18
29	c	520	LMG	C31-C32-C33-C34
31	j	103	LMT	O5'-C5'-C6'-O6'
28	a	417	SQD	C29-C30-C31-C32
40	c	516	DGD	C2B-C3B-C4B-C5B
24	b	604	CLA	O1D-CGD-O2D-CED
33	B	639	PG4	O3-C5-C6-O4
28	x	101	SQD	C24-C25-C26-C27
32	D	410	LHG	C32-C33-C34-C35
40	C	517	DGD	C4B-C5B-C6B-C7B
40	H	103	DGD	C9B-CAB-CBB-CCB
24	d	405	CLA	C10-C11-C12-C13
40	C	516	DGD	C4D-C5D-C6D-O5D
29	d	412	LMG	C17-C18-C19-C20
29	d	412	LMG	C40-C41-C42-C43
31	J	103	LMT	C6-C7-C8-C9
31	f	101	LMT	C11-C10-C9-C8
31	C	533	LMT	C9-C10-C11-C12
29	z	101	LMG	C35-C36-C37-C38
32	e	101	LHG	C13-C14-C15-C16
28	A	616	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
34	E	107	PGE	O1-C1-C2-O2
33	H	107	PG4	O3-C5-C6-O4
29	a	414	LMG	C22-C23-C24-C25
28	l	102	SQD	C29-C30-C31-C32
27	d	407	PL9	C39-C41-C42-C43
28	A	616	SQD	O6-C44-C45-C46
28	a	417	SQD	O6-C44-C45-C46
28	b	633	SQD	C44-C45-C46-O48
28	h	105	SQD	O6-C44-C45-C46
40	d	408	DGD	O1G-C1G-C2G-C3G
34	b	647	PGE	O2-C3-C4-O3
40	h	104	DGD	CDB-CEB-CFB-CGB
24	B	602	CLA	C3-C5-C6-C7
34	E	107	PGE	O2-C3-C4-O3
39	L	101	1PE	OH4-C13-C23-OH3
34	h	108	PGE	O2-C3-C4-O3
40	C	518	DGD	C9B-CAB-CBB-CCB
24	B	606	CLA	C1-C2-C3-C4
24	b	606	CLA	C1-C2-C3-C4
29	A	613	LMG	C38-C39-C40-C41
38	C	521	HTG	C2'-C3'-C4'-C5'
27	A	611	PL9	C28-C29-C31-C32
32	A	618	LHG	C9-C10-C11-C12
32	E	101	LHG	C12-C13-C14-C15
31	C	533	LMT	O5'-C5'-C6'-O6'
31	A	617	LMT	C5-C6-C7-C8
24	c	506	CLA	C16-C17-C18-C19
32	a	419	LHG	O6-C4-C5-O7
28	a	424	SQD	C25-C26-C27-C28
29	b	621	LMG	C38-C39-C40-C41
35	T	105	P6G	O7-C8-C9-O10
26	T	102	BCR	C23-C24-C25-C26
44	V	216	2PE	O10-C11-C12-O13
43	V	203	HEC	C4B-C3B-CAB-CBB
24	C	513	CLA	C8-C10-C11-C12
38	b	624	HTG	C1'-C2'-C3'-C4'
28	l	102	SQD	C14-C15-C16-C17
29	a	414	LMG	C19-C20-C21-C22
31	C	533	LMT	C6-C7-C8-C9
31	b	622	LMT	C2-C3-C4-C5
40	c	518	DGD	C3B-C4B-C5B-C6B
40	h	104	DGD	C9B-CAB-CBB-CCB

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Mol	Chain	Res	Type	Atoms
31	m	101	LMT	C9-C10-C11-C12
28	a	424	SQD	C30-C31-C32-C33
31	B	622	LMT	C4-C5-C6-C7
40	C	517	DGD	C5B-C6B-C7B-C8B
40	D	408	DGD	C8A-C9A-CAA-CBA
28	h	105	SQD	C17-C18-C19-C20
31	t	103	LMT	C6-C7-C8-C9
40	D	408	DGD	CDB-CEB-CFB-CGB
24	B	611	CLA	C16-C17-C18-C19
28	b	633	SQD	O47-C45-C46-O48
28	x	101	SQD	O47-C45-C46-O48
29	B	634	LMG	O7-C8-C9-O8
29	z	101	LMG	O1-C7-C8-O7
40	d	408	DGD	O1G-C1G-C2G-O2G
27	a	412	PL9	C4-C3-C7-C8
38	a	418	HTG	O5-C1-S1-C1'
38	c	531	HTG	O5-C1-S1-C1'
29	B	621	LMG	C36-C37-C38-C39
32	l	101	LHG	C32-C33-C34-C35
33	j	104	PG4	C8-C7-O4-C6
34	J	107	PGE	O1-C1-C2-O2
39	e	105	1PE	OH2-C12-C22-OH3
28	h	105	SQD	C25-C26-C27-C28
40	C	517	DGD	CDB-CEB-CFB-CGB
34	O	309	PGE	O2-C3-C4-O3
29	z	101	LMG	C14-C15-C16-C17
24	A	607	CLA	C11-C12-C13-C14
24	D	403	CLA	C2C-C3C-CAC-CBC
29	C	520	LMG	C40-C41-C42-C43
40	H	103	DGD	C6B-C7B-C8B-C9B
40	c	516	DGD	CCA-CDA-CEA-CFA
31	j	103	LMT	C2-C3-C4-C5
28	a	424	SQD	C14-C15-C16-C17
29	C	520	LMG	C15-C16-C17-C18
31	Y	101	LMT	C2-C3-C4-C5
38	c	531	HTG	C2'-C3'-C4'-C5'
33	V	212	PG4	O2-C3-C4-O3
39	B	653	1PE	OH4-C13-C23-OH3
29	b	621	LMG	C40-C41-C42-C43
28	A	622	SQD	C16-C17-C18-C19
38	c	531	HTG	C3'-C4'-C5'-C6'
40	c	518	DGD	C6A-C7A-C8A-C9A

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Mol	Chain	Res	Type	Atoms
33	e	103	PG4	O2-C3-C4-O3
31	c	521	LMT	C5-C6-C7-C8
32	e	101	LHG	C26-C27-C28-C29
31	m	102	LMT	O5'-C5'-C6'-O6'
29	B	634	LMG	C31-C32-C33-C34
35	I	106	P6G	C14-C15-O16-C17
30	D	412	GOL	O2-C2-C3-O3
30	O	305	GOL	O2-C2-C3-O3
30	V	208	GOL	O1-C1-C2-O2
30	V	208	GOL	O2-C2-C3-O3
40	h	104	DGD	O2G-C1B-C2B-C3B
33	j	104	PG4	C3-C4-O3-C5
34	c	537	PGE	C1-C2-O2-C3
34	c	538	PGE	C3-C4-O3-C5
34	h	109	PGE	C3-C4-O3-C5
34	o	309	PGE	C6-C5-O3-C4
29	C	526	LMG	C23-C24-C25-C26
33	E	102	PG4	C3-C4-O3-C5
34	O	309	PGE	O1-C1-C2-O2
35	T	105	P6G	O16-C17-C18-O19
33	B	643	PG4	C4-C3-O2-C2
34	B	648	PGE	C1-C2-O2-C3
35	C	541	P6G	C18-C17-O16-C15
35	D	417	P6G	C2-C3-O4-C5
39	x	104	1PE	C13-C23-OH3-C22
29	c	519	LMG	C39-C40-C41-C42
40	C	516	DGD	C7B-C8B-C9B-CAB
29	c	519	LMG	C22-C23-C24-C25
33	C	537	PG4	C1-C2-O2-C3
34	C	539	PGE	C3-C4-O3-C5
34	c	540	PGE	C1-C2-O2-C3
28	a	413	SQD	C24-C23-O48-C46
39	V	217	1PE	C23-C13-OH4-C24
32	D	411	LHG	C10-C11-C12-C13
24	c	512	CLA	C16-C17-C18-C20
33	H	106	PG4	O3-C5-C6-O4
32	a	419	LHG	C28-C29-C30-C31
35	A	623	P6G	C12-C11-O10-C9
24	B	614	CLA	C13-C15-C16-C17
26	b	620	BCR	C7-C8-C9-C34
32	a	419	LHG	C29-C30-C31-C32
34	B	648	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
24	B	616	CLA	C12-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C15
24	b	605	CLA	C6-C7-C8-C10
33	b	635	PG4	C4-C3-O2-C2
35	T	105	P6G	C15-C14-O13-C12
35	b	649	P6G	C14-C15-O16-C17
45	i	107	PE8	C21-C20-O19-C18
32	A	618	LHG	C24-C25-C26-C27
33	e	104	PG4	C8-C7-O4-C6
33	j	104	PG4	C4-C3-O2-C2
34	H	108	PGE	C6-C5-O3-C4
35	E	110	P6G	C5-C6-O7-C8
24	b	617	CLA	C5-C6-C7-C8
26	c	527	BCR	C7-C8-C9-C10
34	D	415	PGE	C1-C2-O2-C3
34	b	646	PGE	C4-C3-O2-C2
35	d	415	P6G	C15-C14-O13-C12
28	h	105	SQD	C45-C44-O6-C1
29	C	520	LMG	C8-C7-O1-C1
29	c	520	LMG	C8-C7-O1-C1
40	C	517	DGD	C5D-C6D-O5D-C1E
40	D	408	DGD	C5D-C6D-O5D-C1E
40	c	517	DGD	C2G-C3G-O3G-C1D
40	c	517	DGD	C5D-C6D-O5D-C1E
33	B	640	PG4	C5-C6-O4-C7
33	C	536	PG4	C1-C2-O2-C3
34	A	620	PGE	C4-C3-O2-C2
34	C	540	PGE	C3-C4-O3-C5
34	E	105	PGE	C6-C5-O3-C4
35	B	652	P6G	C18-C17-O16-C15
31	Y	101	LMT	C3'-C4'-O1B-C1B
24	B	609	CLA	C13-C15-C16-C17
40	C	517	DGD	C3A-C4A-C5A-C6A
33	h	106	PG4	C3-C4-O3-C5
33	i	101	PG4	C6-C5-O3-C4
34	B	649	PGE	C6-C5-O3-C4
35	D	416	P6G	C15-C14-O13-C12
28	A	616	SQD	C27-C28-C29-C30
28	a	413	SQD	O10-C23-O48-C46
34	B	649	PGE	C1-C2-O2-C3
30	C	528	GOL	C1-C2-C3-O3
30	D	412	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
30	V	208	GOL	O1-C1-C2-C3
28	x	101	SQD	C29-C30-C31-C32
29	A	613	LMG	C14-C15-C16-C17
40	D	408	DGD	C8B-C9B-CAB-CBB
34	B	650	PGE	O2-C3-C4-O3
44	V	216	2PE	O13-C14-C15-O16
29	z	101	LMG	C36-C37-C38-C39
32	e	101	LHG	C14-C15-C16-C17
24	C	503	CLA	C8-C10-C11-C12
33	j	104	PG4	C5-C6-O4-C7
35	T	105	P6G	C6-C5-O4-C3
28	A	622	SQD	C44-C45-O47-C7
32	a	419	LHG	C4-C5-O7-C7
33	V	209	PG4	C5-C6-O4-C7
33	c	533	PG4	O2-C3-C4-O3
33	H	105	PG4	C3-C4-O3-C5
33	b	637	PG4	C5-C6-O4-C7
34	O	309	PGE	C4-C3-O2-C2
34	o	308	PGE	C6-C5-O3-C4
34	t	105	PGE	C6-C5-O3-C4
35	A	624	P6G	C8-C9-O10-C11
39	e	105	1PE	C14-C24-OH4-C13
32	l	101	LHG	C10-C11-C12-C13
24	C	507	CLA	C16-C17-C18-C19
33	B	643	PG4	C8-C7-O4-C6
33	J	104	PG4	C4-C3-O2-C2
34	B	645	PGE	C3-C4-O3-C5
35	I	106	P6G	C18-C17-O16-C15
33	E	103	PG4	C3-C4-O3-C5
34	E	107	PGE	C3-C4-O3-C5
35	T	105	P6G	C11-C12-O13-C14
39	V	217	1PE	C15-C25-OH5-C14
39	x	104	1PE	C16-C26-OH6-C15
34	I	105	PGE	C6-C5-O3-C4
34	c	540	PGE	C3-C4-O3-C5
33	B	643	PG4	O1-C1-C2-O2
34	E	109	PGE	O1-C1-C2-O2
34	h	110	PGE	O1-C1-C2-O2
35	b	648	P6G	O1-C2-C3-O4
45	i	107	PE8	O22-C23-C24-O25
31	C	533	LMT	C1-C2-C3-C4
28	h	105	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	V	212	PG4	C8-C7-O4-C6
33	X	101	PG4	C5-C6-O4-C7
33	b	635	PG4	C3-C4-O3-C5
34	b	643	PGE	C4-C3-O2-C2
35	A	623	P6G	C18-C17-O16-C15
35	B	652	P6G	C15-C14-O13-C12
40	d	408	DGD	CCB-CDB-CEB-CFB
28	F	104	SQD	C29-C30-C31-C32
40	h	104	DGD	C5B-C6B-C7B-C8B
28	x	101	SQD	C44-C45-C46-O48
29	z	101	LMG	O1-C7-C8-C9
29	C	519	LMG	C11-C10-O7-C8
24	c	509	CLA	C15-C16-C17-C18
33	H	104	PG4	C6-C5-O3-C4
33	c	533	PG4	C1-C2-O2-C3
33	e	104	PG4	C5-C6-O4-C7
31	m	101	LMT	C2-C3-C4-C5
34	O	310	PGE	C4-C3-O2-C2
24	b	605	CLA	C13-C15-C16-C17
29	J	101	LMG	C35-C36-C37-C38
33	b	636	PG4	C6-C5-O3-C4
38	C	531	HTG	C3'-C4'-C5'-C6'
38	C	522	HTG	C2-C1-S1-C1'
38	a	418	HTG	C2-C1-S1-C1'
38	c	522	HTG	C2-C1-S1-C1'
24	b	616	CLA	C5-C6-C7-C8
40	C	518	DGD	C2B-C3B-C4B-C5B
34	o	306	PGE	C6-C5-O3-C4
36	E	111	EDO	O1-C1-C2-O2
31	b	622	LMT	O5B-C5B-C6B-O6B
28	A	612	SQD	O6-C44-C45-O47
28	F	104	SQD	O47-C45-C46-O48
28	h	105	SQD	O6-C44-C45-O47
29	C	520	LMG	O1-C7-C8-O7
29	a	414	LMG	O7-C8-C9-O8
29	z	101	LMG	O7-C8-C9-O8
40	D	408	DGD	O2G-C2G-C3G-O3G
24	D	405	CLA	C16-C17-C18-C19
28	F	104	SQD	C11-C10-C9-C8
33	I	102	PG4	C5-C6-O4-C7
45	i	107	PE8	C2-C3-O4-C5
29	C	520	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	d	412	LMG	C15-C16-C17-C18
32	e	101	LHG	C10-C11-C12-C13
40	C	516	DGD	C8B-C9B-CAB-CBB
28	x	101	SQD	C14-C15-C16-C17
28	x	101	SQD	C26-C27-C28-C29
29	C	520	LMG	C30-C31-C32-C33
34	a	422	PGE	C1-C2-O2-C3
34	h	110	PGE	C6-C5-O3-C4
33	b	636	PG4	O3-C5-C6-O4
31	b	622	LMT	C6-C7-C8-C9
24	c	509	CLA	C10-C11-C12-C13
24	B	605	CLA	C3-C5-C6-C7
34	b	647	PGE	C1-C2-O2-C3
34	o	308	PGE	C4-C3-O2-C2
38	C	530	HTG	C1'-C2'-C3'-C4'
43	v	202	HEC	C4B-C3B-CAB-CBB
29	C	526	LMG	C15-C16-C17-C18
34	b	645	PGE	C1-C2-O2-C3
39	B	654	1PE	C13-C23-OH3-C22
24	B	617	CLA	C2-C1-O2A-CGA
34	t	104	PGE	O2-C3-C4-O3
33	I	104	PG4	C1-C2-O2-C3
33	C	534	PG4	C6-C5-O3-C4
29	A	613	LMG	C22-C23-C24-C25
29	b	621	LMG	C29-C30-C31-C32
41	e	107	HEM	C3D-CAD-CBD-CGD
33	E	102	PG4	O4-C7-C8-O5
34	i	105	PGE	O3-C5-C6-O4
29	z	101	LMG	C24-C25-C26-C27
35	b	648	P6G	O13-C14-C15-O16
29	b	621	LMG	C32-C33-C34-C35
40	C	517	DGD	C7A-C8A-C9A-CAA
29	C	520	LMG	C11-C12-C13-C14
32	B	632	LHG	C10-C11-C12-C13
45	i	107	PE8	O4-C5-C6-O7
34	E	109	PGE	C3-C4-O3-C5
35	d	416	P6G	C9-C8-O7-C6
38	C	529	HTG	C4'-C5'-C6'-C7'
32	d	411	LHG	C14-C15-C16-C17
38	B	631	HTG	C4'-C5'-C6'-C7'
29	B	634	LMG	C4-C5-C6-O5
34	h	107	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
33	V	212	PG4	C1-C2-O2-C3
38	B	624	HTG	C4-C5-C6-O6
28	l	102	SQD	C35-C36-C37-C38
29	j	101	LMG	C40-C41-C42-C43
30	T	103	GOL	O1-C1-C2-O2
30	o	304	GOL	O1-C1-C2-O2
31	M	102	LMT	C2-C1-O1'-C1'
24	A	609	CLA	C3-C5-C6-C7
31	Y	101	LMT	C5'-C4'-O1B-C1B
26	A	610	BCR	C36-C18-C19-C20
31	b	622	LMT	O5B-C1B-O1B-C4'
33	b	637	PG4	C4-C3-O2-C2
35	b	649	P6G	C18-C17-O16-C15
29	J	101	LMG	C36-C37-C38-C39
38	c	522	HTG	C2'-C3'-C4'-C5'
24	C	507	CLA	C4-C3-C5-C6
31	c	521	LMT	C9-C10-C11-C12
29	A	613	LMG	C29-C30-C31-C32
40	d	408	DGD	C8B-C9B-CAB-CBB
24	C	501	CLA	C2A-CAA-CBA-CGA
29	B	621	LMG	C12-C13-C14-C15
34	h	109	PGE	C4-C3-O2-C2
33	C	534	PG4	O4-C7-C8-O5
33	H	105	PG4	O1-C1-C2-O2
33	I	104	PG4	O1-C1-C2-O2
34	D	415	PGE	O3-C5-C6-O4
31	A	617	LMT	C4-C5-C6-C7
24	B	612	CLA	C12-C13-C15-C16
24	C	506	CLA	C6-C7-C8-C10
24	B	617	CLA	C10-C11-C12-C13
34	o	309	PGE	C4-C3-O2-C2
34	t	104	PGE	C4-C3-O2-C2
28	a	413	SQD	C13-C14-C15-C16
28	a	424	SQD	C27-C28-C29-C30
40	c	518	DGD	C8A-C9A-CAA-CBA
34	H	110	PGE	O2-C3-C4-O3
33	J	105	PG4	C3-C4-O3-C5
34	V	214	PGE	C6-C5-O3-C4
34	h	108	PGE	C6-C5-O3-C4
29	a	414	LMG	C17-C18-C19-C20
32	d	411	LHG	C18-C19-C20-C21
28	F	104	SQD	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
29	b	621	LMG	C14-C15-C16-C17
32	e	101	LHG	C2-C3-O3-P
34	B	644	PGE	C6-C5-O3-C4
40	H	103	DGD	CDB-CEB-CFB-CGB
40	c	518	DGD	CDB-CEB-CFB-CGB
29	d	412	LMG	C39-C40-C41-C42
40	h	104	DGD	C7A-C8A-C9A-CAA
39	x	104	1PE	C23-C13-OH4-C24
35	d	415	P6G	C8-C9-O10-C11
33	i	101	PG4	C1-C2-O2-C3
29	a	414	LMG	C31-C32-C33-C34
24	B	612	CLA	C14-C13-C15-C16
24	b	605	CLA	C6-C7-C8-C9
29	A	613	LMG	O8-C28-C29-C30
40	d	408	DGD	C2A-C3A-C4A-C5A
31	M	101	LMT	O5'-C5'-C6'-O6'
28	A	622	SQD	O5-C5-C6-S
28	a	424	SQD	O5-C5-C6-S
28	x	101	SQD	O5-C5-C6-S
34	C	539	PGE	O2-C3-C4-O3
28	b	633	SQD	C18-C19-C20-C21
29	j	101	LMG	C39-C40-C41-C42
40	c	517	DGD	C9B-CAB-CBB-CCB
31	F	102	LMT	C9-C10-C11-C12
40	h	104	DGD	CBA-CCA-CDA-CEA
34	Y	102	PGE	O1-C1-C2-O2
34	E	106	PGE	C4-C3-O2-C2
28	A	616	SQD	O10-C23-O48-C46
29	A	613	LMG	O7-C8-C9-O8
29	d	412	LMG	O1-C7-C8-O7
32	e	101	LHG	O7-C5-C6-O8
40	D	408	DGD	O1G-C1G-C2G-O2G
28	F	104	SQD	C18-C19-C20-C21
40	c	517	DGD	C4B-C5B-C6B-C7B
40	D	408	DGD	CFA-CGA-CHA-CIA
24	c	501	CLA	CBD-CGD-O2D-CED
32	e	101	LHG	C16-C17-C18-C19
28	A	612	SQD	O6-C44-C45-C46
28	F	104	SQD	C44-C45-C46-O48
28	a	424	SQD	O6-C44-C45-C46
29	d	412	LMG	O1-C7-C8-C9
29	C	519	LMG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
40	H	103	DGD	O2G-C1B-C2B-C3B
34	o	307	PGE	C4-C3-O2-C2
40	d	408	DGD	C9A-CAA-CBA-CCA
38	c	531	HTG	C1'-C2'-C3'-C4'
33	B	638	PG4	C8-C7-O4-C6
32	D	411	LHG	C30-C31-C32-C33
40	d	408	DGD	CBA-CCA-CDA-CEA
24	B	602	CLA	CAD-CBD-CGD-O2D
24	B	606	CLA	CAD-CBD-CGD-O2D
24	C	502	CLA	CAD-CBD-CGD-O2D
24	C	504	CLA	CAD-CBD-CGD-O2D
24	b	602	CLA	CAD-CBD-CGD-O2D
24	b	606	CLA	CAD-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O2D
24	c	504	CLA	CAD-CBD-CGD-O2D
24	c	506	CLA	CAD-CBD-CGD-O2D
40	H	103	DGD	C3B-C4B-C5B-C6B
29	a	414	LMG	O10-C28-O8-C9
24	c	504	CLA	C8-C10-C11-C12
40	c	518	DGD	C4A-C5A-C6A-C7A
29	C	519	LMG	C28-C29-C30-C31
35	D	417	P6G	C14-C15-O16-C17
29	c	519	LMG	C40-C41-C42-C43
32	e	101	LHG	C11-C10-C9-C8
28	x	101	SQD	C19-C20-C21-C22
38	C	530	HTG	C4'-C5'-C6'-C7'
29	C	520	LMG	O10-C28-O8-C9
32	D	410	LHG	C26-C27-C28-C29
35	C	541	P6G	C8-C9-O10-C11
28	a	413	SQD	C11-C10-C9-C8
29	C	520	LMG	C14-C15-C16-C17
24	B	602	CLA	CAD-CBD-CGD-O1D
24	B	606	CLA	CAD-CBD-CGD-O1D
24	B	617	CLA	CHA-CBD-CGD-O1D
24	C	502	CLA	CAD-CBD-CGD-O1D
24	C	504	CLA	CAD-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O1D
24	C	509	CLA	CHA-CBD-CGD-O2D
24	b	602	CLA	CAD-CBD-CGD-O1D
24	b	611	CLA	CHA-CBD-CGD-O2D
24	c	502	CLA	CAD-CBD-CGD-O1D
24	c	504	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	c	506	CLA	CAD-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O1D
24	c	509	CLA	CHA-CBD-CGD-O2D
25	d	401	PHO	CHA-CBD-CGD-O2D
32	B	632	LHG	C4-O6-P-O5
32	D	410	LHG	C4-O6-P-O4
32	a	419	LHG	C4-O6-P-O5
32	d	410	LHG	C3-O3-P-O4
32	e	101	LHG	C4-O6-P-O5
32	l	101	LHG	C4-O6-P-O5
33	e	104	PG4	C3-C4-O3-C5
34	H	109	PGE	C3-C4-O3-C5
29	C	526	LMG	C21-C22-C23-C24
33	H	104	PG4	O2-C3-C4-O3
29	C	526	LMG	C14-C15-C16-C17
29	z	101	LMG	C16-C17-C18-C19
24	B	602	CLA	C4-C3-C5-C6
26	B	620	BCR	C5-C6-C7-C8
26	t	102	BCR	C23-C24-C25-C26
28	x	101	SQD	C25-C26-C27-C28
33	I	102	PG4	C8-C7-O4-C6
28	a	417	SQD	C15-C16-C17-C18
32	D	411	LHG	C2-C3-O3-P
32	d	411	LHG	C2-C3-O3-P
33	J	105	PG4	O4-C7-C8-O5
33	b	635	PG4	O1-C1-C2-O2
34	E	105	PGE	O1-C1-C2-O2
34	J	108	PGE	O3-C5-C6-O4
34	a	423	PGE	O3-C5-C6-O4
34	b	644	PGE	O1-C1-C2-O2
34	b	645	PGE	O1-C1-C2-O2
34	b	646	PGE	O1-C1-C2-O2
34	i	106	PGE	O3-C5-C6-O4
35	d	416	P6G	O1-C2-C3-O4
35	T	105	P6G	C5-C6-O7-C8
29	B	634	LMG	C15-C16-C17-C18
40	d	408	DGD	CAB-CBB-CCB-CDB
28	b	633	SQD	O47-C7-C8-C9
33	I	103	PG4	O3-C5-C6-O4
35	E	110	P6G	O13-C14-C15-O16
35	E	110	P6G	C8-C9-O10-C11
35	c	541	P6G	C18-C17-O16-C15

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Mol	Chain	Res	Type	Atoms
32	d	411	LHG	C24-C25-C26-C27
35	B	652	P6G	O13-C14-C15-O16
35	E	110	P6G	C18-C17-O16-C15
31	A	617	LMT	C7-C8-C9-C10
31	a	401	LMT	C3-C4-C5-C6
30	B	627	GOL	O1-C1-C2-O2
30	C	523	GOL	O1-C1-C2-O2
30	b	625	GOL	O2-C2-C3-O3
30	c	528	GOL	O2-C2-C3-O3
35	A	624	P6G	O13-C14-C15-O16
27	A	611	PL9	C4-C3-C7-C8
30	b	625	GOL	C1-C2-C3-O3
32	B	632	LHG	C7-C8-C9-C10
29	z	101	LMG	C7-C8-O7-C10
33	B	640	PG4	C1-C2-O2-C3
34	O	308	PGE	C1-C2-O2-C3
28	a	424	SQD	C24-C25-C26-C27
32	B	632	LHG	C11-C12-C13-C14
40	C	516	DGD	C2B-C3B-C4B-C5B
28	A	622	SQD	C32-C33-C34-C35
28	l	102	SQD	C25-C26-C27-C28
32	d	409	LHG	C11-C10-C9-C8
38	a	418	HTG	C4'-C5'-C6'-C7'
29	C	519	LMG	C30-C31-C32-C33
29	a	414	LMG	C16-C17-C18-C19
29	b	621	LMG	C36-C37-C38-C39
33	b	634	PG4	C6-C5-O3-C4
32	A	618	LHG	O6-C4-C5-C6
40	c	516	DGD	C3B-C4B-C5B-C6B
38	B	624	HTG	O5-C5-C6-O6
38	c	530	HTG	O5-C5-C6-O6
24	C	508	CLA	C11-C10-C8-C9
24	B	617	CLA	C6-C7-C8-C10
24	C	508	CLA	C11-C10-C8-C7
24	D	404	CLA	C12-C13-C15-C16
24	a	407	CLA	C4C-C3C-CAC-CBC
33	V	211	PG4	O4-C7-C8-O5
33	i	102	PG4	O1-C1-C2-O2
33	I	104	PG4	C4-C3-O2-C2
31	a	401	LMT	O5'-C5'-C6'-O6'
40	h	104	DGD	CBB-CCB-CDB-CEB
24	c	510	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	b	649	P6G	C11-C12-O13-C14
32	D	409	LHG	C25-C26-C27-C28
40	c	517	DGD	C2E-C1E-O5D-C6D
39	B	653	1PE	C12-C22-OH3-C23
33	E	102	PG4	C5-C6-O4-C7
34	a	422	PGE	C6-C5-O3-C4
34	b	638	PGE	C6-C5-O3-C4
38	b	631	HTG	S1-C1'-C2'-C3'
32	A	618	LHG	C11-C10-C9-C8
33	V	210	PG4	O2-C3-C4-O3
28	a	424	SQD	C12-C13-C14-C15
38	B	630	HTG	C3'-C4'-C5'-C6'
32	A	618	LHG	O7-C5-C6-O8
40	C	518	DGD	C3B-C4B-C5B-C6B
29	b	621	LMG	C12-C13-C14-C15
34	H	110	PGE	C3-C4-O3-C5
35	T	105	P6G	C14-C15-O16-C17
33	I	103	PG4	O2-C3-C4-O3
40	c	517	DGD	C4A-C5A-C6A-C7A
28	a	424	SQD	C11-C12-C13-C14
33	i	103	PG4	C3-C4-O3-C5
44	V	216	2PE	C9-C8-O7-C6
28	l	102	SQD	C12-C13-C14-C15
44	V	216	2PE	O22-C23-C24-O25
34	i	106	PGE	O1-C1-C2-O2
35	E	110	P6G	O1-C2-C3-O4
39	L	101	1PE	OH2-C12-C22-OH3
28	A	616	SQD	C29-C30-C31-C32
28	A	622	SQD	C34-C35-C36-C37
32	l	101	LHG	C12-C13-C14-C15
35	T	105	P6G	O10-C11-C12-O13
34	B	644	PGE	O2-C3-C4-O3
24	d	403	CLA	C4C-C3C-CAC-CBC
32	E	101	LHG	C25-C26-C27-C28
33	B	638	PG4	C6-C5-O3-C4
33	V	210	PG4	C5-C6-O4-C7
24	C	513	CLA	CBA-CGA-O2A-C1
29	B	621	LMG	O8-C28-C29-C30
36	e	106	EDO	O1-C1-C2-O2
40	d	408	DGD	C7B-C8B-C9B-CAB
40	D	408	DGD	C2G-C3G-O3G-C1D
40	c	516	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
45	i	107	PE8	O19-C20-C21-O22
33	C	534	PG4	C8-C7-O4-C6
24	b	602	CLA	C4-C3-C5-C6
31	b	622	LMT	C2B-C1B-O1B-C4'
35	j	106	P6G	C6-C5-O4-C3
27	a	412	PL9	C2-C3-C7-C8
34	V	215	PGE	C1-C2-O2-C3
33	B	642	PG4	O1-C1-C2-O2
31	m	101	LMT	C2-C1-O1'-C1'
31	u	203	LMT	C2-C1-O1'-C1'
34	Y	102	PGE	C6-C5-O3-C4
24	B	616	CLA	C14-C13-C15-C16
24	C	506	CLA	C11-C12-C13-C14
24	D	405	CLA	C11-C10-C8-C9
24	b	612	CLA	C14-C13-C15-C16
28	A	616	SQD	C24-C23-O48-C46
29	C	520	LMG	C29-C28-O8-C9
29	a	414	LMG	C29-C28-O8-C9
27	A	611	PL9	C31-C32-C33-C34
33	X	103	PG4	C3-C4-O3-C5
38	B	623	HTG	C2'-C3'-C4'-C5'
33	B	638	PG4	O2-C3-C4-O3
34	H	108	PGE	C4-C3-O2-C2
35	T	105	P6G	C18-C17-O16-C15
43	v	202	HEC	CAD-CBD-CGD-O2D
33	i	103	PG4	C8-C7-O4-C6
39	j	107	1PE	C12-C22-OH3-C23
45	i	107	PE8	C24-C23-O22-C21
24	B	602	CLA	C2-C3-C5-C6
24	c	511	CLA	CBA-CGA-O2A-C1
24	b	615	CLA	C16-C17-C18-C19
32	d	409	LHG	C26-C27-C28-C29
24	D	405	CLA	C11-C10-C8-C7
24	a	410	CLA	C6-C7-C8-C10
24	C	513	CLA	O1A-CGA-O2A-C1
32	A	618	LHG	C29-C30-C31-C32
33	E	103	PG4	O2-C3-C4-O3
34	J	106	PGE	C4-C3-O2-C2
33	c	532	PG4	C6-C5-O3-C4
35	D	418	P6G	C15-C14-O13-C12
34	J	106	PGE	O3-C5-C6-O4
34	V	214	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
28	h	105	SQD	C14-C15-C16-C17
24	C	507	CLA	C16-C17-C18-C20
24	D	405	CLA	C16-C17-C18-C20
39	e	105	1PE	OH4-C13-C23-OH3
34	b	641	PGE	C1-C2-O2-C3
35	A	624	P6G	C12-C11-O10-C9
34	H	111	PGE	O2-C3-C4-O3
33	E	102	PG4	C6-C5-O3-C4
35	D	416	P6G	C14-C15-O16-C17
44	V	216	2PE	C24-C23-O22-C21
28	A	622	SQD	C11-C10-C9-C8
28	a	417	SQD	C33-C34-C35-C36
24	a	410	CLA	C3-C5-C6-C7
29	C	520	LMG	C18-C19-C20-C21
34	H	110	PGE	C6-C5-O3-C4
31	A	617	LMT	C11-C10-C9-C8
41	e	107	HEM	CAD-CBD-CGD-O1D
28	F	104	SQD	C16-C17-C18-C19
28	a	417	SQD	C24-C25-C26-C27
34	H	108	PGE	C1-C2-O2-C3
35	A	623	P6G	C15-C14-O13-C12
33	c	535	PG4	C8-C7-O4-C6
29	C	526	LMG	C12-C13-C14-C15
29	C	526	LMG	C20-C21-C22-C23
31	b	622	LMT	C9-C10-C11-C12
40	h	104	DGD	C6B-C7B-C8B-C9B
43	v	202	HEC	CAD-CBD-CGD-O1D
29	A	613	LMG	C32-C33-C34-C35
34	O	310	PGE	C1-C2-O2-C3
43	V	203	HEC	CAD-CBD-CGD-O1D
24	C	510	CLA	C8-C10-C11-C12
27	D	407	PL9	C39-C41-C42-C43
27	a	412	PL9	C39-C41-C42-C43
29	j	101	LMG	C36-C37-C38-C39
40	D	408	DGD	C6A-C7A-C8A-C9A
38	C	531	HTG	O5-C5-C6-O6
44	V	216	2PE	C5-C6-O7-C8
24	c	509	CLA	C11-C10-C8-C9
30	v	204	GOL	O1-C1-C2-C3
32	d	411	LHG	O1-C1-C2-C3
40	C	516	DGD	CAB-CBB-CCB-CDB
29	c	519	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
32	A	618	LHG	C30-C31-C32-C33
28	a	417	SQD	C25-C26-C27-C28
40	D	408	DGD	CCB-CDB-CEB-CFB
40	d	408	DGD	C1G-C2G-O2G-C1B
34	b	644	PGE	O2-C3-C4-O3
35	D	416	P6G	C6-C5-O4-C3
29	b	621	LMG	C31-C32-C33-C34
36	V	218	EDO	O1-C1-C2-O2
36	a	425	EDO	O1-C1-C2-O2
34	A	621	PGE	C3-C4-O3-C5
35	b	648	P6G	C5-C6-O7-C8
29	d	412	LMG	C42-C43-C44-C45
29	B	634	LMG	C33-C34-C35-C36
30	C	528	GOL	O2-C2-C3-O3
30	D	413	GOL	O2-C2-C3-O3
30	U	201	GOL	O1-C1-C2-O2
34	B	645	PGE	C4-C3-O2-C2
40	C	517	DGD	C2E-C1E-O5D-C6D
38	c	523	HTG	C4-C5-C6-O6
33	c	532	PG4	C8-C7-O4-C6
24	B	602	CLA	C8-C10-C11-C12
24	B	604	CLA	C5-C6-C7-C8
28	A	612	SQD	C30-C31-C32-C33
40	C	517	DGD	C6B-C7B-C8B-C9B
34	B	646	PGE	C1-C2-O2-C3
34	a	422	PGE	C3-C4-O3-C5
26	B	618	BCR	C5-C6-C7-C8
26	K	101	BCR	C1-C6-C7-C8
26	b	618	BCR	C1-C6-C7-C8
32	A	618	LHG	C7-C8-C9-C10
29	C	526	LMG	C36-C37-C38-C39
40	h	104	DGD	CCB-CDB-CEB-CFB
31	A	617	LMT	C2-C3-C4-C5
34	b	642	PGE	O2-C3-C4-O3
35	j	106	P6G	C15-C14-O13-C12
31	C	533	LMT	C5-C6-C7-C8
33	V	213	PG4	O2-C3-C4-O3
44	V	216	2PE	O19-C20-C21-O22
31	Y	101	LMT	O5'-C5'-C6'-O6'
24	A	609	CLA	C12-C13-C15-C16
24	b	612	CLA	C12-C13-C15-C16
24	c	503	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
40	C	516	DGD	C6B-C7B-C8B-C9B
24	C	501	CLA	C16-C17-C18-C20
32	l	101	LHG	C17-C18-C19-C20
41	e	107	HEM	CAA-CBA-CGA-O1A
41	e	107	HEM	CAD-CBD-CGD-O2D
34	C	539	PGE	C1-C2-O2-C3
39	V	217	1PE	C16-C26-OH6-C15
28	a	417	SQD	C11-C12-C13-C14
29	c	519	LMG	C36-C37-C38-C39
34	J	108	PGE	C1-C2-O2-C3
39	j	107	1PE	C14-C24-OH4-C13
24	b	617	CLA	C3-C5-C6-C7
40	C	518	DGD	O6D-C5D-C6D-O5D
29	C	526	LMG	C32-C33-C34-C35
33	U	202	PG4	O1-C1-C2-O2
33	i	103	PG4	O4-C7-C8-O5
34	E	106	PGE	O1-C1-C2-O2
34	Y	102	PGE	O3-C5-C6-O4
34	J	108	PGE	C4-C3-O2-C2
45	i	107	PE8	C17-C18-O19-C20
43	V	203	HEC	CAD-CBD-CGD-O2D
27	a	412	PL9	C45-C44-C46-C47
35	A	624	P6G	C6-C5-O4-C3
24	b	602	CLA	C2-C3-C5-C6
40	C	518	DGD	C4A-C5A-C6A-C7A
28	a	413	SQD	C24-C25-C26-C27
38	a	418	HTG	O5-C5-C6-O6
24	b	616	CLA	C13-C15-C16-C17
29	C	526	LMG	C13-C14-C15-C16
39	e	105	1PE	C24-C14-OH5-C25
39	x	104	1PE	C14-C24-OH4-C13
24	c	512	CLA	C13-C15-C16-C17
31	m	102	LMT	C7-C8-C9-C10
40	H	103	DGD	CCB-CDB-CEB-CFB
33	V	210	PG4	C4-C3-O2-C2
28	a	417	SQD	C28-C29-C30-C31
27	A	611	PL9	C20-C19-C21-C22
27	a	412	PL9	C15-C14-C16-C17
27	a	412	PL9	C20-C19-C21-C22
40	D	408	DGD	C2A-C3A-C4A-C5A
24	B	603	CLA	C13-C15-C16-C17
33	H	107	PG4	O4-C7-C8-O5

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Mol	Chain	Res	Type	Atoms
33	b	637	PG4	O1-C1-C2-O2
29	d	412	LMG	C16-C17-C18-C19
24	B	613	CLA	C8-C10-C11-C12
34	B	650	PGE	C3-C4-O3-C5
34	i	106	PGE	C4-C3-O2-C2
29	B	621	LMG	C18-C19-C20-C21
40	c	518	DGD	C7A-C8A-C9A-CAA
28	A	612	SQD	C11-C10-C9-C8
34	i	105	PGE	C1-C2-O2-C3
24	c	511	CLA	O1A-CGA-O2A-C1
38	b	623	HTG	C2'-C3'-C4'-C5'
33	B	642	PG4	C1-C2-O2-C3
33	c	534	PG4	C4-C3-O2-C2
33	C	537	PG4	C3-C4-O3-C5
30	C	528	GOL	O1-C1-C2-O2
30	c	528	GOL	O1-C1-C2-O2
30	v	207	GOL	O1-C1-C2-O2
32	D	411	LHG	C28-C29-C30-C31
29	C	519	LMG	C20-C21-C22-C23
36	B	658	EDO	O1-C1-C2-O2
35	I	106	P6G	C2-C3-O4-C5
28	A	622	SQD	C18-C19-C20-C21
28	h	105	SQD	C13-C14-C15-C16
35	C	541	P6G	C5-C6-O7-C8
35	d	415	P6G	C18-C17-O16-C15
40	D	408	DGD	CAB-CBB-CCB-CDB
33	c	533	PG4	O1-C1-C2-O2
33	d	414	PG4	O1-C1-C2-O2
40	C	516	DGD	O1B-C1B-O2G-C2G
25	A	608	PHO	CHA-CBD-CGD-O1D
25	a	409	PHO	CHA-CBD-CGD-O1D
29	b	621	LMG	O8-C28-C29-C30
32	l	101	LHG	C11-C12-C13-C14
35	I	106	P6G	O10-C11-C12-O13
24	A	606	CLA	C16-C17-C18-C20
24	a	408	CLA	C11-C12-C13-C14
28	A	622	SQD	C11-C12-C13-C14
28	A	622	SQD	O47-C45-C46-O48
41	e	107	HEM	CAA-CBA-CGA-O2A
40	c	517	DGD	C7A-C8A-C9A-CAA
24	b	602	CLA	C11-C10-C8-C7
32	D	409	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	b	634	PG4	C8-C7-O4-C6
24	C	505	CLA	C11-C10-C8-C9
24	a	408	CLA	C6-C7-C8-C9
33	x	102	PG4	C4-C3-O2-C2
28	h	105	SQD	C10-C11-C12-C13
34	D	415	PGE	C6-C5-O3-C4
28	a	417	SQD	C45-C44-O6-C1
28	b	633	SQD	C45-C44-O6-C1
40	C	516	DGD	C5D-C6D-O5D-C1E
24	C	509	CLA	C2-C1-O2A-CGA
24	D	404	CLA	C2-C1-O2A-CGA
24	c	509	CLA	C2-C1-O2A-CGA
24	d	404	CLA	C2-C1-O2A-CGA
28	A	622	SQD	C12-C13-C14-C15
24	A	606	CLA	C4C-C3C-CAC-CBC
33	J	105	PG4	C8-C7-O4-C6
24	b	616	CLA	C3A-C2A-CAA-CBA
35	I	106	P6G	C9-C8-O7-C6
32	e	101	LHG	C9-C10-C11-C12
35	E	110	P6G	C9-C8-O7-C6
33	K	102	PG4	O3-C5-C6-O4
38	C	532	HTG	C3'-C4'-C5'-C6'
32	D	409	LHG	C24-C25-C26-C27
38	a	418	HTG	C2'-C3'-C4'-C5'
40	c	516	DGD	C2E-C1E-O5D-C6D
29	a	414	LMG	C36-C37-C38-C39
24	c	512	CLA	O2A-C1-C2-C3
29	a	414	LMG	C34-C35-C36-C37
33	i	104	PG4	C3-C4-O3-C5
34	o	307	PGE	C1-C2-O2-C3
33	X	103	PG4	C8-C7-O4-C6
32	d	410	LHG	C26-C27-C28-C29
34	c	536	PGE	O2-C3-C4-O3
31	b	622	LMT	C7-C8-C9-C10
34	H	109	PGE	C6-C5-O3-C4
28	a	413	SQD	C35-C36-C37-C38
28	x	101	SQD	O48-C23-C24-C25
31	a	401	LMT	C4'-C5'-C6'-O6'
29	B	634	LMG	C42-C43-C44-C45
38	C	521	HTG	C3'-C4'-C5'-C6'
35	D	416	P6G	C9-C8-O7-C6
24	B	606	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	B	621	LMG	C7-C8-C9-O8
29	c	519	LMG	O1-C7-C8-C9
30	A	615	GOL	O2-C2-C3-O3
40	c	517	DGD	C6B-C7B-C8B-C9B
39	x	104	1PE	OH4-C13-C23-OH3
29	B	621	LMG	O9-C10-O7-C8
29	B	621	LMG	C13-C14-C15-C16
28	A	616	SQD	C33-C34-C35-C36
40	c	516	DGD	C7A-C8A-C9A-CAA
35	B	651	P6G	C9-C8-O7-C6
29	c	520	LMG	C14-C15-C16-C17
36	H	112	EDO	O1-C1-C2-O2
33	H	106	PG4	C5-C6-O4-C7
24	B	616	CLA	C11-C10-C8-C9
24	B	607	CLA	C6-C7-C8-C10
24	C	502	CLA	C16-C17-C18-C19
29	c	520	LMG	C11-C12-C13-C14
34	b	639	PGE	O3-C5-C6-O4
35	d	415	P6G	C5-C6-O7-C8
28	A	622	SQD	C19-C20-C21-C22
26	A	610	BCR	C17-C18-C19-C20
35	D	416	P6G	O10-C11-C12-O13
24	C	503	CLA	C6-C7-C8-C10
44	V	216	2PE	C12-C11-O10-C9
33	c	534	PG4	C1-C2-O2-C3
24	C	505	CLA	C2B-C3B-CAB-CBB
24	c	510	CLA	C2B-C3B-CAB-CBB
24	d	403	CLA	C2B-C3B-CAB-CBB
26	b	620	BCR	C1-C6-C7-C8
34	b	640	PGE	O2-C3-C4-O3
35	d	415	P6G	O4-C5-C6-O7
33	I	103	PG4	C1-C2-O2-C3
35	C	541	P6G	C2-C3-O4-C5
28	l	102	SQD	C30-C31-C32-C33
45	i	107	PE8	C6-C5-O4-C3
24	C	509	CLA	C3-C5-C6-C7
24	a	410	CLA	C5-C6-C7-C8
40	C	517	DGD	O6E-C1E-O5D-C6D
40	c	517	DGD	O6E-C1E-O5D-C6D
24	B	605	CLA	CBD-CGD-O2D-CED
28	a	417	SQD	C26-C27-C28-C29
33	U	202	PG4	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
33	D	414	PG4	C1-C2-O2-C3
33	I	102	PG4	O3-C5-C6-O4
24	B	614	CLA	C16-C17-C18-C19
24	b	613	CLA	C13-C15-C16-C17
33	C	535	PG4	O2-C3-C4-O3
35	I	106	P6G	O4-C5-C6-O7
29	c	519	LMG	O7-C10-C11-C12
24	c	510	CLA	C2-C3-C5-C6
33	e	103	PG4	O1-C1-C2-O2
34	V	215	PGE	O3-C5-C6-O4
29	C	519	LMG	O9-C10-O7-C8
33	i	103	PG4	O3-C5-C6-O4
38	C	521	HTG	C2'-C1'-S1-C1
38	C	531	HTG	C2'-C1'-S1-C1
38	c	522	HTG	C2'-C1'-S1-C1
38	c	530	HTG	C2'-C1'-S1-C1
38	c	531	HTG	C2'-C1'-S1-C1
34	O	308	PGE	C3-C4-O3-C5
33	c	534	PG4	O2-C3-C4-O3
40	c	518	DGD	C2A-C1A-O1G-C1G
29	C	526	LMG	C24-C25-C26-C27
35	D	416	P6G	O7-C8-C9-O10
24	b	608	CLA	C3-C5-C6-C7
28	a	424	SQD	C10-C11-C12-C13
40	c	518	DGD	O1A-C1A-O1G-C1G
33	I	103	PG4	C4-C3-O2-C2
33	K	102	PG4	C6-C5-O3-C4
24	C	512	CLA	CAA-CBA-CGA-O2A
29	C	526	LMG	O7-C10-C11-C12
40	C	518	DGD	O1G-C1A-C2A-C3A
33	V	209	PG4	C4-C3-O2-C2
35	A	624	P6G	O10-C11-C12-O13
28	F	104	SQD	C33-C34-C35-C36
29	j	101	LMG	C35-C36-C37-C38
29	z	101	LMG	C31-C32-C33-C34
24	B	602	CLA	CAA-CBA-CGA-O2A
40	c	518	DGD	O1G-C1A-C2A-C3A
33	C	536	PG4	O3-C5-C6-O4
33	b	636	PG4	O2-C3-C4-O3
33	x	102	PG4	O2-C3-C4-O3
29	a	414	LMG	C30-C31-C32-C33
44	V	216	2PE	O7-C8-C9-O10

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Mol	Chain	Res	Type	Atoms
32	A	618	LHG	C26-C27-C28-C29
34	c	536	PGE	C3-C4-O3-C5
33	X	103	PG4	O3-C5-C6-O4
33	a	421	PG4	O3-C5-C6-O4
31	C	533	LMT	C5'-C4'-O1B-C1B
29	A	613	LMG	C15-C16-C17-C18
34	E	107	PGE	C6-C5-O3-C4
35	b	649	P6G	C5-C6-O7-C8
28	a	413	SQD	O47-C7-C8-C9
33	C	536	PG4	C6-C5-O3-C4
34	E	104	PGE	O3-C5-C6-O4
32	d	410	LHG	C32-C33-C34-C35
31	m	102	LMT	C2-C1-O1'-C1'
24	C	506	CLA	C15-C16-C17-C18
24	D	403	CLA	C15-C16-C17-C18
34	B	646	PGE	C3-C4-O3-C5
34	D	415	PGE	C4-C3-O2-C2
24	D	404	CLA	C14-C13-C15-C16
24	a	410	CLA	C6-C7-C8-C9
24	B	616	CLA	C13-C15-C16-C17
32	E	101	LHG	O7-C7-C8-C9
38	B	623	HTG	C3'-C4'-C5'-C6'
24	C	513	CLA	C4-C3-C5-C6
33	b	636	PG4	C8-C7-O4-C6
28	A	616	SQD	O5-C1-O6-C44
28	h	105	SQD	O5-C1-O6-C44
40	C	516	DGD	O6E-C1E-O5D-C6D
28	h	105	SQD	O48-C23-C24-C25
33	i	101	PG4	C8-C7-O4-C6
29	C	526	LMG	C35-C36-C37-C38
26	b	620	BCR	C7-C8-C9-C10
35	B	651	P6G	C14-C15-O16-C17
35	d	416	P6G	C8-C9-O10-C11
32	B	632	LHG	C5-C6-O8-C23
24	c	501	CLA	C2A-CAA-CBA-CGA
28	A	616	SQD	C2-C1-O6-C44
24	B	602	CLA	C10-C11-C12-C13
33	V	210	PG4	C6-C5-O3-C4
36	O	311	EDO	O1-C1-C2-O2
36	c	542	EDO	O1-C1-C2-O2
40	d	408	DGD	C9B-CAB-CBB-CCB
24	B	603	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
33	B	636	PG4	O4-C7-C8-O5
34	c	537	PGE	O3-C5-C6-O4
30	v	207	GOL	O1-C1-C2-C3
31	Y	101	LMT	O5B-C1B-O1B-C4'
24	a	410	CLA	C13-C15-C16-C17
28	h	105	SQD	O49-C7-C8-C9
32	B	632	LHG	C17-C18-C19-C20
32	l	101	LHG	C16-C17-C18-C19
24	C	504	CLA	C6-C7-C8-C10
24	a	408	CLA	C11-C10-C8-C7
24	b	613	CLA	C11-C10-C8-C7
38	c	531	HTG	O5-C5-C6-O6
33	C	537	PG4	C5-C6-O4-C7
34	b	646	PGE	C6-C5-O3-C4
29	d	412	LMG	C9-C8-O7-C10
29	z	101	LMG	C9-C8-O7-C10
32	a	419	LHG	C6-C5-O7-C7
35	b	648	P6G	O10-C11-C12-O13
28	x	101	SQD	C13-C14-C15-C16
32	d	409	LHG	C32-C33-C34-C35
35	d	416	P6G	C2-C3-O4-C5
33	B	639	PG4	O2-C3-C4-O3
35	A	623	P6G	O4-C5-C6-O7
28	A	616	SQD	C7-C8-C9-C10
31	F	102	LMT	O1'-C1-C2-C3
33	c	535	PG4	O2-C3-C4-O3
34	E	105	PGE	C4-C3-O2-C2
38	h	101	HTG	S1-C1'-C2'-C3'
33	E	102	PG4	C1-C2-O2-C3
29	z	101	LMG	C39-C40-C41-C42
28	b	633	SQD	O49-C7-C8-C9
32	d	410	LHG	C34-C35-C36-C37
33	b	637	PG4	O3-C5-C6-O4
29	C	526	LMG	O9-C10-C11-C12
28	a	413	SQD	C12-C13-C14-C15
33	B	642	PG4	C5-C6-O4-C7
34	H	109	PGE	C4-C3-O2-C2
34	o	307	PGE	C6-C5-O3-C4
35	j	106	P6G	C8-C9-O10-C11
24	B	617	CLA	C6-C7-C8-C9
24	C	506	CLA	C6-C7-C8-C9
24	b	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	z	101	LMG	O7-C10-C11-C12
35	c	541	P6G	C8-C9-O10-C11
33	B	640	PG4	O3-C5-C6-O4
34	B	647	PGE	O2-C3-C4-O3
35	b	649	P6G	O7-C8-C9-O10
40	D	408	DGD	C3B-C4B-C5B-C6B
28	a	413	SQD	C32-C33-C34-C35
24	c	512	CLA	C3-C5-C6-C7
24	a	410	CLA	C4-C3-C5-C6
24	c	510	CLA	C4-C3-C5-C6
24	C	512	CLA	CAA-CBA-CGA-O1A
40	C	518	DGD	O1A-C1A-C2A-C3A
32	d	411	LHG	C13-C14-C15-C16
28	a	417	SQD	O5-C5-C6-S
31	u	203	LMT	C3-C4-C5-C6
33	i	104	PG4	C6-C5-O3-C4
45	i	107	PE8	C18-C17-O16-C15
30	v	204	GOL	O1-C1-C2-O2
32	e	101	LHG	O7-C7-C8-C9
28	x	101	SQD	C32-C33-C34-C35
33	b	637	PG4	O2-C3-C4-O3
40	H	103	DGD	O1B-C1B-C2B-C3B
31	j	103	LMT	C3'-C4'-O1B-C1B
40	d	408	DGD	CCA-CDA-CEA-CFA
38	b	631	HTG	C4'-C5'-C6'-C7'
34	E	107	PGE	C4-C3-O2-C2
24	c	512	CLA	CAA-CBA-CGA-O2A
28	A	612	SQD	O47-C7-C8-C9
33	C	537	PG4	O2-C3-C4-O3
35	A	623	P6G	O7-C8-C9-O10
33	b	634	PG4	C5-C6-O4-C7
33	x	102	PG4	O3-C5-C6-O4
39	V	217	1PE	OH4-C13-C23-OH3
29	c	520	LMG	C36-C37-C38-C39
28	l	102	SQD	C44-C45-C46-O48
24	D	403	CLA	C4C-C3C-CAC-CBC
28	a	413	SQD	O49-C7-C8-C9
29	c	519	LMG	O9-C10-C11-C12
40	c	518	DGD	O1A-C1A-C2A-C3A
27	A	611	PL9	C15-C14-C16-C17
33	X	101	PG4	O3-C5-C6-O4
31	M	101	LMT	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
33	V	212	PG4	O3-C5-C6-O4
34	a	423	PGE	O2-C3-C4-O3
35	D	416	P6G	C5-C6-O7-C8
24	A	606	CLA	CAD-CBD-CGD-O2D
24	B	610	CLA	CAD-CBD-CGD-O2D
24	D	405	CLA	CAD-CBD-CGD-O2D
24	b	611	CLA	CAD-CBD-CGD-O2D
24	d	405	CLA	CAD-CBD-CGD-O2D
25	A	608	PHO	CAD-CBD-CGD-O2D
24	a	408	CLA	C2C-C3C-CAC-CBC
33	c	534	PG4	C8-C7-O4-C6
34	j	105	PGE	O2-C3-C4-O3
45	i	107	PE8	O10-C11-C12-O13
28	h	105	SQD	O10-C23-C24-C25
35	D	418	P6G	C12-C11-O10-C9
34	B	646	PGE	C4-C3-O2-C2
31	c	521	LMT	O5B-C5B-C6B-O6B
24	d	403	CLA	C15-C16-C17-C18
34	B	647	PGE	C3-C4-O3-C5
29	d	412	LMG	C18-C19-C20-C21
29	z	101	LMG	O9-C10-C11-C12
32	E	101	LHG	O9-C7-C8-C9
32	e	101	LHG	O9-C7-C8-C9
33	c	532	PG4	C1-C2-O2-C3
33	c	535	PG4	C5-C6-O4-C7
44	V	216	2PE	O16-C17-C18-O19
40	d	408	DGD	C8A-C9A-CAA-CBA
33	J	104	PG4	O1-C1-C2-O2
34	a	423	PGE	O1-C1-C2-O2
24	B	613	CLA	C13-C15-C16-C17
24	a	410	CLA	C15-C16-C17-C18
29	a	414	LMG	O8-C28-C29-C30
34	B	645	PGE	O2-C3-C4-O3
34	b	641	PGE	O2-C3-C4-O3
35	d	416	P6G	O13-C14-C15-O16
44	V	216	2PE	O4-C5-C6-O7
40	c	518	DGD	O6D-C5D-C6D-O5D
33	V	210	PG4	C3-C4-O3-C5
28	A	622	SQD	O47-C7-C8-C9
29	d	412	LMG	O7-C10-C11-C12
41	E	113	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

156 monomers are involved in 318 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	k	101	BCR	6	0
38	C	529	HTG	1	0
24	c	512	CLA	2	0
28	A	616	SQD	1	0
26	c	515	BCR	4	0
24	c	506	CLA	3	0
24	B	614	CLA	1	0
38	o	301	HTG	1	0
33	I	104	PG4	2	0
24	C	508	CLA	1	0
30	c	529	GOL	7	0
24	B	616	CLA	1	0
43	V	203	HEC	1	0
24	B	606	CLA	2	0
26	d	406	BCR	3	0
24	B	607	CLA	3	0
29	d	412	LMG	2	0
24	C	501	CLA	1	0
24	B	604	CLA	2	0
30	b	629	GOL	1	0
25	A	608	PHO	1	0
28	A	622	SQD	2	0
24	A	606	CLA	4	0
26	B	620	BCR	4	0
24	c	510	CLA	3	0
36	D	419	EDO	3	0
26	C	525	BCR	1	0
24	b	607	CLA	1	0
29	B	634	LMG	6	0
32	d	411	LHG	1	0
24	b	610	CLA	4	0
32	D	411	LHG	1	0
26	D	406	BCR	2	0
24	B	610	CLA	4	0
27	a	412	PL9	11	0
28	A	612	SQD	2	0
24	C	511	CLA	1	0
26	T	102	BCR	8	0
32	D	409	LHG	1	0
24	D	403	CLA	3	0
29	b	621	LMG	2	0
38	C	531	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	A	611	PL9	7	0
24	b	615	CLA	3	0
29	A	613	LMG	3	0
30	A	614	GOL	1	0
29	C	526	LMG	3	0
26	K	101	BCR	2	0
26	h	103	BCR	3	0
34	o	308	PGE	2	0
32	d	410	LHG	1	0
24	D	404	CLA	2	0
38	C	532	HTG	1	0
24	b	602	CLA	2	0
24	b	614	CLA	1	0
26	A	610	BCR	3	0
30	A	615	GOL	3	0
24	d	405	CLA	1	0
34	B	646	PGE	2	0
26	C	514	BCR	1	0
26	t	102	BCR	5	0
31	M	102	LMT	2	0
24	b	617	CLA	1	0
24	B	602	CLA	11	0
24	A	609	CLA	1	0
30	t	101	GOL	1	0
38	h	101	HTG	1	0
30	d	413	GOL	1	0
32	l	101	LHG	1	0
24	d	404	CLA	2	0
24	C	505	CLA	2	0
24	b	609	CLA	1	0
24	c	502	CLA	2	0
31	J	103	LMT	1	0
30	D	402	GOL	1	0
28	b	633	SQD	2	0
33	H	106	PG4	2	0
24	B	611	CLA	1	0
26	b	618	BCR	1	0
32	d	409	LHG	1	0
28	x	101	SQD	2	0
35	B	652	P6G	1	0
30	C	528	GOL	10	0
29	z	101	LMG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	C	503	CLA	1	0
38	C	521	HTG	1	0
24	c	503	CLA	2	0
24	B	615	CLA	2	0
26	B	619	BCR	4	0
30	c	525	GOL	2	0
24	C	512	CLA	3	0
29	B	621	LMG	1	0
34	O	308	PGE	3	0
26	c	514	BCR	1	0
30	O	305	GOL	1	0
24	a	408	CLA	1	0
40	d	408	DGD	0	1
41	e	107	HEM	4	0
25	D	401	PHO	1	0
35	T	105	P6G	2	0
24	c	505	CLA	6	0
30	C	523	GOL	4	0
24	c	509	CLA	1	0
40	D	408	DGD	2	0
30	D	412	GOL	1	0
30	T	103	GOL	1	0
24	D	405	CLA	5	0
24	a	407	CLA	4	0
24	d	403	CLA	2	0
29	c	519	LMG	1	0
24	C	502	CLA	3	0
32	e	101	LHG	2	0
24	c	507	CLA	1	0
31	u	203	LMT	3	0
24	B	608	CLA	1	0
29	a	414	LMG	1	0
30	o	305	GOL	1	0
24	C	509	CLA	4	0
24	b	611	CLA	3	0
24	A	607	CLA	1	0
45	i	107	PE8	1	0
26	B	618	BCR	4	0
24	c	504	CLA	3	0
26	c	527	BCR	2	0
24	C	507	CLA	2	0
24	C	510	CLA	3	0

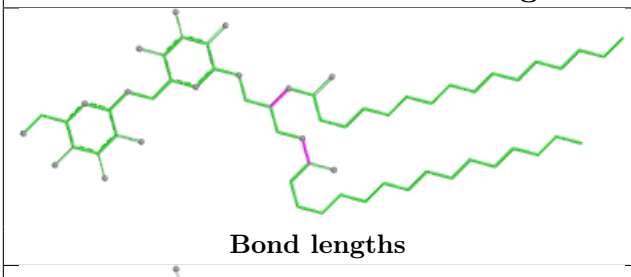
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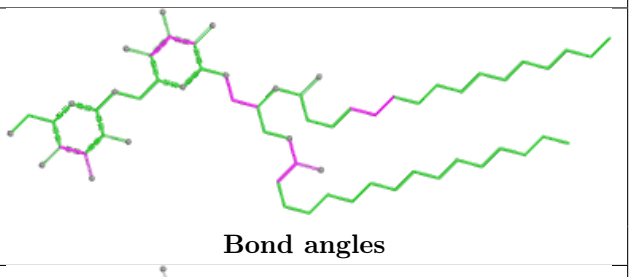
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	606	CLA	1	0
26	H	102	BCR	3	0
33	c	533	PG4	1	0
30	a	416	GOL	1	0
31	B	622	LMT	2	0
26	a	411	BCR	3	0
24	C	504	CLA	2	0
30	a	415	GOL	1	0
26	C	515	BCR	3	0
44	V	216	2PE	3	0
24	b	612	CLA	2	0
30	U	201	GOL	2	0
26	b	620	BCR	5	0
41	E	113	HEM	5	0
38	B	623	HTG	3	0
24	b	604	CLA	2	0
24	a	410	CLA	1	0
26	b	619	BCR	4	0
31	M	101	LMT	3	0
24	C	513	CLA	1	0
31	I	101	LMT	1	0
31	Y	101	LMT	1	0
39	x	104	1PE	1	0
24	c	508	CLA	1	0
25	d	401	PHO	3	0
28	a	424	SQD	1	0
24	b	616	CLA	1	0
24	c	501	CLA	2	0
24	C	506	CLA	5	0
24	b	608	CLA	2	0

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

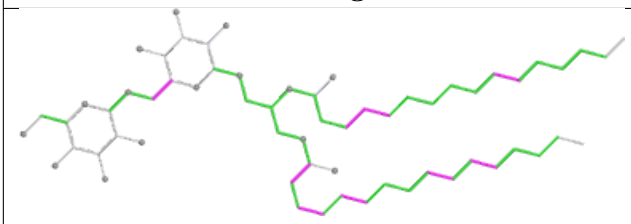
Ligand DGD C 518



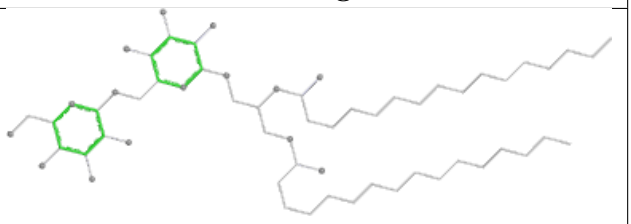
Bond lengths



Bond angles

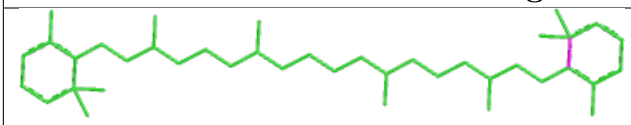


Torsions

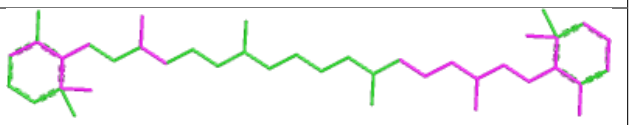


Rings

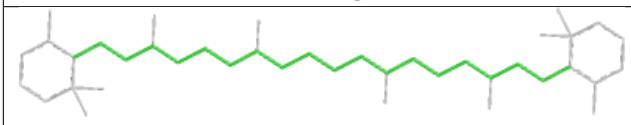
Ligand BCR k 101



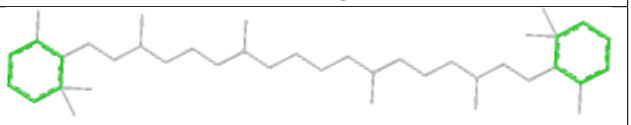
Bond lengths



Bond angles

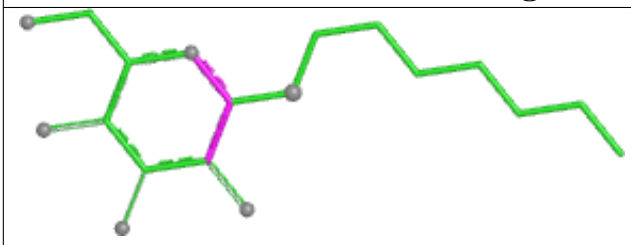


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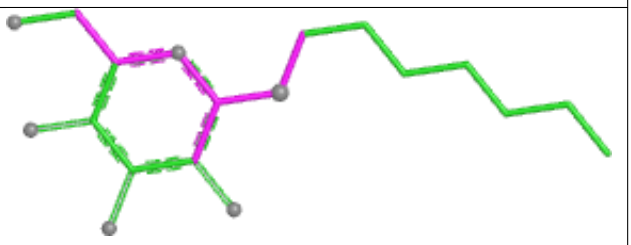


Rings

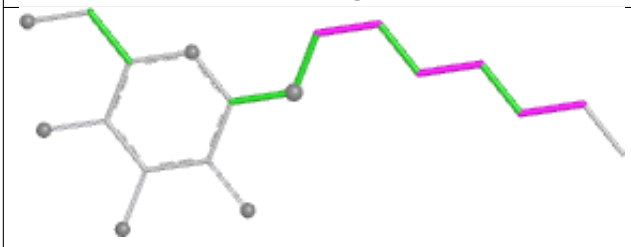
Ligand HTG C 529



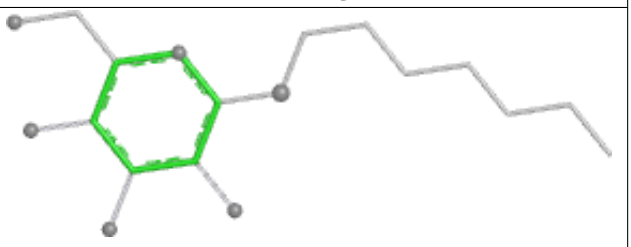
Bond lengths



Bond angles

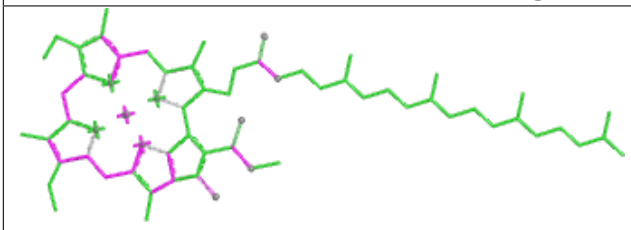


Torsions

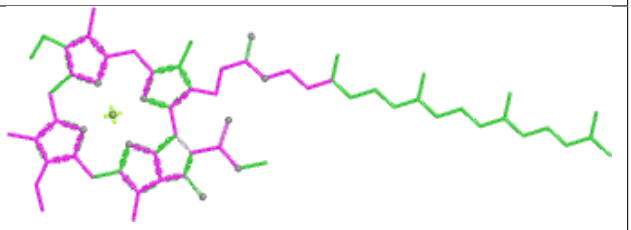


Rings

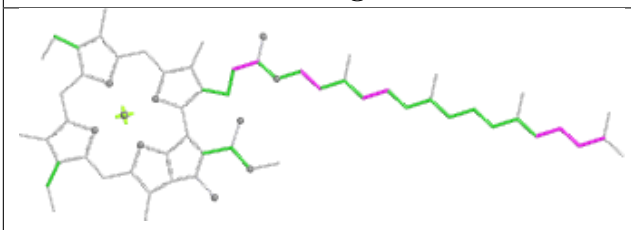
Ligand CLA c 512



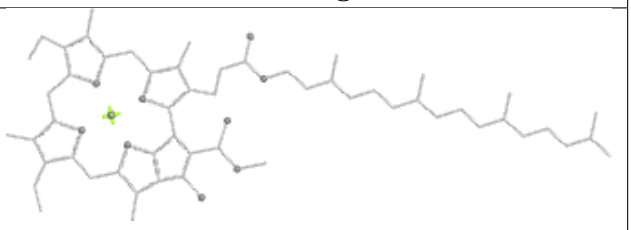
Bond lengths



Bond angles

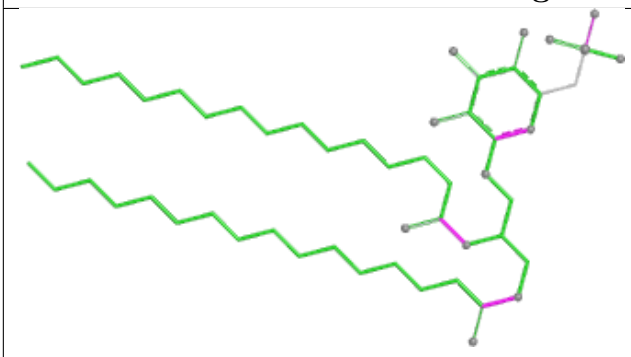


Torsions

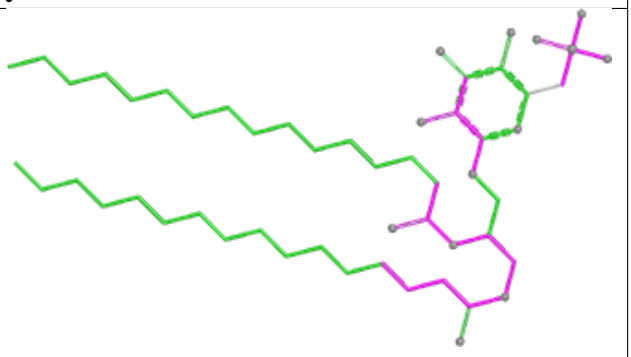


Rings

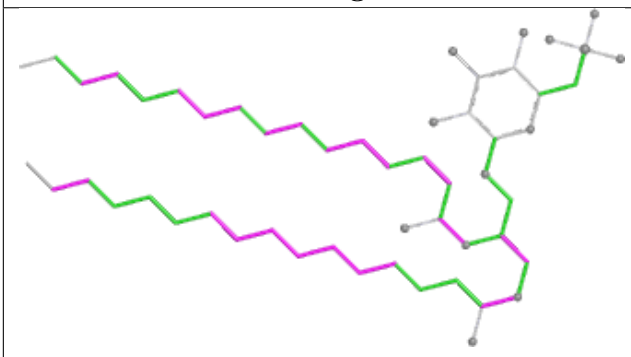
Ligand SQD l 102



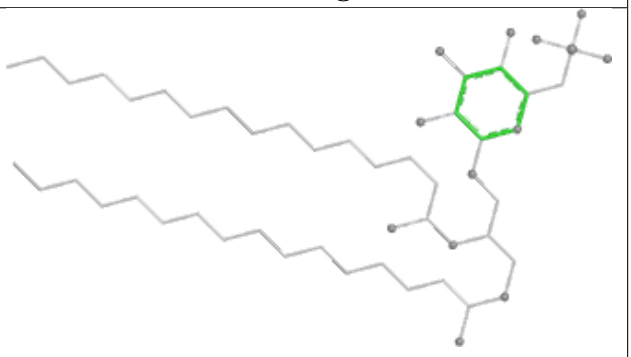
Bond lengths



Bond angles

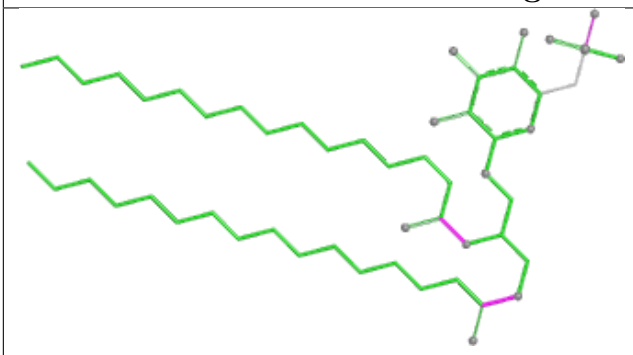


Torsions

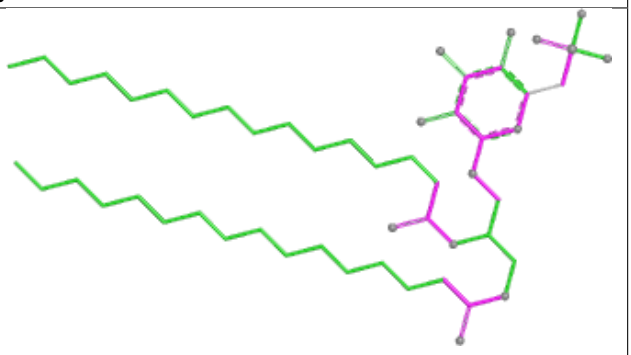


Rings

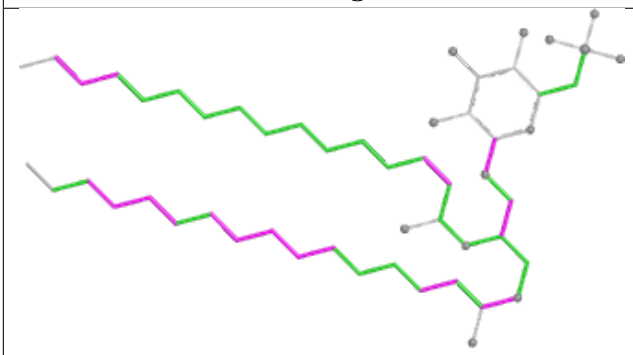
Ligand SQD A 616



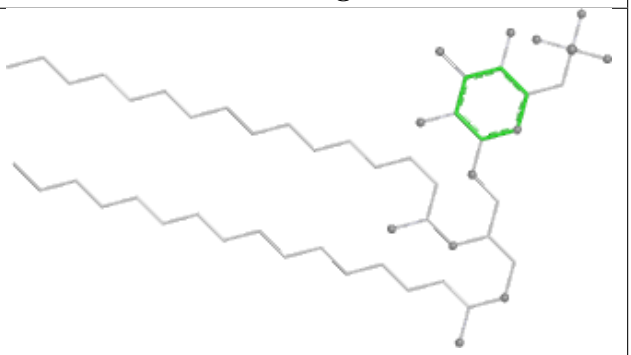
Bond lengths



Bond angles

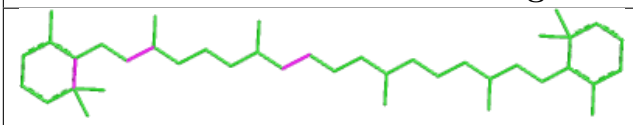


Torsions

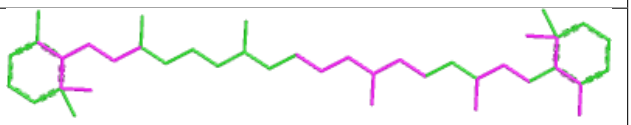


Rings

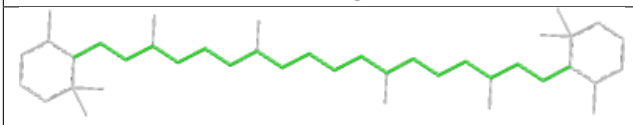
Ligand BCR c 515



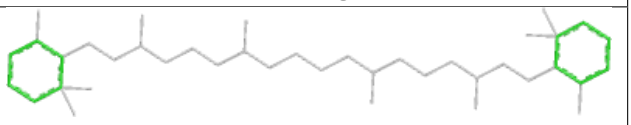
Bond lengths



Bond angles

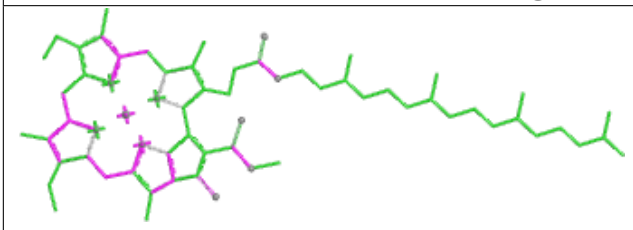


Torsions

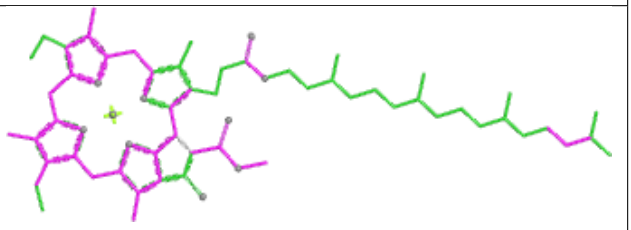


Rings

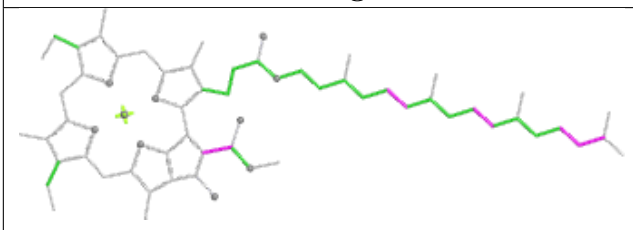
Ligand CLA c 506



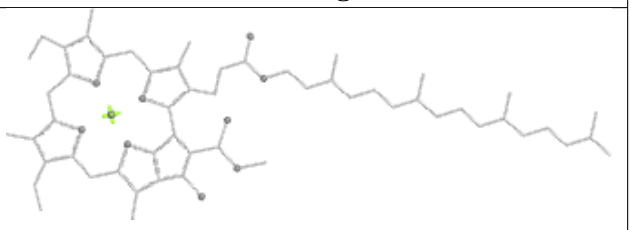
Bond lengths



Bond angles

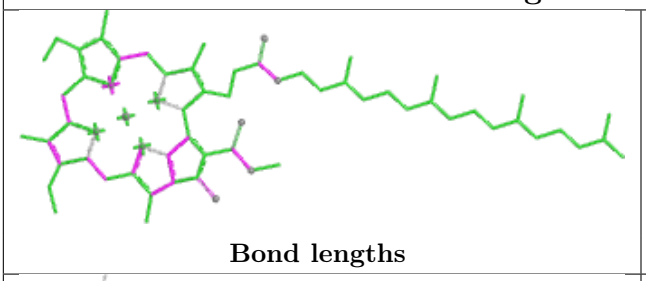


Torsions

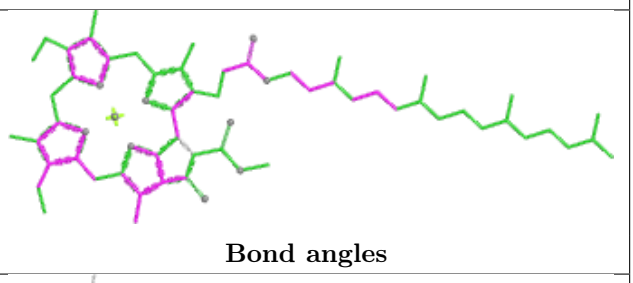


Rings

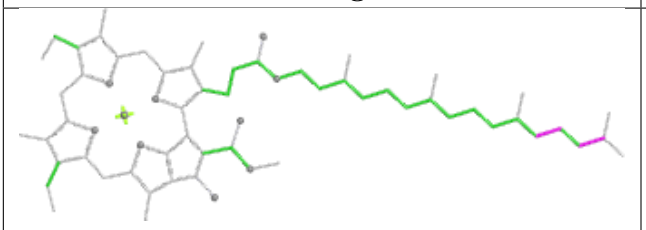
Ligand CLA B 614



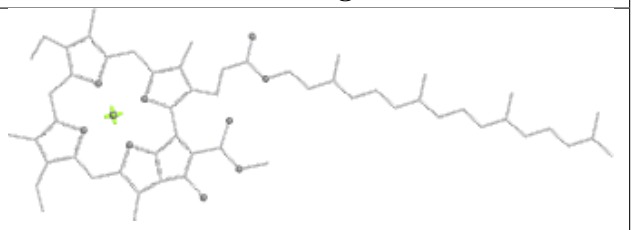
Bond lengths



Bond angles

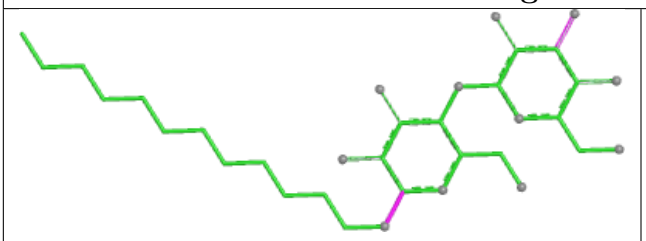


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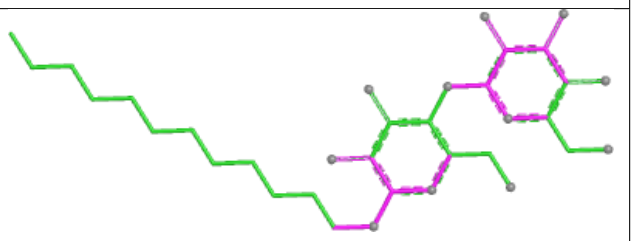


Rings

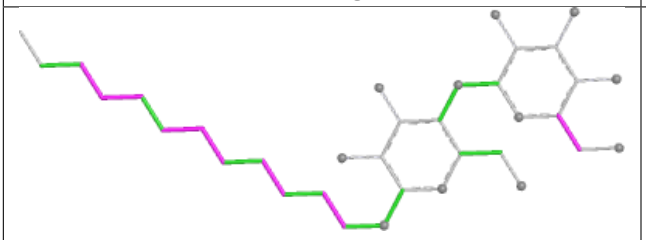
Ligand LMT A 617



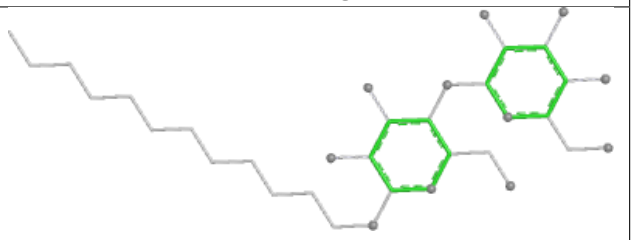
Bond lengths



Bond angles

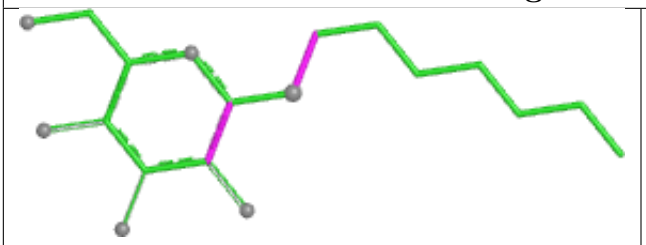


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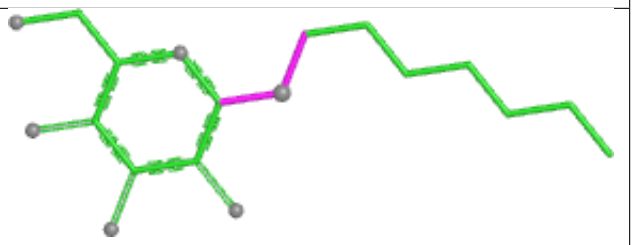


Rings

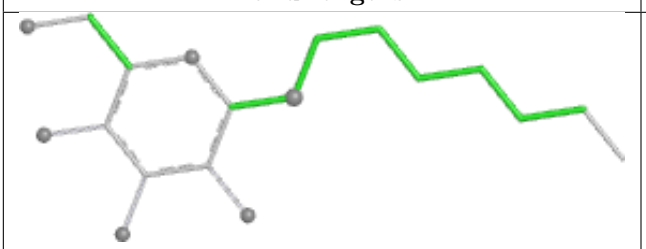
Ligand HTG o 301



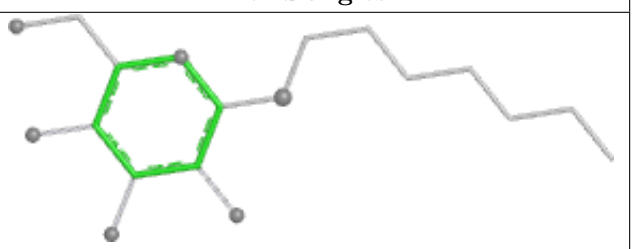
Bond lengths



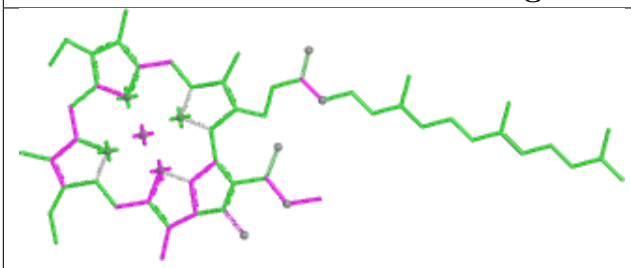
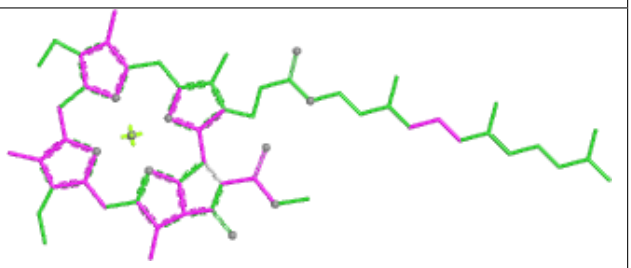
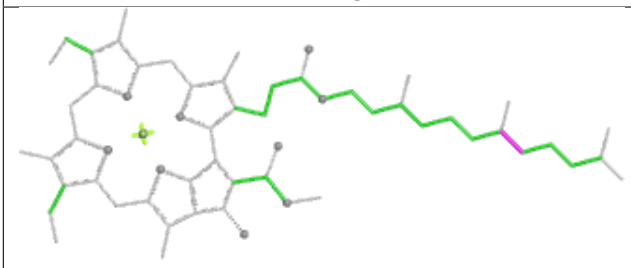
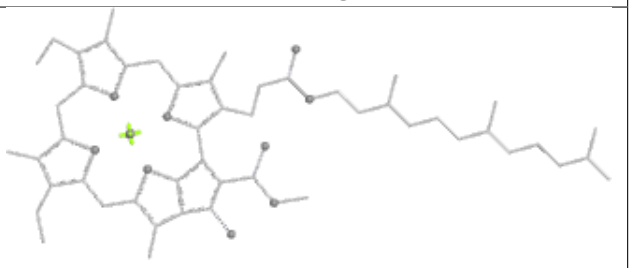
Bond angles

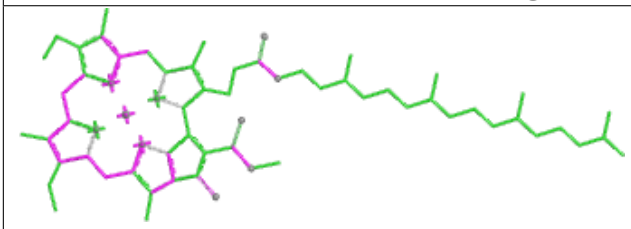
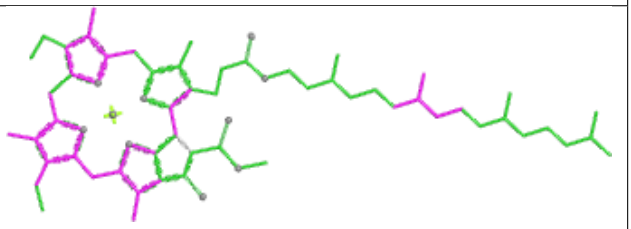
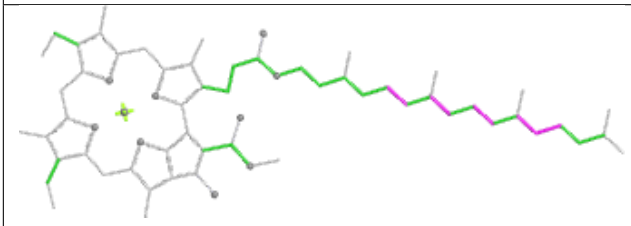
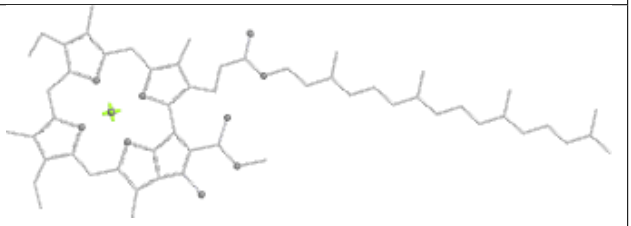


Torsions

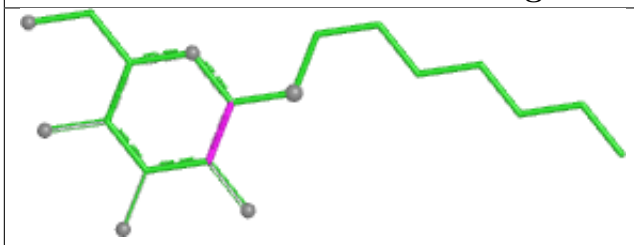


Rings

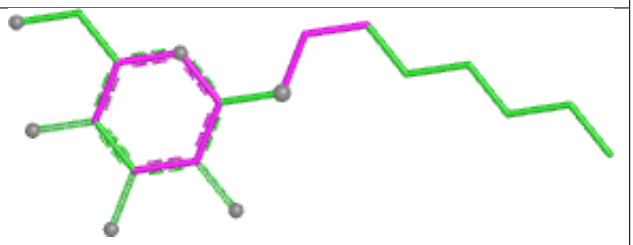
Ligand CLA C 508	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

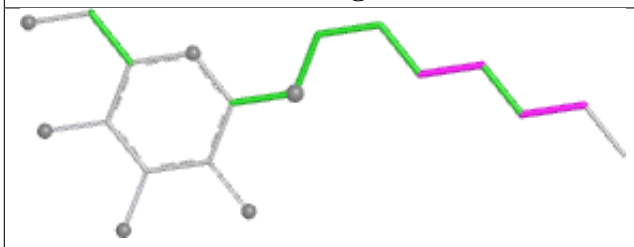
Ligand HTG b 623



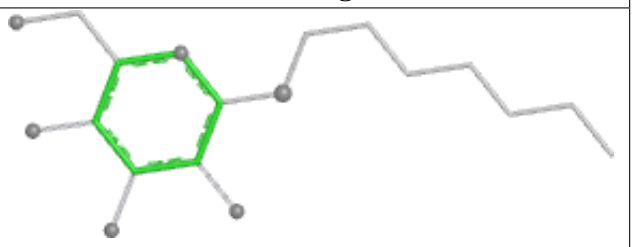
Bond lengths



Bond angles

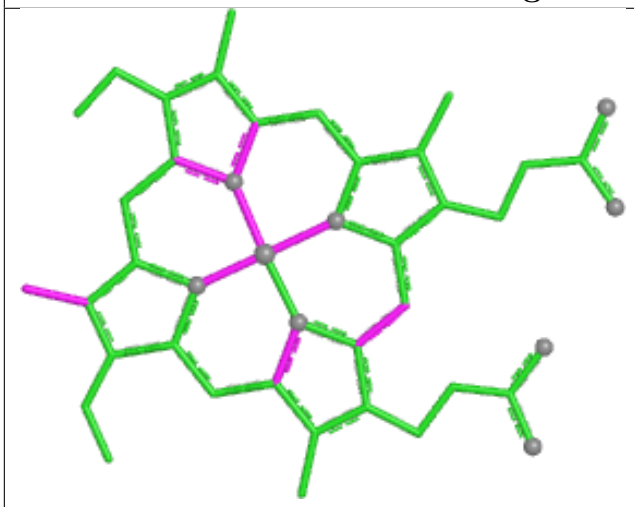


Torsions

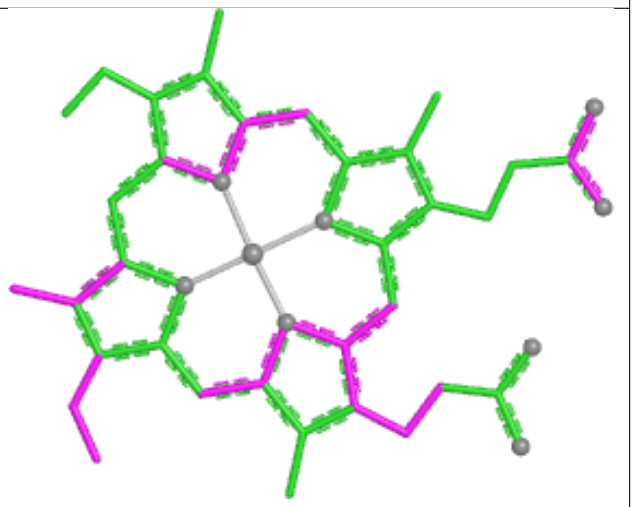


Rings

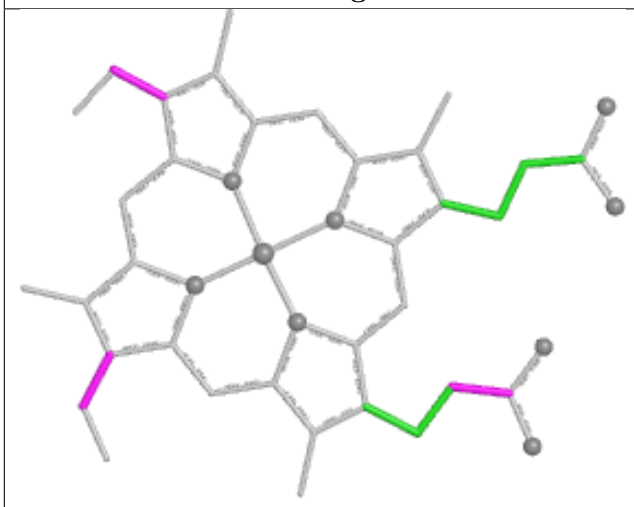
Ligand HEC V 203



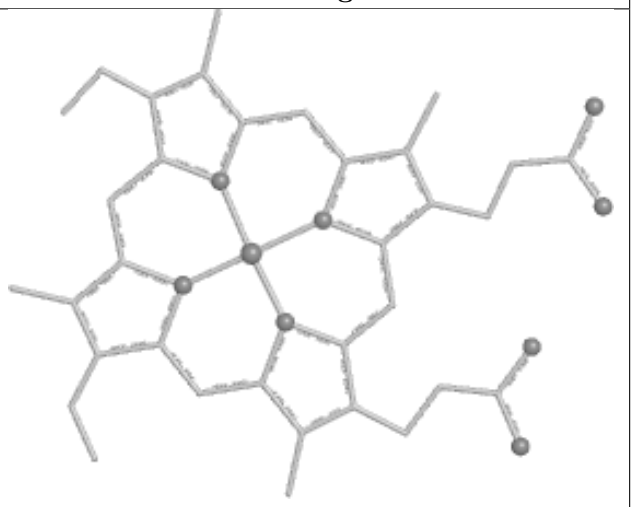
Bond lengths



Bond angles

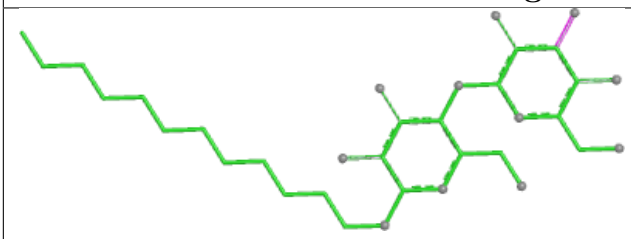


Torsions

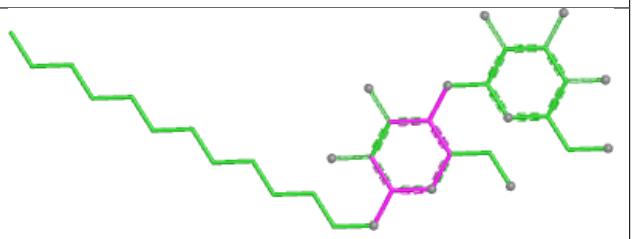


Rings

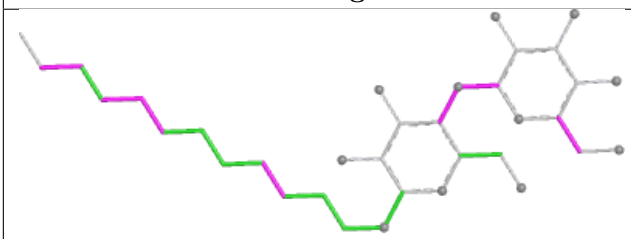
Ligand LMT b 622



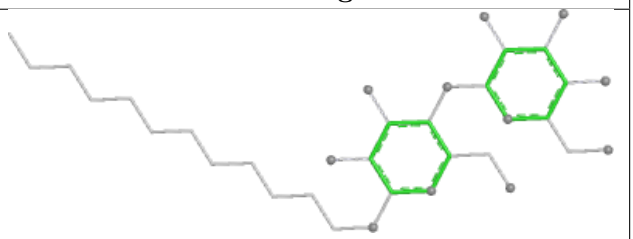
Bond lengths



Bond angles

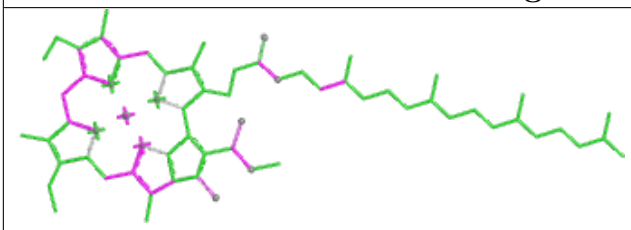


Torsions

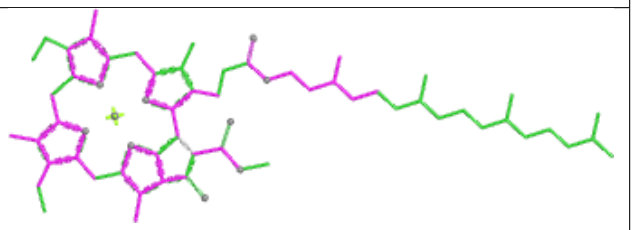


Rings

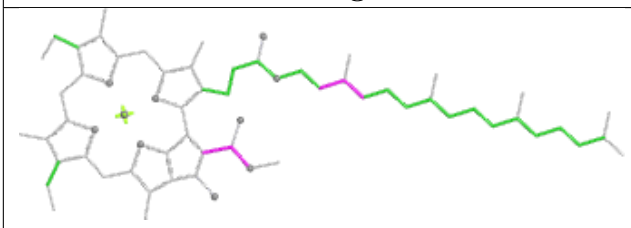
Ligand CLA B 606



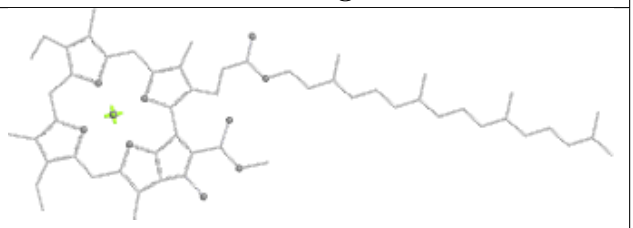
Bond lengths



Bond angles

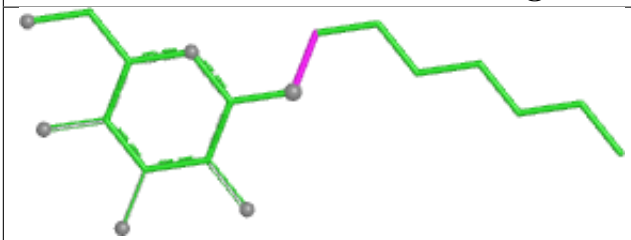


Torsions

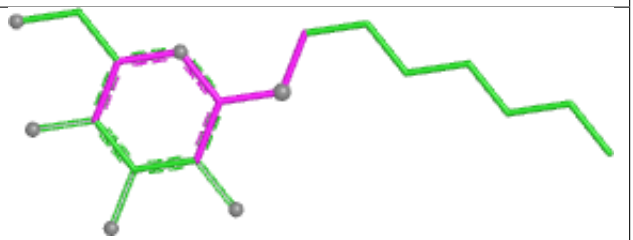


Rings

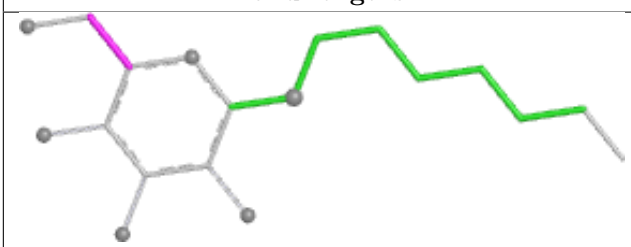
Ligand HTG c 523



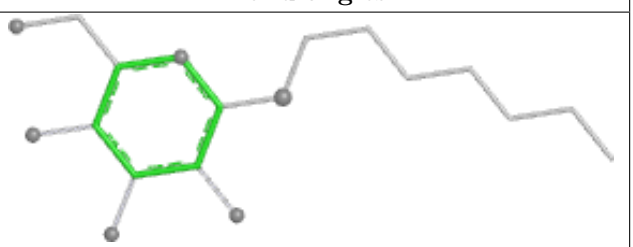
Bond lengths



Bond angles

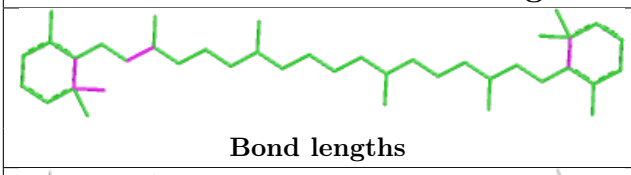


Torsions

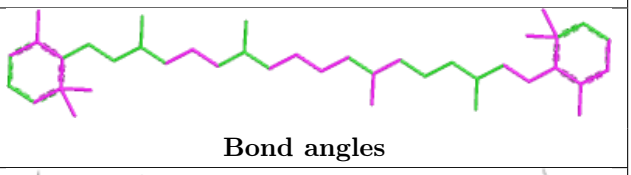


Rings

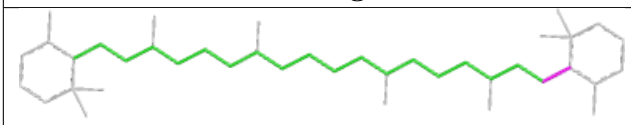
Ligand BCR d 406



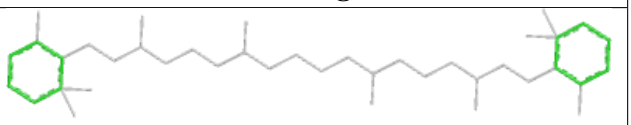
Bond lengths



Bond angles

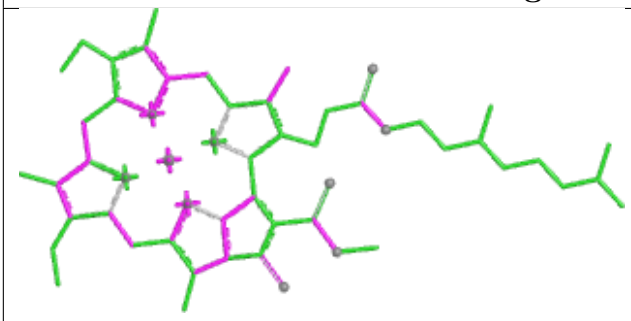


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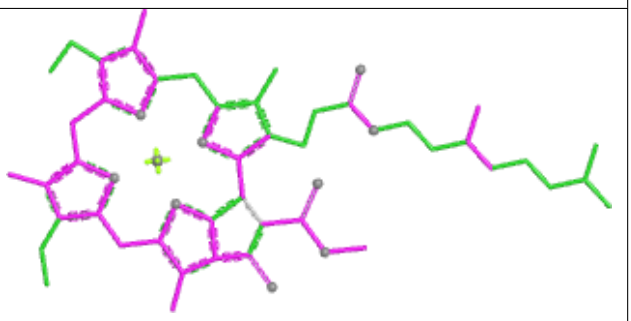


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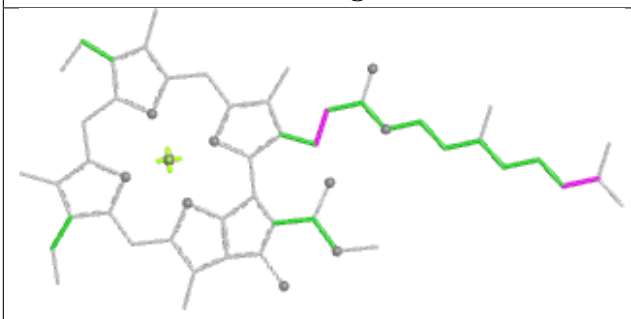
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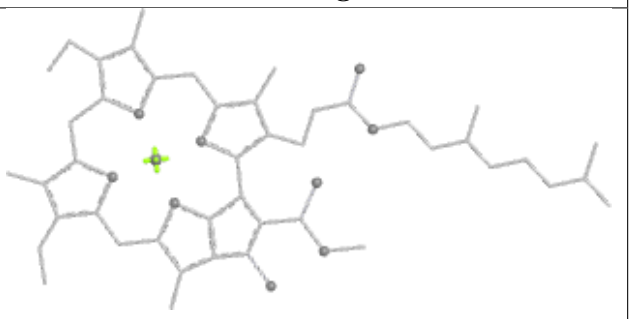
Bond lengths



Bond angles

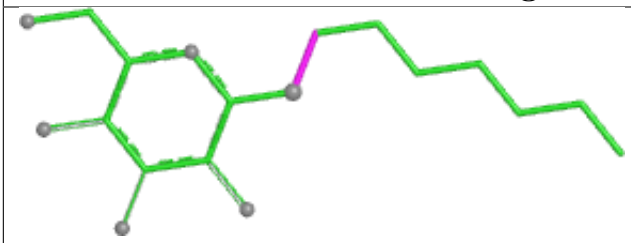


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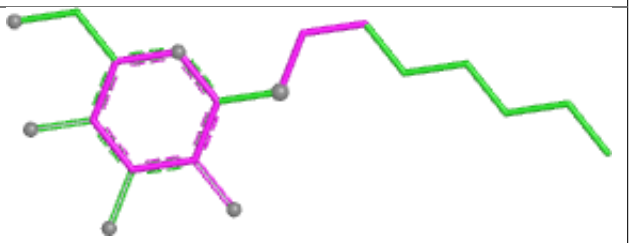


Rings

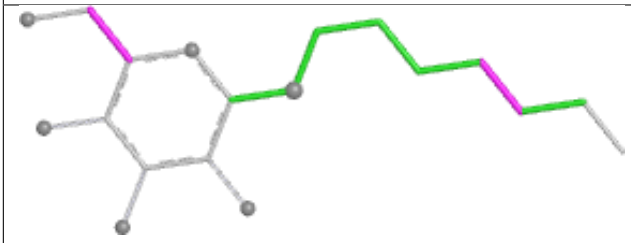
Ligand HTG H 101



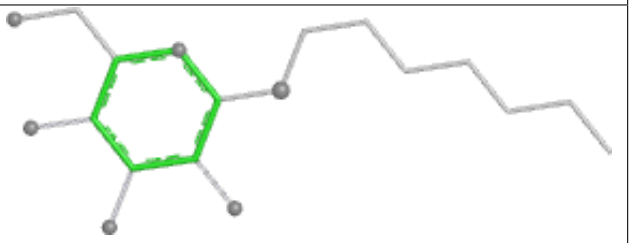
Bond lengths



Bond angles

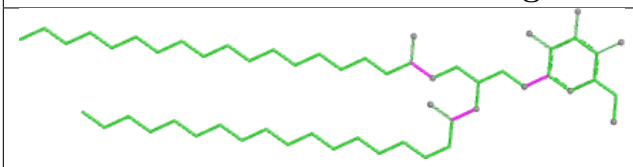


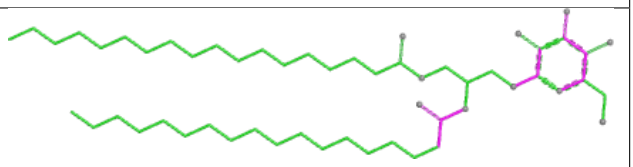
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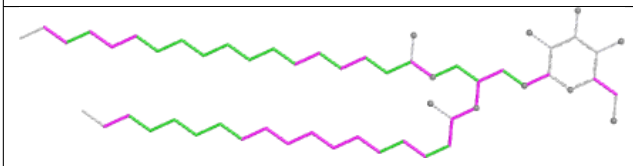


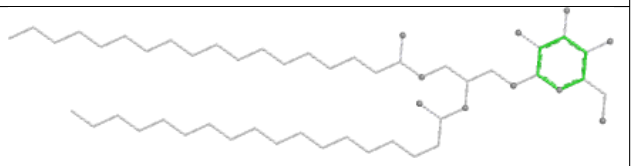
Rings

Ligand LMG d 412

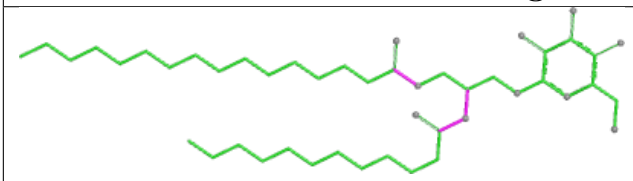

Bond lengths

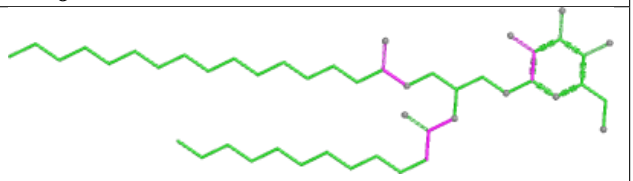

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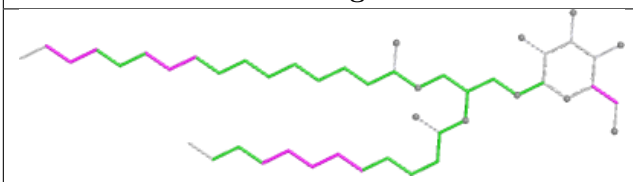

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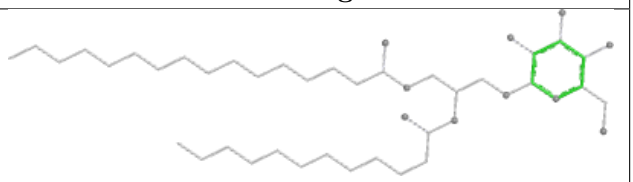

Rings

Ligand LMG j 101

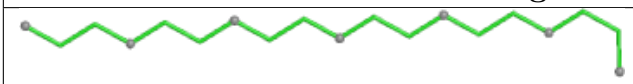

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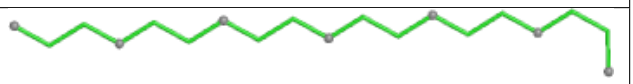

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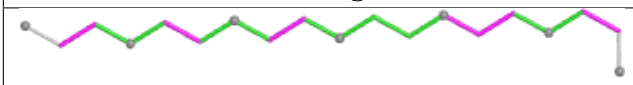

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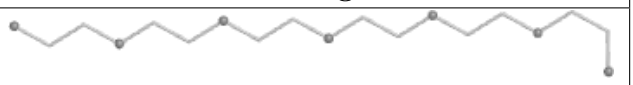

Rings

Ligand P6G b 648

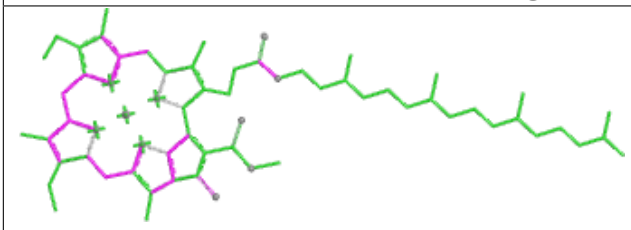

Bond lengths


Bond angles

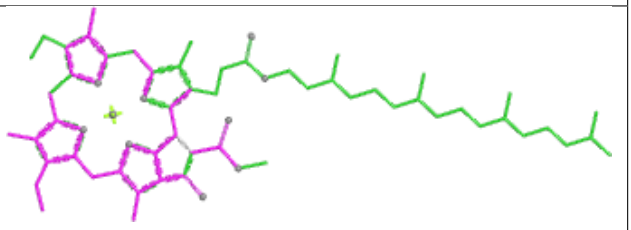

Torsions


Rings

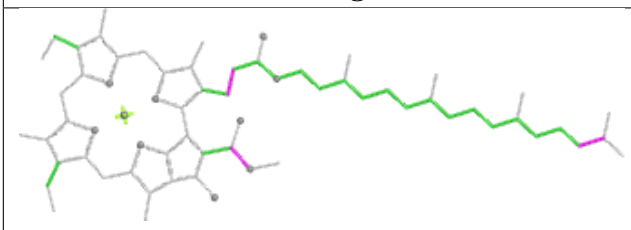
Ligand CLA C 501



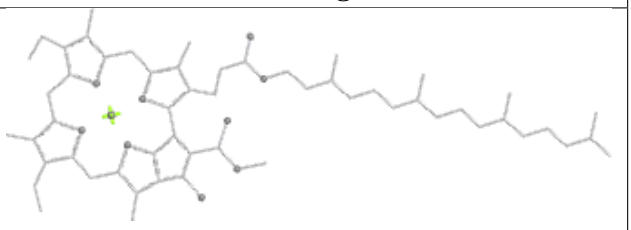
Bond lengths



Bond angles

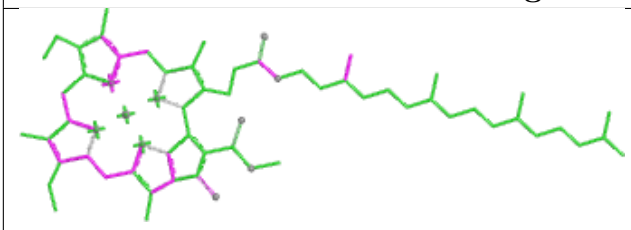


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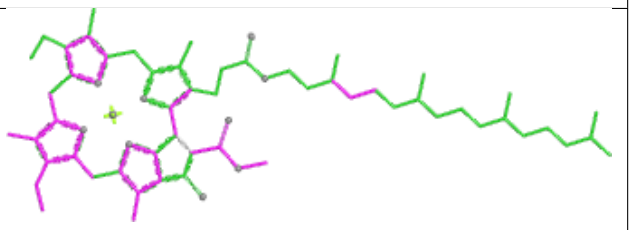


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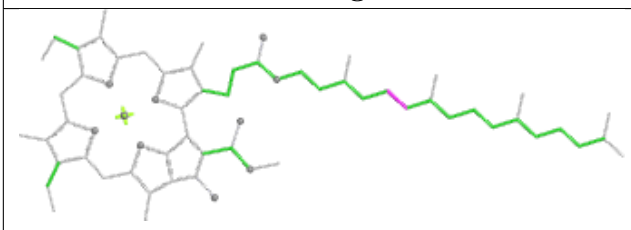
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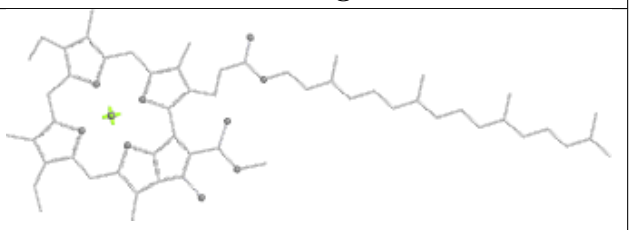
Bond lengths



Bond angles

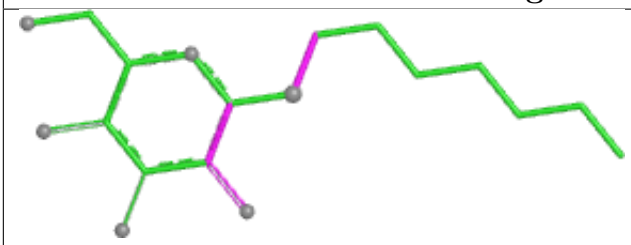


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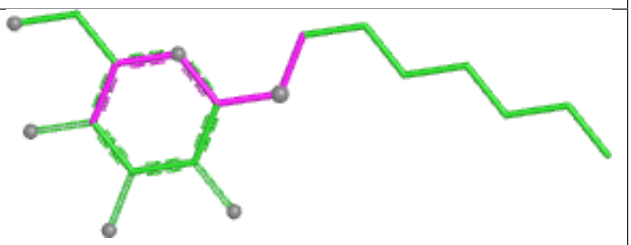


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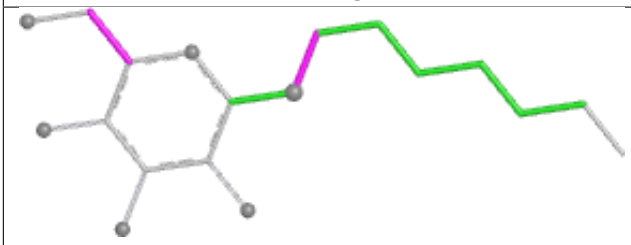
Ligand HTG c 530



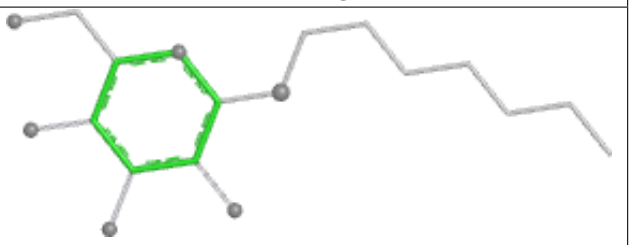
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Bond angles

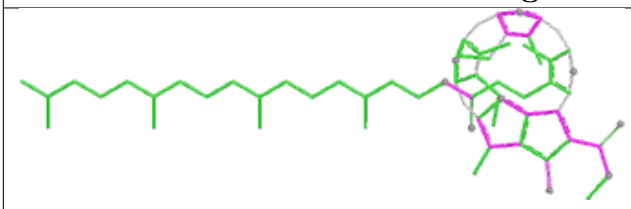


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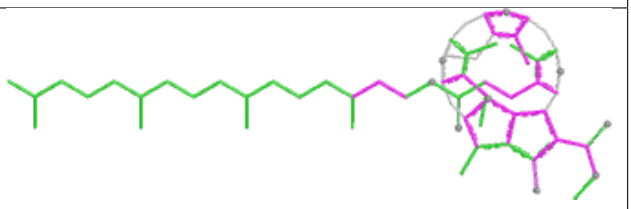


Rings

Ligand PHO A 608



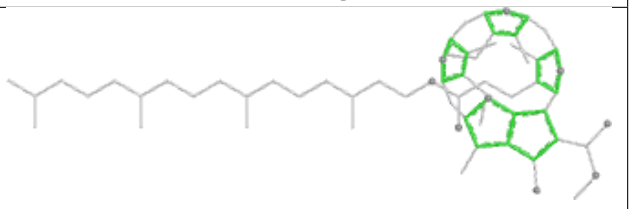
Bond lengths



Bond angles

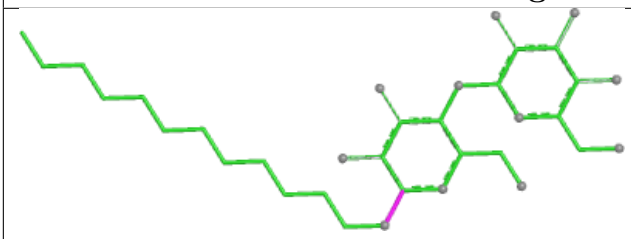


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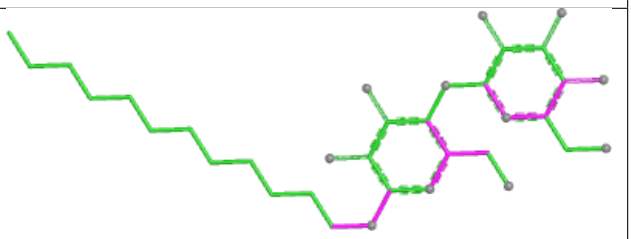


Rings

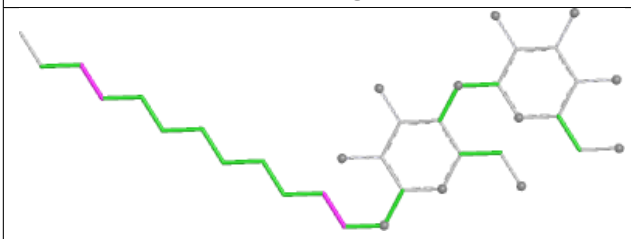
Ligand LMT f 101



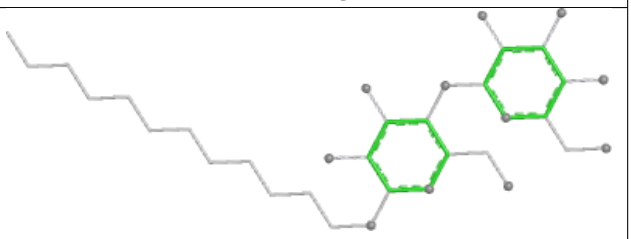
Bond lengths



Bond angles

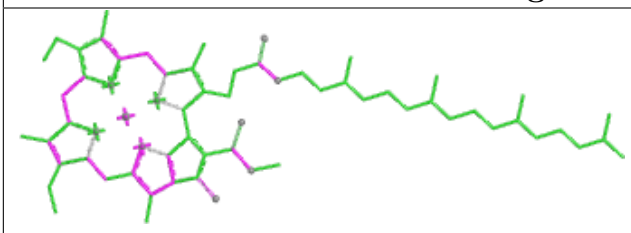


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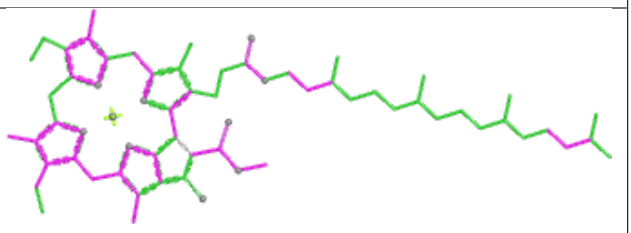


Rings

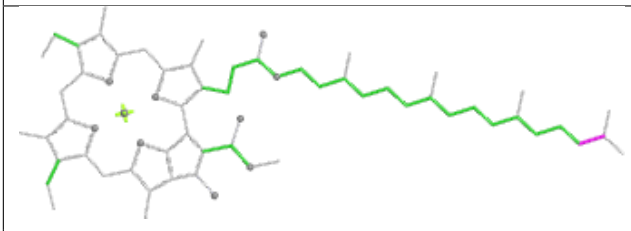
Ligand CLA b 603



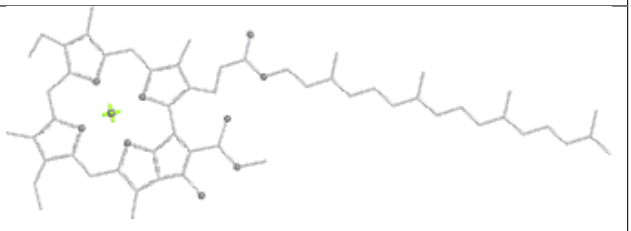
Bond lengths



Bond angles

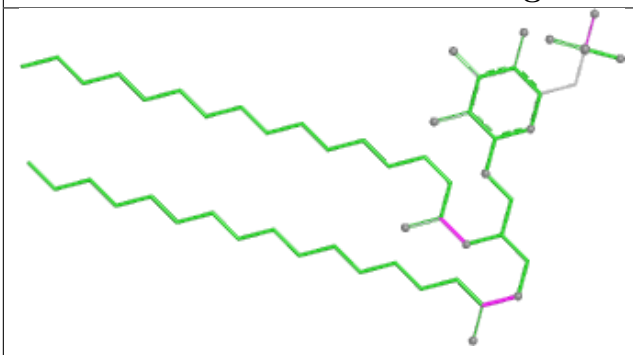


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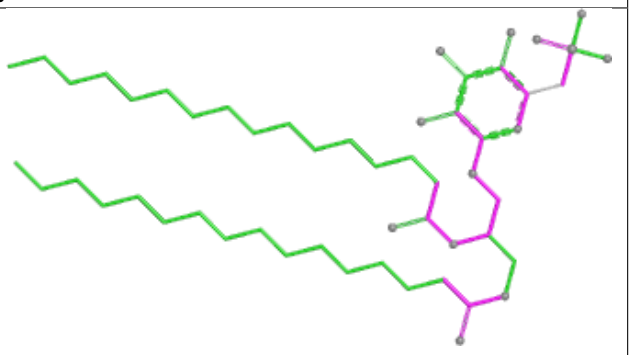


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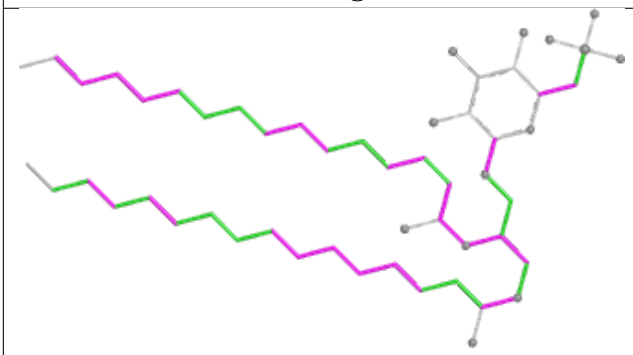
Ligand SQD A 622



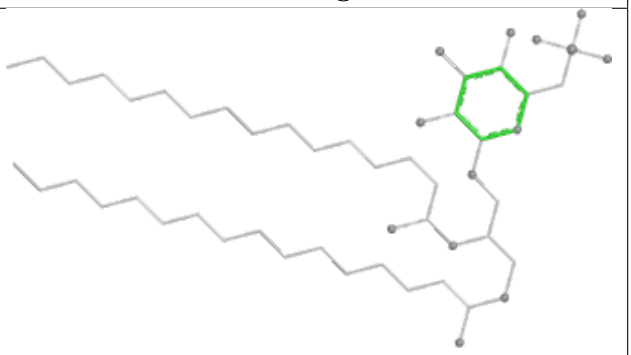
Bond lengths



Bond angles

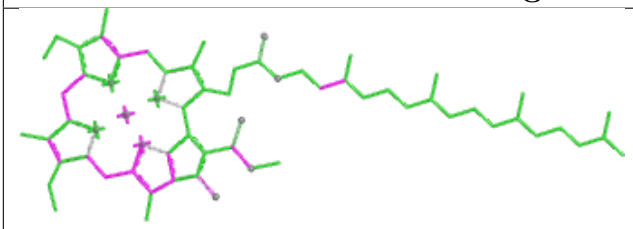


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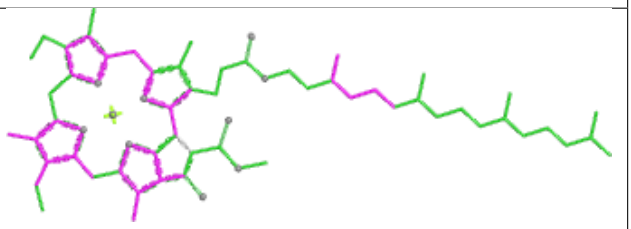


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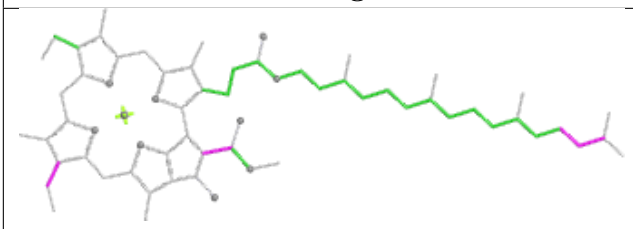
Ligand CLA A 606



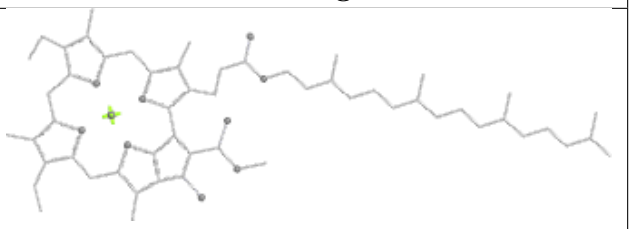
Bond lengths



Bond angles

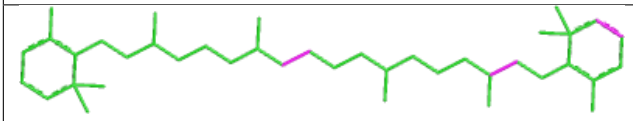


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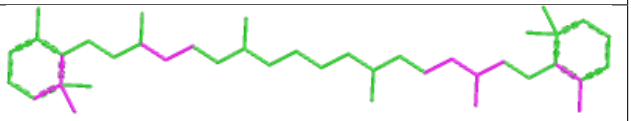


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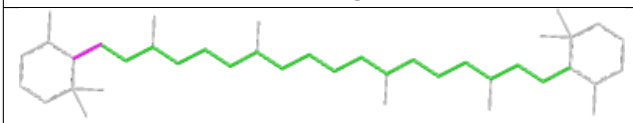
Ligand BCR B 620



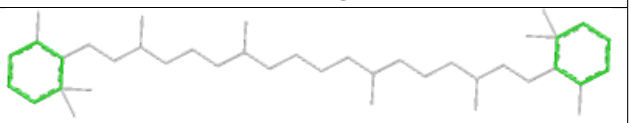
Bond lengths



Bond angles

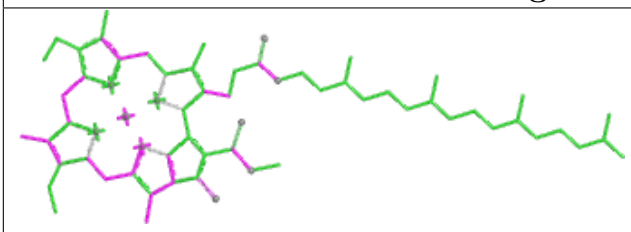


Torsions

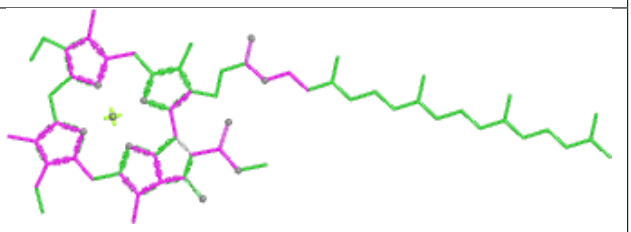


Rings

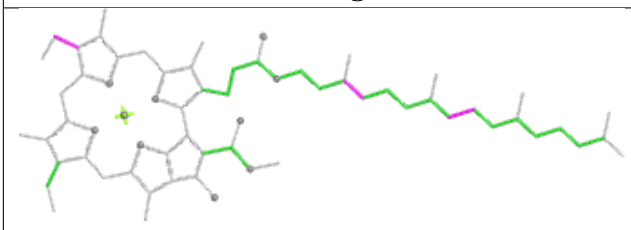
Ligand CLA c 510



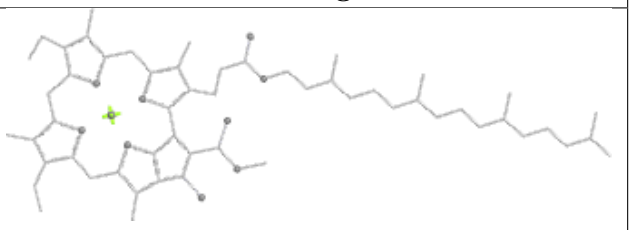
Bond lengths



Bond angles



Torsions

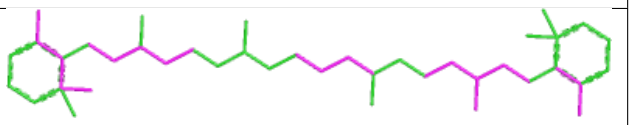


Rings

Ligand BCR C 525



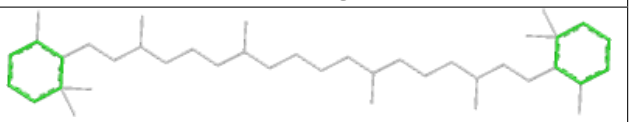
Bond lengths



Bond angles

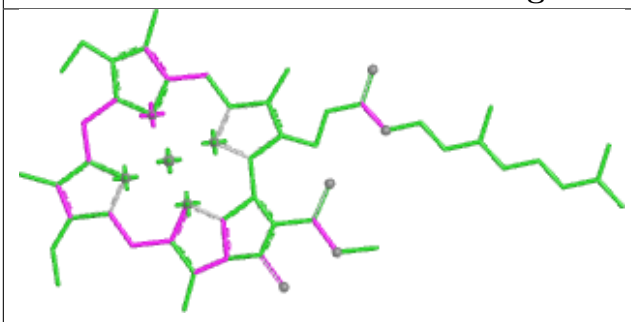


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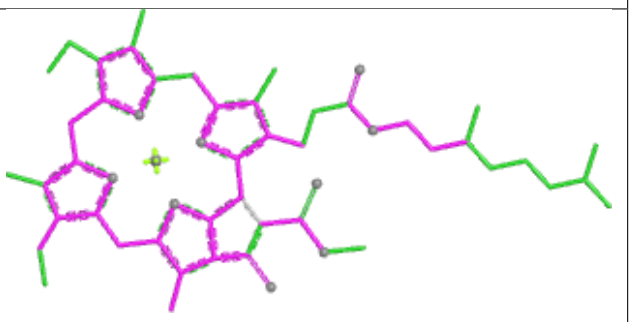


Rings

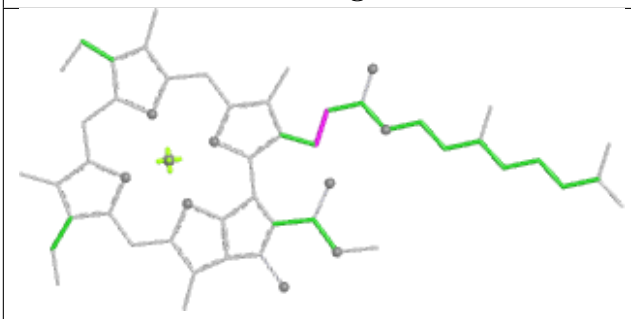
Ligand CLA b 607



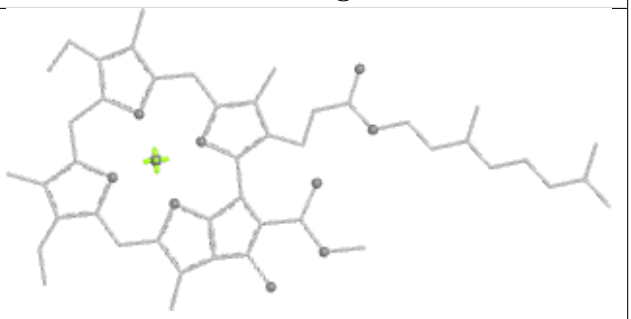
Bond lengths



Bond angles

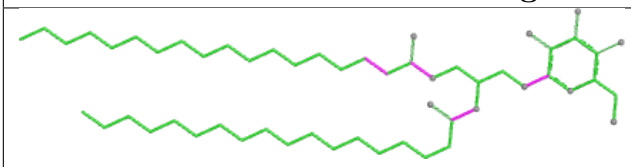


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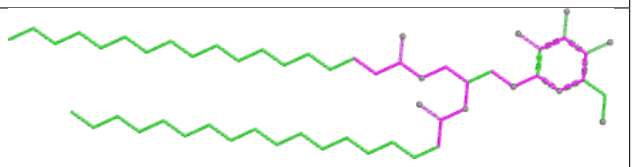


Rings

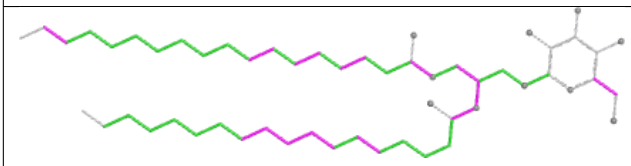
Ligand LMG B 634



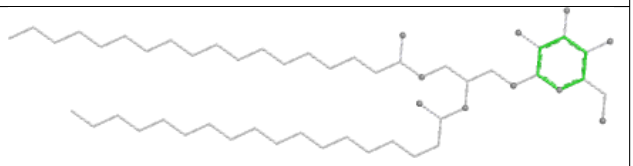
Bond lengths



Bond angles

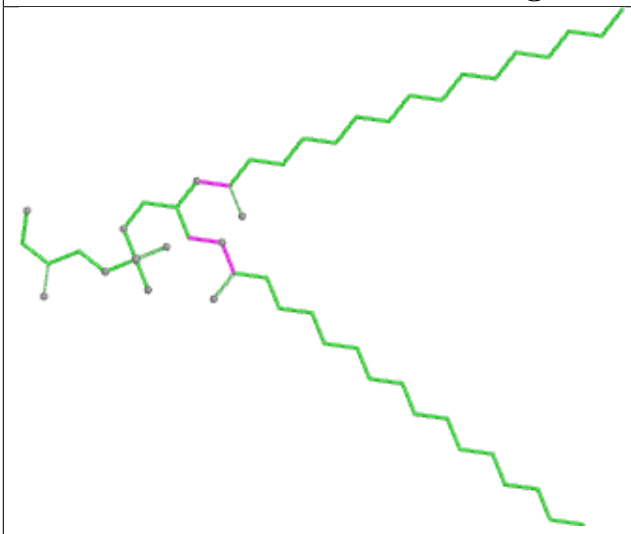


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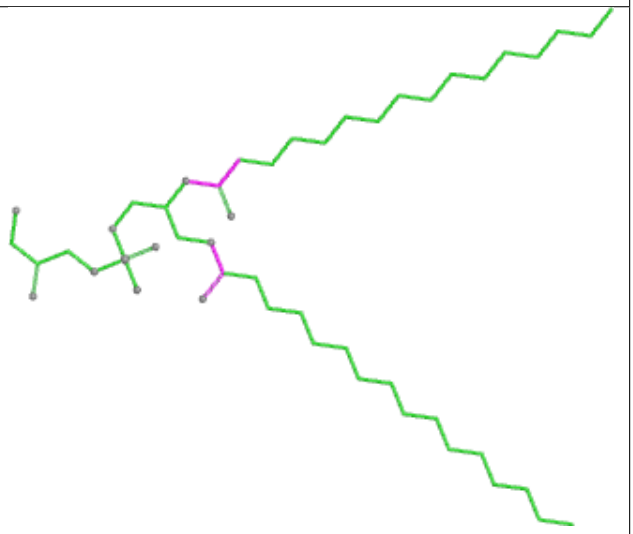


Rings

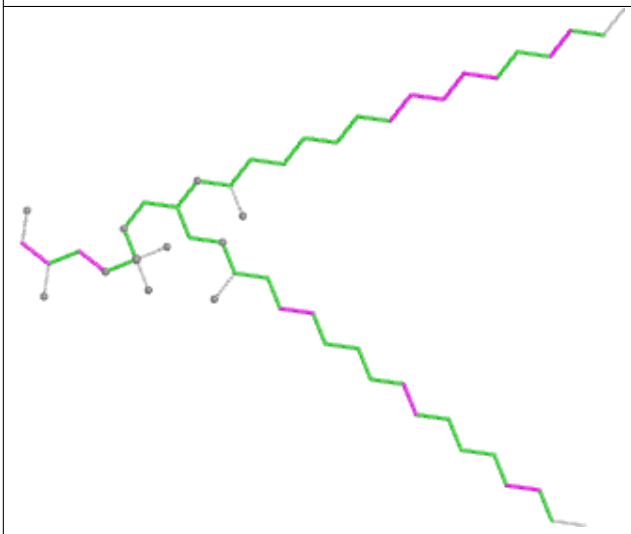
Ligand LHG d 411



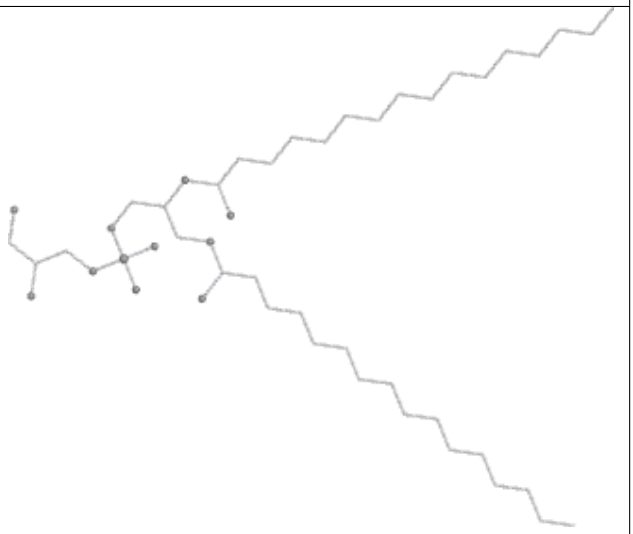
Bond lengths



Bond angles

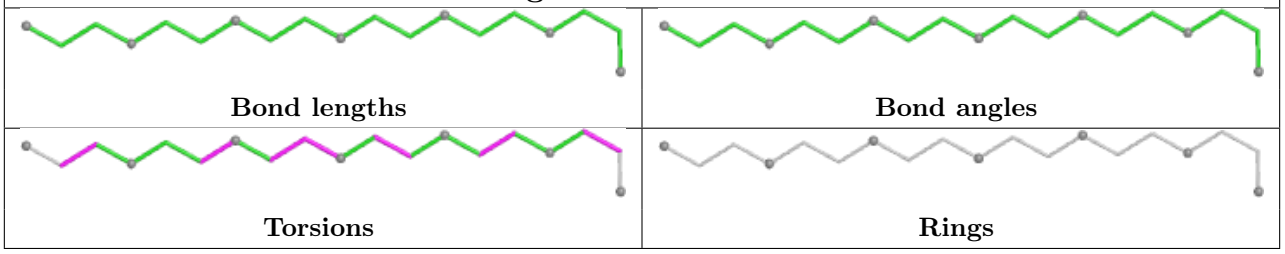


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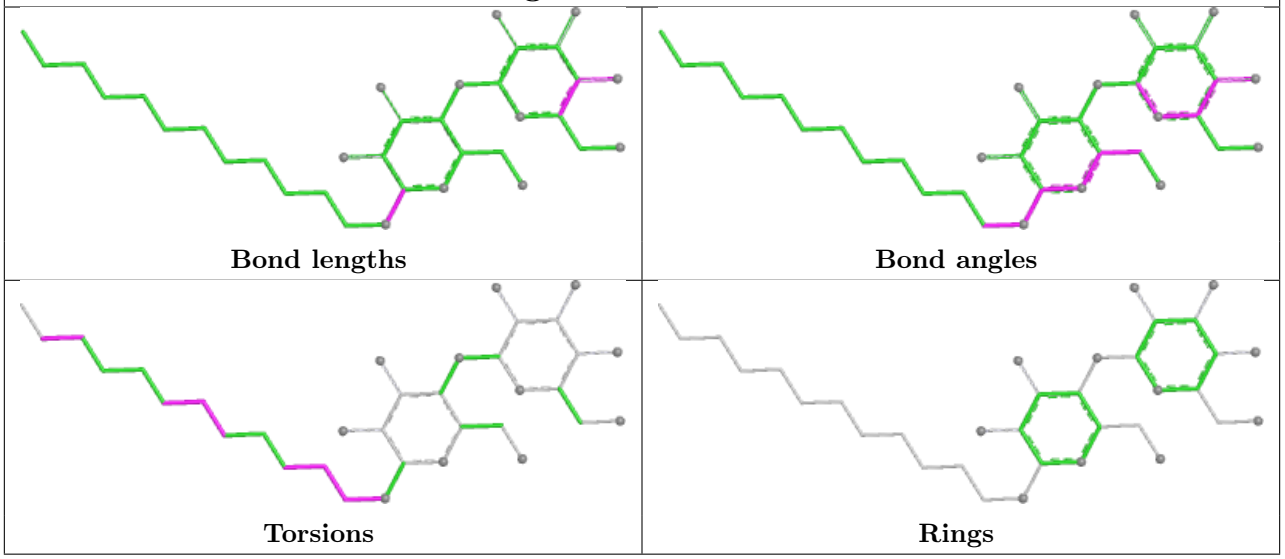


Rings

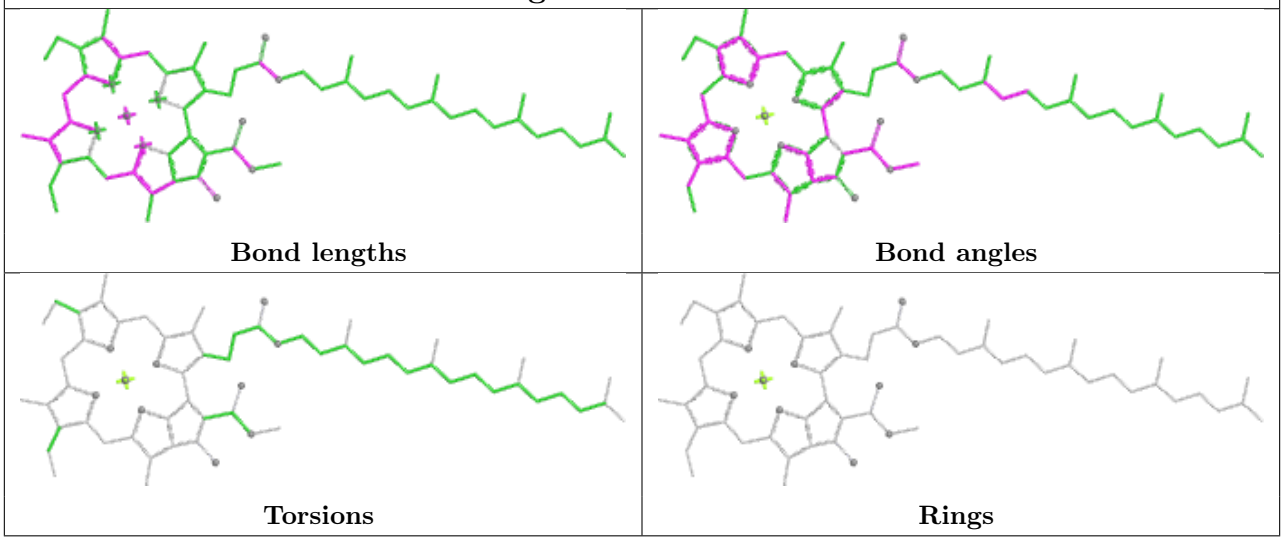
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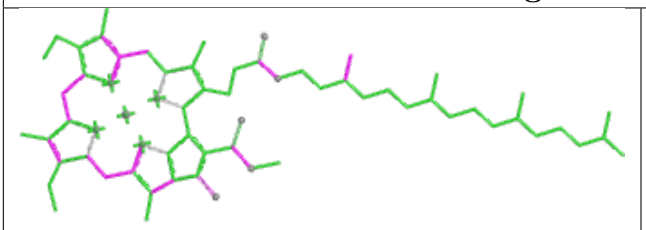
Ligand LMT F 102



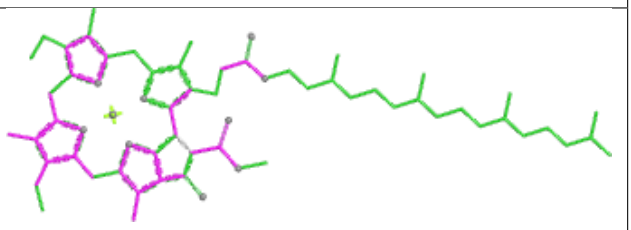
Ligand CLA b 610



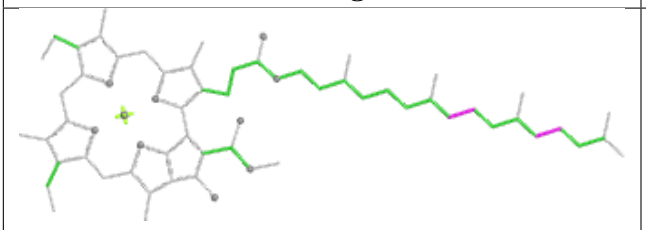
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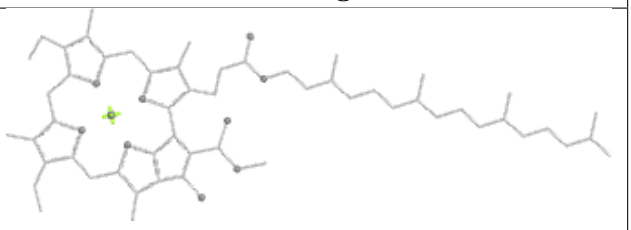
Bond lengths



Bond angles

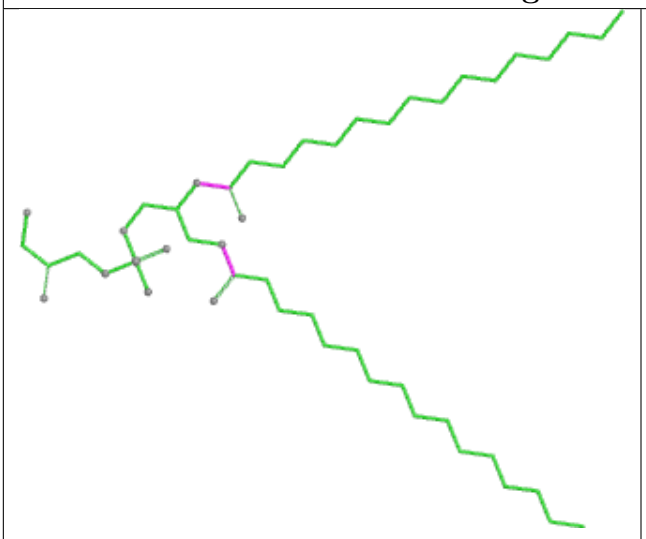


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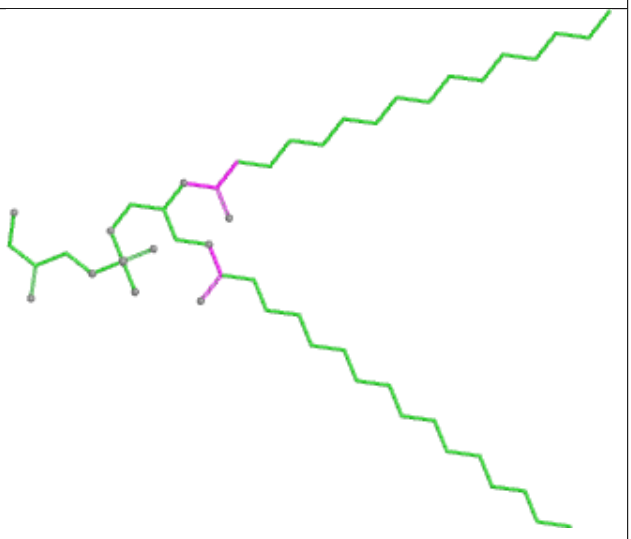


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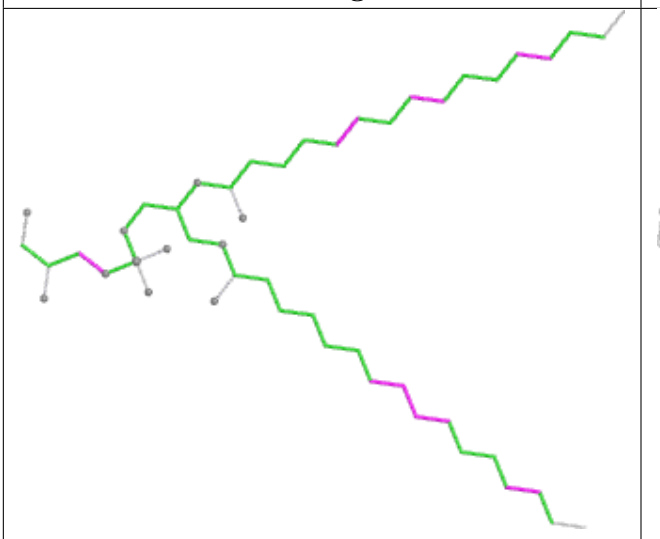
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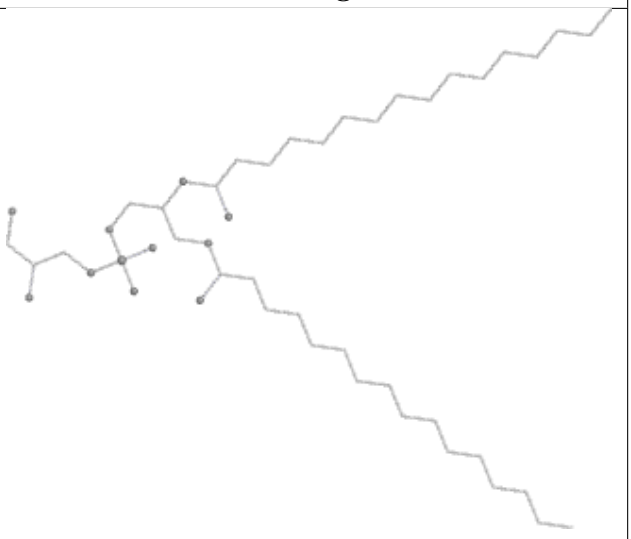
Bond lengths



Bond angles

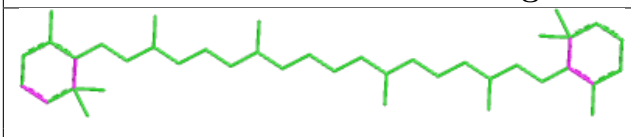


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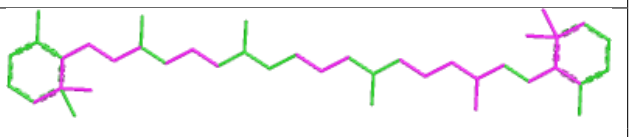


Rings

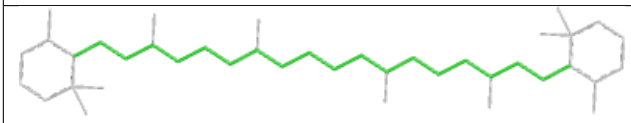
Ligand BCR D 406



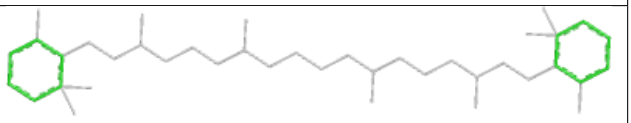
Bond lengths



Bond angles

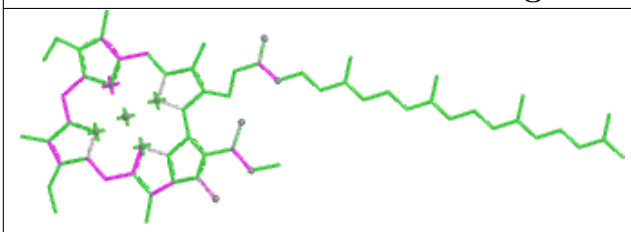


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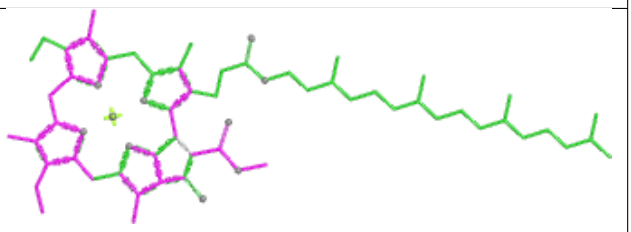


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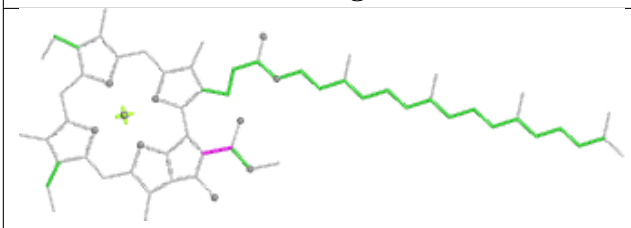
Ligand CLA B 610



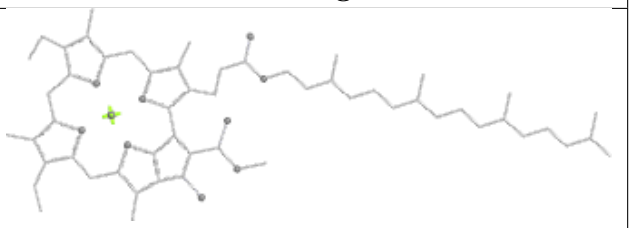
Bond lengths



Bond angles

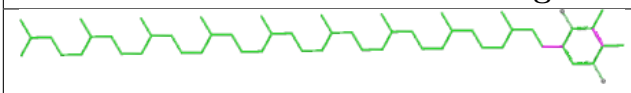


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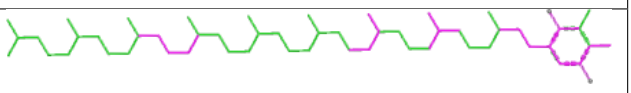


Rings

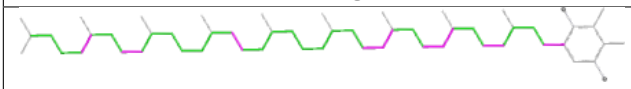
Ligand PL9 a 412



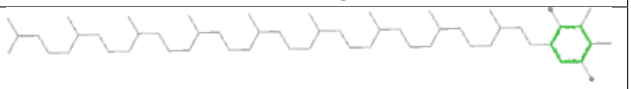
Bond lengths



Bond angles

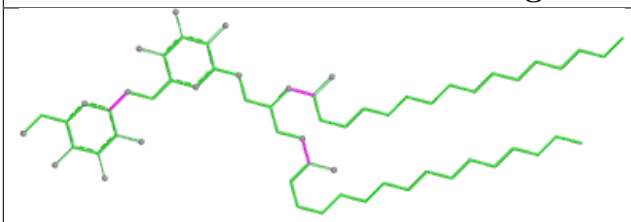


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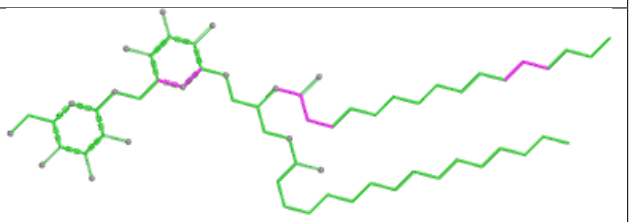


Rings

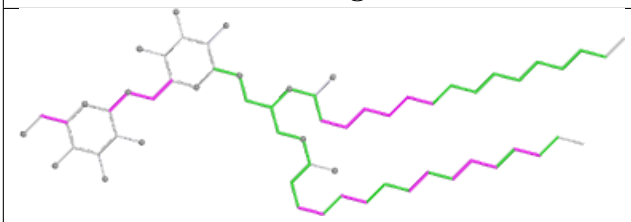
Ligand DGD c 516



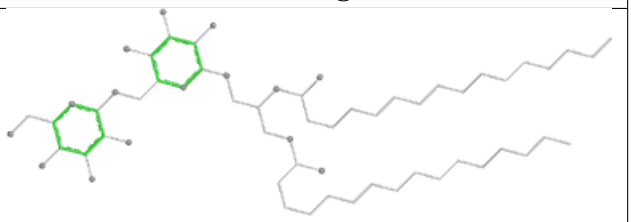
Bond lengths



Bond angles

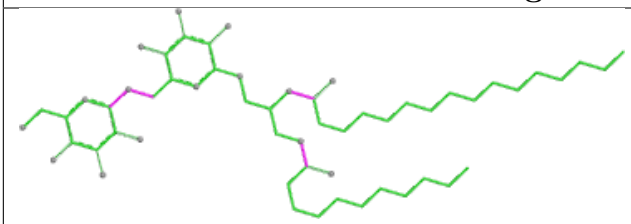


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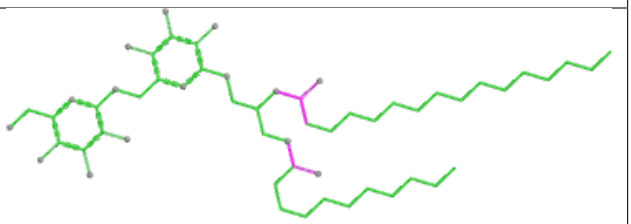


Rings

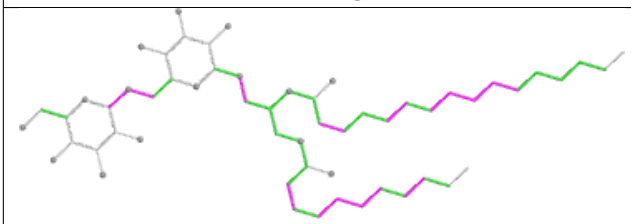
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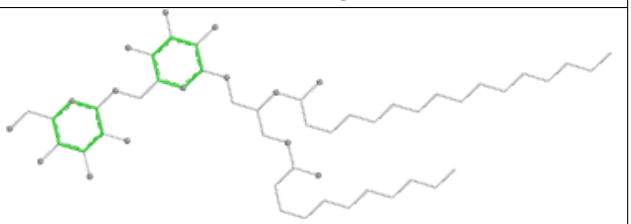
Bond lengths



Bond angles

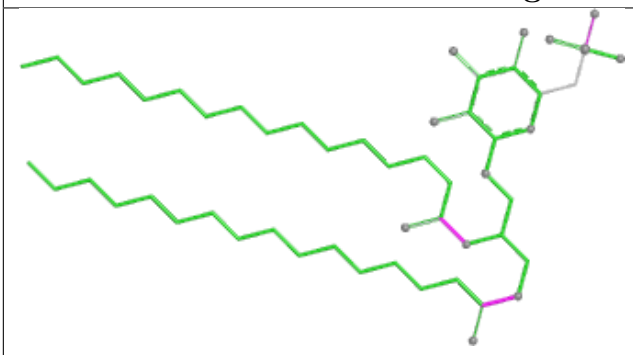


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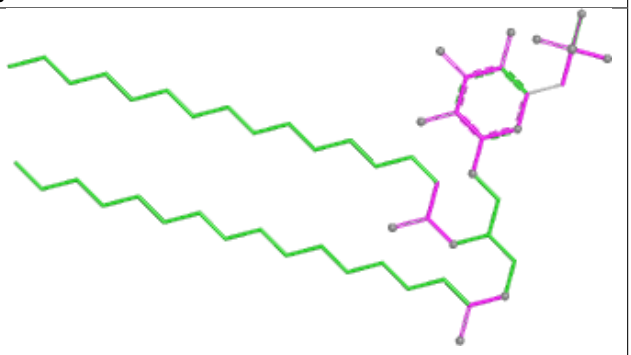


Rings

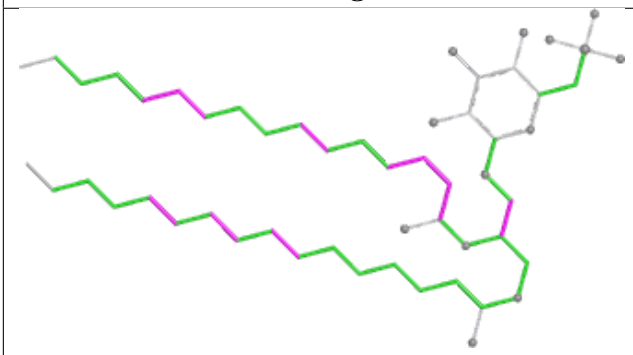
Ligand SQD A 612



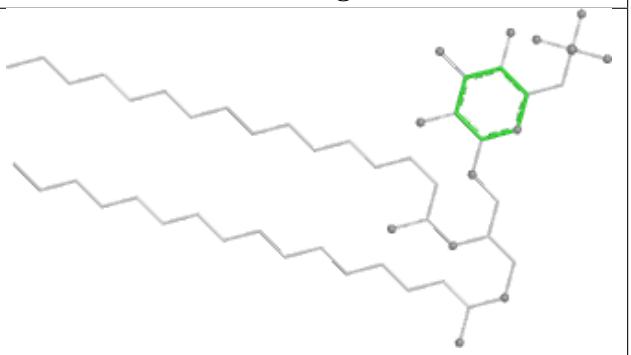
Bond lengths



Bond angles

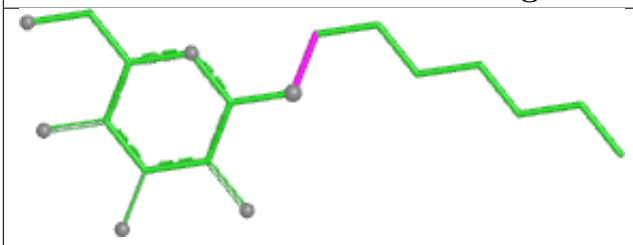


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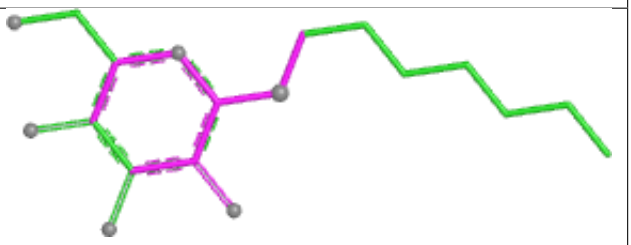


Rings

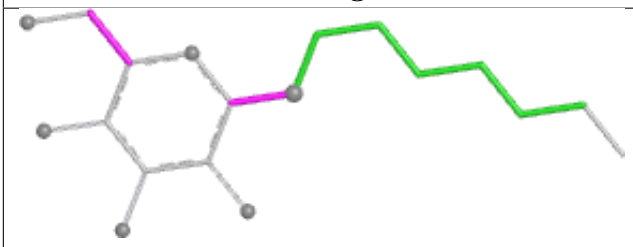
Ligand HTG B 624



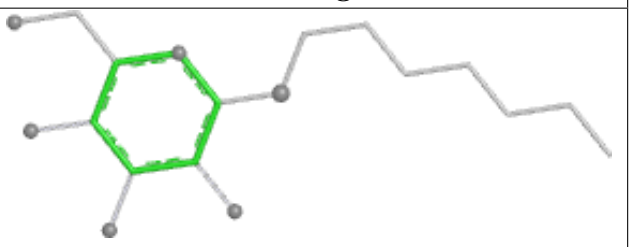
Bond lengths



Bond angles

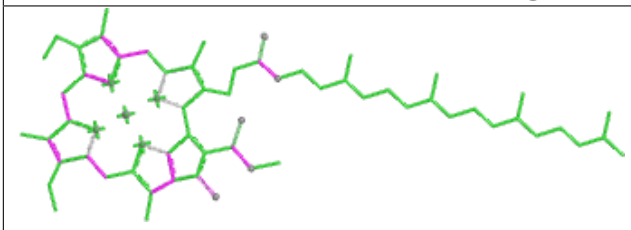


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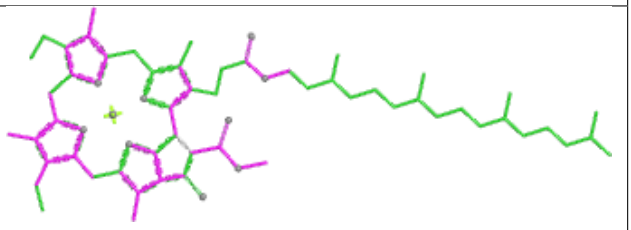


Rings

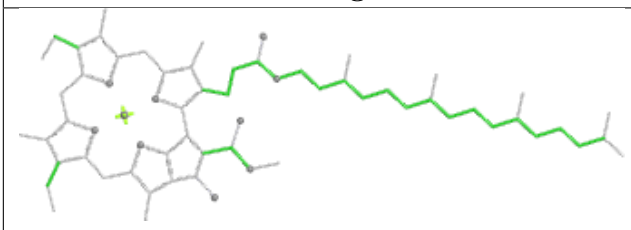
Ligand CLA C 511



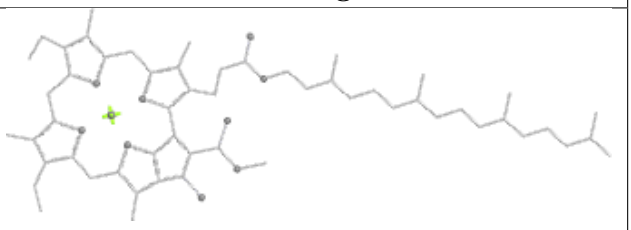
Bond lengths



Bond angles

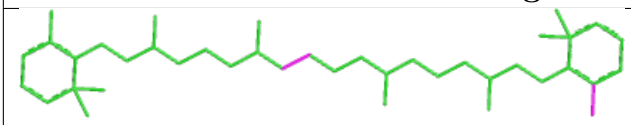


Torsions

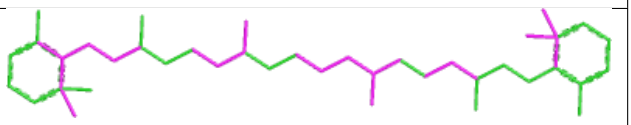


Rings

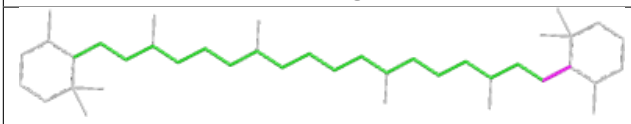
Ligand BCR T 102



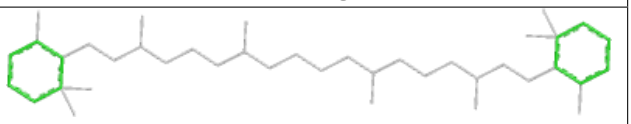
Bond lengths



Bond angles

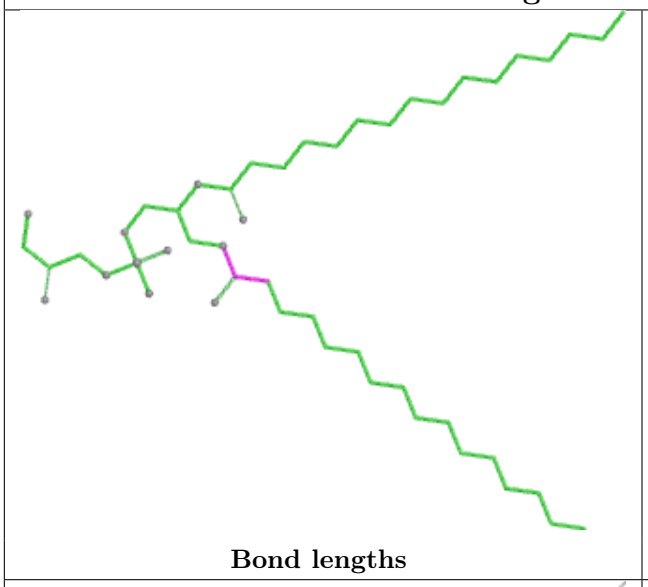


Torsions

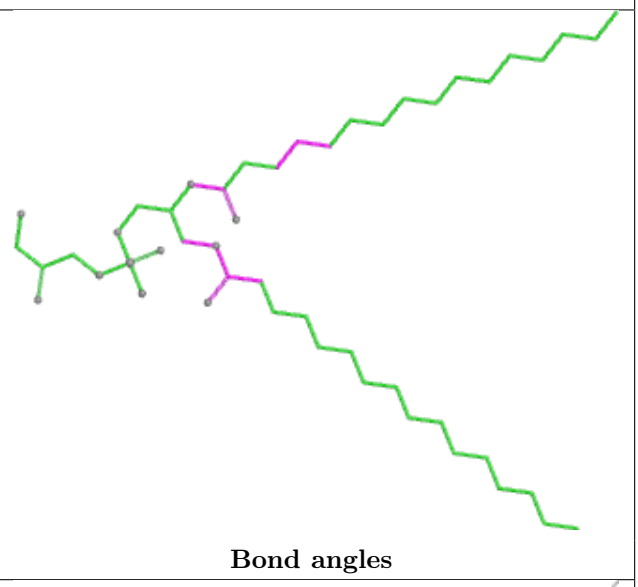


Rings

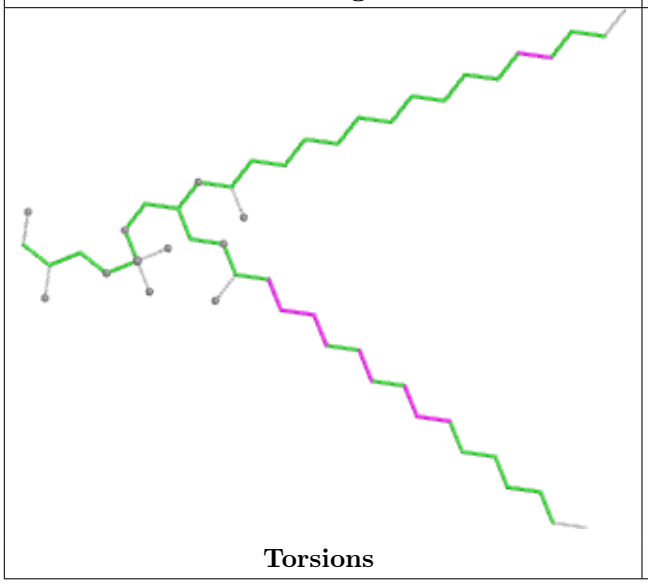
Ligand LHG D 409



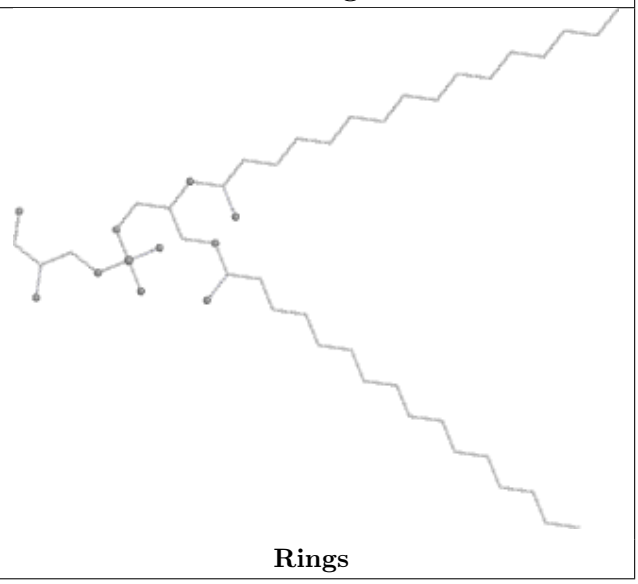
Bond lengths



Bond angles

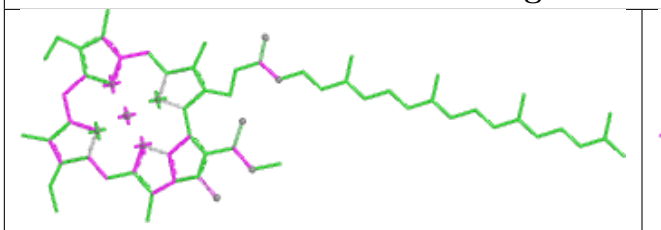


Torsions

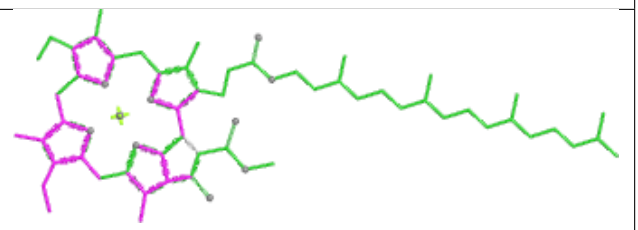


Rings

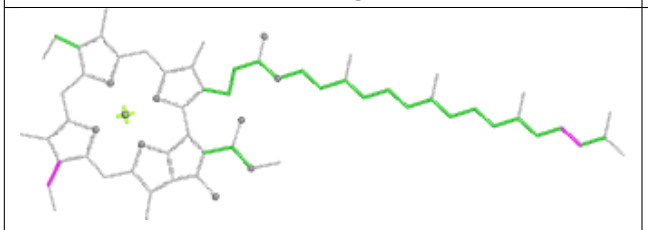
Ligand CLA D 403



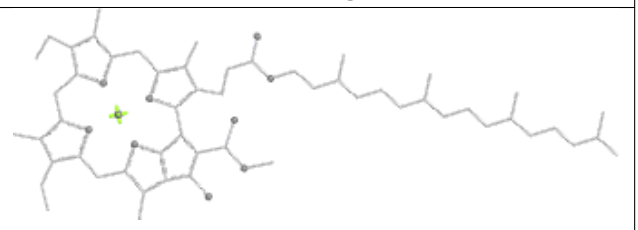
Bond lengths



Bond angles

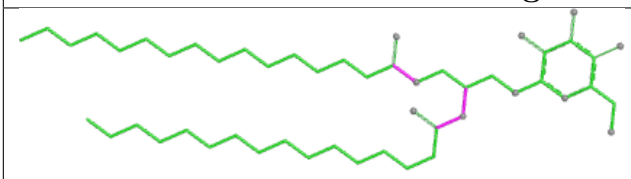


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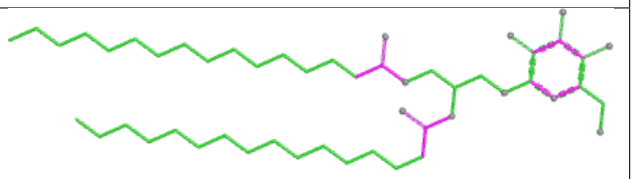


Rings

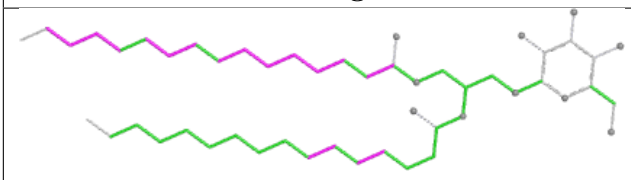
Ligand LMG b 621



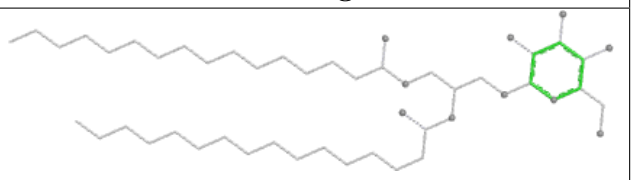
Bond lengths



Bond angles

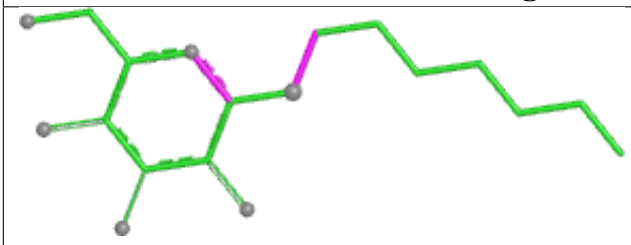


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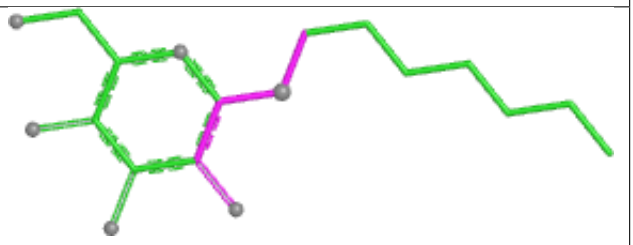


Rings

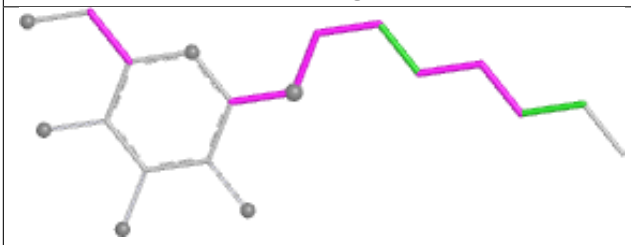
Ligand HTG C 531



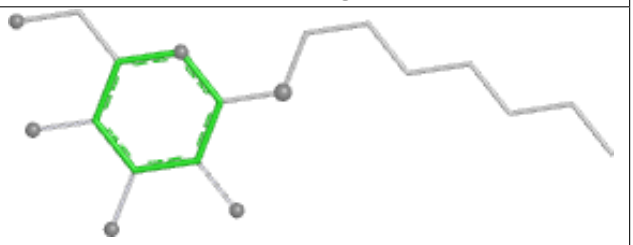
Bond lengths



Bond angles



Torsions

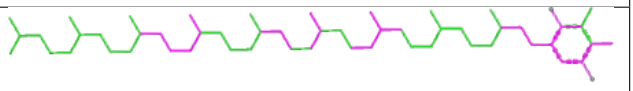


Rings

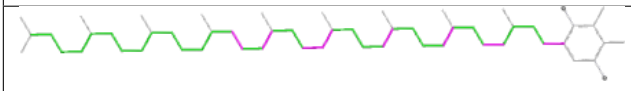
Ligand PL9 A 611



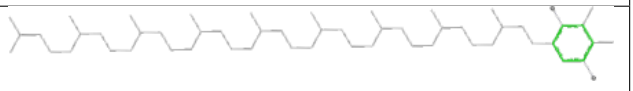
Bond lengths



Bond angles

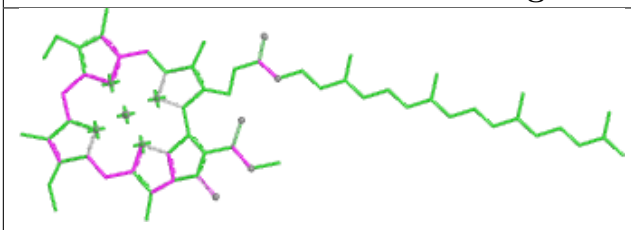


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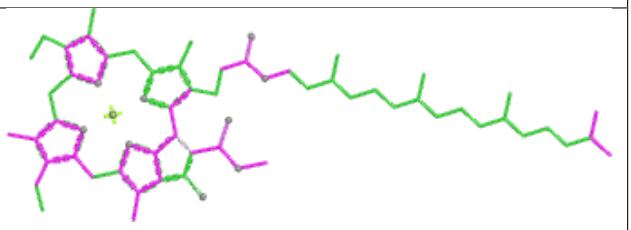


Rings

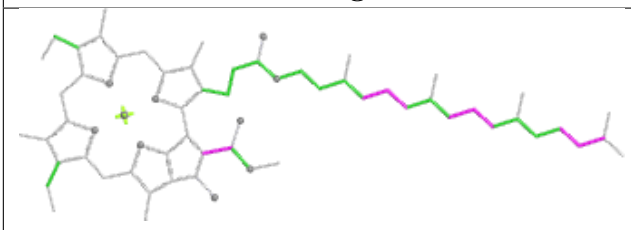
Ligand CLA b 615



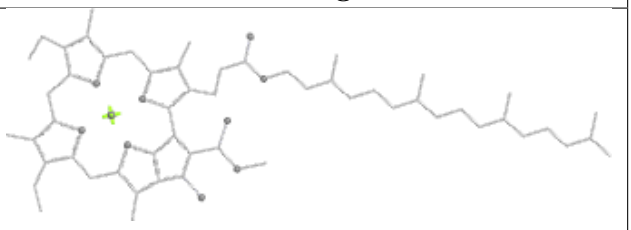
Bond lengths



Bond angles

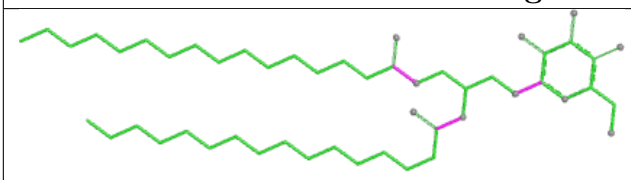


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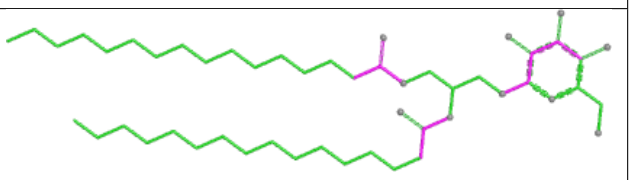


Rings

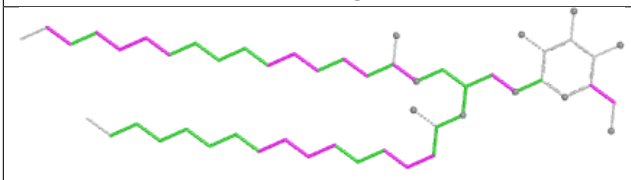
Ligand LMG c 520



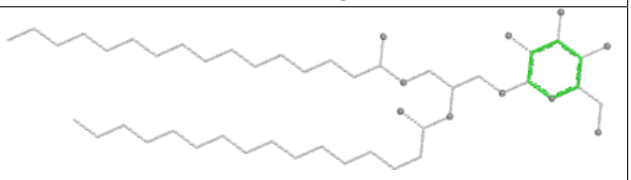
Bond lengths



Bond angles

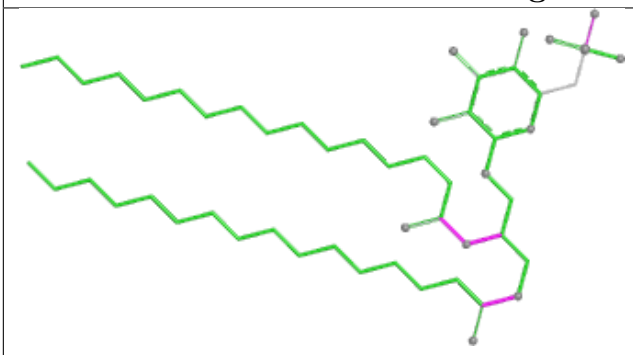


Torsions

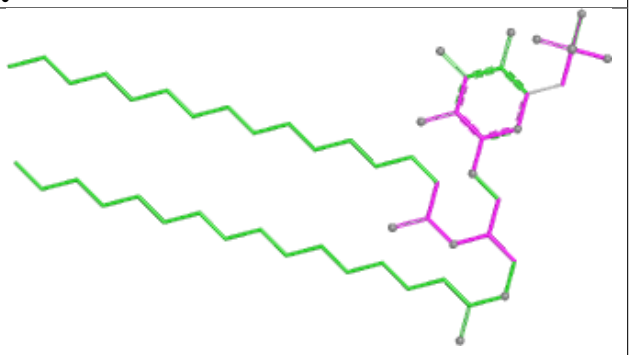


Rings

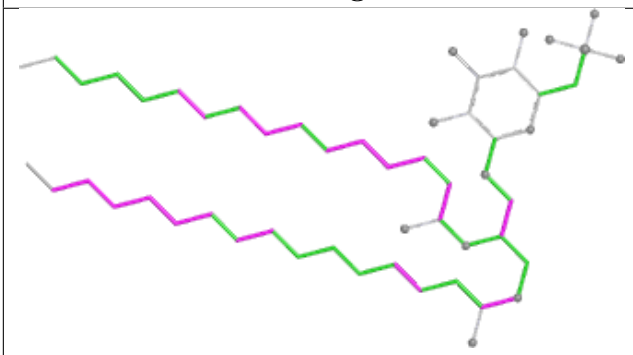
Ligand SQD a 413



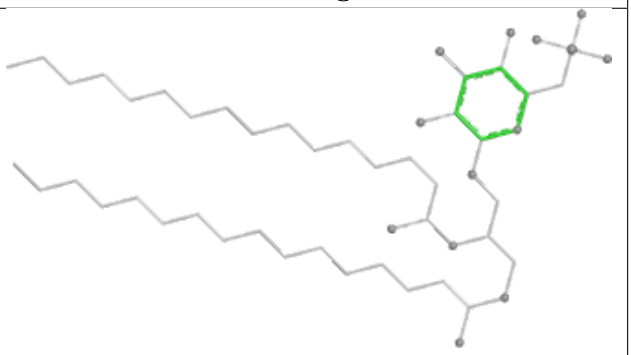
Bond lengths



Bond angles

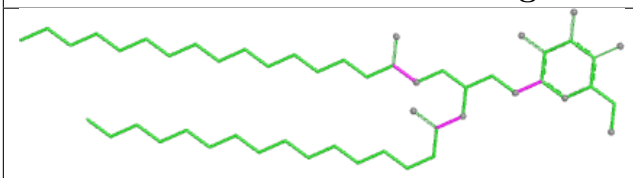


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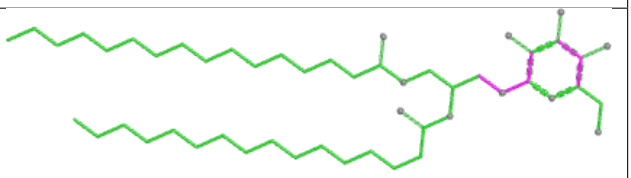


Rings

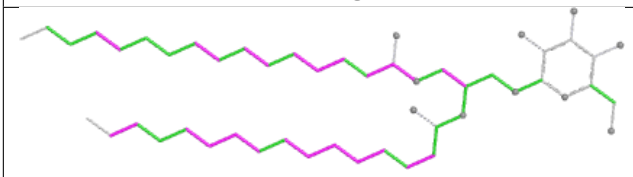
Ligand LMG A 613



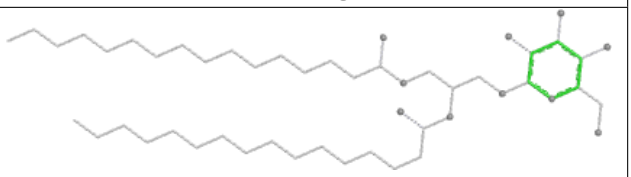
Bond lengths



Bond angles

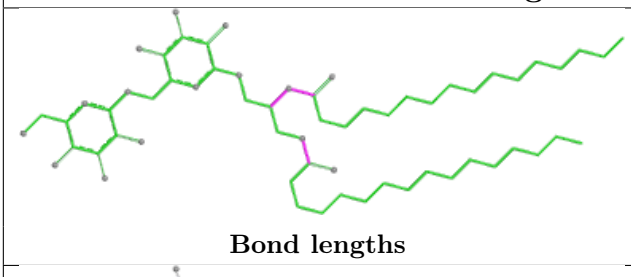


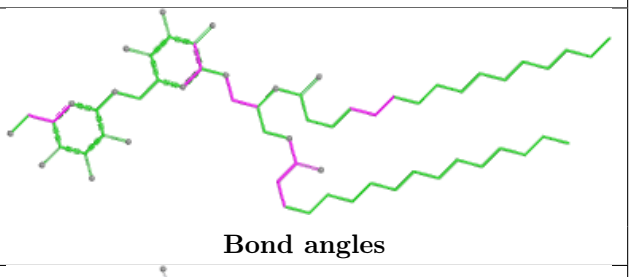
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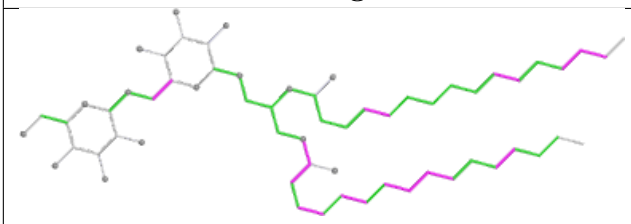


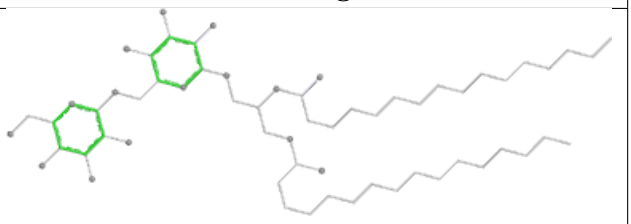
Rings

Ligand DGD c 518

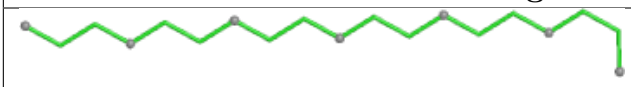

Bond lengths

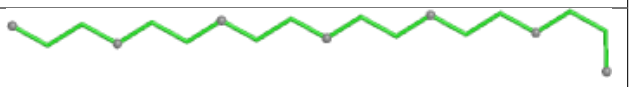

Bond angles


Torsions

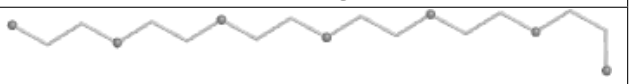

Rings

Ligand P6G B 651

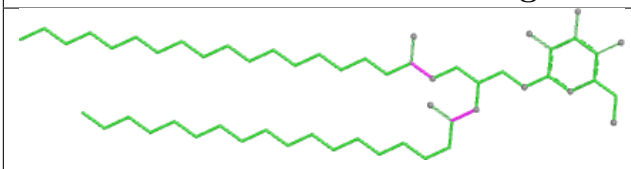

Bond lengths

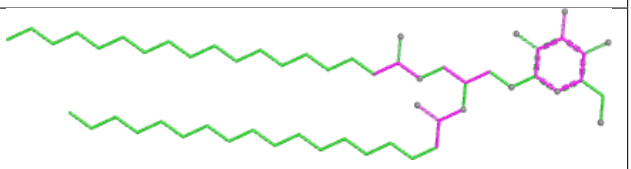

Bond angles

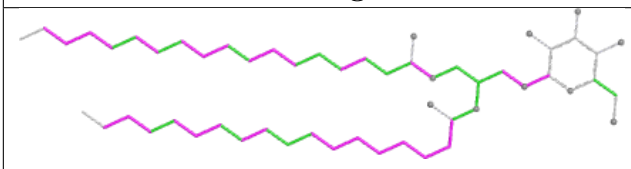

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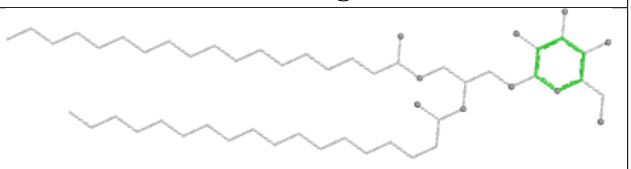

Rings

Ligand LMG C 526

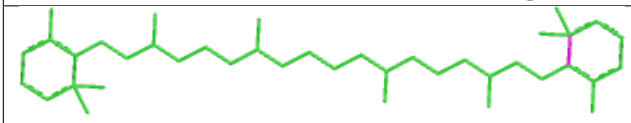

Bond lengths

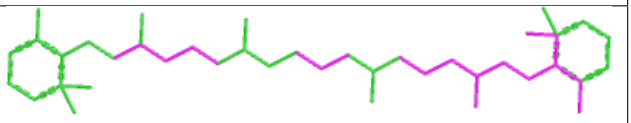

Bond angles

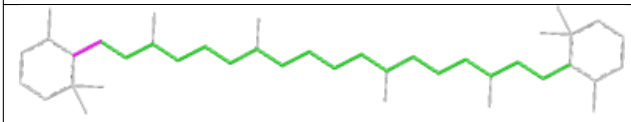

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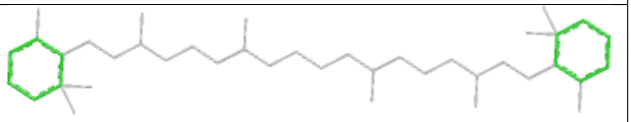

Rings

Ligand BCR K 101


Bond lengths


Bond angles

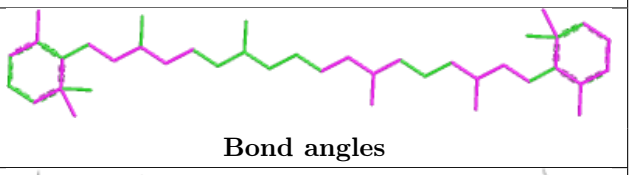

Torsions


Rings

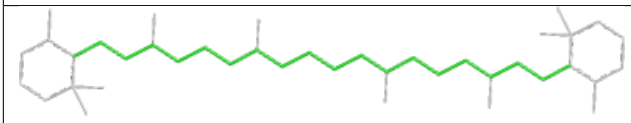
Ligand BCR h 103



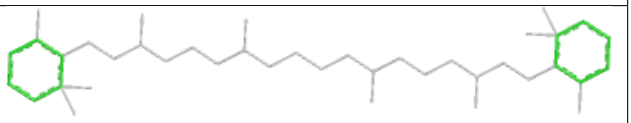
Bond lengths



Bond angles



Torsions



Rings

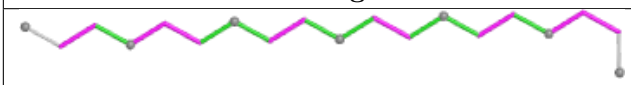
Ligand P6G D 417



Bond lengths



Bond angles

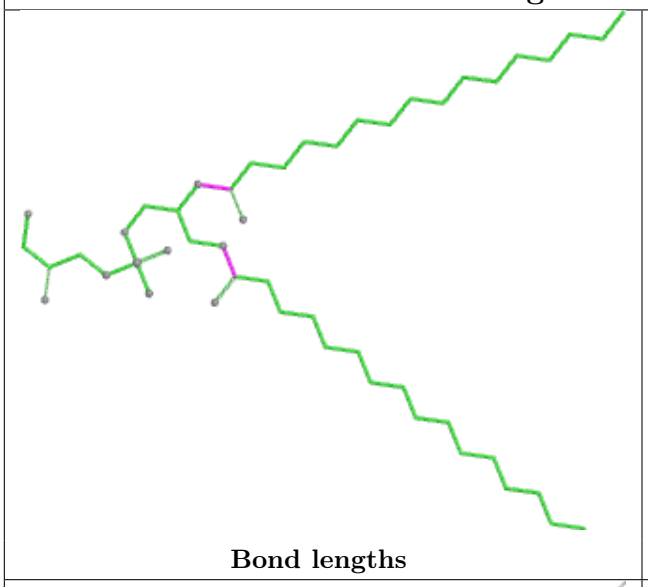


Torsions

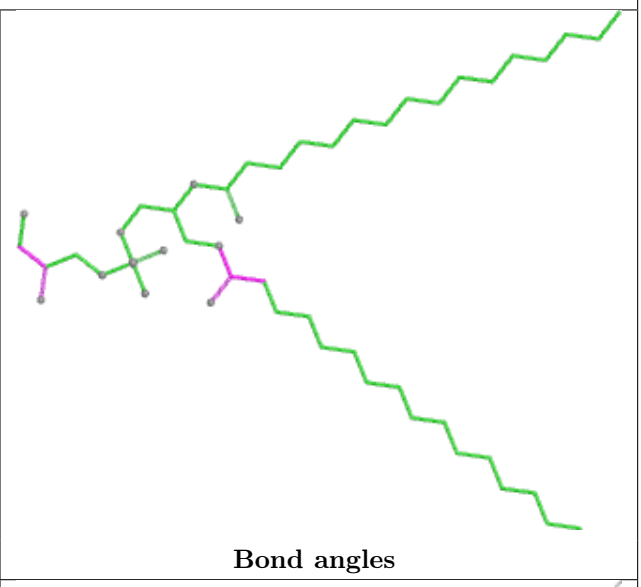


Rings

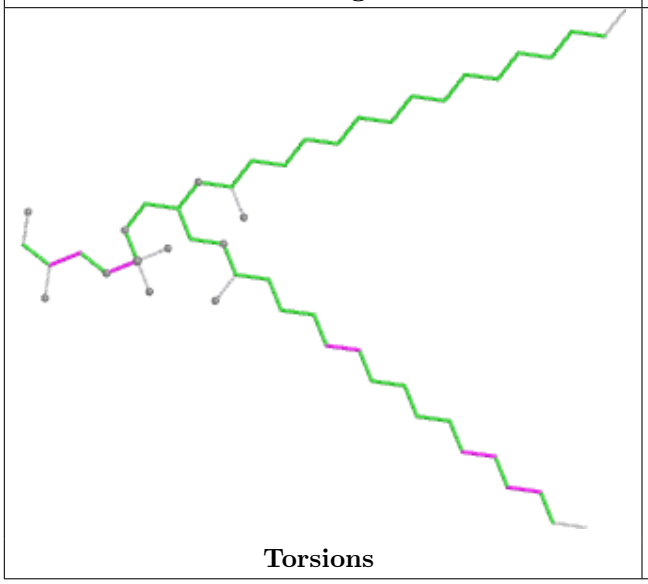
Ligand LHG d 410



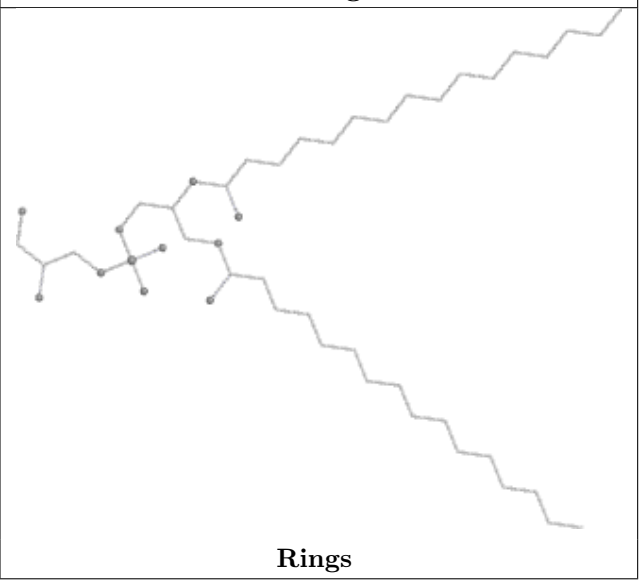
Bond lengths



Bond angles

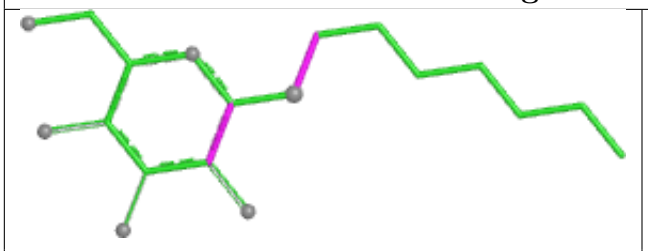


Torsions

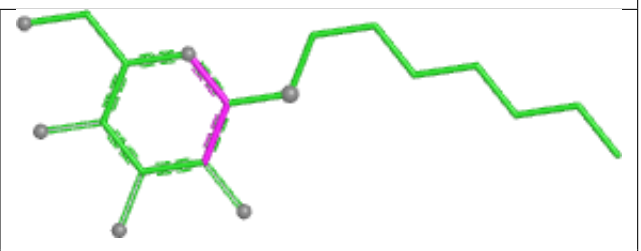


Rings

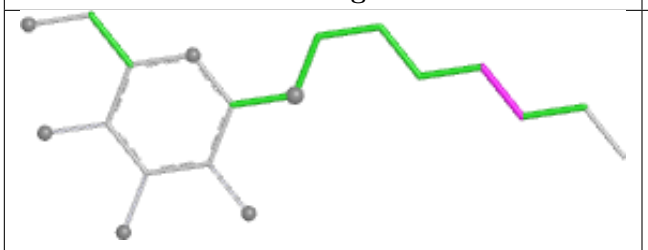
Ligand HTG O 303



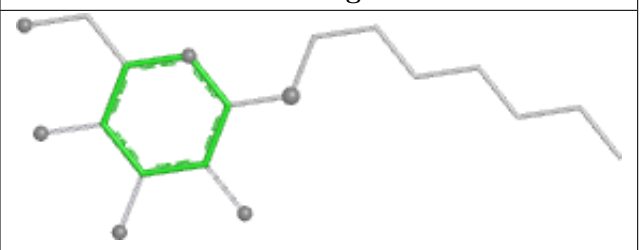
Bond lengths



Bond angles

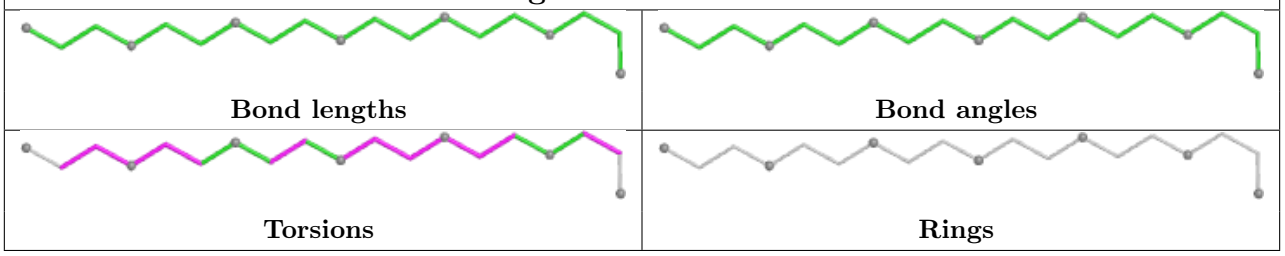


Torsions

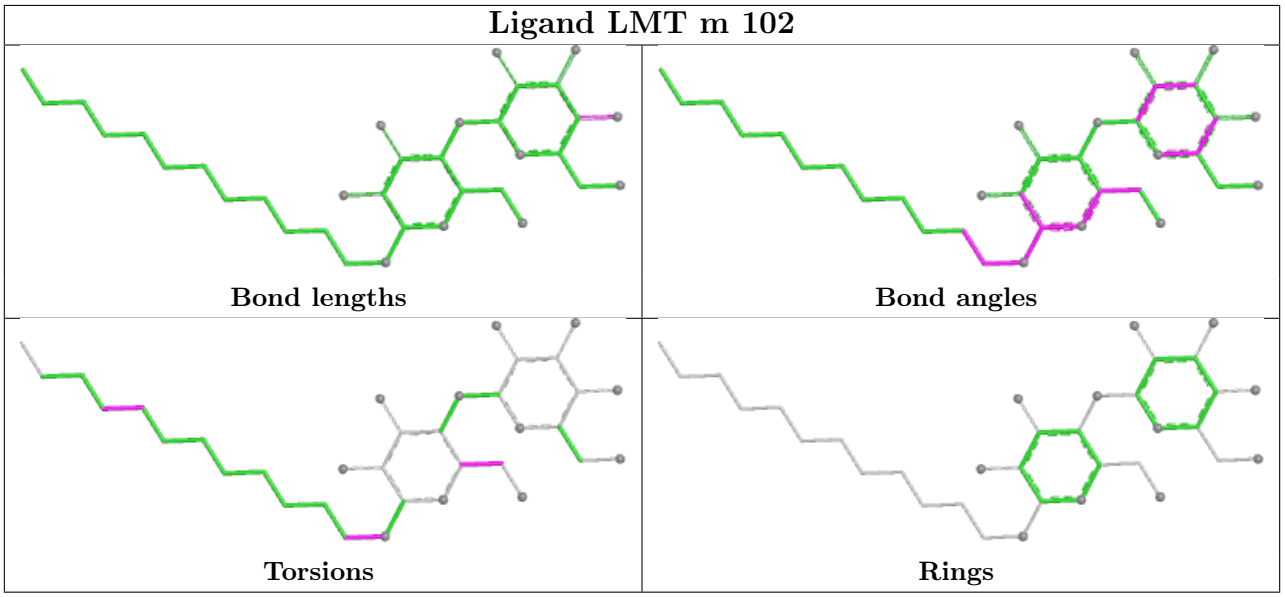


Rings

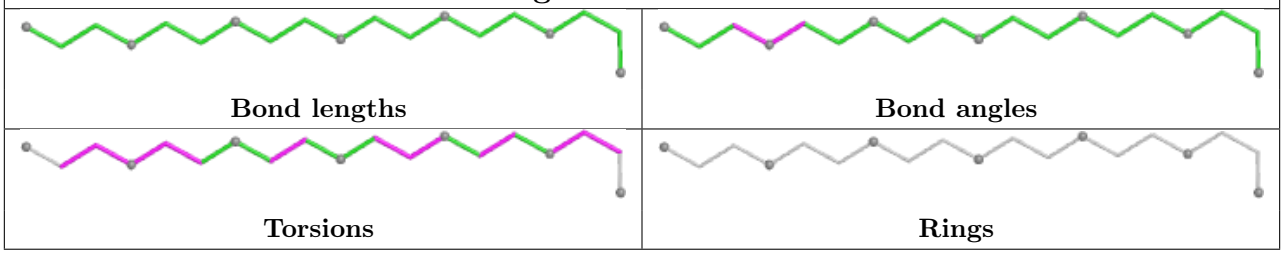
Ligand P6G E 110



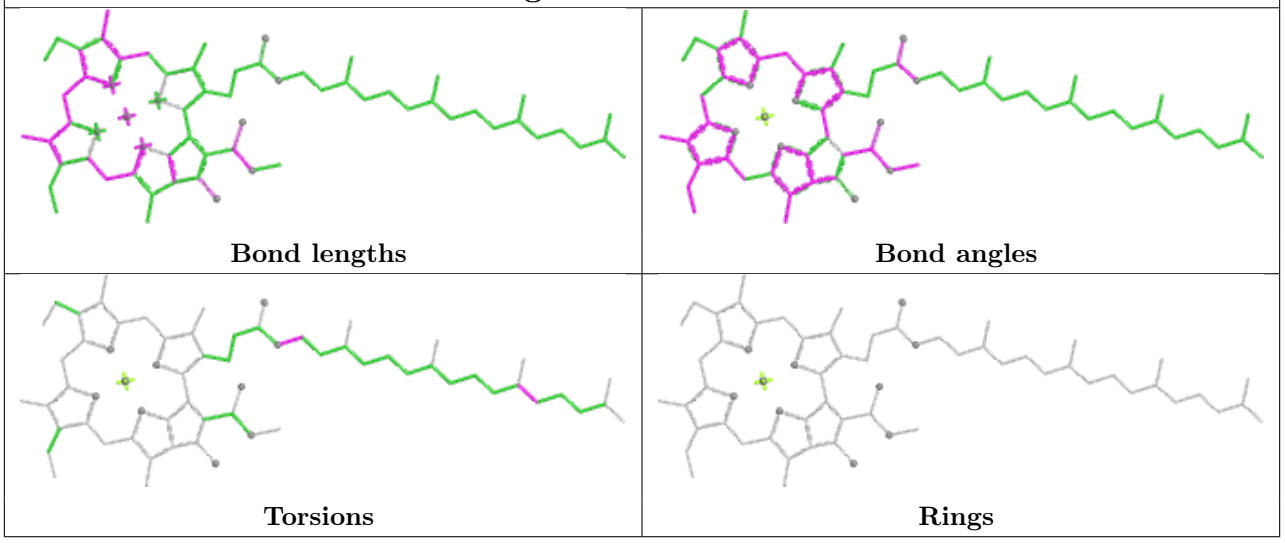
Ligand LMT m 102



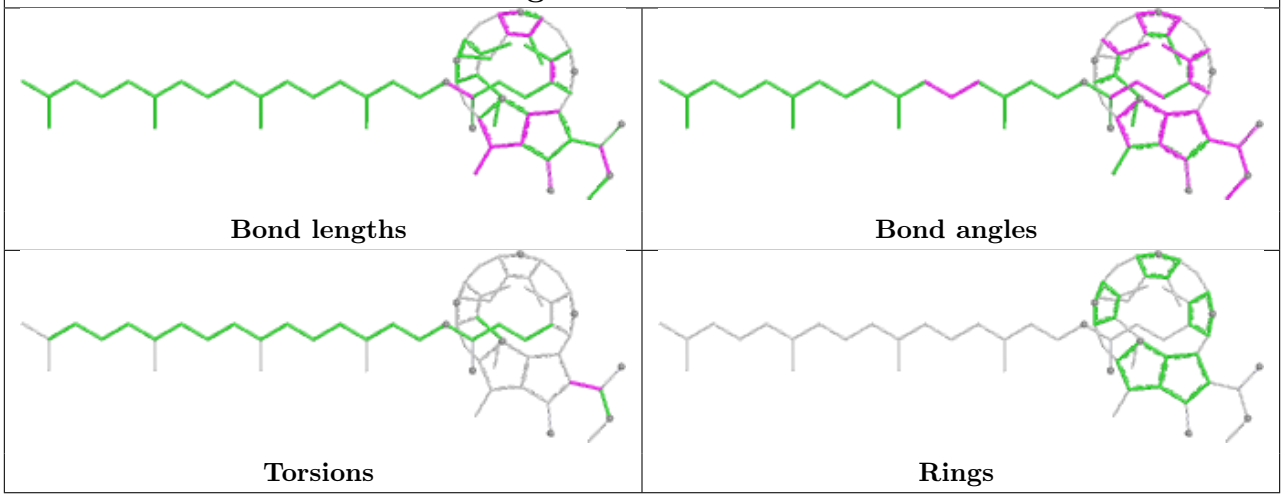
Ligand P6G I 106



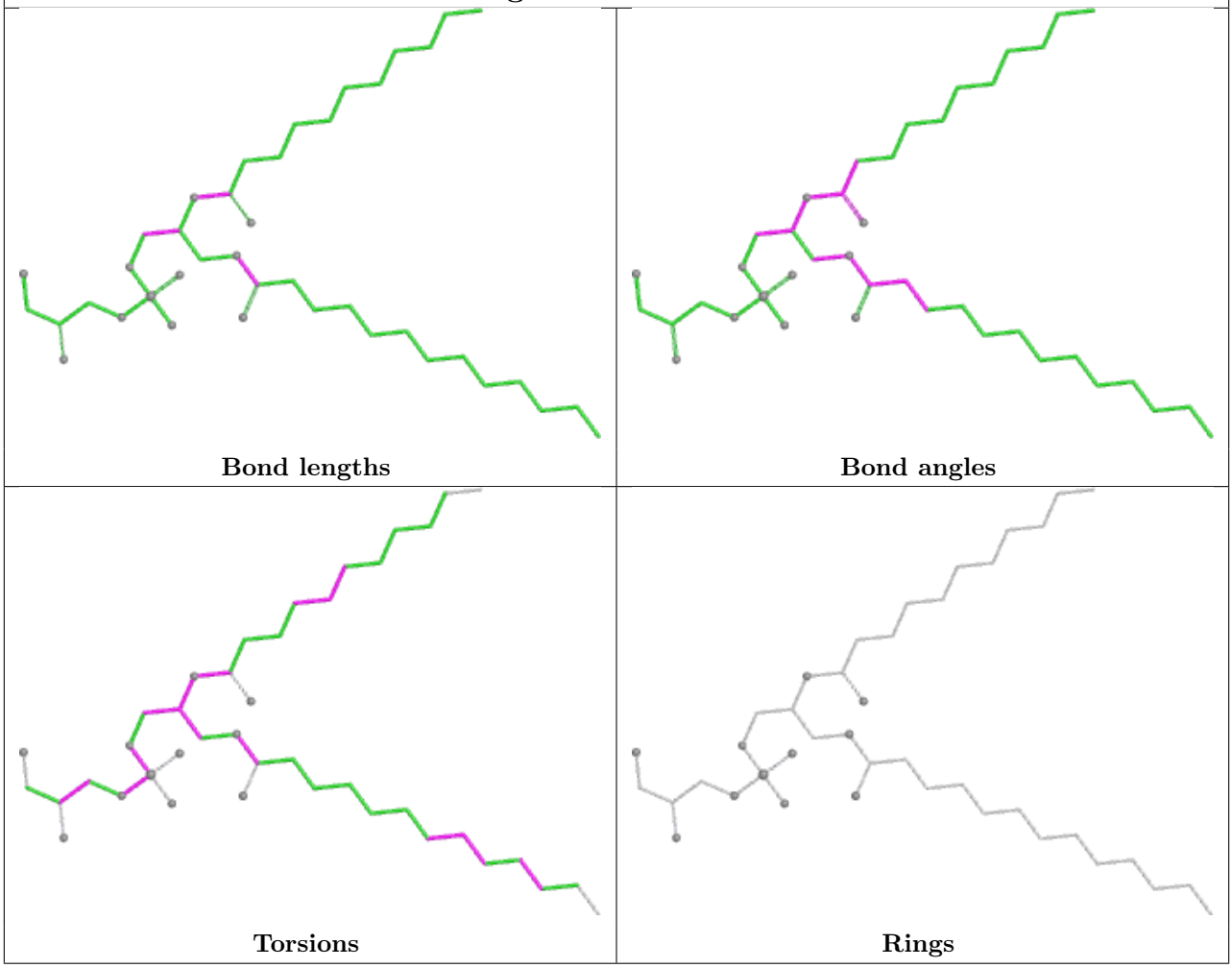
Ligand CLA D 404



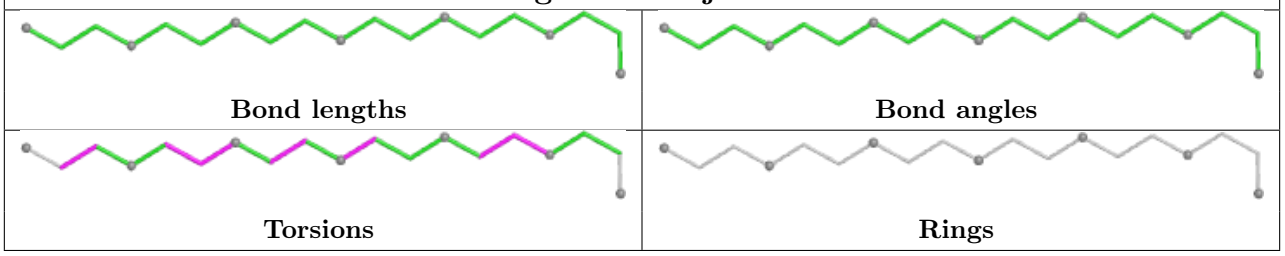
Ligand PHO a 409



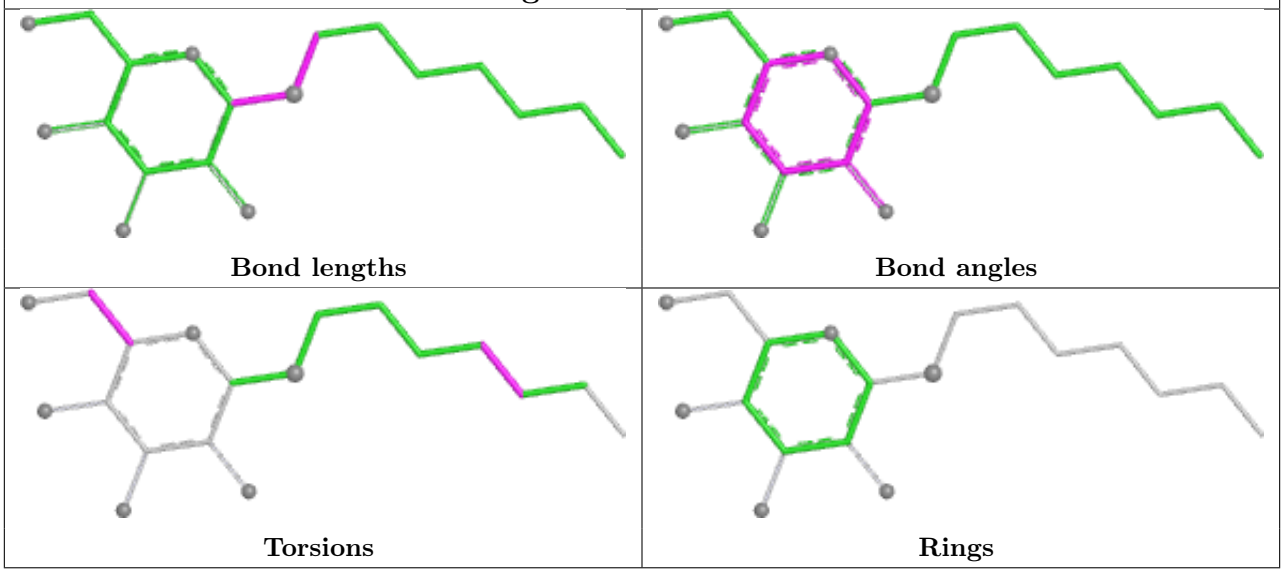
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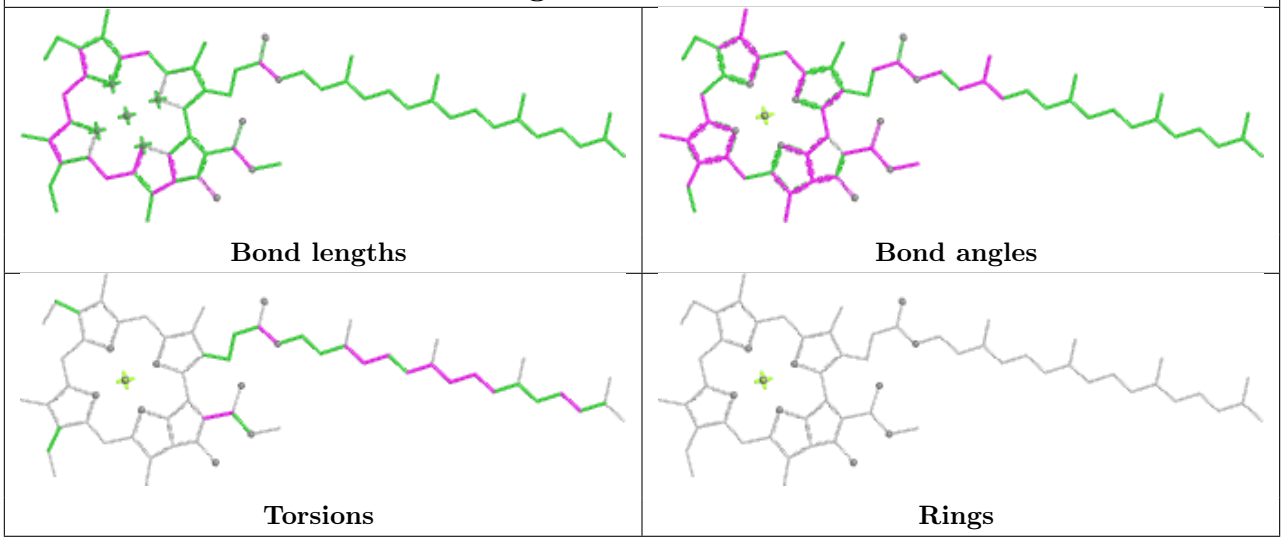
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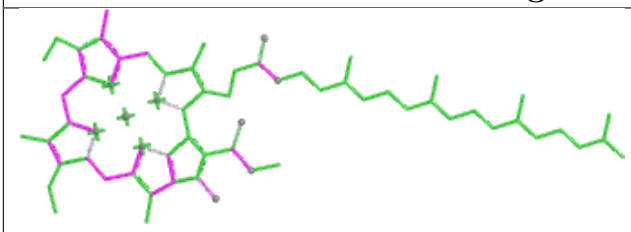
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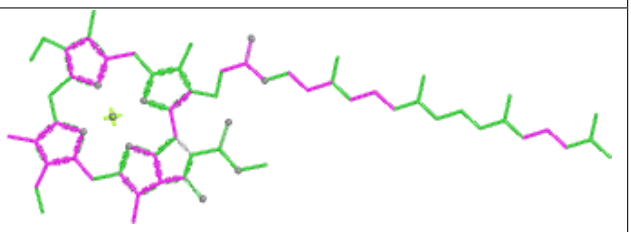
Ligand CLA b 602



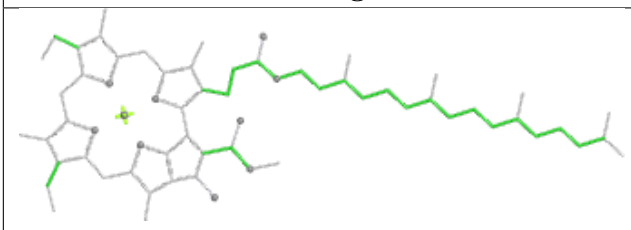
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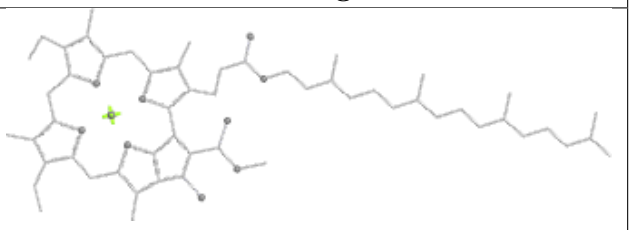
Bond lengths



Bond angles



Torsions

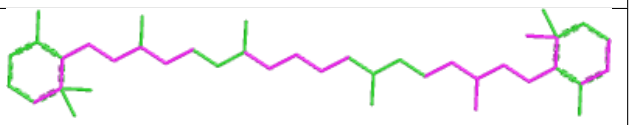


Rings

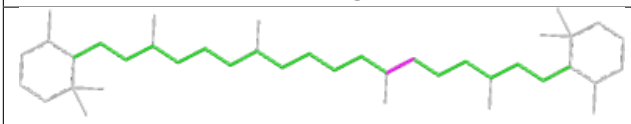
Ligand BCR A 610



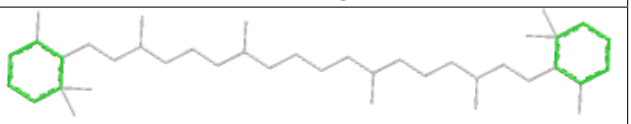
Bond lengths



Bond angles

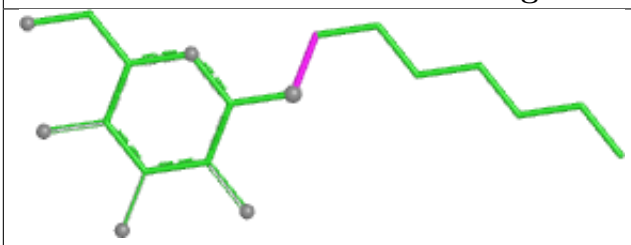


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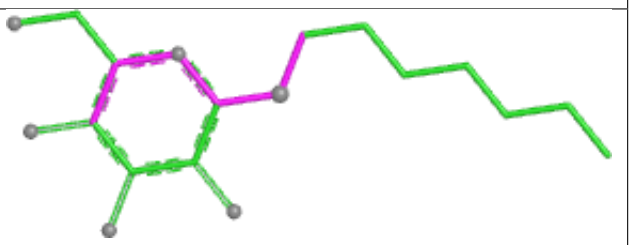


Rings

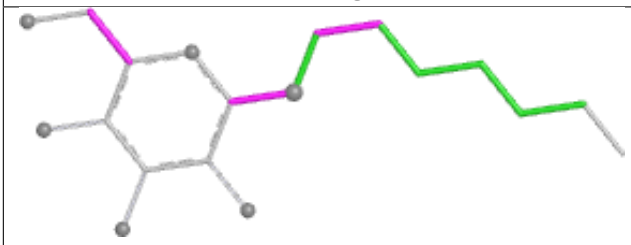
Ligand HTG C 522



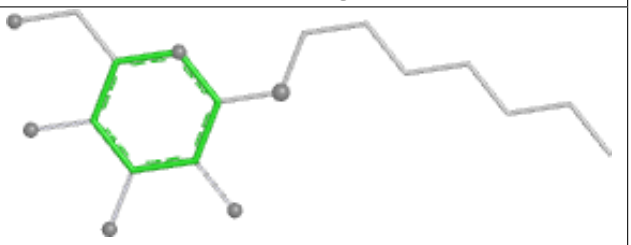
Bond lengths



Bond angles

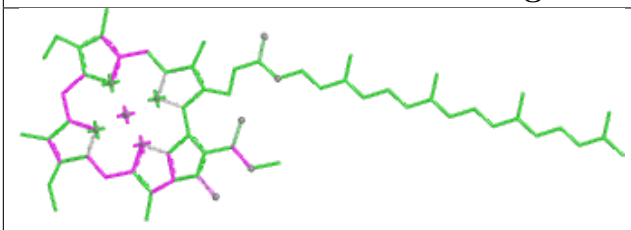


Torsions

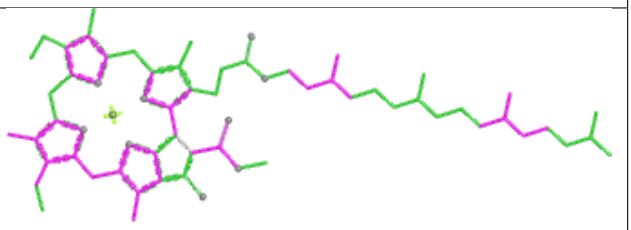


Rings

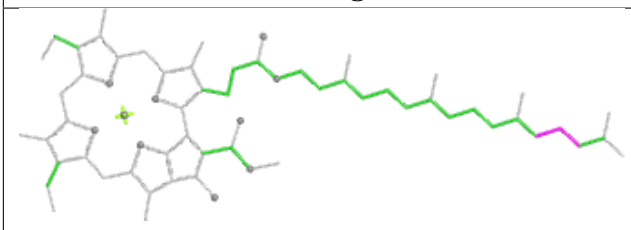
Ligand CLA B 603



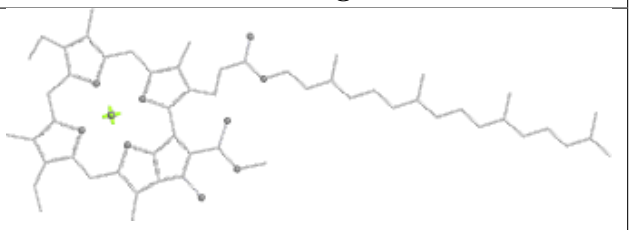
Bond lengths



Bond angles

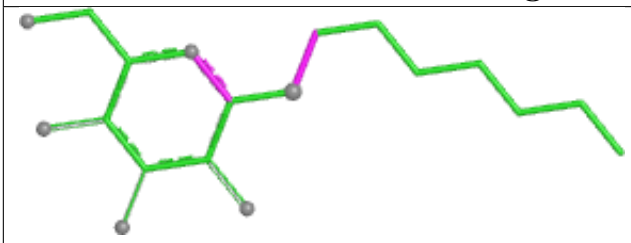


Torsions

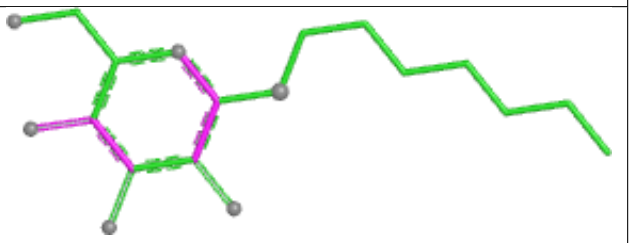


Rings

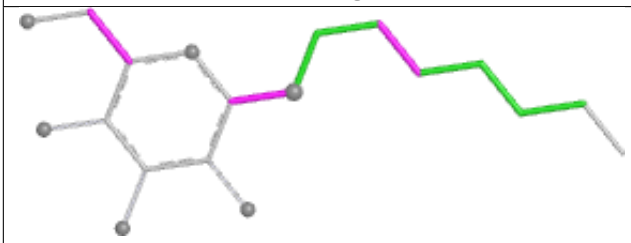
Ligand HTG b 624



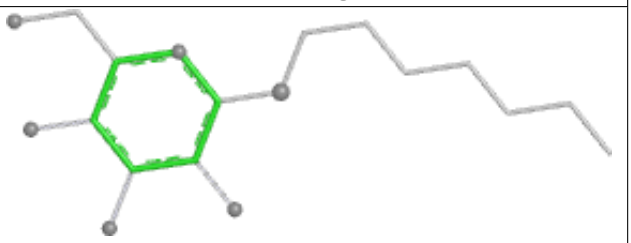
Bond lengths



Bond angles

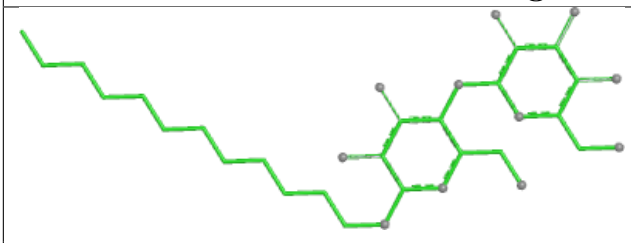


Torsions

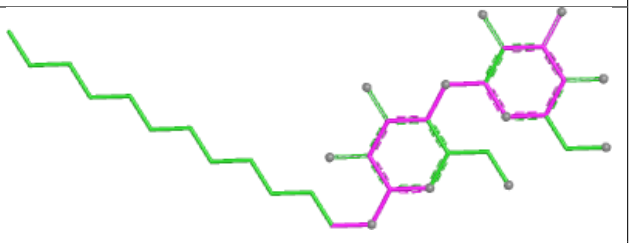


Rings

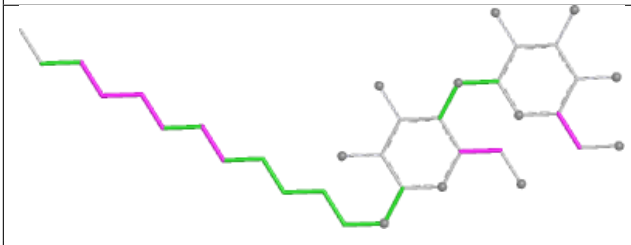
Ligand LMT t 103



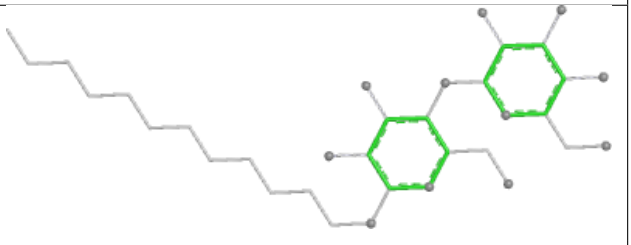
Bond lengths



Bond angles

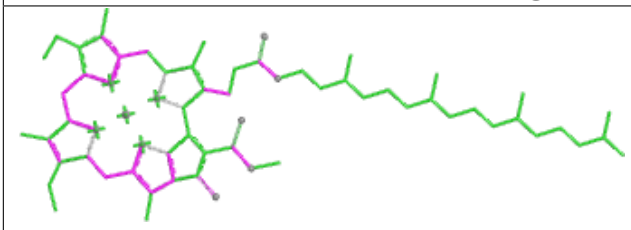


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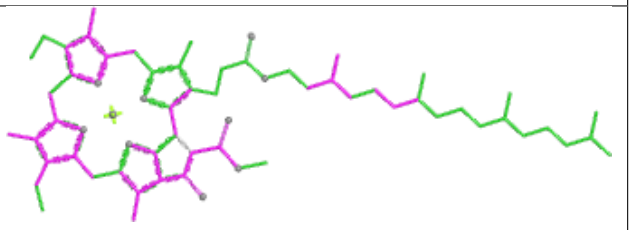


Rings

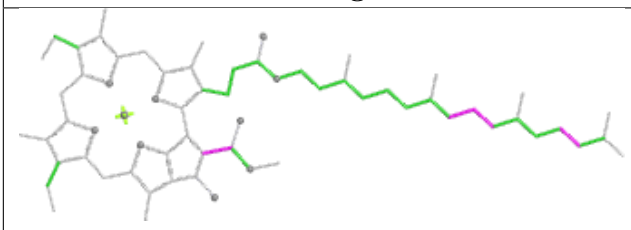
Ligand CLA d 405



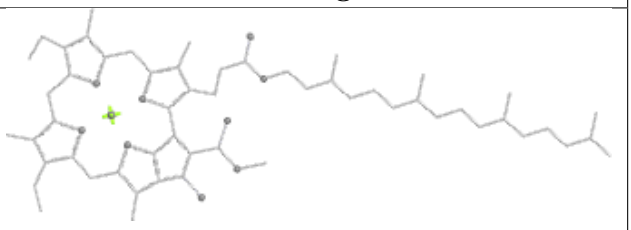
Bond lengths



Bond angles

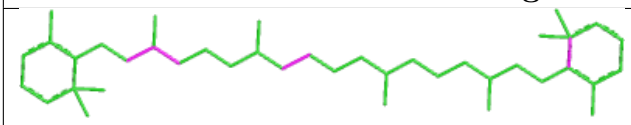


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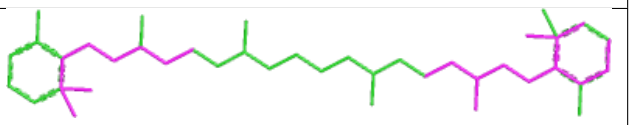


Rings

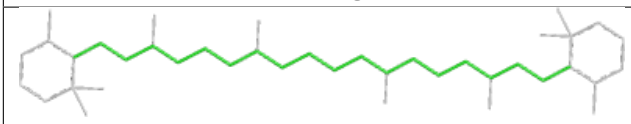
Ligand BCR C 514



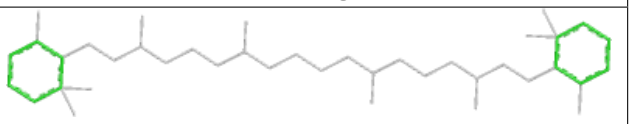
Bond lengths



Bond angles

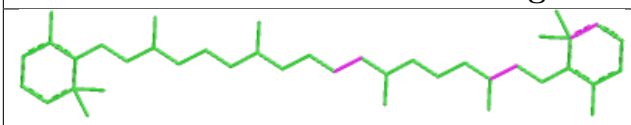


Torsions

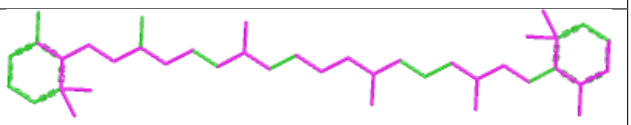


Rings

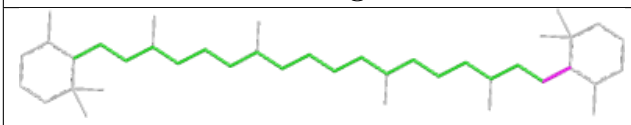
Ligand BCR t 102



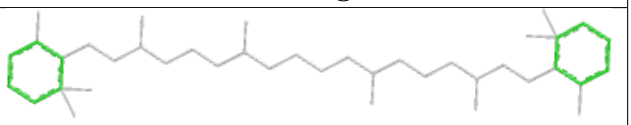
Bond lengths



Bond angles

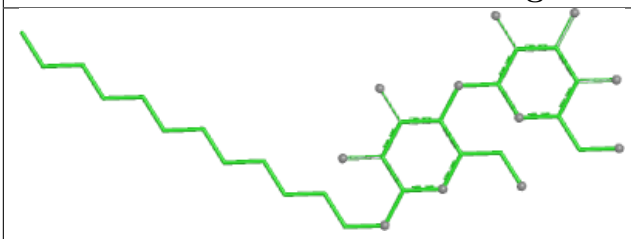


Torsions

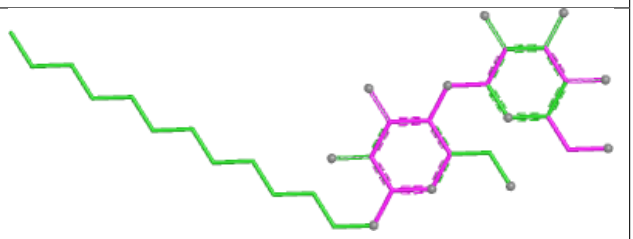


Rings

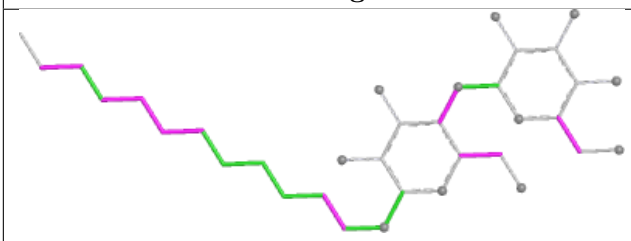
Ligand LMT c 521



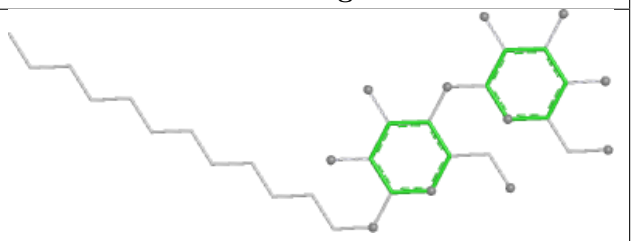
Bond lengths



Bond angles

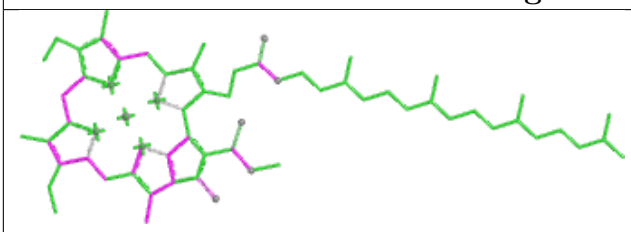


Torsions

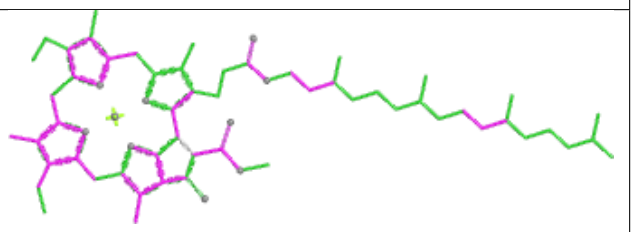


Rings

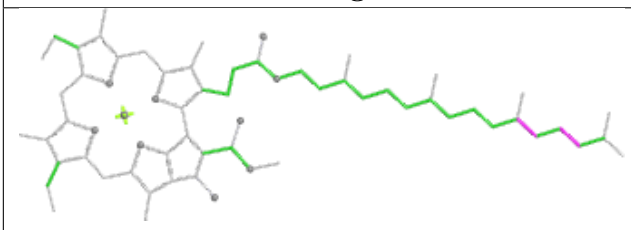
Ligand CLA B 612



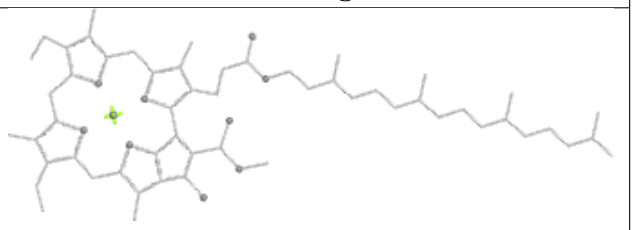
Bond lengths



Bond angles



Torsions



Rings

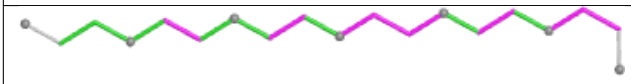
Ligand P6G d 416



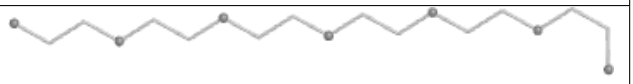
Bond lengths



Bond angles

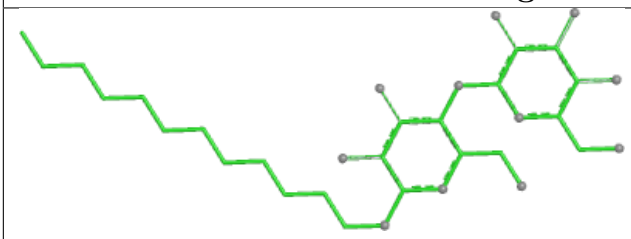


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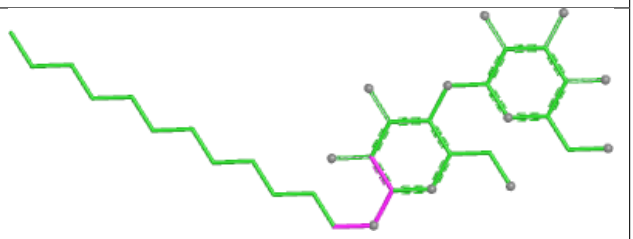


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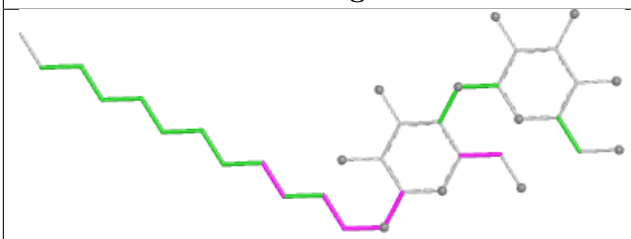
Ligand LMT M 102



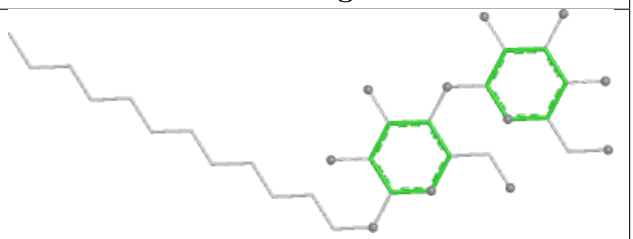
Bond lengths



Bond angles

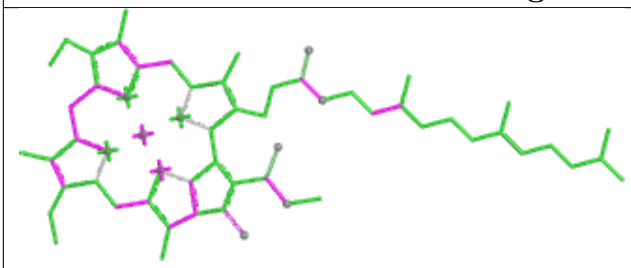


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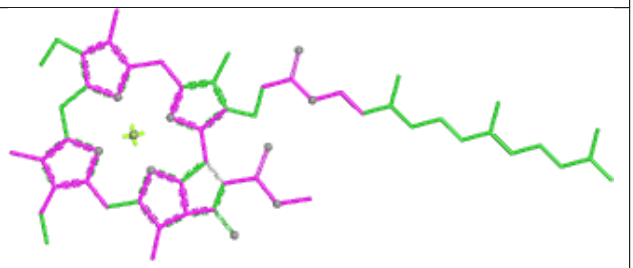


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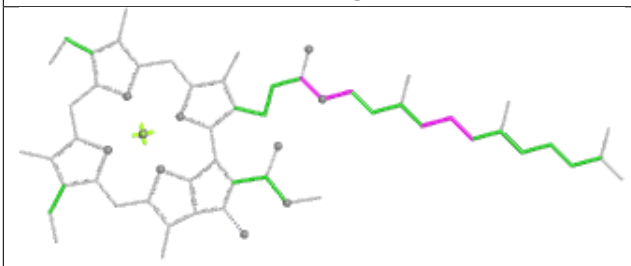
Ligand CLA b 617



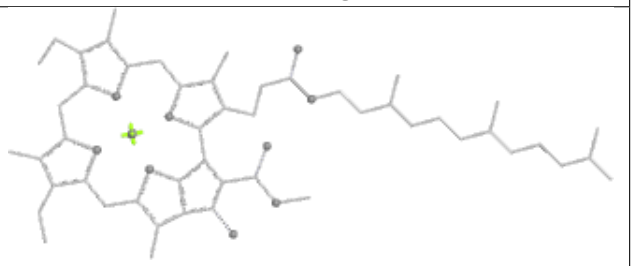
Bond lengths



Bond angles

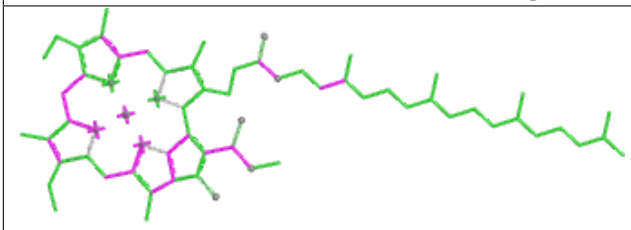


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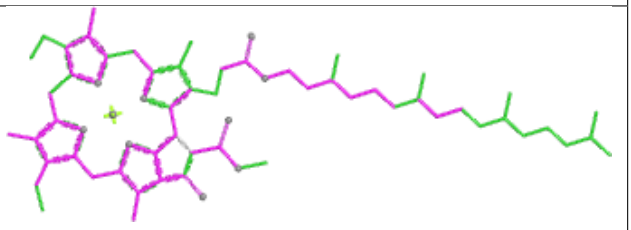


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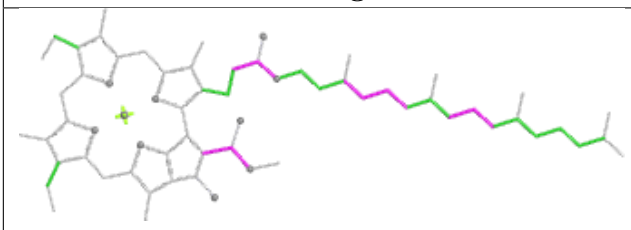
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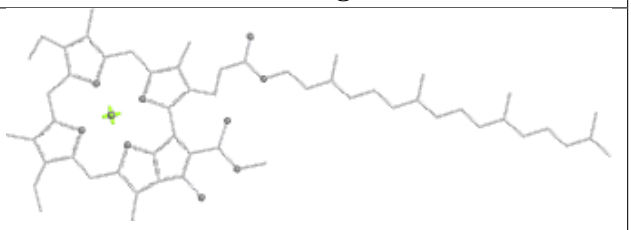
Bond lengths



Bond angles

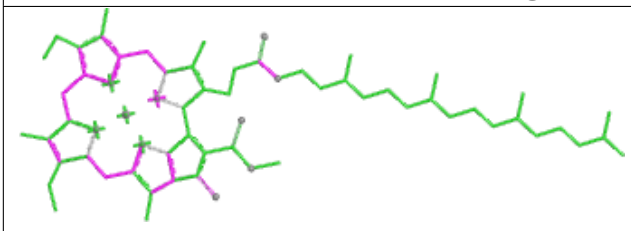


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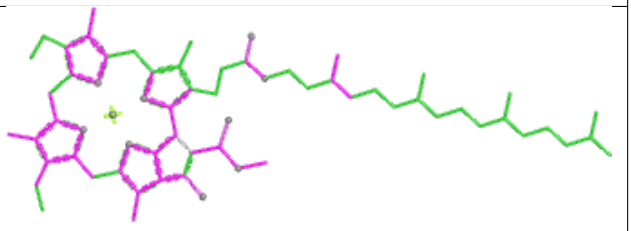


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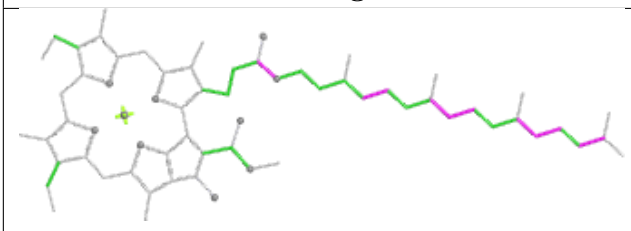
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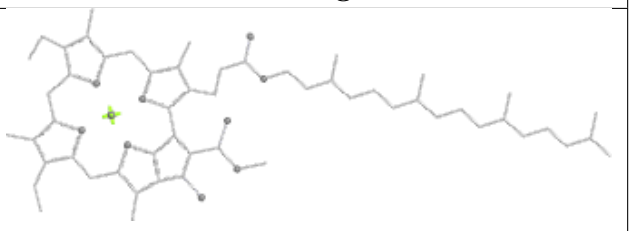
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Bond angles

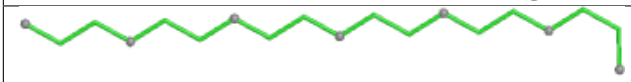


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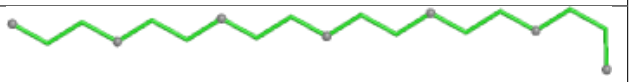


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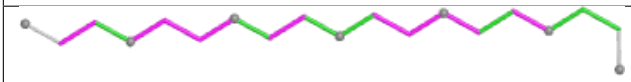
Ligand P6G D 416



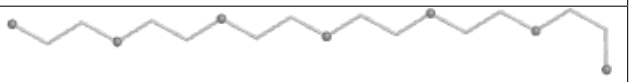
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Bond angles

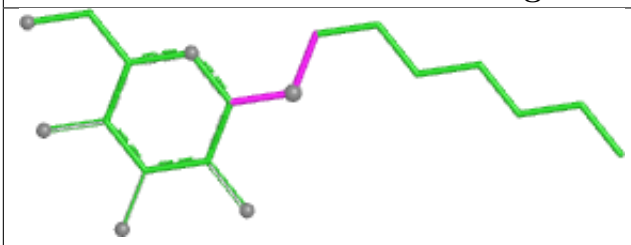


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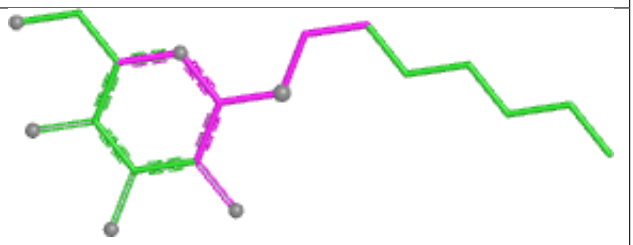


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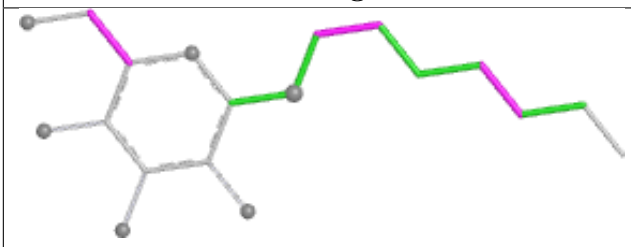
Ligand HTG h 101



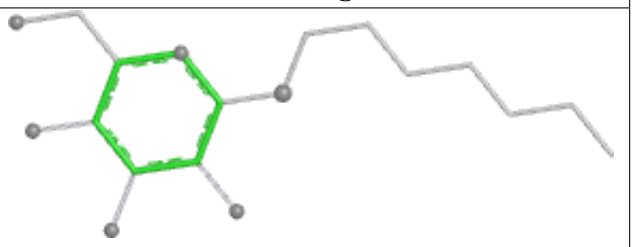
Bond lengths



Bond angles

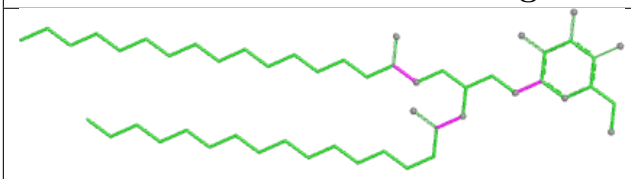


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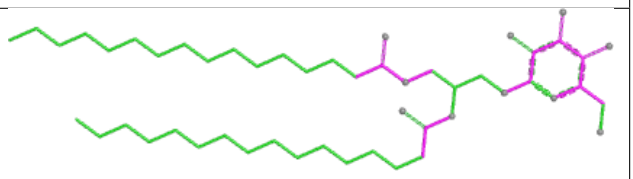


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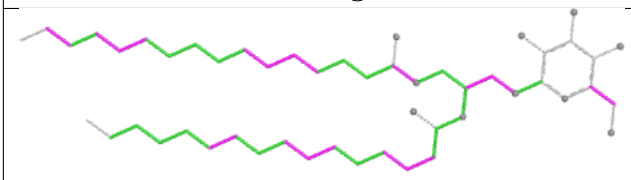
Ligand LMG C 520



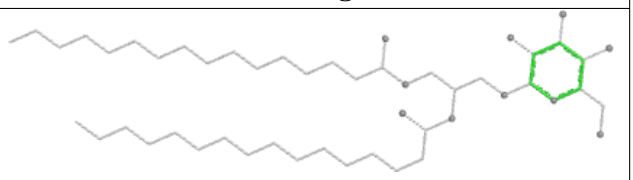
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Bond angles

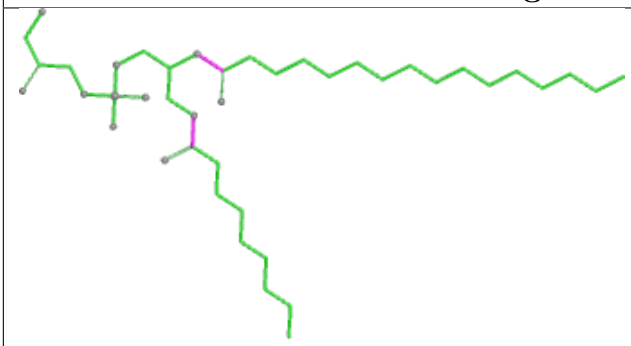


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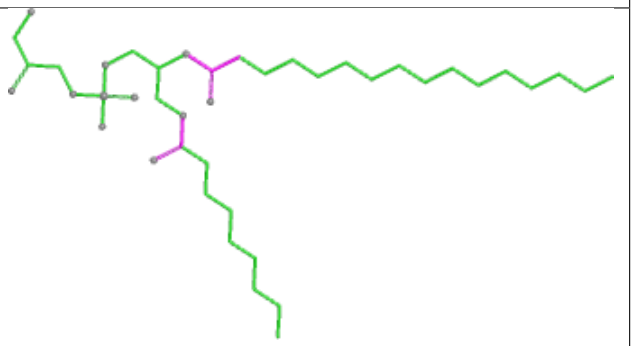


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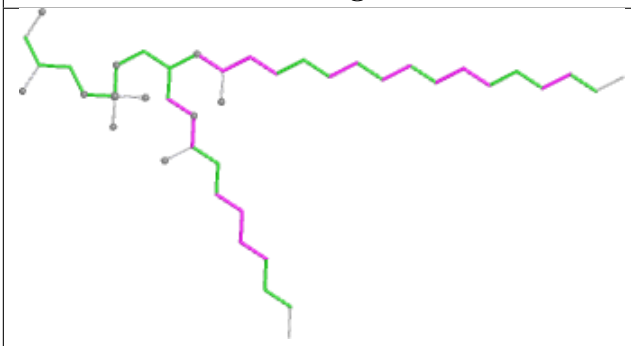
Ligand LHG E 101



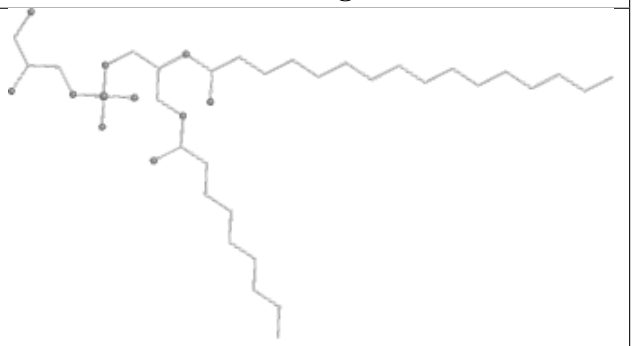
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Bond angles

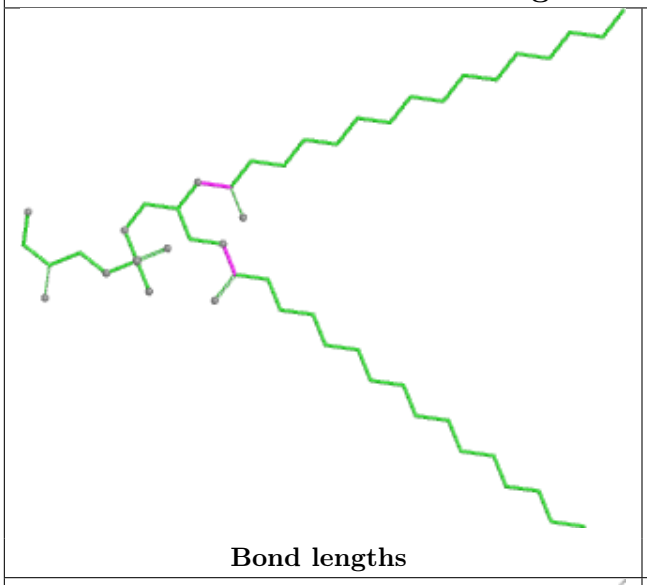


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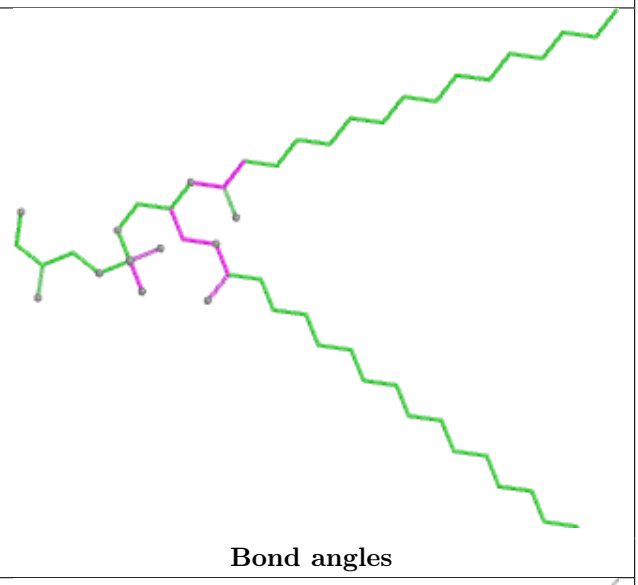


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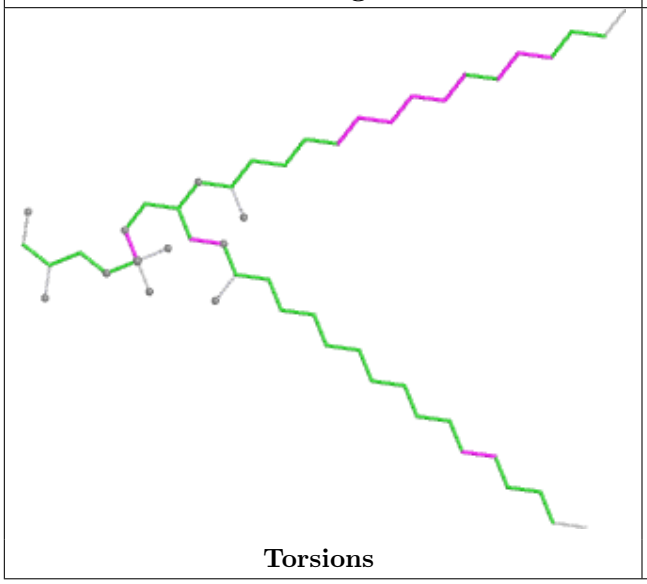
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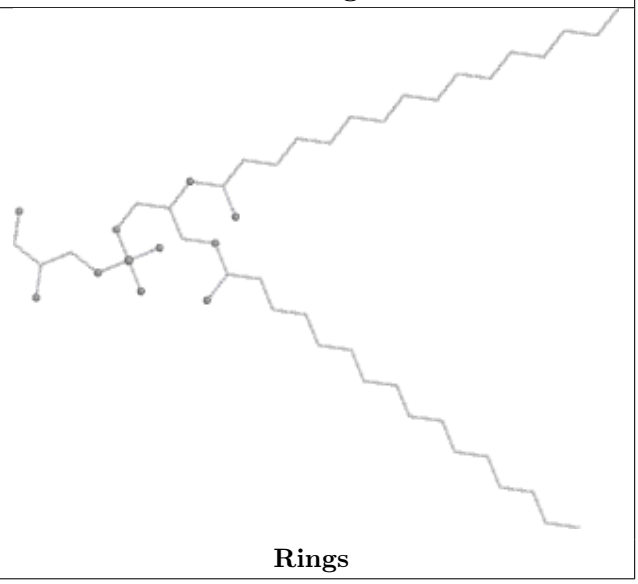
Bond lengths



Bond angles

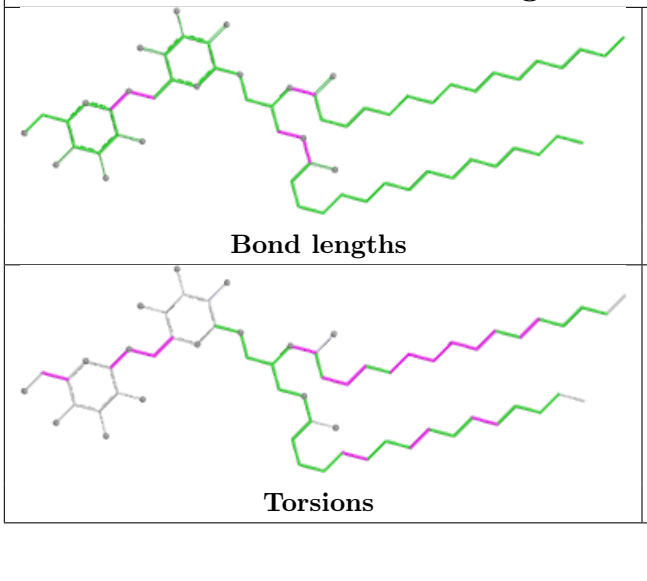


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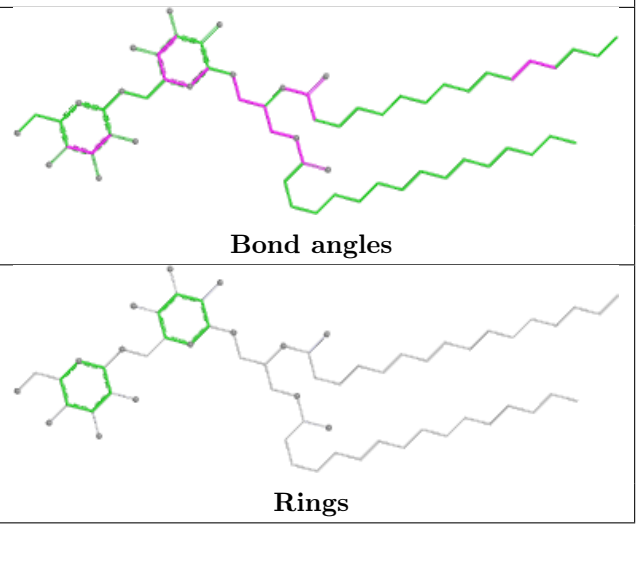


Rings

Ligand DGD C 516



Bond lengths

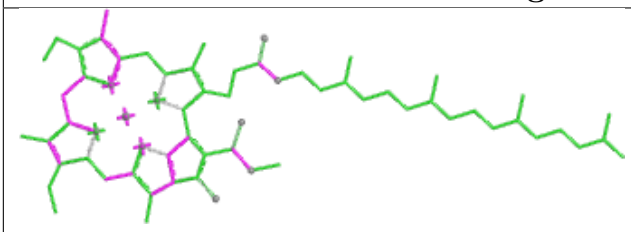


Bond angles

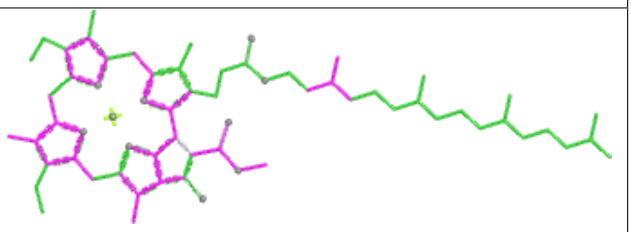
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Rings

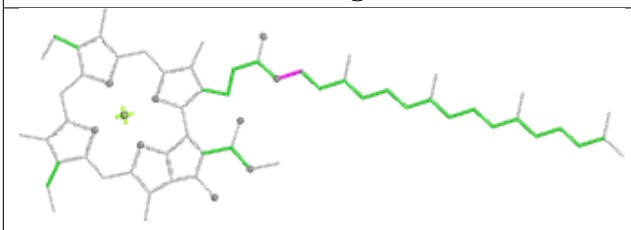
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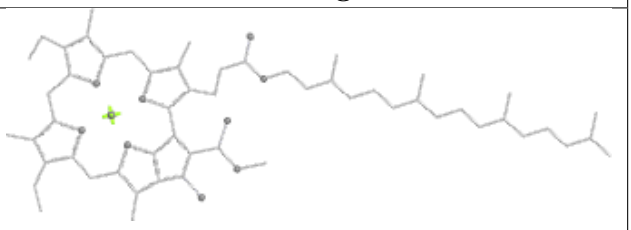
Bond lengths



Bond angles

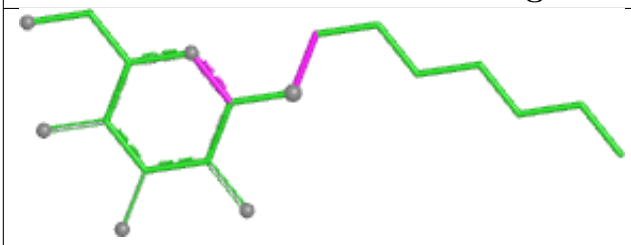


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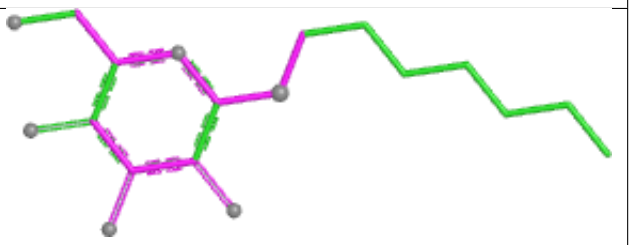


Rings

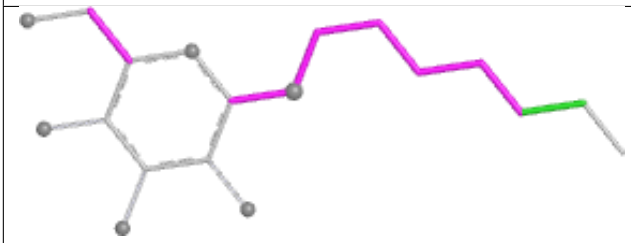
Ligand HTG c 531



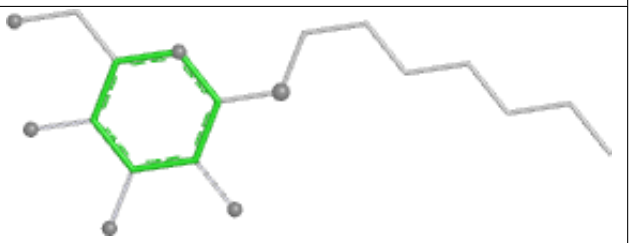
Bond lengths



Bond angles

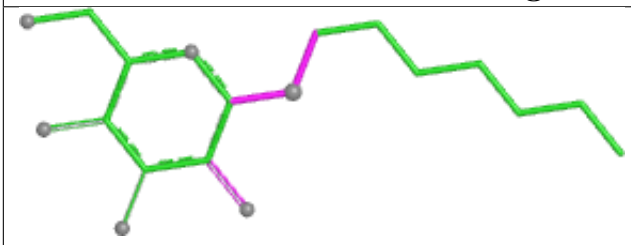


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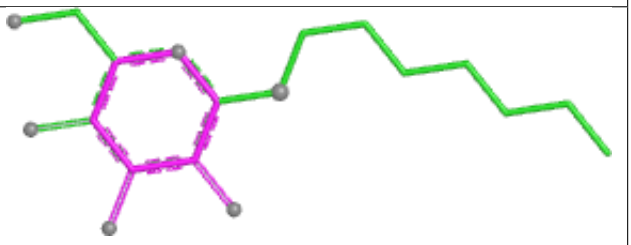


Rings

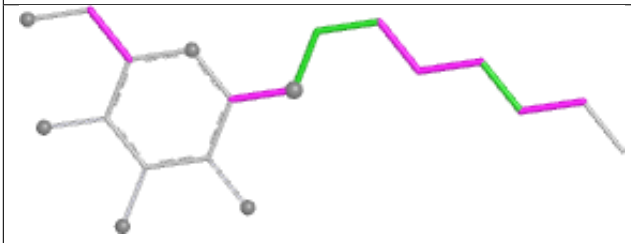
Ligand HTG a 418



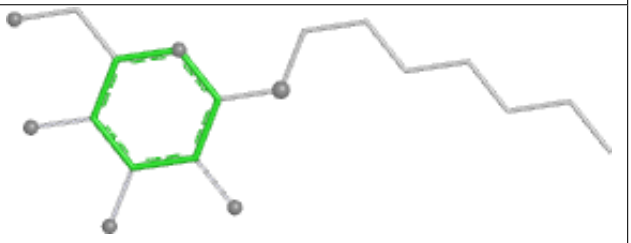
Bond lengths



Bond angles

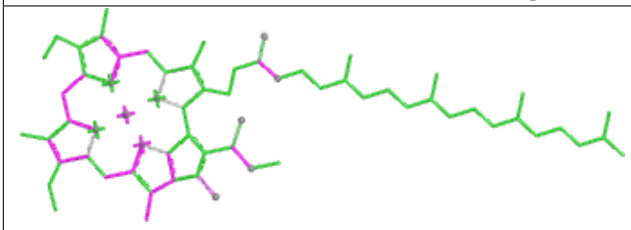


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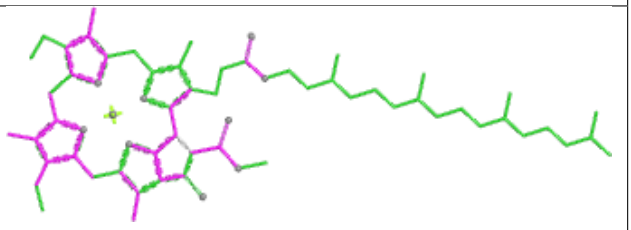


Rings

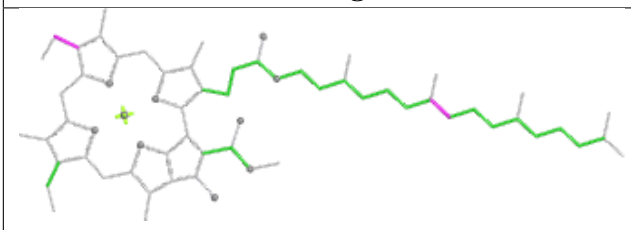
Ligand CLA C 505



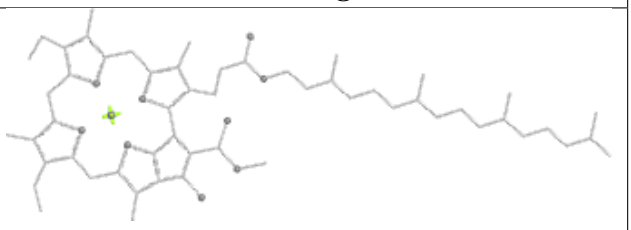
Bond lengths



Bond angles

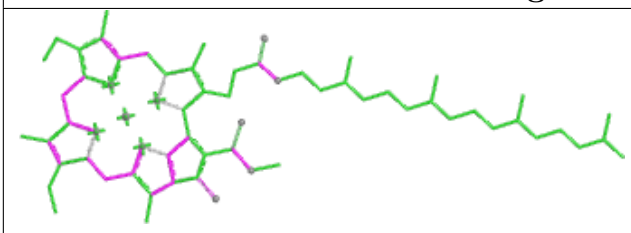


Torsions

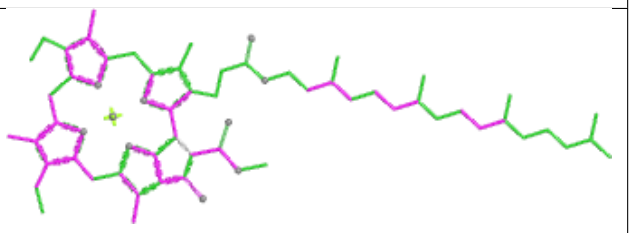


Rings

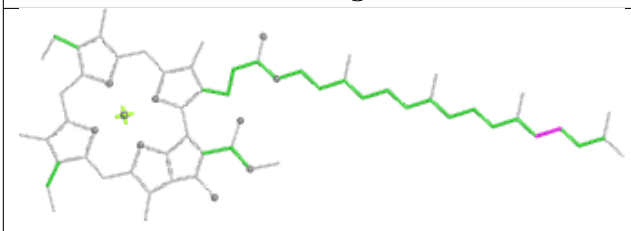
Ligand CLA b 609



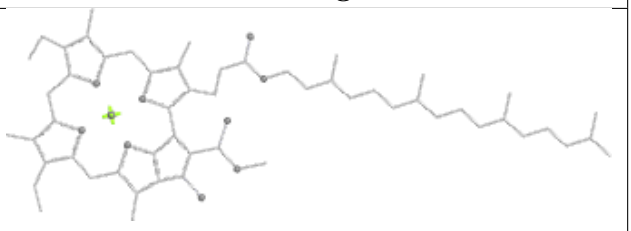
Bond lengths



Bond angles

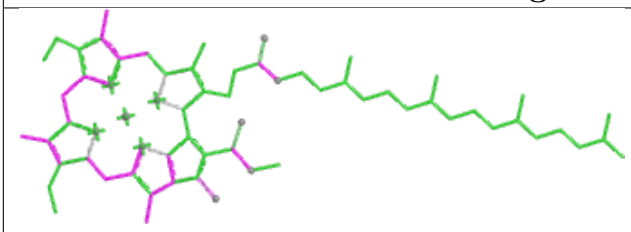


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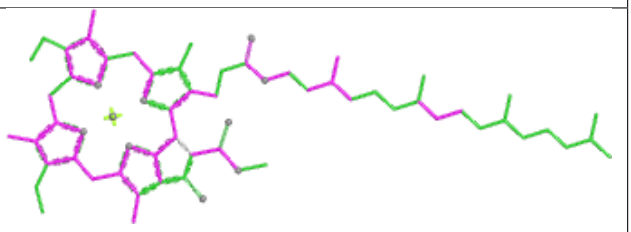


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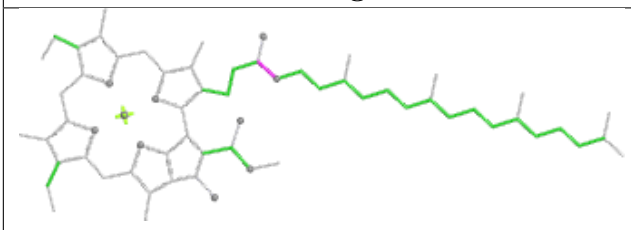
Ligand CLA c 511



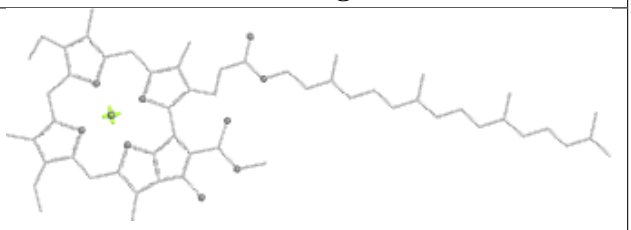
Bond lengths



Bond angles

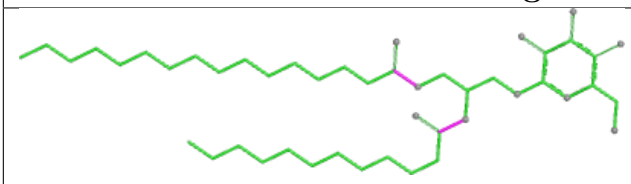


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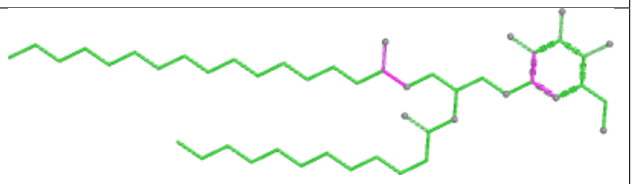


Rings

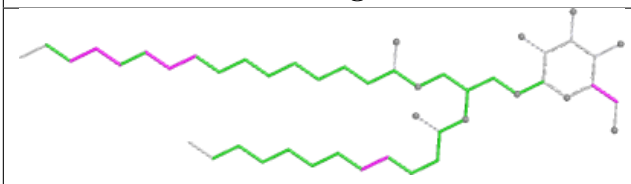
Ligand LMG J 101



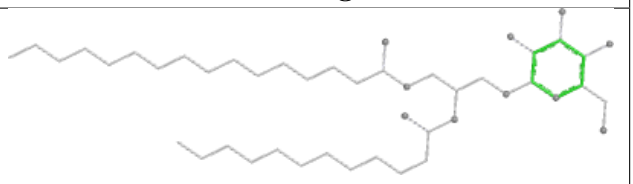
Bond lengths



Bond angles

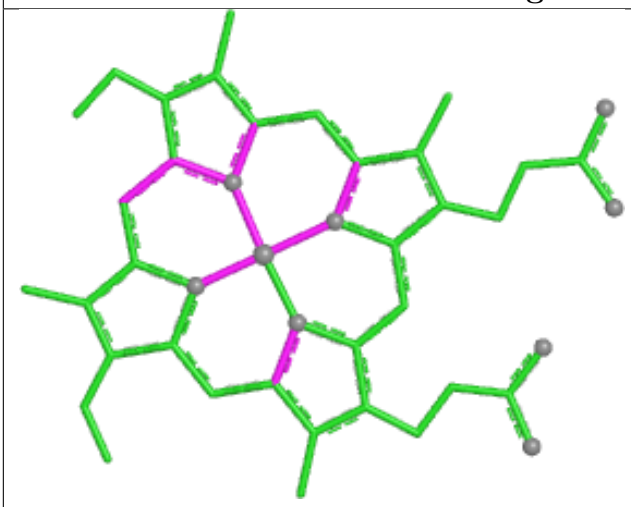


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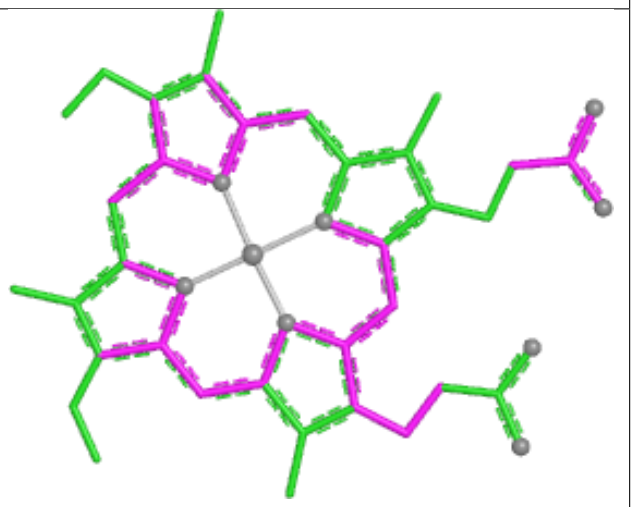


Rings

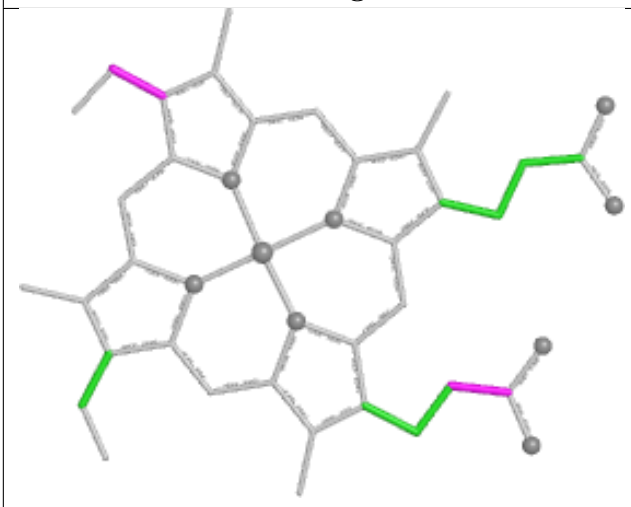
Ligand HEC v 202



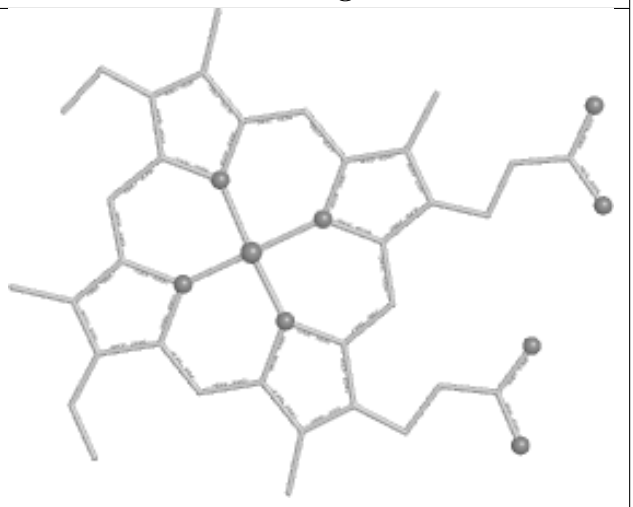
Bond lengths



Bond angles

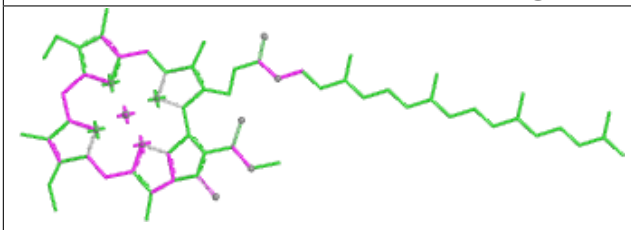


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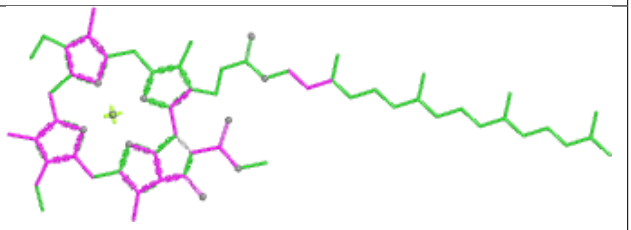


Rings

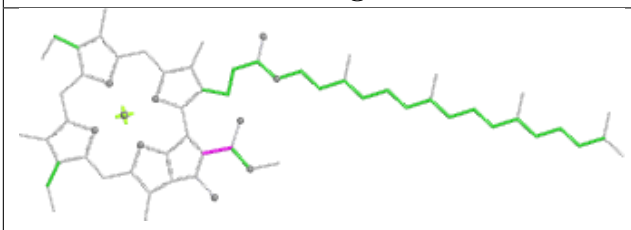
Ligand CLA c 502



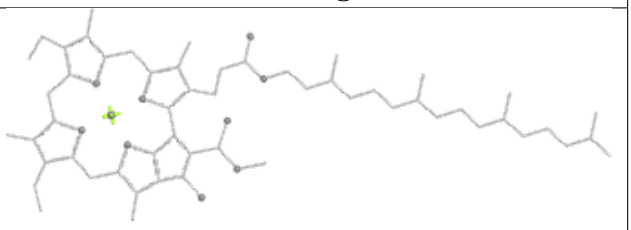
Bond lengths



Bond angles

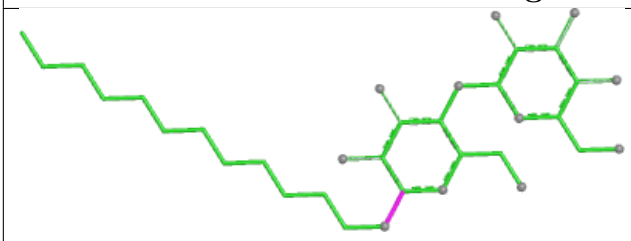


Torsions



Rings

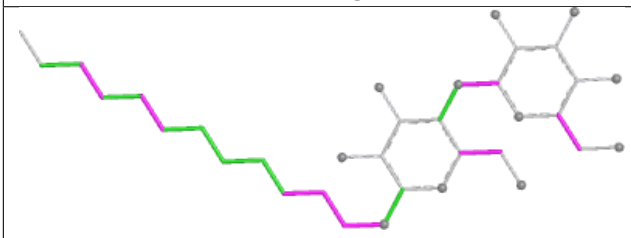
Ligand LMT J 103



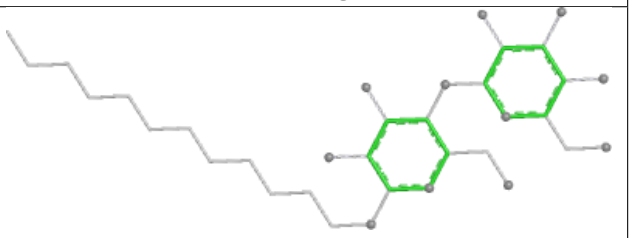
Bond lengths



Bond angles

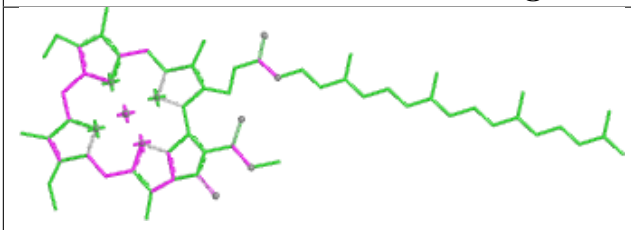


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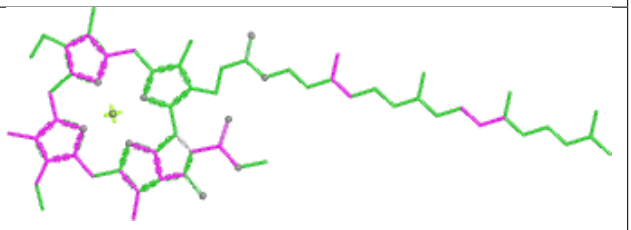


Rings

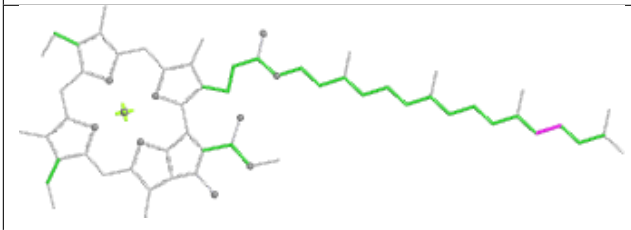
Ligand CLA B 609



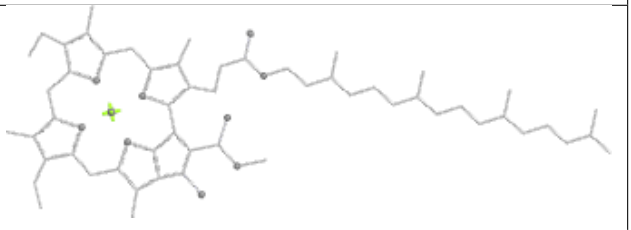
Bond lengths



Bond angles

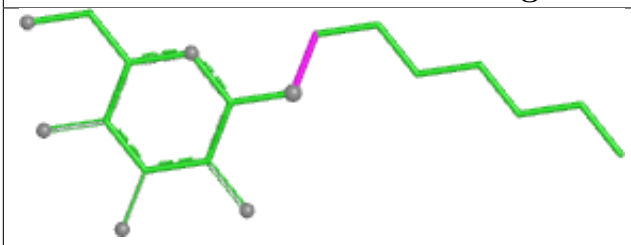


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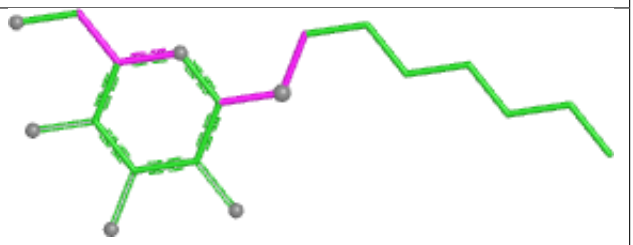


Rings

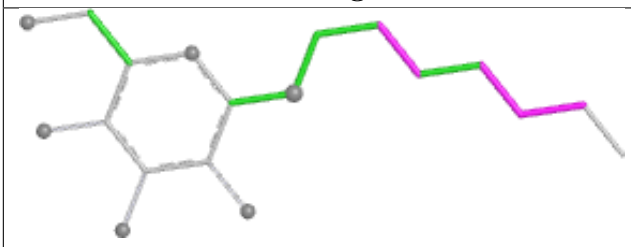
Ligand HTG C 530



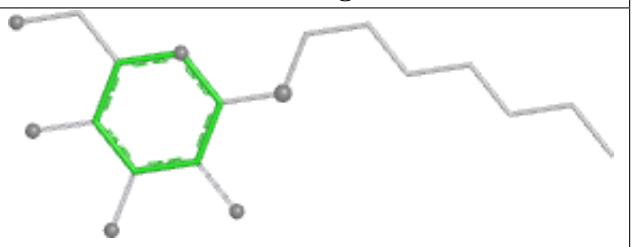
Bond lengths



Bond angles

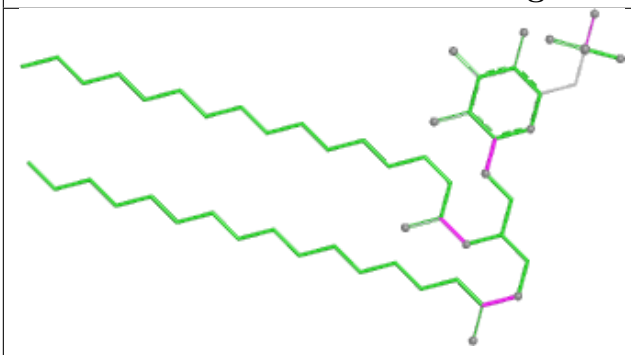


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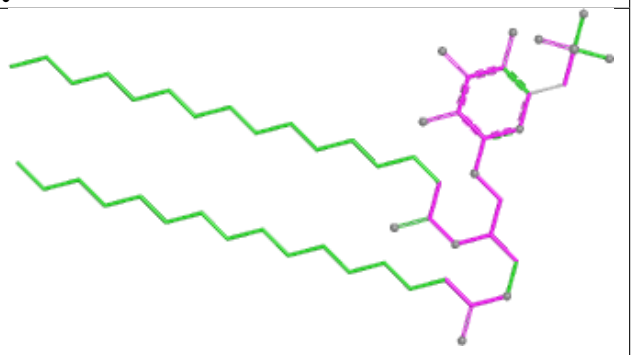


Rings

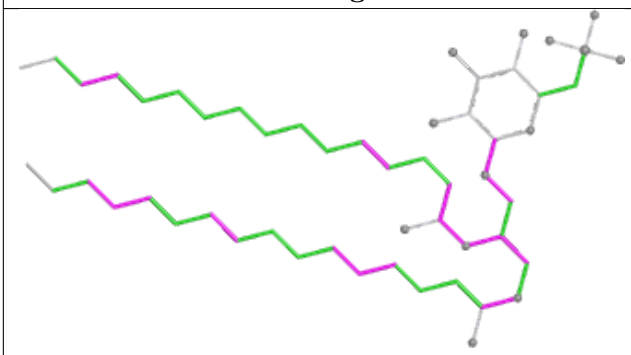
Ligand SQD b 633



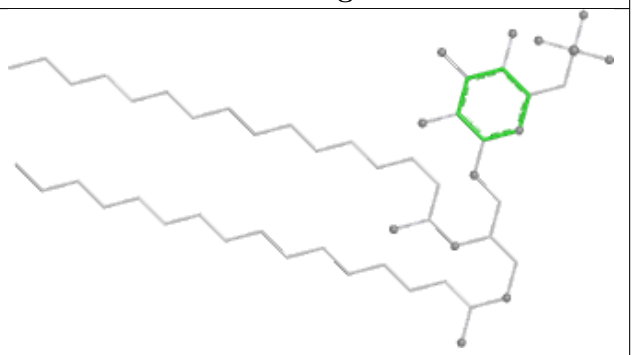
Bond lengths



Bond angles

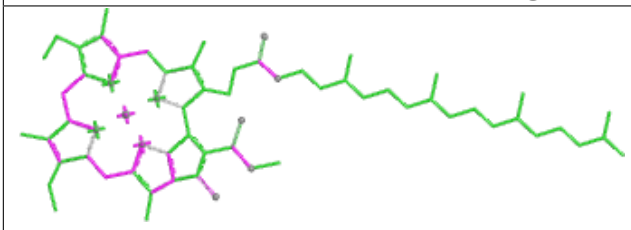


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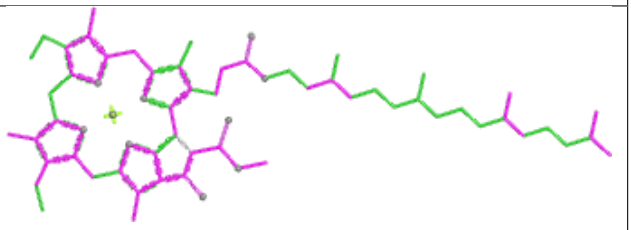


Rings

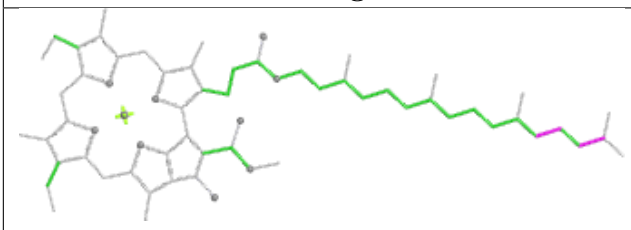
Ligand CLA B 611



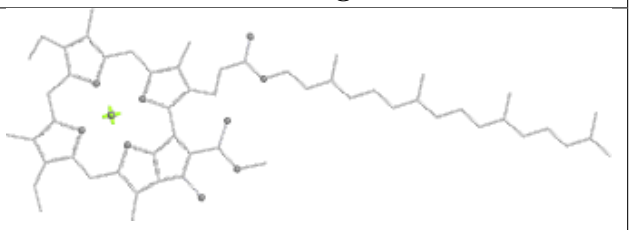
Bond lengths



Bond angles



Torsions

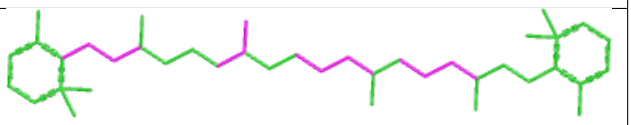


Rings

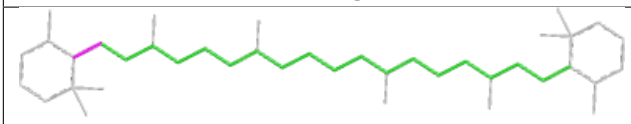
Ligand BCR b 618



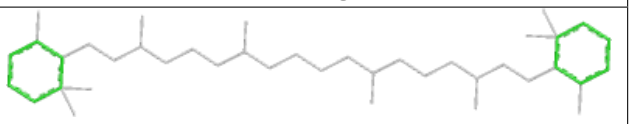
Bond lengths



Bond angles

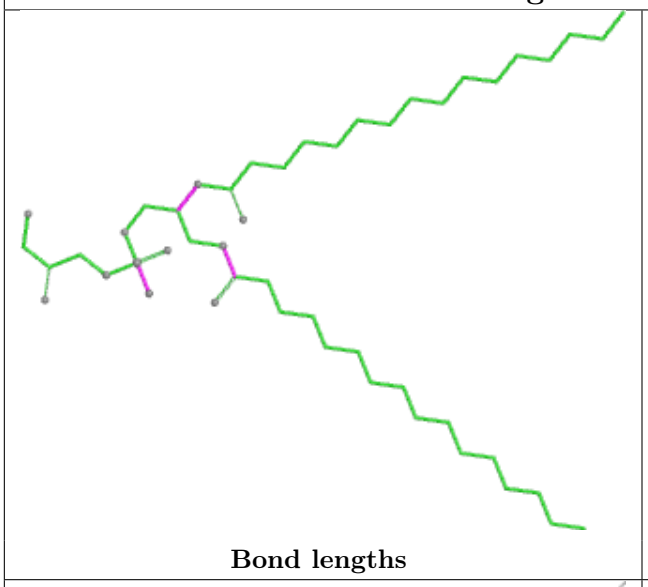


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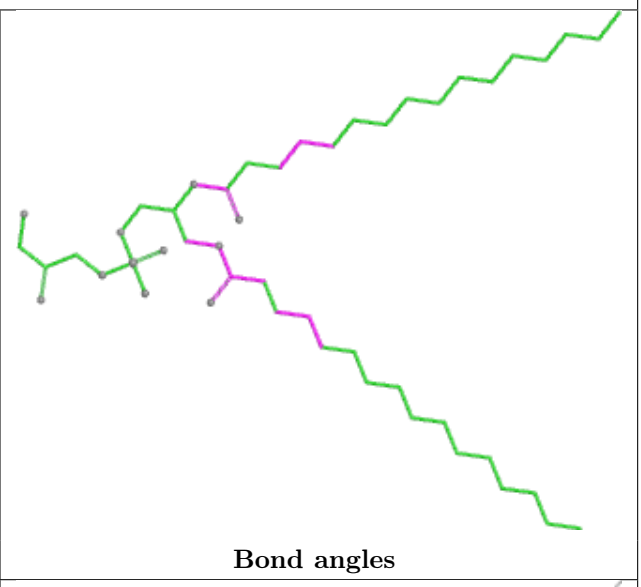


Rings

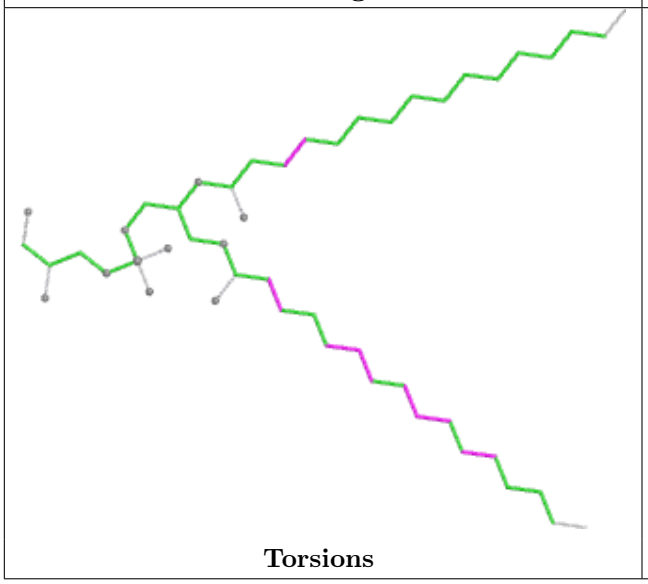
Ligand LHG d 409



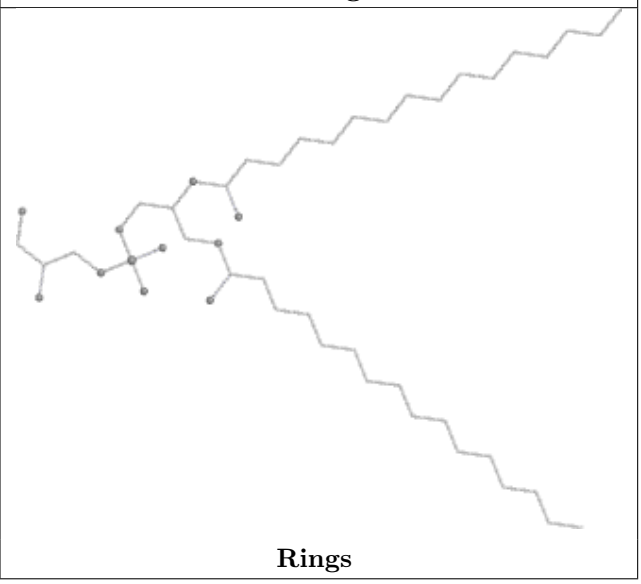
Bond lengths



Bond angles

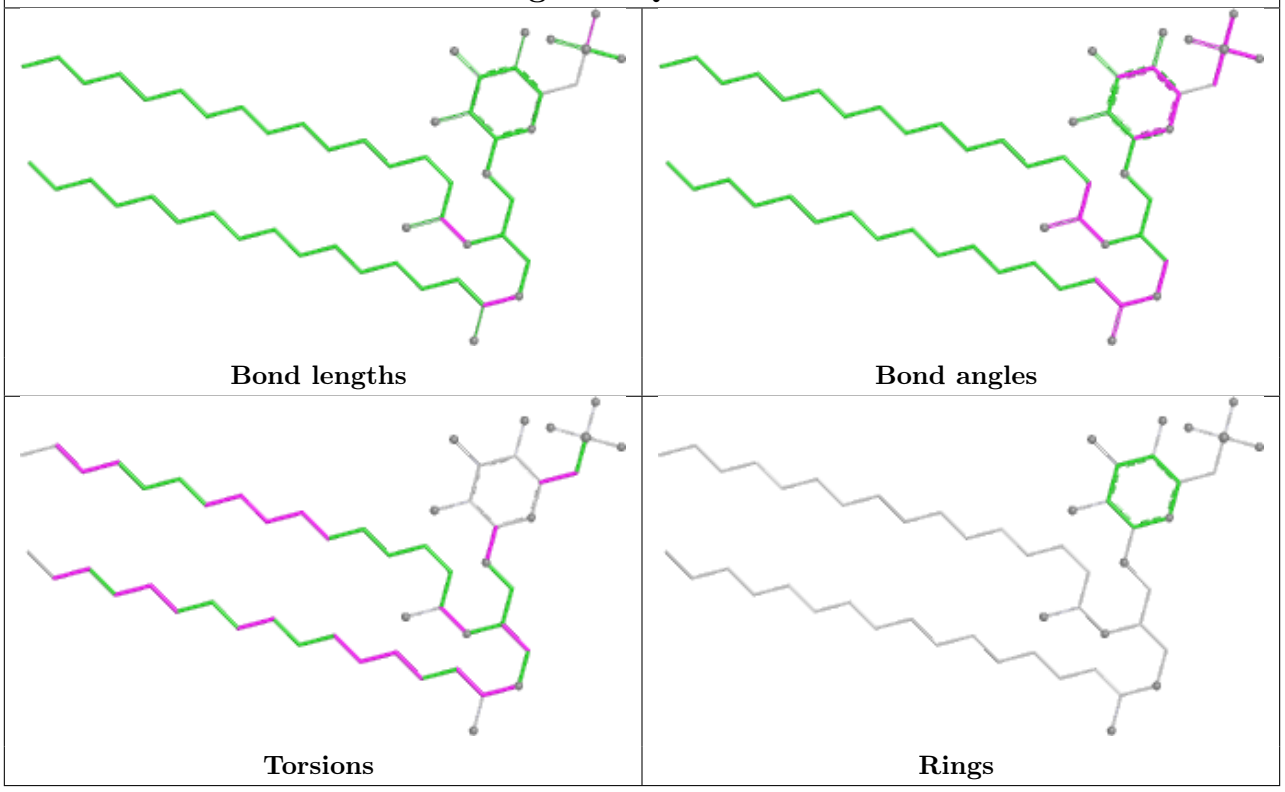


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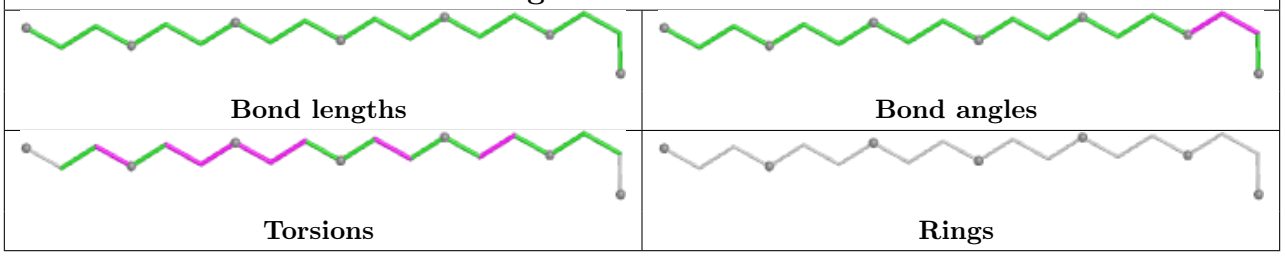


Rings

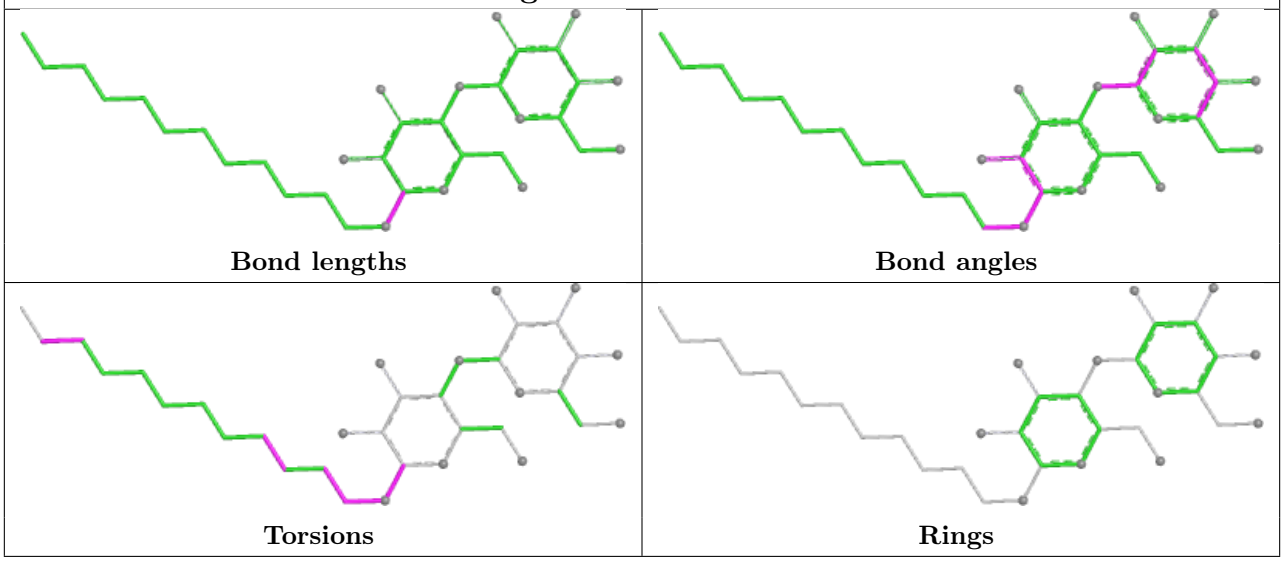
Ligand SQD x 101



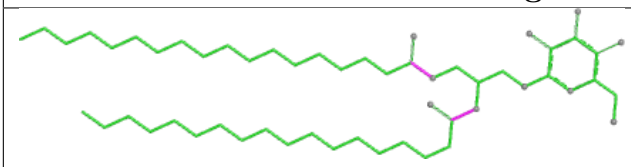
Ligand P6G B 652



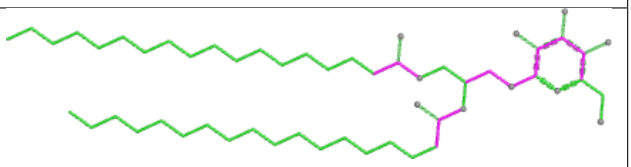
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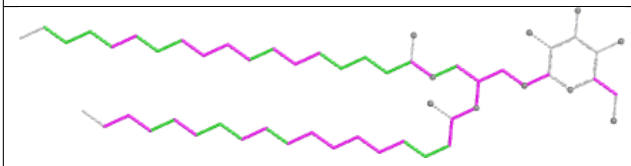
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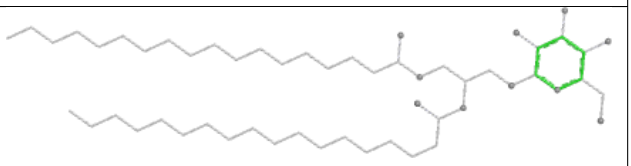
Bond lengths



Bond angles

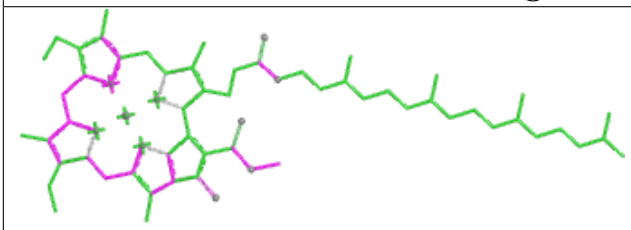


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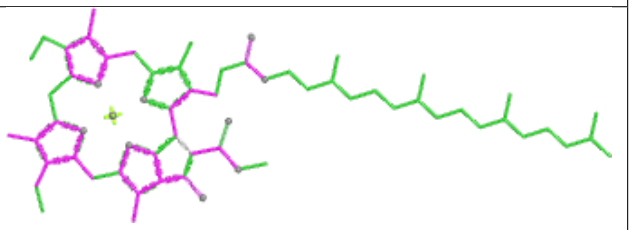


Rings

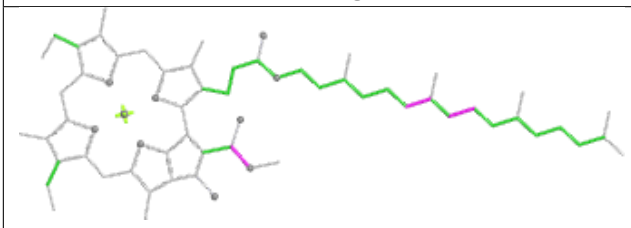
Ligand CLA C 503



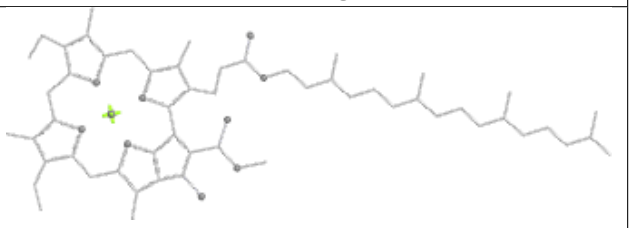
Bond lengths



Bond angles

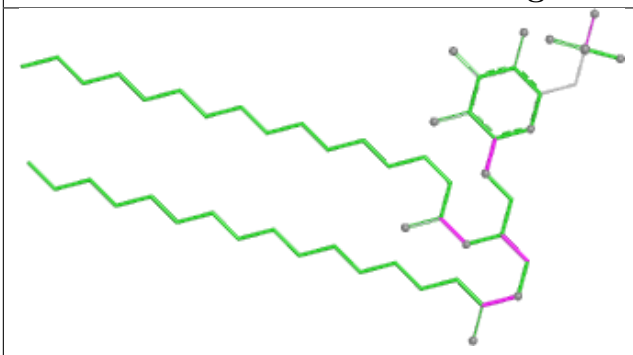


Torsions

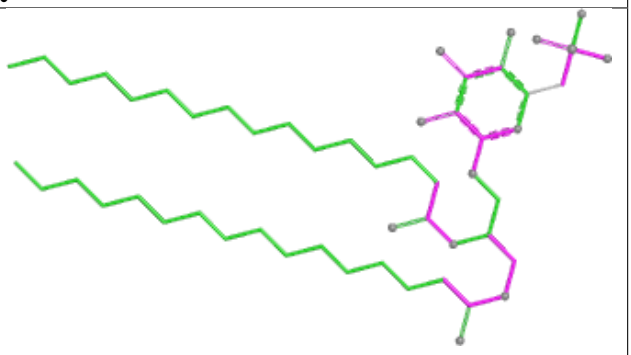


Rings

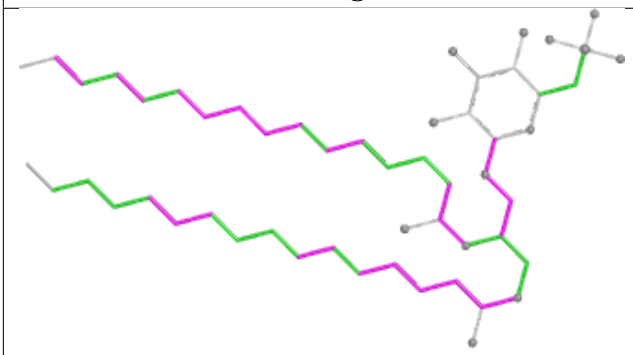
Ligand SQD h 105



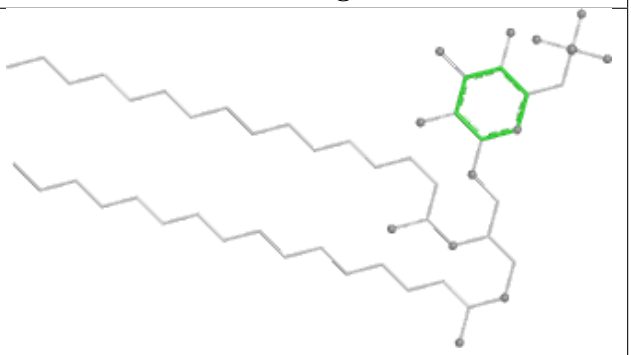
Bond lengths



Bond angles

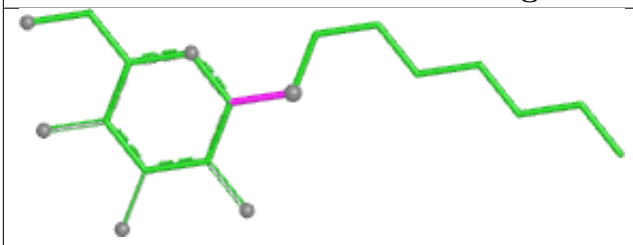


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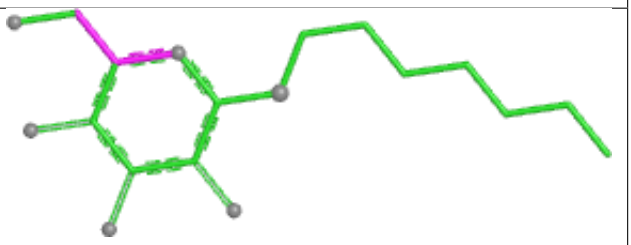


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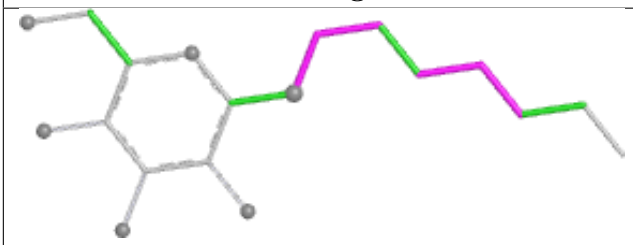
Ligand HTG C 521



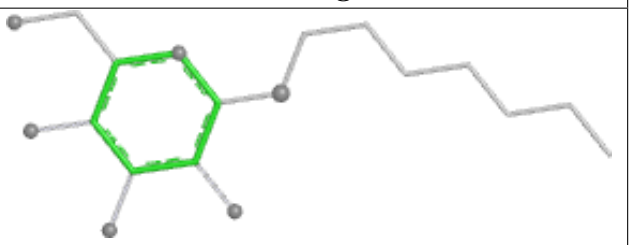
Bond lengths



Bond angles

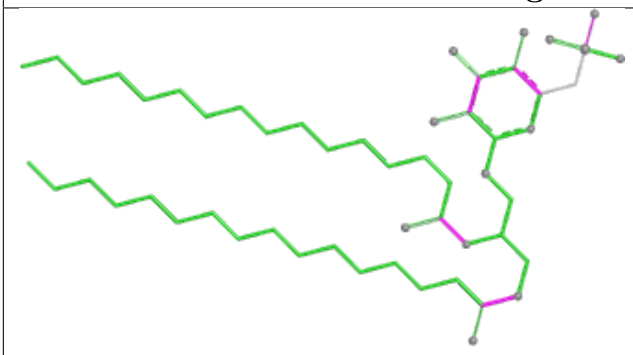


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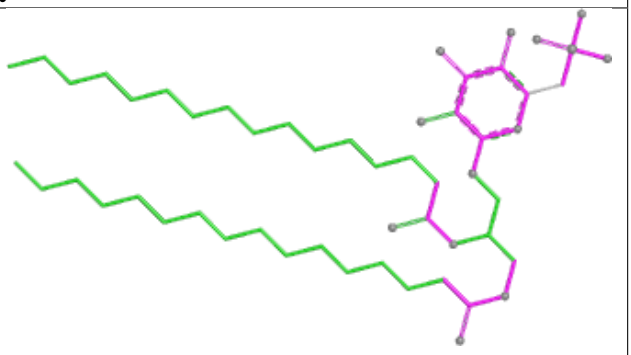


Rings

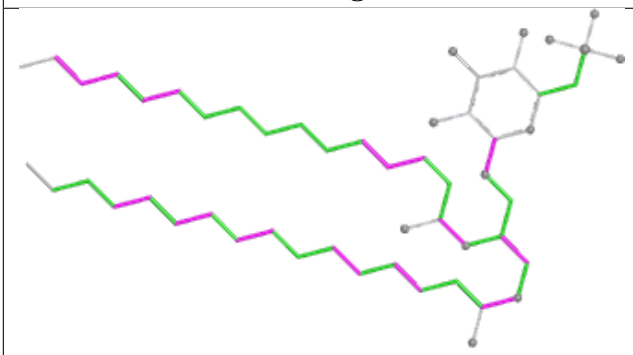
Ligand SQD F 104



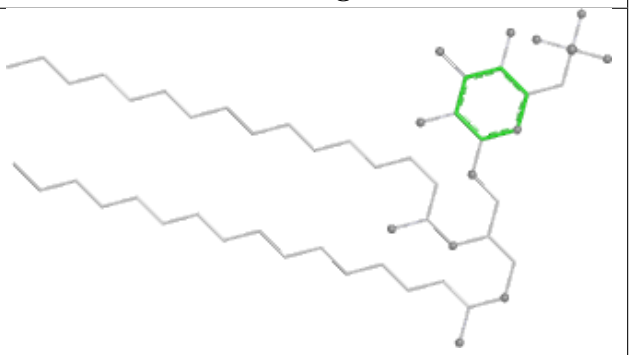
Bond lengths



Bond angles

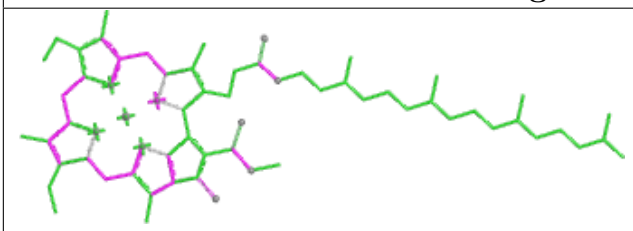


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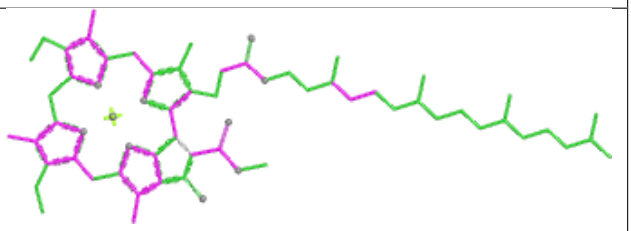


Rings

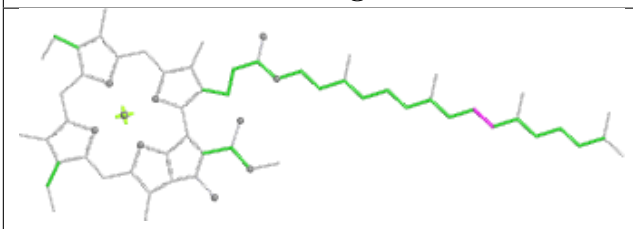
Ligand CLA c 513



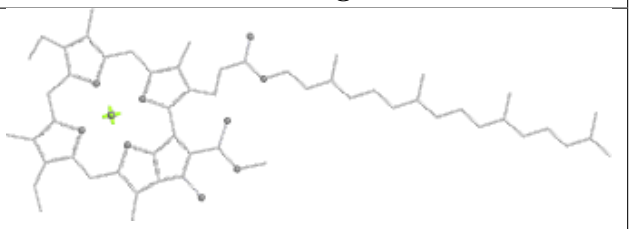
Bond lengths



Bond angles

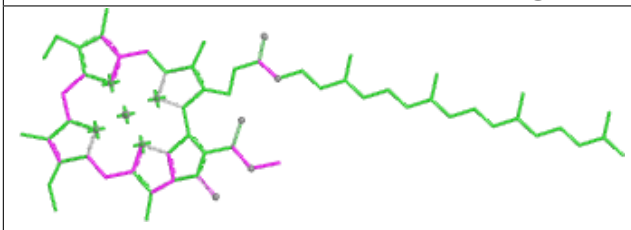


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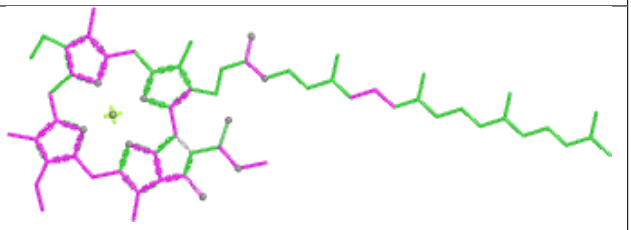


Rings

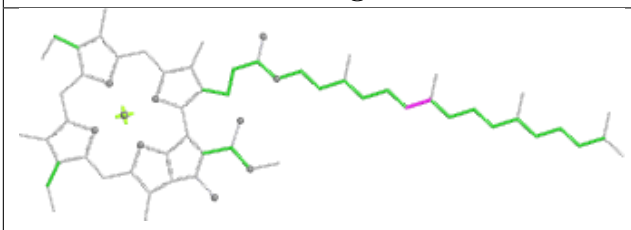
Ligand CLA c 503



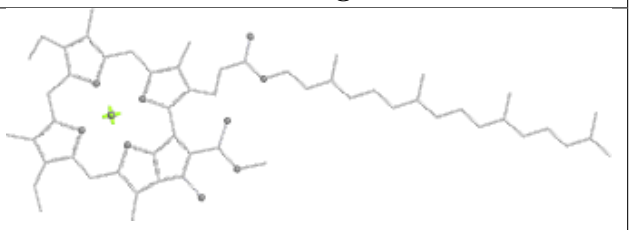
Bond lengths



Bond angles

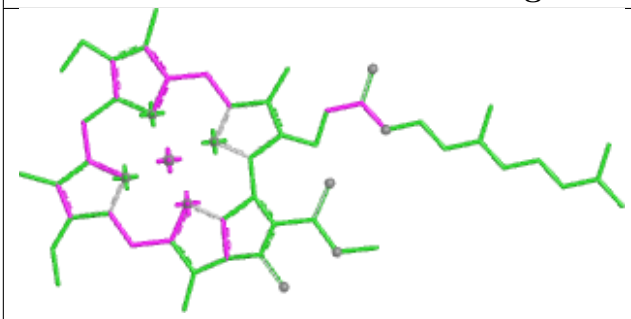


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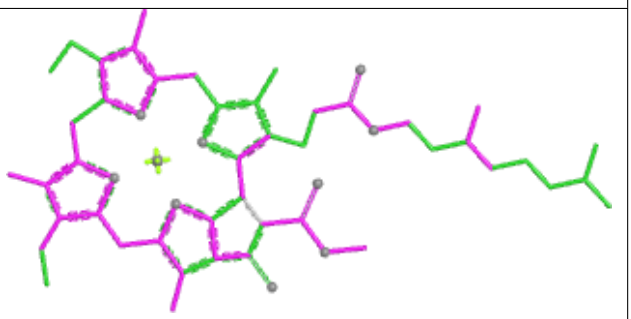


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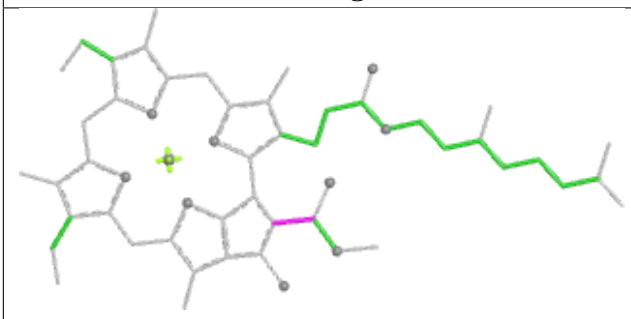
Ligand CLA B 615



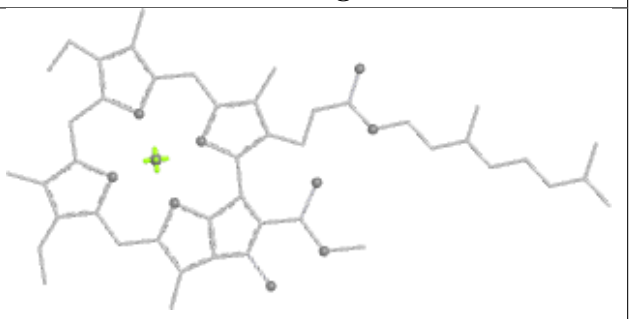
Bond lengths



Bond angles

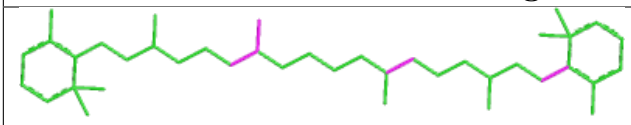


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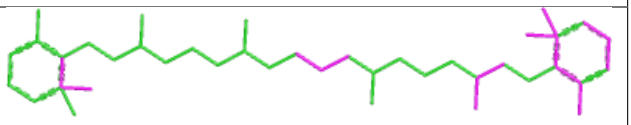


Rings

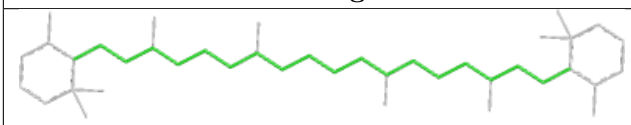
Ligand BCR B 619



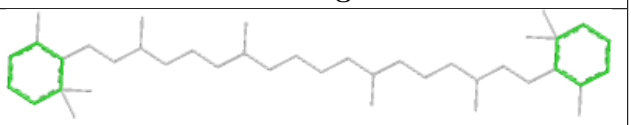
Bond lengths



Bond angles

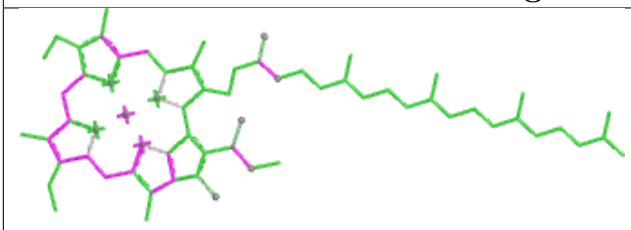


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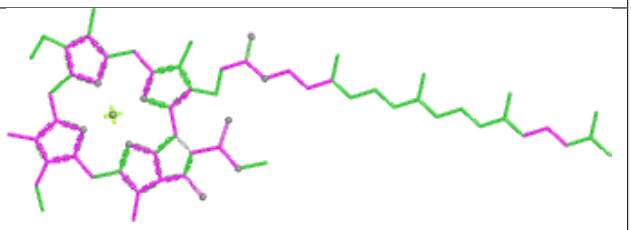


Rings

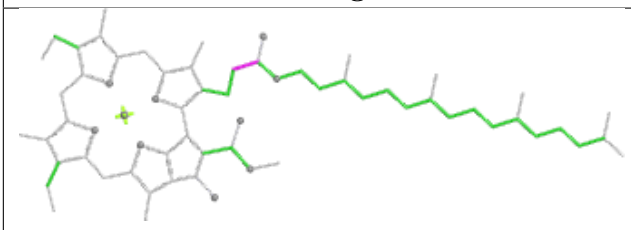
Ligand CLA C 512



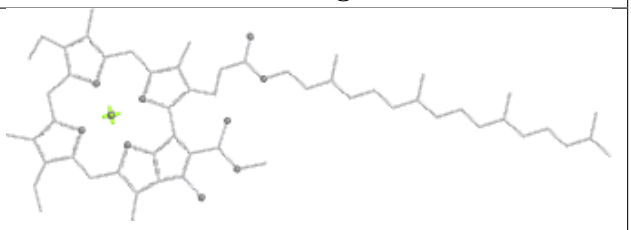
Bond lengths



Bond angles

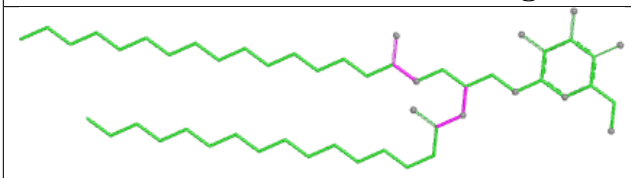


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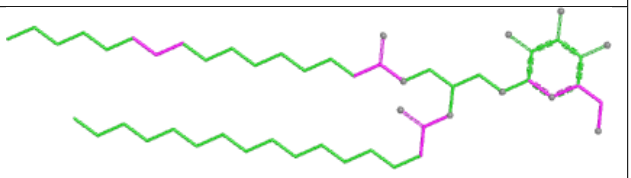


Rings

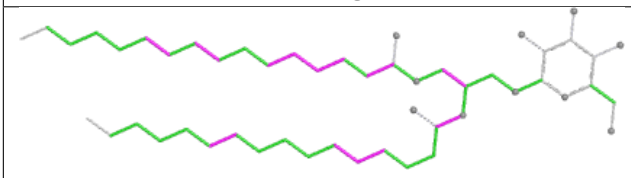
Ligand LMG B 621



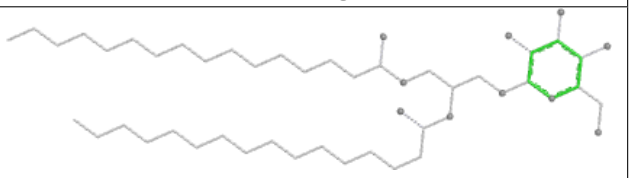
Bond lengths



Bond angles

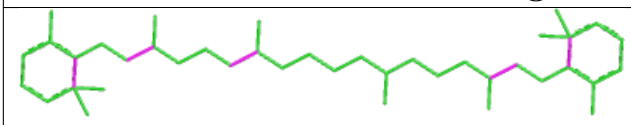


Torsions

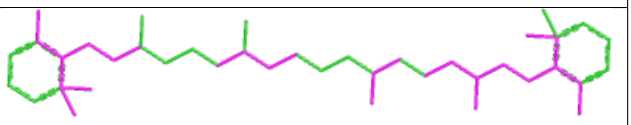


Rings

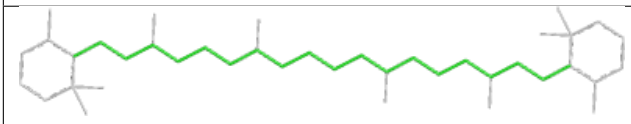
Ligand BCR c 514



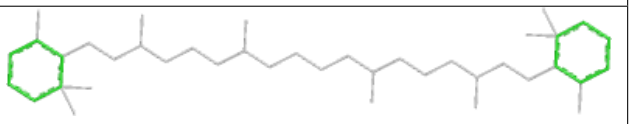
Bond lengths



Bond angles

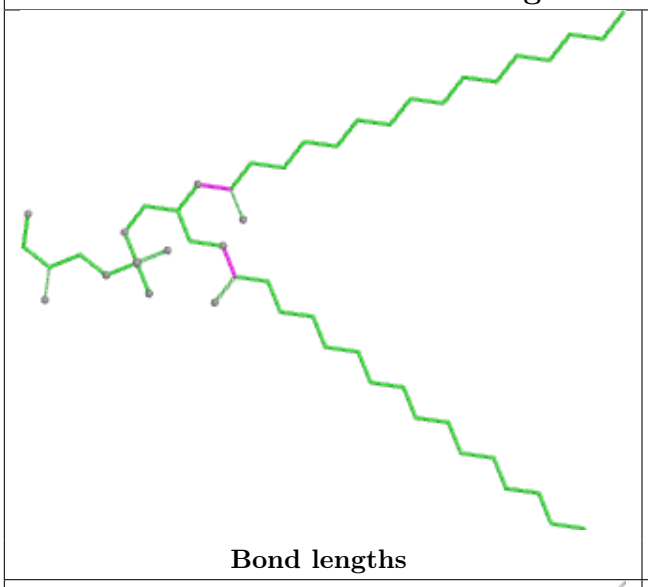


Torsions

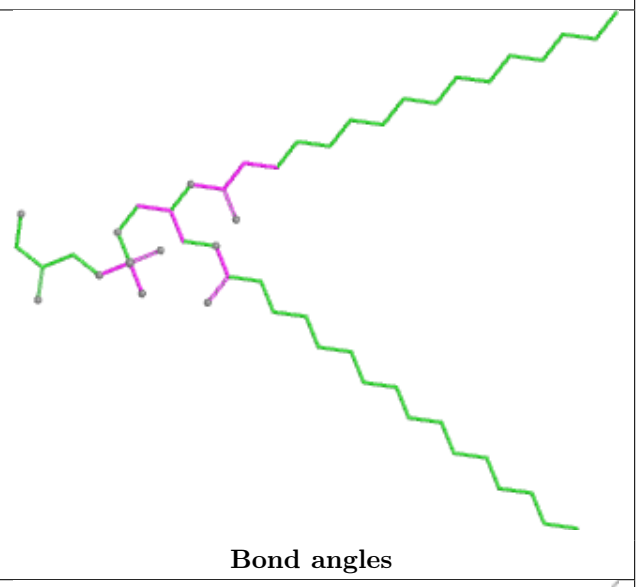


Rings

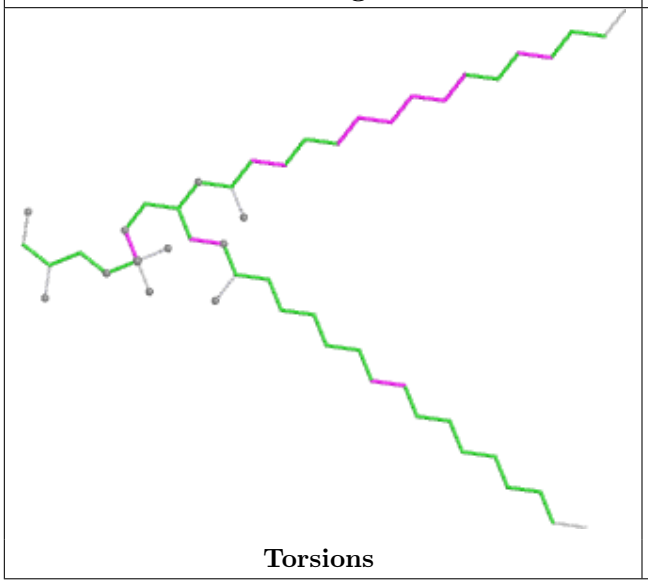
Ligand LHG B 632



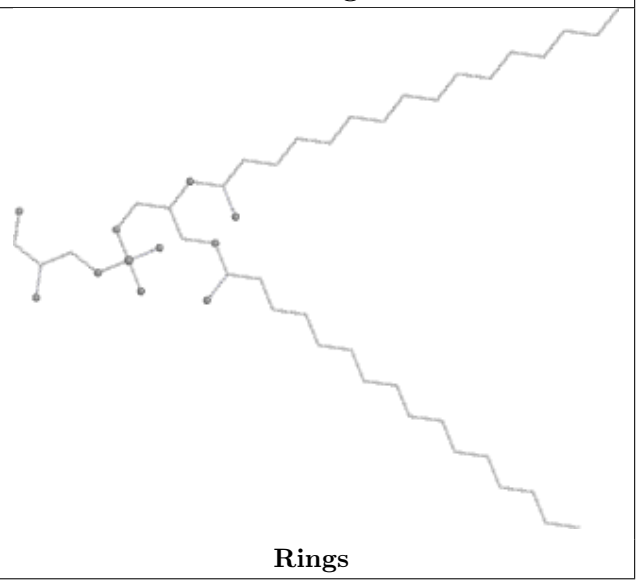
Bond lengths



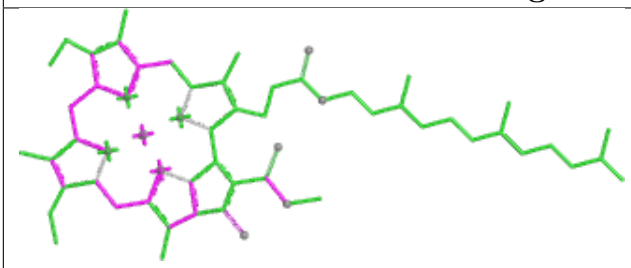
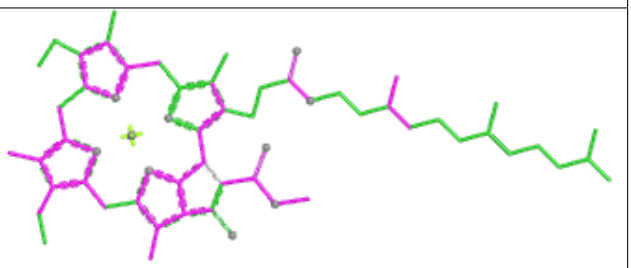
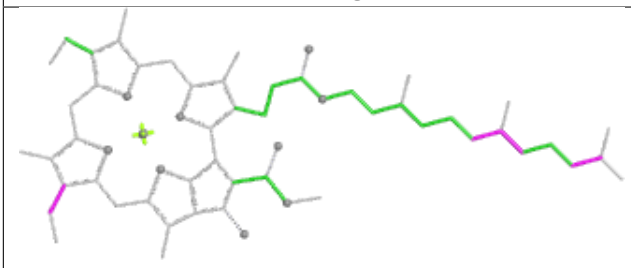
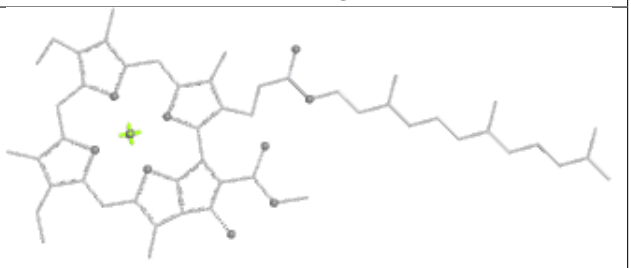
Bond angles

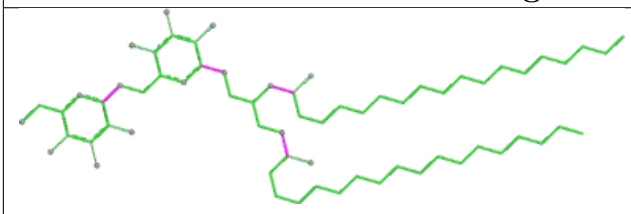
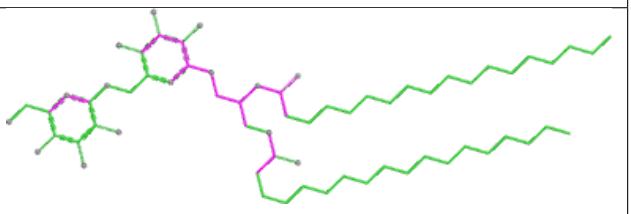
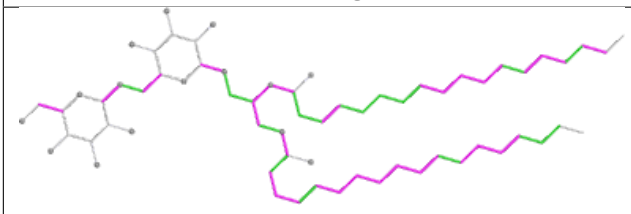
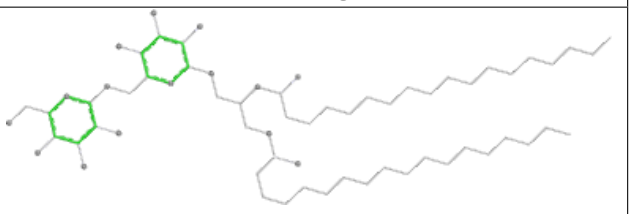


Torsions

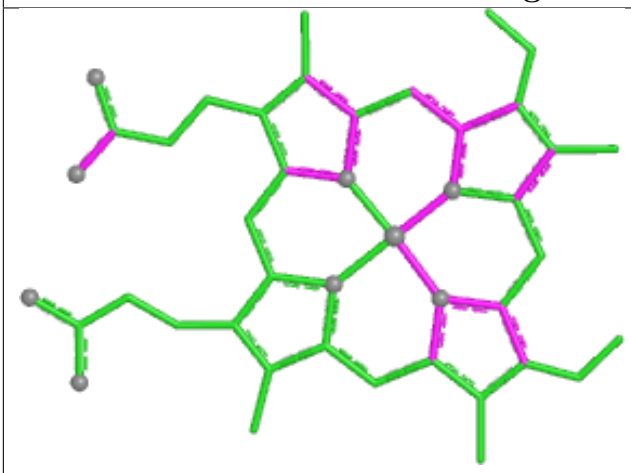


Rings

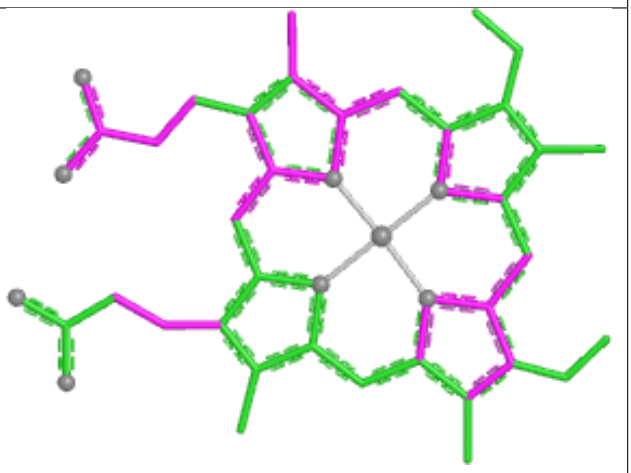
Ligand CLA a 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand DGD d 408	
 Bond lengths	 Bond angles
 Torsions	 Rings

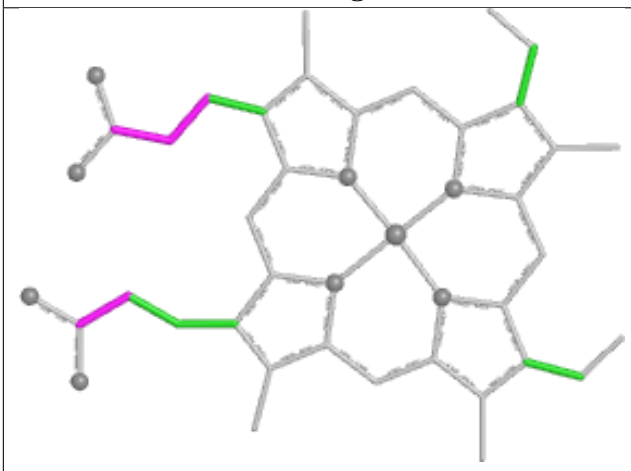
Ligand HEM e 107



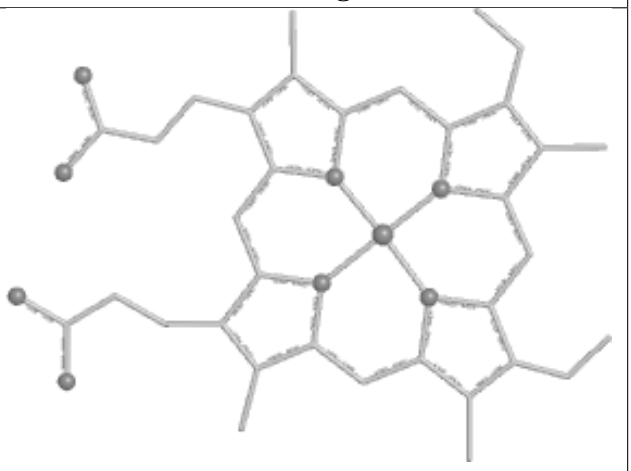
Bond lengths



Bond angles

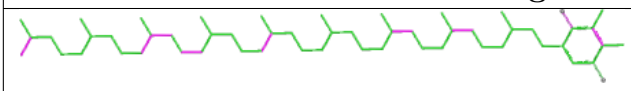


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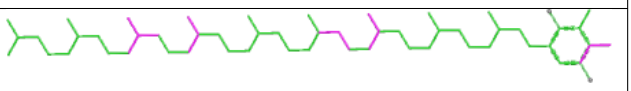


Rings

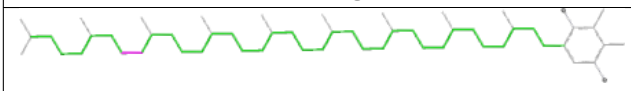
Ligand PL9 D 407



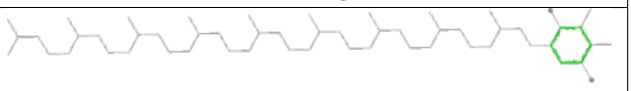
Bond lengths



Bond angles

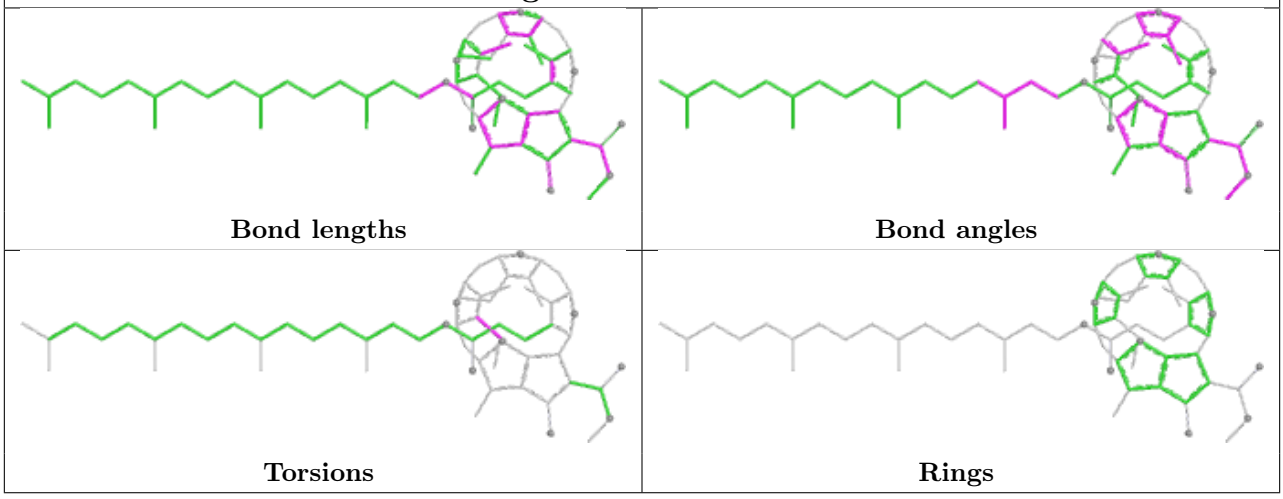


Torsions

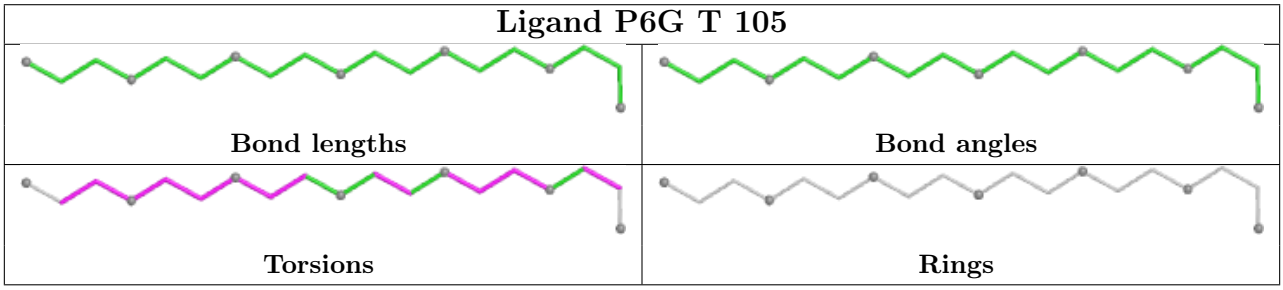


Rings

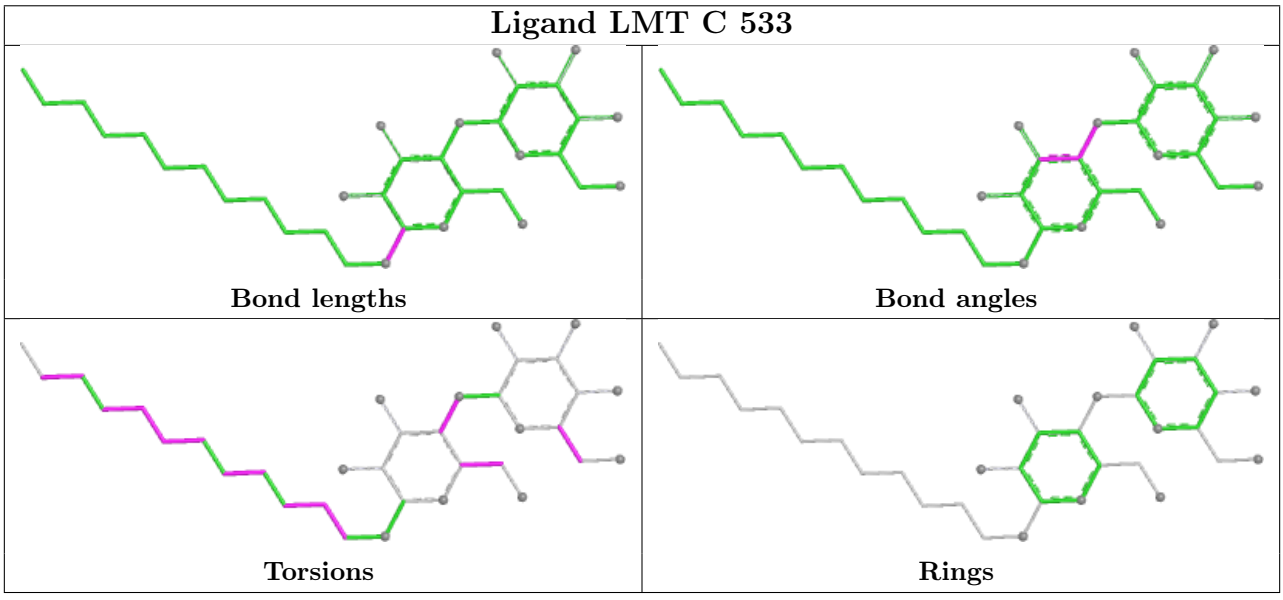
Ligand PHO D 401



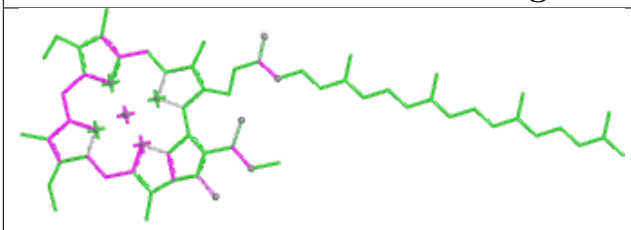
Ligand P6G T 105



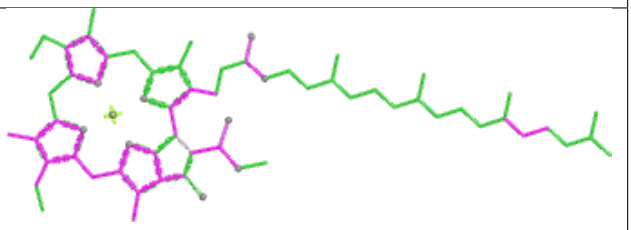
Ligand LMT C 533



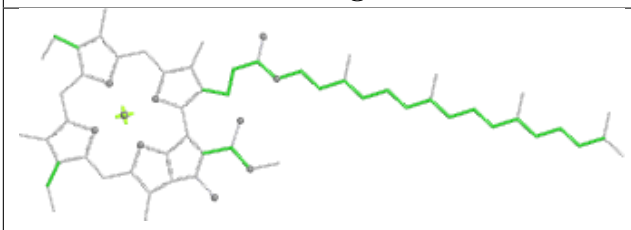
Ligand CLA c 505



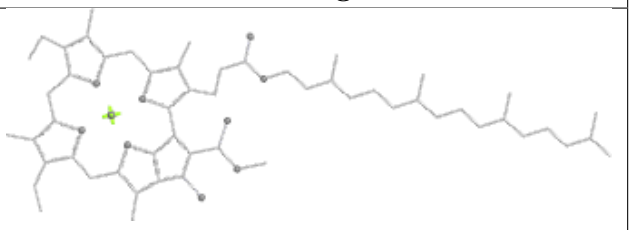
Bond lengths



Bond angles

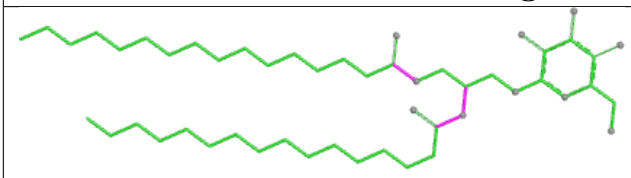


Torsions

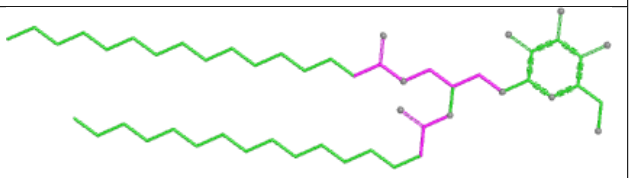


Rings

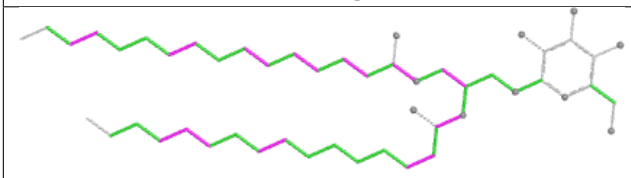
Ligand LMG C 519



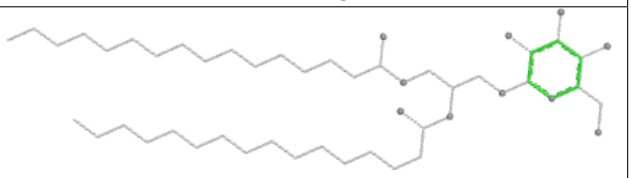
Bond lengths



Bond angles

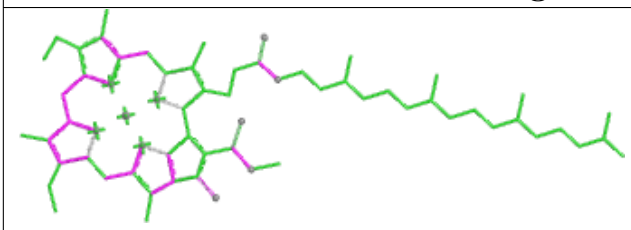


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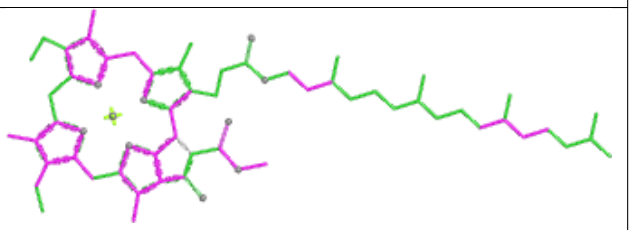


Rings

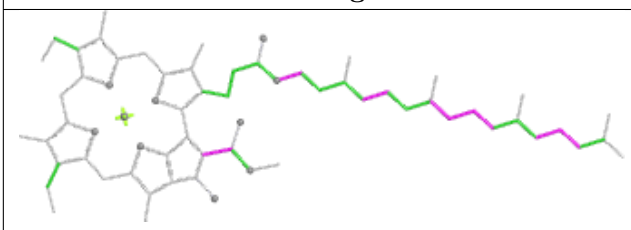
Ligand CLA c 509



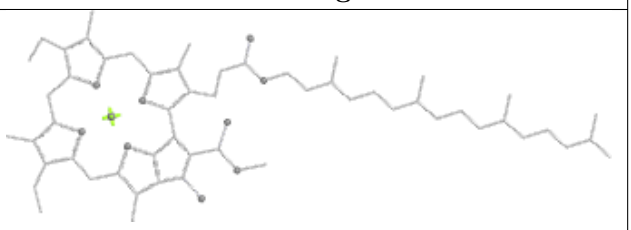
Bond lengths



Bond angles

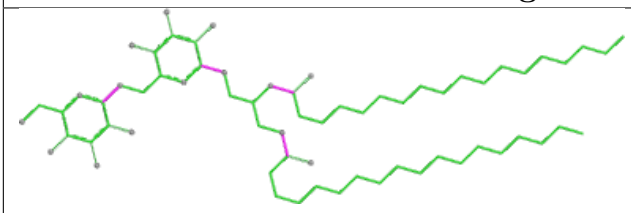


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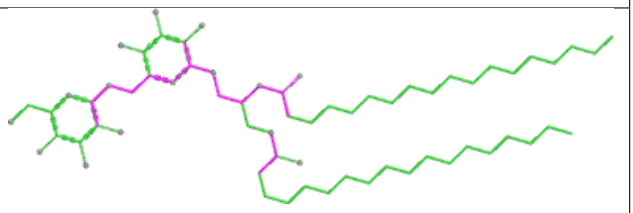


Rings

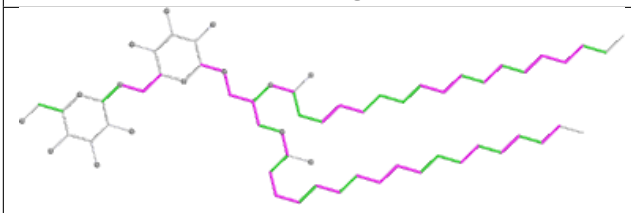
Ligand DGD D 408



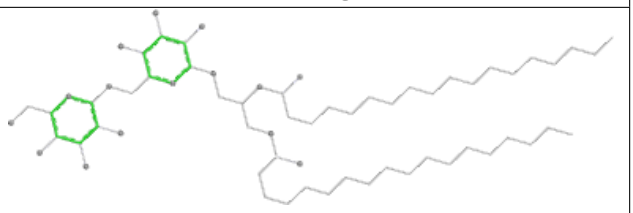
Bond lengths



Bond angles

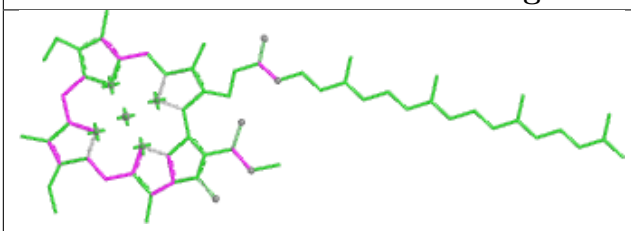


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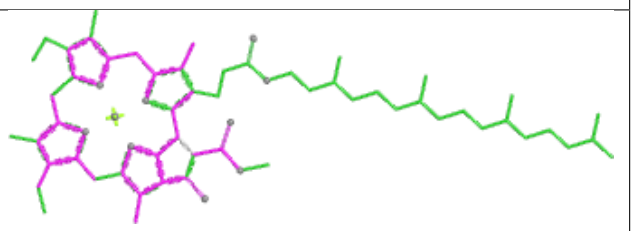


Rings

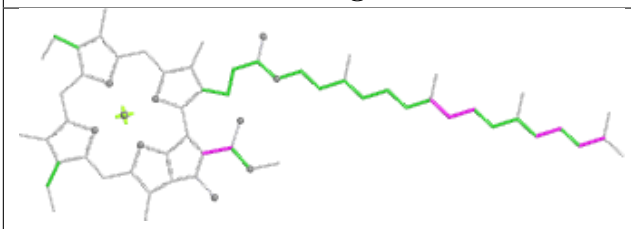
Ligand CLA D 405



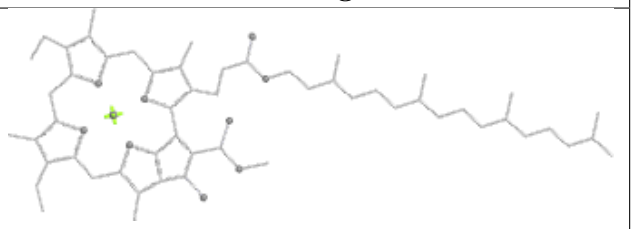
Bond lengths



Bond angles

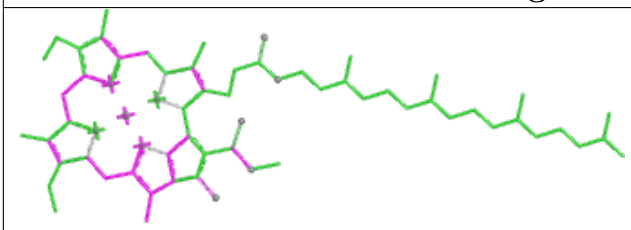


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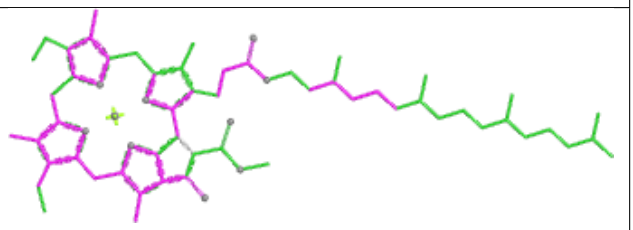


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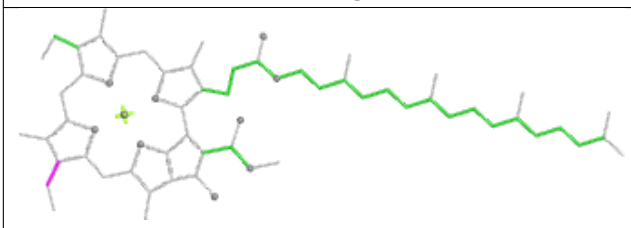
Ligand CLA a 407



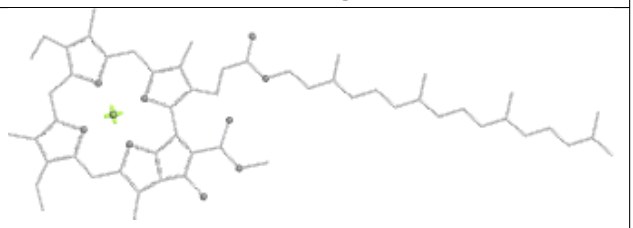
Bond lengths



Bond angles

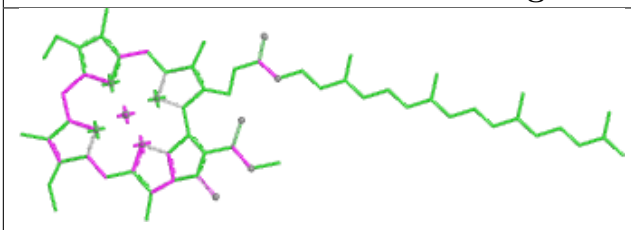


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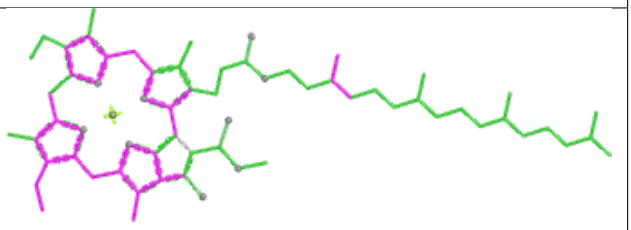


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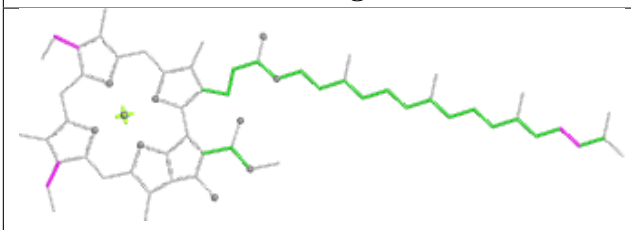
Ligand CLA d 403



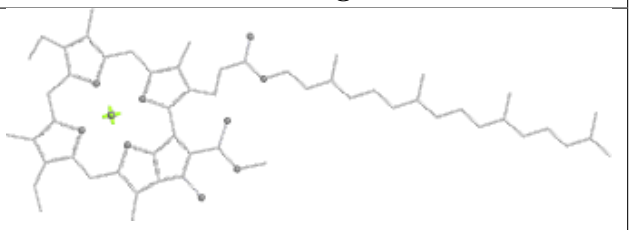
Bond lengths



Bond angles

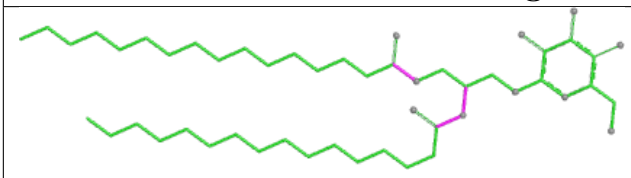


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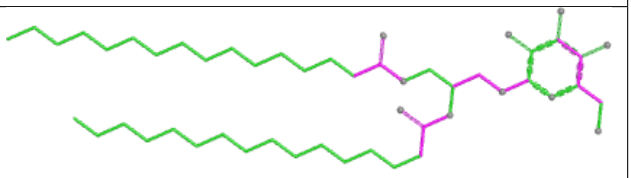


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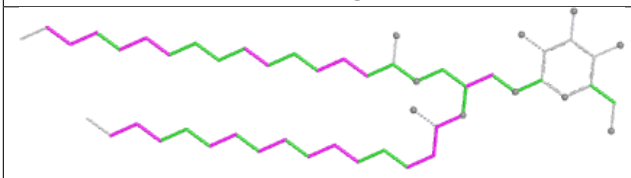
Ligand LMG c 519



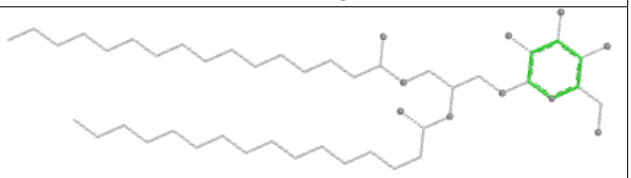
Bond lengths



Bond angles

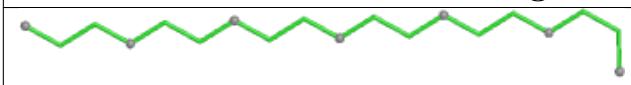


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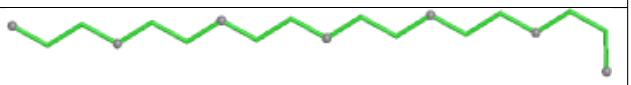


Rings

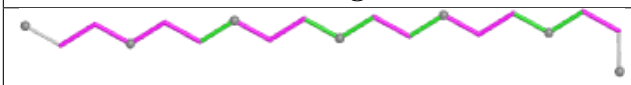
Ligand P6G b 649



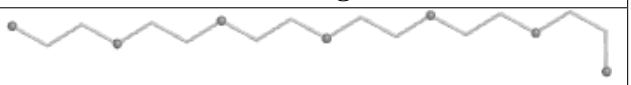
Bond lengths



Bond angles

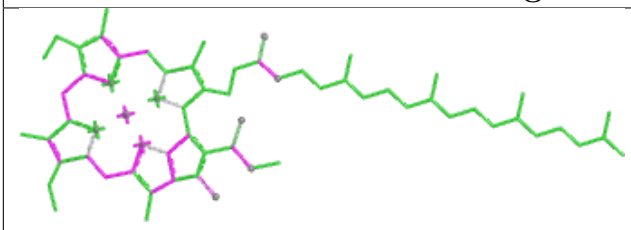


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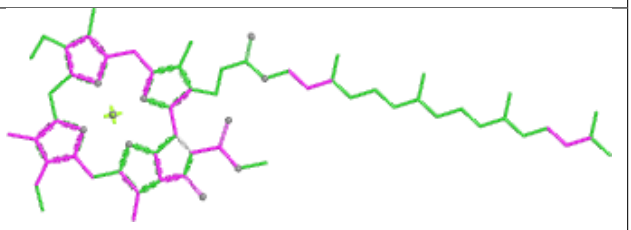


Rings

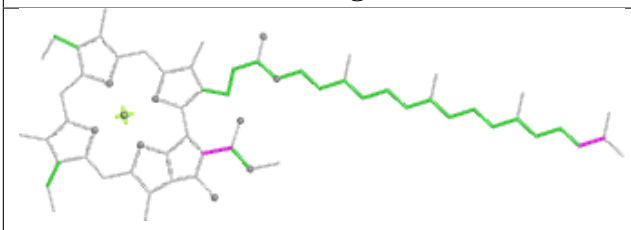
Ligand CLA C 502



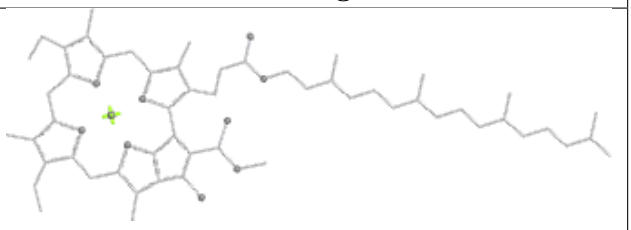
Bond lengths



Bond angles

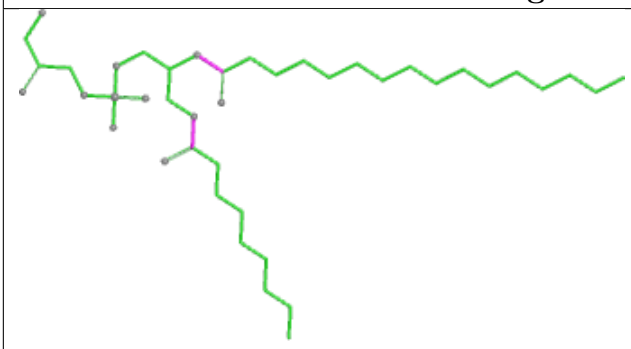


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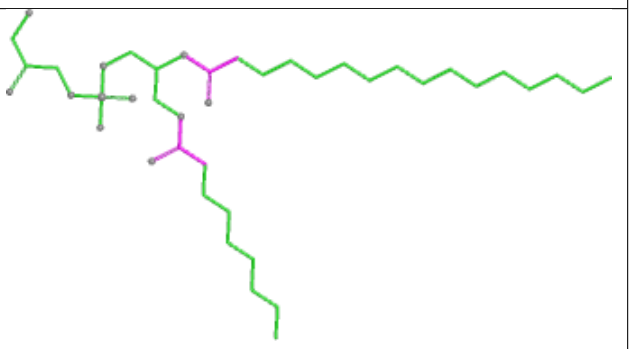


Rings

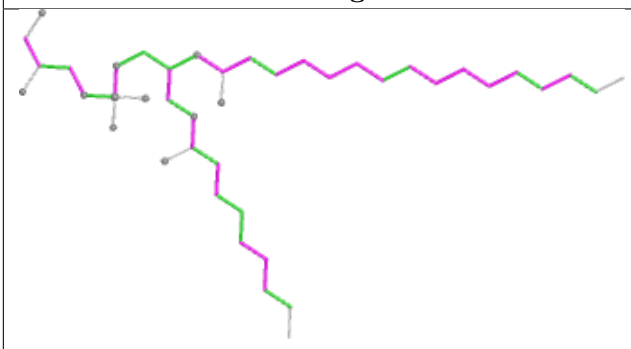
Ligand LHG e 101



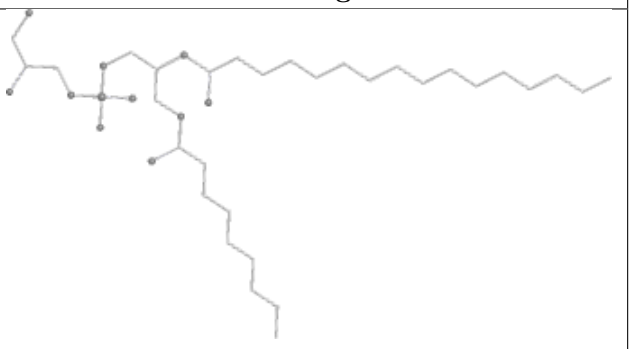
Bond lengths



Bond angles

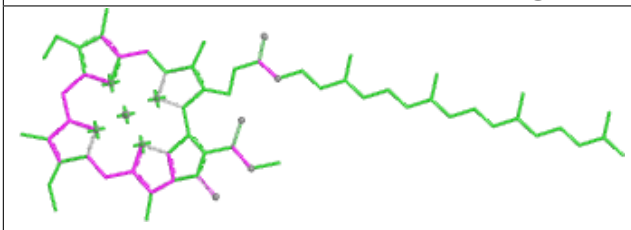


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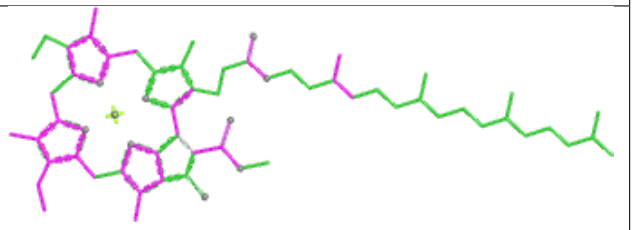


Rings

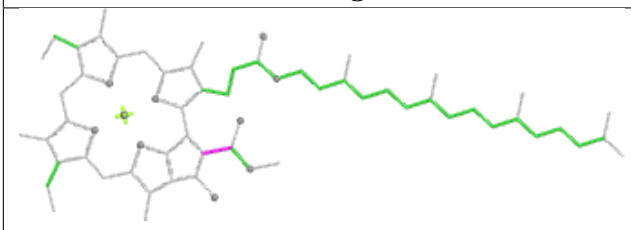
Ligand CLA c 507



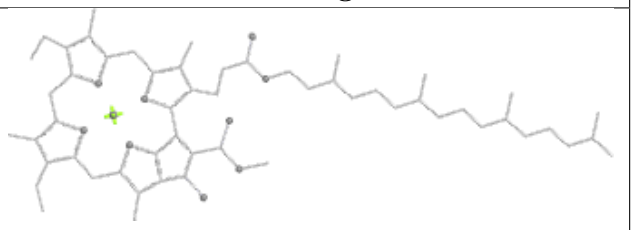
Bond lengths



Bond angles

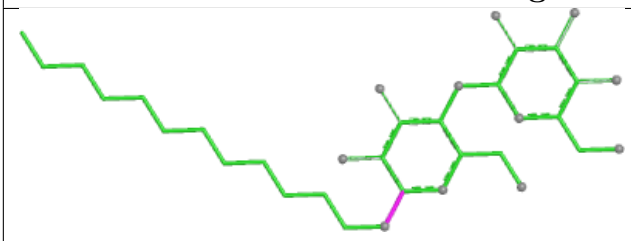


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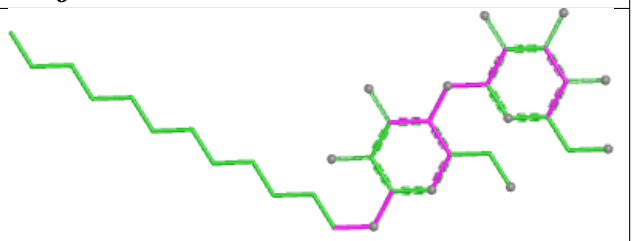


Rings

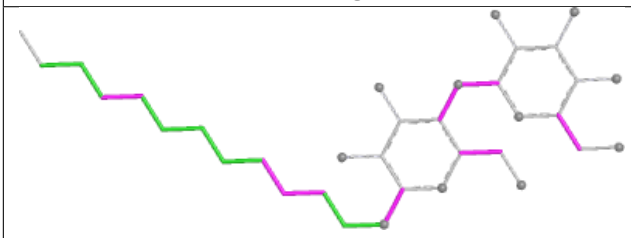
Ligand LMT j 103



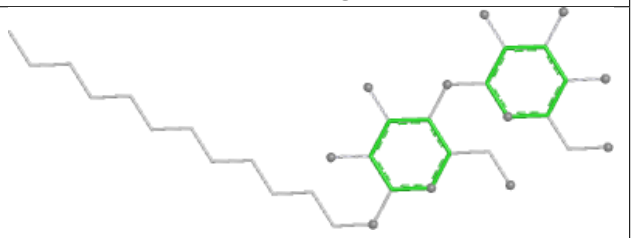
Bond lengths



Bond angles

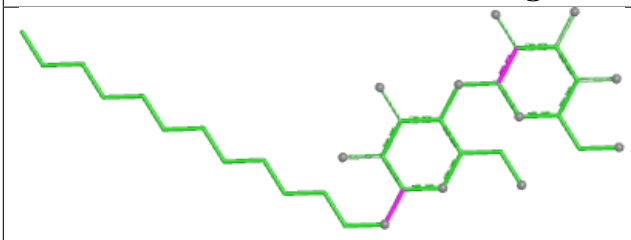


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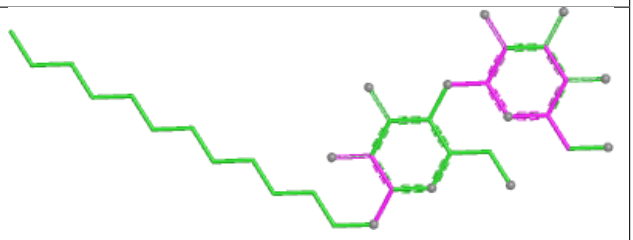


Rings

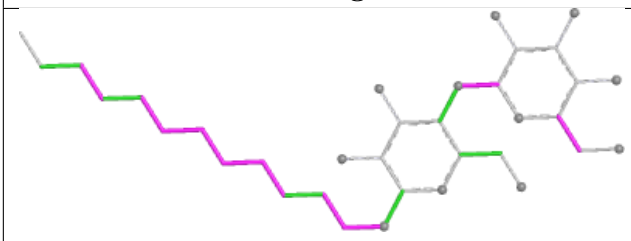
Ligand LMT u 203



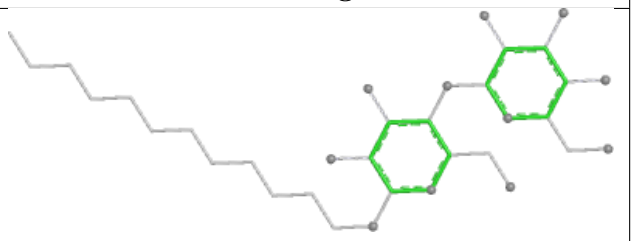
Bond lengths



Bond angles

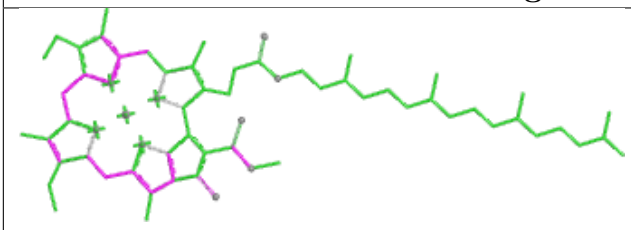


Torsions

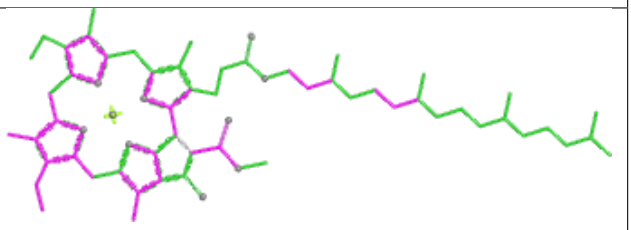


Rings

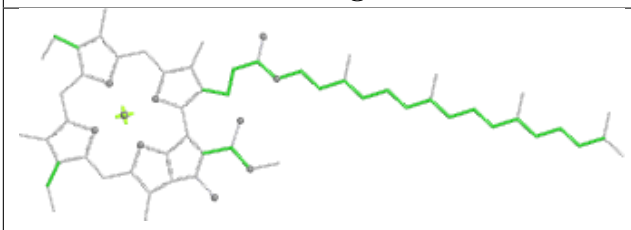
Ligand CLA B 608



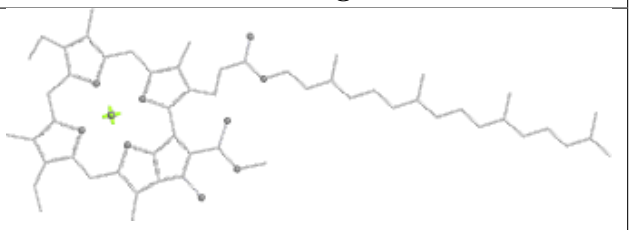
Bond lengths



Bond angles

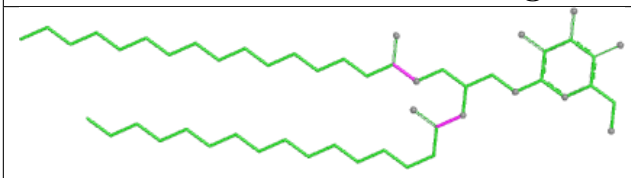


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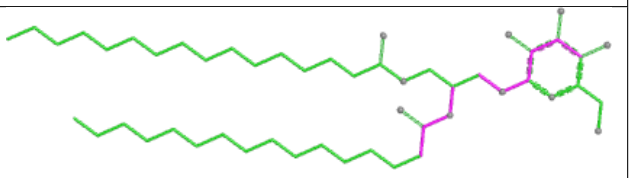


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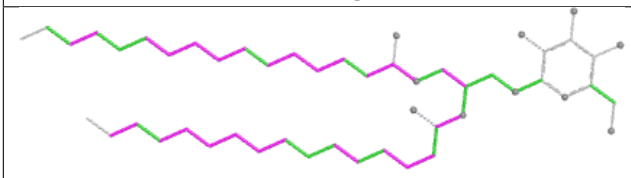
Ligand LMG a 414



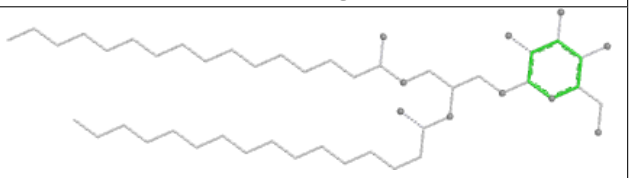
Bond lengths



Bond angles

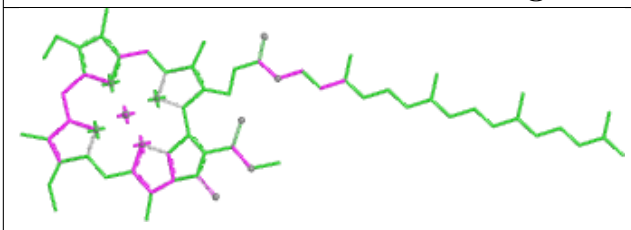


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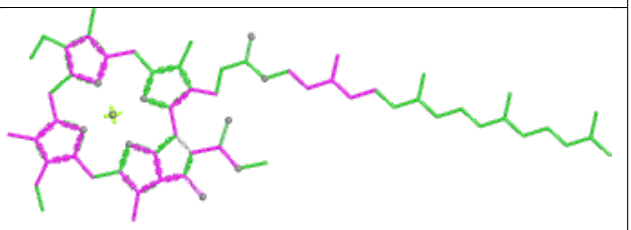


Rings

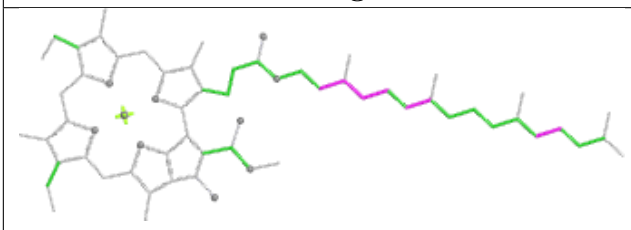
Ligand CLA b 605



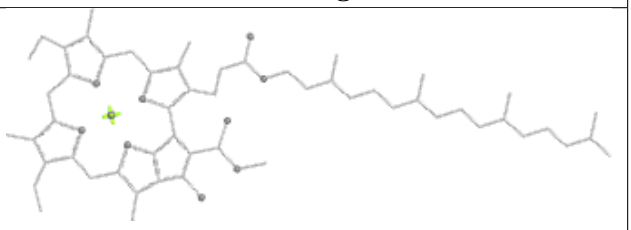
Bond lengths



Bond angles

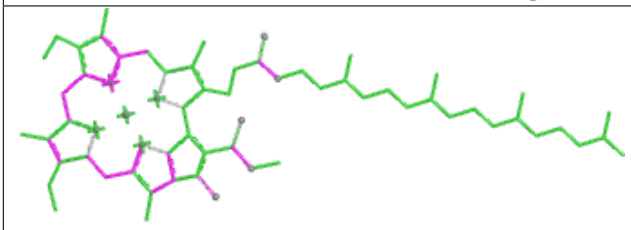


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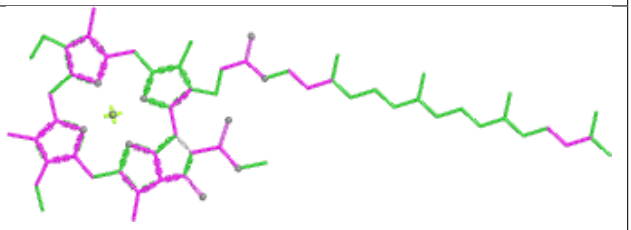


Rings

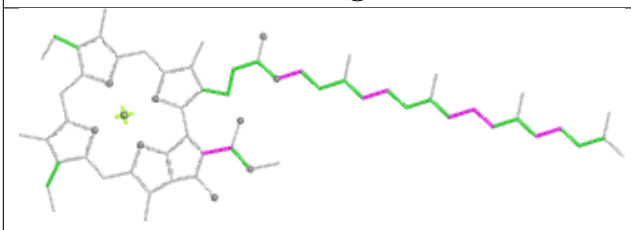
Ligand CLA C 509



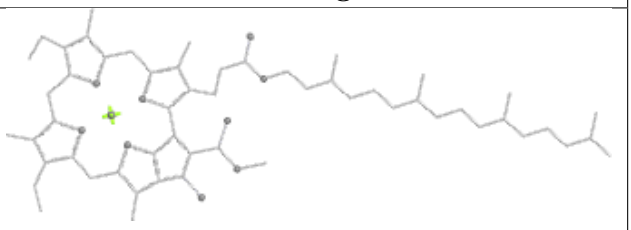
Bond lengths



Bond angles

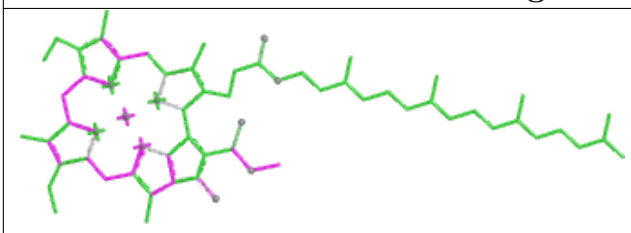


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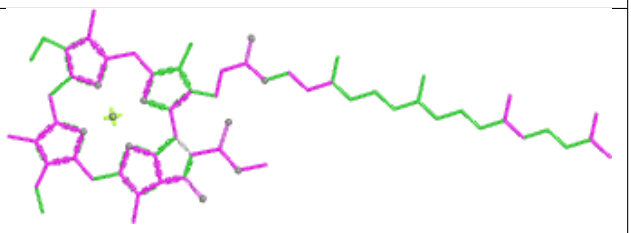


Rings

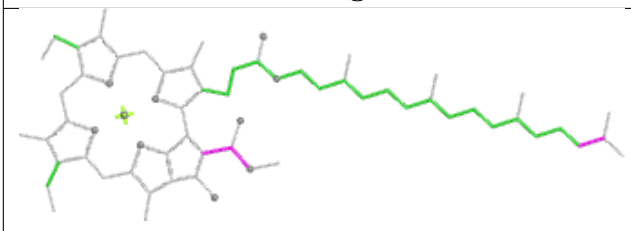
Ligand CLA b 611



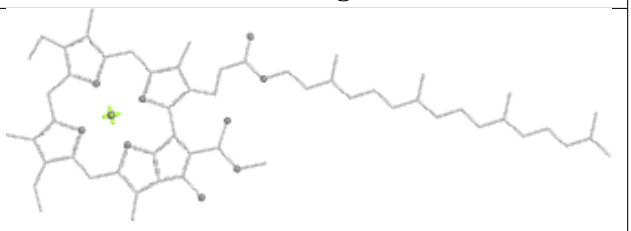
Bond lengths



Bond angles

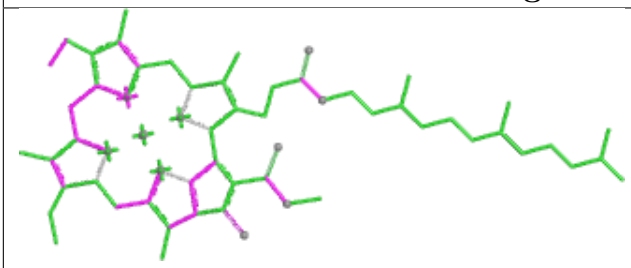


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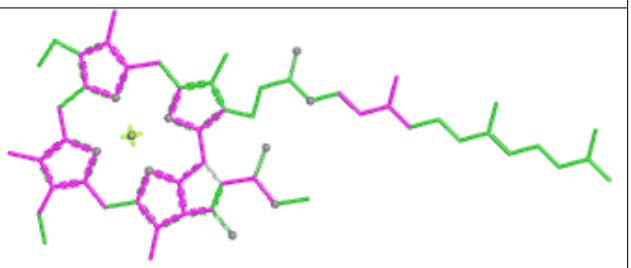


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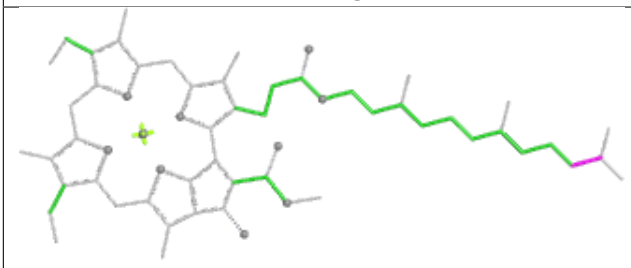
Ligand CLA A 607



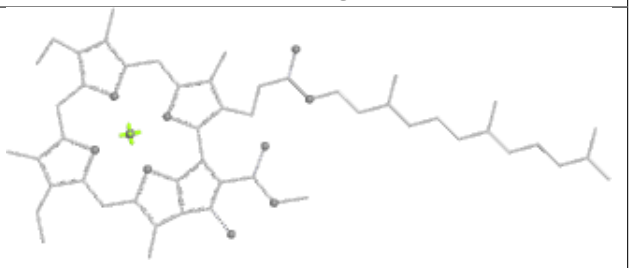
Bond lengths



Bond angles

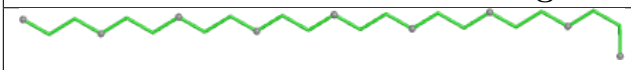


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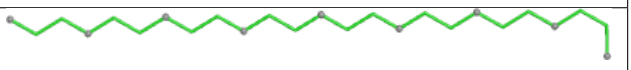


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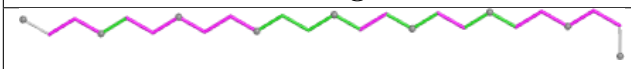
Ligand PE8 i 107



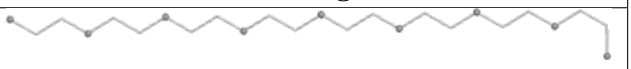
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Bond angles

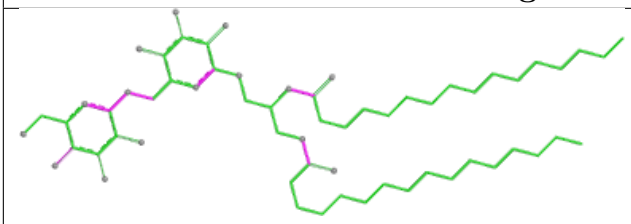


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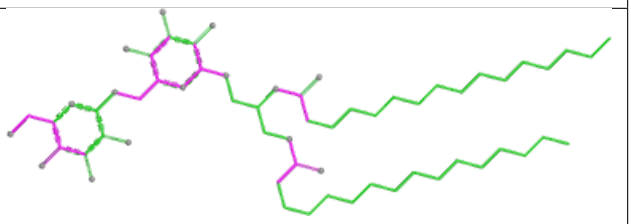


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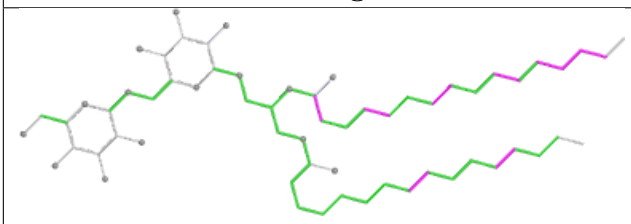
Ligand DGD H 103



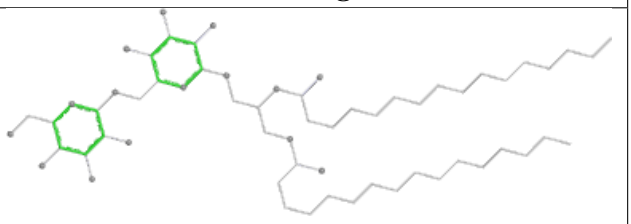
Bond lengths



Bond angles

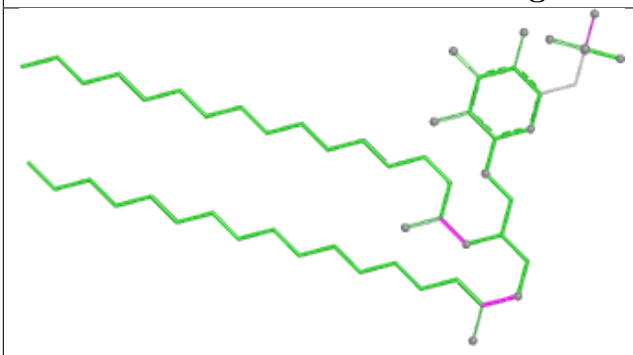


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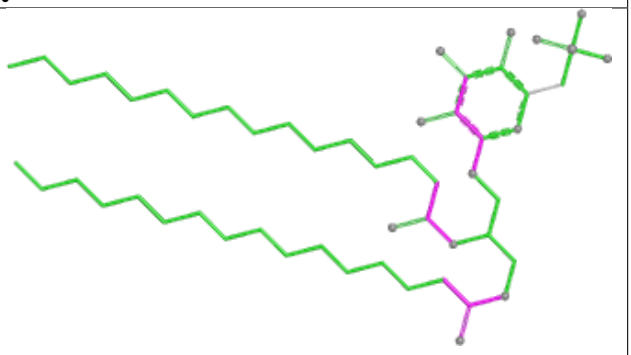


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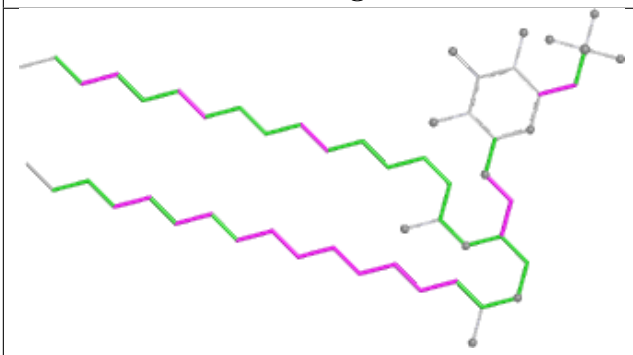
Ligand SQD a 417



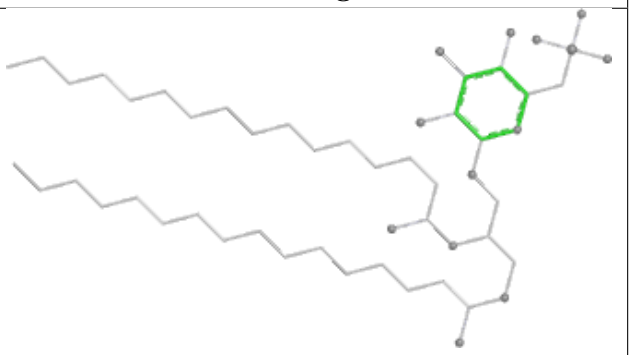
Bond lengths



Bond angles



Torsions

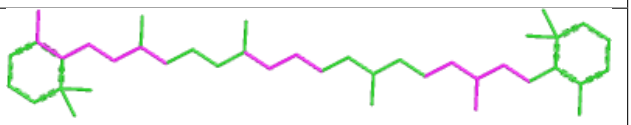


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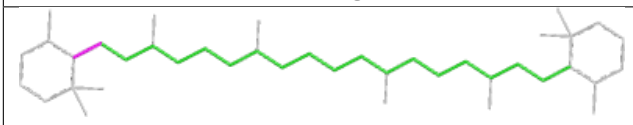
Ligand BCR B 618



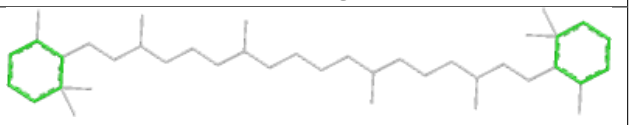
Bond lengths



Bond angles

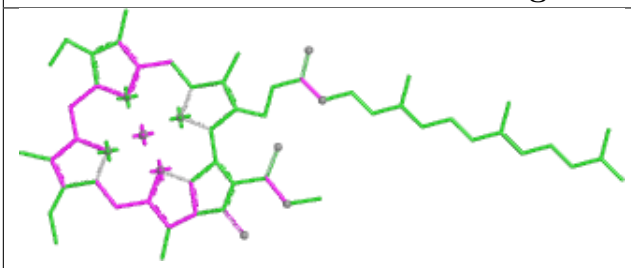


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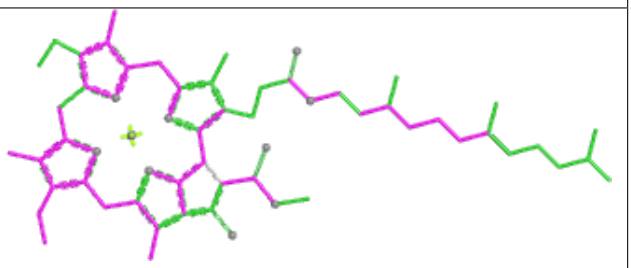


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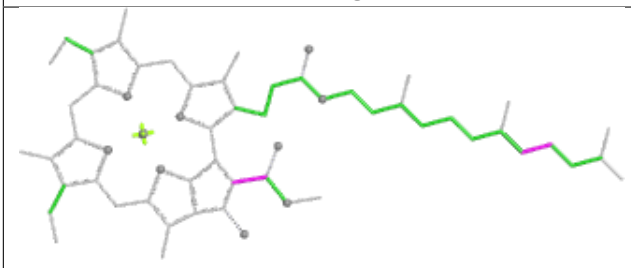
Ligand CLA c 504



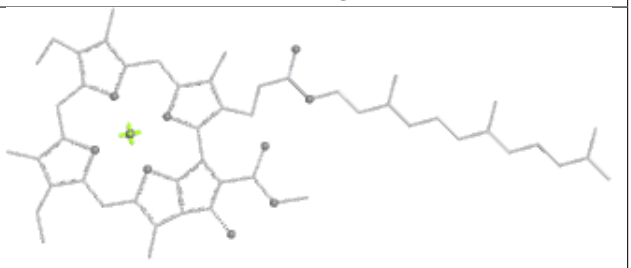
Bond lengths



Bond angles

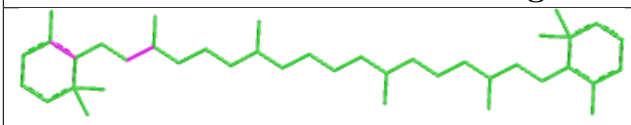


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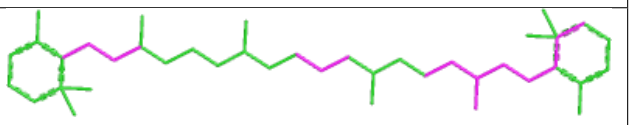


Rings

Ligand BCR c 527



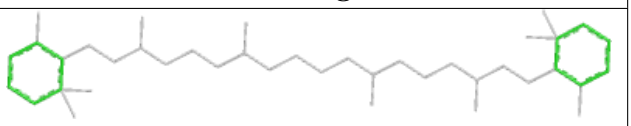
Bond lengths



Bond angles

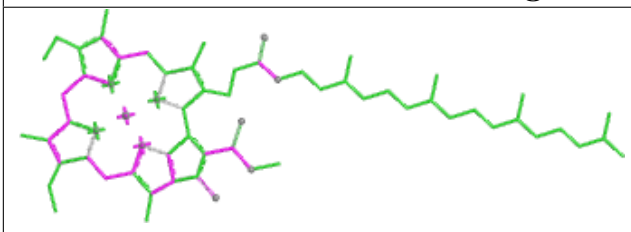


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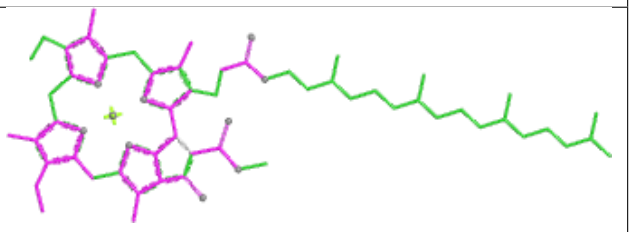


Rings

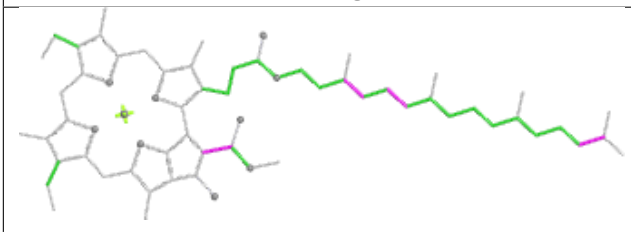
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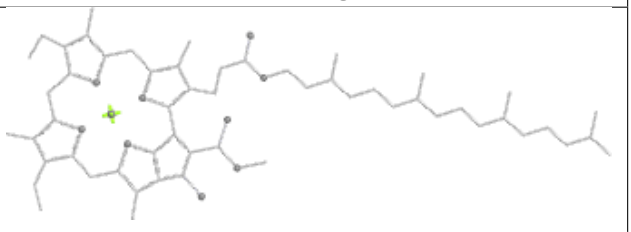
Bond lengths



Bond angles

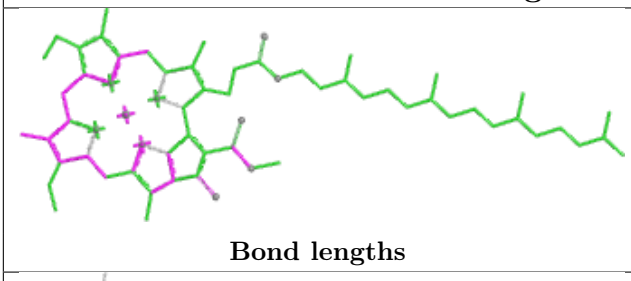


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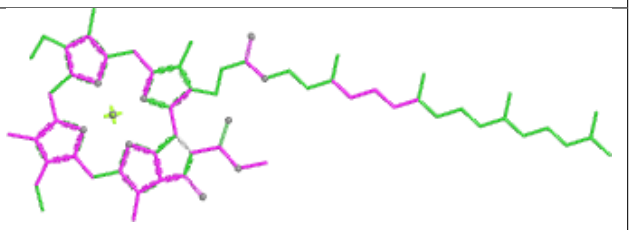


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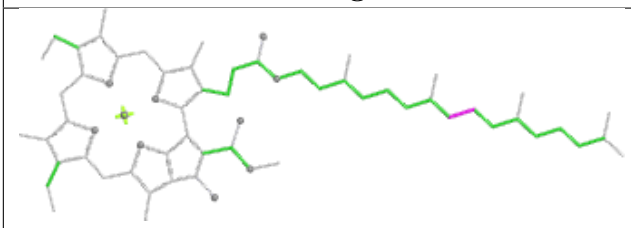
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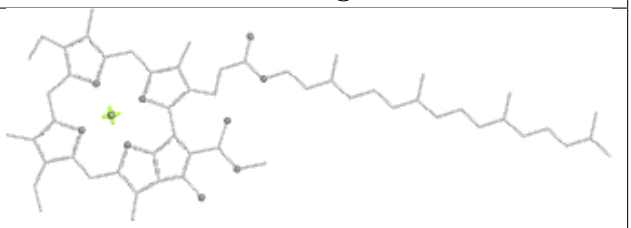
Bond lengths



Bond angles

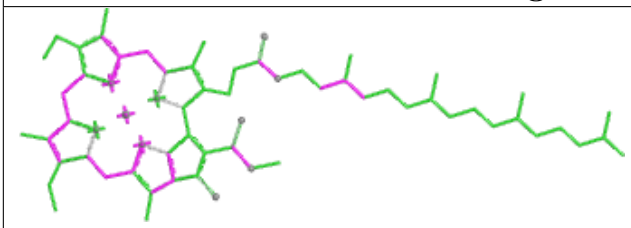


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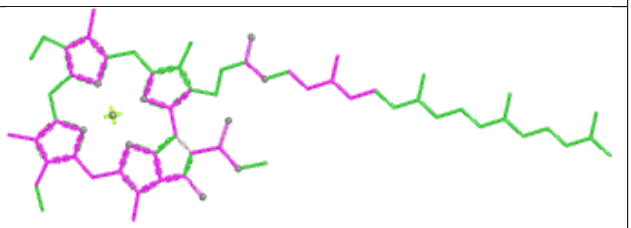


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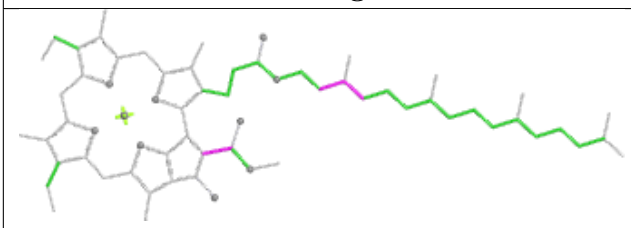
Ligand CLA b 606



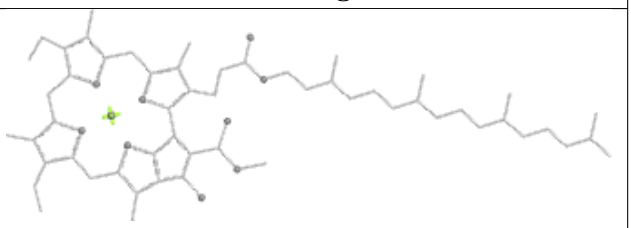
Bond lengths



Bond angles

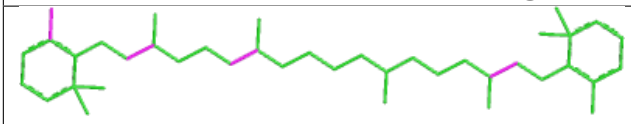


Torsions

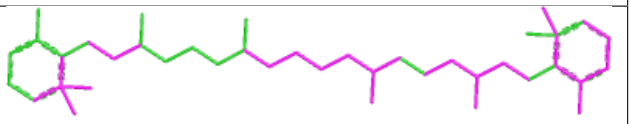


Rings

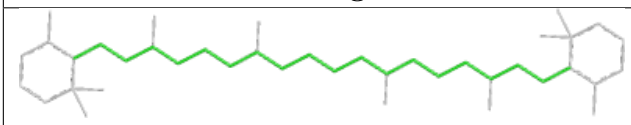
Ligand BCR H 102



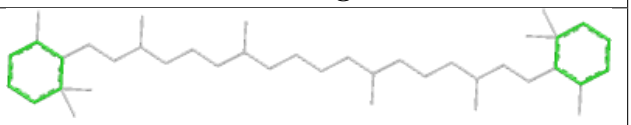
Bond lengths



Bond angles

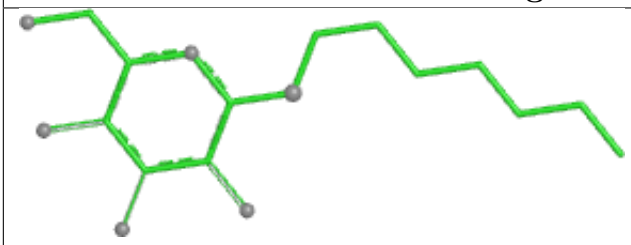


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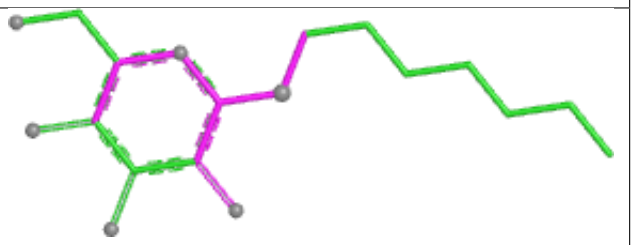


Rings

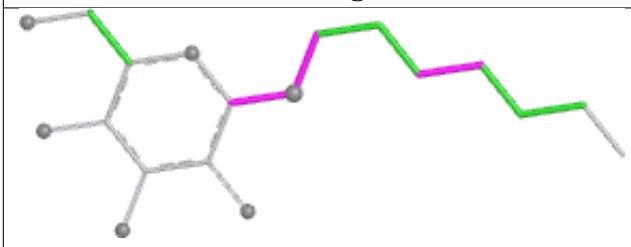
Ligand HTG c 522



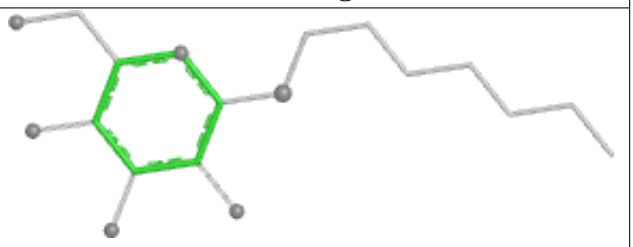
Bond lengths



Bond angles

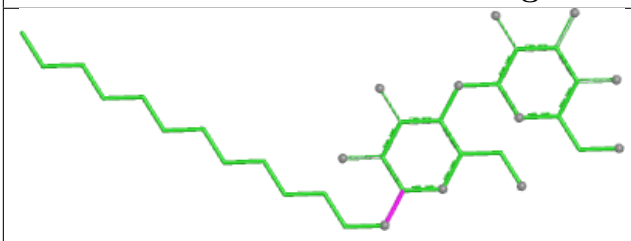


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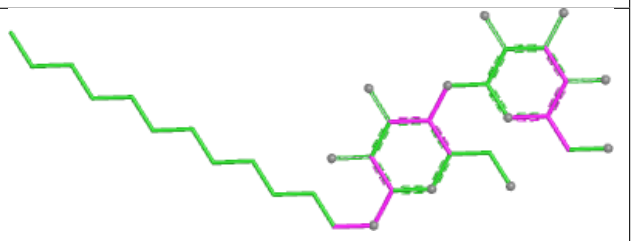


Rings

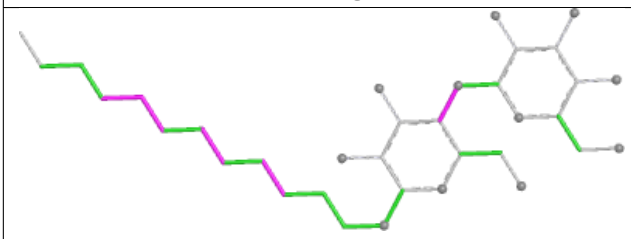
Ligand LMT B 622



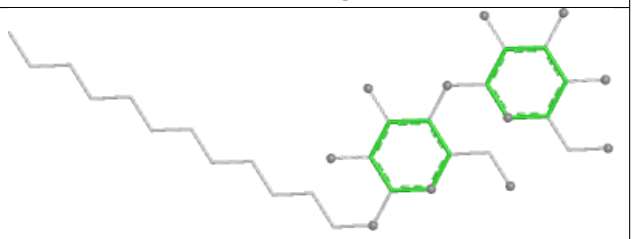
Bond lengths



Bond angles

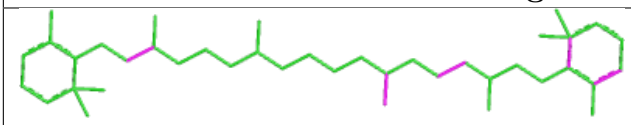


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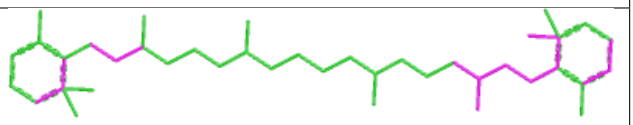


Rings

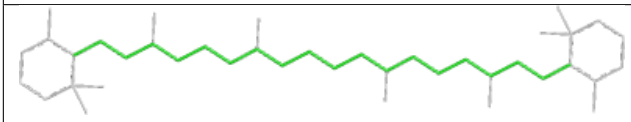
Ligand BCR a 411



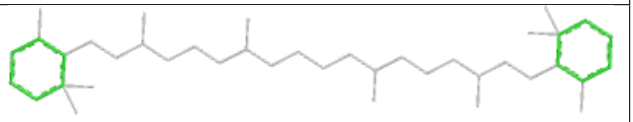
Bond lengths



Bond angles

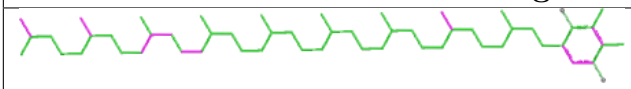


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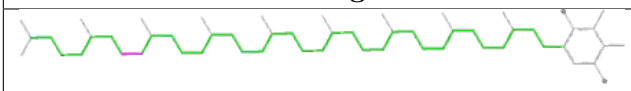


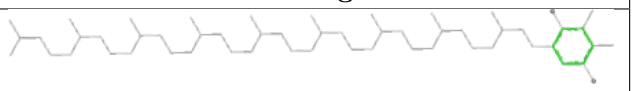
Rings

Ligand PL9 d 407

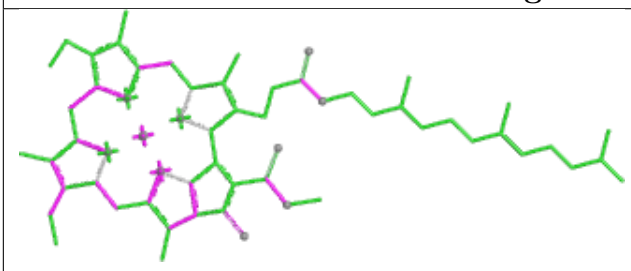

Bond lengths

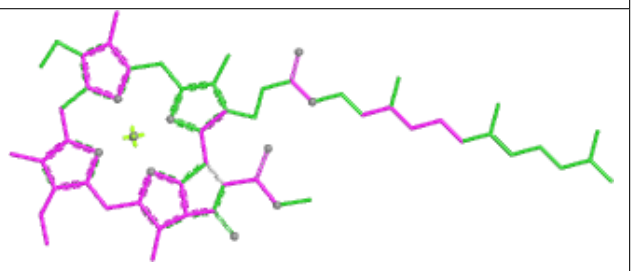

Bond angles

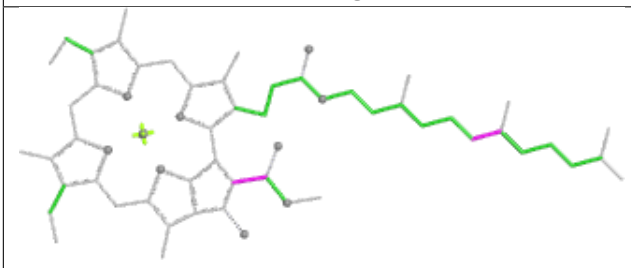

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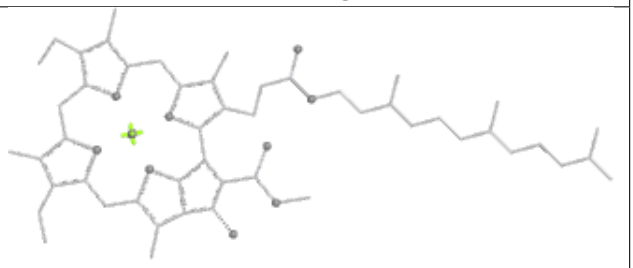

Rings

Ligand CLA C 504

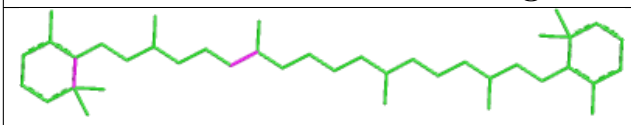

Bond lengths

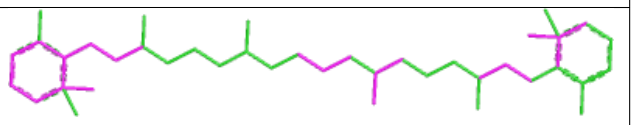

Bond angles


Torsions

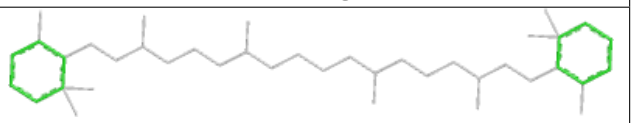

Rings

Ligand BCR C 515

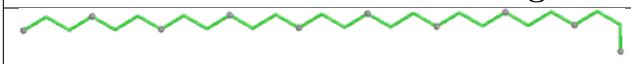

Bond lengths


Bond angles


Torsions


Rings

Ligand 2PE V 216

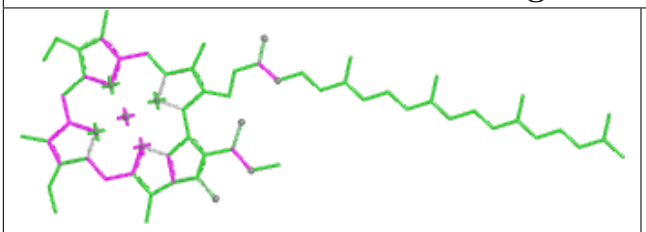

Bond lengths


Bond angles

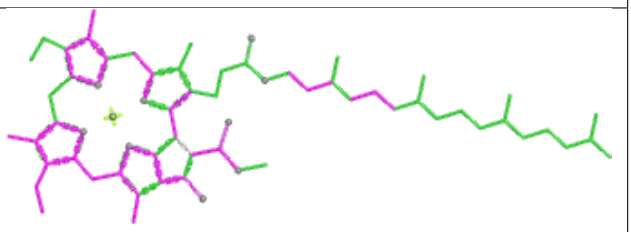

Torsions


Rings

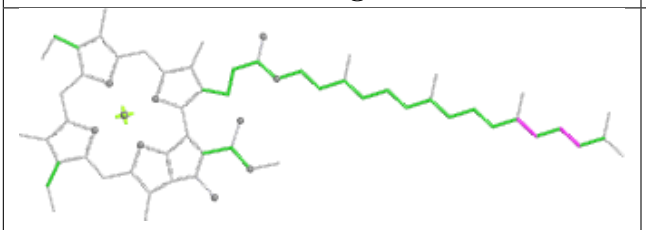
Ligand CLA b 612



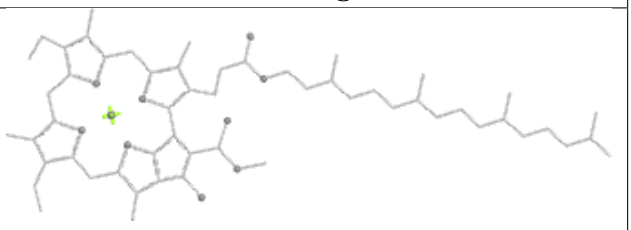
Bond lengths



Bond angles

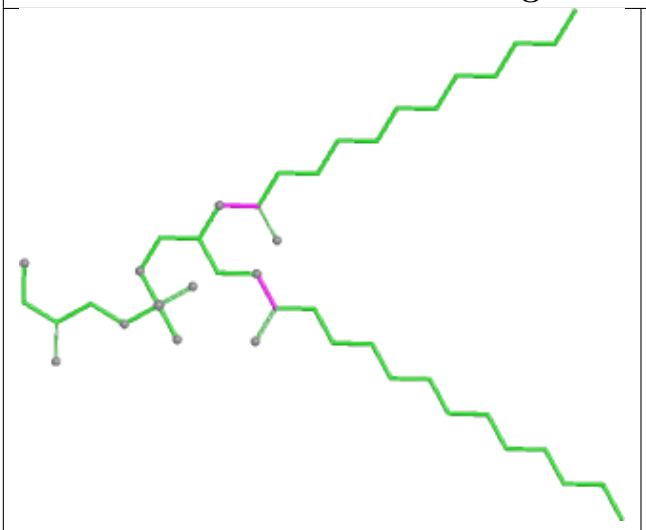


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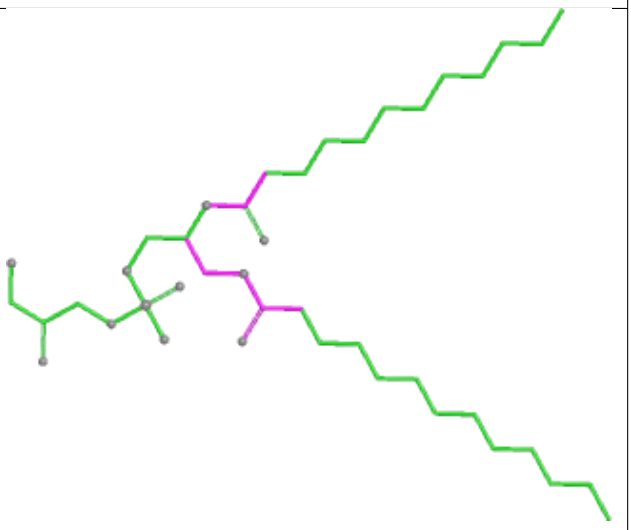


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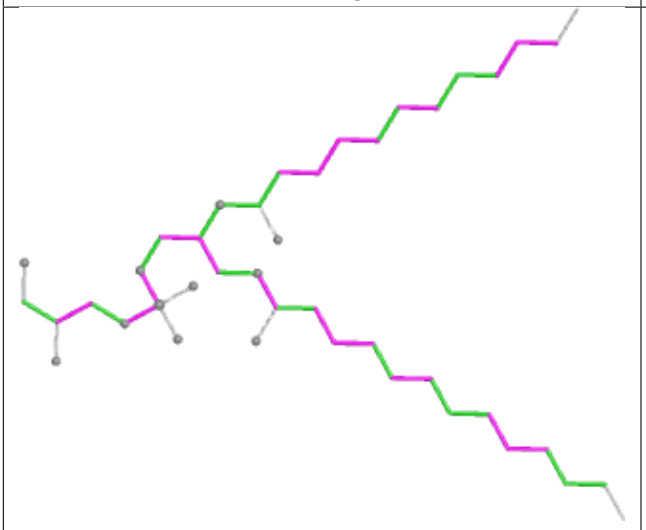
Ligand LHG A 618



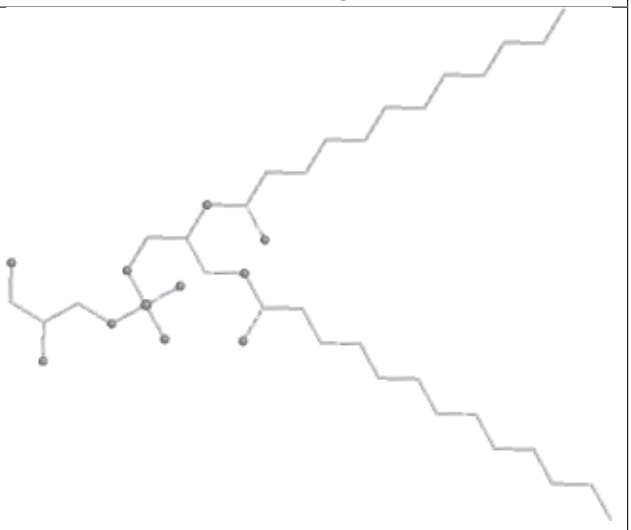
Bond lengths



Bond angles



Torsions

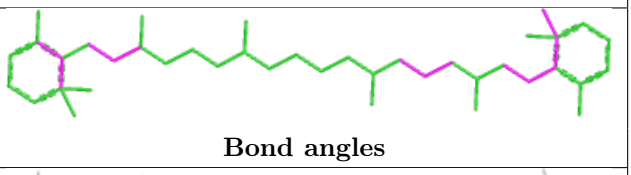


Rings

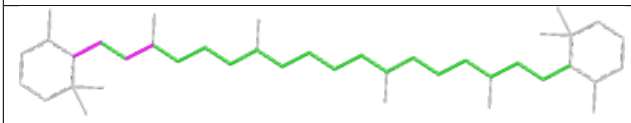
Ligand BCR b 620



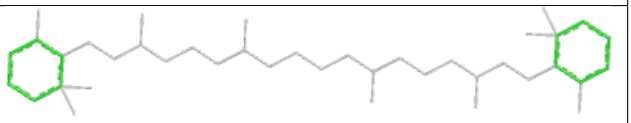
Bond lengths



Bond angles



Torsions



Rings

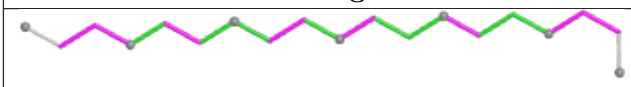
Ligand P6G C 541



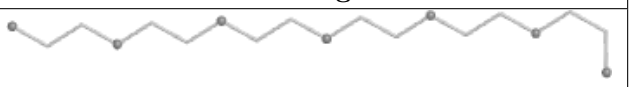
Bond lengths



Bond angles

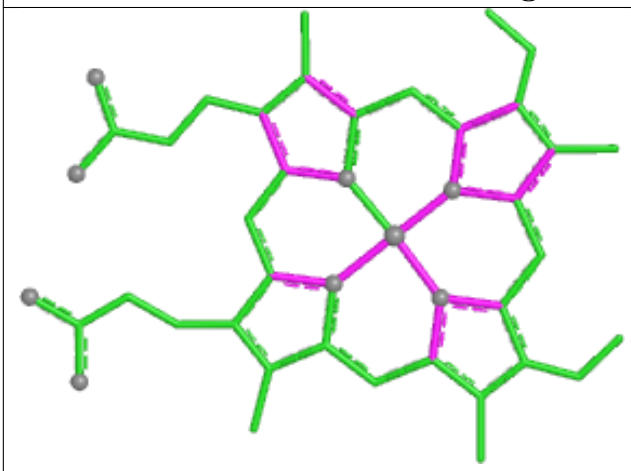


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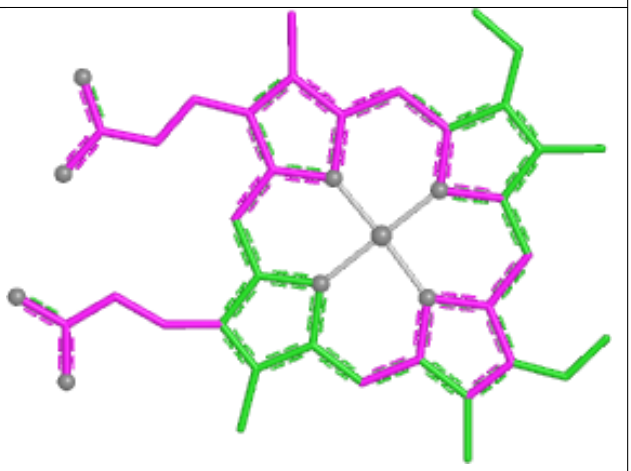


Rings

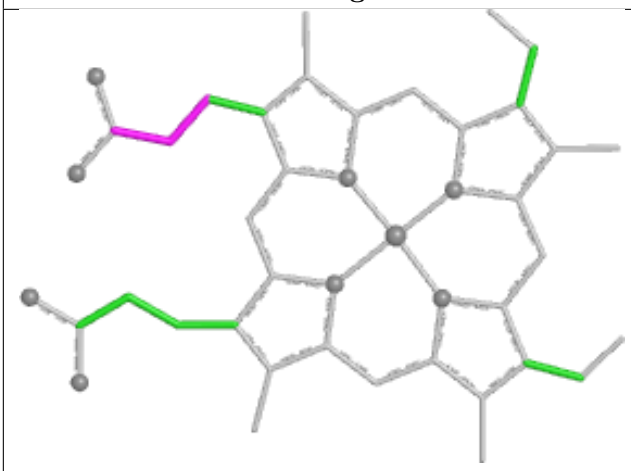
Ligand HEM E 113



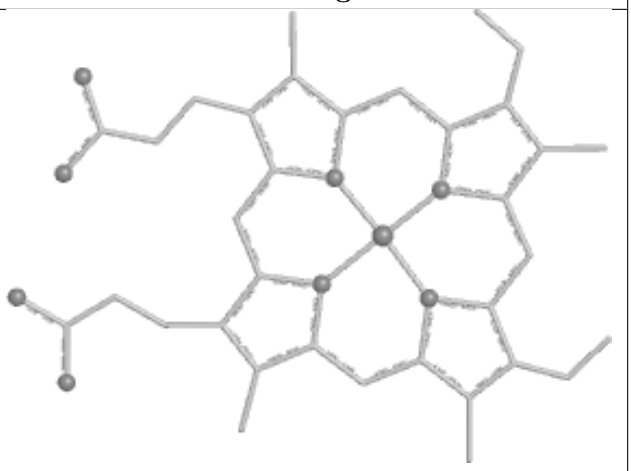
Bond lengths



Bond angles

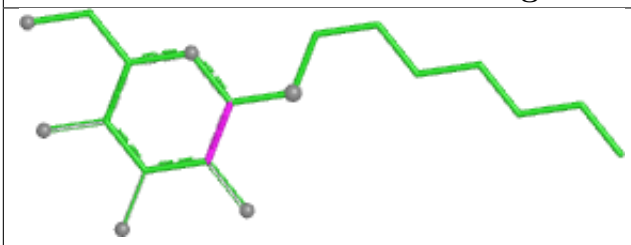


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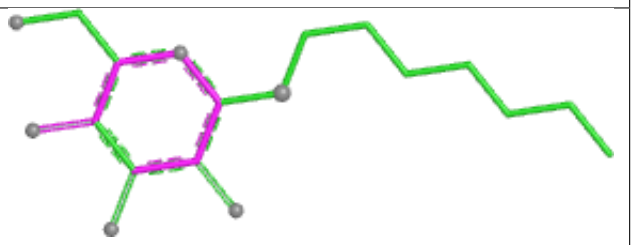


Rings

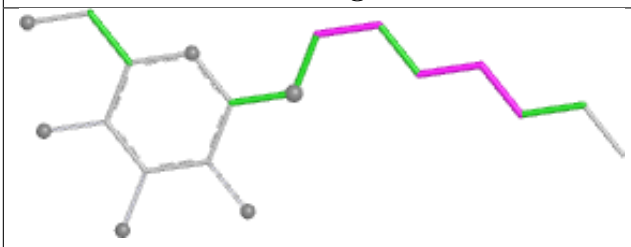
Ligand HTG B 623



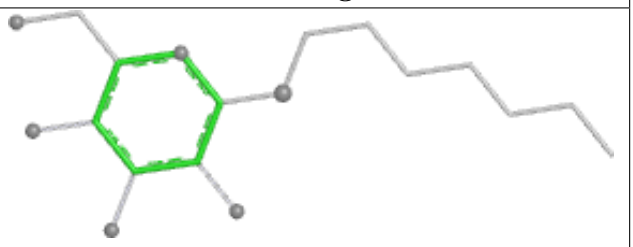
Bond lengths



Bond angles

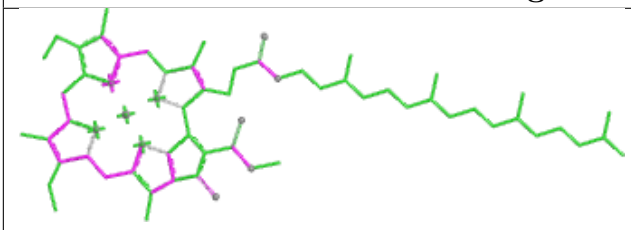


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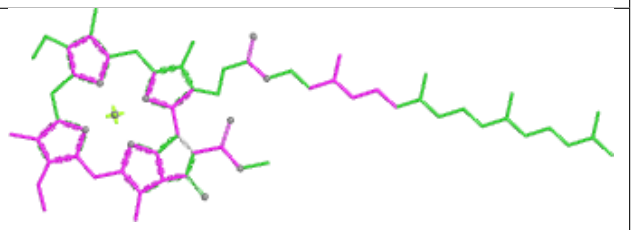


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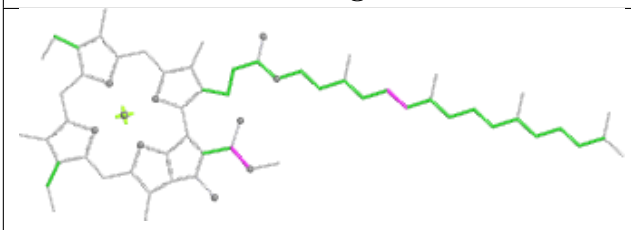
Ligand CLA b 604



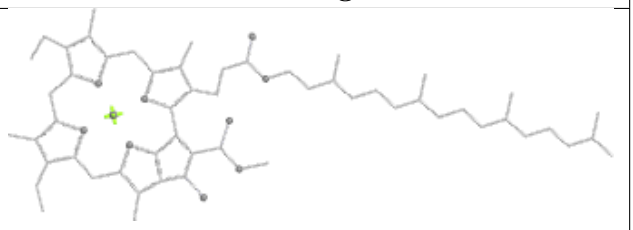
Bond lengths



Bond angles

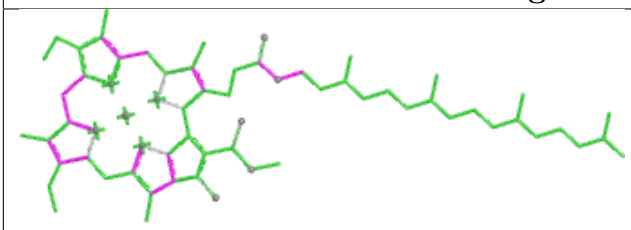


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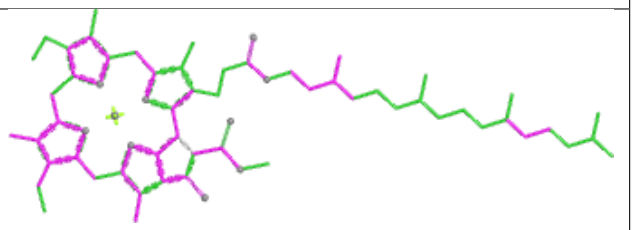


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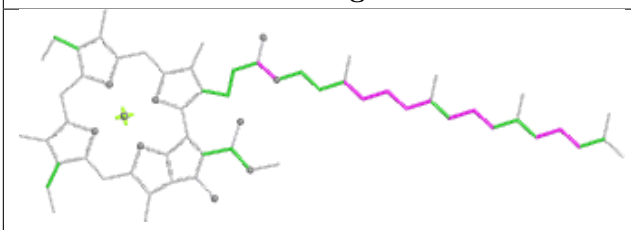
Ligand CLA a 410



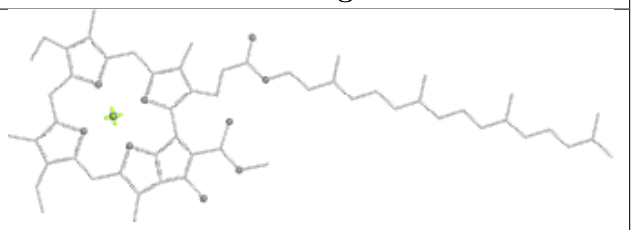
Bond lengths



Bond angles



Torsions

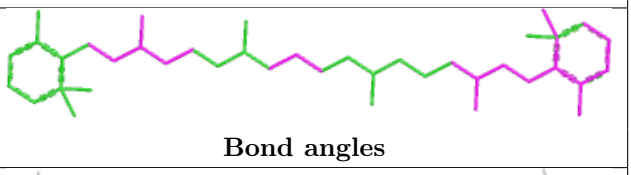


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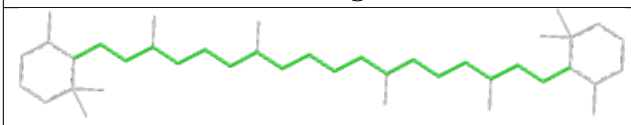
Ligand BCR b 619



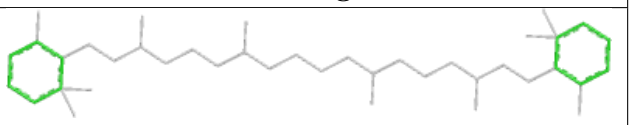
Bond lengths



Bond angles

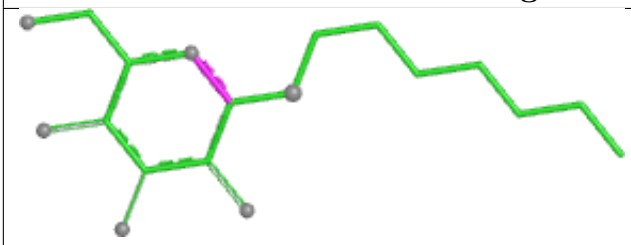


Torsions

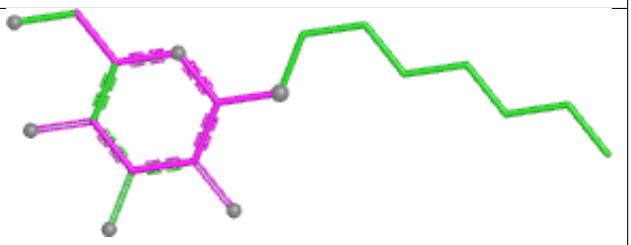


Rings

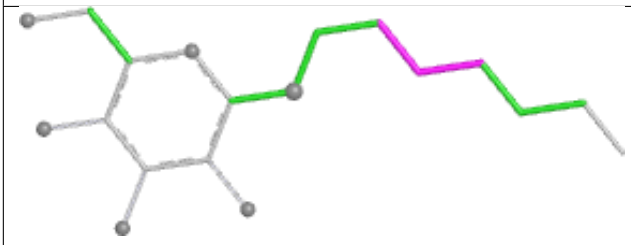
Ligand HTG V 204



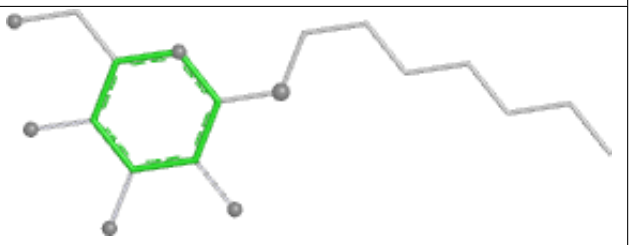
Bond lengths



Bond angles

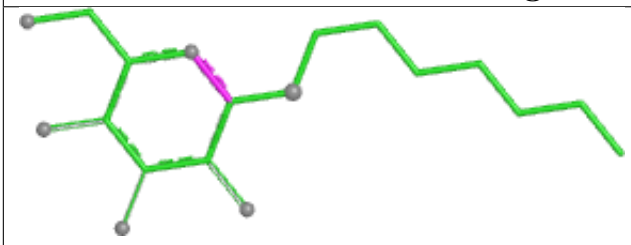


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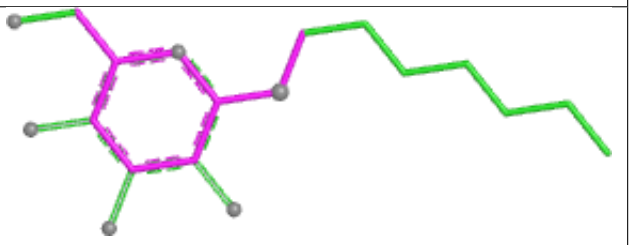


Rings

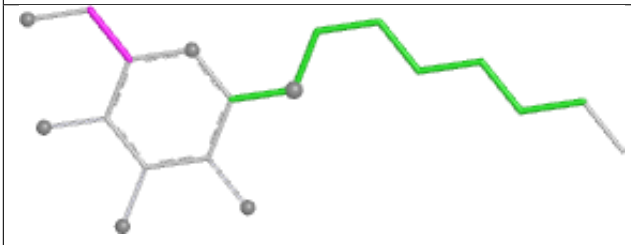
Ligand HTG b 632



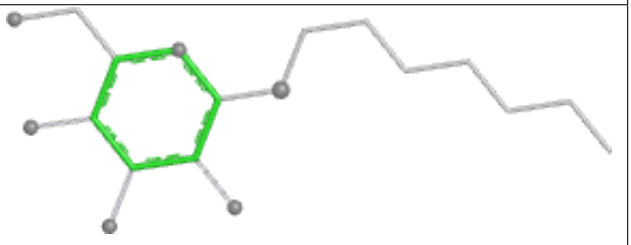
Bond lengths



Bond angles

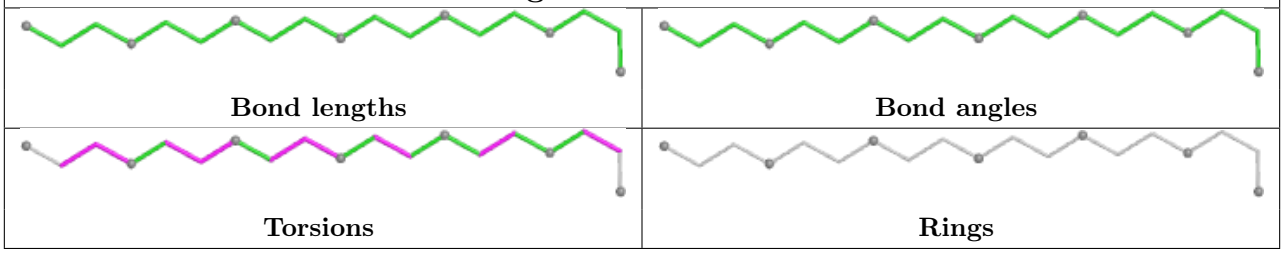


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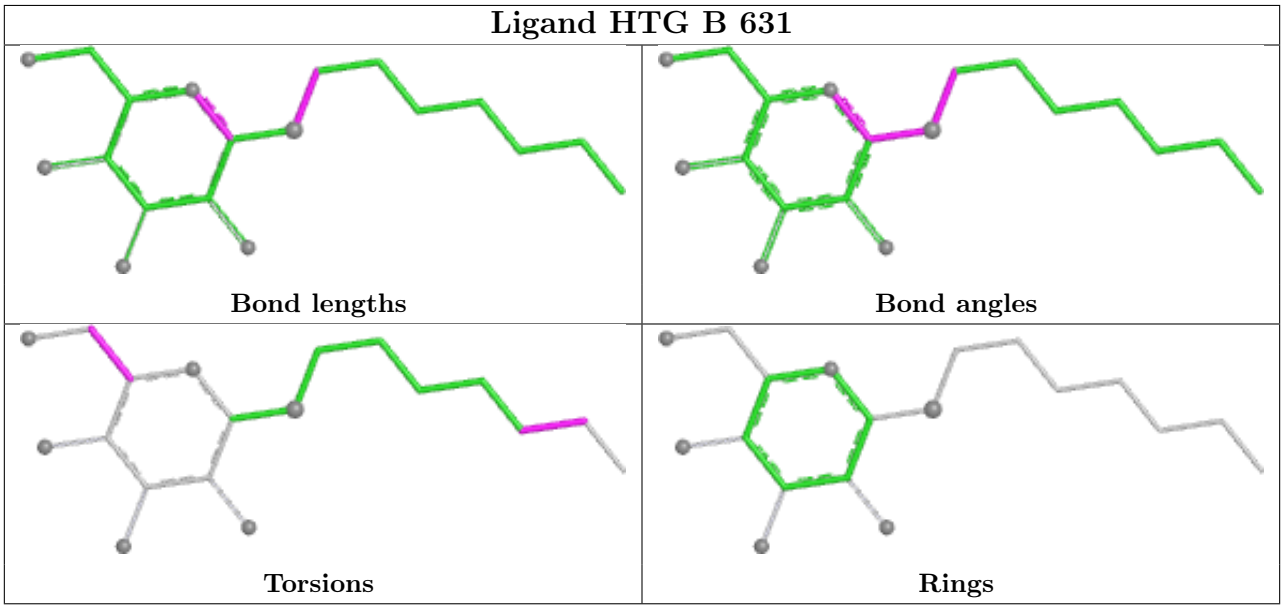


Rings

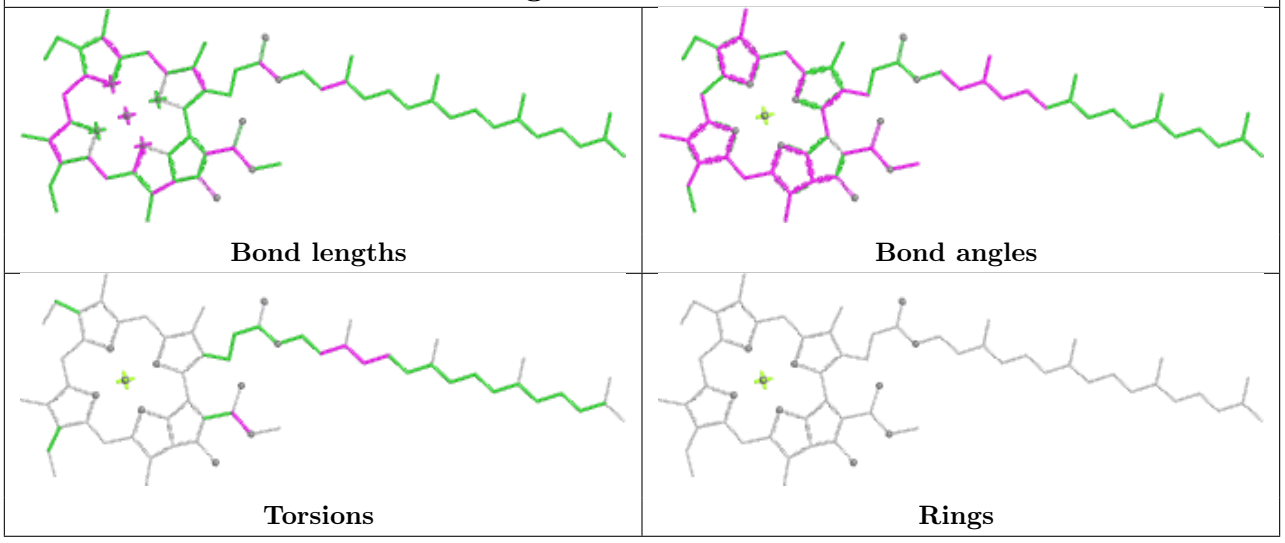
Ligand P6G A 623



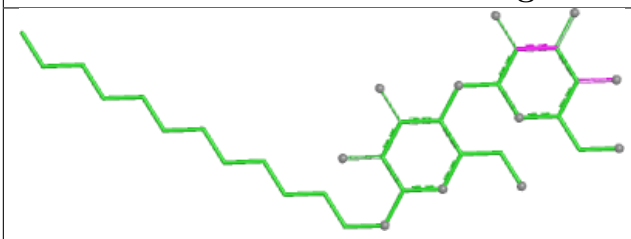
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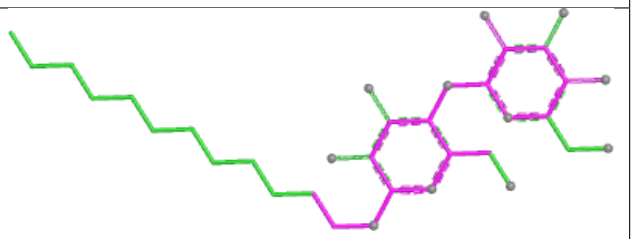
Ligand CLA B 605



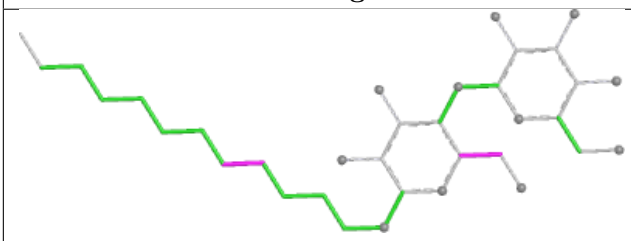
Ligand LMT M 101



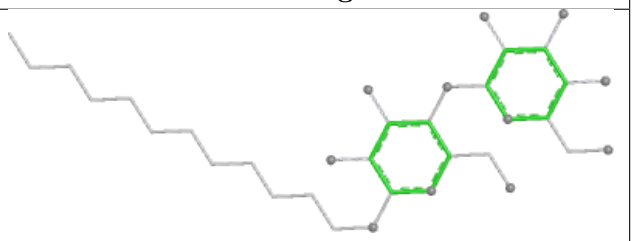
Bond lengths



Bond angles

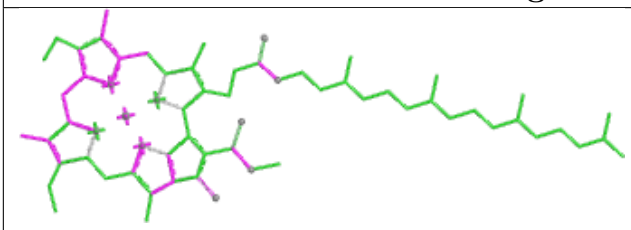


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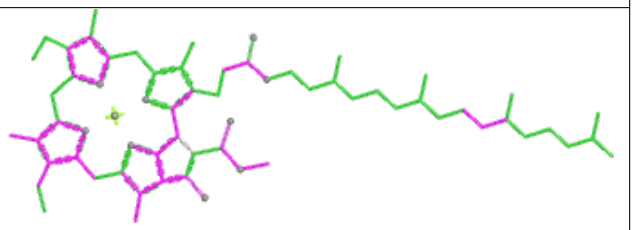


Rings

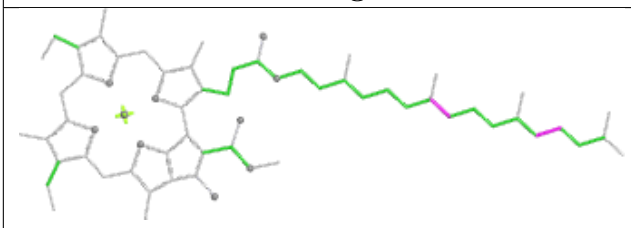
Ligand CLA b 613



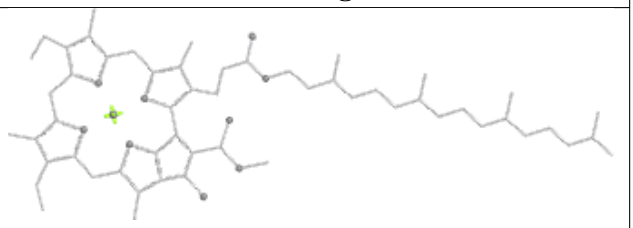
Bond lengths



Bond angles

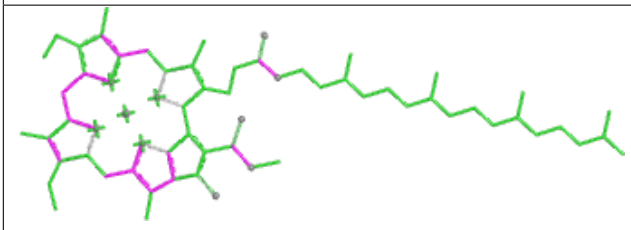


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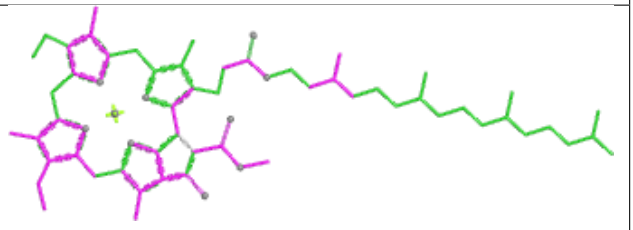


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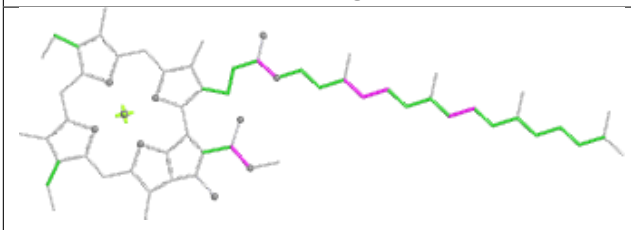
Ligand CLA C 513



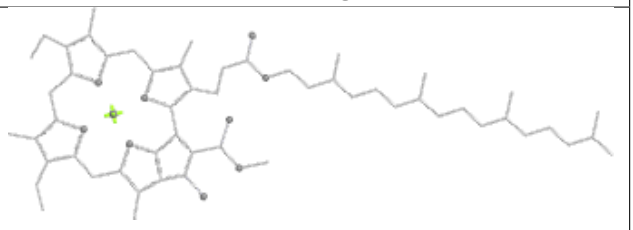
Bond lengths



Bond angles

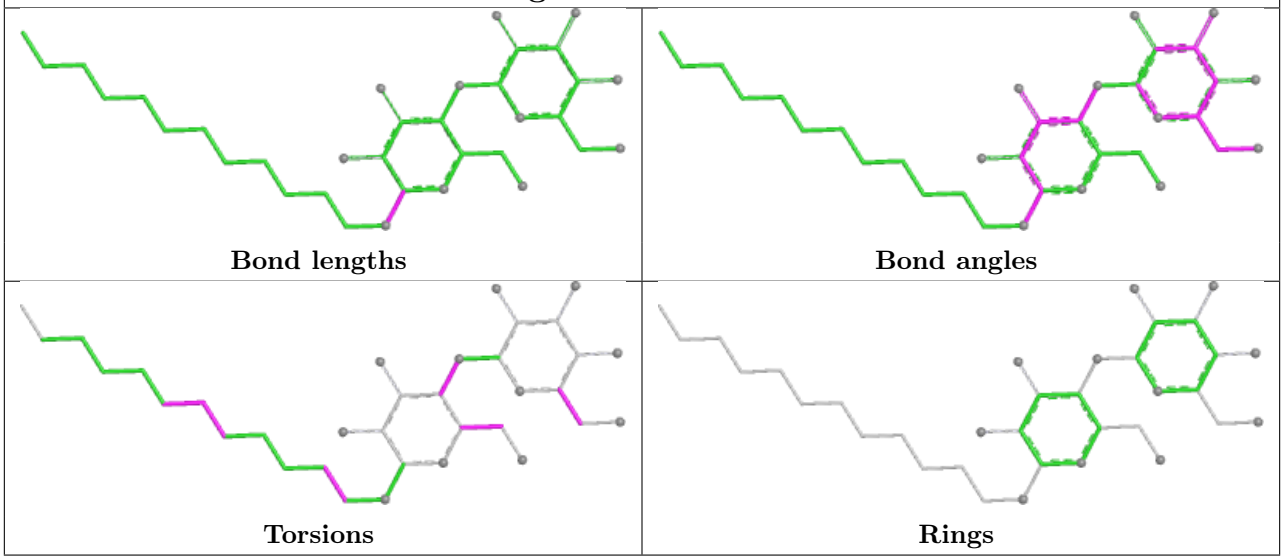


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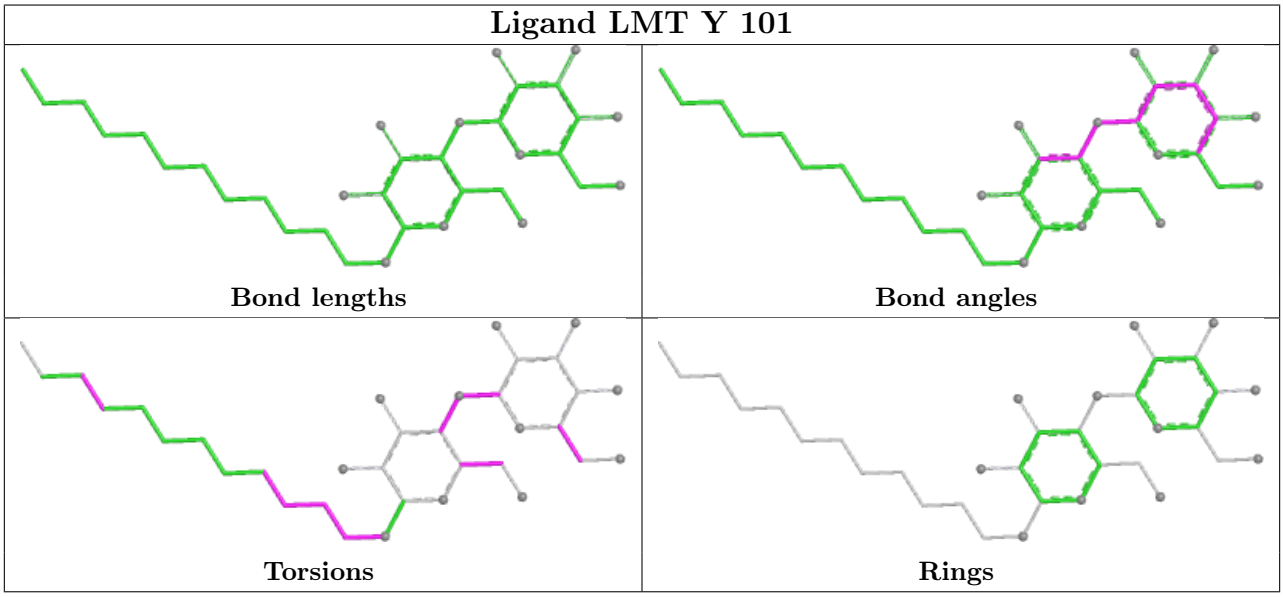


Rings

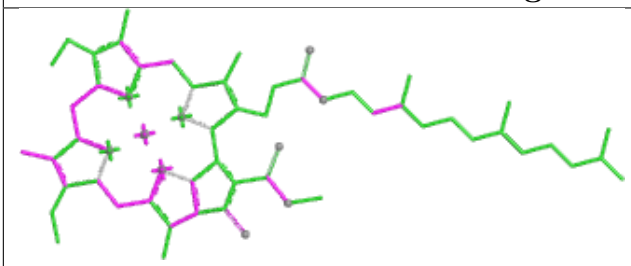
Ligand LMT I 101



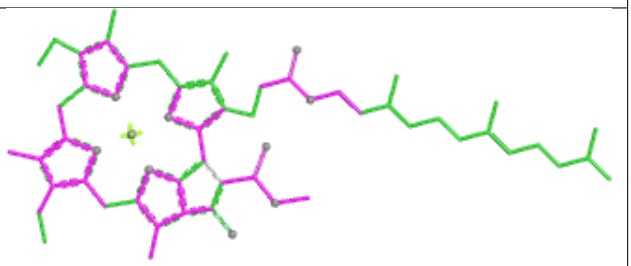
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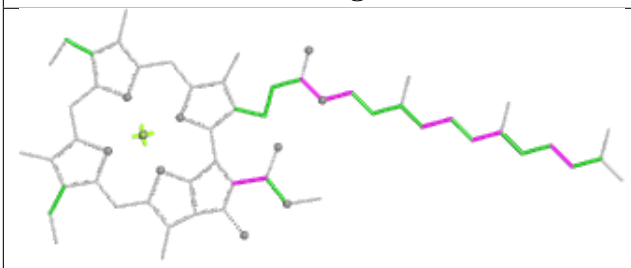
Ligand CLA B 617



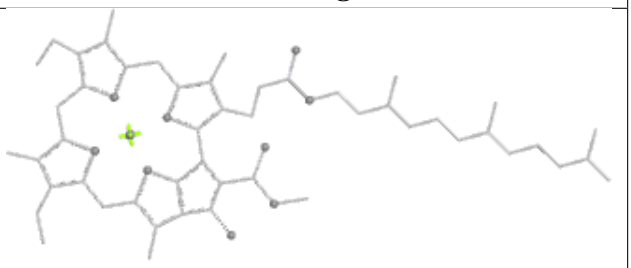
Bond lengths



Bond angles

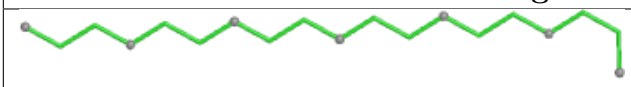


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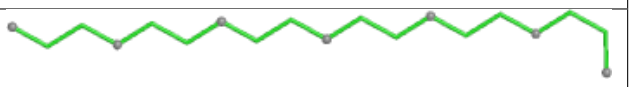


Rings

Ligand P6G c 541



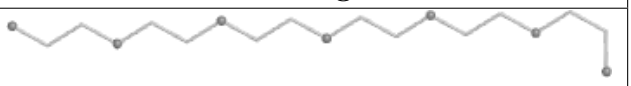
Bond lengths



Bond angles

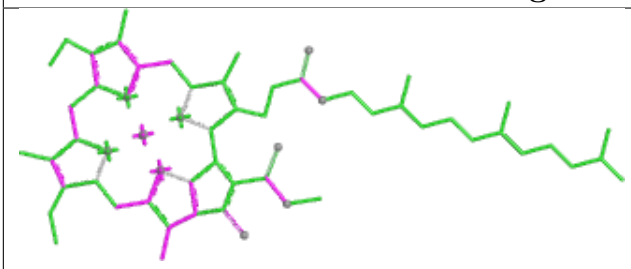


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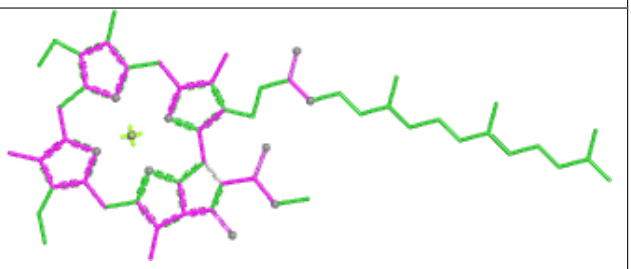


Rings

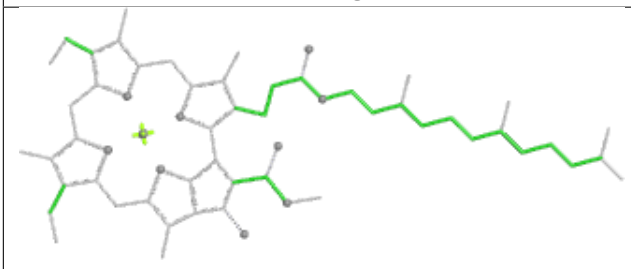
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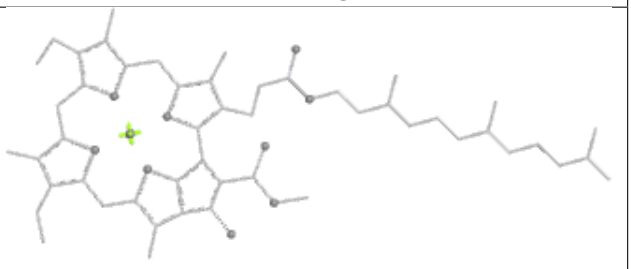
Bond lengths



Bond angles

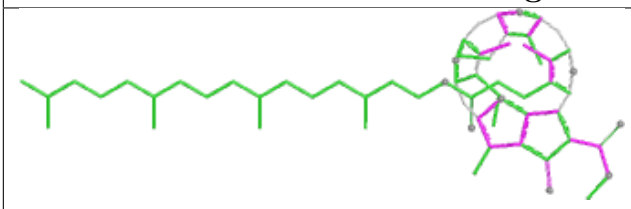


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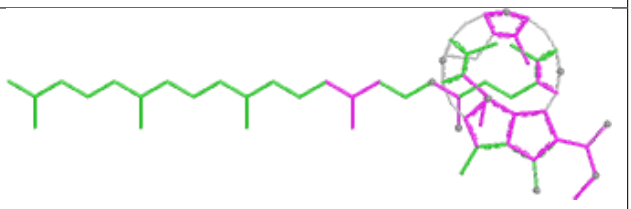


Rings

Ligand PHO d 401



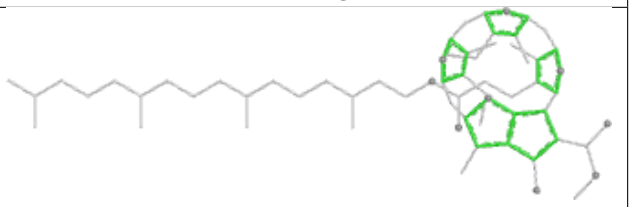
Bond lengths



Bond angles

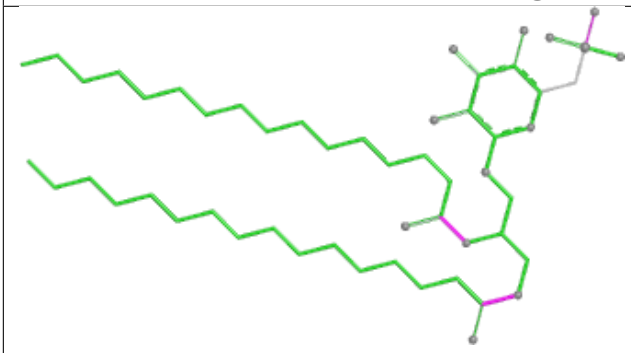


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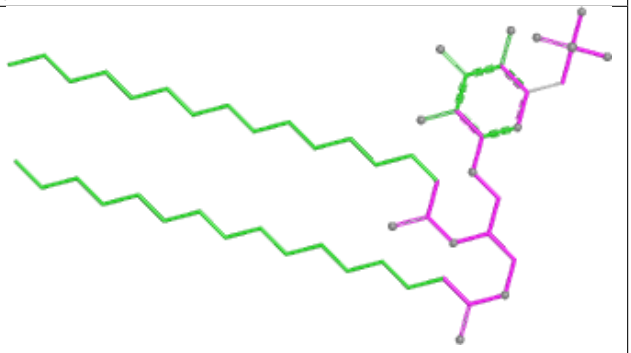


Rings

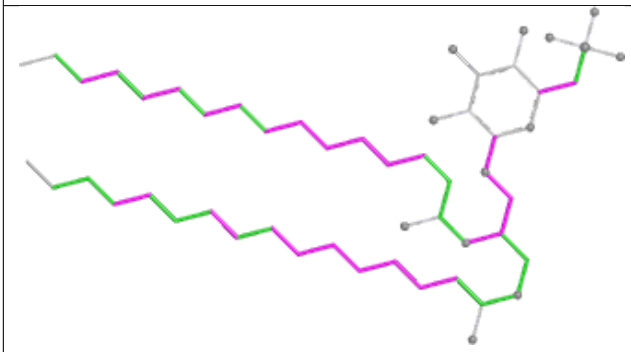
Ligand SQD a 424



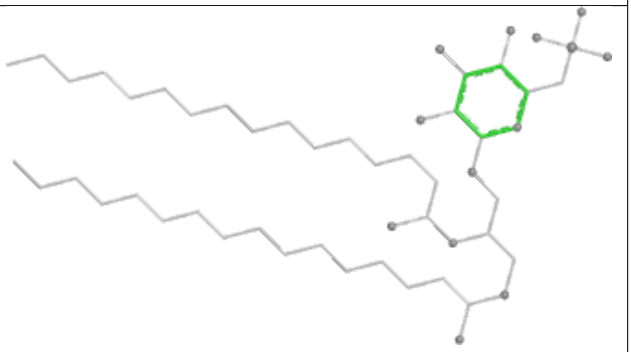
Bond lengths



Bond angles

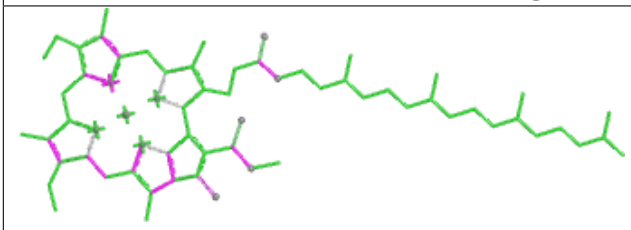


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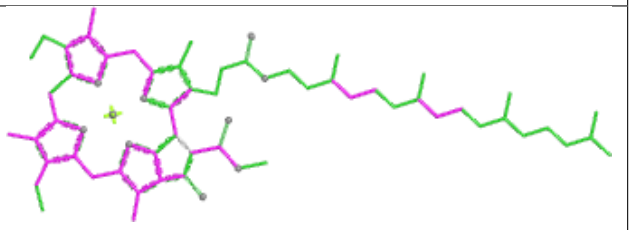


Rings

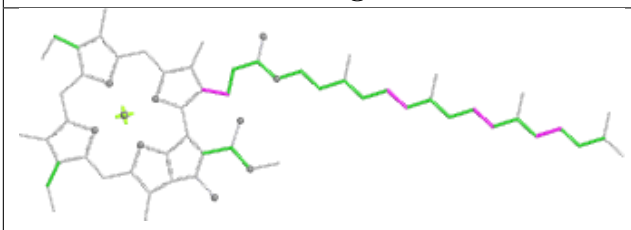
Ligand CLA b 616



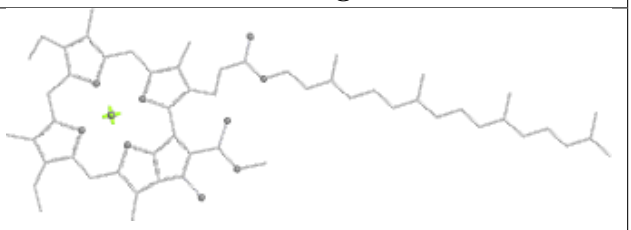
Bond lengths



Bond angles



Torsions



Rings

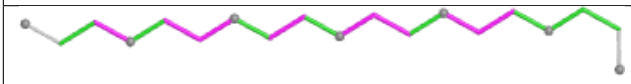
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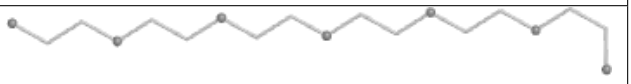
Bond lengths



Bond angles

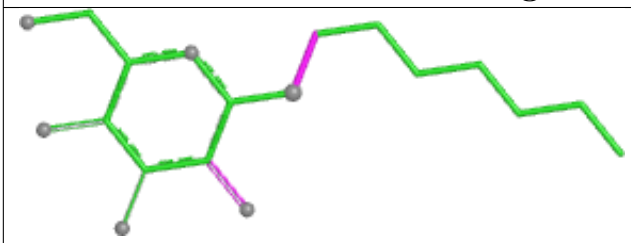


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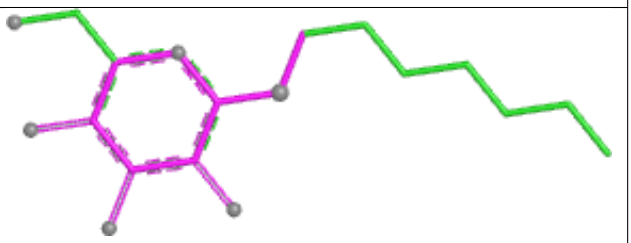


Rings

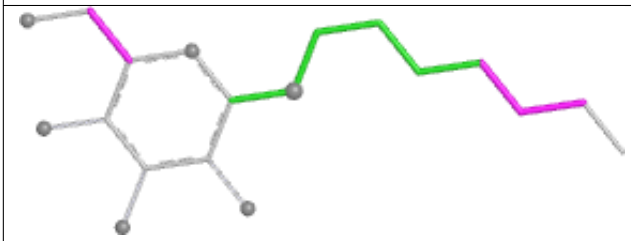
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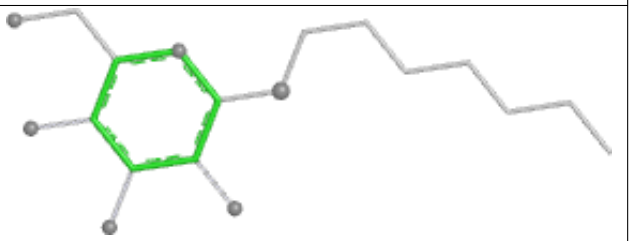
Bond lengths



Bond angles

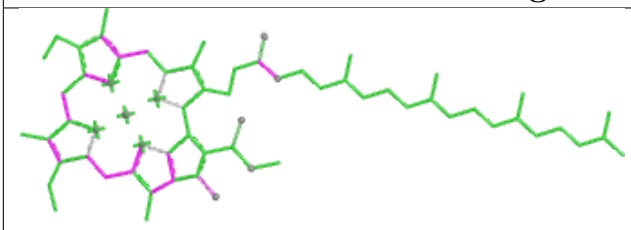


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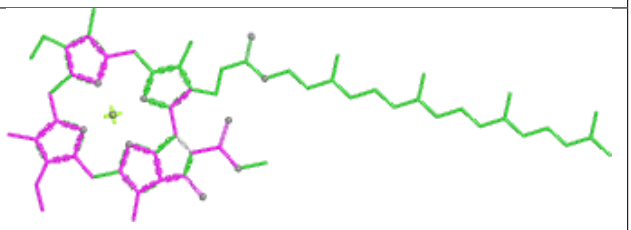


Rings

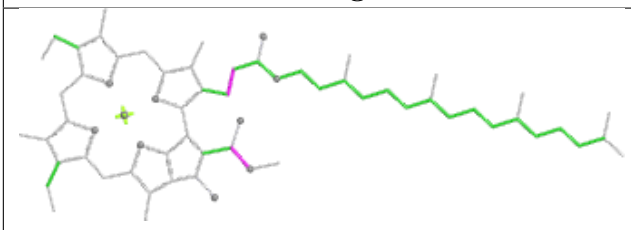
Ligand CLA c 501



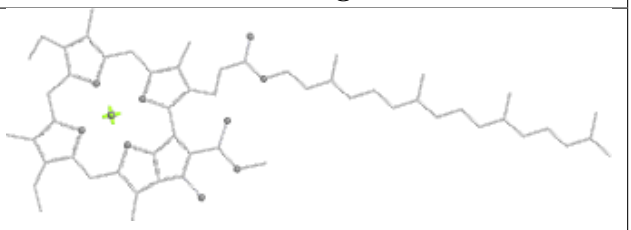
Bond lengths



Bond angles

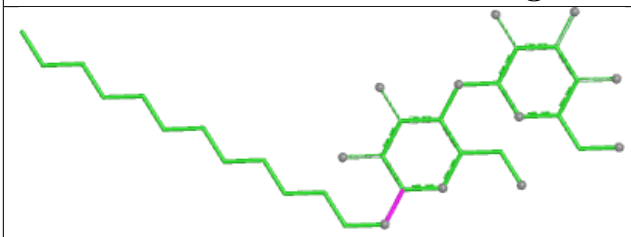


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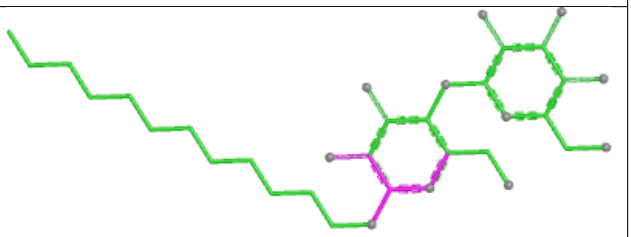


Rings

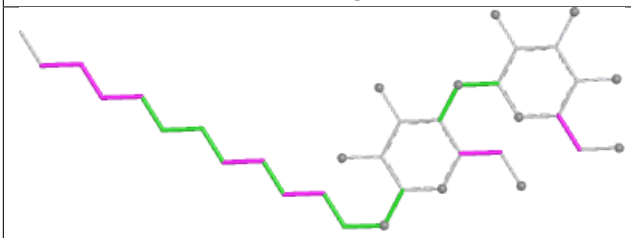
Ligand LMT a 401



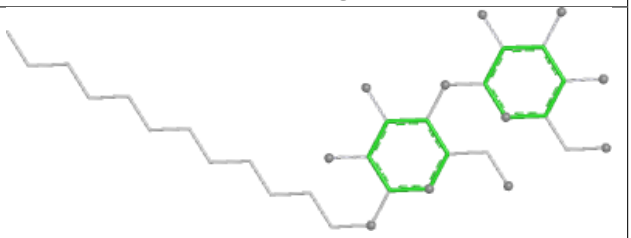
Bond lengths



Bond angles

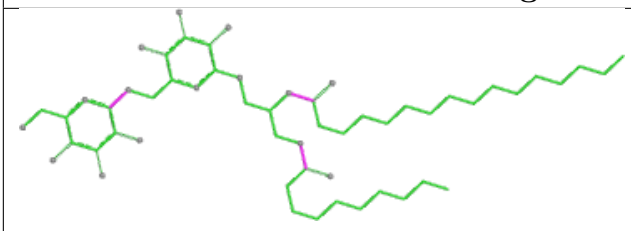


Torsions

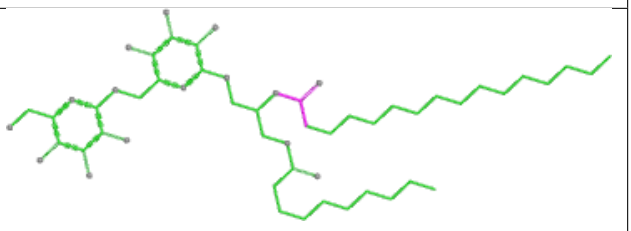


Rings

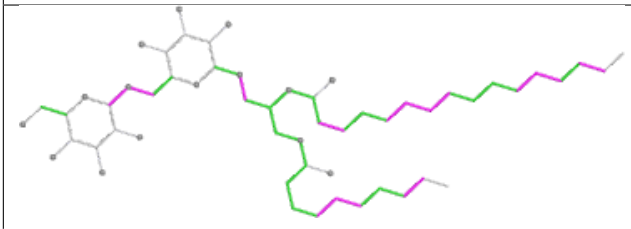
Ligand DGD C 517



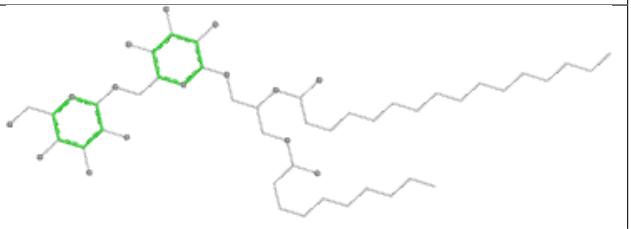
Bond lengths



Bond angles

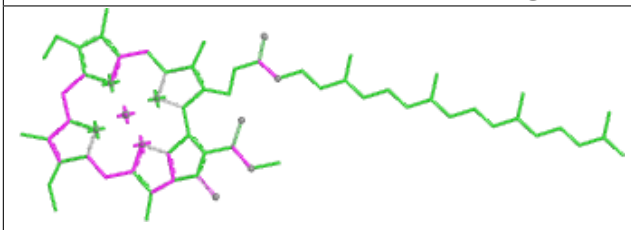


Torsions

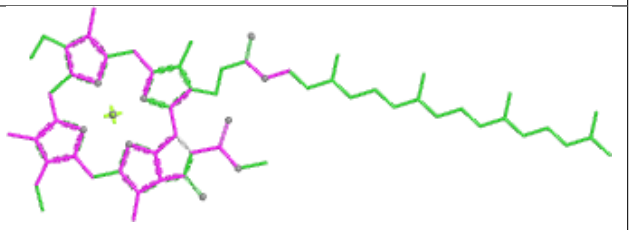


Rings

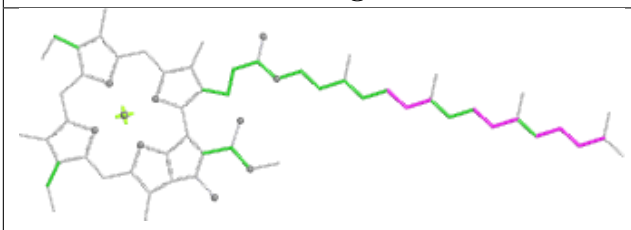
Ligand CLA C 506



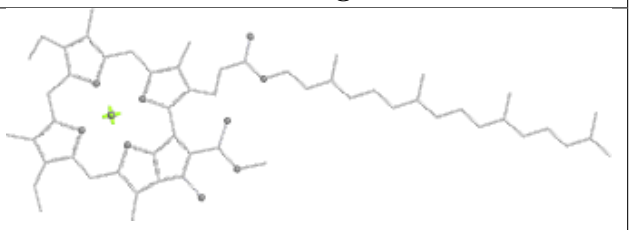
Bond lengths



Bond angles

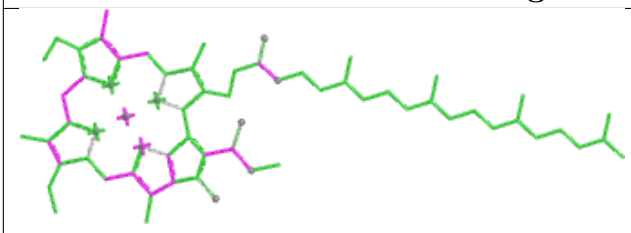


Torsions

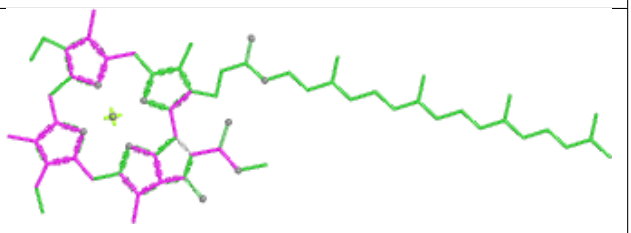


Rings

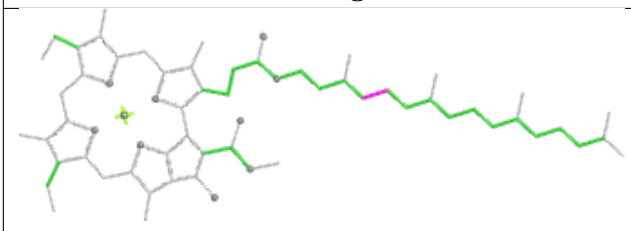
Ligand CLA b 608



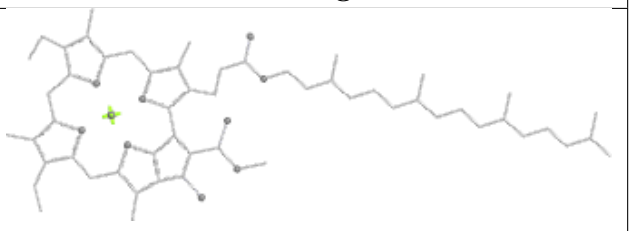
Bond lengths



Bond angles

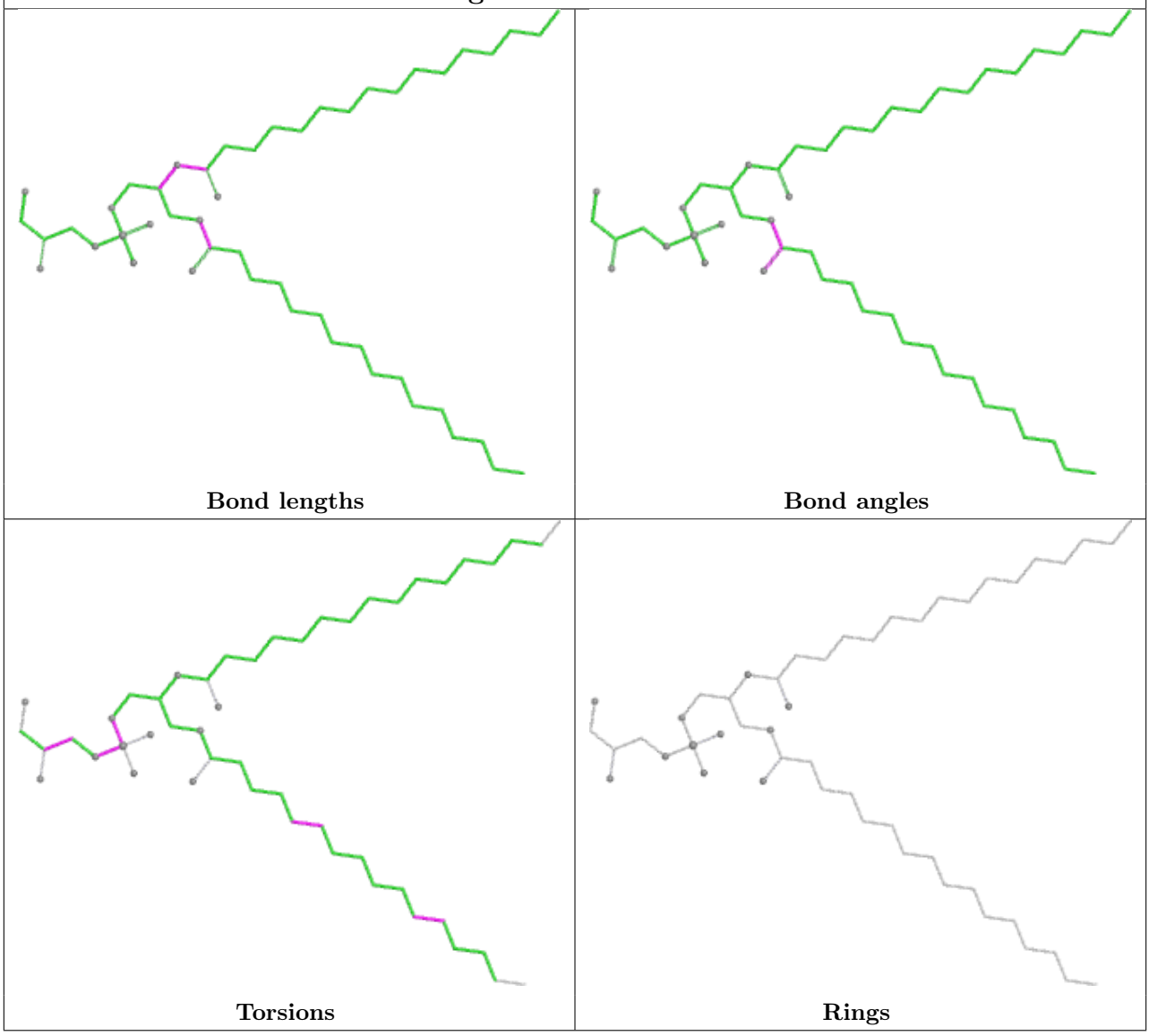


Torsions

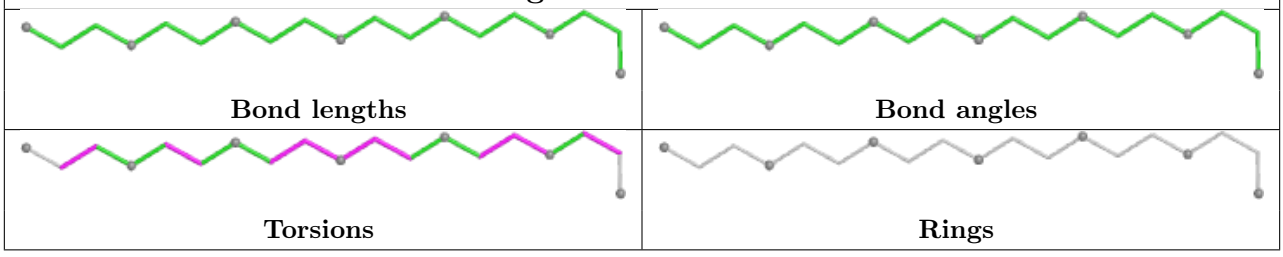


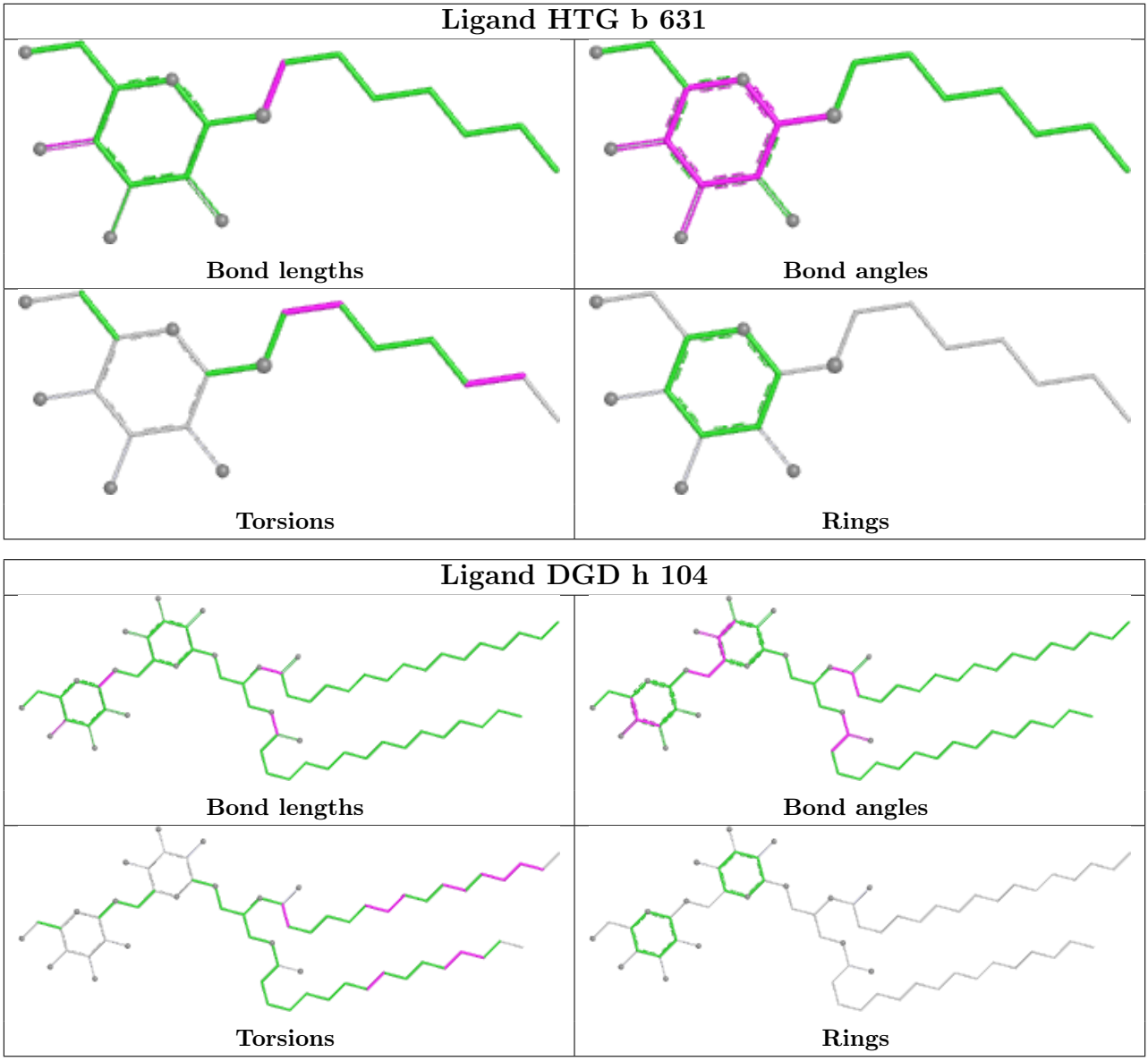
Rings

Ligand LHG D 410



Ligand P6G A 624





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	334/344 (97%)	-0.89	0 100 100	15, 22, 46, 78	4 (1%)
1	a	334/344 (97%)	-0.86	0 100 100	16, 24, 52, 89	4 (1%)
2	B	504/506 (99%)	-0.83	1 (0%) 91 92	14, 26, 57, 92	11 (2%)
2	b	506/506 (100%)	-0.75	2 (0%) 88 90	14, 29, 71, 129	10 (1%)
3	C	451/458 (98%)	-0.82	0 100 100	19, 31, 46, 87	5 (1%)
3	c	458/458 (100%)	-0.76	2 (0%) 88 90	20, 35, 50, 108	4 (0%)
4	D	341/342 (99%)	-0.96	0 100 100	16, 23, 40, 114	1 (0%)
4	d	341/342 (99%)	-0.90	0 100 100	17, 26, 44, 110	2 (0%)
5	E	81/83 (97%)	-0.57	0 100 100	19, 40, 66, 92	3 (3%)
5	e	81/83 (97%)	-0.45	0 100 100	22, 45, 75, 118	2 (2%)
6	F	34/44 (77%)	-0.68	0 100 100	26, 33, 63, 82	0
6	f	32/44 (72%)	-0.54	0 100 100	30, 38, 78, 117	0
7	H	65/65 (100%)	-0.72	1 (1%) 72 75	19, 33, 47, 123	2 (3%)
7	h	65/65 (100%)	-0.55	2 (3%) 51 55	26, 38, 56, 116	1 (1%)
8	I	37/38 (97%)	-0.72	0 100 100	28, 35, 75, 91	0
8	i	37/38 (97%)	-0.70	0 100 100	27, 34, 67, 89	0
9	J	39/40 (97%)	-0.42	0 100 100	20, 36, 108, 130	2 (5%)
9	j	39/40 (97%)	-0.43	0 100 100	29, 43, 75, 89	0
10	K	37/37 (100%)	-0.63	0 100 100	31, 37, 56, 70	0
10	k	37/37 (100%)	-0.59	0 100 100	36, 44, 64, 75	0
11	L	37/37 (100%)	-0.89	0 100 100	11, 21, 70, 92	1 (2%)
11	l	37/37 (100%)	-0.81	0 100 100	13, 22, 70, 95	2 (5%)
12	M	33/36 (91%)	-0.86	0 100 100	11, 22, 44, 88	2 (6%)
12	m	34/36 (94%)	-0.79	0 100 100	12, 24, 75, 98	1 (2%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	O	245/245 (100%)	-0.70	1 (0%) 88 90	18, 32, 69, 128	6 (2%)
13	o	245/245 (100%)	-0.68	1 (0%) 88 90	18, 34, 84, 136	5 (2%)
14	T	29/32 (90%)	-0.93	0 100 100	18, 22, 47, 101	1 (3%)
14	t	29/32 (90%)	-0.77	0 100 100	19, 22, 44, 81	1 (3%)
15	U	97/104 (93%)	-0.82	0 100 100	21, 31, 58, 95	2 (2%)
15	u	97/104 (93%)	-0.85	0 100 100	24, 31, 47, 84	0
16	V	137/137 (100%)	-0.85	0 100 100	16, 29, 46, 66	2 (1%)
16	v	137/137 (100%)	-0.74	0 100 100	20, 38, 58, 73	1 (0%)
17	Y	29/30 (96%)	-0.02	1 (3%) 48 51	36, 47, 76, 109	1 (3%)
17	y	29/30 (96%)	-0.10	0 100 100	40, 56, 81, 92	1 (3%)
18	X	40/41 (97%)	-0.39	0 100 100	23, 40, 100, 118	1 (2%)
18	x	40/41 (97%)	-0.24	0 100 100	36, 43, 112, 132	0
19	Z	62/62 (100%)	-0.38	0 100 100	37, 47, 86, 94	0
19	z	62/62 (100%)	0.14	2 (3%) 50 54	50, 62, 101, 117	0
All	All	5272/5362 (98%)	-0.76	13 (0%) 91 92	11, 30, 65, 136	78 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
19	z	62	VAL	3.5
7	h	65	LEU	3.2
7	h	66	GLY	2.9
3	c	17	ALA	2.4
19	z	3	ILE	2.4
13	o	3	ALA	2.3
2	b	486	LEU	2.3
3	c	18	ALA	2.2
2	b	499	VAL	2.1
13	O	56	PRO	2.1
7	H	65	LEU	2.1
2	B	494	GLY	2.0
17	Y	18	VAL	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MHS	D	336	11/12	0.97	0.05	23,28,37,38	0
8	FME	I	1	10/11	0.98	0.06	26,32,40,44	0
12	FME	M	1	10/11	0.98	0.05	27,32,64,68	0
14	FME	T	1[A]	10/11	0.98	0.05	21,25,47,47	7
14	FME	T	1[B]	10/11	0.98	0.05	21,25,32,35	7
12	FME	m	1[A]	10/11	0.98	0.07	24,30,61,84	7
12	FME	m	1[B]	10/11	0.98	0.07	30,33,55,66	7
14	FME	t	1[A]	10/11	0.98	0.04	20,24,39,42	7
14	FME	t	1[B]	10/11	0.98	0.04	20,24,31,36	7
4	MHS	d	336	11/12	0.99	0.05	27,32,44,44	0
8	FME	i	1	10/11	0.99	0.04	30,33,36,37	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
39	1PE	B	653	16/16	0.70	0.12	103,121,137,148	0
38	HTG	C	530	19/19	0.71	0.10	98,124,143,150	0
34	PGE	f	105	10/10	0.73	0.10	91,98,114,127	0
34	PGE	D	415	10/10	0.75	0.11	86,105,110,122	0
34	PGE	o	307	10/10	0.75	0.11	90,112,130,142	0
34	PGE	c	536	10/10	0.76	0.13	87,105,124,125	0
31	LMT	C	533	35/35	0.77	0.11	72,121,170,191	0
34	PGE	E	108	10/10	0.78	0.15	52,65,68,73	10
34	PGE	E	105	10/10	0.78	0.12	90,96,116,118	0
36	EDO	B	656	4/4	0.80	0.22	78,87,100,107	0
36	EDO	c	542	4/4	0.80	0.15	88,91,102,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	PGE	H	110	10/10	0.80	0.08	91,103,116,118	0
33	PG4	B	643	13/13	0.80	0.10	75,92,114,118	0
34	PGE	V	215	10/10	0.81	0.12	66,90,103,111	0
38	HTG	C	529	19/19	0.81	0.11	70,102,136,144	0
28	SQD	h	105	54/54	0.81	0.11	76,100,195,214	0
38	HTG	a	418	19/19	0.81	0.12	53,84,123,124	0
34	PGE	c	540	10/10	0.81	0.10	82,92,110,113	0
39	1PE	V	217	16/16	0.81	0.12	63,93,120,133	0
36	EDO	V	218	4/4	0.82	0.12	87,88,88,96	0
34	PGE	J	107	10/10	0.82	0.09	87,137,168,170	0
34	PGE	O	310	10/10	0.82	0.12	58,81,122,137	0
31	LMT	j	103	35/35	0.82	0.09	68,114,162,168	0
35	P6G	C	541	19/19	0.82	0.11	79,103,127,142	0
30	GOL	O	307	6/6	0.82	0.10	116,117,120,123	0
36	EDO	H	112	4/4	0.82	0.13	70,85,94,95	0
30	GOL	v	205	6/6	0.83	0.13	102,122,135,152	0
34	PGE	b	646	10/10	0.83	0.10	70,102,120,121	0
38	HTG	C	531	19/19	0.83	0.10	72,109,139,142	0
34	PGE	h	109	10/10	0.83	0.10	84,97,111,113	0
34	PGE	o	306	10/10	0.83	0.11	70,92,102,103	0
30	GOL	C	527	6/6	0.83	0.10	96,108,112,135	0
31	LMT	u	203	35/35	0.84	0.13	42,77,115,137	0
35	P6G	D	418	19/19	0.84	0.10	68,99,126,131	0
34	PGE	E	107	10/10	0.84	0.11	73,106,142,143	0
39	1PE	x	104	16/16	0.84	0.11	85,105,130,136	0
44	2PE	V	216	28/28	0.84	0.11	44,91,110,123	0
33	PG4	e	103	13/13	0.85	0.08	72,107,125,136	0
34	PGE	J	106	10/10	0.85	0.09	85,121,129,138	0
34	PGE	B	650	10/10	0.85	0.10	88,109,126,128	0
34	PGE	O	309	10/10	0.85	0.12	62,86,111,111	0
31	LMT	Y	101	35/35	0.85	0.09	61,118,170,188	0
33	PG4	C	534	13/13	0.85	0.10	81,103,119,119	0
34	PGE	b	645	10/10	0.85	0.09	106,110,126,134	0
35	P6G	E	110	19/19	0.85	0.11	49,95,111,122	0
39	1PE	j	107	16/16	0.85	0.09	74,106,155,159	0
33	PG4	E	102	13/13	0.85	0.12	62,81,106,120	0
33	PG4	H	104	13/13	0.85	0.10	83,98,117,119	0
34	PGE	b	647	10/10	0.86	0.08	77,97,109,109	0
33	PG4	c	535	13/13	0.86	0.10	69,89,109,115	0
33	PG4	B	640	13/13	0.86	0.09	66,86,95,99	0
33	PG4	e	104	13/13	0.86	0.10	78,94,120,120	0
33	PG4	B	642	13/13	0.86	0.11	66,86,115,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
34	PGE	C	540	10/10	0.86	0.09	74,83,102,111	0
28	SQD	A	622	54/54	0.86	0.11	63,85,136,187	0
34	PGE	V	214	10/10	0.86	0.12	50,86,96,98	0
33	PG4	V	212	13/13	0.86	0.12	82,96,120,123	0
34	PGE	E	106	10/10	0.86	0.10	85,95,111,116	0
35	P6G	c	541	19/19	0.86	0.11	43,61,68,72	19
40	DGD	d	408	66/66	0.86	0.10	57,89,155,184	0
33	PG4	b	634	13/13	0.86	0.10	78,90,111,123	0
33	PG4	C	538	13/13	0.87	0.10	65,93,115,123	0
34	PGE	h	108	10/10	0.87	0.10	70,75,101,105	0
33	PG4	b	637	13/13	0.87	0.10	74,97,124,130	0
34	PGE	b	639	10/10	0.87	0.09	79,97,111,119	0
34	PGE	b	644	10/10	0.87	0.09	83,100,113,125	0
34	PGE	H	111	10/10	0.87	0.08	82,100,121,127	0
38	HTG	c	530	19/19	0.87	0.11	66,104,128,145	0
33	PG4	c	534	13/13	0.87	0.13	69,85,99,112	0
33	PG4	H	107	13/13	0.87	0.09	68,83,105,110	0
35	P6G	b	649	19/19	0.87	0.09	71,103,125,128	0
33	PG4	V	211	13/13	0.87	0.12	54,89,114,120	0
34	PGE	c	539	10/10	0.87	0.10	80,90,104,104	0
31	LMT	F	102	35/35	0.87	0.10	43,81,105,126	0
33	PG4	V	213	13/13	0.88	0.09	68,80,103,112	0
33	PG4	X	102	13/13	0.88	0.11	77,95,113,114	0
33	PG4	X	103	13/13	0.88	0.09	78,99,111,115	0
36	EDO	o	311	4/4	0.88	0.09	81,83,83,86	0
33	PG4	a	420	13/13	0.88	0.08	79,94,105,106	0
34	PGE	i	106	10/10	0.88	0.08	78,95,100,103	0
34	PGE	j	105	10/10	0.88	0.10	73,109,124,125	0
33	PG4	D	414	13/13	0.88	0.12	86,95,105,110	0
38	HTG	c	523	19/19	0.88	0.09	65,86,104,106	0
34	PGE	b	640	10/10	0.88	0.08	61,88,103,118	0
38	HTG	c	531	19/19	0.88	0.09	59,99,122,124	0
38	HTG	h	101	19/19	0.88	0.10	62,86,123,141	0
31	LMT	m	101	35/35	0.88	0.10	45,62,75,92	0
31	LMT	c	521	35/35	0.88	0.10	54,77,95,101	0
33	PG4	A	619	13/13	0.88	0.09	83,96,112,112	0
33	PG4	C	535	13/13	0.88	0.13	66,74,108,121	0
40	DGD	D	408	66/66	0.88	0.10	56,88,142,175	0
30	GOL	y	101	6/6	0.88	0.08	82,90,98,101	0
34	PGE	B	646	10/10	0.88	0.09	83,95,114,119	0
34	PGE	H	109	10/10	0.89	0.08	84,95,102,105	0
36	EDO	B	658	4/4	0.89	0.07	82,84,89,110	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
36	EDO	E	111	4/4	0.89	0.10	66,83,90,97	0
33	PG4	J	105	13/13	0.89	0.10	75,88,110,115	0
34	PGE	c	537	10/10	0.89	0.09	96,106,120,123	0
33	PG4	d	414	13/13	0.89	0.09	65,79,85,87	0
34	PGE	I	105	10/10	0.89	0.12	60,83,95,99	0
38	HTG	C	522	19/19	0.89	0.09	50,83,100,110	0
28	SQD	a	424	54/54	0.89	0.10	63,83,134,198	0
30	GOL	e	102	6/6	0.89	0.10	79,91,112,117	0
30	GOL	o	303	6/6	0.89	0.10	79,96,110,126	0
38	HTG	H	101	19/19	0.89	0.09	50,94,122,122	0
34	PGE	h	110	10/10	0.89	0.09	71,99,111,117	0
33	PG4	E	103	13/13	0.89	0.07	59,76,89,105	0
32	LHG	e	101	42/49	0.89	0.10	60,105,123,171	0
33	PG4	H	105	13/13	0.89	0.11	72,87,126,147	0
34	PGE	a	423	10/10	0.89	0.08	78,91,107,107	0
34	PGE	t	104	10/10	0.89	0.07	60,79,99,100	0
39	1PE	B	654	16/16	0.89	0.09	46,68,92,105	0
31	LMT	f	101	35/35	0.89	0.09	54,85,110,119	0
39	1PE	e	105	16/16	0.89	0.09	77,93,116,121	0
33	PG4	I	103	13/13	0.89	0.09	73,97,121,129	0
33	PG4	c	533	13/13	0.89	0.10	77,90,105,109	0
33	PG4	J	104	13/13	0.89	0.10	74,82,107,108	0
34	PGE	H	108	10/10	0.89	0.10	66,86,129,136	0
35	P6G	j	106	19/19	0.89	0.09	50,74,98,112	0
33	PG4	B	641	13/13	0.90	0.09	74,97,107,115	0
32	LHG	A	618	42/49	0.90	0.09	49,90,145,167	0
34	PGE	x	103	10/10	0.90	0.09	81,98,110,112	0
32	LHG	a	419	41/49	0.90	0.11	52,85,176,193	0
33	PG4	x	102	13/13	0.90	0.09	79,95,107,108	0
34	PGE	A	621	10/10	0.90	0.08	66,116,120,129	0
33	PG4	H	106	13/13	0.90	0.12	38,53,67,74	13
30	GOL	f	104	6/6	0.90	0.07	94,115,135,150	0
34	PGE	J	108	10/10	0.90	0.07	80,98,116,120	0
30	GOL	T	103	6/6	0.90	0.11	62,79,91,111	0
36	EDO	B	657	4/4	0.90	0.10	93,95,100,102	0
33	PG4	b	635	13/13	0.90	0.08	58,76,103,109	0
36	EDO	D	419	4/4	0.90	0.14	66,70,78,97	0
33	PG4	B	637	13/13	0.90	0.10	68,82,106,106	0
33	PG4	B	638	13/13	0.90	0.10	66,84,114,130	0
33	PG4	V	209	13/13	0.90	0.11	51,84,95,101	0
29	LMG	d	412	55/55	0.90	0.11	47,77,119,137	0
34	PGE	E	109	10/10	0.90	0.10	51,93,103,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
38	HTG	B	624	19/19	0.90	0.08	47,103,125,143	0
33	PG4	i	101	13/13	0.91	0.08	71,84,95,98	0
33	PG4	j	104	13/13	0.91	0.09	78,97,113,116	0
31	LMT	J	103	35/35	0.91	0.08	47,78,115,134	0
29	LMG	c	520	51/55	0.91	0.08	47,76,100,124	0
36	EDO	a	425	4/4	0.91	0.07	74,78,96,120	0
34	PGE	B	645	10/10	0.91	0.09	68,81,89,93	0
33	PG4	a	421	13/13	0.91	0.07	76,89,99,102	0
34	PGE	i	105	10/10	0.91	0.09	70,81,89,92	0
34	PGE	B	649	10/10	0.91	0.09	66,82,101,105	0
28	SQD	F	104	54/54	0.91	0.11	55,80,110,135	0
33	PG4	C	536	13/13	0.91	0.11	66,72,93,103	0
34	PGE	a	422	10/10	0.91	0.09	72,75,85,92	0
34	PGE	o	308	10/10	0.91	0.10	48,87,100,104	0
34	PGE	o	309	10/10	0.91	0.08	53,78,92,97	0
38	HTG	b	624	19/19	0.91	0.09	54,91,117,133	0
33	PG4	b	636	13/13	0.91	0.08	71,79,90,93	0
27	PL9	a	412	55/55	0.91	0.09	46,69,101,108	0
35	P6G	B	652	19/19	0.91	0.09	42,84,105,109	0
33	PG4	c	532	13/13	0.91	0.09	70,78,98,101	0
34	PGE	b	641	10/10	0.91	0.07	99,104,114,125	0
33	PG4	K	102	13/13	0.91	0.09	56,70,102,109	0
39	1PE	L	101	16/16	0.91	0.09	56,72,99,100	0
35	P6G	I	106	19/19	0.91	0.09	56,81,119,121	0
27	PL9	A	611	55/55	0.91	0.10	39,63,96,107	0
33	PG4	B	639	13/13	0.91	0.09	64,79,104,115	0
29	LMG	C	526	55/55	0.91	0.10	47,83,115,124	0
30	GOL	b	626	6/6	0.91	0.09	42,46,50,54	0
30	GOL	c	529	6/6	0.91	0.20	27,31,39,40	6
34	PGE	c	538	10/10	0.91	0.11	68,102,115,129	0
45	PE8	i	107	25/25	0.91	0.11	44,66,104,122	0
33	PG4	X	101	13/13	0.92	0.09	63,89,105,108	0
30	GOL	u	201	6/6	0.92	0.08	43,70,71,77	0
34	PGE	b	643	10/10	0.92	0.10	70,85,103,116	0
33	PG4	h	106	13/13	0.92	0.07	67,76,106,108	0
38	HTG	B	631	19/19	0.92	0.08	46,90,129,147	0
28	SQD	x	101	54/54	0.92	0.09	62,84,132,147	0
35	P6G	A	624	19/19	0.92	0.08	70,85,105,113	0
33	PG4	i	102	13/13	0.92	0.07	65,71,81,82	0
29	LMG	z	101	55/55	0.92	0.10	49,95,120,160	0
38	HTG	C	532	19/19	0.92	0.08	57,85,128,156	0
32	LHG	E	101	42/49	0.92	0.10	54,80,100,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	GOL	B	633	6/6	0.92	0.09	69,71,84,97	0
34	PGE	B	644	10/10	0.92	0.10	58,71,117,137	0
38	HTG	b	632	19/19	0.92	0.09	49,79,119,135	0
35	P6G	b	648	19/19	0.92	0.09	59,66,80,84	0
30	GOL	B	635	6/6	0.92	0.08	46,67,79,83	0
30	GOL	d	413	6/6	0.92	0.08	74,88,114,116	0
35	P6G	d	415	19/19	0.92	0.09	51,64,88,97	0
34	PGE	O	308	10/10	0.92	0.11	31,62,83,96	0
36	EDO	A	625	4/4	0.92	0.08	70,71,80,80	0
34	PGE	B	648	10/10	0.92	0.10	55,75,82,93	0
33	PG4	U	202	13/13	0.92	0.09	52,80,100,102	0
29	LMG	B	634	55/55	0.92	0.10	39,69,141,167	0
36	EDO	C	542	4/4	0.92	0.07	77,84,88,96	0
33	PG4	V	210	13/13	0.92	0.09	53,84,115,120	0
30	GOL	D	413	6/6	0.92	0.09	58,67,76,84	0
30	GOL	m	103	6/6	0.92	0.09	47,69,88,116	0
36	EDO	J	109	4/4	0.92	0.10	78,79,85,96	0
30	GOL	O	305	6/6	0.92	0.08	55,65,71,77	0
28	SQD	l	102	54/54	0.93	0.08	46,71,104,172	0
34	PGE	B	647	10/10	0.93	0.07	78,92,122,122	0
30	GOL	v	207	6/6	0.93	0.08	63,73,86,86	0
30	GOL	c	528	6/6	0.93	0.09	78,79,88,89	0
31	LMT	B	622	35/35	0.93	0.08	46,73,107,123	0
30	GOL	D	412	6/6	0.93	0.07	55,80,95,102	0
33	PG4	B	636	13/13	0.93	0.08	71,98,116,121	0
33	PG4	I	102	13/13	0.93	0.07	62,73,97,112	0
30	GOL	B	626	6/6	0.93	0.10	34,41,49,61	0
33	PG4	I	104	13/13	0.93	0.08	65,73,90,93	0
31	LMT	I	101	35/35	0.93	0.09	57,83,111,113	0
30	GOL	O	304	6/6	0.93	0.07	60,69,79,88	0
31	LMT	M	101	35/35	0.93	0.07	34,51,70,73	0
31	LMT	M	102	35/35	0.93	0.07	43,59,82,96	0
38	HTG	c	522	19/19	0.93	0.08	60,74,96,106	0
35	P6G	d	416	19/19	0.93	0.09	43,61,100,111	0
28	SQD	b	633	54/54	0.93	0.08	46,66,104,116	0
31	LMT	b	622	35/35	0.93	0.07	49,76,124,132	0
36	EDO	B	655	4/4	0.93	0.09	45,50,57,88	0
28	SQD	a	417	54/54	0.93	0.08	40,64,93,101	0
33	PG4	i	103	13/13	0.93	0.07	74,85,98,105	0
30	GOL	C	523	6/6	0.93	0.16	35,46,56,62	0
30	GOL	a	416	6/6	0.93	0.08	39,57,72,77	0
34	PGE	A	620	7/10	0.93	0.07	68,77,83,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
33	PG4	C	537	13/13	0.93	0.08	67,76,92,108	0
36	EDO	E	112	4/4	0.93	0.11	84,94,96,100	0
30	GOL	u	202	6/6	0.93	0.09	50,56,61,63	0
34	PGE	T	104	7/10	0.93	0.09	76,77,96,103	0
30	GOL	v	203	6/6	0.93	0.10	66,79,82,98	0
36	EDO	X	104	4/4	0.93	0.08	73,80,83,88	0
38	HTG	V	204	19/19	0.94	0.08	36,52,89,102	0
31	LMT	a	401	35/35	0.94	0.07	37,52,75,83	0
35	P6G	T	105	19/19	0.94	0.09	42,59,85,88	0
36	EDO	I	107	4/4	0.94	0.07	84,89,91,96	0
30	GOL	O	302	6/6	0.94	0.06	51,55,67,70	0
28	SQD	A	616	54/54	0.94	0.07	39,65,102,107	0
30	GOL	C	528	6/6	0.94	0.19	24,27,36,38	6
34	PGE	C	539	10/10	0.94	0.10	56,73,94,96	0
34	PGE	Y	102	10/10	0.94	0.08	61,84,103,104	0
36	EDO	i	108	4/4	0.94	0.08	70,71,76,87	0
30	GOL	v	206	6/6	0.94	0.07	50,54,66,75	0
29	LMG	a	414	51/55	0.94	0.07	42,64,80,90	0
34	PGE	E	104	10/10	0.94	0.07	67,76,99,106	0
38	HTG	C	521	19/19	0.94	0.08	53,65,84,85	0
31	LMT	t	103	35/35	0.94	0.08	32,75,110,117	0
35	P6G	B	651	19/19	0.94	0.07	49,63,77,81	0
34	PGE	h	107	10/10	0.94	0.07	67,78,92,95	0
30	GOL	o	304	6/6	0.94	0.07	45,53,55,62	0
34	PGE	b	642	10/10	0.94	0.07	51,65,87,92	0
29	LMG	C	520	51/55	0.94	0.08	38,79,108,121	0
35	P6G	D	416	19/19	0.95	0.07	38,60,84,87	0
34	PGE	b	638	10/10	0.95	0.07	55,77,90,93	0
31	LMT	A	617	35/35	0.95	0.08	37,55,92,105	0
30	GOL	t	101	6/6	0.95	0.10	44,49,56,62	0
33	PG4	i	104	13/13	0.95	0.07	56,71,90,91	0
24	CLA	b	602	65/65	0.95	0.07	28,47,99,111	0
30	GOL	U	201	6/6	0.95	0.08	40,67,78,98	0
34	PGE	t	105	7/10	0.95	0.06	58,79,84,87	0
26	BCR	C	514	40/40	0.95	0.06	31,41,50,57	0
35	P6G	A	623	19/19	0.95	0.08	48,60,95,96	0
26	BCR	c	514	40/40	0.95	0.06	39,51,58,60	0
30	GOL	O	306	6/6	0.95	0.09	39,45,55,97	0
30	GOL	A	615	6/6	0.95	0.07	34,54,62,66	0
30	GOL	o	305	6/6	0.95	0.07	51,56,61,62	0
36	EDO	o	310	4/4	0.95	0.07	60,65,77,90	0
30	GOL	a	415	6/6	0.96	0.06	29,39,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
26	BCR	t	102	40/40	0.96	0.06	21,29,48,53	0
31	LMT	m	102	35/35	0.96	0.06	28,50,66,82	0
26	BCR	D	406	40/40	0.96	0.06	23,28,60,65	0
29	LMG	c	519	51/55	0.96	0.06	34,67,104,112	0
30	GOL	D	402	6/6	0.96	0.10	31,37,43,44	0
30	GOL	d	402	6/6	0.96	0.07	35,39,45,48	0
35	P6G	D	417	19/19	0.96	0.08	35,56,89,111	0
26	BCR	a	411	40/40	0.96	0.05	20,25,31,32	0
38	HTG	b	631	19/19	0.96	0.07	41,48,77,98	0
24	CLA	c	513	65/65	0.96	0.07	37,51,89,99	0
36	EDO	O	311	4/4	0.96	0.12	42,54,57,72	0
30	GOL	F	101	6/6	0.96	0.08	43,48,50,54	0
33	PG4	l	103	13/13	0.96	0.06	48,64,71,74	0
26	BCR	d	406	40/40	0.96	0.05	28,36,70,82	0
30	GOL	A	614	6/6	0.96	0.06	33,37,38,44	0
36	EDO	d	417	4/4	0.96	0.09	46,49,52,58	0
29	LMG	A	613	51/55	0.96	0.06	45,60,82,95	0
30	GOL	B	625	6/6	0.96	0.06	32,36,38,50	0
26	BCR	h	103	40/40	0.96	0.06	25,35,50,53	0
37	CA	B	601	1/1	0.96	0.11	82,82,82,82	0
37	CA	h	102	1/1	0.96	0.05	97,97,97,97	0
38	HTG	B	623	19/19	0.96	0.09	28,40,74,88	0
29	LMG	C	519	51/55	0.96	0.08	29,59,104,117	0
38	HTG	B	630	19/19	0.96	0.07	38,50,78,82	0
26	BCR	k	101	40/40	0.96	0.06	34,40,51,54	0
30	GOL	V	208	6/6	0.96	0.06	65,70,82,83	0
24	CLA	C	512	65/65	0.97	0.05	31,39,74,85	0
30	GOL	T	101	6/6	0.97	0.06	52,52,56,59	0
26	BCR	H	102	40/40	0.97	0.05	23,33,52,55	0
29	LMG	B	621	51/55	0.97	0.05	27,39,54,88	0
30	GOL	V	201	6/6	0.97	0.06	28,30,35,39	0
36	EDO	e	106	4/4	0.97	0.06	72,76,79,89	0
30	GOL	V	205	6/6	0.97	0.05	26,34,37,43	0
30	GOL	V	207	6/6	0.97	0.06	44,49,52,55	0
26	BCR	K	101	40/40	0.97	0.05	27,36,45,47	0
26	BCR	T	102	40/40	0.97	0.05	20,29,45,60	0
24	CLA	C	513	65/65	0.97	0.05	33,44,73,92	0
30	GOL	b	625	6/6	0.97	0.05	34,39,44,54	0
26	BCR	b	618	40/40	0.97	0.04	19,26,33,37	0
32	LHG	D	409	49/49	0.97	0.05	25,35,45,55	0
30	GOL	b	627	6/6	0.97	0.05	40,47,52,54	0
30	GOL	b	628	6/6	0.97	0.07	32,34,35,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	GOL	b	629	6/6	0.97	0.12	36,42,45,50	0
30	GOL	c	525	6/6	0.97	0.06	47,49,64,80	0
26	BCR	b	619	40/40	0.97	0.05	21,28,47,57	0
29	LMG	b	621	51/55	0.97	0.05	28,39,53,103	0
26	BCR	b	620	40/40	0.97	0.05	24,32,45,48	0
24	CLA	B	602	65/65	0.97	0.07	27,39,92,115	0
26	BCR	c	515	40/40	0.97	0.05	26,35,47,55	0
29	LMG	j	101	47/55	0.97	0.06	26,35,80,91	0
38	HTG	b	623	19/19	0.97	0.08	26,42,77,81	0
26	BCR	c	527	40/40	0.97	0.05	34,42,53,59	0
24	CLA	b	613	65/65	0.97	0.05	20,25,32,41	0
24	CLA	c	503	65/65	0.97	0.05	26,35,42,52	0
24	CLA	c	504	60/65	0.97	0.05	25,31,67,75	0
24	CLA	c	506	65/65	0.97	0.06	26,37,83,95	0
30	GOL	B	627	6/6	0.97	0.06	35,44,48,48	0
24	CLA	c	507	65/65	0.97	0.06	28,34,50,59	0
27	PL9	D	407	55/55	0.97	0.05	17,22,33,48	0
24	CLA	c	511	65/65	0.97	0.05	28,36,47,52	0
28	SQD	A	612	54/54	0.97	0.06	31,55,78,87	0
24	CLA	c	512	65/65	0.97	0.05	30,44,74,79	0
24	CLA	C	503	65/65	0.97	0.05	26,30,38,43	0
25	PHO	d	401	64/64	0.97	0.04	20,25,31,41	0
28	SQD	a	413	54/54	0.97	0.06	33,54,92,96	0
26	BCR	A	610	40/40	0.97	0.04	20,25,32,35	0
26	BCR	B	619	40/40	0.97	0.05	20,26,50,62	0
40	DGD	H	103	62/66	0.97	0.05	21,31,45,54	0
40	DGD	c	517	57/66	0.97	0.05	27,34,75,108	0
24	CLA	C	506	65/65	0.97	0.06	28,39,97,106	0
40	DGD	h	104	62/66	0.97	0.06	25,35,49,55	0
26	BCR	C	515	40/40	0.97	0.04	28,33,52,59	0
26	BCR	C	525	40/40	0.97	0.05	26,33,39,41	0
24	CLA	b	609	65/65	0.98	0.04	22,27,37,44	0
24	CLA	b	610	65/65	0.98	0.04	23,30,35,44	0
24	CLA	b	611	65/65	0.98	0.04	23,28,38,44	0
24	CLA	b	612	65/65	0.98	0.04	18,24,37,42	0
24	CLA	A	609	65/65	0.98	0.06	19,24,109,130	0
24	CLA	b	614	65/65	0.98	0.04	19,23,48,54	0
24	CLA	b	615	65/65	0.98	0.05	18,26,94,117	0
24	CLA	b	616	65/65	0.98	0.05	22,29,47,56	0
29	LMG	J	101	47/55	0.98	0.05	23,29,74,83	0
24	CLA	b	617	60/65	0.98	0.06	26,31,82,92	0
24	CLA	c	501	65/65	0.98	0.04	27,35,49,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	c	502	65/65	0.98	0.04	24,30,41,50	0
22	CL	V	202	1/1	0.98	0.05	68,68,68,68	0
24	CLA	B	603	65/65	0.98	0.04	21,26,33,38	0
24	CLA	c	505	65/65	0.98	0.04	25,29,44,50	0
24	CLA	B	604	65/65	0.98	0.04	19,23,34,41	0
24	CLA	B	605	65/65	0.98	0.04	17,21,55,58	0
24	CLA	c	508	60/65	0.98	0.04	23,29,52,62	0
24	CLA	c	509	65/65	0.98	0.04	25,33,52,53	0
24	CLA	c	510	65/65	0.98	0.04	26,32,41,48	0
24	CLA	B	606	65/65	0.98	0.04	18,22,34,38	0
30	GOL	B	628	6/6	0.98	0.06	34,40,48,49	0
32	LHG	B	632	49/49	0.98	0.05	20,30,52,61	0
30	GOL	B	629	6/6	0.98	0.07	31,39,60,64	0
32	LHG	D	411	49/49	0.98	0.06	23,31,81,89	0
24	CLA	B	607	55/65	0.98	0.04	19,25,33,49	0
24	CLA	B	608	65/65	0.98	0.04	16,20,32,38	0
32	LHG	d	409	49/49	0.98	0.05	27,37,48,52	0
32	LHG	d	410	49/49	0.98	0.04	21,27,42,51	0
32	LHG	d	411	49/49	0.98	0.05	26,31,79,84	0
24	CLA	d	403	65/65	0.98	0.03	17,20,29,38	0
32	LHG	l	101	49/49	0.98	0.04	23,30,49,62	0
24	CLA	d	404	65/65	0.98	0.04	17,21,37,43	0
24	CLA	d	405	65/65	0.98	0.06	25,33,91,101	0
25	PHO	A	608	64/64	0.98	0.04	17,19,26,26	0
25	PHO	D	401	64/64	0.98	0.04	17,23,31,41	0
25	PHO	a	409	64/64	0.98	0.04	17,21,26,32	0
24	CLA	B	609	65/65	0.98	0.04	19,24,33,40	0
24	CLA	B	610	65/65	0.98	0.04	22,27,33,37	0
26	BCR	B	618	40/40	0.98	0.04	21,25,33,34	0
37	CA	O	301	1/1	0.98	0.05	53,53,53,53	0
37	CA	b	601	1/1	0.98	0.09	72,72,72,72	0
24	CLA	B	611	65/65	0.98	0.04	20,24,38,51	0
26	BCR	B	620	40/40	0.98	0.04	22,31,46,50	0
24	CLA	B	612	65/65	0.98	0.04	16,21,35,39	0
24	CLA	B	613	65/65	0.98	0.04	17,23,30,39	0
24	CLA	B	614	65/65	0.98	0.04	17,21,48,64	0
24	CLA	B	615	55/65	0.98	0.04	17,23,55,82	0
24	CLA	B	616	65/65	0.98	0.04	21,27,48,56	0
24	CLA	C	501	65/65	0.98	0.04	25,30,48,57	0
30	GOL	V	206	6/6	0.98	0.07	33,35,42,42	0
24	CLA	C	502	65/65	0.98	0.04	21,27,37,54	0
23	BCT	A	605	4/4	0.98	0.05	27,31,35,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
24	CLA	C	504	60/65	0.98	0.04	20,26,70,81	0
38	HTG	O	303	19/19	0.98	0.06	27,31,50,65	0
24	CLA	C	505	65/65	0.98	0.05	23,29,47,52	0
23	BCT	a	406	4/4	0.98	0.05	27,28,31,49	0
24	CLA	C	507	65/65	0.98	0.04	27,33,48,64	0
24	CLA	C	508	60/65	0.98	0.04	23,29,51,61	0
24	CLA	C	509	65/65	0.98	0.05	27,33,50,57	0
24	CLA	C	510	65/65	0.98	0.05	22,29,41,48	0
30	GOL	b	630	6/6	0.98	0.06	30,39,52,53	0
24	CLA	C	511	65/65	0.98	0.05	26,33,40,45	0
30	GOL	c	526	6/6	0.98	0.04	24,28,29,32	0
23	BCT	m	104[A]	4/4	0.98	0.05	18,34,38,38	4
23	BCT	m	104[B]	4/4	0.98	0.05	7,13,18,19	4
38	HTG	o	301	19/19	0.98	0.05	25,32,41,63	0
24	CLA	D	403	65/65	0.98	0.04	14,18,28,44	0
24	CLA	D	404	65/65	0.98	0.04	13,18,35,40	0
24	CLA	D	405	65/65	0.98	0.05	22,29,91,98	0
30	GOL	f	103	6/6	0.98	0.04	50,53,56,56	0
27	PL9	d	407	55/55	0.98	0.04	19,24,31,39	0
24	CLA	a	407	65/65	0.98	0.04	17,20,27,41	0
24	CLA	a	410	65/65	0.98	0.06	20,25,98,113	0
40	DGD	C	516	62/66	0.98	0.05	20,31,90,104	0
40	DGD	C	517	56/66	0.98	0.05	21,31,74,88	0
40	DGD	C	518	62/66	0.98	0.05	20,30,71,80	0
24	CLA	A	606	65/65	0.98	0.04	14,18,27,44	0
24	CLA	b	603	65/65	0.98	0.04	21,28,39,43	0
40	DGD	c	516	62/66	0.98	0.05	23,35,77,86	0
24	CLA	b	604	65/65	0.98	0.04	22,28,38,45	0
40	DGD	c	518	62/66	0.98	0.05	25,36,65,81	0
24	CLA	b	605	65/65	0.98	0.04	17,23,53,59	0
24	CLA	b	606	65/65	0.98	0.04	20,25,33,39	0
41	HEM	e	107	43/43	0.98	0.06	40,47,74,103	0
24	CLA	b	607	55/65	0.98	0.04	22,27,36,49	0
24	CLA	b	608	65/65	0.98	0.04	17,22,31,37	0
24	CLA	a	408	60/65	0.99	0.04	18,25,73,85	0
30	GOL	v	204	6/6	0.99	0.05	30,36,41,50	0
24	CLA	A	607	60/65	0.99	0.04	17,20,66,78	0
37	CA	c	524	1/1	0.99	0.06	45,45,45,45	0
22	CL	v	201	1/1	0.99	0.03	72,72,72,72	0
37	CA	o	302	1/1	0.99	0.04	55,55,55,55	0
24	CLA	B	617	60/65	0.99	0.05	21,27,90,107	0
41	HEM	E	113	43/43	0.99	0.05	35,42,61,68	0

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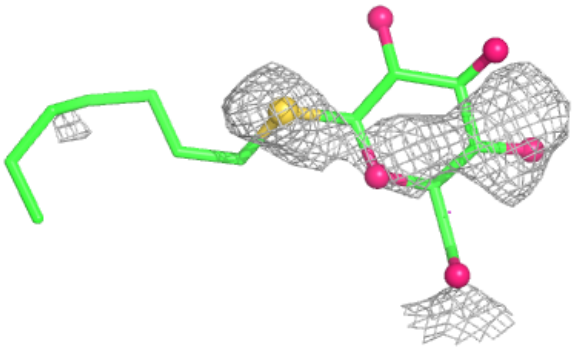
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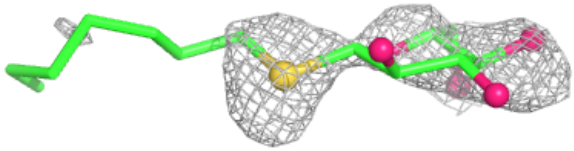
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	GOL	C	524	6/6	0.99	0.03	21,22,24,26	0
42	MG	J	102	1/1	0.99	0.05	27,27,27,27	0
42	MG	j	102	1/1	0.99	0.08	35,35,35,35	0
43	HEC	V	203	43/43	0.99	0.04	20,24,27,29	0
43	HEC	v	202	43/43	0.99	0.04	26,31,34,38	0
32	LHG	D	410	49/49	0.99	0.04	21,27,41,48	0
22	CL	A	604	1/1	0.99	0.02	21,21,21,21	0
22	CL	A	603	1/1	1.00	0.04	23,23,23,23	0
42	MG	F	103	1/1	1.00	0.03	32,32,32,32	0
20	OEX	A	601	10/10	1.00	0.02	20,21,24,26	0
42	MG	f	102	1/1	1.00	0.01	45,45,45,45	0
20	OEX	a	402	10/10	1.00	0.02	23,24,26,27	0
22	CL	a	404	1/1	1.00	0.04	28,28,28,28	0
22	CL	a	405	1/1	1.00	0.02	25,25,25,25	0
21	FE2	A	602	1/1	1.00	0.02	25,25,25,25	0
21	FE2	a	403	1/1	1.00	0.02	25,25,25,25	0

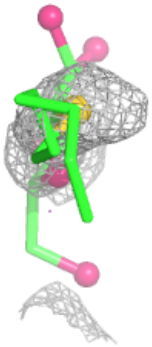
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HTG C 530:

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

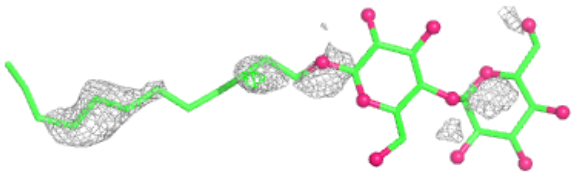


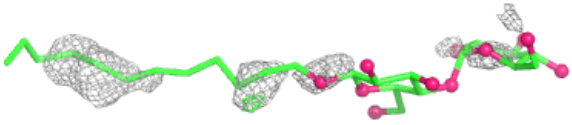


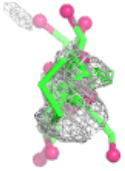


Electron density around LMT C 533:

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

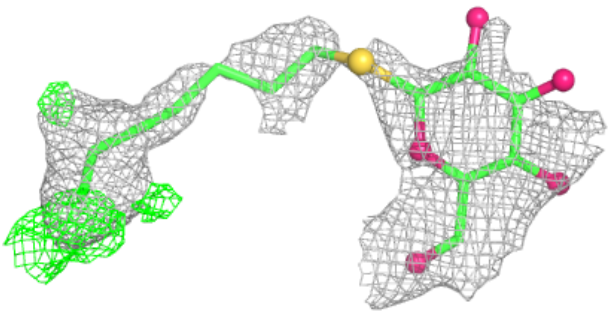


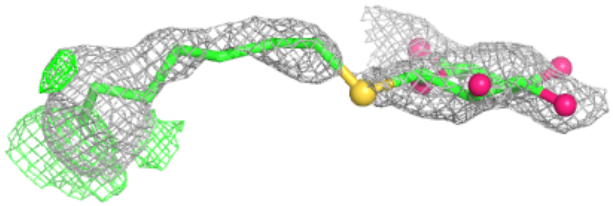


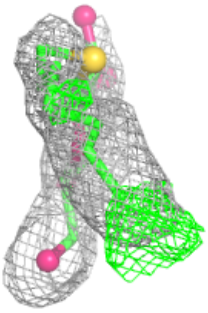


Electron density around HTG C 529:

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

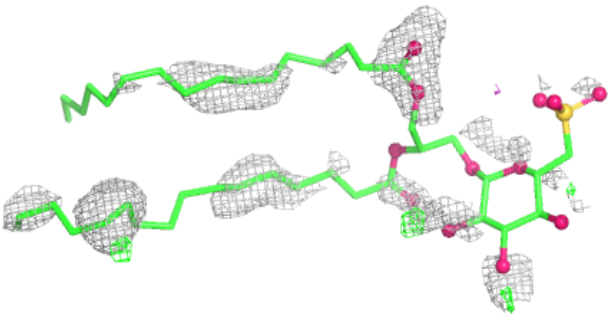


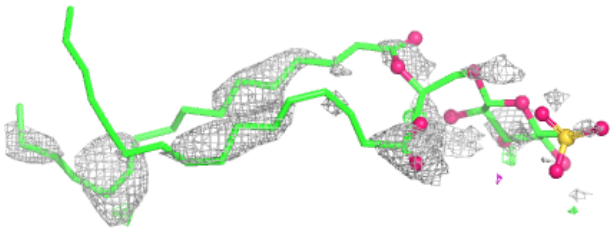


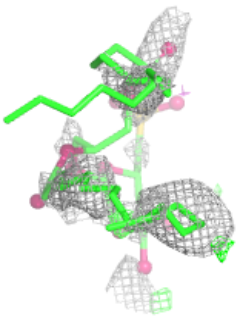


Electron density around SQD h 105:

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

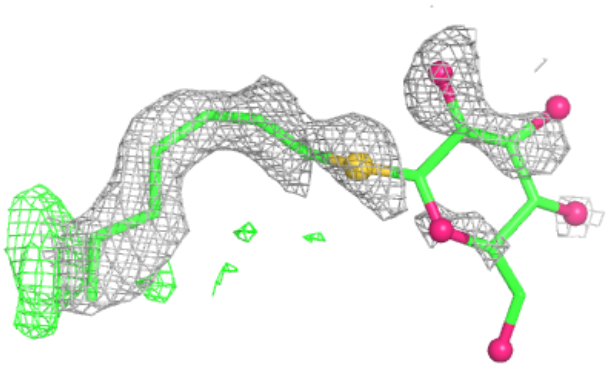


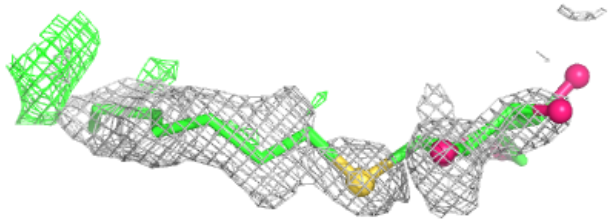


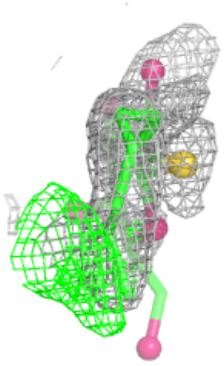


Electron density around HTG a 418:

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

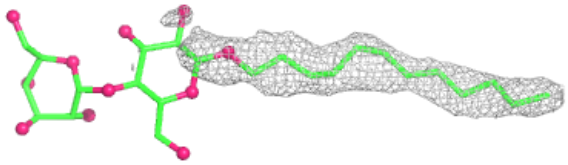




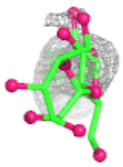


Electron density around LMT j 103:

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

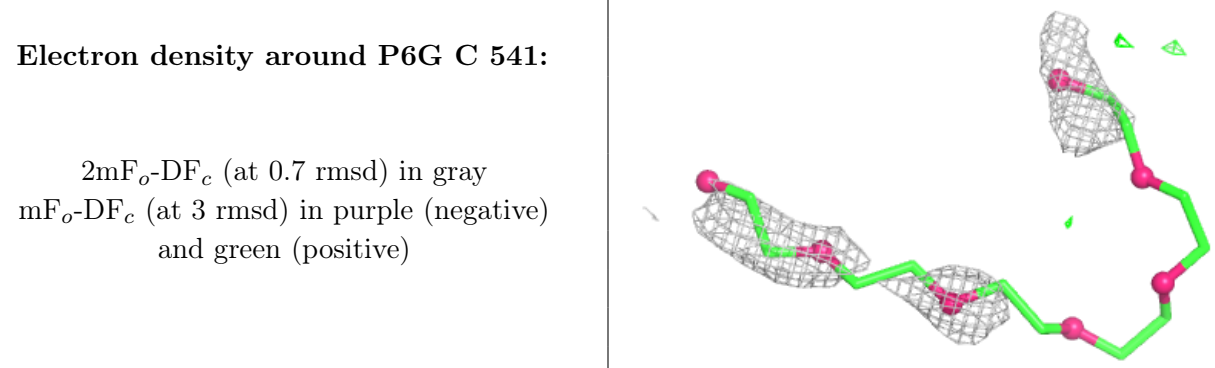


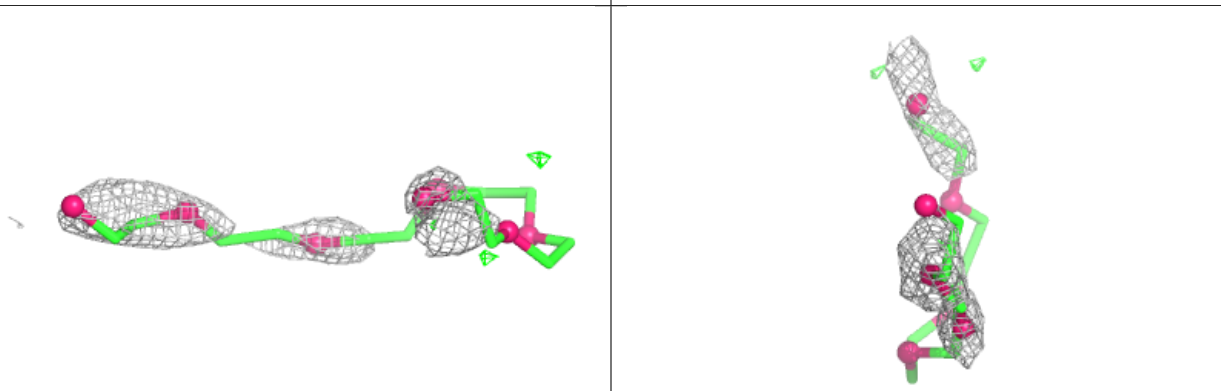




Electron density around P6G C 541:

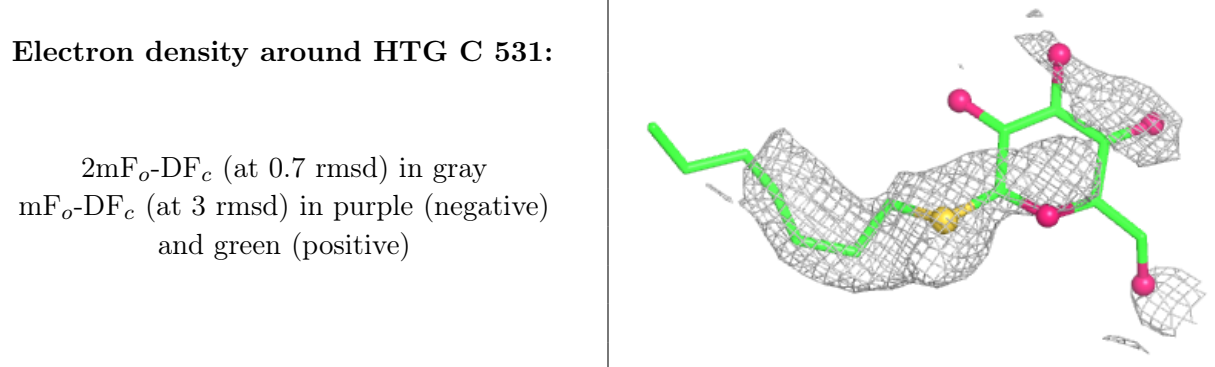
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

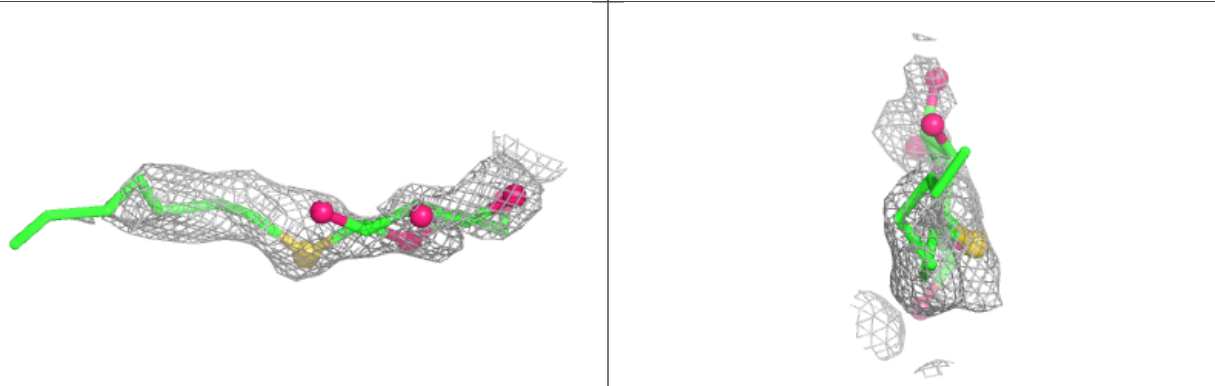




Electron density around HTG C 531:

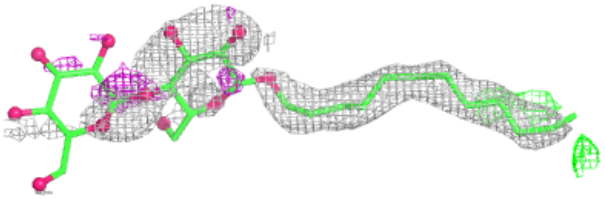
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

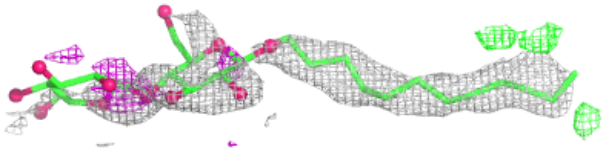


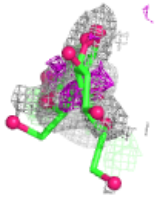


Electron density around LMT u 203:

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

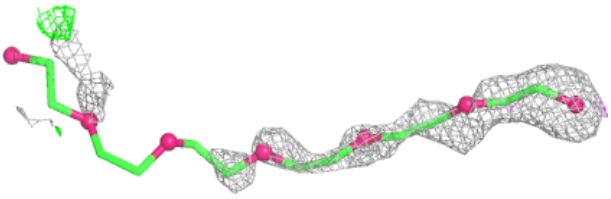


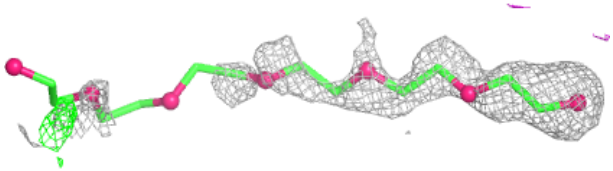


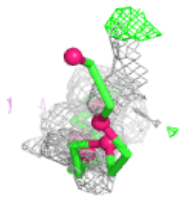


Electron density around P6G D 418:

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

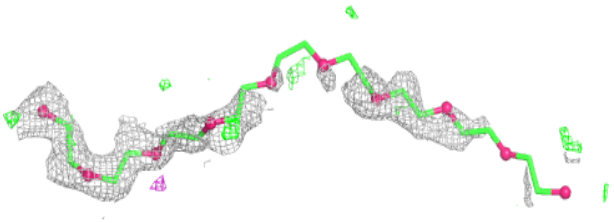


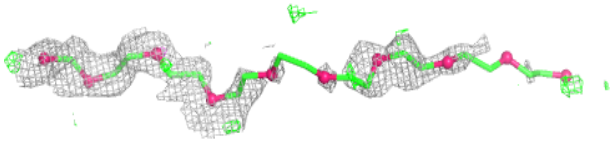


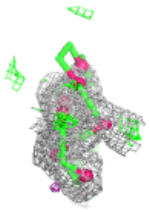


Electron density around 2PE V 216:

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

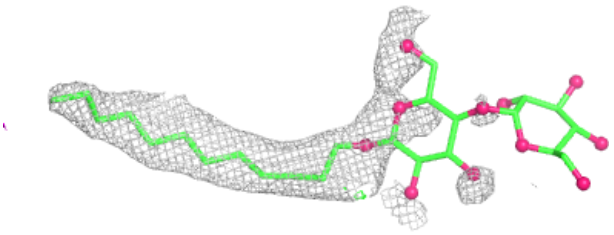


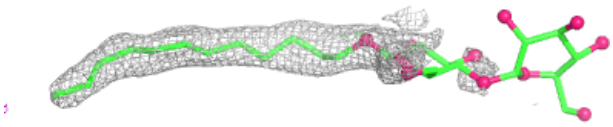


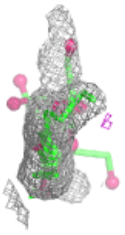


Electron density around LMT Y 101:

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

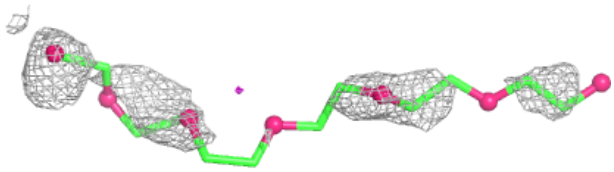


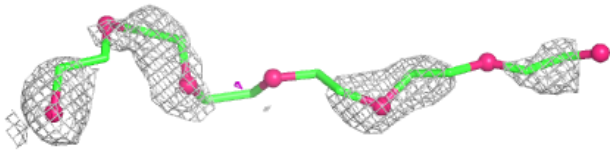


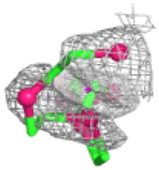


Electron density around P6G E 110:

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

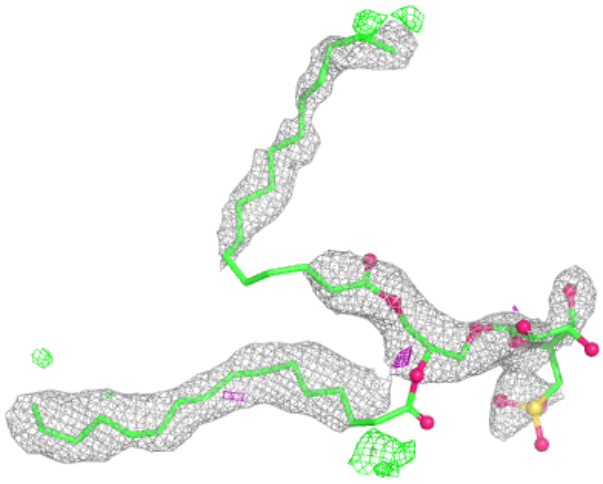


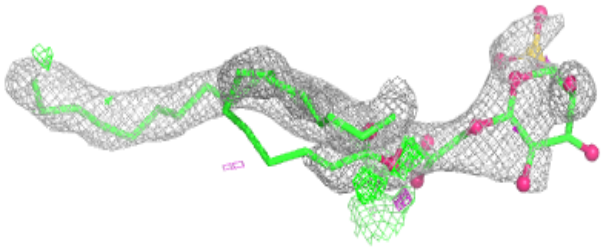


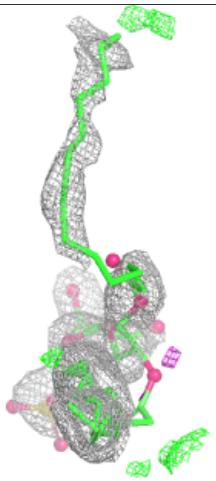


Electron density around SQD A 622:

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

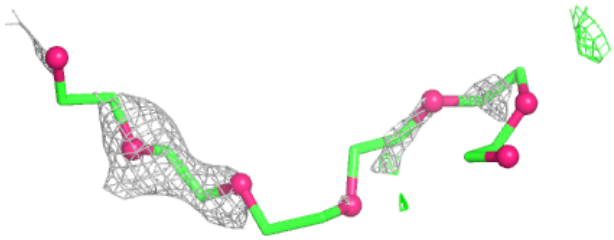


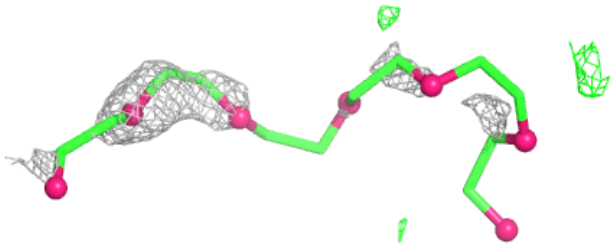


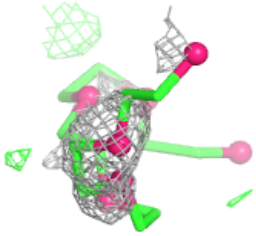


Electron density around P6G c 541:

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

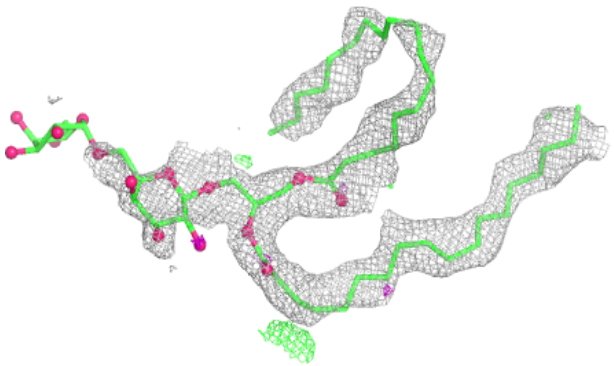


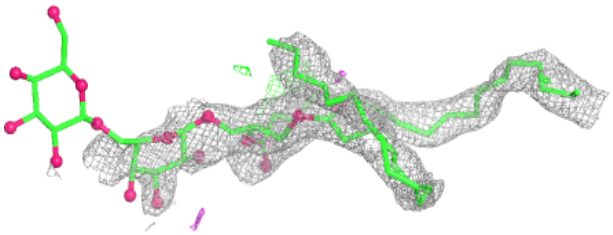


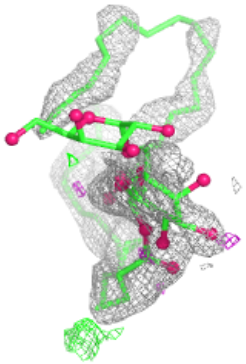


Electron density around DGD d 408:

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

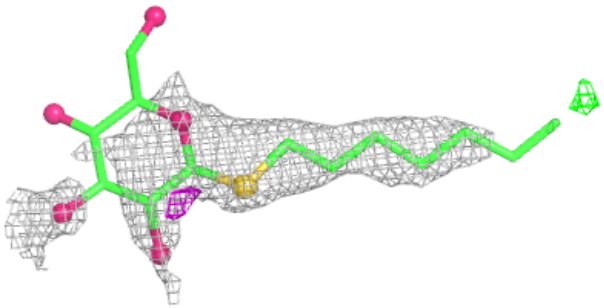


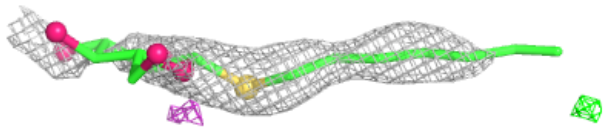


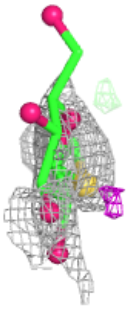


Electron density around HTG c 530:

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

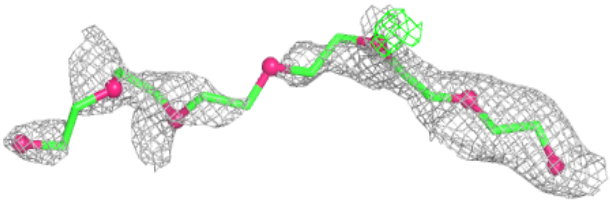


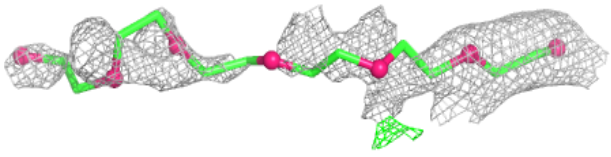


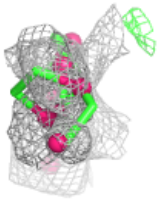


Electron density around P6G b 649:

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

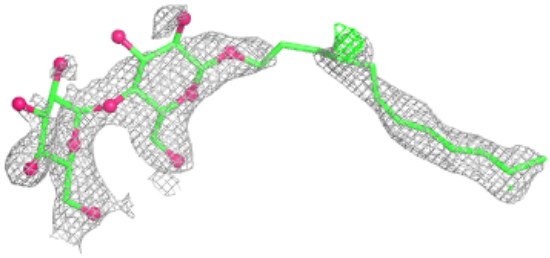


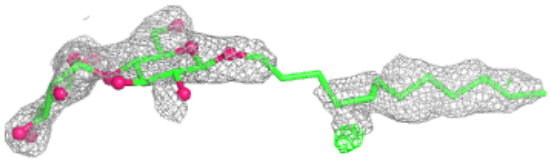


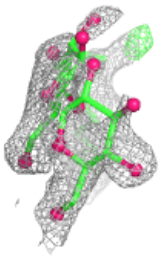


Electron density around LMT F 102:

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

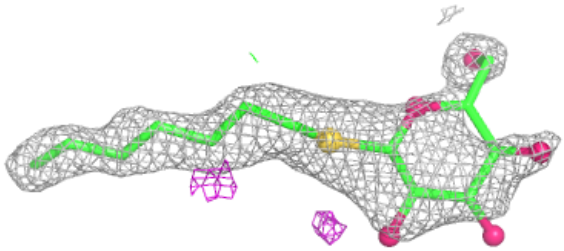


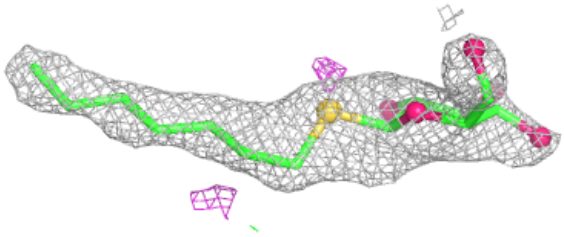


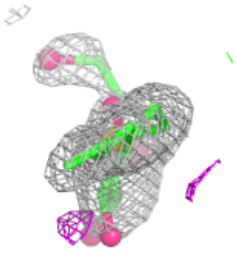


Electron density around HTG c 523:

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

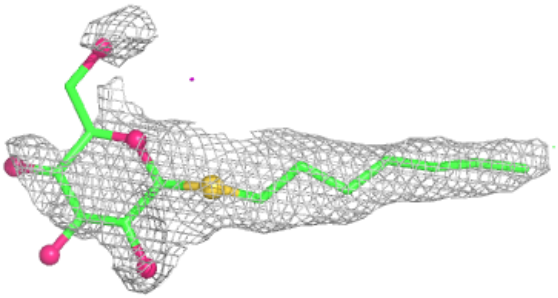


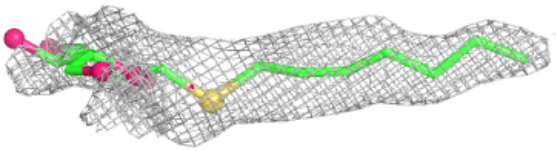


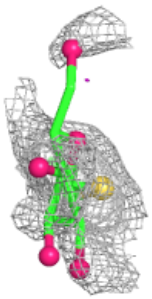


Electron density around HTG c 531:

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

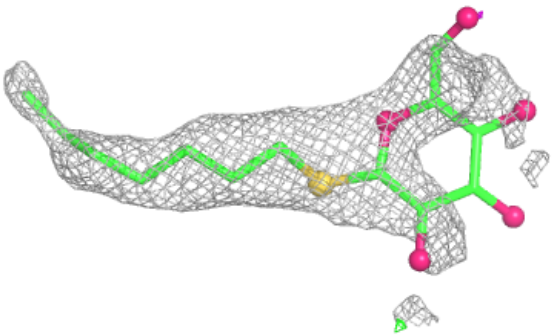


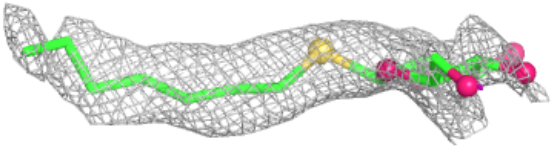


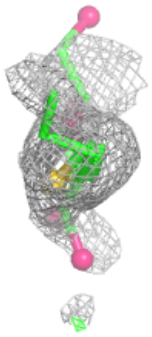


Electron density around HTG h 101:

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

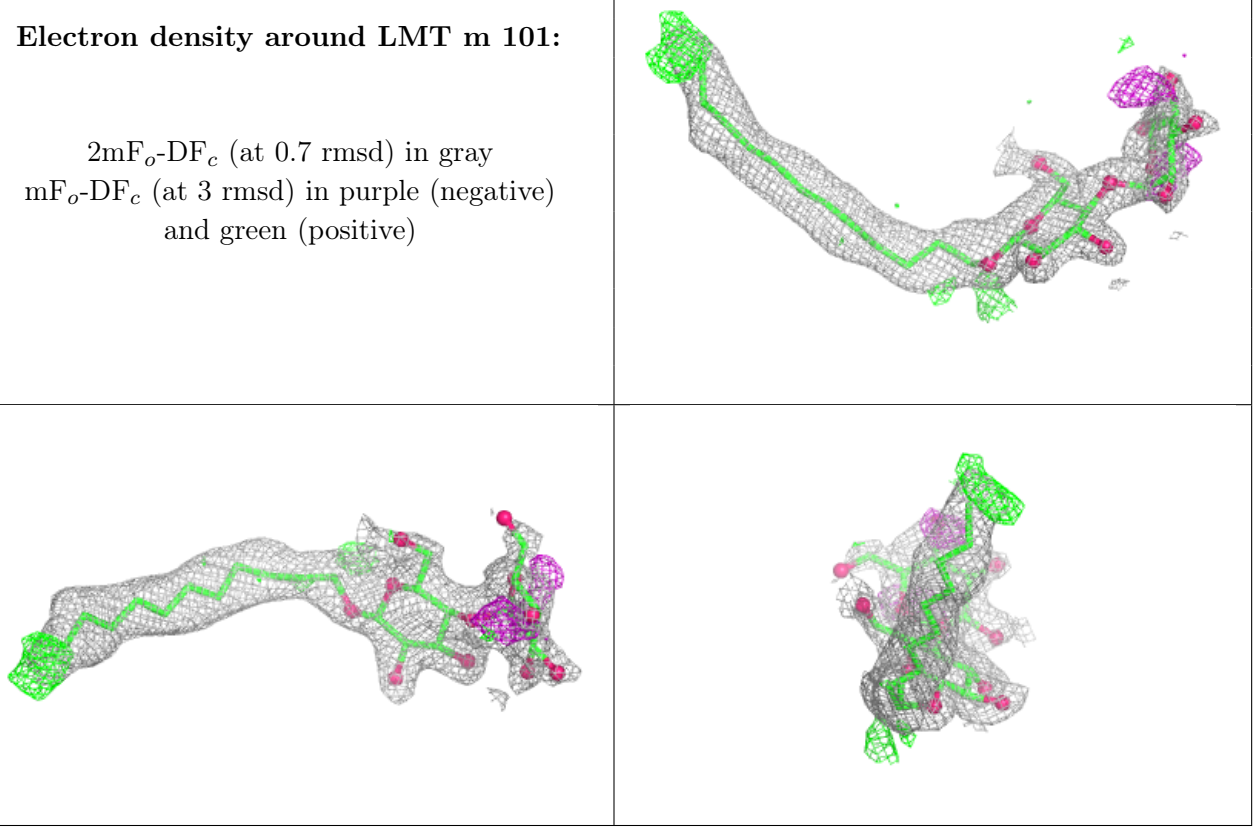






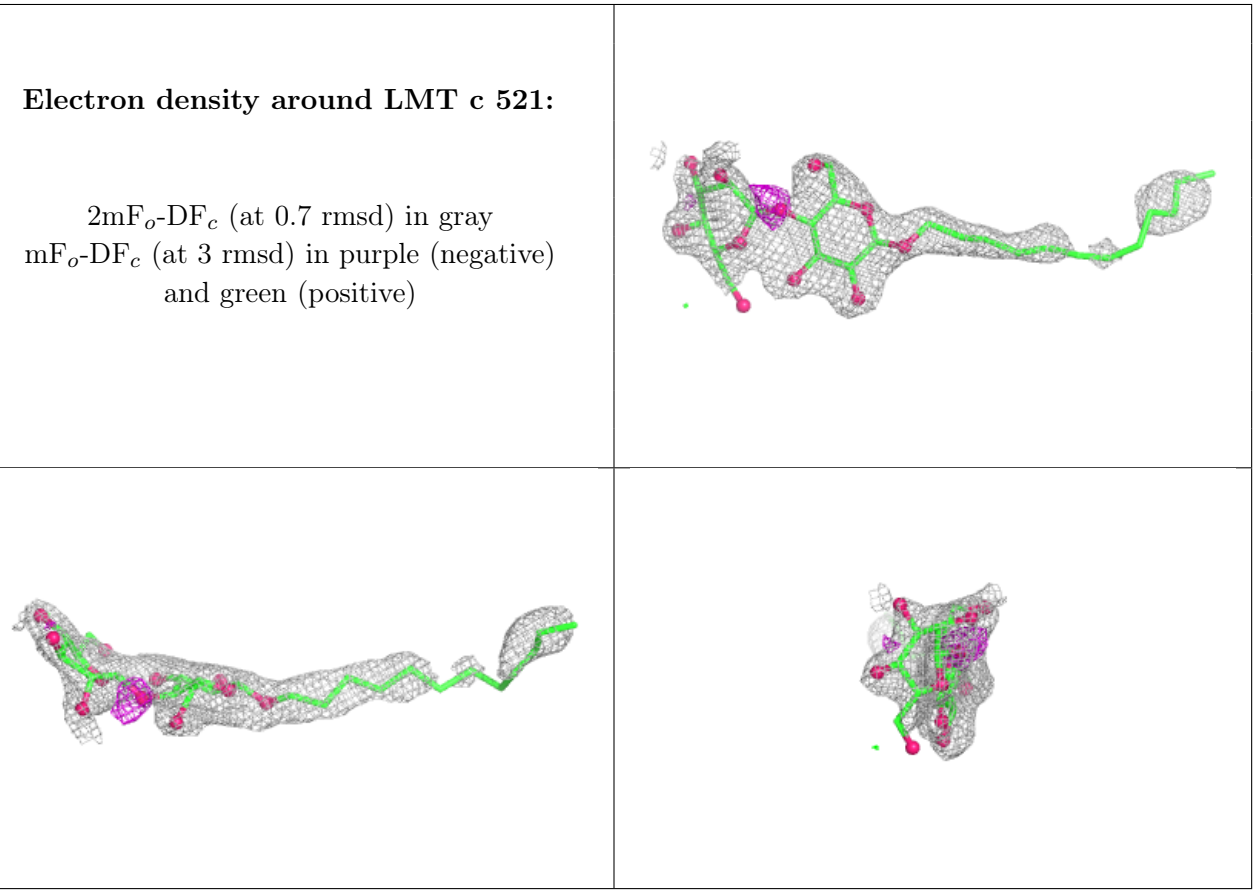
Electron density around LMT m 101:

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



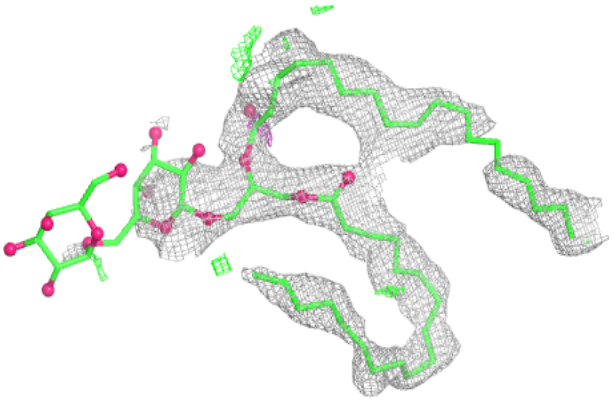
Electron density around LMT c 521:

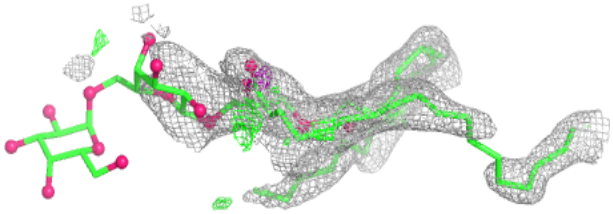
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

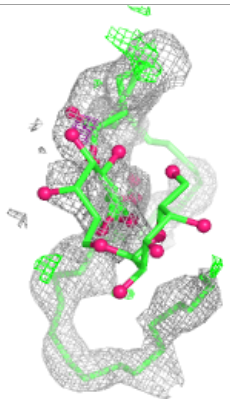


Electron density around DGD D 408:

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

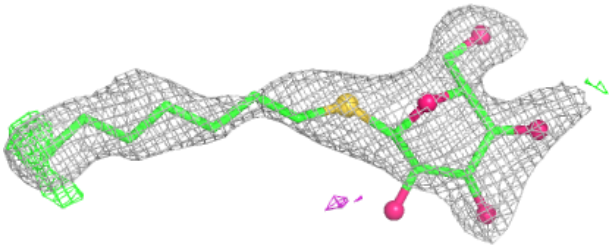


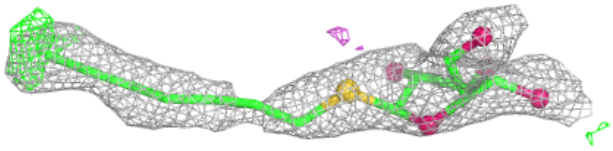


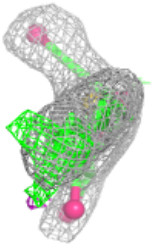


Electron density around HTG C 522:

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

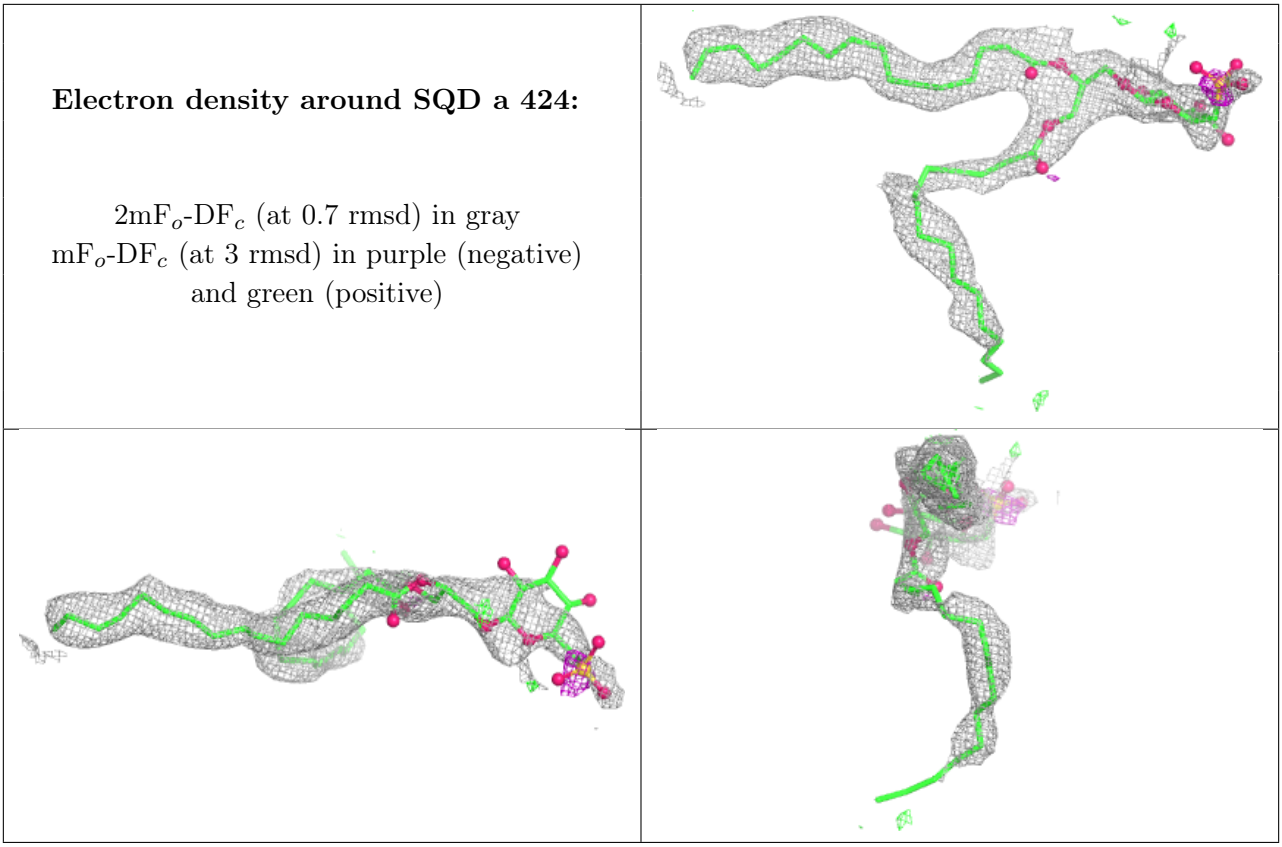






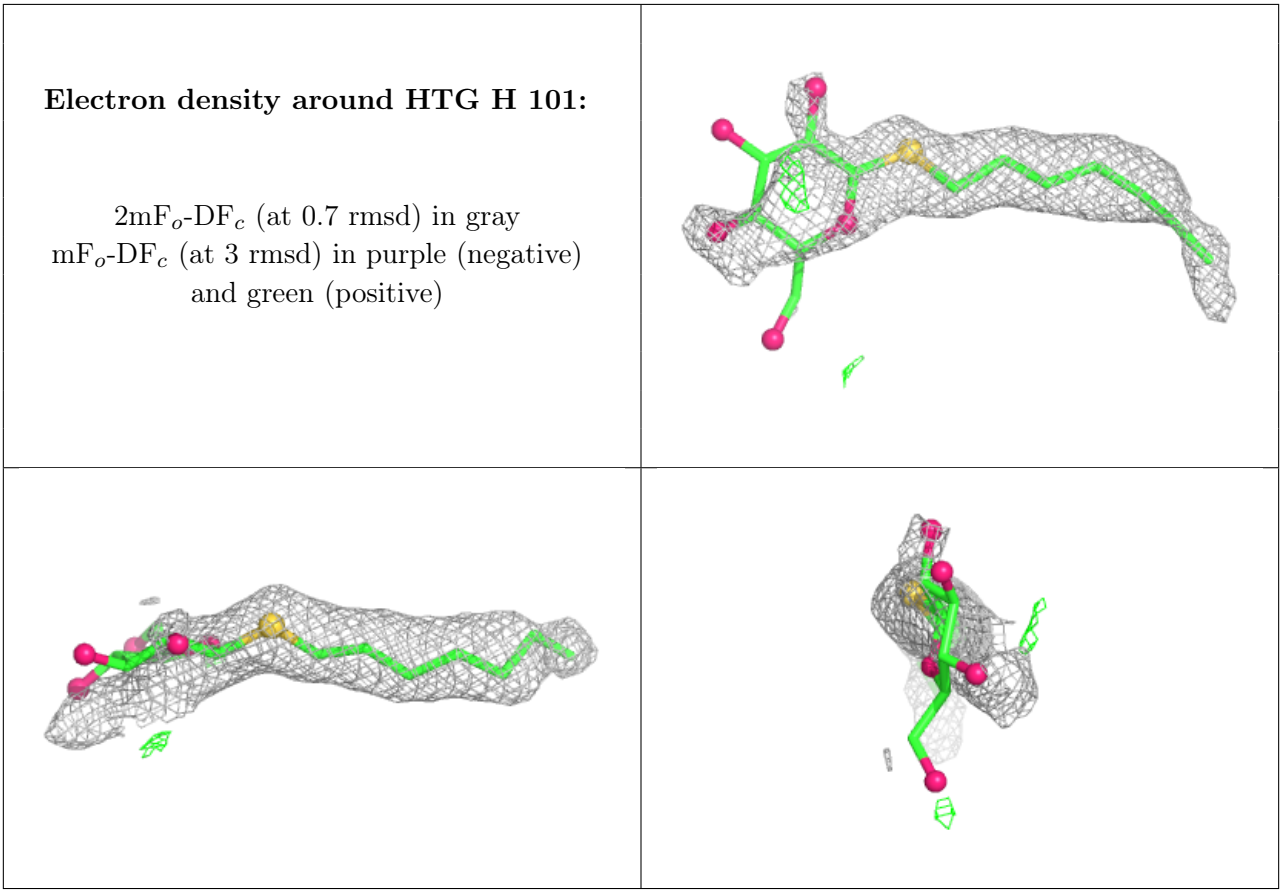
Electron density around SQD a 424:

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



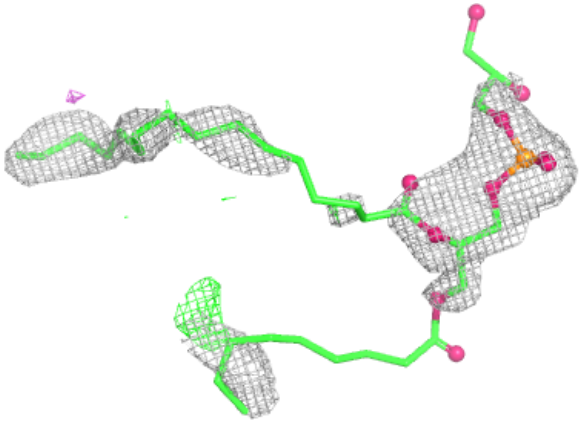
Electron density around HTG H 101:

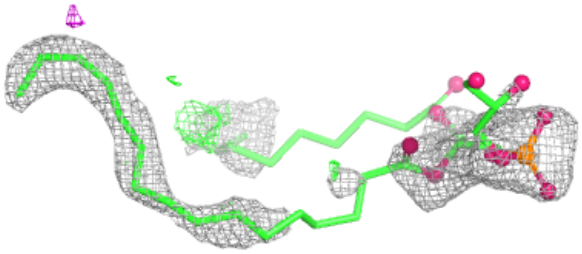
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

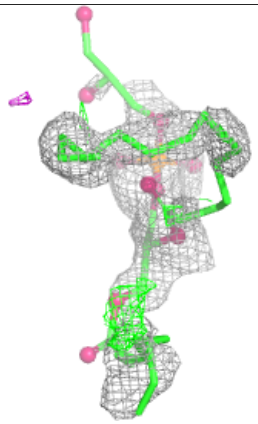


Electron density around LHG e 101:

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

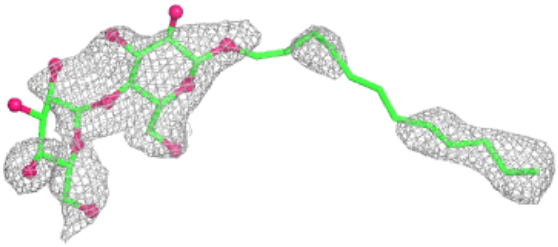


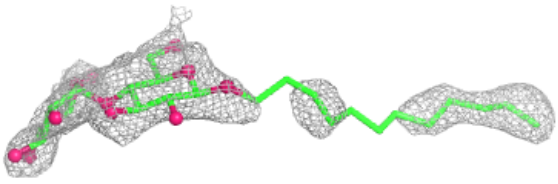


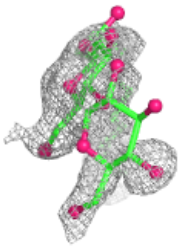


Electron density around LMT f 101:

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

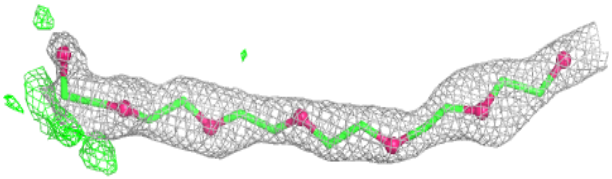


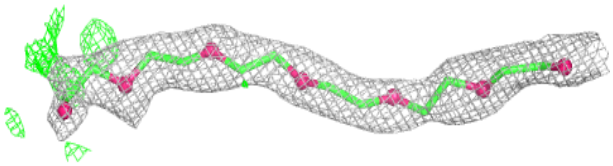


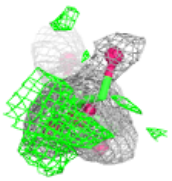


Electron density around P6G j 106:

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

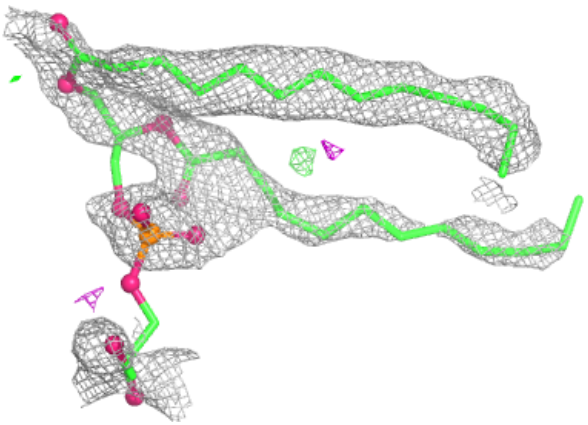


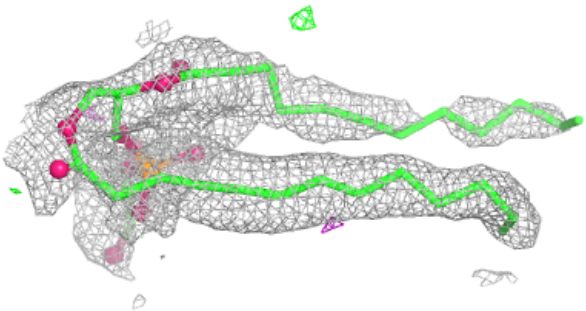


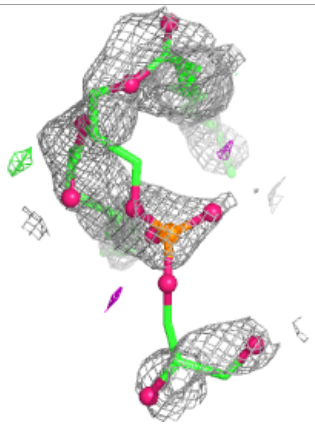


Electron density around LHG A 618:

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

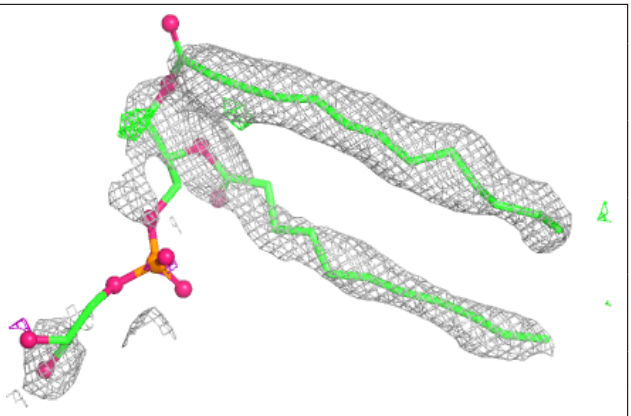


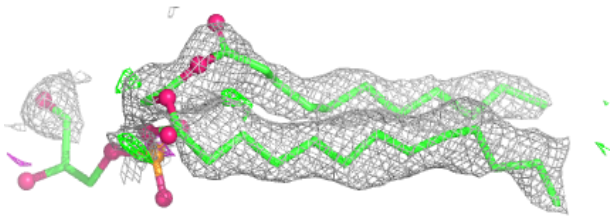


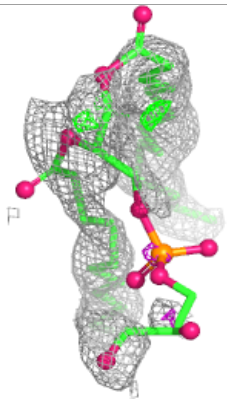


Electron density around LHG a 419:

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

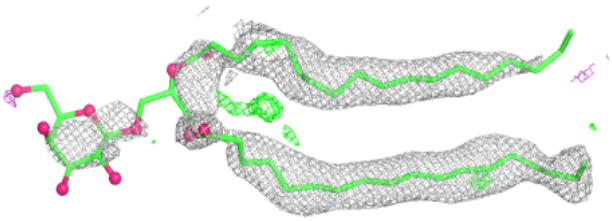


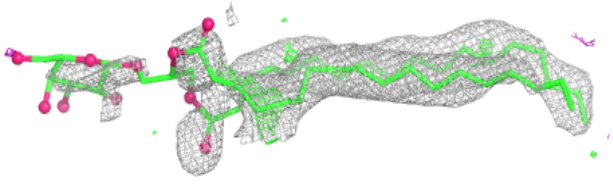


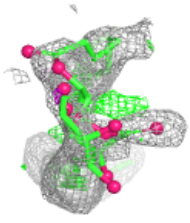


Electron density around LMG d 412:

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

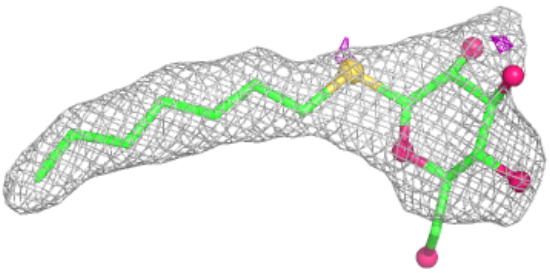


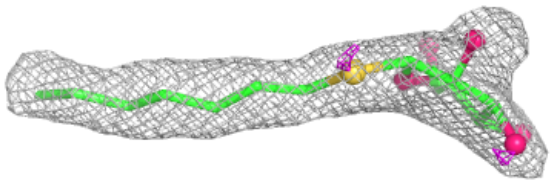


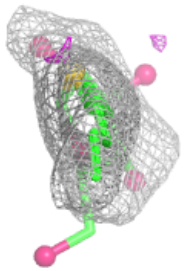


Electron density around HTG B 624:

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

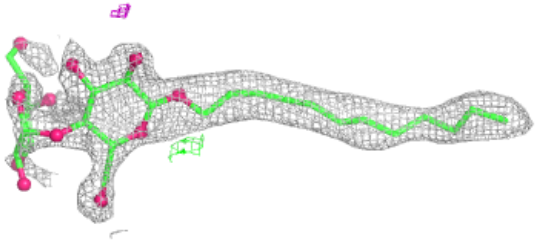


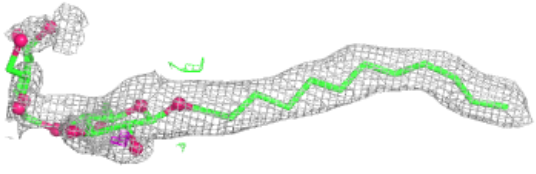


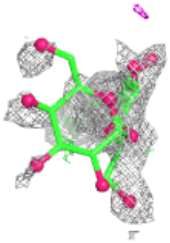


Electron density around LMT J 103:

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

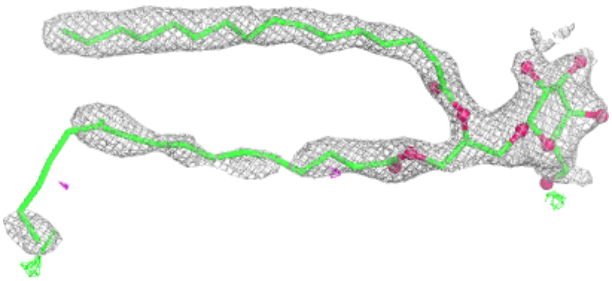


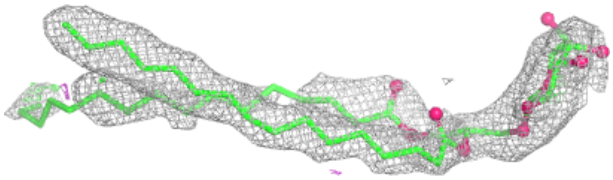


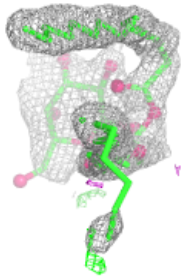


Electron density around LMG c 520:

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

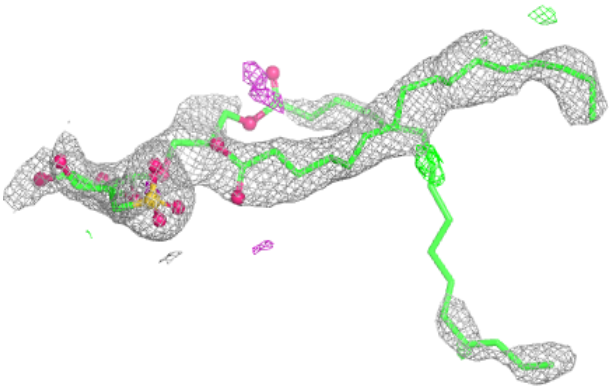


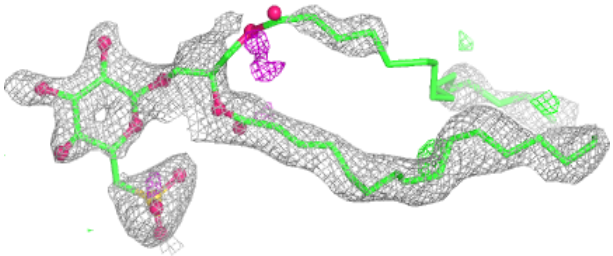


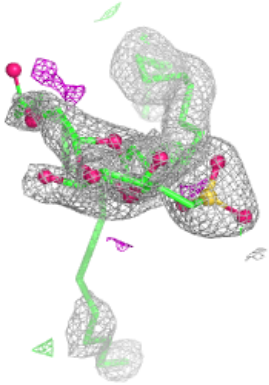


Electron density around SQD F 104:

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

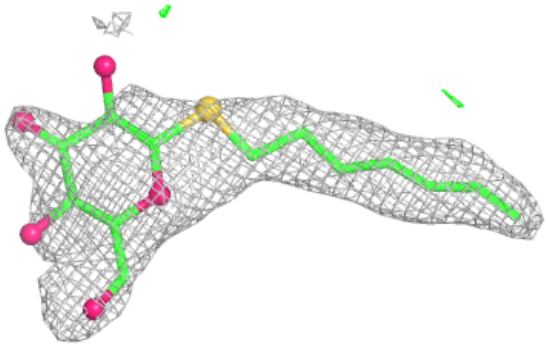


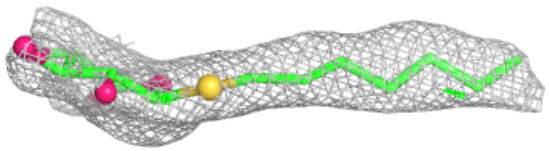


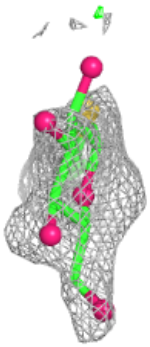


Electron density around HTG b 624:

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

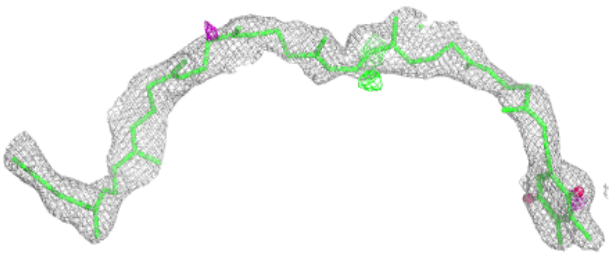


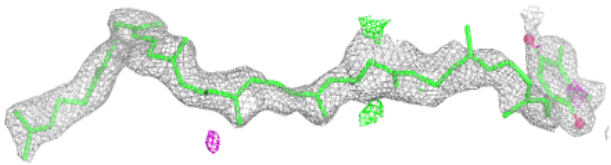


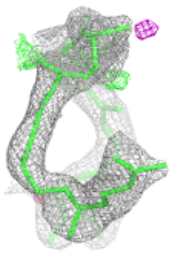


Electron density around PL9 a 412:

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

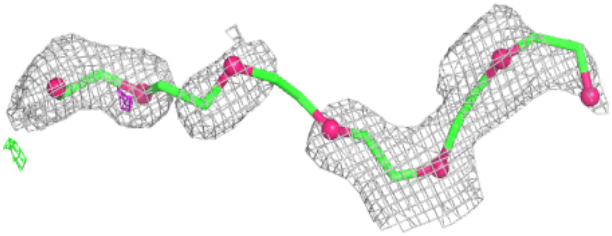


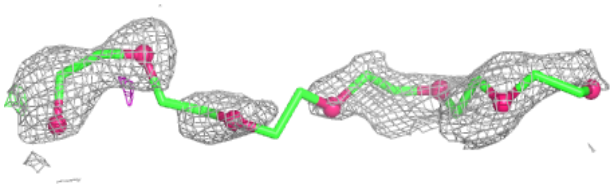


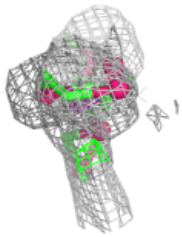


Electron density around P6G B 652:

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

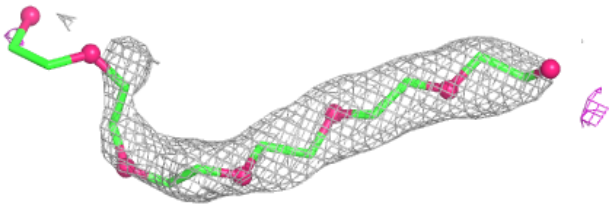


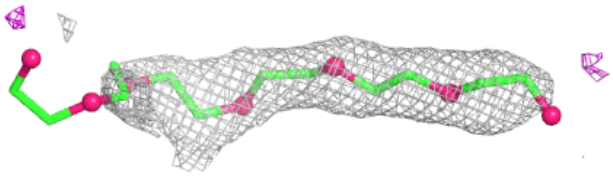


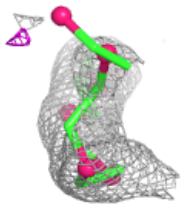


Electron density around P6G I 106:

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

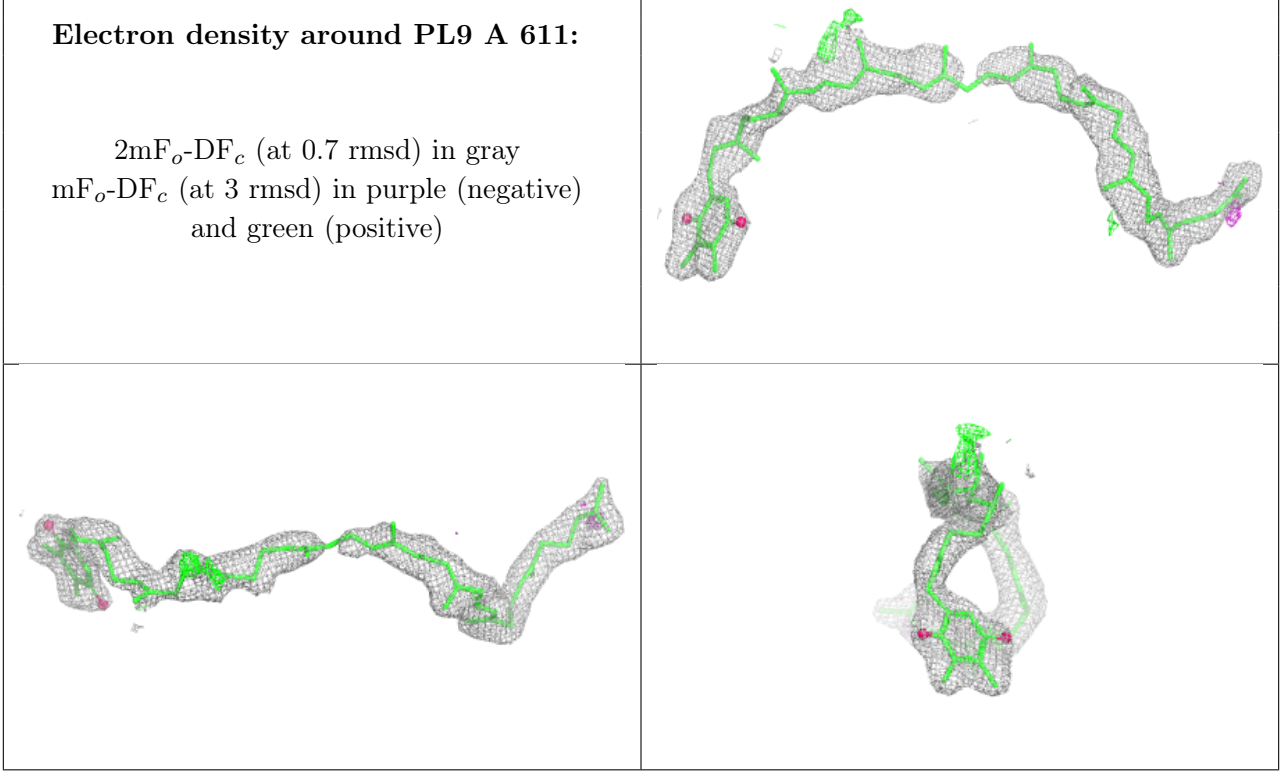






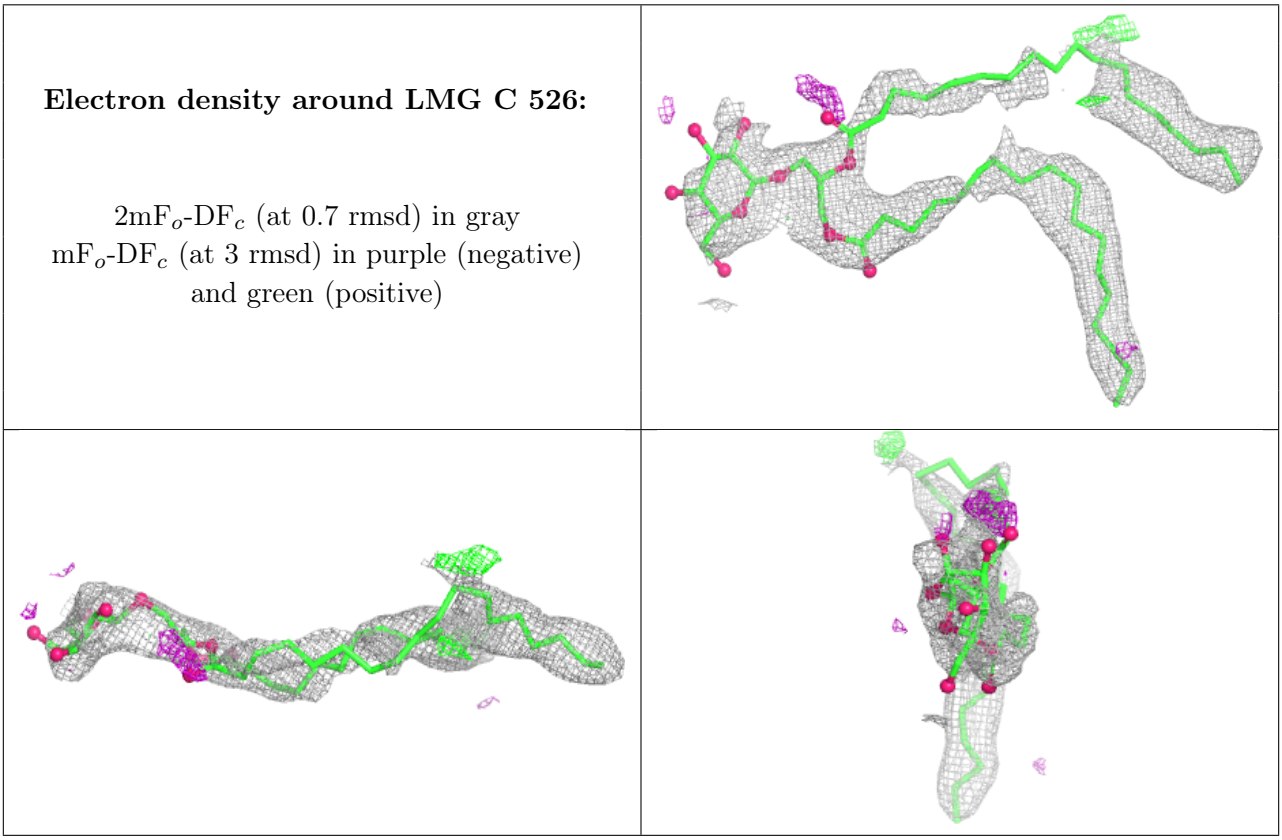
Electron density around PL9 A 611:

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



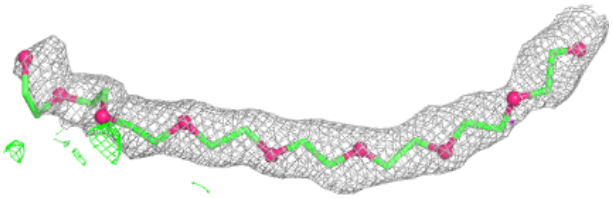
Electron density around LMG C 526:

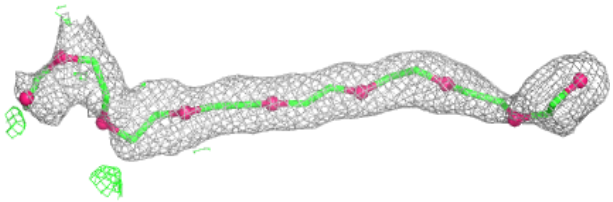
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

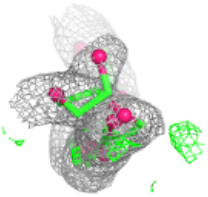


Electron density around PE8 i 107:

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

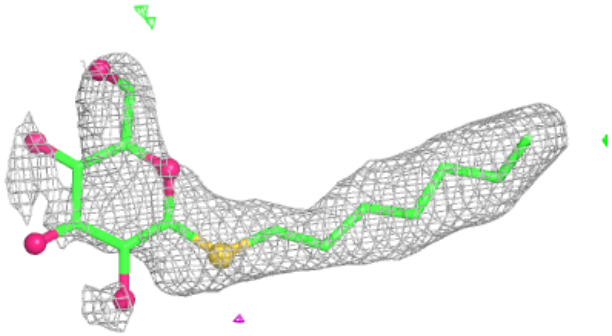


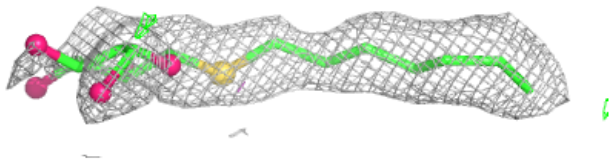


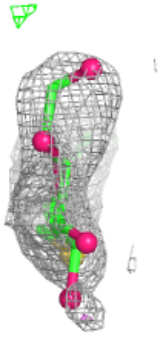


Electron density around HTG B 631:

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

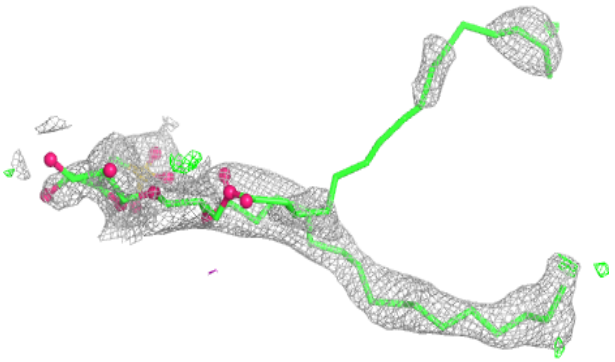


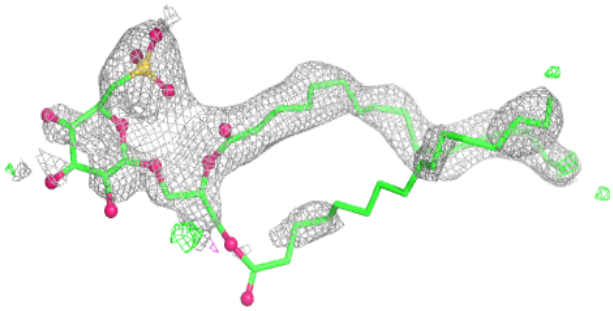


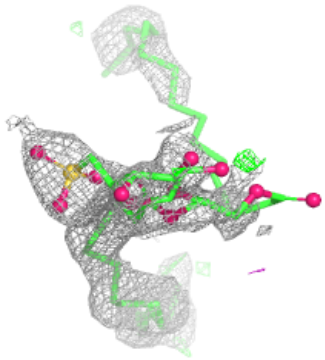


Electron density around SQD x 101:

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

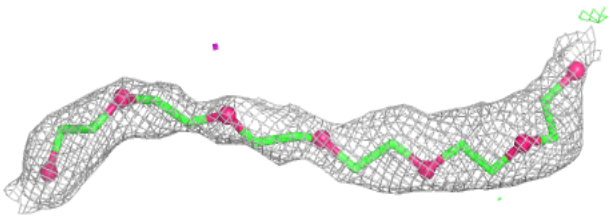


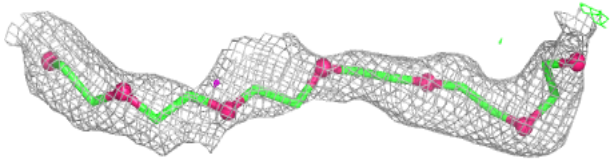


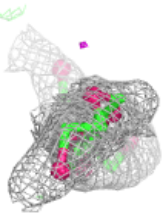


Electron density around P6G A 624:

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

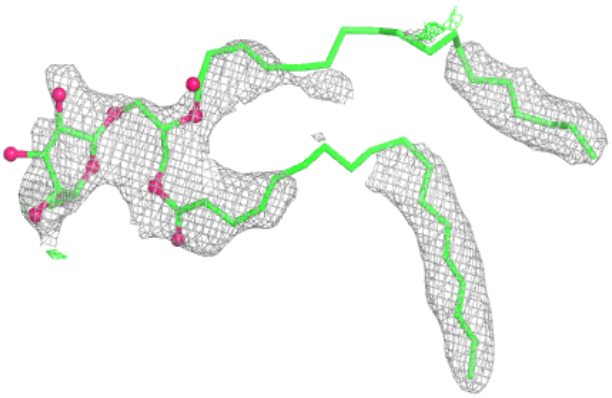


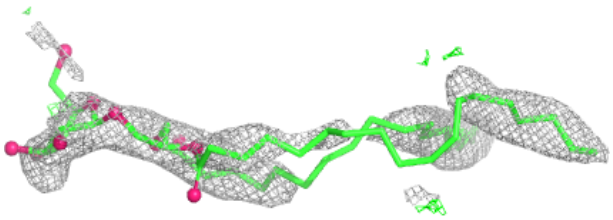


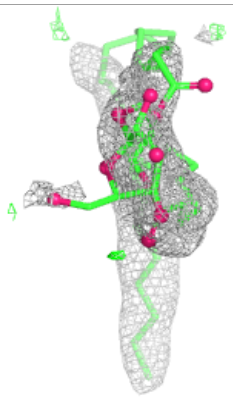


Electron density around LMG z 101:

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

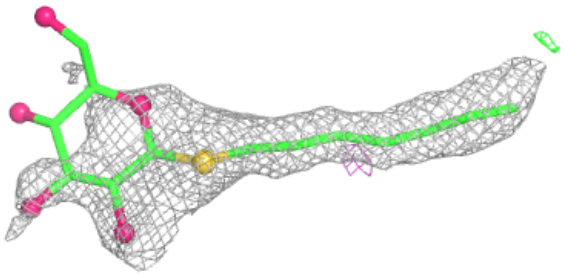


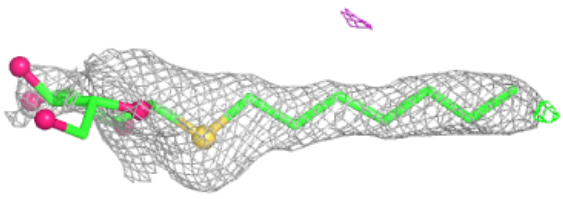


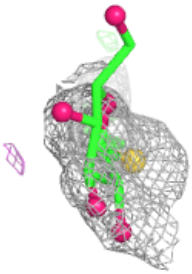


Electron density around HTG C 532:

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

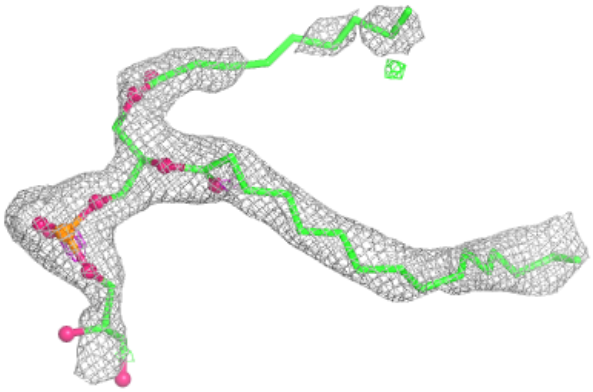


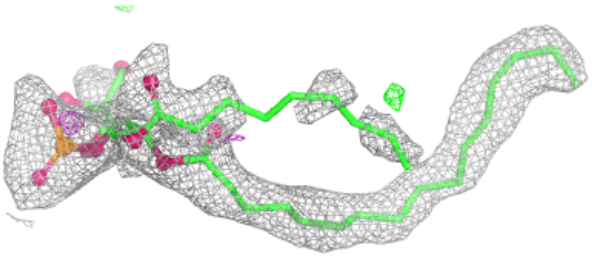


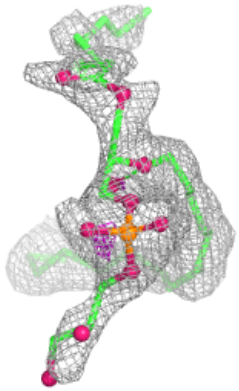


Electron density around LHG E 101:

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

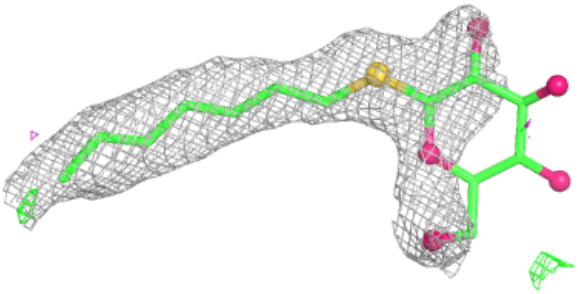


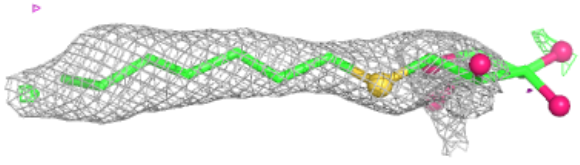


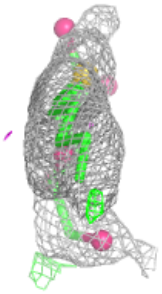


Electron density around HTG b 632:

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

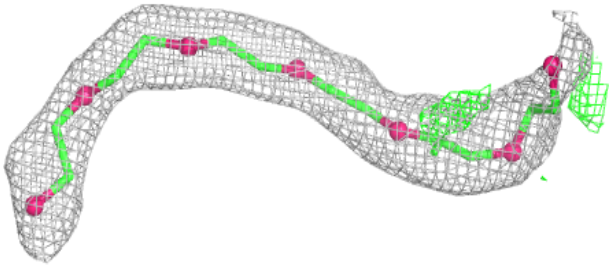


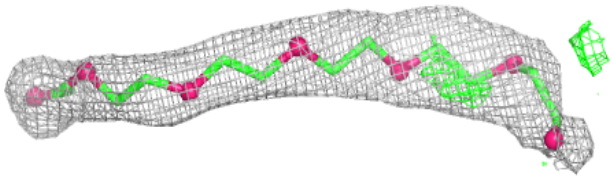


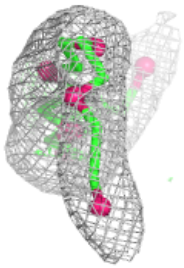


Electron density around P6G b 648:

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

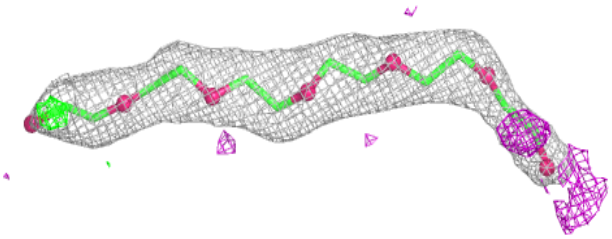


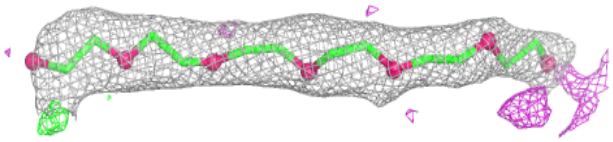


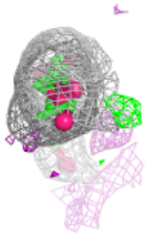


Electron density around P6G d 415:

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

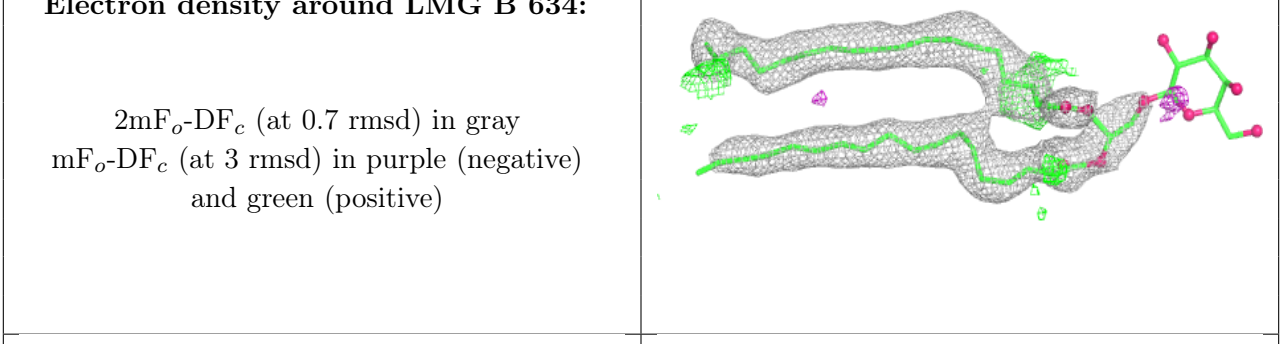


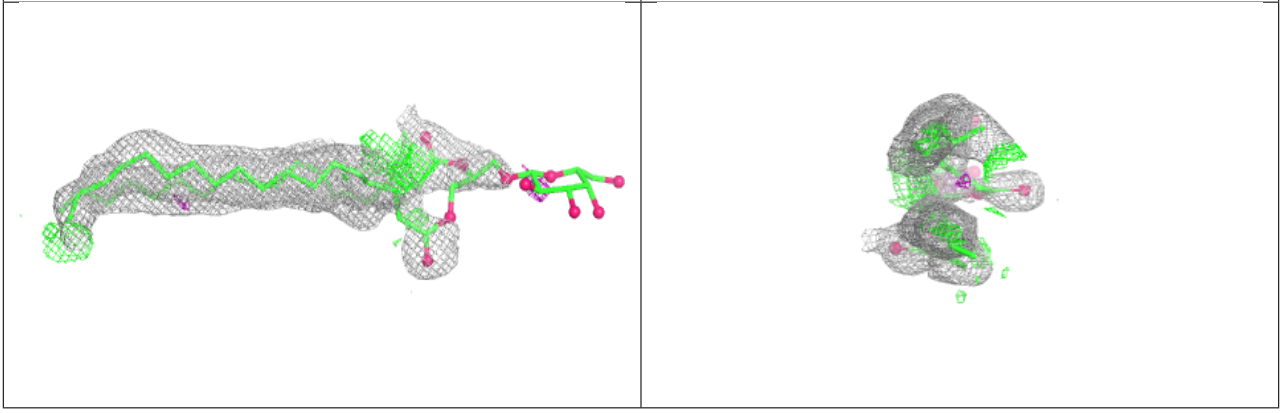




Electron density around LMG B 634:

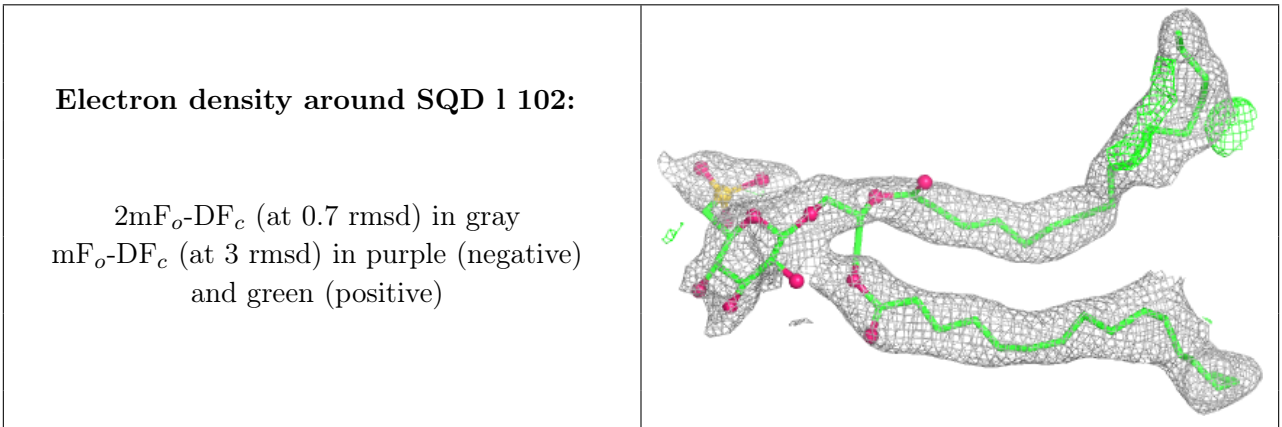
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

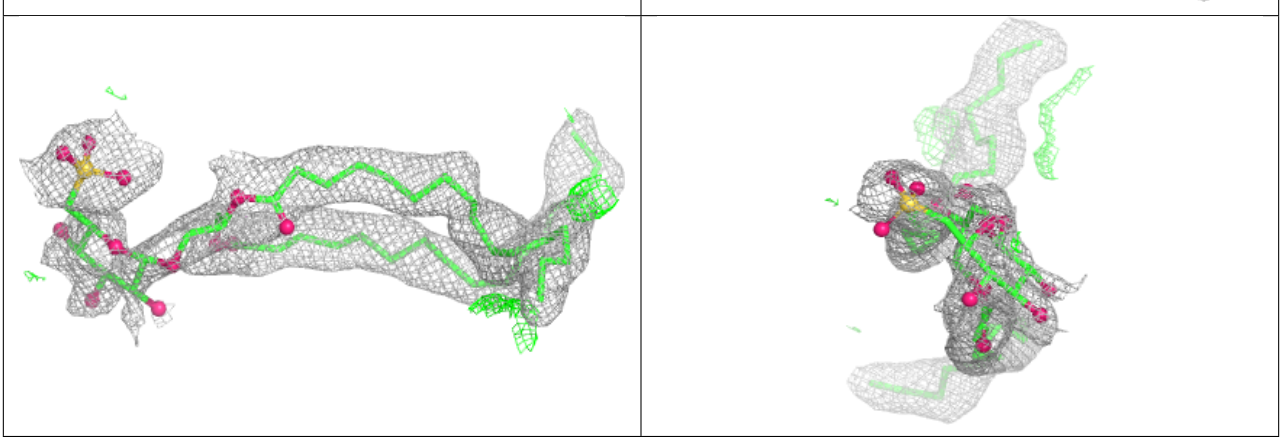




Electron density around SQD l 102:

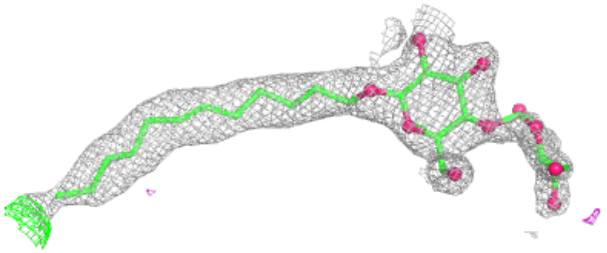
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

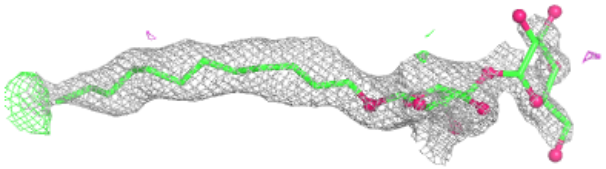


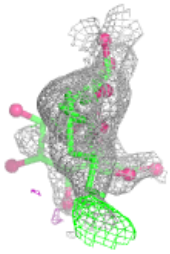


Electron density around LMT B 622:

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

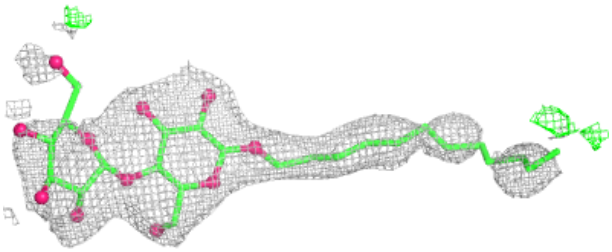


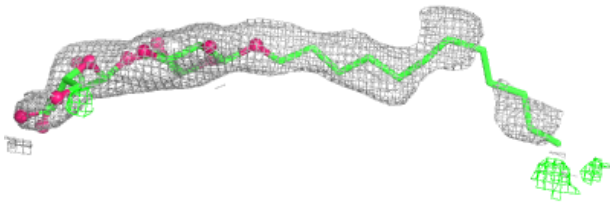


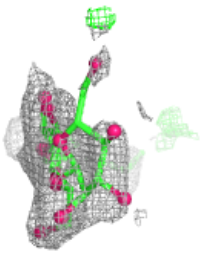


Electron density around LMT I 101:

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

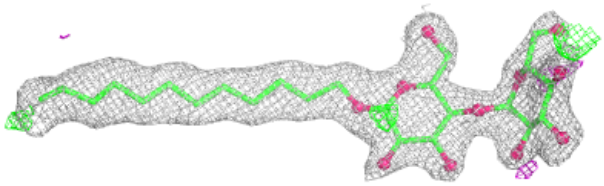


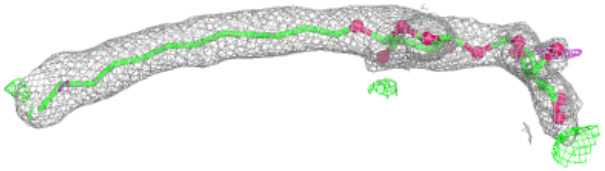


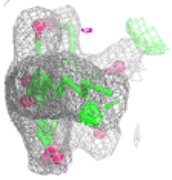


Electron density around LMT M 101:

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

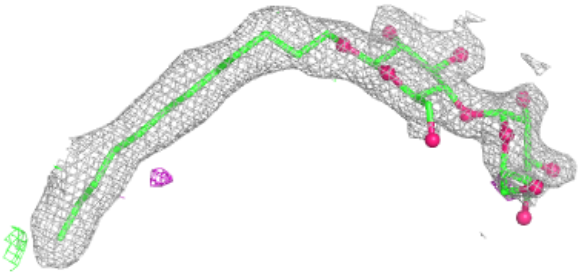


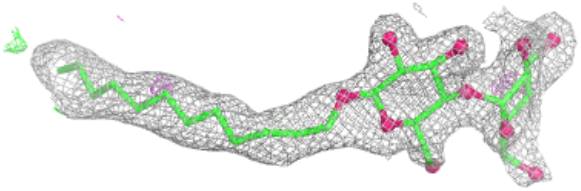


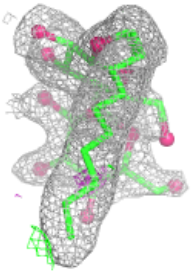


Electron density around LMT M 102:

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

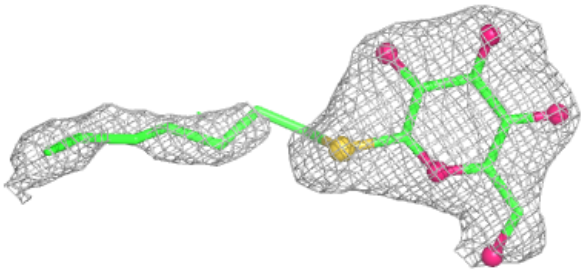


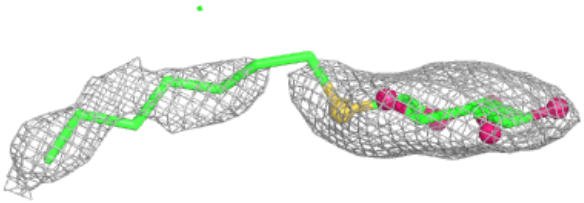


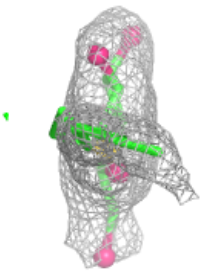


Electron density around HTG c 522:

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

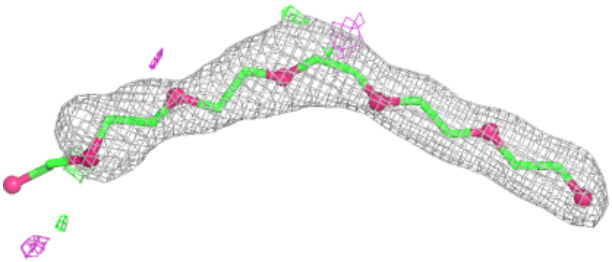


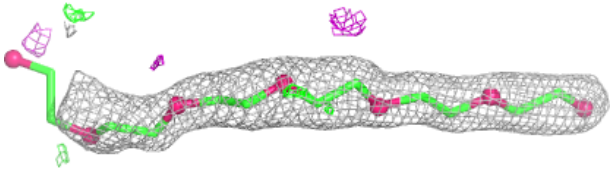


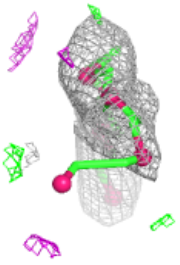


Electron density around P6G d 416:

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







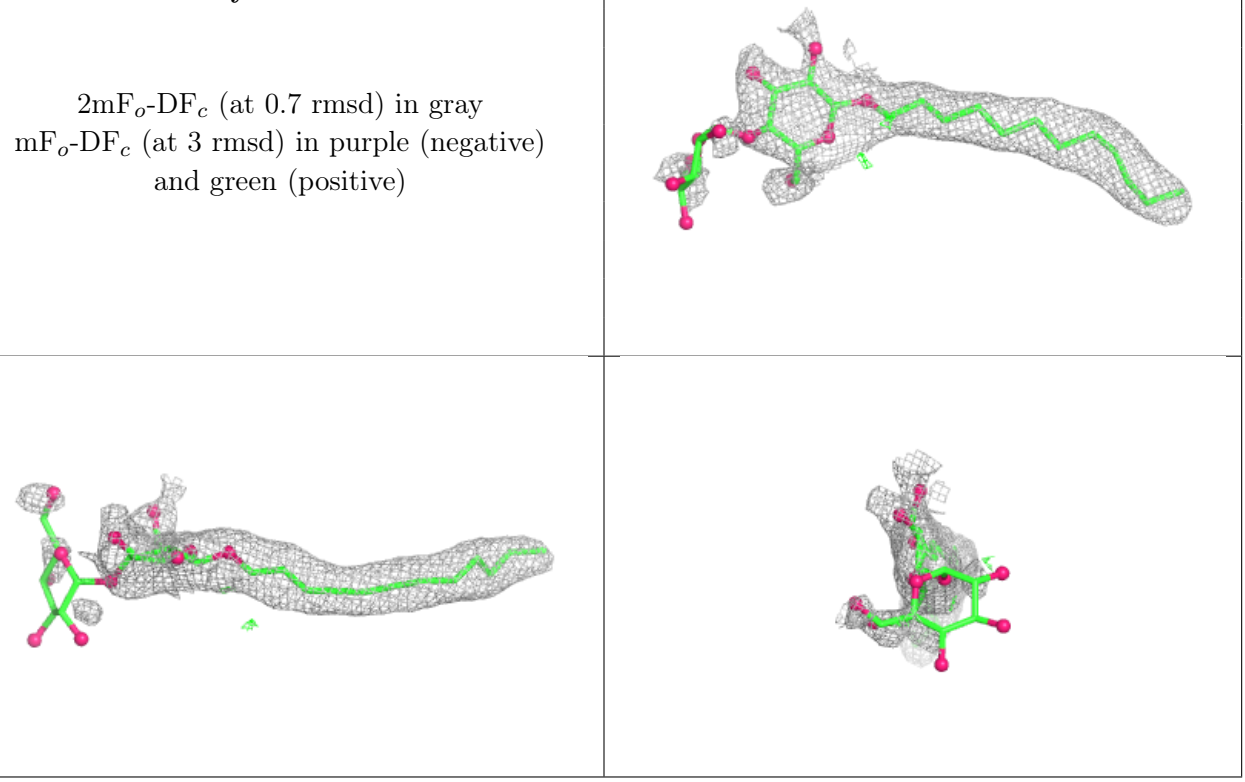
Electron density around SQD b 633:

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



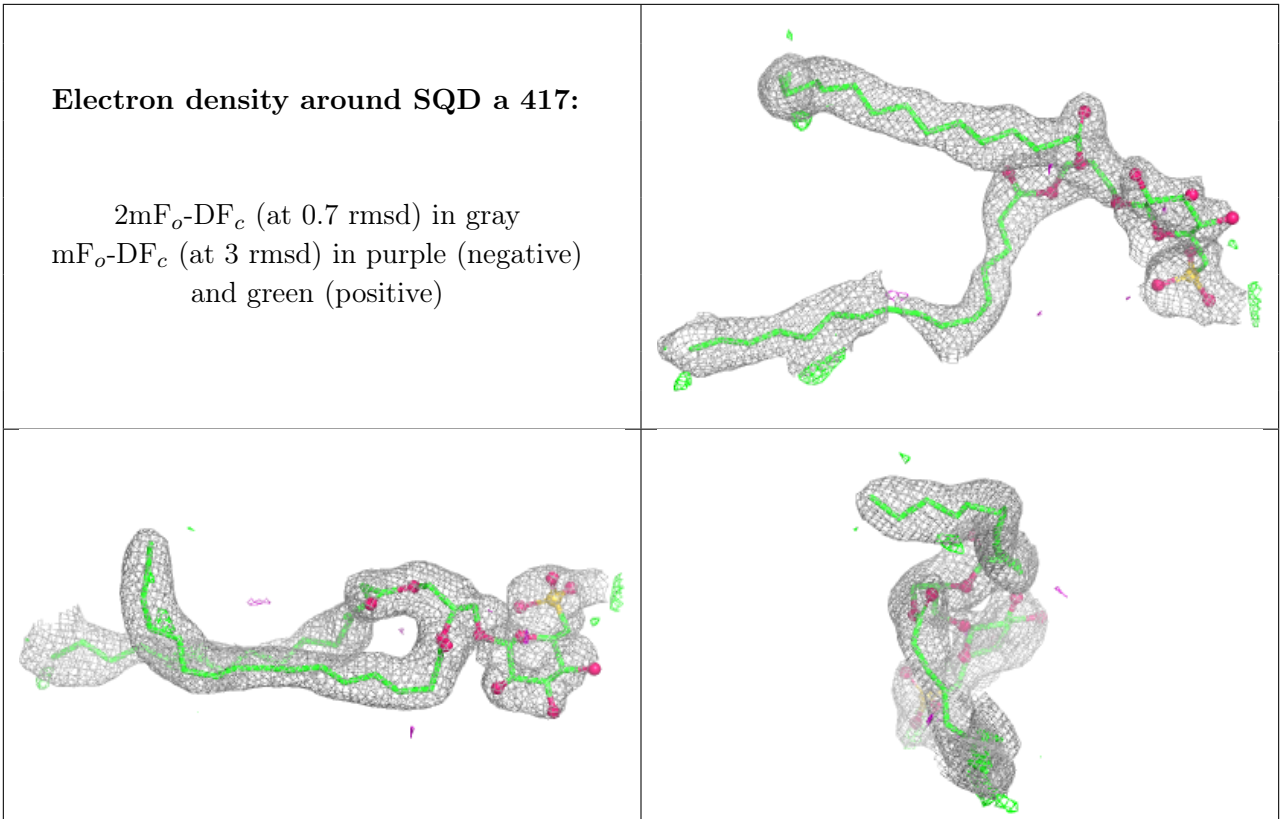
Electron density around LMT b 622:

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



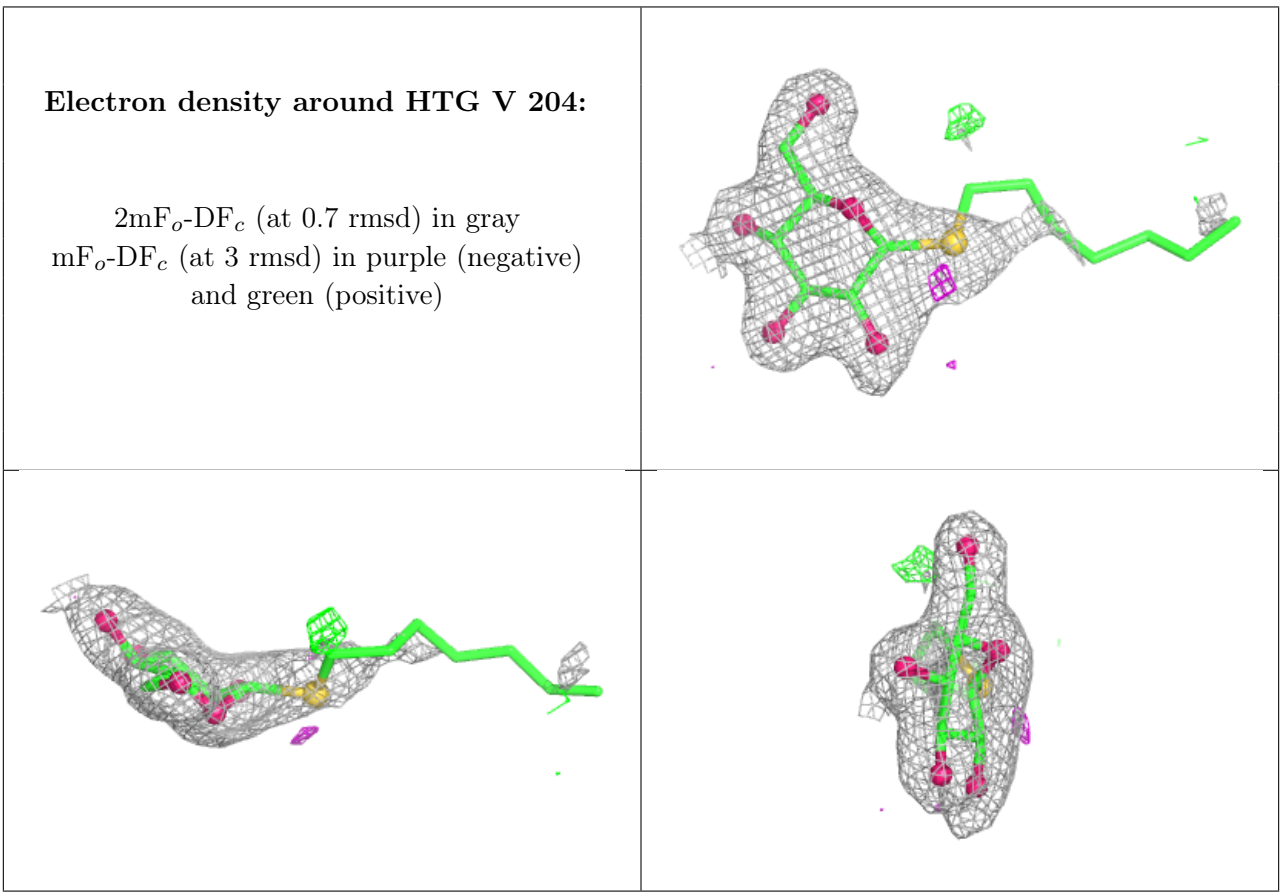
Electron density around SQD a 417:

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



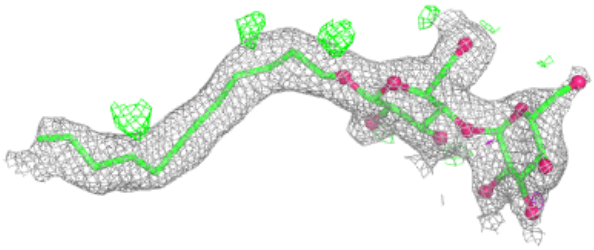
Electron density around HTG V 204:

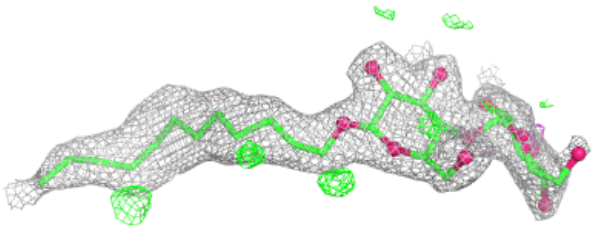
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

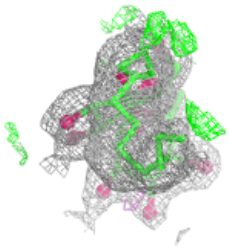


Electron density around LMT a 401:

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

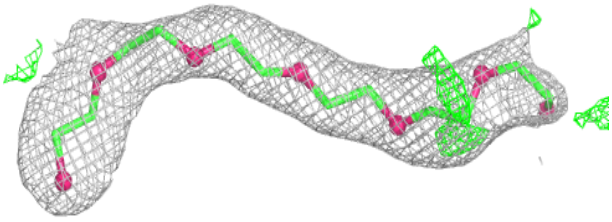


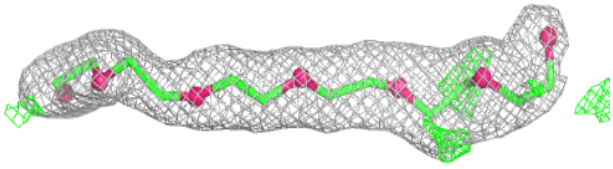


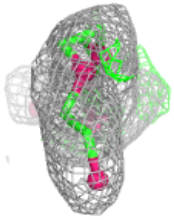


Electron density around P6G T 105:

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

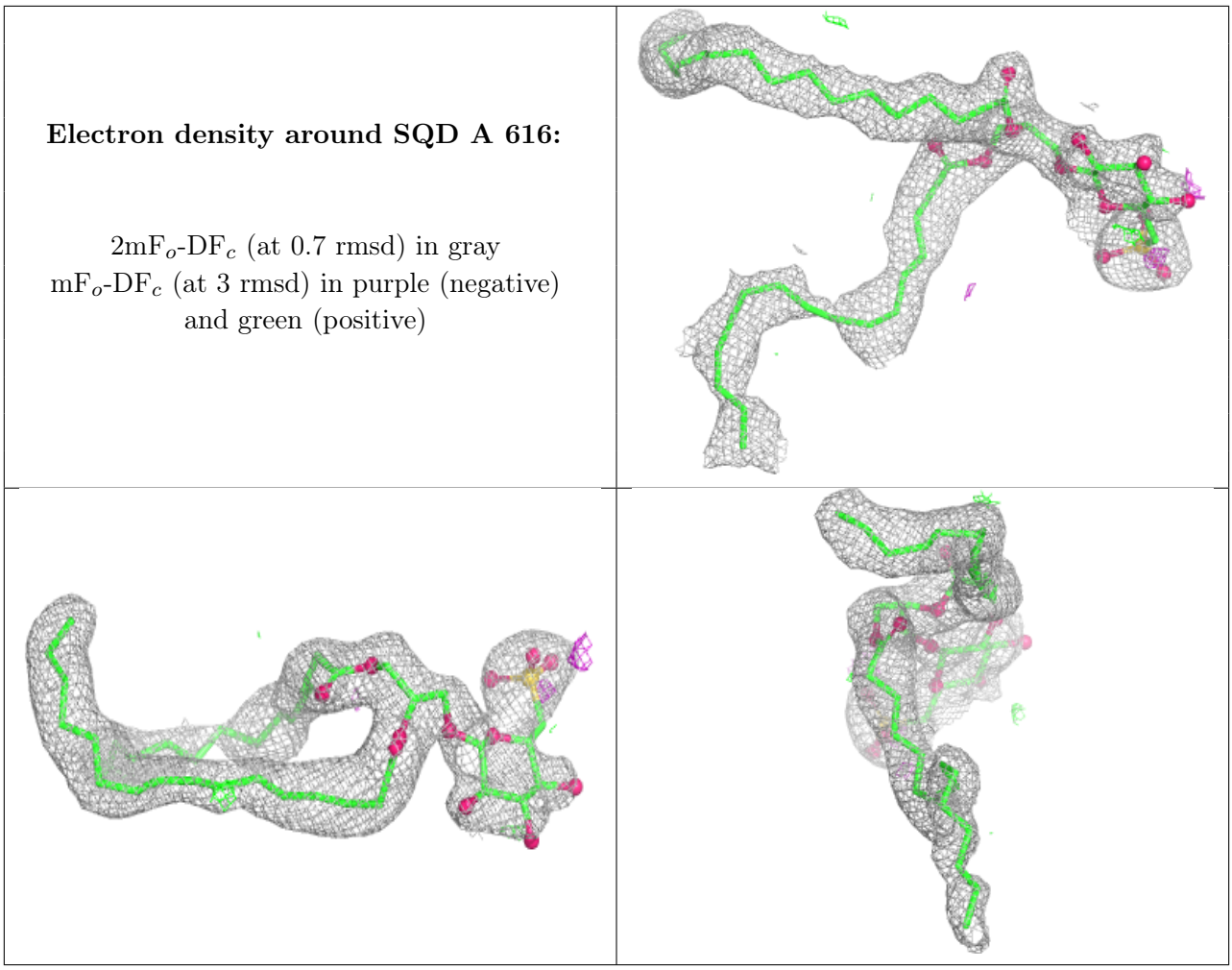






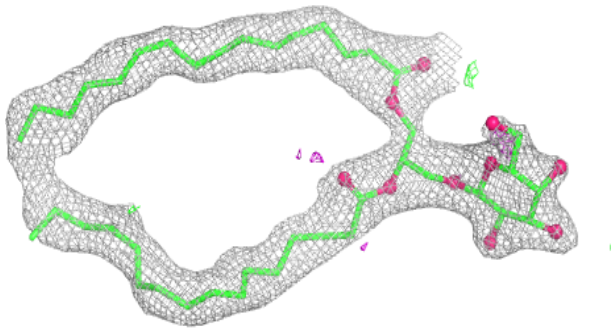
Electron density around SQD A 616:

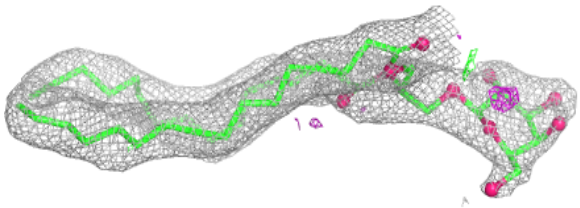
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

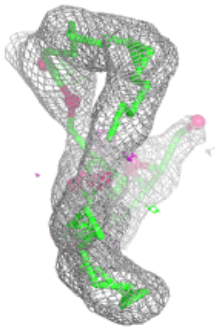


Electron density around LMG a 414:

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

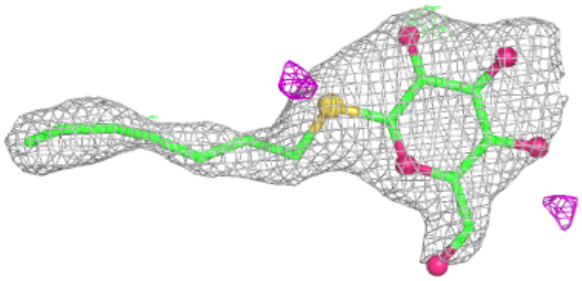


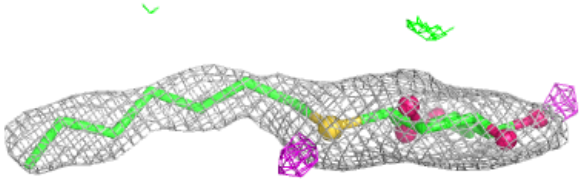


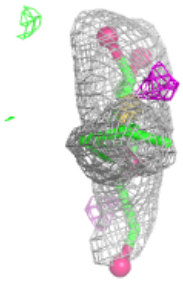


Electron density around HTG C 521:

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

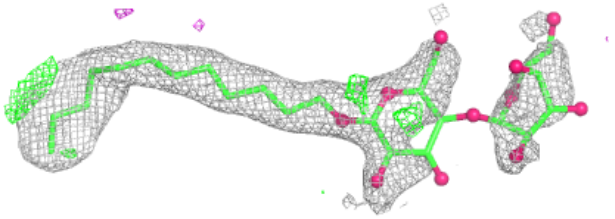


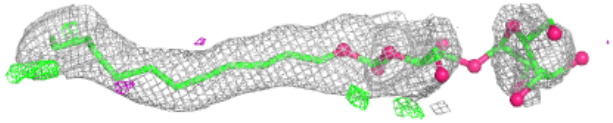


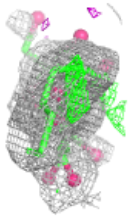


Electron density around LMT t 103:

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

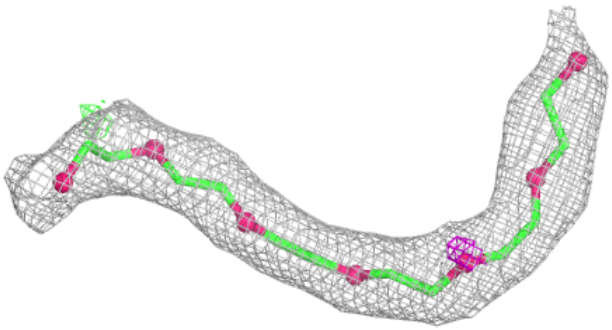


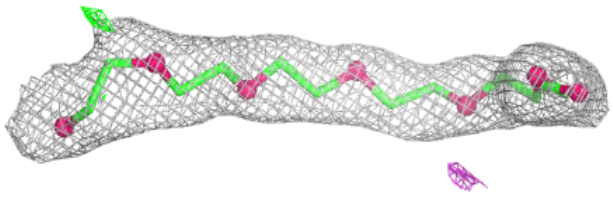


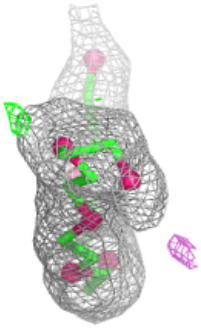


Electron density around P6G B 651:

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

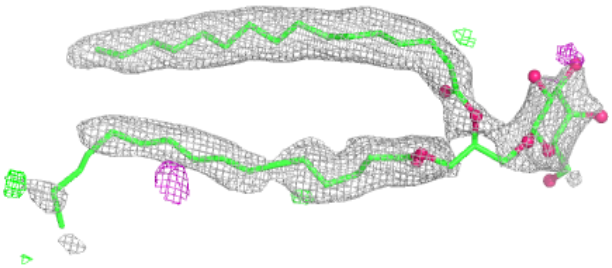


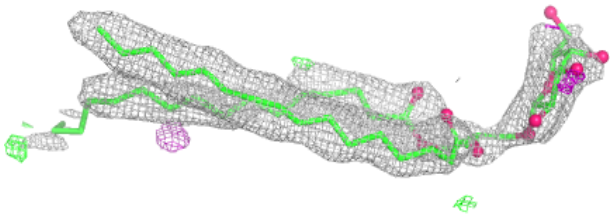


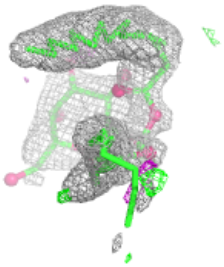


Electron density around LMG C 520:

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

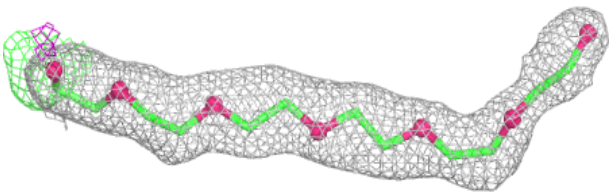


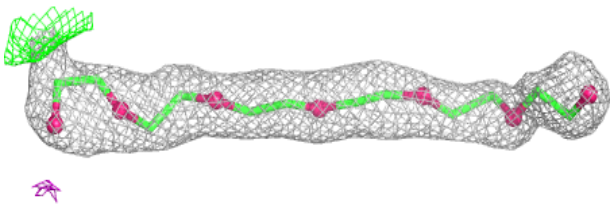


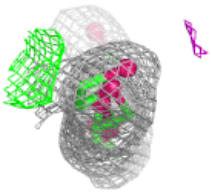


Electron density around P6G D 416:

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

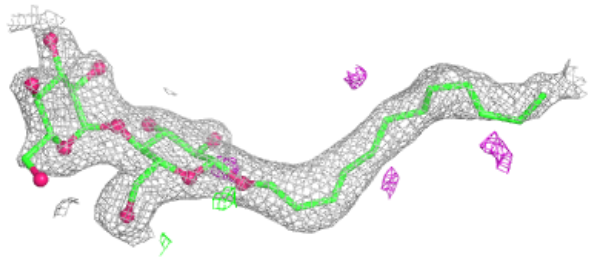


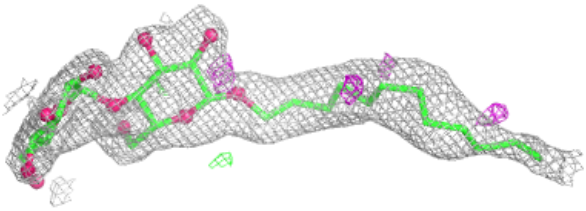


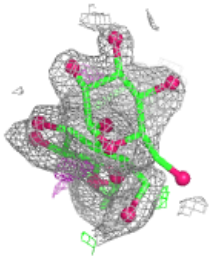


Electron density around LMT A 617:

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

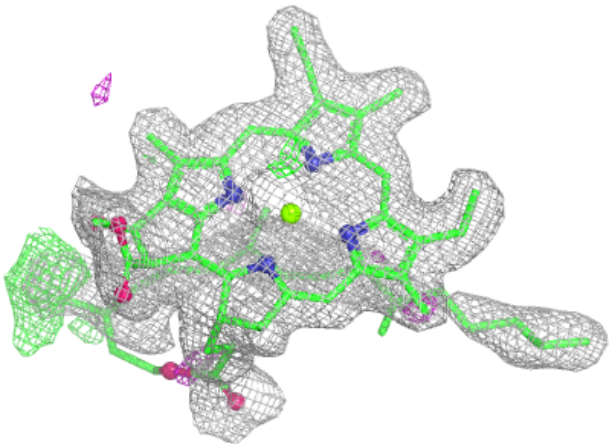


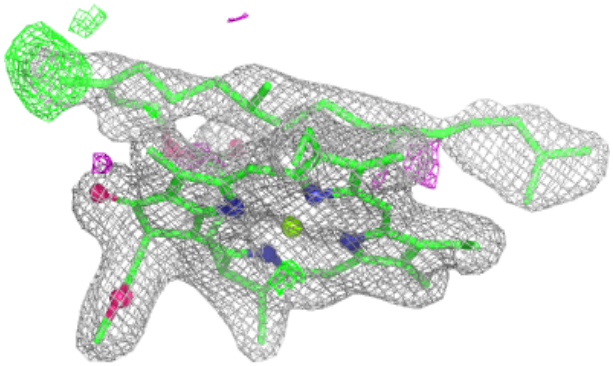


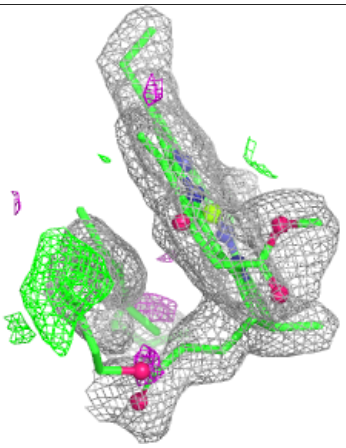


Electron density around CLA b 602:

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

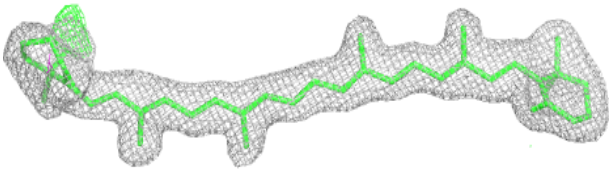


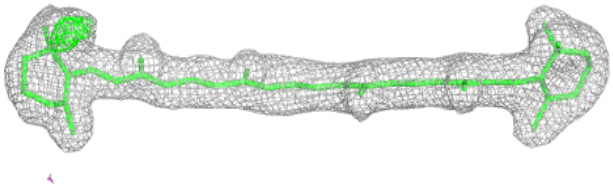


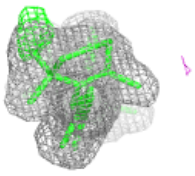


Electron density around BCR C 514:

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

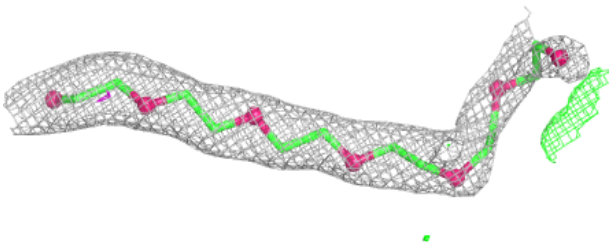


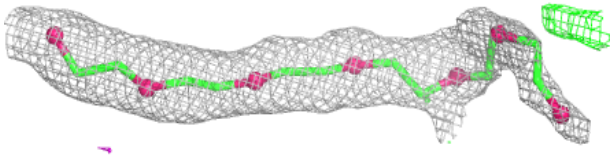


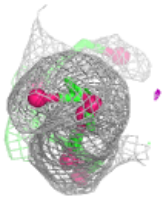


Electron density around P6G A 623:

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

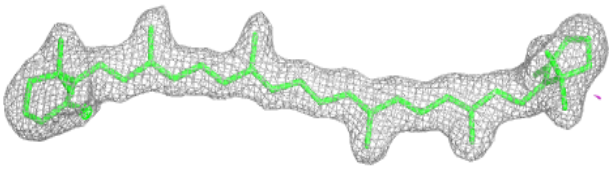


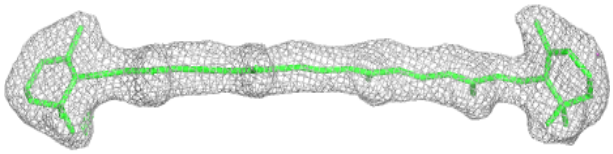


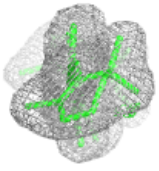


Electron density around BCR c 514:

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

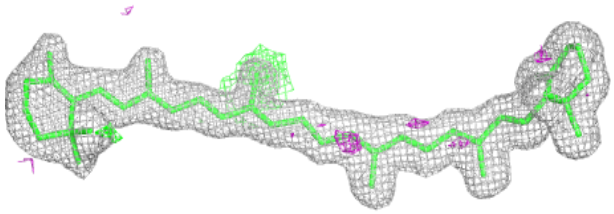


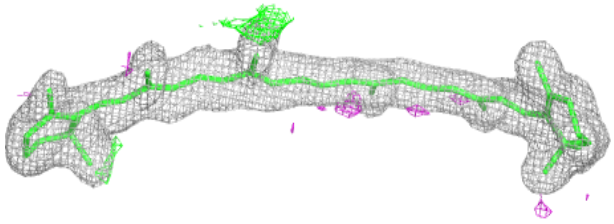


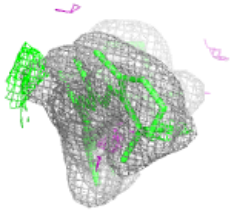


Electron density around BCR t 102:

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

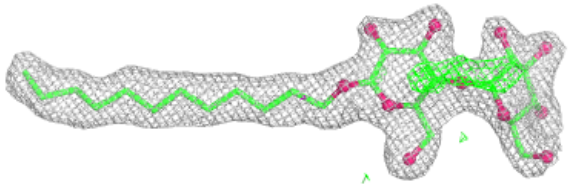


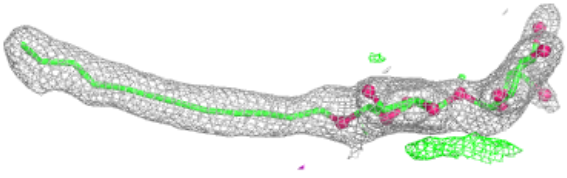


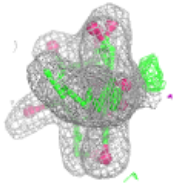


Electron density around LMT m 102:

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

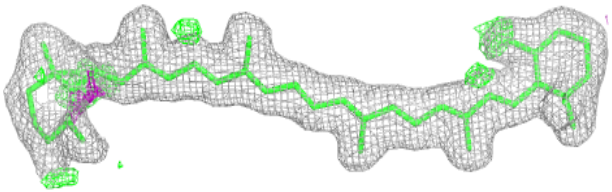


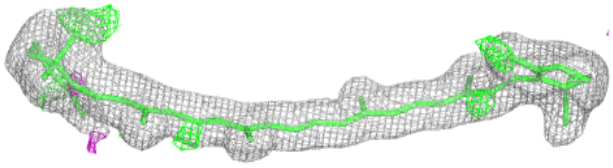


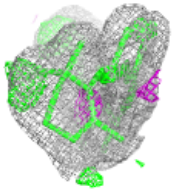


Electron density around BCR D 406:

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

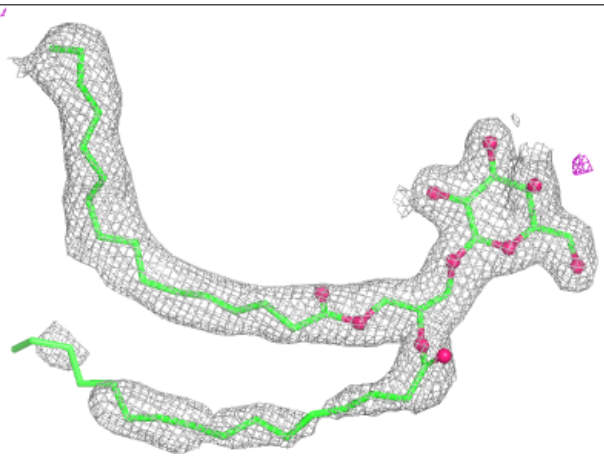


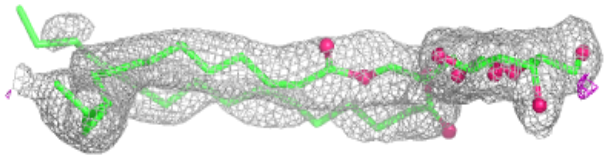


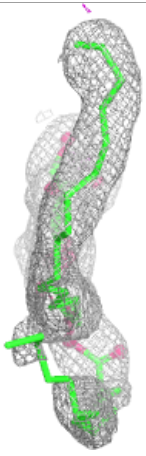


Electron density around LMG c 519:

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

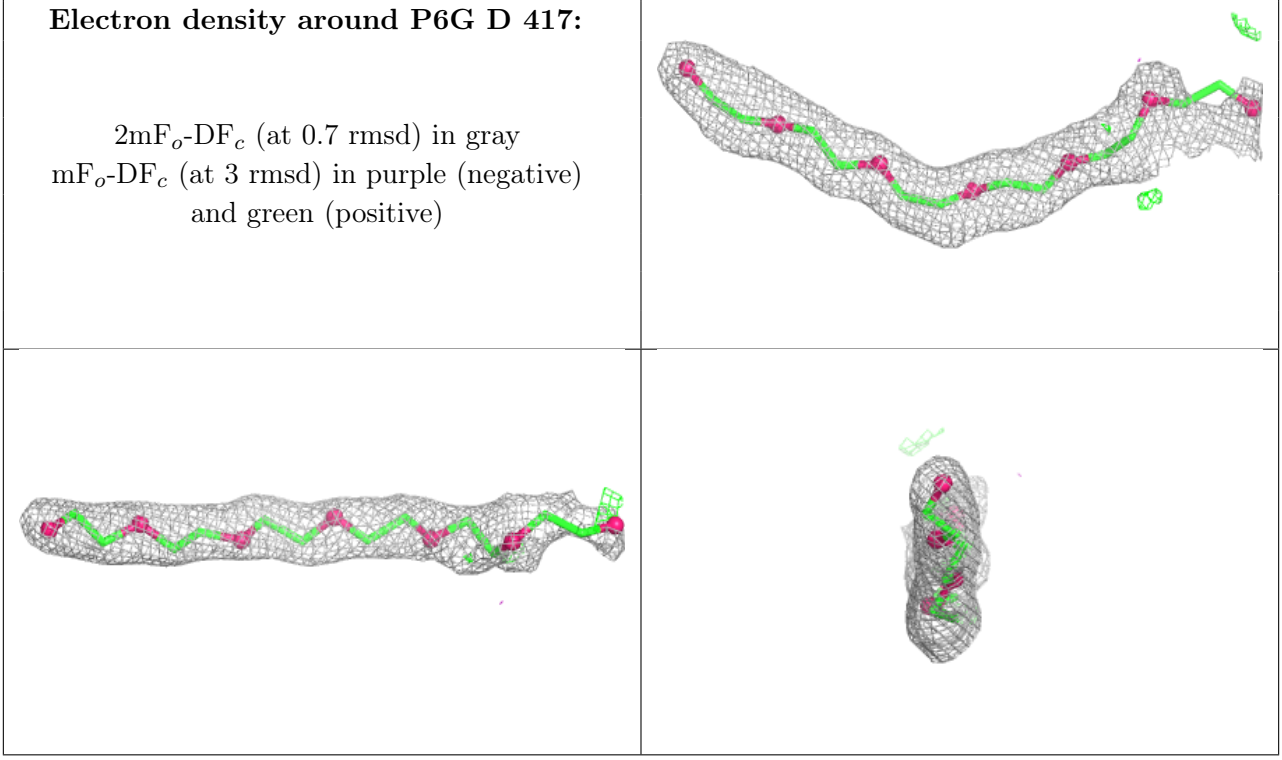






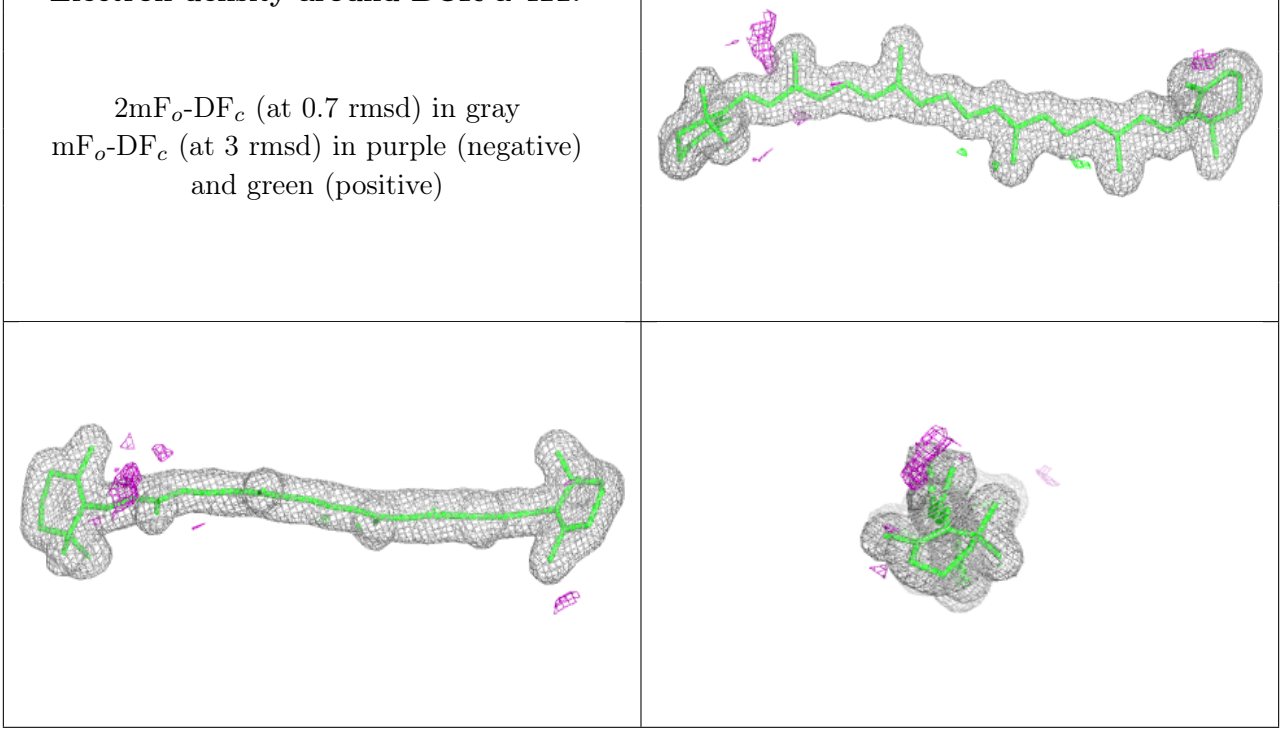
Electron density around P6G D 417:

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



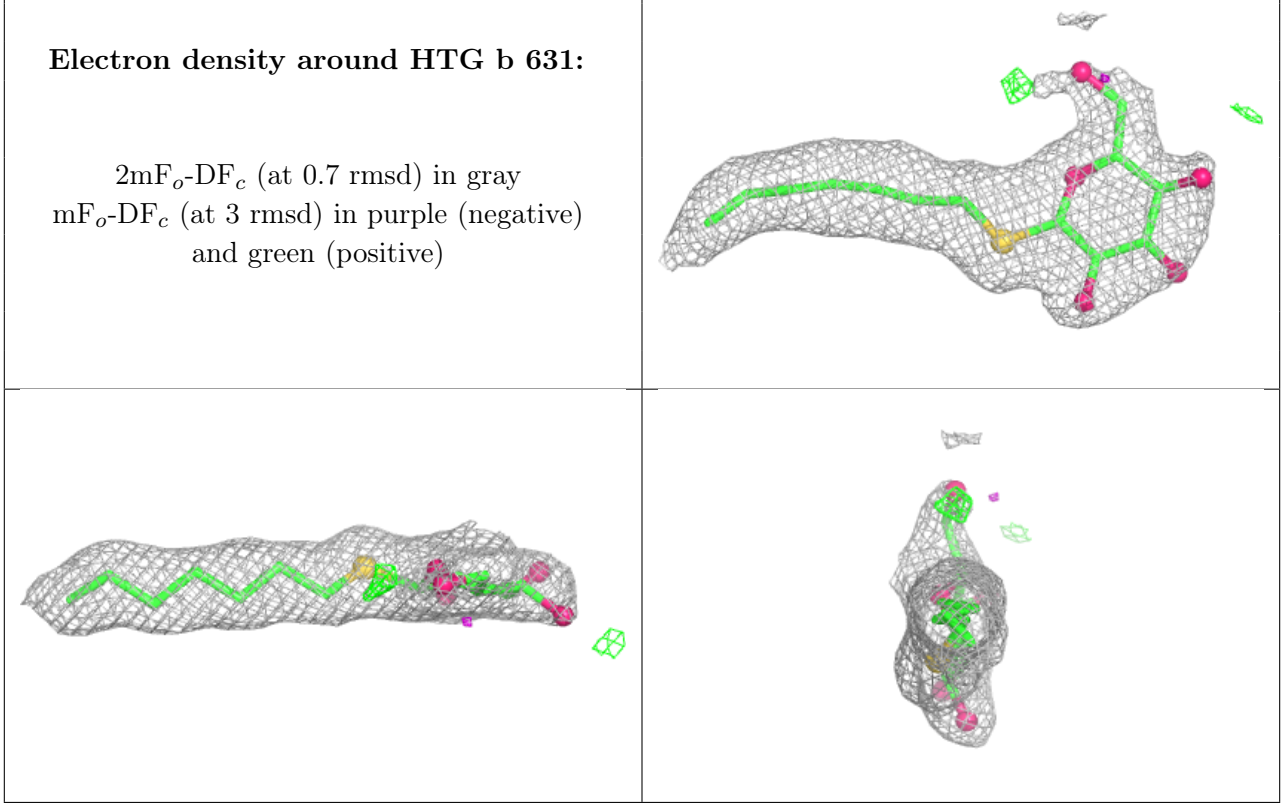
Electron density around BCR a 411:

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



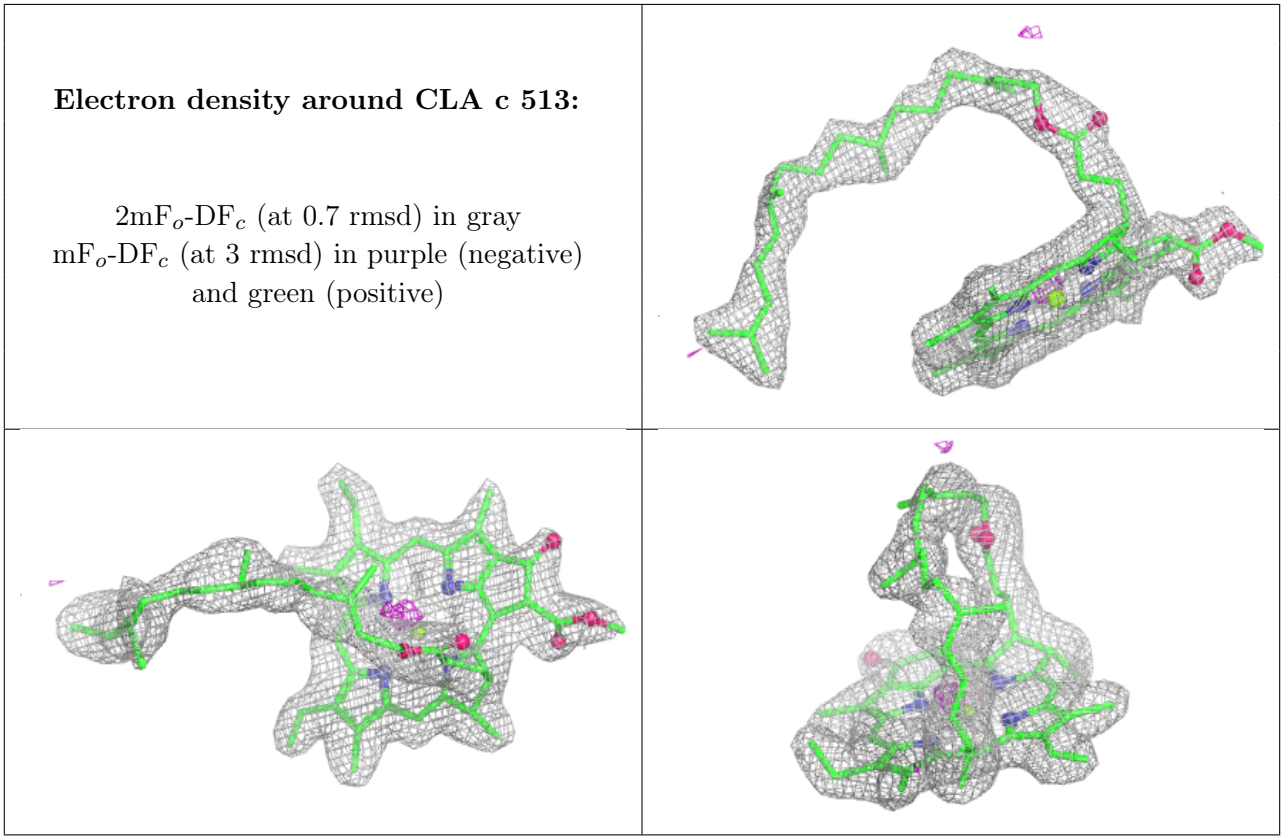
Electron density around HTG b 631:

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



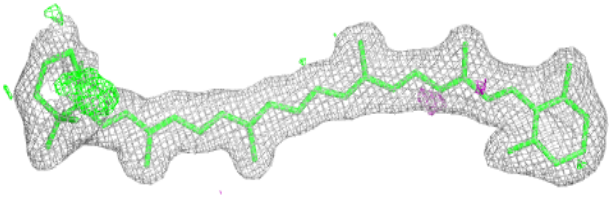
Electron density around CLA c 513:

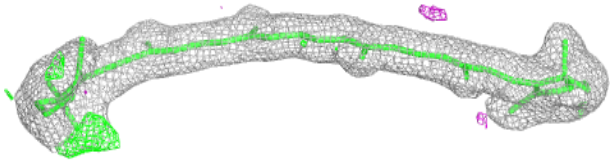
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

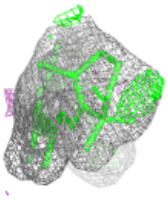


Electron density around BCR d 406:

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

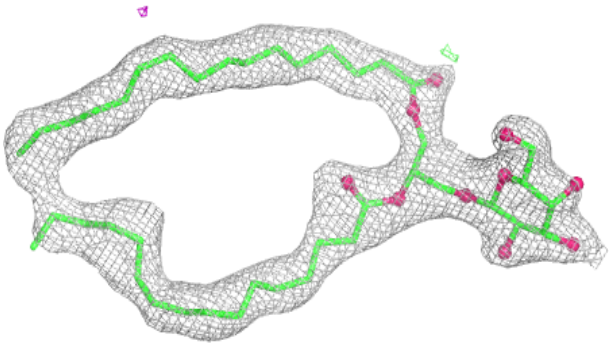


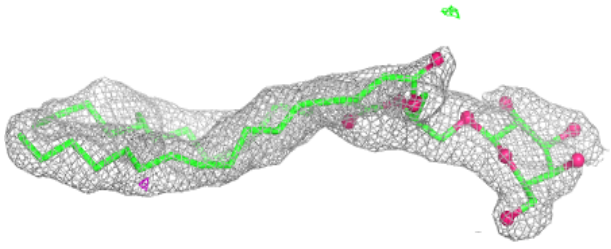


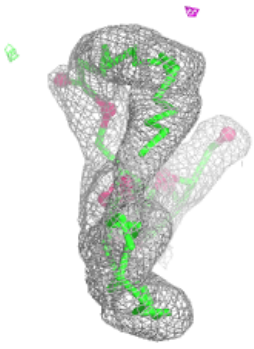


Electron density around LMG A 613:

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

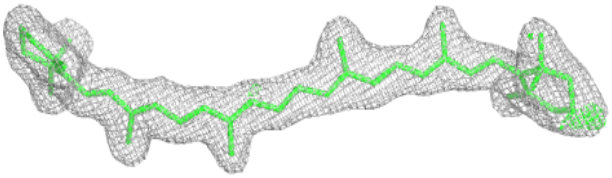


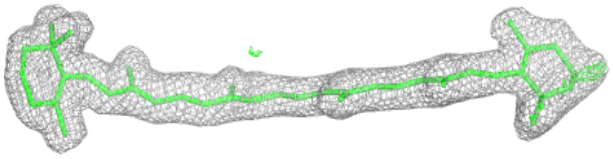


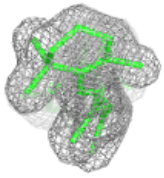


Electron density around BCR h 103:

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

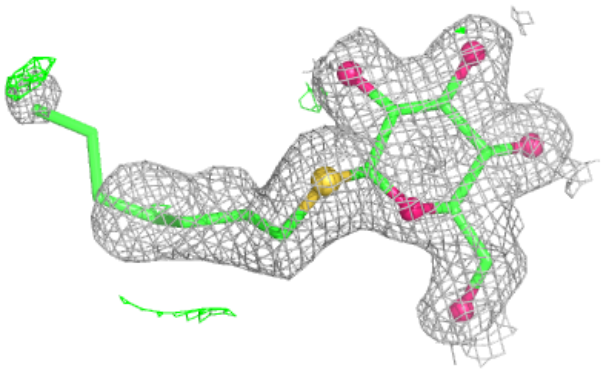


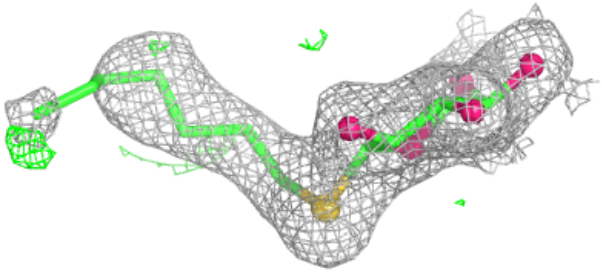


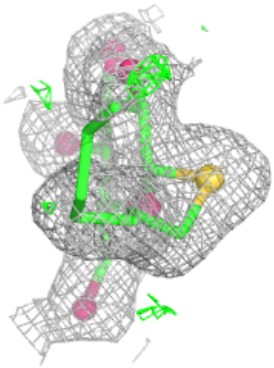


Electron density around HTG B 623:

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

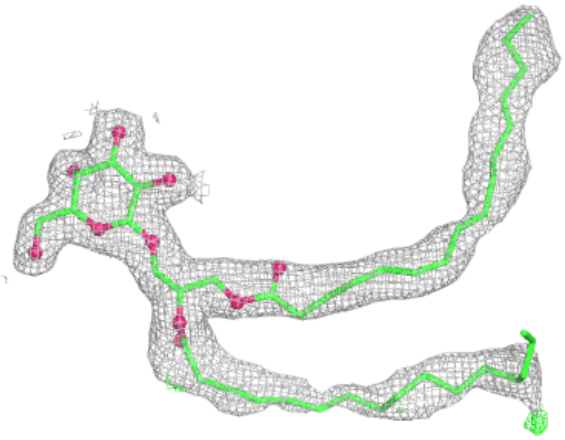


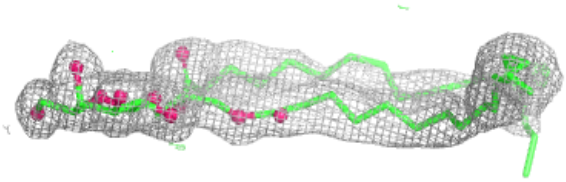


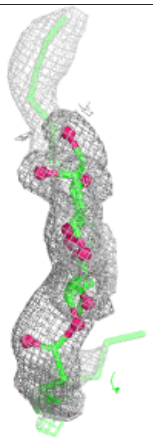


Electron density around LMG C 519:

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

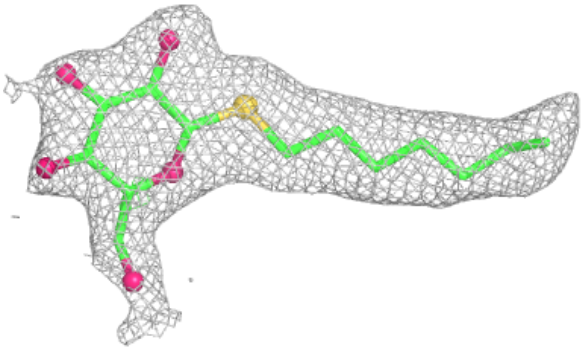


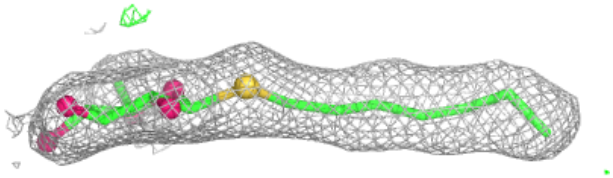


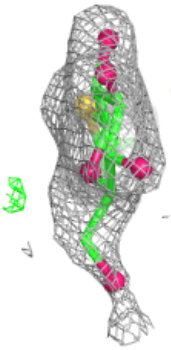


Electron density around HTG B 630:

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

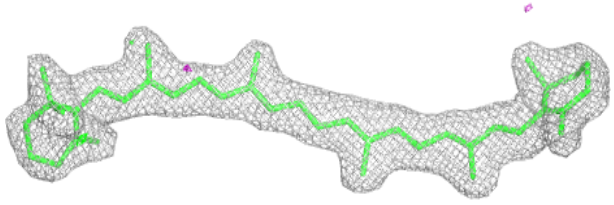


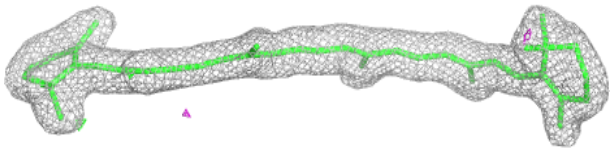


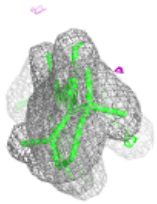


Electron density around BCR k 101:

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

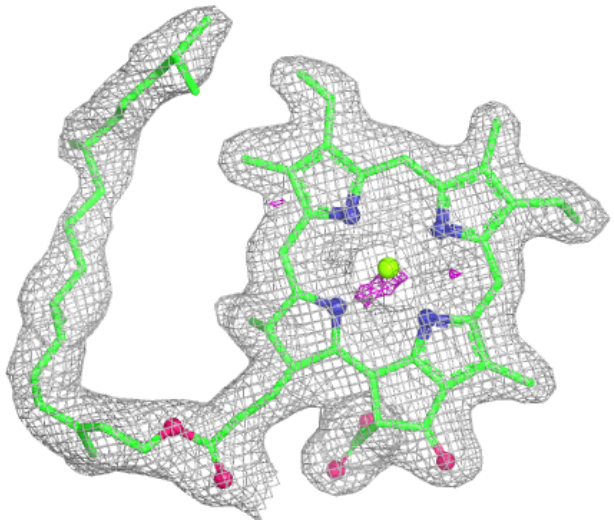


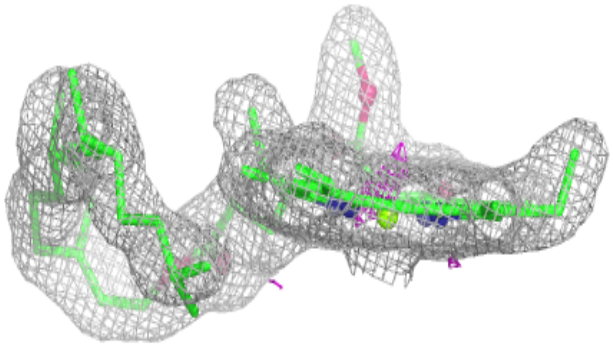


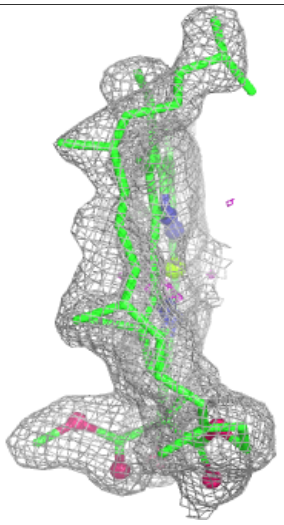


Electron density around CLA C 512:

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

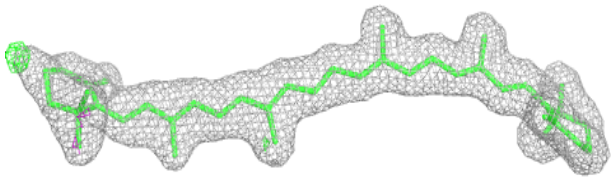


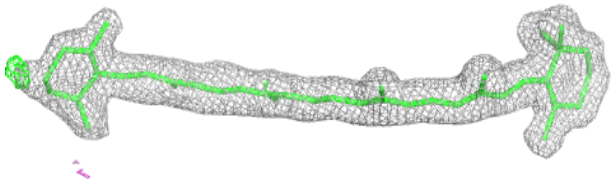


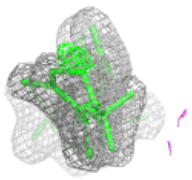


Electron density around BCR H 102:

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

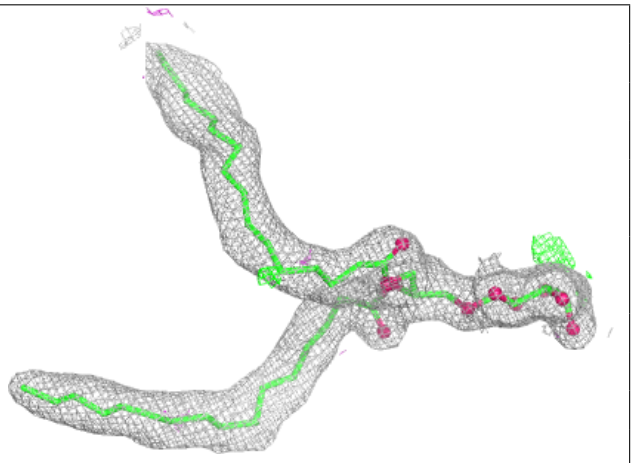


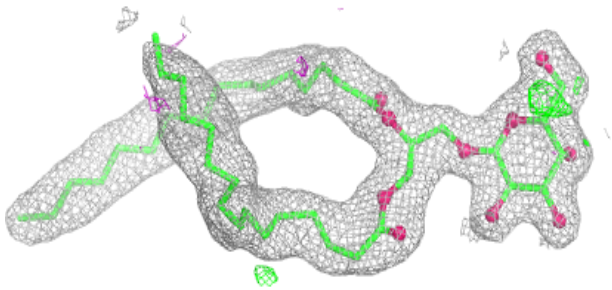


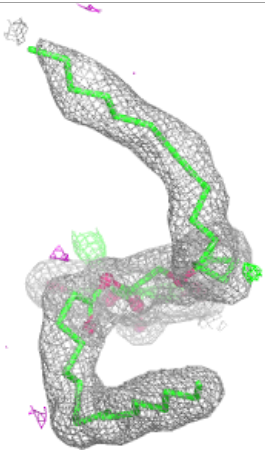


Electron density around LMG B 621:

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

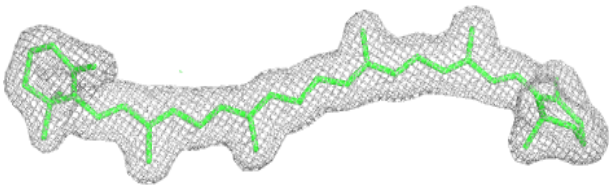


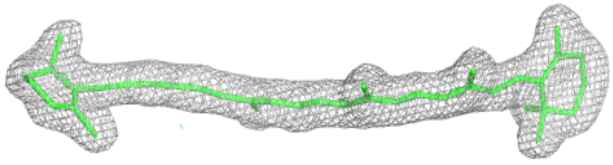


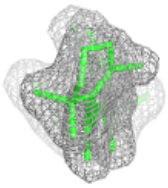


Electron density around BCR K 101:

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

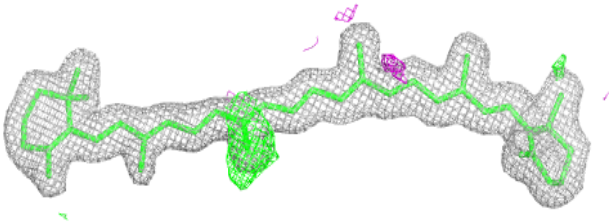


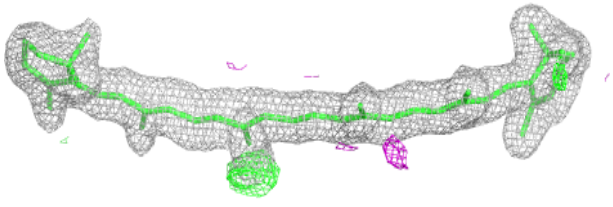


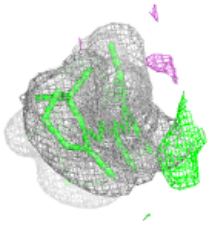


Electron density around BCR T 102:

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

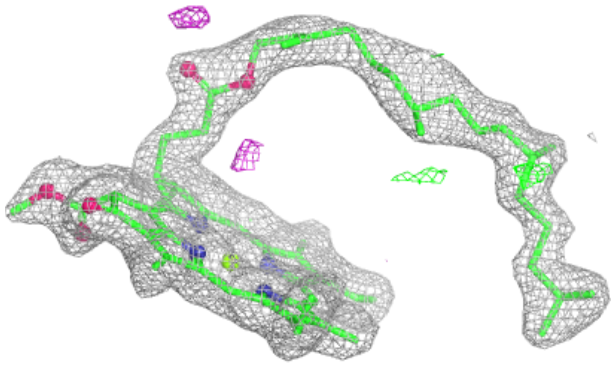


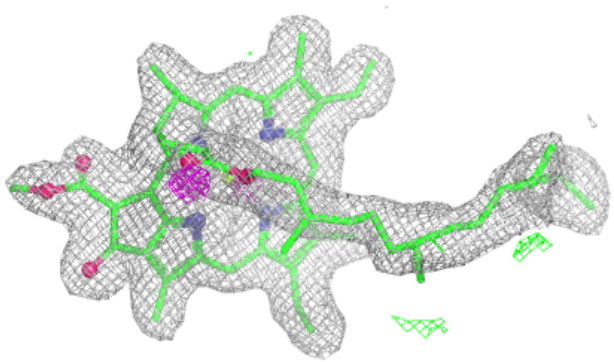


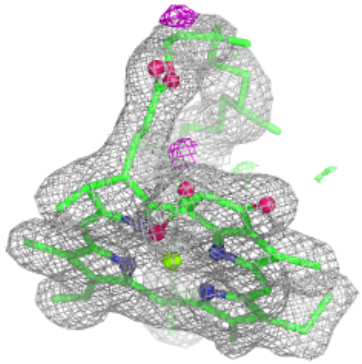


Electron density around CLA C 513:

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

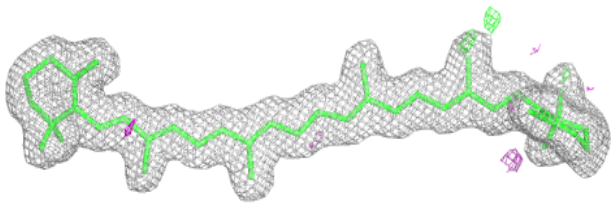


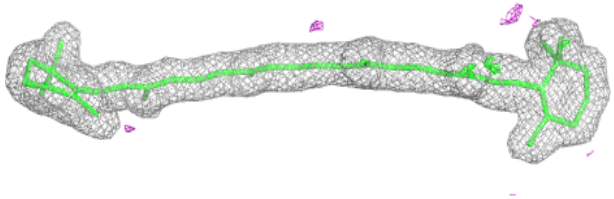


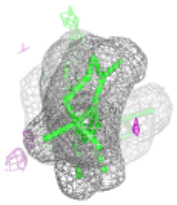


Electron density around BCR b 618:

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

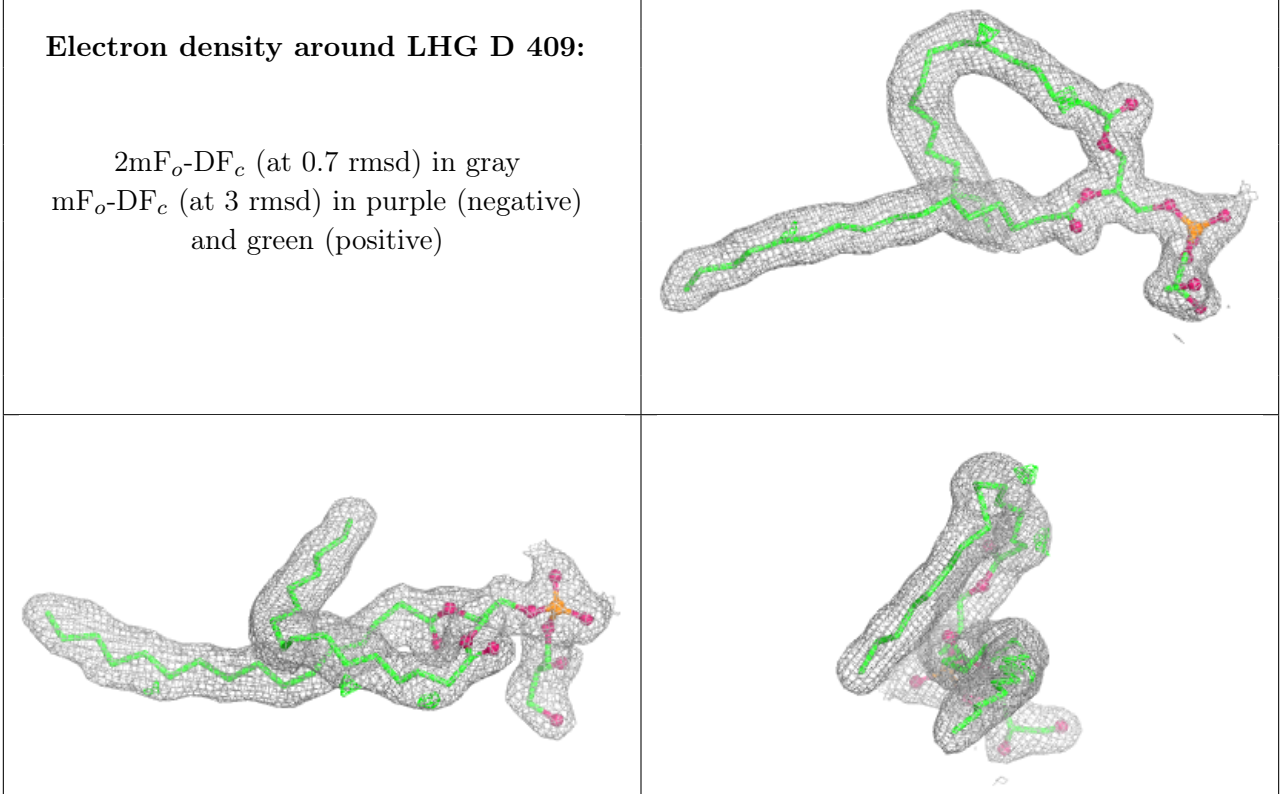






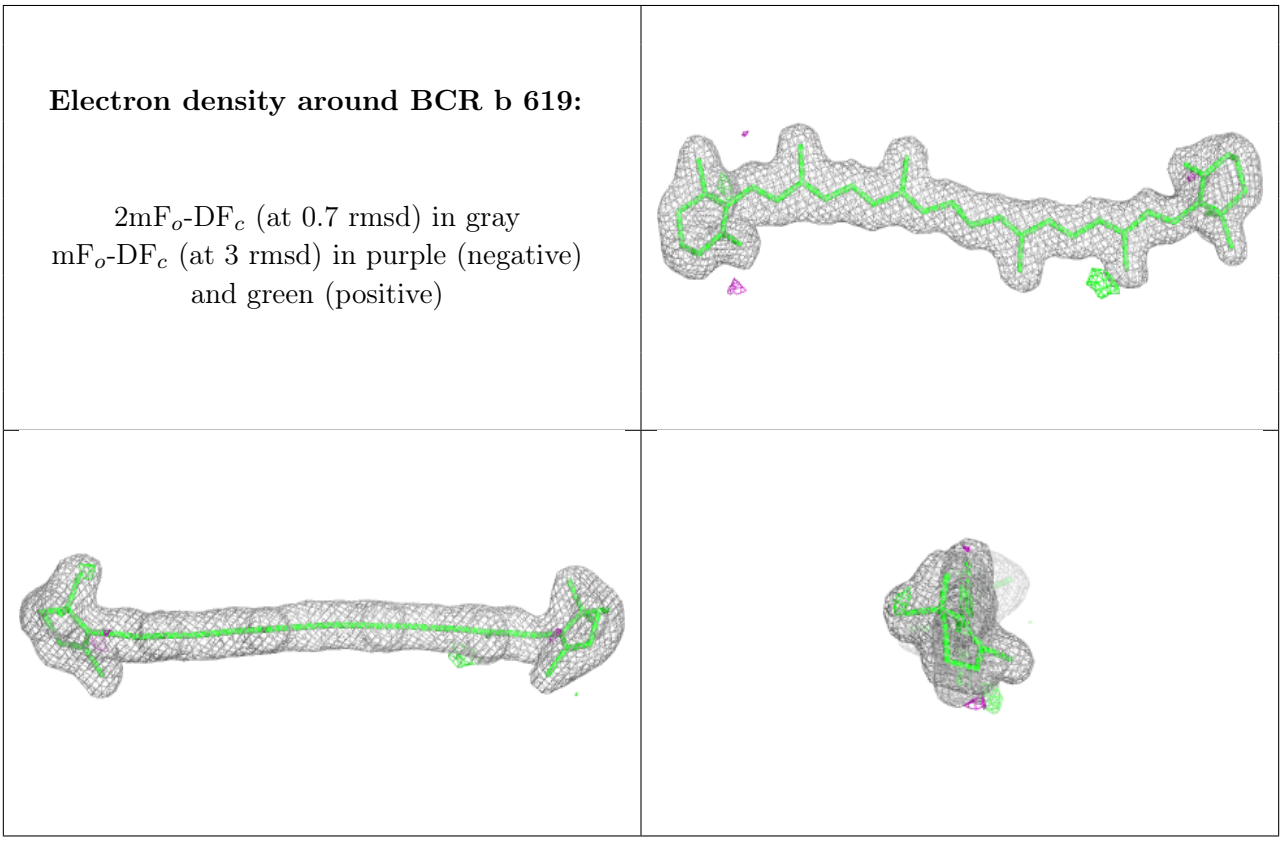
Electron density around LHG D 409:

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



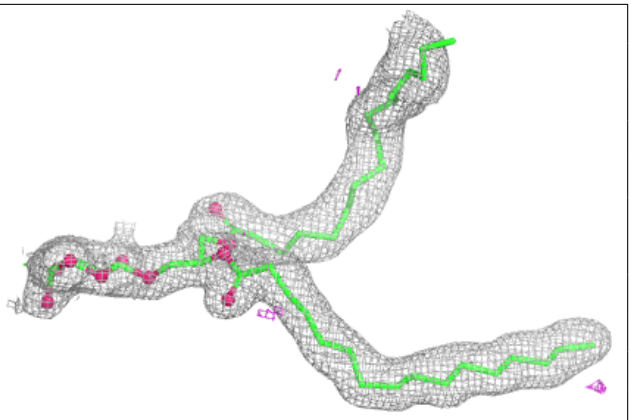
Electron density around BCR b 619:

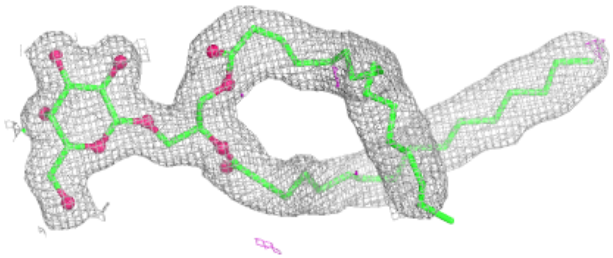
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

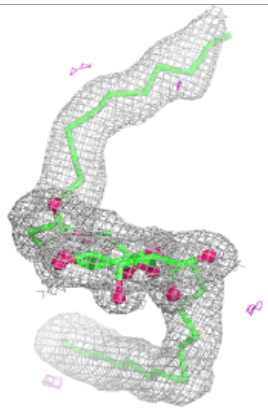


Electron density around LMG b 621:

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

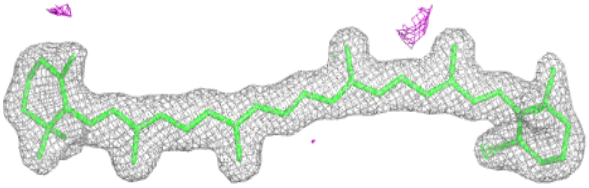


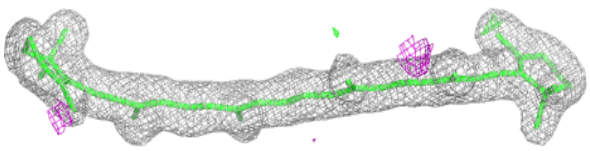


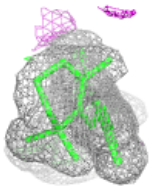


Electron density around BCR b 620:

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

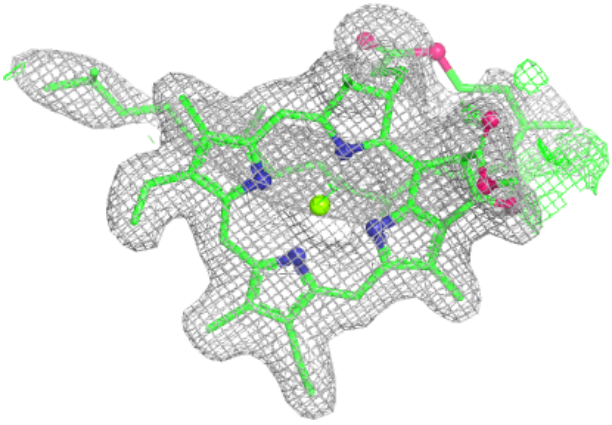


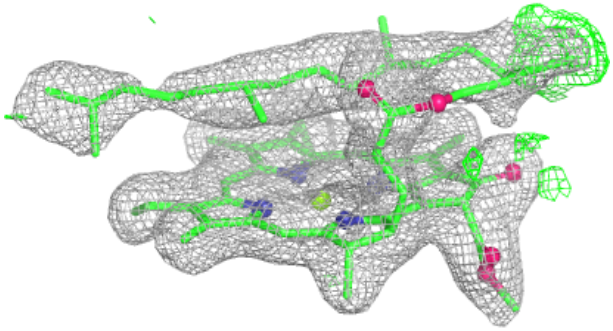


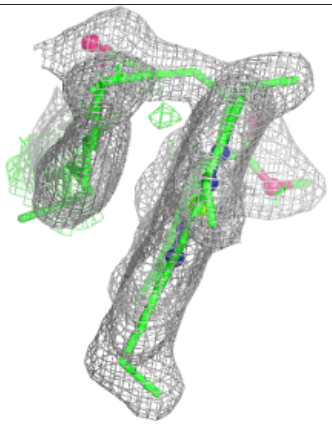


Electron density around CLA B 602:

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

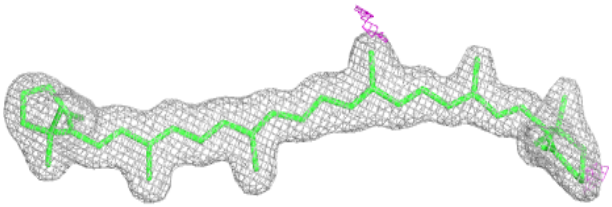


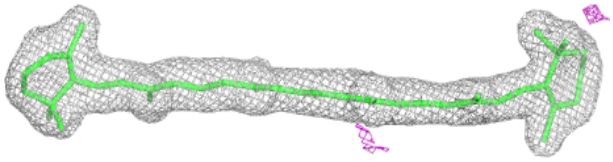


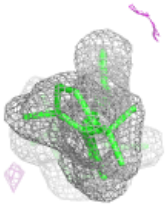


Electron density around BCR c 515:

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

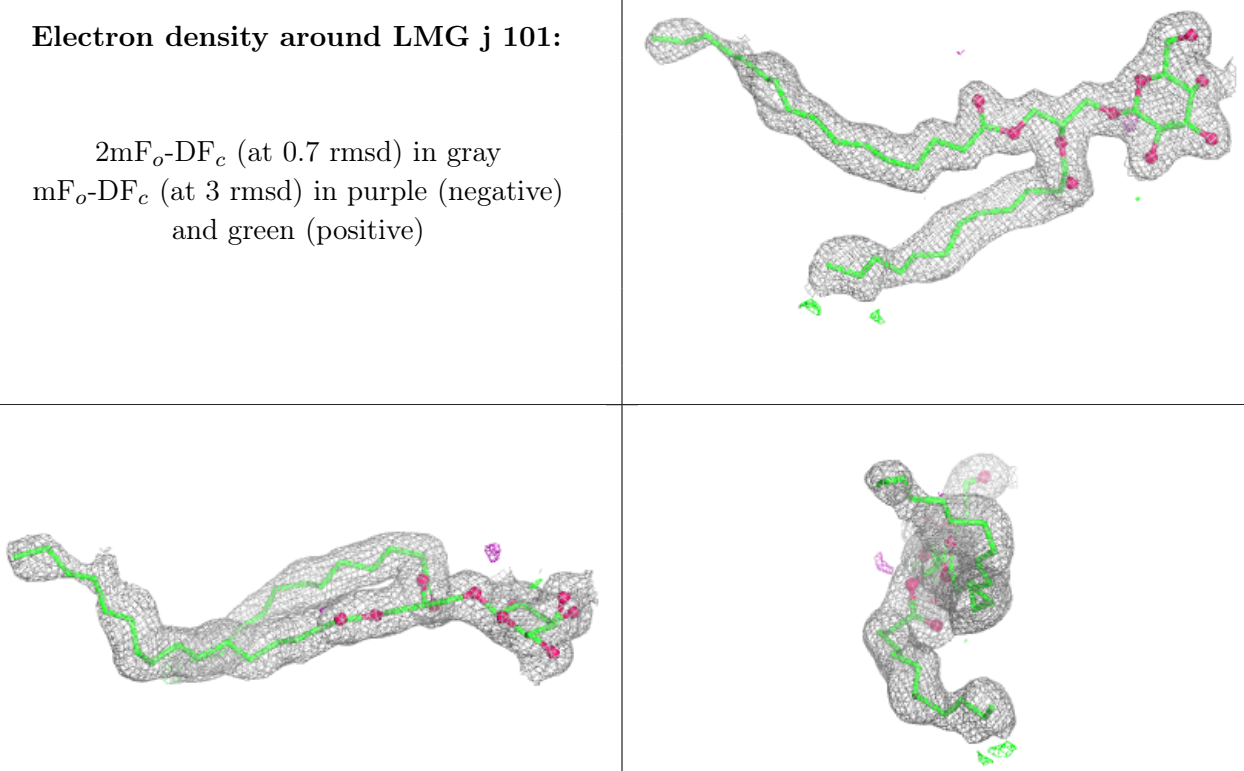






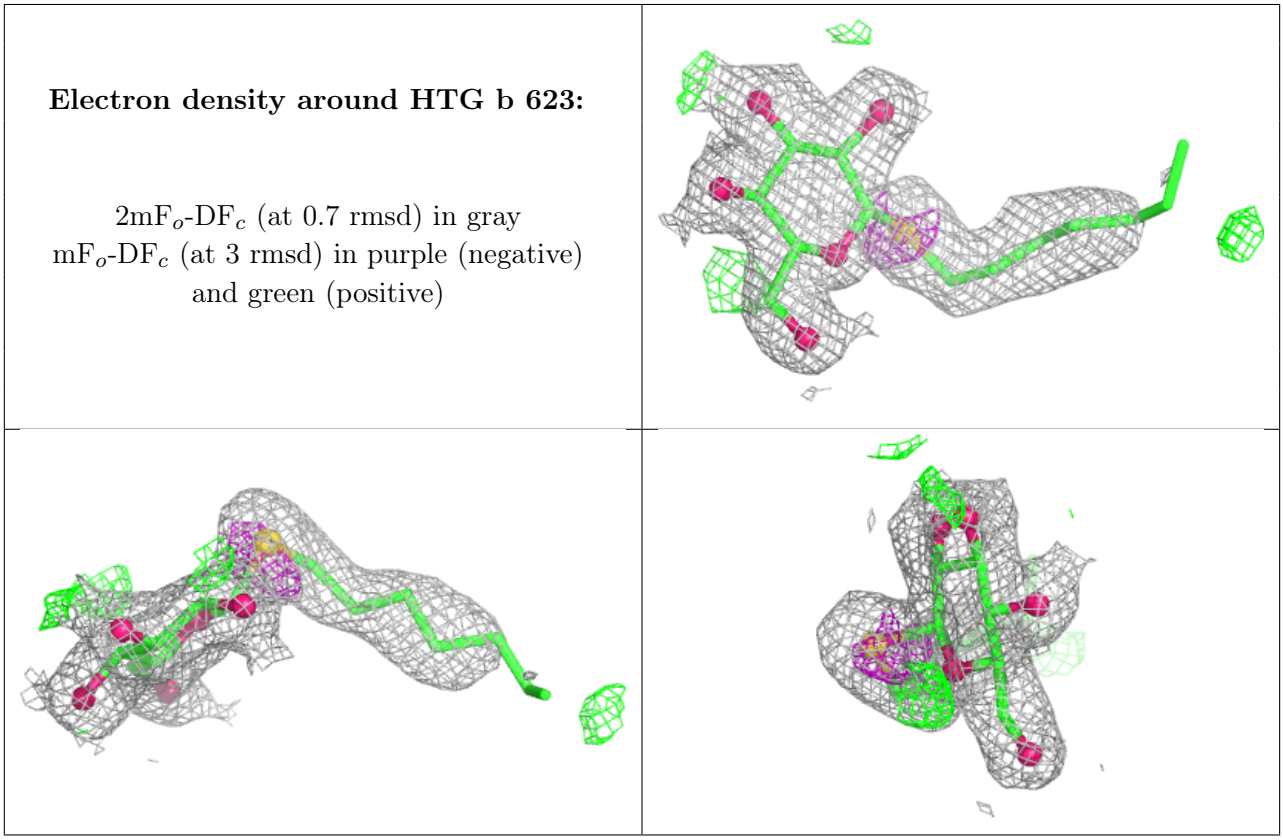
Electron density around LMG j 101:

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



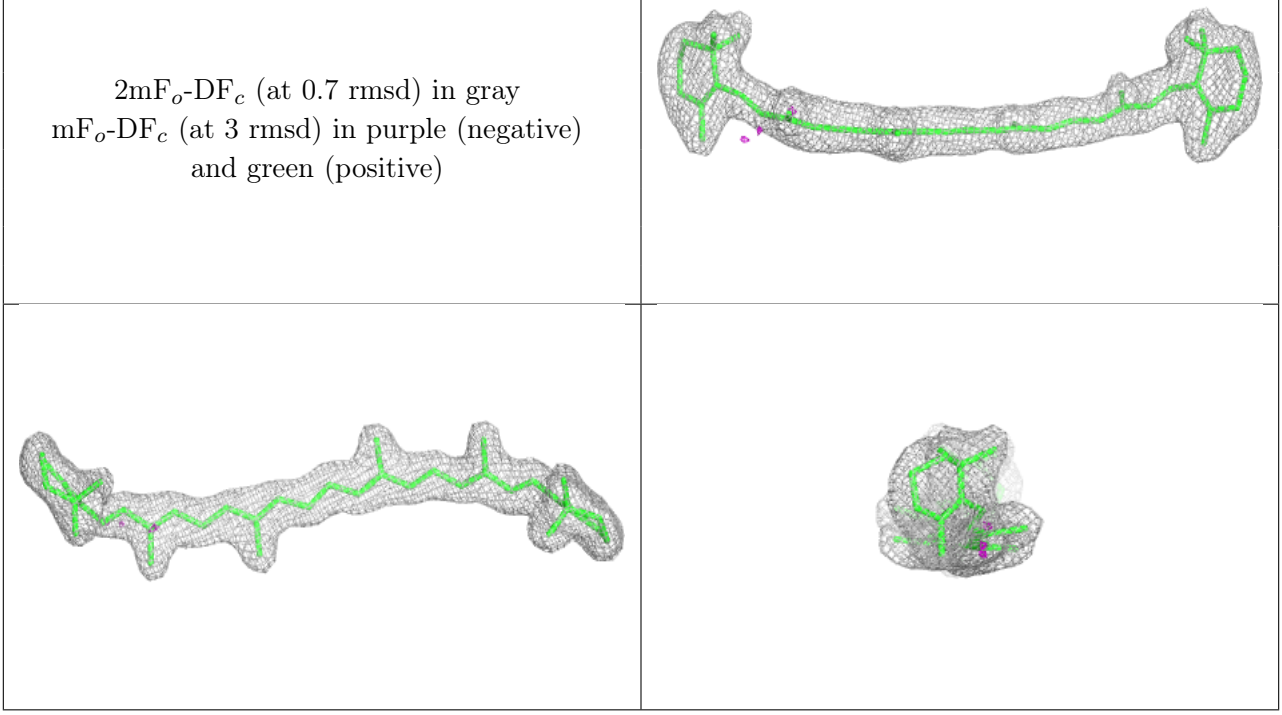
Electron density around HTG b 623:

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



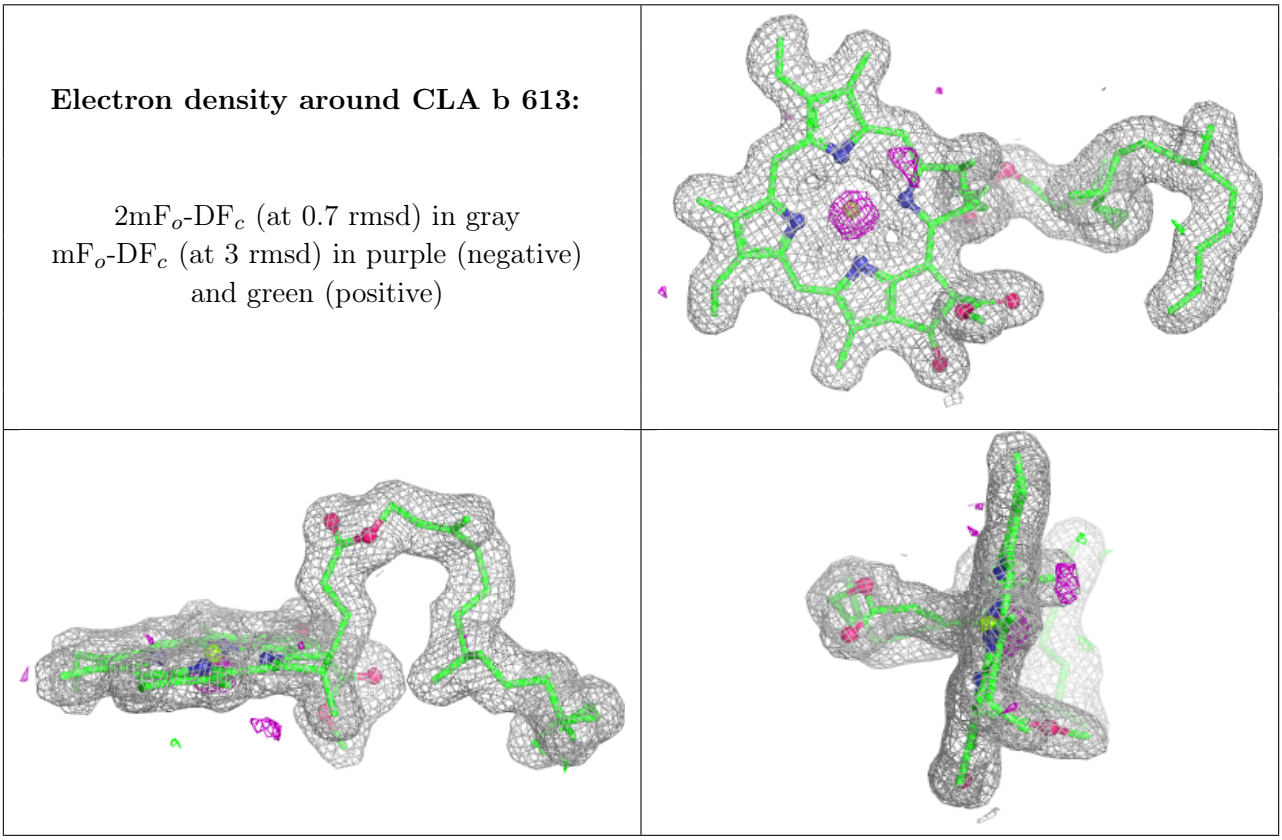
Electron density around BCR c 527:

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



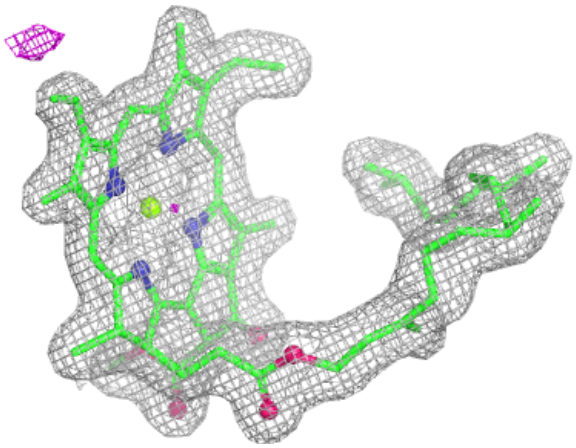
Electron density around CLA b 613:

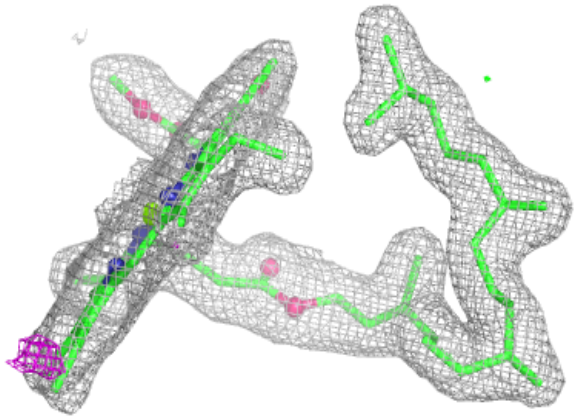
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

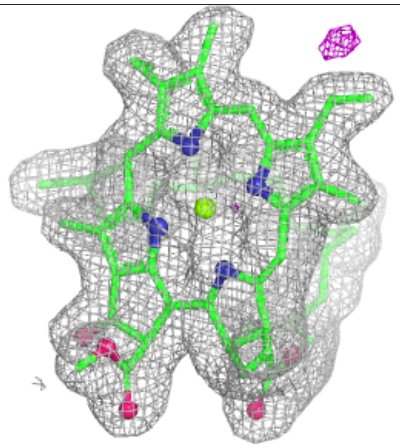


Electron density around CLA c 503:

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

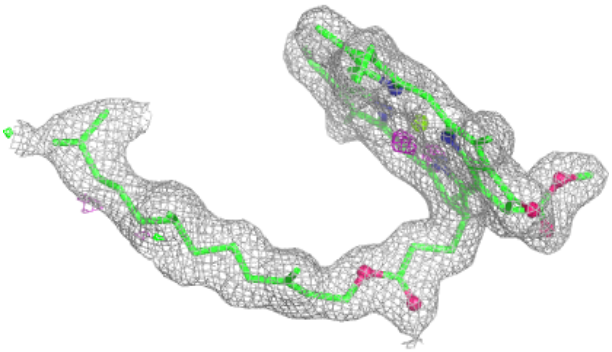


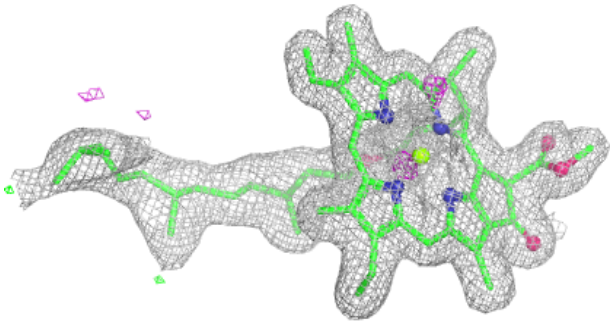


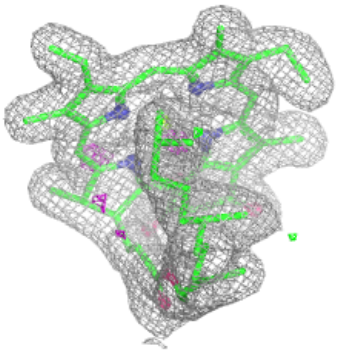


Electron density around CLA c 504:

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

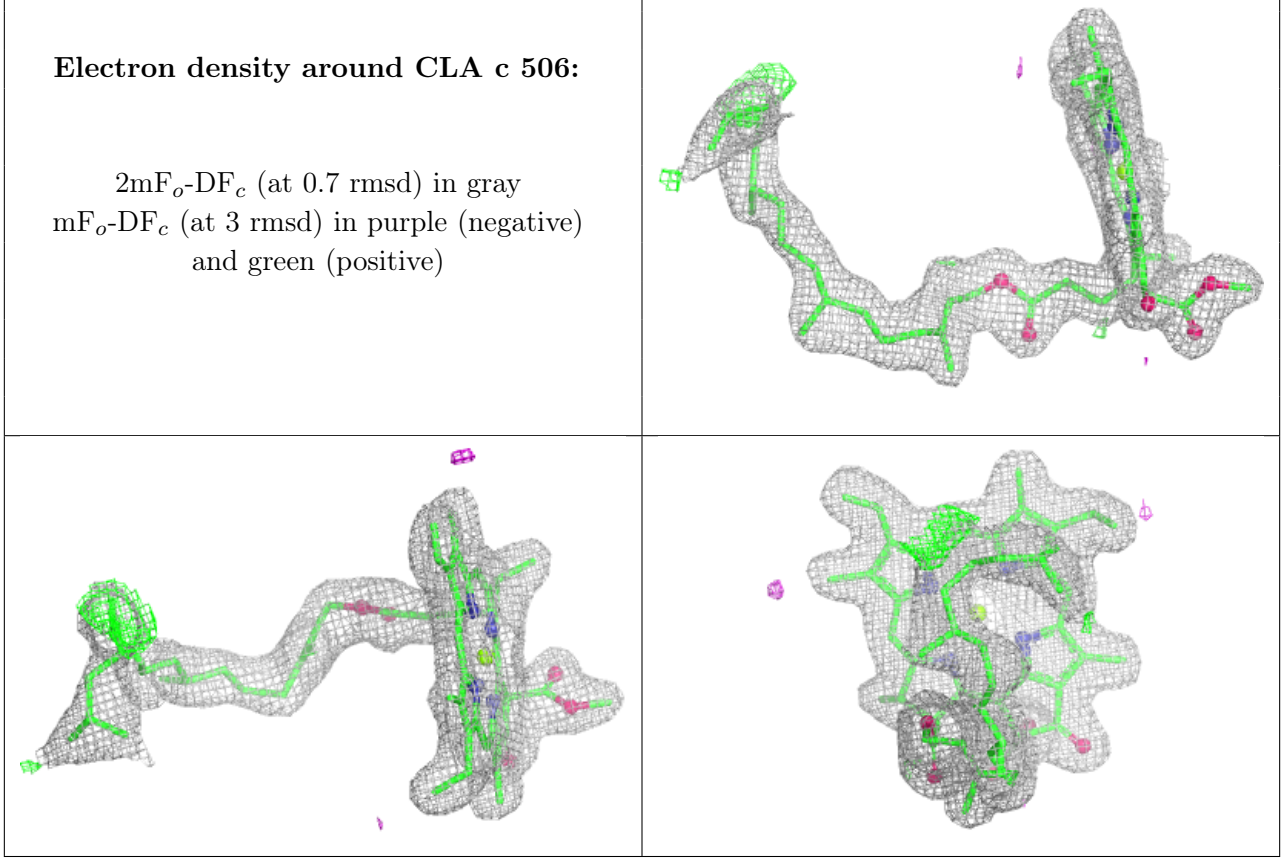






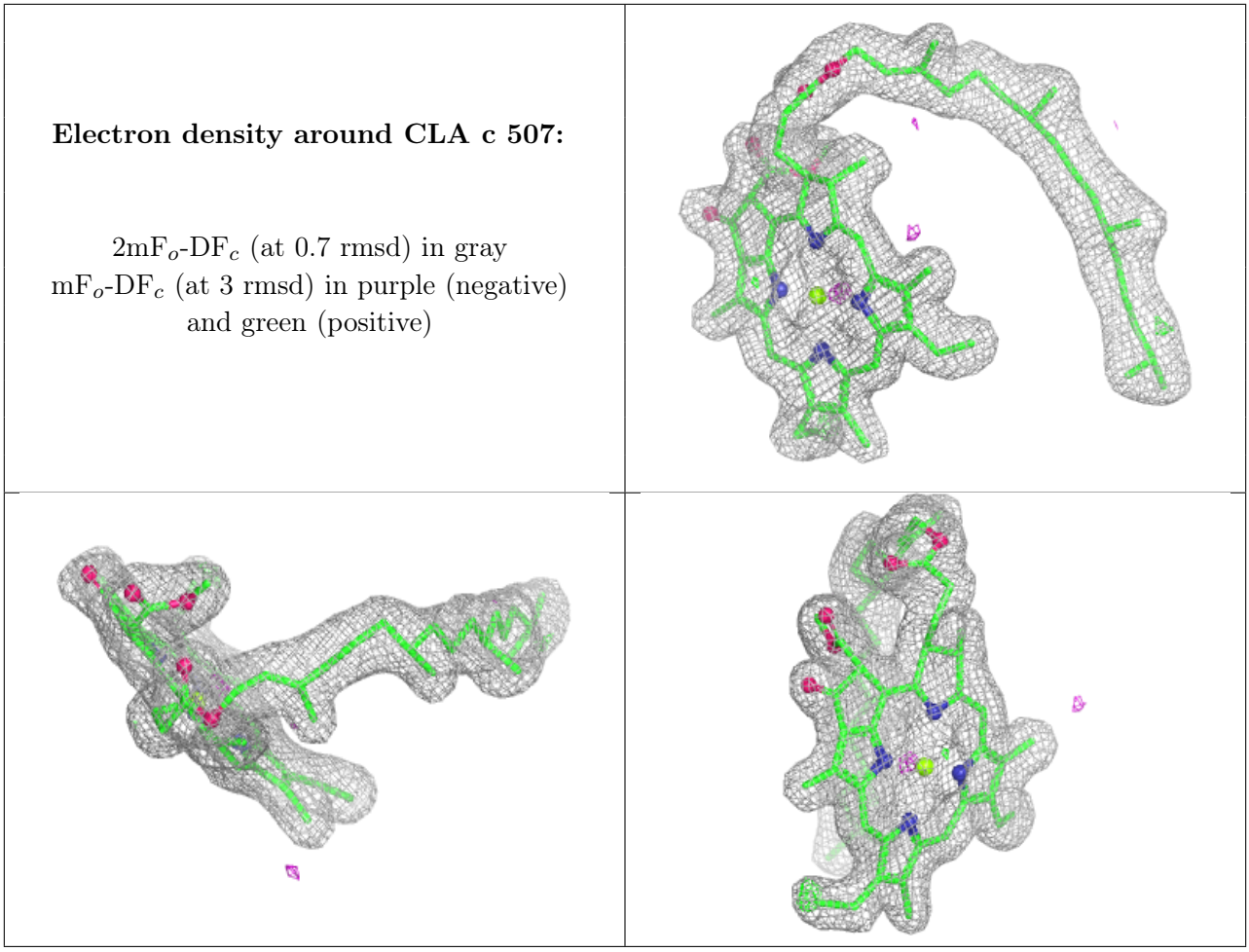
Electron density around CLA c 506:

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



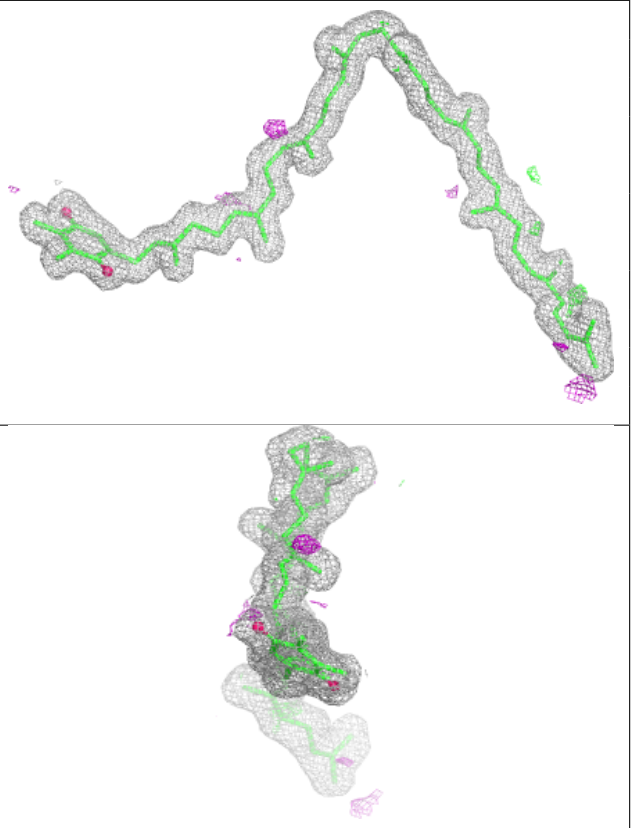
Electron density around CLA c 507:

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



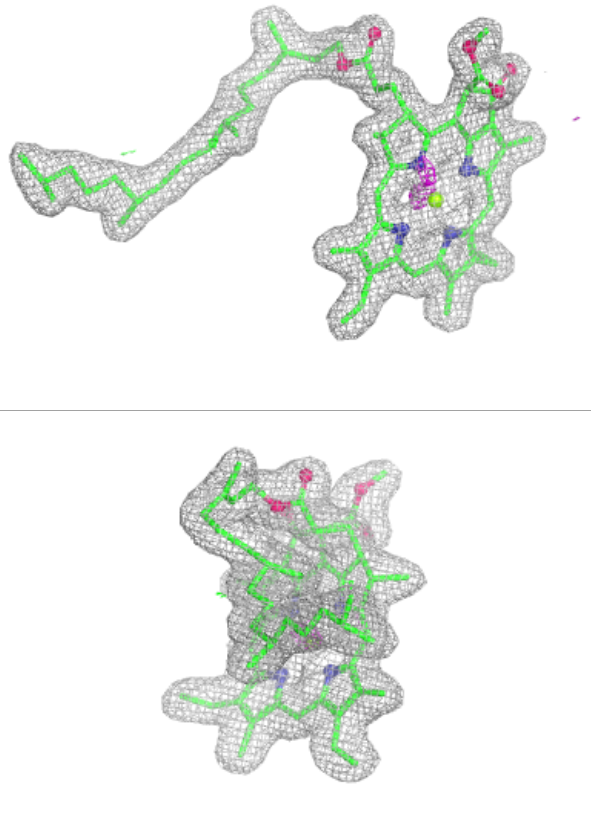
Electron density around PL9 D 407:

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



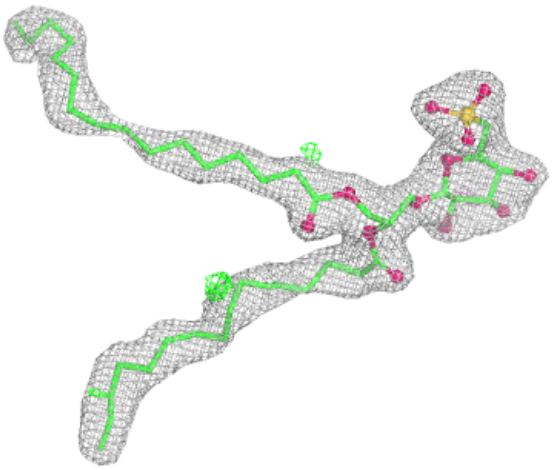
Electron density around CLA c 511:

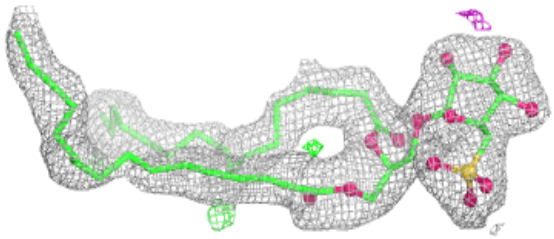
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

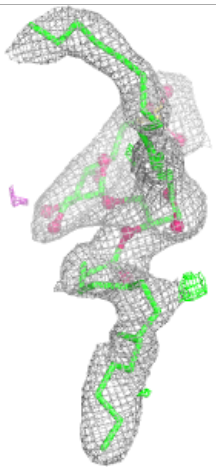


Electron density around SQD A 612:

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

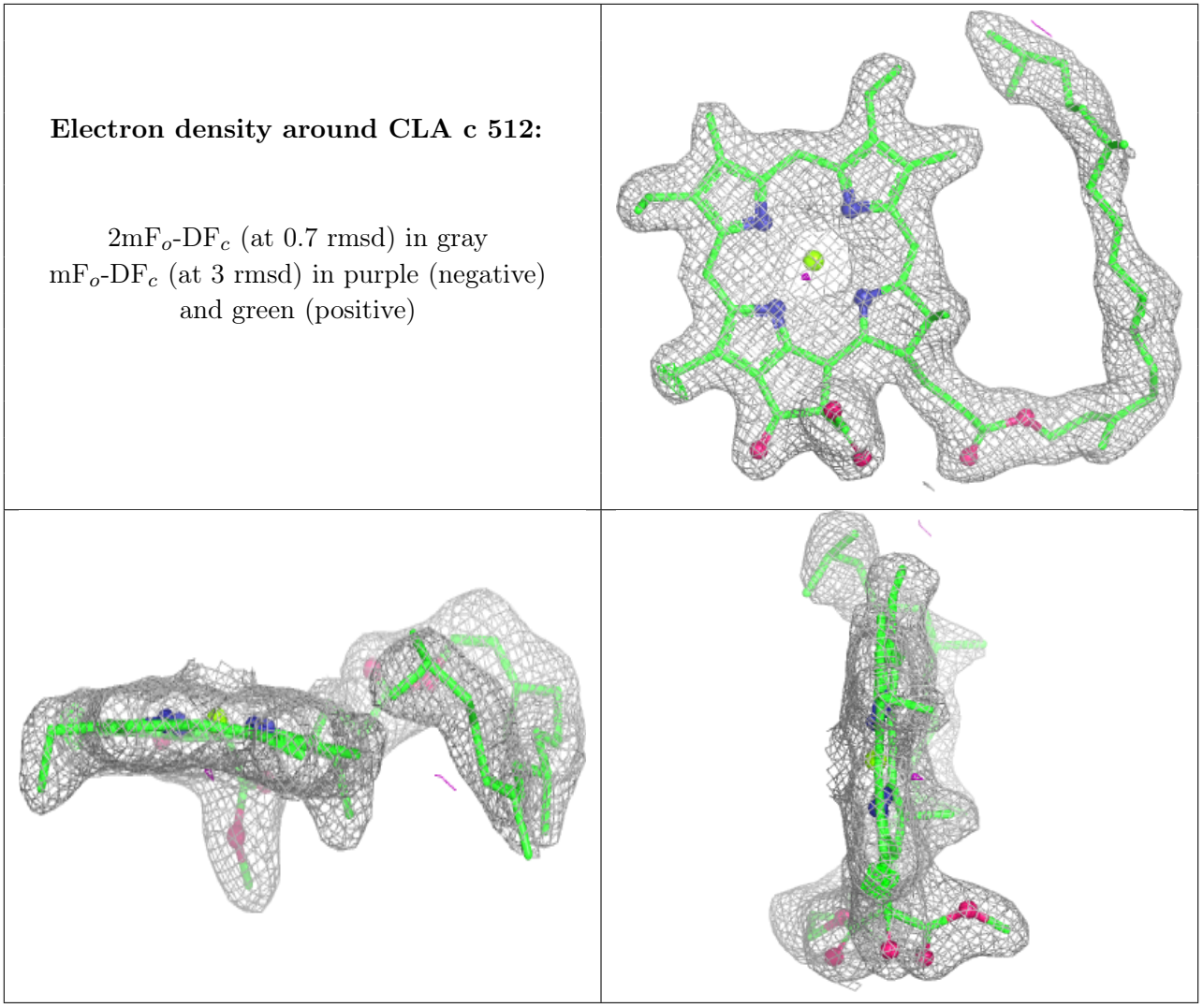






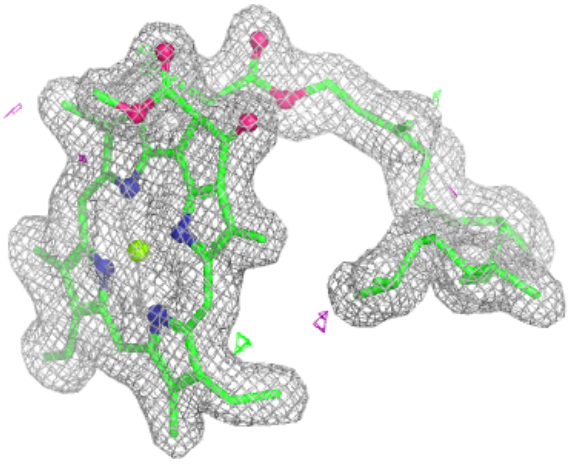
Electron density around CLA c 512:

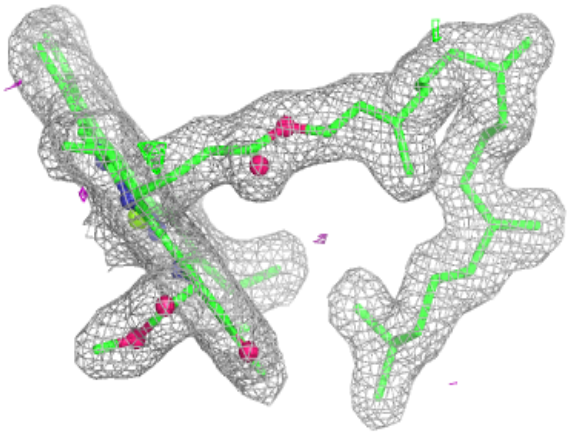
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

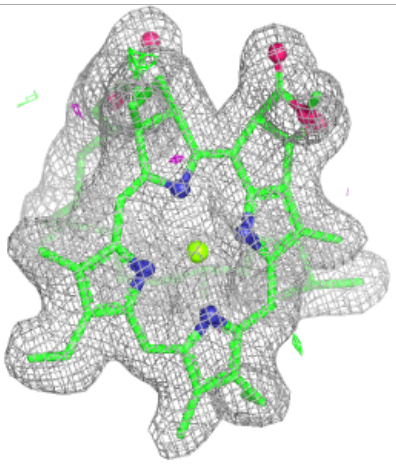


Electron density around CLA C 503:

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

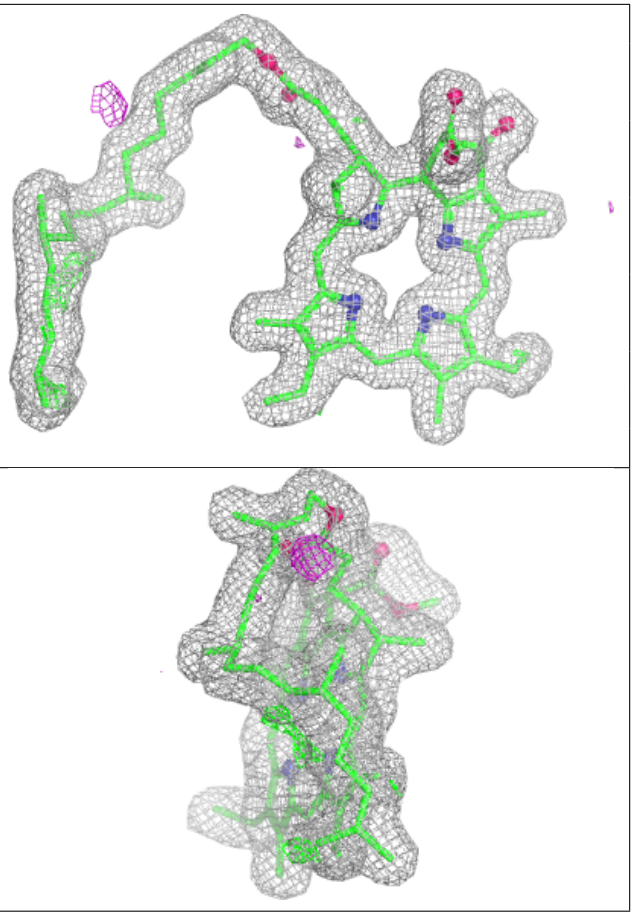






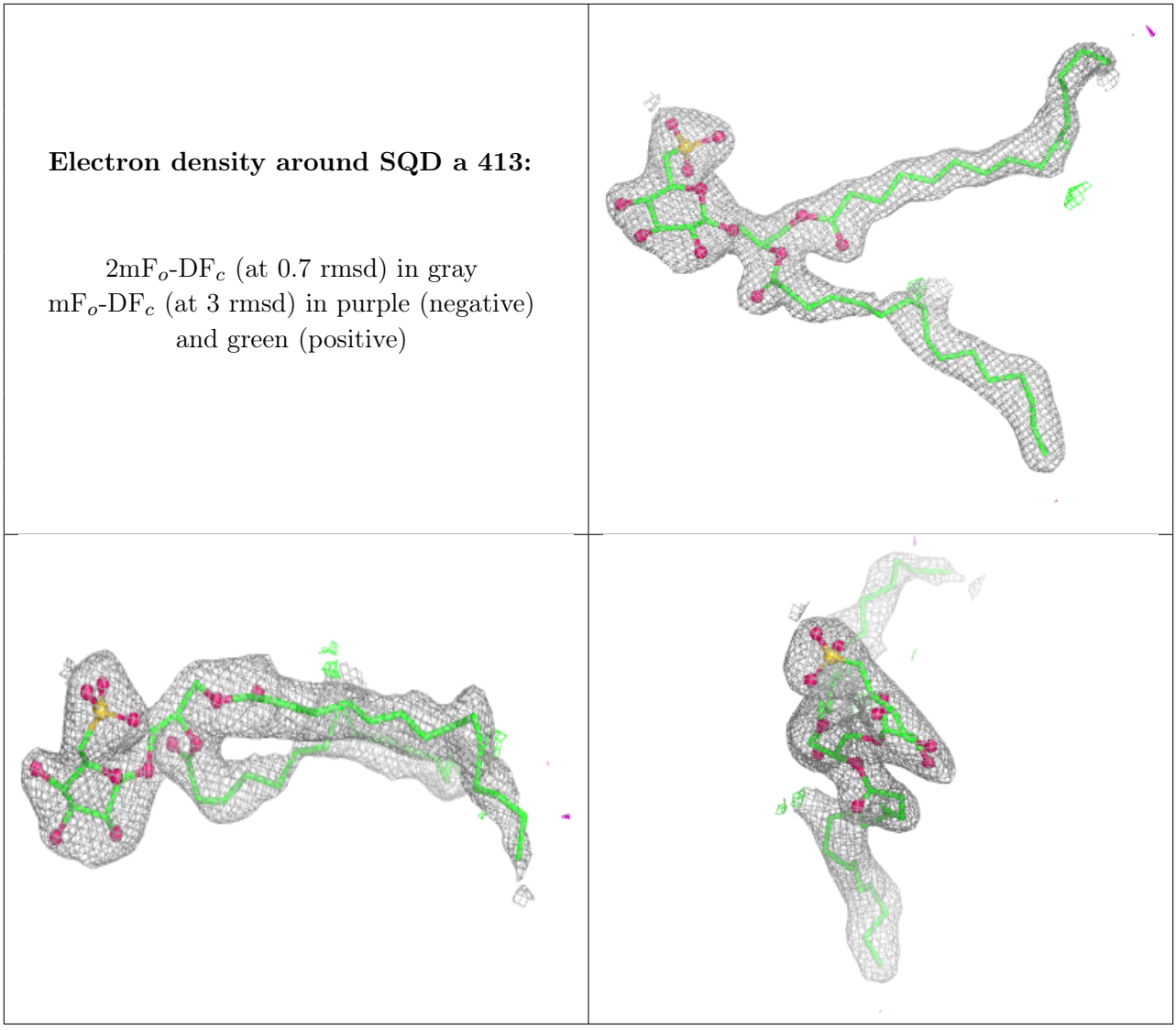
Electron density around PHO d 401:

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



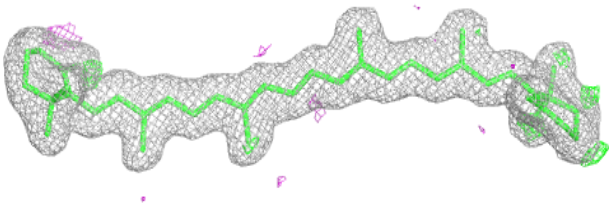
Electron density around SQD a 413:

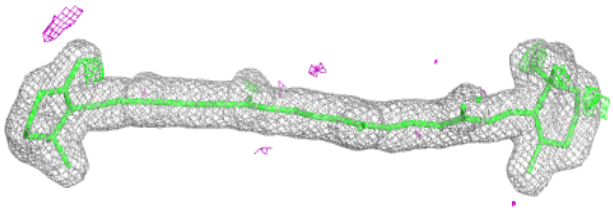
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

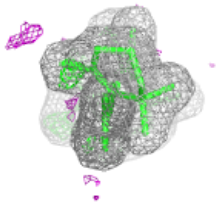


Electron density around BCR A 610:

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

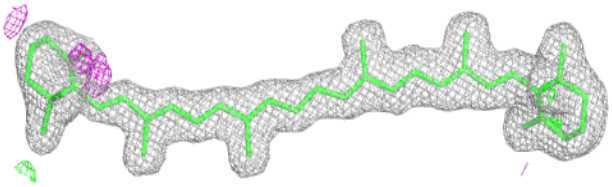


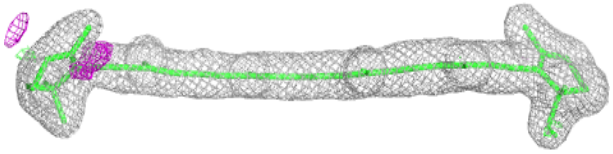


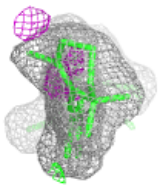


Electron density around BCR B 619:

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

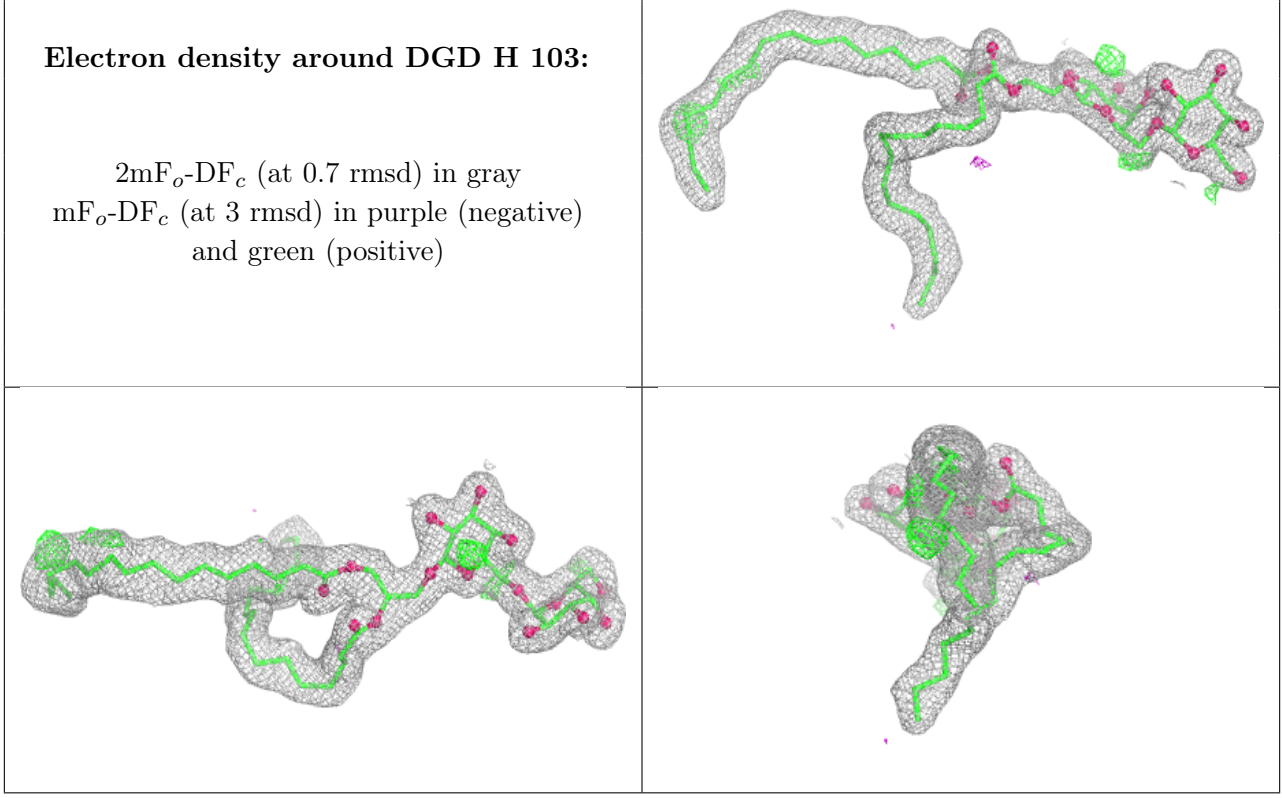






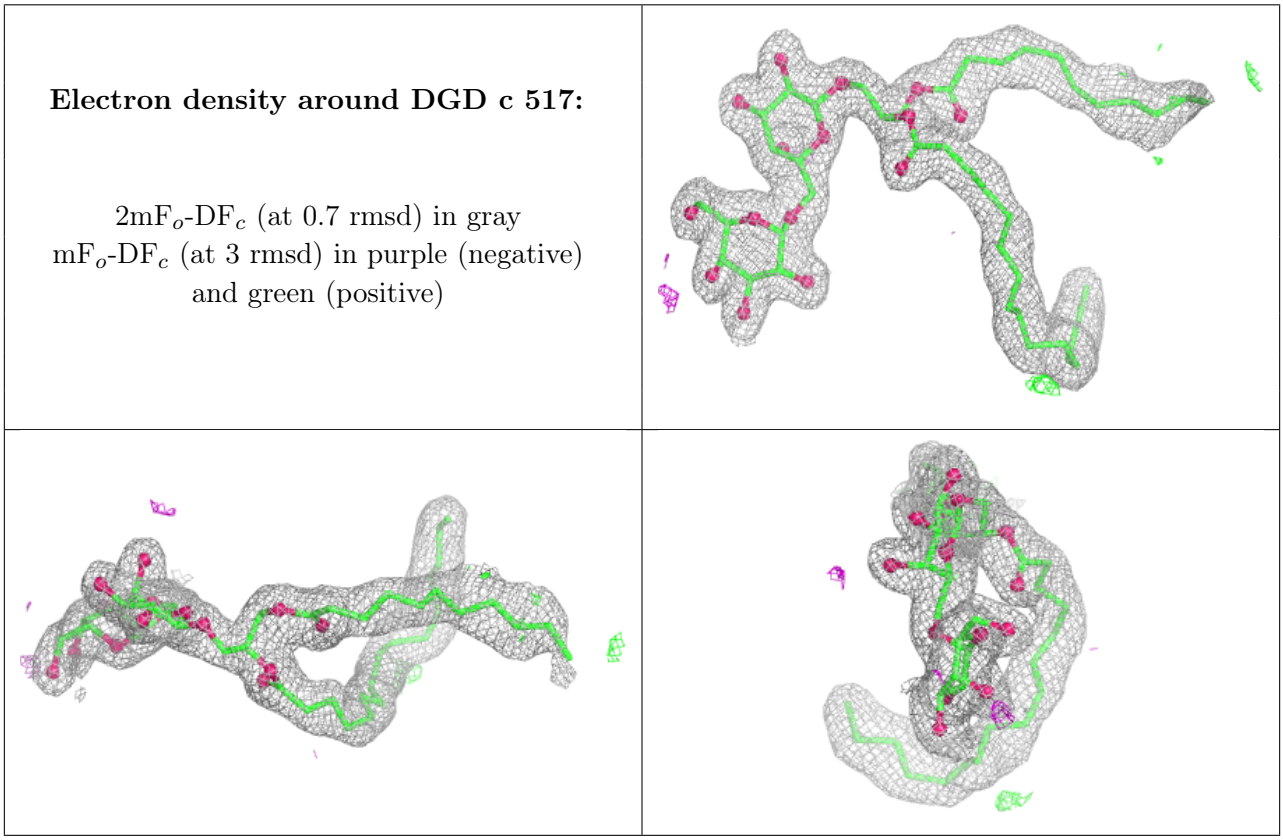
Electron density around DGD H 103:

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



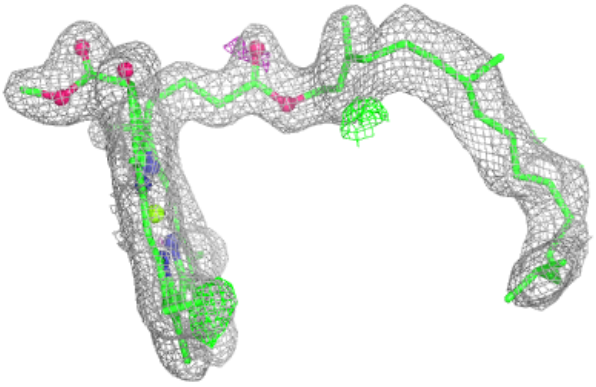
Electron density around DGD c 517:

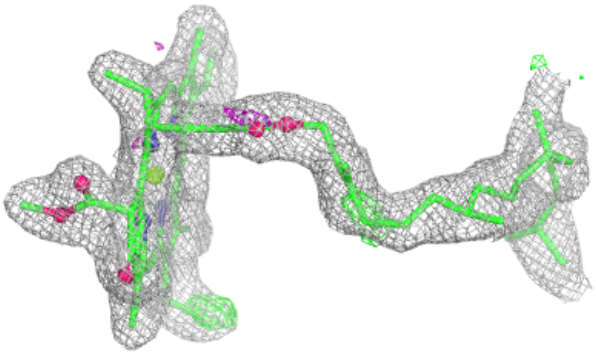
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

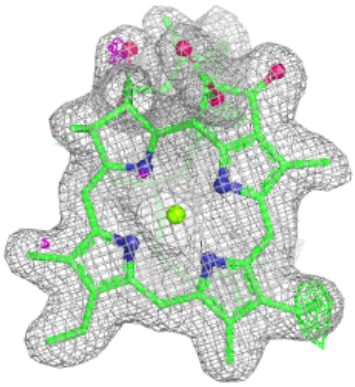


Electron density around CLA C 506:

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

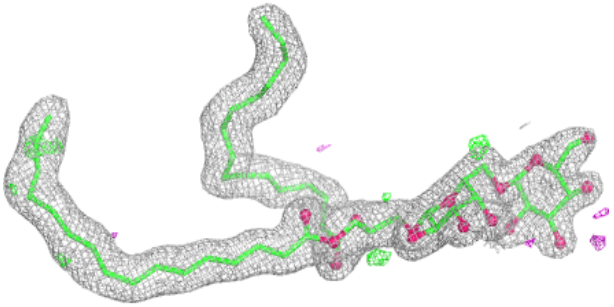


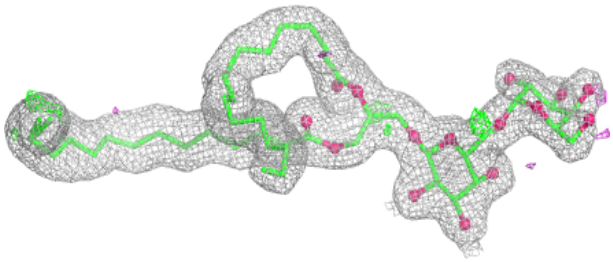


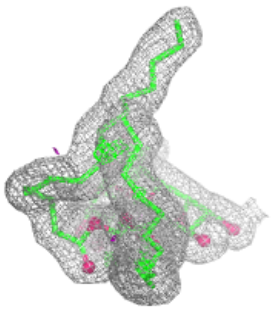


Electron density around DGD h 104:

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

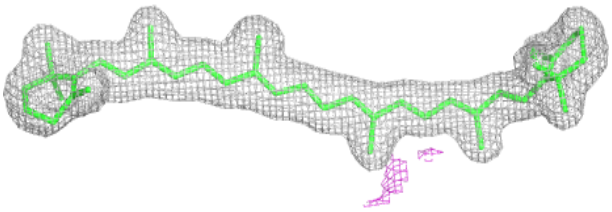


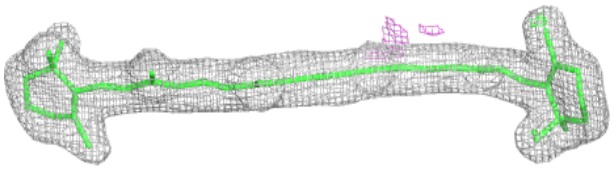


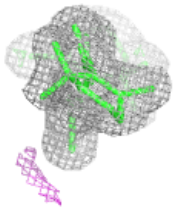


Electron density around BCR C 515:

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

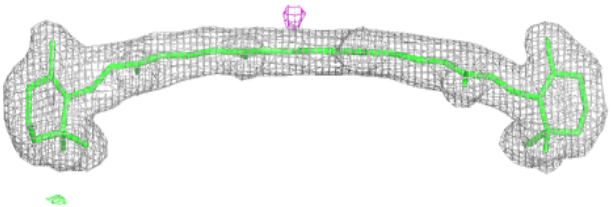


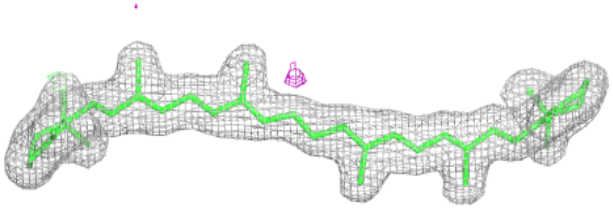


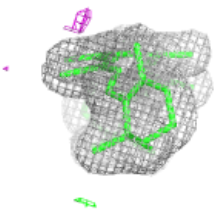


Electron density around BCR C 525:

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

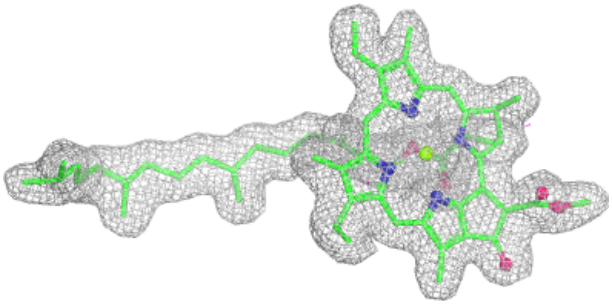


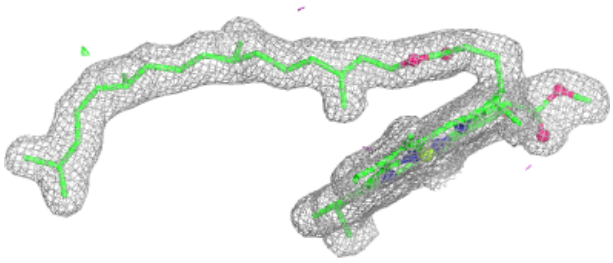


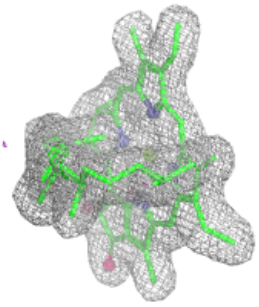


Electron density around CLA b 609:

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

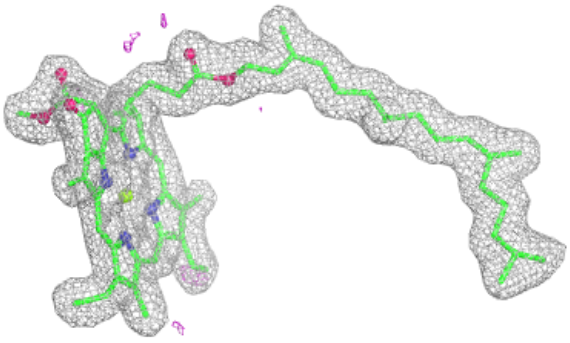


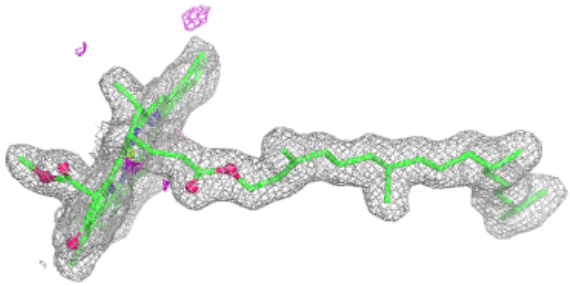


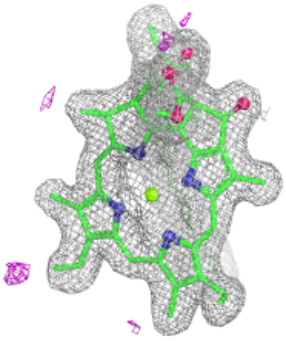


Electron density around CLA b 610:

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

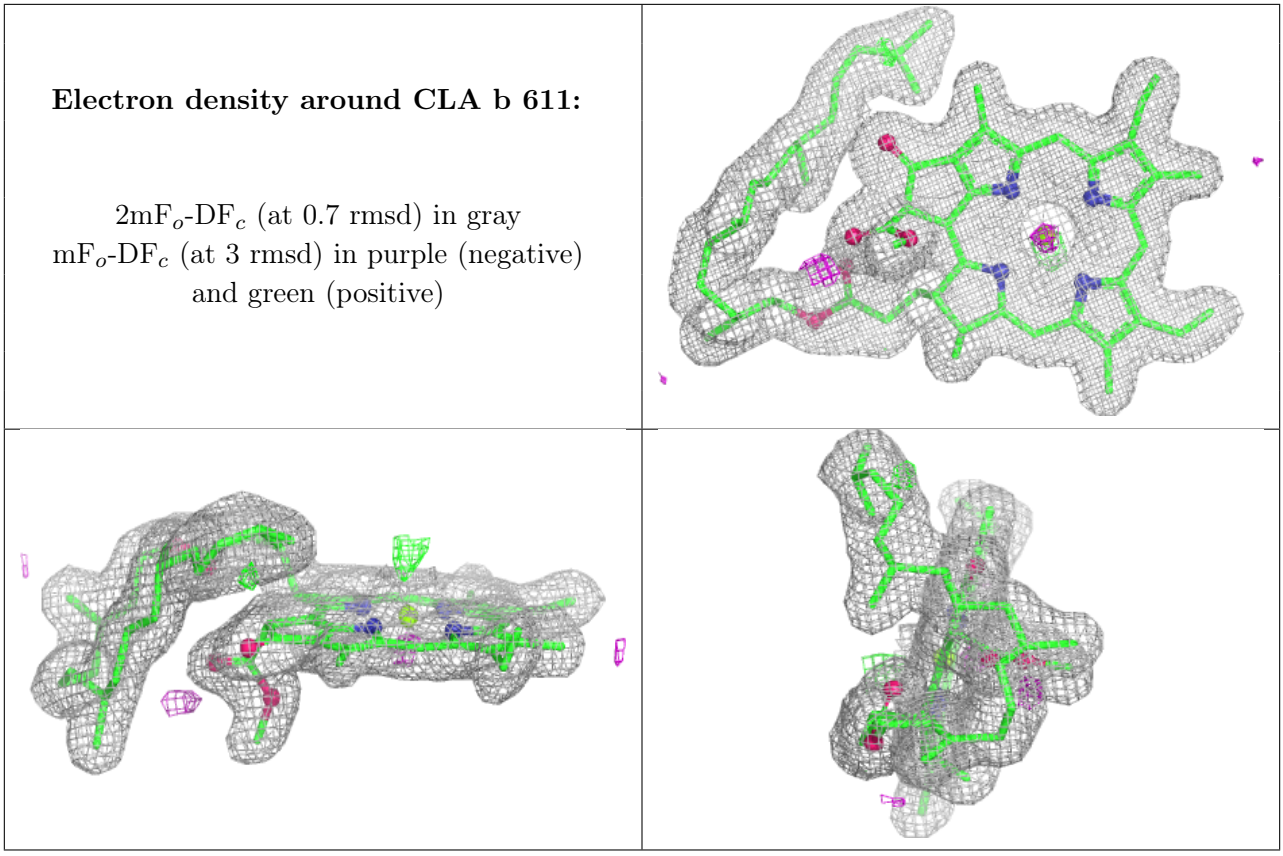






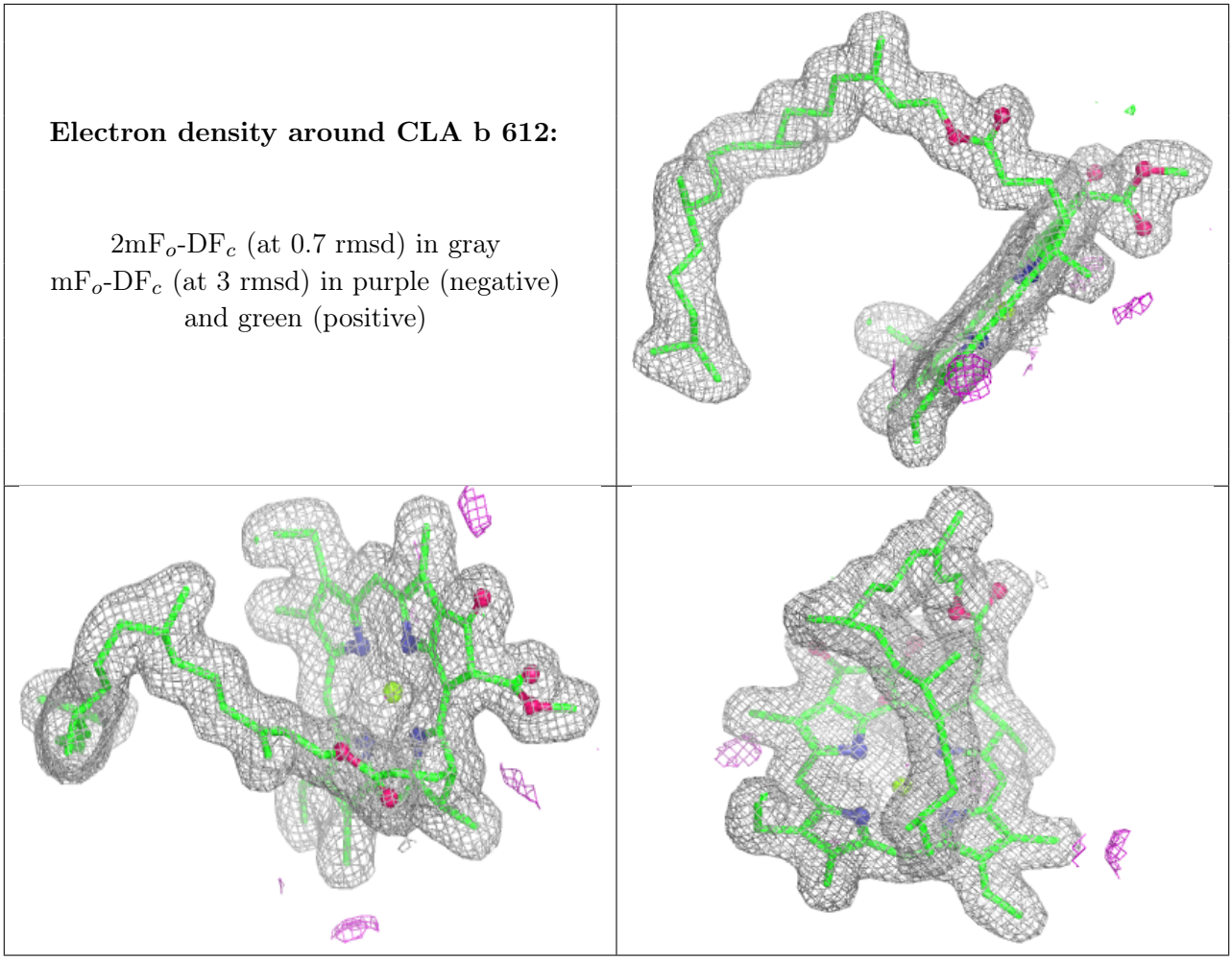
Electron density around CLA b 611:

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



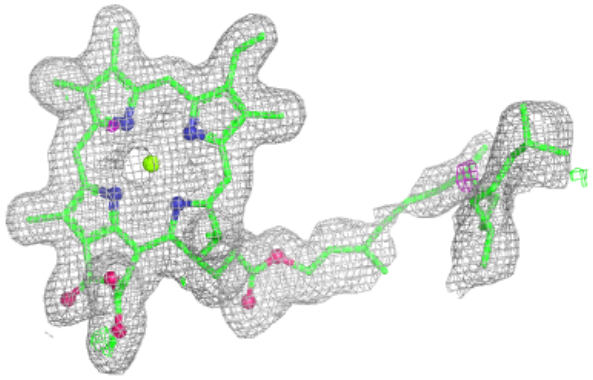
Electron density around CLA b 612:

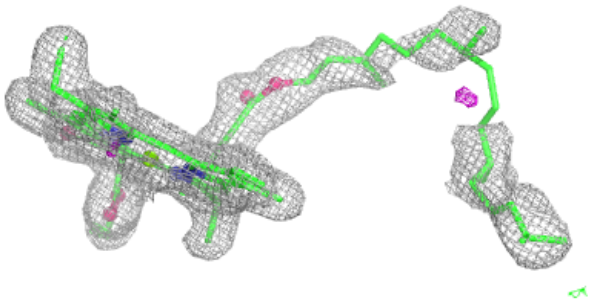
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

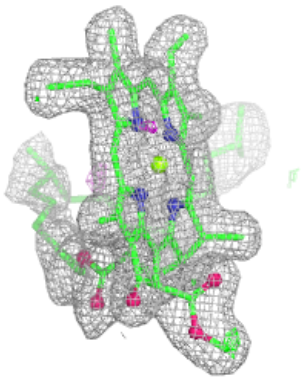


Electron density around CLA A 609:

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

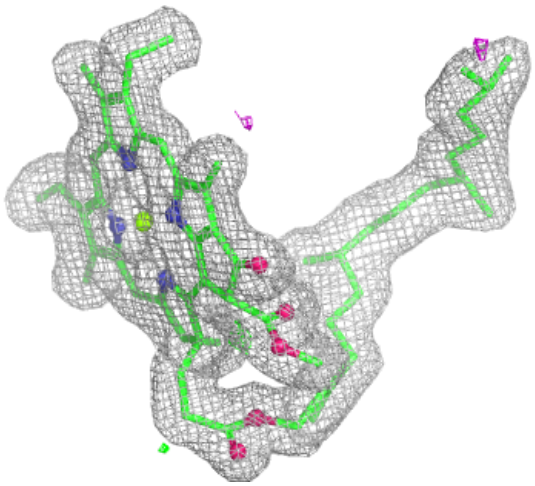


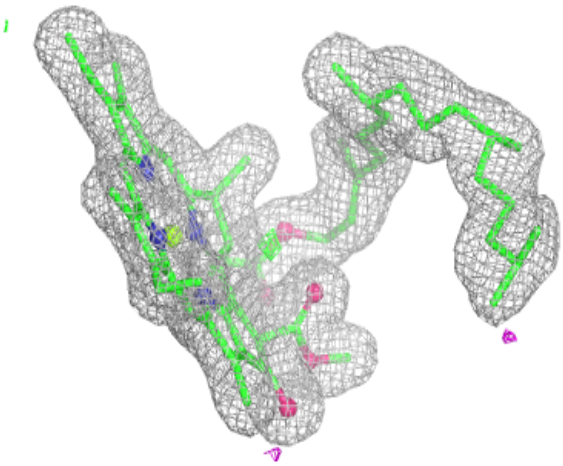


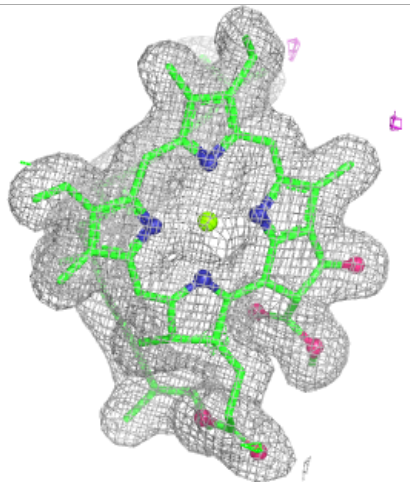


Electron density around CLA b 614:

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

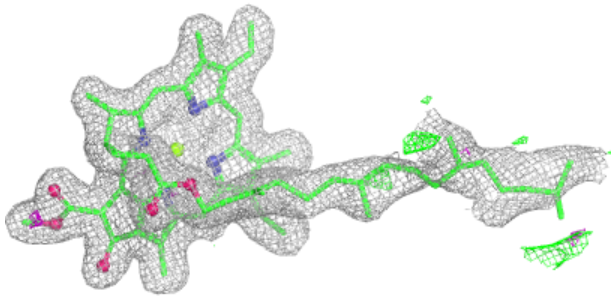


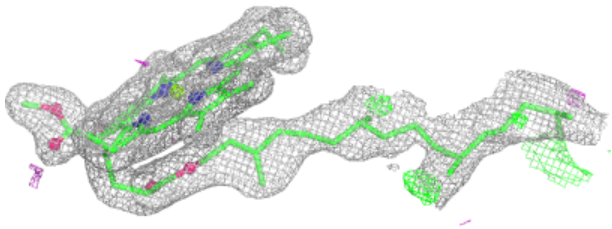


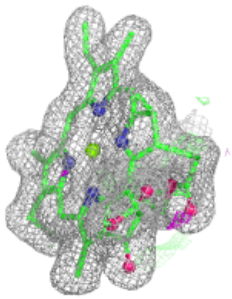


Electron density around CLA b 615:

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

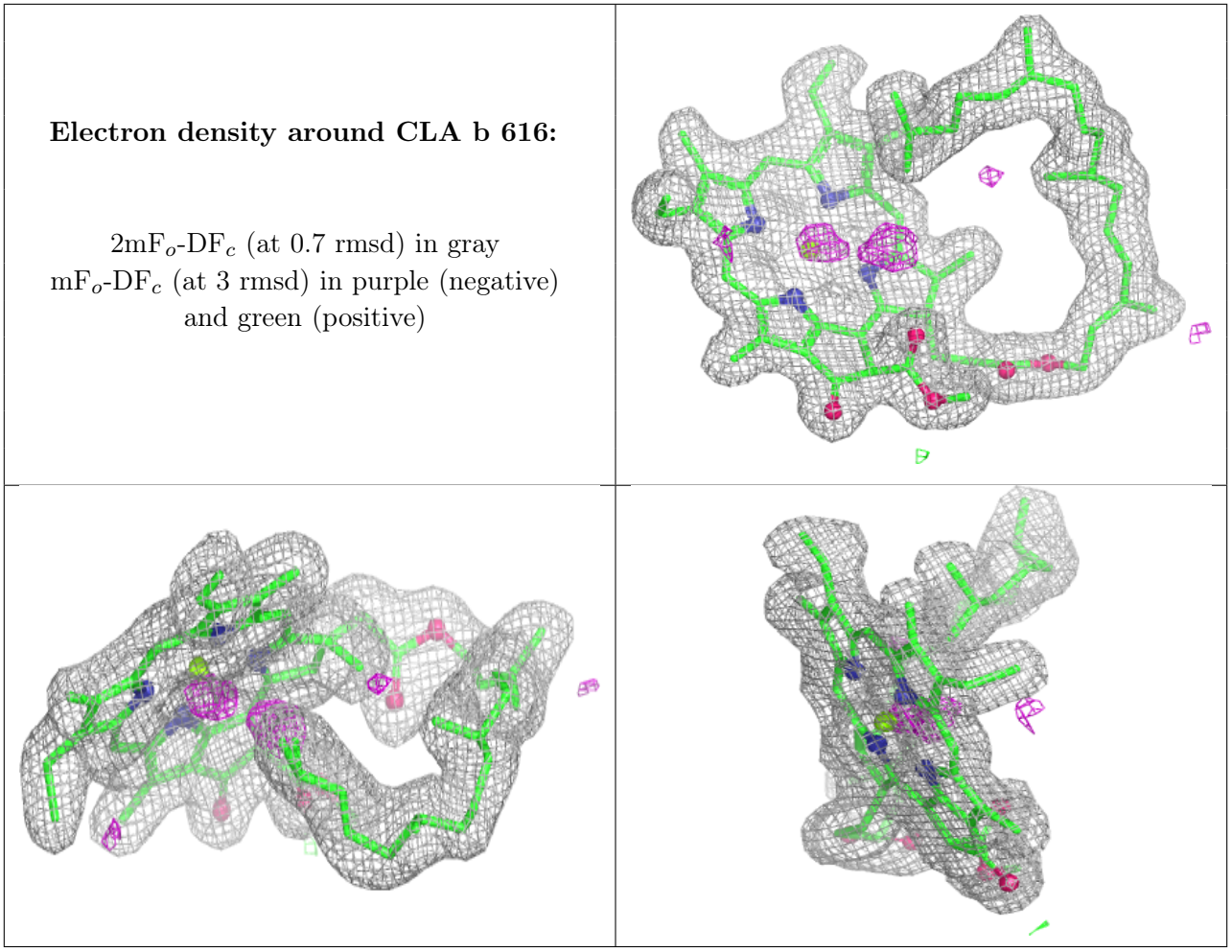






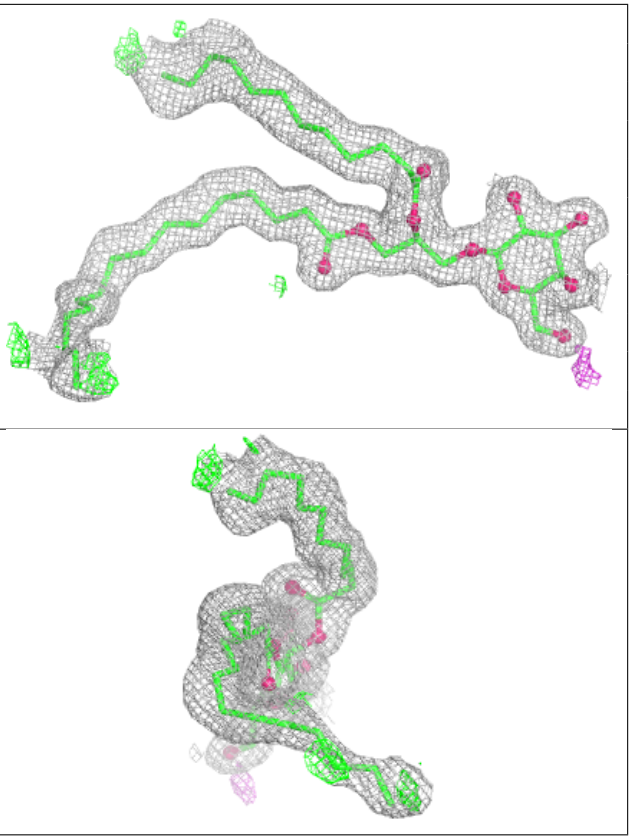
Electron density around CLA b 616:

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



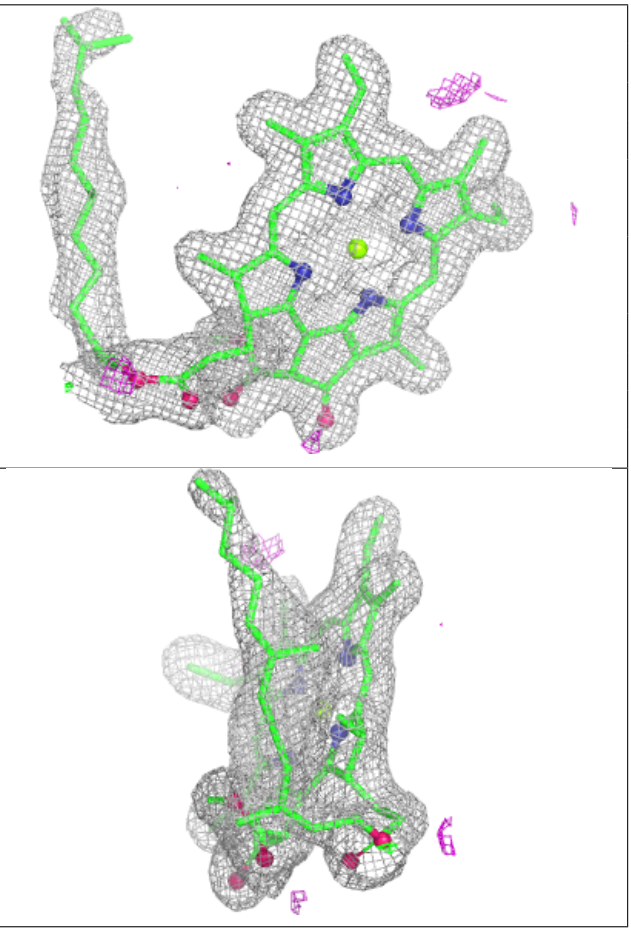
Electron density around LMG J 101:

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



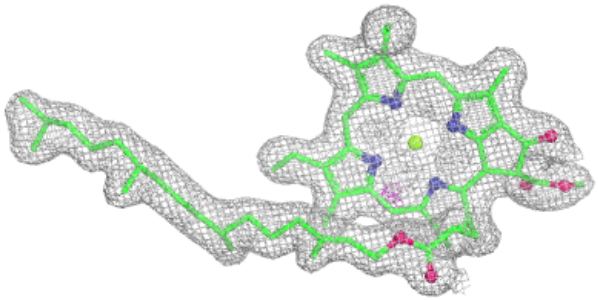
Electron density around CLA b 617:

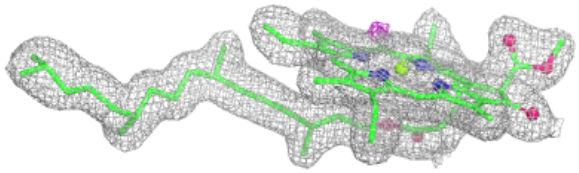
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

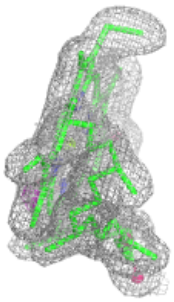


Electron density around CLA c 501:

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

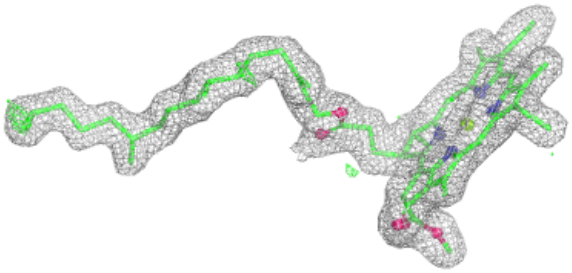


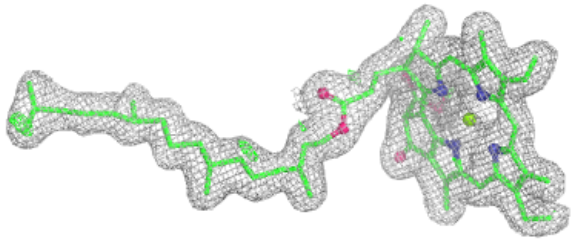


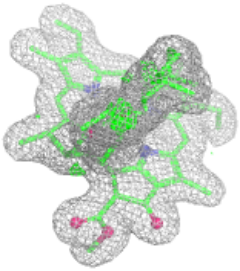


Electron density around CLA c 502:

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

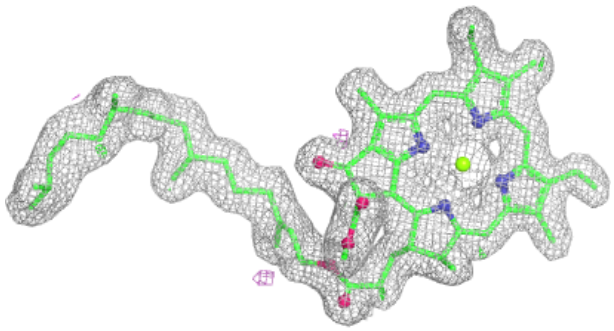


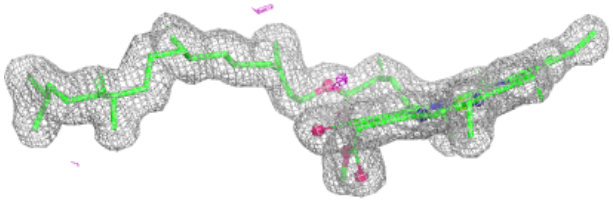


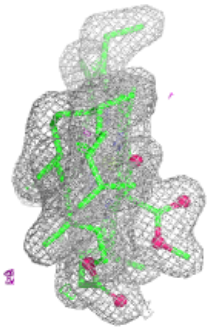


Electron density around CLA B 603:

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

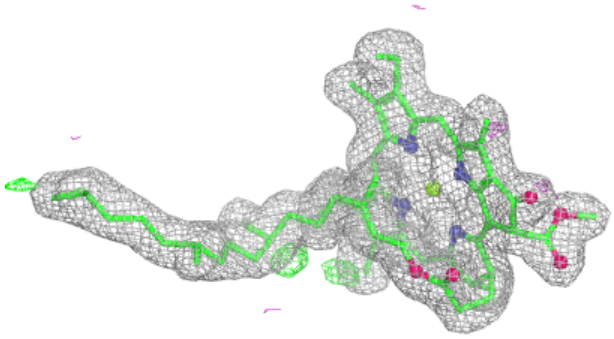


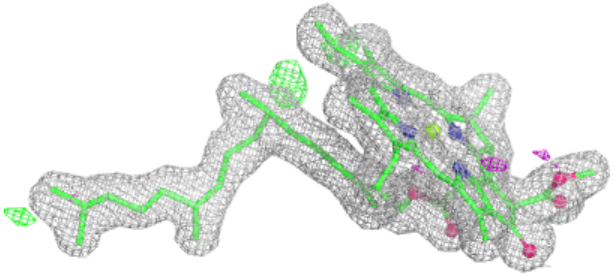


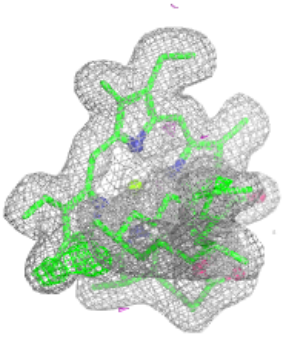


Electron density around CLA c 505:

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

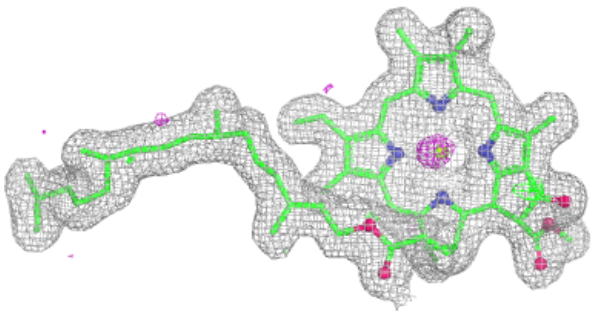


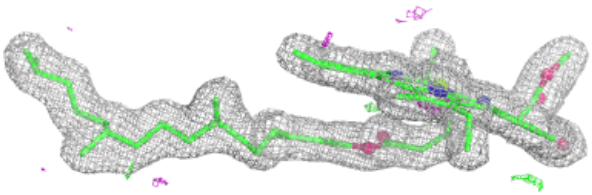


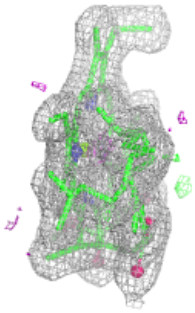


Electron density around CLA B 604:

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

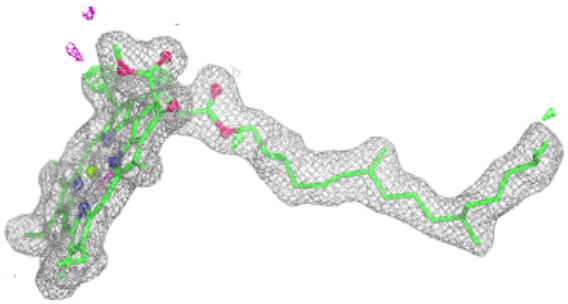


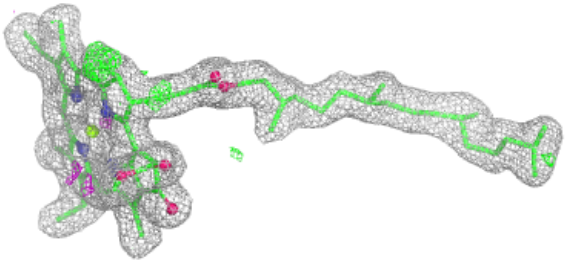




Electron density around CLA B 605:

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

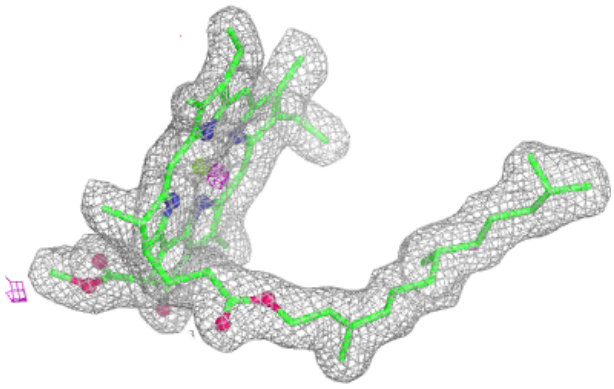


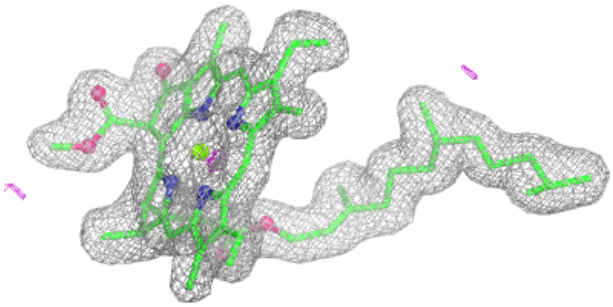


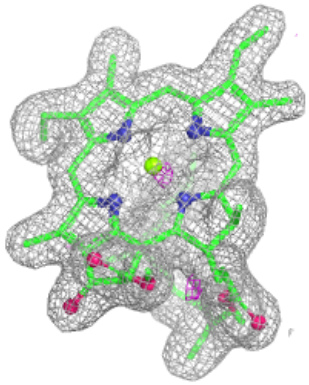


Electron density around CLA c 508:

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

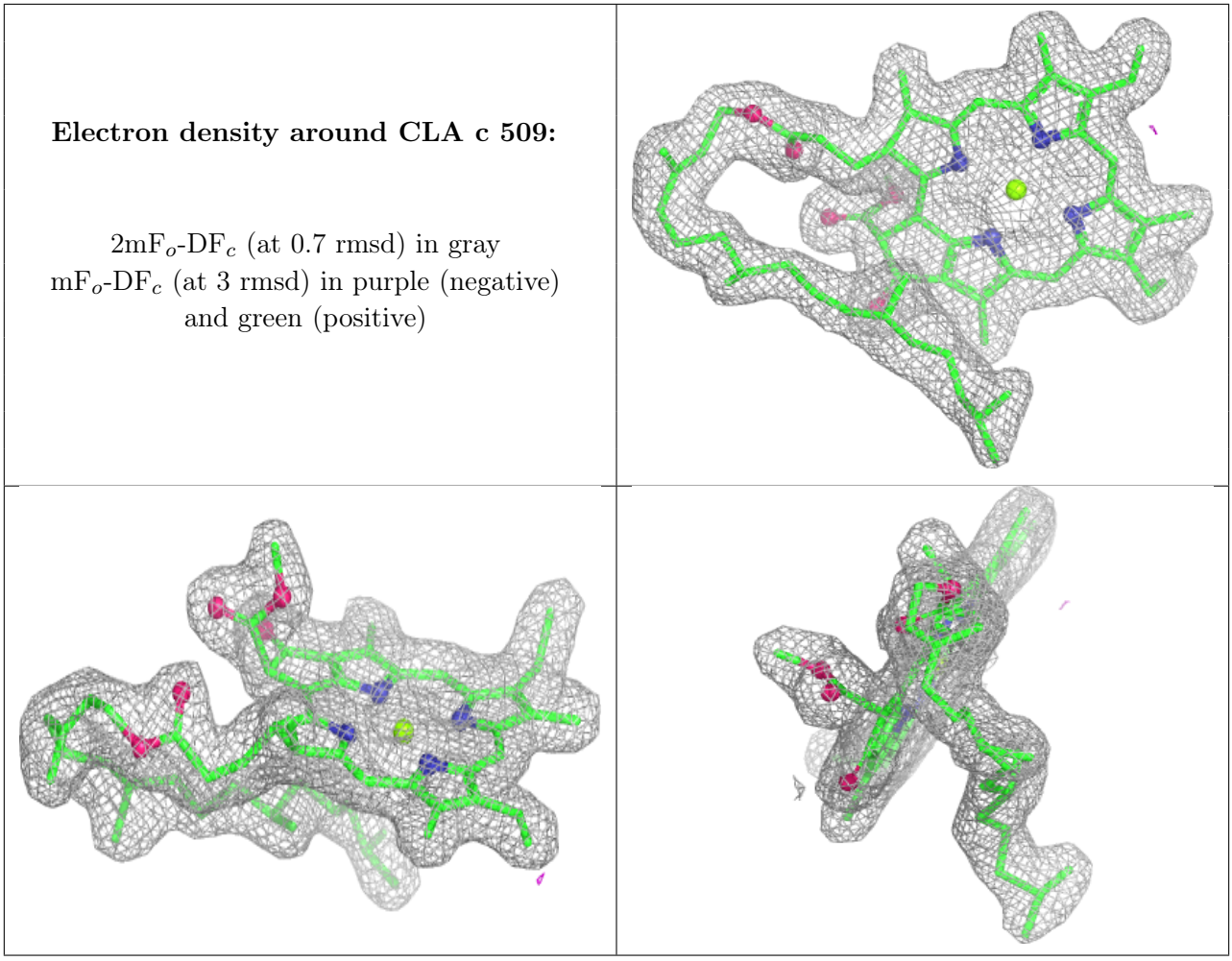






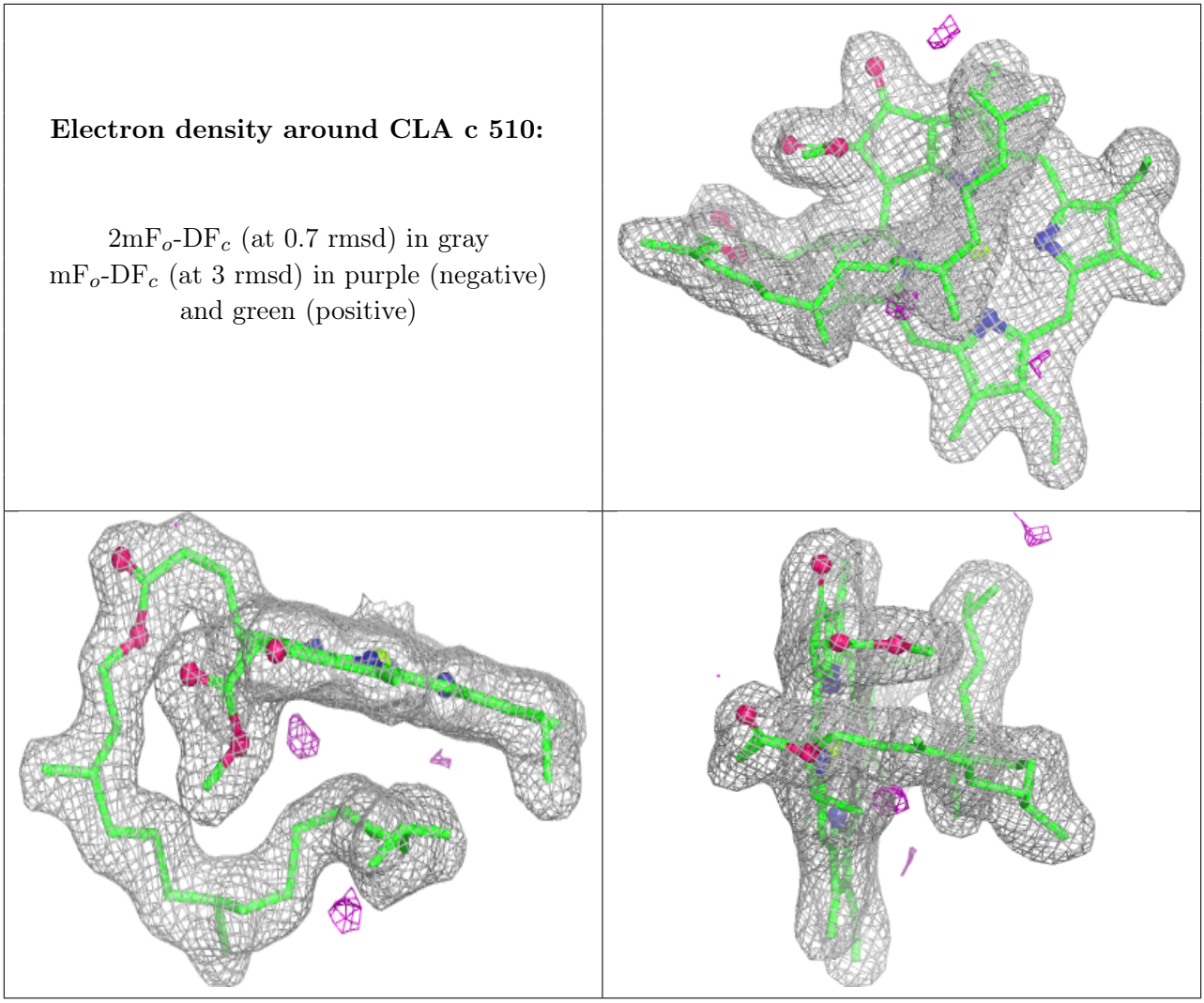
Electron density around CLA c 509:

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



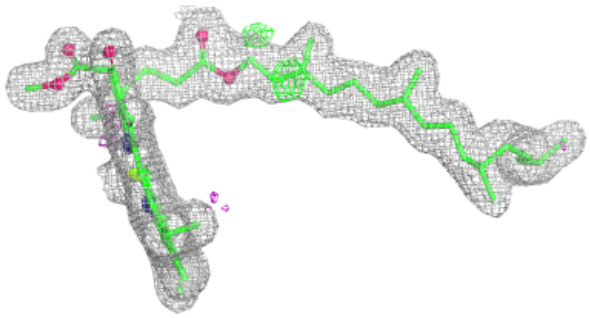
Electron density around CLA c 510:

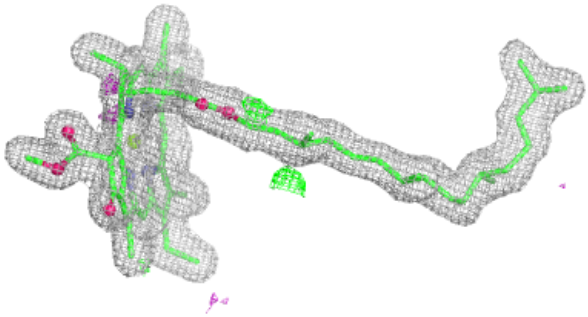
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

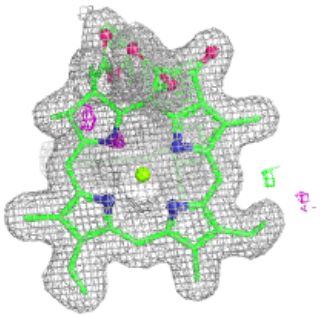


Electron density around CLA B 606:

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



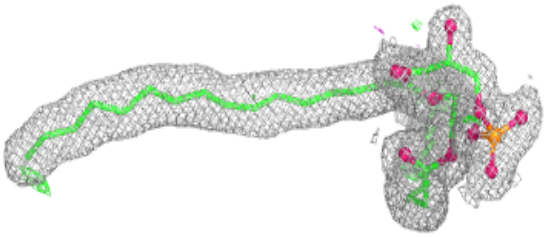


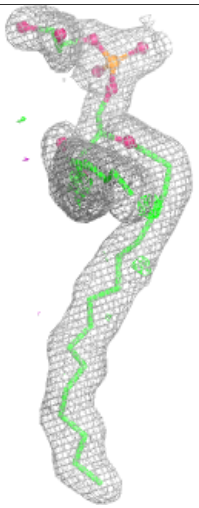


Electron density around LHG B 632:

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

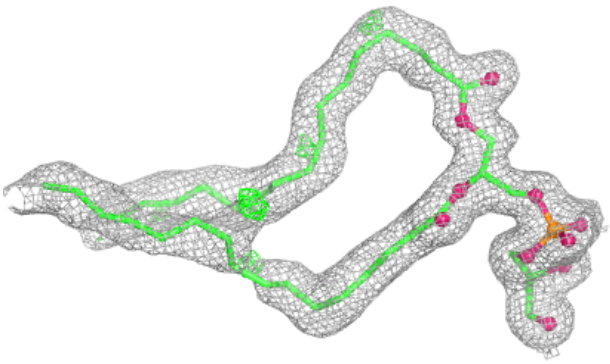


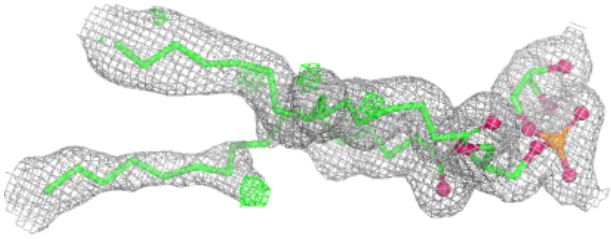


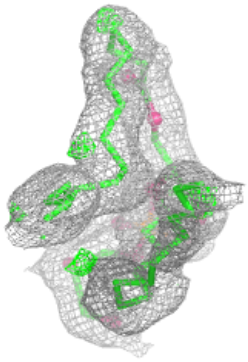


Electron density around LHG D 411:

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

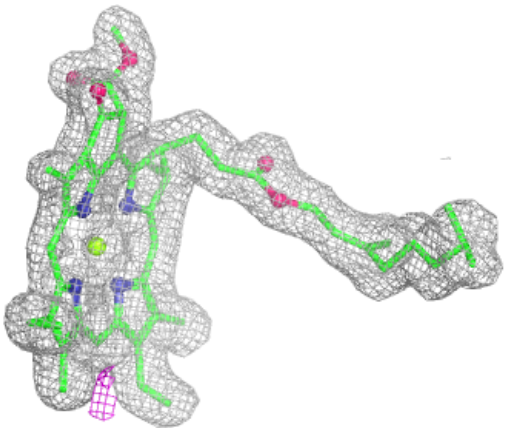


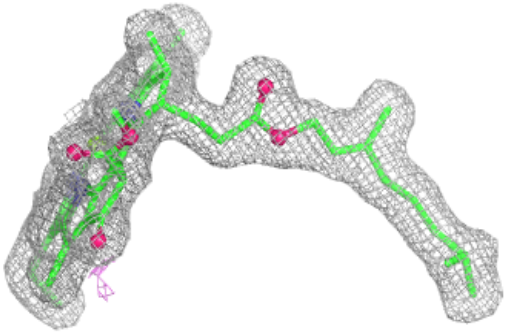


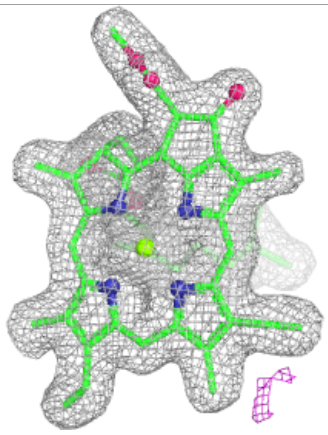


Electron density around CLA B 607:

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

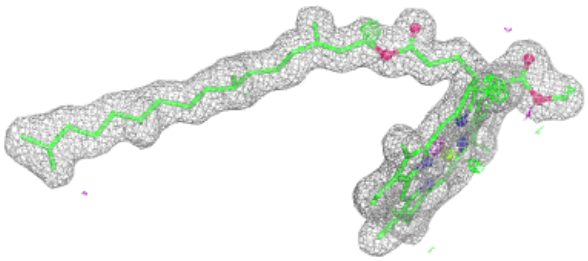


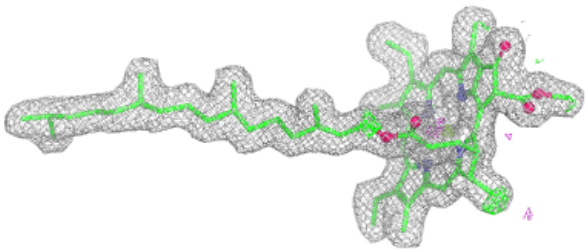


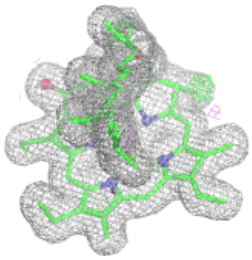


Electron density around CLA B 608:

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

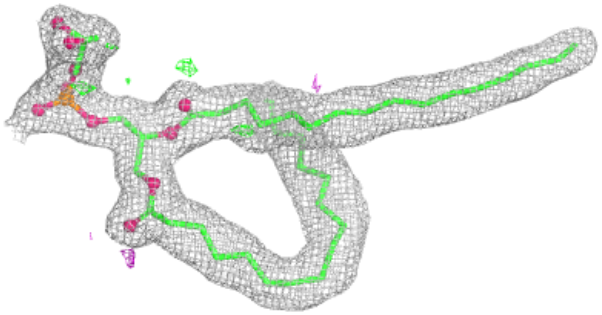


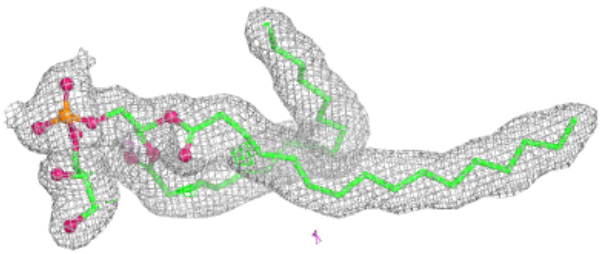




Electron density around LHG d 409:

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

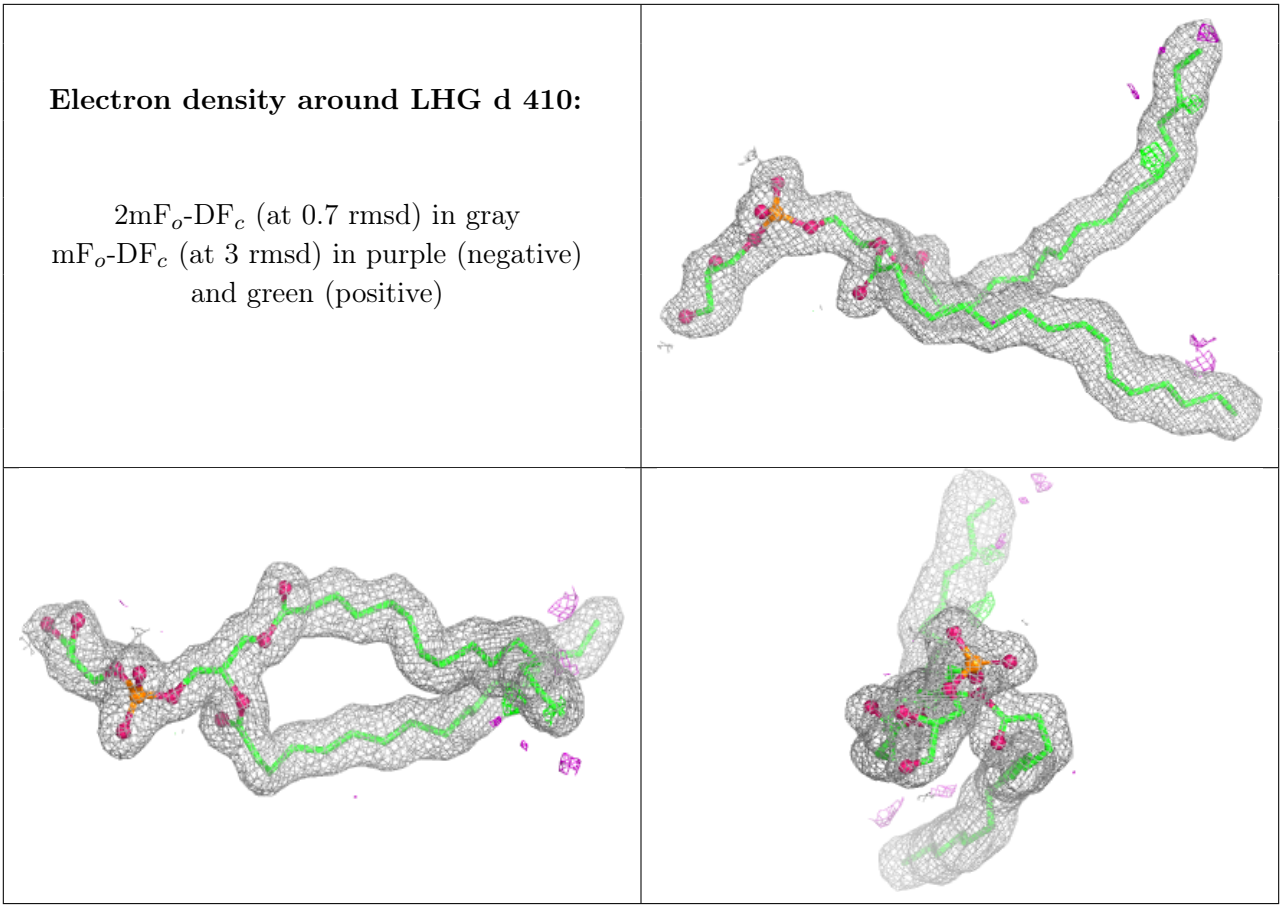






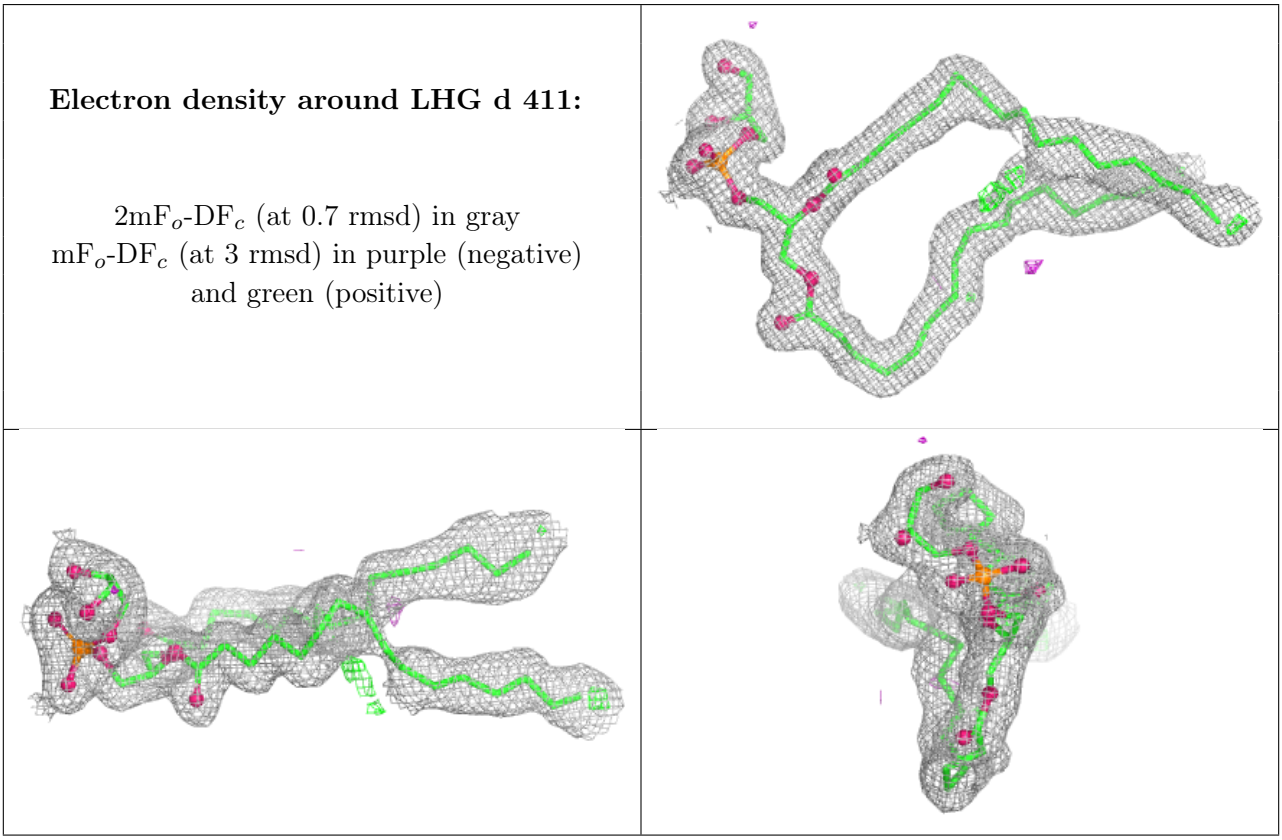
Electron density around LHG d 410:

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



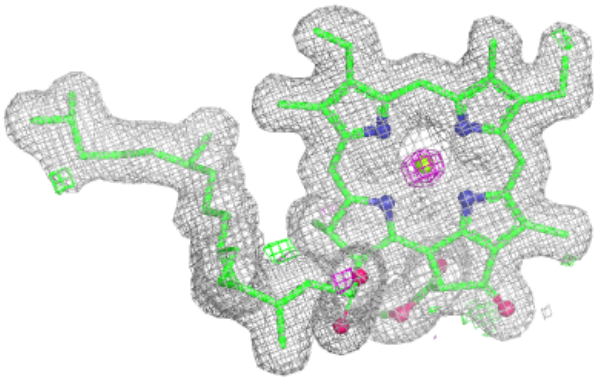
Electron density around LHG d 411:

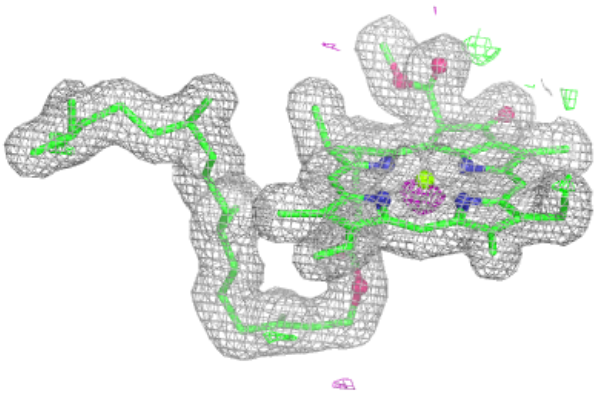
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

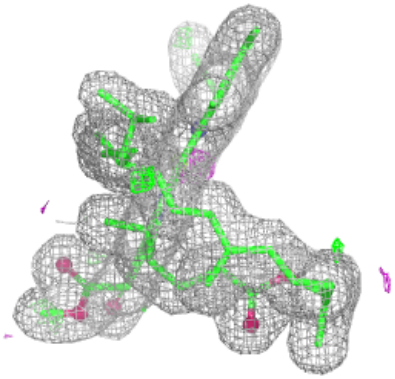


Electron density around CLA d 403:

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

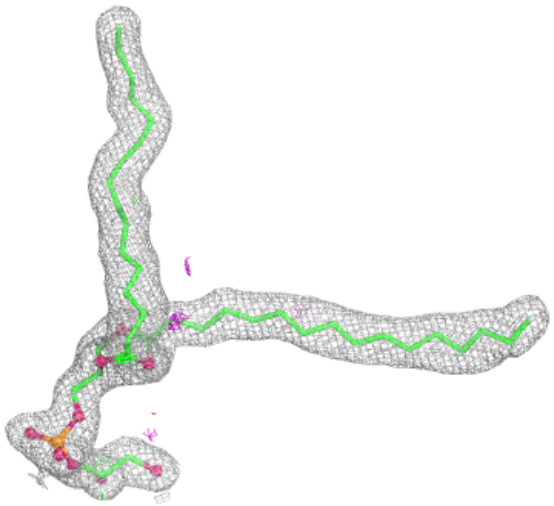


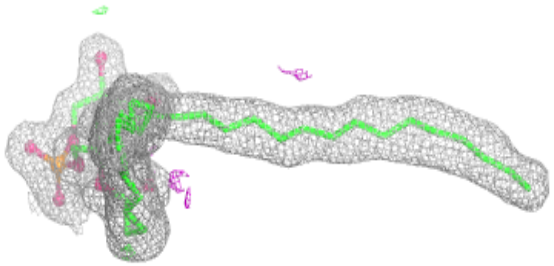


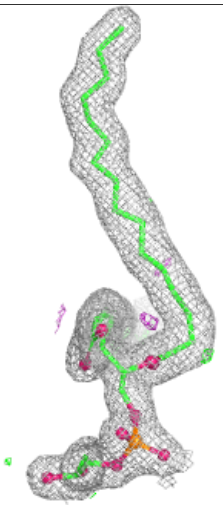


Electron density around LHG l 101:

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

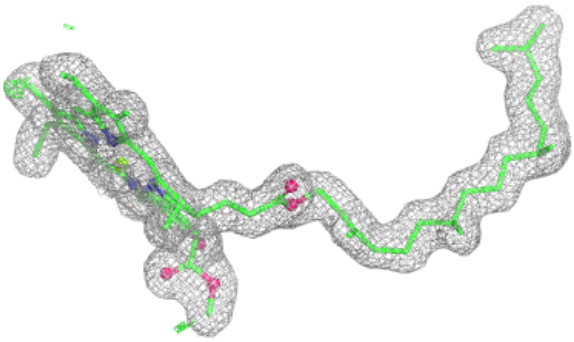


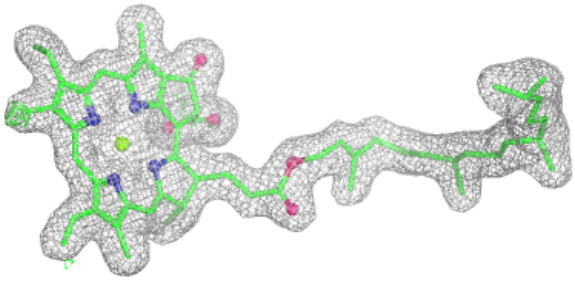


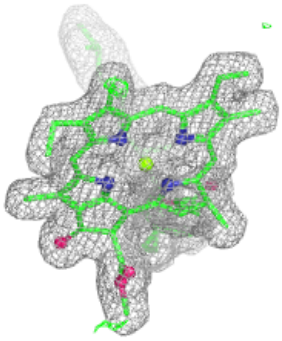


Electron density around CLA d 404:

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

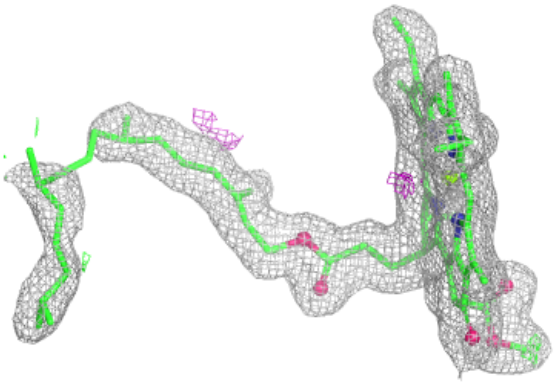


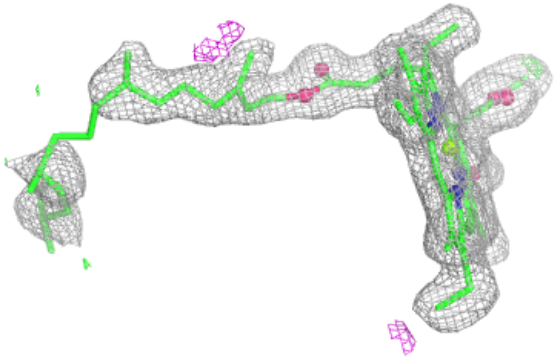


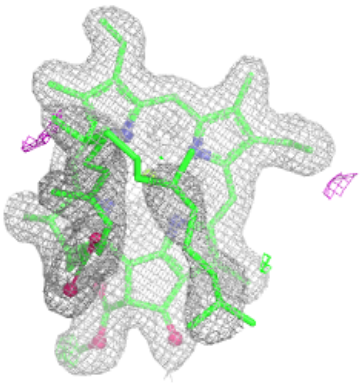


Electron density around CLA d 405:

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

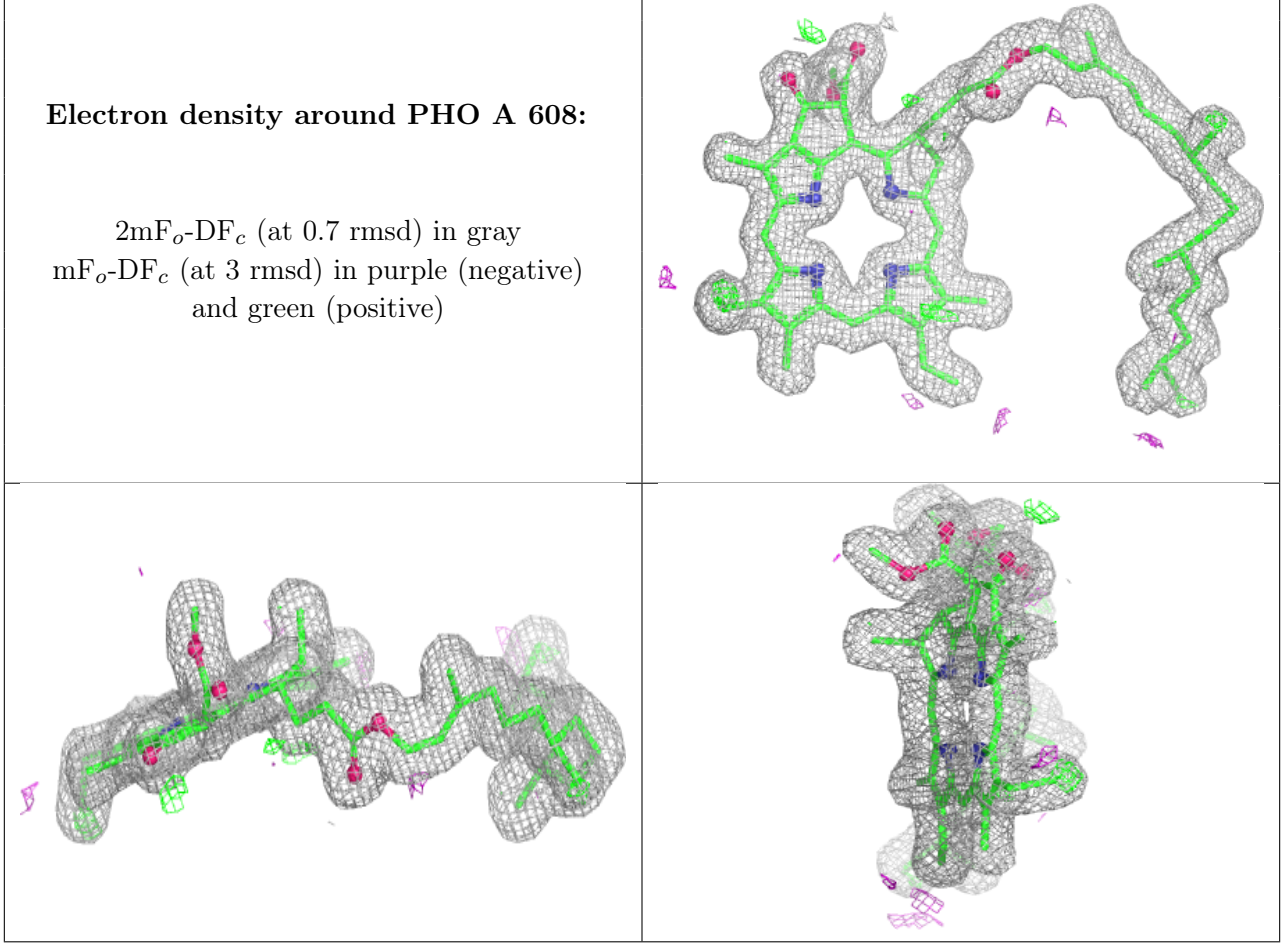






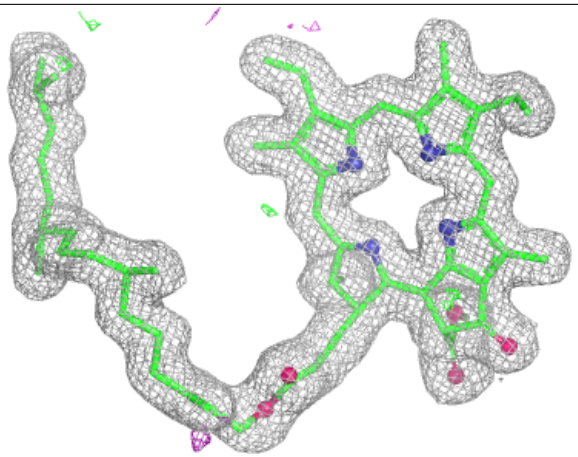
Electron density around PHO A 608:

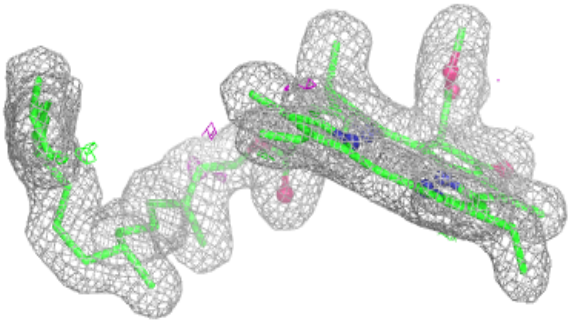
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

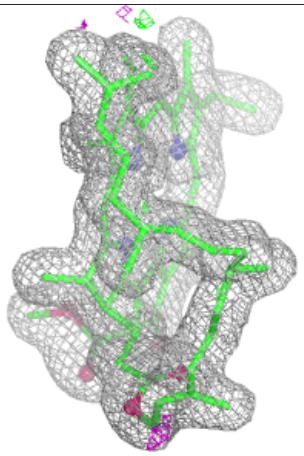


Electron density around PHO D 401:

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

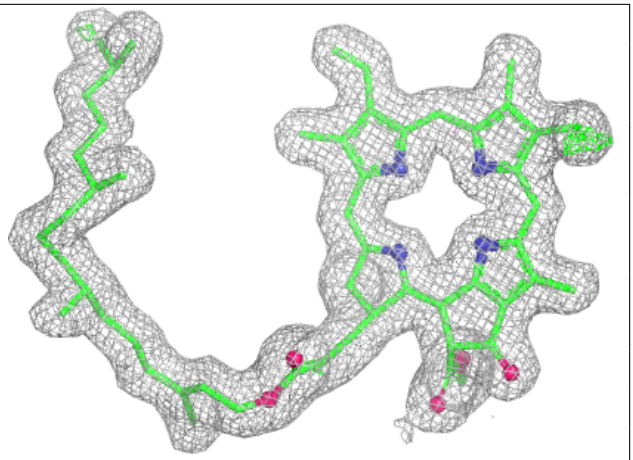


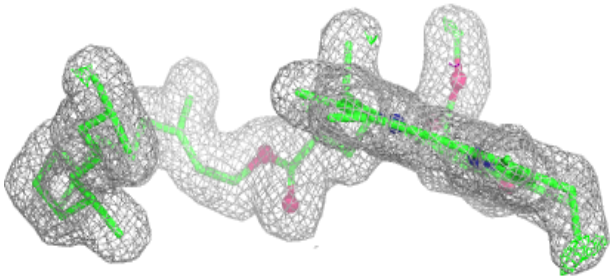


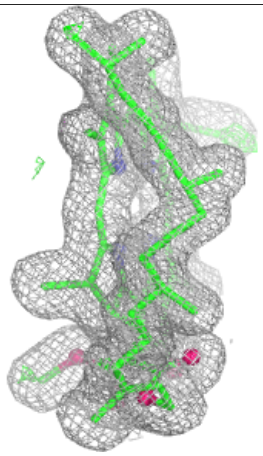


Electron density around PHO a 409:

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

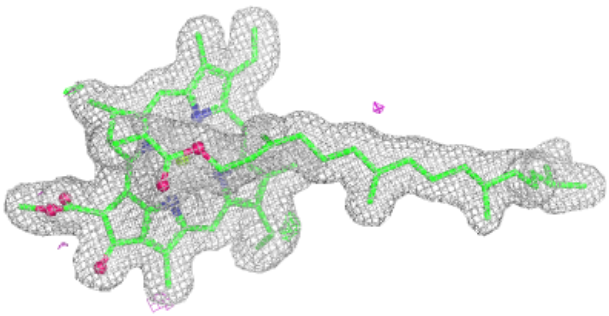


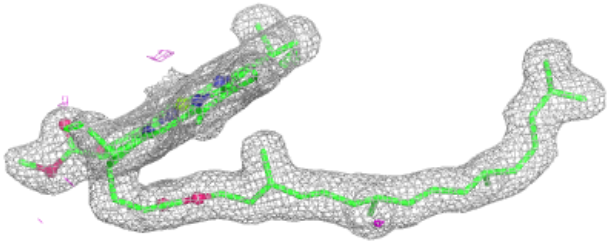


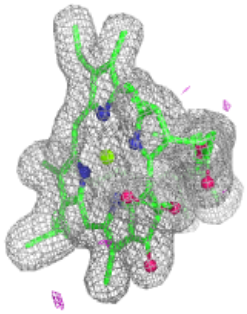


Electron density around CLA B 609:

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

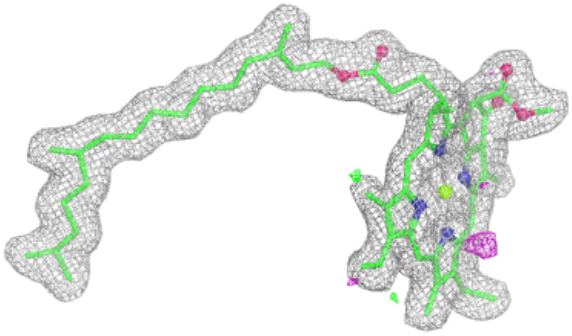


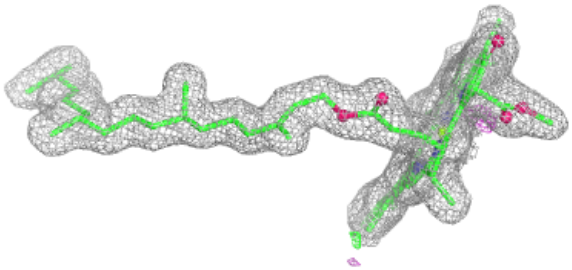


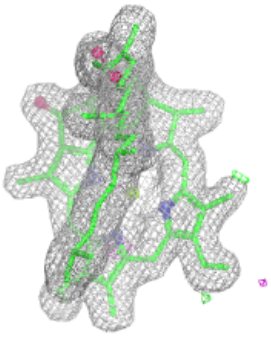


Electron density around CLA B 610:

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

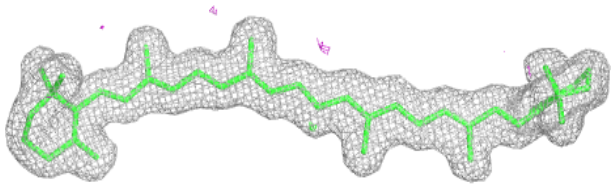


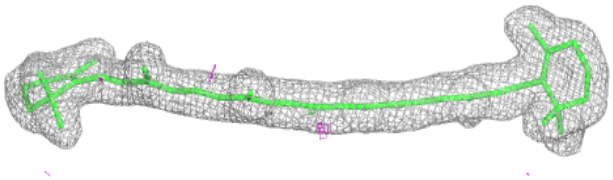


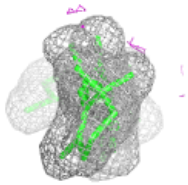


Electron density around BCR B 618:

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

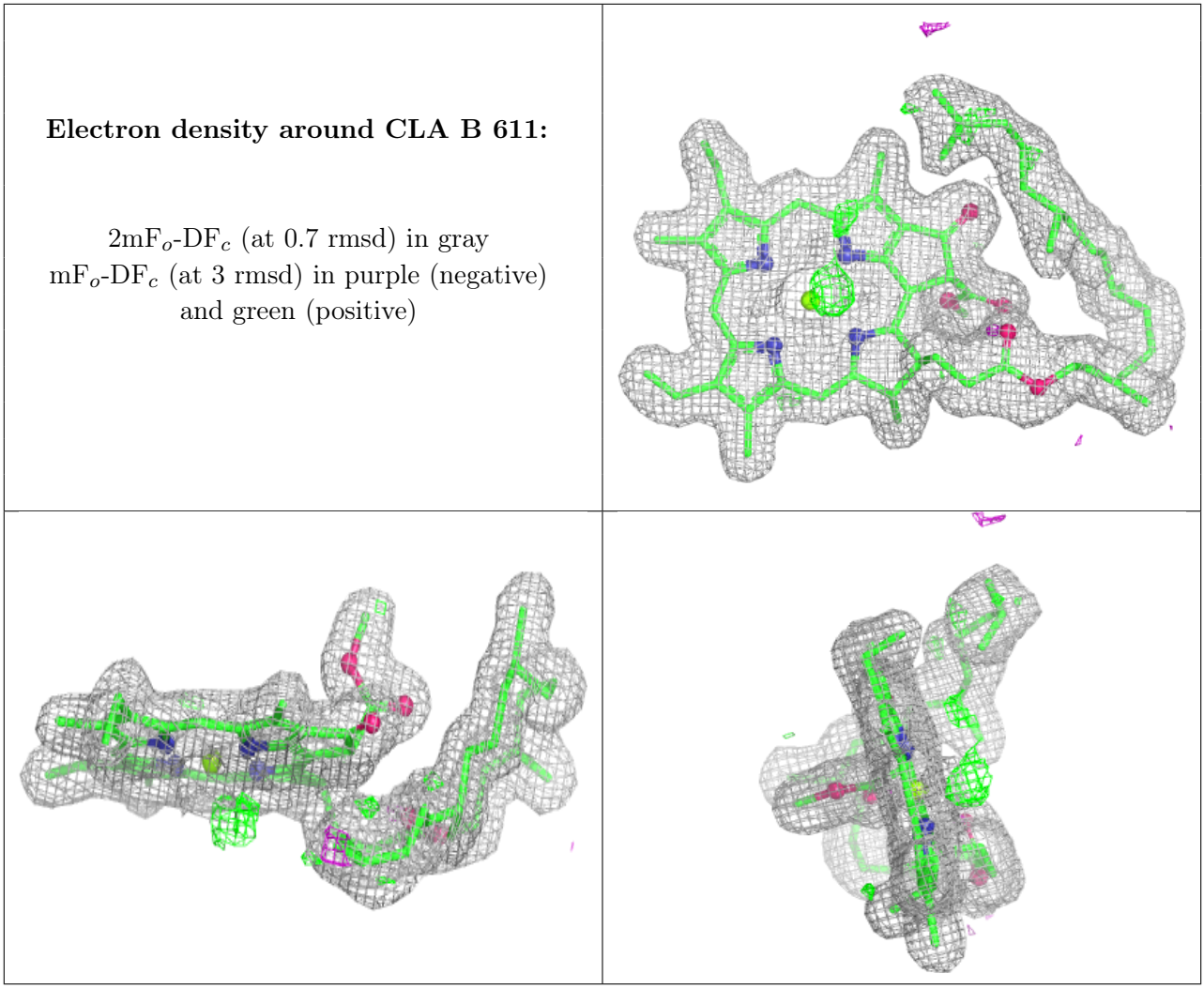






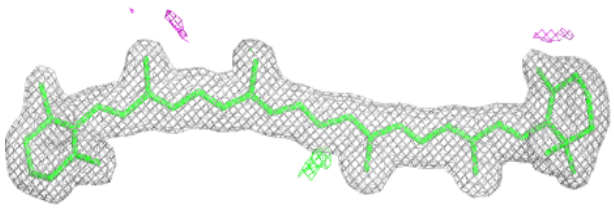
Electron density around CLA B 611:

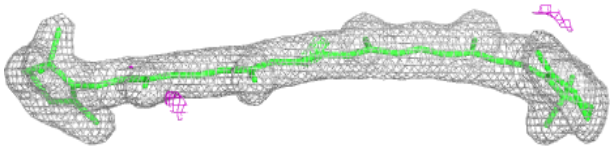
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

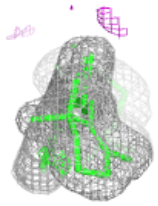


Electron density around BCR B 620:

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

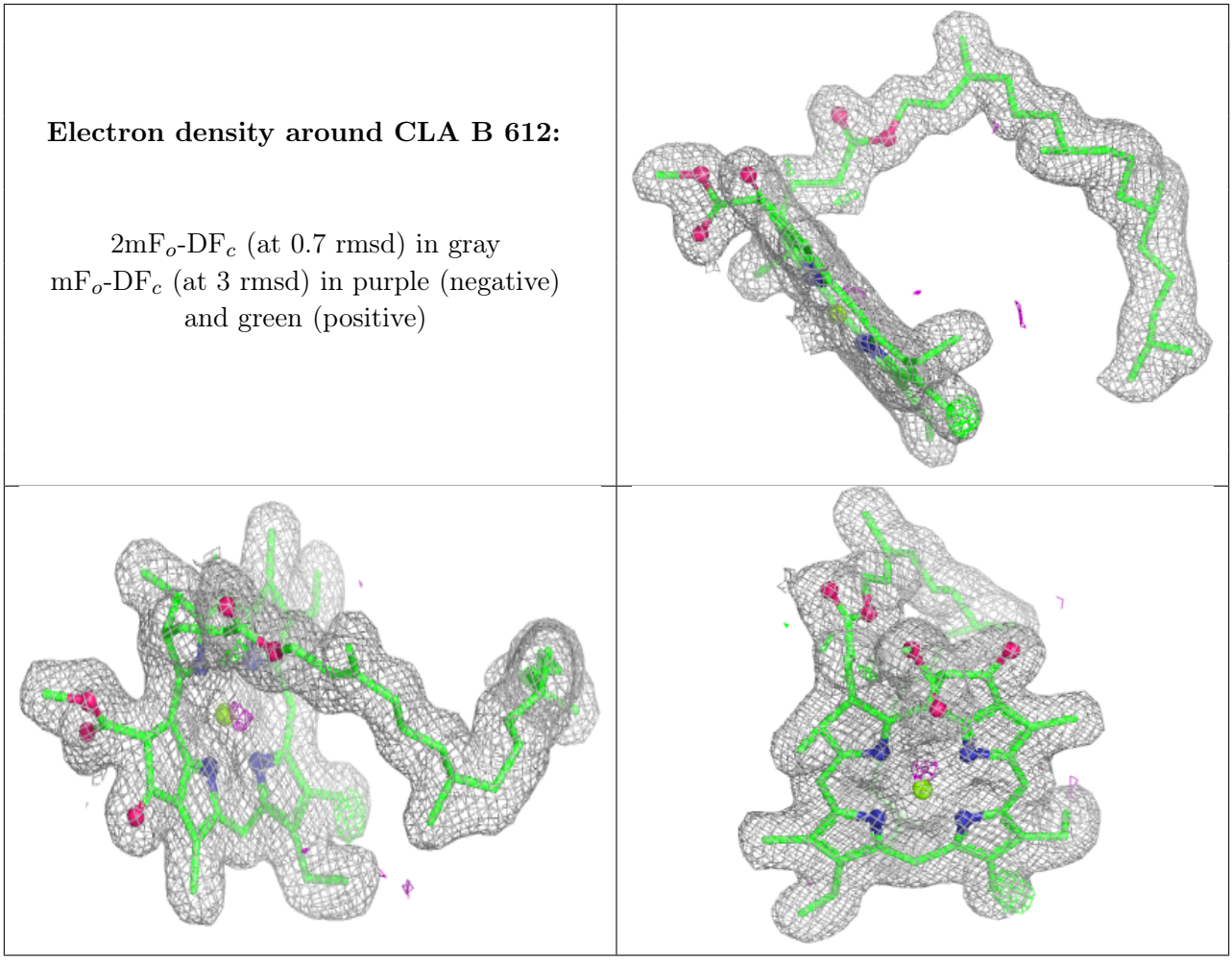






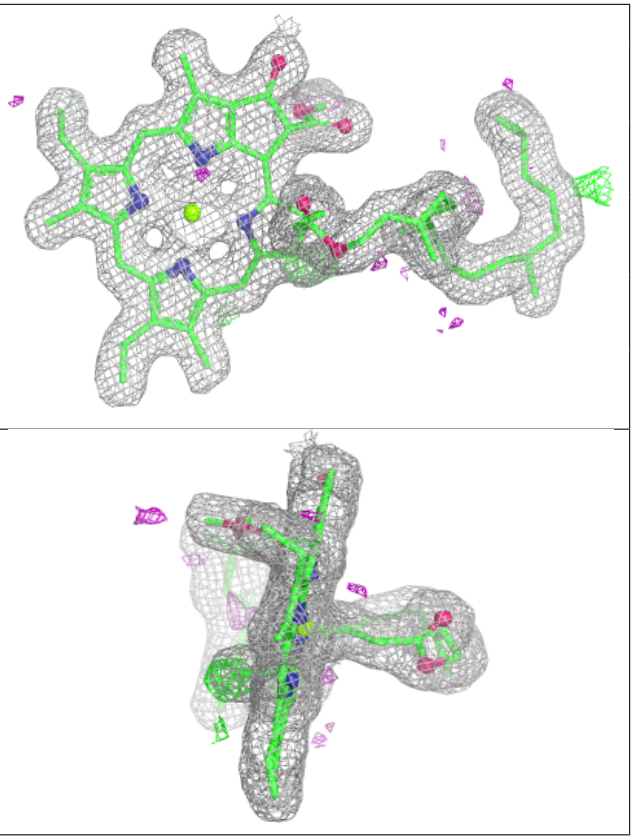
Electron density around CLA B 612:

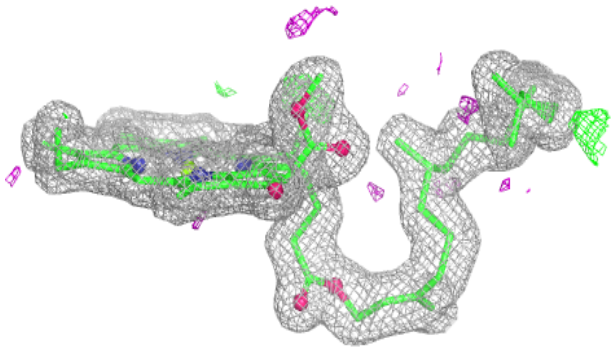
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CLA B 613:

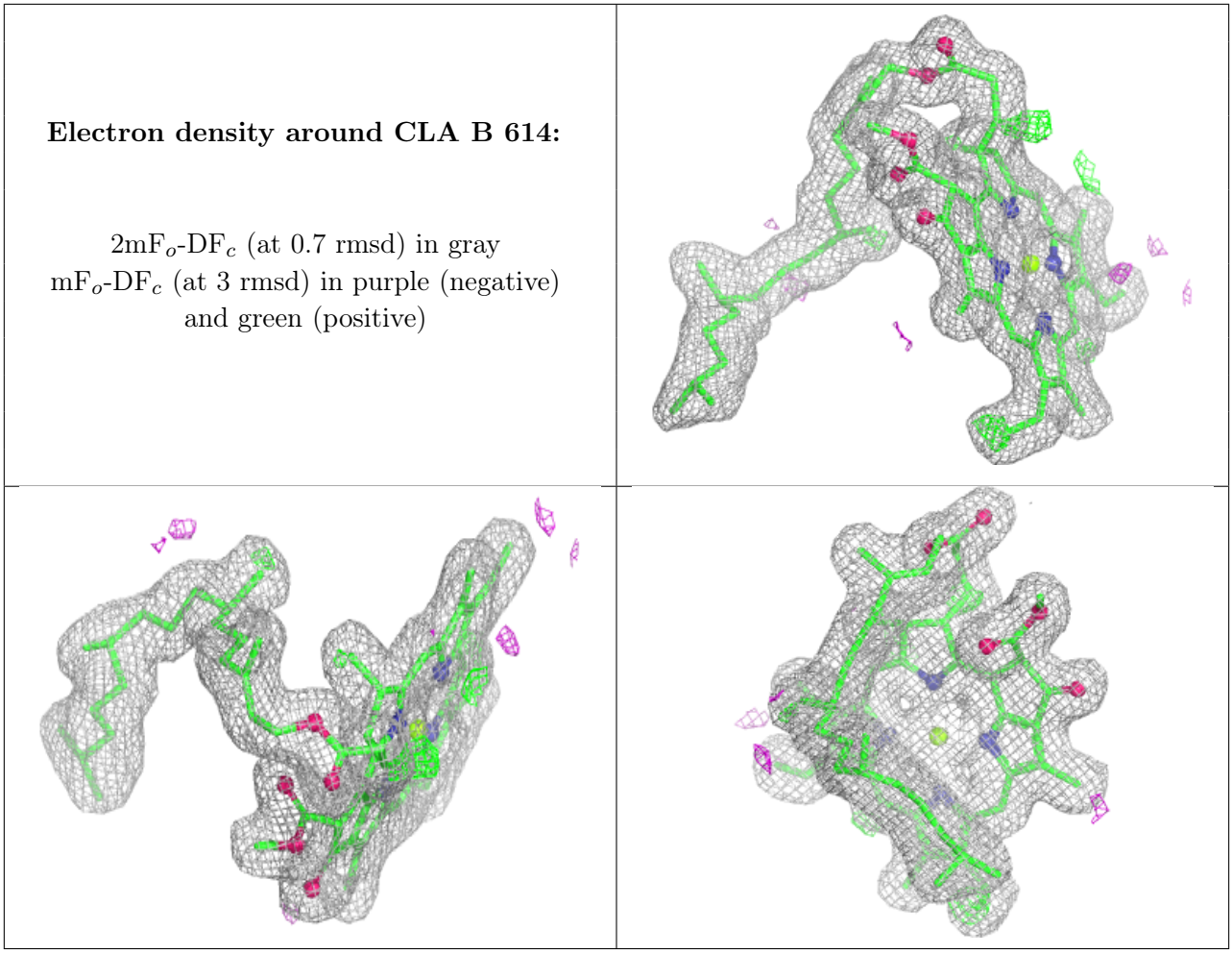
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





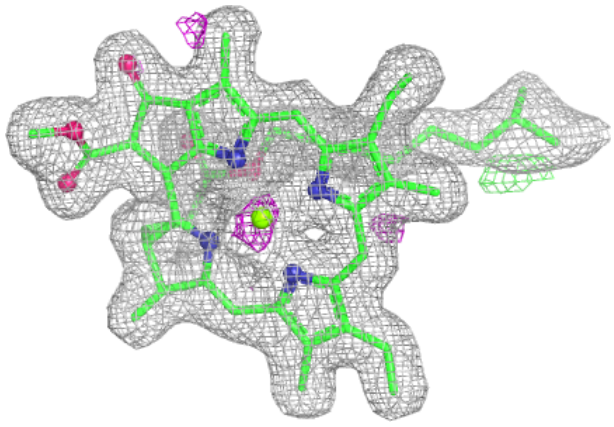
Electron density around CLA B 614:

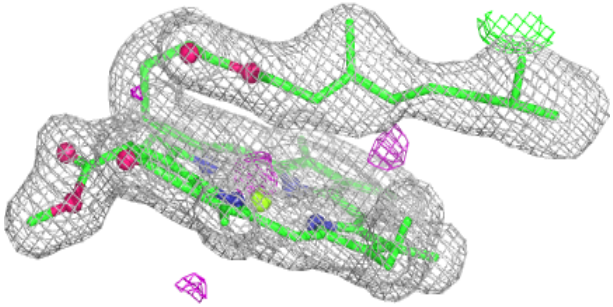
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

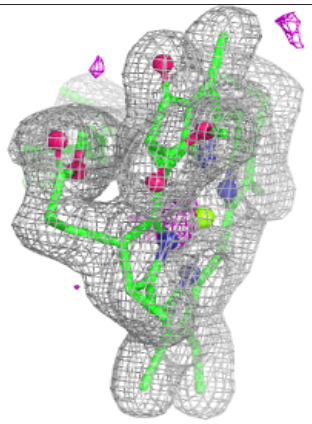


Electron density around CLA B 615:

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

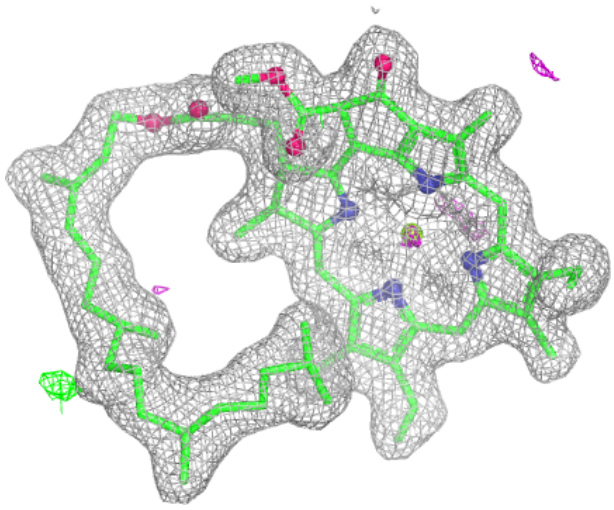


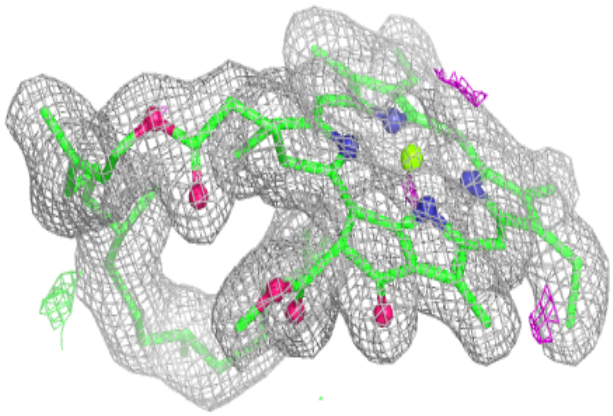


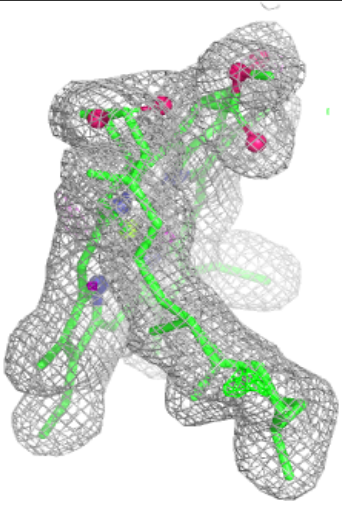


Electron density around CLA B 616:

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

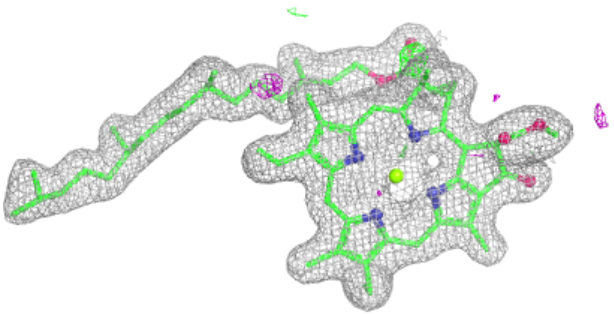


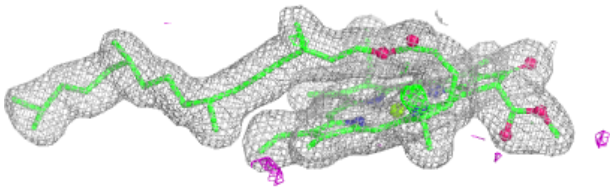


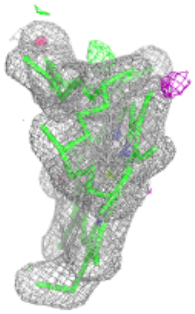


Electron density around CLA C 501:

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

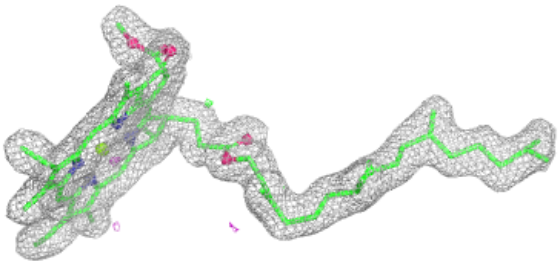


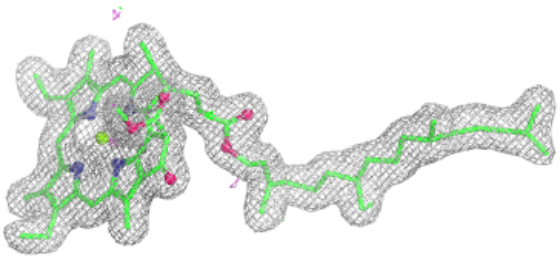


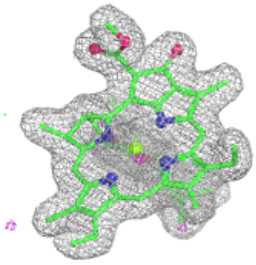


Electron density around CLA C 502:

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

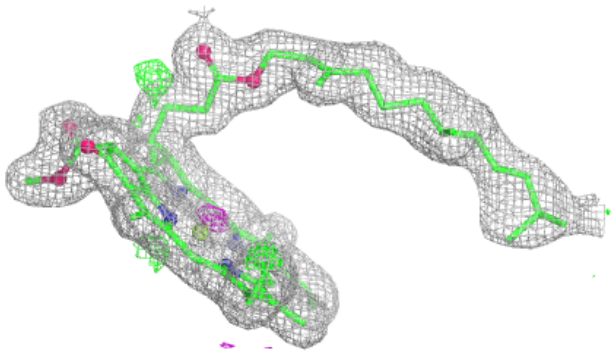


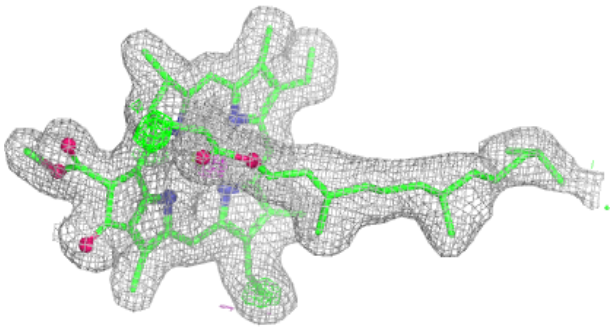


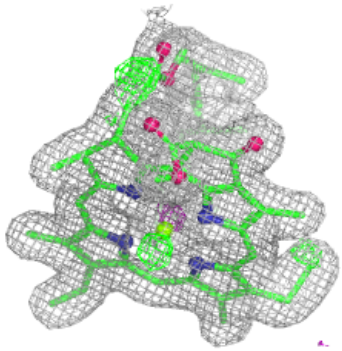


Electron density around CLA C 504:

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

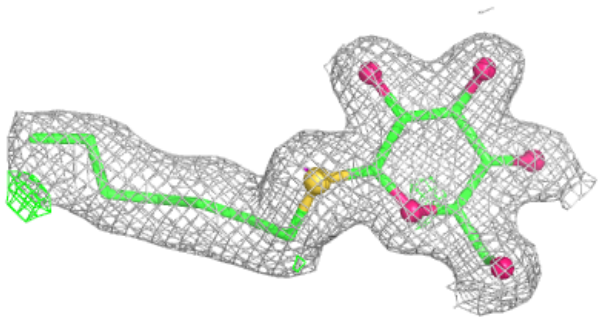


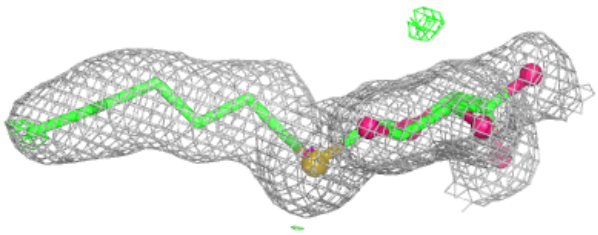


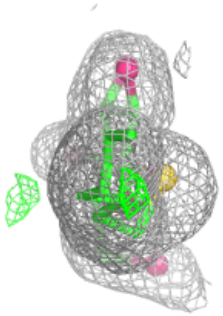


Electron density around HTG O 303:

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

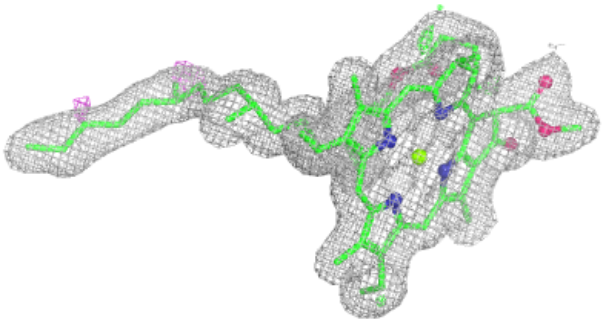


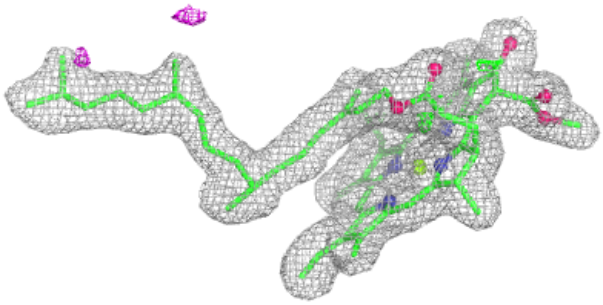


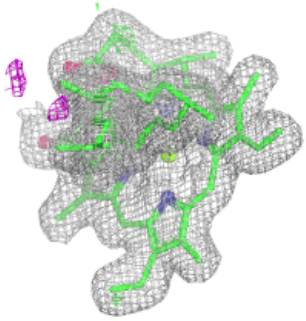


Electron density around CLA C 505:

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

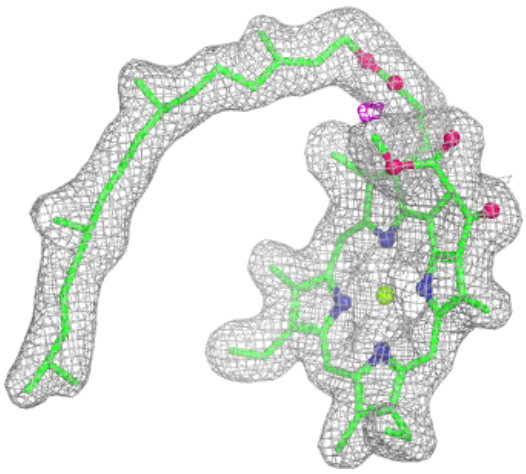


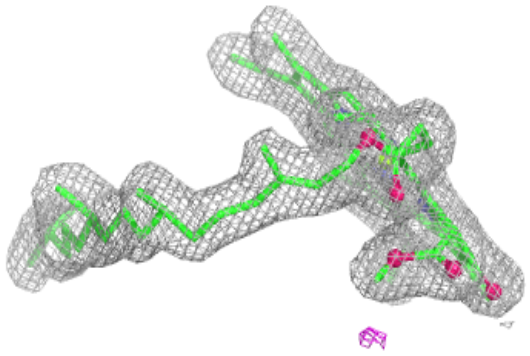


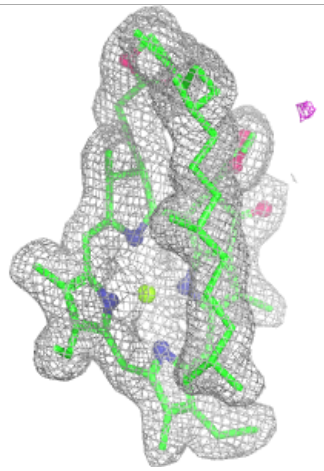


Electron density around CLA C 507:

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

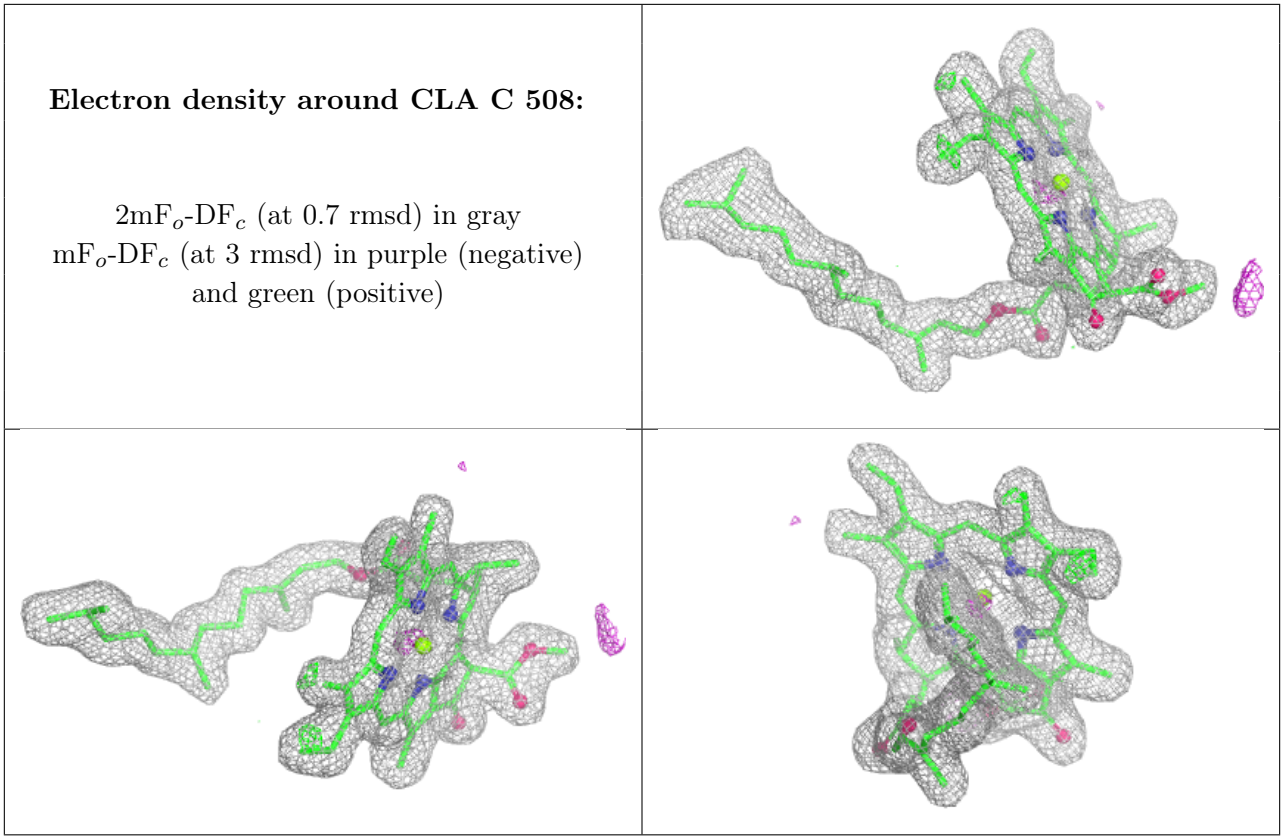






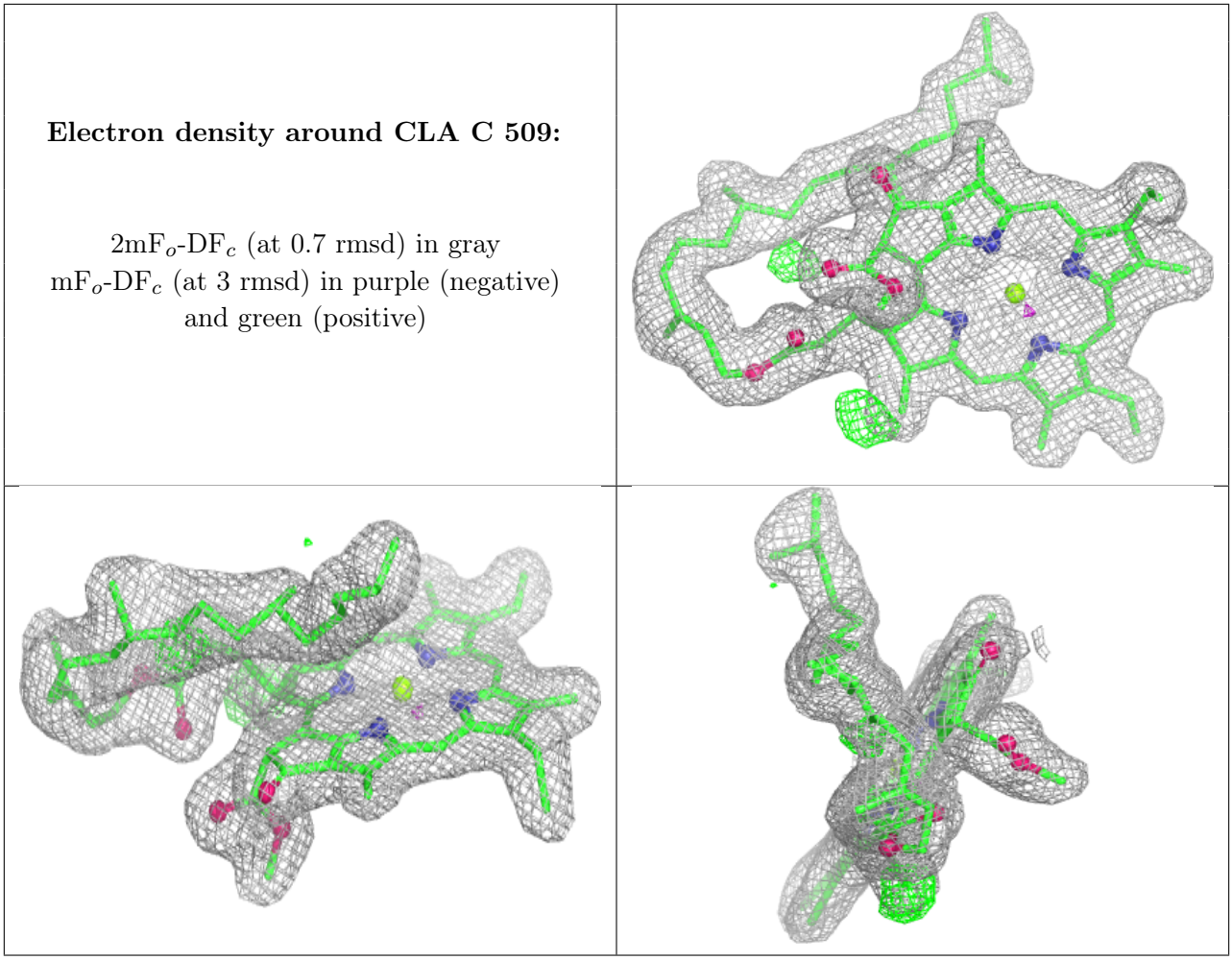
Electron density around CLA C 508:

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



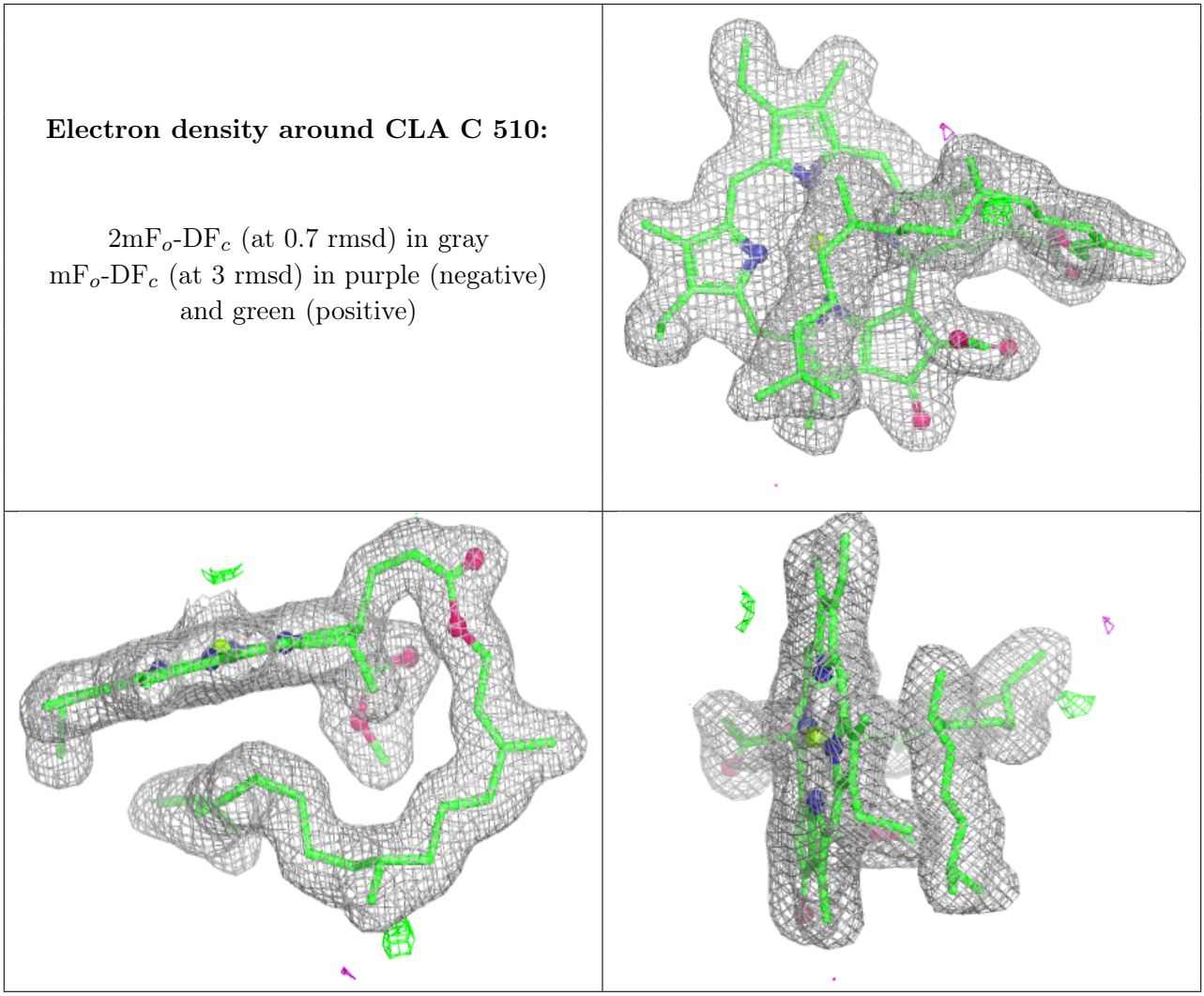
Electron density around CLA C 509:

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



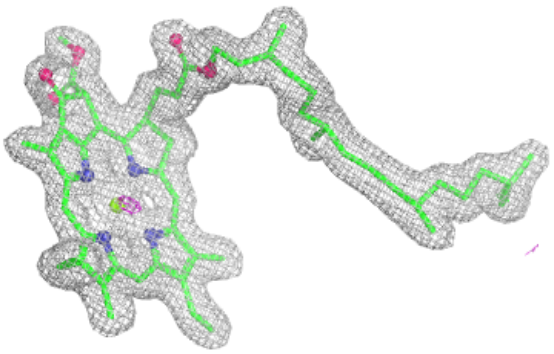
Electron density around CLA C 510:

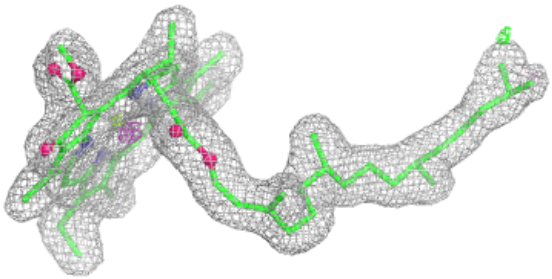
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

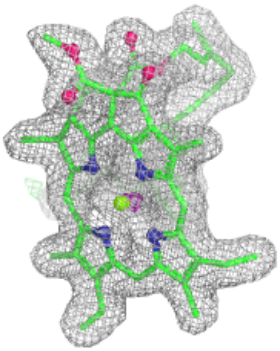


Electron density around CLA C 511:

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

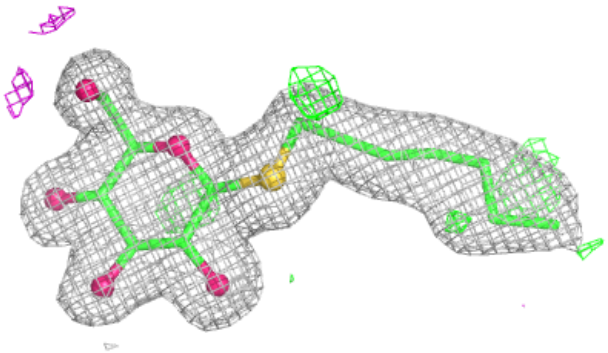


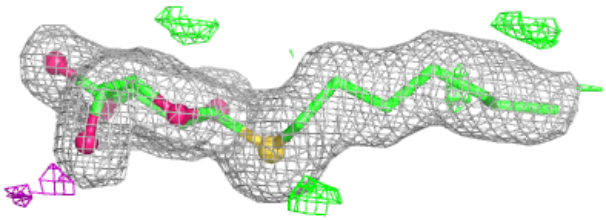


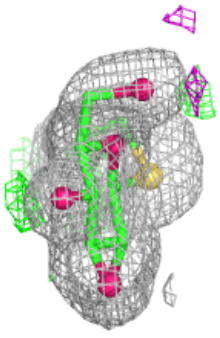


Electron density around HTG o 301:

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

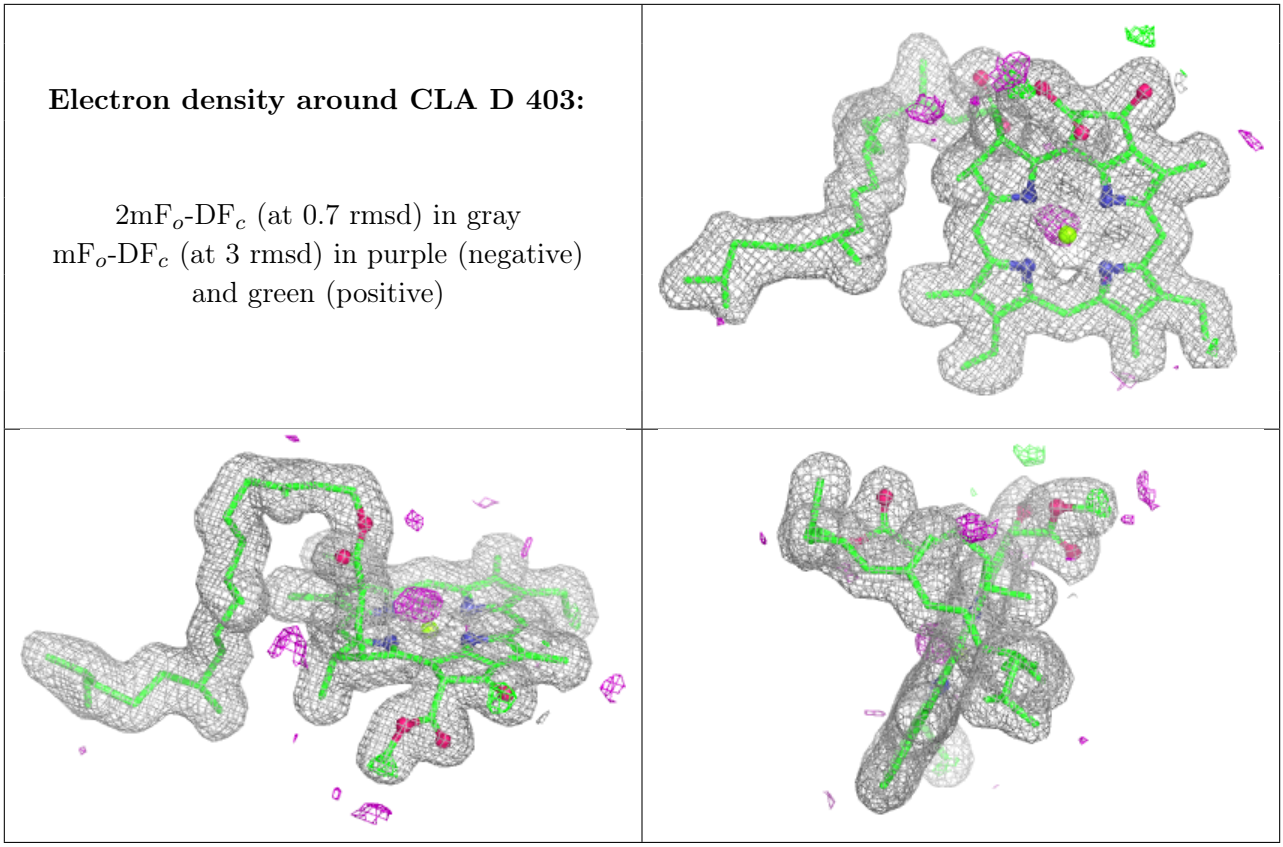






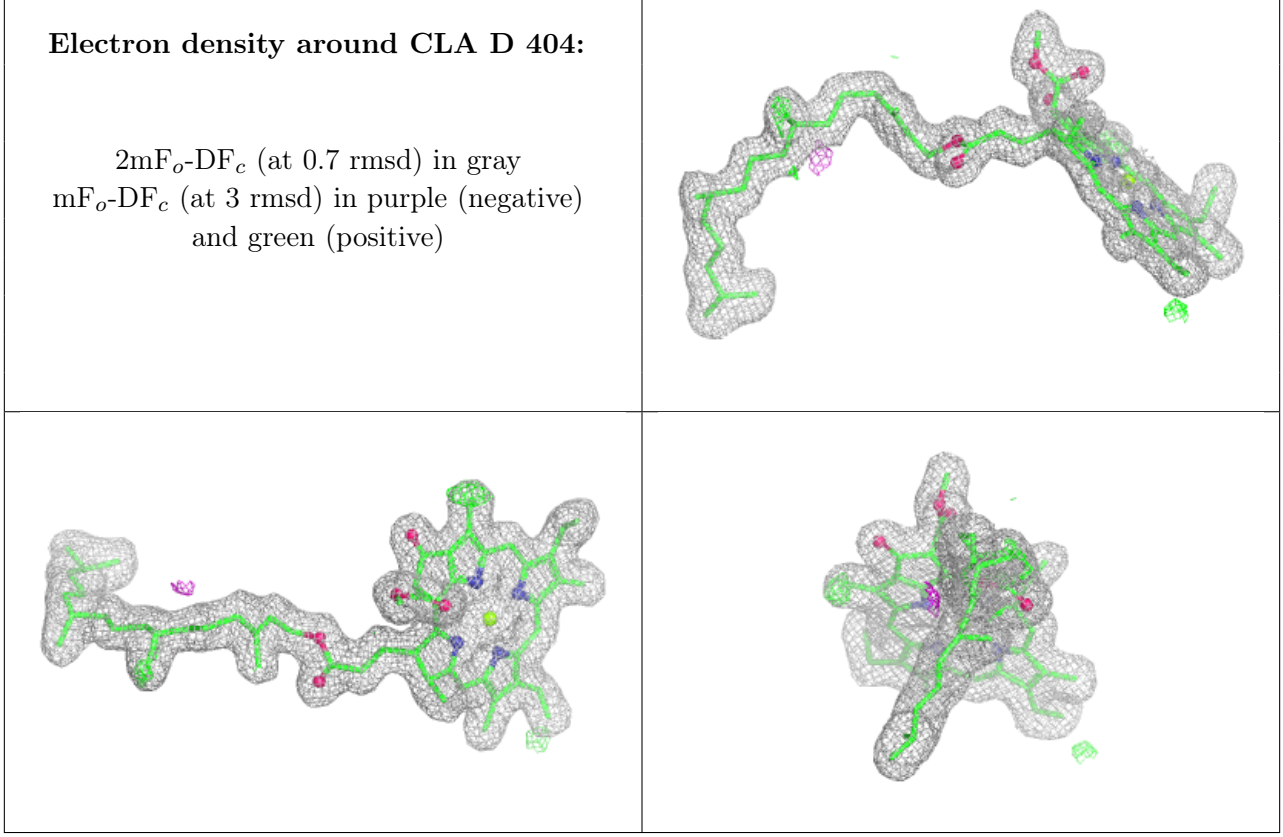
Electron density around CLA D 403:

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



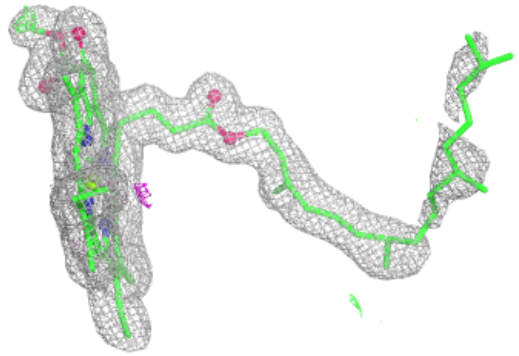
Electron density around CLA D 404:

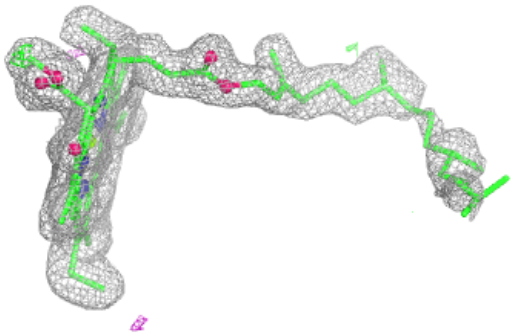
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

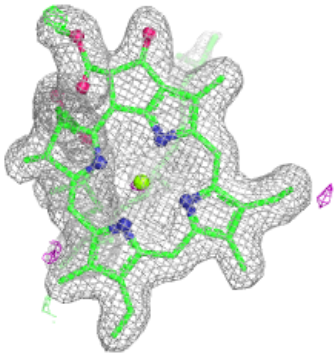


Electron density around CLA D 405:

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

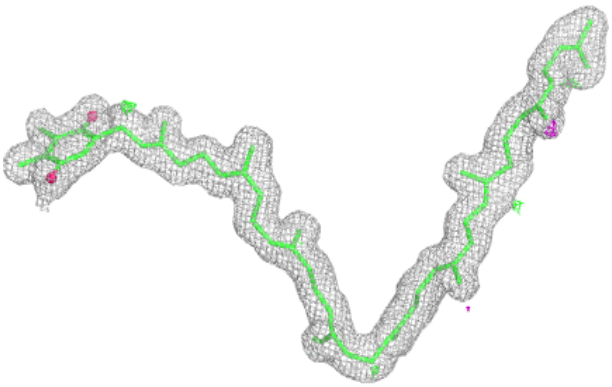


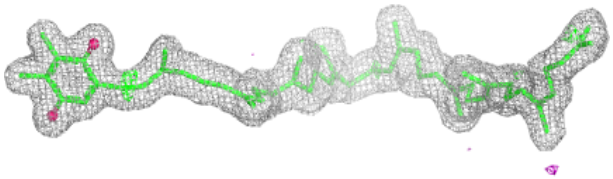


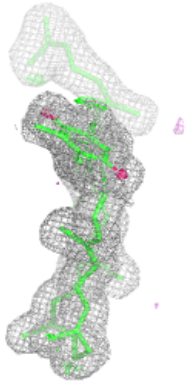


Electron density around PL9 d 407:

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

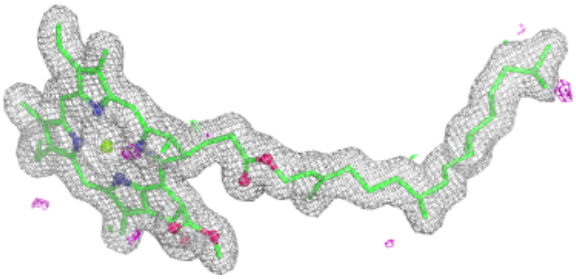


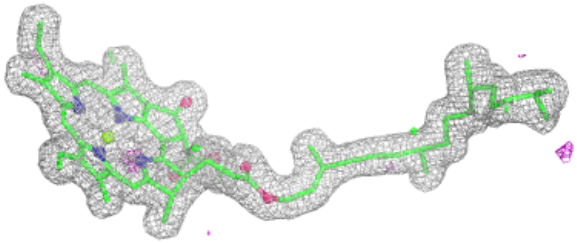


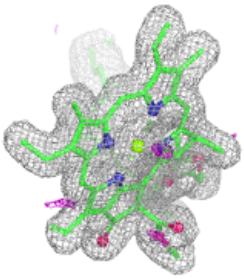


Electron density around CLA a 407:

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

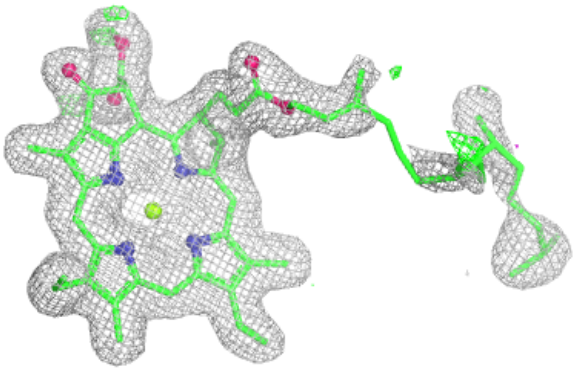


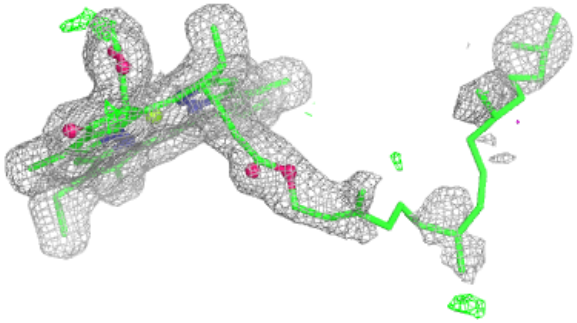


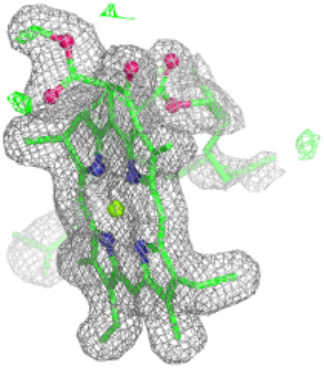


Electron density around CLA a 410:

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

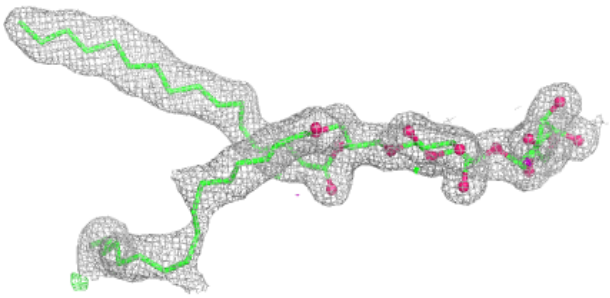


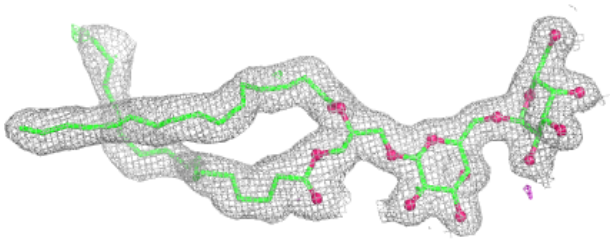


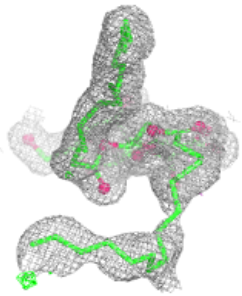


Electron density around DGD C 516:

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

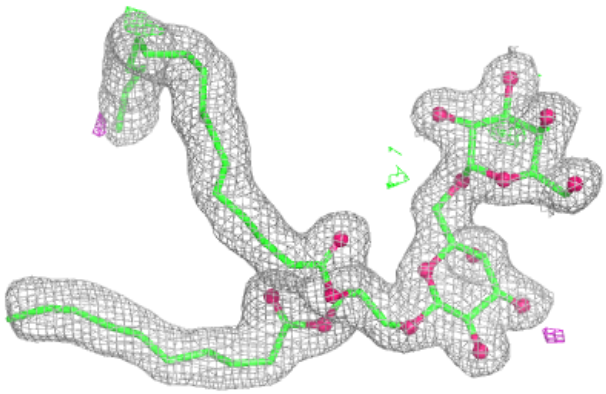


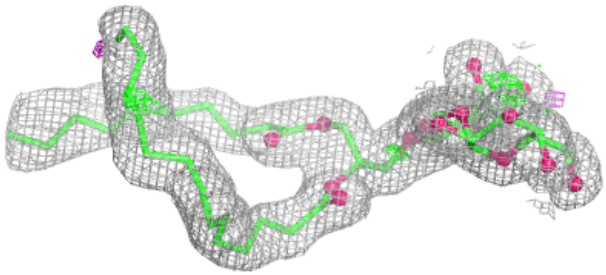


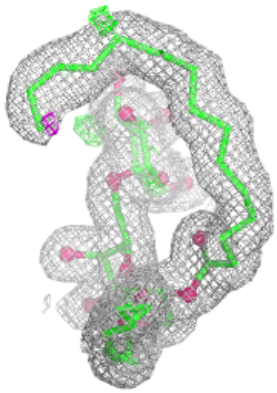


Electron density around DGD C 517:

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

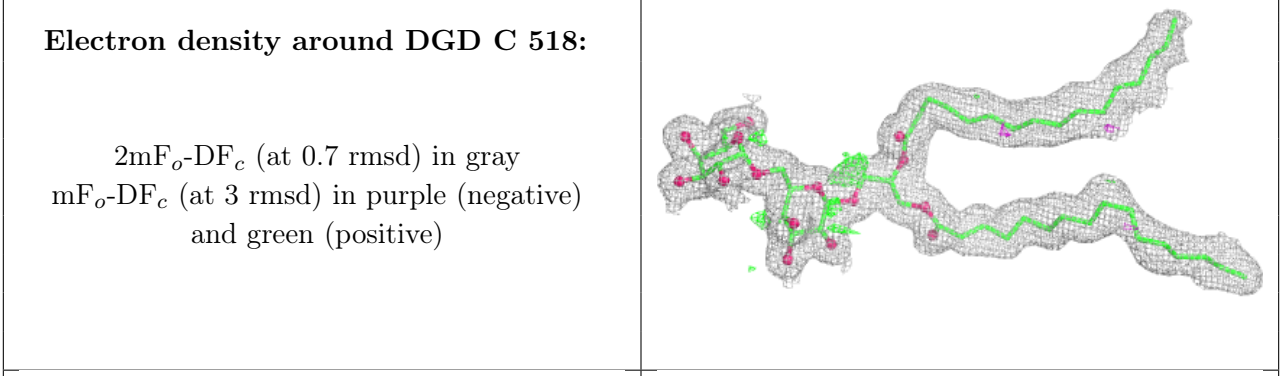


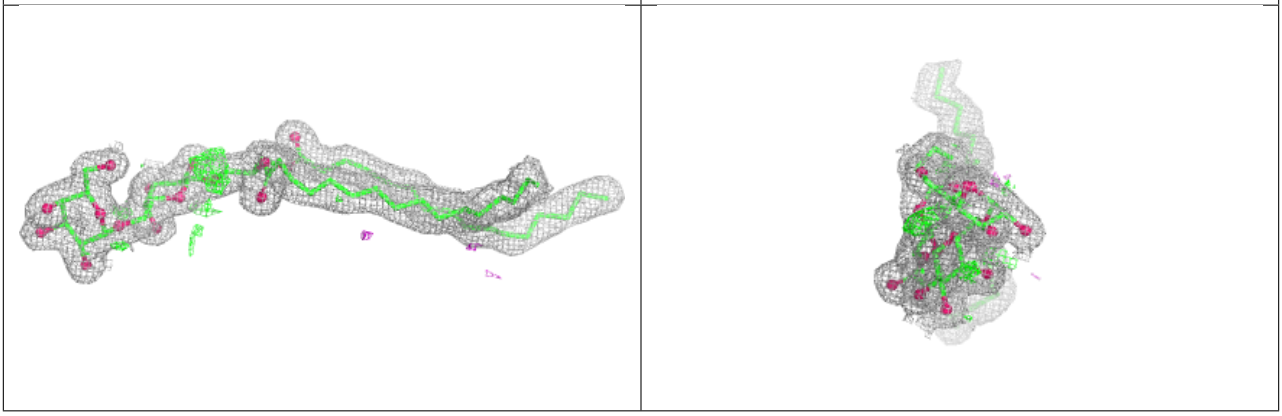




Electron density around DGD C 518:

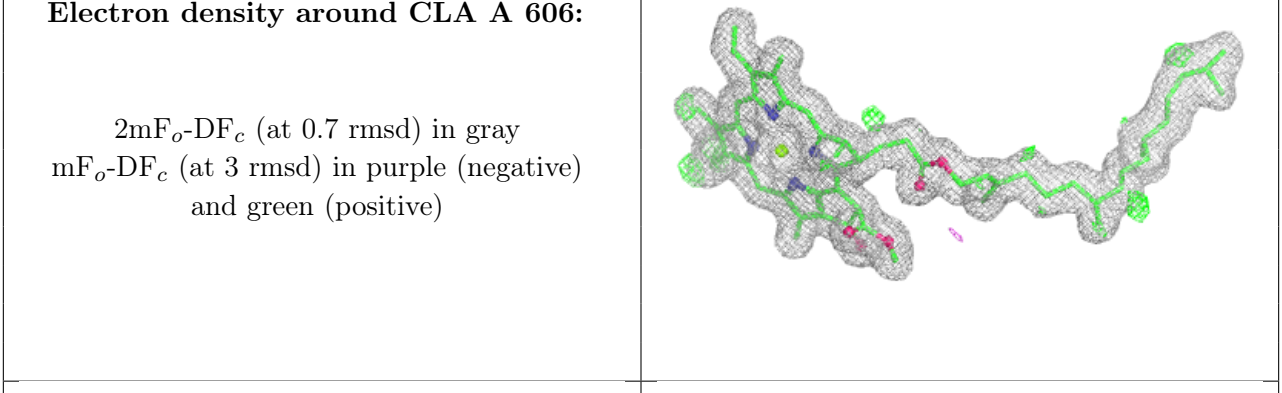
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

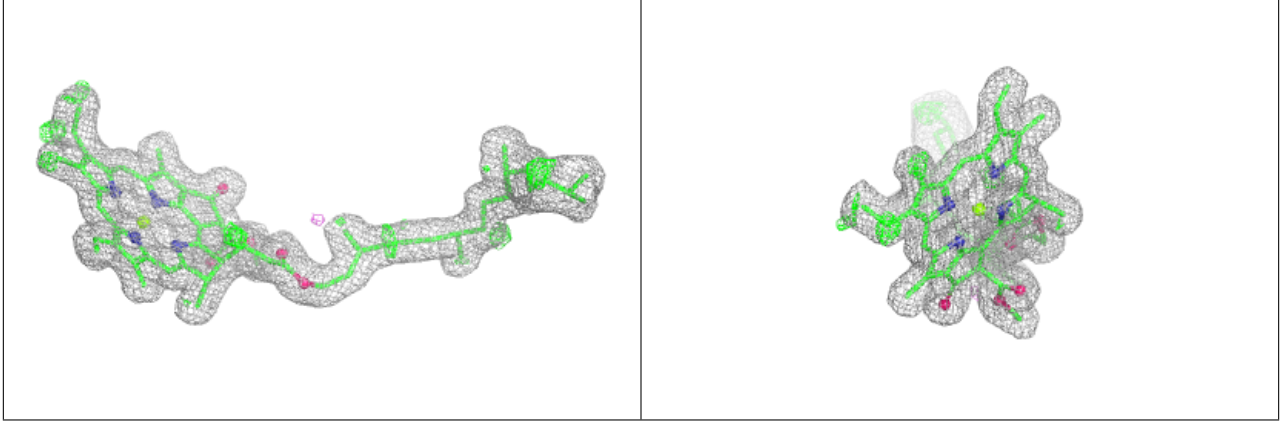




Electron density around CLA A 606:

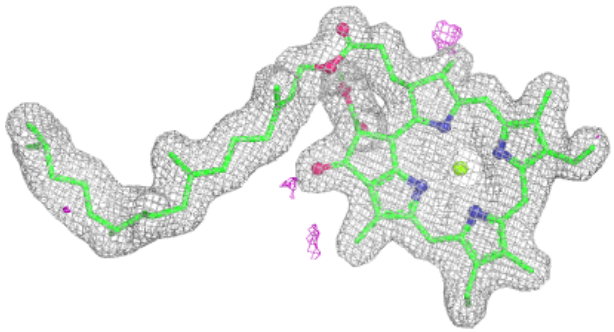
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

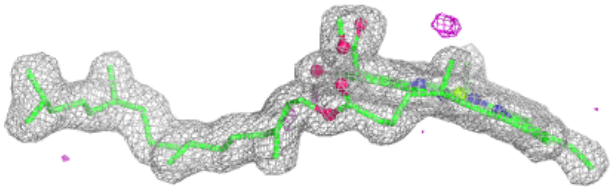




Electron density around CLA b 603:

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

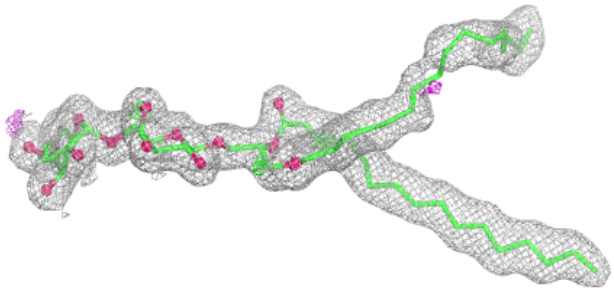


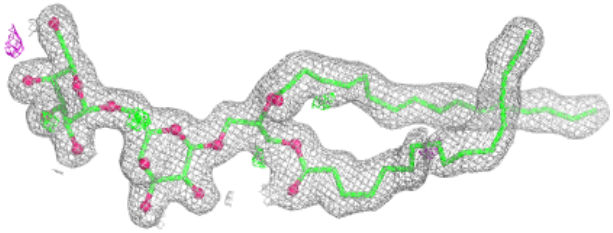


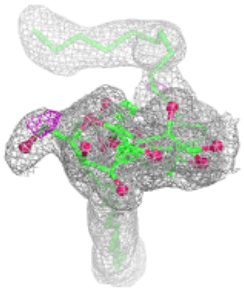


Electron density around DGD c 516:

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

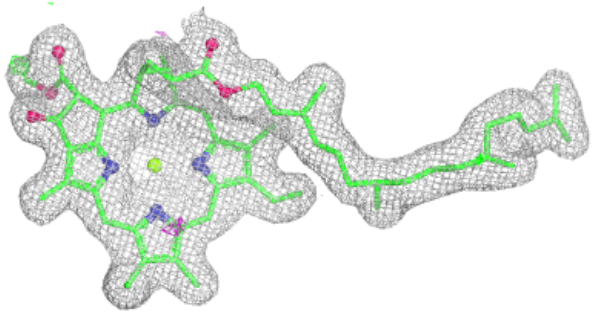






Electron density around CLA b 604:

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

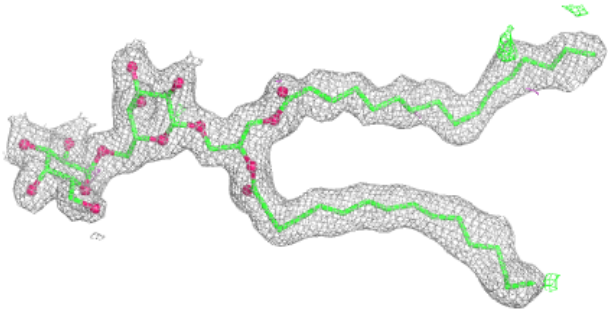


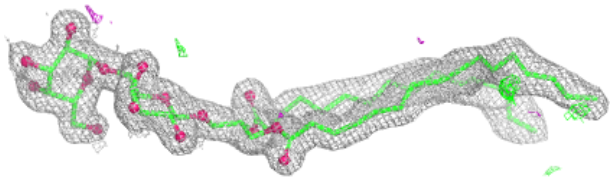


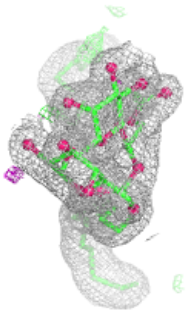


Electron density around DGD c 518:

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

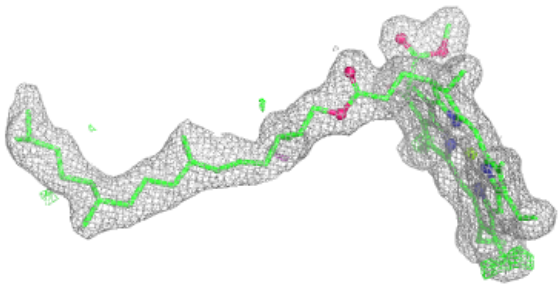


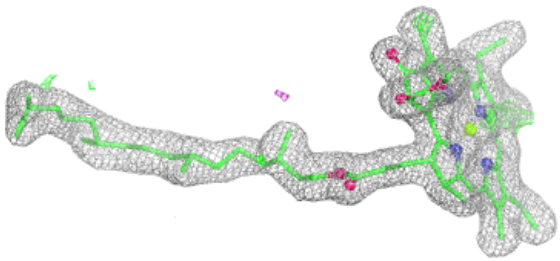


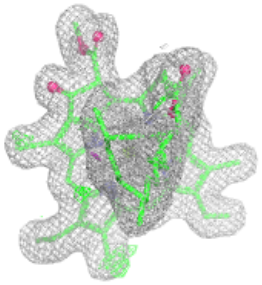


Electron density around CLA b 605:

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

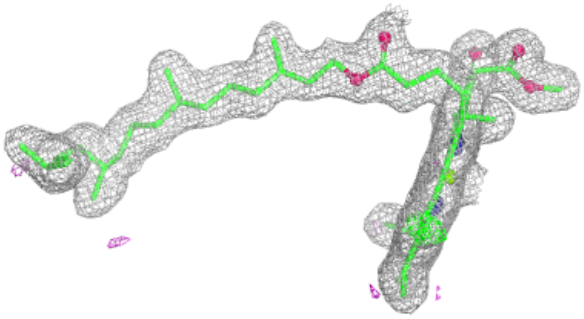


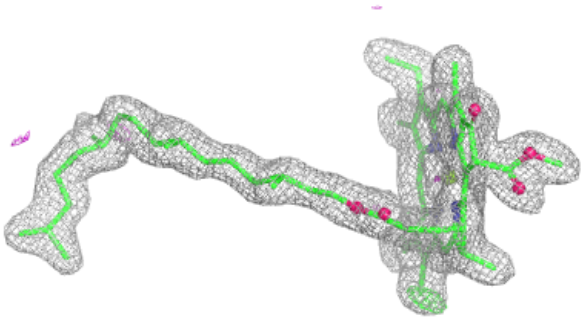


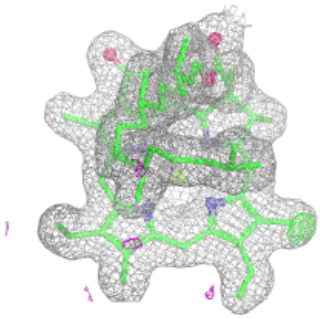


Electron density around CLA b 606:

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

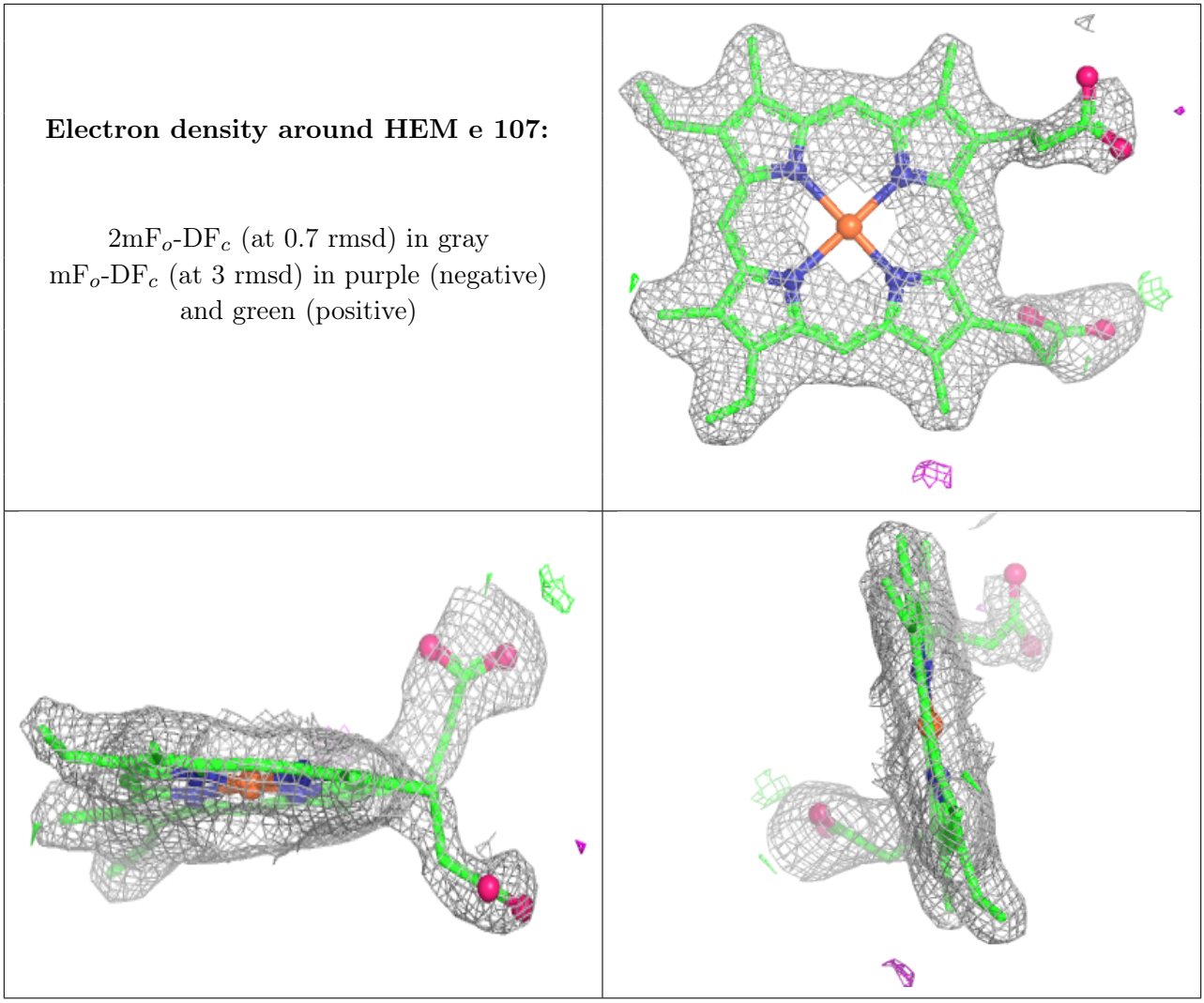






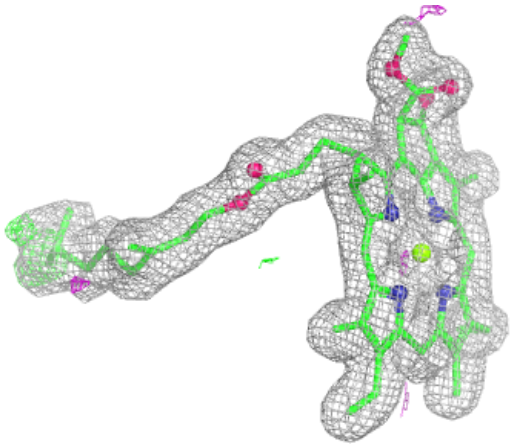
Electron density around HEM e 107:

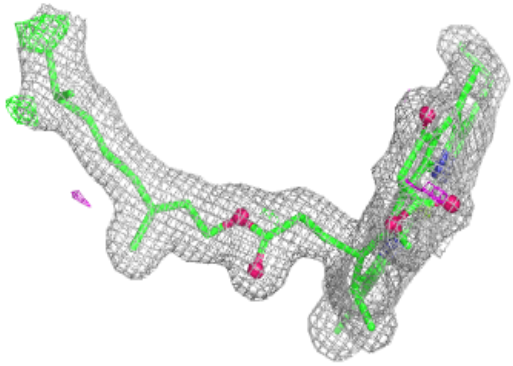
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

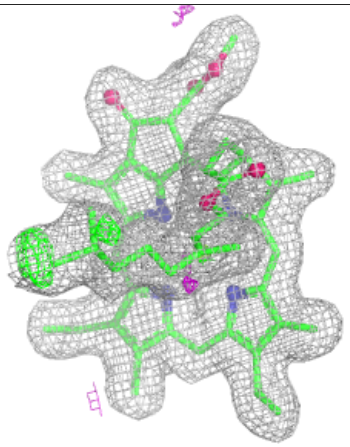


Electron density around CLA b 607:

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

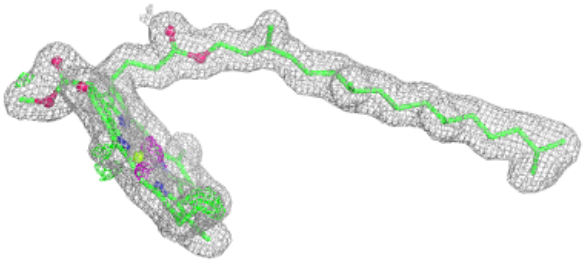


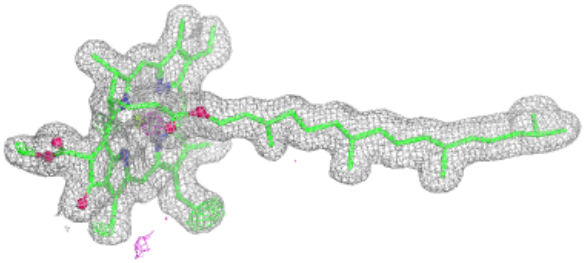


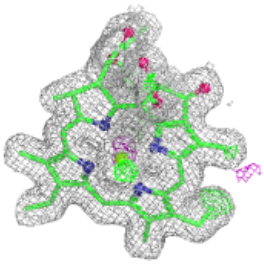


Electron density around CLA b 608:

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

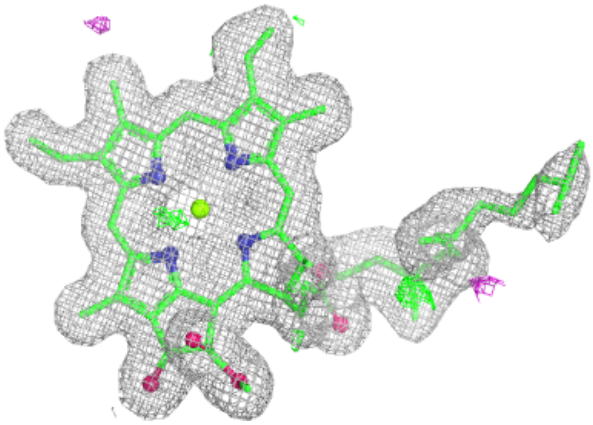


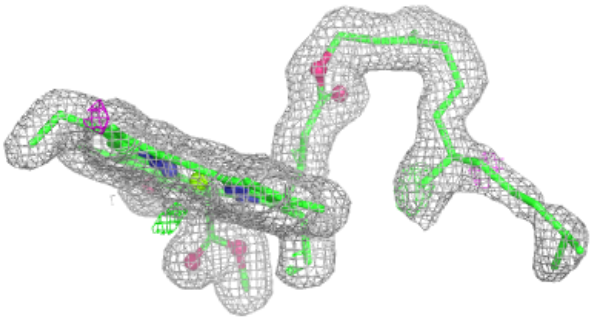


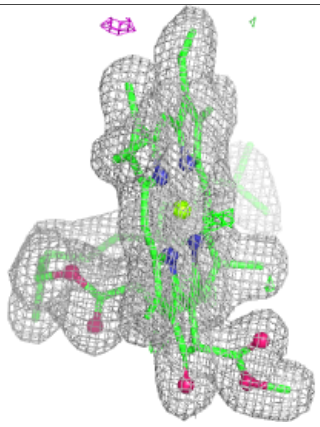


Electron density around CLA a 408:

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

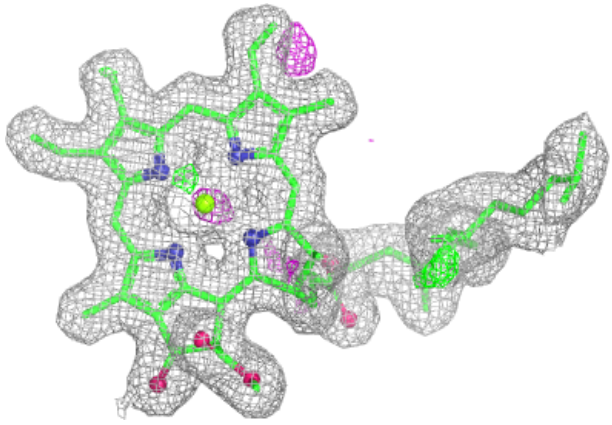


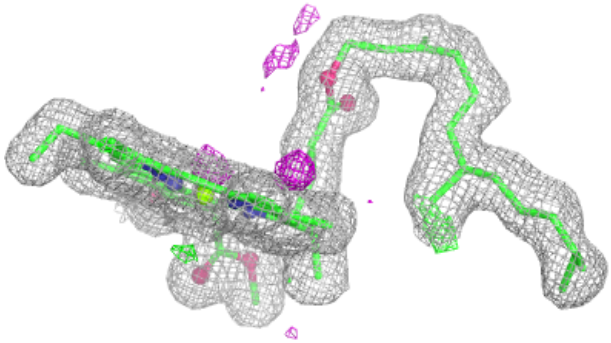


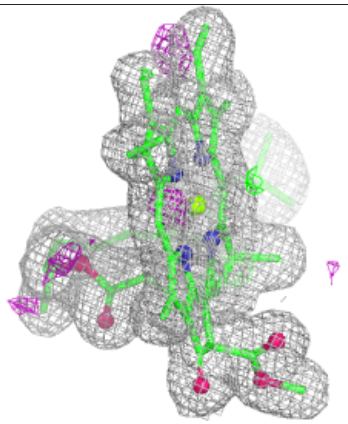


Electron density around CLA A 607:

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

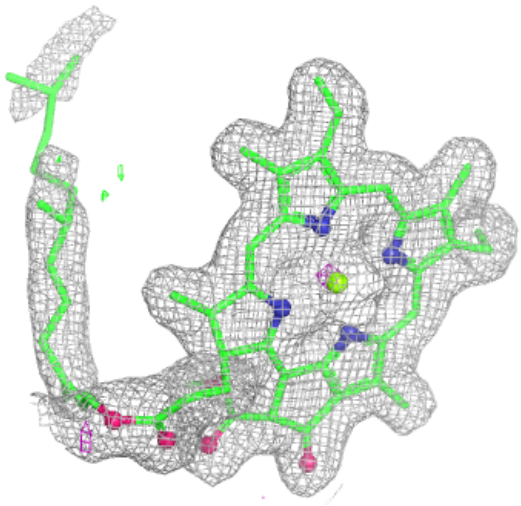


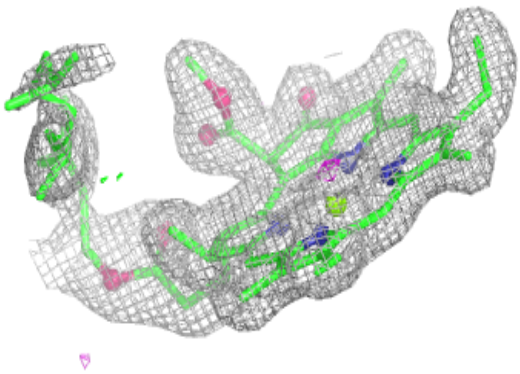


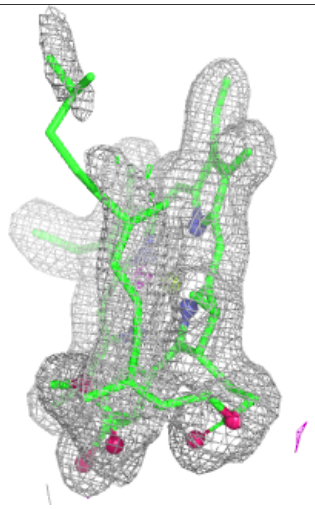


Electron density around CLA B 617:

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

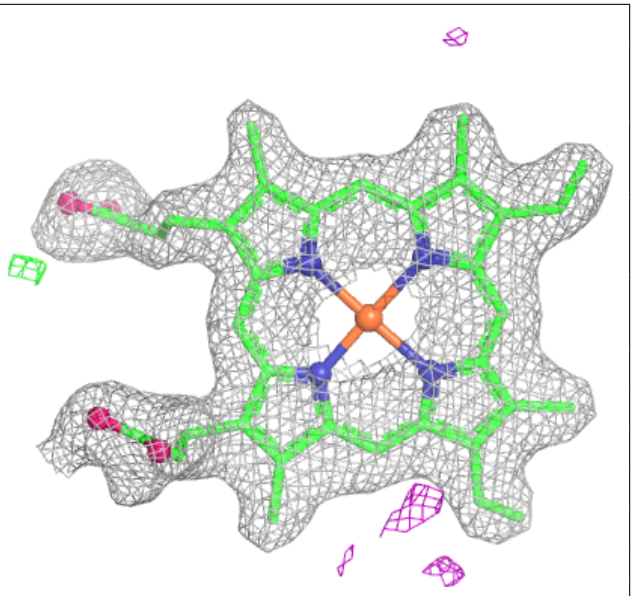


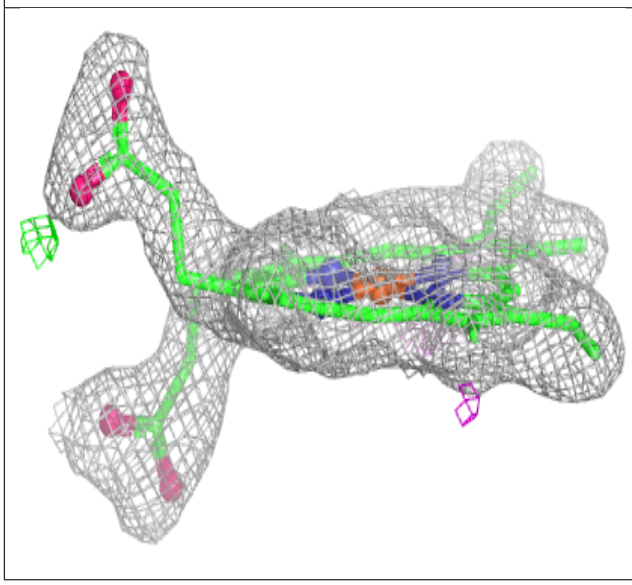




Electron density around HEM E 113:

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

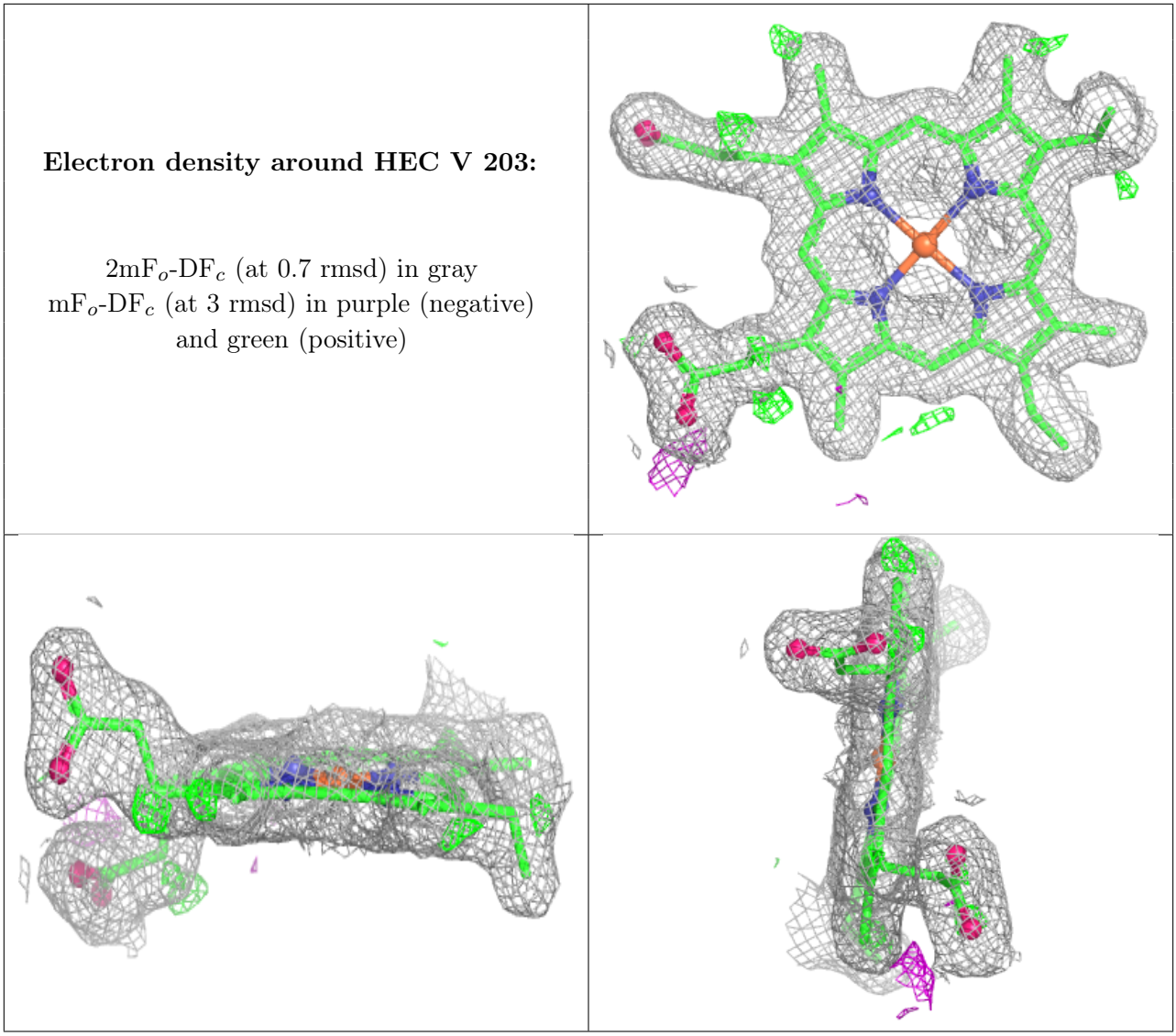






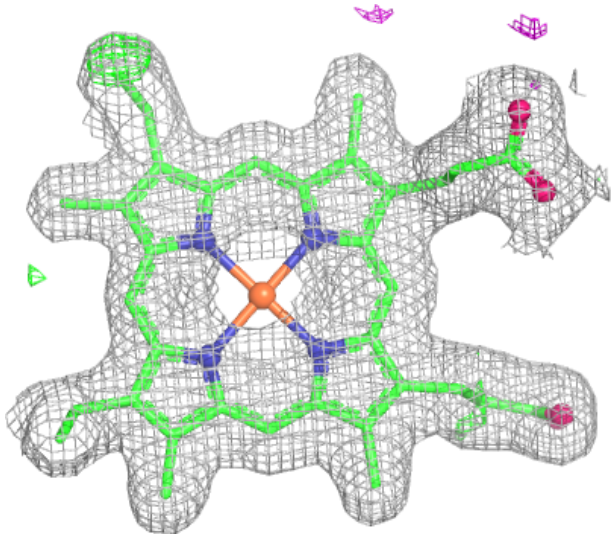
Electron density around HEC V 203:

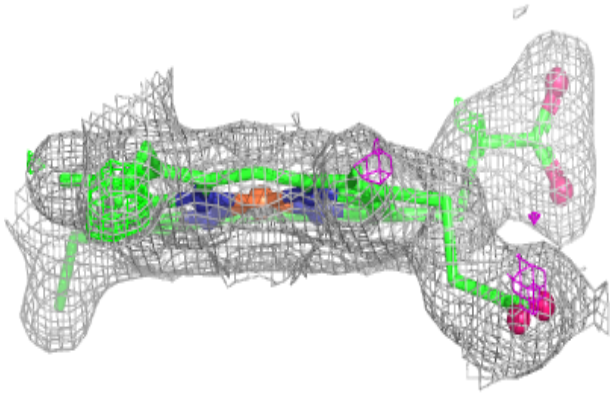
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

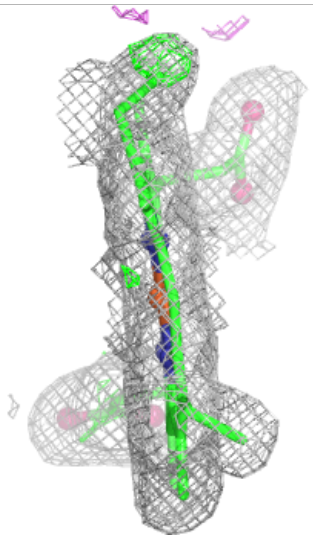


Electron density around HEC v 202:

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

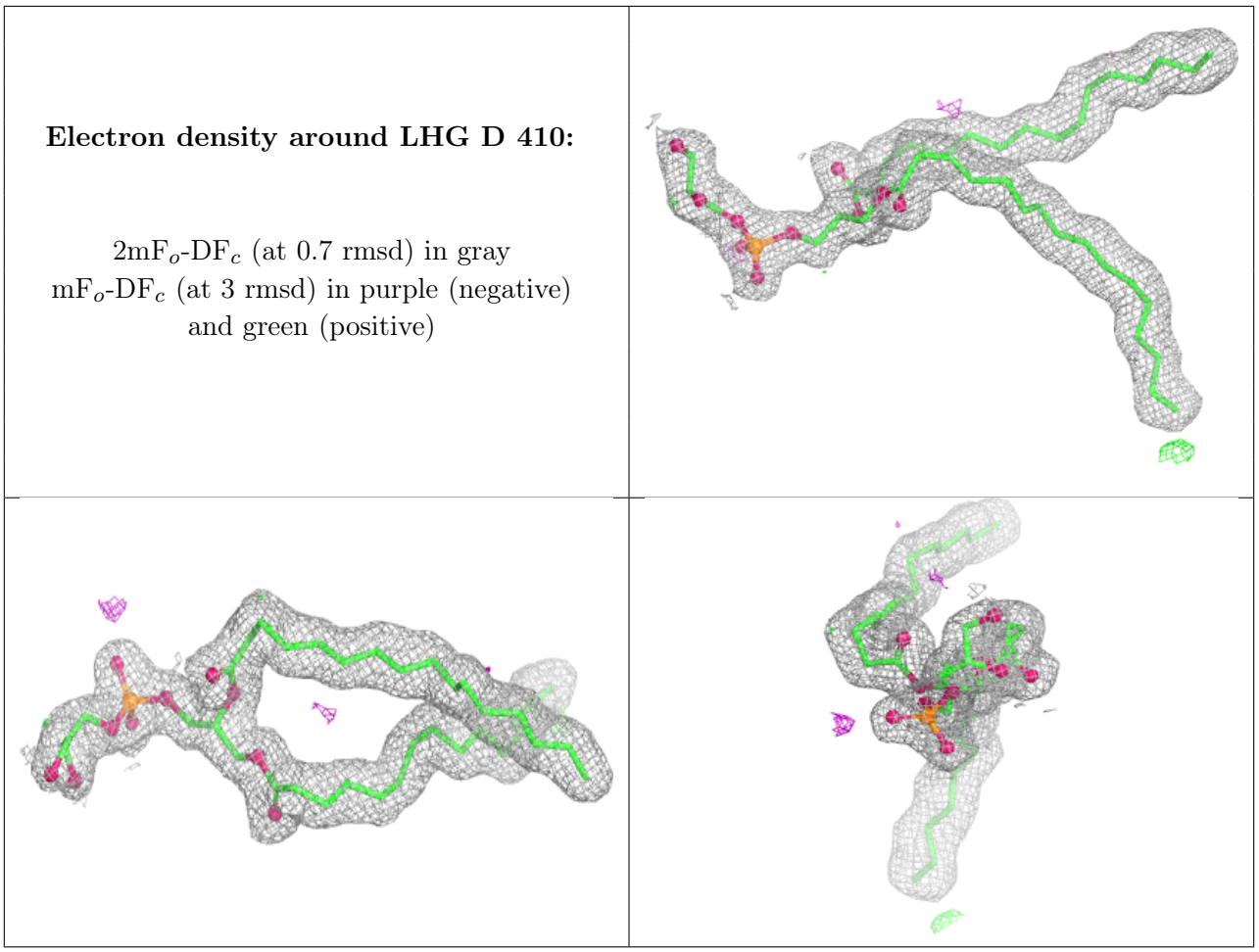






Electron density around LHG D 410:

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



6.5 Other polymers

There are no such residues in this entry.